



Full wwPDB X-ray Structure Validation Report i

May 25, 2020 – 09:23 am BST

PDB ID : 5XAZ
Title : Crystal structure of full length native tylp, a tetr regulator from streptomyces fradiae
Authors : Ray, S.; Panjikar, S.; Anand, R.
Deposited on : 2017-03-15
Resolution : 2.30 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 i symbol.

The following versions of software and data (see references ①) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

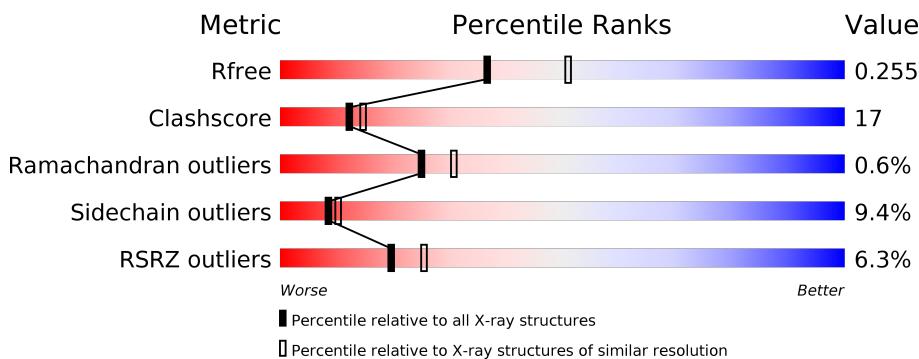
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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.



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Mol	Chain	Length	Quality of chain				
1	G	228	7%	66%	19%	7%	7%
1	H	228	5%	69%	19%	•	7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13820 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 Gamma-butyrolactone receptor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total 1709	C 1067	N 318	O 319	S 5	0	0	0
1	H	211	Total 1620	C 1015	N 296	O 304	S 5	0	0	0
1	B	223	Total 1709	C 1067	N 318	O 319	S 5	0	0	0
1	C	213	Total 1634	C 1024	N 299	O 306	S 5	0	0	0
1	D	220	Total 1702	C 1062	N 318	O 316	S 6	0	1	0
1	E	213	Total 1643	C 1030	N 304	O 304	S 5	0	1	0
1	F	222	Total 1701	C 1063	N 317	O 316	S 5	0	0	0
1	G	213	Total 1643	C 1030	N 304	O 304	S 5	0	1	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	ALA	ARG	engineered mutation	UNP Q9XCC7
A	227	LEU	-	expression tag	UNP Q9XCC7
A	228	GLU	-	expression tag	UNP Q9XCC7
A	229	HIS	-	expression tag	UNP Q9XCC7
H	113	ALA	ARG	engineered mutation	UNP Q9XCC7
H	227	LEU	-	expression tag	UNP Q9XCC7
H	228	GLU	-	expression tag	UNP Q9XCC7
H	229	HIS	-	expression tag	UNP Q9XCC7
B	113	ALA	ARG	engineered mutation	UNP Q9XCC7
B	227	LEU	-	expression tag	UNP Q9XCC7
B	228	GLU	-	expression tag	UNP Q9XCC7
B	229	HIS	-	expression tag	UNP Q9XCC7
C	113	ALA	ARG	engineered mutation	UNP Q9XCC7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	227	LEU	-	expression tag	UNP Q9XCC7
C	228	GLU	-	expression tag	UNP Q9XCC7
C	229	HIS	-	expression tag	UNP Q9XCC7
D	113	ALA	ARG	engineered mutation	UNP Q9XCC7
D	227	LEU	-	expression tag	UNP Q9XCC7
D	228	GLU	-	expression tag	UNP Q9XCC7
D	229	HIS	-	expression tag	UNP Q9XCC7
E	113	ALA	ARG	engineered mutation	UNP Q9XCC7
E	227	LEU	-	expression tag	UNP Q9XCC7
E	228	GLU	-	expression tag	UNP Q9XCC7
E	229	HIS	-	expression tag	UNP Q9XCC7
F	113	ALA	ARG	engineered mutation	UNP Q9XCC7
F	227	LEU	-	expression tag	UNP Q9XCC7
F	228	GLU	-	expression tag	UNP Q9XCC7
F	229	HIS	-	expression tag	UNP Q9XCC7
G	113	ALA	ARG	engineered mutation	UNP Q9XCC7
G	227	LEU	-	expression tag	UNP Q9XCC7
G	228	GLU	-	expression tag	UNP Q9XCC7
G	229	HIS	-	expression tag	UNP Q9XCC7

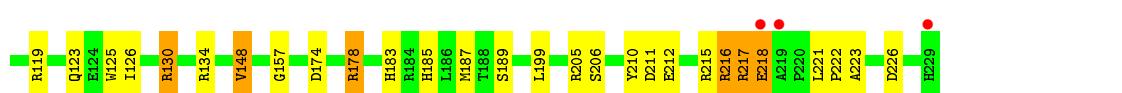
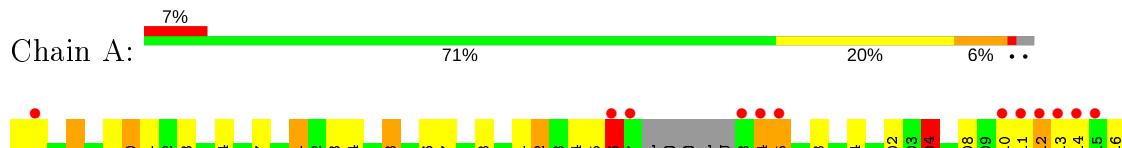
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	58	Total O 58 58	0	0
2	H	58	Total O 58 58	0	0
2	B	68	Total O 68 68	0	0
2	C	57	Total O 57 57	0	0
2	D	62	Total O 62 62	0	0
2	E	45	Total O 45 45	0	0
2	F	62	Total O 62 62	0	0
2	G	49	Total O 49 49	0	0

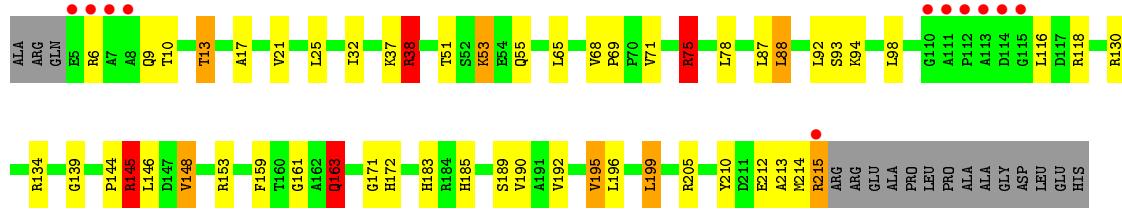
3 Residue-property plots [\(i\)](#)

These plots are drawn for all protein, RNA and DNA 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.

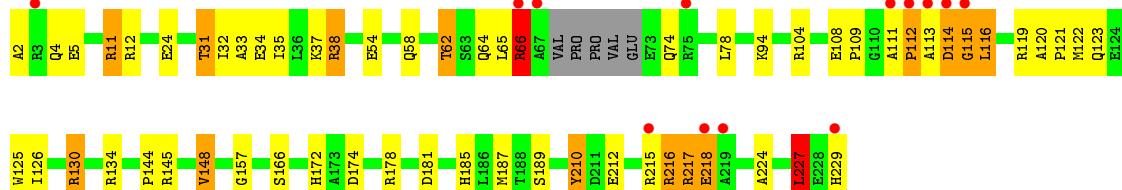
- Molecule 1: Gamma-butyrolactone receptor protein



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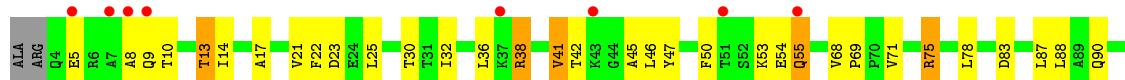


- Molecule 1: Gamma-butyrolactone receptor protein



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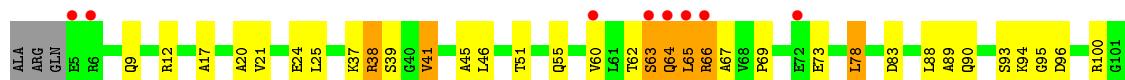




