



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:15 PM UTC

PDB ID : 7BM5 / pdb_00007bm5
Title : Crystal structure of Fab1, the Fab fragment of the anti-BamA monoclonal antibody MAB1
Authors : White, P.; Storek, K.M.; Rutherford, S.T.; Radford, S.E.
Deposited on : 2021-01-19
Resolution : 2.95 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:

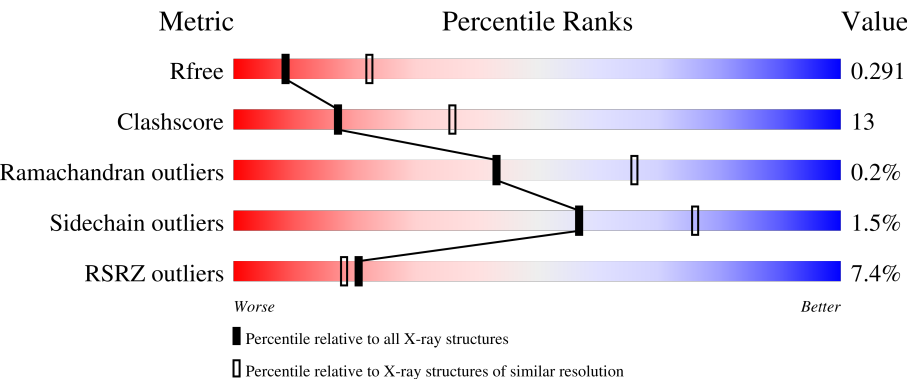
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
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 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	215	2% 72% 26% ..
1	C	215	8% 71% 22% 6%
1	E	215	13% 66% 21% 12%
1	G	215	13% 70% 19% 9%
1	J	215	4% 74% 23% ..

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Mol	Chain	Length	Quality of chain
1	L	215	4% 74% 22% • •
2	B	228	3% 70% 24% • 5%
2	D	228	7% 70% 21% 9%
2	F	228	9% 67% 21% • 11%
2	H	228	6% 73% 23% • •
2	I	228	7% 56% 11% 33%
2	K	228	5% 72% 21% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18443 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 Fab1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	212	Total	C	N	O	S	0	0	0
			1643	1030	278	330	5			
1	A	212	Total	C	N	O	S	0	0	0
			1633	1024	274	330	5			
1	C	203	Total	C	N	O	S	0	0	0
			1547	967	260	315	5			
1	E	190	Total	C	N	O	S	0	0	0
			1446	905	242	293	6			
1	J	212	Total	C	N	O	S	0	0	0
			1631	1021	275	330	5			
1	G	196	Total	C	N	O	S	0	0	0
			1489	935	247	303	4			

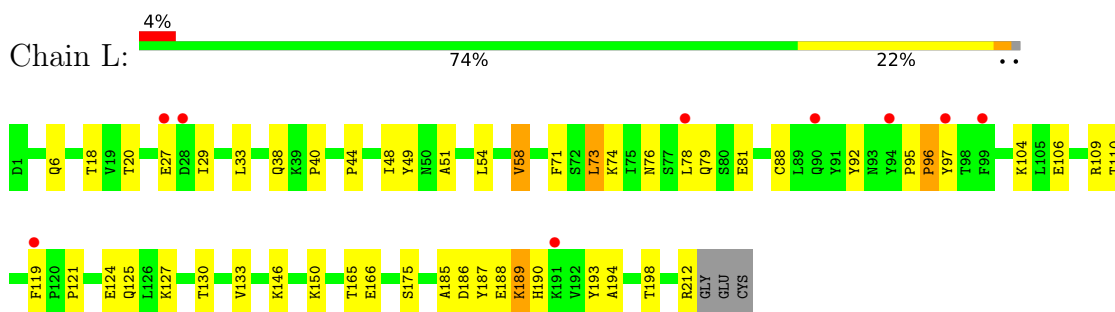
- Molecule 2 is a protein called Fab1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	0	0
			1658	1052	280	319	7			
2	B	216	Total	C	N	O	S	0	0	0
			1631	1037	274	313	7			
2	D	208	Total	C	N	O	S	0	0	0
			1545	979	259	300	7			
2	F	204	Total	C	N	O	S	0	0	0
			1503	950	253	293	7			
2	K	216	Total	C	N	O	S	0	0	0
			1605	1023	269	306	7			
2	I	153	Total	C	N	O	S	0	0	0
			1112	706	188	212	6			

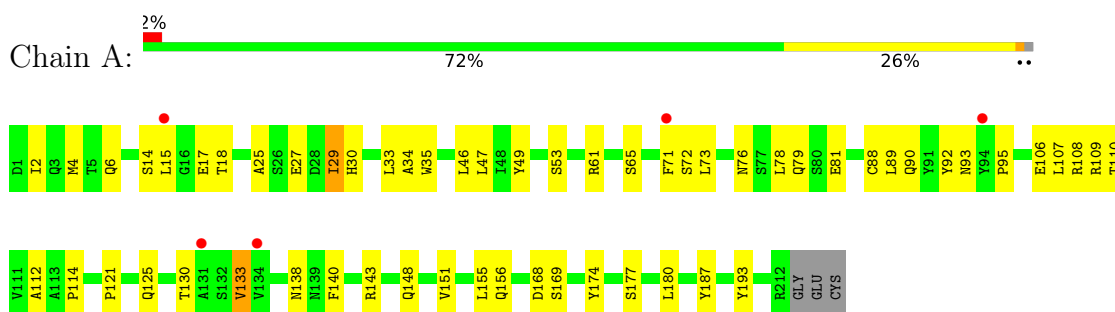
3 Residue-property plots [i](#)

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.

