



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:10 AM UTC

PDB ID : 5HEU / pdb_00005heu
Title : Pentameric ligand-gated ion channel ELIC mutant A257Y
Authors : Bertozzi, C.; Dutzler, R.
Deposited on : 2016-01-06
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

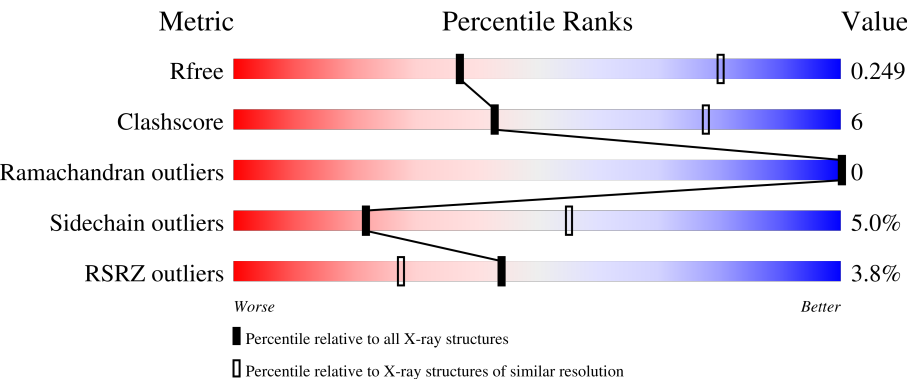
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	3% 77% 17% • 5%
1	B	322	4% 76% 17% • 5%
1	C	322	2% 77% 17% • 5%
1	D	322	2% 80% 13% • 5%
1	E	322	2% 76% 17% • 5%

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Mol	Chain	Length	Quality of chain
1	F	322	2% 76% 18% • 5%
1	G	322	6% 76% 18% • 5%
1	H	322	3% 76% 17% • 5%
1	I	322	4% 77% 16% • 5%
1	J	322	7% 75% 20% • 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24980 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
			2498	1627	416	449	6			
1	B	307	Total	C	N	O	S	0	0	0
			2498	1627	416	449	6			
1	C	307	Total	C	N	O	S	0	0	0
			2498	1627	416	449	6			
1	D	307	Total	C	N	O	S	0	0	0
			2498	1627	416	449	6			
1	E	307	Total	C	N	O	S	0	0	0
			2498	1627	416	449	6			
1	F	307	Total	C	N	O	S	0	0	0
			2498	1627	416	449	6			
1	G	307	Total	C	N	O	S	0	0	0
			2498	1627	416	449	6			
1	H	307	Total	C	N	O	S	0	0	0
			2498	1627	416	449	6			
1	I	307	Total	C	N	O	S	0	0	0
			2498	1627	416	449	6			
1	J	307	Total	C	N	O	S	0	0	0
			2498	1627	416	449	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	ALA	TYR	engineered mutation	UNP E0SJQ4
B	258	ALA	TYR	engineered mutation	UNP E0SJQ4
C	258	ALA	TYR	engineered mutation	UNP E0SJQ4
D	258	ALA	TYR	engineered mutation	UNP E0SJQ4
E	258	ALA	TYR	engineered mutation	UNP E0SJQ4
F	258	ALA	TYR	engineered mutation	UNP E0SJQ4
G	258	ALA	TYR	engineered mutation	UNP E0SJQ4
H	258	ALA	TYR	engineered mutation	UNP E0SJQ4
I	258	ALA	TYR	engineered mutation	UNP E0SJQ4

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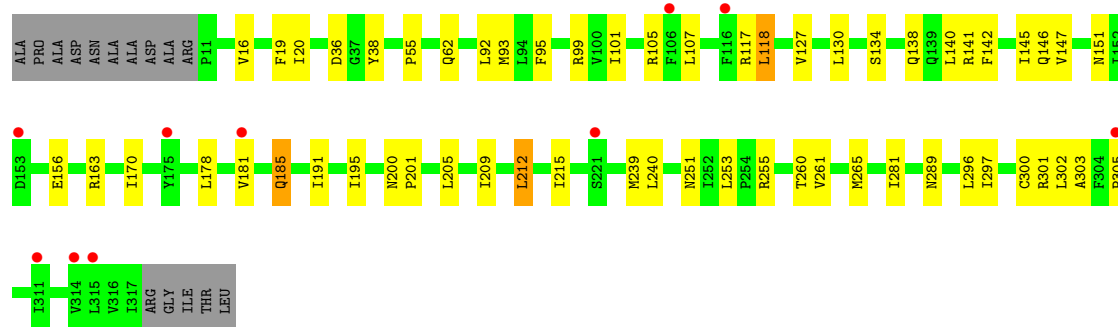
Chain	Residue	Modelled	Actual	Comment	Reference
J	258	ALA	TYR	engineered mutation	UNP E0SJQ4

3 Residue-property plots [i](#)

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

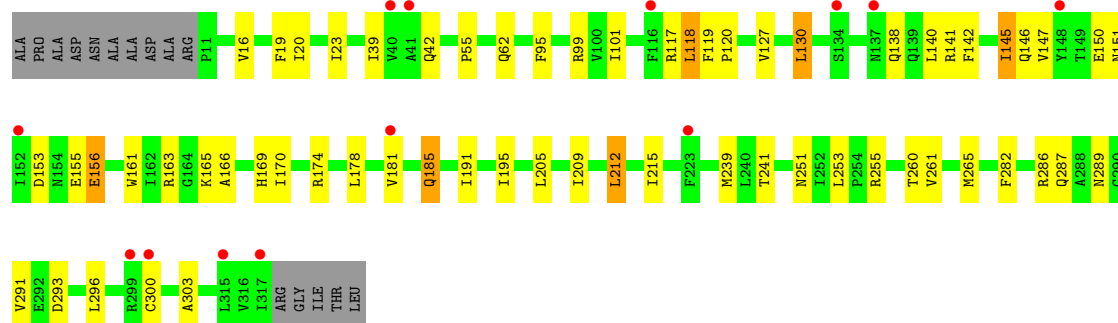
- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain A: 



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

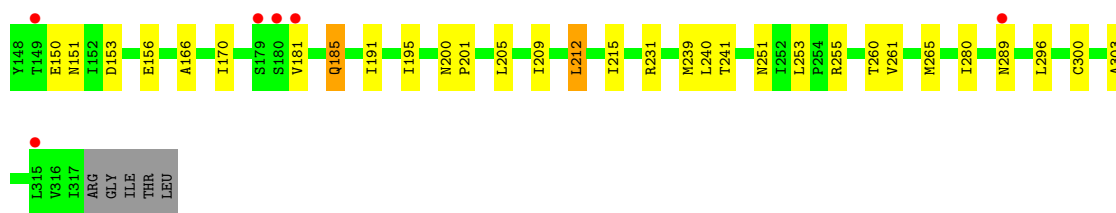
Chain B: 