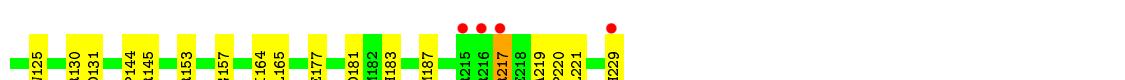
- Molecule 1: Gamma-butyrolactone receptor protein



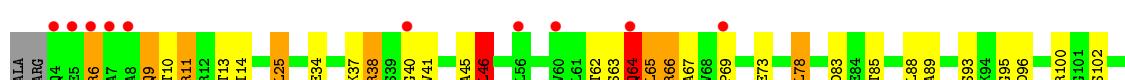
- Molecule 1: Gamma-butyrolactone receptor protein

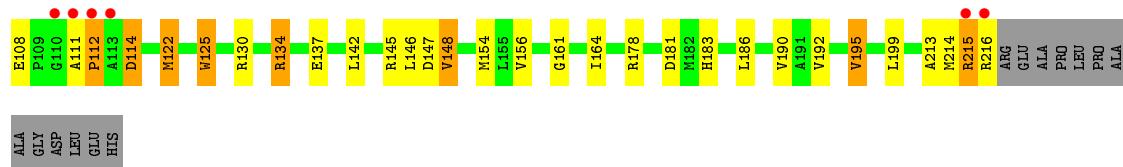


- Molecule 1: Gamma-butyrolactone receptor protein



- Molecule 1: Gamma-butyrolactone receptor protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.48Å 71.57Å 158.58Å 90.00° 102.92° 90.00°	Depositor
Resolution (Å)	19.81 – 2.30 19.81 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.81-2.30) 99.4 (19.81-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	3.08 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R , R_{free}	0.204 , 0.253 0.208 , 0.255	Depositor DCC
R_{free} test set	992 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.4	EDS
L-test for twinning ²	$< L > = 0.46$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13820	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.10 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.4642e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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 i

5.1 Standard geometry i

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	1.04	1/1731 (0.1%)	1.15	9/2343 (0.4%)
1	B	1.04	2/1731 (0.1%)	1.10	11/2343 (0.5%)
1	C	0.96	0/1656	1.04	7/2245 (0.3%)
1	D	0.96	1/1722 (0.1%)	1.11	8/2326 (0.3%)
1	E	0.99	1/1669 (0.1%)	1.09	10/2262 (0.4%)
1	F	0.98	3/1723 (0.2%)	1.08	10/2332 (0.4%)
1	G	1.00	1/1669 (0.1%)	1.11	12/2262 (0.5%)
1	H	0.89	0/1642	1.05	7/2227 (0.3%)
All	All	0.98	9/13543 (0.1%)	1.09	74/18340 (0.4%)

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	G	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	125	TRP	CD2-CE2	8.28	1.51	1.41
1	A	125	TRP	CD2-C \bar{E} 2	6.64	1.49	1.41
1	E	125	TRP	CD2-CE2	6.32	1.49	1.41
1	F	102	SER	CB-OG	-6.21	1.34	1.42
1	G	125	TRP	CD2-CE2	6.05	1.48	1.41
1	F	177	GLU	CD-OE2	5.93	1.32	1.25
1	B	125	TRP	CD2-C \bar{E} 2	5.37	1.47	1.41
1	D	102	SER	CB-OG	-5.24	1.35	1.42
1	B	210	TYR	CG-CD2	5.23	1.46	1.39

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	178	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	H	145	ARG	NE-CZ-NH1	-10.19	115.20	120.30
1	D	178	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	F	153	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	F	6	ARG	NE-CZ-NH1	-9.10	115.75	120.30
1	G	122	MET	CG-SD-CE	-9.00	85.80	100.20
1	E	178	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	E	111	ALA	C-N-CD	-8.72	101.43	120.60
1	C	153	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	D	104	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	B	12	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	D	104	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	G	114	ASP	CB-CG-OD2	8.18	125.67	118.30
1	A	104	ARG	NE-CZ-NH1	8.03	124.32	120.30
1	A	130	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	E	83	ASP	CB-CG-OD1	7.66	125.20	118.30
1	C	75	ARG	CG-CD-NE	-7.58	95.89	111.80
1	D	88	LEU	CB-CG-CD1	-7.33	98.54	111.00
1	A	119	ARG	NE-CZ-NH1	-7.30	116.65	120.30
1	G	114	ASP	CB-CG-OD1	-6.79	112.18	118.30
1	D	11	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	B	119	ARG	NE-CZ-NH1	-6.51	117.05	120.30
1	E	114	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	A	66	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	B	104	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	H	75	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	H	153	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	6	ARG	NE-CZ-NH1	-6.41	117.10	120.30
1	F	104	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	G	25	LEU	C-N-CA	-6.38	108.90	122.30
1	G	83	ASP	CB-CG-OD1	6.34	124.00	118.30
1	A	134	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	E	114	ASP	CB-CG-OD1	6.08	123.77	118.30
1	F	83	ASP	CB-CG-OD1	6.07	123.76	118.30
1	B	66	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	F	12	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	A	38	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	C	205	ARG	NE-CZ-NH1	-5.95	117.32	120.30
1	B	130	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	H	205	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	B	119	ARG	NE-CZ-NH2	5.79	123.20	120.30
1	G	46	LEU	CB-CG-CD1	5.75	120.78	111.00
1	F	165	LEU	CB-CG-CD1	-5.70	101.31	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	181	ASP	CB-CG-OD1	5.69	123.42	118.30
1	E	178	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	E	181	ASP	CB-CG-OD1	5.64	123.37	118.30
1	E	197	VAL	CG1-CB-CG2	5.59	119.84	110.90
1	B	11	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	G	11	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	12	ARG	CG-CD-NE	-5.48	100.30	111.80
1	G	46	LEU	CA-CB-CG	5.43	127.80	115.30
1	F	153	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	H	163	GLN	N-CA-CB	-5.35	100.98	110.60
1	E	78	LEU	CB-CG-CD1	5.33	120.06	111.00
1	G	145	ARG	CG-CD-NE	-5.30	100.67	111.80
1	B	181	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	F	6	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	C	198	ARG	NE-CZ-NH1	-5.27	117.67	120.30
1	G	147	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	C	214	MET	CG-SD-CE	5.24	108.58	100.20
1	F	104	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	D	12	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	217	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	134	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	D	104	ARG	CD-NE-CZ	5.17	130.84	123.60
1	G	78	LEU	CB-CG-CD1	5.16	119.77	111.00
1	B	227	LEU	CA-CB-CG	5.13	127.10	115.30
1	F	108	GLU	CB-CA-C	-5.13	100.14	110.40
1	C	83	ASP	CB-CG-OD1	5.07	122.87	118.30
1	H	195	VAL	CG1-CB-CG2	5.07	119.02	110.90
1	E	64	GLN	N-CA-C	-5.05	97.36	111.00
1	A	119	ARG	NE-CZ-NH2	5.03	122.82	120.30
1	H	38	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	C	163	GLN	N-CA-CB	-5.01	101.58	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	40	GLY	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	1709	0	1741	102	0
1	B	1709	0	1741	70	0
1	C	1634	0	1669	39	0
1	D	1702	0	1736	49	0
1	E	1643	0	1684	62	1
1	F	1701	0	1734	46	0
1	G	1643	0	1683	60	0
1	H	1620	0	1655	52	0
2	A	58	0	0	7	0
2	B	68	0	0	19	0
2	C	57	0	0	3	0
2	D	62	0	0	11	0
2	E	45	0	0	4	0
2	F	62	0	0	12	0
2	G	49	0	0	5	0
2	H	58	0	0	8	1
All	All	13820	0	13643	459	1

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 17.