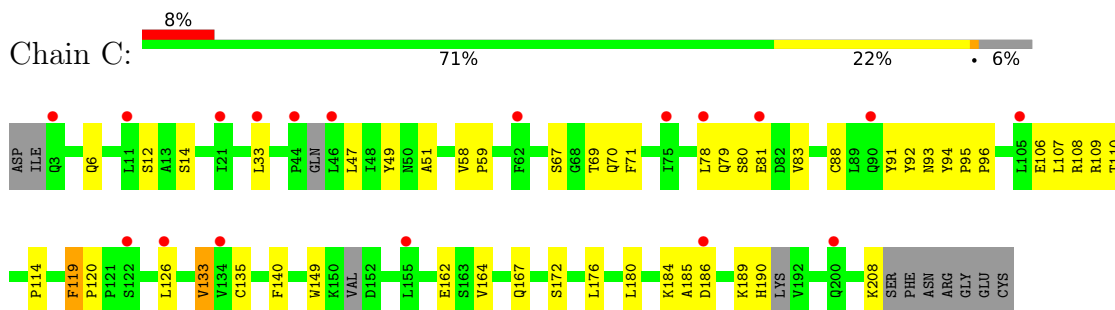
- Molecule 1: Fab1 light chain



- Molecule 1: Fab1 light chain

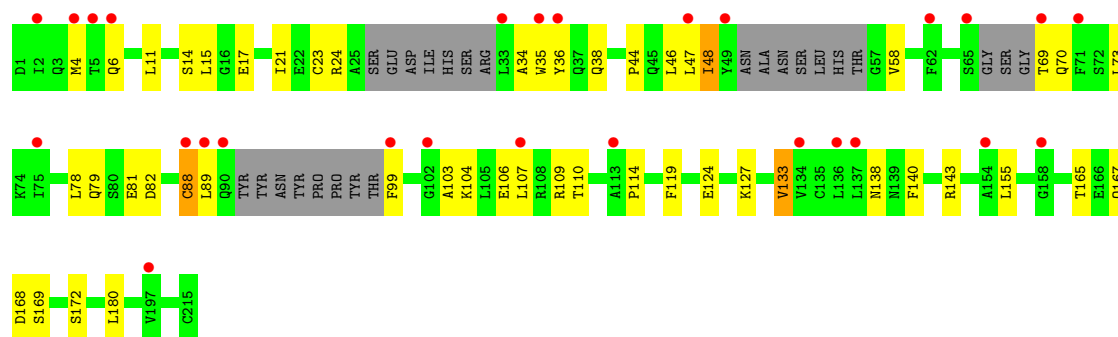


- Molecule 1: Fab1 light chain

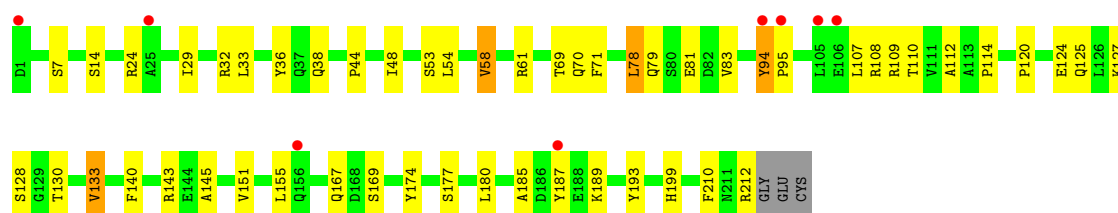


- Molecule 1: Fab1 light chain

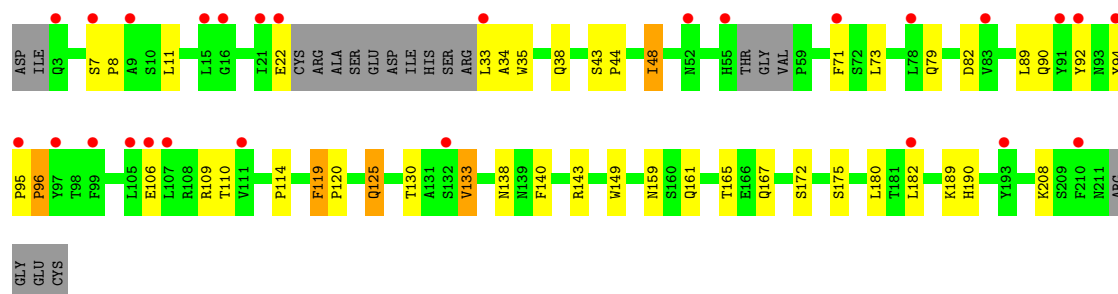




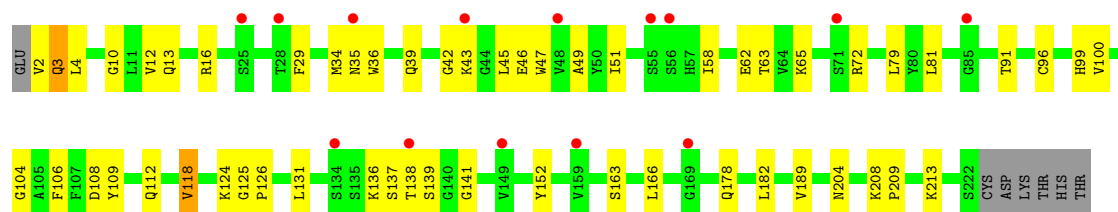
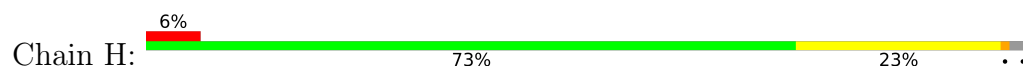
• Molecule 1: Fab1 light chain



