Full wwPDB X-ray Structure Validation Report

Oct 2, 2021 – 02:10 PM EDT

PDB ID	:	3KLE
Title	:	Crystal structure of AZT-resistant HIV-1 Reverse Transcriptase crosslinked to a DSDNA with a bound excision product, AZTPPPPA
Authors	:	Tu, X.; Das, K.; Sarafianos, S.G.; Arnold, E.
Deposited on	:	2009-11-07
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

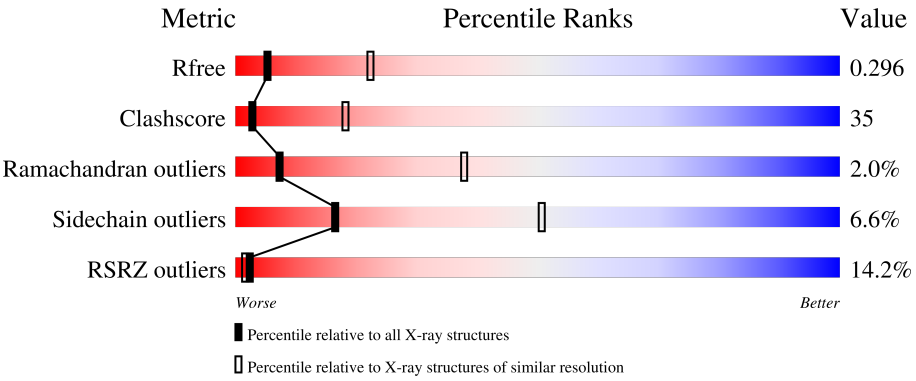
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	562	.% 41% 53% 6%
1	E	562	.% 40% 53% 6%
1	I	562	16% 39% 55% 6%
1	M	562	33% 41% 53% 6%
2	B	437	3% 46% 46% 5% .

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Mol	Chain	Length	Quality of chain
2	F	437	3% 41% 48% 6%
2	J	437	20% 43% 48% 5%
2	N	437	38% 43% 48% 5%
3	C	27	33% 56% 7%
3	G	27	26% 63% 7%
3	K	27	30% 59% 7%
3	O	27	15% 33% 56% 7%
4	D	21	43% 43% 14%
4	H	21	52% 33% 14%
4	L	21	5% 38% 52% 10%
4	P	21	10% 38% 52% 10%
5	Q	2	50% 50%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 36120 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	560	Total	C	N	O	S	0	0	0
			4560	2953	762	838	7			
1	E	560	Total	C	N	O	S	0	0	0
			4560	2953	762	838	7			
1	I	560	Total	C	N	O	S	0	0	0
			4560	2953	762	838	7			
1	M	560	Total	C	N	O	S	0	0	0
			4560	2953	762	838	7			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	41	LEU	MET	engineered mutation	UNP P03366
A	67	ASN	ASP	engineered mutation	UNP P03366
A	70	ARG	LYS	engineered mutation	UNP P03366
A	215	TYR	THR	engineered mutation	UNP P03366
A	219	GLN	LYS	engineered mutation	UNP P03366
A	258	CYS	GLN	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366
A	559	VAL	ILE	see remark 999	UNP P03366
E	-1	MET	-	expression tag	UNP P03366
E	0	VAL	-	expression tag	UNP P03366
E	41	LEU	MET	engineered mutation	UNP P03366
E	67	ASN	ASP	engineered mutation	UNP P03366
E	70	ARG	LYS	engineered mutation	UNP P03366
E	215	TYR	THR	engineered mutation	UNP P03366
E	219	GLN	LYS	engineered mutation	UNP P03366
E	258	CYS	GLN	engineered mutation	UNP P03366
E	280	SER	CYS	engineered mutation	UNP P03366
E	559	VAL	ILE	see remark 999	UNP P03366
I	-1	MET	-	expression tag	UNP P03366

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Chain	Residue	Modelled	Actual	Comment	Reference
I	0	VAL	-	expression tag	UNP P03366
I	41	LEU	MET	engineered mutation	UNP P03366
I	67	ASN	ASP	engineered mutation	UNP P03366
I	70	ARG	LYS	engineered mutation	UNP P03366
I	215	TYR	THR	engineered mutation	UNP P03366
I	219	GLN	LYS	engineered mutation	UNP P03366
I	258	CYS	GLN	engineered mutation	UNP P03366
I	280	SER	CYS	engineered mutation	UNP P03366
I	559	VAL	ILE	see remark 999	UNP P03366
M	-1	MET	-	expression tag	UNP P03366
M	0	VAL	-	expression tag	UNP P03366
M	41	LEU	MET	engineered mutation	UNP P03366
M	67	ASN	ASP	engineered mutation	UNP P03366
M	70	ARG	LYS	engineered mutation	UNP P03366
M	215	TYR	THR	engineered mutation	UNP P03366
M	219	GLN	LYS	engineered mutation	UNP P03366
M	258	CYS	GLN	engineered mutation	UNP P03366
M	280	SER	CYS	engineered mutation	UNP P03366
M	559	VAL	ILE	see remark 999	UNP P03366

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	425	Total	C	N	O	S	0	0	0
			3462	2248	576	632	6			
2	F	419	Total	C	N	O	S	0	0	0
			3434	2232	570	626	6			
2	J	419	Total	C	N	O	S	0	0	0
			3434	2232	570	626	6			
2	N	419	Total	C	N	O	S	0	0	0
			3434	2232	570	626	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366
B	429	GLY	-	expression tag	UNP P03366
B	430	GLY	-	expression tag	UNP P03366
B	431	HIS	-	expression tag	UNP P03366
B	432	HIS	-	expression tag	UNP P03366
B	433	HIS	-	expression tag	UNP P03366
B	434	HIS	-	expression tag	UNP P03366

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Chain	Residue	Modelled	Actual	Comment	Reference
B	435	HIS	-	expression tag	UNP P03366
B	436	HIS	-	expression tag	UNP P03366
B	437	HIS	-	expression tag	UNP P03366
F	280	SER	CYS	engineered mutation	UNP P03366
F	429	GLY	-	expression tag	UNP P03366
F	430	GLY	-	expression tag	UNP P03366
F	431	HIS	-	expression tag	UNP P03366
F	432	HIS	-	expression tag	UNP P03366
F	433	HIS	-	expression tag	UNP P03366
F	434	HIS	-	expression tag	UNP P03366
F	435	HIS	-	expression tag	UNP P03366
F	436	HIS	-	expression tag	UNP P03366
F	437	HIS	-	expression tag	UNP P03366
J	280	SER	CYS	engineered mutation	UNP P03366
J	429	GLY	-	expression tag	UNP P03366
J	430	GLY	-	expression tag	UNP P03366
J	431	HIS	-	expression tag	UNP P03366
J	432	HIS	-	expression tag	UNP P03366
J	433	HIS	-	expression tag	UNP P03366
J	434	HIS	-	expression tag	UNP P03366
J	435	HIS	-	expression tag	UNP P03366
J	436	HIS	-	expression tag	UNP P03366
J	437	HIS	-	expression tag	UNP P03366
N	280	SER	CYS	engineered mutation	UNP P03366
N	429	GLY	-	expression tag	UNP P03366
N	430	GLY	-	expression tag	UNP P03366
N	431	HIS	-	expression tag	UNP P03366
N	432	HIS	-	expression tag	UNP P03366
N	433	HIS	-	expression tag	UNP P03366
N	434	HIS	-	expression tag	UNP P03366
N	435	HIS	-	expression tag	UNP P03366
N	436	HIS	-	expression tag	UNP P03366
N	437	HIS	-	expression tag	UNP P03366

- Molecule 3 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	25	Total	C	N	O	P	0	0	0
			515	243	102	146	24			
3	G	25	Total	C	N	O	P	0	0	0
			515	243	102	146	24			
3	K	25	Total	C	N	O	P	0	0	0
			515	243	102	146	24			

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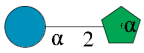
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	O	25	Total	C	N	O	P	0	0	0
			515	243	102	146	24			

- Molecule 4 is a DNA chain called DNA (5'-D(*AP*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MRG)P*CP*GP*CP*CP*(2DA))-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	21	Total	C	N	O	P	S	0	0	0
			427	205	77	124	20	1			
4	H	21	Total	C	N	O	P	S	0	0	0
			427	205	77	124	20	1			
4	L	21	Total	C	N	O	P	S	0	0	0
			427	205	77	124	20	1			
4	P	21	Total	C	N	O	P	S	0	0	0
			427	205	77	124	20	1			

- Molecule 5 is an oligosaccharide called alpha-D-fructofuranose-(2-1)-alpha-D-glucopyranose.

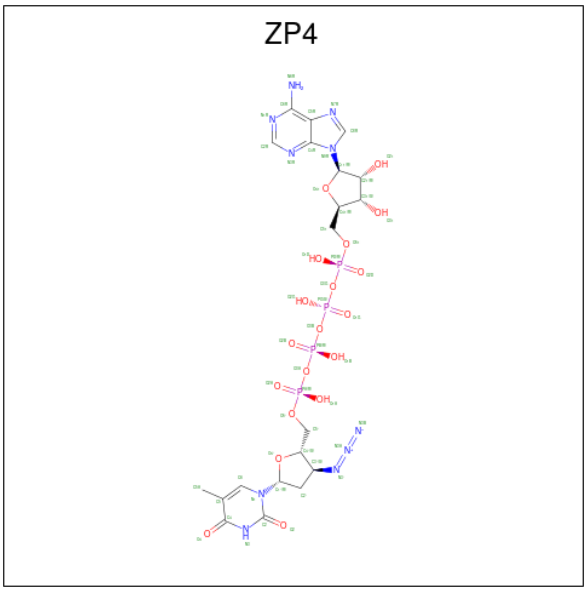


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	Q	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

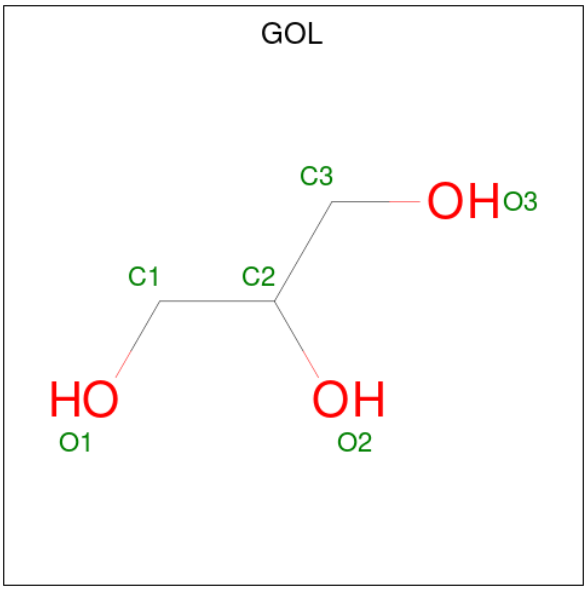
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		
6	E	2	Total	Mg	0	0
			2	2		
6	I	2	Total	Mg	0	0
			2	2		
6	M	2	Total	Mg	0	0
			2	2		

- Molecule 7 is [[[[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-dihydroxy-oxolan-2-yl]methoxy-hydroxy-phosphoryl]oxy-hydroxy-phosphoryl]oxy-hydroxy-phosphoryl] [(2S,3S,5R)-3-azido-5-(5-methyl-2,4-dioxo-pyrimidin-1-yl)oxolan-2-yl]methyl hydrogen phosphate (three-letter code: ZP4) (formula: $C_{20}H_{28}N_{10}O_{19}P_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			53	20	10	19	4		
7	E	1	Total	C	N	O	P	0	0
			53	20	10	19	4		
7	I	1	Total	C	N	O	P	0	0
			53	20	10	19	4		
7	M	1	Total	C	N	O	P	0	0
			53	20	10	19	4		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 6 3 3	0	0
8	F	1	Total C O 6 3 3	0	0

- Molecule 9 is water.

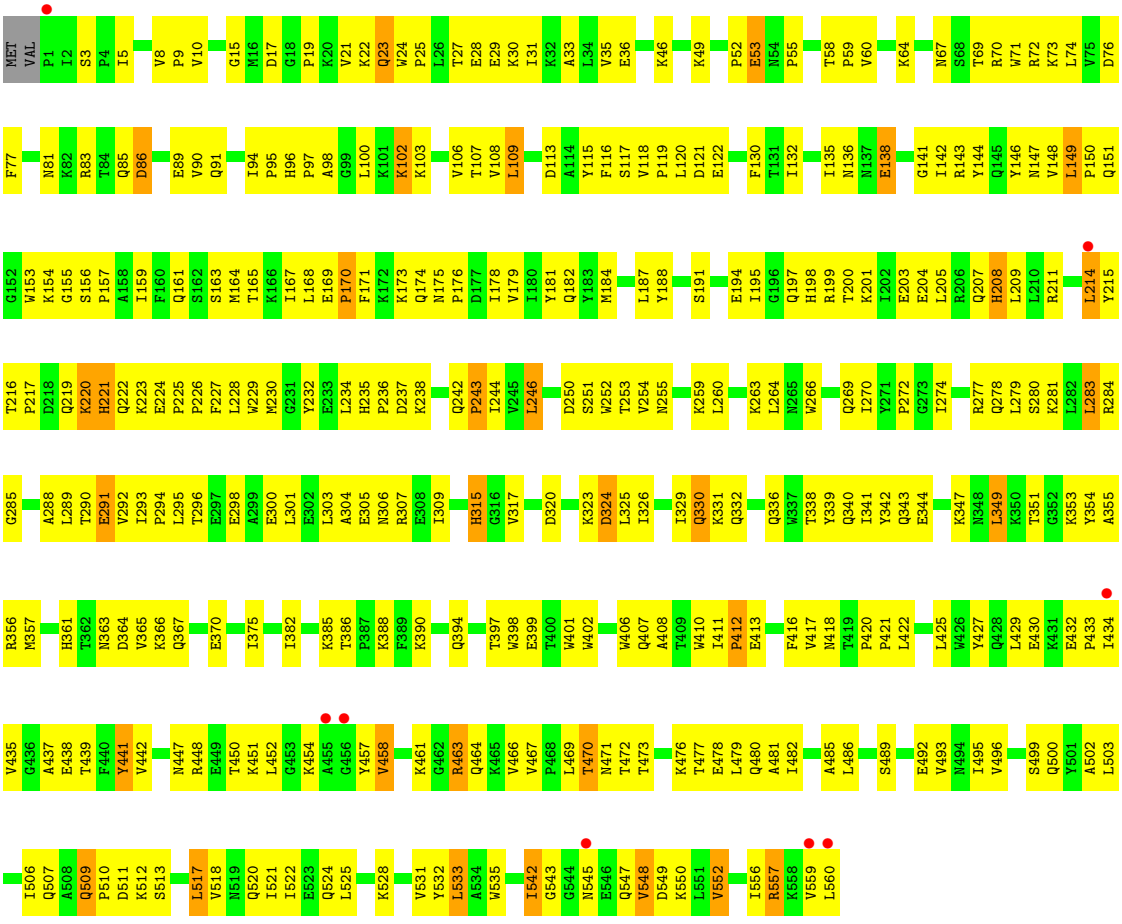
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	18	Total O 18 18	0	0
9	B	10	Total O 10 10	0	0
9	E	12	Total O 12 12	0	0
9	F	10	Total O 10 10	0	0
9	I	5	Total O 5 5	0	0
9	J	14	Total O 14 14	0	0
9	M	3	Total O 3 3	0	0
9	N	8	Total O 8 8	0	0
9	C	2	Total O 2 2	0	0
9	D	2	Total O 2 2	0	0
9	G	1	Total O 1 1	0	0
9	H	1	Total O 1 1	0	0
9	K	1	Total O 1 1	0	0
9	L	1	Total O 1 1	0	0
9	O	4	Total O 4 4	0	0
9	P	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

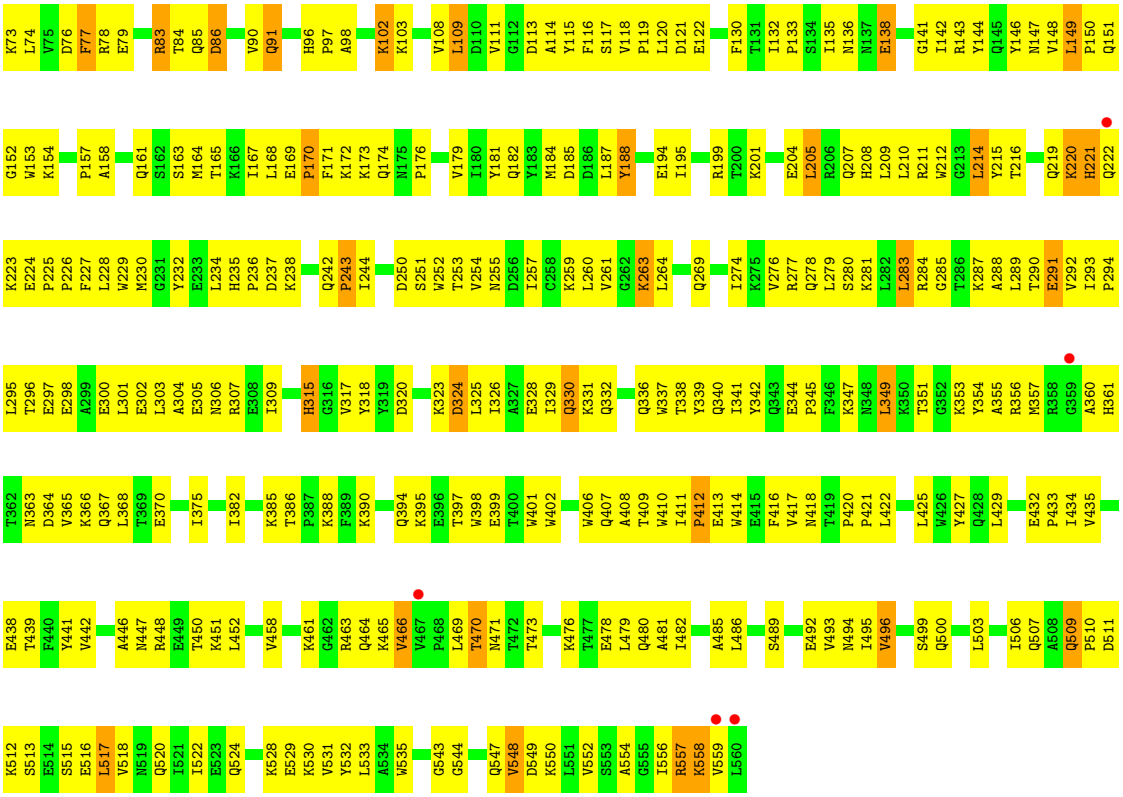
• Molecule 1: Reverse transcriptase/ribonuclease H

Chain A:



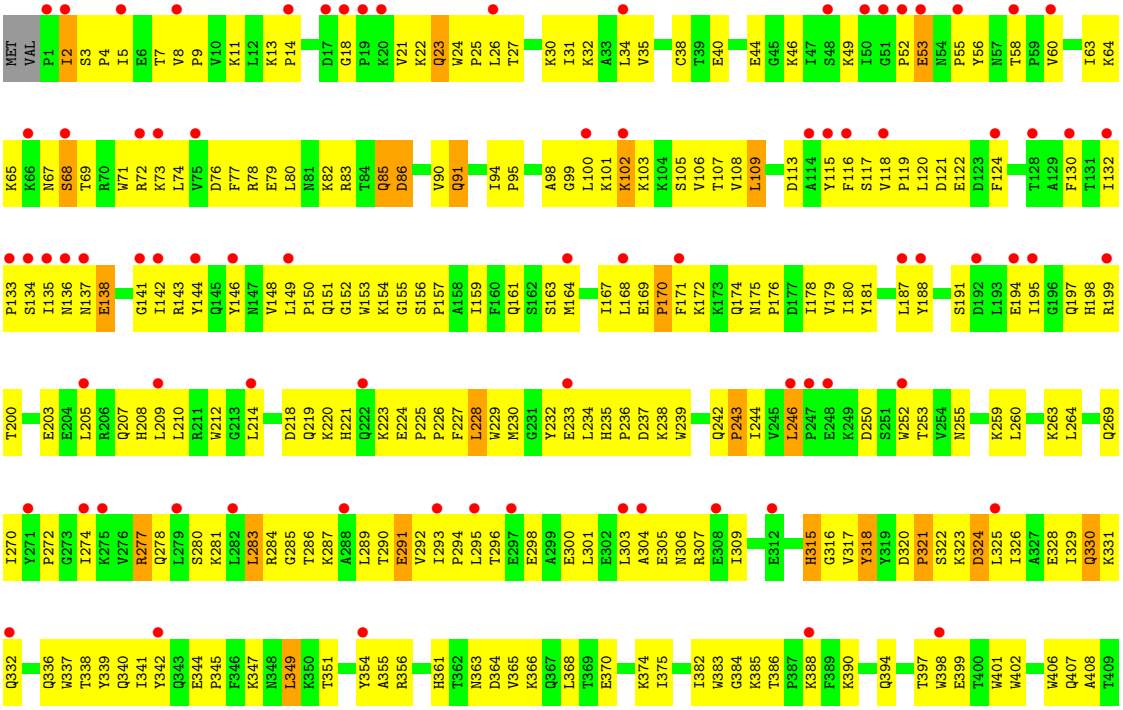
• Molecule 1: Reverse transcriptase/ribonuclease H

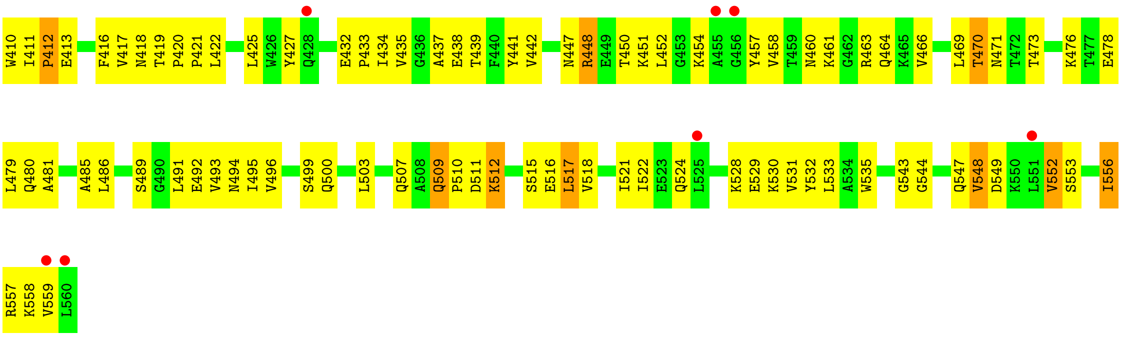
Chain E:



• Molecule 1: Reverse transcriptase/ribonuclease H

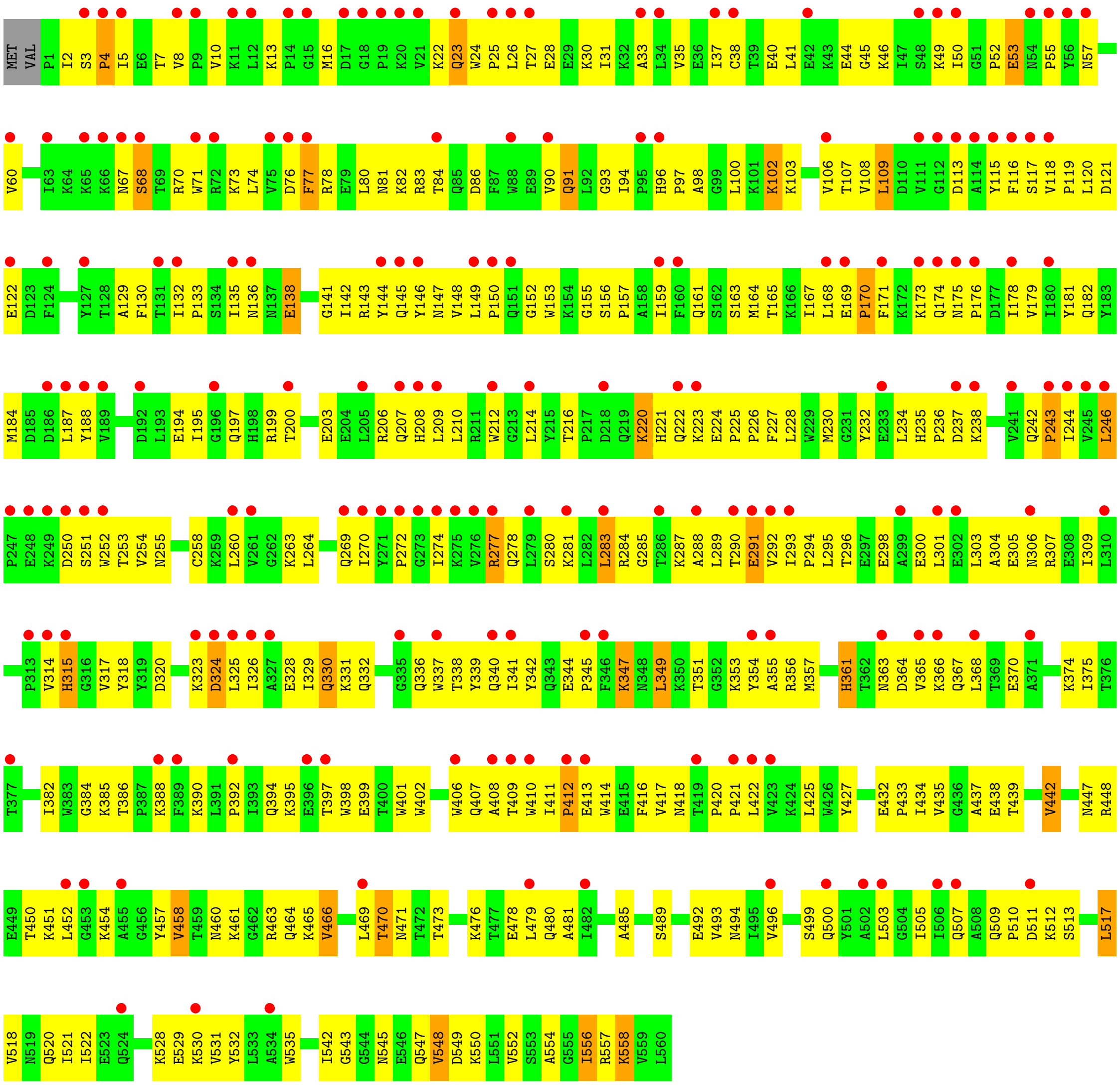
Chain I:





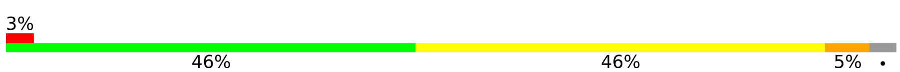
• Molecule 1: Reverse transcriptase/ribonuclease H

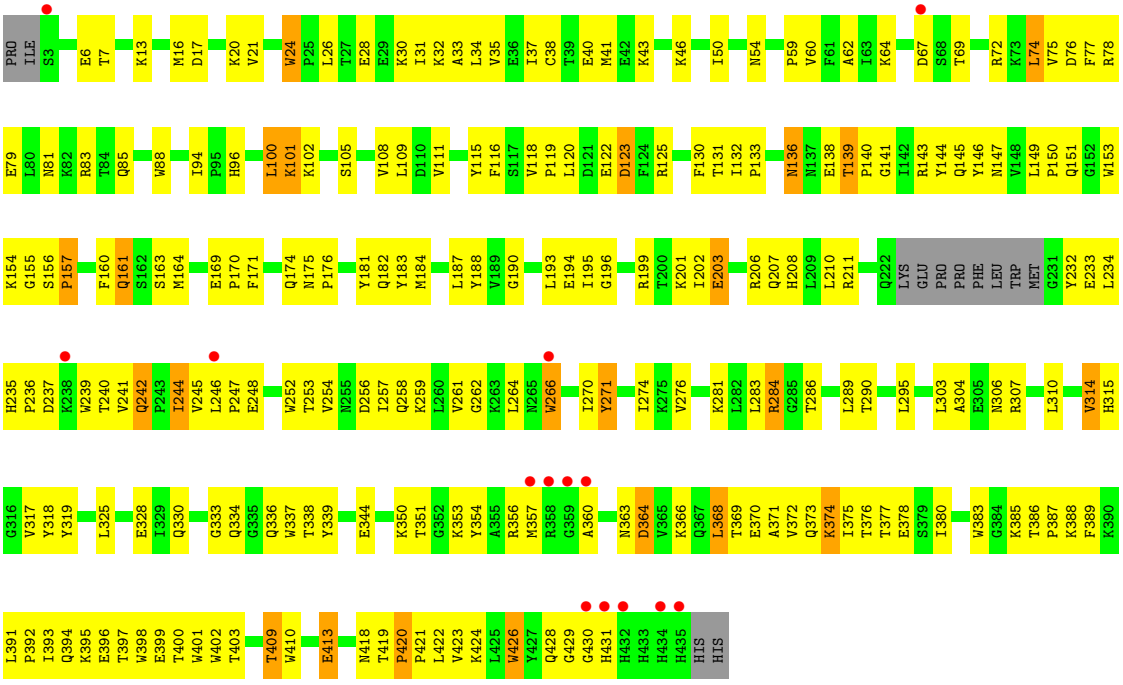
Chain M:



• Molecule 2: p51 RT

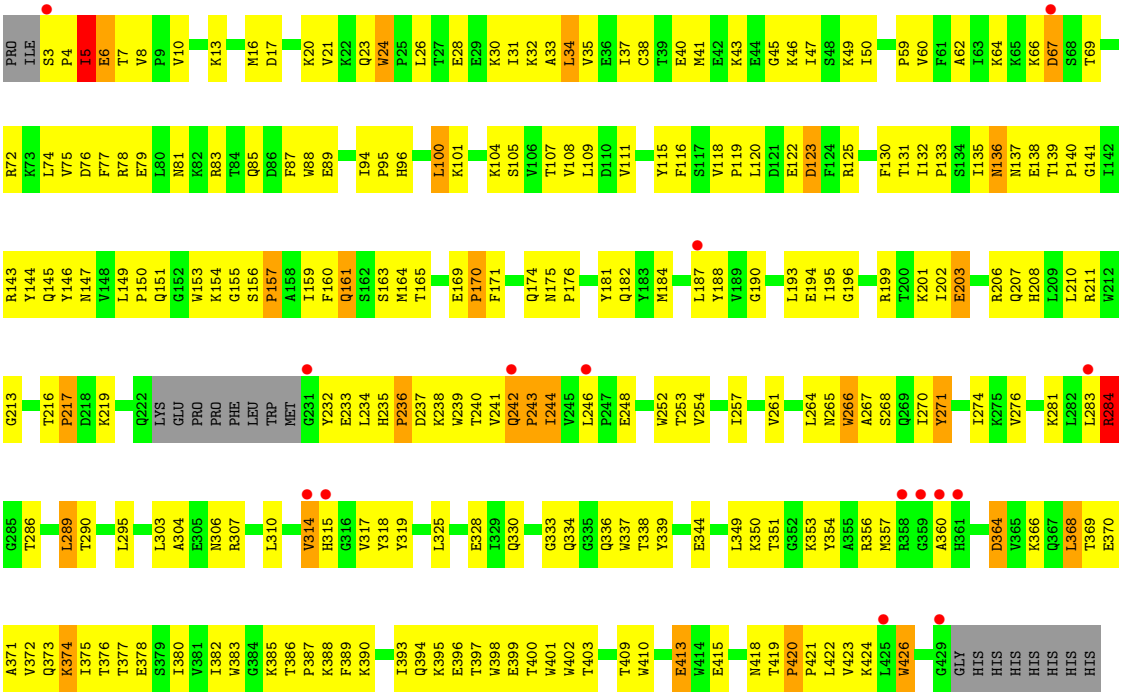
Chain B:





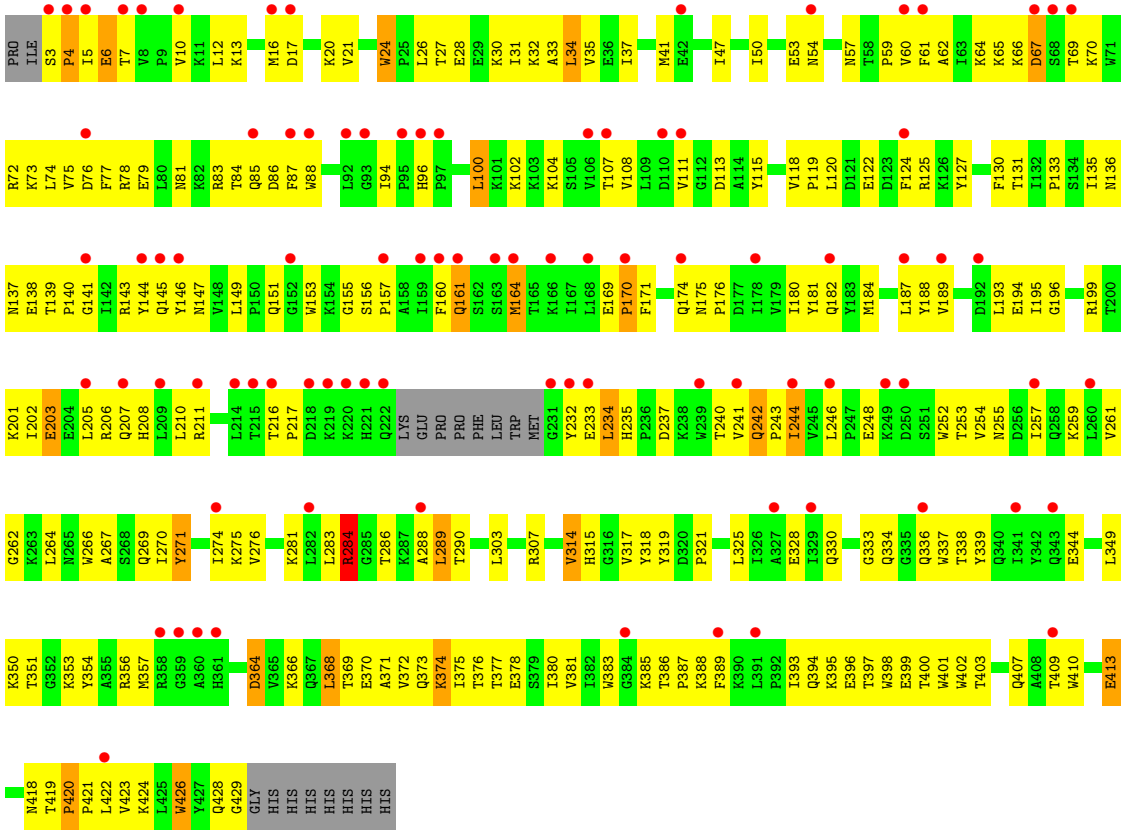
• Molecule 2: p51 RT

Chain F:



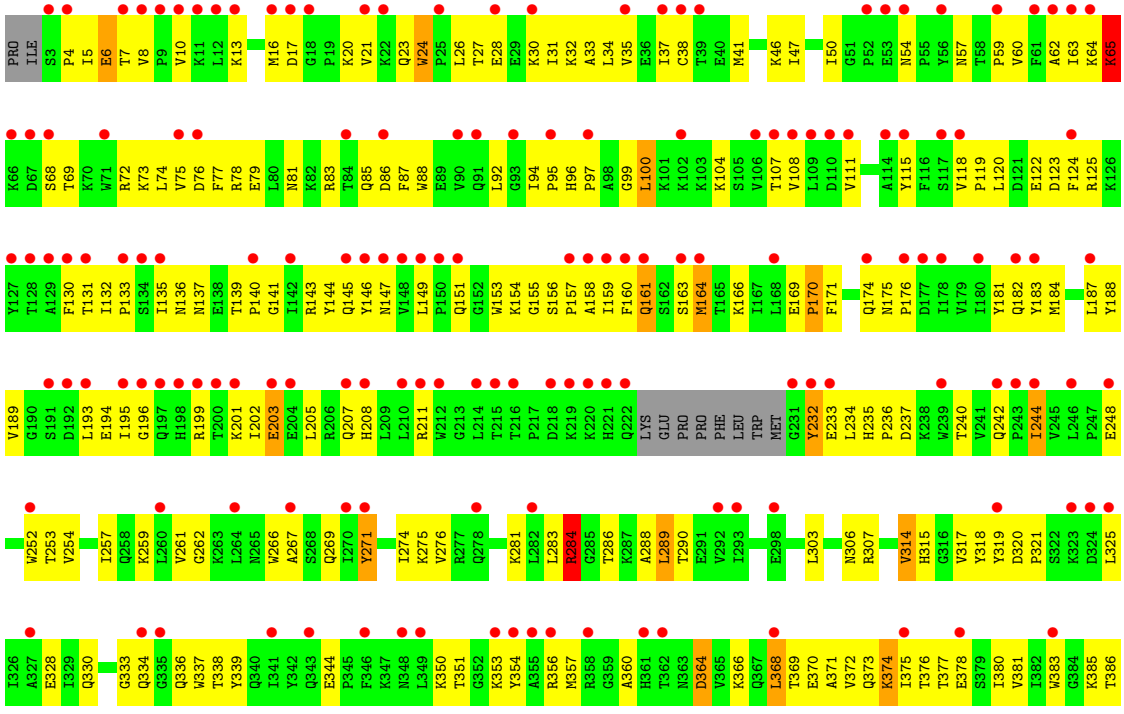
• Molecule 2: p51 RT

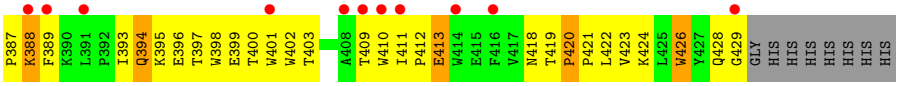
Chain J:



• Molecule 2: p51 RT

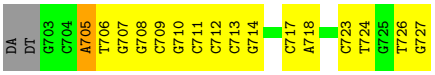
Chain N:





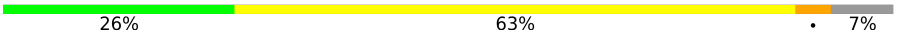
• Molecule 3: DNA (25-MER)

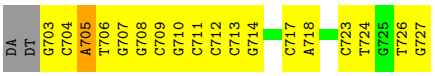
Chain C:



• Molecule 3: DNA (25-MER)

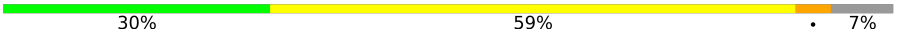
Chain G:

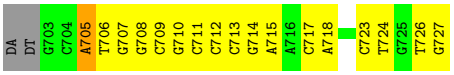




• Molecule 3: DNA (25-MER)

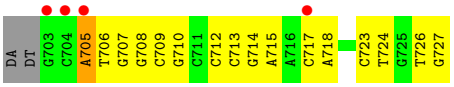
Chain K:





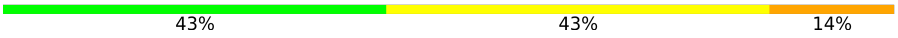
• Molecule 3: DNA (25-MER)

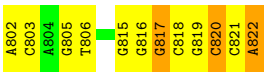
Chain O:



• Molecule 4: DNA (5'-D(*AP*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MRG)P*CP*GP*CP*CP*(2DA))-3')

Chain D:



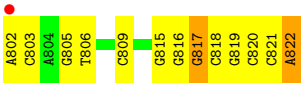


• Molecule 4: DNA (5'-D(*AP*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MRG)P*CP*GP*CP*CP*(2DA))-3')

Chain H:

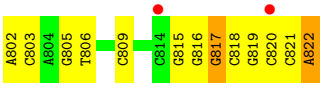
• Molecule 4: DNA (5'-D(*AP*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MRG)P*CP*GP*CP*CP*(2DA))-3')

Chain L:



• Molecule 4: DNA (5'-D(*AP*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MRG)P*CP*GP*CP*CP*(2DA))-3')

Chain P:



• Molecule 5: alpha-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain Q:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.74Å 283.33Å 155.23Å 90.00° 89.73° 90.00°	Depositor
Resolution (Å)	24.83 – 3.20 24.83 – 3.18	Depositor EDS
% Data completeness (in resolution range)	90.4 (24.83-3.20) 88.8 (24.83-3.18)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 3.17Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.280 , 0.308 0.270 , 0.296	Depositor DCC
R_{free} test set	1993 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å^2)	73.0	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 12.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.279 for h,-k,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	36120	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZP4, 2DA, Z9N, GOL, MG, MRG, GLC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.56	0/4679	0.70	2/6357 (0.0%)
1	E	0.59	0/4679	0.71	2/6357 (0.0%)
1	I	0.42	0/4679	0.61	0/6357
1	M	0.42	0/4679	0.61	2/6357 (0.0%)
2	B	0.63	0/3559	0.71	0/4838
2	F	0.62	0/3531	0.71	0/4800
2	J	0.44	0/3531	0.64	0/4800
2	N	0.42	0/3531	0.62	0/4800
3	C	0.88	0/579	0.93	0/893
3	G	0.96	0/579	0.93	0/893
3	K	0.56	0/579	0.81	0/893
3	O	0.56	0/579	0.81	0/893
4	D	0.92	0/424	0.90	0/649
4	H	0.87	0/424	0.93	0/649
4	L	0.56	0/424	0.88	0/649
4	P	0.53	0/424	0.85	0/649
All	All	0.55	0/36880	0.69	6/50834 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
3	G	0	1
3	K	0	1
3	O	0	1
4	D	0	1
4	H	0	1
All	All	0	6

