Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:24 pm BST

PDB ID	:	5HEO
Title	:	Pentameric ligand-gated ion channel ELIC mutant P254G
Authors	:	Bertozzi, C.; Dutzler, R.
Deposited on	:	2016-01-06
Resolution	:	3.30 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 ⓘ symbol.

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

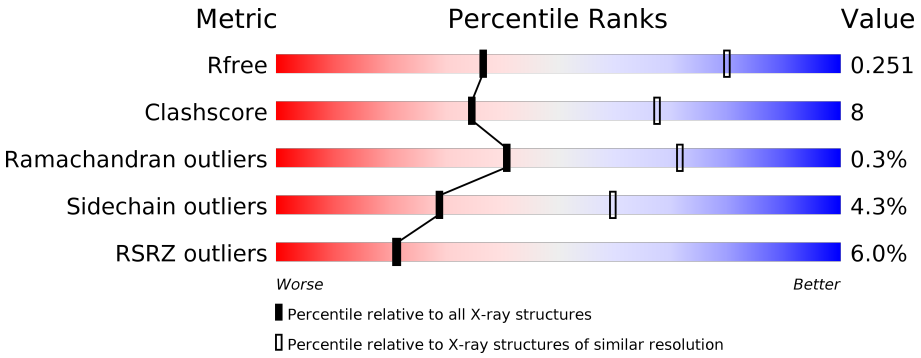
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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.

Mol	Chain	Length	Quality of chain
1	A	322	4% 74% 21% • 5%
1	B	322	4% 71% 23% • 5%
1	C	322	6% 75% 20% • 5%
1	D	322	4% 75% 19% • 5%
1	E	322	4% 71% 23% • 5%
1	F	322	7% 70% 24% • 5%

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Mol	Chain	Length	Quality of chain
1	G	322	9% 74% 20% • 5%
1	H	322	7% 70% 23% • 5%
1	I	322	6% 75% 19% • 5%
1	J	322	6% 72% 22% • 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25020 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-aminobutyric-acid receptor subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	B	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	C	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	D	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	E	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	F	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	G	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	H	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	I	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	J	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	GLY	PRO	engineered mutation	UNP E0SJQ4
B	254	GLY	PRO	engineered mutation	UNP E0SJQ4
C	254	GLY	PRO	engineered mutation	UNP E0SJQ4
D	254	GLY	PRO	engineered mutation	UNP E0SJQ4
E	254	GLY	PRO	engineered mutation	UNP E0SJQ4
F	254	GLY	PRO	engineered mutation	UNP E0SJQ4
G	254	GLY	PRO	engineered mutation	UNP E0SJQ4
H	254	GLY	PRO	engineered mutation	UNP E0SJQ4
I	254	GLY	PRO	engineered mutation	UNP E0SJQ4

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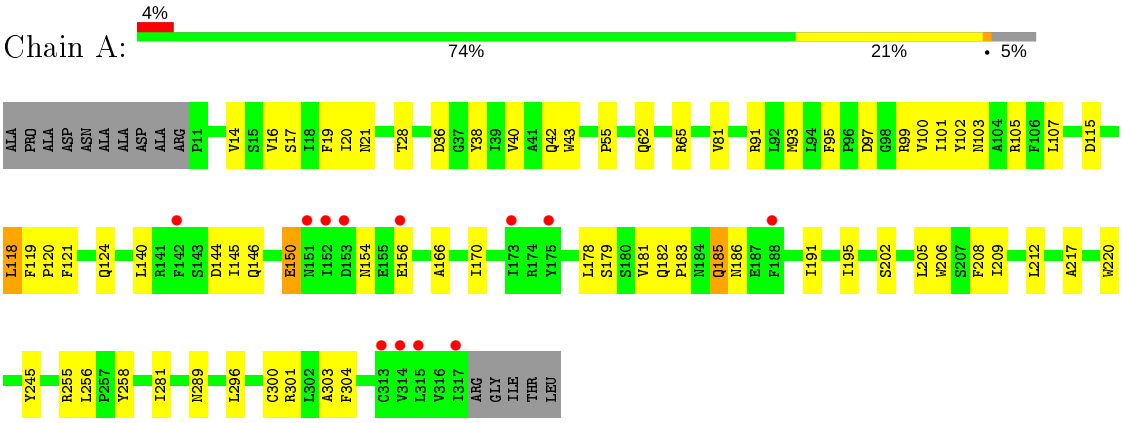
Chain	Residue	Modelled	Actual	Comment	Reference
J	254	GLY	PRO	engineered mutation	UNP E0SJQ4

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.

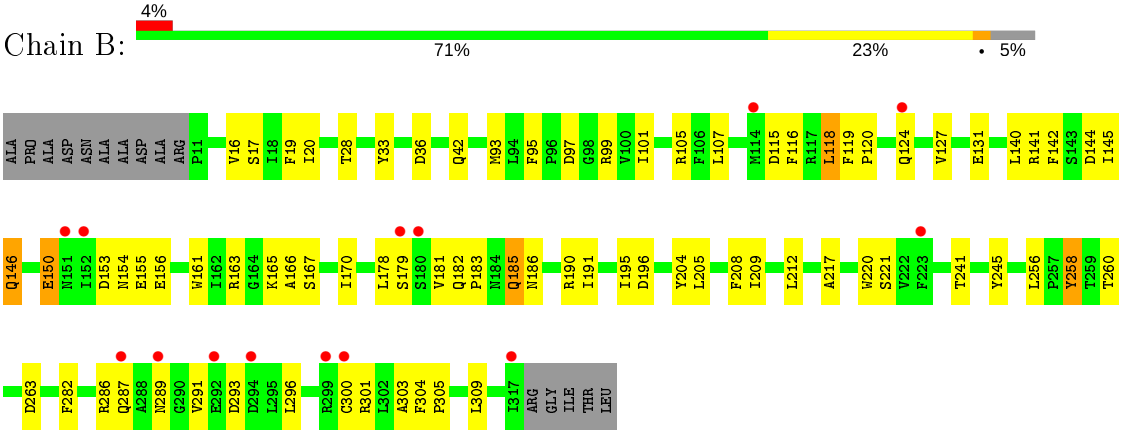
- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain A:



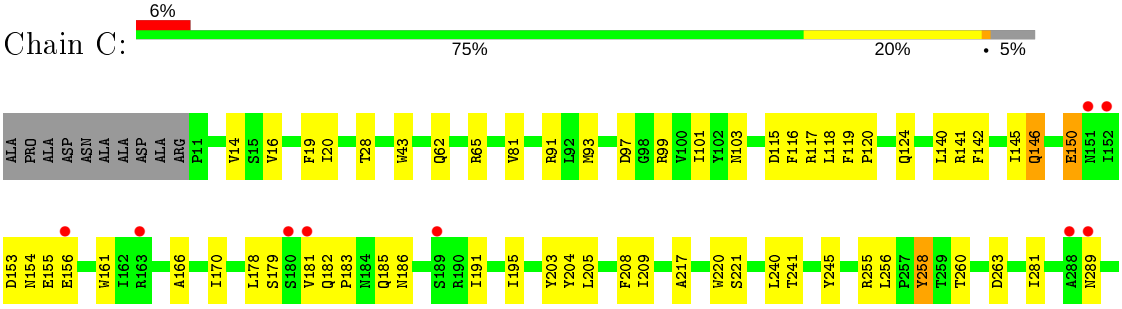
- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

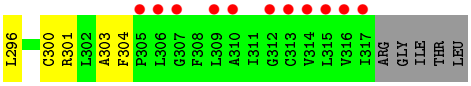
Chain B:



- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

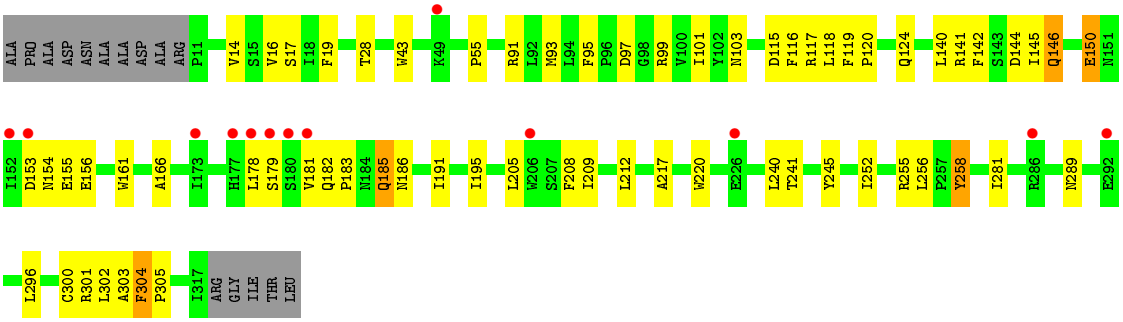
Chain C:





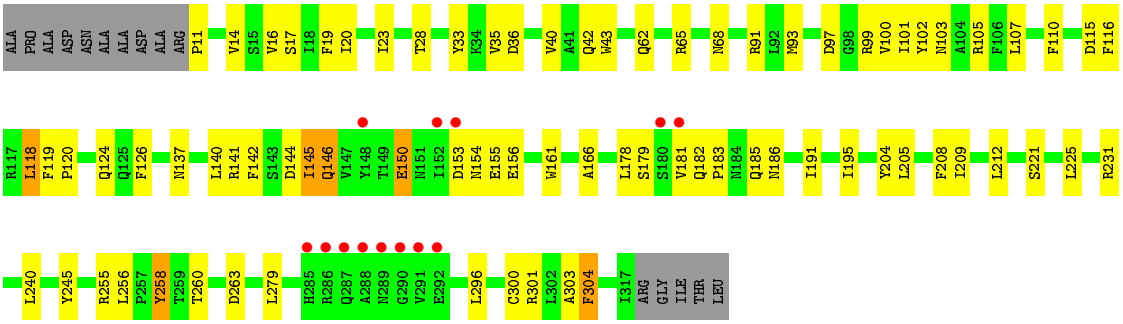
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain D:



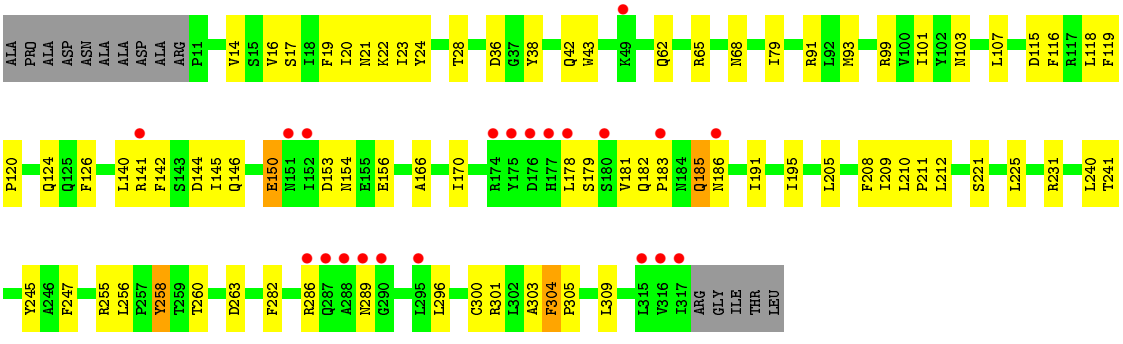
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain E:



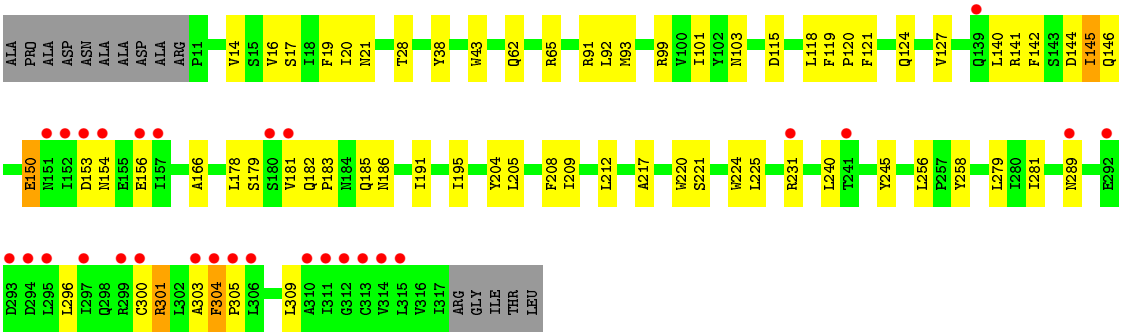
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain F:



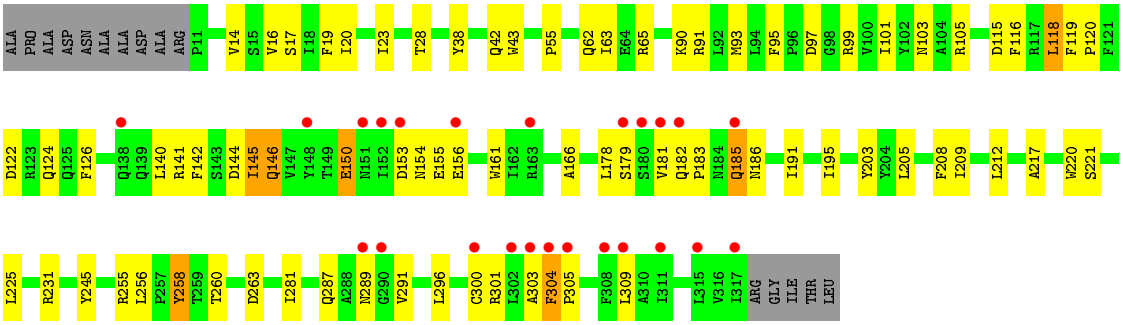
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain G:



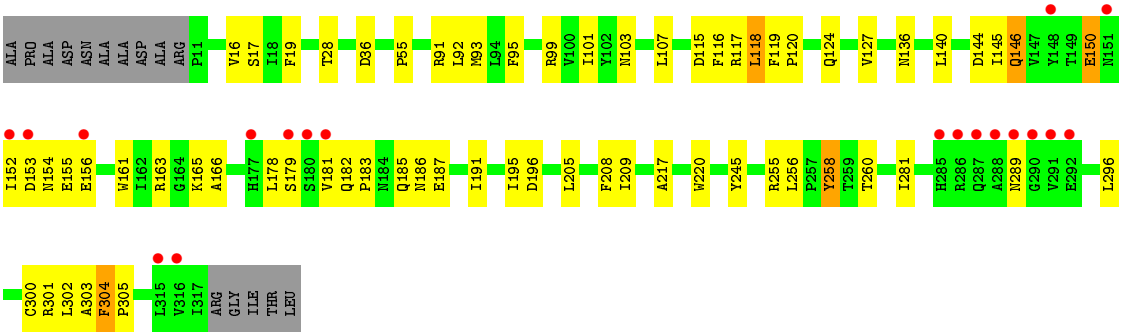
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain H:



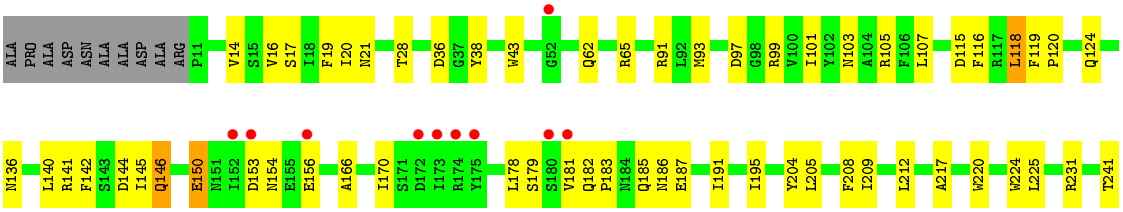
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

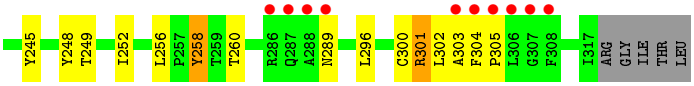
Chain I:



• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain J:




Y245
Y248
T249
I252
L256
P257
Y258
T259
T260
R286
Q287
A288
N289
L296
C300
R301
L302
A303
F304
P305
L306
G307
F308
I317
ARG
GLY
ILE
THR
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	104.95Å 266.57Å 110.69Å 90.00° 109.33° 90.00°	Depositor
Resolution (Å)	29.89 – 3.30 49.52 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.89-3.30) 99.9 (49.52-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.221 , 0.252 0.224 , 0.251	Depositor DCC
R_{free} test set	4333 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	93.6	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 62.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	25020	wwPDB-VP
Average B, all atoms (Å^2)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.26	0/2569	0.45	0/3500
1	B	0.27	0/2569	0.46	0/3500
1	C	0.26	0/2569	0.45	0/3500
1	D	0.27	0/2569	0.45	0/3500
1	E	0.26	0/2569	0.44	0/3500
1	F	0.26	0/2569	0.45	0/3500
1	G	0.27	0/2569	0.46	0/3500
1	H	0.26	0/2569	0.45	0/3500
1	I	0.27	0/2569	0.45	0/3500
1	J	0.27	0/2569	0.45	0/3500
All	All	0.27	0/25690	0.45	0/35000

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2502	0	2474	43	0
1	B	2502	0	2474	53	0
1	C	2502	0	2474	41	0
1	D	2502	0	2474	39	0
1	E	2502	0	2474	49	0
1	F	2502	0	2474	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2502	0	2474	38	0
1	H	2502	0	2474	52	0
1	I	2502	0	2474	42	0
1	J	2502	0	2474	43	0
All	All	25020	0	24740	412	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 8.