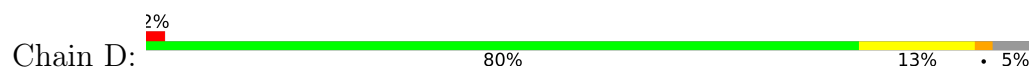
- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

Chain C: 

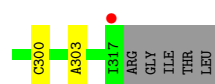
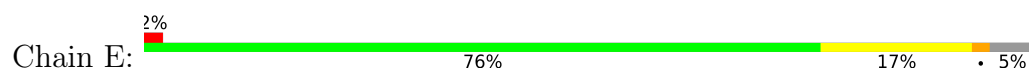




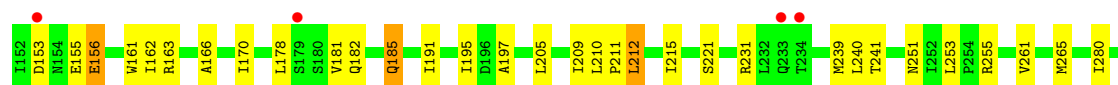
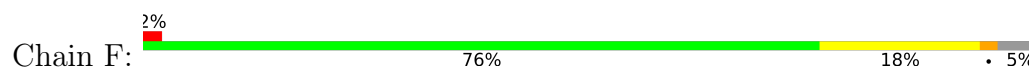
- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



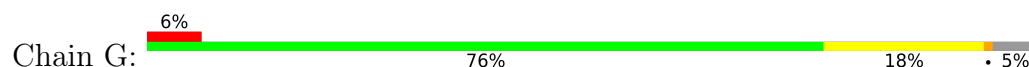
- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

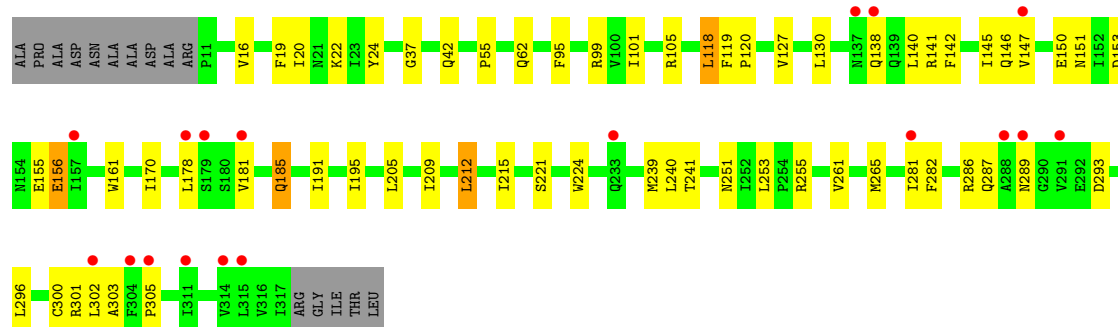


- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

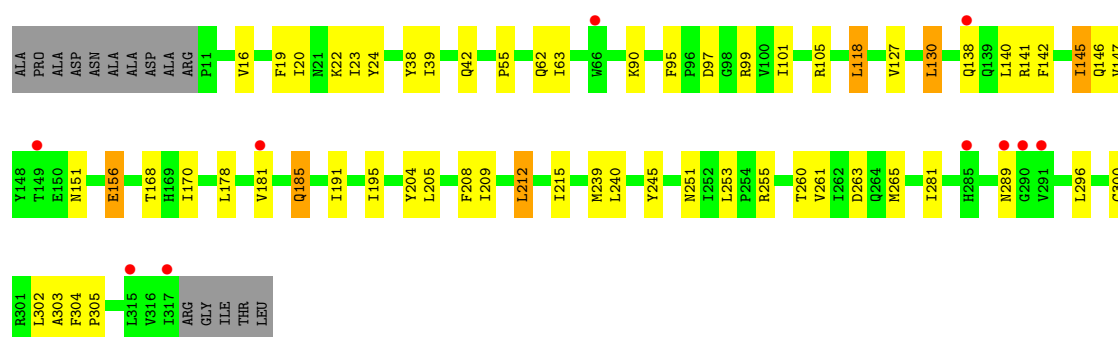
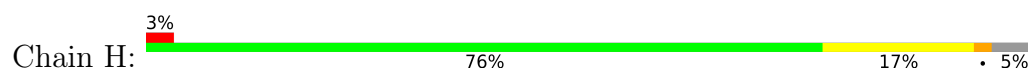


- Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

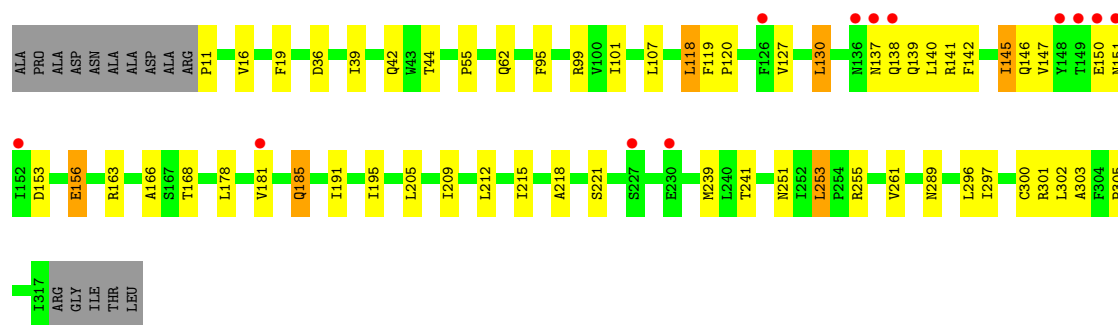
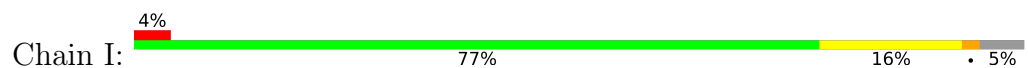