All (459) 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:H:51:THR:HG22	1:H:55:GLN:NE2	1.07	1.38
1:A:111:ALA:HB3	1:A:114:ASP:CB	1.51	1.38
1:B:35:ILE:HA	2:B:304:HOH:O	1.20	1.34
1:H:51:THR:CG2	1:H:55:GLN:NE2	1.91	1.34
1:H:51:THR:CG2	1:H:55:GLN:HE22	1.44	1.24
1:G:64:GLN:OE1	1:G:102:SER:OG	1.56	1.23
1:D:62:THR:HG22	2:D:303:HOH:O	1.41	1.21
1:A:111:ALA:CA	1:A:114:ASP:HB2	1.71	1.20
1:B:64:GLN:HE22	1:B:217:ARG:NH2	1.41	1.18
1:B:172:HIS:HD2	2:B:306:HOH:O	1.26	1.18
1:A:31:THR:HG22	1:A:34:GLU:H	1.09	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:GLN:NE2	1:E:102:SER:OG	1.77	1.16
1:H:214:MET:O	1:H:215:ARG:HB3	1.45	1.16
1:G:6:ARG:HH11	1:G:6:ARG:HG2	1.15	1.12
1:A:111:ALA:N	1:A:114:ASP:HB2	1.64	1.11
1:B:31:THR:HG22	1:B:34:GLU:H	1.10	1.10
1:A:111:ALA:CB	1:A:114:ASP:CB	2.29	1.10
1:A:111:ALA:HB3	1:A:114:ASP:CG	1.71	1.09
1:A:110:GLY:C	1:A:112:PRO:CD	2.21	1.08
1:B:64:GLN:NE2	1:B:217:ARG:HH22	1.51	1.07
1:E:62:THR:HB	1:E:66:ARG:NH1	1.68	1.06
1:C:90:GLN:O	1:C:94:LYS:HG2	1.52	1.05
1:E:62:THR:HB	1:E:66:ARG:HH11	1.12	1.05
1:A:111:ALA:HB3	1:A:114:ASP:CA	1.85	1.04
1:B:64:GLN:NE2	1:B:217:ARG:NH2	2.05	1.03
1:A:110:GLY:C	1:A:112:PRO:HD2	1.77	1.03
1:A:111:ALA:CB	1:A:114:ASP:HB2	1.89	1.02
1:D:122[A]:MET:HE1	1:D:156:VAL:HG11	1.42	1.00
1:E:63:SER:O	1:E:67:ALA:CB	2.10	0.99
1:H:145:ARG:NH1	1:H:145:ARG:HB3	1.78	0.98
1:A:110:GLY:CA	1:A:112:PRO:HD2	1.94	0.97
1:G:65:LEU:HD21	1:G:125:TRP:HA	1.47	0.97
1:A:31:THR:CG2	1:A:34:GLU:H	1.77	0.97
1:E:63:SER:O	1:E:64:GLN:C	1.96	0.96
1:A:111:ALA:N	1:A:112:PRO:HD3	1.80	0.95
1:A:111:ALA:CB	1:A:114:ASP:CG	2.34	0.95
1:B:172:HIS:CD2	2:B:306:HOH:O	2.07	0.92
1:F:6:ARG:NH2	2:F:301:HOH:O	2.02	0.92
1:A:110:GLY:CA	1:A:112:PRO:CD	2.47	0.92
1:A:110:GLY:HA3	1:A:112:PRO:HD2	1.50	0.91
1:F:116:LEU:HD13	1:F:118:ARG:HG3	1.51	0.91
1:E:63:SER:O	1:E:67:ALA:HB2	1.69	0.90
1:A:62:THR:CG2	1:A:66:ARG:HH22	1.84	0.90
1:B:31:THR:CG2	1:B:34:GLU:H	1.86	0.87
1:A:111:ALA:N	1:A:112:PRO:CD	2.30	0.87
1:F:31:THR:HG22	1:F:34:GLU:H	1.41	0.86
1:G:62:THR:CG2	2:G:308:HOH:O	2.23	0.85
1:F:6:ARG:NE	2:F:301:HOH:O	1.90	0.85
1:A:64:GLN:NE2	1:A:217:ARG:HH22	1.75	0.85
1:D:122[A]:MET:CE	1:D:156:VAL:HG11	2.06	0.85
1:C:38:ARG:CG	1:C:38:ARG:HH11	1.89	0.85
1:A:111:ALA:HB3	1:A:114:ASP:OD1	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6:ARG:CZ	2:F:301:HOH:O	2.21	0.85
1:A:31:THR:HG22	1:A:34:GLU:N	1.92	0.84
1:A:64:GLN:HE22	1:A:217:ARG:NH2	1.75	0.84
1:A:112:PRO:HA	1:A:114:ASP:N	1.93	0.83
1:B:62:THR:HG23	1:B:66:ARG:NH2	1.94	0.83
1:E:63:SER:O	1:E:64:GLN:O	1.97	0.83
1:A:112:PRO:CA	1:A:114:ASP:N	2.42	0.83
1:D:74:GLN:CB	1:D:79:GLN:HB3	2.08	0.82
1:F:110:GLY:HA3	2:F:339:HOH:O	1.78	0.82
1:A:111:ALA:HB3	1:A:114:ASP:HA	1.60	0.82
1:A:112:PRO:HA	1:A:114:ASP:H	1.43	0.82
1:E:183[B]:HIS:CD2	2:E:323:HOH:O	2.32	0.82
1:B:62:THR:CG2	1:B:66:ARG:HH22	1.93	0.82
1:H:51:THR:HG22	1:H:55:GLN:CD	2.00	0.81
1:A:110:GLY:HA3	1:A:112:PRO:CD	2.09	0.81
1:A:112:PRO:N	1:A:114:ASP:N	2.29	0.81
1:H:38:ARG:HH11	1:H:38:ARG:CG	1.95	0.80
1:A:111:ALA:CB	1:A:114:ASP:OD1	2.29	0.80
1:C:38:ARG:HG2	1:C:38:ARG:HH11	1.44	0.80
1:E:38:ARG:HH11	1:E:38:ARG:HB3	1.46	0.80
1:B:64:GLN:CD	1:B:217:ARG:HH22	1.85	0.80
1:H:145:ARG:HH11	1:H:145:ARG:CB	1.94	0.80
1:B:123:GLN:HG2	2:B:366:HOH:O	1.82	0.79
1:F:78:LEU:HD13	1:F:187:MET:HE1	1.63	0.79
1:G:6:ARG:NH1	1:G:6:ARG:HG2	1.88	0.79
1:A:78:LEU:HD13	1:A:187:MET:HE1	1.64	0.79
1:G:122:MET:HE1	1:G:156:VAL:HG11	1.66	0.78
1:H:145:ARG:CB	1:H:145:ARG:NH1	2.46	0.78
1:B:78:LEU:HD13	1:B:187:MET:HE1	1.65	0.78
1:A:111:ALA:N	1:A:114:ASP:CB	2.47	0.78
1:D:73:GLU:O	1:D:74:GLN:CB	2.30	0.77
1:D:183:HIS:ND1	2:D:301:HOH:O	2.02	0.77
1:A:64:GLN:HE22	1:A:217:ARG:HH22	1.30	0.77
1:A:78:LEU:HD13	1:A:187:MET:CE	2.15	0.77
1:B:166:SER:HB3	2:B:306:HOH:O	1.85	0.77
1:B:31:THR:HG22	1:B:34:GLU:N	1.94	0.77
1:A:110:GLY:C	1:A:112:PRO:HD3	2.02	0.77
1:H:192:VAL:CG2	1:H:195:VAL:HG13	2.15	0.77
1:B:64:GLN:HE22	1:B:217:ARG:HH21	1.29	0.76
1:A:111:ALA:H	1:A:114:ASP:HB2	1.50	0.76
1:H:75:ARG:NH1	2:H:301:HOH:O	2.09	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:74:GLN:O	1:F:75:ARG:CB	2.30	0.75
1:A:62:THR:CG2	1:A:66:ARG:NH2	2.50	0.75
1:B:78:LEU:HD13	1:B:187:MET:CE	2.16	0.75
1:B:111:ALA:H	1:B:114:ASP:CB	1.99	0.74
1:A:111:ALA:C	1:A:114:ASP:HB2	2.07	0.74
1:A:110:GLY:CA	1:A:112:PRO:HD3	2.17	0.74
1:H:71:VAL:HG13	2:H:315:HOH:O	1.86	0.74
1:A:111:ALA:C	1:A:113:ALA:C	2.45	0.74
1:C:183:HIS:HD2	2:C:326:HOH:O	1.70	0.73
1:D:31:THR:HG22	1:D:34:GLU:H	1.51	0.73
1:A:6:ARG:NE	2:A:301:HOH:O	2.00	0.73
1:D:130:ARG:HH11	1:D:130:ARG:HG2	1.53	0.73
1:G:122:MET:CE	1:G:156:VAL:HG11	2.19	0.73
1:A:62:THR:HG23	1:A:66:ARG:NH2	2.03	0.73
1:F:62:THR:HG22	2:F:307:HOH:O	1.89	0.73
1:A:189:SER:OG	1:H:185:HIS:HD2	1.72	0.72
1:C:10:THR:HA	1:C:13:THR:HG23	1.71	0.72
1:B:62:THR:HG23	1:B:66:ARG:HH22	1.52	0.72
1:E:63:SER:O	1:E:67:ALA:HB3	1.89	0.72
1:H:189:SER:CB	2:H:302:HOH:O	2.37	0.72
1:G:95:GLY:HA2	1:G:100:ARG:HD2	1.71	0.72
1:D:66:ARG:NH1	2:D:303:HOH:O	2.23	0.71
1:A:10:THR:HG22	1:A:223:ALA:H	1.53	0.71
1:F:31:THR:CG2	1:F:34:GLU:H	2.03	0.71
1:G:111:ALA:HB1	1:G:112:PRO:HD2	1.71	0.71
1:D:130:ARG:HD3	1:D:149:ASP:OD2	1.91	0.71
1:A:111:ALA:H	1:A:114:ASP:CB	2.04	0.70
1:G:65:LEU:HD21	1:G:125:TRP:CA	2.21	0.70
1:D:38:ARG:HB2	1:D:38:ARG:HH11	1.57	0.70
1:F:130:ARG:NH1	1:F:131:ASP:OD1	2.24	0.70
1:A:111:ALA:O	1:A:113:ALA:C	2.30	0.70
1:G:11:ARG:NE	2:G:301:HOH:O	1.97	0.70
1:A:112:PRO:CA	1:A:114:ASP:H	2.01	0.69
1:E:215:ARG:O	1:E:216:ARG:HB2	1.92	0.69
1:E:211:ASP:O	1:E:215:ARG:HG2	1.93	0.69
1:B:62:THR:HG22	1:B:66:ARG:HH12	1.57	0.69
1:F:2:ALA:O	1:F:6:ARG:HG3	1.93	0.69
1:H:51:THR:CG2	1:H:55:GLN:CD	2.59	0.68
1:H:38:ARG:HH11	1:H:38:ARG:HG2	1.59	0.68
1:B:111:ALA:H	1:B:114:ASP:HB2	1.59	0.68
1:E:111:ALA:HB1	1:E:112:PRO:HD2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:PRO:N	1:A:114:ASP:HB2	2.09	0.67
1:C:111:ALA:O	1:C:112:PRO:C	2.32	0.67
1:A:111:ALA:O	1:A:112:PRO:C	2.33	0.67
1:F:38:ARG:HH11	1:F:38:ARG:HB2	1.60	0.67
1:B:224:ALA:HA	1:B:227:LEU:HD22	1.77	0.66
1:H:189:SER:OG	2:H:302:HOH:O	2.10	0.66
1:C:137:GLU:CD	2:C:307:HOH:O	2.33	0.66
1:D:164:ILE:CD1	1:E:164:ILE:CD1	2.73	0.66
1:F:111:ALA:O	1:F:113:ALA:O	2.13	0.66
1:G:63:SER:O	1:G:65:LEU:N	2.29	0.65
1:A:112:PRO:CA	1:A:113:ALA:C	2.62	0.65
1:E:62:THR:CG2	2:E:304:HOH:O	2.45	0.65
1:F:78:LEU:HD13	1:F:187:MET:CE	2.25	0.65
1:H:10:THR:HA	1:H:13:THR:HG23	1.77	0.65
1:A:111:ALA:O	1:A:113:ALA:N	2.29	0.65
1:G:38:ARG:HH11	1:G:38:ARG:CG	2.09	0.65
1:A:218:GLU:CD	1:A:218:GLU:O	2.34	0.65
1:B:189:SER:OG	1:C:185:HIS:HD2	1.80	0.65