All (412) 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:B:140:LEU:HD13	1:B:191:ILE:HG13	1.71	0.71
1:A:93:MET:HB3	1:A:101:ILE:HB	1.75	0.69
1:F:115:ASP:O	1:F:124:GLN:NE2	2.25	0.67
1:H:208:PHE:O	1:H:245:TYR:OH	2.11	0.66
1:H:93:MET:HB3	1:H:101:ILE:HB	1.77	0.66
1:I:93:MET:HB3	1:I:101:ILE:HB	1.76	0.66
1:D:93:MET:HB3	1:D:101:ILE:HB	1.77	0.66
1:F:93:MET:HB3	1:F:101:ILE:HB	1.76	0.66
1:C:150:GLU:HG3	1:C:154:ASN:H	1.61	0.66
1:E:150:GLU:HG3	1:E:154:ASN:H	1.61	0.65
1:J:93:MET:HB3	1:J:101:ILE:HB	1.79	0.65
1:E:208:PHE:O	1:E:245:TYR:OH	2.15	0.65
1:C:140:LEU:HD13	1:C:191:ILE:HG13	1.78	0.64
1:C:178:LEU:HD23	1:C:182:GLN:HG3	1.80	0.64
1:E:93:MET:HB3	1:E:101:ILE:HB	1.79	0.64
1:D:140:LEU:HD13	1:D:191:ILE:HG13	1.79	0.64
1:D:300:CYS:HA	1:D:303:ALA:HB3	1.80	0.64
1:C:208:PHE:O	1:C:245:TYR:OH	2.15	0.64
1:J:28:THR:HB	1:J:256:LEU:HD21	1.79	0.64
1:C:115:ASP:O	1:C:124:GLN:NE2	2.29	0.63
1:D:28:THR:HB	1:D:256:LEU:HD21	1.81	0.63
1:F:178:LEU:HD23	1:F:182:GLN:HG3	1.81	0.63
1:H:150:GLU:HG3	1:H:154:ASN:H	1.62	0.63
1:B:150:GLU:HG3	1:B:154:ASN:H	1.62	0.63
1:E:119:PHE:HB3	1:E:120:PRO:HD3	1.82	0.62
1:I:140:LEU:HD13	1:I:191:ILE:HG13	1.80	0.62
1:A:300:CYS:HA	1:A:303:ALA:HB3	1.79	0.62
1:E:115:ASP:O	1:E:124:GLN:NE2	2.28	0.62
1:E:140:LEU:HD13	1:E:191:ILE:HG13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ALA:HB2	1:B:195:ILE:HG12	1.80	0.62
1:B:93:MET:HB3	1:B:101:ILE:HB	1.82	0.62
1:E:28:THR:HB	1:E:256:LEU:HD21	1.81	0.62
1:I:300:CYS:HA	1:I:303:ALA:HB3	1.82	0.62
1:G:115:ASP:O	1:G:124:GLN:NE2	2.26	0.62
1:G:300:CYS:HA	1:G:303:ALA:HB3	1.82	0.61
1:G:93:MET:HB3	1:G:101:ILE:HB	1.82	0.61
1:C:91:ARG:HG2	1:C:103:ASN:HB3	1.82	0.61
1:C:119:PHE:HB3	1:C:120:PRO:HD3	1.82	0.61
1:A:140:LEU:HD13	1:A:191:ILE:HG13	1.83	0.61
1:F:170:ILE:HG12	1:F:191:ILE:HG12	1.82	0.61
1:G:140:LEU:HD13	1:G:191:ILE:HG13	1.83	0.61
1:J:119:PHE:HB3	1:J:120:PRO:HD3	1.83	0.61
1:J:208:PHE:O	1:J:245:TYR:OH	2.18	0.61
1:E:155:GLU:O	1:E:161:TRP:NE1	2.31	0.61
1:H:115:ASP:O	1:H:124:GLN:NE2	2.33	0.61
1:J:140:LEU:HD13	1:J:191:ILE:HG13	1.82	0.61
1:F:140:LEU:HD13	1:F:191:ILE:HG13	1.81	0.61
1:G:150:GLU:HG3	1:G:154:ASN:H	1.66	0.61
1:A:178:LEU:HD23	1:A:182:GLN:HG3	1.83	0.60
1:H:119:PHE:HB3	1:H:120:PRO:HD3	1.83	0.60
1:B:119:PHE:HB3	1:B:120:PRO:HD3	1.83	0.60
1:C:150:GLU:HB2	1:C:153:ASP:HB3	1.83	0.60
1:I:119:PHE:HB3	1:I:120:PRO:HD3	1.84	0.60
1:E:150:GLU:HB2	1:E:153:ASP:HB3	1.83	0.60
1:E:91:ARG:HG2	1:E:103:ASN:HB3	1.82	0.60
1:F:119:PHE:HB3	1:F:120:PRO:HD3	1.83	0.60
1:I:115:ASP:O	1:I:124:GLN:NE2	2.31	0.60
1:B:170:ILE:HG12	1:B:191:ILE:HG12	1.82	0.60
1:G:119:PHE:HB3	1:G:120:PRO:HD3	1.84	0.60
1:J:205:LEU:HD12	1:J:209:ILE:HD12	1.84	0.60
1:H:140:LEU:HD13	1:H:191:ILE:HG13	1.83	0.59
1:C:19:PHE:CE2	1:C:146:GLN:HG3	2.37	0.59
1:F:91:ARG:HG2	1:F:103:ASN:HB3	1.84	0.59
1:F:300:CYS:HA	1:F:303:ALA:HB3	1.83	0.59
1:A:119:PHE:HB3	1:A:120:PRO:HD3	1.83	0.59
1:G:178:LEU:HD23	1:G:182:GLN:HG3	1.84	0.59
1:J:115:ASP:O	1:J:124:GLN:NE2	2.34	0.59
1:C:14:VAL:HG22	1:C:43:TRP:HB3	1.85	0.58
1:C:205:LEU:HD12	1:C:209:ILE:HD12	1.84	0.58
1:D:99:ARG:NH2	1:E:181:VAL:HG21	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:181:VAL:O	1:G:183:PRO:HD3	2.03	0.58
1:E:36:ASP:HB2	1:E:107:LEU:HD13	1.85	0.58
1:B:205:LEU:HD12	1:B:209:ILE:HD12	1.85	0.58
1:J:150:GLU:HG3	1:J:154:ASN:H	1.68	0.58
1:C:28:THR:HB	1:C:256:LEU:HD21	1.84	0.58
1:D:115:ASP:OD2	1:D:117:ARG:NH2	2.25	0.58
1:E:178:LEU:HD23	1:E:182:GLN:HG3	1.86	0.58
1:H:166:ALA:HB2	1:H:195:ILE:HG12	1.86	0.58
1:B:300:CYS:HA	1:B:303:ALA:HB3	1.85	0.57
1:D:119:PHE:HB3	1:D:120:PRO:HD3	1.85	0.57
1:H:28:THR:HB	1:H:256:LEU:HD21	1.87	0.57
1:C:300:CYS:HA	1:C:303:ALA:HB3	1.85	0.57
1:A:170:ILE:HG12	1:A:191:ILE:HG12	1.87	0.57
1:J:36:ASP:HB2	1:J:107:LEU:HD13	1.86	0.57
1:D:14:VAL:HG22	1:D:43:TRP:HB3	1.85	0.57
1:H:300:CYS:HA	1:H:303:ALA:HB3	1.86	0.56
1:B:208:PHE:O	1:B:245:TYR:OH	2.24	0.56
1:B:42:GLN:HE21	1:B:99:ARG:HD2	1.70	0.56
1:E:181:VAL:O	1:E:183:PRO:HD3	2.05	0.56
1:H:205:LEU:HD12	1:H:209:ILE:HD12	1.87	0.56
1:I:99:ARG:NH2	1:J:181:VAL:HG21	2.21	0.56
1:B:241:THR:HA	1:C:240:LEU:HD13	1.88	0.56
1:B:181:VAL:O	1:B:183:PRO:HD3	2.05	0.56
1:D:208:PHE:O	1:D:245:TYR:OH	2.21	0.56
1:D:150:GLU:HG3	1:D:154:ASN:H	1.71	0.56
1:E:300:CYS:HA	1:E:303:ALA:HB3	1.86	0.56
1:F:150:GLU:HG3	1:F:154:ASN:H	1.70	0.56
1:G:205:LEU:HD12	1:G:209:ILE:HD12	1.88	0.56
1:H:99:ARG:NH2	1:I:181:VAL:HG21	2.21	0.56
1:J:300:CYS:HA	1:J:303:ALA:HB3	1.88	0.56
1:A:28:THR:HB	1:A:256:LEU:HD21	1.89	0.55
1:I:19:PHE:CE2	1:I:146:GLN:HG3	2.41	0.55
1:A:99:ARG:NH2	1:B:181:VAL:HG21	2.21	0.55
1:J:181:VAL:O	1:J:183:PRO:HD3	2.06	0.55
1:E:19:PHE:CE2	1:E:146:GLN:HG3	2.41	0.55
1:A:181:VAL:O	1:A:183:PRO:HD3	2.07	0.55
1:H:150:GLU:HB2	1:H:153:ASP:HB3	1.89	0.55
1:F:19:PHE:CE2	1:F:146:GLN:HG3	2.42	0.55
1:G:150:GLU:HB2	1:G:153:ASP:HB3	1.89	0.55
1:I:181:VAL:O	1:I:183:PRO:HD3	2.07	0.55
1:F:99:ARG:NH2	1:G:181:VAL:HG21	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:181:VAL:O	1:H:183:PRO:HD3	2.06	0.54
1:G:221:SER:HB2	1:H:281:ILE:HD11	1.89	0.54
1:F:181:VAL:HG21	1:J:99:ARG:NH2	2.21	0.54
1:H:14:VAL:HG22	1:H:43:TRP:HB3	1.88	0.54
1:C:115:ASP:OD2	1:C:117:ARG:NH2	2.25	0.54
1:C:166:ALA:HB2	1:C:195:ILE:HG12	1.89	0.54
1:D:181:VAL:O	1:D:183:PRO:HD3	2.08	0.54
1:B:99:ARG:NH2	1:C:181:VAL:HG21	2.22	0.54
1:A:91:ARG:HG2	1:A:103:ASN:HB3	1.88	0.54
1:C:181:VAL:O	1:C:183:PRO:HD3	2.08	0.54
1:C:99:ARG:NH2	1:D:181:VAL:HG21	2.23	0.54
1:I:150:GLU:HG3	1:I:154:ASN:H	1.72	0.54
1:A:115:ASP:O	1:A:124:GLN:NE2	2.33	0.53
1:D:115:ASP:O	1:D:124:GLN:NE2	2.29	0.53
1:J:178:LEU:HD23	1:J:182:GLN:HG3	1.89	0.53
1:G:204:TYR:OH	1:H:255:ARG:NH1	2.42	0.53
1:B:28:THR:HB	1:B:256:LEU:HD21	1.89	0.53
1:B:150:GLU:HB2	1:B:153:ASP:HB3	1.91	0.53
1:E:225:LEU:HB2	1:E:231:ARG:HG3	1.90	0.53
1:G:166:ALA:HB2	1:G:195:ILE:HG12	1.91	0.53
1:A:62:GLN:HA	1:A:65:ARG:HG3	1.90	0.52
1:G:225:LEU:HB2	1:G:231:ARG:HG3	1.90	0.52
1:A:42:GLN:HE21	1:A:99:ARG:HD2	1.73	0.52
1:A:42:GLN:NE2	1:A:99:ARG:HD2	2.24	0.52
1:A:81:VAL:O	1:E:105:ARG:NH2	2.42	0.52
1:I:205:LEU:HD12	1:I:209:ILE:HD12	1.91	0.52
1:H:178:LEU:HD23	1:H:182:GLN:HG3	1.90	0.52
1:A:166:ALA:HB2	1:A:195:ILE:HG12	1.91	0.52
1:A:14:VAL:HG22	1:A:43:TRP:HB3	1.91	0.52