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	442	VAL	CB-CA-C	-5.99	100.03	111.40
1	A	542	ILE	CB-CA-C	-5.82	99.95	111.60
1	M	68	SER	CB-CA-C	-5.54	99.57	110.10
1	A	463	ARG	CB-CA-C	-5.51	99.39	110.40
1	E	492	GLU	N-CA-C	-5.31	96.66	111.00
1	E	205	LEU	CA-CB-CG	5.16	127.17	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	705	DA	Sidechain
4	D	820	DC	Sidechain
3	G	705	DA	Sidechain
4	H	820	DC	Sidechain
3	K	705	DA	Sidechain
3	O	705	DA	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4560	0	4627	358	0
1	E	4560	0	4627	359	0
1	I	4560	0	4627	385	0
1	M	4560	0	4628	344	0
2	B	3462	0	3462	236	0
2	F	3434	0	3450	260	0
2	J	3434	0	3450	273	0
2	N	3434	0	3450	253	0
3	C	515	0	280	24	0
3	G	515	0	280	25	0
3	K	515	0	280	27	0
3	O	515	0	280	24	0
4	D	427	0	242	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	427	0	242	11	0
4	L	427	0	242	12	0
4	P	427	0	243	16	0
5	Q	23	0	10	4	0
6	A	2	0	0	0	0
6	E	2	0	0	0	0
6	I	2	0	0	0	0
6	M	2	0	0	0	0
7	A	53	0	24	10	0
7	E	53	0	24	9	0
7	I	53	0	24	4	0
7	M	53	0	24	7	0
8	B	6	0	8	0	0
8	F	6	0	8	0	0
9	A	18	0	0	0	0
9	B	10	0	0	0	0
9	C	2	0	0	0	0
9	D	2	0	0	0	0
9	E	12	0	0	0	0
9	F	10	0	0	1	0
9	G	1	0	0	0	0
9	H	1	0	0	0	0
9	I	5	0	0	1	0
9	J	14	0	0	5	0
9	K	1	0	0	0	0
9	L	1	0	0	0	0
9	M	3	0	0	0	0
9	N	8	0	0	3	0
9	O	4	0	0	0	0
9	P	1	0	0	1	0
All	All	36120	0	34532	2497	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All (2497) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:441:TYR:CD1	1:I:544:GLY:HA3	1.70	1.25
1:I:286:THR:O	1:I:287:LYS:HG2	1.44	1.16
2:F:125:ARG:HD3	2:F:147:ASN:HA	1.29	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:489:SER:HB2	1:I:493:VAL:HG11	1.29	1.14
2:B:79:GLU:HG3	2:B:83:ARG:HH12	0.98	1.14
1:E:489:SER:HB2	1:E:493:VAL:HG11	1.27	1.14
1:E:511:ASP:OD1	1:E:512:LYS:HG3	1.47	1.13
2:J:125:ARG:HD3	2:J:147:ASN:HA	1.27	1.13
1:I:225:PRO:HB2	1:I:226:PRO:HD3	1.16	1.13
1:M:489:SER:HB2	1:M:493:VAL:HG11	1.28	1.13
1:A:489:SER:HB2	1:A:493:VAL:HG11	1.27	1.12
2:B:125:ARG:HD3	2:B:147:ASN:HA	1.31	1.12
2:F:79:GLU:HG3	2:F:83:ARG:HH12	1.02	1.12
1:E:441:TYR:CD1	1:E:544:GLY:HA3	1.85	1.11
2:B:64:LYS:HE3	2:B:69:THR:HA	1.27	1.11
1:A:157:PRO:O	1:A:161:GLN:HG3	1.49	1.11
2:N:65:LYS:HB2	2:N:68:SER:HB2	1.34	1.10
2:N:125:ARG:HD3	2:N:147:ASN:HA	1.32	1.09
2:N:79:GLU:HG3	2:N:83:ARG:HH12	1.02	1.09
2:F:64:LYS:HE3	2:F:69:THR:HA	1.34	1.08
1:M:511:ASP:OD1	1:M:512:LYS:HG3	1.53	1.07
2:J:79:GLU:HG3	2:J:83:ARG:HH12	0.99	1.06
2:J:184:MET:SD	2:J:410:TRP:HB3	1.96	1.05
1:I:511:ASP:OD1	1:I:512:LYS:CG	2.05	1.04
1:I:511:ASP:OD1	1:I:512:LYS:HG3	1.58	1.03
1:M:90:VAL:HG22	2:N:140:PRO:HB2	1.39	1.03
2:B:79:GLU:HG3	2:B:83:ARG:NH1	1.74	1.02
1:E:102:LYS:HD2	1:E:102:LYS:H	1.24	1.02
2:J:79:GLU:HG3	2:J:83:ARG:NH1	1.75	1.02
1:I:274:ILE:HG23	1:I:306:ASN:HD21	1.26	1.01
2:F:79:GLU:HG3	2:F:83:ARG:NH1	1.76	1.01
1:I:441:TYR:HD1	1:I:544:GLY:HA3	1.22	1.00
1:E:52:PRO:HA	1:E:143:ARG:HH22	1.25	1.00
2:N:79:GLU:HG3	2:N:83:ARG:NH1	1.77	1.00
1:A:23:GLN:NE2	1:A:60:VAL:H	1.59	0.99
1:A:102:LYS:H	1:A:102:LYS:HD2	1.27	0.99
2:J:5:ILE:HG13	2:J:6:GLU:H	1.24	0.99
1:I:439:THR:HG21	2:J:289:LEU:HD13	1.43	0.99
1:M:274:ILE:HG23	1:M:306:ASN:HD21	1.26	0.98
1:E:293:ILE:HD12	1:E:294:PRO:HD2	1.46	0.97
1:E:277:ARG:NH1	1:E:336:GLN:HG3	1.80	0.96
1:I:103:LYS:HE3	1:I:179:VAL:HG21	1.47	0.96
1:M:23:GLN:NE2	1:M:60:VAL:H	1.64	0.96
1:M:439:THR:HG21	2:N:289:LEU:HD13	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:102:LYS:HD2	1:M:102:LYS:H	1.32	0.94
1:I:67:ASN:O	1:I:68:SER:HB2	1.68	0.93
2:J:5:ILE:HG13	2:J:6:GLU:N	1.81	0.93
1:A:52:PRO:HA	1:A:143:ARG:HH22	1.29	0.93
2:J:79:GLU:CG	2:J:83:ARG:HH12	1.82	0.93
2:B:79:GLU:CG	2:B:83:ARG:HH12	1.82	0.92
2:J:24:TRP:CZ3	2:J:403:THR:HG21	2.05	0.92
1:I:435:VAL:HA	2:J:290:THR:HG21	1.51	0.91
1:M:225:PRO:HB2	1:M:226:PRO:HD3	1.51	0.91
2:B:30:LYS:HE2	2:B:62:ALA:O	1.71	0.91
1:M:157:PRO:O	1:M:161:GLN:HG3	1.69	0.91
1:I:293:ILE:HD12	1:I:294:PRO:HD2	1.51	0.91
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.52	0.91
1:A:293:ILE:HD12	1:A:294:PRO:HD2	1.53	0.90
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.50	0.90
2:F:79:GLU:CG	2:F:83:ARG:HH12	1.85	0.90
2:J:157:PRO:HG2	2:J:184:MET:HA	1.51	0.90
1:E:23:GLN:NE2	1:E:60:VAL:H	1.69	0.90
1:I:23:GLN:NE2	1:I:60:VAL:H	1.69	0.90
1:I:225:PRO:CB	1:I:226:PRO:HD3	2.00	0.90
1:I:225:PRO:HB2	1:I:226:PRO:CD	2.01	0.90
2:N:79:GLU:CG	2:N:83:ARG:HH12	1.85	0.90
2:N:60:VAL:HG12	2:N:75:VAL:HG22	1.54	0.90
1:I:238:LYS:HG2	1:I:315:HIS:ND1	1.87	0.89
1:E:157:PRO:O	1:E:161:GLN:HG3	1.73	0.89
1:M:67:ASN:O	1:M:68:SER:HB2	1.70	0.89
1:M:435:VAL:HA	2:N:290:THR:HG21	1.54	0.89
2:F:60:VAL:HG12	2:F:75:VAL:HG22	1.53	0.88
1:I:155:GLY:O	1:I:159:ILE:HG12	1.73	0.88
1:M:135:ILE:H	1:M:135:ILE:HD12	1.36	0.88
1:E:432:GLU:HG3	1:E:433:PRO:HD2	1.55	0.88
1:I:558:LYS:HG2	1:I:559:VAL:H	1.35	0.88
2:F:244:ILE:HD13	2:F:244:ILE:H	1.38	0.88
1:I:277:ARG:NH1	1:I:336:GLN:HG3	1.89	0.88
2:J:60:VAL:HG12	2:J:75:VAL:HG22	1.55	0.88
2:N:64:LYS:HE3	2:N:69:THR:HA	1.56	0.88
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.53	0.87
1:E:439:THR:HG21	2:F:289:LEU:HD13	1.56	0.87
2:N:111:VAL:HG11	2:N:187:LEU:HD22	1.53	0.87
1:A:260:LEU:HD21	1:A:303:LEU:HD23	1.54	0.87
1:M:103:LYS:HE3	1:M:179:VAL:HG21	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:GLU:HG3	1:A:433:PRO:HD2	1.56	0.87
2:F:261:VAL:HG13	2:F:276:VAL:HG21	1.53	0.87
1:I:157:PRO:O	1:I:161:GLN:HG3	1.74	0.87
1:A:485:ALA:O	1:A:489:SER:HB3	1.74	0.87
2:N:157:PRO:HG2	2:N:184:MET:HA	1.54	0.87
1:E:49:LYS:HE3	1:E:142:ILE:HD12	1.57	0.87
1:M:432:GLU:HG3	1:M:433:PRO:HD2	1.56	0.86
1:A:221:HIS:HE1	1:A:228:LEU:HB2	1.40	0.85
2:F:30:LYS:HE2	2:F:62:ALA:O	1.76	0.85
2:B:244:ILE:H	2:B:244:ILE:HD13	1.41	0.85
1:A:135:ILE:H	1:A:135:ILE:HD12	1.39	0.85
1:E:207:GLN:NE2	1:E:210:LEU:HD23	1.91	0.85
2:N:96:HIS:HE1	2:N:381:VAL:O	1.59	0.85
2:F:111:VAL:HG11	2:F:187:LEU:HD22	1.58	0.85
1:I:224:GLU:O	1:I:227:PHE:CE2	2.30	0.85
1:I:382:ILE:O	2:J:136:ASN:HB2	1.76	0.84
1:A:277:ARG:NH1	1:A:336:GLN:HG3	1.92	0.84
2:F:100:LEU:HD23	2:F:100:LEU:H	1.40	0.84
1:M:293:ILE:HD12	1:M:294:PRO:HD2	1.59	0.84
1:A:171:PHE:HB2	1:A:208:HIS:CD2	2.12	0.84
2:N:171:PHE:HB2	2:N:208:HIS:ND1	1.91	0.84
1:E:529:GLU:O	1:E:530:LYS:HG3	1.78	0.84
1:I:163:SER:O	1:I:167:ILE:HD13	1.77	0.84
1:I:286:THR:C	1:I:287:LYS:HG2	1.97	0.84
2:B:428:GLN:HG2	2:B:429:GLY:H	1.41	0.84
2:J:234:LEU:H	2:J:234:LEU:HD12	1.43	0.84
1:I:224:GLU:O	1:I:227:PHE:CZ	2.30	0.84
2:F:157:PRO:HG2	2:F:184:MET:HA	1.58	0.84
2:B:13:LYS:O	2:B:16:MET:HB2	1.78	0.83
1:E:485:ALA:O	1:E:489:SER:HB3	1.78	0.83
1:E:220:LYS:O	1:E:220:LYS:HD2	1.77	0.83
2:J:244:ILE:H	2:J:244:ILE:HD13	1.40	0.83
2:J:261:VAL:HG13	2:J:276:VAL:HG21	1.61	0.83
2:B:157:PRO:HG2	2:B:184:MET:HA	1.60	0.83
1:I:135:ILE:H	1:I:135:ILE:HD12	1.43	0.82
1:I:432:GLU:HG3	1:I:433:PRO:HD2	1.59	0.82
1:M:503:LEU:O	1:M:507:GLN:HG3	1.79	0.82
2:J:171:PHE:HB2	2:J:208:HIS:ND1	1.93	0.82
1:M:221:HIS:CE1	1:M:228:LEU:H	1.97	0.82
2:J:13:LYS:O	2:J:16:MET:HB2	1.78	0.82
1:E:135:ILE:H	1:E:135:ILE:HD12	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:LEU:H	2:B:100:LEU:HD23	1.43	0.82
2:B:171:PHE:HB2	2:B:208:HIS:ND1	1.95	0.82
1:A:244:ILE:HD11	1:A:263:LYS:HG3	1.62	0.82
1:E:458:VAL:HG12	1:E:548:VAL:HG22	1.61	0.82
1:E:274:ILE:HG23	1:E:306:ASN:HD21	1.41	0.81
1:I:558:LYS:HG2	1:I:559:VAL:N	1.91	0.81
2:N:261:VAL:HG13	2:N:276:VAL:HG21	1.61	0.81
1:E:221:HIS:HE1	1:E:228:LEU:HB2	1.45	0.81
1:M:277:ARG:NH1	1:M:336:GLN:HG3	1.94	0.81
1:M:485:ALA:O	1:M:489:SER:HB3	1.79	0.81
1:A:559:VAL:HG22	1:A:560:LEU:N	1.94	0.81
1:I:199:ARG:NH2	1:I:223:LYS:HB2	1.95	0.81
1:M:23:GLN:HE21	1:M:60:VAL:H	1.24	0.81
1:M:253:THR:HG22	1:M:292:VAL:HG22	1.62	0.81
2:N:96:HIS:CE1	2:N:381:VAL:O	2.32	0.81
1:A:274:ILE:HG23	1:A:306:ASN:HD21	1.45	0.81
1:E:24:TRP:HB2	1:E:25:PRO:HD2	1.62	0.80
2:F:13:LYS:O	2:F:16:MET:HB2	1.81	0.80
1:I:485:ALA:O	1:I:489:SER:HB3	1.81	0.80
1:I:503:LEU:O	1:I:507:GLN:HG3	1.81	0.80
1:I:100:LEU:HD21	1:I:181:TYR:CE1	2.17	0.80
1:I:458:VAL:HG12	1:I:548:VAL:HG22	1.63	0.80
1:M:73:LYS:HE3	1:M:146:TYR:OH	1.81	0.80
1:A:3:SER:OG	1:A:5:ILE:HG22	1.81	0.80
1:I:49:LYS:HE3	1:I:142:ILE:HD12	1.61	0.80
1:I:260:LEU:HD21	1:I:303:LEU:HD23	1.62	0.80
2:J:64:LYS:HE3	2:J:69:THR:HA	1.62	0.80
1:A:557:ARG:O	1:A:557:ARG:HD3	1.81	0.80
1:E:458:VAL:CG1	1:E:548:VAL:HG22	2.11	0.80
1:E:510:PRO:HB2	1:E:522:ILE:HD11	1.64	0.80
2:F:314:VAL:HG22	2:F:315:HIS:N	1.97	0.80
2:J:5:ILE:HD11	5:Q:1:GLC:H4	1.64	0.80
2:J:281:LYS:O	2:J:284:ARG:HB2	1.81	0.80
1:A:171:PHE:HB2	1:A:208:HIS:HD2	1.43	0.79
1:A:27:THR:O	1:A:31:ILE:HG13	1.82	0.79
1:A:221:HIS:H	1:A:221:HIS:CD2	1.96	0.79
1:E:500:GLN:HB3	2:F:422:LEU:HD13	1.63	0.79
2:N:421:PRO:HA	2:N:426:TRP:HE1	1.47	0.79
1:E:425:LEU:HD13	1:E:509:GLN:HE22	1.48	0.79
2:N:13:LYS:O	2:N:16:MET:HB2	1.81	0.79
1:E:503:LEU:O	1:E:507:GLN:HG3	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:261:VAL:HG13	2:B:276:VAL:HG21	1.62	0.79
2:N:69:THR:O	2:N:69:THR:HG22	1.80	0.79
1:A:511:ASP:OD1	1:A:512:LYS:HG3	1.83	0.79
2:F:94:ILE:HD11	2:F:161:GLN:HG2	1.63	0.79
2:F:281:LYS:O	2:F:284:ARG:HB2	1.82	0.79
1:E:278:GLN:HG3	1:E:298:GLU:HB3	1.64	0.79
2:J:3:SER:N	2:J:4:PRO:HD3	1.98	0.79
2:B:281:LYS:O	2:B:284:ARG:HB2	1.83	0.79
1:I:458:VAL:CG1	1:I:548:VAL:HG22	2.13	0.78
1:E:103:LYS:HE3	1:E:179:VAL:HG21	1.64	0.78
4:H:821:DC:H2'	4:H:822:2DA:H8	1.63	0.78
1:E:441:TYR:HD1	1:E:544:GLY:HA3	1.43	0.78
2:J:30:LYS:HE2	2:J:62:ALA:O	1.81	0.78
2:B:194:GLU:OE2	2:B:195:ILE:HG22	1.84	0.78
2:F:171:PHE:HB2	2:F:208:HIS:ND1	1.99	0.78
1:A:503:LEU:O	1:A:507:GLN:HG3	1.84	0.77
2:F:314:VAL:HG22	2:F:315:HIS:H	1.48	0.77
1:M:163:SER:O	1:M:167:ILE:HD13	1.83	0.77
2:J:115:TYR:OH	2:J:157:PRO:HG3	1.84	0.77
1:M:155:GLY:O	1:M:159:ILE:HG12	1.83	0.77
2:B:314:VAL:HG22	2:B:315:HIS:N	2.00	0.77
1:A:103:LYS:HE3	1:A:179:VAL:HG21	1.66	0.77
1:E:52:PRO:HA	1:E:143:ARG:NH2	2.00	0.77
1:M:244:ILE:HD11	1:M:263:LYS:HG3	1.67	0.77
2:N:303:LEU:HD21	2:N:307:ARG:HH21	1.49	0.77
1:I:171:PHE:HB2	1:I:208:HIS:CD2	2.20	0.77
2:J:421:PRO:HA	2:J:426:TRP:HE1	1.49	0.77
2:B:94:ILE:HD11	2:B:161:GLN:HG2	1.66	0.77
1:E:235:HIS:HB2	1:E:238:LYS:O	1.85	0.77
1:A:278:GLN:HG3	1:A:298:GLU:HB3	1.66	0.76
1:A:155:GLY:O	1:A:159:ILE:HG12	1.84	0.76
1:A:280:SER:O	1:A:283:LEU:HD12	1.85	0.76
1:E:73:LYS:HE3	1:E:146:TYR:OH	1.84	0.76
2:F:421:PRO:HA	2:F:426:TRP:HE1	1.50	0.76
2:J:303:LEU:HD21	2:J:307:ARG:HH21	1.49	0.76
1:I:235:HIS:HB3	1:I:236:PRO:HD2	1.67	0.76
1:I:441:TYR:CE1	1:I:544:GLY:HA3	2.19	0.76
2:B:314:VAL:HG22	2:B:315:HIS:H	1.49	0.76
2:B:421:PRO:HA	2:B:426:TRP:HE1	1.49	0.76
1:E:260:LEU:HD21	1:E:303:LEU:HD23	1.67	0.76
2:J:314:VAL:HG22	2:J:315:HIS:H	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LYS:HE3	1:A:142:ILE:HD12	1.67	0.76
1:I:156:SER:N	1:I:157:PRO:HD2	2.01	0.76
2:J:65:LYS:HA	2:J:407:GLN:HE21	1.51	0.76
1:E:3:SER:OG	1:E:5:ILE:HG22	1.84	0.76
1:E:221:HIS:CE1	1:E:228:LEU:H	2.04	0.76
2:N:65:LYS:HB2	2:N:68:SER:CB	2.15	0.76
1:A:27:THR:HB	1:A:30:LYS:HB2	1.67	0.76
1:I:23:GLN:HE21	1:I:60:VAL:H	1.33	0.76
1:M:548:VAL:O	1:M:552:VAL:HG22	1.86	0.75
2:J:314:VAL:HG22	2:J:315:HIS:N	2.01	0.75
1:E:463:ARG:NH1	1:E:463:ARG:HB2	2.02	0.75
1:M:278:GLN:HG3	1:M:298:GLU:HB3	1.68	0.75
1:E:463:ARG:HB2	1:E:463:ARG:HH11	1.51	0.75
2:N:387:PRO:HG2	2:N:389:PHE:CE1	2.22	0.75
3:C:709:DC:H2'	3:C:710:DG:H8	1.51	0.75
2:B:428:GLN:HG2	2:B:429:GLY:N	2.01	0.75
1:A:52:PRO:HA	1:A:143:ARG:NH2	2.01	0.75
4:H:817:MRG:H2'	4:H:818:DC:C6	2.21	0.75
2:F:254:VAL:HG13	2:F:283:LEU:HD22	1.68	0.74
1:E:102:LYS:HD2	1:E:102:LYS:N	2.01	0.74
1:E:548:VAL:O	1:E:552:VAL:HG22	1.86	0.74
2:J:100:LEU:H	2:J:100:LEU:HD23	1.52	0.74
1:A:72:ARG:HG3	1:A:151:GLN:HE22	1.50	0.74
1:E:211:ARG:HD2	2:J:5:ILE:HD13	1.67	0.74
1:I:24:TRP:HB2	1:I:25:PRO:HD2	1.68	0.74
1:I:511:ASP:OD1	1:I:512:LYS:HG2	1.84	0.74
2:B:33:ALA:O	2:B:37:ILE:HG12	1.88	0.74
1:E:27:THR:HB	1:E:30:LYS:HB2	1.69	0.74
2:N:281:LYS:O	2:N:284:ARG:HB2	1.87	0.74
1:E:221:HIS:H	1:E:221:HIS:CD2	2.05	0.74
2:F:303:LEU:HD21	2:F:307:ARG:HH21	1.50	0.74
1:I:207:GLN:NE2	1:I:210:LEU:HD23	2.01	0.74
1:I:463:ARG:HB2	1:I:463:ARG:HH11	1.52	0.74
1:I:463:ARG:HB2	1:I:463:ARG:NH1	2.02	0.74
2:N:314:VAL:HG22	2:N:315:HIS:N	2.02	0.74
1:A:31:ILE:O	1:A:35:VAL:HG23	1.88	0.74
2:B:64:LYS:CE	2:B:69:THR:HG23	2.18	0.74
2:F:194:GLU:OE2	2:F:195:ILE:HG22	1.87	0.74
2:J:387:PRO:HG2	2:J:389:PHE:CE1	2.23	0.74
2:N:314:VAL:HG22	2:N:315:HIS:H	1.52	0.74
1:E:244:ILE:HD11	1:E:263:LYS:HG3	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:447:ASN:HB2	1:E:556:ILE:HG23	1.70	0.74
1:I:510:PRO:HB2	1:I:522:ILE:HD11	1.70	0.74
2:J:33:ALA:O	2:J:37:ILE:HG12	1.88	0.74
1:I:228:LEU:HA	1:I:232:TYR:O	1.88	0.74
1:I:425:LEU:HD13	1:I:509:GLN:HE22	1.51	0.74
2:J:254:VAL:HG13	2:J:283:LEU:HD22	1.69	0.74
4:P:805:DG:H5"	9:P:81:HOH:O	1.88	0.74
1:A:73:LYS:O	1:A:74:LEU:HD23	1.88	0.73
1:A:253:THR:HG22	1:A:292:VAL:HG22	1.70	0.73
1:M:511:ASP:OD1	1:M:512:LYS:CG	2.36	0.73
1:A:24:TRP:HB2	1:A:25:PRO:HD2	1.70	0.73
1:A:458:VAL:HG13	1:A:548:VAL:HG22	1.68	0.73
1:A:73:LYS:HE3	1:A:146:TYR:OH	1.88	0.73
2:B:64:LYS:HE3	2:B:69:THR:CA	2.14	0.73
2:B:369:THR:O	2:B:373:GLN:HG3	1.88	0.73
1:I:101:LYS:CE	1:I:321:PRO:HG3	2.17	0.73
2:N:100:LEU:HD23	2:N:100:LEU:H	1.53	0.73
1:A:425:LEU:HD13	1:A:509:GLN:HE22	1.53	0.73
1:A:156:SER:N	1:A:157:PRO:HD2	2.03	0.73
1:A:510:PRO:HB2	1:A:522:ILE:HD11	1.69	0.73
2:J:234:LEU:HD12	2:J:234:LEU:N	2.03	0.73
1:I:229:TRP:CE2	1:I:230:MET:HG2	2.24	0.73
1:M:510:PRO:HB2	1:M:522:ILE:HD11	1.71	0.73
2:N:33:ALA:O	2:N:37:ILE:HG12	1.89	0.73
1:M:90:VAL:CG2	2:N:140:PRO:HB2	2.17	0.72
2:F:387:PRO:HG2	2:F:389:PHE:CE1	2.24	0.72
2:B:75:VAL:HG11	2:B:77:PHE:CE2	2.24	0.72
1:E:171:PHE:HB2	1:E:208:HIS:CD2	2.24	0.72
2:B:74:LEU:HD12	2:B:75:VAL:N	2.04	0.72
3:C:708:DG:H2'	3:C:709:DC:C6	2.25	0.72
1:A:163:SER:O	1:A:167:ILE:HD13	1.88	0.72
2:B:94:ILE:CD1	2:B:161:GLN:HG2	2.19	0.72
1:A:320:ASP:OD2	1:A:323:LYS:HE2	1.89	0.72
1:E:511:ASP:OD1	1:E:512:LYS:CG	2.35	0.72
1:I:101:LYS:HE3	1:I:321:PRO:CG	2.19	0.72
2:J:115:TYR:CZ	2:J:157:PRO:HG3	2.24	0.72
1:I:90:VAL:HG23	2:J:141:GLY:O	1.88	0.72
2:F:33:ALA:O	2:F:37:ILE:HG12	1.90	0.71
1:M:108:VAL:O	1:M:220:LYS:HB2	1.89	0.71
2:F:94:ILE:CD1	2:F:161:GLN:HG2	2.20	0.71
1:I:27:THR:O	1:I:31:ILE:HG13	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:244:ILE:HD11	1:I:263:LYS:HG3	1.71	0.71
1:I:286:THR:O	1:I:287:LYS:CG	2.32	0.71
3:K:709:DC:H2'	3:K:710:DG:H8	1.55	0.71
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.71	0.71
1:A:221:HIS:H	1:A:221:HIS:HD2	1.38	0.71
1:E:27:THR:O	1:E:31:ILE:HG13	1.90	0.71
2:F:74:LEU:HD12	2:F:75:VAL:N	2.05	0.71
1:M:156:SER:N	1:M:157:PRO:HD2	2.05	0.71
1:M:4:PRO:HD2	1:M:212:TRP:O	1.90	0.71
1:M:116:PHE:HA	1:M:148:VAL:HG21	1.73	0.71
2:N:115:TYR:CZ	2:N:157:PRO:HG3	2.26	0.71
2:N:194:GLU:OE2	2:N:195:ILE:HG22	1.90	0.71
1:I:199:ARG:O	1:I:203:GLU:HG2	1.91	0.71
1:I:100:LEU:CD2	1:I:181:TYR:CE1	2.74	0.71
1:A:533:LEU:N	1:A:533:LEU:HD12	2.06	0.71
4:D:817:MRG:H2'	4:D:818:DC:C6	2.26	0.71
1:I:2:ILE:H	1:I:2:ILE:HD12	1.55	0.70
2:N:62:ALA:O	2:N:63:ILE:CG2	2.39	0.70
1:A:548:VAL:O	1:A:552:VAL:HG22	1.90	0.70
2:F:175:ASN:HD21	2:F:201:LYS:NZ	1.90	0.70
2:B:122:GLU:HA	2:B:125:ARG:HE	1.57	0.70
1:E:277:ARG:NH1	1:E:336:GLN:CG	2.54	0.70
1:I:223:LYS:HG3	1:I:223:LYS:O	1.90	0.70
2:N:244:ILE:HD13	2:N:244:ILE:H	1.55	0.70
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.73	0.70
2:F:64:LYS:CE	2:F:69:THR:HG23	2.22	0.70
1:I:469:LEU:HD21	1:I:480:GLN:HG3	1.73	0.70
2:J:37:ILE:O	2:J:41:MET:HG3	1.90	0.70
2:F:376:THR:O	2:F:380:ILE:HG13	1.91	0.70
2:J:372:VAL:HG13	2:J:389:PHE:CE2	2.26	0.70
1:E:221:HIS:CE1	1:E:228:LEU:HB2	2.25	0.70
1:I:91:GLN:HG3	1:I:161:GLN:HE22	1.56	0.70
1:I:329:ILE:HD11	1:I:375:ILE:HD12	1.72	0.70
1:M:260:LEU:HD21	1:M:303:LEU:HD23	1.73	0.70
4:L:821:DC:H2'	4:L:822:2DA:H8	1.73	0.70
1:I:439:THR:CG2	2:J:289:LEU:HD13	2.20	0.70
1:A:23:GLN:HE21	1:A:60:VAL:H	1.38	0.70
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.27	0.70
1:I:253:THR:HG22	1:I:292:VAL:HG22	1.74	0.70
2:J:72:ARG:HH21	2:J:409:THR:HG22	1.55	0.70
2:N:254:VAL:HG13	2:N:283:LEU:HD22	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:100:LEU:H	2:F:100:LEU:CD2	2.04	0.69
1:I:548:VAL:O	1:I:552:VAL:HG22	1.92	0.69
3:G:723:DC:H2"	3:G:724:DT:O5'	1.92	0.69
1:E:23:GLN:HE21	1:E:60:VAL:H	1.40	0.69
1:I:101:LYS:HE3	1:I:321:PRO:HG3	1.73	0.69
1:I:278:GLN:HG3	1:I:298:GLU:HB3	1.74	0.69
4:P:821:DC:H2'	4:P:822:2DA:H8	1.72	0.69
1:E:280:SER:O	1:E:283:LEU:HD12	1.92	0.69
2:F:372:VAL:HG13	2:F:389:PHE:CE2	2.26	0.69
1:I:435:VAL:CA	2:J:290:THR:HG21	2.23	0.69
2:N:47:ILE:HG22	2:N:146:TYR:HA	1.74	0.69
1:E:394:GLN:HB2	1:E:397:THR:OG1	1.92	0.69
1:I:303:LEU:O	1:I:307:ARG:HB2	1.93	0.69
1:I:451:LYS:O	1:I:471:ASN:HA	1.92	0.69
1:M:458:VAL:HG13	1:M:548:VAL:HG22	1.73	0.69
1:E:277:ARG:HH11	1:E:336:GLN:HG3	1.54	0.69
1:I:558:LYS:HE3	1:I:559:VAL:O	1.92	0.69
1:I:238:LYS:HZ1	1:I:347:LYS:HE2	1.57	0.69
1:A:366:LYS:O	1:A:370:GLU:HG3	1.91	0.69
2:B:303:LEU:HD21	2:B:307:ARG:HH21	1.56	0.69
1:E:65:LYS:NZ	1:E:70:ARG:HH21	1.90	0.69
1:E:451:LYS:O	1:E:471:ASN:HA	1.93	0.69
1:I:441:TYR:CD1	1:I:544:GLY:CA	2.63	0.69
1:M:27:THR:O	1:M:31:ILE:HG13	1.92	0.69
1:M:288:ALA:HB3	1:M:291:GLU:HG3	1.75	0.69
1:M:451:LYS:O	1:M:471:ASN:HA	1.93	0.69
4:P:802:DA:H4'	4:P:803:DC:OP1	1.93	0.69
2:J:94:ILE:HD11	2:J:161:GLN:HG2	1.75	0.69
2:J:194:GLU:OE2	2:J:195:ILE:HG22	1.91	0.69
2:N:156:SER:HB2	2:N:157:PRO:HD3	1.74	0.69
2:F:234:LEU:HD12	2:F:234:LEU:N	2.08	0.69
1:I:101:LYS:HE3	1:I:321:PRO:HD3	1.75	0.69
2:J:243:PRO:HB2	2:J:244:ILE:HD13	1.75	0.69
2:N:371:ALA:O	2:N:375:ILE:HG12	1.92	0.69
2:B:372:VAL:HG13	2:B:389:PHE:CE2	2.27	0.68
1:M:329:ILE:HD11	1:M:375:ILE:HD12	1.74	0.68
1:M:469:LEU:HD21	1:M:480:GLN:HG3	1.75	0.68
2:N:78:ARG:HD3	2:N:411:ILE:HB	1.76	0.68
2:B:254:VAL:HG13	2:B:283:LEU:HD22	1.74	0.68
1:E:3:SER:HB3	1:E:119:PRO:HD3	1.73	0.68
1:E:366:LYS:O	1:E:370:GLU:HG3	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:469:LEU:HD21	1:E:480:GLN:HG3	1.75	0.68
2:F:100:LEU:HD23	2:F:100:LEU:N	2.08	0.68
1:M:303:LEU:O	1:M:307:ARG:HB2	1.94	0.68
3:G:709:DC:H2'	3:G:710:DG:H8	1.59	0.68
1:A:135:ILE:HD12	1:A:135:ILE:N	2.09	0.68
2:F:356:ARG:HG2	2:F:357:MET:H	1.59	0.68
2:F:37:ILE:O	2:F:41:MET:HG3	1.93	0.68
2:N:31:ILE:O	2:N:35:VAL:HG23	1.94	0.68
1:E:171:PHE:HB2	1:E:208:HIS:HD2	1.59	0.68
2:J:376:THR:HG23	2:J:386:THR:HG23	1.74	0.68
2:N:369:THR:O	2:N:373:GLN:HG3	1.94	0.68
2:J:371:ALA:O	2:J:375:ILE:HG12	1.92	0.68
1:A:237:ASP:OD2	1:A:238:LYS:HD3	1.94	0.68
2:N:122:GLU:HA	2:N:125:ARG:HE	1.59	0.68
1:I:209:LEU:HB3	1:I:214:LEU:HB2	1.74	0.68
2:B:100:LEU:H	2:B:100:LEU:CD2	2.06	0.68
1:M:209:LEU:HB3	1:M:214:LEU:HB2	1.76	0.68
2:F:376:THR:HG23	2:F:386:THR:HG23	1.75	0.67
4:P:818:DC:H2'	4:P:819:DG:H8	1.59	0.67
1:A:90:VAL:HG22	2:B:140:PRO:HB2	1.75	0.67
1:A:102:LYS:HD2	1:A:102:LYS:N	2.05	0.67
1:A:235:HIS:HB2	1:A:238:LYS:O	1.94	0.67
2:B:376:THR:O	2:B:380:ILE:HG13	1.94	0.67
3:C:709:DC:H2'	3:C:710:DG:C8	2.28	0.67
3:G:708:DG:H2'	3:G:709:DC:C6	2.29	0.67
4:P:818:DC:H2'	4:P:819:DG:C8	2.29	0.67
1:E:132:ILE:O	1:E:141:GLY:HA3	1.94	0.67
1:E:148:VAL:O	1:E:150:PRO:HD3	1.94	0.67
1:I:103:LYS:HE3	1:I:179:VAL:CG2	2.23	0.67
2:J:31:ILE:O	2:J:35:VAL:HG23	1.94	0.67
1:A:227:PHE:HB2	1:A:234:LEU:HB2	1.76	0.67
1:E:317:VAL:HG11	1:E:347:LYS:HB3	1.75	0.67
2:N:376:THR:HG23	2:N:386:THR:HG23	1.76	0.67
4:L:818:DC:H2'	4:L:819:DG:C8	2.29	0.67
2:N:184:MET:SD	2:N:410:TRP:HB3	2.35	0.67
4:L:818:DC:H2'	4:L:819:DG:H8	1.59	0.67
1:A:70:ARG:HH12	7:A:823:ZP4:C31	2.07	0.67
1:A:221:HIS:CD2	1:A:221:HIS:N	2.62	0.67
1:E:227:PHE:HB2	1:E:234:LEU:HB2	1.76	0.67
1:E:329:ILE:HD11	1:E:375:ILE:HD12	1.77	0.67
1:M:94:ILE:HD11	3:O:708:DG:H21	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:425:LEU:HD13	1:M:509:GLN:HE22	1.59	0.67
1:A:135:ILE:H	1:A:135:ILE:CD1	2.08	0.67
1:E:303:LEU:O	1:E:307:ARG:HB2	1.94	0.67
2:F:64:LYS:HE3	2:F:69:THR:CA	2.20	0.67
3:G:705:DA:H2"	3:G:706:DT:O5'	1.94	0.67
1:A:451:LYS:O	1:A:471:ASN:HA	1.95	0.67
1:A:559:VAL:HG22	1:A:560:LEU:H	1.58	0.67
1:E:136:ASN:OD1	1:E:138:GLU:HG3	1.95	0.67
1:E:277:ARG:HH11	1:E:336:GLN:CG	2.08	0.67
2:J:107:THR:HG23	2:J:232:TYR:HE2	1.58	0.67
2:J:156:SER:HB2	2:J:157:PRO:HD3	1.76	0.67
1:A:148:VAL:O	1:A:150:PRO:HD3	1.95	0.67
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.77	0.66
1:I:280:SER:O	1:I:283:LEU:HD12	1.94	0.66
2:J:72:ARG:HH22	2:J:151:GLN:HB3	1.60	0.66
1:M:184:MET:HG3	4:P:822:2DA:H2'	1.75	0.66
4:D:802:DA:H4'	4:D:803:DC:OP1	1.93	0.66
1:A:518:VAL:O	1:A:522:ILE:HG12	1.94	0.66
1:M:556:ILE:HG13	1:M:557:ARG:N	2.10	0.66
1:E:22:LYS:HG2	1:E:23:GLN:N	2.10	0.66
1:A:559:VAL:CG2	1:A:560:LEU:N	2.58	0.66
1:E:463:ARG:HH11	1:E:463:ARG:CB	2.08	0.66
2:F:75:VAL:HG11	2:F:77:PHE:CE2	2.31	0.66
2:J:66:LYS:O	2:J:67:ASP:HB2	1.94	0.66
1:M:135:ILE:HD12	1:M:135:ILE:N	2.08	0.66
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.76	0.66
1:E:435:VAL:HA	2:F:290:THR:HG21	1.75	0.66
2:J:125:ARG:HG2	2:J:146:TYR:O	1.96	0.66
2:B:371:ALA:O	2:B:375:ILE:HG12	1.96	0.66
2:F:369:THR:O	2:F:373:GLN:HG3	1.96	0.66
1:I:195:ILE:O	1:I:199:ARG:HG2	1.96	0.66
1:I:394:GLN:HB2	1:I:397:THR:OG1	1.95	0.66
2:J:369:THR:O	2:J:373:GLN:HG3	1.96	0.66
1:M:135:ILE:H	1:M:135:ILE:CD1	2.08	0.66
2:J:6:GLU:OE1	2:J:6:GLU:HA	1.95	0.66
2:B:153:TRP:CE2	2:B:155:GLY:HA3	2.31	0.66
2:F:314:VAL:CG2	2:F:315:HIS:H	2.08	0.66
2:N:171:PHE:HB2	2:N:208:HIS:CE1	2.31	0.66
2:J:403:THR:HG23	9:J:449:HOH:O	1.95	0.66
1:M:116:PHE:HA	1:M:148:VAL:CG2	2.26	0.66
2:N:72:ARG:NH1	2:N:151:GLN:OE1	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:372:VAL:HG13	2:N:389:PHE:CE2	2.31	0.66
1:A:559:VAL:CG2	1:A:560:LEU:H	2.09	0.65
2:B:100:LEU:HD23	2:B:100:LEU:N	2.11	0.65
2:F:418:ASN:O	2:F:419:THR:HG23	1.95	0.65
2:J:376:THR:O	2:J:380:ILE:HG13	1.96	0.65
1:M:53:GLU:O	1:M:55:PRO:HD3	1.96	0.65
1:M:195:ILE:O	1:M:199:ARG:HG2	1.96	0.65
1:A:469:LEU:HD21	1:A:480:GLN:HG3	1.79	0.65
2:B:247:PRO:HA	2:B:431:HIS:CA	2.26	0.65
1:E:557:ARG:O	1:E:558:LYS:HG2	1.96	0.65
1:M:408:ALA:HB3	2:N:393:ILE:HB	1.78	0.65
2:N:78:ARG:HA	2:N:81:ASN:HD22	1.60	0.65
4:D:818:DC:H2'	4:D:819:DG:C8	2.31	0.65
1:A:303:LEU:O	1:A:307:ARG:HB2	1.96	0.65
1:M:394:GLN:HB2	1:M:397:THR:OG1	1.96	0.65
2:F:261:VAL:HG13	2:F:276:VAL:CG2	2.25	0.65
1:A:317:VAL:HG11	1:A:347:LYS:HB3	1.78	0.65
2:F:50:ILE:HG21	2:F:145:GLN:OE1	1.95	0.65
1:I:238:LYS:NZ	1:I:347:LYS:HE2	2.12	0.65
1:M:26:LEU:HD12	1:M:133:PRO:HG3	1.78	0.65
2:F:175:ASN:HD21	2:F:201:LYS:CE	2.09	0.65
2:J:234:LEU:H	2:J:234:LEU:CD1	2.09	0.65
3:K:709:DC:H2'	3:K:710:DG:C8	2.32	0.65
2:B:31:ILE:CD1	2:B:133:PRO:HG2	2.26	0.65
2:B:314:VAL:CG2	2:B:315:HIS:H	2.08	0.65
2:F:356:ARG:HG2	2:F:357:MET:N	2.12	0.65
1:I:324:ASP:HA	1:I:385:LYS:HZ1	1.62	0.65
3:O:707:DG:H2"	3:O:708:DG:H5'	1.78	0.65
1:A:557:ARG:O	1:A:557:ARG:CD	2.44	0.65
2:F:319:TYR:OH	2:F:385:LYS:HD3	1.97	0.65
1:E:181:TYR:CE1	2:F:138:GLU:HG2	2.32	0.65
2:J:314:VAL:CG2	2:J:315:HIS:H	2.10	0.65
1:M:70:ARG:HG2	1:M:71:TRP:H	1.59	0.65
1:M:207:GLN:NE2	1:M:210:LEU:HD23	2.12	0.65
2:N:37:ILE:O	2:N:41:MET:HG3	1.96	0.65
3:G:709:DC:H2'	3:G:710:DG:C8	2.32	0.65
1:E:425:LEU:HD13	1:E:509:GLN:NE2	2.12	0.64
1:E:518:VAL:O	1:E:522:ILE:HG12	1.96	0.64
2:F:69:THR:O	2:F:69:THR:HG22	1.97	0.64
1:I:118:VAL:HB	1:I:149:LEU:HD22	1.79	0.64
2:J:78:ARG:HA	2:J:81:ASN:HD22	1.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:130:PHE:CZ	1:M:144:TYR:HB2	2.32	0.64
3:G:707:DG:H2"	3:G:708:DG:H5'	1.79	0.64
1:A:277:ARG:HH11	1:A:336:GLN:HG3	1.60	0.64
2:F:78:ARG:HA	2:F:81:ASN:HD22	1.62	0.64
2:J:169:GLU:HA	2:J:169:GLU:OE2	1.97	0.64
2:J:171:PHE:HB2	2:J:208:HIS:CE1	2.33	0.64
2:J:175:ASN:HD21	2:J:201:LYS:NZ	1.95	0.64
1:M:27:THR:HB	1:M:30:LYS:HB2	1.78	0.64
3:C:723:DC:H2"	3:C:724:DT:O5'	1.96	0.64
1:I:320:ASP:OD2	1:I:323:LYS:HE2	1.97	0.64
1:M:439:THR:CG2	2:N:289:LEU:HD13	2.26	0.64
2:N:72:ARG:HH22	2:N:151:GLN:HB3	1.62	0.64
2:B:156:SER:HB2	2:B:157:PRO:HD3	1.78	0.64
1:E:135:ILE:HD12	1:E:135:ILE:N	2.13	0.64
2:N:8:VAL:HG21	2:N:159:ILE:HD12	1.79	0.64
1:A:217:PRO:HB2	1:A:219:GLN:NE2	2.11	0.64
2:F:371:ALA:O	2:F:375:ILE:HG12	1.97	0.64
1:M:24:TRP:HB2	1:M:25:PRO:HD2	1.79	0.64
1:M:227:PHE:HB2	1:M:234:LEU:HB2	1.80	0.64
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.33	0.64
1:E:463:ARG:HG2	1:E:464:GLN:N	2.13	0.64
1:E:556:ILE:HD12	1:E:556:ILE:N	2.12	0.64
1:I:199:ARG:HH22	1:I:223:LYS:HB2	1.60	0.64
1:M:447:ASN:HA	1:M:556:ILE:HD13	1.80	0.64
4:D:821:DC:H2'	4:D:822:2DA:H8	1.78	0.64
2:B:64:LYS:CE	2:B:69:THR:HA	2.17	0.64
1:E:301:LEU:O	1:E:304:ALA:HB3	1.98	0.64
1:I:229:TRP:NE1	1:I:230:MET:HG2	2.13	0.64
1:I:463:ARG:HH11	1:I:463:ARG:CB	2.10	0.64
2:J:115:TYR:HB3	2:J:149:LEU:HB2	1.78	0.64
1:M:73:LYS:HE3	1:M:146:TYR:CZ	2.32	0.64
1:E:163:SER:O	1:E:167:ILE:HD13	1.96	0.64
1:E:207:GLN:HE22	1:E:210:LEU:HD23	1.63	0.64
1:E:441:TYR:CE1	1:E:544:GLY:HA3	2.30	0.64
1:I:130:PHE:CZ	1:I:144:TYR:HB2	2.33	0.64
1:M:46:LYS:HD3	1:M:116:PHE:HB3	1.79	0.64
1:M:529:GLU:O	1:M:530:LYS:HG3	1.97	0.64
2:B:125:ARG:HG2	2:B:146:TYR:O	1.98	0.64
1:I:90:VAL:HG22	2:J:140:PRO:HB2	1.79	0.64
2:N:153:TRP:CZ2	2:N:155:GLY:HA3	2.33	0.64
2:N:418:ASN:O	2:N:419:THR:HG23	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:723:DC:H2"	3:K:724:DT:O5'	1.97	0.64
2:B:69:THR:HG22	2:B:69:THR:O	1.96	0.64
1:E:64:LYS:HD3	1:E:68:SER:HB3	1.79	0.64
2:F:28:GLU:HA	2:F:135:ILE:HD11	1.80	0.64
1:I:109:LEU:HG	1:I:220:LYS:HD2	1.79	0.64
2:J:118:VAL:HG22	5:Q:1:GLC:H3	1.80	0.64
1:A:324:ASP:HA	1:A:385:LYS:HZ1	1.63	0.63
1:A:394:GLN:HB2	1:A:397:THR:OG1	1.98	0.63
2:F:7:THR:HG22	2:F:119:PRO:HG2	1.80	0.63
1:I:132:ILE:O	1:I:141:GLY:HA3	1.98	0.63
2:J:100:LEU:H	2:J:100:LEU:CD2	2.10	0.63
2:J:195:ILE:HG13	2:J:199:ARG:NH1	2.13	0.63
3:O:709:DC:H2'	3:O:710:DG:H8	1.62	0.63
2:J:122:GLU:HA	2:J:125:ARG:HE	1.63	0.63
2:N:13:LYS:HD3	2:N:86:ASP:HB2	1.80	0.63
2:N:153:TRP:CE2	2:N:155:GLY:HA3	2.33	0.63
2:B:64:LYS:HE2	2:B:69:THR:HG23	1.78	0.63
1:E:27:THR:HB	1:E:30:LYS:CB	2.28	0.63
1:E:209:LEU:HB3	1:E:214:LEU:HB2	1.79	0.63
1:E:255:ASN:HD22	1:E:289:LEU:HD22	1.63	0.63
2:F:31:ILE:O	2:F:35:VAL:HG23	1.97	0.63
1:I:442:VAL:HG11	1:I:485:ALA:HB2	1.80	0.63
1:M:366:LYS:O	1:M:370:GLU:HG3	1.97	0.63
1:A:109:LEU:N	1:A:109:LEU:HD12	2.14	0.63
1:A:221:HIS:CE1	1:A:228:LEU:HB2	2.28	0.63
2:B:153:TRP:CZ2	2:B:155:GLY:HA3	2.33	0.63
2:F:241:VAL:HG13	2:F:351:THR:N	2.13	0.63
3:C:707:DG:H2'	3:C:708:DG:H8	1.63	0.63
1:A:425:LEU:HD13	1:A:509:GLN:NE2	2.13	0.63
2:B:31:ILE:O	2:B:35:VAL:HG23	1.98	0.63
1:E:195:ILE:O	1:E:199:ARG:HG2	1.97	0.63
1:I:277:ARG:HH11	1:I:336:GLN:HG3	1.61	0.63
1:I:324:ASP:HA	1:I:385:LYS:NZ	2.13	0.63
2:N:175:ASN:HD21	2:N:201:LYS:NZ	1.97	0.63
1:I:3:SER:OG	1:I:5:ILE:HG22	1.99	0.63
1:I:500:GLN:HB3	2:J:422:LEU:HD13	1.80	0.63
2:N:377:THR:HA	2:N:380:ILE:HD12	1.80	0.63
2:J:13:LYS:HD3	2:J:86:ASP:HB2	1.79	0.63
2:J:60:VAL:CG1	2:J:75:VAL:HG22	2.29	0.63
1:M:49:LYS:HE3	1:M:142:ILE:HD12	1.81	0.63
4:D:818:DC:H2'	4:D:819:DG:H8	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:LYS:NZ	1:E:130:PHE:CE2	2.60	0.62
1:M:91:GLN:HG3	1:M:161:GLN:HE22	1.63	0.62
1:M:132:ILE:O	1:M:141:GLY:HA3	1.99	0.62
2:N:303:LEU:HD21	2:N:307:ARG:NH2	2.14	0.62
2:B:339:TYR:CD2	2:B:375:ILE:HD12	2.33	0.62
2:B:418:ASN:O	2:B:419:THR:HG23	1.99	0.62
1:M:67:ASN:O	1:M:68:SER:CB	2.44	0.62
2:N:100:LEU:H	2:N:100:LEU:CD2	2.11	0.62
1:A:22:LYS:HG2	1:A:23:GLN:N	2.14	0.62
1:A:237:ASP:O	1:A:238:LYS:HD2	1.99	0.62
1:I:136:ASN:HB3	1:I:138:GLU:HG3	1.81	0.62
1:I:529:GLU:O	1:I:530:LYS:HG3	1.99	0.62
2:J:153:TRP:CZ2	2:J:155:GLY:HA3	2.34	0.62
2:J:244:ILE:H	2:J:244:ILE:CD1	2.12	0.62
2:J:303:LEU:HD21	2:J:307:ARG:NH2	2.14	0.62
2:N:6:GLU:OE1	2:N:6:GLU:HA	1.99	0.62
2:N:314:VAL:CG2	2:N:315:HIS:H	2.13	0.62
3:K:706:DT:H2'	3:K:707:DG:C8	2.34	0.62
2:B:118:VAL:HG13	2:B:119:PRO:HD2	1.81	0.62
2:B:161:GLN:NE2	2:B:161:GLN:HA	2.14	0.62
1:E:398:TRP:CZ2	1:E:411:ILE:HG12	2.34	0.62
2:F:244:ILE:H	2:F:244:ILE:CD1	2.12	0.62
1:A:15:GLY:HA2	2:F:165:THR:HG21	1.82	0.62
1:A:132:ILE:O	1:A:141:GLY:HA3	1.99	0.62
1:A:301:LEU:O	1:A:304:ALA:HB3	2.00	0.62
1:I:49:LYS:CE	1:I:142:ILE:HD12	2.28	0.62
2:B:319:TYR:OH	2:B:385:LYS:HD3	2.00	0.62
1:E:135:ILE:H	1:E:135:ILE:CD1	2.12	0.62
2:F:122:GLU:HA	2:F:125:ARG:HE	1.65	0.62
1:I:31:ILE:O	1:I:35:VAL:HG23	1.98	0.62
2:J:149:LEU:HB3	2:J:156:SER:OG	1.99	0.62
2:N:74:LEU:HD12	2:N:75:VAL:N	2.15	0.62
4:L:802:DA:H4'	4:L:803:DC:OP1	2.00	0.62
1:A:406:TRP:HD1	1:A:407:GLN:HE21	1.47	0.62
2:B:175:ASN:HD21	2:B:201:LYS:NZ	1.98	0.62
2:F:241:VAL:HG13	2:F:351:THR:H	1.65	0.62
2:J:47:ILE:HG22	2:J:146:TYR:HA	1.80	0.62
2:J:418:ASN:O	2:J:419:THR:HG23	1.99	0.62
1:M:94:ILE:CD1	3:O:708:DG:H21	2.12	0.62
2:F:5:ILE:HG23	2:F:6:GLU:N	2.15	0.62
2:F:153:TRP:CE2	2:F:155:GLY:HA3	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:706:DT:H2'	3:G:707:DG:H8	1.64	0.62
1:I:285:GLY:N	3:K:714:DG:OP1	2.32	0.62
1:M:442:VAL:HB	1:M:481:ALA:HB1	1.81	0.62
4:H:818:DC:H2'	4:H:819:DG:C8	2.35	0.62
1:A:324:ASP:HA	1:A:385:LYS:NZ	2.15	0.62
2:B:303:LEU:HD23	2:B:303:LEU:C	2.19	0.62
1:E:164:MET:HE2	1:E:168:LEU:HD11	1.82	0.62
2:F:31:ILE:CD1	2:F:133:PRO:HG2	2.30	0.62
2:F:303:LEU:HD21	2:F:307:ARG:NH2	2.14	0.62
2:J:74:LEU:HD12	2:J:75:VAL:N	2.15	0.62
2:N:69:THR:O	2:N:69:THR:CG2	2.47	0.62
1:E:118:VAL:O	1:E:148:VAL:HG23	2.00	0.61
1:E:253:THR:HG22	1:E:292:VAL:HG22	1.81	0.61
1:E:438:GLU:OE2	1:E:463:ARG:NH1	2.33	0.61
1:I:101:LYS:HE3	1:I:321:PRO:CD	2.29	0.61
2:J:5:ILE:CG1	2:J:6:GLU:H	2.08	0.61
3:K:707:DG:H2"	3:K:708:DG:H5'	1.80	0.61
1:A:103:LYS:HE3	1:A:179:VAL:CG2	2.28	0.61
1:A:116:PHE:C	1:A:148:VAL:HG21	2.21	0.61
1:A:194:GLU:OE1	1:A:194:GLU:HA	1.99	0.61
1:A:195:ILE:O	1:A:199:ARG:HG2	1.99	0.61
1:A:329:ILE:HG12	1:A:339:TYR:HB3	1.82	0.61
1:E:446:ALA:C	1:E:556:ILE:HG21	2.21	0.61
2:F:303:LEU:C	2:F:303:LEU:HD23	2.20	0.61
2:J:24:TRP:CH2	2:J:403:THR:HG21	2.35	0.61
2:J:111:VAL:HG11	2:J:187:LEU:HD22	1.81	0.61
1:M:320:ASP:OD2	1:M:323:LYS:HE2	1.99	0.61
2:N:125:ARG:HG2	2:N:146:TYR:O	2.00	0.61
1:E:303:LEU:O	1:E:303:LEU:HD13	2.01	0.61
2:F:314:VAL:CG2	2:F:315:HIS:N	2.63	0.61
2:N:24:TRP:CZ3	2:N:403:THR:HG21	2.36	0.61
1:A:288:ALA:HB3	1:A:291:GLU:HG3	1.82	0.61
1:E:27:THR:HG22	1:E:30:LYS:H	1.66	0.61
1:I:274:ILE:HG23	1:I:306:ASN:ND2	2.07	0.61
1:I:366:LYS:O	1:I:370:GLU:HG3	2.00	0.61
1:A:64:LYS:HE3	1:A:71:TRP:CZ2	2.36	0.61
1:A:74:LEU:HD13	3:C:705:DA:C5	2.34	0.61
1:E:31:ILE:O	1:E:35:VAL:HG23	2.00	0.61
1:E:382:ILE:O	2:F:136:ASN:HB2	2.01	0.61
2:F:156:SER:HB2	2:F:157:PRO:HD3	1.80	0.61
1:I:425:LEU:HD13	1:I:509:GLN:NE2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:463:ARG:HG2	1:I:464:GLN:N	2.16	0.61
2:B:195:ILE:HG13	2:B:199:ARG:NH1	2.15	0.61
1:A:438:GLU:OE2	1:A:463:ARG:NH1	2.33	0.61
1:A:543:GLY:HA2	2:B:283:LEU:O	2.00	0.61
2:B:101:LYS:HG2	2:B:102:LYS:HG3	1.82	0.61
1:E:288:ALA:HB3	1:E:291:GLU:HG3	1.82	0.61
1:E:408:ALA:HB3	2:F:393:ILE:HB	1.83	0.61
1:E:463:ARG:HG2	1:E:464:GLN:H	1.64	0.61
2:F:426:TRP:H	2:F:426:TRP:HD1	1.48	0.61
1:M:76:ASP:OD1	3:O:705:DA:H4'	2.00	0.61
1:I:31:ILE:HG23	1:I:133:PRO:HG2	1.83	0.61
2:J:336:GLN:NE2	2:J:353:LYS:HD3	2.16	0.61
3:O:709:DC:H2'	3:O:710:DG:C8	2.36	0.61
1:A:435:VAL:HA	2:B:290:THR:HG21	1.81	0.61
2:B:78:ARG:HA	2:B:81:ASN:HD22	1.65	0.61
2:B:376:THR:HG23	2:B:386:THR:HG23	1.82	0.61
2:F:26:LEU:HD12	2:F:31:ILE:HD13	1.82	0.61
1:I:277:ARG:NH1	1:I:336:GLN:CG	2.63	0.61
1:I:398:TRP:CZ2	1:I:411:ILE:HG12	2.36	0.61
1:M:438:GLU:HG2	1:M:461:LYS:HD3	1.83	0.61
1:A:27:THR:HB	1:A:30:LYS:CB	2.30	0.61
1:A:437:ALA:HB1	1:A:492:GLU:O	2.01	0.61
1:I:77:PHE:HB2	1:I:152:GLY:O	2.01	0.61
1:M:235:HIS:HB2	1:M:238:LYS:O	2.01	0.61
2:B:171:PHE:HB2	2:B:208:HIS:CE1	2.35	0.60
1:E:90:VAL:HG22	2:F:140:PRO:HB2	1.83	0.60
1:I:155:GLY:O	1:I:159:ILE:CG1	2.49	0.60
1:I:447:ASN:HB3	1:I:450:THR:OG1	2.00	0.60
1:M:115:TYR:CE2	7:M:823:ZP4:H2'A	2.36	0.60
2:N:244:ILE:HD13	2:N:244:ILE:N	2.15	0.60
3:G:706:DT:H2'	3:G:707:DG:C8	2.36	0.60
2:B:171:PHE:H	2:B:208:HIS:HE1	1.49	0.60
2:J:153:TRP:CE2	2:J:155:GLY:HA3	2.36	0.60
1:A:438:GLU:HG2	1:A:461:LYS:HD3	1.83	0.60
2:B:175:ASN:HD21	2:B:201:LYS:CE	2.14	0.60
1:E:46:LYS:O	1:E:147:ASN:HB2	2.01	0.60
1:M:115:TYR:CD2	7:M:823:ZP4:H2'A	2.36	0.60
2:N:60:VAL:CG1	2:N:75:VAL:HG22	2.28	0.60
2:F:195:ILE:HG13	2:F:199:ARG:NH1	2.16	0.60
1:I:239:TRP:CE2	1:I:316:GLY:HA3	2.36	0.60
1:M:518:VAL:O	1:M:522:ILE:HG12	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:26:LEU:HD12	2:N:31:ILE:HD13	1.83	0.60
3:K:706:DT:H2'	3:K:707:DG:H8	1.66	0.60
3:O:707:DG:H2'	3:O:708:DG:H8	1.66	0.60
1:A:52:PRO:HG2	2:F:318:TYR:CD1	2.35	0.60
1:A:211:ARG:HG3	1:A:211:ARG:HH11	1.67	0.60
1:A:221:HIS:CE1	1:A:228:LEU:H	2.19	0.60
2:B:356:ARG:HG2	2:B:357:MET:H	1.67	0.60
1:I:53:GLU:O	1:I:55:PRO:HD3	2.01	0.60
1:I:221:HIS:H	1:I:221:HIS:CD2	2.20	0.60
1:M:27:THR:HB	1:M:30:LYS:CB	2.32	0.60
2:N:62:ALA:O	2:N:63:ILE:HG23	2.01	0.60
2:N:64:LYS:HE3	2:N:69:THR:CA	2.31	0.60
2:B:242:GLN:NE2	2:B:353:LYS:HE3	2.16	0.60
1:E:339:TYR:CD1	1:E:375:ILE:HD11	2.37	0.60
1:I:67:ASN:O	1:I:68:SER:CB	2.46	0.60
1:I:463:ARG:HG2	1:I:464:GLN:H	1.67	0.60
1:M:238:LYS:HG2	1:M:315:HIS:ND1	2.15	0.60
3:C:706:DT:H2'	3:C:707:DG:C8	2.36	0.60
1:A:109:LEU:HA	1:A:220:LYS:HB2	1.84	0.60
2:B:314:VAL:CG2	2:B:315:HIS:N	2.65	0.60
2:J:428:GLN:HG2	2:J:429:GLY:H	1.65	0.60
1:M:2:ILE:HD11	1:M:45:GLY:O	2.02	0.60
2:N:64:LYS:NZ	2:N:69:THR:O	2.30	0.60
1:A:98:ALA:HB1	1:A:349:LEU:HD22	1.83	0.60
1:E:53:GLU:H	1:E:53:GLU:CD	2.04	0.60
1:E:465:LYS:O	1:E:466:VAL:HG12	2.01	0.60
1:M:274:ILE:HG23	1:M:306:ASN:ND2	2.09	0.60
4:P:817:MRG:H2'	4:P:818:DC:C6	2.37	0.60
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.66	0.60
1:A:398:TRP:CZ2	1:A:411:ILE:HG12	2.37	0.60
1:I:69:THR:O	1:I:69:THR:HG22	2.02	0.60
1:I:218:ASP:HA	1:I:220:LYS:NZ	2.15	0.60
1:M:10:VAL:HG21	1:M:153:TRP:HH2	1.67	0.60
1:M:406:TRP:HD1	1:M:407:GLN:HE21	1.50	0.60
3:C:706:DT:H2'	3:C:707:DG:H8	1.67	0.60
1:A:533:LEU:N	1:A:533:LEU:CD1	2.66	0.59
1:E:229:TRP:CE3	1:E:234:LEU:HD11	2.36	0.59
1:E:329:ILE:HG12	1:E:339:TYR:HB3	1.84	0.59
2:F:234:LEU:HD12	2:F:234:LEU:H	1.66	0.59
2:N:171:PHE:H	2:N:208:HIS:HE1	1.50	0.59
1:A:220:LYS:HD2	1:A:220:LYS:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:VAL:CG1	2:B:75:VAL:HG22	2.28	0.59
2:B:284:ARG:HH11	2:B:284:ARG:HG3	1.67	0.59
1:E:136:ASN:OD1	1:E:138:GLU:CG	2.50	0.59
1:E:174:GLN:C	1:E:176:PRO:HD3	2.22	0.59
1:E:324:ASP:HA	1:E:385:LYS:HZ1	1.67	0.59
1:E:543:GLY:HA2	2:F:283:LEU:O	2.02	0.59
1:I:90:VAL:CG2	2:J:141:GLY:O	2.49	0.59
1:M:398:TRP:CZ2	1:M:411:ILE:HG12	2.37	0.59
3:C:726:DT:H2"	3:C:727:DG:C8	2.37	0.59
2:B:143:ARG:HG2	2:B:143:ARG:HH11	1.68	0.59
1:E:9:PRO:HA	1:E:121:ASP:OD2	2.03	0.59
1:M:28:GLU:HG3	1:M:135:ILE:O	2.02	0.59
1:M:74:LEU:HD13	3:O:705:DA:C5	2.37	0.59
1:M:109:LEU:HD12	1:M:109:LEU:N	2.18	0.59
2:N:169:GLU:HA	2:N:169:GLU:OE2	2.01	0.59
1:A:531:VAL:HG12	1:A:533:LEU:CD1	2.33	0.59
1:E:102:LYS:H	1:E:102:LYS:CD	2.05	0.59
1:I:118:VAL:O	1:I:148:VAL:HG23	2.02	0.59
1:I:174:GLN:C	1:I:176:PRO:HD3	2.22	0.59
1:I:406:TRP:HD1	1:I:407:GLN:HE21	1.50	0.59
2:J:100:LEU:HD23	2:J:100:LEU:N	2.17	0.59
2:J:171:PHE:H	2:J:208:HIS:HE1	1.51	0.59
2:J:261:VAL:HG13	2:J:276:VAL:CG2	2.31	0.59
1:M:194:GLU:OE1	1:M:194:GLU:HA	2.02	0.59
4:H:802:DA:H4'	4:H:803:DC:OP1	2.01	0.59
1:A:174:GLN:C	1:A:176:PRO:HD3	2.22	0.59
1:E:438:GLU:HG2	1:E:461:LYS:HD3	1.83	0.59
2:F:125:ARG:HG2	2:F:146:TYR:O	2.02	0.59
2:J:175:ASN:HD21	2:J:201:LYS:CE	2.15	0.59
3:O:706:DT:H2'	3:O:707:DG:C8	2.38	0.59
1:A:320:ASP:O	1:A:343:GLN:NE2	2.36	0.59
1:E:293:ILE:CD1	1:E:294:PRO:HD2	2.29	0.59
2:F:171:PHE:H	2:F:208:HIS:HE1	1.51	0.59
1:I:303:LEU:O	1:I:303:LEU:HD13	2.03	0.59
1:M:148:VAL:O	1:M:150:PRO:HD3	2.03	0.59
1:M:438:GLU:OE2	1:M:463:ARG:NH1	2.35	0.59
2:N:4:PRO:HB2	2:N:7:THR:HG23	1.84	0.59
2:N:100:LEU:HD23	2:N:100:LEU:N	2.17	0.59
2:B:37:ILE:O	2:B:41:MET:HG3	2.03	0.59
1:I:438:GLU:OE2	1:I:463:ARG:NH1	2.35	0.59
2:N:175:ASN:HD21	2:N:201:LYS:CE	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:406:TRP:HD1	1:E:407:GLN:HE21	1.49	0.59
1:I:277:ARG:HH11	1:I:336:GLN:CG	2.15	0.59
1:M:410:TRP:HZ3	2:N:401:TRP:CE2	2.21	0.59
1:M:447:ASN:CA	1:M:556:ILE:HD13	2.32	0.59
1:A:102:LYS:H	1:A:102:LYS:CD	2.06	0.59
1:A:277:ARG:NH1	1:A:336:GLN:CG	2.66	0.59
4:L:817:MRG:H2'	4:L:818:DC:C6	2.37	0.59
1:A:283:LEU:HD12	1:A:283:LEU:H	1.66	0.59
1:E:76:ASP:OD1	3:G:705:DA:H4'	2.03	0.58
1:I:518:VAL:O	1:I:522:ILE:HG12	2.03	0.58
2:J:337:TRP:HB2	2:J:354:TYR:HB3	1.85	0.58
3:K:726:DT:H2"	3:K:727:DG:C8	2.37	0.58
1:I:438:GLU:HG2	1:I:461:LYS:HD3	1.86	0.58
1:M:103:LYS:HE3	1:M:179:VAL:CG2	2.32	0.58
2:N:337:TRP:HB2	2:N:354:TYR:HB3	1.86	0.58
1:E:531:VAL:HG12	1:E:532:TYR:N	2.16	0.58
2:N:376:THR:O	2:N:380:ILE:HG13	2.04	0.58
3:O:708:DG:H2'	3:O:709:DC:C6	2.37	0.58
2:B:241:VAL:HG13	2:B:351:THR:H	1.67	0.58
1:E:79:GLU:O	1:E:83:ARG:HD2	2.03	0.58
1:E:221:HIS:HE1	1:E:228:LEU:CB	2.16	0.58
1:I:418:ASN:O	1:I:420:PRO:HD3	2.04	0.58
2:J:303:LEU:HD23	2:J:303:LEU:C	2.23	0.58
1:A:277:ARG:HH11	1:A:336:GLN:CG	2.15	0.58
1:I:98:ALA:HB1	1:I:349:LEU:HD22	1.85	0.58
1:M:329:ILE:HG12	1:M:339:TYR:HB3	1.84	0.58