1:D:31:THR:CG2	1:D:34:GLU:H	2.10	0.64
1:D:145:ARG:HD3	2:D:360:HOH:O	1.97	0.64
1:A:24:GLU:CD	1:A:38:ARG:HH22	2.01	0.64
1:G:65:LEU:CD2	1:G:125:TRP:HA	2.26	0.64
1:D:78:LEU:HD13	1:D:187:MET:HE1	1.78	0.64
1:A:10:THR:HG21	1:A:226:ASP:OD2	1.97	0.64
1:F:61:LEU:HA	1:F:102:SER:HB2	1.79	0.64
1:B:157:GLY:O	1:C:161:GLY:HA3	1.97	0.63
1:C:38:ARG:NH1	1:C:38:ARG:HG2	2.09	0.63
1:C:8:ALA:HA	2:C:352:HOH:O	1.98	0.63
1:F:118:ARG:HD2	2:F:356:HOH:O	1.98	0.63
1:A:6:ARG:NH2	2:A:301:HOH:O	2.26	0.63
1:D:64:GLN:HG3	1:D:99:VAL:HG22	1.79	0.63
1:A:64:GLN:NE2	1:A:217:ARG:NH2	2.40	0.62
1:A:62:THR:HG22	1:A:66:ARG:HH12	1.64	0.62
1:E:95:GLY:HA2	1:E:100:ARG:HD2	1.82	0.62
1:B:114:ASP:O	1:B:116:LEU:N	2.30	0.62
1:B:166:SER:CB	2:B:306:HOH:O	2.44	0.62
1:H:214:MET:HA	1:H:214:MET:CE	2.30	0.62
1:C:54:GLU:OE1	1:C:115:GLY:O	2.18	0.61
1:B:111:ALA:HB1	1:B:112:PRO:HD2	1.81	0.61
1:C:214:MET:O	1:C:215:ARG:HD3	2.00	0.61
1:H:214:MET:HA	1:H:214:MET:HE2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:HIS:HE1	2:B:349:HOH:O	1.82	0.61
1:G:130:ARG:HG3	1:G:148:VAL:HG13	1.82	0.60
1:H:183:HIS:HD2	2:H:332:HOH:O	1.81	0.60
1:E:60:VAL:O	1:E:63:SER:HB3	2.01	0.60
1:G:41:VAL:HG13	1:G:45:ALA:HB3	1.84	0.60
1:G:38:ARG:HH11	1:G:38:ARG:HG2	1.66	0.60
1:F:28:GLU:OE1	1:F:111:ALA:HB3	2.02	0.60
1:C:90:GLN:O	1:C:94:LYS:CG	2.40	0.59
1:G:63:SER:C	1:G:65:LEU:N	2.53	0.59
1:D:122[B]:MET:HE2	1:D:122[B]:MET:HA	1.84	0.59
1:E:134:ARG:NH1	1:E:137:GLU:HB3	2.17	0.59
1:E:192:VAL:CG2	1:E:195:VAL:HG13	2.31	0.59
1:H:196:LEU:HA	1:H:199:LEU:HD22	1.85	0.59
1:E:9:GLN:HG2	1:E:12:ARG:NH1	2.17	0.59
1:B:37:LYS:HE3	2:B:325:HOH:O	2.02	0.58
1:E:108:GLU:CG	1:E:108:GLU:O	2.50	0.58
1:G:63:SER:HB3	1:G:67:ALA:CB	2.33	0.58
1:A:64:GLN:CD	1:A:217:ARG:HH22	2.06	0.58
1:A:111:ALA:C	1:A:114:ASP:N	2.56	0.58
1:B:111:ALA:HB3	1:B:114:ASP:HB2	1.85	0.58
1:E:203:ALA:O	1:E:207:ILE:HG23	2.03	0.58
1:F:104:ARG:O	1:F:108:GLU:HG3	2.02	0.58
1:G:38:ARG:HB3	1:G:38:ARG:HH11	1.67	0.58
1:F:183:HIS:ND1	2:F:303:HOH:O	2.24	0.58
1:E:38:ARG:NH1	1:E:38:ARG:HB3	2.18	0.58
1:B:38:ARG:NH2	2:B:301:HOH:O	2.31	0.58
1:E:64:GLN:NE2	1:E:102:SER:HG	1.99	0.57
1:H:38:ARG:NH1	1:H:38:ARG:CG	2.62	0.57
1:C:50:PHE:HB3	1:C:55:GLN:CG	2.34	0.57
1:G:215:ARG:O	1:G:216:ARG:HG3	2.04	0.57
1:G:62:THR:HG21	2:G:308:HOH:O	1.95	0.57
1:A:189:SER:OG	1:H:185:HIS:CD2	2.57	0.57
1:D:130:ARG:CD	1:D:149:ASP:OD2	2.53	0.57
1:F:164:ILE:CD1	1:G:164:ILE:CD1	2.83	0.57
1:A:157:GLY:O	1:H:161:GLY:HA3	2.05	0.57
1:E:46:LEU:HD23	1:E:46:LEU:C	2.24	0.57
1:H:51:THR:H	1:H:55:GLN:NE2	2.02	0.57
1:A:215:ARG:O	1:A:216:ARG:CB	2.53	0.56
1:B:185:HIS:HE1	2:B:363:HOH:O	1.87	0.56
1:E:17:ALA:CB	1:E:39:SER:HB3	2.35	0.56
1:G:137:GLU:HB2	1:G:142:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ASP:OD2	1:A:178:ARG:HD2	2.06	0.56
1:E:65:LEU:C	1:E:67:ALA:H	2.09	0.56
1:H:38:ARG:HH11	1:H:38:ARG:HG3	1.70	0.56
1:C:41:VAL:HG13	1:C:42:THR:N	2.21	0.56
1:D:174:ASP:OD2	1:D:178:ARG:HD2	2.05	0.56
1:D:157:GLY:O	1:E:161:GLY:HA3	2.06	0.56
1:H:38:ARG:NH1	1:H:38:ARG:HG2	2.17	0.56
1:D:120:ALA:N	1:D:121:PRO:CD	2.68	0.56
1:B:24:GLU:OE2	1:B:38:ARG:NH2	2.39	0.56
1:E:38:ARG:CB	1:E:38:ARG:HH11	2.16	0.56
1:H:192:VAL:HG22	1:H:195:VAL:HG13	1.88	0.56
1:C:69:PRO:HG2	1:C:213:ALA:HB1	1.88	0.55
1:D:164:ILE:HD11	1:E:164:ILE:HD13	1.87	0.55
1:B:62:THR:CG2	1:B:66:ARG:NH2	2.57	0.55
1:E:130:ARG:HG3	1:E:148:VAL:CG1	2.36	0.55
1:G:63:SER:HB3	1:G:67:ALA:HB2	1.88	0.55
1:F:3:ARG:HB2	1:F:3:ARG:CZ	2.36	0.55
1:H:189:SER:HB3	2:H:302:HOH:O	2.03	0.55
1:H:68:VAL:HG13	1:H:87:LEU:HD23	1.89	0.54
1:A:62:THR:HG21	1:A:66:ARG:HH22	1.68	0.54
1:H:192:VAL:HG23	1:H:195:VAL:HG13	1.90	0.54
1:H:214:MET:O	1:H:215:ARG:CB	2.30	0.54
1:F:38:ARG:HB2	1:F:38:ARG:NH1	2.22	0.54
1:F:111:ALA:O	1:F:113:ALA:C	2.46	0.54
1:D:164:ILE:CD1	1:E:164:ILE:HD13	2.38	0.54
1:G:38:ARG:HH11	1:G:38:ARG:CB	2.21	0.54
1:B:11:ARG:NE	2:B:303:HOH:O	2.24	0.54
1:G:111:ALA:HB3	1:G:114:ASP:HB3	1.89	0.54
1:B:31:THR:HB	2:B:333:HOH:O	2.07	0.54
1:D:31:THR:HB	2:D:340:HOH:O	2.07	0.54
1:A:185:HIS:HD2	1:H:189:SER:OG	1.91	0.54
1:B:38:ARG:NE	2:B:301:HOH:O	2.04	0.53
1:D:104:ARG:HD3	1:E:109:PRO:HG2	1.89	0.53
1:G:192:VAL:CG2	1:G:195:VAL:HG13	2.37	0.53
1:G:154:MET:HE3	1:G:186:LEU:HD22	1.90	0.53
1:A:111:ALA:HB2	1:A:114:ASP:CG	2.27	0.53
1:A:123:GLN:HG2	2:A:355:HOH:O	2.07	0.53
1:D:130:ARG:HG2	1:D:130:ARG:NH1	2.23	0.53
1:A:111:ALA:CB	1:A:114:ASP:CA	2.73	0.53
1:A:183:HIS:ND1	2:A:303:HOH:O	2.19	0.53
1:D:42:THR:HA	1:D:228:GLU:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:66:ARG:NH1	2:F:307:HOH:O	2.41	0.53
1:F:157:GLY:O	1:G:161:GLY:HA3	2.09	0.53
1:G:10:THR:HG22	2:G:340:HOH:O	2.09	0.53
1:G:96:ASP:O	1:G:100:ARG:HG3	2.08	0.52
1:D:122[B]:MET:HA	1:D:122[B]:MET:CE	2.38	0.52
1:H:144:PRO:O	1:H:145:ARG:HG2	2.10	0.52
1:G:11:ARG:NH2	2:G:301:HOH:O	2.42	0.52
1:F:164:ILE:HD13	1:G:164:ILE:CD1	2.39	0.52
1:B:94:LYS:HG3	1:B:210:TYR:OH	2.09	0.52
1:H:51:THR:HG23	1:H:55:GLN:NE2	2.11	0.52
1:A:74:GLN:NE2	1:A:205:ARG:NH2	2.58	0.52
1:C:68:VAL:HG13	1:C:87:LEU:HD23	1.92	0.52
1:E:177:GLU:OE2	1:E:178:ARG:NH2	2.43	0.52
1:B:38:ARG:HB2	2:B:304:HOH:O	2.09	0.52
1:D:78:LEU:HD13	1:D:187:MET:CE	2.39	0.52
1:C:171:GLY:O	1:C:172:HIS:HB2	2.11	0.51
1:A:112:PRO:CD	1:A:114:ASP:HB2	2.40	0.51
1:E:192:VAL:HG22	1:E:195:VAL:HG13	1.91	0.51
1:B:31:THR:HG23	1:B:33:ALA:H	1.75	0.51
1:D:38:ARG:NH1	1:D:38:ARG:HB2	2.25	0.51
1:A:58:GLN:O	1:A:62:THR:HB	2.09	0.51
1:B:130:ARG:HG2	1:B:148:VAL:HG13	1.92	0.51
1:B:111:ALA:H	1:B:114:ASP:HB3	1.75	0.51
1:H:69:PRO:HG2	1:H:213:ALA:HB1	1.91	0.51
1:E:64:GLN:O	1:E:67:ALA:HB3	2.11	0.51
1:F:3:ARG:NH1	1:F:3:ARG:HB3	2.26	0.51
1:G:89:ALA:O	1:G:93:SER:HB2	2.10	0.51
1:G:63:SER:O	1:G:64:GLN:C	2.48	0.50
1:H:139:GLY:HA3	2:H:320:HOH:O	2.11	0.50
1:A:112:PRO:N	1:A:114:ASP:CB	2.74	0.50
1:E:108:GLU:O	1:E:108:GLU:HG2	2.11	0.50
1:F:3:ARG:CB	1:F:3:ARG:CZ	2.89	0.50
1:H:130:ARG:HE	1:H:134:ARG:NH2	2.10	0.50
1:G:6:ARG:CG	1:G:6:ARG:HH11	2.03	0.50
1:A:61:LEU:HA	1:A:102:SER:HB2	1.93	0.50
1:E:69:PRO:HG3	1:E:213:ALA:HB1	1.93	0.50
1:E:215:ARG:O	1:E:216:ARG:CB	2.59	0.50
1:A:111:ALA:HB2	1:A:114:ASP:OD1	2.10	0.50
1:B:114:ASP:O	1:B:114:ASP:OD2	2.30	0.50
1:B:218:GLU:OE1	1:B:218:GLU:O	2.30	0.50
1:C:111:ALA:O	1:C:112:PRO:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:164:ILE:CD1	1:G:164:ILE:HD13	2.42	0.50
1:B:111:ALA:O	1:B:112:PRO:C	2.50	0.50
1:H:171:GLY:O	1:H:172:HIS:HB2	2.10	0.50
1:A:13:THR:HG21	1:A:222:PRO:HG3	1.94	0.50
1:A:218:GLU:O	1:A:218:GLU:OE1	2.30	0.49
1:D:9:GLN:HG2	1:D:221:LEU:O	2.11	0.49
1:F:164:ILE:HD11	1:G:164:ILE:HD13	1.94	0.49
1:B:5:GLU:HG3	2:B:329:HOH:O	2.12	0.49