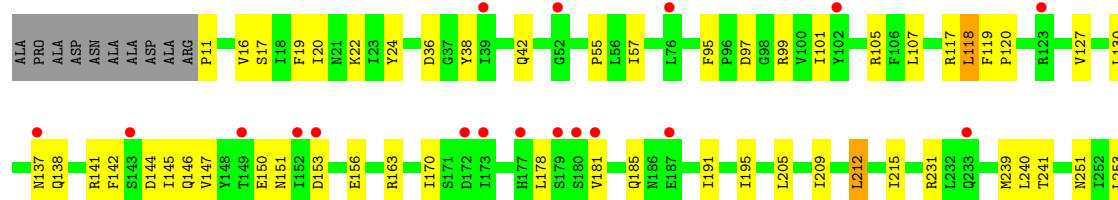
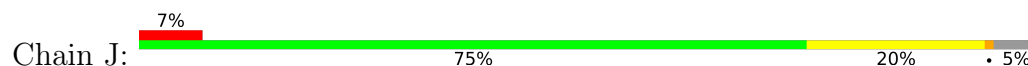
• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1

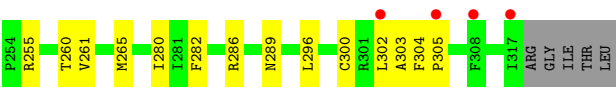


• Molecule 1: Gamma-aminobutyric-acid receptor subunit beta-1



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.00Å 266.61Å 110.71Å 90.00° 110.47° 90.00°	Depositor
Resolution (Å)	29.94 – 3.20 29.94 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.94-3.20) 99.4 (29.94-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.220 , 0.247 0.224 , 0.249	Depositor DCC
R_{free} test set	4694 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	83.0	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 63.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24980	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.13	0/2565	0.34	0/3496
1	B	0.15	0/2565	0.34	0/3496
1	C	0.13	0/2565	0.35	0/3496
1	D	0.13	0/2565	0.34	0/3496
1	E	0.13	0/2565	0.34	0/3496
1	F	0.13	0/2565	0.34	0/3496
1	G	0.14	0/2565	0.36	0/3496
1	H	0.13	0/2565	0.35	0/3496
1	I	0.12	0/2565	0.34	0/3496
1	J	0.14	0/2565	0.35	0/3496
All	All	0.13	0/25650	0.35	0/34960

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	2498	0	2474	32	0
1	B	2498	0	2474	39	0
1	C	2498	0	2474	31	0
1	D	2498	0	2474	26	0
1	E	2498	0	2474	37	0
1	F	2498	0	2474	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2498	0	2474	33	0
1	H	2498	0	2474	36	0
1	I	2498	0	2474	36	0
1	J	2498	0	2474	34	0
All	All	24980	0	24740	306	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 6.

