Full wwPDB X-ray Structure Validation Report (i)

Mar 22, 2016 – 12:59 AM EDT

PDB ID	:	5HEW
Title	:	Pentameric ligand-gated ion channel ELIC mutant T28D
Authors	:	Engeler, S.; Dutzler, R.
Deposited on	:	2016-01-06
Resolution	:	4.50 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
http://wwpdb.org/validation/2016/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:

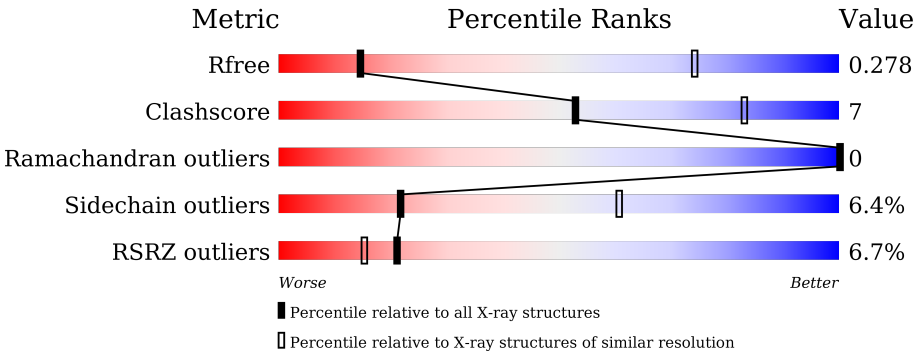
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 4.50 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}	91344	1071 (5.40-3.60)
Clashscore	102246	1003 (5.30-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
Sidechain outliers	100360	1099 (5.40-3.60)
RSRZ outliers	91569	1075 (5.40-3.60)

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. 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	5% 76% 18% • 5%
1	B	322	9% 75% 19% • 5%
1	C	322	7% 72% 23% • 5%
1	D	322	7% 76% 17% • 5%
1	E	322	5% 75% 19% • 5%
1	F	322	9% 75% 20% • 5%

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Mol	Chain	Length	Quality of chain
1	G	322	7% 72% 21% 5%
1	H	322	5% 72% 21% 5%
1	I	322	5% 74% 19% 5%
1	J	322	3% 75% 18% 5%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 25060 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
			2506	1633	416	451	6			
1	B	307	Total	C	N	O	S	0	0	0
			2506	1633	416	451	6			
1	C	307	Total	C	N	O	S	0	0	0
			2506	1633	416	451	6			
1	D	307	Total	C	N	O	S	0	0	0
			2506	1633	416	451	6			
1	E	307	Total	C	N	O	S	0	0	0
			2506	1633	416	451	6			
1	F	307	Total	C	N	O	S	0	0	0
			2506	1633	416	451	6			
1	G	307	Total	C	N	O	S	0	0	0
			2506	1633	416	451	6			
1	H	307	Total	C	N	O	S	0	0	0
			2506	1633	416	451	6			
1	I	307	Total	C	N	O	S	0	0	0
			2506	1633	416	451	6			
1	J	307	Total	C	N	O	S	0	0	0
			2506	1633	416	451	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ASP	THR	engineered mutation	UNP E0SJQ4
B	28	ASP	THR	engineered mutation	UNP E0SJQ4
C	28	ASP	THR	engineered mutation	UNP E0SJQ4
D	28	ASP	THR	engineered mutation	UNP E0SJQ4
E	28	ASP	THR	engineered mutation	UNP E0SJQ4
F	28	ASP	THR	engineered mutation	UNP E0SJQ4
G	28	ASP	THR	engineered mutation	UNP E0SJQ4
H	28	ASP	THR	engineered mutation	UNP E0SJQ4
I	28	ASP	THR	engineered mutation	UNP E0SJQ4

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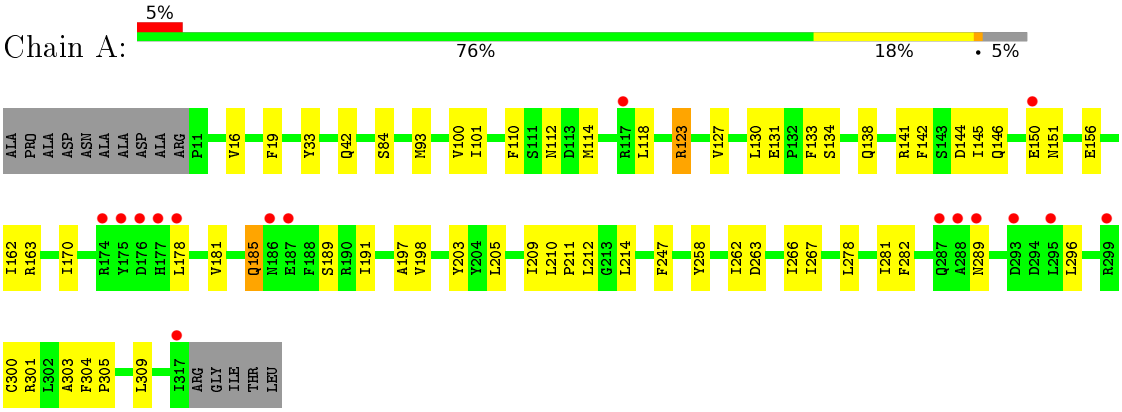
Chain	Residue	Modelled	Actual	Comment	Reference
J	28	ASP	THR	engineered mutation	UNP E0SJQ4

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 errors 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.

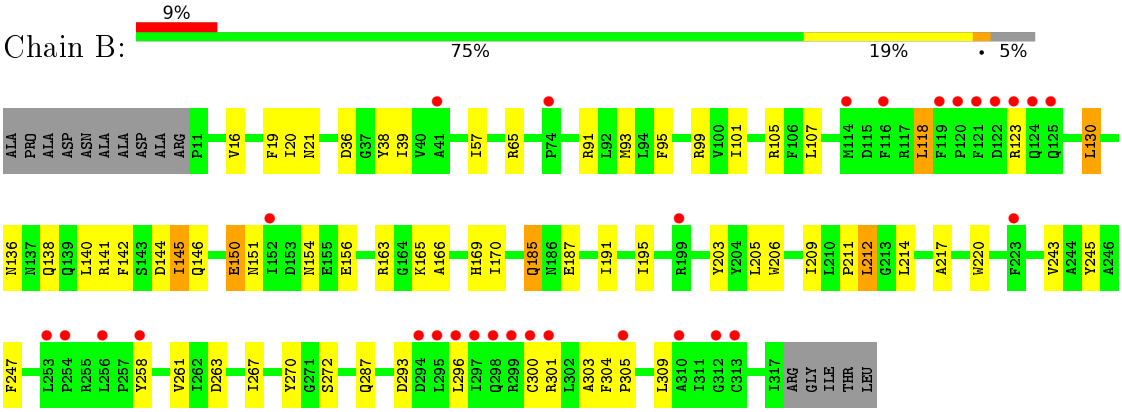
- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain A:



