



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2024 – 02:03 am BST

PDB ID : 2C7F
Title : The Structure of a family 51 arabinofuranosidase, Araf51, from *Clostridium thermocellum* in complex with 1,5- α -L-Arabinotriose.
Authors : Taylor, E.J.; Smith, N.L.; Turkenburg, J.P.; D'Souza, S.; Gilbert, H.J.; Davies, G.J.
Deposited on : 2005-11-23
Resolution : 2.70 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

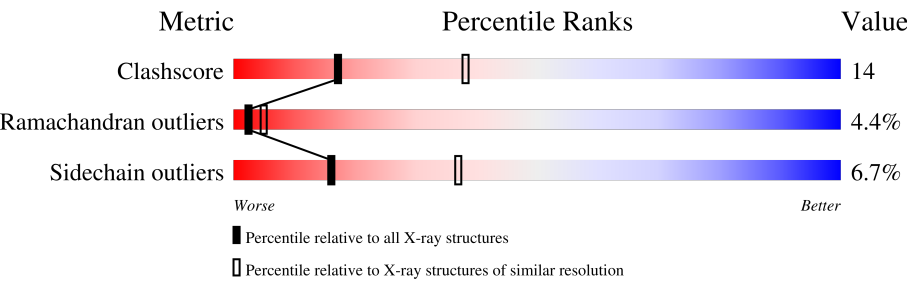
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

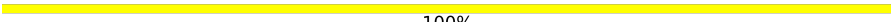
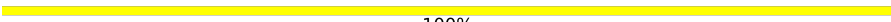

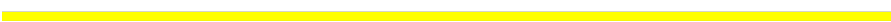
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	513	<div><div>76%</div><div>14%</div><div>.</div><div>.</div><div>.</div></div>
1	B	513	<div><div>75%</div><div>16%</div><div>5%</div><div>.</div><div>.</div><div>.</div></div>
1	C	513	<div><div>72%</div><div>18%</div><div>5%</div><div>.</div><div>.</div><div>.</div></div>
1	D	513	<div><div>75%</div><div>17%</div><div>.</div><div>.</div><div>.</div><div>.</div></div>
1	E	513	<div><div>75%</div><div>16%</div><div>.</div><div>.</div><div>.</div><div>.</div></div>
1	F	513	<div><div>75%</div><div>14%</div><div>6%</div><div>.</div><div>.</div><div>.</div></div>
2	G	3	<div><div>100%</div></div>
2	I	3	<div><div>100%</div></div>

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Mol	Chain	Length	Quality of chain
2	J	3	 100%
2	K	3	 100%
3	H	2	 100%
3	L	2	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24046 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.

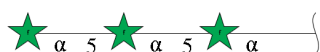
- Molecule 1 is a protein called ALPHA-L-ARABINOFURANOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3971	2523	676	750	22			
1	B	497	Total	C	N	O	S	0	0	0
			3972	2518	680	753	21			
1	C	496	Total	C	N	O	S	0	1	0
			3977	2523	679	753	22			
1	D	499	Total	C	N	O	S	0	0	0
			3978	2522	680	754	22			
1	E	492	Total	C	N	O	S	0	0	1
			3886	2465	663	738	20			
1	F	496	Total	C	N	O	S	0	0	0
			3959	2513	674	751	21			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	173	ALA	GLU	engineered mutation	UNP Q4CJG5
B	173	ALA	GLU	engineered mutation	UNP Q4CJG5
C	173	ALA	GLU	engineered mutation	UNP Q4CJG5
D	173	ALA	GLU	engineered mutation	UNP Q4CJG5
E	173	ALA	GLU	engineered mutation	UNP Q4CJG5
F	173	ALA	GLU	engineered mutation	UNP Q4CJG5

- Molecule 2 is an oligosaccharide called alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose.



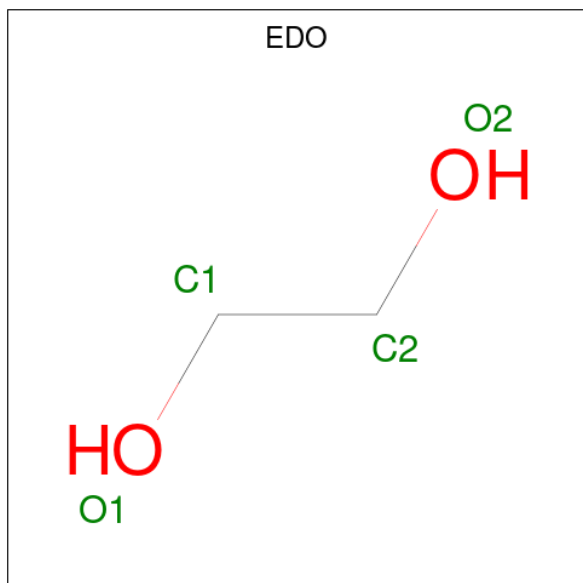
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	G	3	Total	C	O	0	0	0
			28	15	13			
2	I	3	Total	C	O	0	0	0
			28	15	13			
2	J	3	Total	C	O	0	0	0
			28	15	13			
2	K	3	Total	C	O	0	0	0
			28	15	13			

- Molecule 3 is an oligosaccharide called alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	H	2	Total	C	O	0	0	0
			19	10	9			
3	L	2	Total	C	O	0	0	0
			19	10	9			

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

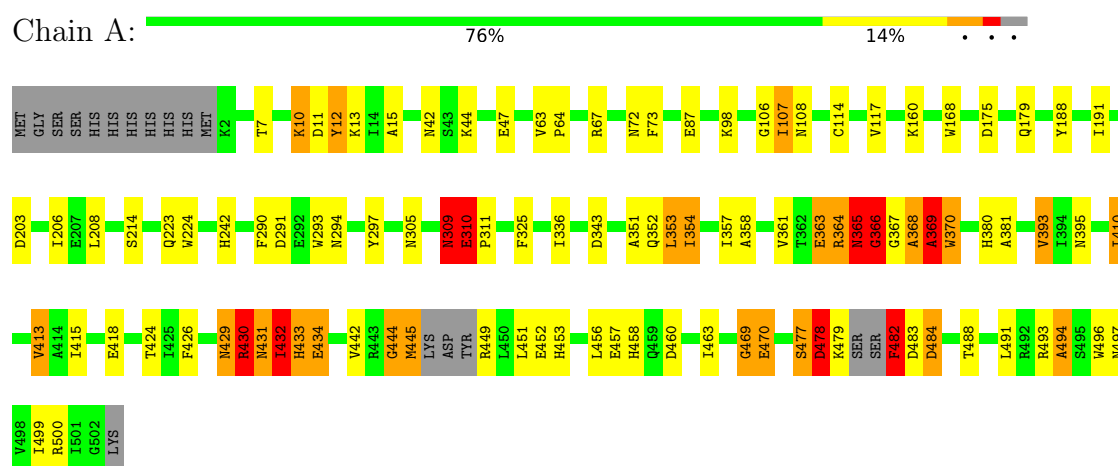
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	26	Total O 26 26	0	0
5	B	16	Total O 16 16	0	0
5	C	19	Total O 19 19	0	0
5	D	21	Total O 21 21	0	0
5	E	15	Total O 15 15	0	0
5	F	20	Total O 20 20	0	0

3 Residue-property plots

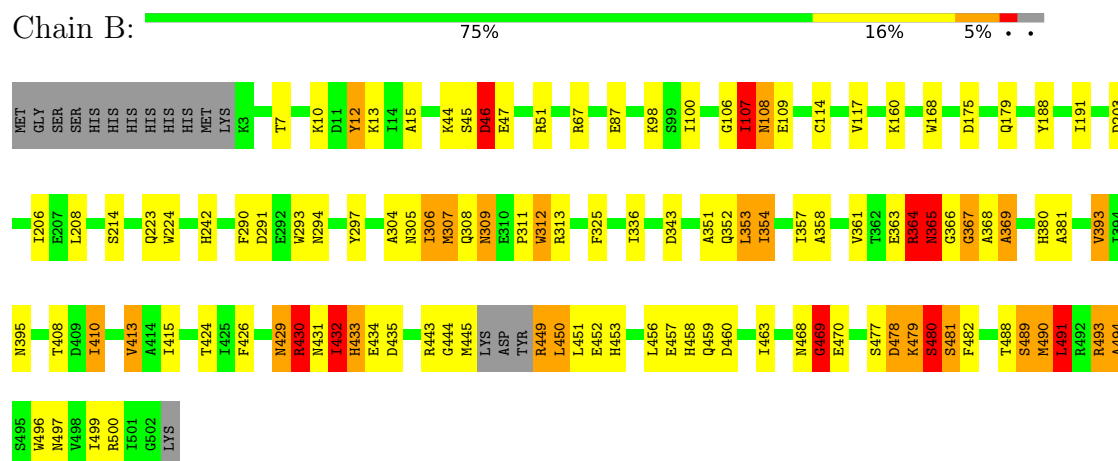
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS failed to run properly.

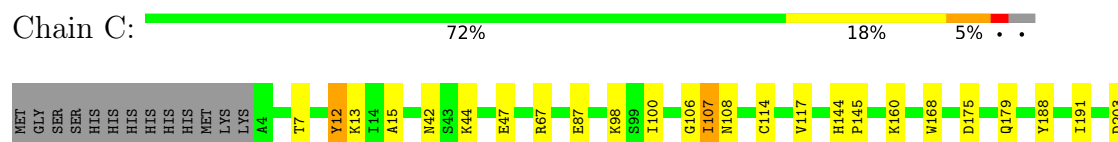
• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE

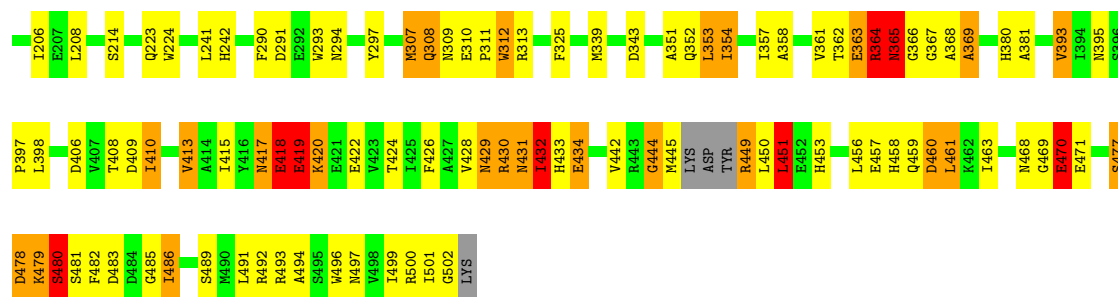


• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE



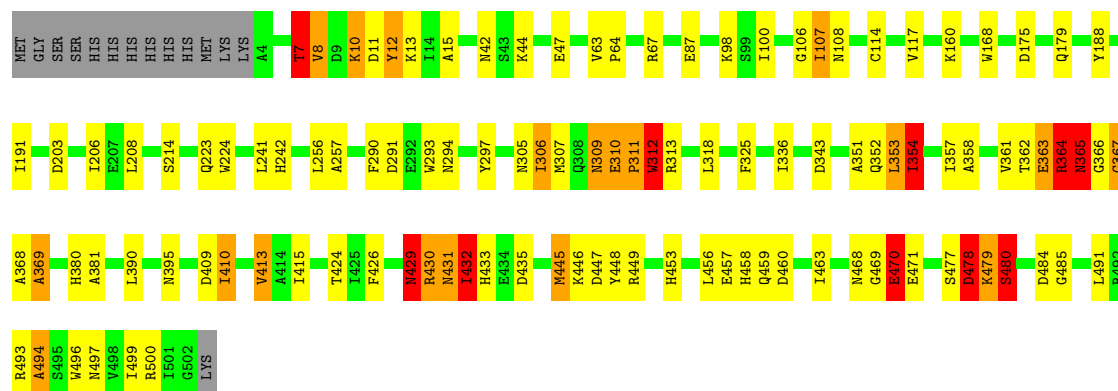
• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE





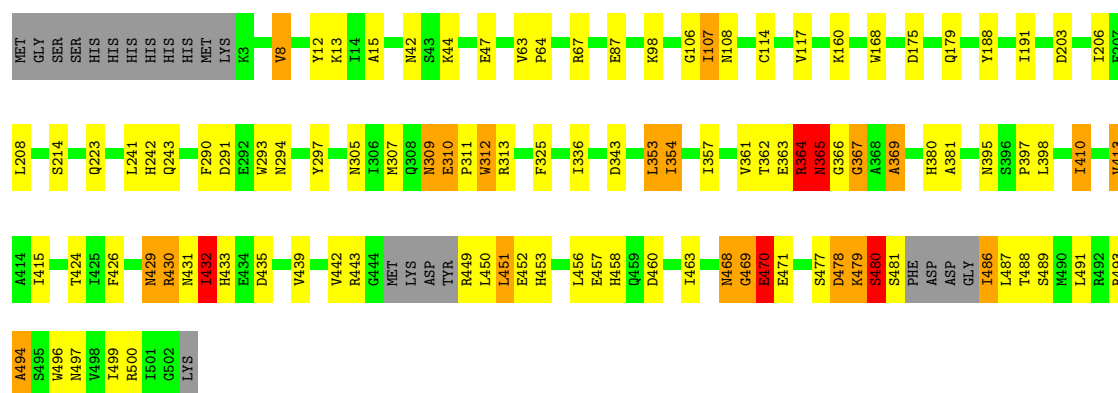
• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE

Chain D: 75% 17%



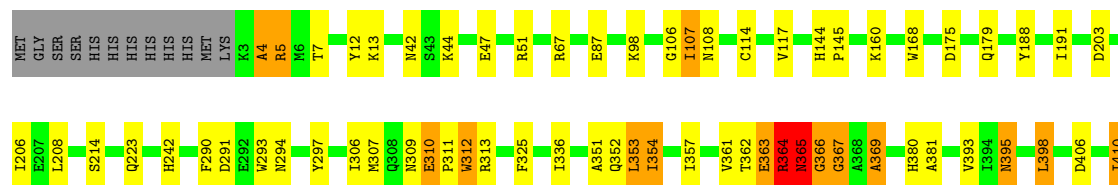
• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE

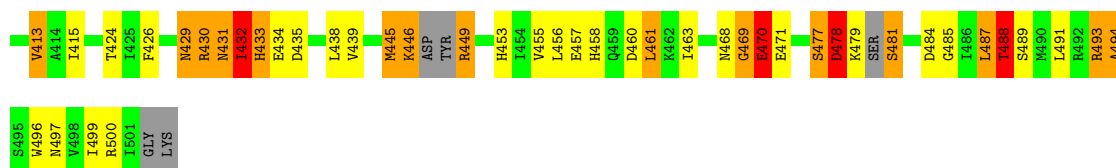
Chain E: 75% 16%




• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE

Chain F: 75% 14% 6%





- Molecule 2: alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose

Chain G:  100%

AHR1
AHR2
AHR3

- Molecule 2: alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose

Chain I:  100%

AHR1
AHR2
AHR3

- Molecule 2: alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose

Chain J:  100%

AHR1
AHR2
AHR3

- Molecule 2: alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose

Chain K:  100%

AHR1
AHR2
AHR3

- Molecule 3: alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose

Chain H:  100%

AHR1
AHR2

- Molecule 3: alpha-L-arabinofuranose-(1-5)-alpha-L-arabinofuranose

Chain L:  100%

AHR1
AHR2

4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	173.34Å 173.34Å 272.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	145.86 – 2.70	Depositor
% Data completeness (in resolution range)	99.7 (145.86-2.70)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.242 , 0.255	Depositor
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.027	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24046	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: EDO, AHR

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	0.35	0/4061	0.57	1/5499 (0.0%)
1	B	0.36	0/4063	0.59	2/5503 (0.0%)
1	C	0.36	0/4068	0.58	0/5514
1	D	0.34	0/4071	0.57	1/5516 (0.0%)
1	E	0.33	0/3973	0.55	0/5382
1	F	0.32	0/4049	0.55	1/5485 (0.0%)
All	All	0.34	0/24285	0.57	5/32899 (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
1	A	0	18
1	B	0	20
1	C	0	17
1	D	0	15
1	E	0	11
1	F	1	17
All	All	1	98

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	ASP	N-CA-C	6.22	127.80	111.00
1	F	461	LEU	CA-CB-CG	5.84	128.74	115.30
1	A	310	GLU	N-CA-C	5.37	125.50	111.00
1	B	491	LEU	CA-CB-CG	5.25	127.36	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	390	LEU	CB-CG-CD2	5.05	119.59	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	479	LYS	CA

All (98) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	223	GLN	Peptide
1	A	309	ASN	Peptide
1	A	353	LEU	Peptide
1	A	365	ASN	Peptide
1	A	366	GLY	Peptide
1	A	367	GLY	Peptide
1	A	368	ALA	Peptide
1	A	369	ALA	Peptide
1	A	393	VAL	Peptide
1	A	429	ASN	Peptide
1	A	430	ARG	Peptide
1	A	431	ASN	Peptide
1	A	433	HIS	Peptide
1	A	444	GLY	Peptide
1	A	469	GLY	Peptide
1	A	478	ASP	Peptide
1	A	482	PHE	Peptide
1	A	72	ASN	Peptide
1	B	107	ILE	Peptide
1	B	109	GLU	Peptide
1	B	223	GLN	Peptide
1	B	304	ALA	Peptide
1	B	306	ILE	Peptide
1	B	307	MET	Peptide
1	B	309	ASN	Peptide
1	B	312	TRP	Peptide
1	B	353	LEU	Peptide
1	B	365	ASN	Peptide
1	B	366	GLY	Peptide
1	B	367	GLY	Peptide
1	B	429	ASN	Peptide
1	B	430	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	B	432	ILE	Peptide
1	B	444	GLY	Peptide
1	B	45	SER	Peptide
1	B	469	GLY	Peptide
1	B	489	SER	Peptide
1	B	491	LEU	Peptide
1	C	223	GLN	Peptide
1	C	307	MET	Peptide
1	C	312	TRP	Peptide
1	C	353	LEU	Peptide
1	C	364	ARG	Peptide
1	C	365	ASN	Peptide
1	C	367	GLY	Peptide
1	C	417	ASN	Peptide
1	C	418	GLU	Peptide
1	C	419	GLU	Peptide
1	C	429	ASN	Peptide
1	C	431	ASN	Peptide
1	C	444	GLY	Peptide
1	C	450	LEU	Peptide
1	C	460	ASP	Peptide
1	C	470	GLU	Peptide
1	C	471	GLU	Peptide
1	D	223	GLN	Peptide
1	D	307	MET	Peptide
1	D	309	ASN	Peptide
1	D	311	PRO	Peptide
1	D	312	TRP	Peptide
1	D	353	LEU	Peptide
1	D	364	ARG	Peptide
1	D	365	ASN	Peptide
1	D	367	GLY	Peptide
1	D	429	ASN	Peptide
1	D	431	ASN	Peptide
1	D	471	GLU	Peptide
1	D	478	ASP	Peptide
1	D	480	SER	Peptide
1	D	7	THR	Peptide
1	E	223	GLN	Peptide
1	E	307	MET	Peptide
1	E	312	TRP	Peptide
1	E	353	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	E	364	ARG	Peptide
1	E	367	GLY	Peptide
1	E	429	ASN	Peptide
1	E	430	ARG	Peptide
1	E	443	ARG	Peptide
1	E	471	GLU	Peptide
1	E	480	SER	Peptide
1	F	223	GLN	Peptide
1	F	307	MET	Peptide
1	F	312	TRP	Peptide
1	F	353	LEU	Peptide
1	F	364	ARG	Peptide
1	F	365	ASN	Peptide
1	F	366	GLY	Peptide
1	F	367	GLY	Peptide
1	F	4	ALA	Peptide
1	F	429	ASN	Peptide
1	F	431	ASN	Peptide
1	F	445	MET	Peptide
1	F	471	GLU	Peptide
1	F	477	SER	Peptide
1	F	478	ASP	Peptide
1	F	487	LEU	Peptide
1	F	488	THR	Peptide

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	3971	0	3869	112	0
1	B	3972	0	3852	113	0
1	C	3977	0	3857	123	0
1	D	3978	0	3854	111	0
1	E	3886	0	3756	98	0
1	F	3959	0	3834	106	0
2	G	28	0	0	0	0
2	I	28	0	0	0	0
2	J	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	28	0	0	0	0
3	H	19	0	0	0	0
3	L	19	0	0	0	0
4	A	12	0	18	0	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
4	D	4	0	6	0	0
4	E	8	0	12	0	0
4	F	4	0	6	0	0
5	A	26	0	0	0	0
5	B	16	0	0	0	0
5	C	19	0	0	0	0
5	D	21	0	0	0	0
5	E	15	0	0	1	0
5	F	20	0	0	0	0
All	All	24046	0	23076	653	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 14.