• Molecule 1: Fab1 light chain

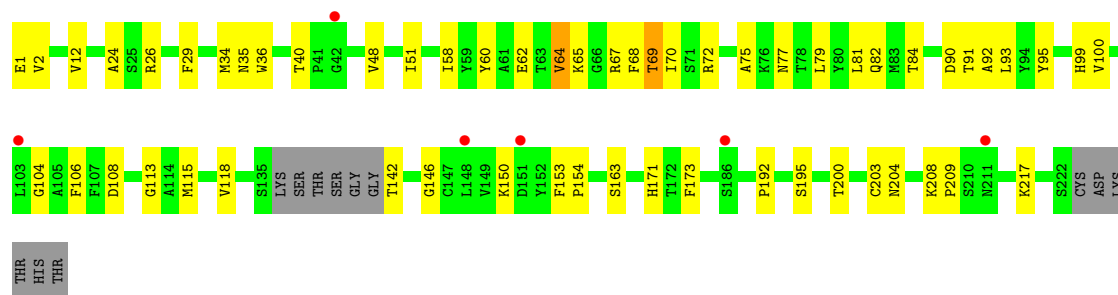


• Molecule 2: Fab1 heavy chain

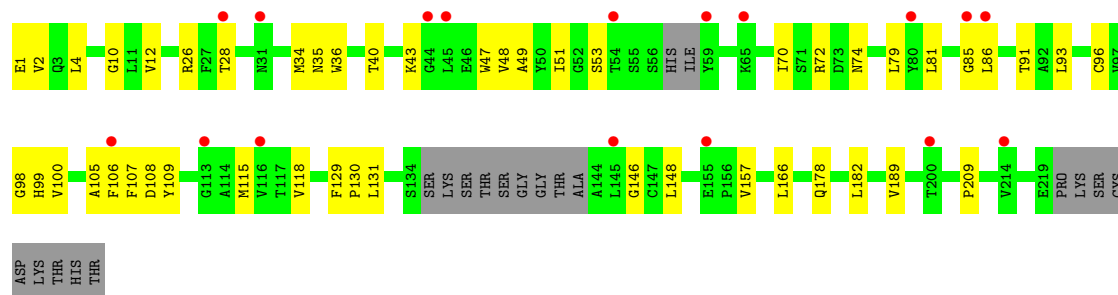


• Molecule 2: Fab1 heavy chain

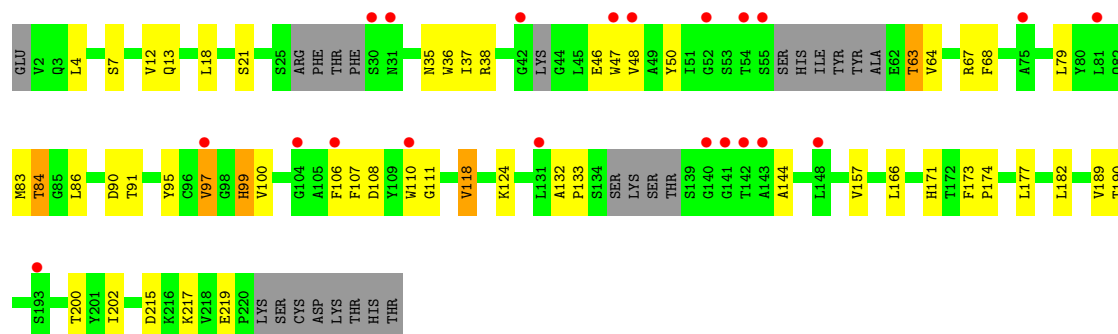




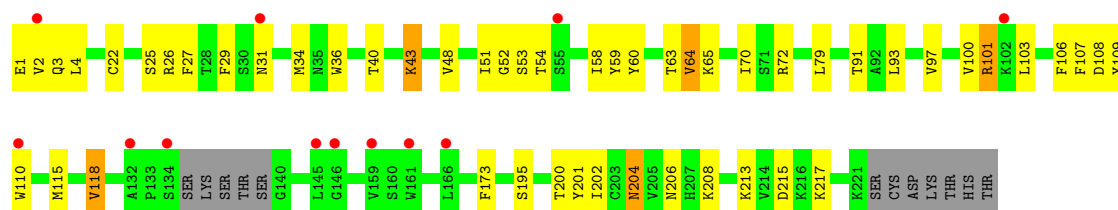
- Molecule 2: Fab1 heavy chain



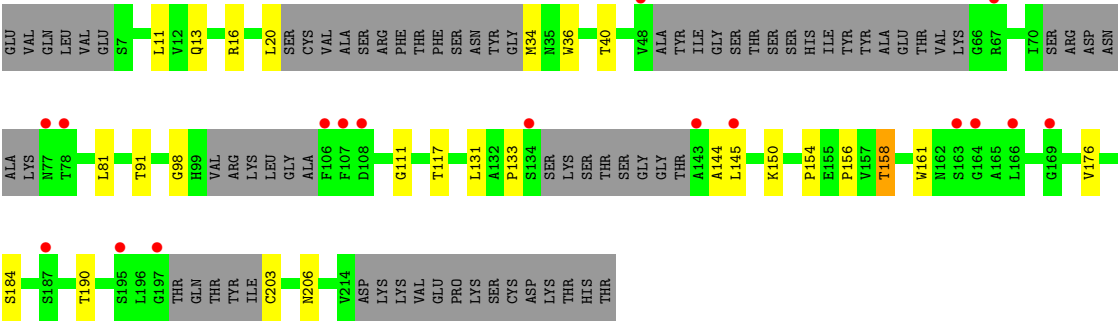
- Molecule 2: Fab1 heavy chain



- Molecule 2: Fab1 heavy chain



- Molecule 2: Fab1 heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.01Å 130.14Å 138.92Å 90.00° 106.06° 90.00°	Depositor
Resolution (Å)	88.42 – 2.95 88.42 – 2.95	Depositor EDS
% Data completeness (in resolution range)	46.1 (88.42-2.95) 46.1 (88.42-2.95)	Depositor EDS
R_{merge}	0.42	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.257 , 0.290 0.263 , 0.291	Depositor DCC
R_{free} test set	1495 reflections (2.25%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 6.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	18443	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.03% 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	0.46	0/1670	0.85	0/2270
1	C	0.49	0/1579	0.89	2/2145 (0.1%)
1	E	0.47	0/1471	0.89	3/1990 (0.2%)
1	G	0.45	0/1521	0.90	4/2068 (0.2%)
1	J	0.47	0/1668	0.90	4/2269 (0.2%)
1	L	0.50	0/1680	0.91	2/2281 (0.1%)
2	B	0.39	0/1671	0.89	2/2275 (0.1%)
2	D	0.40	0/1579	0.81	0/2150
2	F	0.44	1/1535 (0.1%)	0.90	6/2089 (0.3%)
2	H	0.38	0/1699	0.87	3/2313 (0.1%)
2	I	0.39	0/1134	0.75	0/1541
2	K	0.45	0/1645	0.92	2/2243 (0.1%)
All	All	0.44	1/18852 (0.0%)	0.88	28/25634 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	97	VAL	N-CA	5.02	1.51	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	63	THR	CB-CA-C	-8.74	106.48	116.54
1	C	119	PHE	CA-C-N	8.61	129.25	120.38
1	C	119	PHE	C-N-CA	8.61	129.25	120.38
1	G	119	PHE	CA-C-N	7.93	125.37	119.66
1	G	119	PHE	C-N-CA	7.93	125.37	119.66
2	F	97	VAL	N-CA-C	6.45	117.77	108.48
1	L	58	VAL	CA-C-N	6.33	126.25	119.85
1	L	58	VAL	C-N-CA	6.33	126.25	119.85
1	G	48	ILE	N-CA-C	6.17	117.01	108.12
1	E	119	PHE	CA-C-N	5.86	126.42	120.38
1	E	119	PHE	C-N-CA	5.86	126.42	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	64	VAL	N-CA-C	5.86	117.13	111.91
1	E	48	ILE	N-CA-C	5.85	116.54	108.12
1	J	58	VAL	CA-C-N	5.83	125.74	119.85
1	J	58	VAL	C-N-CA	5.83	125.74	119.85
2	H	3	GLN	N-CA-C	-5.80	104.97	112.68
2	F	84	THR	N-CA-C	-5.67	105.18	111.36
2	H	42	GLY	N-CA-C	-5.61	107.04	114.95
2	H	100	VAL	N-CA-C	5.59	115.90	107.80
2	K	101	ARG	N-CA-C	-5.54	106.57	113.55
1	J	94	TYR	CA-C-N	-5.48	114.74	120.38
1	J	94	TYR	C-N-CA	-5.48	114.74	120.38
2	F	132	ALA	CA-C-N	5.33	126.50	119.84
2	F	132	ALA	C-N-CA	5.33	126.50	119.84
2	K	43	LYS	N-CA-C	5.22	118.67	112.72
2	B	146	GLY	N-CA-C	5.21	119.97	111.27
1	G	125	GLN	N-CA-C	-5.09	106.84	113.16
2	F	63	THR	N-CA-C	5.05	115.98	108.31