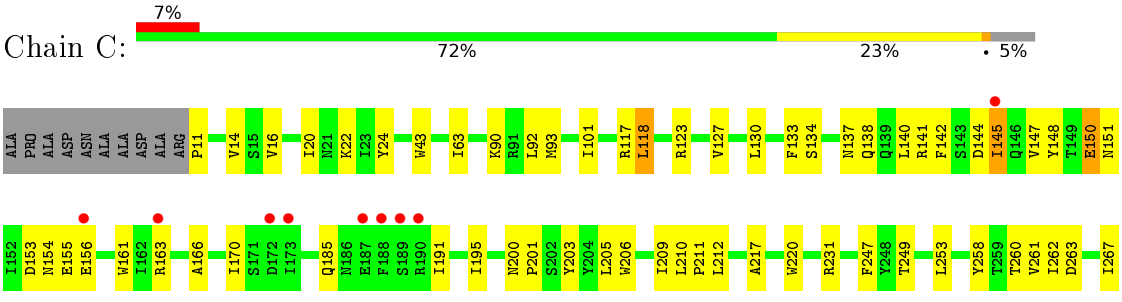
- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

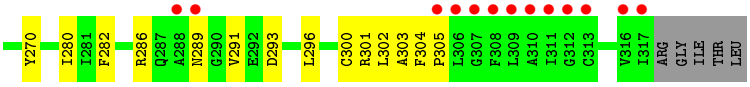
Chain B:



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

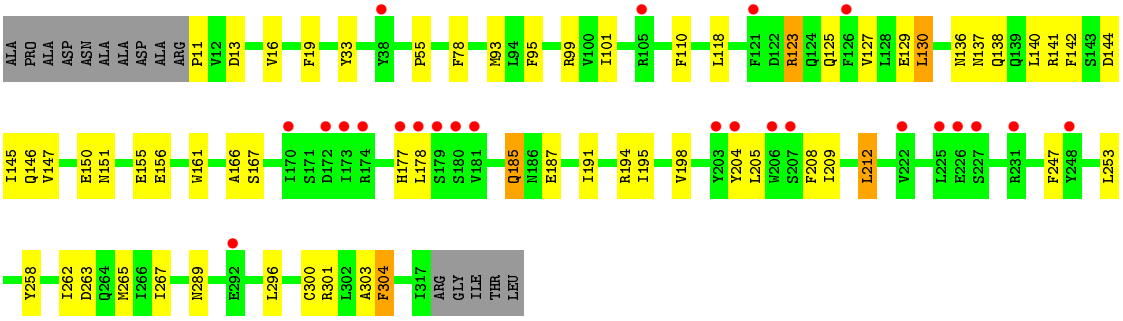
Chain C:





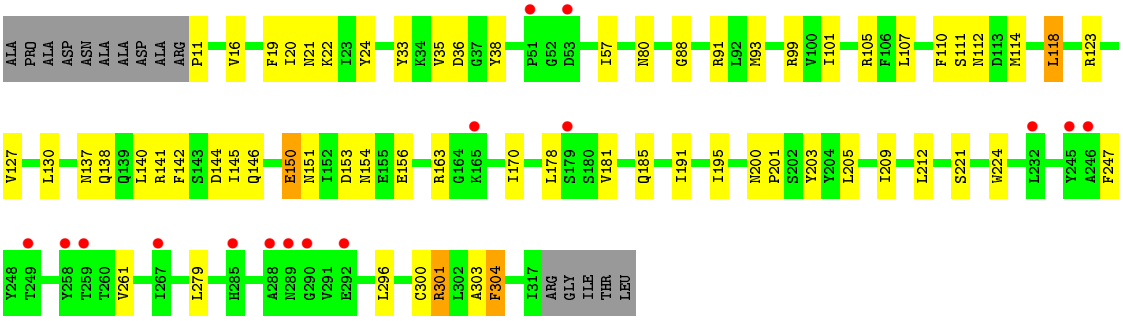
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain D:



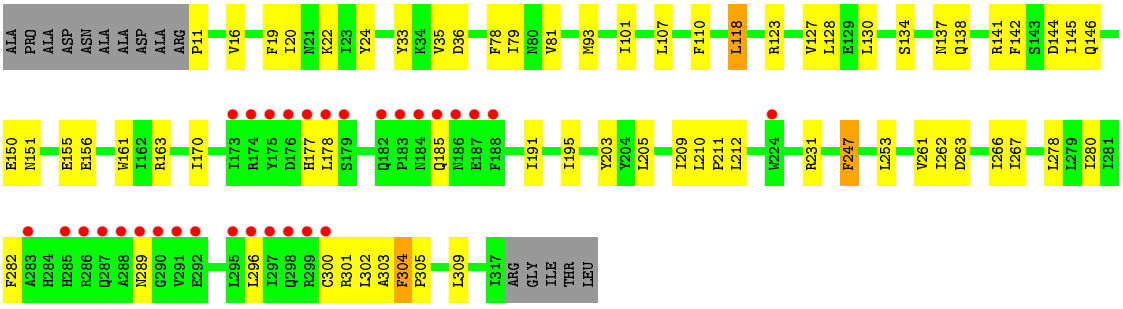
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain E:



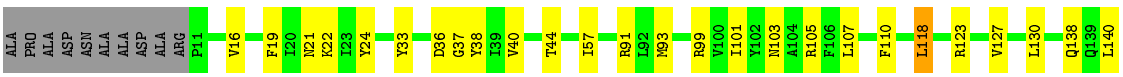
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

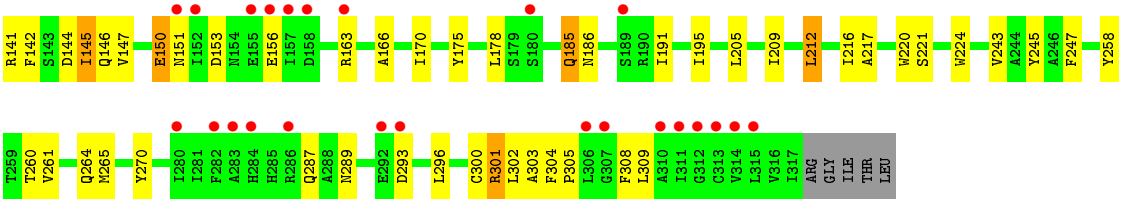
Chain F:



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

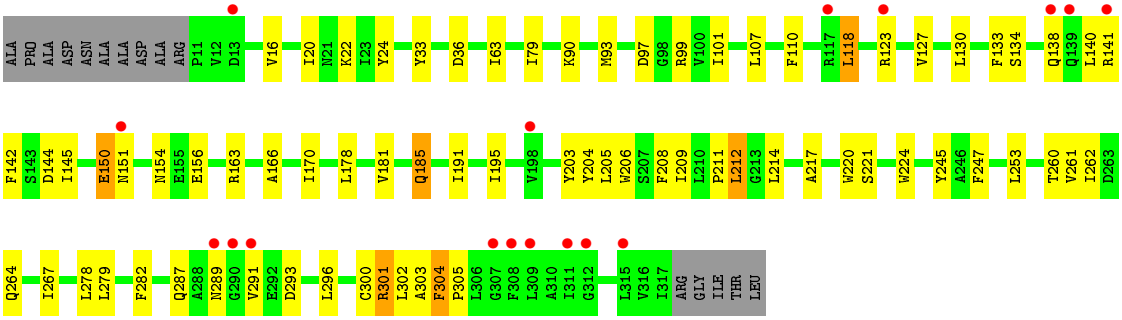
Chain G:





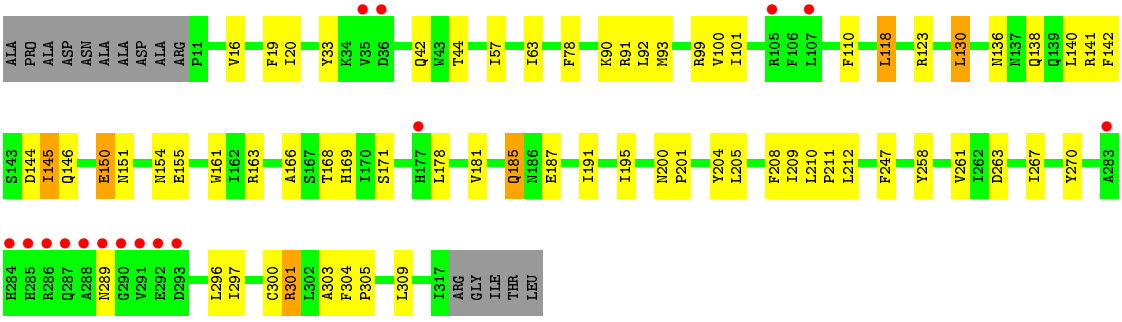
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain H:



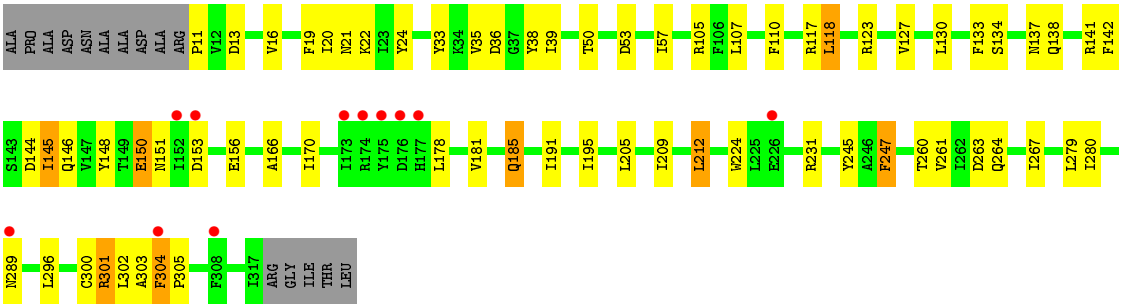
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain I:



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

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	105.45Å 266.96Å 110.20Å 90.00° 110.50° 90.00°	Depositor
Resolution (Å)	29.93 – 4.50 49.39 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.93-4.50) 100.0 (49.39-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.237 , 0.271 0.254 , 0.278	Depositor DCC
R_{free} test set	1727 reflections (5.12%)	DCC
Wilson B-factor (Å^2)	216.4	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 191.3	EDS
Estimated twinning fraction	0.043 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 86212 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	25060	wwPDB-VP
Average B, all atoms (Å^2)	288.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0/2574	0.43	0/3508
1	B	0.27	0/2574	0.43	0/3508
1	C	0.27	0/2574	0.43	0/3508
1	D	0.26	0/2574	0.44	0/3508
1	E	0.26	0/2574	0.43	0/3508
1	F	0.26	0/2574	0.43	0/3508
1	G	0.26	0/2574	0.43	0/3508
1	H	0.26	0/2574	0.43	0/3508
1	I	0.26	0/2574	0.44	0/3508
1	J	0.27	0/2574	0.43	0/3508
All	All	0.26	0/25740	0.43	0/35080

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	2506	0	2475	29	0
1	B	2506	0	2475	39	0
1	C	2506	0	2475	39	0
1	D	2506	0	2475	30	0
1	E	2506	0	2475	35	0
1	F	2506	0	2475	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2506	0	2475	38	0
1	H	2506	0	2475	41	0
1	I	2506	0	2475	41	0
1	J	2506	0	2475	38	0
All	All	25060	0	24750	327	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 7.