2:N:261:VAL:HG13	2:N:276:VAL:CG2	2.32	0.58
2:B:261:VAL:HG13	2:B:276:VAL:CG2	2.33	0.58
1:E:324:ASP:HA	1:E:385:LYS:NZ	2.19	0.58
2:J:5:ILE:CG1	2:J:6:GLU:N	2.60	0.58
2:J:75:VAL:HG11	2:J:77:PHE:CE2	2.38	0.58
2:J:181:TYR:HA	9:J:450:HOH:O	2.04	0.58
1:M:221:HIS:HE1	1:M:228:LEU:H	1.48	0.58
1:M:277:ARG:NH1	1:M:336:GLN:CG	2.67	0.58
1:E:469:LEU:HD12	1:E:469:LEU:N	2.18	0.58
1:A:27:THR:HG22	1:A:30:LYS:H	1.69	0.58
2:F:60:VAL:CG1	2:F:75:VAL:HG22	2.29	0.58
2:N:62:ALA:C	2:N:63:ILE:HG23	2.22	0.58
2:N:149:LEU:HB3	2:N:156:SER:OG	2.03	0.58
4:H:815:DG:H2"	4:H:816:DG:O5'	2.03	0.58
2:F:131:THR:OG1	2:F:143:ARG:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:8:VAL:CG2	2:N:159:ILE:HD12	2.34	0.58
2:B:400:THR:HG22	2:B:401:TRP:CD2	2.39	0.57
2:F:31:ILE:HD11	2:F:133:PRO:HG2	1.84	0.57
1:I:8:VAL:HB	1:I:159:ILE:HD12	1.86	0.57
2:J:244:ILE:HD13	2:J:244:ILE:N	2.16	0.57
1:M:146:TYR:CD2	1:M:150:PRO:HB3	2.39	0.57
2:N:303:LEU:C	2:N:303:LEU:HD23	2.24	0.57
2:N:366:LYS:O	2:N:370:GLU:HG3	2.03	0.57
3:G:726:DT:H2"	3:G:727:DG:C8	2.39	0.57
1:E:277:ARG:HH12	1:E:336:GLN:HG3	1.68	0.57
2:J:17:ASP:OD2	2:J:20:LYS:HE3	2.04	0.57
2:B:72:ARG:HE	2:B:409:THR:HG22	1.68	0.57
2:B:303:LEU:HD21	2:B:307:ARG:NH2	2.19	0.57
1:I:218:ASP:HA	1:I:220:LYS:HZ2	1.69	0.57
2:J:26:LEU:HD12	2:J:31:ILE:HD13	1.87	0.57
1:A:70:ARG:NH2	7:A:823:ZP4:PD	2.78	0.57
1:A:146:TYR:CD2	1:A:150:PRO:HB3	2.39	0.57
1:A:205:LEU:HD13	1:A:209:LEU:HD11	1.86	0.57
2:B:356:ARG:HG2	2:B:357:MET:N	2.19	0.57
1:E:118:VAL:HB	1:E:149:LEU:HD22	1.87	0.57
2:F:64:LYS:HE2	2:F:69:THR:HG23	1.84	0.57
2:F:217:PRO:HG3	9:F:444:HOH:O	2.04	0.57
1:I:181:TYR:CE1	2:J:138:GLU:HG2	2.39	0.57
2:J:284:ARG:HH11	2:J:284:ARG:HG3	1.70	0.57
1:M:44:GLU:OE2	7:M:823:ZP4:N6R	2.37	0.57
2:N:195:ILE:HG13	2:N:199:ARG:NH1	2.20	0.57
1:A:90:VAL:HG23	2:B:141:GLY:O	2.03	0.57
2:F:17:ASP:OD2	2:F:20:LYS:HE3	2.04	0.57
1:I:194:GLU:OE1	1:I:194:GLU:HA	2.04	0.57
1:M:543:GLY:HA2	2:N:283:LEU:O	2.05	0.57
3:K:707:DG:H2'	3:K:708:DG:H8	1.68	0.57
1:A:394:GLN:NE2	1:A:416:PHE:CZ	2.72	0.57
2:F:252:TRP:HB3	2:F:257:ILE:HD11	1.87	0.57
2:F:284:ARG:HH11	2:F:284:ARG:HG3	1.69	0.57
2:N:336:GLN:NE2	2:N:353:LYS:HD3	2.20	0.57
2:B:336:GLN:NE2	2:B:353:LYS:HD3	2.19	0.57
1:E:281:LYS:HE2	1:E:284:ARG:NH1	2.19	0.57
2:F:203:GLU:O	2:F:207:GLN:HG2	2.04	0.57
2:F:248:GLU:HB2	2:F:307:ARG:NH1	2.20	0.57
2:J:274:ILE:N	2:J:274:ILE:HD12	2.19	0.57
2:N:252:TRP:HB3	2:N:257:ILE:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:MET:HE2	1:A:187:LEU:HD21	1.85	0.57
1:A:500:GLN:HB3	2:B:422:LEU:HD13	1.86	0.57
1:A:500:GLN:HG2	1:A:535:TRP:HE1	1.69	0.57
2:B:252:TRP:HB3	2:B:257:ILE:HD11	1.87	0.57
1:E:211:ARG:HD3	5:Q:1:GLC:H2	1.86	0.57
2:F:161:GLN:HA	2:F:161:GLN:NE2	2.20	0.57
1:I:382:ILE:HG23	2:J:136:ASN:OD1	2.05	0.57
1:I:410:TRP:CZ2	1:I:412:PRO:HA	2.39	0.57
1:M:199:ARG:NH2	1:M:223:LYS:HB2	2.20	0.57
2:N:183:TYR:CD2	2:N:380:ILE:HG21	2.40	0.57
2:B:50:ILE:HG21	2:B:145:GLN:OE1	2.04	0.57
1:E:90:VAL:HG23	2:F:141:GLY:O	2.05	0.57
1:I:91:GLN:CG	1:I:161:GLN:HE22	2.18	0.57
1:M:500:GLN:HB3	2:N:422:LEU:HD13	1.87	0.57
2:N:388:LYS:HG2	2:N:413:GLU:HB3	1.87	0.57
2:B:337:TRP:HB2	2:B:354:TYR:HB3	1.85	0.57
2:F:96:HIS:HA	2:F:181:TYR:CE1	2.40	0.57
1:I:100:LEU:HD21	1:I:181:TYR:CZ	2.39	0.57
2:J:203:GLU:O	2:J:207:GLN:HG2	2.05	0.57
1:I:329:ILE:HG12	1:I:339:TYR:HB3	1.86	0.56
1:I:543:GLY:HA2	2:J:283:LEU:O	2.05	0.56
2:J:234:LEU:HA	9:J:445:HOH:O	2.03	0.56
1:M:16:MET:CE	1:M:83:ARG:HG2	2.35	0.56
1:I:52:PRO:HA	1:I:143:ARG:HH22	1.70	0.56
2:J:241:VAL:HG13	2:J:351:THR:H	1.70	0.56
2:N:393:ILE:HD13	2:N:398:TRP:HB2	1.86	0.56
2:N:400:THR:HG22	2:N:401:TRP:CD2	2.40	0.56
3:O:723:DC:H2"	3:O:724:DT:O5'	2.04	0.56
1:E:406:TRP:CD2	2:F:420:PRO:HB3	2.40	0.56
2:F:153:TRP:CZ2	2:F:155:GLY:HA3	2.40	0.56
2:F:171:PHE:HB2	2:F:208:HIS:CE1	2.39	0.56
2:F:194:GLU:OE1	2:F:194:GLU:HA	2.04	0.56
2:F:248:GLU:HB2	2:F:307:ARG:HH12	1.70	0.56
2:F:274:ILE:HD12	2:F:274:ILE:N	2.20	0.56
1:I:32:LYS:NZ	1:I:135:ILE:HG21	2.21	0.56
1:I:242:GLN:HB3	1:I:243:PRO:HD2	1.87	0.56
1:I:252:TRP:CD1	1:I:295:LEU:HD13	2.40	0.56
1:I:557:ARG:NE	3:K:724:DT:OP2	2.39	0.56
1:M:174:GLN:C	1:M:176:PRO:HD3	2.25	0.56
1:M:235:HIS:HB3	1:M:236:PRO:HD2	1.86	0.56
1:M:447:ASN:HB3	1:M:450:THR:OG1	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:17:ASP:OD2	2:N:20:LYS:HE3	2.06	0.56
1:A:252:TRP:CD1	1:A:295:LEU:HD13	2.40	0.56
2:F:232:TYR:CD2	2:F:233:GLU:N	2.73	0.56
1:I:388:LYS:HE3	1:I:413:GLU:OE2	2.05	0.56
1:M:435:VAL:CA	2:N:290:THR:HG21	2.31	0.56
3:C:707:DG:H2'	3:C:708:DG:C8	2.41	0.56
3:O:706:DT:H2'	3:O:707:DG:H8	1.70	0.56
1:A:70:ARG:HH12	7:A:823:ZP4:H31	1.70	0.56
2:B:28:GLU:OE2	2:B:32:LYS:HE3	2.05	0.56
1:E:109:LEU:HD12	1:E:109:LEU:N	2.19	0.56
1:I:156:SER:N	1:I:157:PRO:CD	2.67	0.56
1:M:410:TRP:CZ2	1:M:412:PRO:HA	2.39	0.56
1:M:418:ASN:O	1:M:420:PRO:HD3	2.06	0.56
1:A:242:GLN:HB3	1:A:243:PRO:HD2	1.88	0.56
1:A:407:GLN:HE22	2:B:418:ASN:HA	1.70	0.56
2:B:72:ARG:HH12	2:B:151:GLN:CD	2.09	0.56
1:E:169:GLU:HB3	1:E:170:PRO:HD3	1.87	0.56
1:I:8:VAL:HG13	2:J:53:GLU:OE1	2.06	0.56
1:I:108:VAL:O	1:I:220:LYS:HB2	2.05	0.56
1:I:109:LEU:N	1:I:109:LEU:HD12	2.21	0.56
1:I:228:LEU:HD23	1:I:233:GLU:HG2	1.88	0.56
2:J:252:TRP:HB3	2:J:257:ILE:HD11	1.88	0.56
2:J:314:VAL:CG2	2:J:315:HIS:N	2.67	0.56
2:J:366:LYS:O	2:J:370:GLU:HG3	2.05	0.56
1:M:13:LYS:HE3	1:M:84:THR:O	2.06	0.56
1:A:303:LEU:O	1:A:303:LEU:HD13	2.06	0.56
1:E:65:LYS:HZ2	1:E:70:ARG:HH21	1.53	0.56
1:E:221:HIS:CD2	1:E:221:HIS:N	2.69	0.56
1:I:281:LYS:HE2	1:I:284:ARG:NH1	2.20	0.56
1:M:324:ASP:HA	1:M:385:LYS:NZ	2.21	0.56
1:A:70:ARG:NH2	7:A:823:ZP4:O1D	2.38	0.56
1:A:108:VAL:O	1:A:220:LYS:HB2	2.06	0.56
1:E:407:GLN:HE22	2:F:418:ASN:HA	1.70	0.56
1:I:239:TRP:O	1:I:315:HIS:HA	2.06	0.56
1:I:325:LEU:HD12	1:I:325:LEU:N	2.21	0.56
1:M:7:THR:HG22	1:M:119:PRO:HB2	1.88	0.56
4:H:818:DC:H2'	4:H:819:DG:H8	1.71	0.56
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.06	0.56
1:A:458:VAL:CG1	1:A:548:VAL:HG22	2.36	0.56
1:E:221:HIS:H	1:E:221:HIS:HD2	1.48	0.56
2:F:393:ILE:HD13	2:F:398:TRP:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:426:TRP:CD1	2:F:426:TRP:N	2.66	0.56
1:I:255:ASN:HB2	1:I:289:LEU:HB3	1.87	0.56
2:J:372:VAL:HG13	2:J:389:PHE:CD2	2.40	0.56
1:M:324:ASP:HA	1:M:385:LYS:HZ1	1.71	0.56
1:M:382:ILE:O	2:N:136:ASN:HB2	2.06	0.56
1:A:191:SER:OG	1:A:198:HIS:ND1	2.38	0.55
2:J:6:GLU:HB2	9:J:447:HOH:O	2.06	0.55
2:J:426:TRP:H	2:J:426:TRP:HD1	1.48	0.55
1:M:109:LEU:HA	1:M:220:LYS:HB2	1.88	0.55
1:M:221:HIS:H	1:M:221:HIS:CD2	2.24	0.55
1:A:3:SER:HB3	1:A:119:PRO:HD3	1.88	0.55
2:B:232:TYR:CD2	2:B:233:GLU:N	2.74	0.55
2:N:75:VAL:HG11	2:N:77:PHE:CE2	2.41	0.55
2:N:284:ARG:HH11	2:N:284:ARG:HG3	1.71	0.55
3:C:705:DA:H2"	3:C:706:DT:O5'	2.06	0.55
1:A:339:TYR:CD1	1:A:375:ILE:HD11	2.41	0.55
1:A:410:TRP:CZ2	1:A:412:PRO:HA	2.41	0.55
1:E:222:GLN:N	1:E:224:GLU:OE1	2.40	0.55
2:F:336:GLN:NE2	2:F:353:LYS:HD3	2.21	0.55
2:F:372:VAL:HG13	2:F:389:PHE:CD2	2.40	0.55
1:I:49:LYS:HE3	1:I:142:ILE:HG23	1.88	0.55
2:N:325:LEU:O	2:N:387:PRO:HA	2.06	0.55
2:N:339:TYR:CD2	2:N:375:ILE:HD12	2.41	0.55
1:A:298:GLU:H	1:A:298:GLU:CD	2.10	0.55
2:B:241:VAL:HG13	2:B:351:THR:N	2.21	0.55
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.87	0.55
2:B:423:VAL:O	2:B:423:VAL:HG12	2.07	0.55
1:E:194:GLU:OE1	1:E:194:GLU:HA	2.06	0.55
1:E:410:TRP:CZ2	1:E:412:PRO:HA	2.42	0.55
1:I:115:TYR:CE2	7:I:823:ZP4:H2'A	2.41	0.55
1:I:151:GLN:OE1	7:I:823:ZP4:H2'	2.07	0.55
4:L:816:DG:H2'	4:L:817:MRG:H8	1.88	0.55
3:O:726:DT:H2"	3:O:727:DG:C8	2.40	0.55
2:B:426:TRP:CD1	2:B:426:TRP:N	2.65	0.55
1:E:303:LEU:CD1	1:E:307:ARG:HD2	2.37	0.55
1:I:7:THR:HG22	1:I:119:PRO:HB2	1.88	0.55
1:I:264:LEU:HD12	1:I:306:ASN:ND2	2.22	0.55
2:J:94:ILE:CD1	2:J:161:GLN:HG2	2.36	0.55
1:M:31:ILE:O	1:M:35:VAL:HG23	2.06	0.55
1:M:102:LYS:HD2	1:M:102:LYS:N	2.12	0.55
1:A:421:PRO:O	1:A:422:LEU:HD23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:GLU:OE1	2:B:194:GLU:HA	2.05	0.55
1:E:557:ARG:C	1:E:558:LYS:HG2	2.26	0.55
2:J:377:THR:HA	2:J:380:ILE:HD12	1.88	0.55
1:M:277:ARG:HH11	1:M:336:GLN:HG3	1.72	0.55
2:N:314:VAL:CG2	2:N:315:HIS:N	2.68	0.55
4:D:815:DG:H2"	4:D:816:DG:O5'	2.06	0.55
1:E:418:ASN:O	1:E:420:PRO:HD3	2.07	0.55
1:E:556:ILE:HD12	1:E:556:ILE:H	1.70	0.55
2:J:130:PHE:CZ	2:J:144:TYR:HB2	2.42	0.55
1:M:52:PRO:HA	1:M:143:ARG:HH22	1.71	0.55
1:A:156:SER:N	1:A:157:PRO:CD	2.70	0.55
2:B:131:THR:OG1	2:B:143:ARG:HG2	2.07	0.55
1:E:130:PHE:CZ	1:E:144:TYR:HB2	2.42	0.55
1:E:235:HIS:HB3	1:E:236:PRO:HD2	1.87	0.55
2:F:333:GLY:O	2:F:334:GLN:HB2	2.07	0.55
2:J:400:THR:HG22	2:J:401:TRP:CD2	2.42	0.55
2:N:46:LYS:O	2:N:147:ASN:N	2.38	0.55
2:N:274:ILE:HD12	2:N:274:ILE:N	2.21	0.55
1:E:164:MET:HE2	1:E:187:LEU:HD21	1.88	0.55
2:F:235:HIS:C	2:F:237:ASP:H	2.10	0.55
2:F:243:PRO:HB2	2:F:244:ILE:HD13	1.89	0.55
1:I:109:LEU:HA	1:I:220:LYS:HB2	1.89	0.55
2:N:62:ALA:O	2:N:63:ILE:HG22	2.07	0.55
1:E:232:TYR:N	1:E:242:GLN:HE21	2.04	0.54
1:I:100:LEU:CD2	1:I:181:TYR:CZ	2.89	0.54
1:M:77:PHE:HB2	1:M:152:GLY:O	2.07	0.54
2:N:104:LYS:HA	2:N:237:ASP:OD2	2.06	0.54
2:N:108:VAL:HG22	2:N:188:TYR:CD2	2.42	0.54
1:A:164:MET:CE	1:A:187:LEU:HD21	2.37	0.54
1:A:418:ASN:O	1:A:420:PRO:HD3	2.08	0.54
1:E:441:TYR:CD1	1:E:544:GLY:CA	2.77	0.54
2:J:28:GLU:OE2	2:J:32:LYS:HE3	2.06	0.54
2:N:194:GLU:OE1	2:N:194:GLU:HA	2.07	0.54
2:N:372:VAL:HG13	2:N:389:PHE:CD2	2.42	0.54
1:E:394:GLN:NE2	1:E:416:PHE:CZ	2.75	0.54
1:I:22:LYS:HG2	1:I:23:GLN:N	2.22	0.54
1:I:469:LEU:CD2	1:I:480:GLN:HG3	2.37	0.54
2:J:50:ILE:HG21	2:J:145:GLN:OE1	2.07	0.54
2:J:356:ARG:HG2	2:J:357:MET:H	1.71	0.54
1:A:285:GLY:N	3:C:714:DG:OP1	2.37	0.54
1:A:472:THR:HG21	1:A:477:THR:HG22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:242:GLN:HB3	1:M:243:PRO:HD2	1.90	0.54
1:A:22:LYS:HG2	1:A:23:GLN:H	1.71	0.54
1:A:495:ILE:O	1:A:533:LEU:HA	2.07	0.54
2:F:257:ILE:O	2:F:261:VAL:HG23	2.07	0.54
1:I:26:LEU:HD12	1:I:133:PRO:HG3	1.90	0.54
1:I:72:ARG:NH2	7:I:823:ZP4:O3A	2.41	0.54
1:M:303:LEU:O	1:M:303:LEU:HD13	2.07	0.54
2:N:426:TRP:H	2:N:426:TRP:HD1	1.50	0.54
1:A:118:VAL:O	1:A:148:VAL:HG23	2.07	0.54
1:A:408:ALA:HB3	2:B:393:ILE:HB	1.89	0.54
2:B:96:HIS:HA	2:B:181:TYR:CE1	2.43	0.54
1:I:473:THR:HG21	4:L:809:DC:P	2.48	0.54
2:J:325:LEU:O	2:J:387:PRO:HA	2.08	0.54
1:E:221:HIS:HE1	1:E:228:LEU:H	1.55	0.54
2:F:72:ARG:HH21	2:F:409:THR:HG22	1.72	0.54
2:F:366:LYS:O	2:F:370:GLU:HG3	2.08	0.54
2:F:400:THR:HG22	2:F:401:TRP:CD2	2.43	0.54
1:I:118:VAL:C	1:I:148:VAL:HG23	2.28	0.54
1:I:225:PRO:CB	1:I:226:PRO:CD	2.71	0.54
2:J:94:ILE:HG21	2:J:182:GLN:O	2.07	0.54
2:J:96:HIS:CE1	2:J:381:VAL:O	2.61	0.54
2:N:203:GLU:O	2:N:207:GLN:HG2	2.08	0.54
1:A:23:GLN:HE22	1:A:60:VAL:H	1.48	0.54
1:A:76:ASP:OD1	3:C:705:DA:H4'	2.07	0.54
1:A:246:LEU:HD21	1:A:264:LEU:HD11	1.89	0.54
1:M:255:ASN:HD22	1:M:289:LEU:HD22	1.72	0.54
1:M:283:LEU:H	1:M:283:LEU:HD12	1.72	0.54
1:M:301:LEU:O	1:M:304:ALA:HB3	2.08	0.54
2:N:88:TRP:CE2	2:N:154:LYS:HD2	2.43	0.54
1:E:3:SER:HB2	1:E:117:SER:O	2.08	0.54
1:E:116:PHE:C	1:E:148:VAL:HG21	2.28	0.54
1:E:252:TRP:CD1	1:E:295:LEU:HD13	2.42	0.54
2:F:423:VAL:O	2:F:423:VAL:HG12	2.08	0.54
1:I:116:PHE:C	1:I:148:VAL:HG21	2.28	0.54
1:M:399:GLU:HA	1:M:402:TRP:CD1	2.42	0.54
2:N:59:PRO:HG2	2:N:76:ASP:HB3	1.89	0.54
1:A:237:ASP:C	1:A:238:LYS:HD2	2.28	0.54
1:E:421:PRO:O	1:E:422:LEU:HD23	2.08	0.54
1:I:229:TRP:CE2	1:I:230:MET:CG	2.90	0.54
3:C:726:DT:H2"	3:C:727:DG:OP2	2.07	0.54
1:A:303:LEU:CD1	1:A:307:ARG:HD2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:ARG:NH1	1:A:463:ARG:HB2	2.23	0.53
1:E:442:VAL:HG11	1:E:485:ALA:HB2	1.89	0.53
1:I:3:SER:HB2	1:I:117:SER:O	2.08	0.53
1:A:46:LYS:O	1:A:147:ASN:HB2	2.09	0.53
2:B:328:GLU:O	2:B:339:TYR:HA	2.09	0.53
2:J:325:LEU:HD21	2:J:383:TRP:CE3	2.42	0.53
3:C:707:DG:H2"	3:C:708:DG:H5'	1.89	0.53
1:A:70:ARG:HH22	7:A:823:ZP4:PD	2.31	0.53
1:A:388:LYS:HE3	1:A:413:GLU:OE2	2.08	0.53
2:B:366:LYS:O	2:B:370:GLU:HG3	2.08	0.53
2:F:244:ILE:HD13	2:F:244:ILE:N	2.17	0.53
1:I:510:PRO:O	1:I:522:ILE:HD12	2.08	0.53
1:M:108:VAL:HA	1:M:187:LEU:O	2.09	0.53
2:N:4:PRO:HA	2:N:119:PRO:HG3	1.90	0.53
2:B:244:ILE:H	2:B:244:ILE:CD1	2.16	0.53
2:B:339:TYR:CE2	2:B:375:ILE:HD12	2.43	0.53
2:F:94:ILE:HG21	2:F:182:GLN:O	2.07	0.53
2:F:130:PHE:CZ	2:F:144:TYR:HB2	2.44	0.53
2:F:339:TYR:CD2	2:F:375:ILE:HD12	2.43	0.53
1:I:303:LEU:CD1	1:I:307:ARG:HD2	2.38	0.53
4:P:818:DC:H2"	4:P:819:DG:H5'	1.91	0.53
2:B:333:GLY:O	2:B:334:GLN:HB2	2.08	0.53
2:B:344:GLU:OE1	2:B:344:GLU:HA	2.09	0.53
1:E:164:MET:CE	1:E:168:LEU:HD11	2.39	0.53
1:I:27:THR:HB	1:I:30:LYS:HB2	1.91	0.53
2:N:257:ILE:O	2:N:261:VAL:HG23	2.08	0.53
1:A:9:PRO:HA	1:A:121:ASP:OD2	2.08	0.53
1:A:73:LYS:HE3	1:A:146:TYR:CZ	2.43	0.53
1:E:479:LEU:HB3	1:E:517:LEU:HD13	1.91	0.53
2:F:26:LEU:HB2	2:F:31:ILE:CD1	2.38	0.53
1:I:406:TRP:CE2	2:J:420:PRO:HB3	2.43	0.53
1:M:237:ASP:O	1:M:238:LYS:HD2	2.08	0.53
2:N:356:ARG:HG2	2:N:357:MET:H	1.72	0.53
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.43	0.53
1:E:447:ASN:HB3	1:E:450:THR:OG1	2.09	0.53
1:I:90:VAL:HG22	1:I:90:VAL:O	2.09	0.53
2:J:26:LEU:HB2	2:J:31:ILE:CD1	2.39	0.53
1:M:73:LYS:HE3	1:M:146:TYR:CE1	2.44	0.53
1:M:164:MET:CE	1:M:187:LEU:HD21	2.38	0.53
1:E:255:ASN:HB2	1:E:289:LEU:HB3	1.91	0.53
1:E:300:GLU:OE1	1:E:300:GLU:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:235:HIS:HB2	1:I:238:LYS:O	2.09	0.53
1:M:280:SER:O	1:M:283:LEU:HD12	2.08	0.53
2:N:131:THR:OG1	2:N:143:ARG:HG2	2.08	0.53
3:G:707:DG:H2'	3:G:708:DG:H8	1.73	0.53
1:A:90:VAL:HG22	1:A:90:VAL:O	2.09	0.53
2:B:274:ILE:N	2:B:274:ILE:HD12	2.23	0.53
1:E:181:TYR:CZ	2:F:138:GLU:HG2	2.44	0.53
1:I:298:GLU:H	1:I:298:GLU:CD	2.12	0.53
2:J:113:ASP:N	2:J:151:GLN:HE21	2.07	0.53
2:N:76:ASP:OD1	2:N:411:ILE:HD12	2.09	0.53
2:N:130:PHE:CZ	2:N:144:TYR:HB2	2.43	0.53
3:G:712:DC:H2'	3:G:713:DC:C6	2.44	0.53
4:P:815:DG:H2"	4:P:816:DG:O5'	2.09	0.53
1:A:205:LEU:CD1	1:A:209:LEU:HD11	2.39	0.53
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.90	0.53
1:E:340:GLN:HB3	1:E:351:THR:HG22	1.90	0.53
1:E:399:GLU:HA	1:E:402:TRP:CD1	2.44	0.53
1:E:469:LEU:CD2	1:E:480:GLN:HG3	2.38	0.53
2:F:337:TRP:HB2	2:F:354:TYR:HB3	1.89	0.53
1:I:447:ASN:HB2	1:I:556:ILE:HD13	1.91	0.53
1:I:469:LEU:N	1:I:469:LEU:HD12	2.24	0.53
2:J:194:GLU:OE1	2:J:194:GLU:HA	2.09	0.53
2:J:423:VAL:O	2:J:423:VAL:HG12	2.10	0.53
2:B:257:ILE:O	2:B:261:VAL:HG23	2.09	0.52
1:E:174:GLN:NE2	2:J:6:GLU:OE1	2.42	0.52
1:I:255:ASN:HD22	1:I:289:LEU:HD22	1.74	0.52
2:J:276:VAL:O	2:J:276:VAL:HG22	2.08	0.52
1:M:3:SER:CB	1:M:117:SER:O	2.57	0.52
1:M:90:VAL:HG22	2:N:140:PRO:CB	2.26	0.52
1:M:510:PRO:O	1:M:522:ILE:HD12	2.09	0.52
2:N:28:GLU:OE2	2:N:32:LYS:HE3	2.08	0.52
3:K:708:DG:H2'	3:K:709:DC:C6	2.44	0.52
1:E:242:GLN:HB3	1:E:243:PRO:HD2	1.91	0.52
2:F:235:HIS:O	2:F:237:ASP:N	2.42	0.52
2:B:59:PRO:HG2	2:B:76:ASP:HB3	1.90	0.52
1:E:90:VAL:HG22	1:E:90:VAL:O	2.09	0.52
1:E:215:TYR:CD2	1:E:216:THR:N	2.78	0.52
2:F:421:PRO:O	2:F:424:LYS:N	2.43	0.52
1:I:421:PRO:O	1:I:422:LEU:HD23	2.10	0.52
1:M:40:GLU:O	1:M:44:GLU:HG3	2.09	0.52
1:M:94:ILE:HD11	3:O:708:DG:N2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:255:ASN:HB2	1:M:289:LEU:HB3	1.90	0.52
1:M:361:HIS:CD2	1:M:505:ILE:HG23	2.44	0.52
1:M:388:LYS:HE3	1:M:413:GLU:OE2	2.09	0.52
2:N:115:TYR:OH	2:N:157:PRO:HG3	2.08	0.52
2:N:166:LYS:HB2	9:N:438:HOH:O	2.09	0.52
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.90	0.52
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.44	0.52
2:B:31:ILE:HD11	2:B:133:PRO:HG2	1.92	0.52
2:J:96:HIS:HE1	2:J:381:VAL:O	1.93	0.52
1:M:115:TYR:HB3	1:M:149:LEU:O	2.08	0.52
1:A:531:VAL:HG12	1:A:532:TYR:N	2.24	0.52
2:B:26:LEU:HD12	2:B:31:ILE:HD13	1.90	0.52
1:E:53:GLU:O	1:E:55:PRO:HD3	2.10	0.52
1:E:146:TYR:CD2	1:E:150:PRO:HB3	2.45	0.52
1:E:357:MET:HG2	1:E:367:GLN:HE22	1.75	0.52
2:J:257:ILE:O	2:J:261:VAL:HG23	2.10	0.52
1:M:8:VAL:HB	1:M:159:ILE:HD12	1.91	0.52
1:M:512:LYS:O	1:M:513:SER:HB2	2.10	0.52
2:N:104:LYS:HG3	2:N:237:ASP:OD2	2.09	0.52
2:N:423:VAL:O	2:N:423:VAL:HG12	2.10	0.52
3:O:707:DG:H2'	3:O:708:DG:C8	2.45	0.52
1:A:463:ARG:HG2	1:A:464:GLN:N	2.23	0.52
1:E:214:LEU:CD2	1:E:214:LEU:N	2.73	0.52
1:I:219:GLN:CD	1:I:219:GLN:N	2.63	0.52
1:I:399:GLU:HA	1:I:402:TRP:CD1	2.44	0.52
2:J:242:GLN:NE2	2:J:353:LYS:HE3	2.24	0.52
1:M:558:LYS:HE3	1:M:558:LYS:HA	1.91	0.52
2:N:13:LYS:HZ2	2:N:86:ASP:H	1.57	0.52
1:A:116:PHE:O	1:A:148:VAL:HG21	2.10	0.52
1:A:500:GLN:HG2	1:A:535:TRP:NE1	2.24	0.52
1:A:510:PRO:O	1:A:522:ILE:HD12	2.09	0.52
2:B:199:ARG:O	2:B:202:ILE:HB	2.09	0.52
2:B:377:THR:HA	2:B:380:ILE:HD12	1.91	0.52
1:E:388:LYS:HE3	1:E:413:GLU:OE2	2.09	0.52
2:F:271:TYR:HB2	2:F:274:ILE:CD1	2.39	0.52
1:I:283:LEU:HD12	1:I:283:LEU:H	1.73	0.52
1:I:410:TRP:HZ3	2:J:401:TRP:CE2	2.28	0.52
1:A:181:TYR:CE1	2:B:138:GLU:HG2	2.45	0.52
1:M:3:SER:HB2	1:M:117:SER:O	2.10	0.52
1:A:52:PRO:HD2	1:A:53:GLU:OE1	2.10	0.52
1:A:171:PHE:CZ	1:A:205:LEU:HD23	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LEU:HG	1:A:264:LEU:HD23	1.91	0.52
1:A:300:GLU:OE1	1:A:300:GLU:HA	2.09	0.52
2:B:76:ASP:OD1	2:B:78:ARG:HB2	2.09	0.52
2:B:118:VAL:CG1	2:B:119:PRO:HD2	2.40	0.52
2:F:28:GLU:OE2	2:F:32:LYS:HE3	2.09	0.52
2:F:169:GLU:HA	2:F:169:GLU:OE2	2.08	0.52
1:I:264:LEU:HD12	1:I:306:ASN:HD22	1.73	0.52
2:J:131:THR:OG1	2:J:143:ARG:HG2	2.10	0.52
2:J:161:GLN:NE2	2:J:161:GLN:HA	2.24	0.52
1:M:156:SER:N	1:M:157:PRO:CD	2.72	0.52
1:M:181:TYR:HE2	2:N:136:ASN:HD22	1.56	0.52
1:M:463:ARG:CB	1:M:463:ARG:HH11	2.23	0.52
1:A:542:ILE:HG23	2:B:283:LEU:HD12	1.91	0.52
1:E:53:GLU:CD	1:E:53:GLU:N	2.63	0.52
1:E:298:GLU:H	1:E:298:GLU:CD	2.14	0.52
2:F:74:LEU:HD12	2:F:74:LEU:C	2.30	0.52
1:I:124:PHE:CE2	1:I:153:TRP:CZ2	2.98	0.52
1:I:237:ASP:O	1:I:238:LYS:HD2	2.10	0.52
1:I:384:GLY:O	2:J:28:GLU:N	2.43	0.52
2:J:374:LYS:HE2	2:J:378:GLU:HG3	1.92	0.52
2:J:426:TRP:CD1	2:J:426:TRP:N	2.66	0.52
1:M:38:CYS:SG	1:M:132:ILE:HG13	2.50	0.52
1:M:253:THR:HA	1:M:292:VAL:HA	1.92	0.52
2:N:31:ILE:HD11	2:N:133:PRO:HG2	1.90	0.52
2:B:21:VAL:CG1	2:B:59:PRO:HD3	2.40	0.51
2:B:74:LEU:HD12	2:B:74:LEU:C	2.30	0.51
2:B:372:VAL:HG13	2:B:389:PHE:CD2	2.44	0.51
1:E:115:TYR:OH	1:E:184:MET:HE3	2.10	0.51
1:I:94:ILE:HD11	3:K:708:DG:H21	1.75	0.51
1:I:293:ILE:CD1	1:I:294:PRO:HD2	2.31	0.51
2:J:85:GLN:HA	2:J:88:TRP:CE2	2.45	0.51
2:J:356:ARG:HG2	2:J:357:MET:N	2.25	0.51
2:F:6:GLU:OE1	2:F:6:GLU:HA	2.10	0.51
1:M:339:TYR:CD1	1:M:375:ILE:HD11	2.46	0.51
1:M:458:VAL:HG22	1:M:458:VAL:O	2.10	0.51
1:M:458:VAL:CG1	1:M:548:VAL:HG22	2.38	0.51
2:N:276:VAL:O	2:N:276:VAL:HG22	2.09	0.51
4:L:818:DC:H2"	4:L:819:DG:H5'	1.92	0.51
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.93	0.51
2:B:17:ASP:OD2	2:B:20:LYS:HE3	2.10	0.51
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:GLU:HB2	2:B:307:ARG:NH1	2.26	0.51
2:F:115:TYR:HB3	2:F:149:LEU:HB2	1.92	0.51
2:J:319:TYR:OH	2:J:385:LYS:HD3	2.10	0.51
1:A:293:ILE:CD1	1:A:294:PRO:HD2	2.35	0.51
1:E:109:LEU:HA	1:E:220:LYS:HB2	1.93	0.51
1:E:260:LEU:HG	1:E:264:LEU:HD23	1.91	0.51
1:I:101:LYS:HE2	1:I:321:PRO:HG3	1.91	0.51
1:I:108:VAL:HA	1:I:187:LEU:O	2.10	0.51
2:J:339:TYR:CD2	2:J:375:ILE:HD12	2.45	0.51
1:M:116:PHE:CA	1:M:148:VAL:HG21	2.40	0.51
1:A:255:ASN:HB2	1:A:289:LEU:HB3	1.92	0.51
2:B:376:THR:HB	2:B:410:TRP:CH2	2.45	0.51
1:M:136:ASN:OD1	1:M:138:GLU:HG3	2.10	0.51
1:A:70:ARG:C	1:A:71:TRP:CD1	2.84	0.51
1:A:542:ILE:HG23	2:B:283:LEU:CD1	2.40	0.51
2:B:244:ILE:HD13	2:B:244:ILE:N	2.18	0.51
2:B:266:TRP:CE2	2:B:423:VAL:HG21	2.45	0.51
1:E:27:THR:CG2	1:E:30:LYS:H	2.24	0.51
2:F:328:GLU:O	2:F:339:TYR:HA	2.11	0.51
2:F:344:GLU:OE1	2:F:344:GLU:HA	2.11	0.51
1:I:301:LEU:O	1:I:304:ALA:HB3	2.11	0.51
2:J:248:GLU:HB2	2:J:307:ARG:HH12	1.76	0.51
2:N:30:LYS:HE2	2:N:62:ALA:O	2.10	0.51
2:N:73:LYS:NZ	2:N:130:PHE:CZ	2.79	0.51
2:N:163:SER:HA	9:N:438:HOH:O	2.10	0.51
2:N:356:ARG:HG2	2:N:357:MET:N	2.25	0.51
3:K:707:DG:H2'	3:K:708:DG:C8	2.45	0.51
1:A:331:LYS:HE3	1:A:364:ASP:OD1	2.10	0.51
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.93	0.51
1:I:320:ASP:C	1:I:322:SER:H	2.13	0.51
1:I:394:GLN:NE2	1:I:416:PHE:CZ	2.78	0.51
2:J:73:LYS:HD3	2:J:146:TYR:OH	2.11	0.51
1:M:242:GLN:O	1:M:243:PRO:C	2.49	0.51
1:M:285:GLY:N	3:O:714:DG:OP1	2.39	0.51
1:M:364:ASP:N	1:M:511:ASP:OD2	2.41	0.51
2:N:318:TYR:O	2:N:318:TYR:CD1	2.64	0.51
2:N:388:LYS:HG2	2:N:413:GLU:O	2.11	0.51
2:J:13:LYS:HB2	2:J:16:MET:HG3	1.93	0.51
1:A:70:ARG:NH1	7:A:823:ZP4:H31	2.24	0.51
2:B:17:ASP:O	2:B:83:ARG:CD	2.59	0.51
2:B:40:GLU:O	2:B:43:LYS:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:229:TRP:CE2	1:E:230:MET:HG2	2.46	0.51
1:E:278:GLN:HG3	1:E:298:GLU:CB	2.38	0.51
2:F:325:LEU:HD21	2:F:383:TRP:CE3	2.46	0.51
1:I:95:PRO:HG3	2:J:137:ASN:O	2.11	0.51
1:I:300:GLU:OE1	1:I:300:GLU:HA	2.10	0.51
2:J:350:LYS:HG2	2:J:351:THR:N	2.25	0.51
1:M:300:GLU:OE1	1:M:300:GLU:HA	2.10	0.51
1:M:463:ARG:HG2	1:M:464:GLN:N	2.25	0.51
1:E:2:ILE:HD11	1:E:45:GLY:O	2.11	0.51
2:F:174:GLN:O	2:F:176:PRO:HD3	2.11	0.51
1:A:23:GLN:HE21	1:A:60:VAL:HG22	1.76	0.50
2:B:26:LEU:HB2	2:B:31:ILE:CD1	2.41	0.50
2:B:72:ARG:HH11	2:B:72:ARG:HG3	1.76	0.50
2:B:350:LYS:HG2	2:B:351:THR:N	2.26	0.50
2:F:271:TYR:HB2	2:F:274:ILE:HD13	1.94	0.50
1:I:27:THR:HB	1:I:30:LYS:CB	2.42	0.50
1:I:281:LYS:O	1:I:284:ARG:HB2	2.11	0.50
1:I:339:TYR:CD1	1:I:375:ILE:HD11	2.46	0.50
2:J:232:TYR:CD2	2:J:233:GLU:N	2.79	0.50
2:J:248:GLU:HB2	2:J:307:ARG:NH1	2.25	0.50
1:A:15:GLY:CA	2:F:165:THR:HG21	2.41	0.50
2:B:76:ASP:C	2:B:78:ARG:H	2.14	0.50
2:B:421:PRO:O	2:B:424:LYS:N	2.44	0.50
2:B:428:GLN:CG	2:B:429:GLY:N	2.73	0.50
1:I:148:VAL:O	1:I:150:PRO:HD3	2.11	0.50
2:J:113:ASP:HA	2:J:151:GLN:NE2	2.26	0.50
2:N:244:ILE:H	2:N:244:ILE:CD1	2.24	0.50
4:D:818:DC:H2"	4:D:819:DG:H5'	1.91	0.50
3:G:707:DG:H2'	3:G:708:DG:C8	2.46	0.50
3:K:717:DC:H2"	3:K:718:DA:OP2	2.11	0.50
1:A:200:THR:O	1:A:203:GLU:HB2	2.12	0.50
1:E:114:ALA:N	7:E:823:ZP4:N3A	2.60	0.50
2:F:423:VAL:HB	2:F:426:TRP:CG	2.46	0.50
2:J:108:VAL:HG22	2:J:188:TYR:CD2	2.47	0.50
2:N:95:PRO:O	2:N:181:TYR:HE1	1.94	0.50
2:B:75:VAL:HG11	2:B:77:PHE:CD2	2.46	0.50
1:E:164:MET:CE	1:E:187:LEU:HD21	2.40	0.50
2:J:319:TYR:OH	2:J:321:PRO:HA	2.11	0.50
1:M:22:LYS:HG2	1:M:23:GLN:N	2.25	0.50
3:O:717:DC:H2"	3:O:718:DA:OP2	2.12	0.50
2:B:72:ARG:HH21	2:B:409:THR:HG22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:PRO:HB3	2:B:430:GLY:C	2.32	0.50
1:E:354:TYR:CE1	1:E:356:ARG:HB3	2.47	0.50
2:F:350:LYS:HG2	2:F:351:THR:N	2.26	0.50
1:I:91:GLN:CG	1:I:161:GLN:NE2	2.75	0.50
1:I:354:TYR:CE1	1:I:356:ARG:HB3	2.47	0.50
2:J:59:PRO:HG2	2:J:76:ASP:HB3	1.93	0.50
2:J:72:ARG:HH11	2:J:72:ARG:HG3	1.76	0.50
2:J:274:ILE:HD12	2:J:274:ILE:H	1.76	0.50
1:M:81:ASN:OD1	1:M:153:TRP:HA	2.11	0.50
1:M:206:ARG:HG3	1:M:216:THR:HG21	1.94	0.50
1:M:221:HIS:HE1	1:M:228:LEU:HB2	1.75	0.50
2:N:31:ILE:CD1	2:N:133:PRO:HG2	2.42	0.50
1:E:114:ALA:N	7:E:823:ZP4:N3B	2.59	0.50
1:M:277:ARG:HH11	1:M:336:GLN:CG	2.24	0.50
4:D:816:DG:H2'	4:D:817:MRG:H8	1.92	0.50
1:A:53:GLU:O	1:A:55:PRO:HD3	2.12	0.50
1:A:281:LYS:HE2	1:A:284:ARG:NH1	2.26	0.50
1:A:531:VAL:HG12	1:A:533:LEU:HD12	1.94	0.50
2:F:67:ASP:HB3	2:F:219:LYS:CB	2.42	0.50
2:F:374:LYS:HE2	2:F:378:GLU:OE2	2.12	0.50
2:J:157:PRO:HG2	2:J:184:MET:CA	2.34	0.50
2:J:195:ILE:HG23	9:J:448:HOH:O	2.12	0.50
1:M:260:LEU:HG	1:M:264:LEU:HD23	1.93	0.50
1:M:463:ARG:HH11	1:M:463:ARG:HB3	1.76	0.50
2:N:17:ASP:O	2:N:83:ARG:CD	2.60	0.50
2:N:21:VAL:CG1	2:N:59:PRO:HD3	2.42	0.50
2:N:26:LEU:HB2	2:N:31:ILE:CD1	2.41	0.50
2:N:161:GLN:HA	2:N:161:GLN:NE2	2.27	0.50
3:C:713:DC:H2'	3:C:714:DG:C8	2.47	0.50
1:M:252:TRP:CD1	1:M:295:LEU:HD13	2.47	0.50
1:A:120:LEU:O	1:A:121:ASP:C	2.50	0.50
1:A:232:TYR:OH	1:A:269:GLN:NE2	2.38	0.50
2:B:422:LEU:C	2:B:424:LYS:H	2.14	0.50
1:E:49:LYS:CE	1:E:142:ILE:HD12	2.34	0.50
1:I:454:LYS:HB2	1:I:552:VAL:O	2.12	0.50
2:J:17:ASP:O	2:J:83:ARG:CD	2.60	0.50
1:M:221:HIS:CE1	1:M:228:LEU:HB2	2.47	0.50
2:N:73:LYS:HD3	2:N:146:TYR:OH	2.12	0.50
2:N:248:GLU:HB2	2:N:307:ARG:HH12	1.77	0.50
1:A:406:TRP:CD2	2:B:420:PRO:HB3	2.47	0.49
1:I:9:PRO:HA	1:I:121:ASP:OD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:72:ARG:HD3	1:I:74:LEU:HD21	1.94	0.49
1:A:72:ARG:HG3	1:A:151:GLN:NE2	2.24	0.49
1:A:420:PRO:HA	1:A:421:PRO:C	2.32	0.49
1:A:454:LYS:HB2	1:A:552:VAL:O	2.12	0.49
2:B:75:VAL:CG1	2:B:77:PHE:CD2	2.95	0.49
2:B:203:GLU:O	2:B:207:GLN:HG2	2.11	0.49
1:E:223:LYS:O	1:E:223:LYS:HG3	2.12	0.49
1:I:31:ILE:CG2	1:I:133:PRO:HG2	2.41	0.49
2:J:76:ASP:C	2:J:78:ARG:H	2.15	0.49
1:M:442:VAL:HG11	1:M:485:ALA:HB2	1.94	0.49
2:N:16:MET:HA	2:N:16:MET:CE	2.41	0.49
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.53	0.49
1:E:98:ALA:HB1	1:E:349:LEU:HD22	1.93	0.49
1:E:103:LYS:HE3	1:E:179:VAL:CG2	2.38	0.49
2:F:72:ARG:HE	2:F:409:THR:HG22	1.77	0.49
2:N:118:VAL:HG13	2:N:119:PRO:HD2	1.94	0.49
1:A:406:TRP:CE2	2:B:420:PRO:HB3	2.47	0.49
1:A:479:LEU:HB3	1:A:517:LEU:HD13	1.95	0.49
2:B:271:TYR:HB2	2:B:274:ILE:CD1	2.42	0.49
1:E:447:ASN:CB	1:E:556:ILE:HG23	2.41	0.49
2:F:13:LYS:HB2	2:F:16:MET:HG3	1.95	0.49
2:F:377:THR:HA	2:F:380:ILE:HD12	1.94	0.49
1:I:242:GLN:O	1:I:243:PRO:C	2.50	0.49
2:J:393:ILE:HD13	2:J:398:TRP:HB2	1.94	0.49
1:M:3:SER:OG	1:M:5:ILE:HG22	2.12	0.49
1:M:70:ARG:CG	1:M:71:TRP:H	2.26	0.49
2:N:248:GLU:HB2	2:N:307:ARG:NH1	2.27	0.49
3:K:705:DA:H2"	3:K:706:DT:O5'	2.12	0.49
4:L:815:DG:H2"	4:L:816:DG:O5'	2.12	0.49
1:A:121:ASP:C	1:A:121:ASP:OD1	2.51	0.49
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.95	0.49
1:A:463:ARG:CB	1:A:463:ARG:HH11	2.26	0.49
1:E:441:TYR:HD2	1:E:496:VAL:HG22	1.77	0.49
2:F:59:PRO:HG2	2:F:76:ASP:HB3	1.95	0.49
1:I:408:ALA:HB3	2:J:393:ILE:HB	1.93	0.49
1:I:557:ARG:CZ	3:K:724:DT:OP2	2.60	0.49
9:I:564:HOH:O	2:J:259:LYS:HE2	2.11	0.49
2:J:428:GLN:HG2	2:J:429:GLY:N	2.27	0.49
1:M:363:ASN:HA	1:M:511:ASP:CG	2.32	0.49
4:H:820:DC:H2"	4:H:821:DC:H5'	1.93	0.49
1:E:232:TYR:OH	1:E:269:GLN:NE2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:65:LYS:NZ	7:I:823:ZP4:O1D	2.34	0.49
1:I:237:ASP:C	1:I:238:LYS:HD2	2.32	0.49
2:J:16:MET:HA	2:J:16:MET:CE	2.42	0.49
1:M:169:GLU:HB3	1:M:170:PRO:HD3	1.93	0.49
2:N:232:TYR:CD2	2:N:233:GLU:N	2.81	0.49
3:C:712:DC:H2'	3:C:713:DC:C6	2.48	0.49
1:A:250:ASP:CG	1:A:251:SER:H	2.15	0.49
1:E:364:ASP:N	1:E:511:ASP:OD2	2.46	0.49
2:F:374:LYS:HE2	2:F:378:GLU:HG3	1.95	0.49
2:F:422:LEU:C	2:F:424:LYS:H	2.14	0.49
1:I:495:ILE:O	1:I:533:LEU:HA	2.12	0.49
1:I:503:LEU:HD22	1:I:535:TRP:HB2	1.95	0.49
2:J:64:LYS:CE	2:J:69:THR:HG23	2.43	0.49
1:M:221:HIS:CD2	1:M:221:HIS:N	2.80	0.49
1:M:244:ILE:HG23	1:M:244:ILE:O	2.12	0.49
1:M:503:LEU:HD22	1:M:535:TRP:HB2	1.95	0.49
3:G:723:DC:H2"	3:G:724:DT:C5'	2.42	0.49
1:A:115:TYR:CD2	7:A:823:ZP4:H2'A	2.48	0.49
1:A:476:LYS:O	1:A:479:LEU:HB2	2.13	0.49
2:B:88:TRP:CZ2	2:B:154:LYS:HD2	2.48	0.49
1:E:283:LEU:HD12	1:E:283:LEU:H	1.77	0.49
1:E:305:GLU:O	1:E:309:ILE:HG13	2.13	0.49
1:E:357:MET:HG2	1:E:367:GLN:NE2	2.28	0.49
1:E:503:LEU:HD22	1:E:535:TRP:HB2	1.93	0.49
2:F:10:VAL:HG21	2:F:153:TRP:HH2	1.77	0.49
2:F:241:VAL:HG22	2:F:350:LYS:HG3	1.95	0.49
2:F:318:TYR:CD1	2:F:318:TYR:O	2.66	0.49
2:J:235:HIS:C	2:J:237:ASP:H	2.16	0.49
1:M:2:ILE:HG22	1:M:117:SER:O	2.12	0.49
1:M:10:VAL:HG11	1:M:153:TRP:HZ2	1.77	0.49
2:N:23:GLN:HG2	2:N:133:PRO:HD3	1.95	0.49
2:N:174:GLN:O	2:N:176:PRO:HD3	2.13	0.49
2:N:428:GLN:HG2	2:N:429:GLY:H	1.77	0.49
1:A:355:ALA:O	1:A:356:ARG:C	2.50	0.49
2:B:247:PRO:HA	2:B:431:HIS:N	2.28	0.49
2:F:47:ILE:HG22	2:F:146:TYR:HA	1.95	0.49
1:I:420:PRO:HA	1:I:421:PRO:C	2.33	0.49
1:I:447:ASN:OD1	1:I:450:THR:HG23	2.12	0.49
2:J:83:ARG:HH11	2:J:83:ARG:HG3	1.78	0.49
2:J:84:THR:O	2:J:87:PHE:HB3	2.12	0.49
2:J:125:ARG:HH11	2:J:147:ASN:HB3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:225:PRO:O	1:M:234:LEU:O	2.31	0.49
1:M:394:GLN:NE2	1:M:416:PHE:CZ	2.81	0.49
7:M:823:ZP4:H6	4:P:822:2DA:H2"	1.94	0.49
2:N:115:TYR:OH	2:N:184:MET:O	2.29	0.49
1:E:65:LYS:HZ3	1:E:70:ARG:HH21	1.61	0.49
1:I:264:LEU:CD1	1:I:306:ASN:HD22	2.26	0.49
1:I:437:ALA:HB1	1:I:492:GLU:O	2.12	0.49
1:M:149:LEU:HD21	1:M:159:ILE:CG2	2.43	0.49
1:M:164:MET:HE2	1:M:168:LEU:HD11	1.95	0.49
2:N:376:THR:HB	2:N:410:TRP:CH2	2.48	0.49
1:A:221:HIS:HE1	1:A:228:LEU:CB	2.18	0.48
2:B:368:LEU:O	2:B:372:VAL:HG23	2.13	0.48
1:E:533:LEU:HD12	1:E:533:LEU:N	2.28	0.48
2:F:16:MET:HA	2:F:16:MET:CE	2.42	0.48
1:I:118:VAL:O	1:I:148:VAL:CG2	2.61	0.48
1:M:264:LEU:HD12	1:M:306:ASN:HD22	1.78	0.48
1:M:303:LEU:CD1	1:M:307:ARG:HD2	2.43	0.48
2:N:78:ARG:HD2	2:N:412:PRO:O	2.13	0.48
2:N:328:GLU:O	2:N:339:TYR:HA	2.13	0.48
1:A:58:THR:HG21	1:A:77:PHE:CD1	2.48	0.48
1:A:113:ASP:HB3	1:A:116:PHE:HB2	1.94	0.48
1:A:560:LEU:HB3	2:J:102:LYS:NZ	2.29	0.48
2:B:83:ARG:HH11	2:B:83:ARG:HG3	1.78	0.48
2:B:248:GLU:HB2	2:B:307:ARG:HH12	1.78	0.48
2:B:423:VAL:HB	2:B:426:TRP:CG	2.48	0.48
1:E:355:ALA:O	1:E:356:ARG:C	2.49	0.48
1:E:406:TRP:CE2	2:F:420:PRO:HB3	2.48	0.48
1:E:420:PRO:HA	1:E:421:PRO:C	2.33	0.48
1:E:517:LEU:O	1:E:520:GLN:HB2	2.13	0.48
2:F:72:ARG:HH12	2:F:151:GLN:CD	2.16	0.48
2:F:325:LEU:O	2:F:387:PRO:HA	2.13	0.48
1:I:253:THR:HA	1:I:292:VAL:HA	1.94	0.48
1:M:7:THR:CG2	1:M:119:PRO:HB2	2.44	0.48
1:M:340:GLN:HB3	1:M:351:THR:HG22	1.95	0.48
1:M:556:ILE:HG23	1:M:557:ARG:H	1.78	0.48
2:N:157:PRO:HG2	2:N:184:MET:CA	2.35	0.48
2:B:109:LEU:HD22	2:B:109:LEU:N	2.29	0.48
2:B:139:THR:OG1	2:B:140:PRO:HD2	2.13	0.48
1:E:320:ASP:OD2	1:E:323:LYS:HE2	2.13	0.48
2:F:76:ASP:C	2:F:78:ARG:H	2.16	0.48
1:I:332:GLN:HG3	1:I:338:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:332:GLN:HG3	1:M:338:THR:HG23	1.94	0.48
1:M:425:LEU:HD13	1:M:509:GLN:NE2	2.28	0.48
2:N:174:GLN:C	2:N:176:PRO:HD3	2.33	0.48
1:A:430:GLU:HB2	1:A:532:TYR:HB2	1.95	0.48
1:A:525:LEU:HD23	1:A:531:VAL:HG21	1.96	0.48
2:B:374:LYS:HE2	2:B:378:GLU:HG3	1.96	0.48
1:E:224:GLU:OE1	1:E:224:GLU:N	2.46	0.48
1:E:495:ILE:O	1:E:533:LEU:HA	2.13	0.48
2:F:104:LYS:HG3	2:F:237:ASP:OD2	2.13	0.48
2:F:108:VAL:HG22	2:F:188:TYR:CD2	2.48	0.48
2:F:130:PHE:CE1	2:F:144:TYR:HB2	2.48	0.48
2:F:368:LEU:O	2:F:372:VAL:HG23	2.13	0.48
2:F:396:GLU:O	2:F:397:THR:C	2.48	0.48
1:I:435:VAL:HA	2:J:290:THR:CG2	2.35	0.48
1:I:533:LEU:N	1:I:533:LEU:HD12	2.28	0.48
2:J:21:VAL:CG1	2:J:59:PRO:HD3	2.43	0.48
1:M:305:GLU:O	1:M:309:ILE:HG13	2.13	0.48
1:A:178:ILE:HD12	1:A:191:SER:HB3	1.96	0.48
1:A:225:PRO:HB2	1:A:226:PRO:HD3	1.94	0.48
1:A:357:MET:HG2	1:A:367:GLN:NE2	2.29	0.48
2:B:169:GLU:HA	2:B:169:GLU:OE2	2.12	0.48
2:B:195:ILE:HG23	2:B:196:GLY:N	2.28	0.48
1:E:264:LEU:HD12	1:E:306:ASN:ND2	2.28	0.48
1:E:447:ASN:OD1	1:E:450:THR:HG23	2.13	0.48
1:I:239:TRP:O	1:I:316:GLY:N	2.44	0.48
2:J:115:TYR:HB3	2:J:149:LEU:CB	2.43	0.48
1:M:476:LYS:O	1:M:479:LEU:HB2	2.13	0.48
2:N:85:GLN:HA	2:N:88:TRP:CE2	2.48	0.48
4:P:820:DC:H2"	4:P:821:DC:H5'	1.94	0.48
1:A:222:GLN:N	1:A:224:GLU:OE1	2.46	0.48
1:E:76:ASP:C	1:E:78:ARG:H	2.17	0.48
1:E:108:VAL:C	1:E:109:LEU:HD12	2.34	0.48
1:E:157:PRO:HG2	1:E:158:ALA:H	1.79	0.48
2:F:274:ILE:CD1	2:F:274:ILE:H	2.25	0.48
1:I:239:TRP:CD1	1:I:316:GLY:O	2.67	0.48
1:I:408:ALA:HA	2:J:364:ASP:OD2	2.12	0.48
2:J:422:LEU:C	2:J:424:LYS:H	2.16	0.48
1:M:220:LYS:O	1:M:220:LYS:HD2	2.12	0.48
2:N:62:ALA:C	2:N:63:ILE:CG2	2.81	0.48
1:E:225:PRO:HB2	1:E:226:PRO:HD3	1.96	0.48
2:F:107:THR:HG23	2:F:232:TYR:HE2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:174:GLN:C	2:F:176:PRO:HD3	2.34	0.48
1:I:113:ASP:HB3	1:I:116:PHE:HB2	1.95	0.48
2:J:174:GLN:O	2:J:176:PRO:HD3	2.14	0.48
1:M:136:ASN:OD1	1:M:138:GLU:CG	2.62	0.48
1:M:270:ILE:O	1:M:272:PRO:HD3	2.14	0.48
2:B:271:TYR:HB2	2:B:274:ILE:HD13	1.96	0.48
1:E:442:VAL:HG21	1:E:482:ILE:HG12	1.96	0.48
2:F:271:TYR:N	2:F:271:TYR:CD1	2.82	0.48
2:J:130:PHE:CE1	2:J:144:TYR:HB2	2.48	0.48
1:M:427:TYR:N	1:M:427:TYR:CD1	2.81	0.48
2:N:426:TRP:CD1	2:N:426:TRP:N	2.68	0.48
1:A:219:GLN:CD	1:A:219:GLN:N	2.67	0.48
2:B:426:TRP:H	2:B:426:TRP:HD1	1.50	0.48
1:E:33:ALA:O	1:E:37:ILE:HG12	2.13	0.48
1:I:115:TYR:HB3	1:I:149:LEU:O	2.14	0.48
1:I:120:LEU:O	1:I:121:ASP:C	2.52	0.48
1:I:305:GLU:O	1:I:309:ILE:HG13	2.14	0.48
2:J:195:ILE:HG23	2:J:196:GLY:N	2.29	0.48
2:J:344:GLU:OE1	2:J:344:GLU:HA	2.13	0.48
1:M:325:LEU:N	1:M:325:LEU:HD12	2.29	0.48
1:M:407:GLN:HE22	2:N:418:ASN:HA	1.77	0.48
3:G:726:DT:H2"	3:G:727:DG:OP2	2.13	0.48
1:E:237:ASP:O	1:E:238:LYS:HD2	2.14	0.48
1:E:363:ASN:HA	1:E:511:ASP:CG	2.35	0.48
2:F:104:LYS:HA	2:F:237:ASP:OD2	2.14	0.48
1:I:441:TYR:CE1	1:I:544:GLY:CA	2.94	0.48
2:J:235:HIS:O	2:J:237:ASP:N	2.45	0.48
2:J:274:ILE:H	2:J:274:ILE:CD1	2.27	0.48
2:J:319:TYR:OH	2:J:385:LYS:CD	2.62	0.48
1:M:96:HIS:H	2:N:136:ASN:HD21	1.61	0.48
1:M:175:ASN:HB3	1:M:178:ILE:HG12	1.95	0.48
2:N:78:ARG:HD3	2:N:411:ILE:O	2.14	0.48
2:N:350:LYS:HG2	2:N:351:THR:N	2.28	0.48
1:E:120:LEU:O	1:E:121:ASP:C	2.51	0.47
1:E:478:GLU:CG	1:E:499:SER:HB2	2.44	0.47
1:I:447:ASN:CB	1:I:556:ILE:HD13	2.44	0.47
1:I:476:LYS:O	1:I:479:LEU:HB2	2.14	0.47
2:J:31:ILE:CD1	2:J:133:PRO:HG2	2.44	0.47
1:M:517:LEU:HD22	1:M:521:ILE:HD11	1.96	0.47
2:N:422:LEU:C	2:N:424:LYS:H	2.17	0.47
3:G:713:DC:H2'	3:G:714:DG:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:705:DA:H2"	3:O:706:DT:O5'	2.12	0.47
1:A:357:MET:HG2	1:A:367:GLN:HE22	1.79	0.47
1:A:531:VAL:CG1	1:A:533:LEU:HD11	2.43	0.47
2:B:357:MET:HB3	2:B:360:ALA:HB3	1.96	0.47
2:F:319:TYR:OH	2:F:385:LYS:CD	2.61	0.47
2:F:376:THR:HB	2:F:410:TRP:CH2	2.48	0.47
1:I:3:SER:CB	1:I:117:SER:O	2.62	0.47
1:M:237:ASP:C	1:M:238:LYS:HD2	2.34	0.47
1:M:315:HIS:H	1:M:315:HIS:CD2	2.32	0.47
1:M:363:ASN:HB2	1:M:511:ASP:OD2	2.13	0.47
2:N:38:CYS:SG	2:N:132:ILE:HD11	2.54	0.47
2:N:374:LYS:HE2	2:N:378:GLU:HG3	1.97	0.47
1:A:27:THR:CG2	1:A:30:LYS:H	2.27	0.47
1:A:242:GLN:O	1:A:243:PRO:C	2.53	0.47
1:A:332:GLN:HG3	1:A:338:THR:HG23	1.97	0.47
1:A:354:TYR:CE1	1:A:356:ARG:HB3	2.49	0.47
1:A:447:ASN:OD1	1:A:450:THR:HG23	2.13	0.47
2:B:423:VAL:HB	2:B:426:TRP:CD1	2.49	0.47
1:E:22:LYS:HG2	1:E:23:GLN:H	1.78	0.47
2:F:388:LYS:HG2	2:F:413:GLU:HB3	1.96	0.47
1:I:77:PHE:O	1:I:80:LEU:N	2.48	0.47
1:I:340:GLN:HB3	1:I:351:THR:HG22	1.96	0.47
1:M:298:GLU:CD	1:M:298:GLU:H	2.18	0.47
1:M:528:LYS:HG3	1:M:531:VAL:CG2	2.44	0.47
1:A:90:VAL:CG2	2:B:141:GLY:O	2.63	0.47
1:A:136:ASN:OD1	1:A:138:GLU:CG	2.62	0.47
1:A:211:ARG:HG3	1:A:211:ARG:NH1	2.27	0.47
2:B:94:ILE:HG21	2:B:182:GLN:O	2.14	0.47
2:B:194:GLU:CD	2:B:195:ILE:H	2.18	0.47
2:B:396:GLU:O	2:B:397:THR:C	2.50	0.47
1:E:442:VAL:HB	1:E:481:ALA:HB1	1.96	0.47
2:F:115:TYR:CZ	2:F:157:PRO:HG3	2.49	0.47
1:I:549:ASP:O	1:I:553:SER:OG	2.31	0.47
2:J:174:GLN:C	2:J:176:PRO:HD3	2.35	0.47
2:J:271:TYR:HB2	2:J:274:ILE:CD1	2.44	0.47
2:J:328:GLU:O	2:J:339:TYR:HA	2.14	0.47
1:M:479:LEU:HB3	1:M:517:LEU:HD13	1.96	0.47
2:N:13:LYS:HB2	2:N:16:MET:HG3	1.96	0.47
2:N:83:ARG:HH11	2:N:83:ARG:HG3	1.80	0.47
2:N:274:ILE:HD12	2:N:274:ILE:H	1.79	0.47
2:B:274:ILE:HD12	2:B:274:ILE:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:LEU:O	2:B:387:PRO:HA	2.14	0.47
1:E:250:ASP:CG	1:E:251:SER:H	2.18	0.47
1:E:395:LYS:HD3	1:E:414:TRP:CZ2	2.49	0.47
2:F:244:ILE:HD11	2:F:271:TYR:OH	2.14	0.47
1:I:167:ILE:O	1:I:170:PRO:HD2	2.15	0.47
2:J:368:LEU:O	2:J:372:VAL:HG23	2.14	0.47
1:M:315:HIS:CD2	1:M:315:HIS:N	2.81	0.47
2:N:13:LYS:NZ	2:N:86:ASP:H	2.11	0.47
2:N:195:ILE:HG23	2:N:196:GLY:N	2.30	0.47
1:A:463:ARG:HB2	1:A:463:ARG:HH11	1.79	0.47
2:B:339:TYR:CG	2:B:375:ILE:HD12	2.49	0.47
1:E:27:THR:CG2	1:E:29:GLU:HB3	2.45	0.47
1:E:244:ILE:HG23	1:E:244:ILE:O	2.14	0.47
2:J:96:HIS:HA	2:J:181:TYR:CE1	2.49	0.47
1:M:116:PHE:CE1	1:M:146:TYR:HE2	2.32	0.47
3:G:717:DC:H2"	3:G:718:DA:OP2	2.14	0.47
1:A:171:PHE:CE2	1:A:205:LEU:HD23	2.50	0.47
1:A:175:ASN:HB3	1:A:178:ILE:HG12	1.97	0.47
1:A:511:ASP:OD1	1:A:511:ASP:C	2.53	0.47
1:E:85:GLN:O	1:E:85:GLN:HG3	2.13	0.47
1:E:242:GLN:O	1:E:243:PRO:C	2.52	0.47
1:E:510:PRO:O	1:E:522:ILE:HD12	2.14	0.47
1:I:221:HIS:H	1:I:221:HIS:HD2	1.62	0.47
1:I:246:LEU:HD11	1:I:264:LEU:HD22	1.97	0.47
1:I:303:LEU:HD13	1:I:307:ARG:HD2	1.96	0.47
1:I:325:LEU:HD13	1:I:385:LYS:HE2	1.97	0.47
1:I:364:ASP:N	1:I:511:ASP:OD2	2.46	0.47
2:J:271:TYR:N	2:J:271:TYR:CD1	2.82	0.47
1:M:116:PHE:HE1	1:M:146:TYR:CE2	2.32	0.47
1:M:232:TYR:OH	1:M:269:GLN:NE2	2.45	0.47
1:M:420:PRO:HA	1:M:421:PRO:C	2.35	0.47
2:N:402:TRP:CZ2	2:N:403:THR:HG22	2.49	0.47
4:H:818:DC:H2"	4:H:819:DG:H5'	1.95	0.47
1:A:109:LEU:N	1:A:109:LEU:CD1	2.78	0.47
1:A:305:GLU:O	1:A:309:ILE:HG13	2.15	0.47
2:F:72:ARG:HH11	2:F:72:ARG:HG3	1.80	0.47
2:F:118:VAL:HG13	2:F:119:PRO:HD2	1.96	0.47
1:I:34:LEU:HB3	1:I:132:ILE:HD12	1.96	0.47
1:I:78:ARG:O	1:I:82:LYS:HG3	2.15	0.47
2:J:208:HIS:HD2	2:J:208:HIS:O	1.98	0.47
1:M:115:TYR:CZ	7:M:823:ZP4:H2'A	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:225:PRO:HB2	1:M:226:PRO:CD	2.35	0.47
1:M:290:THR:O	1:M:291:GLU:C	2.52	0.47
2:N:92:LEU:HB2	2:N:158:ALA:HB1	1.95	0.47
1:A:33:ALA:O	1:A:36:GLU:HB3	2.14	0.47
1:A:118:VAL:HB	1:A:149:LEU:HD22	1.97	0.47
1:I:285:GLY:O	1:I:287:LYS:HG2	2.15	0.47
1:I:434:ILE:N	1:I:434:ILE:HD12	2.30	0.47
2:J:318:TYR:CD1	2:J:318:TYR:O	2.68	0.47
2:J:374:LYS:HE2	2:J:378:GLU:OE2	2.15	0.47
1:M:225:PRO:CB	1:M:226:PRO:HD3	2.31	0.47
1:M:354:TYR:CE1	1:M:356:ARG:HB3	2.50	0.47
3:C:717:DC:H2"	3:C:718:DA:OP2	2.14	0.47
3:K:712:DC:H2'	3:K:713:DC:C6	2.50	0.47