All (653) 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:C:478:ASP:CB	1:C:479:LYS:HB2	1.30	1.62
1:A:431:ASN:HA	1:A:432:ILE:CG2	1.39	1.53
1:E:431:ASN:CB	1:E:432:ILE:HG22	1.35	1.52
1:C:478:ASP:HB3	1:C:479:LYS:CB	1.46	1.45
1:A:431:ASN:CA	1:A:432:ILE:HG22	1.43	1.43
1:C:478:ASP:CA	1:C:479:LYS:HB2	1.50	1.35
1:B:450:LEU:HD12	1:B:451:LEU:N	1.48	1.26
1:F:445:MET:CA	1:F:446:LYS:HB2	1.61	1.25
1:E:431:ASN:HA	1:E:432:ILE:CB	1.62	1.23
1:A:478:ASP:CB	1:A:479:LYS:HB3	1.70	1.22
1:D:429:ASN:HA	1:D:430:ARG:CB	1.70	1.22
1:F:477:SER:HB2	1:F:478:ASP:OD1	1.42	1.19
1:F:4:ALA:HB1	1:F:5:ARG:CB	1.72	1.18
1:B:450:LEU:HD12	1:B:450:LEU:C	1.52	1.18
1:C:478:ASP:CB	1:C:479:LYS:CB	2.10	1.18
1:E:431:ASN:CA	1:E:432:ILE:HB	1.72	1.18
1:E:431:ASN:CB	1:E:432:ILE:CG2	2.23	1.17
1:E:432:ILE:H	1:E:493:ARG:HB2	1.09	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:ASP:HB3	1:A:479:LYS:HB3	1.15	1.13
1:E:431:ASN:HB2	1:E:432:ILE:HG22	1.27	1.12
1:F:445:MET:HA	1:F:446:LYS:HB2	1.12	1.12
1:B:469:GLY:HA2	1:B:470:GLU:HB2	1.21	1.11
1:B:449:ARG:HG2	1:B:449:ARG:HH11	1.07	1.10
1:E:429:ASN:O	1:E:431:ASN:O	1.67	1.10
1:B:469:GLY:HA2	1:B:470:GLU:CB	1.81	1.09
1:F:4:ALA:CB	1:F:5:ARG:CB	2.30	1.09
1:B:107:ILE:HG13	1:B:108:ASN:H	1.10	1.08
1:D:429:ASN:HA	1:D:430:ARG:HB3	1.27	1.08
1:C:418:GLU:HG3	1:C:419:GLU:CB	1.83	1.07
1:D:409:ASP:O	1:D:429:ASN:HB2	1.54	1.07
1:F:478:ASP:HB3	1:F:479:LYS:HA	1.26	1.07
1:B:449:ARG:HH11	1:B:449:ARG:CG	1.67	1.07
1:F:477:SER:CB	1:F:478:ASP:OD1	2.02	1.07
1:C:418:GLU:CG	1:C:419:GLU:HB3	1.85	1.06
1:E:431:ASN:HB3	1:E:432:ILE:CG2	1.82	1.05
1:A:478:ASP:HA	1:A:479:LYS:HB2	1.36	1.05
1:A:444:GLY:CA	1:A:445:MET:HB2	1.88	1.04
1:B:490:MET:O	1:B:491:LEU:HD23	1.56	1.03
1:F:4:ALA:CA	1:F:5:ARG:CB	2.37	1.03
1:D:431:ASN:HA	1:D:432:ILE:HG22	1.37	1.02
1:C:444:GLY:HA3	1:C:445:MET:HB2	1.40	1.02
1:E:431:ASN:HB3	1:E:432:ILE:HG22	1.07	1.02
1:A:444:GLY:HA3	1:A:445:MET:HB2	1.40	1.00
1:C:485:GLY:HA2	1:C:486:ILE:O	1.59	1.00
1:F:445:MET:CB	1:F:446:LYS:HB2	1.91	1.00
1:B:450:LEU:C	1:B:450:LEU:CD1	2.30	0.99
1:A:478:ASP:HB3	1:A:479:LYS:CB	1.92	0.99
1:C:478:ASP:HB3	1:C:479:LYS:HB3	1.38	0.99
1:C:478:ASP:HA	1:C:479:LYS:HB2	1.40	0.98
1:A:442:VAL:HG22	1:A:445:MET:HB3	1.45	0.97
1:B:107:ILE:HG13	1:B:108:ASN:N	1.73	0.97
1:E:429:ASN:O	1:E:431:ASN:N	1.99	0.96
1:D:429:ASN:CA	1:D:430:ARG:HB3	1.94	0.96
1:A:353:LEU:C	1:A:354:ILE:HG12	1.86	0.95
1:C:478:ASP:CA	1:C:479:LYS:CB	2.40	0.95
1:E:431:ASN:CA	1:E:432:ILE:CB	2.34	0.94
1:B:450:LEU:CD1	1:B:451:LEU:N	2.30	0.94
1:E:432:ILE:H	1:E:493:ARG:CB	1.80	0.93
1:C:444:GLY:HA3	1:C:445:MET:CB	1.98	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4:ALA:HA	1:F:5:ARG:CB	1.96	0.93
1:F:398:LEU:HD12	1:F:406:ASP:CA	1.99	0.92
1:A:478:ASP:CB	1:A:479:LYS:CB	2.46	0.92
1:B:431:ASN:C	1:B:432:ILE:HG22	1.89	0.92
1:B:449:ARG:N	1:B:482:PHE:CE2	2.38	0.91
1:C:418:GLU:HG3	1:C:419:GLU:HB3	0.95	0.91
1:A:478:ASP:CA	1:A:479:LYS:CB	2.48	0.90
1:D:305:ASN:O	1:D:309:ASN:HB2	1.71	0.89
1:F:478:ASP:HB3	1:F:479:LYS:CA	2.02	0.89
1:F:478:ASP:CB	1:F:479:LYS:HA	2.02	0.89
1:A:431:ASN:HA	1:A:432:ILE:CB	2.03	0.88
1:B:449:ARG:N	1:B:482:PHE:HE2	1.72	0.88
1:B:449:ARG:HG2	1:B:449:ARG:NH1	1.83	0.88
1:D:7:THR:C	1:D:8:VAL:CG2	2.43	0.87
1:A:478:ASP:HA	1:A:479:LYS:CB	2.05	0.87
1:B:432:ILE:HG12	1:B:432:ILE:O	1.75	0.87
1:D:429:ASN:HA	1:D:430:ARG:HB2	1.55	0.87
1:A:478:ASP:CA	1:A:479:LYS:HB2	2.05	0.86
1:F:445:MET:HA	1:F:446:LYS:CB	2.03	0.86
1:B:469:GLY:CA	1:B:470:GLU:CB	2.53	0.85
1:F:432:ILE:O	1:F:433:HIS:CD2	2.30	0.85
1:A:310:GLU:H	1:A:311:PRO:HD3	1.41	0.85
1:D:309:ASN:HB3	1:D:310:GLU:HB2	1.57	0.85
1:E:431:ASN:HA	1:E:432:ILE:HB	0.86	0.84
1:B:480:SER:HA	1:B:481:SER:CB	2.07	0.84
1:F:398:LEU:CD1	1:F:406:ASP:HB3	2.07	0.84
1:F:398:LEU:HD12	1:F:406:ASP:CB	2.08	0.84
1:A:305:ASN:O	1:A:309:ASN:HB2	1.78	0.83
1:F:398:LEU:HD12	1:F:406:ASP:HA	1.57	0.83
1:B:431:ASN:C	1:B:432:ILE:CG2	2.46	0.83
1:F:445:MET:HB3	1:F:446:LYS:CB	2.08	0.83
1:D:7:THR:C	1:D:8:VAL:HG23	1.98	0.82
1:B:368:ALA:O	1:B:369:ALA:HB3	1.77	0.82
1:E:431:ASN:CA	1:E:432:ILE:CG2	2.57	0.82
1:B:353:LEU:HB3	1:B:354:ILE:HG13	1.61	0.82
1:A:431:ASN:OD1	1:A:433:HIS:HB2	1.78	0.82
1:F:445:MET:CB	1:F:446:LYS:CB	2.58	0.81
1:A:432:ILE:HD13	1:A:432:ILE:O	1.81	0.80
1:B:7:THR:CG2	1:B:393:VAL:HB	2.11	0.80
1:B:431:ASN:O	1:B:432:ILE:CG2	2.30	0.80
1:D:309:ASN:ND2	1:D:310:GLU:HG3	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:LEU:C	1:B:354:ILE:HG12	2.01	0.80
1:E:431:ASN:HA	1:E:432:ILE:CG2	2.11	0.80
1:B:432:ILE:O	1:B:432:ILE:CG1	2.30	0.80
1:C:7:THR:CG2	1:C:393:VAL:HB	2.12	0.79
1:B:368:ALA:O	1:B:369:ALA:CB	2.30	0.79
1:B:306:ILE:O	1:B:306:ILE:CG2	2.30	0.79
1:F:445:MET:CA	1:F:446:LYS:CB	2.50	0.79
1:B:431:ASN:O	1:B:432:ILE:HG23	1.83	0.79
1:E:432:ILE:N	1:E:493:ARG:HB2	1.93	0.78
1:E:431:ASN:O	1:E:494:ALA:N	2.13	0.78
1:A:393:VAL:HG21	1:D:12:TYR:CE1	2.19	0.78
1:E:397:PRO:C	1:E:398:LEU:HD23	2.04	0.78
1:D:7:THR:CA	1:D:8:VAL:HG23	2.13	0.78
1:D:7:THR:HA	1:D:8:VAL:HG23	1.66	0.77
1:C:417:ASN:HA	1:C:418:GLU:HB3	1.65	0.77
1:A:7:THR:CG2	1:A:393:VAL:HG12	2.14	0.77
1:F:431:ASN:HD21	1:F:434:GLU:CG	1.98	0.77
1:C:417:ASN:HA	1:C:418:GLU:CB	2.15	0.76
1:D:431:ASN:CA	1:D:432:ILE:HG22	2.16	0.76
1:A:431:ASN:CB	1:A:432:ILE:HG22	2.15	0.76
1:B:469:GLY:CA	1:B:470:GLU:HB2	2.10	0.76
1:F:398:LEU:HD13	1:F:406:ASP:C	2.06	0.76
1:F:398:LEU:CD1	1:F:406:ASP:CA	2.64	0.75
1:E:486:ILE:CG2	1:E:487:LEU:N	2.49	0.75
1:F:7:THR:CG2	1:F:393:VAL:HB	2.16	0.75
1:A:7:THR:HG22	1:A:393:VAL:HG12	1.66	0.75
1:B:449:ARG:CG	1:B:449:ARG:NH1	2.40	0.75
1:F:398:LEU:HD12	1:F:406:ASP:HB3	1.66	0.74
1:D:353:LEU:C	1:D:354:ILE:HG12	2.08	0.74
1:E:353:LEU:HB3	1:E:354:ILE:HG12	1.69	0.74
1:B:429:ASN:O	1:B:494:ALA:HA	1.88	0.74
1:D:310:GLU:H	1:D:311:PRO:HD3	1.50	0.74
1:F:363:GLU:O	1:F:364:ARG:HB2	1.87	0.74
1:A:431:ASN:OD1	1:A:434:GLU:HB2	1.88	0.74
1:B:306:ILE:O	1:B:306:ILE:HG22	1.86	0.74
1:F:353:LEU:HB3	1:F:354:ILE:HG12	1.70	0.74
1:C:363:GLU:O	1:C:364:ARG:HB2	1.87	0.73
1:A:12:TYR:CE2	1:D:12:TYR:CE2	2.77	0.73
1:A:444:GLY:N	1:A:445:MET:HB2	2.03	0.73
1:B:480:SER:HA	1:B:481:SER:HB2	1.69	0.73
1:F:435:ASP:OD1	1:F:493:ARG:HG2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ILE:HG23	1:A:413:VAL:HG22	1.71	0.73
1:B:433:HIS:H	1:B:493:ARG:HB2	1.54	0.73
1:F:336:ILE:HG23	1:F:413:VAL:HG22	1.71	0.72
1:F:4:ALA:O	1:F:438:LEU:HA	1.89	0.72
1:E:243:GLN:NE2	5:E:701:HOH:O	2.21	0.72
1:E:336:ILE:HG23	1:E:413:VAL:HG22	1.71	0.72
1:C:469:GLY:HA2	1:C:470:GLU:HB3	1.72	0.72
1:F:469:GLY:HA2	1:F:470:GLU:CB	2.20	0.71
1:F:431:ASN:HA	1:F:432:ILE:HG22	1.72	0.71
1:A:353:LEU:O	1:A:354:ILE:HG12	1.91	0.71
1:E:469:GLY:HA2	1:E:470:GLU:CB	2.20	0.71
1:F:469:GLY:HA2	1:F:470:GLU:HB3	1.71	0.71
1:D:336:ILE:HG23	1:D:413:VAL:HG22	1.71	0.71
1:B:336:ILE:HG23	1:B:413:VAL:HG22	1.71	0.71
1:C:469:GLY:HA2	1:C:470:GLU:CB	2.20	0.71
1:D:409:ASP:O	1:D:429:ASN:CB	2.37	0.70
1:D:309:ASN:C	1:D:310:GLU:CG	2.60	0.70
1:C:478:ASP:HA	1:C:479:LYS:CB	2.13	0.70
1:D:469:GLY:HA2	1:D:470:GLU:CB	2.20	0.70
1:E:469:GLY:HA2	1:E:470:GLU:HB3	1.72	0.70
1:F:431:ASN:C	1:F:432:ILE:HG22	2.12	0.70
1:B:12:TYR:CE2	1:C:12:TYR:CE2	2.80	0.70
1:D:469:GLY:HA2	1:D:470:GLU:HB3	1.73	0.69
1:E:450:LEU:HD22	1:E:481:SER:HA	1.74	0.69
1:D:100:ILE:HG12	1:D:312:TRP:O	1.92	0.69
1:A:310:GLU:N	1:A:311:PRO:HD3	2.08	0.69
1:B:431:ASN:OD1	1:B:434:GLU:N	2.22	0.69
1:F:431:ASN:ND2	1:F:434:GLU:CG	2.55	0.69
1:C:353:LEU:C	1:C:354:ILE:HG12	2.13	0.69
1:C:431:ASN:HD21	1:C:434:GLU:HG3	1.58	0.69
1:E:486:ILE:HG22	1:E:487:LEU:N	2.07	0.69
1:C:485:GLY:CA	1:C:486:ILE:O	2.38	0.69
1:F:477:SER:CA	1:F:478:ASP:OD1	2.41	0.69
1:F:398:LEU:CD1	1:F:406:ASP:C	2.61	0.68
1:F:477:SER:C	1:F:478:ASP:OD1	2.31	0.68
1:F:431:ASN:ND2	1:F:434:GLU:HG3	2.08	0.68
1:D:479:LYS:O	1:D:480:SER:HB2	1.94	0.68
1:B:106:GLY:C	1:B:107:ILE:CG2	2.62	0.67
1:A:431:ASN:HA	1:A:432:ILE:HG22	0.70	0.67
1:D:311:PRO:HB2	1:D:312:TRP:CD1	2.28	0.67
1:C:417:ASN:HA	1:C:418:GLU:HG2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:361:VAL:O	1:F:369:ALA:HA	1.94	0.67
1:D:309:ASN:CG	1:D:310:GLU:HG3	2.16	0.67
1:C:100:ILE:HG12	1:C:312:TRP:O	1.95	0.67
1:C:419:GLU:HG3	1:C:420:LYS:HB2	1.75	0.66
1:D:309:ASN:O	1:D:310:GLU:CG	2.43	0.66
1:D:361:VAL:O	1:D:369:ALA:HA	1.94	0.66
1:C:444:GLY:CA	1:C:445:MET:CB	2.73	0.66
1:F:431:ASN:O	1:F:433:HIS:N	2.28	0.66
1:A:393:VAL:HG21	1:D:12:TYR:CZ	2.31	0.66
1:C:361:VAL:O	1:C:369:ALA:HA	1.95	0.66
1:C:417:ASN:OD1	1:C:418:GLU:N	2.30	0.65
1:F:398:LEU:HD11	1:F:406:ASP:HB3	1.78	0.65
1:A:442:VAL:CG2	1:A:445:MET:HB3	2.22	0.65
1:A:42:ASN:ND2	1:A:366:GLY:O	2.22	0.65
1:C:429:ASN:CG	1:C:429:ASN:O	2.33	0.65
1:E:361:VAL:O	1:E:369:ALA:HA	1.95	0.65
1:B:361:VAL:O	1:B:369:ALA:HA	1.96	0.65
1:C:431:ASN:ND2	1:C:431:ASN:O	2.30	0.65
1:F:5:ARG:CB	1:F:395:ASN:O	2.45	0.65
1:A:444:GLY:H	1:A:445:MET:HB2	1.62	0.65
1:D:363:GLU:O	1:D:364:ARG:HB2	1.97	0.65
1:F:445:MET:HB3	1:F:446:LYS:HB3	1.79	0.65
1:D:353:LEU:O	1:D:354:ILE:HG12	1.96	0.65
1:D:380:HIS:HD2	1:D:496:TRP:HE1	1.45	0.65
1:E:410:ILE:HD11	1:E:491:LEU:HD12	1.79	0.65
1:F:365:ASN:OD1	1:F:365:ASN:N	2.30	0.64
1:A:444:GLY:HA3	1:A:445:MET:CB	2.21	0.64
1:C:429:ASN:C	1:C:431:ASN:H	2.00	0.64
1:D:7:THR:OG1	1:D:8:VAL:N	2.30	0.64
1:E:431:ASN:HB2	1:E:433:HIS:H	1.63	0.64
1:C:451:LEU:HD12	1:C:501:ILE:C	2.17	0.64
1:F:410:ILE:HD11	1:F:491:LEU:HD12	1.80	0.64
1:B:380:HIS:HD2	1:B:496:TRP:HE1	1.45	0.64
1:D:410:ILE:HD11	1:D:491:LEU:HD12	1.80	0.64
1:E:380:HIS:HD2	1:E:496:TRP:HE1	1.46	0.64
1:C:410:ILE:HD11	1:C:491:LEU:HD12	1.79	0.63
1:E:431:ASN:O	1:E:493:ARG:HA	1.97	0.63
1:C:417:ASN:O	1:C:422:GLU:N	2.26	0.63