All (327) 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:J:170:ILE:HG12	1:J:191:ILE:HG12	1.72	0.71
1:I:93:MET:HB3	1:I:101:ILE:HB	1.75	0.69
1:G:170:ILE:HG12	1:G:191:ILE:HG12	1.76	0.67
1:B:170:ILE:HG12	1:B:191:ILE:HG12	1.76	0.67
1:B:300:CYS:HA	1:B:303:ALA:HB3	1.77	0.66
1:B:165:LYS:HG3	1:I:163:ARG:HB3	1.78	0.65
1:A:170:ILE:HG12	1:A:191:ILE:HG12	1.79	0.65
1:E:36:ASP:HB2	1:E:107:LEU:HD13	1.79	0.65
1:G:300:CYS:HA	1:G:303:ALA:HB3	1.80	0.63
1:I:300:CYS:HA	1:I:303:ALA:HB3	1.79	0.63
1:F:300:CYS:HA	1:F:303:ALA:HB3	1.79	0.62
1:F:93:MET:HB3	1:F:101:ILE:HB	1.81	0.61
1:A:281:ILE:HD11	1:E:221:SER:HB2	1.82	0.61
1:F:170:ILE:HG12	1:F:191:ILE:HG12	1.82	0.61
1:A:300:CYS:HA	1:A:303:ALA:HB3	1.84	0.59
1:D:300:CYS:HA	1:D:303:ALA:HB3	1.83	0.59
1:J:300:CYS:HA	1:J:303:ALA:HB3	1.85	0.58
1:C:300:CYS:HA	1:C:303:ALA:HB3	1.85	0.58
1:H:93:MET:HB3	1:H:101:ILE:HB	1.84	0.58
1:J:39:ILE:HD11	1:J:130:LEU:HD11	1.85	0.58
1:B:93:MET:HB3	1:B:101:ILE:HB	1.85	0.58
1:C:11:PRO:HA	1:C:137:ASN:O	2.04	0.58
1:E:205:LEU:HD23	1:E:209:ILE:HD12	1.84	0.58
1:G:57:ILE:HD13	1:H:134:SER:HB3	1.86	0.57
1:D:205:LEU:HD23	1:D:209:ILE:HD12	1.86	0.57
1:G:205:LEU:HD23	1:G:209:ILE:HD12	1.86	0.57
1:I:140:LEU:HD13	1:I:191:ILE:HG13	1.87	0.57
1:D:93:MET:HB3	1:D:101:ILE:HB	1.86	0.56
1:I:91:ARG:HB3	1:J:133:PHE:HE2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:ASP:HB2	1:F:107:LEU:HD13	1.87	0.56
1:G:33:TYR:CE1	1:G:110:PHE:HB2	2.40	0.56
1:G:93:MET:HB3	1:G:101:ILE:HB	1.87	0.56
1:H:205:LEU:HD23	1:H:209:ILE:HD12	1.87	0.56
1:F:205:LEU:HD23	1:F:209:ILE:HD12	1.88	0.56
1:H:300:CYS:HA	1:H:303:ALA:HB3	1.86	0.55
1:H:63:ILE:HD12	1:H:90:LYS:HG3	1.88	0.55
1:B:205:LEU:HD23	1:B:209:ILE:HD12	1.87	0.55
1:C:118:LEU:HA	1:C:261:VAL:HG23	1.88	0.55
1:B:140:LEU:HD13	1:B:191:ILE:HG13	1.89	0.55
1:B:169:HIS:HA	1:I:168:THR:O	2.07	0.55
1:E:300:CYS:HA	1:E:303:ALA:HB3	1.87	0.54
1:B:166:ALA:HB2	1:B:195:ILE:HG12	1.89	0.54
1:A:205:LEU:HD23	1:A:209:ILE:HD12	1.88	0.54
1:J:36:ASP:HB2	1:J:107:LEU:HD13	1.89	0.54
1:I:150:GLU:HG3	1:I:154:ASN:H	1.73	0.54
1:B:150:GLU:HG3	1:B:154:ASN:H	1.73	0.54
1:E:150:GLU:HG3	1:E:154:ASN:H	1.72	0.54
1:D:33:TYR:CE1	1:D:110:PHE:HB2	2.43	0.53
1:C:14:VAL:HG22	1:C:43:TRP:HB3	1.89	0.53
1:I:205:LEU:HD23	1:I:209:ILE:HD12	1.90	0.53
1:F:305:PRO:O	1:F:309:LEU:HG	2.10	0.52
1:B:19:PHE:CE2	1:B:146:GLN:HG3	2.44	0.52
1:I:63:ILE:HD12	1:I:90:LYS:HG3	1.91	0.52
1:E:150:GLU:HG3	1:E:153:ASP:HB3	1.92	0.52
1:J:19:PHE:CE2	1:J:146:GLN:HG3	2.45	0.52
1:C:93:MET:HB3	1:C:101:ILE:HB	1.91	0.51
1:C:170:ILE:HG12	1:C:191:ILE:HG12	1.92	0.51
1:E:33:TYR:CE1	1:E:110:PHE:HB2	2.46	0.51
1:F:11:PRO:HA	1:F:137:ASN:O	2.11	0.51
1:H:118:LEU:HA	1:H:261:VAL:HG23	1.92	0.51
1:A:134:SER:HB3	1:E:57:ILE:HD13	1.93	0.51
1:I:44:THR:HA	1:I:99:ARG:HA	1.93	0.51
1:G:36:ASP:HB2	1:G:107:LEU:HD13	1.93	0.50
1:A:93:MET:HB3	1:A:101:ILE:HB	1.94	0.50
1:I:136:ASN:HB2	1:I:187:GLU:O	2.12	0.50
1:J:141:ARG:HG3	1:J:142:PHE:CD2	2.47	0.50
1:B:36:ASP:HB2	1:B:107:LEU:HD13	1.93	0.49
1:J:33:TYR:CE1	1:J:110:PHE:HB2	2.47	0.49
1:D:140:LEU:HD13	1:D:191:ILE:HG13	1.94	0.49
1:G:141:ARG:HG3	1:G:142:PHE:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:33:TYR:CE1	1:H:110:PHE:HB2	2.47	0.49
1:H:206:TRP:O	1:H:211:PRO:HD3	2.13	0.49
1:G:287:GLN:HG3	1:G:293:ASP:HB2	1.94	0.49
1:E:141:ARG:HG3	1:E:142:PHE:CD2	2.48	0.49
1:H:170:ILE:HG12	1:H:191:ILE:HG12	1.93	0.49
1:D:136:ASN:HB2	1:D:187:GLU:O	2.12	0.49
1:D:147:VAL:HG21	1:D:195:ILE:HD13	1.95	0.48
1:E:19:PHE:CE2	1:E:146:GLN:HG3	2.48	0.48
1:H:221:SER:HA	1:H:224:TRP:HD1	1.78	0.48
1:J:205:LEU:HD23	1:J:209:ILE:HD12	1.94	0.48
1:J:20:ILE:HD12	1:J:195:ILE:HD11	1.95	0.48
1:D:166:ALA:HB2	1:D:195:ILE:HG12	1.95	0.48
1:E:38:TYR:CZ	1:E:105:ARG:HD3	2.49	0.48
1:F:253:LEU:HD21	1:F:262:ILE:HD12	1.94	0.48
1:G:212:LEU:HD12	1:G:265:MET:HB3	1.95	0.48
1:F:19:PHE:CE2	1:F:146:GLN:HG3	2.48	0.48
1:B:169:HIS:CG	1:I:168:THR:HG1	2.30	0.48
1:B:145:ILE:HG13	1:B:166:ALA:HB3	1.96	0.48
1:G:212:LEU:CD1	1:G:265:MET:HB3	2.44	0.48
1:I:19:PHE:CE2	1:I:146:GLN:HG3	2.48	0.48
1:B:21:ASN:HD21	1:B:38:TYR:HE1	1.60	0.48
1:C:150:GLU:HG3	1:C:154:ASN:H	1.79	0.48
1:E:224:TRP:CE2	1:E:301:ARG:HG2	2.49	0.48
1:D:263:ASP:O	1:D:267:ILE:HG12	2.14	0.47
1:H:287:GLN:HB2	1:H:291:VAL:HB	1.96	0.47
1:G:221:SER:HA	1:G:224:TRP:HD1	1.79	0.47
1:H:253:LEU:HD21	1:H:262:ILE:HD12	1.96	0.47
1:I:263:ASP:O	1:I:267:ILE:HG12	2.14	0.47
1:B:305:PRO:O	1:B:309:LEU:HG	2.15	0.47
1:B:185:GLN:H	1:B:185:GLN:HG3	1.50	0.47
1:G:91:ARG:HB3	1:H:133:PHE:HE2	1.78	0.47
1:H:141:ARG:HG3	1:H:142:PHE:CD2	2.49	0.47
1:H:150:GLU:HG3	1:H:154:ASN:H	1.79	0.47
1:J:150:GLU:HG3	1:J:153:ASP:HB3	1.95	0.47
1:H:203:TYR:HB2	1:I:258:TYR:HA	1.97	0.47
1:A:19:PHE:CE2	1:A:146:GLN:HG3	2.50	0.47
1:H:204:TYR:O	1:H:208:PHE:HB2	2.14	0.47
1:H:22:LYS:HE3	1:H:24:TYR:CD1	2.50	0.47
1:I:57:ILE:HD13	1:J:134:SER:HB3	1.97	0.47
1:A:203:TYR:HB2	1:B:258:TYR:HA	1.97	0.47
1:B:170:ILE:HB	1:I:169:HIS:ND1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:141:ARG:HG3	1:F:142:PHE:CD2	2.49	0.47
1:D:141:ARG:HG3	1:D:142:PHE:CD2	2.50	0.47
1:C:205:LEU:HD23	1:C:209:ILE:HD12	1.97	0.47
1:F:33:TYR:CE1	1:F:110:PHE:HB2	2.50	0.47