1:A:255:ASN:HD22	1:A:289:LEU:HD22	1.80	0.47
2:B:271:TYR:N	2:B:271:TYR:CD1	2.83	0.47
1:I:479:LEU:HB3	1:I:517:LEU:HD13	1.96	0.47
2:J:104:LYS:HA	2:J:237:ASP:OD2	2.15	0.47
1:M:171:PHE:HB2	1:M:208:HIS:CD2	2.50	0.47
1:M:315:HIS:H	1:M:315:HIS:HD2	1.63	0.47
1:M:410:TRP:CZ3	2:N:401:TRP:CE2	3.02	0.47
2:B:244:ILE:HG12	2:B:310:LEU:HD13	1.98	0.46
1:E:290:THR:O	1:E:291:GLU:C	2.52	0.46
2:F:195:ILE:HG23	2:F:196:GLY:N	2.30	0.46
1:I:98:ALA:O	1:I:349:LEU:CD2	2.63	0.46
2:J:76:ASP:OD1	2:J:78:ARG:HB2	2.16	0.46
1:M:447:ASN:OD1	1:M:450:THR:HG23	2.14	0.46
1:A:28:GLU:HA	1:A:31:ILE:HD12	1.97	0.46
1:A:72:ARG:HD3	1:A:74:LEU:HD21	1.97	0.46
2:B:319:TYR:OH	2:B:385:LYS:CD	2.63	0.46
2:F:17:ASP:O	2:F:83:ARG:CD	2.63	0.46
2:J:3:SER:N	2:J:4:PRO:CD	2.71	0.46
2:J:10:VAL:HG22	2:J:87:PHE:CZ	2.49	0.46
2:J:253:THR:O	2:J:257:ILE:HG12	2.15	0.46
1:M:16:MET:HE1	1:M:83:ARG:HG2	1.97	0.46
1:M:28:GLU:HA	1:M:31:ILE:HD12	1.97	0.46
1:M:384:GLY:O	2:N:27:THR:HA	2.16	0.46
1:M:452:LEU:HD23	1:M:470:THR:O	2.15	0.46
1:M:558:LYS:HA	1:M:558:LYS:CE	2.45	0.46
2:N:28:GLU:HA	2:N:135:ILE:HD11	1.97	0.46
2:N:271:TYR:HB2	2:N:274:ILE:CD1	2.44	0.46
1:A:290:THR:O	1:A:291:GLU:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:21:VAL:CG1	2:F:59:PRO:HD3	2.46	0.46
1:I:181:TYR:CZ	2:J:138:GLU:HG2	2.49	0.46
1:I:448:ARG:HD3	3:K:724:DT:H5"	1.97	0.46
1:I:480:GLN:HA	1:I:480:GLN:HE21	1.80	0.46
1:M:328:GLU:HG3	1:M:390:LYS:HB2	1.98	0.46
1:M:457:TYR:CD1	1:M:457:TYR:C	2.88	0.46
1:A:225:PRO:O	1:A:234:LEU:O	2.34	0.46
2:B:16:MET:HA	2:B:16:MET:CE	2.45	0.46
1:I:98:ALA:O	1:I:349:LEU:HD21	2.16	0.46
1:I:244:ILE:O	1:I:244:ILE:HG23	2.15	0.46
2:J:216:THR:O	2:J:217:PRO:C	2.53	0.46
1:M:46:LYS:O	1:M:147:ASN:HB2	2.16	0.46
1:M:480:GLN:HA	1:M:480:GLN:HE21	1.80	0.46
1:E:164:MET:HG3	1:E:164:MET:O	2.14	0.46
1:E:285:GLY:O	1:E:287:LYS:HG2	2.15	0.46
2:F:242:GLN:NE2	2:F:353:LYS:HE3	2.30	0.46
2:F:253:THR:O	2:F:257:ILE:HG12	2.15	0.46
1:I:103:LYS:HB3	1:I:191:SER:O	2.15	0.46
1:I:320:ASP:O	1:I:322:SER:N	2.48	0.46
2:J:84:THR:HG21	2:J:124:PHE:CZ	2.51	0.46
2:J:118:VAL:HG13	2:J:119:PRO:HD2	1.97	0.46
1:M:437:ALA:HB1	1:M:492:GLU:O	2.15	0.46
1:A:23:GLN:NE2	1:A:60:VAL:HG22	2.29	0.46
1:A:303:LEU:HD13	1:A:307:ARG:HD2	1.98	0.46
1:A:303:LEU:HD11	1:A:307:ARG:NH1	2.31	0.46
1:E:153:TRP:O	1:E:154:LYS:C	2.54	0.46
2:F:38:CYS:SG	2:F:132:ILE:HD11	2.55	0.46
2:F:76:ASP:OD1	2:F:78:ARG:HB2	2.15	0.46
2:F:85:GLN:HA	2:F:88:TRP:CE2	2.50	0.46
2:F:261:VAL:CG1	2:F:276:VAL:HG21	2.37	0.46
1:I:342:TYR:HA	1:I:349:LEU:HB2	1.97	0.46
1:I:439:THR:HA	1:I:494:ASN:HB2	1.98	0.46
1:M:16:MET:HE2	1:M:83:ARG:HG2	1.98	0.46
1:A:326:ILE:O	1:A:341:ILE:HA	2.16	0.46
1:E:49:LYS:HG3	1:E:142:ILE:HG23	1.98	0.46
1:E:441:TYR:CD2	1:E:496:VAL:HG22	2.50	0.46
1:E:511:ASP:OD1	1:E:511:ASP:C	2.55	0.46
1:E:524:GLN:O	1:E:528:LYS:HG2	2.15	0.46
2:F:402:TRP:CZ2	2:F:403:THR:HG22	2.51	0.46
1:M:90:VAL:HG23	2:N:141:GLY:O	2.16	0.46
1:M:108:VAL:C	1:M:109:LEU:HD12	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:143:ARG:HG2	2:N:143:ARG:HH11	1.81	0.46
2:N:314:VAL:HG13	2:N:317:VAL:HG13	1.98	0.46
2:N:423:VAL:HB	2:N:426:TRP:CG	2.50	0.46
4:D:820:DC:H2"	4:D:821:DC:H5'	1.96	0.46
3:K:713:DC:H2'	3:K:714:DG:C8	2.51	0.46
3:O:726:DT:H2"	3:O:727:DG:OP2	2.15	0.46
1:A:136:ASN:OD1	1:A:138:GLU:HG3	2.15	0.46
1:A:222:GLN:H	1:A:224:GLU:CD	2.18	0.46
1:A:479:LEU:HD22	1:A:521:ILE:CD1	2.45	0.46
1:E:332:GLN:OE1	1:E:332:GLN:HA	2.16	0.46
2:F:423:VAL:HB	2:F:426:TRP:CD1	2.50	0.46
1:I:290:THR:O	1:I:291:GLU:C	2.54	0.46
1:M:118:VAL:HB	1:M:149:LEU:HD22	1.98	0.46
1:M:264:LEU:HD12	1:M:306:ASN:ND2	2.31	0.46
1:A:67:ASN:C	1:A:69:THR:N	2.69	0.46
1:E:114:ALA:HB3	7:E:823:ZP4:N3'	2.30	0.46
1:E:235:HIS:O	1:E:318:TYR:HE2	1.98	0.46
1:E:332:GLN:HG3	1:E:338:THR:HG23	1.98	0.46
1:E:476:LYS:O	1:E:479:LEU:HB2	2.16	0.46
2:F:303:LEU:HD23	2:F:304:ALA:N	2.31	0.46
1:I:105:SER:HB3	1:I:198:HIS:CG	2.51	0.46
1:I:337:TRP:CZ3	1:I:368:LEU:HD23	2.51	0.46
2:J:388:LYS:HG2	2:J:413:GLU:HB3	1.96	0.46
1:M:23:GLN:NE2	1:M:60:VAL:N	2.47	0.46
1:M:258:CYS:HG	4:P:817:MRG:H24	1.63	0.46
1:M:460:ASN:ND2	2:N:288:ALA:HB2	2.30	0.46
2:N:253:THR:O	2:N:257:ILE:HG12	2.16	0.46
2:B:318:TYR:CD1	2:B:318:TYR:O	2.69	0.46
1:E:331:LYS:HE3	1:E:364:ASP:OD1	2.14	0.46
2:F:13:LYS:HZ1	2:F:85:GLN:H	1.64	0.46
2:F:366:LYS:O	2:F:369:THR:HB	2.16	0.46
1:I:146:TYR:CD2	1:I:150:PRO:HB3	2.51	0.46
1:M:57:ASN:HA	1:M:129:ALA:O	2.16	0.46
1:M:384:GLY:O	2:N:27:THR:HG22	2.16	0.46
2:N:339:TYR:CG	2:N:375:ILE:HD12	2.51	0.46
1:A:325:LEU:HD13	1:A:385:LYS:HE2	1.97	0.45
2:B:330:GLN:HB2	2:B:338:THR:OG1	2.16	0.45
1:E:10:VAL:CG1	1:E:11:LYS:N	2.78	0.45
1:E:222:GLN:H	1:E:224:GLU:CD	2.20	0.45
1:E:479:LEU:HD23	1:E:479:LEU:HA	1.82	0.45
2:F:203:GLU:OE2	2:F:206:ARG:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:236:PRO:HG2	1:I:237:ASP:OD1	2.15	0.45
2:J:314:VAL:HG13	2:J:317:VAL:HG13	1.98	0.45
1:M:465:LYS:O	1:M:466:VAL:HG12	2.16	0.45
2:N:10:VAL:HG22	2:N:87:PHE:CZ	2.51	0.45
2:N:169:GLU:HB2	2:N:170:PRO:HD3	1.98	0.45
2:N:396:GLU:O	2:N:397:THR:C	2.55	0.45
4:H:816:DG:H2'	4:H:817:MRG:H8	1.97	0.45
1:A:115:TYR:OH	1:A:184:MET:HE3	2.16	0.45
2:B:325:LEU:HB3	2:B:387:PRO:HA	1.98	0.45
2:B:395:LYS:O	2:B:399:GLU:HG3	2.16	0.45
2:F:160:PHE:CD2	2:F:164:MET:HB2	2.51	0.45
2:F:325:LEU:O	2:F:388:LYS:N	2.43	0.45
1:I:315:HIS:N	1:I:315:HIS:CD2	2.83	0.45
1:I:427:TYR:OH	1:I:510:PRO:HD2	2.15	0.45
2:J:339:TYR:CE2	2:J:375:ILE:HD12	2.51	0.45
2:J:423:VAL:HB	2:J:426:TRP:CG	2.50	0.45
1:M:76:ASP:C	1:M:78:ARG:H	2.19	0.45
1:M:120:LEU:O	1:M:121:ASP:C	2.54	0.45
1:M:222:GLN:N	1:M:224:GLU:OE1	2.49	0.45
2:N:395:LYS:O	2:N:399:GLU:HG3	2.15	0.45
1:E:250:ASP:OD2	1:E:250:ASP:N	2.50	0.45
1:E:325:LEU:N	1:E:325:LEU:HD12	2.30	0.45
1:E:416:PHE:CD1	1:E:417:VAL:N	2.85	0.45
1:I:478:GLU:CD	1:I:499:SER:HB2	2.36	0.45
2:J:61:PHE:CD2	2:J:403:THR:HB	2.51	0.45
2:J:73:LYS:NZ	2:J:146:TYR:OH	2.48	0.45
2:N:199:ARG:O	2:N:202:ILE:HB	2.16	0.45
2:N:325:LEU:HD21	2:N:383:TRP:CE3	2.51	0.45
1:A:229:TRP:CE3	1:A:234:LEU:HD11	2.52	0.45
1:A:441:TYR:N	1:A:441:TYR:CD2	2.82	0.45
1:E:70:ARG:HH22	7:E:823:ZP4:PD	2.40	0.45
1:E:86:ASP:OD1	1:E:86:ASP:N	2.50	0.45
1:E:264:LEU:CD1	1:E:306:ASN:HD22	2.30	0.45
2:F:101:LYS:HD3	2:F:382:ILE:HG23	1.98	0.45
2:F:105:SER:O	2:F:190:GLY:HA2	2.16	0.45
1:I:553:SER:O	1:I:556:ILE:HG23	2.17	0.45
2:J:376:THR:HB	2:J:410:TRP:CH2	2.51	0.45
1:M:164:MET:HE2	1:M:187:LEU:HD21	1.99	0.45
1:M:325:LEU:HD13	1:M:385:LYS:HE2	1.98	0.45
1:M:330:GLN:HE21	1:M:330:GLN:HB2	1.53	0.45
1:M:421:PRO:O	1:M:422:LEU:HD23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:423:VAL:HB	2:N:426:TRP:CD1	2.51	0.45
3:O:712:DC:H2'	3:O:713:DC:C6	2.51	0.45
1:A:250:ASP:N	1:A:250:ASP:OD2	2.50	0.45
2:B:85:GLN:HA	2:B:88:TRP:CE2	2.51	0.45
2:B:143:ARG:HG2	2:B:143:ARG:NH1	2.31	0.45
2:B:274:ILE:HA	2:B:306:ASN:OD1	2.16	0.45
1:E:328:GLU:HG3	1:E:390:LYS:HB2	1.99	0.45
2:F:115:TYR:OH	2:F:157:PRO:HG3	2.17	0.45
2:F:125:ARG:HH11	2:F:147:ASN:HB3	1.82	0.45
1:I:32:LYS:HZ2	1:I:135:ILE:HG21	1.81	0.45
1:I:153:TRP:O	1:I:154:LYS:C	2.54	0.45
1:I:169:GLU:HB3	1:I:170:PRO:HD3	1.98	0.45
2:J:242:GLN:OE1	2:J:353:LYS:HG3	2.16	0.45
1:M:228:LEU:HD22	1:M:242:GLN:NE2	2.32	0.45
1:M:337:TRP:CZ3	1:M:368:LEU:HD23	2.52	0.45
2:N:368:LEU:O	2:N:372:VAL:HG23	2.16	0.45
3:K:714:DG:H2"	3:K:715:DA:C8	2.51	0.45
1:A:106:VAL:HG12	1:A:107:THR:N	2.32	0.45
2:B:6:GLU:OE1	2:B:6:GLU:HA	2.17	0.45
2:B:130:PHE:CE1	2:B:144:TYR:HB2	2.52	0.45
1:E:108:VAL:O	1:E:220:LYS:HB2	2.17	0.45
1:E:118:VAL:C	1:E:148:VAL:HG23	2.37	0.45
1:E:315:HIS:CD2	1:E:315:HIS:N	2.84	0.45
2:F:236:PRO:HA	2:F:239:TRP:CD2	2.52	0.45
2:F:274:ILE:N	2:F:274:ILE:CD1	2.80	0.45
1:I:11:LYS:N	1:I:85:GLN:OE1	2.49	0.45
1:I:315:HIS:CD2	1:I:315:HIS:H	2.35	0.45
1:I:355:ALA:O	1:I:356:ARG:C	2.53	0.45
2:J:69:THR:HG22	2:J:69:THR:O	2.15	0.45
2:J:241:VAL:HG13	2:J:351:THR:N	2.32	0.45
2:J:423:VAL:HB	2:J:426:TRP:CD1	2.51	0.45
1:M:149:LEU:HD21	1:M:159:ILE:HG22	1.99	0.45
2:N:76:ASP:C	2:N:78:ARG:H	2.20	0.45
3:O:707:DG:H2"	3:O:708:DG:C5'	2.46	0.45
3:O:713:DC:H2'	3:O:714:DG:C8	2.52	0.45
1:A:27:THR:HG22	1:A:29:GLU:HB3	1.98	0.45
1:A:264:LEU:HD12	1:A:306:ASN:HD22	1.81	0.45
1:A:442:VAL:HG21	1:A:482:ILE:HG12	1.98	0.45
2:B:235:HIS:C	2:B:237:ASP:H	2.19	0.45
2:B:274:ILE:CD1	2:B:274:ILE:H	2.29	0.45
1:E:24:TRP:C	1:E:24:TRP:CD1	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:398:TRP:CH2	1:E:411:ILE:HG12	2.51	0.45
1:E:480:GLN:O	1:E:481:ALA:C	2.55	0.45
2:F:109:LEU:HD22	2:F:109:LEU:N	2.32	0.45
2:F:216:THR:O	2:F:217:PRO:C	2.54	0.45
2:F:274:ILE:HD12	2:F:274:ILE:H	1.80	0.45
2:J:72:ARG:HH21	2:J:409:THR:CG2	2.27	0.45
1:M:480:GLN:HA	1:M:480:GLN:NE2	2.31	0.45
2:N:130:PHE:CE1	2:N:144:TYR:HB2	2.51	0.45
1:E:121:ASP:C	1:E:121:ASP:OD1	2.55	0.45
1:E:209:LEU:O	1:E:212:TRP:N	2.47	0.45
1:E:264:LEU:HD12	1:E:306:ASN:HD22	1.81	0.45
1:E:315:HIS:CD2	1:E:315:HIS:H	2.35	0.45
1:E:326:ILE:O	1:E:341:ILE:HA	2.17	0.45
2:F:174:GLN:HG3	2:F:175:ASN:OD1	2.16	0.45
2:F:244:ILE:HG12	2:F:310:LEU:HD13	1.99	0.45
1:I:2:ILE:HG22	1:I:3:SER:H	1.82	0.45
1:I:250:ASP:N	1:I:250:ASP:OD2	2.50	0.45
2:J:84:THR:HG21	2:J:124:PHE:CE1	2.51	0.45
2:J:234:LEU:N	2:J:234:LEU:CD1	2.73	0.45
1:M:357:MET:HG2	1:M:367:GLN:HE22	1.82	0.45
2:N:320:ASP:HA	2:N:321:PRO:HD2	1.78	0.45
1:A:27:THR:CG2	1:A:29:GLU:HB3	2.47	0.45
1:A:103:LYS:CE	1:A:179:VAL:HG21	2.42	0.45
1:A:108:VAL:C	1:A:109:LEU:HD12	2.36	0.45
1:A:264:LEU:HD12	1:A:306:ASN:ND2	2.32	0.45
1:A:457:TYR:CD1	1:A:457:TYR:C	2.90	0.45
2:B:24:TRP:CZ3	2:B:403:THR:HG21	2.52	0.45
2:B:54:ASN:HB3	2:B:143:ARG:HH21	1.82	0.45
2:B:303:LEU:HD23	2:B:304:ALA:N	2.31	0.45
1:E:409:THR:O	2:F:364:ASP:HB3	2.17	0.45
2:F:75:VAL:HG11	2:F:77:PHE:CD2	2.51	0.45
1:I:480:GLN:HA	1:I:480:GLN:NE2	2.32	0.45
1:M:434:ILE:HD12	1:M:434:ILE:N	2.32	0.45
2:N:10:VAL:HG11	2:N:124:PHE:CE1	2.51	0.45
2:N:234:LEU:HD12	2:N:234:LEU:H	1.81	0.45
1:A:264:LEU:CD1	1:A:306:ASN:HD22	2.30	0.45
1:A:295:LEU:HB3	1:A:300:GLU:HG2	1.99	0.45
1:A:480:GLN:NE2	1:A:480:GLN:HA	2.32	0.45
2:B:366:LYS:O	2:B:369:THR:HB	2.17	0.45
1:E:108:VAL:HA	1:E:187:LEU:O	2.17	0.45
1:E:188:TYR:CD1	1:E:188:TYR:C	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:531:VAL:CG1	1:E:532:TYR:N	2.80	0.45
1:I:108:VAL:C	1:I:109:LEU:HD12	2.37	0.45
1:M:93:GLY:N	2:N:137:ASN:OD1	2.49	0.45
1:M:473:THR:HG21	4:P:809:DC:P	2.57	0.45
3:G:712:DC:H2"	3:G:713:DC:O5'	2.16	0.45
1:A:81:ASN:HB3	1:A:154:LYS:CD	2.47	0.44
1:A:96:HIS:ND1	1:A:97:PRO:HD2	2.32	0.44
2:B:402:TRP:CZ2	2:B:403:THR:HG22	2.52	0.44
1:I:398:TRP:CH2	1:I:411:ILE:HG12	2.53	0.44
2:J:325:LEU:O	2:J:388:LYS:N	2.42	0.44
2:J:396:GLU:O	2:J:397:THR:C	2.55	0.44
2:J:421:PRO:O	2:J:424:LYS:N	2.49	0.44
1:M:244:ILE:CD1	1:M:263:LYS:HG3	2.43	0.44
1:M:293:ILE:CD1	1:M:294:PRO:HD2	2.39	0.44
1:A:342:TYR:HA	1:A:349:LEU:HB2	1.98	0.44
1:A:478:GLU:CD	1:A:499:SER:HB2	2.38	0.44
1:A:512:LYS:O	1:A:513:SER:HB2	2.17	0.44
1:E:446:ALA:O	1:E:556:ILE:HG21	2.17	0.44
1:I:433:PRO:HD3	2:J:255:ASN:OD1	2.18	0.44
1:I:511:ASP:OD1	1:I:511:ASP:C	2.56	0.44
2:J:189:VAL:HG21	2:J:205:LEU:HD13	1.99	0.44
1:M:355:ALA:O	1:M:356:ARG:C	2.54	0.44
1:A:24:TRP:CD1	1:A:24:TRP:C	2.91	0.44
1:A:72:ARG:CD	1:A:74:LEU:HD21	2.48	0.44
1:A:342:TYR:OH	1:A:390:LYS:HD2	2.17	0.44
2:B:374:LYS:HE2	2:B:378:GLU:OE2	2.17	0.44
1:E:90:VAL:CG2	2:F:141:GLY:O	2.65	0.44
2:F:163:SER:O	2:F:164:MET:C	2.55	0.44
1:I:4:PRO:HD2	1:I:212:TRP:O	2.16	0.44
1:I:103:LYS:CE	1:I:179:VAL:HG21	2.34	0.44
1:I:164:MET:HE2	1:I:168:LEU:HD11	1.98	0.44
2:N:72:ARG:HH22	2:N:151:GLN:CB	2.30	0.44
2:N:160:PHE:CD2	2:N:164:MET:HB2	2.52	0.44
2:N:234:LEU:HD12	2:N:234:LEU:N	2.32	0.44
2:N:271:TYR:N	2:N:271:TYR:CD1	2.85	0.44
4:P:805:DG:H1'	4:P:806:DT:H5'	1.99	0.44
4:P:816:DG:H2'	4:P:817:MRG:H8	1.99	0.44
1:A:72:ARG:HG2	1:A:74:LEU:HD21	2.00	0.44
2:B:72:ARG:HE	2:B:409:THR:CG2	2.30	0.44
1:E:109:LEU:N	1:E:109:LEU:CD1	2.80	0.44
2:F:241:VAL:HG12	2:F:351:THR:OG1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:315:HIS:H	1:I:315:HIS:HD2	1.66	0.44
1:M:115:TYR:CG	7:M:823:ZP4:H2'A	2.52	0.44
2:N:274:ILE:H	2:N:274:ILE:CD1	2.30	0.44
1:A:439:THR:CG2	2:B:289:LEU:HD13	2.33	0.44
1:E:96:HIS:ND1	1:E:97:PRO:HD2	2.32	0.44
2:F:339:TYR:CE2	2:F:375:ILE:HD12	2.53	0.44
1:I:8:VAL:CG1	2:J:53:GLU:OE1	2.66	0.44
1:I:40:GLU:O	1:I:44:GLU:HG3	2.18	0.44
1:I:382:ILE:HA	2:J:136:ASN:HA	1.99	0.44
1:M:50:ILE:CG2	1:M:145:GLN:HB3	2.46	0.44
3:K:726:DT:H2"	3:K:727:DG:OP2	2.16	0.44
1:E:27:THR:HG22	1:E:29:GLU:HB3	1.98	0.44
1:E:478:GLU:CD	1:E:499:SER:HB2	2.38	0.44
2:F:157:PRO:HG2	2:F:184:MET:CA	2.38	0.44
1:I:100:LEU:O	1:I:318:TYR:HB3	2.18	0.44
2:J:118:VAL:HG22	5:Q:1:GLC:C3	2.45	0.44
1:M:49:LYS:HE3	1:M:142:ILE:HG23	2.00	0.44
1:M:209:LEU:HB3	1:M:214:LEU:CB	2.46	0.44
1:M:270:ILE:HG23	1:M:314:VAL:CG2	2.48	0.44
1:M:342:TYR:HA	1:M:349:LEU:HB2	1.99	0.44
1:M:447:ASN:CB	1:M:556:ILE:HD13	2.47	0.44
4:L:820:DC:H2"	4:L:821:DC:H5'	1.98	0.44
1:A:85:GLN:O	1:A:85:GLN:HG3	2.14	0.44
1:A:224:GLU:OE1	1:A:224:GLU:N	2.51	0.44
2:B:203:GLU:OE2	2:B:206:ARG:HD2	2.18	0.44
1:E:115:TYR:CG	7:E:823:ZP4:H2'A	2.52	0.44
1:E:253:THR:HA	1:E:292:VAL:HA	1.99	0.44
1:E:295:LEU:HB3	1:E:300:GLU:HG2	2.00	0.44
2:F:83:ARG:HH11	2:F:83:ARG:HG3	1.83	0.44
1:I:260:LEU:HG	1:I:264:LEU:HD23	1.99	0.44
1:I:374:LYS:O	1:I:374:LYS:HD3	2.17	0.44
1:I:442:VAL:HB	1:I:481:ALA:HB1	2.00	0.44
2:J:203:GLU:OE2	2:J:206:ARG:HD2	2.18	0.44
2:J:259:LYS:O	2:J:262:GLY:N	2.51	0.44
1:M:295:LEU:HB3	1:M:300:GLU:HG2	1.99	0.44
1:M:325:LEU:C	1:M:326:ILE:HD12	2.37	0.44
2:N:339:TYR:CE2	2:N:375:ILE:HD12	2.52	0.44
1:A:164:MET:HE2	1:A:168:LEU:HD11	2.00	0.44
1:A:254:VAL:HG12	1:A:255:ASN:N	2.32	0.44
1:A:480:GLN:HA	1:A:480:GLN:HE21	1.82	0.44
2:B:160:PHE:CD2	2:B:164:MET:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:THR:OG1	2:B:256:ASP:OD1	2.34	0.44
1:E:50:ILE:HG13	1:E:143:ARG:HB3	2.00	0.44
1:E:73:LYS:CE	1:E:146:TYR:OH	2.61	0.44
1:E:225:PRO:O	1:E:234:LEU:O	2.36	0.44
1:E:337:TRP:CZ3	1:E:368:LEU:HD23	2.53	0.44
2:F:75:VAL:CG1	2:F:77:PHE:CD2	3.01	0.44
2:F:238:LYS:HE2	2:F:238:LYS:HB2	1.80	0.44
1:I:91:GLN:HG2	1:I:161:GLN:NE2	2.33	0.44
1:I:330:GLN:HE21	1:I:330:GLN:HB2	1.57	0.44
1:I:452:LEU:HD23	1:I:470:THR:O	2.18	0.44
2:J:125:ARG:HH11	2:J:147:ASN:CB	2.31	0.44
2:J:206:ARG:O	2:J:210:LEU:CD1	2.65	0.44
1:M:4:PRO:HD2	1:M:212:TRP:C	2.37	0.44
1:M:33:ALA:O	1:M:37:ILE:HG12	2.18	0.44
1:M:96:HIS:ND1	1:M:97:PRO:HD2	2.33	0.44
1:M:98:ALA:HB1	1:M:349:LEU:HD22	2.00	0.44
1:M:223:LYS:O	1:M:223:LYS:HG3	2.17	0.44
2:N:122:GLU:HA	2:N:125:ARG:HH21	1.83	0.44
2:N:330:GLN:HB2	2:N:338:THR:OG1	2.18	0.44
2:N:374:LYS:HE2	2:N:378:GLU:OE2	2.17	0.44
1:A:53:GLU:CD	1:A:53:GLU:H	2.20	0.44
1:A:100:LEU:HA	1:A:100:LEU:HD23	1.78	0.44
1:A:173:LYS:O	1:A:176:PRO:HD3	2.18	0.44
2:B:246:LEU:O	2:B:307:ARG:NH1	2.51	0.44
2:B:325:LEU:O	2:B:388:LYS:N	2.45	0.44
2:B:339:TYR:CE2	2:B:375:ILE:HG23	2.53	0.44
1:E:115:TYR:CZ	7:E:823:ZP4:H1'	2.53	0.44
2:F:23:GLN:HG2	2:F:133:PRO:HD3	1.99	0.44
2:F:325:LEU:HB3	2:F:387:PRO:HA	2.00	0.44
1:I:232:TYR:OH	1:I:269:GLN:NE2	2.48	0.44
1:I:331:LYS:HB3	1:I:421:PRO:HG2	2.00	0.44
1:I:478:GLU:CG	1:I:499:SER:HB2	2.48	0.44
2:J:271:TYR:HB2	2:J:274:ILE:HD13	1.99	0.44
2:N:76:ASP:OD1	2:N:78:ARG:HB2	2.18	0.44
1:A:164:MET:HG3	1:A:164:MET:O	2.17	0.43
1:A:416:PHE:CD1	1:A:417:VAL:N	2.86	0.43
1:A:427:TYR:OH	1:A:510:PRO:HD2	2.18	0.43
1:A:434:ILE:N	1:A:434:ILE:HD12	2.33	0.43
1:E:22:LYS:CG	1:E:23:GLN:N	2.79	0.43
1:E:70:ARG:NH2	7:E:823:ZP4:O1D	2.51	0.43
1:E:439:THR:HA	1:E:494:ASN:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:26:LEU:HB2	2:F:31:ILE:HD11	1.99	0.43
2:F:234:LEU:H	2:F:234:LEU:CD1	2.30	0.43
1:I:106:VAL:HG12	1:I:107:THR:N	2.33	0.43
1:I:136:ASN:O	1:I:137:ASN:CB	2.66	0.43
1:M:70:ARG:NH2	7:M:823:ZP4:H31	2.33	0.43
1:M:454:LYS:HB2	1:M:552:VAL:O	2.18	0.43
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.98	0.43
1:E:439:THR:CG2	2:F:289:LEU:HD13	2.37	0.43
2:F:252:TRP:CG	2:F:295:LEU:HD11	2.52	0.43
2:J:7:THR:HG22	2:J:119:PRO:HG2	2.00	0.43
2:J:330:GLN:HB2	2:J:338:THR:OG1	2.18	0.43
1:M:303:LEU:HD13	1:M:307:ARG:HD2	2.00	0.43
1:M:329:ILE:O	1:M:392:PRO:HD3	2.17	0.43
2:N:244:ILE:HD11	2:N:271:TYR:OH	2.18	0.43
1:A:17:ASP:CG	2:F:95:PRO:HB3	2.39	0.43
1:A:138:GLU:HG3	1:A:138:GLU:H	1.52	0.43
2:B:234:LEU:HD12	2:B:234:LEU:N	2.33	0.43
1:E:303:LEU:HD13	1:E:307:ARG:HD2	1.99	0.43
1:E:363:ASN:OD1	1:E:365:VAL:N	2.51	0.43
1:E:512:LYS:O	1:E:513:SER:HB2	2.18	0.43
2:F:234:LEU:N	2:F:234:LEU:CD1	2.78	0.43
1:I:255:ASN:O	1:I:259:LYS:HG3	2.18	0.43
1:I:281:LYS:HE2	1:I:284:ARG:CZ	2.48	0.43
1:I:511:ASP:C	1:I:512:LYS:CG	2.87	0.43
2:J:274:ILE:N	2:J:274:ILE:CD1	2.81	0.43
1:M:91:GLN:HG3	1:M:161:GLN:NE2	2.32	0.43
1:M:478:GLU:CD	1:M:499:SER:HB2	2.39	0.43
2:N:57:ASN:OD1	2:N:143:ARG:NH1	2.51	0.43
2:N:125:ARG:HH11	2:N:147:ASN:HB3	1.81	0.43
2:N:357:MET:HB3	2:N:360:ALA:HB3	2.00	0.43
1:A:94:ILE:HD11	3:C:708:DG:H21	1.84	0.43
1:A:332:GLN:OE1	1:A:332:GLN:HA	2.18	0.43
2:B:174:GLN:O	2:B:176:PRO:HD3	2.18	0.43
2:B:237:ASP:C	2:B:239:TRP:H	2.20	0.43
2:F:46:LYS:HD2	2:F:116:PHE:HB3	2.01	0.43
1:I:135:ILE:H	1:I:135:ILE:CD1	2.20	0.43
1:M:91:GLN:CG	1:M:161:GLN:NE2	2.81	0.43
1:M:374:LYS:O	1:M:374:LYS:HD3	2.18	0.43
1:M:479:LEU:HA	1:M:479:LEU:HD23	1.76	0.43
2:N:72:ARG:HH21	2:N:409:THR:HG22	1.83	0.43
2:N:174:GLN:HG3	2:N:175:ASN:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:344:GLU:OE1	2:N:344:GLU:HA	2.17	0.43
1:A:165:THR:HA	1:A:182:GLN:HE22	1.83	0.43
1:A:479:LEU:HD23	1:A:479:LEU:HA	1.74	0.43
1:E:79:GLU:OE2	1:E:83:ARG:NH1	2.51	0.43
1:E:219:GLN:OE1	7:E:823:ZP4:H41	2.19	0.43
1:E:315:HIS:H	1:E:315:HIS:HD2	1.66	0.43
1:I:49:LYS:NZ	1:I:142:ILE:HD12	2.34	0.43
1:I:209:LEU:HB3	1:I:214:LEU:CB	2.46	0.43
1:I:232:TYR:HE1	1:I:269:GLN:NE2	2.16	0.43
2:J:244:ILE:HD11	2:J:271:TYR:OH	2.19	0.43
1:M:250:ASP:CG	1:M:251:SER:H	2.21	0.43
1:M:398:TRP:CH2	1:M:411:ILE:HG12	2.54	0.43
1:M:494:ASN:OD1	1:M:532:TYR:HB3	2.19	0.43
1:A:489:SER:OG	1:A:528:LYS:HE3	2.18	0.43
2:B:174:GLN:C	2:B:176:PRO:HD3	2.39	0.43
2:B:202:ILE:HD13	2:B:202:ILE:HA	1.80	0.43
2:B:314:VAL:HG13	2:B:317:VAL:HG13	2.01	0.43
1:E:465:LYS:O	1:E:466:VAL:CG1	2.67	0.43
1:E:547:GLN:O	1:E:548:VAL:C	2.56	0.43
1:I:317:VAL:O	1:I:349:LEU:HD23	2.18	0.43
1:I:448:ARG:HD3	3:K:724:DT:C5'	2.49	0.43
2:J:246:LEU:HD11	2:J:264:LEU:HD21	2.00	0.43
1:M:113:ASP:HB3	1:M:116:PHE:HB2	1.99	0.43
1:M:230:MET:C	4:P:821:DC:H5"	2.39	0.43
1:M:342:TYR:OH	1:M:390:LYS:HD2	2.19	0.43
2:N:208:HIS:O	2:N:208:HIS:HD2	2.02	0.43
2:N:420:PRO:HB2	2:N:421:PRO:HD2	2.01	0.43
3:O:714:DG:H2"	3:O:715:DA:C8	2.53	0.43
1:A:95:PRO:HD2	1:A:230:MET:HE1	1.99	0.43
1:A:253:THR:HA	1:A:292:VAL:HA	1.99	0.43
2:B:123:ASP:OD2	2:B:123:ASP:N	2.51	0.43
2:F:5:ILE:CG2	2:F:6:GLU:N	2.80	0.43
2:F:30:LYS:O	2:F:34:LEU:HB2	2.19	0.43
2:F:232:TYR:CG	2:F:233:GLU:N	2.84	0.43
1:I:13:LYS:HE2	1:I:86:ASP:OD1	2.19	0.43
1:I:79:GLU:O	1:I:83:ARG:HG3	2.19	0.43
1:I:101:LYS:HG2	1:I:321:PRO:HD3	2.00	0.43
1:I:205:LEU:O	1:I:208:HIS:HB3	2.19	0.43
1:I:270:ILE:O	1:I:272:PRO:HD3	2.19	0.43
2:J:333:GLY:O	2:J:334:GLN:HB2	2.18	0.43
1:M:91:GLN:CG	1:M:161:GLN:HE22	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:703:DG:H4'	3:G:704:DC:OP2	2.18	0.43
2:B:388:LYS:HG2	2:B:413:GLU:HB3	2.01	0.43
1:I:164:MET:CE	1:I:187:LEU:HD21	2.48	0.43
2:J:125:ARG:NH1	2:J:147:ASN:HB3	2.34	0.43
2:J:395:LYS:O	2:J:399:GLU:HG3	2.18	0.43
2:N:94:ILE:HG21	2:N:182:GLN:O	2.18	0.43
3:C:710:DG:H2'	3:C:711:DC:C6	2.53	0.43
1:A:201:LYS:O	1:A:204:GLU:HB2	2.19	0.43
2:B:157:PRO:HG2	2:B:184:MET:CA	2.40	0.43
1:E:91:GLN:HG3	1:E:161:GLN:HE22	1.84	0.43
1:I:7:THR:CG2	1:I:119:PRO:HB2	2.49	0.43
1:I:175:ASN:HB3	1:I:178:ILE:HG12	2.00	0.43
1:I:221:HIS:CD2	1:I:221:HIS:N	2.83	0.43
2:J:374:LYS:O	2:J:374:LYS:HE3	2.19	0.43
1:M:181:TYR:HE2	2:N:136:ASN:ND2	2.15	0.43
1:M:432:GLU:CG	1:M:433:PRO:HD2	2.39	0.43
2:N:325:LEU:HB3	2:N:387:PRO:HA	2.00	0.43
1:A:89:GLU:HG3	3:C:708:DG:OP1	2.19	0.43
1:A:217:PRO:HB3	7:A:823:ZP4:O41	2.19	0.43
1:A:330:GLN:HE21	1:A:330:GLN:HB2	1.50	0.43
1:A:427:TYR:CD1	1:A:427:TYR:N	2.87	0.43
1:A:502:ALA:O	1:A:503:LEU:C	2.57	0.43
1:E:118:VAL:O	1:E:148:VAL:CG2	2.67	0.43
1:E:406:TRP:HE1	2:F:418:ASN:CG	2.21	0.43
1:E:427:TYR:N	1:E:427:TYR:CD1	2.87	0.43
1:I:21:VAL:HG13	1:I:58:THR:HA	2.00	0.43
1:I:328:GLU:HG3	1:I:390:LYS:HB2	2.01	0.43
1:I:451:LYS:HA	1:I:451:LYS:HD3	1.83	0.43
1:M:109:LEU:N	1:M:109:LEU:CD1	2.82	0.43
2:N:319:TYR:OH	2:N:321:PRO:HA	2.18	0.43
3:G:707:DG:H2"	3:G:708:DG:C5'	2.49	0.43
4:L:816:DG:H2'	4:L:817:MRG:C8	2.48	0.43
2:B:246:LEU:HD11	2:B:264:LEU:HD21	2.00	0.42
1:E:201:LYS:O	1:E:204:GLU:HB2	2.18	0.42
1:E:225:PRO:HD2	1:E:226:PRO:HD3	2.00	0.42
2:F:276:VAL:O	2:F:276:VAL:HG22	2.19	0.42
1:I:46:LYS:HD3	1:I:116:PHE:HB3	1.99	0.42
1:I:416:PHE:CD1	1:I:417:VAL:N	2.86	0.42
1:I:417:VAL:HG22	1:I:419:THR:HG22	2.01	0.42
2:J:174:GLN:HG3	2:J:175:ASN:OD1	2.19	0.42
2:J:420:PRO:HB2	2:J:421:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:90:VAL:HG22	1:M:90:VAL:O	2.19	0.42
1:A:155:GLY:O	1:A:159:ILE:CG1	2.62	0.42
1:A:266:TRP:CE2	4:D:820:DC:H4'	2.54	0.42
1:E:164:MET:HE3	1:E:168:LEU:HD21	2.01	0.42
1:E:429:LEU:HD11	1:E:506:ILE:HG22	2.01	0.42
2:F:8:VAL:HB	2:F:159:ILE:HD12	2.00	0.42
1:I:99:GLY:HA2	1:I:383:TRP:NE1	2.34	0.42
1:I:238:LYS:HB3	1:I:315:HIS:HB2	2.00	0.42
1:I:303:LEU:HD11	1:I:307:ARG:NH1	2.34	0.42
1:I:317:VAL:HG11	1:I:347:LYS:HB3	2.00	0.42
1:I:479:LEU:HD23	1:I:479:LEU:HA	1.77	0.42
2:J:366:LYS:O	2:J:369:THR:HB	2.20	0.42
1:M:246:LEU:HD11	1:M:264:LEU:HD22	2.01	0.42
1:M:439:THR:HA	1:M:494:ASN:HB2	2.01	0.42
2:N:374:LYS:O	2:N:374:LYS:HE3	2.19	0.42
3:C:712:DC:H2"	3:C:713:DC:O5'	2.18	0.42
1:A:454:LYS:HA	1:A:467:VAL:O	2.20	0.42
1:A:542:ILE:O	1:A:545:ASN:HB3	2.19	0.42
2:B:245:VAL:O	2:B:245:VAL:HG13	2.19	0.42
1:M:357:MET:HG2	1:M:367:GLN:NE2	2.33	0.42
2:N:88:TRP:CZ2	2:N:154:LYS:HD2	2.54	0.42
1:A:64:LYS:HE3	1:A:71:TRP:CE2	2.54	0.42
1:A:229:TRP:CE2	1:A:230:MET:HG2	2.54	0.42
1:A:549:ASP:O	1:A:550:LYS:C	2.58	0.42
2:B:210:LEU:HD12	2:B:210:LEU:N	2.34	0.42
1:E:325:LEU:C	1:E:326:ILE:HD12	2.40	0.42
1:E:452:LEU:HD23	1:E:470:THR:O	2.20	0.42
2:F:24:TRP:CZ3	2:F:403:THR:HG21	2.54	0.42
2:F:66:LYS:O	2:F:67:ASP:HB2	2.19	0.42
1:I:486:LEU:HB3	1:I:524:GLN:HG2	2.01	0.42
2:J:70:LYS:HD3	2:J:70:LYS:HA	1.78	0.42
1:M:285:GLY:O	1:M:287:LYS:HG2	2.19	0.42
1:M:365:VAL:HG11	1:M:401:TRP:CD1	2.55	0.42
1:M:409:THR:O	2:N:364:ASP:HB3	2.20	0.42
3:K:711:DC:H2'	3:K:712:DC:C6	2.55	0.42
1:A:86:ASP:OD1	1:A:86:ASP:N	2.53	0.42
1:A:130:PHE:CE1	1:A:144:TYR:HB2	2.54	0.42
1:A:325:LEU:C	1:A:326:ILE:HD12	2.40	0.42
1:A:398:TRP:CH2	1:A:411:ILE:HG12	2.54	0.42
2:B:122:GLU:HA	2:B:125:ARG:HH21	1.85	0.42
2:B:391:LEU:HA	2:B:392:PRO:HD2	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:420:PRO:HB2	2:B:421:PRO:HD2	2.01	0.42
1:E:111:VAL:HG11	1:E:214:LEU:HD13	2.01	0.42
1:E:113:ASP:HA	7:E:823:ZP4:N3B	2.34	0.42
1:E:171:PHE:CE2	1:E:205:LEU:HD23	2.54	0.42
1:E:354:TYR:HE1	1:E:356:ARG:HB3	1.84	0.42
1:E:360:ALA:O	1:E:513:SER:HA	2.19	0.42
2:F:49:LYS:HG2	2:F:144:TYR:CE1	2.55	0.42
2:F:330:GLN:HB2	2:F:338:THR:OG1	2.19	0.42
1:I:517:LEU:HD22	1:I:521:ILE:HD11	2.02	0.42
2:J:199:ARG:O	2:J:202:ILE:HB	2.19	0.42
1:M:528:LYS:HA	1:M:528:LYS:HD3	1.58	0.42
1:A:8:VAL:HB	1:A:159:ILE:HD12	2.02	0.42
2:B:350:LYS:O	2:B:351:THR:HG23	2.19	0.42
1:E:204:GLU:HG2	2:J:3:SER:O	2.19	0.42
2:F:246:LEU:HD11	2:F:264:LEU:HD21	2.01	0.42
2:J:143:ARG:HG2	2:J:143:ARG:HH11	1.85	0.42
1:M:169:GLU:O	1:M:173:LYS:HG3	2.20	0.42
1:M:254:VAL:HG21	1:M:287:LYS:HB3	2.01	0.42
1:M:264:LEU:CD1	1:M:306:ASN:HD22	2.33	0.42
1:M:331:LYS:HB3	1:M:421:PRO:HG2	2.02	0.42
1:M:511:ASP:OD1	1:M:511:ASP:C	2.58	0.42
2:N:135:ILE:C	2:N:137:ASN:N	2.73	0.42
2:N:189:VAL:HG21	2:N:205:LEU:HD13	2.01	0.42
1:A:58:THR:HG21	1:A:77:PHE:HD1	1.85	0.42
1:A:67:ASN:C	1:A:69:THR:H	2.22	0.42
1:A:325:LEU:HD12	1:A:325:LEU:N	2.33	0.42
2:B:108:VAL:HB	2:B:232:TYR:OH	2.18	0.42
2:B:419:THR:HA	2:B:420:PRO:HD2	1.90	0.42
1:E:24:TRP:CZ2	3:G:704:DC:OP1	2.72	0.42
1:E:489:SER:OG	1:E:528:LYS:NZ	2.49	0.42
1:E:549:ASP:O	1:E:550:LYS:C	2.57	0.42
2:F:194:GLU:CD	2:F:195:ILE:H	2.23	0.42
2:F:420:PRO:HB2	2:F:421:PRO:HD2	2.01	0.42
1:I:18:GLY:HA3	1:I:56:TYR:CE1	2.54	0.42
1:I:252:TRP:CD1	1:I:295:LEU:CD1	3.03	0.42
1:I:354:TYR:HE1	1:I:356:ARG:HB3	1.84	0.42
2:J:350:LYS:O	2:J:351:THR:HG23	2.19	0.42
2:J:420:PRO:CB	2:J:421:PRO:HD2	2.50	0.42
1:M:155:GLY:O	1:M:159:ILE:CG1	2.61	0.42
1:M:517:LEU:O	1:M:520:GLN:HB2	2.20	0.42
1:M:547:GLN:O	1:M:548:VAL:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:259:LYS:O	2:N:262:GLY:N	2.53	0.42
2:N:419:THR:HA	2:N:420:PRO:HD2	1.86	0.42
2:N:420:PRO:CB	2:N:421:PRO:HD2	2.50	0.42
1:A:197:GLN:O	1:A:200:THR:HB	2.19	0.42
1:A:478:GLU:CG	1:A:499:SER:HB2	2.50	0.42
1:A:480:GLN:HE21	1:A:480:GLN:CA	2.30	0.42
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.54	0.42
1:E:18:GLY:HA3	1:E:56:TYR:CE1	2.55	0.42
1:E:26:LEU:HD12	1:E:133:PRO:HG3	2.02	0.42
1:E:138:GLU:HG3	1:E:138:GLU:H	1.54	0.42
1:E:260:LEU:HD23	1:E:279:LEU:HD22	2.02	0.42
1:E:365:VAL:HG11	1:E:401:TRP:CD1	2.54	0.42
2:F:206:ARG:O	2:F:210:LEU:CD1	2.68	0.42
2:F:241:VAL:CG1	2:F:351:THR:OG1	2.67	0.42
1:I:91:GLN:HG3	1:I:161:GLN:NE2	2.29	0.42
1:I:100:LEU:HD23	1:I:181:TYR:CZ	2.55	0.42
1:I:116:PHE:CE1	1:I:146:TYR:HE2	2.37	0.42
1:I:116:PHE:HE1	1:I:146:TYR:HE2	1.67	0.42
1:I:528:LYS:HA	1:I:528:LYS:HD3	1.62	0.42
1:I:531:VAL:HG12	1:I:532:TYR:N	2.35	0.42
2:J:4:PRO:HG3	2:J:119:PRO:HB3	2.01	0.42
1:M:77:PHE:HB3	1:M:80:LEU:HB3	2.02	0.42
1:M:480:GLN:HE21	1:M:480:GLN:CA	2.31	0.42
1:A:81:ASN:HB3	1:A:154:LYS:HD2	2.02	0.42
1:A:486:LEU:HB3	1:A:524:GLN:HG2	2.01	0.42
1:E:65:LYS:O	1:E:66:LYS:C	2.58	0.42
1:E:74:LEU:HD13	3:G:705:DA:C5	2.55	0.42
1:E:330:GLN:HE21	1:E:330:GLN:HB2	1.54	0.42
1:E:331:LYS:HB3	1:E:421:PRO:HG2	2.01	0.42
1:E:338:THR:HA	1:E:353:LYS:HA	2.02	0.42
1:E:486:LEU:HB3	1:E:524:GLN:HG2	2.01	0.42
2:F:72:ARG:HH21	2:F:409:THR:CG2	2.33	0.42
2:F:395:LYS:O	2:F:399:GLU:HG3	2.20	0.42
1:I:76:ASP:OD1	3:K:705:DA:H4'	2.19	0.42
1:I:384:GLY:O	2:J:27:THR:HA	2.20	0.42
1:I:491:LEU:HD12	1:I:491:LEU:HA	1.93	0.42
2:J:26:LEU:HB2	2:J:31:ILE:HD11	2.01	0.42
2:J:31:ILE:HD11	2:J:133:PRO:HG2	2.01	0.42
2:J:402:TRP:CZ2	2:J:403:THR:HG22	2.54	0.42
1:M:106:VAL:HG12	1:M:107:THR:N	2.34	0.42
1:M:480:GLN:O	1:M:481:ALA:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:72:ARG:HH11	2:N:72:ARG:HG3	1.84	0.42
1:A:21:VAL:HG13	1:A:58:THR:HA	2.01	0.42
1:A:382:ILE:O	2:B:136:ASN:HB2	2.19	0.42
1:A:398:TRP:O	1:A:401:TRP:HB3	2.20	0.42
2:B:31:ILE:HD12	2:B:133:PRO:HG2	2.01	0.42
1:E:301:LEU:O	1:E:305:GLU:HG3	2.20	0.42
1:E:302:GLU:O	1:E:306:ASN:HB2	2.20	0.42
1:E:510:PRO:HB2	1:E:522:ILE:CD1	2.43	0.42
1:I:229:TRP:CD1	1:I:230:MET:HG2	2.55	0.42
2:J:107:THR:HG23	2:J:232:TYR:CE2	2.47	0.42
2:J:169:GLU:HB2	2:J:170:PRO:HD3	2.02	0.42
1:M:50:ILE:HG21	1:M:145:GLN:HB3	2.01	0.42
1:M:109:LEU:HA	1:M:220:LYS:CB	2.48	0.42
1:M:165:THR:HA	1:M:182:GLN:HE22	1.84	0.42
1:M:528:LYS:HG3	1:M:531:VAL:HG21	2.02	0.42
2:N:50:ILE:HG21	2:N:145:GLN:OE1	2.19	0.42
2:N:54:ASN:HB3	2:N:143:ARG:HH21	1.85	0.42
2:N:333:GLY:O	2:N:334:GLN:HB2	2.20	0.42
3:C:708:DG:H2'	3:C:709:DC:H6	1.82	0.42
1:A:260:LEU:HD23	1:A:279:LEU:HD22	2.02	0.41
1:A:329:ILE:HD11	1:A:375:ILE:CD1	2.48	0.41
1:E:434:ILE:HD12	1:E:434:ILE:N	2.35	0.41
1:E:473:THR:OG1	1:E:476:LYS:HG3	2.20	0.41
2:F:314:VAL:HG13	2:F:317:VAL:HG13	2.02	0.41
1:I:398:TRP:O	1:I:401:TRP:HB3	2.20	0.41
1:I:557:ARG:NH2	3:K:724:DT:OP2	2.53	0.41
2:J:135:ILE:C	2:J:137:ASN:N	2.73	0.41
1:M:317:VAL:HG11	1:M:347:LYS:HB3	2.01	0.41
1:M:326:ILE:O	1:M:341:ILE:HA	2.20	0.41
1:M:463:ARG:NH1	1:M:463:ARG:CB	2.83	0.41
2:N:107:THR:HG23	2:N:232:TYR:HE2	1.85	0.41
1:A:49:LYS:CE	1:A:142:ILE:HD12	2.42	0.41
1:A:49:LYS:HG3	1:A:142:ILE:HG23	2.03	0.41
1:A:242:GLN:HB3	1:A:243:PRO:CD	2.50	0.41
1:A:338:THR:HA	1:A:353:LYS:HA	2.03	0.41
1:A:517:LEU:O	1:A:520:GLN:HB2	2.20	0.41
1:A:524:GLN:O	1:A:528:LYS:HG2	2.19	0.41
1:E:157:PRO:HG3	3:G:707:DG:O4'	2.20	0.41
1:E:242:GLN:HB3	1:E:243:PRO:CD	2.49	0.41
1:E:342:TYR:HA	1:E:349:LEU:HB2	2.01	0.41
1:E:533:LEU:N	1:E:533:LEU:CD1	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:88:TRP:CZ2	2:F:154:LYS:HD2	2.55	0.41
2:F:125:ARG:HH11	2:F:147:ASN:CB	2.33	0.41
2:F:210:LEU:N	2:F:210:LEU:HD12	2.35	0.41
1:I:13:LYS:HA	1:I:14:PRO:HD3	1.93	0.41
1:I:34:LEU:HD12	1:I:34:LEU:H	1.85	0.41
1:I:73:LYS:HE3	1:I:146:TYR:OH	2.20	0.41
1:I:172:LYS:HE2	1:I:180:ILE:HB	2.02	0.41
1:M:73:LYS:O	1:M:74:LEU:HD23	2.19	0.41
1:M:100:LEU:O	1:M:318:TYR:HB3	2.19	0.41
1:M:109:LEU:HD23	1:M:216:THR:HG21	2.01	0.41
1:M:197:GLN:O	1:M:200:THR:HB	2.21	0.41
1:M:281:LYS:HE2	1:M:284:ARG:NH1	2.35	0.41
2:N:271:TYR:HB2	2:N:274:ILE:HD13	2.01	0.41
1:A:259:LYS:HA	4:D:819:DG:H5'	2.03	0.41
1:E:254:VAL:HB	1:E:288:ALA:O	2.20	0.41
1:E:528:LYS:HA	1:E:528:LYS:HD3	1.90	0.41
2:F:274:ILE:HA	2:F:306:ASN:OD1	2.19	0.41
2:F:339:TYR:CE2	2:F:375:ILE:HG23	2.55	0.41
1:I:69:THR:O	1:I:69:THR:CG2	2.67	0.41
1:I:480:GLN:HE21	1:I:480:GLN:CA	2.31	0.41
2:J:160:PHE:CD2	2:J:164:MET:HB2	2.55	0.41
2:J:169:GLU:OE2	2:J:169:GLU:CA	2.66	0.41
1:M:242:GLN:HB3	1:M:243:PRO:CD	2.50	0.41
2:N:235:HIS:C	2:N:237:ASP:H	2.23	0.41
1:A:30:LYS:O	1:A:31:ILE:C	2.57	0.41
1:A:97:PRO:O	1:A:100:LEU:HB2	2.20	0.41
1:A:221:HIS:HD2	1:A:221:HIS:N	2.09	0.41
1:A:278:GLN:HG3	1:A:298:GLU:CB	2.41	0.41
2:B:64:LYS:CE	2:B:69:THR:CG2	2.94	0.41
2:B:163:SER:O	2:B:164:MET:C	2.58	0.41
1:E:257:ILE:O	1:E:260:LEU:HB3	2.19	0.41
2:F:135:ILE:C	2:F:137:ASN:N	2.73	0.41
2:F:270:ILE:HB	2:F:271:TYR:CD1	2.55	0.41
1:I:63:ILE:HG21	1:I:74:LEU:HD11	2.02	0.41
1:I:178:ILE:HD12	1:I:191:SER:HB3	2.02	0.41
1:I:363:ASN:OD1	1:I:365:VAL:N	2.54	0.41
2:J:242:GLN:NE2	2:J:242:GLN:O	2.54	0.41
2:N:26:LEU:HB2	2:N:31:ILE:HD11	2.02	0.41
2:N:94:ILE:HD11	2:N:161:GLN:HG2	2.01	0.41
3:K:707:DG:H2"	3:K:708:DG:C5'	2.48	0.41
1:A:531:VAL:CG1	1:A:533:LEU:CD1	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:LYS:HE3	1:E:84:THR:O	2.21	0.41
1:E:30:LYS:O	1:E:31:ILE:C	2.58	0.41
1:E:188:TYR:O	1:E:188:TYR:HD1	2.04	0.41
2:F:146:TYR:CD2	2:F:150:PRO:HB3	2.55	0.41
2:F:374:LYS:O	2:F:374:LYS:HE3	2.20	0.41
2:F:420:PRO:CB	2:F:421:PRO:HD2	2.50	0.41
1:I:153:TRP:O	1:I:155:GLY:N	2.53	0.41
1:I:277:ARG:HH12	1:I:336:GLN:HG3	1.80	0.41
1:M:199:ARG:HH22	1:M:223:LYS:HB2	1.85	0.41
1:A:3:SER:HB2	1:A:117:SER:O	2.21	0.41
2:B:244:ILE:HD11	2:B:271:TYR:OH	2.19	0.41
2:B:270:ILE:HB	2:B:271:TYR:CD1	2.56	0.41
1:E:342:TYR:OH	1:E:390:LYS:HD2	2.20	0.41
2:F:357:MET:HB3	2:F:360:ALA:HB3	2.03	0.41
1:I:11:LYS:O	1:I:85:GLN:HB3	2.20	0.41
1:I:227:PHE:HB2	1:I:234:LEU:HB2	2.03	0.41
2:J:270:ILE:HB	2:J:271:TYR:CD1	2.55	0.41
1:M:332:GLN:HA	1:M:332:GLN:OE1	2.20	0.41
1:M:402:TRP:HB2	1:M:409:THR:HG23	2.02	0.41
1:M:416:PHE:CD1	1:M:417:VAL:N	2.88	0.41
2:N:267:ALA:O	2:N:269:GLN:N	2.53	0.41
2:N:274:ILE:N	2:N:274:ILE:CD1	2.84	0.41
2:N:274:ILE:HA	2:N:306:ASN:OD1	2.21	0.41
2:N:393:ILE:HG12	2:N:394:GLN:N	2.36	0.41
4:L:805:DG:H1'	4:L:806:DT:H5'	2.03	0.41
1:A:223:LYS:O	1:A:223:LYS:HG3	2.20	0.41
2:B:105:SER:O	2:B:190:GLY:HA2	2.20	0.41
1:E:17:ASP:CG	1:E:18:GLY:H	2.23	0.41
1:E:489:SER:OG	1:E:528:LYS:HE3	2.20	0.41
2:F:339:TYR:CG	2:F:375:ILE:HD12	2.56	0.41
2:F:390:LYS:NZ	2:F:415:GLU:OE2	2.53	0.41
1:I:100:LEU:HD21	1:I:181:TYR:CD1	2.54	0.41
1:I:285:GLY:O	1:I:286:THR:C	2.58	0.41
1:I:332:GLN:HA	1:I:332:GLN:OE1	2.21	0.41
1:M:115:TYR:C	1:M:117:SER:H	2.24	0.41
1:M:338:THR:HA	1:M:353:LYS:HA	2.03	0.41
1:M:517:LEU:O	1:M:521:ILE:HG13	2.21	0.41
2:N:108:VAL:HB	2:N:232:TYR:OH	2.20	0.41
1:A:169:GLU:HB3	1:A:170:PRO:HD3	2.01	0.41
2:B:46:LYS:HE2	2:B:116:PHE:HB3	2.02	0.41
2:B:337:TRP:CZ3	2:B:368:LEU:HG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:GLU:O	1:E:44:GLU:HG3	2.20	0.41
1:E:65:LYS:HZ3	1:E:70:ARG:NH2	2.18	0.41
1:E:235:HIS:O	1:E:318:TYR:CE2	2.73	0.41
1:I:326:ILE:O	1:I:341:ILE:HA	2.20	0.41
1:I:515:SER:O	1:I:516:GLU:C	2.58	0.41
2:J:180:ILE:HA	2:J:188:TYR:O	2.20	0.41
2:J:350:LYS:HG2	2:J:351:THR:H	1.86	0.41
1:A:270:ILE:O	1:A:272:PRO:HD3	2.21	0.41
1:A:315:HIS:CD2	1:A:315:HIS:N	2.88	0.41
1:A:363:ASN:OD1	1:A:363:ASN:C	2.59	0.41
2:B:181:TYR:CE2	2:B:183:TYR:HB2	2.56	0.41
2:B:258:GLN:HG2	2:B:283:LEU:HD13	2.03	0.41
1:E:194:GLU:O	1:E:195:ILE:C	2.59	0.41
1:E:234:LEU:HA	1:E:234:LEU:HD23	1.78	0.41
1:E:432:GLU:CG	1:E:433:PRO:HD2	2.38	0.41
1:E:441:TYR:CD2	1:E:496:VAL:CG2	3.03	0.41
1:E:446:ALA:HA	1:E:556:ILE:HG12	2.03	0.41
2:F:143:ARG:HG2	2:F:143:ARG:HH11	1.86	0.41
2:F:202:ILE:HD13	2:F:202:ILE:HA	1.85	0.41
1:I:102:LYS:HB3	1:I:102:LYS:HE2	1.76	0.41
1:I:207:GLN:HE22	1:I:210:LEU:HD23	1.83	0.41
1:I:365:VAL:HG11	1:I:401:TRP:CD1	2.56	0.41
2:J:12:LEU:HD22	2:J:127:TYR:CZ	2.55	0.41
2:J:267:ALA:O	2:J:270:ILE:N	2.54	0.41
2:J:339:TYR:CE2	2:J:375:ILE:HG23	2.56	0.41
1:M:116:PHE:CE1	1:M:146:TYR:CE2	3.09	0.41
2:N:88:TRP:CD1	2:N:154:LYS:HB2	2.56	0.41
2:N:366:LYS:O	2:N:369:THR:HB	2.21	0.41
3:O:712:DC:H2"	3:O:713:DC:O5'	2.21	0.41
1:A:303:LEU:HD11	1:A:307:ARG:HH11	1.85	0.41
1:A:438:GLU:CD	1:A:463:ARG:NH1	2.74	0.41
1:A:473:THR:OG1	1:A:476:LYS:HG3	2.20	0.41
2:B:235:HIS:O	2:B:237:ASP:N	2.50	0.41
2:B:274:ILE:N	2:B:274:ILE:CD1	2.84	0.41
2:F:123:ASP:OD2	2:F:123:ASP:N	2.53	0.41
1:I:109:LEU:N	1:I:109:LEU:CD1	2.83	0.41
2:J:54:ASN:HB3	2:J:143:ARG:HH21	1.86	0.41
3:C:711:DC:H2'	3:C:712:DC:C6	2.56	0.41
3:G:711:DC:H2'	3:G:712:DC:C6	2.56	0.41
4:H:817:MRG:H2'	4:H:818:DC:H6	1.79	0.41
1:A:8:VAL:O	1:A:121:ASP:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ASN:O	1:A:69:THR:N	2.54	0.40
1:A:452:LEU:HD23	1:A:470:THR:O	2.21	0.40
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.56	0.40
2:B:252:TRP:CG	2:B:295:LEU:HD11	2.55	0.40
1:E:72:ARG:HG3	1:E:151:GLN:HE22	1.86	0.40
1:E:173:LYS:O	1:E:176:PRO:HD3	2.20	0.40
1:E:259:LYS:HA	4:H:819:DG:H5'	2.03	0.40
2:F:349:LEU:HD23	2:F:349:LEU:HA	1.87	0.40
1:I:480:GLN:O	1:I:481:ALA:C	2.59	0.40
1:I:533:LEU:N	1:I:533:LEU:CD1	2.83	0.40
1:I:547:GLN:O	1:I:548:VAL:C	2.59	0.40
2:J:57:ASN:OD1	2:J:143:ARG:NH1	2.53	0.40
2:J:267:ALA:C	2:J:269:GLN:N	2.73	0.40
2:N:24:TRP:CH2	2:N:403:THR:HG21	2.55	0.40
2:N:74:LEU:HD12	2:N:74:LEU:C	2.42	0.40
2:N:194:GLU:CD	2:N:195:ILE:H	2.24	0.40
1:A:70:ARG:NH1	7:A:823:ZP4:C31	2.81	0.40
1:A:215:TYR:CD2	1:A:216:THR:N	2.89	0.40
1:A:219:GLN:HE21	7:A:823:ZP4:H41	1.86	0.40
2:B:244:ILE:HD11	2:B:271:TYR:CE1	2.56	0.40
1:E:515:SER:O	1:E:516:GLU:C	2.59	0.40
1:I:94:ILE:HA	1:I:95:PRO:HD3	1.98	0.40
1:I:164:MET:O	1:I:164:MET:HG3	2.21	0.40
1:I:235:HIS:CB	1:I:236:PRO:HD2	2.40	0.40
1:I:457:TYR:CD1	1:I:457:TYR:C	2.94	0.40
1:I:460:ASN:ND2	2:J:288:ALA:HB2	2.36	0.40
2:J:325:LEU:HB3	2:J:387:PRO:HA	2.02	0.40
2:J:349:LEU:HD23	2:J:349:LEU:HA	1.88	0.40
1:M:78:ARG:O	1:M:82:LYS:HG3	2.20	0.40
1:M:200:THR:O	1:M:203:GLU:HB2	2.20	0.40
1:M:557:ARG:HG2	1:M:558:LYS:N	2.36	0.40
2:N:166:LYS:HD2	9:N:438:HOH:O	2.21	0.40
3:G:709:DC:H2"	3:G:710:DG:H5'	2.03	0.40
1:A:232:TYR:N	1:A:242:GLN:HE21	2.20	0.40
1:A:547:GLN:O	1:A:548:VAL:C	2.60	0.40
1:E:77:PHE:HB2	1:E:152:GLY:O	2.21	0.40
1:E:165:THR:HA	1:E:182:GLN:HE22	1.87	0.40
1:E:261:VAL:HG13	1:E:276:VAL:HG11	2.02	0.40
1:E:339:TYR:CG	1:E:375:ILE:HD11	2.56	0.40
2:F:10:VAL:HG22	2:F:87:PHE:CZ	2.57	0.40
2:F:40:GLU:O	2:F:43:LYS:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:169:GLU:HB2	2:F:170:PRO:HD3	2.03	0.40
1:I:38:CYS:SG	1:I:132:ILE:HG13	2.61	0.40
1:I:64:LYS:HE3	1:I:71:TRP:CH2	2.56	0.40
1:I:197:GLN:O	1:I:200:THR:HB	2.22	0.40
1:I:208:HIS:O	1:I:212:TRP:HD1	2.04	0.40
1:I:342:TYR:OH	1:I:390:LYS:HD2	2.22	0.40
2:J:30:LYS:O	2:J:34:LEU:HB2	2.21	0.40
2:J:339:TYR:CG	2:J:375:ILE:HD12	2.56	0.40
2:N:78:ARG:NH1	2:N:411:ILE:HG22	2.37	0.40
4:D:805:DG:H1'	4:D:806:DT:H5'	2.03	0.40
1:A:73:LYS:C	1:A:74:LEU:HD23	2.42	0.40
1:A:315:HIS:CD2	1:A:315:HIS:H	2.40	0.40
2:B:259:LYS:O	2:B:262:GLY:N	2.54	0.40
2:B:363:ASN:O	2:B:364:ASP:C	2.59	0.40
1:E:281:LYS:HE2	1:E:284:ARG:CZ	2.51	0.40
1:E:559:VAL:O	1:E:559:VAL:HG13	2.22	0.40
2:F:203:GLU:O	2:F:203:GLU:OE1	2.39	0.40
2:F:265:ASN:O	2:F:268:SER:OG	2.34	0.40
2:F:267:ALA:O	2:F:270:ILE:N	2.54	0.40
1:I:94:ILE:CD1	3:K:708:DG:H21	2.34	0.40
1:M:37:ILE:O	1:M:41:LEU:HG	2.21	0.40
1:M:395:LYS:HD3	1:M:414:TRP:CZ2	2.55	0.40
1:M:549:ASP:O	1:M:550:LYS:C	2.59	0.40
1:A:194:GLU:O	1:A:195:ILE:C	2.60	0.40
1:A:203:GLU:O	1:A:207:GLN:HB2	2.22	0.40
1:A:363:ASN:OD1	1:A:365:VAL:N	2.55	0.40
2:B:83:ARG:NH1	2:B:83:ARG:HG3	2.36	0.40
1:E:184:MET:HB3	1:E:185:ASP:H	1.58	0.40
2:F:43:LYS:C	2:F:45:GLY:H	2.25	0.40
2:F:89:GLU:HG2	2:F:89:GLU:O	2.22	0.40
2:F:266:TRP:CE2	2:F:423:VAL:HG21	2.56	0.40
1:M:363:ASN:OD1	1:M:365:VAL:N	2.55	0.40
1:M:542:ILE:O	1:M:545:ASN:HB3	2.21	0.40
2:N:97:PRO:C	2:N:99:GLY:H	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	558/562 (99%)	469 (84%)	81 (14%)	8 (1%)	11	46
1	E	558/562 (99%)	461 (83%)	85 (15%)	12 (2%)	6	35
1	I	558/562 (99%)	476 (85%)	69 (12%)	13 (2%)	6	34
1	M	558/562 (99%)	474 (85%)	70 (12%)	14 (2%)	5	32
2	B	421/437 (96%)	362 (86%)	53 (13%)	6 (1%)	11	46
2	F	415/437 (95%)	361 (87%)	42 (10%)	12 (3%)	4	28
2	J	415/437 (95%)	366 (88%)	43 (10%)	6 (1%)	11	46
2	N	415/437 (95%)	360 (87%)	47 (11%)	8 (2%)	8	39
All	All	3898/3996 (98%)	3329 (85%)	490 (13%)	79 (2%)	7	38