All (306) 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:F:300:CYS:HA	1:F:303:ALA:HB3	1.76	0.68
1:H:251:ASN:O	1:H:255:ARG:NH1	2.28	0.67
1:B:170:ILE:HG12	1:B:191:ILE:HG12	1.77	0.66
1:A:300:CYS:HA	1:A:303:ALA:HB3	1.77	0.66
1:D:300:CYS:HA	1:D:303:ALA:HB3	1.79	0.64
1:A:170:ILE:HG12	1:A:191:ILE:HG12	1.80	0.63
1:H:300:CYS:HA	1:H:303:ALA:HB3	1.79	0.62
1:I:251:ASN:O	1:I:255:ARG:NH1	2.33	0.62
1:I:300:CYS:HA	1:I:303:ALA:HB3	1.80	0.62
1:I:205:LEU:HD23	1:I:209:ILE:HD12	1.82	0.62
1:B:300:CYS:HA	1:B:303:ALA:HB3	1.81	0.62
1:H:212:LEU:HD12	1:H:265:MET:HE2	1.81	0.62
1:E:300:CYS:HA	1:E:303:ALA:HB3	1.81	0.61
1:E:251:ASN:O	1:E:255:ARG:NH1	2.34	0.61
1:D:205:LEU:HD23	1:D:209:ILE:HD12	1.83	0.61
1:A:205:LEU:HD23	1:A:209:ILE:HD12	1.82	0.61
1:B:174:ARG:NH2	1:I:139:GLN:OE1	2.34	0.61
1:G:251:ASN:O	1:G:255:ARG:NH1	2.33	0.61
1:J:300:CYS:HA	1:J:303:ALA:HB3	1.83	0.60
1:C:300:CYS:HA	1:C:303:ALA:HB3	1.82	0.60
1:B:205:LEU:HD23	1:B:209:ILE:HD12	1.85	0.59
1:B:118:LEU:HA	1:B:261:VAL:HG23	1.83	0.58
1:F:170:ILE:HG12	1:F:191:ILE:HG12	1.84	0.58
1:B:251:ASN:O	1:B:255:ARG:NH1	2.36	0.58
1:F:251:ASN:O	1:F:255:ARG:NH1	2.36	0.58
1:G:300:CYS:HA	1:G:303:ALA:HB3	1.84	0.58
1:D:118:LEU:HA	1:D:261:VAL:HG23	1.85	0.58
1:A:251:ASN:O	1:A:255:ARG:NH1	2.37	0.57
1:J:251:ASN:O	1:J:255:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:ASN:O	1:D:255:ARG:NH1	2.37	0.57
1:J:205:LEU:HD23	1:J:209:ILE:HD12	1.87	0.57
1:I:118:LEU:HA	1:I:261:VAL:HG23	1.87	0.57
1:H:118:LEU:HA	1:H:261:VAL:HG23	1.87	0.57
1:F:118:LEU:HA	1:F:261:VAL:HG23	1.86	0.56
1:G:205:LEU:HD23	1:G:209:ILE:HD12	1.87	0.56
1:H:215:ILE:HG12	1:I:239:MET:HE3	1.87	0.56
1:H:170:ILE:HG12	1:H:191:ILE:HG12	1.87	0.56
1:C:118:LEU:HA	1:C:261:VAL:HG23	1.86	0.56
1:C:212:LEU:HD12	1:C:265:MET:HE2	1.87	0.56
1:C:251:ASN:O	1:C:255:ARG:NH1	2.39	0.56
1:E:212:LEU:HD12	1:E:265:MET:HE2	1.86	0.56
1:F:205:LEU:HD23	1:F:209:ILE:HD12	1.88	0.56
1:F:240:LEU:HD13	1:J:241:THR:HA	1.88	0.56
1:B:166:ALA:HB2	1:B:195:ILE:HG12	1.87	0.55
1:D:156:GLU:CD	1:D:156:GLU:H	2.15	0.55
1:D:118:LEU:H	1:D:118:LEU:HD12	1.72	0.55
1:H:205:LEU:HD23	1:H:209:ILE:HD12	1.89	0.55
1:E:118:LEU:HA	1:E:261:VAL:HG23	1.90	0.54
1:E:36:ASP:HB2	1:E:107:LEU:HD13	1.90	0.54
1:D:170:ILE:HG12	1:D:191:ILE:HG12	1.90	0.54
1:E:249:THR:HG23	1:E:253:LEU:HD23	1.90	0.54
1:J:212:LEU:HD12	1:J:265:MET:HE2	1.90	0.54
1:B:212:LEU:HD12	1:B:265:MET:HE2	1.91	0.54
1:C:170:ILE:HG12	1:C:191:ILE:HG12	1.89	0.54
1:C:205:LEU:HD23	1:C:209:ILE:HD12	1.90	0.53
1:J:118:LEU:HA	1:J:261:VAL:HG23	1.90	0.53
1:I:156:GLU:CD	1:I:156:GLU:H	2.16	0.53
1:D:166:ALA:HB2	1:D:195:ILE:HG12	1.90	0.53
1:C:39:ILE:HD11	1:C:130:LEU:HD11	1.91	0.53
1:E:155:GLU:O	1:E:161:TRP:NE1	2.39	0.53
1:E:170:ILE:HG12	1:E:191:ILE:HG12	1.89	0.53
1:I:19:PHE:CE2	1:I:146:GLN:HG3	2.44	0.53
1:A:118:LEU:HA	1:A:261:VAL:HG23	1.91	0.52
1:F:181:VAL:HG21	1:J:99:ARG:NH2	2.24	0.52
1:F:209:ILE:HG23	1:F:265:MET:HE1	1.92	0.51
1:I:39:ILE:HD11	1:I:130:LEU:HD11	1.92	0.51
1:D:99:ARG:NH2	1:E:181:VAL:HG21	2.26	0.51
1:E:19:PHE:CE2	1:E:146:GLN:HG3	2.46	0.51
1:J:170:ILE:HG12	1:J:191:ILE:HG12	1.93	0.51
1:D:147:VAL:HG21	1:D:195:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:39:ILE:HD11	1:H:130:LEU:HD11	1.92	0.51
1:E:150:GLU:HG3	1:E:153:ASP:HB3	1.92	0.51
1:G:99:ARG:NH2	1:H:181:VAL:HG21	2.26	0.51
1:B:215:ILE:HG12	1:C:239:MET:HE3	1.92	0.50
1:G:170:ILE:HG12	1:G:191:ILE:HG12	1.94	0.50
1:G:287:GLN:HG3	1:G:293:ASP:HB2	1.92	0.50
1:H:22:LYS:HE3	1:H:24:TYR:CD1	2.47	0.50
1:B:19:PHE:CE2	1:B:146:GLN:HG3	2.47	0.50
1:D:19:PHE:CE2	1:D:146:GLN:HG3	2.46	0.50
1:G:155:GLU:O	1:G:161:TRP:NE1	2.43	0.50
1:A:20:ILE:HD12	1:A:195:ILE:HD11	1.94	0.49
1:A:147:VAL:HG21	1:A:195:ILE:HD13	1.93	0.49
1:D:39:ILE:HD11	1:D:130:LEU:HD11	1.95	0.49
1:F:22:LYS:HE3	1:F:24:TYR:CD1	2.47	0.49
1:J:141:ARG:HG3	1:J:142:PHE:CD2	2.47	0.49
1:A:141:ARG:HG3	1:A:142:PHE:CD2	2.48	0.49
1:F:118:LEU:HD12	1:F:118:LEU:H	1.77	0.49
1:B:39:ILE:HD11	1:B:130:LEU:HD11	1.94	0.49
1:B:140:LEU:HD13	1:B:191:ILE:HG13	1.93	0.49
1:B:141:ARG:HG3	1:B:142:PHE:CD2	2.47	0.49
1:H:20:ILE:HD12	1:H:195:ILE:HD11	1.93	0.49
1:C:118:LEU:HD12	1:C:118:LEU:H	1.78	0.49
1:H:99:ARG:NH2	1:I:181:VAL:HG21	2.28	0.49
1:C:231:ARG:HB3	1:C:280:ILE:HD13	1.95	0.49
1:H:141:ARG:HG3	1:H:142:PHE:CD2	2.48	0.48
1:I:141:ARG:HG3	1:I:142:PHE:CD2	2.48	0.48
1:F:140:LEU:HD13	1:F:191:ILE:HG13	1.95	0.48
1:F:141:ARG:HG3	1:F:142:PHE:CD2	2.47	0.48
1:I:36:ASP:HB2	1:I:107:LEU:HD13	1.94	0.48
1:G:118:LEU:HA	1:G:261:VAL:HG23	1.94	0.48
1:G:141:ARG:HG3	1:G:142:PHE:CD2	2.48	0.48
1:F:19:PHE:CE2	1:F:146:GLN:HG3	2.49	0.48
1:J:36:ASP:HB2	1:J:107:LEU:HD13	1.95	0.48
1:B:241:THR:HA	1:C:240:LEU:HD13	1.96	0.48
1:F:215:ILE:HG12	1:G:239:MET:HE3	1.96	0.48
1:H:19:PHE:CE2	1:H:146:GLN:HG3	2.49	0.48
1:A:239:MET:HE3	1:E:215:ILE:HG12	1.94	0.48
1:D:141:ARG:HG3	1:D:142:PHE:CD2	2.49	0.47