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	1633	0	1570	44	1
1	C	1547	0	1468	45	0
1	E	1446	0	1391	39	0
1	G	1489	0	1416	36	0
1	J	1631	0	1559	37	1
1	L	1643	0	1592	43	0
2	B	1631	0	1598	49	0
2	D	1545	0	1494	33	0
2	F	1503	0	1453	44	0
2	H	1658	0	1626	40	0
2	I	1112	0	1075	17	0
2	K	1605	0	1558	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	18443	0	17800	456	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (456) 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:G:95:PRO:HG2	1:G:96:PRO:HD3	1.20	1.16
1:E:4:MET:HE1	1:E:23:CYS:SG	1.98	1.03
2:B:51:ILE:HD13	2:B:72:ARG:HG2	1.37	1.02
1:L:6:GLN:NE2	1:L:88:CYS:SG	2.33	1.02
1:G:95:PRO:CG	1:G:96:PRO:HD3	1.98	0.93
1:C:58:VAL:HG22	1:C:59:PRO:HD2	1.52	0.92
2:I:11:LEU:HD12	2:I:154:PRO:HG3	1.53	0.90
1:C:58:VAL:CG2	1:C:59:PRO:HD2	2.01	0.90
2:B:91:THR:HG22	2:B:118:VAL:H	1.39	0.88
1:E:4:MET:CE	1:E:23:CYS:SG	2.63	0.86
2:K:202:ILE:HD12	2:K:204:ASN:HD21	1.40	0.84
2:D:91:THR:HG22	2:D:118:VAL:H	1.41	0.83
2:F:91:THR:HG22	2:F:118:VAL:H	1.40	0.83
2:B:62:GLU:HA	2:B:65:LYS:HE3	1.60	0.82
1:G:95:PRO:HG2	1:G:96:PRO:CD	2.08	0.82
1:E:78:LEU:HD12	1:E:78:LEU:O	1.80	0.81
2:F:35:ASN:HB2	2:F:97:VAL:HB	1.64	0.80
1:L:33:LEU:HB3	1:L:51:ALA:HB2	1.62	0.80
1:G:8:PRO:HD3	1:G:22:GLU:HB2	1.61	0.80
2:K:206:ASN:HD22	2:K:213:LYS:HD3	1.47	0.80
2:H:2:VAL:HG12	2:H:3:GLN:H	1.47	0.80
2:K:3:GLN:HG3	2:K:26:ARG:HG3	1.63	0.80
1:G:90:GLN:HE21	1:G:92:TYR:HB3	1.48	0.79
2:K:4:LEU:HD21	2:K:27:PHE:HZ	1.48	0.79
1:L:40:PRO:HB3	1:L:166:GLU:HG2	1.65	0.77
1:G:7:SER:N	1:G:8:PRO:HD2	1.99	0.77
2:K:3:GLN:NE2	2:K:26:ARG:NH1	2.33	0.76
2:H:91:THR:HG22	2:H:118:VAL:H	1.48	0.75
1:E:4:MET:HE3	1:E:24:ARG:O	1.87	0.75
1:L:29:ILE:HG23	1:L:92:TYR:HB2	1.68	0.75
2:K:202:ILE:CD1	2:K:204:ASN:HD21	1.99	0.75
1:J:69:THR:HG23	1:J:70:GLN:HG2	1.68	0.74
2:K:29:PHE:O	2:K:72:ARG:NH2	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:31:ASN:O	2:K:101:ARG:NH1	2.20	0.74
2:K:202:ILE:HD12	2:K:204:ASN:ND2	2.03	0.74
1:L:78:LEU:HD12	1:L:78:LEU:O	1.87	0.73
1:C:78:LEU:HD12	1:C:78:LEU:O	1.88	0.73
2:B:51:ILE:HG23	2:B:72:ARG:HD2	1.71	0.73
2:K:2:VAL:HG22	2:K:109:TYR:HB2	1.71	0.72
1:A:78:LEU:HD12	1:A:78:LEU:O	1.90	0.71
1:L:121:PRO:HD3	1:L:133:VAL:HG22	1.72	0.71
1:J:38:GLN:HB2	1:J:44:PRO:HB3	1.71	0.71
2:K:2:VAL:HG22	2:K:109:TYR:CB	2.20	0.71
2:H:35:ASN:HB2	2:H:49:ALA:O	1.91	0.70
2:H:12:VAL:HG12	2:H:13:GLN:N	2.06	0.70
2:B:51:ILE:CD1	2:B:72:ARG:HG2	2.17	0.69
1:G:106:GLU:OE2	1:G:143:ARG:NH2	2.24	0.69
1:L:104:LYS:NZ	1:L:106:GLU:OE2	2.27	0.68
1:C:69:THR:HG23	1:C:70:GLN:HG3	1.74	0.68
2:D:26:ARG:NH2	2:K:100:VAL:O	2.25	0.68
1:E:81:GLU:N	1:E:81:GLU:OE1	2.27	0.68
2:I:158:THR:HG23	2:I:206:ASN:HB3	1.75	0.67
1:G:8:PRO:HB2	1:G:11:LEU:HD11	1.77	0.67
2:I:91:THR:HG23	2:I:117:THR:HA	1.77	0.67
2:I:161:TRP:HA	2:I:203:CYS:HA	1.77	0.67
2:B:51:ILE:CG2	2:B:72:ARG:HD2	2.26	0.66
1:C:95:PRO:CB	1:C:96:PRO:CD	2.74	0.66
1:A:4:MET:HE3	1:A:25:ALA:HB2	1.78	0.66
2:F:63:THR:OG1	2:F:64:VAL:N	2.25	0.66
1:E:133:VAL:HG13	1:E:180:LEU:HB3	1.77	0.65
2:F:68:PHE:CE2	2:F:83:MET:HG2	2.32	0.65
2:B:51:ILE:HD13	2:B:72:ARG:CG	2.20	0.65
1:A:61:ARG:HH12	1:A:79:GLN:HG2	1.61	0.65
2:K:200:THR:HG23	2:K:217:LYS:HE2	1.78	0.65
2:K:3:GLN:NE2	2:K:26:ARG:HH11	1.94	0.65
2:K:100:VAL:HG21	2:K:106:PHE:CE2	2.33	0.64
2:H:51:ILE:HG13	2:H:58:ILE:HG22	1.80	0.64
1:A:6:GLN:NE2	1:A:88:CYS:SG	2.71	0.63
1:A:49:TYR:HB2	2:B:106:PHE:CE2	2.33	0.63
2:F:35:ASN:HD21	2:F:99:HIS:CE1	2.16	0.63
1:A:133:VAL:HG13	1:A:180:LEU:HB3	1.80	0.63
2:D:34:MET:HB3	2:D:79:LEU:HD22	1.81	0.63
2:I:144:ALA:HB2	2:I:190:THR:HG22	1.80	0.63
1:E:104:LYS:NZ	1:E:106:GLU:OE2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:12:VAL:HG21	2:F:18:LEU:HD22	1.81	0.62
1:J:133:VAL:HG13	1:J:180:LEU:HB3	1.82	0.62
2:B:51:ILE:HG13	2:B:58:ILE:HG12	1.81	0.62
1:C:93:ASN:OD1	1:C:93:ASN:O	2.18	0.62
1:C:126:LEU:O	1:C:184:LYS:HD2	1.98	0.62
1:A:14:SER:HA	1:A:108:ARG:HB2	1.82	0.62
2:F:215:ASP:OD2	2:I:16:ARG:NE	2.29	0.62
1:L:185:ALA:O	1:L:189:LYS:HD3	1.99	0.61
2:I:11:LEU:HD12	2:I:154:PRO:CG	2.29	0.61
2:F:12:VAL:HG12	2:F:13:GLN:N	2.14	0.61
2:F:95:TYR:HB3	2:F:110:TRP:HE3	1.64	0.61
2:H:62:GLU:O	2:H:65:LYS:HG3	1.99	0.61
2:D:178:GLN:HG2	2:D:182:LEU:O	2.01	0.61
2:I:20:LEU:HD12	2:I:81:LEU:HD23	1.82	0.61
1:C:133:VAL:HG13	1:C:180:LEU:HB3	1.81	0.61
1:C:164:VAL:HG22	1:C:176:LEU:HD13	1.81	0.61
2:K:2:VAL:HG12	2:K:2:VAL:O	2.01	0.61
1:E:140:PHE:HE1	1:E:143:ARG:HA	1.65	0.61
1:J:81:GLU:OE1	1:J:169:SER:HB2	2.01	0.61
1:E:34:ALA:HB3	1:E:89:LEU:HB3	1.83	0.60
2:B:40:THR:HG22	2:B:92:ALA:HB2	1.83	0.60
2:K:100:VAL:HG11	2:K:106:PHE:CE1	2.37	0.60
1:L:95:PRO:HB2	1:L:96:PRO:HD3	1.83	0.60
2:K:22:CYS:HB3	2:K:79:LEU:HB3	1.84	0.60
1:C:91:TYR:HB2	2:D:105:ALA:HB3	1.83	0.60
1:E:24:ARG:HG3	1:E:70:GLN:OE1	2.01	0.60
2:B:100:VAL:HG11	2:B:106:PHE:CE2	2.36	0.60
2:B:104:GLY:HA3	2:B:106:PHE:CE1	2.36	0.60
2:D:2:VAL:HG12	2:D:2:VAL:O	2.00	0.60
2:I:34:MET:N	2:I:98:GLY:HA2	2.17	0.60
1:A:177:SER:HB3	2:B:173:PHE:CE2	2.37	0.60
1:E:167:GLN:HE21	1:E:172:SER:HB3	1.68	0.59
2:F:217:LYS:HZ3	2:F:219:GLU:CD	2.10	0.59
1:C:58:VAL:HG22	1:C:59:PRO:CD	2.31	0.59
2:F:4:LEU:HB2	2:F:111:GLY:HA2	1.85	0.59
1:E:114:PRO:HB3	1:E:140:PHE:HB3	1.84	0.59
1:G:7:SER:N	1:G:8:PRO:CD	2.66	0.59
1:A:29:ILE:HG22	1:A:92:TYR:HB3	1.83	0.59
1:E:38:GLN:HA	1:E:44:PRO:HA	1.84	0.58
1:E:99:PHE:CE2	2:F:37:ILE:HD13	2.39	0.58
2:H:12:VAL:CG1	2:H:13:GLN:N	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:78:LEU:HD12	1:J:78:LEU:O	2.04	0.58
2:I:133:PRO:HD3	2:I:145:LEU:HB3	1.86	0.58
1:L:187:TYR:O	1:L:193:TYR:OH	2.22	0.58
2:D:10:GLY:HA3	2:D:209:PRO:HG3	1.85	0.57
1:L:48:ILE:HD12	1:L:73:LEU:HD12	1.87	0.57
1:E:48:ILE:HD12	1:E:73:LEU:HD12	1.85	0.57
1:A:106:GLU:OE2	1:A:143:ARG:NH2	2.37	0.57
1:C:78:LEU:HD12	1:C:78:LEU:C	2.30	0.57
2:I:150:LYS:HG3	2:I:184:SER:OG	2.04	0.57
2:H:178:GLN:HG2	2:H:182:LEU:O	2.05	0.57
1:G:159:ASN:HD22	1:G:182:LEU:HD21	1.70	0.57
2:B:192:PRO:HG2	2:B:195:SER:HB3	1.85	0.57
2:F:217:LYS:NZ	2:F:219:GLU:OE2	2.27	0.57
1:E:47:LEU:HD22	1:E:58:VAL:HG21	1.87	0.56
2:B:67:ARG:NH2	2:B:90:ASP:OD2	2.38	0.56
2:D:72:ARG:NH1	2:D:74:ASN:OD1	2.39	0.56
2:D:35:ASN:HD21	2:D:99:HIS:CE1	2.23	0.56
2:K:4:LEU:HD21	2:K:27:PHE:CZ	2.35	0.56
1:L:124:GLU:HA	1:L:127:LYS:HE2	1.87	0.56
1:L:150:LYS:HB3	1:L:194:ALA:HB3	1.87	0.55
1:J:167:GLN:HG3	1:J:174:TYR:CE1	2.41	0.55
2:F:200:THR:HG23	2:F:217:LYS:HE2	1.87	0.55
1:A:130:THR:HG21	2:B:150:LYS:HZ3	1.71	0.55
1:L:188:GLU:HA	1:L:212:ARG:HH12	1.71	0.55
1:J:83:VAL:HG22	1:J:107:LEU:HG	1.88	0.55
1:E:15:LEU:HD21	1:E:107:LEU:HD13	1.89	0.55
1:A:138:ASN:O	1:A:174:TYR:O	2.24	0.55
1:G:133:VAL:HG13	1:G:180:LEU:HB3	1.88	0.55
2:I:13:GLN:HB2	2:I:16:ARG:HD2	1.89	0.55
1:C:58:VAL:HG23	1:C:59:PRO:HD2	1.84	0.54