1:C:417:ASN:CG	1:C:418:GLU:HG2	2.18	0.63
1:E:439:VAL:HG12	1:E:488:THR:HG22	1.80	0.63
1:B:429:ASN:OD1	1:B:431:ASN:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ILE:HD11	1:A:491:LEU:HD12	1.80	0.63
1:A:429:ASN:O	1:A:494:ALA:HA	1.97	0.63
1:A:380:HIS:HD2	1:A:496:TRP:HE1	1.46	0.63
1:C:478:ASP:HB3	1:C:479:LYS:CA	2.25	0.63
1:E:429:ASN:O	1:E:431:ASN:C	2.36	0.63
1:C:380:HIS:HD2	1:C:496:TRP:HE1	1.46	0.63
1:E:305:ASN:O	1:E:309:ASN:HB2	1.98	0.63
1:A:431:ASN:C	1:A:432:ILE:HG22	2.19	0.62
1:B:410:ILE:HD11	1:B:491:LEU:HD12	1.80	0.62
1:D:100:ILE:CG1	1:D:312:TRP:O	2.46	0.62
1:A:469:GLY:HA2	1:A:470:GLU:HB2	1.81	0.62
1:D:410:ILE:HD12	1:D:429:ASN:HB3	1.81	0.62
1:B:7:THR:HG22	1:B:393:VAL:HB	1.79	0.62
1:B:106:GLY:C	1:B:107:ILE:HG23	2.19	0.62
1:A:453:HIS:ND1	1:A:499:ILE:HG12	2.14	0.62
1:D:309:ASN:ND2	1:D:310:GLU:OE2	2.32	0.62
1:C:408:THR:O	1:C:430:ARG:HD3	2.00	0.62
1:C:453:HIS:ND1	1:C:499:ILE:HG12	2.14	0.62
1:D:453:HIS:ND1	1:D:499:ILE:HG12	2.15	0.62
1:B:353:LEU:O	1:B:354:ILE:HG12	1.99	0.62
1:B:380:HIS:CD2	1:B:496:TRP:HE1	2.18	0.62
1:D:380:HIS:CD2	1:D:496:TRP:HE1	2.18	0.62
1:E:380:HIS:CD2	1:E:496:TRP:HE1	2.18	0.62
1:A:432:ILE:H	1:A:494:ALA:N	1.98	0.62
1:D:309:ASN:CB	1:D:310:GLU:HG3	2.29	0.62
1:D:353:LEU:HB3	1:D:354:ILE:HG13	1.80	0.62
1:E:429:ASN:C	1:E:431:ASN:N	2.50	0.62
1:B:410:ILE:HD12	1:B:429:ASN:HB2	1.81	0.62
1:B:453:HIS:ND1	1:B:499:ILE:HG12	2.15	0.62
1:E:453:HIS:ND1	1:E:499:ILE:HG12	2.15	0.61
1:C:478:ASP:CG	1:C:479:LYS:HB2	2.17	0.61
1:A:380:HIS:CD2	1:A:496:TRP:HE1	2.18	0.61
1:C:7:THR:HG22	1:C:393:VAL:HB	1.81	0.61
1:E:429:ASN:O	1:E:429:ASN:CG	2.39	0.61
1:F:453:HIS:ND1	1:F:499:ILE:HG12	2.16	0.61
1:A:442:VAL:HG22	1:A:445:MET:CB	2.26	0.61
1:A:449:ARG:O	1:A:449:ARG:HG2	1.98	0.61
1:A:478:ASP:HB3	1:A:479:LYS:CA	2.31	0.61
1:B:480:SER:HA	1:B:481:SER:HB3	1.82	0.61
1:E:431:ASN:HB2	1:E:432:ILE:CG2	2.15	0.61
1:F:398:LEU:CD1	1:F:406:ASP:CB	2.72	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:431:ASN:HA	1:C:432:ILE:HB	1.83	0.61
1:F:431:ASN:O	1:F:431:ASN:CG	2.38	0.61
1:C:380:HIS:CD2	1:C:496:TRP:HE1	2.18	0.60
1:C:419:GLU:HG3	1:C:419:GLU:O	2.01	0.60
1:B:408:THR:O	1:B:430:ARG:HD2	2.01	0.60
1:C:417:ASN:HA	1:C:418:GLU:CG	2.31	0.60
1:C:479:LYS:O	1:C:480:SER:CB	2.49	0.60
1:B:480:SER:CA	1:B:481:SER:HB2	2.31	0.59
1:C:100:ILE:CG1	1:C:312:TRP:O	2.50	0.59
1:E:365:ASN:N	1:E:365:ASN:OD1	2.35	0.59
1:C:479:LYS:O	1:C:480:SER:HB3	2.03	0.59
1:F:429:ASN:O	1:F:494:ALA:N	2.35	0.59
1:F:432:ILE:O	1:F:433:HIS:HD2	1.85	0.59
1:B:51:ARG:HH22	1:B:367:GLY:HA3	1.68	0.59
1:D:309:ASN:O	1:D:310:GLU:HG3	2.03	0.59
1:A:353:LEU:HB3	1:A:354:ILE:HG13	1.83	0.59
1:A:368:ALA:O	1:A:369:ALA:HB3	2.01	0.59
1:E:8:VAL:HG22	1:E:442:VAL:HG23	1.85	0.59
1:A:310:GLU:H	1:A:311:PRO:CD	2.16	0.58
1:B:353:LEU:HB3	1:B:354:ILE:CG1	2.32	0.58
1:F:431:ASN:CA	1:F:432:ILE:HG22	2.32	0.58
1:E:431:ASN:C	1:E:494:ALA:N	2.57	0.58
1:D:309:ASN:HB3	1:D:310:GLU:CB	2.31	0.58
1:E:362:THR:HG22	1:E:369:ALA:HB2	1.84	0.58
1:A:410:ILE:HD12	1:A:429:ASN:HB2	1.86	0.58
1:C:362:THR:HG22	1:C:369:ALA:HB2	1.85	0.58
1:F:353:LEU:CB	1:F:354:ILE:HG12	2.34	0.58
1:F:410:ILE:HD12	1:F:429:ASN:HB2	1.86	0.58
1:E:432:ILE:N	1:E:493:ARG:C	2.57	0.58
1:A:469:GLY:HA2	1:A:470:GLU:CB	2.34	0.58
1:B:469:GLY:HA2	1:B:470:GLU:HB3	1.80	0.58
1:D:445:MET:HB2	1:D:447:ASP:H	1.68	0.58
1:D:429:ASN:CB	1:D:430:ARG:HB3	2.34	0.58
1:E:398:LEU:HD23	1:E:398:LEU:N	2.16	0.58
1:A:434:GLU:H	1:A:493:ARG:HB3	1.68	0.57
1:E:431:ASN:C	1:E:494:ALA:H	2.07	0.57
1:F:362:THR:HG22	1:F:369:ALA:HB2	1.85	0.57
1:F:455:VAL:HG23	1:F:497:ASN:OD1	2.03	0.57
1:F:453:HIS:CE1	1:F:497:ASN:ND2	2.72	0.57
1:D:362:THR:HG22	1:D:369:ALA:HB2	1.85	0.57
1:E:353:LEU:CB	1:E:354:ILE:HG12	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:432:ILE:H	1:E:493:ARG:CA	2.17	0.57
1:A:442:VAL:HG13	1:A:445:MET:C	2.25	0.57
1:C:431:ASN:HA	1:C:432:ILE:HG22	1.85	0.57
1:C:417:ASN:OD1	1:C:420:LYS:HB3	2.04	0.57
1:C:417:ASN:O	1:C:422:GLU:O	2.23	0.57
1:C:417:ASN:OD1	1:C:418:GLU:CG	2.53	0.56
1:D:309:ASN:C	1:D:310:GLU:HG3	2.24	0.56
1:F:458:HIS:HD2	1:F:460:ASP:H	1.53	0.56
1:B:51:ARG:HH12	1:B:367:GLY:CA	2.18	0.56
1:B:481:SER:HB3	1:B:488:THR:O	2.06	0.56
1:C:491:LEU:HD22	1:C:497:ASN:ND2	2.21	0.56
1:A:431:ASN:CA	1:A:432:ILE:CB	2.78	0.56
1:A:478:ASP:CG	1:A:479:LYS:HB3	2.25	0.56
1:F:380:HIS:CD2	1:F:496:TRP:HE1	2.24	0.56
1:B:100:ILE:HG12	1:B:312:TRP:O	2.05	0.56
1:C:339:MET:HE1	1:C:413:VAL:CG1	2.36	0.56
1:C:419:GLU:O	1:C:419:GLU:CG	2.53	0.56
1:B:477:SER:HB2	1:B:478:ASP:OD1	2.06	0.56
1:E:458:HIS:HD2	1:E:460:ASP:H	1.54	0.56
1:B:469:GLY:CA	1:B:470:GLU:HB3	2.35	0.56
1:C:431:ASN:HA	1:C:432:ILE:CB	2.36	0.56
1:B:429:ASN:O	1:B:494:ALA:CA	2.54	0.55
1:B:458:HIS:HD2	1:B:460:ASP:H	1.54	0.55
1:B:480:SER:CA	1:B:481:SER:CB	2.81	0.55
1:E:431:ASN:HB2	1:E:433:HIS:N	2.21	0.55
1:D:458:HIS:HD2	1:D:460:ASP:H	1.54	0.55
1:B:491:LEU:HD22	1:B:497:ASN:ND2	2.21	0.55
1:B:354:ILE:H	1:B:358:ALA:CB	2.20	0.55
1:A:458:HIS:HD2	1:A:460:ASP:H	1.54	0.55
1:D:257:ALA:HA	1:D:430:ARG:NH1	2.21	0.55
1:B:353:LEU:C	1:B:354:ILE:CG1	2.73	0.55
1:D:305:ASN:O	1:D:309:ASN:CB	2.48	0.55
1:F:398:LEU:CD1	1:F:406:ASP:HA	2.32	0.55
1:D:310:GLU:N	1:D:311:PRO:HD3	2.22	0.55
1:E:491:LEU:HD22	1:E:497:ASN:ND2	2.21	0.55
1:F:449:ARG:O	1:F:449:ARG:HG2	2.05	0.55
1:D:491:LEU:HD22	1:D:497:ASN:ND2	2.22	0.54
1:E:8:VAL:HG22	1:E:8:VAL:O	2.06	0.54
1:B:393:VAL:HG22	1:C:12:TYR:OH	2.08	0.54
1:B:431:ASN:OD1	1:B:434:GLU:HB2	2.07	0.54
1:D:309:ASN:O	1:D:310:GLU:HG2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:LEU:HD22	1:A:497:ASN:ND2	2.22	0.54
1:A:429:ASN:C	1:A:431:ASN:H	2.11	0.54
1:A:432:ILE:H	1:A:493:ARG:C	2.11	0.54
1:D:42:ASN:ND2	1:D:366:GLY:O	2.41	0.54
1:D:445:MET:HG3	1:D:448:TYR:CG	2.42	0.54
1:A:393:VAL:CG2	1:D:12:TYR:CE1	2.90	0.54
1:B:100:ILE:CG1	1:B:312:TRP:O	2.56	0.53
1:B:12:TYR:OH	1:C:393:VAL:HG22	2.08	0.53
1:F:7:THR:HG23	1:F:393:VAL:HB	1.91	0.53
1:C:398:LEU:HD23	1:C:398:LEU:N	2.22	0.53
1:C:431:ASN:HA	1:C:432:ILE:CG2	2.38	0.53
1:D:7:THR:C	1:D:8:VAL:HG22	2.27	0.53
1:E:311:PRO:HB2	1:E:312:TRP:CD1	2.44	0.53
1:F:311:PRO:HB2	1:F:312:TRP:CD1	2.43	0.53
1:C:417:ASN:CA	1:C:418:GLU:HG2	2.38	0.53
1:D:354:ILE:H	1:D:358:ALA:CB	2.22	0.53
1:E:397:PRO:O	1:E:398:LEU:HD23	2.09	0.53
1:D:309:ASN:ND2	1:D:310:GLU:CG	2.69	0.52
1:B:432:ILE:O	1:B:433:HIS:CD2	2.63	0.52
1:C:397:PRO:C	1:C:398:LEU:HD23	2.30	0.52
1:F:51:ARG:HH12	1:F:367:GLY:HA3	1.74	0.52
1:C:42:ASN:ND2	1:C:366:GLY:O	2.39	0.52
1:E:468:ASN:O	1:E:469:GLY:O	2.27	0.52
1:E:435:ASP:OD1	1:E:493:ARG:HG2	2.10	0.52
1:A:433:HIS:N	1:A:493:ARG:HB2	2.25	0.52
1:C:449:ARG:HA	1:C:482:PHE:CD2	2.45	0.52
1:C:477:SER:HB2	1:C:478:ASP:OD1	2.09	0.52
1:D:429:ASN:CG	1:D:429:ASN:O	2.48	0.51
1:B:431:ASN:O	1:B:433:HIS:HB2	2.10	0.51
1:F:7:THR:HG22	1:F:393:VAL:HB	1.91	0.51
1:F:491:LEU:HD22	1:F:497:ASN:ND2	2.24	0.51
1:D:431:ASN:CG	1:D:431:ASN:O	2.48	0.51
1:A:477:SER:HB2	1:A:478:ASP:OD1	2.10	0.51
1:B:364:ARG:O	1:B:365:ASN:C	2.49	0.51
1:D:364:ARG:O	1:D:365:ASN:C	2.49	0.51
1:C:354:ILE:H	1:C:358:ALA:CB	2.23	0.51
1:A:432:ILE:H	1:A:493:ARG:CA	2.24	0.51
1:D:67:ARG:HD2	1:D:291:ASP:HB2	1.93	0.51
1:D:353:LEU:C	1:D:354:ILE:CG1	2.75	0.51
1:F:398:LEU:CD1	1:F:406:ASP:O	2.59	0.51
1:D:429:ASN:HB2	1:D:430:ARG:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ASP:OD1	1:B:214:SER:OG	2.29	0.50
1:C:175:ASP:OD1	1:C:214:SER:OG	2.28	0.50
1:C:451:LEU:CD1	1:C:501:ILE:C	2.80	0.50
1:A:188:TYR:HA	1:A:191:ILE:HG22	1.93	0.50
1:B:67:ARG:HD2	1:B:291:ASP:HB2	1.93	0.50
1:E:8:VAL:O	1:E:8:VAL:CG2	2.59	0.50
1:B:188:TYR:HA	1:B:191:ILE:HG22	1.93	0.50
1:C:417:ASN:OD1	1:C:418:GLU:HG2	2.11	0.50
1:A:393:VAL:CG2	1:D:12:TYR:CZ	2.94	0.50
1:B:429:ASN:O	1:B:494:ALA:N	2.43	0.50
1:B:478:ASP:HB3	1:B:479:LYS:CB	2.42	0.50
1:C:188:TYR:HA	1:C:191:ILE:HG22	1.93	0.50
1:E:67:ARG:HD2	1:E:291:ASP:HB2	1.93	0.50
1:B:480:SER:HB2	1:B:489:SER:HA	1.93	0.50
1:D:188:TYR:HA	1:D:191:ILE:HG22	1.93	0.50
1:F:4:ALA:CB	1:F:395:ASN:O	2.60	0.50
1:C:307:MET:O	1:C:308:GLN:HB2	2.12	0.50
1:E:429:ASN:O	1:E:429:ASN:OD1	2.30	0.50
1:E:429:ASN:O	1:E:431:ASN:CA	2.60	0.50
1:F:432:ILE:HD13	1:F:433:HIS:CD2	2.47	0.50
1:C:429:ASN:C	1:C:431:ASN:N	2.65	0.50
1:F:67:ARG:HD2	1:F:291:ASP:HB2	1.94	0.50
1:F:431:ASN:O	1:F:431:ASN:OD1	2.30	0.50
1:C:429:ASN:O	1:C:429:ASN:OD1	2.30	0.49
1:D:445:MET:SD	1:D:445:MET:N	2.85	0.49
1:E:8:VAL:CG2	1:E:442:VAL:HG23	2.42	0.49
1:A:361:VAL:O	1:A:369:ALA:HA	2.12	0.49
1:A:451:LEU:HB2	1:A:500:ARG:O	2.12	0.49
1:B:51:ARG:HH12	1:B:367:GLY:HA2	1.76	0.49
1:F:188:TYR:HA	1:F:191:ILE:HG22	1.93	0.49
1:F:398:LEU:HD13	1:F:406:ASP:O	2.10	0.49
1:D:175:ASP:OD1	1:D:214:SER:OG	2.28	0.49
1:E:449:ARG:O	1:E:449:ARG:HG2	2.12	0.49
1:F:431:ASN:HD21	1:F:434:GLU:HG3	1.73	0.49
1:E:478:ASP:HB3	1:E:479:LYS:CB	2.43	0.49
1:B:432:ILE:O	1:B:432:ILE:CD1	2.59	0.49
1:C:458:HIS:HD2	1:C:460:ASP:H	1.61	0.49
1:A:10:LYS:HD2	1:A:11:ASP:OD1	2.12	0.49
1:C:339:MET:CE	1:C:413:VAL:CG1	2.90	0.49
1:F:453:HIS:CE1	1:F:497:ASN:HD22	2.31	0.49
1:A:67:ARG:HD2	1:A:291:ASP:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:LEU:HB3	1:A:354:ILE:CG1	2.41	0.49
1:B:354:ILE:H	1:B:358:ALA:HB2	1.77	0.49
1:C:67:ARG:HD2	1:C:291:ASP:HB2	1.93	0.49
1:C:480:SER:HB2	1:C:489:SER:HA	1.95	0.49
1:A:363:GLU:O	1:A:364:ARG:HB2	2.13	0.49
1:C:7:THR:HG23	1:C:393:VAL:HB	1.93	0.49
1:A:442:VAL:HG11	1:A:482:PHE:HZ	1.78	0.49
1:B:479:LYS:O	1:B:480:SER:HB3	2.12	0.49
1:C:431:ASN:O	1:C:431:ASN:CG	2.48	0.49
1:D:431:ASN:O	1:D:431:ASN:OD1	2.30	0.49
1:F:42:ASN:ND2	1:F:366:GLY:O	2.29	0.49
1:F:175:ASP:OD1	1:F:214:SER:OG	2.27	0.49
1:B:450:LEU:CD1	1:B:451:LEU:H	2.22	0.48
1:E:188:TYR:HA	1:E:191:ILE:HG22	1.93	0.48