1:C:93:MET:HB3	1:C:101:ILE:HB	1.92	0.52
1:D:91:ARG:HG2	1:D:103:ASN:HB3	1.92	0.52
1:B:42:GLN:NE2	1:B:99:ARG:HD2	2.26	0.51
1:A:281:ILE:HD11	1:E:221:SER:HB2	1.91	0.51
1:A:181:VAL:HG21	1:E:99:ARG:NH2	2.25	0.51
1:D:166:ALA:HB2	1:D:195:ILE:HG12	1.92	0.51
1:F:181:VAL:O	1:F:183:PRO:HD3	2.09	0.51
1:B:167:SER:HB3	1:I:165:LYS:HG3	1.92	0.51
1:I:28:THR:HB	1:I:256:LEU:HD21	1.92	0.51
1:D:205:LEU:HD12	1:D:209:ILE:HD12	1.93	0.51
1:B:19:PHE:CE2	1:B:146:GLN:HG3	2.46	0.51
1:A:205:LEU:HD12	1:A:209:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:208:PHE:O	1:G:245:TYR:OH	2.26	0.51
1:J:91:ARG:HG2	1:J:103:ASN:HB3	1.93	0.51
1:J:150:GLU:HB2	1:J:153:ASP:HB3	1.93	0.51
1:B:155:GLU:O	1:B:161:TRP:NE1	2.42	0.51
1:D:116:PHE:HB2	1:D:258:TYR:HE1	1.75	0.51
1:I:115:ASP:OD2	1:I:117:ARG:NH2	2.24	0.51
1:B:165:LYS:NZ	1:I:196:ASP:HB2	2.26	0.50
1:B:204:TYR:OH	1:C:255:ARG:NH1	2.44	0.50
1:B:165:LYS:HZ2	1:I:196:ASP:HB2	1.76	0.50
1:F:42:GLN:HE21	1:F:99:ARG:HD2	1.76	0.50
1:I:36:ASP:HB2	1:I:107:LEU:HD13	1.93	0.50
1:I:95:PHE:HB2	1:I:99:ARG:HB2	1.93	0.50
1:J:17:SER:HA	1:J:144:ASP:O	2.12	0.50
1:F:221:SER:HB2	1:G:281:ILE:HD11	1.94	0.50
1:H:42:GLN:HE21	1:H:99:ARG:HD2	1.75	0.50
1:B:196:ASP:OD2	1:I:165:LYS:HD3	2.11	0.50
1:F:28:THR:HB	1:F:256:LEU:HD21	1.93	0.50
1:G:121:PHE:CE1	1:G:205:LEU:HD11	2.47	0.50
1:G:91:ARG:HG2	1:G:103:ASN:HB3	1.93	0.49
1:H:38:TYR:CZ	1:H:105:ARG:HD3	2.46	0.49
1:B:217:ALA:HA	1:B:220:TRP:CE3	2.47	0.49
1:B:119:PHE:HB2	1:B:260:THR:HB	1.93	0.49
1:A:182:GLN:CD	1:A:182:GLN:H	2.15	0.49
1:F:255:ARG:NH1	1:J:204:TYR:OH	2.46	0.49
1:H:42:GLN:NE2	1:H:99:ARG:HD2	2.27	0.49
1:C:119:PHE:HB2	1:C:260:THR:HB	1.93	0.49
1:I:116:PHE:HB2	1:I:258:TYR:HE1	1.78	0.49
1:A:208:PHE:O	1:A:245:TYR:OH	2.26	0.49
1:B:116:PHE:HB2	1:B:258:TYR:HE1	1.77	0.49
1:E:166:ALA:HB2	1:E:195:ILE:HG12	1.95	0.49
1:A:97:ASP:OD2	1:A:99:ARG:NH1	2.46	0.49
1:B:115:ASP:O	1:B:124:GLN:NE2	2.42	0.49
1:E:62:GLN:HA	1:E:65:ARG:HG3	1.93	0.49
1:A:186:ASN:OD1	1:A:186:ASN:N	2.46	0.48
1:H:91:ARG:HG2	1:H:103:ASN:HB3	1.94	0.48
1:I:186:ASN:OD1	1:I:186:ASN:N	2.46	0.48
1:J:166:ALA:HB2	1:J:195:ILE:HG12	1.95	0.48
1:E:97:ASP:OD2	1:E:99:ARG:NH1	2.47	0.48
1:H:260:THR:H	1:H:263:ASP:HB2	1.77	0.48
1:C:170:ILE:HG12	1:C:191:ILE:HG12	1.93	0.48
1:H:119:PHE:HB2	1:H:260:THR:HB	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:178:LEU:HD23	1:I:182:GLN:HG3	1.95	0.48
1:A:150:GLU:HG3	1:A:154:ASN:H	1.78	0.48
1:E:141:ARG:HG2	1:E:142:PHE:CD2	2.48	0.48
1:F:23:ILE:HG21	1:F:126:PHE:CD2	2.48	0.48
1:F:116:PHE:HB2	1:F:258:TYR:HE1	1.78	0.48
1:A:36:ASP:HB2	1:A:107:LEU:HD13	1.96	0.48
1:F:141:ARG:HG2	1:F:142:PHE:HD2	1.77	0.48
1:B:17:SER:HA	1:B:144:ASP:O	2.14	0.48
1:J:186:ASN:N	1:J:186:ASN:OD1	2.46	0.48
1:E:182:GLN:H	1:E:182:GLN:CD	2.17	0.48
1:G:182:GLN:CD	1:G:182:GLN:H	2.17	0.48
1:B:178:LEU:HD23	1:B:182:GLN:HG3	1.95	0.48
1:D:150:GLU:HB2	1:D:153:ASP:HB3	1.94	0.48
1:I:17:SER:HA	1:I:144:ASP:O	2.14	0.47
1:C:241:THR:HA	1:D:240:LEU:HD13	1.96	0.47
1:A:255:ARG:NH1	1:E:204:TYR:OH	2.47	0.47
1:J:225:LEU:HB2	1:J:231:ARG:HG3	1.96	0.47
1:F:182:GLN:H	1:F:182:GLN:CD	2.16	0.47
1:F:240:LEU:HD13	1:J:241:THR:HA	1.96	0.47
1:A:121:PHE:CE1	1:A:205:LEU:HD11	2.50	0.47
1:F:205:LEU:HD12	1:F:209:ILE:HD12	1.95	0.47
1:G:99:ARG:NH2	1:H:181:VAL:HG21	2.29	0.47
1:F:36:ASP:HB2	1:F:107:LEU:HD13	1.96	0.47
1:C:182:GLN:CD	1:C:182:GLN:H	2.17	0.47
1:J:38:TYR:CZ	1:J:105:ARG:HD3	2.49	0.47
1:A:21:ASN:HD21	1:A:38:TYR:HE1	1.63	0.47
1:D:19:PHE:CE2	1:D:146:GLN:HG3	2.50	0.47
1:E:119:PHE:HB2	1:E:260:THR:HB	1.96	0.47
1:G:21:ASN:HD21	1:G:38:TYR:HE1	1.61	0.47
1:B:182:GLN:CD	1:B:182:GLN:H	2.16	0.47
1:J:62:GLN:HA	1:J:65:ARG:HG3	1.96	0.47
1:D:178:LEU:HD23	1:D:182:GLN:HG3	1.96	0.47
1:H:186:ASN:OD1	1:H:186:ASN:N	2.47	0.47
1:E:186:ASN:OD1	1:E:186:ASN:N	2.48	0.47
1:F:42:GLN:NE2	1:F:99:ARG:HD2	2.29	0.47
1:H:20:ILE:HD12	1:H:195:ILE:HD11	1.97	0.47
1:D:182:GLN:H	1:D:182:GLN:CD	2.17	0.47
1:H:212:LEU:HB2	1:H:245:TYR:CE2	2.50	0.47
1:B:221:SER:HB2	1:C:281:ILE:HD11	1.96	0.46
1:D:186:ASN:OD1	1:D:186:ASN:N	2.46	0.46
1:E:17:SER:HA	1:E:144:ASP:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:186:ASN:N	1:F:186:ASN:OD1	2.47	0.46
1:H:155:GLU:O	1:H:161:TRP:NE1	2.48	0.46
1:H:19:PHE:CE2	1:H:146:GLN:HG3	2.50	0.46
1:J:14:VAL:HG22	1:J:43:TRP:HB3	1.96	0.46
1:H:221:SER:HB2	1:I:281:ILE:HD11	1.98	0.46
1:E:205:LEU:HD12	1:E:209:ILE:HD12	1.98	0.46
1:G:17:SER:HA	1:G:144:ASP:O	2.15	0.46
1:H:116:PHE:HB2	1:H:258:TYR:HE1	1.78	0.46
1:H:141:ARG:HG2	1:H:142:PHE:CD2	2.50	0.46
1:F:21:ASN:HD21	1:F:38:TYR:HE1	1.63	0.46
1:A:212:LEU:HB2	1:A:245:TYR:CE2	2.50	0.46
1:F:208:PHE:O	1:F:245:TYR:OH	2.27	0.46
1:B:282:PHE:CZ	1:B:286:ARG:HG3	2.51	0.46
1:F:65:ARG:HA	1:F:68:ASN:ND2	2.29	0.46
1:G:14:VAL:HG22	1:G:43:TRP:HB3	1.98	0.46
1:I:182:GLN:H	1:I:182:GLN:CD	2.19	0.46
1:B:185:GLN:OE1	1:B:185:GLN:N	2.44	0.46
1:G:224:TRP:CE2	1:G:301:ARG:HG2	2.50	0.46
1:D:252:ILE:HG23	1:E:255:ARG:HB2	1.98	0.46
1:E:260:THR:H	1:E:263:ASP:HB2	1.81	0.46
1:J:182:GLN:CD	1:J:182:GLN:H	2.19	0.46
1:I:166:ALA:HB2	1:I:195:ILE:HG12	1.98	0.46
1:J:119:PHE:HB2	1:J:260:THR:HB	1.98	0.46
1:B:97:ASP:OD2	1:B:99:ARG:NH1	2.49	0.45
1:C:155:GLU:O	1:C:161:TRP:NE1	2.47	0.45
1:F:150:GLU:HB2	1:F:153:ASP:HB3	1.97	0.45
1:B:186:ASN:OD1	1:B:186:ASN:N	2.48	0.45
1:D:155:GLU:O	1:D:161:TRP:NE1	2.46	0.45
1:G:28:THR:HB	1:G:256:LEU:HD21	1.96	0.45
1:J:19:PHE:CE2	1:J:146:GLN:HG3	2.51	0.45
1:G:186:ASN:OD1	1:G:186:ASN:N	2.48	0.45
1:H:17:SER:HA	1:H:144:ASP:O	2.17	0.45
1:J:116:PHE:HB2	1:J:258:TYR:HE1	1.82	0.45
1:B:291:VAL:HG12	1:B:293:ASP:H	1.80	0.45
1:C:178:LEU:HA	1:C:178:LEU:HD12	1.83	0.45
1:E:141:ARG:HG2	1:E:142:PHE:HD2	1.81	0.45
1:I:150:GLU:HB2	1:I:153:ASP:HB3	1.99	0.45
1:I:118:LEU:HD12	1:I:118:LEU:H	1.82	0.45
1:B:260:THR:H	1:B:263:ASP:HB2	1.82	0.45
1:F:62:GLN:HA	1:F:65:ARG:HG3	1.99	0.45
1:J:21:ASN:HD21	1:J:38:TYR:HE1	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ARG:HH11	1:I:152:ILE:HD12	1.82	0.45
1:E:279:LEU:HD22	1:E:304:PHE:CE1	2.52	0.45
1:A:185:GLN:N	1:A:185:GLN:OE1	2.44	0.44
1:B:20:ILE:HD12	1:B:195:ILE:HD11	1.98	0.44
1:B:36:ASP:HB2	1:B:107:LEU:HD13	2.00	0.44
1:J:136:ASN:HB2	1:J:187:GLU:O	2.17	0.44
1:A:38:TYR:CZ	1:A:105:ARG:HD3	2.52	0.44
1:C:221:SER:HB2	1:D:281:ILE:HD11	1.99	0.44