1:C:167:GLN:HE21	1:C:172:SER:HB3	1.73	0.54
1:C:14:SER:HA	1:C:108:ARG:HB2	1.88	0.54
1:J:44:PRO:HG2	2:K:110:TRP:HE1	1.72	0.54
2:K:3:GLN:HB3	2:K:25:SER:HB2	1.88	0.54
1:A:4:MET:SD	1:A:90:GLN:HB3	2.47	0.54
2:F:37:ILE:HD12	2:F:110:TRP:CH2	2.42	0.54
1:C:83:VAL:HB	1:C:107:LEU:HG	1.90	0.54
1:L:104:LYS:HB2	2:H:43:LYS:HZ1	1.73	0.54
1:L:78:LEU:HD12	1:L:78:LEU:C	2.33	0.53
1:E:35:TRP:HB2	1:E:48:ILE:HB	1.90	0.53
2:K:40:THR:HB	2:K:43:LYS:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:10:GLY:HA3	2:H:209:PRO:HG3	1.89	0.53
1:E:6:GLN:NE2	1:E:103:ALA:HB2	2.24	0.53
2:H:104:GLY:HA3	2:H:106:PHE:CE2	2.43	0.53
1:E:109:ARG:HG2	1:E:110:THR:N	2.23	0.53
1:J:114:PRO:HB3	1:J:140:PHE:HB3	1.91	0.53
2:D:100:VAL:HG21	2:D:106:PHE:CZ	2.44	0.53
1:G:33:LEU:HD13	1:G:71:PHE:CD1	2.44	0.53
1:L:29:ILE:HG23	1:L:92:TYR:CB	2.38	0.53
2:F:100:VAL:HG11	2:F:106:PHE:CE2	2.44	0.53
2:B:200:THR:HG23	2:B:217:LYS:HE2	1.91	0.53
1:A:65:SER:HB2	1:A:72:SER:OG	2.09	0.52
1:A:81:GLU:OE1	1:A:81:GLU:N	2.39	0.52
1:L:33:LEU:HD13	1:L:71:PHE:CD2	2.45	0.52
2:H:166:LEU:HD21	2:H:189:VAL:HG21	1.91	0.52
1:E:140:PHE:CD1	1:E:140:PHE:C	2.87	0.52
2:B:34:MET:HB3	2:B:79:LEU:HD22	1.91	0.52
1:E:99:PHE:CZ	2:F:37:ILE:HD13	2.44	0.52
1:A:29:ILE:HG22	1:A:92:TYR:CB	2.39	0.52
1:G:138:ASN:ND2	2:I:190:THR:HG21	2.23	0.52
2:H:13:GLN:HB3	2:H:16:ARG:HG3	1.92	0.52
2:H:138:THR:OG1	2:H:139:SER:N	2.41	0.52
2:F:12:VAL:HG11	2:F:86:LEU:CD1	2.40	0.52
2:F:202:ILE:HD11	2:F:215:ASP:HB3	1.91	0.52
1:C:186:ASP:OD1	1:C:190:HIS:ND1	2.33	0.52
1:A:121:PRO:HD3	1:A:133:VAL:HB	1.91	0.52
1:C:95:PRO:HB2	1:C:96:PRO:HD2	1.92	0.52
2:K:29:PHE:CD1	2:K:34:MET:HE3	2.44	0.52
1:E:69:THR:HG23	1:E:70:GLN:HG2	1.90	0.52
1:C:80:SER:O	1:C:83:VAL:HG12	2.09	0.51
1:A:187:TYR:O	1:A:193:TYR:OH	2.26	0.51
1:L:79:GLN:HB3	1:L:81:GLU:OE2	2.11	0.51
1:C:83:VAL:HG23	1:C:106:GLU:HA	1.92	0.51
1:E:88:CYS:O	1:E:99:PHE:HA	2.11	0.51
1:J:29:ILE:HG22	1:J:29:ILE:O	2.10	0.51
1:J:44:PRO:HG2	2:K:110:TRP:CZ2	2.45	0.51
1:L:54:LEU:HG	1:L:58:VAL:HG13	1.92	0.51
1:J:48:ILE:HG23	1:J:53:SER:O	2.11	0.51
2:B:93:LEU:HD21	2:B:113:GLY:HA3	1.92	0.51
2:K:3:GLN:CB	2:K:25:SER:HB2	2.40	0.51
1:C:49:TYR:C	1:C:51:ALA:H	2.16	0.51
1:E:36:TYR:OH	2:F:107:PHE:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:GLN:HG2	1:G:82:ASP:CG	2.36	0.51
1:J:94:TYR:HB2	1:J:95:PRO:HD3	1.93	0.51
2:K:2:VAL:CG2	2:K:109:TYR:HB2	2.39	0.51
1:C:109:ARG:HG2	1:C:110:THR:N	2.26	0.50
2:F:166:LEU:HD21	2:F:189:VAL:HG21	1.93	0.50
2:K:202:ILE:CD1	2:K:204:ASN:ND2	2.68	0.50
2:H:34:MET:HB3	2:H:79:LEU:HD22	1.93	0.50
1:J:140:PHE:CE2	1:J:143:ARG:HA	2.46	0.50
2:F:12:VAL:CG1	2:F:13:GLN:N	2.74	0.50
2:K:213:LYS:NZ	2:K:215:ASP:OD1	2.44	0.50
2:B:93:LEU:HA	2:B:115:MET:HA	1.94	0.50
1:L:97:TYR:HD2	2:H:47:TRP:CE2	2.29	0.50
1:C:6:GLN:NE2	1:C:88:CYS:SG	2.85	0.50
2:K:108:ASP:OD1	2:K:109:TYR:N	2.44	0.50
2:H:4:LEU:HD13	2:H:109:TYR:CD2	2.47	0.50
1:E:155:LEU:HD12	1:E:155:LEU:N	2.27	0.50
1:A:33:LEU:HD13	1:A:34:ALA:N	2.27	0.49
1:A:90:GLN:HE22	1:A:93:ASN:HB3	1.76	0.49
2:D:1:GLU:HA	2:K:31:ASN:O	2.12	0.49
1:L:125:GLN:HG2	1:L:130:THR:O	2.12	0.49
2:H:12:VAL:CG1	2:H:13:GLN:H	2.26	0.49
1:L:146:LYS:HB3	1:L:198:THR:HB	1.94	0.49
2:B:29:PHE:CD1	2:B:34:MET:HE3	2.46	0.49
1:C:95:PRO:CB	1:C:96:PRO:HD2	2.41	0.49
1:E:24:ARG:HA	1:E:70:GLN:OE1	2.12	0.49
1:G:38:GLN:HA	1:G:44:PRO:HA	1.95	0.49
2:B:35:ASN:HD21	2:B:99:HIS:CD2	2.31	0.49
2:D:1:GLU:O	2:D:1:GLU:HG2	2.11	0.49
2:B:36:TRP:HD1	2:B:70:ILE:HD12	1.78	0.49
2:K:103:LEU:HB3	2:K:106:PHE:HE2	1.76	0.48
2:H:39:GLN:HB2	2:H:45:LEU:HD13	1.94	0.48
1:J:125:GLN:HG2	1:J:130:THR:O	2.13	0.48
1:J:125:GLN:O	1:J:128:SER:OG	2.26	0.48
1:G:167:GLN:HE21	1:G:172:SER:HB3	1.79	0.48
2:B:100:VAL:HG12	2:B:108:ASP:HB2	1.95	0.48
1:C:78:LEU:HD11	1:C:107:LEU:HD22	1.95	0.48
2:K:97:VAL:HG13	2:K:110:TRP:HE3	1.78	0.48
2:B:208:LYS:HB2	2:B:209:PRO:HD3	1.96	0.48
2:K:3:GLN:OE1	2:K:3:GLN:HA	2.14	0.48
1:C:96:PRO:HA	2:D:47:TRP:CZ3	2.48	0.48
1:A:151:VAL:HG21	1:A:156:GLN:NE2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:29:PHE:O	2:H:72:ARG:NH2	2.43	0.47
1:A:130:THR:HG21	2:B:150:LYS:NZ	2.28	0.47
2:D:4:LEU:HD23	2:D:96:CYS:SG	2.54	0.47
2:F:12:VAL:CG2	2:F:18:LEU:HD22	2.43	0.47
1:A:125:GLN:HG2	1:A:130:THR:O	2.14	0.47
1:E:4:MET:HE2	1:E:4:MET:HB3	1.75	0.47
1:E:14:SER:N	1:E:17:GLU:OE2	2.40	0.47
2:K:97:VAL:HG13	2:K:110:TRP:CE3	2.49	0.47
1:E:38:GLN:HB2	1:E:44:PRO:HB3	1.95	0.47
2:B:100:VAL:CG1	2:B:108:ASP:HB2	2.44	0.47
1:C:12:SER:OG	1:C:108:ARG:NH2	2.47	0.47
1:C:185:ALA:O	1:C:189:LYS:HG3	2.15	0.47
1:G:95:PRO:CB	1:G:96:PRO:HD3	2.42	0.47
1:G:165:THR:HG22	1:G:175:SER:H	1.79	0.47
1:L:6:GLN:HE22	1:L:88:CYS:N	2.12	0.47
2:B:36:TRP:O	2:B:48:VAL:HG22	2.15	0.47
2:K:60:TYR:CE2	2:K:70:ILE:HG22	2.50	0.47
1:L:95:PRO:CB	1:L:96:PRO:HD3	2.44	0.47
2:D:36:TRP:O	2:D:48:VAL:HG22	2.14	0.47
1:C:94:TYR:N	1:C:95:PRO:CD	2.78	0.47
1:J:29:ILE:HG22	1:J:32:ARG:HB2	1.97	0.47
1:G:94:TYR:N	1:G:95:PRO:HD2	2.29	0.47
2:B:24:ALA:HB3	2:B:77:ASN:HB3	1.97	0.47
2:B:67:ARG:O	2:B:84:THR:OG1	2.29	0.47
2:B:69:THR:HG23	2:B:82:GLN:HB3	1.97	0.47
1:C:47:LEU:HD22	1:C:58:VAL:HG21	1.95	0.46
2:K:60:TYR:CZ	2:K:70:ILE:HG22	2.51	0.46
2:F:38:ARG:NH1	2:F:90:ASP:HA	2.30	0.46
1:J:44:PRO:HG2	2:K:110:TRP:NE1	2.30	0.46
1:C:79:GLN:OE1	1:C:81:GLU:HB3	2.15	0.46
2:D:108:ASP:OD1	2:D:109:TYR:N	2.47	0.46
2:F:36:TRP:HE1	2:F:79:LEU:HG	1.81	0.46
2:K:53:SER:HA	2:K:72:ARG:CZ	2.45	0.46
1:C:119:PHE:HA	1:C:120:PRO:HD2	1.80	0.46
2:B:60:TYR:CE2	2:B:70:ILE:HG22	2.50	0.46
2:B:142:THR:HG22	2:B:192:PRO:HA	1.97	0.46
2:D:98:GLY:O	2:D:107:PHE:HB3	2.15	0.46
2:K:3:GLN:HE21	2:K:26:ARG:HH11	1.63	0.46
1:G:161:GLN:HG2	2:I:176:VAL:HG21	1.97	0.46
2:H:4:LEU:HD23	2:H:96:CYS:SG	2.55	0.46
1:E:168:ASP:OD1	1:E:169:SER:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:143:ARG:HB3	1:J:174:TYR:CD2	2.51	0.46
1:L:20:THR:HG22	1:L:74:LYS:HG2	1.96	0.46
1:L:49:TYR:C	1:L:51:ALA:H	2.24	0.46
2:D:28:THR:HG23	2:K:59:TYR:CZ	2.51	0.46
2:H:12:VAL:HG12	2:H:13:GLN:H	1.80	0.46
1:A:49:TYR:HB2	2:B:106:PHE:CZ	2.49	0.46
1:A:109:ARG:NH1	1:A:112:ALA:HB2	2.30	0.46
1:A:79:GLN:HG3	1:A:81:GLU:OE1	2.15	0.45
1:E:35:TRP:CE2	1:E:73:LEU:HB2	2.51	0.45
2:F:35:ASN:OD1	2:F:50:TYR:HD1	1.98	0.45
1:L:27:GLU:O	1:L:27:GLU:HG2	2.16	0.45
1:G:35:TRP:CG	1:G:73:LEU:HD12	2.51	0.45
1:A:2:ILE:HD13	1:A:27:GLU:CB	2.45	0.45
1:C:79:GLN:HG3	1:C:81:GLU:H	1.81	0.45
2:F:35:ASN:HB2	2:F:97:VAL:CB	2.42	0.45
1:G:119:PHE:CD2	2:I:131:LEU:HD13	2.52	0.45
2:D:131:LEU:HD11	2:D:148:LEU:HB2	1.99	0.45
2:F:36:TRP:O	2:F:48:VAL:HG22	2.17	0.45
2:F:37:ILE:HG12	2:F:47:TRP:HA	1.98	0.45
2:K:1:GLU:HB3	2:K:3:GLN:NE2	2.31	0.45
1:L:109:ARG:NH1	1:L:110:THR:O	2.49	0.45
1:A:138:ASN:OD1	2:B:171:HIS:CE1	2.69	0.45
1:E:138:ASN:HD21	2:F:171:HIS:CD2	2.34	0.45