1:D:118:ARG:HD3	2:D:319:HOH:O	2.11	0.49
1:H:92:LEU:HD21	1:H:163:GLN:HG2	1.95	0.49
1:A:111:ALA:O	1:A:113:ALA:O	2.29	0.49
1:B:31:THR:HG23	1:B:33:ALA:N	2.27	0.49
1:A:11:ARG:NE	2:A:302:HOH:O	2.16	0.49
1:D:38:ARG:NH2	2:D:302:HOH:O	2.04	0.49
1:G:192:VAL:HG22	1:G:195:VAL:HG13	1.94	0.49
1:C:111:ALA:HB1	1:C:112:PRO:HD2	1.94	0.48
1:A:94:LYS:HG3	1:A:210:TYR:OH	2.14	0.48
1:D:32:ILE:HG12	2:D:333:HOH:O	2.13	0.48
1:H:118:ARG:NH2	2:H:304:HOH:O	2.30	0.48
1:G:62:THR:O	1:G:66:ARG:HB2	2.14	0.48
1:A:130:ARG:HG2	1:A:148:VAL:HG13	1.96	0.48
1:E:89:ALA:O	1:E:93:SER:HB2	2.13	0.48
1:A:6:ARG:CZ	2:A:301:HOH:O	2.44	0.48
1:B:144:PRO:O	1:B:145:ARG:HB2	2.14	0.48
1:G:85:THR:HG21	1:G:183[B]:HIS:CD2	2.49	0.48
1:B:62:THR:HG22	1:B:66:ARG:NH1	2.27	0.47
1:C:41:VAL:HG13	1:C:45:ALA:HB3	1.95	0.47
1:F:144:PRO:O	1:F:145:ARG:HB2	2.14	0.47
1:G:130:ARG:HG3	1:G:148:VAL:CG1	2.43	0.47
1:B:62:THR:HG21	1:B:66:ARG:HH22	1.78	0.47
1:E:62:THR:CB	1:E:66:ARG:NH1	2.60	0.47
1:E:130:ARG:HG3	1:E:148:VAL:HG13	1.96	0.47
1:A:104:ARG:O	1:A:108:GLU:HG3	2.15	0.47
1:A:112:PRO:HD3	1:A:114:ASP:CB	2.44	0.47
1:G:69:PRO:HG3	1:G:213:ALA:HB1	1.96	0.47
1:A:2:ALA:O	1:A:6:ARG:HG3	2.15	0.47
1:E:65:LEU:HD23	1:E:65:LEU:N	2.29	0.47
1:C:50:PHE:HB3	1:C:55:GLN:HG2	1.96	0.47
1:E:41:VAL:HG13	1:E:45:ALA:HB3	1.96	0.47
1:E:90:GLN:OE1	1:E:94:LYS:HE2	2.15	0.47
1:H:88:LEU:HD13	1:H:159:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:GLN:O	1:B:62:THR:HB	2.15	0.46
1:D:164:ILE:HD13	1:E:164:ILE:CD1	2.44	0.46
1:B:111:ALA:N	1:B:114:ASP:CB	2.74	0.46
1:B:215:ARG:O	1:B:216:ARG:CB	2.64	0.46
1:B:35:ILE:CA	2:B:304:HOH:O	2.08	0.46
1:B:120:ALA:HB3	1:B:121:PRO:HD3	1.96	0.46
1:H:92:LEU:HD21	1:H:163:GLN:CG	2.45	0.46
1:A:112:PRO:HD3	1:A:114:ASP:HB2	1.96	0.46
1:G:65:LEU:HD23	1:G:125:TRP:CD1	2.51	0.46
1:B:189:SER:OG	1:C:185:HIS:CD2	2.65	0.46
1:B:2:ALA:HB3	2:B:329:HOH:O	2.15	0.46
1:C:32:ILE:HD11	1:C:53:LYS:N	2.30	0.46
1:G:62:THR:HB	1:G:66:ARG:HE	1.80	0.46
1:B:113:ALA:C	1:B:115:GLY:N	2.68	0.46
1:D:104:ARG:HD2	1:D:108:GLU:OE1	2.16	0.46
1:G:62:THR:OG1	1:G:62:THR:O	2.29	0.46
1:B:111:ALA:N	1:B:114:ASP:HB2	2.30	0.45
1:C:130:ARG:HE	1:C:134:ARG:NH2	2.14	0.45
1:D:177:GLU:HG2	2:D:355:HOH:O	2.16	0.45
1:B:24:GLU:CD	1:B:38:ARG:HH22	2.19	0.45
1:A:74:GLN:NE2	1:A:205:ARG:HH22	2.14	0.45
1:C:130:ARG:HE	1:C:134:ARG:HH21	1.63	0.45
1:A:31:THR:HB	2:A:340:HOH:O	2.16	0.45
1:B:174:ASP:OD2	1:B:178:ARG:HD2	2.16	0.45
1:C:22:PHE:CE1	1:C:30:THR:HG21	2.51	0.45
1:D:46:LEU:HD23	1:D:46:LEU:C	2.36	0.45
1:A:31:THR:HG23	1:A:33:ALA:H	1.81	0.45
1:C:38:ARG:HH11	1:C:38:ARG:HG3	1.75	0.45
1:G:122:MET:HE2	1:G:156:VAL:HG11	1.98	0.45
1:A:112:PRO:N	1:A:113:ALA:C	2.68	0.45
1:A:111:ALA:CB	1:A:114:ASP:HA	2.39	0.45
1:E:96:ASP:O	1:E:100:ARG:HG3	2.17	0.44
1:B:54:GLU:HG3	1:B:116:LEU:HD23	2.00	0.44
1:D:3:ARG:HB3	1:D:3:ARG:CZ	2.47	0.44
1:E:63:SER:O	1:E:67:ALA:N	2.50	0.44
1:C:23:ASP:OD2	1:C:100:ARG:HD3	2.18	0.44
1:F:62:THR:CG2	2:F:307:HOH:O	2.58	0.44
1:G:111:ALA:HB1	1:G:112:PRO:CD	2.46	0.44
1:C:41:VAL:CG1	1:C:42:THR:N	2.80	0.44
1:C:5:GLU:HG3	1:C:5:GLU:O	2.16	0.44
1:C:17:ALA:O	1:C:21:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:112:PRO:HA	1:F:113:ALA:HA	1.57	0.44
1:F:3:ARG:NH1	1:F:3:ARG:CB	2.80	0.44
1:A:31:THR:HG23	1:A:33:ALA:N	2.33	0.44
1:C:116:LEU:HA	1:C:116:LEU:HD12	1.84	0.44
1:D:118:ARG:O	1:D:121:PRO:HD2	2.17	0.44
1:E:146:LEU:HD13	1:E:190:VAL:HG22	2.00	0.44
1:E:62:THR:O	1:E:62:THR:OG1	2.29	0.44
1:G:38:ARG:NH1	1:G:38:ARG:HG2	2.31	0.44
1:D:11:ARG:NE	2:D:304:HOH:O	2.23	0.43
1:A:112:PRO:HA	1:A:113:ALA:HA	1.48	0.43
1:A:75:ARG:HG2	1:A:75:ARG:H	1.55	0.43
1:F:219:ALA:HA	1:F:220:PRO:HD3	1.78	0.43
1:F:229:HIS:HE1	2:F:353:HOH:O	2.00	0.43
1:G:214:MET:HA	1:G:214:MET:HE2	2.00	0.43
1:C:14:ILE:HD11	1:C:41:VAL:HG11	2.00	0.43
1:D:185:HIS:HD2	1:E:189:SER:OG	2.01	0.43
1:E:214:MET:O	1:E:216:ARG:N	2.51	0.43
1:A:47:TYR:HH	1:B:2:ALA:N	2.17	0.43
1:G:178:ARG:HD3	1:G:178:ARG:HA	1.59	0.43
1:G:199:LEU:HA	1:G:199:LEU:HD23	1.76	0.43
1:A:62:THR:HG22	1:A:66:ARG:NH1	2.30	0.42
1:D:130:ARG:NH1	1:D:134:ARG:CZ	2.82	0.42
1:E:110:GLY:O	1:E:111:ALA:C	2.55	0.42
1:A:27:TYR:CD1	1:A:116:LEU:HD22	2.54	0.42
1:E:20:ALA:O	1:E:24:GLU:HG3	2.19	0.42
1:G:14:ILE:HD13	1:G:46:LEU:HA	2.01	0.42
1:D:212:GLU:HG3	1:D:216:ARG:NH1	2.35	0.42
1:B:62:THR:HG23	1:B:66:ARG:CZ	2.48	0.42
1:D:122[A]:MET:CE	1:D:156:VAL:CG1	2.89	0.42
1:E:171:GLY:O	1:E:172:HIS:HB2	2.19	0.42
1:E:21:VAL:HG22	1:E:38:ARG:HD3	2.02	0.42
1:C:96:ASP:HA	1:C:97:PRO:HD3	1.73	0.42
1:A:185:HIS:CD2	1:H:189:SER:OG	2.71	0.42
1:D:137:GLU:HB2	1:D:142:LEU:HD12	2.02	0.42
1:E:143:LEU:HD11	2:E:321:HOH:O	2.18	0.42
1:F:111:ALA:O	1:F:113:ALA:CA	2.68	0.42
1:E:65:LEU:C	1:E:67:ALA:N	2.72	0.42
1:G:65:LEU:O	1:G:66:ARG:CB	2.66	0.42
1:E:51:THR:HG23	1:E:55:GLN:OE1	2.19	0.41
1:F:28:GLU:OE1	1:F:111:ALA:CB	2.67	0.41
1:F:58:GLN:O	1:F:62:THR:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:92:LEU:CD2	1:H:163:GLN:HG2	2.49	0.41
1:B:122:MET:HA	1:B:122:MET:HE2	2.01	0.41
1:C:36:LEU:HD21	1:C:46:LEU:HB2	2.01	0.41
1:E:111:ALA:CB	1:E:112:PRO:HD2	2.32	0.41
1:C:47:TYR:HA	1:C:50:PHE:O	2.21	0.41
1:F:31:THR:HG22	1:F:34:GLU:CB	2.51	0.41
1:A:112:PRO:CD	1:A:114:ASP:CB	2.98	0.41
1:B:111:ALA:N	1:B:114:ASP:HB3	2.33	0.41
1:E:183[B]:HIS:HE1	2:E:324:HOH:O	2.02	0.41
1:B:126:ILE:O	1:B:130:ARG:HB2	2.21	0.41
1:D:61:LEU:HA	1:D:102:SER:HB2	2.03	0.41
1:F:118:ARG:HD3	2:F:323:HOH:O	2.21	0.41
1:F:31:THR:HB	2:F:322:HOH:O	2.20	0.41
1:H:146:LEU:HD11	1:H:190:VAL:HA	2.03	0.41
1:H:17:ALA:O	1:H:21:VAL:HG23	2.20	0.41
1:G:134:ARG:HD2	1:G:134:ARG:HA	1.81	0.41
1:H:32:ILE:HD11	1:H:53:LYS:N	2.36	0.41
1:H:94:LYS:HE3	1:H:210:TYR:CE2	2.56	0.41
1:G:146:LEU:HD13	1:G:190:VAL:HG22	2.03	0.41
1:G:34:GLU:OE2	1:G:38:ARG:HD2	2.20	0.41
1:H:130:ARG:HG3	1:H:148:VAL:HG13	2.02	0.41
1:A:46:LEU:C	1:A:46:LEU:HD23	2.41	0.41
1:D:183:HIS:CE1	2:D:301:HOH:O	2.60	0.41
1:F:9:GLN:HG3	1:F:221:LEU:O	2.21	0.41
1:G:122:MET:O	1:G:122:MET:HE3	2.21	0.41
1:A:126:ILE:O	1:A:130:ARG:HB2	2.20	0.41
1:G:6:ARG:HB2	1:G:9:GLN:HB2	2.02	0.41
1:B:32:ILE:HG12	2:B:343:HOH:O	2.20	0.40
1:A:9:GLN:HG2	1:A:221:LEU:O	2.20	0.40
1:B:108:GLU:HA	1:B:109:PRO:HD3	1.91	0.40
1:B:11:ARG:NH2	2:B:303:HOH:O	2.48	0.40
1:E:154:MET:HB3	1:E:154:MET:HE3	1.88	0.40
1:F:98:LEU:HD12	1:F:217:ARG:HH12	1.86	0.40
1:H:116:LEU:HD12	1:H:116:LEU:HA	1.97	0.40
1:C:38:ARG:NH1	1:C:38:ARG:CG	2.58	0.40
1:D:31:THR:HG23	1:D:33:ALA:N	2.36	0.40
1:A:199:LEU:HA	1:A:199:LEU:HD23	1.91	0.40
1:F:64:GLN:OE1	1:F:217:ARG:NH2	2.47	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:ILE:CG2	2:H:352:HOH:O[2_645]	1.93	0.27