1:F:225:LEU:HB2	1:F:231:ARG:HG3	1.98	0.44
1:C:141:ARG:HG2	1:C:142:PHE:CD2	2.52	0.44
1:G:217:ALA:HA	1:G:220:TRP:CE3	2.52	0.44
1:I:300:CYS:O	1:I:304:PHE:HB2	2.17	0.44
1:J:20:ILE:HD12	1:J:195:ILE:HD11	1.99	0.44
1:C:186:ASN:N	1:C:186:ASN:OD1	2.48	0.44
1:F:166:ALA:HB2	1:F:195:ILE:HG12	2.00	0.44
1:F:300:CYS:O	1:F:304:PHE:HB2	2.17	0.44
1:H:141:ARG:HG2	1:H:142:PHE:HD2	1.81	0.44
1:B:305:PRO:O	1:B:309:LEU:HG	2.17	0.44
1:D:141:ARG:HG2	1:D:142:PHE:CD2	2.52	0.44
1:E:33:TYR:CE1	1:E:110:PHE:HB2	2.53	0.44
1:C:260:THR:H	1:C:263:ASP:HB2	1.82	0.44
1:D:185:GLN:N	1:D:185:GLN:OE1	2.43	0.44
1:G:92:LEU:HD23	1:G:92:LEU:HA	1.91	0.44
1:I:119:PHE:HB2	1:I:260:THR:HB	2.00	0.44
1:A:121:PHE:HE1	1:A:205:LEU:HD11	1.83	0.43
1:D:300:CYS:O	1:D:304:PHE:HB2	2.17	0.43
1:E:23:ILE:HG21	1:E:126:PHE:CD2	2.53	0.43
1:E:65:ARG:HA	1:E:68:ASN:ND2	2.33	0.43
1:H:300:CYS:O	1:H:304:PHE:HB2	2.18	0.43
1:I:19:PHE:CD2	1:I:146:GLN:HG3	2.53	0.43
1:C:20:ILE:HD12	1:C:195:ILE:HD11	2.00	0.43
1:G:145:ILE:O	1:G:145:ILE:HG13	2.18	0.43
1:G:19:PHE:CE2	1:G:146:GLN:HG3	2.53	0.43
1:H:185:GLN:OE1	1:H:185:GLN:N	2.43	0.43
1:A:42:GLN:HA	1:A:100:VAL:O	2.19	0.43
1:J:97:ASP:OD2	1:J:99:ARG:NH1	2.52	0.43
1:B:105:ARG:NH2	1:C:81:VAL:O	2.51	0.43
1:F:305:PRO:O	1:F:309:LEU:HG	2.18	0.43
1:I:92:LEU:HD23	1:I:92:LEU:HA	1.91	0.43
1:G:212:LEU:HB2	1:G:245:TYR:CE2	2.53	0.43
1:C:97:ASP:OD2	1:C:99:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:LEU:HD12	1:E:118:LEU:H	1.84	0.43
1:E:178:LEU:HD12	1:E:178:LEU:HA	1.84	0.43
1:J:208:PHE:CE1	1:J:249:THR:HA	2.53	0.43
1:E:40:VAL:HA	1:E:102:TYR:O	2.19	0.43
1:H:182:GLN:CD	1:H:182:GLN:H	2.21	0.43
1:C:204:TYR:O	1:C:208:PHE:HB2	2.18	0.43
1:G:141:ARG:HG2	1:G:142:PHE:CD2	2.54	0.43
1:H:55:PRO:HB3	1:H:95:PHE:CD1	2.54	0.43
1:H:118:LEU:O	1:H:122:ASP:N	2.52	0.43
1:B:33:TYR:OH	1:B:127:VAL:N	2.46	0.43
1:D:217:ALA:HA	1:D:220:TRP:CE3	2.54	0.42
1:D:93:MET:HG2	1:D:95:PHE:CE2	2.54	0.42
1:E:14:VAL:HG22	1:E:43:TRP:HB3	2.01	0.42
1:F:20:ILE:HD12	1:F:195:ILE:HD11	2.00	0.42
1:F:212:LEU:HB2	1:F:245:TYR:CE2	2.54	0.42
1:A:202:SER:O	1:A:206:TRP:HD1	2.03	0.42
1:F:185:GLN:OE1	1:F:185:GLN:N	2.43	0.42
1:H:305:PRO:O	1:H:309:LEU:HG	2.19	0.42
1:B:165:LYS:HD3	1:I:163:ARG:HB3	2.01	0.42
1:C:141:ARG:HG2	1:C:142:PHE:HD2	1.85	0.42
1:F:241:THR:HA	1:G:240:LEU:HD13	2.02	0.42
1:H:225:LEU:HB2	1:H:231:ARG:HG3	2.01	0.42
1:H:23:ILE:HG21	1:H:126:PHE:CD2	2.54	0.42
1:I:136:ASN:HB2	1:I:187:GLU:O	2.19	0.42
1:J:141:ARG:HG2	1:J:142:PHE:CD2	2.54	0.42
1:E:116:PHE:HB2	1:E:258:TYR:HE1	1.84	0.42
1:J:217:ALA:HA	1:J:220:TRP:CE3	2.54	0.42
1:A:20:ILE:HD12	1:A:195:ILE:HD11	2.01	0.42
1:A:217:ALA:HA	1:A:220:TRP:CE3	2.55	0.42
1:D:141:ARG:HG2	1:D:142:PHE:HD2	1.84	0.42
1:D:97:ASP:OD2	1:D:99:ARG:NH1	2.52	0.42
1:F:119:PHE:HB2	1:F:260:THR:HB	2.02	0.42
1:B:119:PHE:CB	1:B:260:THR:HB	2.49	0.42
1:B:141:ARG:HG2	1:B:142:PHE:CD2	2.55	0.42
1:C:62:GLN:HA	1:C:65:ARG:HG3	2.02	0.42
1:D:55:PRO:HB3	1:D:95:PHE:CD1	2.54	0.42
1:E:20:ILE:HD12	1:E:195:ILE:HD11	2.02	0.42
1:F:178:LEU:HD12	1:F:178:LEU:HA	1.84	0.42
1:F:14:VAL:HG22	1:F:43:TRP:HB3	2.02	0.42
1:A:17:SER:HA	1:A:144:ASP:O	2.20	0.42
1:D:17:SER:HA	1:D:144:ASP:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:THR:HA	1:E:240:LEU:HD13	2.01	0.42
1:H:19:PHE:CD2	1:H:146:GLN:HG3	2.55	0.42
1:H:95:PHE:HE2	1:H:101:ILE:HD12	1.85	0.42
1:C:217:ALA:HA	1:C:220:TRP:CE3	2.55	0.42
1:I:302:LEU:C	1:I:305:PRO:HD2	2.40	0.42
1:E:145:ILE:O	1:E:145:ILE:HG13	2.19	0.41
1:I:55:PRO:HB3	1:I:95:PHE:CD1	2.54	0.41
1:B:131:GLU:OE2	1:B:190:ARG:NE	2.43	0.41
1:G:305:PRO:O	1:G:309:LEU:HG	2.19	0.41
1:I:91:ARG:HG2	1:I:103:ASN:HB3	2.01	0.41
1:A:55:PRO:HB3	1:A:95:PHE:CD1	2.55	0.41
1:A:95:PHE:HB2	1:A:99:ARG:HB2	2.02	0.41
1:E:11:PRO:HA	1:E:137:ASN:O	2.21	0.41
1:F:22:LYS:HE3	1:F:24:TYR:CD1	2.55	0.41
1:F:79:ILE:HA	1:F:79:ILE:HD13	1.91	0.41
1:G:62:GLN:HA	1:G:65:ARG:HG3	2.02	0.41
1:H:217:ALA:HA	1:H:220:TRP:CE3	2.55	0.41
1:H:203:TYR:CE2	1:I:255:ARG:HG3	2.56	0.41
1:B:118:LEU:HD12	1:B:118:LEU:H	1.85	0.41
1:B:287:GLN:HG3	1:B:293:ASP:HB2	2.02	0.41
1:B:95:PHE:HB2	1:B:99:ARG:HB2	2.03	0.41
1:E:212:LEU:HB2	1:E:245:TYR:CE2	2.56	0.41
1:G:20:ILE:HD12	1:G:195:ILE:HD11	2.02	0.41
1:H:95:PHE:HB2	1:H:99:ARG:HB2	2.02	0.41
1:J:118:LEU:H	1:J:118:LEU:HD12	1.85	0.41
1:J:302:LEU:C	1:J:305:PRO:HD2	2.41	0.41
1:B:212:LEU:HB2	1:B:245:TYR:CE2	2.56	0.41
1:C:203:TYR:CE2	1:D:255:ARG:HG3	2.56	0.41
1:G:279:LEU:HD22	1:G:304:PHE:CE1	2.55	0.41
1:I:208:PHE:O	1:I:245:TYR:OH	2.32	0.41
1:J:224:TRP:CE2	1:J:301:ARG:HG2	2.55	0.41
1:A:19:PHE:CE2	1:A:146:GLN:HG3	2.56	0.41
1:F:260:THR:H	1:F:263:ASP:HB2	1.86	0.41
1:H:145:ILE:O	1:H:145:ILE:HG13	2.21	0.41
1:A:118:LEU:H	1:A:118:LEU:HD12	1.86	0.41
1:A:40:VAL:HA	1:A:102:TYR:O	2.20	0.41
1:F:17:SER:HA	1:F:144:ASP:O	2.21	0.41
1:I:217:ALA:HA	1:I:220:TRP:CE3	2.56	0.41
1:D:212:LEU:HB2	1:D:245:TYR:CE2	2.56	0.41
1:E:42:GLN:HA	1:E:100:VAL:O	2.21	0.41
1:J:170:ILE:HG12	1:J:191:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:212:LEU:HB2	1:J:245:TYR:CE2	2.56	0.41
1:E:35:VAL:HB	1:E:110:PHE:CE1	2.56	0.40
1:H:287:GLN:CB	1:H:291:VAL:HB	2.51	0.40
1:H:62:GLN:HA	1:H:65:ARG:HG3	2.03	0.40
1:I:155:GLU:O	1:I:161:TRP:NE1	2.51	0.40
1:B:178:LEU:HA	1:B:178:LEU:HD12	1.84	0.40
1:C:116:PHE:HB2	1:C:258:TYR:HE1	1.87	0.40
1:F:210:LEU:HB3	1:F:211:PRO:HD3	2.03	0.40
1:F:282:PHE:CZ	1:F:286:ARG:HG3	2.56	0.40
1:D:302:LEU:C	1:D:305:PRO:HD2	2.42	0.40
1:F:247:PHE:CD1	1:J:248:TYR:HA	2.56	0.40
1:H:97:ASP:OD2	1:H:99:ARG:NH1	2.55	0.40
1:F:255:ARG:HB2	1:J:252:ILE:HG23	2.04	0.40
1:H:63:ILE:HD12	1:H:90:LYS:HG3	2.03	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	305/322 (95%)	288 (94%)	16 (5%)	1 (0%)	41	71
1	B	305/322 (95%)	288 (94%)	16 (5%)	1 (0%)	41	71
1	C	305/322 (95%)	288 (94%)	16 (5%)	1 (0%)	41	71
1	D	305/322 (95%)	289 (95%)	15 (5%)	1 (0%)	41	71
1	E	305/322 (95%)	288 (94%)	16 (5%)	1 (0%)	41	71
1	F	305/322 (95%)	289 (95%)	15 (5%)	1 (0%)	41	71
1	G	305/322 (95%)	288 (94%)	16 (5%)	1 (0%)	41	71
1	H	305/322 (95%)	288 (94%)	16 (5%)	1 (0%)	41	71
1	I	305/322 (95%)	288 (94%)	16 (5%)	1 (0%)	41	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	J	305/322 (95%)	287 (94%)	17 (6%)	1 (0%)	41 71
All	All	3050/3220 (95%)	2881 (94%)	159 (5%)	10 (0%)	41 71