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	THR
2	B	314	VAL
1	E	77	PHE
2	F	314	VAL
1	A	448	ARG
1	E	296	THR
1	E	448	ARG
2	F	136	ASN
2	F	193	LEU
1	I	122	GLU
1	I	296	THR
2	J	314	VAL
2	N	232	TYR
2	N	314	VAL
1	A	122	GLU
1	A	470	THR
2	B	136	ASN

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Mol	Chain	Res	Type
2	B	193	LEU
1	E	122	GLU
1	E	345	PRO
1	E	470	THR
1	E	554	ALA
2	F	284	ARG
1	I	318	TYR
1	I	345	PRO
1	I	448	ARG
2	J	193	LEU
2	J	284	ARG
1	M	77	PHE
1	M	122	GLU
1	M	296	THR
1	M	345	PRO
1	M	448	ARG
1	M	470	THR
1	M	554	ALA
2	N	193	LEU
1	A	291	GLU
2	B	236	PRO
1	E	291	GLU
1	E	297	GLU
2	F	5	ILE
2	F	217	PRO
1	I	277	ARG
1	I	412	PRO
1	I	470	THR
2	J	4	PRO
1	M	4	PRO
1	M	277	ARG
1	M	347	LYS
1	M	412	PRO
2	N	65	LYS
2	N	236	PRO
1	A	412	PRO
2	B	170	PRO
1	E	412	PRO
2	F	170	PRO
2	F	243	PRO
1	I	85	GLN
1	I	243	PRO