2:F:144:ALA:HB2	2:F:190:THR:HG22	1.98	0.45
2:H:2:VAL:HG21	2:H:112:GLN:HG3	1.97	0.45
1:A:15:LEU:HD21	1:A:107:LEU:HD13	1.99	0.45
1:J:61:ARG:HH12	1:J:79:GLN:HG2	1.80	0.45
2:K:206:ASN:CG	2:K:208:LYS:HZ2	2.20	0.45
1:J:38:GLN:HA	1:J:44:PRO:HA	1.99	0.45
2:D:36:TRP:HD1	2:D:70:ILE:HD12	1.82	0.45
1:C:92:TYR:O	1:C:92:TYR:CG	2.70	0.44
1:E:167:GLN:NE2	1:E:172:SER:HB3	2.32	0.44
1:G:90:GLN:NE2	1:G:92:TYR:HB3	2.26	0.44
2:H:124:LYS:NZ	2:H:125:GLY:O	2.49	0.44
1:G:7:SER:H	1:G:8:PRO:HD2	1.81	0.44
2:K:1:GLU:O	2:K:1:GLU:HG2	2.17	0.44
2:K:100:VAL:HG21	2:K:106:PHE:CZ	2.51	0.44
2:H:2:VAL:HG12	2:H:3:GLN:N	2.24	0.44
1:G:95:PRO:CG	1:G:96:PRO:CD	2.81	0.44
1:A:29:ILE:HD11	1:A:71:PHE:CE1	2.53	0.44
1:C:33:LEU:HD13	1:C:71:PHE:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:24:ARG:HG3	1:J:70:GLN:OE1	2.18	0.44
1:G:125:GLN:HG2	1:G:130:THR:O	2.17	0.44
2:B:29:PHE:HD1	2:B:34:MET:HE3	1.83	0.44
2:K:195:SER:OG	2:K:201:TYR:OH	2.21	0.44
2:B:163:SER:H	2:B:204:ASN:HD21	1.66	0.44
2:D:12:VAL:HG11	2:D:86:LEU:HD22	1.99	0.44
1:L:190:HIS:O	1:L:212:ARG:NH2	2.51	0.44
1:A:30:HIS:HD2	1:A:92:TYR:CE1	2.36	0.44
2:F:67:ARG:O	2:F:84:THR:OG1	2.29	0.44
1:G:133:VAL:HG22	1:G:149:TRP:CH2	2.53	0.44
1:C:114:PRO:HB3	1:C:140:PHE:HB3	2.00	0.44
1:G:114:PRO:HB3	1:G:140:PHE:HB3	2.00	0.44
1:L:18:THR:HG22	1:L:76:ASN:HA	1.98	0.43
1:J:151:VAL:HG22	1:J:193:TYR:HD1	1.83	0.43
2:D:51:ILE:HD13	2:D:72:ARG:HG2	2.00	0.43
2:D:131:LEU:HB2	2:D:146:GLY:C	2.42	0.43
1:L:186:ASP:HA	1:L:189:LYS:HG2	1.99	0.43
1:C:162:GLU:HB3	1:C:176:LEU:HD11	2.01	0.43
1:J:187:TYR:CZ	1:J:212:ARG:HD2	2.54	0.43
1:G:43:SER:OG	2:I:111:GLY:O	2.31	0.43
1:G:189:LYS:HG2	1:G:190:HIS:CD2	2.53	0.43
2:B:36:TRP:CD1	2:B:81:LEU:HB2	2.52	0.43
2:K:36:TRP:O	2:K:48:VAL:HG22	2.18	0.43
2:I:36:TRP:CG	2:I:81:LEU:HD22	2.53	0.43
2:F:100:VAL:CG1	2:F:108:ASP:HB2	2.49	0.43
2:K:36:TRP:HD1	2:K:70:ILE:HD12	1.83	0.43
2:D:93:LEU:HD23	2:D:115:MET:HB2	2.00	0.43
2:D:109:TYR:HD1	2:K:54:THR:HG21	1.84	0.43
1:L:119:PHE:HB3	2:H:131:LEU:HD22	2.00	0.43
1:L:165:THR:HG22	1:L:175:SER:H	1.83	0.43
1:G:109:ARG:HG2	1:G:110:THR:N	2.34	0.43
2:K:91:THR:HG22	2:K:118:VAL:H	1.83	0.43
1:G:119:PHE:HA	1:G:120:PRO:HD2	1.88	0.43
2:F:95:TYR:HB3	2:F:110:TRP:CE3	2.50	0.43
1:A:14:SER:N	1:A:17:GLU:OE2	2.35	0.43
2:K:34:MET:HB3	2:K:79:LEU:HD22	2.00	0.43
2:H:46:GLU:OE2	2:H:63:THR:HG21	2.19	0.43
2:H:137:SER:HB2	2:H:141:GLY:HA3	2.01	0.43
1:E:124:GLU:HA	1:E:127:LYS:HE2	2.01	0.43
1:J:124:GLU:HA	1:J:127:LYS:HE2	2.01	0.43
1:L:97:TYR:CD2	2:H:47:TRP:CE2	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:140:PHE:HE2	1:J:143:ARG:HA	1.84	0.43
2:K:206:ASN:OD1	2:K:208:LYS:NZ	2.35	0.43
1:L:54:LEU:CG	1:L:58:VAL:HG13	2.49	0.42
1:E:46:LEU:HD22	2:F:107:PHE:O	2.19	0.42
2:K:93:LEU:HA	2:K:115:MET:HA	2.00	0.42
2:H:29:PHE:CE1	2:H:34:MET:HG3	2.54	0.42
1:C:67:SER:HA	1:C:71:PHE:CE1	2.53	0.42
1:C:92:TYR:O	1:C:92:TYR:CD1	2.73	0.42
1:C:95:PRO:HB2	1:C:96:PRO:CD	2.46	0.42
1:G:33:LEU:HG	1:G:89:LEU:O	2.19	0.42
2:F:7:SER:O	2:F:21:SER:OG	2.29	0.42
2:K:52:GLY:O	2:K:72:ARG:HD3	2.19	0.42
1:L:6:GLN:NE2	1:L:88:CYS:CB	2.83	0.42
2:H:4:LEU:HD13	2:H:109:TYR:CE2	2.54	0.42
2:B:1:GLU:O	2:B:26:ARG:HD2	2.19	0.42
2:F:37:ILE:HD12	2:F:110:TRP:HH2	1.84	0.42
2:F:37:ILE:HG23	2:F:46:GLU:C	2.44	0.42
2:K:64:VAL:O	2:K:64:VAL:HG13	2.19	0.42
1:L:97:TYR:HD2	2:H:47:TRP:CZ2	2.37	0.42
2:H:36:TRP:CD1	2:H:81:LEU:HB2	2.55	0.42
1:A:30:HIS:CD2	1:A:92:TYR:CE1	3.08	0.42
1:A:33:LEU:HD22	1:A:89:LEU:O	2.19	0.42
1:J:14:SER:HA	1:J:108:ARG:HB2	2.01	0.42
2:B:93:LEU:HD22	2:B:95:TYR:CZ	2.54	0.42
1:L:187:TYR:O	1:L:212:ARG:NH1	2.48	0.42
1:A:109:ARG:HG2	1:A:110:THR:N	2.34	0.42
2:B:100:VAL:HG21	2:B:106:PHE:CE2	2.54	0.42
2:D:53:SER:O	2:D:72:ARG:NH1	2.52	0.42
1:A:2:ILE:HD13	1:A:27:GLU:HB2	2.02	0.42
2:B:75:ALA:C	2:B:77:ASN:H	2.28	0.42
2:H:126:PRO:HB3	2:H:152:TYR:HB3	2.02	0.42
1:A:168:ASP:OD1	1:A:169:SER:N	2.52	0.42
1:C:208:LYS:HA	1:C:208:LYS:HD3	1.86	0.42
1:J:109:ARG:NH1	1:J:110:THR:O	2.53	0.42
2:F:37:ILE:HG23	2:F:46:GLU:O	2.19	0.42
1:C:58:VAL:CG2	1:C:59:PRO:CD	2.88	0.42
1:J:33:LEU:HD13	1:J:71:PHE:CD2	2.54	0.42
1:J:36:TYR:OH	2:K:107:PHE:O	2.22	0.42
1:J:120:PRO:HB3	1:J:210:PHE:CE2	2.55	0.42
2:B:100:VAL:HG21	2:B:106:PHE:CZ	2.55	0.42
2:F:91:THR:CG2	2:F:118:VAL:HG22	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:LEU:CD1	1:C:107:LEU:HD22	2.49	0.42
1:J:177:SER:HB3	2:K:173:PHE:CE2	2.55	0.42
2:D:49:ALA:HB1	2:D:70:ILE:HG21	2.01	0.42
2:D:85:GLY:C	2:D:86:LEU:HD12	2.45	0.42
1:L:54:LEU:CD1	1:L:58:VAL:HG13	2.50	0.41
2:H:29:PHE:O	2:H:29:PHE:CG	2.72	0.41
2:H:208:LYS:HB2	2:H:209:PRO:HD3	2.01	0.41
2:K:29:PHE:HD1	2:K:34:MET:HE3	1.84	0.41
2:K:31:ASN:HB3	2:K:101:ARG:CZ	2.50	0.41
1:J:185:ALA:O	1:J:189:LYS:HG2	2.19	0.41
1:A:35:TRP:O	1:A:47:LEU:HB2	2.21	0.41
1:A:81:GLU:HG3	1:A:169:SER:O	2.19	0.41
1:A:114:PRO:HB3	1:A:140:PHE:HB3	2.01	0.41
2:D:129:PHE:HA	2:D:130:PRO:HD3	1.80	0.41
2:H:104:GLY:HA3	2:H:106:PHE:CD2	2.55	0.41
2:H:163:SER:H	2:H:204:ASN:HD21	1.67	0.41
1:J:145:ALA:HB2	1:J:199:HIS:HD2	1.84	0.41
2:K:60:TYR:HB2	2:K:65:LYS:HG3	2.02	0.41
1:A:177:SER:HB3	2:B:173:PHE:CD2	2.55	0.41
2:F:133:PRO:HB3	2:F:144:ALA:O	2.20	0.41
1:J:44:PRO:HG2	2:K:110:TRP:HZ2	1.86	0.41
2:K:51:ILE:HG13	2:K:58:ILE:HG12	2.02	0.41
2:H:213:LYS:HE3	2:H:213:LYS:HB2	1.87	0.41
1:L:38:GLN:HB2	1:L:44:PRO:HB3	2.03	0.41
2:H:108:ASP:OD1	2:H:109:TYR:N	2.53	0.41
1:C:135:CYS:HB2	1:C:149:TRP:CZ2	2.56	0.41
2:B:64:VAL:HG11	2:B:68:PHE:CE2	2.56	0.41
2:D:40:THR:OG1	2:D:43:LYS:O	2.39	0.41
2:D:166:LEU:HD21	2:D:189:VAL:HG21	2.02	0.41
2:F:173:PHE:HA	2:F:174:PRO:HD3	1.94	0.41
1:C:167:GLN:NE2	1:C:172:SER:HB3	2.36	0.41
1:E:165:THR:HG23	2:F:173:PHE:CD2	2.55	0.41
2:K:91:THR:CG2	2:K:118:VAL:H	2.34	0.41
1:G:182:LEU:HA	1:G:182:LEU:HD23	1.89	0.40
2:B:12:VAL:HG23	2:B:118:VAL:HG22	2.03	0.40
2:D:4:LEU:HD13	2:D:109:TYR:CD2	2.56	0.40
2:F:124:LYS:HD2	2:F:182:LEU:HD21	2.04	0.40
2:K:4:LEU:HD23	2:K:4:LEU:HA	1.84	0.40
1:L:6:GLN:HE21	1:L:88:CYS:CB	2.31	0.40
1:L:29:ILE:CG2	1:L:92:TYR:HB2	2.45	0.40
1:A:18:THR:HG22	1:A:76:ASN:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LEU:HD21	1:A:49:TYR:HB3	2.03	0.40
1:A:148:GLN:HB3	1:A:155:LEU:HD11	2.02	0.40
1:J:109:ARG:NH1	1:J:112:ALA:HB2	2.35	0.40
1:G:208:LYS:HA	1:G:208:LYS:HD3	1.81	0.40
1:G:34:ALA:HA	1:G:48:ILE:O	2.21	0.40
2:B:153:PHE:HA	2:B:154:PRO:HA	1.86	0.40
2:K:91:THR:CG2	2:K:118:VAL:HG22	2.51	0.40
1:E:11:LEU:HD22	1:E:21:ILE:HD13	2.04	0.40
1:E:79:GLN:O	1:E:82:ASP:HB2	2.21	0.40
1:J:54:LEU:HG	1:J:58:VAL:HG13	2.03	0.40
2:B:93:LEU:HB2	2:B:115:MET:HE2	2.04	0.40
2:B:163:SER:H	2:B:204:ASN:ND2	2.20	0.40
2:D:36:TRP:NE1	2:D:81:LEU:HB2	2.36	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:SER:OG	1:J:189:LYS:NZ[1_455]	2.06	0.14