1:I:99:ARG:CZ	1:J:181:VAL:HG21	2.45	0.47
1:G:178:LEU:HA	1:G:178:LEU:HD12	1.76	0.46
1:C:203:TYR:HB2	1:D:258:TYR:HA	1.97	0.46
1:D:19:PHE:CE2	1:D:146:GLN:HG3	2.51	0.46
1:E:20:ILE:HD12	1:E:195:ILE:HD11	1.96	0.46
1:E:22:LYS:HE3	1:E:24:TYR:CD1	2.51	0.46
1:A:163:ARG:HA	1:A:163:ARG:HD3	1.70	0.46
1:B:203:TYR:HB2	1:C:258:TYR:HA	1.96	0.46
1:H:178:LEU:HA	1:H:178:LEU:HD12	1.78	0.46
1:H:300:CYS:O	1:H:304:PHE:HB2	2.15	0.46
1:I:141:ARG:HG3	1:I:142:PHE:CD2	2.50	0.46
1:I:305:PRO:O	1:I:309:LEU:HG	2.16	0.46
1:J:11:PRO:HA	1:J:137:ASN:O	2.16	0.46
1:J:22:LYS:HE3	1:J:24:TYR:CD1	2.51	0.46
1:C:166:ALA:HB2	1:C:195:ILE:HG12	1.97	0.46
1:I:155:GLU:O	1:I:161:TRP:NE1	2.49	0.46
1:A:141:ARG:HG3	1:A:142:PHE:CD2	2.51	0.46
1:A:281:ILE:CD1	1:E:221:SER:HB2	2.46	0.46
1:A:263:ASP:O	1:A:267:ILE:HG12	2.16	0.46
1:G:216:ILE:HD13	1:G:308:PHE:CZ	2.51	0.46
1:B:141:ARG:HG3	1:B:142:PHE:CD2	2.51	0.46
1:B:20:ILE:HD12	1:B:195:ILE:HD11	1.97	0.46
1:I:178:LEU:HD12	1:I:178:LEU:HA	1.79	0.46
1:B:39:ILE:HD11	1:B:130:LEU:HD11	1.97	0.46
1:E:178:LEU:HD12	1:E:178:LEU:HA	1.80	0.46
1:H:140:LEU:HD13	1:H:191:ILE:HG13	1.98	0.46
1:I:145:ILE:HG13	1:I:166:ALA:HB3	1.97	0.46
1:I:91:ARG:HB3	1:J:133:PHE:CE2	2.48	0.46
1:J:300:CYS:O	1:J:304:PHE:HB2	2.16	0.46
1:C:217:ALA:HA	1:C:220:TRP:CE3	2.51	0.46
1:C:140:LEU:HD13	1:C:191:ILE:HG13	1.98	0.45
1:D:155:GLU:O	1:D:161:TRP:NE1	2.49	0.45
1:A:262:ILE:O	1:A:266:ILE:HG12	2.15	0.45
1:C:141:ARG:HG3	1:C:142:PHE:CD2	2.51	0.45
1:F:278:LEU:O	1:F:282:PHE:N	2.37	0.45
1:E:170:ILE:HG12	1:E:191:ILE:HG12	1.98	0.45
1:I:204:TYR:O	1:I:208:PHE:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:279:LEU:HD22	1:E:304:PHE:CE1	2.51	0.45
1:G:243:VAL:HA	1:G:270:TYR:OH	2.17	0.45
1:A:214:LEU:HD23	1:B:270:TYR:HB3	1.99	0.45
1:D:185:GLN:HG3	1:D:185:GLN:H	1.53	0.45
1:F:177:HIS:NE2	1:J:148:TYR:HE2	2.15	0.45
1:G:175:TYR:O	1:G:186:ASN:HB2	2.17	0.45
1:H:163:ARG:HD3	1:H:163:ARG:HA	1.79	0.45
1:H:205:LEU:HA	1:H:209:ILE:HB	1.98	0.45
1:A:258:TYR:HA	1:E:203:TYR:HB2	1.97	0.45
1:H:36:ASP:HB2	1:H:107:LEU:HD13	1.99	0.45
1:J:50:THR:OG1	1:J:53:ASP:HA	2.17	0.45
1:F:163:ARG:HA	1:F:163:ARG:HD3	1.71	0.45
1:F:178:LEU:HD12	1:F:178:LEU:HA	1.74	0.45
1:A:181:VAL:HG21	1:E:99:ARG:NH2	2.32	0.45
1:C:148:TYR:HE2	1:D:177:HIS:HE2	1.64	0.45
1:H:166:ALA:HB2	1:H:195:ILE:HG12	1.98	0.45
1:I:33:TYR:CE1	1:I:110:PHE:HB2	2.52	0.45
1:J:178:LEU:HD12	1:J:178:LEU:HA	1.79	0.45
1:A:33:TYR:CE1	1:A:110:PHE:HB2	2.52	0.45
1:B:220:TRP:NE1	1:B:272:SER:OG	2.43	0.45
1:C:145:ILE:HG13	1:C:166:ALA:HB3	1.98	0.45
1:D:123:ARG:HE	1:D:198:VAL:HG22	1.82	0.45
1:G:150:GLU:HG3	1:G:153:ASP:HB3	1.99	0.45
1:B:136:ASN:HB2	1:B:187:GLU:O	2.16	0.44
1:A:133:PHE:HE2	1:E:91:ARG:HB3	1.82	0.44
1:G:212:LEU:HD23	1:G:245:TYR:CD2	2.52	0.44
1:H:20:ILE:HD12	1:H:195:ILE:HD11	1.98	0.44
1:F:35:VAL:HG21	1:F:128:LEU:HD11	2.00	0.44
1:J:145:ILE:HG13	1:J:166:ALA:HB3	1.98	0.44
1:C:231:ARG:HB3	1:C:280:ILE:HD13	2.00	0.44
1:A:162:ILE:HD13	1:A:197:ALA:HB2	2.00	0.44
1:C:253:LEU:HD21	1:C:262:ILE:HD12	1.99	0.44
1:F:262:ILE:O	1:F:266:ILE:HG12	2.17	0.44
1:G:145:ILE:HG13	1:G:166:ALA:HB3	1.98	0.44
1:A:185:GLN:H	1:A:185:GLN:HG3	1.44	0.44
1:B:38:TYR:CZ	1:B:105:ARG:HD3	2.53	0.44
1:C:155:GLU:O	1:C:161:TRP:NE1	2.48	0.44
1:B:214:LEU:HD23	1:C:270:TYR:HB3	1.99	0.44
1:J:117:ARG:O	1:J:260:THR:HA	2.17	0.44
1:C:205:LEU:HA	1:C:209:ILE:HB	1.99	0.44
1:F:22:LYS:HE3	1:F:24:TYR:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:185:GLN:H	1:G:185:GLN:HG3	1.51	0.44
1:H:217:ALA:HA	1:H:220:TRP:CE3	2.53	0.44
1:J:21:ASN:HD21	1:J:38:TYR:HE1	1.65	0.44
1:C:263:ASP:O	1:C:267:ILE:HG12	2.18	0.44
1:F:300:CYS:O	1:F:304:PHE:HB2	2.17	0.44
1:G:118:LEU:HA	1:G:261:VAL:HG23	1.99	0.44
1:I:20:ILE:HD12	1:I:195:ILE:HD11	2.00	0.44
1:A:112:ASN:O	1:A:114:MET:HG3	2.18	0.43
1:C:150:GLU:HG3	1:C:153:ASP:HB3	1.99	0.43
1:C:20:ILE:HD12	1:C:195:ILE:HD11	1.99	0.43
1:B:217:ALA:HA	1:B:220:TRP:CE3	2.54	0.43
1:C:117:ARG:O	1:C:260:THR:HA	2.19	0.43
1:B:118:LEU:HA	1:B:261:VAL:HG23	2.00	0.43
1:B:95:PHE:HB2	1:B:99:ARG:HB2	2.00	0.43
1:B:57:ILE:HD13	1:C:134:SER:HB3	2.00	0.43
1:H:212:LEU:HD23	1:H:245:TYR:CD2	2.54	0.43
1:H:291:VAL:HG12	1:H:293:ASP:H	1.82	0.43
1:H:279:LEU:HD22	1:H:304:PHE:CE1	2.53	0.43
1:I:42:GLN:HA	1:I:100:VAL:O	2.19	0.43
1:E:221:SER:HA	1:E:224:TRP:HD1	1.83	0.43
1:G:140:LEU:HD13	1:G:191:ILE:HG13	1.99	0.43
1:F:203:TYR:HB2	1:G:258:TYR:HA	2.00	0.43
1:J:38:TYR:CZ	1:J:105:ARG:HD3	2.53	0.43
1:B:263:ASP:O	1:B:267:ILE:HG12	2.19	0.43
1:E:140:LEU:HD13	1:E:191:ILE:HG13	2.00	0.43
1:G:21:ASN:HD21	1:G:38:TYR:HE1	1.67	0.43
1:G:217:ALA:HA	1:G:220:TRP:CE3	2.54	0.43
1:G:99:ARG:NH2	1:H:181:VAL:HG21	2.34	0.43
1:F:263:ASP:O	1:F:267:ILE:HG12	2.18	0.43
1:F:78:PHE:HB2	1:F:81:VAL:HB	2.00	0.43
1:A:278:LEU:O	1:A:282:PHE:N	2.43	0.43
1:C:63:ILE:HD12	1:C:90:LYS:HG3	2.01	0.43
1:H:214:LEU:HD23	1:I:270:TYR:HB3	1.99	0.43
1:I:185:GLN:H	1:I:185:GLN:HG3	1.53	0.43
1:I:210:LEU:HB3	1:I:211:PRO:HD3	2.01	0.43
1:F:247:PHE:HE2	1:J:247:PHE:CD2	2.37	0.43
1:D:253:LEU:HD21	1:D:262:ILE:HD12	2.01	0.42
1:E:11:PRO:HA	1:E:137:ASN:O	2.19	0.42
1:I:169:HIS:NE2	1:I:171:SER:HB3	2.33	0.42
1:F:20:ILE:HD12	1:F:195:ILE:HD11	2.00	0.42