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Mol	Chain	Res	Type
1	I	291	GLU
1	M	291	GLU
2	N	170	PRO
2	N	284	ARG
2	F	236	PRO
2	J	170	PRO
1	M	243	PRO
2	N	420	PRO
2	F	213	GLY
2	F	420	PRO
2	J	420	PRO
1	A	170	PRO
1	A	243	PRO
1	E	170	PRO
1	E	243	PRO
1	I	321	PRO
2	B	420	PRO
2	F	4	PRO
1	I	170	PRO
1	M	170	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	500/502 (100%)	465 (93%)	35 (7%)	15	48
1	E	500/502 (100%)	470 (94%)	30 (6%)	19	54
1	I	500/502 (100%)	471 (94%)	29 (6%)	20	55
1	M	500/502 (100%)	475 (95%)	25 (5%)	24	60
2	B	375/397 (94%)	348 (93%)	27 (7%)	14	47
2	F	375/397 (94%)	347 (92%)	28 (8%)	13	45
2	J	375/397 (94%)	348 (93%)	27 (7%)	14	47
2	N	375/397 (94%)	345 (92%)	30 (8%)	12	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3500/3596 (97%)	3269 (93%)	231 (7%)	16 51

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	PRO
1	A	23	GLN
1	A	53	GLU
1	A	83	ARG
1	A	86	ASP
1	A	91	GLN
1	A	102	LYS
1	A	109	LEU
1	A	138	GLU
1	A	149	LEU
1	A	188	TYR
1	A	208	HIS
1	A	214	LEU
1	A	220	LYS
1	A	221	HIS
1	A	246	LEU
1	A	283	LEU
1	A	315	HIS
1	A	324	ASP
1	A	330	GLN
1	A	344	GLU
1	A	349	LEU
1	A	361	HIS
1	A	386	THR
1	A	441	TYR
1	A	458	VAL
1	A	466	VAL
1	A	496	VAL
1	A	509	GLN
1	A	517	LEU
1	A	533	LEU
1	A	548	VAL
1	A	552	VAL
1	A	556	ILE
1	A	557	ARG
2	B	24	TRP
2	B	34	LEU