1:B:282:PHE:CZ	1:B:286:ARG:HG3	2.50	0.47
1:E:55:PRO:HB3	1:E:95:PHE:CD1	2.50	0.47
1:E:155:GLU:C	1:E:161:TRP:HE1	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ASP:HB2	1:A:107:LEU:HD13	1.95	0.47
1:C:141:ARG:HG3	1:C:142:PHE:CD2	2.49	0.47
1:G:215:ILE:HG12	1:H:239:MET:HE3	1.96	0.47
1:B:150:GLU:HG3	1:B:153:ASP:HB3	1.96	0.47
1:E:141:ARG:HG3	1:E:142:PHE:CD2	2.49	0.47
1:I:215:ILE:HG12	1:J:239:MET:HE3	1.97	0.47
1:E:156:GLU:CD	1:E:156:GLU:H	2.22	0.47
1:G:150:GLU:HG3	1:G:153:ASP:HB3	1.96	0.47
1:J:150:GLU:HG3	1:J:153:ASP:HB3	1.95	0.47
1:J:302:LEU:C	1:J:305:PRO:HD2	2.40	0.47
1:B:117:ARG:O	1:B:260:THR:HA	2.14	0.47
1:B:147:VAL:HG21	1:B:195:ILE:HD13	1.97	0.46
1:F:212:LEU:HD12	1:F:265:MET:HE2	1.97	0.46
1:G:241:THR:HA	1:H:240:LEU:HD13	1.97	0.46
1:D:215:ILE:HG12	1:E:239:MET:HE3	1.97	0.46
1:I:42:GLN:HG3	1:I:101:ILE:HG12	1.96	0.46
1:B:20:ILE:HD12	1:B:195:ILE:HD11	1.97	0.46
1:C:215:ILE:HG12	1:D:239:MET:HE3	1.97	0.46
1:H:147:VAL:HG21	1:H:195:ILE:HD13	1.96	0.46
1:J:22:LYS:HE3	1:J:24:TYR:CD1	2.51	0.46
1:F:150:GLU:HG3	1:F:153:ASP:HB3	1.97	0.46
1:A:281:ILE:HD11	1:E:221:SER:HB2	1.98	0.46
1:A:163:ARG:HD3	1:A:163:ARG:HA	1.72	0.46
1:C:19:PHE:CE2	1:C:146:GLN:HG3	2.51	0.46
1:I:118:LEU:HD12	1:I:118:LEU:H	1.81	0.46
1:C:42:GLN:HG3	1:C:101:ILE:HG12	1.98	0.46
1:B:118:LEU:HD12	1:B:118:LEU:H	1.81	0.45
1:B:156:GLU:CD	1:B:156:GLU:H	2.23	0.45
1:B:23:ILE:HD11	1:B:195:ILE:HD12	1.99	0.45
1:B:145:ILE:HG13	1:B:166:ALA:HB3	1.99	0.45
1:C:99:ARG:NH2	1:D:181:VAL:HG21	2.31	0.45
1:E:39:ILE:HD11	1:E:130:LEU:HD11	1.97	0.45
1:J:42:GLN:HG3	1:J:101:ILE:HG12	1.98	0.45
1:B:99:ARG:NH2	1:C:181:VAL:HG21	2.32	0.45
1:G:19:PHE:CE2	1:G:146:GLN:HG3	2.51	0.45
1:J:38:TYR:CZ	1:J:105:ARG:HD3	2.51	0.45
1:F:145:ILE:HG13	1:F:166:ALA:HB3	1.98	0.45
1:F:163:ARG:HD3	1:F:163:ARG:HA	1.74	0.45
1:I:150:GLU:HG3	1:I:153:ASP:HB3	1.98	0.45
1:D:178:LEU:HD12	1:D:178:LEU:HA	1.83	0.45
1:J:17:SER:HA	1:J:144:ASP:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:117:ARG:O	1:J:260:THR:HA	2.16	0.45
1:J:231:ARG:HB3	1:J:280:ILE:HD13	1.98	0.45
1:B:163:ARG:HD3	1:B:163:ARG:HA	1.74	0.45
1:H:55:PRO:HB3	1:H:95:PHE:CD1	2.52	0.45
1:C:117:ARG:O	1:C:260:THR:HA	2.17	0.45
1:J:19:PHE:CE2	1:J:146:GLN:HG3	2.51	0.44
1:C:147:VAL:HG21	1:C:195:ILE:HD13	1.99	0.44
1:F:99:ARG:NH2	1:G:181:VAL:HG21	2.32	0.44
1:A:185:GLN:H	1:A:185:GLN:HG3	1.48	0.44
1:C:166:ALA:HB2	1:C:195:ILE:HG12	1.98	0.44
1:E:11:PRO:HA	1:E:137:ASN:O	2.18	0.44
1:H:23:ILE:HD11	1:H:195:ILE:HD12	1.98	0.44
1:H:97:ASP:OD2	1:H:99:ARG:NH1	2.50	0.44
1:A:38:TYR:CZ	1:A:105:ARG:HD3	2.53	0.44
1:H:140:LEU:HD13	1:H:191:ILE:HG13	1.99	0.44
1:G:282:PHE:CZ	1:G:286:ARG:HG3	2.53	0.44
1:I:147:VAL:HG21	1:I:195:ILE:HD13	1.99	0.44
1:A:19:PHE:CE2	1:A:146:GLN:HG3	2.53	0.44
1:A:240:LEU:HD13	1:E:241:THR:HA	1.99	0.44
1:D:145:ILE:HG13	1:D:166:ALA:HB3	2.00	0.44
1:E:147:VAL:HG21	1:E:195:ILE:HD13	2.00	0.44
1:G:221:SER:HB2	1:H:281:ILE:HD11	2.00	0.44
1:I:99:ARG:NH2	1:J:181:VAL:HG21	2.33	0.44
1:A:99:ARG:NH2	1:B:181:VAL:HG21	2.33	0.44
1:A:302:LEU:C	1:A:305:PRO:HD2	2.42	0.44
1:C:185:GLN:H	1:C:185:GLN:HG3	1.52	0.44
1:H:178:LEU:HD12	1:H:178:LEU:HA	1.76	0.44
1:B:155:GLU:O	1:B:161:TRP:NE1	2.48	0.43
1:E:119:PHE:HB3	1:E:120:PRO:HD3	2.01	0.43
1:F:36:ASP:HB2	1:F:107:LEU:HD13	2.00	0.43
1:F:93:MET:HB3	1:F:101:ILE:HB	1.99	0.43
1:E:38:TYR:CZ	1:E:105:ARG:HD3	2.54	0.43
1:E:118:LEU:HD12	1:E:118:LEU:H	1.84	0.43
1:F:210:LEU:HB3	1:F:211:PRO:HD3	2.01	0.43
1:I:166:ALA:HB2	1:I:195:ILE:HG12	2.00	0.43
1:I:253:LEU:HD12	1:I:253:LEU:HA	1.88	0.43
1:J:11:PRO:HA	1:J:137:ASN:O	2.18	0.43
1:A:55:PRO:HB3	1:A:95:PHE:CD1	2.54	0.43
1:F:119:PHE:HB3	1:F:120:PRO:HD3	2.01	0.43
1:F:58:VAL:HG13	1:F:62:GLN:HB3	2.01	0.43
1:F:97:ASP:OD2	1:F:99:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:TYR:CZ	1:C:105:ARG:HD3	2.54	0.43
1:E:178:LEU:HD12	1:E:178:LEU:HA	1.81	0.43
1:G:22:LYS:HE3	1:G:24:TYR:CD1	2.54	0.43
1:I:241:THR:HA	1:J:240:LEU:HD13	2.01	0.43
1:A:93:MET:HB3	1:A:101:ILE:HB	2.01	0.43
1:A:140:LEU:HD13	1:A:191:ILE:HG13	2.01	0.43
1:B:119:PHE:HB3	1:B:120:PRO:HD3	2.01	0.43
1:A:181:VAL:HG21	1:E:99:ARG:NH2	2.33	0.42
1:H:38:TYR:CZ	1:H:105:ARG:HD3	2.53	0.42
1:J:97:ASP:OD2	1:J:99:ARG:NH1	2.52	0.42
1:E:22:LYS:HE3	1:E:24:TYR:CD1	2.54	0.42
1:J:282:PHE:CZ	1:J:286:ARG:HG3	2.54	0.42
1:F:162:ILE:HD13	1:F:197:ALA:HB2	2.01	0.42
1:G:20:ILE:HD12	1:G:195:ILE:HD11	2.00	0.42
1:H:185:GLN:H	1:H:185:GLN:HG3	1.52	0.42
1:I:119:PHE:HB3	1:I:120:PRO:HD3	2.01	0.42
1:I:178:LEU:HA	1:I:178:LEU:HD12	1.75	0.42
1:A:209:ILE:HG23	1:A:265:MET:HE1	2.01	0.42
1:B:291:VAL:HG12	1:B:293:ASP:H	1.84	0.42
1:F:241:THR:HA	1:G:240:LEU:HD13	2.02	0.42
1:G:55:PRO:HB3	1:G:95:PHE:CD1	2.55	0.42
1:C:150:GLU:HG3	1:C:153:ASP:HB3	2.00	0.42
1:E:20:ILE:HD12	1:E:195:ILE:HD11	2.01	0.42
1:H:260:THR:H	1:H:263:ASP:HB2	1.84	0.42
1:I:145:ILE:HG13	1:I:166:ALA:HB3	2.01	0.42
1:F:185:GLN:H	1:F:185:GLN:HG3	1.56	0.42