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	179	SER
1	A	179	SER
1	B	179	SER
1	C	179	SER
1	D	179	SER
1	E	179	SER
1	F	179	SER
1	G	179	SER
1	I	179	SER
1	J	179	SER

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	274/283 (97%)	263 (96%)	11 (4%)	31 61
1	B	274/283 (97%)	262 (96%)	12 (4%)	28 59
1	C	274/283 (97%)	262 (96%)	12 (4%)	28 59
1	D	274/283 (97%)	262 (96%)	12 (4%)	28 59
1	E	274/283 (97%)	263 (96%)	11 (4%)	31 61
1	F	274/283 (97%)	263 (96%)	11 (4%)	31 61
1	G	274/283 (97%)	262 (96%)	12 (4%)	28 59
1	H	274/283 (97%)	262 (96%)	12 (4%)	28 59
1	I	274/283 (97%)	261 (95%)	13 (5%)	26 57
1	J	274/283 (97%)	262 (96%)	12 (4%)	28 59
All	All	2740/2830 (97%)	2622 (96%)	118 (4%)	29 59

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	118	LEU
1	A	145	ILE
1	A	150	GLU
1	A	156	GLU
1	A	185	GLN
1	A	258	TYR
1	A	289	ASN
1	A	296	LEU
1	A	301	ARG
1	A	304	PHE
1	B	16	VAL
1	B	118	LEU
1	B	145	ILE
1	B	146	GLN
1	B	150	GLU
1	B	156	GLU
1	B	185	GLN
1	B	258	TYR
1	B	289	ASN
1	B	296	LEU
1	B	301	ARG
1	B	304	PHE
1	C	16	VAL
1	C	118	LEU
1	C	145	ILE
1	C	146	GLN
1	C	150	GLU
1	C	156	GLU
1	C	185	GLN
1	C	258	TYR
1	C	289	ASN
1	C	296	LEU
1	C	301	ARG
1	C	304	PHE
1	D	16	VAL
1	D	118	LEU
1	D	145	ILE
1	D	146	GLN
1	D	150	GLU
1	D	156	GLU
1	D	185	GLN

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Mol	Chain	Res	Type
1	D	258	TYR
1	D	289	ASN
1	D	296	LEU
1	D	301	ARG
1	D	304	PHE
1	E	16	VAL
1	E	118	LEU
1	E	145	ILE
1	E	146	GLN
1	E	150	GLU
1	E	156	GLU
1	E	185	GLN
1	E	258	TYR
1	E	296	LEU
1	E	301	ARG
1	E	304	PHE
1	F	16	VAL
1	F	118	LEU
1	F	145	ILE
1	F	150	GLU
1	F	156	GLU
1	F	185	GLN
1	F	258	TYR
1	F	289	ASN
1	F	296	LEU
1	F	301	ARG
1	F	304	PHE
1	G	16	VAL
1	G	118	LEU
1	G	127	VAL
1	G	145	ILE
1	G	150	GLU
1	G	156	GLU
1	G	185	GLN
1	G	258	TYR
1	G	289	ASN
1	G	296	LEU
1	G	301	ARG
1	G	304	PHE
1	H	16	VAL
1	H	118	LEU
1	H	145	ILE