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Mol	Chain	Res	Type
2	B	67	ASP
2	B	74	LEU
2	B	100	LEU
2	B	101	LYS
2	B	120	LEU
2	B	123	ASP
2	B	139	THR
2	B	157	PRO
2	B	161	GLN
2	B	203	GLU
2	B	211	ARG
2	B	240	THR
2	B	242	GLN
2	B	244	ILE
2	B	266	TRP
2	B	271	TYR
2	B	284	ARG
2	B	286	THR
2	B	364	ASP
2	B	368	LEU
2	B	374	LYS
2	B	394	GLN
2	B	409	THR
2	B	413	GLU
2	B	426	TRP
1	E	23	GLN
1	E	53	GLU
1	E	83	ARG
1	E	86	ASP
1	E	91	GLN
1	E	102	LYS
1	E	109	LEU
1	E	138	GLU
1	E	149	LEU
1	E	172	LYS
1	E	188	TYR
1	E	214	LEU
1	E	220	LYS
1	E	221	HIS
1	E	263	LYS
1	E	283	LEU
1	E	315	HIS

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Mol	Chain	Res	Type
1	E	324	ASP
1	E	330	GLN
1	E	344	GLU
1	E	349	LEU
1	E	361	HIS
1	E	386	THR
1	E	466	VAL
1	E	496	VAL
1	E	509	GLN
1	E	517	LEU
1	E	548	VAL
1	E	557	ARG
1	E	558	LYS
2	F	3	SER
2	F	5	ILE
2	F	6	GLU
2	F	24	TRP
2	F	34	LEU
2	F	67	ASP
2	F	100	LEU
2	F	120	LEU
2	F	123	ASP
2	F	139	THR
2	F	157	PRO
2	F	161	GLN
2	F	203	GLU
2	F	211	ARG
2	F	240	THR
2	F	242	GLN
2	F	244	ILE
2	F	266	TRP
2	F	271	TYR
2	F	284	ARG
2	F	286	THR
2	F	289	LEU
2	F	364	ASP
2	F	368	LEU
2	F	374	LYS
2	F	394	GLN
2	F	413	GLU
2	F	426	TRP
1	I	2	ILE

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Mol	Chain	Res	Type
1	I	23	GLN
1	I	53	GLU
1	I	68	SER
1	I	86	ASP
1	I	91	GLN
1	I	102	LYS
1	I	109	LEU
1	I	134	SER
1	I	138	GLU
1	I	188	TYR
1	I	228	LEU
1	I	246	LEU
1	I	283	LEU
1	I	315	HIS
1	I	324	ASP
1	I	330	GLN
1	I	344	GLU
1	I	349	LEU
1	I	361	HIS
1	I	386	THR
1	I	466	VAL
1	I	496	VAL
1	I	509	GLN
1	I	512	LYS
1	I	517	LEU
1	I	548	VAL
1	I	552	VAL
1	I	556	ILE
2	J	6	GLU
2	J	24	TRP
2	J	34	LEU
2	J	67	ASP
2	J	100	LEU
2	J	120	LEU
2	J	139	THR
2	J	161	GLN
2	J	164	MET
2	J	203	GLU
2	J	211	ARG
2	J	234	LEU
2	J	240	THR
2	J	242	GLN

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Mol	Chain	Res	Type
2	J	244	ILE
2	J	266	TRP
2	J	271	TYR
2	J	275	LYS
2	J	284	ARG
2	J	286	THR
2	J	289	LEU
2	J	364	ASP
2	J	368	LEU
2	J	374	LYS
2	J	394	GLN
2	J	413	GLU
2	J	426	TRP
1	M	23	GLN
1	M	53	GLU
1	M	86	ASP
1	M	91	GLN
1	M	102	LYS
1	M	109	LEU
1	M	138	GLU
1	M	188	TYR
1	M	220	LYS
1	M	246	LEU
1	M	283	LEU
1	M	315	HIS
1	M	324	ASP
1	M	330	GLN
1	M	344	GLU
1	M	349	LEU
1	M	361	HIS
1	M	386	THR
1	M	458	VAL
1	M	466	VAL
1	M	496	VAL
1	M	517	LEU
1	M	548	VAL
1	M	556	ILE
1	M	558	LYS
2	N	5	ILE
2	N	6	GLU
2	N	24	TRP
2	N	34	LEU

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Mol	Chain	Res	Type
2	N	65	LYS
2	N	100	LEU
2	N	120	LEU
2	N	123	ASP
2	N	139	THR
2	N	161	GLN
2	N	164	MET
2	N	203	GLU
2	N	211	ARG
2	N	240	THR
2	N	242	GLN
2	N	244	ILE
2	N	266	TRP
2	N	271	TYR
2	N	275	LYS
2	N	284	ARG
2	N	286	THR
2	N	289	LEU
2	N	364	ASP
2	N	368	LEU
2	N	374	LYS
2	N	385	LYS
2	N	388	LYS
2	N	394	GLN
2	N	413	GLU
2	N	426	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	161	GLN
1	A	182	GLN
1	A	197	GLN
1	A	207	GLN
1	A	208	HIS
1	A	219	GLN
1	A	221	HIS
1	A	242	GLN
1	A	269	GLN
1	A	330	GLN
1	A	334	GLN

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Mol	Chain	Res	Type
1	A	340	GLN
1	A	407	GLN
1	A	471	ASN
1	A	480	GLN
1	A	487	GLN
1	A	509	GLN
1	A	519	ASN
1	A	520	GLN
1	A	547	GLN
2	B	174	GLN
2	B	175	ASN
2	B	197	GLN
2	B	208	HIS
2	B	278	GLN
2	B	315	HIS
2	B	336	GLN
2	B	394	GLN
2	B	407	GLN
1	E	23	GLN
1	E	161	GLN
1	E	174	GLN
1	E	182	GLN
1	E	197	GLN
1	E	207	GLN
1	E	208	HIS
1	E	221	HIS
1	E	242	GLN
1	E	255	ASN
1	E	269	GLN
1	E	330	GLN
1	E	340	GLN
1	E	407	GLN
1	E	471	ASN
1	E	480	GLN
1	E	487	GLN
1	E	509	GLN
1	E	519	ASN
1	E	520	GLN
1	E	547	GLN
2	F	161	GLN
2	F	174	GLN
2	F	175	ASN

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Mol	Chain	Res	Type
2	F	197	GLN
2	F	208	HIS
2	F	255	ASN
2	F	278	GLN
2	F	315	HIS
2	F	336	GLN
2	F	394	GLN
2	F	407	GLN
1	I	23	GLN
1	I	161	GLN
1	I	182	GLN
1	I	207	GLN
1	I	208	HIS
1	I	221	HIS
1	I	242	GLN
1	I	330	GLN
1	I	334	GLN
1	I	340	GLN
1	I	407	GLN
1	I	471	ASN
1	I	480	GLN
1	I	487	GLN
1	I	509	GLN
1	I	519	ASN
1	I	520	GLN
1	I	547	GLN
2	J	81	ASN
2	J	96	HIS
2	J	161	GLN
2	J	174	GLN
2	J	175	ASN
2	J	197	GLN
2	J	208	HIS
2	J	278	GLN
2	J	315	HIS
2	J	336	GLN
2	J	394	GLN
2	J	407	GLN
1	M	23	GLN
1	M	161	GLN
1	M	182	GLN
1	M	197	GLN

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Mol	Chain	Res	Type
1	M	207	GLN
1	M	221	HIS
1	M	315	HIS
1	M	330	GLN
1	M	334	GLN
1	M	340	GLN
1	M	407	GLN
1	M	471	ASN
1	M	480	GLN
1	M	487	GLN
1	M	509	GLN
1	M	519	ASN
1	M	520	GLN
1	M	547	GLN
2	N	81	ASN
2	N	96	HIS
2	N	174	GLN
2	N	175	ASN
2	N	197	GLN
2	N	208	HIS
2	N	269	GLN
2	N	278	GLN
2	N	315	HIS
2	N	336	GLN
2	N	394	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	MRG	H	817	1,3,4	22,28,29	1.83	2 (9%)	23,39,42	3.92	7 (30%)
4	2DA	L	822	3,4	17,22,23	0.64	0	13,31,34	1.07	1 (7%)
4	MRG	L	817	1,3,4	22,28,29	1.52	3 (13%)	23,39,42	3.92	8 (34%)
4	2DA	P	822	3,4	17,22,23	0.59	0	13,31,34	1.02	1 (7%)
4	MRG	D	817	1,3,4	22,28,29	1.69	3 (13%)	23,39,42	3.93	8 (34%)
4	2DA	D	822	3,4	17,22,23	0.93	0	13,31,34	1.24	2 (15%)
4	MRG	P	817	3,4	22,28,29	1.65	3 (13%)	23,39,42	3.93	8 (34%)
4	2DA	H	822	3,4	17,22,23	0.77	0	13,31,34	1.12	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MRG	H	817	1,3,4	-	3/8/26/27	0/3/3/3
4	2DA	L	822	3,4	-	0/3/18/19	0/3/3/3
4	MRG	L	817	1,3,4	-	3/8/26/27	0/3/3/3
4	2DA	P	822	3,4	-	0/3/18/19	0/3/3/3
4	MRG	D	817	1,3,4	-	3/8/26/27	0/3/3/3
4	2DA	D	822	3,4	-	0/3/18/19	0/3/3/3
4	MRG	P	817	3,4	-	4/8/26/27	0/3/3/3
4	2DA	H	822	3,4	-	0/3/18/19	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	817	MRG	C21-N2	-6.25	1.33	1.45
4	D	817	MRG	C21-N2	-5.67	1.34	1.45
4	P	817	MRG	C21-N2	-5.61	1.34	1.45
4	L	817	MRG	C21-N2	-5.14	1.35	1.45
4	P	817	MRG	C6-N1	4.08	1.40	1.33
4	H	817	MRG	C6-N1	4.02	1.40	1.33
4	D	817	MRG	C6-N1	3.91	1.39	1.33
4	L	817	MRG	C6-N1	3.70	1.39	1.33
4	D	817	MRG	C8-N7	-2.13	1.30	1.34
4	P	817	MRG	C8-N7	-2.11	1.30	1.34
4	L	817	MRG	C8-N7	-2.03	1.31	1.34

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	817	MRG	C21-N2-C2	-13.79	99.92	123.75
4	P	817	MRG	C21-N2-C2	-13.71	100.06	123.75
4	L	817	MRG	C21-N2-C2	-13.68	100.11	123.75
4	H	817	MRG	C21-N2-C2	-13.48	100.45	123.75
4	H	817	MRG	C5-C6-N1	-9.09	111.00	123.43
4	P	817	MRG	C5-C6-N1	-8.85	111.33	123.43
4	L	817	MRG	C5-C6-N1	-8.79	111.41	123.43
4	D	817	MRG	C5-C6-N1	-8.71	111.52	123.43
4	L	817	MRG	C6-N1-C2	5.66	125.31	115.18
4	H	817	MRG	C6-N1-C2	5.66	125.31	115.18
4	P	817	MRG	C6-N1-C2	5.64	125.28	115.18
4	D	817	MRG	C6-N1-C2	5.63	125.26	115.18
4	H	817	MRG	C23-C22-C21	-4.25	99.00	112.65
4	P	817	MRG	C23-C22-C21	-4.21	99.11	112.65
4	L	817	MRG	C23-C22-C21	-4.20	99.16	112.65
4	D	817	MRG	C23-C22-C21	-4.03	99.71	112.65
4	H	817	MRG	C2-N3-C4	-3.28	111.56	115.28
4	L	817	MRG	C2-N3-C4	-3.09	111.76	115.28
4	D	817	MRG	C2-N3-C4	-2.89	111.99	115.28
4	P	817	MRG	C2-N3-C4	-2.85	112.04	115.28
4	H	822	2DA	C5-C6-N6	2.54	124.21	120.35
4	H	817	MRG	O3'-C3'-C2'	-2.50	101.94	110.90
4	L	822	2DA	C5-C6-N6	2.45	124.07	120.35
4	P	822	2DA	C5-C6-N6	2.42	124.03	120.35
4	D	817	MRG	C22-C21-N2	2.30	117.68	111.49
4	D	817	MRG	C22-C23-S24	2.29	120.32	112.96
4	D	822	2DA	C5-C6-N6	2.27	123.80	120.35
4	L	817	MRG	C22-C21-N2	2.25	117.53	111.49
4	D	817	MRG	O3'-C3'-C2'	-2.22	102.95	110.90
4	P	817	MRG	C6-C5-C4	-2.20	118.70	120.80
4	P	817	MRG	C22-C21-N2	2.17	117.31	111.49
4	D	822	2DA	C4'-O4'-C1'	-2.09	107.83	109.81
4	L	817	MRG	C6-C5-C4	-2.08	118.81	120.80
4	P	817	MRG	C22-C23-S24	2.08	119.63	112.96
4	L	817	MRG	C22-C23-S24	2.06	119.59	112.96
4	H	817	MRG	C22-C23-S24	2.04	119.52	112.96

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	817	MRG	N3-C2-N2-C21
4	D	817	MRG	N1-C2-N2-C21

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Mol	Chain	Res	Type	Atoms
4	D	817	MRG	N2-C21-C22-C23
4	H	817	MRG	N3-C2-N2-C21
4	H	817	MRG	N1-C2-N2-C21
4	H	817	MRG	N2-C21-C22-C23
4	L	817	MRG	N3-C2-N2-C21
4	L	817	MRG	N1-C2-N2-C21
4	L	817	MRG	N2-C21-C22-C23
4	P	817	MRG	N3-C2-N2-C21
4	P	817	MRG	N1-C2-N2-C21
4	P	817	MRG	N2-C21-C22-C23
4	P	817	MRG	C21-C22-C23-S24

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	817	MRG	3	0
4	L	822	2DA	1	0
4	L	817	MRG	3	0
4	P	822	2DA	3	0
4	D	817	MRG	2	0
4	D	822	2DA	1	0
4	P	817	MRG	3	0
4	H	822	2DA	1	0

5.5 Carbohydrates (i)

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GLC	Q	1	5	11,11,12	0.84	1 (9%)	15,15,17	1.32	3 (20%)
5	Z9N	Q	2	5	11,12,12	0.99	1 (9%)	10,18,18	0.97	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GLC	Q	1	5	-	2/2/19/22	0/1/1/1
5	Z9N	Q	2	5	-	0/5/24/24	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	2	Z9N	O2-C2	2.56	1.45	1.40
5	Q	1	GLC	C2-C3	2.08	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Q	1	GLC	C1-C2-C3	3.11	113.48	109.67
5	Q	1	GLC	O5-C5-C6	2.27	110.76	107.20
5	Q	1	GLC	C1-O5-C5	2.23	115.22	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Q	1	GLC	O5-C5-C6-O6
5	Q	1	GLC	C4-C5-C6-O6

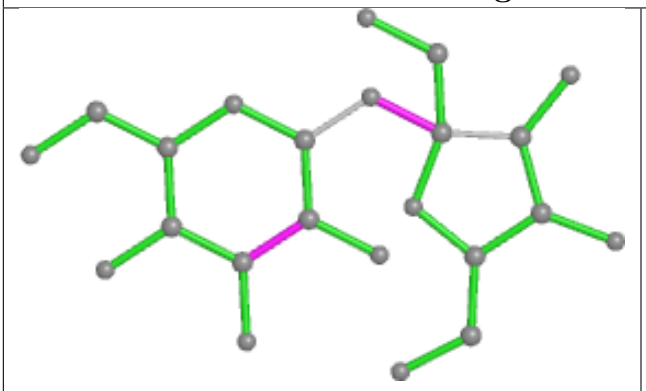
There are no ring outliers.

1 monomer is involved in 4 short contacts:

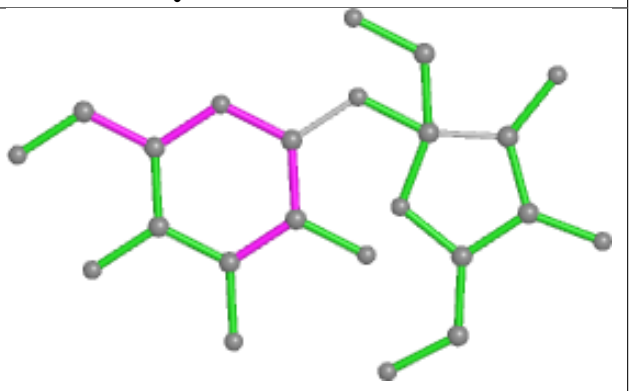
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Q	1	GLC	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

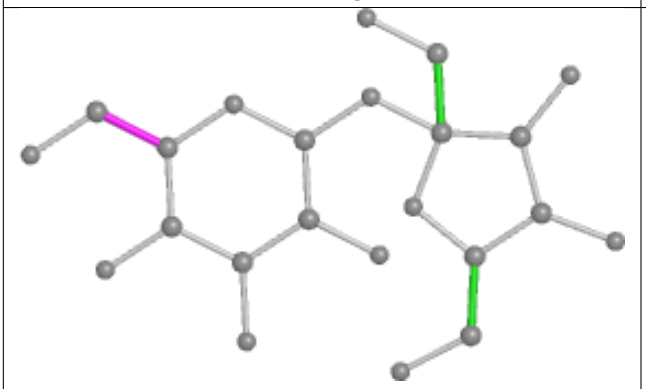
Oligosaccharide Chain Q



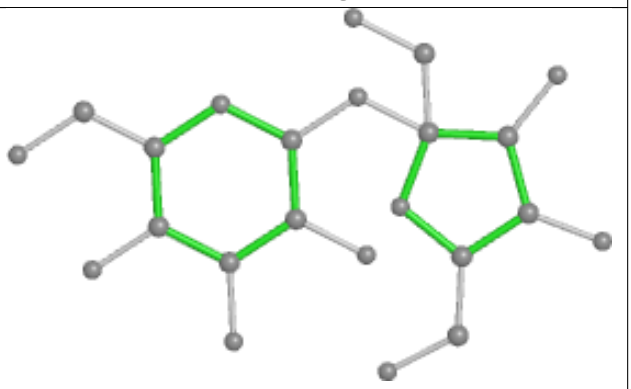
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	GOL	F	438	-	5,5,5	0.52	0	5,5,5	0.34	0
7	ZP4	I	823	6	44,57,57	1.17	5 (11%)	48,88,88	2.47	8 (16%)
7	ZP4	A	823	6	44,57,57	1.22	5 (11%)	48,88,88	2.49	8 (16%)
8	GOL	B	438	-	5,5,5	0.64	0	5,5,5	0.33	0
7	ZP4	M	823	6	44,57,57	1.23	5 (11%)	48,88,88	2.52	6 (12%)
7	ZP4	E	823	6	44,57,57	1.17	6 (13%)	48,88,88	2.53	7 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	F	438	-	-	4/4/4/4	-
7	ZP4	I	823	6	-	5/34/69/69	0/5/5/5
7	ZP4	A	823	6	-	6/34/69/69	0/5/5/5
8	GOL	B	438	-	-	4/4/4/4	-
7	ZP4	M	823	6	-	6/34/69/69	0/5/5/5
7	ZP4	E	823	6	-	6/34/69/69	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	823	ZP4	C4-N3	3.92	1.39	1.33
7	I	823	ZP4	C4-N3	3.27	1.38	1.33
7	A	823	ZP4	C5R-C4R	3.16	1.49	1.40
7	A	823	ZP4	C2R-N3R	3.15	1.37	1.32
7	I	823	ZP4	C5R-C4R	3.06	1.49	1.40
7	A	823	ZP4	O41-C11	2.96	1.45	1.41
7	M	823	ZP4	O41-C11	2.95	1.45	1.41
7	E	823	ZP4	C5R-C4R	2.93	1.48	1.40
7	M	823	ZP4	C5R-C4R	2.92	1.48	1.40
7	E	823	ZP4	O41-C11	2.86	1.45	1.41
7	I	823	ZP4	O41-C11	2.84	1.45	1.41
7	A	823	ZP4	C4-N3	2.73	1.37	1.33
7	E	823	ZP4	C6-C5	-2.64	1.32	1.40
7	M	823	ZP4	C2R-N3R	2.59	1.36	1.32
7	I	823	ZP4	C2R-N3R	2.50	1.36	1.32
7	E	823	ZP4	C2R-N3R	2.44	1.36	1.32
7	M	823	ZP4	C4-C5	2.35	1.46	1.41
7	E	823	ZP4	C4-N3	2.17	1.36	1.33
7	A	823	ZP4	C6-C5	-2.14	1.34	1.40
7	I	823	ZP4	C6-C5	-2.06	1.34	1.40
7	E	823	ZP4	C6R-C5R	2.01	1.50	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	823	ZP4	C4-N3-C2	14.39	127.29	115.14
7	I	823	ZP4	C4-N3-C2	14.23	127.16	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	E	823	ZP4	C4-N3-C2	14.23	127.15	115.14
7	A	823	ZP4	C4-N3-C2	13.94	126.91	115.14
7	M	823	ZP4	N3R-C2R-N1R	-3.79	122.75	128.68
7	E	823	ZP4	N3R-C2R-N1R	-3.78	122.77	128.68
7	I	823	ZP4	N3R-C2R-N1R	-3.75	122.82	128.68
7	E	823	ZP4	PD-O3G-PG	-3.72	120.07	132.83
7	M	823	ZP4	PD-O3G-PG	-3.66	120.28	132.83
7	A	823	ZP4	PD-O3G-PG	-3.64	120.33	132.83
7	A	823	ZP4	PG-O3B-PB	-3.62	120.40	132.83
7	M	823	ZP4	C31-C21-C11	3.60	106.40	100.98
7	A	823	ZP4	N3R-C2R-N1R	-3.55	123.12	128.68
7	E	823	ZP4	C31-C21-C11	3.55	106.32	100.98
7	M	823	ZP4	PG-O3B-PB	-3.41	121.13	132.83
7	E	823	ZP4	PG-O3B-PB	-3.40	121.16	132.83
7	A	823	ZP4	C31-C21-C11	3.34	106.01	100.98
7	I	823	ZP4	C31-C21-C11	2.97	105.44	100.98
7	A	823	ZP4	C4R-C5R-N7R	-2.97	106.31	109.40
7	I	823	ZP4	PG-O3B-PB	-2.96	122.67	132.83
7	I	823	ZP4	PD-O3G-PG	-2.87	122.99	132.83
7	E	823	ZP4	C4R-C5R-N7R	-2.84	106.44	109.40
7	I	823	ZP4	C4R-C5R-N7R	-2.77	106.51	109.40
7	M	823	ZP4	C4R-C5R-N7R	-2.68	106.61	109.40
7	A	823	ZP4	C5A-C5-C6	2.19	123.30	118.68
7	I	823	ZP4	C5A-C5-C6	2.15	123.21	118.68
7	E	823	ZP4	C2R-N1R-C6R	2.12	122.38	118.75
7	A	823	ZP4	PB-O3A-PA	-2.08	125.69	132.83
7	I	823	ZP4	C2R-N1R-C6R	2.05	122.26	118.75

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	823	ZP4	C4'-C3'-N3'-N3A
7	E	823	ZP4	C4'-C3'-N3'-N3A
7	I	823	ZP4	C4'-C3'-N3'-N3A
7	M	823	ZP4	C4'-C3'-N3'-N3A
8	B	438	GOL	O1-C1-C2-C3
8	B	438	GOL	C1-C2-C3-O3
8	F	438	GOL	C1-C2-C3-O3
7	A	823	ZP4	O41-C41-C51-O51
7	E	823	ZP4	O41-C41-C51-O51
7	M	823	ZP4	O41-C41-C51-O51

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Mol	Chain	Res	Type	Atoms
8	F	438	GOL	O1-C1-C2-C3
7	A	823	ZP4	C2'-C3'-N3'-N3A
8	B	438	GOL	O1-C1-C2-O2
7	A	823	ZP4	C31-C41-C51-O51
7	E	823	ZP4	C31-C41-C51-O51
8	F	438	GOL	O1-C1-C2-O2
8	F	438	GOL	O2-C2-C3-O3
8	B	438	GOL	O2-C2-C3-O3
7	I	823	ZP4	O41-C41-C51-O51
7	A	823	ZP4	PA-O3A-PB-O2B
7	I	823	ZP4	PA-O3A-PB-O2B
7	M	823	ZP4	C31-C41-C51-O51
7	M	823	ZP4	C2'-C3'-N3'-N3A
7	E	823	ZP4	PA-O3A-PB-O2B
7	E	823	ZP4	C2'-C3'-N3'-N3A
7	I	823	ZP4	C2'-C3'-N3'-N3A
7	M	823	ZP4	PA-O3A-PB-O1B
7	M	823	ZP4	PA-O3A-PB-O2B
7	A	823	ZP4	PA-O3A-PB-O1B
7	E	823	ZP4	PA-O3A-PB-O1B
7	I	823	ZP4	PA-O3A-PB-O1B

There are no ring outliers.

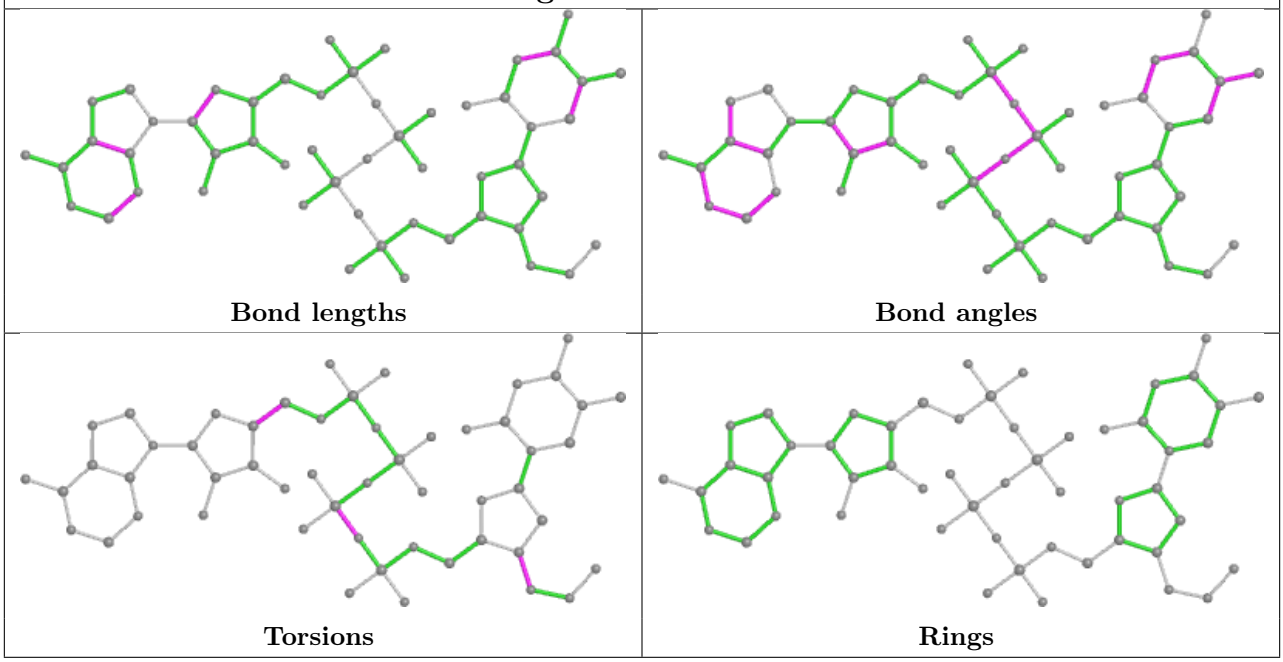
4 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	823	ZP4	4	0
7	A	823	ZP4	10	0
7	M	823	ZP4	7	0
7	E	823	ZP4	9	0

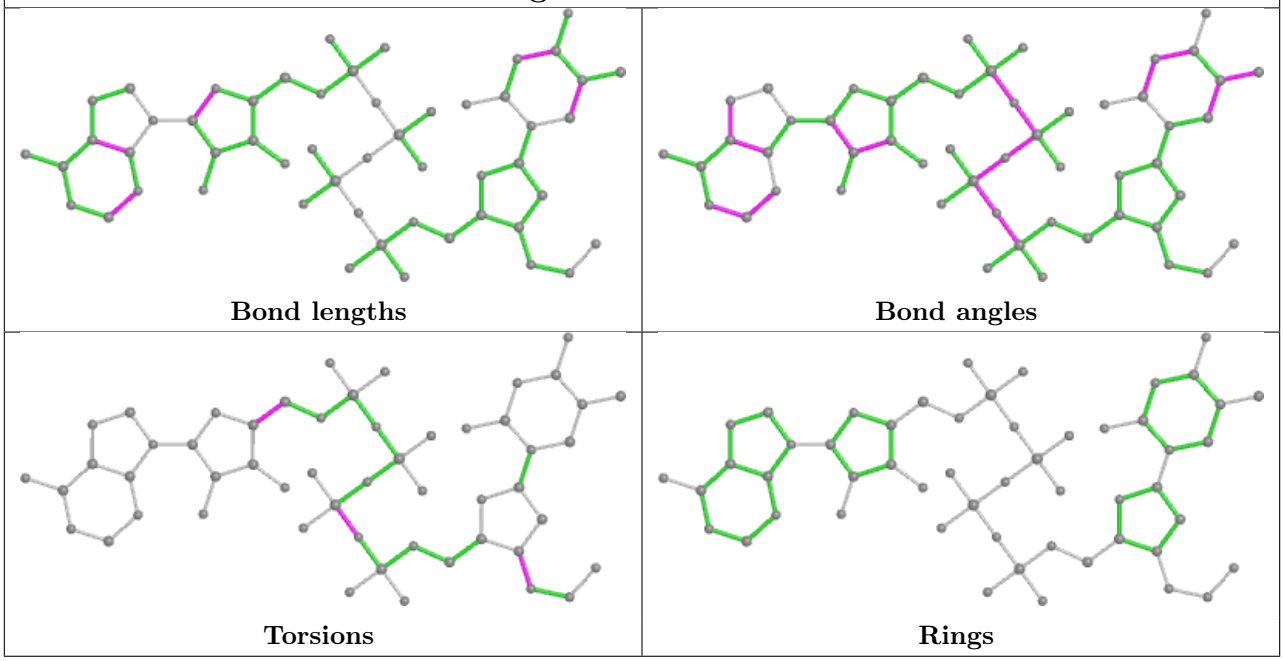
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.