1:A:117:ARG:O	1:A:260:THR:HA	2.20	0.42
1:I:55:PRO:HB3	1:I:95:PHE:CD1	2.55	0.42
1:A:134:SER:HB3	1:E:57:ILE:HD13	2.01	0.42
1:D:297:ILE:O	1:D:301:ARG:HB2	2.19	0.42
1:E:163:ARG:HD3	1:E:163:ARG:HA	1.75	0.42
1:F:130:LEU:HD23	1:F:130:LEU:HA	1.91	0.42
1:G:37:GLY:O	1:G:105:ARG:HD2	2.20	0.42
1:G:140:LEU:HD13	1:G:191:ILE:HG13	2.02	0.42
1:H:302:LEU:C	1:H:305:PRO:HD2	2.44	0.42
1:J:147:VAL:HG21	1:J:195:ILE:HD13	2.02	0.42
1:B:55:PRO:HB3	1:B:95:PHE:CD1	2.55	0.42
1:F:178:LEU:HD12	1:F:178:LEU:HA	1.78	0.42
1:G:42:GLN:HG3	1:G:101:ILE:HG12	2.01	0.42
1:H:209:ILE:HG23	1:H:265:MET:HE1	2.02	0.42
1:I:185:GLN:H	1:I:185:GLN:HG3	1.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:PHE:HB3	1:C:120:PRO:HD3	2.01	0.42
1:H:204:TYR:O	1:H:208:PHE:HB2	2.19	0.42
1:I:218:ALA:O	1:I:221:SER:OG	2.32	0.42
1:J:300:CYS:O	1:J:304:PHE:HB2	2.20	0.42
1:A:118:LEU:HD12	1:A:118:LEU:H	1.85	0.41
1:B:165:LYS:HG3	1:I:163:ARG:HB3	2.01	0.41
1:E:130:LEU:HD23	1:E:130:LEU:HA	1.89	0.41
1:F:231:ARG:HB3	1:F:280:ILE:HD13	2.01	0.41
1:G:185:GLN:H	1:G:185:GLN:HG3	1.53	0.41
1:B:178:LEU:HD12	1:B:178:LEU:HA	1.78	0.41
1:C:140:LEU:HD13	1:C:191:ILE:HG13	2.02	0.41
1:D:155:GLU:O	1:D:161:TRP:NE1	2.53	0.41
1:G:119:PHE:HB3	1:G:120:PRO:HD3	2.01	0.41
1:J:55:PRO:HB3	1:J:95:PHE:CD1	2.56	0.41
1:A:215:ILE:HG12	1:B:239:MET:HE3	2.02	0.41
1:C:92:LEU:HD23	1:C:92:LEU:HA	1.94	0.41
1:H:99:ARG:CZ	1:I:181:VAL:HG21	2.51	0.41
1:H:156:GLU:CD	1:H:156:GLU:H	2.29	0.41
1:J:20:ILE:HD12	1:J:195:ILE:HD11	2.01	0.41
1:A:178:LEU:HD12	1:A:178:LEU:HA	1.79	0.41
1:I:11:PRO:HA	1:I:137:ASN:O	2.20	0.41
1:I:44:THR:HA	1:I:99:ARG:HA	2.02	0.41
1:I:130:LEU:HD23	1:I:130:LEU:HA	1.90	0.41
1:B:42:GLN:HG3	1:B:101:ILE:HG12	2.03	0.41
1:C:241:THR:HA	1:D:240:LEU:HD13	2.03	0.41
1:D:117:ARG:O	1:D:260:THR:HA	2.20	0.41
1:E:37:GLY:O	1:E:105:ARG:HD2	2.21	0.41
1:F:156:GLU:CD	1:F:156:GLU:H	2.29	0.41
1:F:182:GLN:H	1:F:182:GLN:CD	2.28	0.41
1:G:156:GLU:CD	1:G:156:GLU:H	2.28	0.41
1:J:119:PHE:HB3	1:J:120:PRO:HD3	2.03	0.41
1:A:200:ASN:HA	1:A:201:PRO:HD3	1.94	0.41
1:B:155:GLU:C	1:B:161:TRP:HE1	2.27	0.41
1:B:287:GLN:HG3	1:B:293:ASP:HB2	2.03	0.41
1:C:22:LYS:HE3	1:C:24:TYR:CD1	2.55	0.41
1:D:302:LEU:C	1:D:305:PRO:HD2	2.46	0.41
1:G:147:VAL:HG21	1:G:195:ILE:HD13	2.02	0.41
1:I:297:ILE:O	1:I:301:ARG:HB2	2.21	0.41
1:A:297:ILE:O	1:A:301:ARG:HB2	2.19	0.41
1:D:16:VAL:HA	1:D:40:VAL:O	2.21	0.41
1:D:14:VAL:HG22	1:D:43:TRP:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:212:LEU:HD12	1:G:265:MET:HE2	2.01	0.41
1:B:185:GLN:H	1:B:185:GLN:HG3	1.49	0.41
1:F:134:SER:HB3	1:J:57:ILE:HD13	2.03	0.41
1:G:178:LEU:HD12	1:G:178:LEU:HA	1.79	0.41
1:H:42:GLN:HG3	1:H:101:ILE:HG12	2.03	0.41
1:I:140:LEU:HD13	1:I:191:ILE:HG13	2.03	0.41
1:B:169:HIS:HA	1:I:168:THR:O	2.19	0.41
1:C:20:ILE:HD12	1:C:195:ILE:HD11	2.02	0.41
1:E:205:LEU:HD23	1:E:209:ILE:HD12	2.03	0.41
1:F:239:MET:HE3	1:J:215:ILE:HG12	2.02	0.41
1:G:224:TRP:CE2	1:G:301:ARG:HG2	2.56	0.41
1:A:92:LEU:HD23	1:A:92:LEU:HA	1.96	0.40
1:C:200:ASN:HA	1:C:201:PRO:HD3	1.92	0.40
1:E:287:GLN:CB	1:E:291:VAL:HB	2.51	0.40
1:F:20:ILE:HD12	1:F:195:ILE:HD11	2.02	0.40
1:I:302:LEU:C	1:I:305:PRO:HD2	2.46	0.40
1:J:163:ARG:HD3	1:J:163:ARG:HA	1.74	0.40
1:C:26:VAL:HG22	1:C:33:TYR:HB3	2.02	0.40
1:D:300:CYS:O	1:D:304:PHE:HB2	2.21	0.40
1:H:300:CYS:O	1:H:304:PHE:HB2	2.20	0.40
1:A:212:LEU:HD12	1:A:265:MET:HE2	2.03	0.40
1:B:287:GLN:HB2	1:B:291:VAL:HB	2.03	0.40
1:E:282:PHE:CZ	1:E:286:ARG:HG3	2.57	0.40
1:F:155:GLU:O	1:F:161:TRP:NE1	2.52	0.40
1:H:145:ILE:HD12	1:H:168:THR:HG23	2.04	0.40
1:H:212:LEU:HD23	1:H:245:TYR:CD2	2.57	0.40
1:J:178:LEU:HD12	1:J:178:LEU:HA	1.79	0.40
1:E:185:GLN:H	1:E:185:GLN:HG3	1.53	0.40
1:F:221:SER:HB2	1:G:281:ILE:HD11	2.02	0.40
1:G:302:LEU:C	1:G:305:PRO:HD2	2.47	0.40
1:H:63:ILE:HD12	1:H:90:LYS:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	284 (93%)	21 (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%)	284 (93%)	21 (7%)	0	100	100
1	E	305/322 (95%)	283 (93%)	22 (7%)	0	100	100
1	F	305/322 (95%)	284 (93%)	21 (7%)	0	100	100
1	G	305/322 (95%)	284 (93%)	21 (7%)	0	100	100
1	H	305/322 (95%)	284 (93%)	21 (7%)	0	100	100
1	I	305/322 (95%)	284 (93%)	21 (7%)	0	100	100
1	J	305/322 (95%)	283 (93%)	22 (7%)	0	100	100
All	All	3050/3220 (95%)	2838 (93%)	212 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/283 (97%)	260 (95%)	14 (5%)	21	54
1	B	274/283 (97%)	260 (95%)	14 (5%)	21	54
1	C	274/283 (97%)	260 (95%)	14 (5%)	21	54
1	D	274/283 (97%)	261 (95%)	13 (5%)	23	57
1	E	274/283 (97%)	261 (95%)	13 (5%)	23	57
1	F	274/283 (97%)	261 (95%)	13 (5%)	23	57
1	G	274/283 (97%)	260 (95%)	14 (5%)	21	54
1	H	274/283 (97%)	260 (95%)	14 (5%)	21	54
1	I	274/283 (97%)	260 (95%)	14 (5%)	21	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	274/283 (97%)	261 (95%)	13 (5%)	23	57
All	All	2740/2830 (97%)	2604 (95%)	136 (5%)	22	55