1:C:206:TRP:O	1:C:211:PRO:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:GLY:O	1:G:105:ARG:HD2	2.19	0.42
1:D:166:ALA:CB	1:D:195:ILE:HG12	2.49	0.42
1:E:93:MET:HB3	1:E:101:ILE:HB	2.01	0.42
1:G:44:THR:HA	1:G:99:ARG:HA	2.00	0.42
1:I:166:ALA:HB2	1:I:195:ILE:HG12	2.01	0.42
1:B:212:LEU:HD23	1:B:245:TYR:CD2	2.55	0.42
1:D:212:LEU:CD1	1:D:265:MET:HB3	2.50	0.42
1:F:210:LEU:HB3	1:F:211:PRO:HD3	2.02	0.42
1:I:92:LEU:HD23	1:I:92:LEU:HA	1.88	0.42
1:B:206:TRP:O	1:B:211:PRO:HD3	2.20	0.42
1:D:78:PHE:CE1	1:D:130:LEU:HG	2.55	0.42
1:F:118:LEU:HA	1:F:261:VAL:HG23	2.02	0.42
1:G:163:ARG:HA	1:G:163:ARG:HD3	1.78	0.42
1:G:224:TRP:CE2	1:G:301:ARG:HG2	2.55	0.42
1:J:212:LEU:HD23	1:J:245:TYR:CD2	2.55	0.42
1:J:231:ARG:HB3	1:J:280:ILE:HD13	2.00	0.42
1:B:91:ARG:HB3	1:C:133:PHE:HE2	1.85	0.42
1:D:55:PRO:HB3	1:D:95:PHE:CD1	2.55	0.42
1:D:99:ARG:NH2	1:E:181:VAL:HG21	2.34	0.42
1:B:163:ARG:HD3	1:B:163:ARG:HA	1.73	0.41
1:D:129:GLU:HA	1:D:191:ILE:O	2.20	0.41
1:G:147:VAL:HG21	1:G:195:ILE:HD13	2.02	0.41
1:G:305:PRO:O	1:G:309:LEU:HG	2.19	0.41
1:G:40:VAL:HG22	1:G:103:ASN:OD1	2.20	0.41
1:H:302:LEU:C	1:H:305:PRO:HD2	2.40	0.41
1:J:185:GLN:H	1:J:185:GLN:HG3	1.48	0.41
1:J:224:TRP:CE2	1:J:301:ARG:HG2	2.55	0.41
1:D:204:TYR:O	1:D:208:PHE:HB2	2.20	0.41
1:F:134:SER:HB3	1:J:57:ILE:HD13	2.02	0.41
1:F:231:ARG:HB3	1:F:280:ILE:HD13	2.02	0.41
1:H:99:ARG:NH2	1:I:181:VAL:HG21	2.35	0.41
1:A:123:ARG:HE	1:A:198:VAL:HG22	1.85	0.41
1:A:305:PRO:O	1:A:309:LEU:HG	2.20	0.41
1:C:302:LEU:C	1:C:305:PRO:HD2	2.40	0.41
1:J:118:LEU:HA	1:J:261:VAL:HG23	2.01	0.41
1:A:42:GLN:HA	1:A:100:VAL:O	2.21	0.41
1:C:249:THR:O	1:C:253:LEU:HB2	2.21	0.41
1:C:92:LEU:HD23	1:C:92:LEU:HA	1.87	0.41
1:H:224:TRP:CE2	1:H:301:ARG:HG2	2.56	0.41
1:J:13:ASP:HB3	1:J:141:ARG:HD2	2.01	0.41
1:B:287:GLN:HG3	1:B:293:ASP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:ARG:HA	1:C:163:ARG:HD3	1.72	0.41
1:C:282:PHE:CZ	1:C:286:ARG:HG3	2.56	0.41
1:E:35:VAL:HB	1:E:110:PHE:CE1	2.56	0.41
1:E:21:ASN:HD21	1:E:38:TYR:HE1	1.68	0.41
1:H:97:ASP:OD2	1:H:99:ARG:NH1	2.54	0.41
1:H:79:ILE:HA	1:H:79:ILE:HD13	1.95	0.41
1:B:130:LEU:HA	1:B:130:LEU:HD23	1.90	0.41
1:D:178:LEU:HA	1:D:178:LEU:HD12	1.80	0.41
1:F:79:ILE:HA	1:F:79:ILE:HD13	1.94	0.41
1:J:263:ASP:O	1:J:267:ILE:HG12	2.21	0.41
1:J:260:THR:O	1:J:264:GLN:HG3	2.19	0.41
1:J:279:LEU:HD22	1:J:304:PHE:CE1	2.56	0.41
1:A:178:LEU:HD12	1:A:178:LEU:HA	1.80	0.41
1:C:210:LEU:HB3	1:C:211:PRO:HD3	2.03	0.41
1:D:13:ASP:HB3	1:D:141:ARG:HD2	2.02	0.41
1:E:200:ASN:HA	1:E:201:PRO:HD3	1.95	0.41
1:I:200:ASN:HA	1:I:201:PRO:HD3	1.91	0.41
1:J:35:VAL:HB	1:J:110:PHE:CE1	2.56	0.41
1:B:243:VAL:HA	1:B:270:TYR:OH	2.20	0.41
1:D:167:SER:OG	1:D:194:ARG:HB2	2.20	0.41
1:D:125:GLN:OE1	1:D:194:ARG:HD3	2.21	0.41
1:E:80:ASN:HB2	1:E:111:SER:O	2.20	0.41
1:G:19:PHE:CE2	1:G:146:GLN:HG3	2.56	0.41
1:G:260:THR:O	1:G:264:GLN:HG3	2.21	0.41
1:G:302:LEU:C	1:G:305:PRO:HD2	2.41	0.41
1:C:22:LYS:HE3	1:C:24:TYR:CD1	2.56	0.40
1:F:155:GLU:C	1:F:161:TRP:HE1	2.24	0.40
1:H:267:ILE:H	1:H:267:ILE:HG12	1.77	0.40
1:H:278:LEU:O	1:H:282:PHE:N	2.43	0.40
1:I:130:LEU:HD23	1:I:130:LEU:HA	1.89	0.40
1:I:118:LEU:HA	1:I:261:VAL:HG23	2.03	0.40
1:I:297:ILE:O	1:I:301:ARG:HB2	2.22	0.40
1:A:210:LEU:HB3	1:A:211:PRO:HD3	2.03	0.40
1:C:147:VAL:HG21	1:C:195:ILE:HD13	2.02	0.40
1:C:200:ASN:HA	1:C:201:PRO:HD3	1.91	0.40
1:D:300:CYS:O	1:D:304:PHE:HB2	2.21	0.40
1:E:112:ASN:O	1:E:114:MET:HG3	2.21	0.40
1:E:300:CYS:O	1:E:304:PHE:HB2	2.21	0.40
1:A:84:SER:OG	1:E:88:GLY:HA2	2.21	0.40
1:H:260:THR:O	1:H:264:GLN:HG3	2.20	0.40
1:I:78:PHE:CE1	1:I:130:LEU:HG	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:130:LEU:HA	1:J:130:LEU:HD23	1.87	0.40
1:J:302:LEU:C	1:J:305:PRO:HD2	2.41	0.40
1:A:131:GLU:HG3	1:A:189:SER:O	2.21	0.40
1:D:11:PRO:HA	1:D:137:ASN:O	2.20	0.40
1:E:118:LEU:HA	1:E:261:VAL:HG23	2.02	0.40
1:F:302:LEU:C	1:F:305:PRO:HD2	2.41	0.40
1:H:185:GLN:H	1:H:185:GLN:HG3	1.47	0.40
1:C:291:VAL:HG12	1:C:293:ASP:H	1.85	0.40
1:I:163:ARG:HD3	1:I:163:ARG:HA	1.83	0.40
1:E:163:ARG:HA	1:E:163:ARG:HD3	1.82	0.40
1:G:22:LYS:HE3	1:G:24:TYR:CD1	2.56	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%)	285 (93%)	20 (7%)	0	100	100
1	B	305/322 (95%)	284 (93%)	21 (7%)	0	100	100
1	C	305/322 (95%)	284 (93%)	21 (7%)	0	100	100
1	D	305/322 (95%)	285 (93%)	20 (7%)	0	100	100
1	E	305/322 (95%)	286 (94%)	19 (6%)	0	100	100
1	F	305/322 (95%)	285 (93%)	20 (7%)	0	100	100
1	G	305/322 (95%)	285 (93%)	20 (7%)	0	100	100
1	H	305/322 (95%)	285 (93%)	20 (7%)	0	100	100
1	I	305/322 (95%)	285 (93%)	20 (7%)	0	100	100
1	J	305/322 (95%)	284 (93%)	21 (7%)	0	100	100
All	All	3050/3220 (95%)	2848 (93%)	202 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	275/284 (97%)	257 (94%)	18 (6%)	21	60
1	B	275/284 (97%)	258 (94%)	17 (6%)	23	62
1	C	275/284 (97%)	257 (94%)	18 (6%)	21	60
1	D	275/284 (97%)	257 (94%)	18 (6%)	21	60
1	E	275/284 (97%)	258 (94%)	17 (6%)	23	62
1	F	275/284 (97%)	257 (94%)	18 (6%)	21	60
1	G	275/284 (97%)	257 (94%)	18 (6%)	21	60
1	H	275/284 (97%)	257 (94%)	18 (6%)	21	60
1	I	275/284 (97%)	259 (94%)	16 (6%)	25	64
1	J	275/284 (97%)	258 (94%)	17 (6%)	23	62
All	All	2750/2840 (97%)	2575 (94%)	175 (6%)	22	61