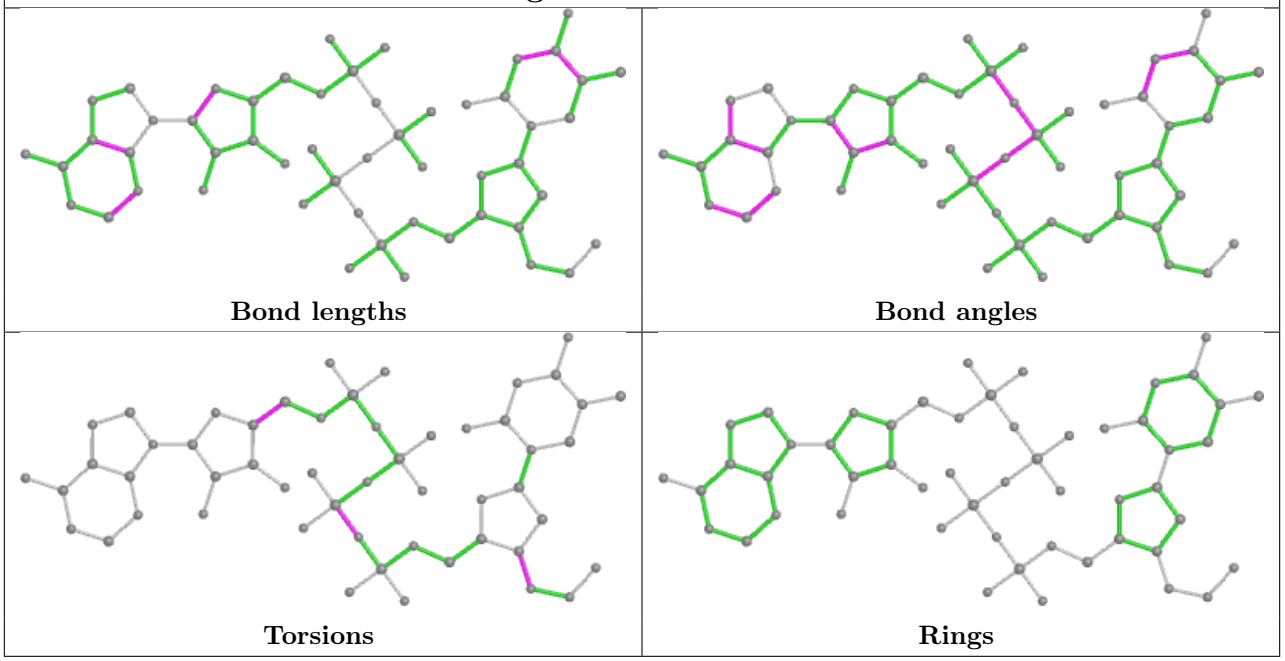
Ligand ZP4 I 823



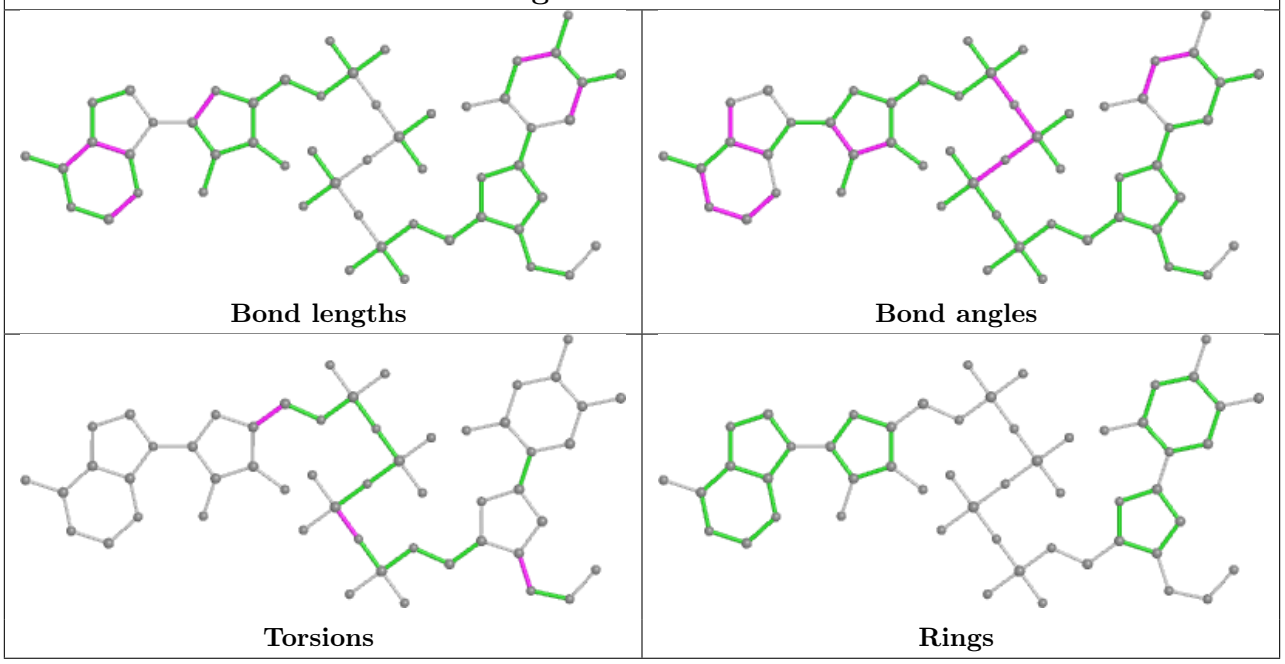
Ligand ZP4 A 823



Ligand ZP4 M 823



Ligand ZP4 E 823



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	560/562 (99%)	0.16	8 (1%) 75 63	31, 60, 76, 87	0
1	E	560/562 (99%)	0.18	8 (1%) 75 63	35, 62, 78, 88	0
1	I	560/562 (99%)	0.81	88 (15%) 2 1	100, 115, 121, 124	0
1	M	560/562 (99%)	1.72	187 (33%) 0 0	109, 129, 134, 137	0
2	B	425/437 (97%)	0.32	14 (3%) 46 30	22, 54, 84, 97	0
2	F	419/437 (95%)	0.30	15 (3%) 42 27	29, 58, 84, 91	0
2	J	419/437 (95%)	1.08	89 (21%) 0 1	102, 115, 121, 126	0
2	N	419/437 (95%)	2.05	167 (39%) 0 0	117, 129, 133, 137	0
3	C	25/27 (92%)	-0.08	0 100 100	29, 62, 82, 92	0
3	G	25/27 (92%)	-0.14	0 100 100	32, 65, 84, 89	0
3	K	25/27 (92%)	-0.32	0 100 100	111, 117, 123, 125	0
3	O	25/27 (92%)	0.67	4 (16%) 1 1	127, 130, 135, 139	0
4	D	19/21 (90%)	-0.08	0 100 100	40, 58, 87, 89	0
4	H	19/21 (90%)	-0.14	0 100 100	42, 62, 88, 96	0
4	L	19/21 (90%)	-0.09	1 (5%) 26 14	105, 115, 123, 123	0
4	P	19/21 (90%)	0.40	2 (10%) 6 3	124, 131, 134, 134	0
All	All	4098/4188 (97%)	0.78	583 (14%) 2 1	22, 94, 131, 139	0

All (583) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	325	LEU	15.1
2	N	21	VAL	13.1
2	N	108	VAL	11.0
2	N	159	ILE	11.0
2	N	3	SER	10.5

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Mol	Chain	Res	Type	RSRZ
2	J	360	ALA	10.3
2	N	10	VAL	10.0
1	M	252	TRP	9.5
2	N	107	THR	9.5
1	M	368	LEU	9.5
1	M	114	ALA	9.4
1	M	112	GLY	9.3
1	M	149	LEU	9.2
1	I	1	PRO	9.1
2	J	220	LYS	8.7
2	J	231	GLY	8.7
1	M	26	LEU	8.6
2	N	18	GLY	8.3
2	N	111	VAL	8.3
2	N	9	PRO	8.2
1	M	132	ILE	8.0
1	M	131	THR	8.0
2	F	67	ASP	7.9
2	N	429	GLY	7.8
2	J	221	HIS	7.8
2	N	221	HIS	7.8
2	N	109	LEU	7.6
1	M	75	VAL	7.6
2	N	409	THR	7.6
2	N	8	VAL	7.4
2	N	212	TRP	7.4
1	I	560	LEU	7.3
2	N	147	ASN	7.2
2	N	161	GLN	7.2
1	M	187	LEU	7.1
2	J	61	PHE	7.1
1	M	50	ILE	7.0
2	N	130	PHE	7.0
1	M	17	ASP	7.0
1	M	21	VAL	6.9
2	N	219	LYS	6.7
1	M	113	ASP	6.7
2	N	54	ASN	6.7
2	N	211	ARG	6.6
2	N	145	GLN	6.6
1	M	96	HIS	6.5
2	N	389	PHE	6.5

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Mol	Chain	Res	Type	RSRZ
1	M	67	ASN	6.5
2	J	361	HIS	6.5
1	M	115	TYR	6.4
2	N	324	ASP	6.3
1	A	560	LEU	6.3
2	N	95	PRO	6.3
1	M	269	GLN	6.2
2	J	7	THR	6.2
2	N	76	ASP	6.2
2	N	207	GLN	6.2
1	M	12	LEU	6.2
3	O	704	DC	6.1
1	M	150	PRO	6.1
1	I	19	PRO	6.0
2	B	431	HIS	6.0
1	M	63	ILE	6.0
1	M	55	PRO	6.0
1	M	19	PRO	5.9
1	M	116	PHE	5.9
2	N	355	ALA	5.9
1	M	273	GLY	5.8
2	N	178	ILE	5.7
1	M	246	LEU	5.6
2	N	160	PHE	5.6
2	N	117	SER	5.5
1	M	363	ASN	5.5
1	M	325	LEU	5.5
2	N	68	SER	5.5
1	M	84	THR	5.4
1	M	366	LYS	5.4
2	N	218	ASP	5.4
1	I	149	LEU	5.4
1	M	168	LEU	5.4
2	N	7	THR	5.4
2	N	71	TRP	5.4
2	N	127	TYR	5.4
1	M	186	ASP	5.4
1	M	212	TRP	5.4
1	M	3	SER	5.3
1	I	118	VAL	5.3
1	I	5	ILE	5.3
2	N	192	ASP	5.2

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Mol	Chain	Res	Type	RSRZ
1	I	246	LEU	5.2
2	J	207	GLN	5.2
1	M	247	PRO	5.1
2	N	195	ILE	5.1
1	M	38	CYS	5.1
2	N	56	TYR	5.0
1	M	306	ASN	5.0
2	J	93	GLY	5.0
1	M	214	LEU	5.0
1	M	34	LEU	4.9
1	M	412	PRO	4.9
1	M	276	VAL	4.9
2	N	12	LEU	4.9
2	N	124	PHE	4.9
2	J	68	SER	4.9
2	J	67	ASP	4.9
1	M	135	ILE	4.9
2	N	246	LEU	4.9
1	E	1	PRO	4.9
2	J	107	THR	4.9
1	M	174	GLN	4.9
1	M	111	VAL	4.9
1	M	25	PRO	4.8
1	M	365	VAL	4.8
2	N	17	ASP	4.8
2	N	110	ASP	4.8
2	N	146	TYR	4.8
2	B	360	ALA	4.8
2	F	314	VAL	4.8
1	M	245	VAL	4.8
1	E	559	VAL	4.7
1	M	389	PHE	4.7
2	J	159	ILE	4.7
2	N	134	SER	4.7
2	J	161	GLN	4.7
1	M	249	LYS	4.7
1	M	117	SER	4.6
2	J	97	PRO	4.6
2	N	11	LYS	4.6
2	N	62	ALA	4.6
2	J	146	TYR	4.6
2	J	164	MET	4.6

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Mol	Chain	Res	Type	RSRZ
1	I	26	LEU	4.6
2	B	67	ASP	4.6
2	J	3	SER	4.5
2	N	408	ALA	4.5
1	M	71	TRP	4.5
1	M	244	ILE	4.5
2	J	88	TRP	4.4
1	M	205	LEU	4.4
2	J	359	GLY	4.4
1	M	279	LEU	4.4
1	M	314	VAL	4.4
1	M	275	LYS	4.4
2	J	222	GLN	4.4
1	I	114	ALA	4.3
1	M	302	GLU	4.3
2	N	215	THR	4.3
2	N	216	THR	4.3
1	M	423	VAL	4.3
2	B	359	GLY	4.3
1	M	397	THR	4.3
2	N	164	MET	4.3
1	I	252	TRP	4.3
1	M	20	LYS	4.3
1	M	60	VAL	4.3
1	M	136	ASN	4.3
2	N	197	GLN	4.2
2	N	150	PRO	4.2
1	M	290	THR	4.2
1	I	130	PHE	4.2
1	I	73	LYS	4.2
1	I	293	ILE	4.2
2	J	95	PRO	4.2
2	N	133	PRO	4.2
1	M	122	GLU	4.2
1	E	2	ILE	4.2
1	I	195	ILE	4.1
1	M	388	LYS	4.1
2	N	335	GLY	4.1
1	I	342	TYR	4.1
1	M	237	ASP	4.1
2	N	151	GLN	4.1
2	N	39	THR	4.0

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Mol	Chain	Res	Type	RSRZ
2	N	131	THR	4.0
1	M	88	TRP	4.0
2	N	67	ASP	4.0
1	M	68	SER	4.0
2	N	191	SER	4.0
1	M	335	GLY	4.0
1	M	251	SER	4.0
1	I	66	LYS	4.0
2	N	203	GLU	4.0
2	N	220	LYS	4.0
2	F	360	ALA	4.0
1	I	18	GLY	4.0
1	I	288	ALA	4.0
2	B	434	HIS	4.0
2	N	52	PRO	3.9
1	M	324	ASP	3.9
1	M	54	ASN	3.9
1	M	408	ALA	3.9
2	N	383	TRP	3.9
1	M	354	TYR	3.9
1	E	68	SER	3.9
1	I	295	LEU	3.9
2	N	334	GLN	3.9
1	M	196	GLY	3.9
1	M	27	THR	3.9
1	M	192	ASP	3.9
1	M	56	TYR	3.9
1	I	188	TYR	3.9
2	N	128	THR	3.9
2	N	204	GLU	3.8
1	M	14	PRO	3.8
1	I	303	LEU	3.8
2	N	292	VAL	3.8
2	N	270	ILE	3.8
2	N	158	ALA	3.8
1	I	192	ASP	3.8
2	J	215	THR	3.8
2	N	75	VAL	3.8
2	J	288	ALA	3.7
2	N	323	LYS	3.7
2	N	28	GLU	3.7
2	B	358	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	560	LEU	3.7
2	N	182	GLN	3.7
2	F	231	GLY	3.7
2	J	145	GLN	3.7
2	F	359	GLY	3.7
2	N	368	LEU	3.7
1	M	11	LYS	3.7
2	J	160	PHE	3.7
2	N	239	TRP	3.7
2	J	168	LEU	3.7
2	J	144	TYR	3.7
2	J	219	LYS	3.7
1	M	151	GLN	3.7
2	N	180	ILE	3.6
2	N	30	LYS	3.6
2	N	140	PRO	3.6
1	I	60	VAL	3.6
2	N	176	PRO	3.6
1	M	455	ALA	3.6
2	J	274	ILE	3.6
2	B	3	SER	3.6
1	M	146	TYR	3.6
2	N	343	GLN	3.6
2	N	410	TRP	3.5
2	N	244	ILE	3.5
2	N	401	TRP	3.5
1	M	8	VAL	3.5
2	N	25	PRO	3.5
1	I	275	LYS	3.5
2	J	5	ILE	3.5
1	I	128	THR	3.4
2	N	115	TYR	3.4
1	I	135	ILE	3.4
1	M	283	LEU	3.4
1	I	132	ILE	3.4
2	N	348	ASN	3.4
1	M	313	PRO	3.4
2	F	358	ARG	3.4
1	I	55	PRO	3.4
2	N	199	ARG	3.4
2	N	319	TYR	3.4
2	N	375	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
3	O	703	DG	3.3
1	M	169	GLU	3.3
1	M	340	GLN	3.3
1	M	502	ALA	3.3
1	I	187	LEU	3.3
1	M	175	ASN	3.3
1	A	1	PRO	3.3
1	M	57	ASN	3.3
1	I	325	LEU	3.3
2	F	315	HIS	3.3
2	N	356	ARG	3.3
2	N	293	ILE	3.2
1	A	455	ALA	3.2
2	N	59	PRO	3.2
2	N	232	TYR	3.2
1	M	127	TYR	3.2
1	M	506	ILE	3.2
1	M	188	TYR	3.2
2	N	53	GLU	3.2
1	I	455	ALA	3.2
1	M	207	GLN	3.2
2	J	182	GLN	3.2
1	M	23	GLN	3.2
1	I	102	LYS	3.1
2	J	10	VAL	3.1
2	J	4	PRO	3.1
1	I	271	TYR	3.1
2	J	92	LEU	3.1
1	I	17	ASP	3.1
1	I	116	PHE	3.1
1	M	18	GLY	3.1
2	B	432	HIS	3.1
1	M	410	TRP	3.1
1	M	271	TYR	3.1
1	M	524	GLN	3.1
1	I	20	LYS	3.1
2	J	87	PHE	3.1
1	M	4	PRO	3.1
2	F	283	LEU	3.1
2	J	409	THR	3.1
1	I	297	GLU	3.1
1	M	241	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
2	N	38	CYS	3.1
1	M	37	ILE	3.1
1	M	180	ILE	3.1
1	M	293	ILE	3.1
2	N	63	ILE	3.1
2	J	233	GLU	3.1
1	I	247	PRO	3.0
1	I	456	GLY	3.0
2	N	61	PHE	3.0
2	N	260	LEU	3.0
2	N	391	LEU	3.0
1	I	146	TYR	3.0
1	I	171	PHE	3.0
2	N	327	ALA	3.0
2	J	76	ASP	3.0
2	N	129	ALA	3.0
1	I	72	ARG	3.0
3	O	705	DA	3.0
2	N	242	GLN	3.0
1	I	141	GLY	3.0
2	N	346	PHE	3.0
1	M	106	VAL	3.0
2	N	349	LEU	3.0
1	M	511	ASP	3.0
2	N	210	LEU	3.0
2	N	264	LEU	3.0
2	J	124	PHE	3.0
1	M	413	GLU	3.0
2	J	141	GLY	2.9
1	I	168	LEU	2.9
1	M	288	ALA	2.9
2	J	106	VAL	2.9
2	J	187	LEU	2.9
1	I	199	ARG	2.9
1	M	5	ILE	2.9
2	J	241	VAL	2.9
1	I	194	GLU	2.9
1	M	248	GLU	2.9
2	J	246	LEU	2.9
2	J	17	ASP	2.9
1	M	208	HIS	2.9
1	M	406	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
2	J	189	VAL	2.9
1	M	209	LEU	2.9
1	M	189	VAL	2.8
1	I	205	LEU	2.8
2	N	37	ILE	2.8
1	I	282	LEU	2.8
2	N	231	GLY	2.8
1	I	75	VAL	2.8
2	N	163	SER	2.8
1	I	58	THR	2.8
1	M	261	VAL	2.8
1	I	52	PRO	2.8
1	I	332	GLN	2.8
2	N	222	GLN	2.8
1	I	279	LEU	2.8
1	M	173	LYS	2.8
1	I	53	GLU	2.8
1	M	9	PRO	2.8
2	J	214	LEU	2.8
1	M	48	SER	2.8
1	M	223	LYS	2.8
2	N	411	ILE	2.8
1	M	274	ILE	2.8
1	M	66	LYS	2.8
1	M	530	LYS	2.8
1	M	33	ALA	2.8
1	M	222	GLN	2.8
1	I	164	MET	2.8
2	J	96	HIS	2.7
1	M	503	LEU	2.7
2	F	3	SER	2.7
2	J	389	PHE	2.7
2	N	416	PHE	2.7
1	I	68	SER	2.7
2	N	243	PRO	2.7
2	N	149	LEU	2.7
1	M	496	VAL	2.7
2	N	248	GLU	2.7
2	N	114	ALA	2.7
1	M	49	LYS	2.7
1	M	65	LYS	2.7
1	M	171	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	M	272	PRO	2.7
1	A	559	VAL	2.7
2	B	266	TRP	2.7
1	M	299	ALA	2.7
1	M	218	ASP	2.7
1	M	469	LEU	2.7
2	J	157	PRO	2.6
2	N	362	THR	2.6
2	J	166	LYS	2.6
1	I	8	VAL	2.6
1	I	48	SER	2.6
1	I	214	LEU	2.6
1	M	250	ASP	2.6
1	M	281	LYS	2.6
2	J	422	LEU	2.6
2	N	102	LYS	2.6
1	M	377	THR	2.6
2	J	216	THR	2.6
1	I	34	LEU	2.6
2	N	200	THR	2.6
1	M	452	LEU	2.6
2	N	353	LYS	2.6
1	M	159	ILE	2.6
1	E	222	GLN	2.6
1	I	248	GLU	2.6
2	J	152	GLY	2.6
1	M	200	THR	2.6
2	J	111	VAL	2.5
2	N	358	ARG	2.5
1	M	292	VAL	2.5
2	J	110	ASP	2.5
1	I	144	TYR	2.5
1	M	291	GLU	2.5
1	I	304	ALA	2.5
1	M	90	VAL	2.5
2	J	232	TYR	2.5
2	J	60	VAL	2.5
2	N	13	LYS	2.5
1	I	133	PRO	2.5
1	M	355	ALA	2.5
1	M	421	PRO	2.5
2	N	157	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	J	211	ARG	2.5
2	N	97	PRO	2.5
2	N	354	TYR	2.5
1	M	534	ALA	2.5
1	M	371	ALA	2.5
1	M	72	ARG	2.5
2	N	148	VAL	2.5
1	M	118	VAL	2.4
1	M	301	LEU	2.4
1	M	453	GLY	2.4
1	I	428	GLN	2.4
2	J	343	GLN	2.4
2	J	358	ARG	2.4
1	A	456	GLY	2.4
2	N	16	MET	2.4
2	N	90	VAL	2.4
2	J	244	ILE	2.4
2	J	336	GLN	2.4
2	B	238	LYS	2.4
1	M	286	THR	2.4
1	E	359	GLY	2.4
2	F	425	LEU	2.4
1	M	77	PHE	2.4
2	J	16	MET	2.4
4	L	802	DA	2.4
1	I	388	LYS	2.4
1	I	222	GLN	2.4
1	I	525	LEU	2.4
2	F	246	LEU	2.4
2	N	388	LYS	2.4
2	N	135	ILE	2.4
2	N	86	ASP	2.4
2	N	414	TRP	2.4
2	J	282	LEU	2.4
1	M	15	GLY	2.4
1	M	500	GLN	2.4
1	M	392	PRO	2.4
2	N	177	ASP	2.4
2	N	93	GLY	2.4
2	N	4	PRO	2.4
2	N	208	HIS	2.4
1	M	145	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	136	ASN	2.4
2	J	8	VAL	2.3
2	B	357	MET	2.3
2	N	298	GLU	2.3
1	M	178	ILE	2.3
2	J	209	LEU	2.3
2	N	66	LYS	2.3
1	I	354	TYR	2.3
1	M	124	PHE	2.3
2	J	391	LEU	2.3
2	N	361	HIS	2.3
2	F	242	GLN	2.3
1	I	551	LEU	2.3
2	J	250	ASP	2.3
1	I	559	VAL	2.3
2	J	178	ILE	2.3
2	N	187	LEU	2.3
2	N	118	VAL	2.3
2	J	384	GLY	2.3
1	I	134	SER	2.3
2	J	260	LEU	2.3
4	P	814	DC	2.3
2	B	430	GLY	2.3
1	I	50	ILE	2.3
1	I	142	ILE	2.3
1	I	274	ILE	2.3
2	N	183	TYR	2.3
1	M	409	THR	2.3
1	I	14	PRO	2.3
1	I	398	TRP	2.3
1	M	160	PHE	2.3
2	B	435	HIS	2.3
1	I	2	ILE	2.2
2	J	329	ILE	2.2
1	M	327	ALA	2.2
2	N	282	LEU	2.2
1	I	209	LEU	2.2
1	M	337	TRP	2.2
2	N	35	VAL	2.2
1	A	545	ASN	2.2
2	N	196	GLY	2.2
2	J	69	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	N	168	LEU	2.2
1	M	396	GLU	2.2
1	M	144	TYR	2.2
1	M	315	HIS	2.2
1	M	243	PRO	2.2
2	B	246	LEU	2.2
1	M	176	PRO	2.2
2	J	85	GLN	2.2
2	J	174	GLN	2.2
2	N	91	GLN	2.2
1	I	308	GLU	2.2
1	M	326	ILE	2.2
1	M	482	ILE	2.2
2	N	106	VAL	2.2
1	I	51	GLY	2.2
1	M	277	ARG	2.2
1	A	434	ILE	2.2
2	F	429	GLY	2.2
2	J	239	TRP	2.2
2	J	327	ALA	2.2
2	N	267	ALA	2.1
3	O	717	DC	2.1
2	N	201	LYS	2.1
1	A	214	LEU	2.1
1	I	312	GLU	2.1
1	M	323	LYS	2.1
4	P	820	DC	2.1
2	F	361	HIS	2.1
1	M	270	ILE	2.1
1	M	422	LEU	2.1
2	N	252	TRP	2.1
2	N	278	GLN	2.1
2	N	198	HIS	2.1
1	M	310	LEU	2.1
1	M	95	PRO	2.1
1	I	233	GLU	2.1
2	J	249	LYS	2.1
2	N	64	LYS	2.1
2	J	192	ASP	2.1
2	J	341	ILE	2.1
1	I	100	LEU	2.1
2	N	214	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	346	PHE	2.1
1	M	233	GLU	2.1
2	N	271	TYR	2.1
2	N	142	ILE	2.1
2	J	205	LEU	2.1
1	M	419	THR	2.1
2	J	163	SER	2.1
1	M	238	LYS	2.0
1	M	42	GLU	2.0
1	M	345	PRO	2.0
1	I	124	PHE	2.0
2	J	42	GLU	2.0
1	E	467	VAL	2.0
2	N	193	LEU	2.0
2	N	341	ILE	2.0
2	N	22	LYS	2.0
2	J	218	ASP	2.0
2	N	174	GLN	2.0
2	N	233	GLU	2.0
2	J	54	ASN	2.0
1	M	507	GLN	2.0
2	N	378	GLU	2.0
1	M	76	ASP	2.0
1	M	341	ILE	2.0
2	J	170	PRO	2.0
2	N	84	THR	2.0
1	I	115	TYR	2.0
2	J	257	ILE	2.0
1	I	137	ASN	2.0
1	M	260	LEU	2.0
1	M	479	LEU	2.0
2	F	187	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	2DA	P	822	20/21	0.46	0.37	131,132,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MRG	P	817	26/27	0.76	0.16	125,132,138,143	0
4	MRG	L	817	26/27	0.79	0.20	117,120,123,124	0
4	2DA	L	822	20/21	0.90	0.18	112,114,115,115	0
4	MRG	H	817	26/27	0.95	0.21	49,55,62,63	0
4	MRG	D	817	26/27	0.96	0.24	46,51,54,55	0
4	2DA	H	822	20/21	0.96	0.21	46,52,61,61	0
4	2DA	D	822	20/21	0.96	0.22	41,45,48,50	0

6.3 Carbohydrates (i)

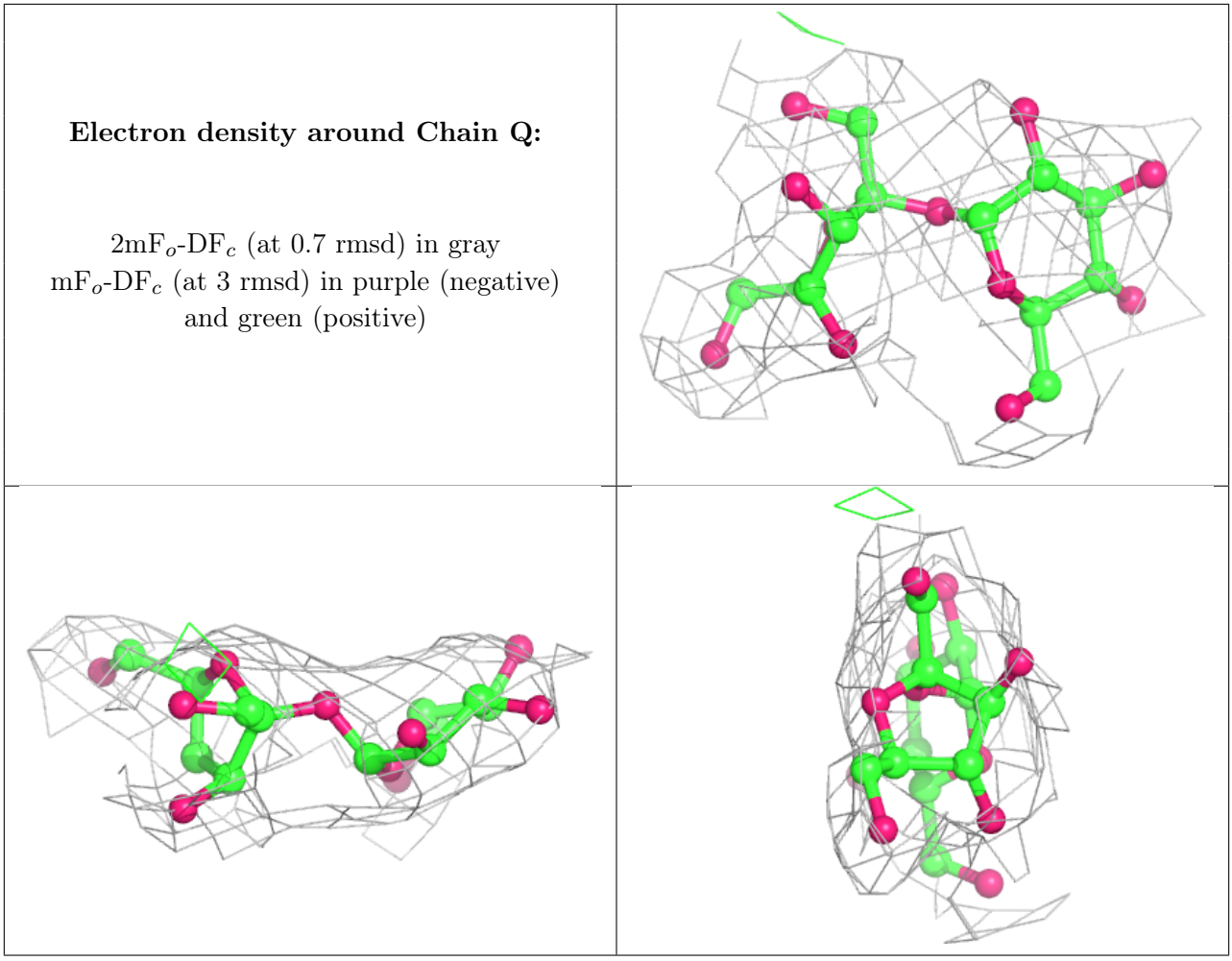
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GLC	Q	1	11/12	0.78	0.22	96,99,100,100	0
5	Z9N	Q	2	12/12	0.78	0.20	94,99,100,101	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain Q:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	M	600	1/1	0.43	0.15	123,123,123,123	0
8	GOL	F	438	6/6	0.68	0.28	69,71,73,74	0
7	ZP4	M	823	53/53	0.71	0.27	128,135,138,139	0
8	GOL	B	438	6/6	0.79	0.37	61,65,67,67	0
6	MG	M	602	1/1	0.82	0.29	94,94,94,94	0
7	ZP4	I	823	53/53	0.89	0.19	107,121,125,126	0
7	ZP4	E	823	53/53	0.91	0.25	50,75,91,94	0
7	ZP4	A	823	53/53	0.92	0.27	45,69,92,94	0
6	MG	A	602	1/1	0.95	0.15	24,24,24,24	0
6	MG	E	602	1/1	0.95	0.22	13,13,13,13	0

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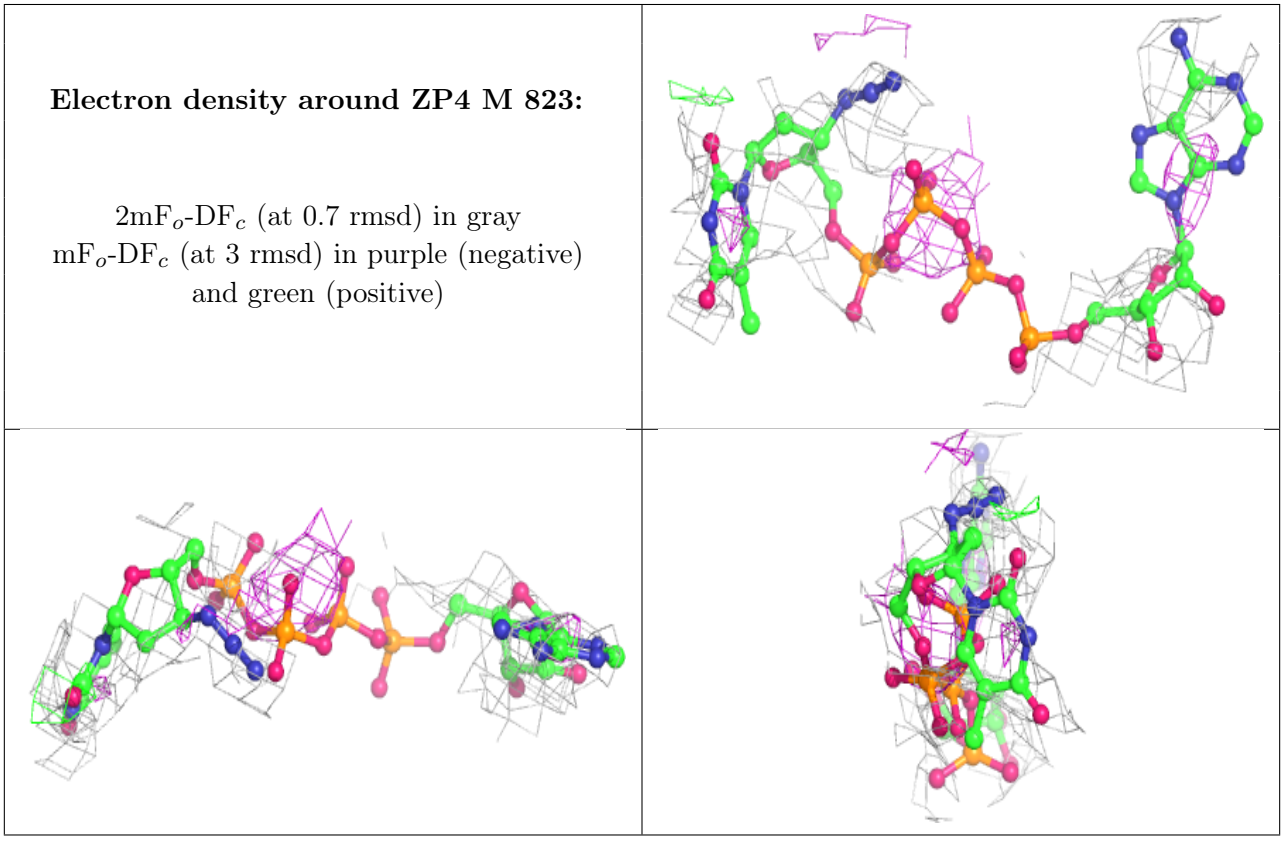
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	I	600	1/1	0.96	0.26	96,96,96,96	0
6	MG	I	602	1/1	0.96	0.19	64,64,64,64	0
6	MG	A	600	1/1	0.97	0.18	27,27,27,27	0
6	MG	E	600	1/1	0.99	0.21	28,28,28,28	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

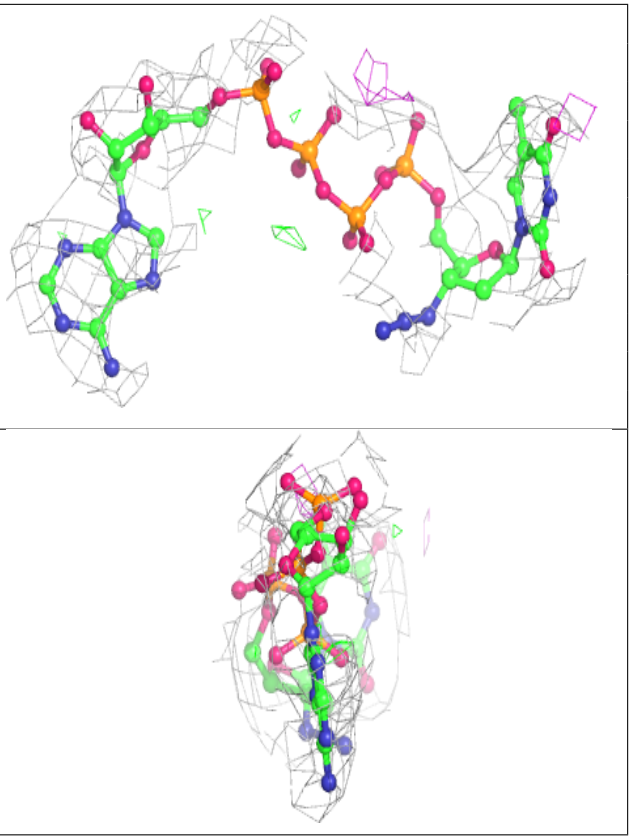
Electron density around ZP4 M 823:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



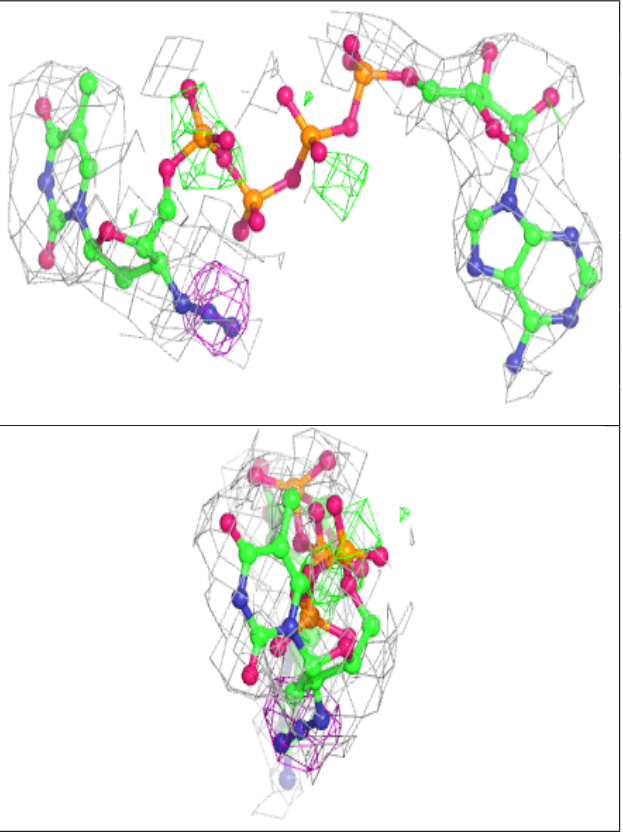
Electron density around ZP4 I 823:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



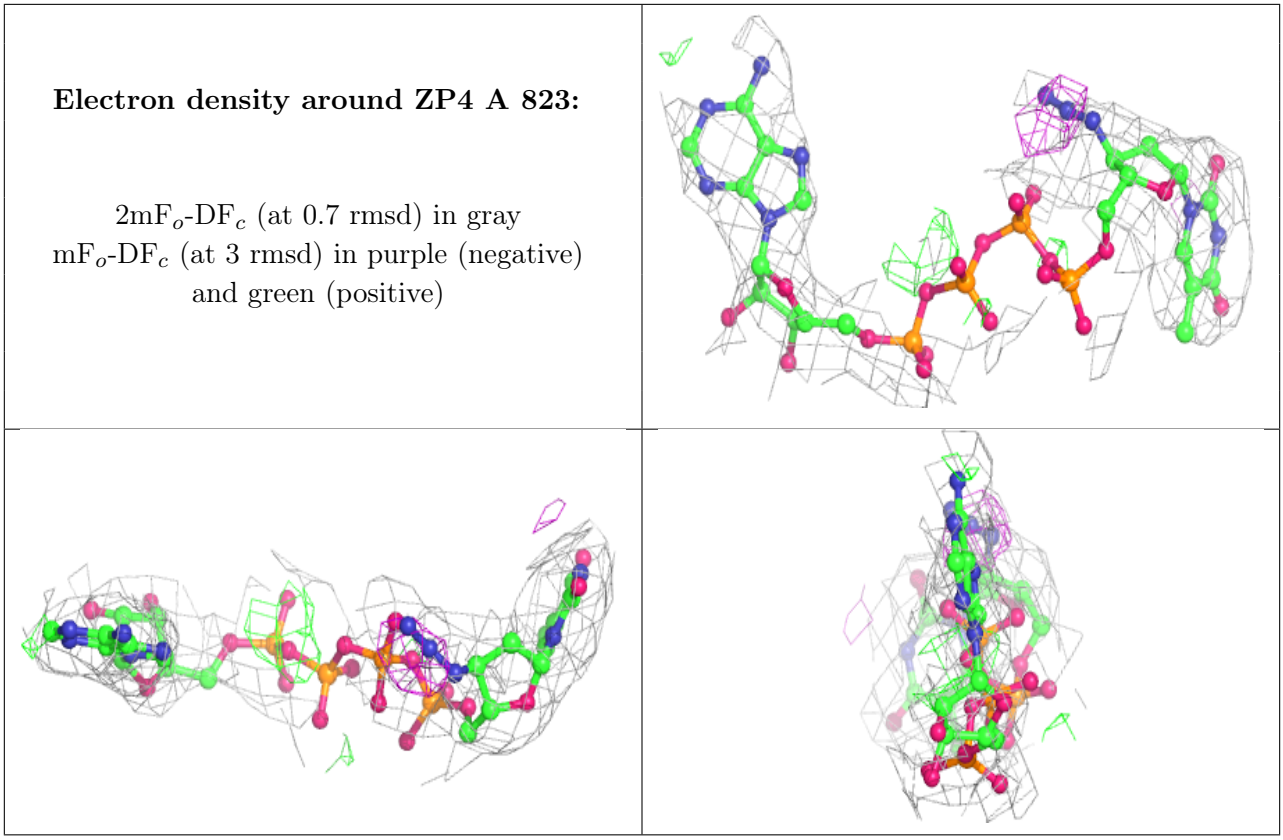
Electron density around ZP4 E 823:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ZP4 A 823:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.