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Mol	Chain	Res	Type
1	H	146	GLN
1	H	150	GLU
1	H	156	GLU
1	H	185	GLN
1	H	258	TYR
1	H	289	ASN
1	H	296	LEU
1	H	301	ARG
1	H	304	PHE
1	I	16	VAL
1	I	118	LEU
1	I	127	VAL
1	I	145	ILE
1	I	146	GLN
1	I	150	GLU
1	I	156	GLU
1	I	185	GLN
1	I	258	TYR
1	I	289	ASN
1	I	296	LEU
1	I	301	ARG
1	I	304	PHE
1	J	16	VAL
1	J	118	LEU
1	J	145	ILE
1	J	146	GLN
1	J	150	GLU
1	J	156	GLU
1	J	185	GLN
1	J	258	TYR
1	J	289	ASN
1	J	296	LEU
1	J	301	ARG
1	J	304	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	B	42	GLN
1	F	42	GLN
1	H	42	GLN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	307/322 (95%)	-0.03	12 (3%)	39	37	52, 98, 193, 283	0
1	B	307/322 (95%)	0.22	14 (4%)	32	30	57, 93, 201, 263	0
1	C	307/322 (95%)	0.16	20 (6%)	18	18	53, 94, 211, 347	0
1	D	307/322 (95%)	0.11	13 (4%)	36	34	46, 94, 192, 270	0
1	E	307/322 (95%)	-0.03	13 (4%)	36	34	57, 97, 184, 303	0
1	F	307/322 (95%)	0.10	21 (6%)	17	17	59, 102, 186, 254	0
1	G	307/322 (95%)	0.24	29 (9%)	8	9	53, 91, 207, 272	0
1	H	307/322 (95%)	0.28	24 (7%)	13	12	57, 95, 201, 297	0
1	I	307/322 (95%)	0.05	19 (6%)	20	20	53, 94, 196, 306	0
1	J	307/322 (95%)	0.11	20 (6%)	18	18	64, 103, 224, 277	0
All	All	3070/3220 (95%)	0.12	185 (6%)	21	21	46, 96, 202, 347	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	152	ILE	16.3
1	C	181	VAL	14.0
1	E	289	ASN	13.2
1	H	180	SER	13.1
1	H	181	VAL	11.4
1	C	289	ASN	11.1
1	A	152	ILE	9.8
1	J	152	ILE	9.7
1	I	289	ASN	9.6
1	D	180	SER	8.8
1	C	180	SER	8.2
1	D	179	SER	7.7
1	G	180	SER	7.1

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Mol	Chain	Res	Type	RSRZ
1	A	151	ASN	7.1
1	H	289	ASN	7.0
1	B	152	ILE	6.8
1	H	151	ASN	6.8
1	I	288	ALA	6.8
1	E	180	SER	6.4
1	C	313	CYS	6.4
1	E	290	GLY	6.2
1	I	287	GLN	6.1
1	F	317	ILE	6.1
1	A	153	ASP	6.0
1	F	152	ILE	5.9
1	G	152	ILE	5.8
1	C	317	ILE	5.7
1	G	292	GLU	5.7
1	G	313	CYS	5.7
1	E	287	GLN	5.6
1	C	306	LEU	5.6
1	G	304	PHE	5.6
1	I	180	SER	5.6
1	C	152	ILE	5.4
1	H	156	GLU	5.2
1	J	305	PRO	5.2
1	J	153	ASP	5.1
1	G	156	GLU	5.1
1	F	177	HIS	5.1
1	B	180	SER	5.1
1	B	317	ILE	5.0
1	J	289	ASN	5.0
1	E	288	ALA	4.9
1	I	181	VAL	4.9
1	D	226	GLU	4.9
1	G	289	ASN	4.8
1	A	175	TYR	4.7
1	J	181	VAL	4.7
1	D	177	HIS	4.7
1	G	315	LEU	4.7
1	J	304	PHE	4.6
1	I	153	ASP	4.6
1	I	286	ARG	4.6
1	B	300	CYS	4.3
1	F	151	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	174	ARG	4.2
1	C	151	ASN	4.2
1	J	156	GLU	4.2
1	H	315	LEU	4.2
1	I	179	SER	4.2
1	G	305	PRO	4.2
1	F	287	GLN	4.1
1	C	316	VAL	4.1
1	C	305	PRO	4.0
1	H	304	PHE	4.0
1	F	178	LEU	4.0
1	I	148	TYR	3.9
1	D	181	VAL	3.9
1	G	157	ILE	3.9
1	F	289	ASN	3.9
1	I	285	HIS	3.9
1	B	299	ARG	3.8
1	F	288	ALA	3.7
1	H	153	ASP	3.7
1	F	180	SER	3.7
1	G	294	ASP	3.6
1	I	291	VAL	3.6
1	I	177	HIS	3.5
1	I	292	GLU	3.5
1	G	314	VAL	3.5
1	E	152	ILE	3.5
1	G	153	ASP	3.4
1	H	179	SER	3.4
1	F	290	GLY	3.4
1	I	290	GLY	3.4
1	E	291	VAL	3.4
1	H	185	GLN	3.4
1	G	312	GLY	3.3
1	B	151	ASN	3.3
1	I	151	ASN	3.3
1	C	314	VAL	3.3
1	H	290	GLY	3.3
1	C	288	ALA	3.3
1	C	315	LEU	3.2
1	E	292	GLU	3.2
1	G	151	ASN	3.2
1	G	306	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	148	TYR	3.1
1	D	153	ASP	3.1
1	G	303	ALA	3.1
1	G	300	CYS	3.1
1	E	181	VAL	3.1
1	C	310	ALA	3.1
1	D	206	TRP	3.1
1	H	302	LEU	3.0
1	H	138	GLN	3.0
1	B	294	ASP	3.0
1	B	289	ASN	3.0
1	J	172	ASP	2.9
1	H	317	ILE	2.9
1	I	152	ILE	2.9
1	C	156	GLU	2.9
1	F	175	TYR	2.9
1	E	153	ASP	2.8
1	D	152	ILE	2.8
1	H	308	PHE	2.8
1	A	156	GLU	2.8
1	J	303	ALA	2.8
1	D	286	ARG	2.8
1	G	311	ILE	2.7
1	A	315	LEU	2.7
1	J	306	LEU	2.7
1	C	309	LEU	2.7
1	I	315	LEU	2.7
1	C	163	ARG	2.7
1	J	173	ILE	2.7
1	C	312	GLY	2.7
1	B	223	PHE	2.7
1	H	303	ALA	2.6
1	A	317	ILE	2.6
1	D	292	GLU	2.6
1	J	175	TYR	2.6
1	F	316	VAL	2.6
1	G	293	ASP	2.6
1	J	286	ARG	2.5
1	F	286	ARG	2.5
1	J	308	PHE	2.5
1	C	189	SER	2.4
1	G	310	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	307	GLY	2.4
1	F	141	ARG	2.4
1	F	183	PRO	2.4
1	H	182	GLN	2.4
1	J	288	ALA	2.4
1	A	313	CYS	2.4
1	I	156	GLU	2.4
1	G	181	VAL	2.3
1	B	287	GLN	2.3
1	A	314	VAL	2.3
1	J	52	GLY	2.3
1	B	179	SER	2.3
1	B	292	GLU	2.3
1	E	286	ARG	2.3
1	E	285	HIS	2.3
1	F	295	LEU	2.3
1	H	309	LEU	2.2
1	G	241	THR	2.2
1	H	300	CYS	2.2
1	D	178	LEU	2.2
1	F	176	ASP	2.2
1	G	299	ARG	2.2
1	D	173	ILE	2.2
1	G	231	ARG	2.2
1	C	307	GLY	2.1
1	G	297	ILE	2.1
1	J	287	GLN	2.1
1	J	174	ARG	2.1
1	A	142	PHE	2.1
1	H	311	ILE	2.1
1	G	139	GLN	2.1
1	I	316	VAL	2.1
1	F	49	LYS	2.1
1	G	154	ASN	2.1
1	F	315	LEU	2.1
1	B	124	GLN	2.0
1	H	163	ARG	2.0
1	E	148	TYR	2.0
1	H	305	PRO	2.0
1	B	114	MET	2.0
1	G	295	LEU	2.0
1	F	186	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	49	LYS	2.0
1	J	180	SER	2.0
1	A	173	ILE	2.0
1	A	188	PHE	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.