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	210/215 (98%)	202 (96%)	7 (3%)	1 (0%)	24	49
1	C	195/215 (91%)	189 (97%)	6 (3%)	0	100	100
1	E	180/215 (84%)	178 (99%)	2 (1%)	0	100	100
1	G	190/215 (88%)	181 (95%)	8 (4%)	1 (0%)	24	49
1	J	210/215 (98%)	202 (96%)	8 (4%)	0	100	100
1	L	210/215 (98%)	203 (97%)	6 (3%)	1 (0%)	24	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	212/228 (93%)	205 (97%)	7 (3%)	0	100	100
2	D	202/228 (89%)	195 (96%)	7 (4%)	0	100	100
2	F	194/228 (85%)	187 (96%)	7 (4%)	0	100	100
2	H	219/228 (96%)	214 (98%)	5 (2%)	0	100	100
2	I	139/228 (61%)	130 (94%)	8 (6%)	1 (1%)	18	40
2	K	212/228 (93%)	202 (95%)	10 (5%)	0	100	100
All	All	2373/2658 (89%)	2288 (96%)	81 (3%)	4 (0%)	43	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	96	PRO
1	A	95	PRO
1	G	96	PRO
2	I	156	PRO

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	184/188 (98%)	181 (98%)	3 (2%)	55	75
1	C	173/188 (92%)	172 (99%)	1 (1%)	78	89
1	E	162/188 (86%)	160 (99%)	2 (1%)	63	79
1	G	166/188 (88%)	165 (99%)	1 (1%)	78	89
1	J	183/188 (97%)	179 (98%)	4 (2%)	45	69
1	L	186/188 (99%)	184 (99%)	2 (1%)	65	80
2	B	181/193 (94%)	178 (98%)	3 (2%)	53	73
2	D	169/193 (88%)	168 (99%)	1 (1%)	78	89
2	F	165/193 (86%)	161 (98%)	4 (2%)	43	67
2	H	184/193 (95%)	181 (98%)	3 (2%)	55	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	122/193 (63%)	120 (98%)	2 (2%)	55	75
2	K	174/193 (90%)	170 (98%)	4 (2%)	44	67
All	All	2049/2286 (90%)	2019 (98%)	30 (2%)	57	76