1:F:4:ALA:HB1	1:F:395:ASN:O	2.13	0.48
1:A:175:ASP:OD1	1:A:214:SER:OG	2.28	0.48
1:A:310:GLU:N	1:A:311:PRO:CD	2.76	0.48
1:B:353:LEU:CB	1:B:354:ILE:HG13	2.38	0.48
1:F:429:ASN:OD1	1:F:431:ASN:HB3	2.13	0.48
1:A:293:TRP:O	1:A:294:ASN:HB2	2.14	0.48
1:B:293:TRP:O	1:B:294:ASN:HB2	2.13	0.48
1:E:480:SER:HB2	1:E:489:SER:HA	1.95	0.48
1:A:431:ASN:OD1	1:A:431:ASN:O	2.30	0.48
1:E:456:LEU:HB3	1:E:496:TRP:HB3	1.95	0.48
1:A:444:GLY:HA3	1:A:445:MET:SD	2.53	0.48
1:D:366:GLY:HA3	1:D:367:GLY:HA2	1.49	0.48
1:E:42:ASN:ND2	1:E:366:GLY:O	2.45	0.48
1:A:456:LEU:HB3	1:A:496:TRP:HB3	1.96	0.48
1:C:354:ILE:H	1:C:358:ALA:HB2	1.79	0.48
1:E:486:ILE:HG23	1:E:487:LEU:H	1.78	0.48
1:B:456:LEU:HB3	1:B:496:TRP:HB3	1.95	0.47
1:E:175:ASP:OD1	1:E:214:SER:OG	2.29	0.47
1:E:424:THR:HG23	1:E:500:ARG:HG2	1.96	0.47
1:A:368:ALA:O	1:A:369:ALA:CB	2.62	0.47
1:B:354:ILE:N	1:B:358:ALA:HB1	2.29	0.47
1:B:435:ASP:OD1	1:B:493:ARG:HG2	2.14	0.47
1:D:456:LEU:HB3	1:D:496:TRP:HB3	1.95	0.47
1:F:435:ASP:OD1	1:F:493:ARG:CG	2.62	0.47
1:C:456:LEU:HB3	1:C:496:TRP:HB3	1.95	0.47
1:A:451:LEU:HA	1:A:451:LEU:HD23	1.57	0.47
1:C:417:ASN:OD1	1:C:418:GLU:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:THR:HG23	1:B:500:ARG:HG2	1.97	0.47
1:E:432:ILE:N	1:E:493:ARG:CA	2.77	0.47
1:F:453:HIS:HE1	1:F:497:ASN:HD22	1.63	0.47
1:C:424:THR:HG23	1:C:500:ARG:HG2	1.96	0.47
1:F:456:LEU:HB3	1:F:496:TRP:HB3	1.97	0.47
1:D:354:ILE:H	1:D:358:ALA:HB2	1.79	0.47
1:F:424:THR:HG23	1:F:500:ARG:HG2	1.97	0.47
1:B:12:TYR:HE2	1:C:12:TYR:CE2	2.32	0.47
1:B:479:LYS:O	1:B:480:SER:CB	2.62	0.47
1:C:293:TRP:O	1:C:294:ASN:HB2	2.15	0.47
1:A:305:ASN:O	1:A:309:ASN:CB	2.57	0.47
1:B:51:ARG:NH2	1:B:367:GLY:HA3	2.29	0.47
1:E:431:ASN:N	1:E:431:ASN:OD1	2.46	0.47
1:A:351:ALA:HA	1:A:352:GLN:HA	1.69	0.46
1:D:256:LEU:O	1:D:430:ARG:NH1	2.48	0.46
1:D:293:TRP:O	1:D:294:ASN:HB2	2.15	0.46
1:F:293:TRP:O	1:F:294:ASN:HB2	2.14	0.46
1:A:429:ASN:O	1:A:494:ALA:N	2.48	0.46
1:A:424:THR:HG23	1:A:500:ARG:HG2	1.97	0.46
1:D:309:ASN:HD22	1:D:310:GLU:CG	2.28	0.46
1:D:453:HIS:CE1	1:D:499:ILE:HG12	2.51	0.46
1:D:354:ILE:N	1:D:358:ALA:HB1	2.31	0.46
1:D:429:ASN:O	1:D:494:ALA:HA	2.16	0.46
1:F:431:ASN:ND2	1:F:434:GLU:HG2	2.29	0.46
1:A:354:ILE:H	1:A:358:ALA:CB	2.28	0.46
1:A:453:HIS:CE1	1:A:499:ILE:HG12	2.51	0.46
1:C:353:LEU:HB3	1:C:354:ILE:HG13	1.98	0.46
1:C:449:ARG:O	1:C:501:ILE:HG23	2.14	0.46
1:F:351:ALA:HA	1:F:352:GLN:HA	1.68	0.46
1:C:431:ASN:C	1:C:433:HIS:H	2.16	0.46
1:D:306:ILE:HG21	1:D:318:LEU:CD2	2.45	0.46
1:D:424:THR:HG23	1:D:500:ARG:HG2	1.97	0.46
1:E:203:ASP:O	1:E:206:ILE:HG12	2.16	0.46
1:B:203:ASP:O	1:B:206:ILE:HG12	2.16	0.46
1:E:293:TRP:O	1:E:294:ASN:HB2	2.14	0.46
1:E:479:LYS:O	1:E:480:SER:HB3	2.14	0.46
1:F:481:SER:OG	1:F:481:SER:O	2.34	0.46
1:B:432:ILE:O	1:B:432:ILE:HD13	2.16	0.46
1:C:106:GLY:O	1:C:108:ASN:N	2.49	0.46
1:D:429:ASN:CA	1:D:430:ARG:CB	2.52	0.46
1:D:431:ASN:C	1:D:433:HIS:H	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:203:ASP:O	1:F:206:ILE:HG12	2.16	0.46
1:B:453:HIS:CE1	1:B:499:ILE:HG12	2.51	0.45
1:C:432:ILE:HD13	1:C:432:ILE:O	2.16	0.45
1:C:354:ILE:N	1:C:358:ALA:HB1	2.31	0.45
1:C:428:VAL:CG1	1:C:429:ASN:N	2.79	0.45
1:D:484:ASP:HA	1:D:485:GLY:HA2	1.53	0.45
1:A:106:GLY:O	1:A:108:ASN:N	2.49	0.45
1:A:203:ASP:O	1:A:206:ILE:HG12	2.16	0.45
1:E:479:LYS:O	1:E:480:SER:CB	2.64	0.45
1:D:106:GLY:O	1:D:108:ASN:N	2.49	0.45
1:D:363:GLU:HB2	1:D:367:GLY:C	2.37	0.45
1:D:447:ASP:CA	1:D:448:TYR:HB2	2.47	0.45
1:E:453:HIS:CE1	1:E:499:ILE:HG12	2.52	0.45
1:A:431:ASN:OD1	1:A:431:ASN:C	2.53	0.45
1:B:311:PRO:HB2	1:B:312:TRP:CD1	2.51	0.45
1:B:430:ARG:O	1:B:430:ARG:HG3	2.16	0.45
1:C:453:HIS:CE1	1:C:499:ILE:HG12	2.51	0.45
1:B:7:THR:HG23	1:B:393:VAL:HB	1.92	0.45
1:D:203:ASP:O	1:D:206:ILE:HG12	2.17	0.45
1:C:478:ASP:CG	1:C:479:LYS:CB	2.81	0.45
1:D:7:THR:O	1:D:8:VAL:HG22	2.17	0.45
1:F:453:HIS:CE1	1:F:499:ILE:HG12	2.52	0.45
1:A:429:ASN:O	1:A:494:ALA:CA	2.63	0.45
1:B:168:TRP:HB2	1:B:208:LEU:HD23	1.99	0.45
1:C:203:ASP:O	1:C:206:ILE:HG12	2.17	0.45
1:C:325:PHE:CZ	1:C:457:GLU:HA	2.52	0.45
1:D:306:ILE:CG2	1:D:318:LEU:HD21	2.46	0.45
1:B:381:ALA:HA	1:B:426:PHE:CE2	2.52	0.44
1:E:325:PHE:CZ	1:E:457:GLU:HA	2.53	0.44
1:F:432:ILE:O	1:F:432:ILE:HD13	2.18	0.44
1:E:106:GLY:O	1:E:108:ASN:N	2.50	0.44
1:F:106:GLY:O	1:F:108:ASN:N	2.50	0.44
1:A:429:ASN:C	1:A:431:ASN:N	2.70	0.44
1:B:351:ALA:HA	1:B:352:GLN:HA	1.68	0.44
1:E:429:ASN:C	1:E:431:ASN:H	2.17	0.44
1:F:487:LEU:HG	1:F:488:THR:CA	2.47	0.44
1:A:325:PHE:CZ	1:A:457:GLU:HA	2.53	0.44
1:A:168:TRP:HB2	1:A:208:LEU:HD23	2.00	0.44
1:C:444:GLY:HA3	1:C:445:MET:HB3	1.93	0.44
1:E:450:LEU:HD22	1:E:481:SER:CA	2.43	0.44
1:B:306:ILE:O	1:B:306:ILE:HG23	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:TRP:HB2	1:C:208:LEU:HD23	2.00	0.44
1:D:309:ASN:HD22	1:D:310:GLU:CD	2.20	0.44
1:C:398:LEU:HD13	1:C:406:ASP:HB3	1.98	0.44
1:D:168:TRP:HB2	1:D:208:LEU:HD23	2.00	0.44
1:D:365:ASN:OD1	1:D:365:ASN:N	2.51	0.44
1:E:168:TRP:HB2	1:E:208:LEU:HD23	2.00	0.44
1:F:325:PHE:CZ	1:F:457:GLU:HA	2.53	0.44
1:A:431:ASN:O	1:A:431:ASN:CG	2.55	0.44
1:B:429:ASN:OD1	1:B:431:ASN:HB3	2.18	0.44
1:C:417:ASN:CA	1:C:418:GLU:CB	2.93	0.44
1:C:451:LEU:HD12	1:C:502:GLY:N	2.33	0.44
1:C:478:ASP:HA	1:C:479:LYS:CG	2.48	0.44
1:D:381:ALA:HA	1:D:426:PHE:CE2	2.53	0.44
1:B:12:TYR:CE2	1:C:12:TYR:HE2	2.33	0.43
1:C:339:MET:CE	1:C:413:VAL:HG11	2.48	0.43
1:D:325:PHE:CZ	1:D:457:GLU:HA	2.53	0.43
1:F:168:TRP:HB2	1:F:208:LEU:HD23	2.00	0.43
1:F:381:ALA:HA	1:F:426:PHE:CE2	2.53	0.43
1:F:481:SER:O	1:F:488:THR:CA	2.66	0.43
1:A:381:ALA:HA	1:A:426:PHE:CE2	2.54	0.43
1:C:381:ALA:HA	1:C:426:PHE:CE2	2.54	0.43
1:E:486:ILE:CG2	1:E:487:LEU:H	2.29	0.43
1:A:452:GLU:OE2	1:A:500:ARG:NH1	2.52	0.43
1:D:309:ASN:HB3	1:D:310:GLU:HG3	2.00	0.43
1:E:364:ARG:O	1:E:365:ASN:C	2.56	0.43
1:E:478:ASP:HA	1:E:479:LYS:CB	2.49	0.43
1:B:325:PHE:CZ	1:B:457:GLU:HA	2.53	0.43
1:B:478:ASP:HA	1:B:479:LYS:CB	2.49	0.43
1:F:4:ALA:O	1:F:439:VAL:N	2.45	0.43
1:A:354:ILE:H	1:A:358:ALA:HB2	1.83	0.42
1:B:450:LEU:CD1	1:B:452:GLU:N	2.81	0.42
1:B:478:ASP:CA	1:B:479:LYS:CB	2.97	0.42
1:E:478:ASP:CA	1:E:479:LYS:CB	2.97	0.42
1:C:417:ASN:OD1	1:C:417:ASN:C	2.57	0.42
1:A:354:ILE:N	1:A:358:ALA:HB1	2.34	0.42
1:D:100:ILE:HG13	1:D:312:TRP:O	2.18	0.42
1:F:380:HIS:HD2	1:F:496:TRP:NE1	2.17	0.42
1:C:451:LEU:HD12	1:C:501:ILE:CA	2.49	0.42
1:B:353:LEU:CB	1:B:354:ILE:CG1	2.97	0.42
1:A:63:VAL:HA	1:A:64:PRO:HD3	1.92	0.42
1:D:435:ASP:OD1	1:D:493:ARG:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:HIS:HA	1:F:145:PRO:HD3	1.95	0.42
1:A:458:HIS:CD2	1:A:460:ASP:H	2.36	0.42
1:D:351:ALA:HA	1:D:352:GLN:HA	1.69	0.42
1:E:381:ALA:HA	1:E:426:PHE:CE2	2.54	0.42
1:E:458:HIS:CD2	1:E:460:ASP:H	2.36	0.42
1:F:429:ASN:O	1:F:494:ALA:HA	2.19	0.42
1:E:309:ASN:O	1:E:310:GLU:HG2	2.20	0.42
1:C:417:ASN:CB	1:C:418:GLU:HG2	2.50	0.42
1:D:15:ALA:HB2	1:D:343:ASP:HB3	2.02	0.42
1:A:431:ASN:O	1:A:434:GLU:O	2.37	0.41
1:A:482:PHE:HD1	1:A:482:PHE:HA	1.68	0.41
1:D:114:CYS:HA	1:D:117:VAL:HG22	2.01	0.41
1:D:368:ALA:O	1:D:369:ALA:HB3	2.19	0.41
1:E:366:GLY:HA3	1:E:367:GLY:HA2	1.37	0.41
1:B:214:SER:O	1:B:242:HIS:HB2	2.20	0.41
1:C:241:LEU:C	1:C:242:HIS:HD2	2.23	0.41
1:F:458:HIS:CD2	1:F:460:ASP:H	2.36	0.41
1:A:10:LYS:H	1:A:10:LYS:HG3	1.62	0.41
1:A:380:HIS:HD2	1:A:496:TRP:NE1	2.16	0.41
1:B:434:GLU:C	1:B:493:ARG:HB3	2.41	0.41
1:D:431:ASN:O	1:D:433:HIS:N	2.38	0.41
1:A:214:SER:O	1:A:242:HIS:HB2	2.21	0.41
1:E:214:SER:O	1:E:242:HIS:HB2	2.20	0.41
1:F:114:CYS:HA	1:F:117:VAL:HG22	2.01	0.41
1:B:15:ALA:HB2	1:B:343:ASP:HB3	2.02	0.41
1:C:214:SER:O	1:C:242:HIS:HB2	2.20	0.41
1:C:409:ASP:O	1:C:430:ARG:HB3	2.21	0.41
1:E:241:LEU:C	1:E:242:HIS:HD2	2.24	0.41
1:F:214:SER:O	1:F:242:HIS:HB2	2.20	0.41
1:A:114:CYS:HA	1:A:117:VAL:HG22	2.01	0.41
1:D:214:SER:O	1:D:242:HIS:HB2	2.21	0.41
1:A:369:ALA:O	1:A:370:TRP:HB3	2.19	0.41
1:C:15:ALA:HB2	1:C:343:ASP:HB3	2.02	0.41
1:D:10:LYS:HD2	1:D:11:ASP:OD1	2.21	0.41
1:F:306:ILE:O	1:F:306:ILE:HG22	2.21	0.41
1:A:7:THR:HG21	1:A:393:VAL:HG12	2.01	0.41
1:A:431:ASN:CA	1:A:432:ILE:CG2	2.30	0.41
1:C:461:LEU:HD12	1:C:461:LEU:HA	1.88	0.41
1:E:432:ILE:N	1:E:493:ARG:CB	2.64	0.41
1:C:144:HIS:HA	1:C:145:PRO:HD3	1.96	0.40
1:D:380:HIS:HD2	1:D:496:TRP:NE1	2.15	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ALA:HB2	1:A:343:ASP:HB3	2.02	0.40
1:B:114:CYS:HA	1:B:117:VAL:HG22	2.02	0.40
1:C:368:ALA:O	1:C:369:ALA:HB3	2.21	0.40
1:D:63:VAL:HA	1:D:64:PRO:HD3	1.92	0.40
1:E:15:ALA:HB2	1:E:343:ASP:HB3	2.02	0.40
1:E:63:VAL:HA	1:E:64:PRO:HD3	1.92	0.40
1:E:114:CYS:HA	1:E:117:VAL:HG22	2.02	0.40
1:E:451:LEU:O	1:E:452:GLU:HB3	2.21	0.40
1:A:353:LEU:HG	1:A:354:ILE:HG12	2.03	0.40
1:C:114:CYS:HA	1:C:117:VAL:HG22	2.02	0.40
1:C:311:PRO:HB2	1:C:312:TRP:CD1	2.56	0.40
1:C:351:ALA:HA	1:C:352:GLN:HA	1.68	0.40
1:C:451:LEU:CD1	1:C:502:GLY:N	2.84	0.40
1:D:241:LEU:C	1:D:242:HIS:HD2	2.25	0.40
1:D:477:SER:HB2	1:D:478:ASP:OD1	2.21	0.40
1:A:433:HIS:HB3	1:A:434:GLU:HG3	2.02	0.40
1:C:353:LEU:O	1:C:354:ILE:HG12	2.20	0.40
1:E:477:SER:HB2	1:E:478:ASP:OD1	2.22	0.40
1:D:431:ASN:C	1:D:432:ILE:HG22	2.42	0.40
1:F:431:ASN:HD21	1:F:434:GLU:HG2	1.81	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	490/513 (96%)	445 (91%)	26 (5%)	19 (4%)	3	6
1	B	493/513 (96%)	440 (89%)	28 (6%)	25 (5%)	2	3
1	C	493/513 (96%)	438 (89%)	30 (6%)	25 (5%)	2	3
1	D	497/513 (97%)	445 (90%)	31 (6%)	21 (4%)	3	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	484/513 (94%)	438 (90%)	27 (6%)	19 (4%)	3	6
1	F	490/513 (96%)	442 (90%)	27 (6%)	21 (4%)	2	5
All	All	2947/3078 (96%)	2648 (90%)	169 (6%)	130 (4%)	2	5