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	219/228 (96%)	211 (96%)	6 (3%)	2 (1%)	17 20
1	B	219/228 (96%)	212 (97%)	4 (2%)	3 (1%)	11 11
1	C	211/228 (92%)	199 (94%)	11 (5%)	1 (0%)	29 35
1	D	215/228 (94%)	209 (97%)	6 (3%)	0	100 100
1	E	212/228 (93%)	199 (94%)	11 (5%)	2 (1%)	17 20
1	F	218/228 (96%)	206 (94%)	11 (5%)	1 (0%)	29 35
1	G	212/228 (93%)	202 (95%)	8 (4%)	2 (1%)	17 20
1	H	209/228 (92%)	202 (97%)	7 (3%)	0	100 100
All	All	1715/1824 (94%)	1640 (96%)	64 (4%)	11 (1%)	25 31

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ARG
1	B	112	PRO
1	B	216	ARG
1	C	112	PRO
1	E	112	PRO
1	E	216	ARG
1	B	115	GLY
1	F	75	ARG
1	G	64	GLN
1	G	112	PRO
1	A	112	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	175/182 (96%)	160 (91%)	15 (9%)	10 12
1	B	175/182 (96%)	161 (92%)	14 (8%)	12 15
1	C	170/182 (93%)	153 (90%)	17 (10%)	7 9
1	D	175/182 (96%)	161 (92%)	14 (8%)	12 15
1	E	171/182 (94%)	151 (88%)	20 (12%)	5 6
1	F	174/182 (96%)	161 (92%)	13 (8%)	13 17
1	G	171/182 (94%)	153 (90%)	18 (10%)	7 8
1	H	169/182 (93%)	150 (89%)	19 (11%)	6 6
All	All	1380/1456 (95%)	1250 (91%)	130 (9%)	8 10