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	118	LEU
1	A	123	ARG
1	A	127	VAL
1	A	130	LEU
1	A	138	GLN
1	A	144	ASP
1	A	145	ILE
1	A	150	GLU
1	A	151	ASN
1	A	156	GLU
1	A	185	GLN
1	A	212	LEU
1	A	247	PHE

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Mol	Chain	Res	Type
1	A	289	ASN
1	A	296	LEU
1	A	301	ARG
1	A	304	PHE
1	B	16	VAL
1	B	65	ARG
1	B	118	LEU
1	B	123	ARG
1	B	130	LEU
1	B	138	GLN
1	B	144	ASP
1	B	145	ILE
1	B	150	GLU
1	B	151	ASN
1	B	156	GLU
1	B	185	GLN
1	B	212	LEU
1	B	247	PHE
1	B	296	LEU
1	B	301	ARG
1	B	304	PHE
1	C	16	VAL
1	C	118	LEU
1	C	123	ARG
1	C	127	VAL
1	C	130	LEU
1	C	138	GLN
1	C	144	ASP
1	C	145	ILE
1	C	150	GLU
1	C	151	ASN
1	C	156	GLU
1	C	185	GLN
1	C	212	LEU
1	C	247	PHE
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	123	ARG

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Mol	Chain	Res	Type
1	D	127	VAL
1	D	130	LEU
1	D	138	GLN
1	D	144	ASP
1	D	145	ILE
1	D	150	GLU
1	D	151	ASN
1	D	156	GLU
1	D	185	GLN
1	D	212	LEU
1	D	247	PHE
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	123	ARG
1	E	127	VAL
1	E	130	LEU
1	E	138	GLN
1	E	144	ASP
1	E	145	ILE
1	E	150	GLU
1	E	151	ASN
1	E	156	GLU
1	E	185	GLN
1	E	212	LEU
1	E	247	PHE
1	E	296	LEU
1	E	301	ARG
1	E	304	PHE
1	F	16	VAL
1	F	118	LEU
1	F	123	ARG
1	F	127	VAL
1	F	130	LEU
1	F	138	GLN
1	F	144	ASP
1	F	145	ILE
1	F	150	GLU
1	F	151	ASN

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Mol	Chain	Res	Type
1	F	156	GLU
1	F	185	GLN
1	F	212	LEU
1	F	247	PHE
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	123	ARG
1	G	127	VAL
1	G	130	LEU
1	G	138	GLN
1	G	144	ASP
1	G	145	ILE
1	G	150	GLU
1	G	151	ASN
1	G	156	GLU
1	G	185	GLN
1	G	212	LEU
1	G	247	PHE
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	123	ARG
1	H	127	VAL
1	H	130	LEU
1	H	138	GLN
1	H	144	ASP
1	H	145	ILE
1	H	150	GLU
1	H	151	ASN
1	H	156	GLU
1	H	185	GLN
1	H	212	LEU
1	H	247	PHE
1	H	289	ASN
1	H	296	LEU

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Mol	Chain	Res	Type
1	H	301	ARG
1	H	304	PHE
1	I	16	VAL
1	I	118	LEU
1	I	123	ARG
1	I	130	LEU
1	I	138	GLN
1	I	144	ASP
1	I	145	ILE
1	I	150	GLU
1	I	151	ASN
1	I	185	GLN
1	I	212	LEU
1	I	247	PHE
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	123	ARG
1	J	127	VAL
1	J	138	GLN
1	J	144	ASP
1	J	145	ILE
1	J	150	GLU
1	J	151	ASN
1	J	156	GLU
1	J	185	GLN
1	J	212	LEU
1	J	247	PHE
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. There are no such sidechains identified.