All (130) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	TRP
1	A	309	ASN
1	A	310	GLU
1	A	354	ILE
1	A	365	ASN
1	A	370	TRP
1	A	430	ARG
1	A	432	ILE
1	A	434	GLU
1	A	478	ASP
1	B	46	ASP
1	B	108	ASN
1	B	224	TRP
1	B	305	ASN
1	B	309	ASN
1	B	313	ARG
1	B	354	ILE
1	B	365	ASN
1	B	430	ARG
1	B	433	HIS
1	B	479	LYS
1	B	480	SER
1	B	481	SER
1	B	490	MET
1	C	224	TRP
1	C	313	ARG
1	C	354	ILE
1	C	419	GLU
1	C	430	ARG
1	C	432	ILE
1	C	451	LEU
1	C	478	ASP
1	C	479	LYS
1	C	480	SER

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Mol	Chain	Res	Type
1	C	481	SER
1	C	486	ILE
1	D	8	VAL
1	D	224	TRP
1	D	310	GLU
1	D	313	ARG
1	D	354	ILE
1	D	365	ASN
1	D	432	ILE
1	D	446	LYS
1	D	478	ASP
1	D	479	LYS
1	D	480	SER
1	E	365	ASN
1	E	430	ARG
1	E	432	ILE
1	E	479	LYS
1	E	480	SER
1	F	5	ARG
1	F	365	ASN
1	F	430	ARG
1	F	478	ASP
1	F	488	THR
1	A	107	ILE
1	A	363	GLU
1	B	107	ILE
1	B	363	GLU
1	B	369	ALA
1	B	478	ASP
1	C	107	ILE
1	C	309	ASN
1	C	364	ARG
1	C	365	ASN
1	C	420	LYS
1	C	470	GLU
1	D	363	GLU
1	D	470	GLU
1	E	309	ASN
1	E	310	GLU
1	E	313	ARG
1	E	469	GLY
1	E	470	GLU