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	10	THR
1	A	31	THR
1	A	62	THR
1	A	65	LEU
1	A	66	ARG
1	A	74	GLN
1	A	75	ARG
1	A	104	ARG
1	A	148	VAL
1	A	178	ARG
1	A	206	SER
1	A	211	ASP
1	A	212	GLU
1	A	218	GLU
1	H	6	ARG
1	H	9	GLN
1	H	13	THR
1	H	25	LEU

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Mol	Chain	Res	Type
1	H	37	LYS
1	H	38	ARG
1	H	53	LYS
1	H	65	LEU
1	H	75	ARG
1	H	78	LEU
1	H	88	LEU
1	H	93	SER
1	H	98	LEU
1	H	145	ARG
1	H	148	VAL
1	H	163	GLN
1	H	199	LEU
1	H	212	GLU
1	H	215	ARG
1	B	4	GLN
1	B	31	THR
1	B	38	ARG
1	B	62	THR
1	B	65	LEU
1	B	66	ARG
1	B	74	GLN
1	B	114	ASP
1	B	116	LEU
1	B	148	VAL
1	B	212	GLU
1	B	217	ARG
1	B	218	GLU
1	B	227	LEU
1	C	9	GLN
1	C	13	THR
1	C	25	LEU
1	C	38	ARG
1	C	41	VAL
1	C	55	GLN
1	C	71	VAL
1	C	75	ARG
1	C	78	LEU
1	C	88	LEU
1	C	94	LYS
1	C	146	LEU
1	C	148	VAL