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	73	LEU
1	L	189	LYS
2	H	99	HIS
2	H	118	VAL
2	H	136	LYS
1	A	29	ILE
1	A	73	LEU
1	A	133	VAL
1	C	133	VAL
1	E	88	CYS
1	E	133	VAL
1	J	7	SER
1	J	78	LEU
1	J	133	VAL
1	J	155	LEU
1	G	133	VAL
2	B	2	VAL
2	B	69	THR
2	B	203	CYS
2	D	157	VAL
2	F	99	HIS
2	F	118	VAL
2	F	157	VAL
2	F	177	LEU
2	K	63	THR
2	K	64	VAL
2	K	118	VAL
2	K	204	ASN
2	I	40	THR
2	I	158	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	79	GLN
2	H	77	ASN
2	H	204	ASN
1	A	30	HIS
1	A	125	GLN
1	A	211	ASN
1	C	38	GLN
1	C	55	HIS
1	C	90	GLN
1	C	93	ASN
1	E	76	ASN
1	E	167	GLN
1	J	38	GLN
1	J	139	ASN
1	J	161	GLN
1	G	90	GLN
2	B	31	ASN
2	B	35	ASN
2	B	77	ASN
2	B	99	HIS
2	D	35	ASN
2	D	39	GLN
2	D	77	ASN
2	D	99	HIS
2	D	171	HIS
2	F	35	ASN
2	F	99	HIS
2	F	171	HIS
2	K	3	GLN
2	K	39	GLN
2	I	162	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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	212/215 (98%)	0.40	5 (2%) 59 51	17, 29, 50, 59	0
1	C	203/215 (94%)	0.90	18 (8%) 15 14	27, 44, 69, 74	0
1	E	190/215 (88%)	0.93	27 (14%) 6 6	30, 54, 81, 94	0
1	G	196/215 (91%)	0.91	27 (13%) 6 6	35, 52, 83, 95	0
1	J	212/215 (98%)	0.36	8 (3%) 44 36	21, 29, 42, 66	0
1	L	212/215 (98%)	0.44	9 (4%) 40 33	18, 31, 56, 66	0
2	B	216/228 (94%)	0.36	6 (2%) 55 47	17, 28, 53, 75	0
2	D	208/228 (91%)	0.67	17 (8%) 17 15	29, 46, 58, 72	0
2	F	204/228 (89%)	0.87	21 (10%) 12 11	24, 53, 76, 91	0
2	H	221/228 (96%)	0.55	14 (6%) 26 22	18, 32, 62, 91	0
2	I	153/228 (67%)	0.67	17 (11%) 10 9	31, 46, 71, 90	0
2	K	216/228 (94%)	0.56	12 (5%) 30 25	19, 32, 53, 77	0
All	All	2443/2658 (91%)	0.63	181 (7%) 20 18	17, 39, 71, 95	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	48	VAL	5.3
1	L	94	TYR	4.6
1	G	15	LEU	4.6
1	A	94	TYR	4.4
1	E	99	PHE	4.3
1	L	97	TYR	4.3
2	F	110	TRP	4.2
1	G	3	GLN	4.2
2	I	164	GLY	4.1
2	K	145	LEU	3.9
1	G	107	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
2	F	54	THR	3.8
1	L	78	LEU	3.8
1	G	55	HIS	3.7
1	E	71	PHE	3.6
1	C	105	LEU	3.6
2	D	59	TYR	3.6
2	D	31	ASN	3.5
2	I	67	ARG	3.5
1	C	90	GLN	3.5
2	I	145	LEU	3.4
2	B	103	LEU	3.3
2	F	140	GLY	3.3
2	I	187	SER	3.3
1	E	90	GLN	3.3
1	E	65	SER	3.3
2	F	52	GLY	3.2
1	C	134	VAL	3.1
2	I	197	GLY	3.1
1	C	46	LEU	3.1
2	H	25	SER	3.1
2	B	186	SER	3.1
1	C	78	LEU	3.1
2	I	169	GLY	3.1
1	C	81	GLU	3.1
1	E	89	LEU	3.1
1	E	136	LEU	3.1
1	G	99	PHE	3.0
2	F	47	TRP	3.0
2	K	55	SER	3.0
1	E	2	ILE	3.0
1	A	134	VAL	2.9
2	I	143	ALA	2.9
1	E	69	THR	2.9
2	F	141	GLY	2.9
1	C	3	GLN	2.9
2	I	108	ASP	2.9
1	C	126	LEU	2.8
2	K	166	LEU	2.8
1	G	193	TYR	2.8
2	F	106	PHE	2.8
2	H	56	SER	2.8
2	F	55	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	16	GLY	2.8
1	E	33	LEU	2.8
2	H	169	GLY	2.8
2	D	155	GLU	2.7
2	F	143	ALA	2.7
1	J	94	TYR	2.7
1	E	5	THR	2.7
1	L	99	PHE	2.7
2	I	77	ASN	2.7
1	G	111	VAL	2.7
1	G	97	TYR	2.7
1	G	52	ASN	2.7
1	J	1	ASP	2.7
1	E	75	ILE	2.7
2	F	75	ALA	2.7
1	E	47	LEU	2.7
2	F	193	SER	2.7
1	C	11	LEU	2.6
2	D	214	VAL	2.6
1	A	131	ALA	2.6
1	C	200	GLN	2.6
2	F	30	SER	2.6
1	C	155	LEU	2.6
1	E	4	MET	2.6
1	J	105	LEU	2.5
2	H	85	GLY	2.5
2	H	149	VAL	2.5
1	G	95	PRO	2.5
1	E	113	ALA	2.5
1	G	132	SER	2.5
2	D	45	LEU	2.5
1	E	154	ALA	2.5
2	K	132	ALA	2.5
2	H	43	LYS	2.5
1	C	186	ASP	2.5
1	C	21	ILE	2.5
1	C	122	SER	2.5
1	G	21	ILE	2.5
2	H	159	VAL	2.5
1	G	94	TYR	2.5
1	G	106	GLU	2.5
1	E	6	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	15	LEU	2.4
1	G	33	LEU	2.4
2	D	86	LEU	2.4
2	D	85	GLY	2.4
1	G	91	TYR	2.4
2	B	42	GLY	2.4
1	E	62	PHE	2.4
2	H	134	SER	2.4
1	J	187	TYR	2.4
2	H	28	THR	2.4
2	D	65	LYS	2.3
1	E	88	CYS	2.3
2	K	161	TRP	2.3
2	I	134	SER	2.3
2	I	163	SER	2.3
1	G	92	TYR	2.3
2	D	200	THR	2.3
2	F	142	THR	2.3
2	D	44	GLY	2.3
2	F	104	GLY	2.3
1	J	156	GLN	2.3
1	C	33	LEU	2.3
2	F	97	VAL	2.3
2	K	2	VAL	2.3
2	D	106	PHE	2.3
1	G	9	ALA	2.3
1	E	107	LEU	2.3
1	E	36	TYR	2.3
2	K	31	ASN	2.3
1	L	191	LYS	2.3
2	H	71	SER	2.3
1	A	71	PHE	2.2
1	G	210	PHE	2.2
2	H	48	VAL	2.2
1	G	71	PHE	2.2
2	H	35	ASN	2.2
2	B	148	LEU	2.2
2	F	31	ASN	2.2
1	L	28	ASP	2.2
2	D	80	TYR	2.2
1	E	158	GLY	2.2
2	D	113	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	102	GLY	2.2
2	D	145	LEU	2.2
1	L	27	GLU	2.2
1	E	134	VAL	2.2
2	D	28	THR	2.2
2	F	42	GLY	2.2
2	K	110	TRP	2.2
2	K	102	LYS	2.2
2	K	146	GLY	2.2
2	F	81	LEU	2.2
1	L	90	GLN	2.1
2	I	78	THR	2.1
2	I	166	LEU	2.1
2	H	55	SER	2.1
2	K	134	SER	2.1
2	I	195	SER	2.1
1	C	44	PRO	2.1
2	D	116	VAL	2.1
2	K	159	VAL	2.1
2	F	148	LEU	2.1
1	C	75	ILE	2.1
2	B	211	ASN	2.1
1	L	119	PHE	2.1
2	B	151	ASP	2.1
1	J	25	ALA	2.1
1	G	22	GLU	2.1
2	I	48	VAL	2.1
1	J	95	PRO	2.1
1	G	78	LEU	2.1
2	I	107	PHE	2.1
2	H	138	THR	2.1
2	D	54	THR	2.1
1	E	35	TRP	2.1
1	E	197	VAL	2.0
2	F	131	LEU	2.0
1	C	62	PHE	2.0
2	I	106	PHE	2.0
1	E	49	TYR	2.0
1	G	7	SER	2.0
1	E	137	LEU	2.0
1	G	105	LEU	2.0
1	G	182	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	106	GLU	2.0
1	G	83	VAL	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.