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Mol	Chain	Res	Type
1	E	478	ASP
1	F	309	ASN
1	F	310	GLU
1	F	313	ARG
1	F	364	ARG
1	F	470	GLU
1	A	364	ARG
1	A	484	ASP
1	B	307	MET
1	B	308	GLN
1	B	494	ALA
1	C	363	GLU
1	C	369	ALA
1	C	418	GLU
1	D	107	ILE
1	D	312	TRP
1	D	369	ALA
1	E	107	ILE
1	E	363	GLU
1	E	364	ARG
1	E	369	ALA
1	F	107	ILE
1	F	363	GLU
1	F	369	ALA
1	F	494	ALA
1	A	297	TYR
1	A	366	GLY
1	A	369	ALA
1	A	494	ALA
1	B	364	ARG
1	C	297	TYR
1	C	494	ALA
1	D	364	ARG
1	D	494	ALA
1	E	297	TYR
1	E	494	ALA
1	F	432	ILE
1	F	433	HIS
1	F	485	GLY
1	A	357	ILE
1	B	297	TYR
1	B	357	ILE

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Mol	Chain	Res	Type
1	C	357	ILE
1	D	297	TYR
1	D	357	ILE
1	D	449	ARG
1	E	357	ILE
1	F	297	TYR
1	F	357	ILE
1	B	469	GLY
1	C	310	GLU
1	F	469	GLY
1	E	354	ILE
1	F	354	ILE

5.3.2 Protein sidechains ⓘ

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	428/450 (95%)	400 (94%)	28 (6%)	17	38
1	B	427/450 (95%)	397 (93%)	30 (7%)	15	35
1	C	428/450 (95%)	395 (92%)	33 (8%)	13	30
1	D	428/450 (95%)	400 (94%)	28 (6%)	17	38
1	E	415/450 (92%)	392 (94%)	23 (6%)	21	46
1	F	425/450 (94%)	396 (93%)	29 (7%)	16	36
All	All	2551/2700 (94%)	2380 (93%)	171 (7%)	16	37

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	12	TYR
1	A	13	LYS
1	A	44	LYS
1	A	47	GLU
1	A	73	PHE

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Mol	Chain	Res	Type
1	A	87	GLU
1	A	98	LYS
1	A	107	ILE
1	A	160	LYS
1	A	179	GLN
1	A	290	PHE
1	A	365	ASN
1	A	395	ASN
1	A	410	ILE
1	A	413	VAL
1	A	415	ILE
1	A	418	GLU
1	A	430	ARG
1	A	432	ILE
1	A	445	MET
1	A	463	ILE
1	A	470	GLU
1	A	477	SER
1	A	482	PHE
1	A	483	ASP
1	A	484	ASP
1	A	488	THR
1	B	10	LYS
1	B	12	TYR
1	B	13	LYS
1	B	44	LYS
1	B	46	ASP
1	B	47	GLU
1	B	87	GLU
1	B	98	LYS
1	B	107	ILE
1	B	160	LYS
1	B	179	GLN
1	B	290	PHE
1	B	364	ARG
1	B	365	ASN
1	B	393	VAL
1	B	395	ASN
1	B	410	ILE
1	B	413	VAL
1	B	415	ILE
1	B	430	ARG

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Mol	Chain	Res	Type
1	B	432	ILE
1	B	443	ARG
1	B	445	MET
1	B	449	ARG
1	B	450	LEU
1	B	459	GLN
1	B	463	ILE
1	B	468	ASN
1	B	480	SER
1	B	493	ARG
1	C	12	TYR
1	C	13	LYS
1	C	44	LYS
1	C	47	GLU
1	C	87	GLU
1	C	98	LYS
1	C	107	ILE
1	C	160	LYS
1	C	179	GLN
1	C	290	PHE
1	C	308	GLN
1	C	365	ASN
1	C	393	VAL
1	C	395	ASN
1	C	410	ILE
1	C	413	VAL
1	C	415	ILE
1	C	419	GLU
1	C	432	ILE
1	C	434	GLU
1	C	442	VAL
1	C	449	ARG
1	C	451	LEU
1	C	459	GLN
1	C	461	LEU
1	C	463	ILE
1	C	468	ASN
1	C	470	GLU
1	C	477	SER
1	C	480	SER
1	C	483	ASP
1	C	492	ARG

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Mol	Chain	Res	Type
1	C	493	ARG
1	D	7	THR
1	D	10	LYS
1	D	12	TYR
1	D	13	LYS
1	D	44	LYS
1	D	47	GLU
1	D	87	GLU
1	D	98	LYS
1	D	107	ILE
1	D	160	LYS
1	D	179	GLN
1	D	290	PHE
1	D	306	ILE
1	D	354	ILE
1	D	365	ASN
1	D	395	ASN
1	D	410	ILE
1	D	413	VAL
1	D	415	ILE
1	D	429	ASN
1	D	430	ARG
1	D	432	ILE
1	D	445	MET
1	D	459	GLN
1	D	463	ILE
1	D	468	ASN
1	D	470	GLU
1	D	480	SER
1	E	8	VAL
1	E	12	TYR
1	E	13	LYS
1	E	44	LYS
1	E	47	GLU
1	E	87	GLU
1	E	98	LYS
1	E	107	ILE
1	E	160	LYS
1	E	179	GLN
1	E	290	PHE
1	E	365	ASN
1	E	395	ASN

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Mol	Chain	Res	Type
1	E	410	ILE
1	E	413	VAL
1	E	415	ILE
1	E	432	ILE
1	E	451	LEU
1	E	463	ILE
1	E	468	ASN
1	E	470	GLU
1	E	480	SER
1	E	486	ILE
1	F	12	TYR
1	F	13	LYS
1	F	44	LYS
1	F	47	GLU
1	F	87	GLU
1	F	98	LYS
1	F	107	ILE
1	F	160	LYS
1	F	179	GLN
1	F	290	PHE
1	F	310	GLU
1	F	365	ASN
1	F	395	ASN
1	F	398	LEU
1	F	410	ILE
1	F	413	VAL
1	F	415	ILE
1	F	430	ARG
1	F	432	ILE
1	F	446	LYS
1	F	449	ARG
1	F	461	LEU
1	F	463	ILE
1	F	468	ASN
1	F	470	GLU
1	F	481	SER
1	F	484	ASP
1	F	489	SER
1	F	493	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	242	HIS
1	A	243	GLN
1	A	380	HIS
1	A	458	HIS
1	B	72	ASN
1	B	242	HIS
1	B	243	GLN
1	B	380	HIS
1	B	433	HIS
1	B	458	HIS
1	C	242	HIS
1	C	243	GLN
1	C	308	GLN
1	C	309	ASN
1	C	380	HIS
1	C	431	ASN
1	C	458	HIS
1	D	242	HIS
1	D	243	GLN
1	D	309	ASN
1	D	380	HIS
1	D	458	HIS
1	E	72	ASN
1	E	242	HIS
1	E	243	GLN
1	E	380	HIS
1	E	458	HIS
1	E	468	ASN
1	F	72	ASN
1	F	242	HIS
1	F	243	GLN
1	F	380	HIS
1	F	431	ASN
1	F	433	HIS
1	F	453	HIS
1	F	458	HIS
1	F	497	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

16 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
2	AHR	G	1	2	10,10,10	0.58	0	13,14,14	1.33	3 (23%)
2	AHR	G	2	2	9,9,10	0.51	0	10,12,14	1.24	1 (10%)
2	AHR	G	3	2	9,9,10	1.64	1 (11%)	10,12,14	1.76	3 (30%)
3	AHR	H	1	3	10,10,10	0.53	0	13,14,14	1.30	2 (15%)
3	AHR	H	2	3	9,9,10	1.65	1 (11%)	10,12,14	1.73	3 (30%)
2	AHR	I	1	2	10,10,10	0.60	0	13,14,14	1.23	2 (15%)
2	AHR	I	2	2	9,9,10	0.54	0	10,12,14	1.27	1 (10%)
2	AHR	I	3	2	9,9,10	1.65	1 (11%)	10,12,14	1.69	3 (30%)
2	AHR	J	1	2	10,10,10	0.60	0	13,14,14	1.32	2 (15%)
2	AHR	J	2	2	9,9,10	0.57	0	10,12,14	1.31	1 (10%)
2	AHR	J	3	2	9,9,10	1.64	1 (11%)	10,12,14	1.70	3 (30%)
2	AHR	K	1	2	10,10,10	0.57	0	13,14,14	1.37	2 (15%)
2	AHR	K	2	2	9,9,10	0.66	0	10,12,14	1.37	1 (10%)
2	AHR	K	3	2	9,9,10	1.64	1 (11%)	10,12,14	1.68	2 (20%)
3	AHR	L	1	3	10,10,10	0.56	0	13,14,14	1.29	2 (15%)
3	AHR	L	2	3	9,9,10	1.62	1 (11%)	10,12,14	1.71	3 (30%)

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
2	AHR	G	1	2	-	0/2/18/18	0/1/1/1
2	AHR	G	2	2	-	2/2/15/18	0/1/1/1
2	AHR	G	3	2	-	0/2/15/18	0/1/1/1
3	AHR	H	1	3	-	2/2/18/18	0/1/1/1
3	AHR	H	2	3	-	0/2/15/18	0/1/1/1
2	AHR	I	1	2	-	1/2/18/18	0/1/1/1
2	AHR	I	2	2	-	2/2/15/18	0/1/1/1
2	AHR	I	3	2	-	0/2/15/18	0/1/1/1
2	AHR	J	1	2	-	2/2/18/18	0/1/1/1
2	AHR	J	2	2	-	2/2/15/18	0/1/1/1
2	AHR	J	3	2	-	0/2/15/18	0/1/1/1
2	AHR	K	1	2	-	2/2/18/18	0/1/1/1
2	AHR	K	2	2	-	2/2/15/18	0/1/1/1
2	AHR	K	3	2	-	0/2/15/18	0/1/1/1
3	AHR	L	1	3	-	2/2/18/18	0/1/1/1
3	AHR	L	2	3	-	0/2/15/18	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	3	AHR	O5-C5	-4.72	1.22	1.42
2	I	3	AHR	O5-C5	-4.70	1.22	1.42
3	H	2	AHR	O5-C5	-4.70	1.22	1.42
2	J	3	AHR	O5-C5	-4.70	1.22	1.42
2	K	3	AHR	O5-C5	-4.67	1.22	1.42
3	L	2	AHR	O5-C5	-4.65	1.22	1.42

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	2	AHR	O5-C5-C4	3.18	122.20	111.29
2	G	3	AHR	O4-C4-C3	3.17	107.51	104.70
2	K	3	AHR	O5-C5-C4	3.17	122.16	111.29
2	I	3	AHR	O4-C4-C3	3.16	107.50	104.70
2	K	3	AHR	O4-C4-C3	3.15	107.50	104.70
2	J	3	AHR	O5-C5-C4	3.14	122.08	111.29
3	H	2	AHR	O5-C5-C4	3.13	122.04	111.29
2	J	3	AHR	O4-C4-C3	3.10	107.45	104.70
2	G	3	AHR	O5-C5-C4	3.09	121.91	111.29
2	I	3	AHR	O5-C5-C4	3.04	121.71	111.29
3	H	2	AHR	O4-C4-C3	2.96	107.33	104.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	2	AHR	O4-C4-C3	2.94	107.30	104.70
2	I	1	AHR	C1-C2-C3	2.93	105.97	102.30
2	J	1	AHR	C1-C2-C3	2.93	105.97	102.30
2	G	1	AHR	C1-C2-C3	2.87	105.89	102.30
2	K	1	AHR	O4-C1-C2	2.80	107.90	104.46
2	K	1	AHR	C1-C2-C3	2.78	105.78	102.30
2	J	2	AHR	C1-C2-C3	2.77	105.85	101.63
2	K	2	AHR	C1-C2-C3	2.73	105.79	101.63
2	G	1	AHR	O4-C1-C2	2.73	107.82	104.46
3	H	1	AHR	C1-C2-C3	2.69	105.67	102.30
3	L	1	AHR	C1-C2-C3	2.67	105.64	102.30
2	J	1	AHR	O4-C1-C2	2.64	107.71	104.46
2	G	2	AHR	C1-C2-C3	2.60	105.59	101.63
2	I	2	AHR	C1-C2-C3	2.57	105.54	101.63
2	G	3	AHR	C1-C2-C3	2.46	105.38	101.63
3	H	2	AHR	C1-C2-C3	2.41	105.29	101.63
2	I	1	AHR	O4-C1-C2	2.34	107.34	104.46
3	L	2	AHR	C1-C2-C3	2.23	105.03	101.63
3	H	1	AHR	O4-C1-C2	2.17	107.13	104.46
2	I	3	AHR	C1-C2-C3	2.11	104.85	101.63
2	G	1	AHR	C2-C3-C4	2.11	106.74	102.64
3	L	1	AHR	O4-C1-C2	2.06	107.00	104.46
2	J	3	AHR	C1-C2-C3	2.02	104.71	101.63

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	1	AHR	O4-C4-C5-O5
2	G	2	AHR	O4-C4-C5-O5
2	I	2	AHR	O4-C4-C5-O5
2	J	2	AHR	O4-C4-C5-O5
2	K	2	AHR	O4-C4-C5-O5
3	H	1	AHR	O4-C4-C5-O5
3	L	1	AHR	O4-C4-C5-O5
2	K	1	AHR	C3-C4-C5-O5
2	K	2	AHR	C3-C4-C5-O5
2	I	2	AHR	C3-C4-C5-O5
2	G	2	AHR	C3-C4-C5-O5
2	J	2	AHR	C3-C4-C5-O5
3	H	1	AHR	C3-C4-C5-O5
3	L	1	AHR	C3-C4-C5-O5