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Mol	Chain	Res	Type
1	C	163	GLN
1	C	212	GLU
1	C	215	ARG
1	C	216	ARG
1	D	3	ARG
1	D	4	GLN
1	D	31	THR
1	D	38	ARG
1	D	62	THR
1	D	66	ARG
1	D	94	LYS
1	D	104	ARG
1	D	148	VAL
1	D	163	GLN
1	D	178	ARG
1	D	181	ASP
1	D	190	VAL
1	D	217	ARG
1	E	25	LEU
1	E	37	LYS
1	E	38	ARG
1	E	41	VAL
1	E	63	SER
1	E	65	LEU
1	E	66	ARG
1	E	73	GLU
1	E	78	LEU
1	E	88	LEU
1	E	116	LEU
1	E	145	ARG
1	E	176	LEU
1	E	190	VAL
1	E	195	VAL
1	E	197	VAL
1	E	207	ILE
1	E	215	ARG
1	E	216	ARG
1	E	217	ARG
1	F	3	ARG
1	F	4	GLN
1	F	31	THR
1	F	38	ARG

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Mol	Chain	Res	Type
1	F	62	THR
1	F	66	ARG
1	F	74	GLN
1	F	76	LEU
1	F	88	LEU
1	F	104	ARG
1	F	116	LEU
1	F	181	ASP
1	F	217	ARG
1	G	6	ARG
1	G	9	GLN
1	G	13	THR
1	G	25	LEU
1	G	37	LYS
1	G	38	ARG
1	G	46	LEU
1	G	64	GLN
1	G	65	LEU
1	G	66	ARG
1	G	73	GLU
1	G	78	LEU
1	G	88	LEU
1	G	108	GLU
1	G	134	ARG
1	G	148	VAL
1	G	195	VAL
1	G	215	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	74	GLN
1	A	185	HIS
1	H	49	HIS
1	H	55	GLN
1	H	163	GLN
1	H	183	HIS
1	H	185	HIS
1	B	64	GLN
1	B	185	HIS
1	B	229	HIS

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Mol	Chain	Res	Type
1	C	183	HIS
1	C	185	HIS
1	D	185	HIS
1	E	64	GLN
1	E	74	GLN
1	F	74	GLN
1	F	185	HIS
1	F	229	HIS
1	G	64	GLN
1	G	74	GLN

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

5.5 Carbohydrates [\(i\)](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [\(i\)](#)

There are no ligands in this entry.

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 i

6.1 Protein, DNA and RNA chains i

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, 95th 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	223/228 (97%)	-0.10	15 (6%) 17 23	15, 24, 62, 138	0
1	B	223/228 (97%)	-0.14	13 (5%) 23 29	13, 24, 62, 129	0
1	C	213/228 (93%)	-0.02	15 (7%) 16 21	16, 31, 78, 130	0
1	D	220/228 (96%)	-0.23	11 (5%) 28 35	16, 24, 56, 96	0
1	E	213/228 (93%)	-0.00	16 (7%) 14 19	16, 29, 70, 100	0
1	F	222/228 (97%)	-0.14	12 (5%) 25 32	14, 24, 62, 134	0
1	G	213/228 (93%)	0.04	16 (7%) 14 19	16, 30, 69, 104	0
1	H	211/228 (92%)	-0.04	11 (5%) 27 34	16, 32, 71, 98	0
All	All	1738/1824 (95%)	-0.08	109 (6%) 20 25	13, 26, 69, 138	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	113	ALA	11.2
1	G	112	PRO	10.4
1	F	112	PRO	10.1
1	A	113	ALA	10.0
1	G	111	ALA	9.5
1	F	111	ALA	9.2
1	H	113	ALA	8.4
1	G	113	ALA	7.9
1	D	67	ALA	7.6
1	A	114	ASP	7.3
1	E	66	ARG	7.2
1	A	75	ARG	7.1
1	A	112	PRO	6.8
1	C	216	ARG	6.5
1	E	65	LEU	6.3
1	B	112	PRO	6.2

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Mol	Chain	Res	Type	RSRZ
1	F	74	GLN	5.7
1	G	4	GLN	5.5
1	B	75	ARG	5.4
1	E	111	ALA	5.3
1	C	112	PRO	5.2
1	H	112	PRO	5.0
1	A	74	GLN	4.9
1	E	113	ALA	4.9
1	B	114	ASP	4.9
1	H	111	ALA	4.8
1	C	55	GLN	4.8
1	D	216	ARG	4.8
1	A	111	ALA	4.7
1	C	110	GLY	4.6
1	H	215	ARG	4.5
1	H	110	GLY	4.5
1	D	75	ARG	4.4
1	C	7	ALA	4.4
1	F	216	ARG	4.4
1	F	114	ASP	4.3
1	C	5	GLU	4.2
1	G	5	GLU	4.2
1	E	64	GLN	4.2
1	G	6	ARG	4.2
1	E	217	ARG	4.2
1	E	5	GLU	4.0
1	H	6	ARG	4.0
1	G	7	ALA	4.0
1	B	67	ALA	3.9
1	E	72	GLU	3.9
1	D	229	HIS	3.9
1	A	67	ALA	3.9
1	C	113	ALA	3.9
1	D	66	ARG	3.8
1	C	8	ALA	3.8
1	G	8	ALA	3.7
1	A	229	HIS	3.7
1	F	229	HIS	3.7
1	D	114	ASP	3.7
1	G	64	GLN	3.7
1	C	215	ARG	3.6
1	E	216	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	215	ARG	3.6
1	F	113	ALA	3.4
1	E	112	PRO	3.4
1	B	111	ALA	3.3
1	E	63	SER	3.3
1	B	115	GLY	3.2
1	A	115	GLY	3.2
1	E	110	GLY	3.1
1	C	115	GLY	3.1
1	C	111	ALA	3.1
1	D	110	GLY	3.0
1	G	110	GLY	3.0
1	B	215	ARG	3.0
1	A	219	ALA	2.9
1	G	216	ARG	2.9
1	B	219	ALA	2.8
1	E	6	ARG	2.8
1	F	66	ARG	2.8
1	E	60	VAL	2.7
1	H	5	GLU	2.6
1	H	8	ALA	2.6
1	D	74	GLN	2.5
1	H	114	ASP	2.5
1	G	60	VAL	2.5
1	C	9	GLN	2.4
1	A	3	ARG	2.4
1	B	218	GLU	2.4
1	B	3	ARG	2.3
1	F	215	ARG	2.3
1	G	215	ARG	2.3
1	H	115	GLY	2.3
1	B	66	ARG	2.3
1	A	110	GLY	2.3
1	F	217	ARG	2.3
1	H	7	ALA	2.3
1	G	40	GLY	2.3
1	A	73	GLU	2.2
1	B	229	HIS	2.2
1	A	218	GLU	2.2
1	D	215	ARG	2.2
1	A	66	ARG	2.2
1	G	56	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	75	ARG	2.1
1	G	69	PRO	2.1
1	E	120	ALA	2.1
1	C	37	LYS	2.1
1	D	3	ARG	2.1
1	D	73	GLU	2.0
1	F	3	ARG	2.0
1	C	43	LYS	2.0
1	C	51	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

6.3 Carbohydrates [\(i\)](#)

There are no carbohydrates in this entry.

6.4 Ligands [\(i\)](#)

There are no ligands in this entry.

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.