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%)	-0.15	16 (5%)	31	24	224, 287, 369, 400	0
1	B	307/322 (95%)	0.21	30 (9%)	10	8	216, 277, 363, 417	0
1	C	307/322 (95%)	-0.12	22 (7%)	18	14	220, 286, 370, 408	0
1	D	307/322 (95%)	0.14	24 (7%)	16	12	219, 281, 368, 438	0
1	E	307/322 (95%)	-0.19	16 (5%)	31	24	224, 286, 358, 406	0
1	F	307/322 (95%)	0.15	30 (9%)	10	8	221, 288, 368, 431	0
1	G	307/322 (95%)	0.15	24 (7%)	16	12	216, 275, 373, 416	0
1	H	307/322 (95%)	-0.10	17 (5%)	29	22	217, 277, 364, 404	0
1	I	307/322 (95%)	-0.10	16 (5%)	31	24	218, 277, 363, 407	0
1	J	307/322 (95%)	-0.25	11 (3%)	46	37	218, 282, 373, 411	0
All	All	3070/3220 (95%)	-0.03	206 (6%)	21	15	216, 282, 368, 438	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	177	HIS	14.6
1	F	176	ASP	12.2
1	E	290	GLY	11.7
1	E	289	ASN	11.3
1	G	157	ILE	10.0
1	C	289	ASN	9.4
1	F	178	LEU	8.7
1	F	174	ARG	8.6
1	I	292	GLU	8.5
1	F	186	ASN	8.3
1	F	175	TYR	7.9
1	H	123	ARG	7.8
1	F	184	ASN	7.5

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Mol	Chain	Res	Type	RSRZ
1	I	291	VAL	7.5
1	C	189	SER	7.3
1	G	156	GLU	7.1
1	I	290	GLY	7.1
1	A	176	ASP	6.2
1	D	226	GLU	6.1
1	C	309	LEU	6.0
1	F	299	ARG	5.9
1	C	312	GLY	5.8
1	B	116	PHE	5.8
1	D	180	SER	5.8
1	C	187	GLU	5.8
1	H	290	GLY	5.8
1	I	289	ASN	5.7
1	G	314	VAL	5.6
1	E	288	ALA	5.5
1	B	254	PRO	5.4
1	F	183	PRO	5.3
1	G	292	GLU	5.2
1	H	289	ASN	5.1
1	D	231	ARG	5.1
1	E	259	THR	5.1
1	D	207	SER	5.0
1	I	287	GLN	5.0
1	B	313	CYS	5.0
1	A	175	TYR	4.9
1	B	124	GLN	4.9
1	D	206	TRP	4.6
1	I	293	ASP	4.6
1	G	152	ILE	4.5
1	A	177	HIS	4.5
1	G	293	ASP	4.5
1	H	312	GLY	4.5
1	J	174	ARG	4.3
1	B	297	ILE	4.2
1	B	120	PRO	4.1
1	C	316	VAL	4.1
1	D	38	TYR	4.0
1	D	179	SER	3.9
1	F	286	ARG	3.9
1	A	289	ASN	3.9
1	G	312	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	312	GLY	3.9
1	G	307	GLY	3.8
1	J	308	PHE	3.8
1	F	292	GLU	3.8
1	C	308	PHE	3.8
1	F	224	TRP	3.8
1	F	298	GLN	3.8
1	B	114	MET	3.7
1	G	313	CYS	3.7
1	D	105	ARG	3.7
1	C	306	LEU	3.6
1	H	117	ARG	3.6
1	B	298	GLN	3.6
1	F	289	ASN	3.6
1	C	313	CYS	3.5
1	I	288	ALA	3.5
1	J	175	TYR	3.5
1	H	13	ASP	3.5
1	G	283	ALA	3.5
1	F	182	GLN	3.4
1	F	187	GLU	3.4
1	F	179	SER	3.4
1	J	289	ASN	3.4
1	I	283	ALA	3.4
1	D	177	HIS	3.4
1	H	138	GLN	3.3
1	A	186	ASN	3.3
1	B	258	TYR	3.3
1	H	308	PHE	3.3
1	B	294	ASP	3.3
1	D	225	LEU	3.3
1	G	180	SER	3.3
1	A	174	ARG	3.2
1	F	297	ILE	3.2
1	G	315	LEU	3.2
1	E	258	TYR	3.2
1	B	299	ARG	3.2
1	C	172	ASP	3.2
1	F	288	ALA	3.2
1	F	300	CYS	3.2
1	D	174	ARG	3.2
1	H	311	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	J	226	GLU	3.2
1	B	122	ASP	3.2
1	C	188	PHE	3.2
1	H	139	GLN	3.1
1	G	282	PHE	3.1
1	I	285	HIS	3.1
1	C	173	ILE	3.1
1	B	300	CYS	3.1
1	B	152	ILE	3.1
1	E	285	HIS	3.1
1	F	295	LEU	3.0
1	B	125	GLN	3.0
1	A	299	ARG	3.0
1	G	163	ARG	3.0
1	D	121	PHE	3.0
1	C	317	ILE	3.0
1	I	36	ASP	3.0
1	J	177	HIS	3.0
1	F	185	GLN	3.0
1	H	141	ARG	2.9
1	C	305	PRO	2.9
1	A	295	LEU	2.9
1	F	283	ALA	2.9
1	D	178	LEU	2.8
1	I	177	HIS	2.8
1	B	296	LEU	2.8
1	F	287	GLN	2.8
1	A	117	ARG	2.8
1	A	293	ASP	2.8
1	A	287	GLN	2.8
1	A	178	LEU	2.8
1	C	310	ALA	2.8
1	G	306	LEU	2.8
1	C	307	GLY	2.7
1	G	311	ILE	2.7
1	F	285	HIS	2.7
1	C	163	ARG	2.7
1	B	123	ARG	2.7
1	G	189	SER	2.7
1	B	253	LEU	2.7
1	G	151	ASN	2.7
1	A	317	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	121	PHE	2.7
1	J	153	ASP	2.7
1	H	309	LEU	2.7
1	I	107	LEU	2.7
1	F	290	GLY	2.6
1	I	105	ARG	2.6
1	B	119	PHE	2.6
1	F	296	LEU	2.6
1	F	173	ILE	2.6
1	E	292	GLU	2.5
1	I	286	ARG	2.5
1	B	305	PRO	2.5
1	G	280	ILE	2.5
1	A	150	GLU	2.5
1	G	286	ARG	2.5
1	E	53	ASP	2.5
1	B	295	LEU	2.5
1	H	315	LEU	2.5
1	I	284	HIS	2.5
1	D	170	ILE	2.5
1	E	51	PRO	2.5
1	E	165	LYS	2.5
1	H	151	ASN	2.5
1	J	152	ILE	2.5
1	D	292	GLU	2.5
1	F	188	PHE	2.5
1	C	288	ALA	2.5
1	J	176	ASP	2.5
1	J	173	ILE	2.4
1	E	267	ILE	2.4
1	C	311	ILE	2.4
1	G	284	HIS	2.4
1	D	181	VAL	2.4
1	D	126	PHE	2.3
1	B	223	PHE	2.3
1	E	232	LEU	2.3
1	E	179	SER	2.3
1	B	301	ARG	2.3
1	E	245	TYR	2.3
1	G	158	ASP	2.3
1	D	227	SER	2.3
1	C	190	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	288	ALA	2.2
1	B	74	PRO	2.2
1	B	41	ALA	2.2
1	C	145	ILE	2.2
1	D	172	ASP	2.2
1	E	249	THR	2.2
1	E	246	ALA	2.2
1	I	35	VAL	2.2
1	J	304	PHE	2.1
1	A	187	GLU	2.1
1	H	307	GLY	2.1
1	D	222	VAL	2.1
1	D	204	TYR	2.1
1	G	310	ALA	2.1
1	C	156	GLU	2.1
1	B	199	ARG	2.1
1	F	291	VAL	2.1
1	B	310	ALA	2.1
1	G	155	GLU	2.1
1	D	173	ILE	2.1
1	H	198	VAL	2.1
1	D	203	TYR	2.1
1	B	256	LEU	2.0
1	H	291	VAL	2.0
1	D	248	TYR	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.