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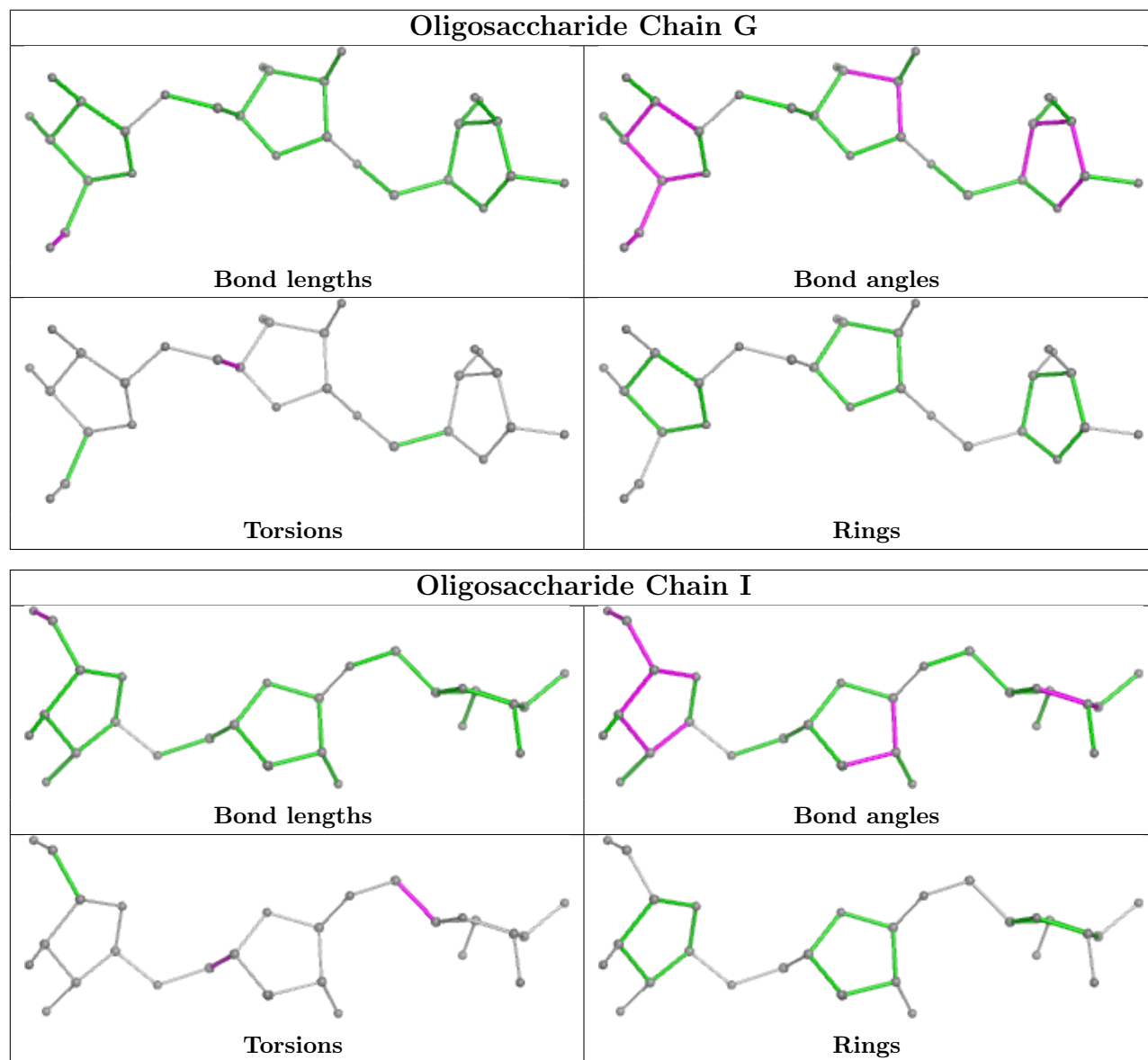
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Mol	Chain	Res	Type	Atoms
2	J	1	AHR	C3-C4-C5-O5
2	J	1	AHR	O4-C4-C5-O5
2	I	1	AHR	C3-C4-C5-O5

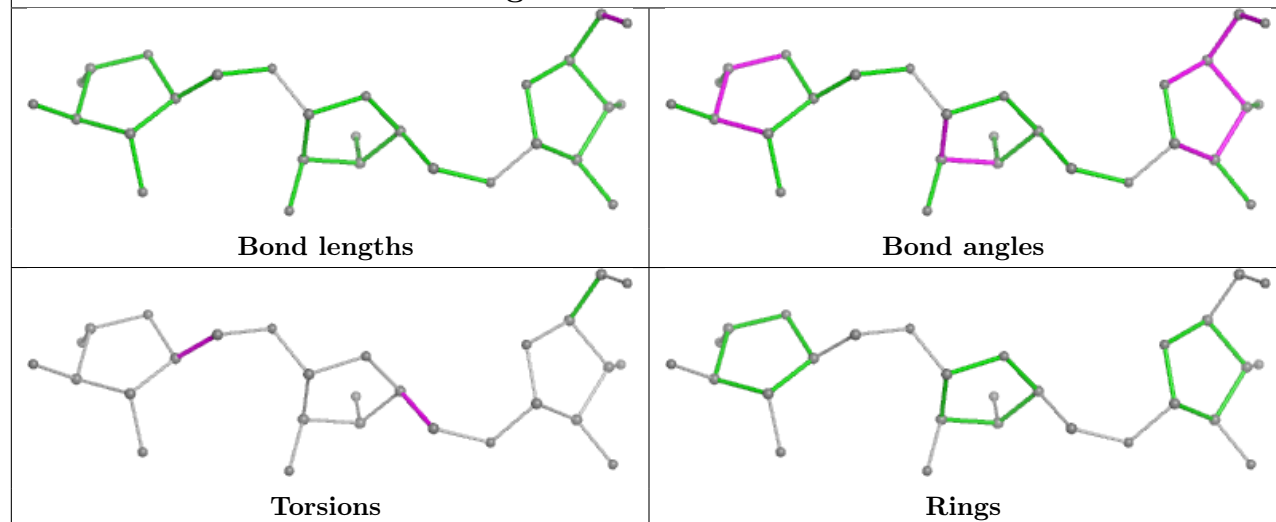
There are no ring outliers.

No monomer is involved in short contacts.

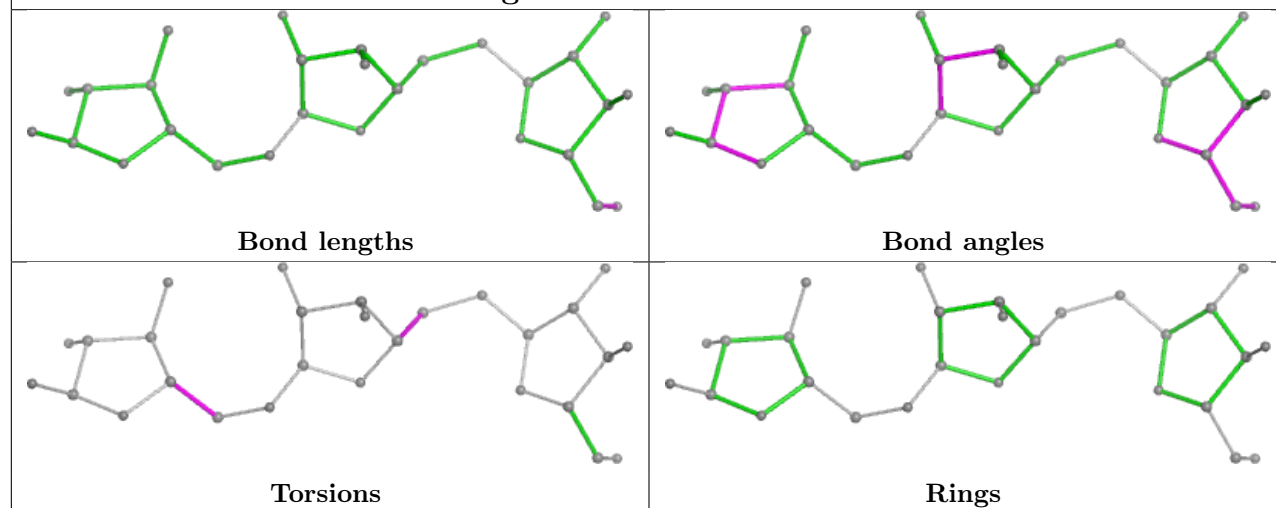
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

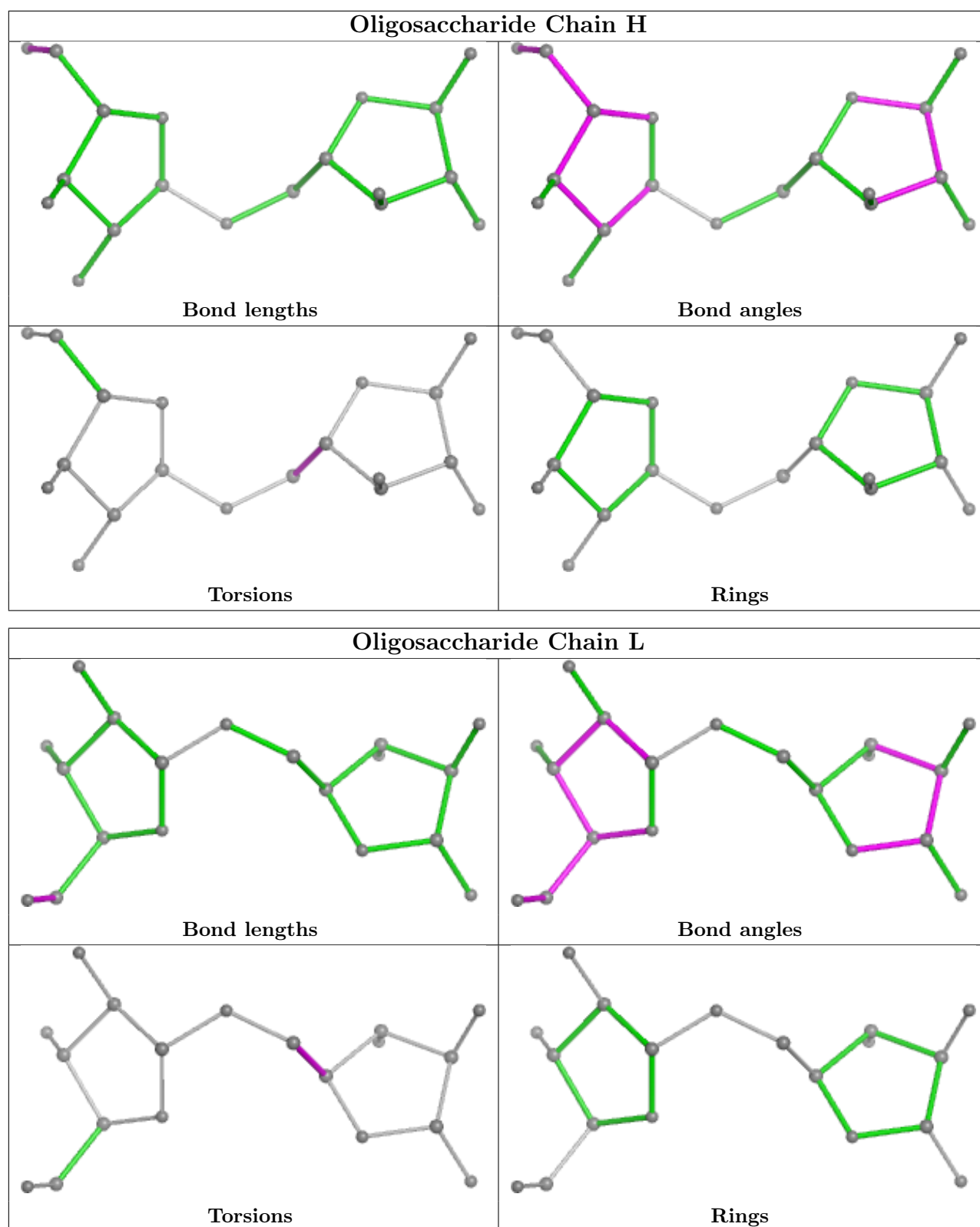


Oligosaccharide Chain J



Oligosaccharide Chain K





5.6 Ligand geometry [i](#)

9 ligands 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	EDO	A	604	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	E	604	-	3,3,3	0.50	0	2,2,2	0.25	0
4	EDO	E	605	-	3,3,3	0.57	0	2,2,2	0.41	0
4	EDO	C	604	-	3,3,3	0.45	0	2,2,2	0.36	0
4	EDO	A	606	-	3,3,3	0.49	0	2,2,2	0.27	0
4	EDO	F	603	-	3,3,3	0.81	0	2,2,2	0.68	0
4	EDO	B	603	-	3,3,3	0.51	0	2,2,2	0.21	0
4	EDO	A	605	-	3,3,3	0.49	0	2,2,2	0.23	0
4	EDO	D	604	-	3,3,3	0.46	0	2,2,2	0.35	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
4	EDO	A	604	-	-	0/1/1/1	-
4	EDO	E	604	-	-	0/1/1/1	-
4	EDO	E	605	-	-	1/1/1/1	-
4	EDO	C	604	-	-	1/1/1/1	-
4	EDO	A	606	-	-	1/1/1/1	-
4	EDO	F	603	-	-	1/1/1/1	-
4	EDO	B	603	-	-	1/1/1/1	-
4	EDO	A	605	-	-	1/1/1/1	-
4	EDO	D	604	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	606	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	603	EDO	O1-C1-C2-O2
4	C	604	EDO	O1-C1-C2-O2
4	D	604	EDO	O1-C1-C2-O2
4	E	605	EDO	O1-C1-C2-O2
4	F	603	EDO	O1-C1-C2-O2
4	A	605	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.