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	62	GLN
1	A	118	LEU
1	A	127	VAL
1	A	130	LEU
1	A	138	GLN
1	A	145	ILE
1	A	151	ASN
1	A	156	GLU
1	A	185	GLN
1	A	212	LEU
1	A	253	LEU
1	A	289	ASN
1	A	296	LEU
1	B	16	VAL
1	B	62	GLN
1	B	118	LEU
1	B	127	VAL
1	B	130	LEU
1	B	138	GLN
1	B	145	ILE
1	B	151	ASN
1	B	156	GLU
1	B	185	GLN
1	B	212	LEU
1	B	253	LEU
1	B	289	ASN
1	B	296	LEU
1	C	16	VAL
1	C	62	GLN
1	C	118	LEU
1	C	127	VAL
1	C	130	LEU
1	C	138	GLN
1	C	145	ILE
1	C	151	ASN

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Mol	Chain	Res	Type
1	C	156	GLU
1	C	185	GLN
1	C	212	LEU
1	C	253	LEU
1	C	289	ASN
1	C	296	LEU
1	D	16	VAL
1	D	118	LEU
1	D	127	VAL
1	D	130	LEU
1	D	138	GLN
1	D	145	ILE
1	D	151	ASN
1	D	156	GLU
1	D	185	GLN
1	D	212	LEU
1	D	253	LEU
1	D	289	ASN
1	D	296	LEU
1	E	16	VAL
1	E	62	GLN
1	E	118	LEU
1	E	127	VAL
1	E	130	LEU
1	E	138	GLN
1	E	145	ILE
1	E	151	ASN
1	E	156	GLU
1	E	185	GLN
1	E	212	LEU
1	E	253	LEU
1	E	296	LEU
1	F	16	VAL
1	F	118	LEU
1	F	127	VAL
1	F	130	LEU
1	F	138	GLN
1	F	145	ILE
1	F	151	ASN
1	F	156	GLU
1	F	185	GLN
1	F	212	LEU

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Mol	Chain	Res	Type
1	F	253	LEU
1	F	289	ASN
1	F	296	LEU
1	G	16	VAL
1	G	62	GLN
1	G	118	LEU
1	G	127	VAL
1	G	130	LEU
1	G	138	GLN
1	G	145	ILE
1	G	151	ASN
1	G	156	GLU
1	G	185	GLN
1	G	212	LEU
1	G	253	LEU
1	G	289	ASN
1	G	296	LEU
1	H	16	VAL
1	H	62	GLN
1	H	118	LEU
1	H	127	VAL
1	H	130	LEU
1	H	138	GLN
1	H	145	ILE
1	H	151	ASN
1	H	156	GLU
1	H	185	GLN
1	H	212	LEU
1	H	253	LEU
1	H	289	ASN
1	H	296	LEU
1	I	16	VAL
1	I	62	GLN
1	I	118	LEU
1	I	127	VAL
1	I	130	LEU
1	I	138	GLN
1	I	145	ILE
1	I	151	ASN
1	I	156	GLU
1	I	185	GLN
1	I	212	LEU

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Mol	Chain	Res	Type
1	I	253	LEU
1	I	289	ASN
1	I	296	LEU
1	J	16	VAL
1	J	118	LEU
1	J	127	VAL
1	J	130	LEU
1	J	138	GLN
1	J	145	ILE
1	J	151	ASN
1	J	156	GLU
1	J	185	GLN
1	J	212	LEU
1	J	253	LEU
1	J	289	ASN
1	J	296	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	251	ASN
1	A	264	GLN
1	A	287	GLN
1	B	62	GLN
1	B	136	ASN
1	B	186	ASN
1	B	251	ASN
1	B	264	GLN
1	C	62	GLN
1	C	124	GLN
1	C	136	ASN
1	C	138	GLN
1	C	186	ASN
1	C	251	ASN
1	D	136	ASN
1	D	185	GLN
1	D	186	ASN
1	D	251	ASN
1	D	264	GLN
1	E	62	GLN
1	E	136	ASN

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Mol	Chain	Res	Type
1	E	185	GLN
1	E	186	ASN
1	E	251	ASN
1	E	264	GLN
1	F	185	GLN
1	F	186	ASN
1	F	251	ASN
1	F	264	GLN
1	G	136	ASN
1	G	186	ASN
1	G	251	ASN
1	G	264	GLN
1	H	136	ASN
1	H	251	ASN
1	H	264	GLN
1	I	62	GLN
1	I	186	ASN
1	I	251	ASN
1	I	264	GLN
1	J	136	ASN
1	J	251	ASN
1	J	264	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 oligosaccharides 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

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, 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	307/322 (95%)	0.09	10 (3%)	49	30	48, 89, 175, 246	0
1	B	307/322 (95%)	0.25	13 (4%)	40	25	49, 81, 194, 258	0
1	C	307/322 (95%)	0.12	8 (2%)	57	37	44, 84, 201, 252	0
1	D	307/322 (95%)	0.12	7 (2%)	61	41	45, 84, 177, 271	0
1	E	307/322 (95%)	0.09	8 (2%)	57	37	51, 87, 178, 325	0
1	F	307/322 (95%)	0.06	8 (2%)	57	37	45, 86, 184, 276	0
1	G	307/322 (95%)	0.21	18 (5%)	28	18	50, 80, 176, 262	0
1	H	307/322 (95%)	0.10	10 (3%)	49	30	45, 86, 201, 255	0
1	I	307/322 (95%)	0.21	12 (3%)	43	27	46, 78, 181, 288	0
1	J	307/322 (95%)	0.23	22 (7%)	21	14	52, 84, 199, 282	0
All	All	3070/3220 (95%)	0.15	116 (3%)	44	27	44, 84, 190, 325	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	289	ASN	5.7
1	G	137	ASN	4.3
1	D	153	ASP	4.1
1	I	148	TYR	4.1
1	A	153	ASP	4.0
1	H	291	VAL	4.0
1	I	137	ASN	3.9
1	J	52	GLY	3.9
1	F	148	TYR	3.9
1	H	290	GLY	3.8
1	G	315	LEU	3.7
1	J	187	GLU	3.7
1	C	181	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	137	ASN	3.7
1	A	181	VAL	3.7
1	B	317	ILE	3.5
1	J	305	PRO	3.5
1	J	153	ASP	3.5
1	G	179	SER	3.4
1	I	181	VAL	3.4
1	A	315	LEU	3.4
1	B	181	VAL	3.4
1	G	314	VAL	3.4
1	D	152	ILE	3.4
1	D	149	THR	3.3
1	E	181	VAL	3.2
1	I	230	GLU	3.1
1	I	126	PHE	3.1
1	J	181	VAL	3.1
1	G	311	ILE	3.1
1	B	152	ILE	3.0
1	J	149	THR	3.0
1	E	149	THR	3.0
1	G	289	ASN	3.0
1	H	289	ASN	3.0
1	B	299	ARG	2.9
1	G	305	PRO	2.9
1	B	223	PHE	2.9
1	G	138	GLN	2.9
1	F	315	LEU	2.9
1	B	148	TYR	2.9
1	F	179	SER	2.9
1	H	138	GLN	2.8
1	H	285	HIS	2.8
1	J	137	ASN	2.8
1	H	315	LEU	2.8
1	G	147	VAL	2.8
1	H	66	TRP	2.8
1	G	304	PHE	2.8
1	J	39	ILE	2.8
1	J	102	TYR	2.8
1	I	152	ILE	2.8
1	J	317	ILE	2.8
1	J	177	HIS	2.7
1	F	306	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	149	THR	2.7
1	I	227	SER	2.7
1	E	76	LEU	2.7
1	I	138	GLN	2.7
1	E	317	ILE	2.6
1	B	300	CYS	2.6
1	J	173	ILE	2.6
1	C	180	SER	2.5
1	C	121	PHE	2.5
1	G	302	LEU	2.5
1	I	136	ASN	2.5
1	J	172	ASP	2.5
1	J	302	LEU	2.5
1	D	126	PHE	2.5
1	G	178	LEU	2.5
1	C	137	ASN	2.4
1	A	305	PRO	2.4
1	J	233	GLN	2.4
1	B	116	PHE	2.4
1	D	315	LEU	2.4
1	F	153	ASP	2.4
1	J	152	ILE	2.4
1	A	221	SER	2.4
1	J	76	LEU	2.4
1	B	315	LEU	2.3
1	C	315	LEU	2.3
1	G	181	VAL	2.3
1	F	234	THR	2.3
1	J	143	SER	2.3
1	E	177	HIS	2.3
1	C	149	THR	2.3
1	A	311	ILE	2.3
1	G	288	ALA	2.3
1	I	149	THR	2.3
1	A	116	PHE	2.3
1	A	314	VAL	2.2
1	B	40	VAL	2.2
1	F	233	GLN	2.2
1	G	281	ILE	2.2
1	G	157	ILE	2.2
1	E	137	ASN	2.2
1	I	151	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	179	SER	2.1
1	E	147	VAL	2.1
1	G	291	VAL	2.1
1	J	179	SER	2.1
1	J	123	ARG	2.1
1	D	11	PRO	2.1
1	D	180	SER	2.1
1	J	308	PHE	2.1
1	H	181	VAL	2.1
1	I	150	GLU	2.1
1	B	134	SER	2.1
1	E	145	ILE	2.1
1	H	317	ILE	2.1
1	A	175	TYR	2.1
1	B	41	ALA	2.0
1	A	106	PHE	2.0
1	F	138	GLN	2.0
1	J	180	SER	2.0
1	G	233	GLN	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 oligosaccharides 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.