



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:29 PM UTC

PDB ID : 4RGN / pdb_00004rgn
Title : Structure of Staphylococcal Enterotoxin B bound to two neutralizing antibodies, 14G8 and 6D3
Authors : Franklin, M.C.; Dutta, K.; Varshney, A.K.; Goger, M.J.; Fries, B.C.
Deposited on : 2014-09-30
Resolution : 2.70 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

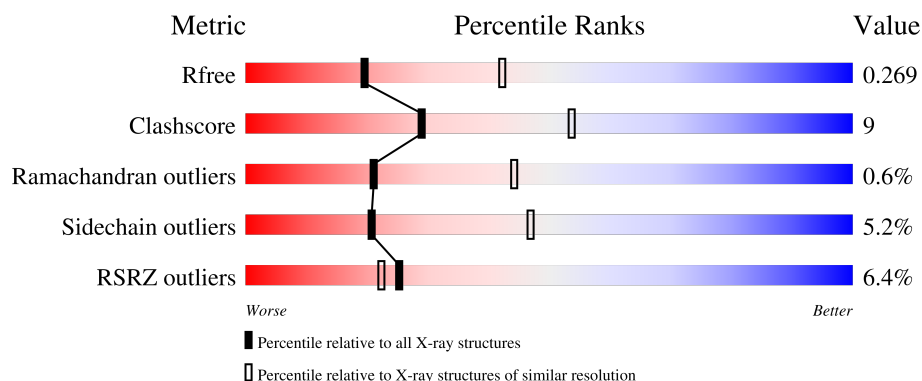
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	245	
1	S	245	
2	B	222	
2	H	222	
3	C	214	

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Mol	Chain	Length	Quality of chain
3	L	214	 77% 20% •
4	D	221	 17% 71% 21% • 5%
4	F	221	 16% 69% 23% • 5%
5	E	220	 9% 80% 19% •
5	G	220	 11% 83% 16% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16749 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 Enterotoxin type B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1789	1149	285	345	10			
1	S	220	Total	C	N	O	S	0	0	0
			1842	1181	297	354	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP P01552
A	-4	SER	-	expression tag	UNP P01552
A	-3	GLU	-	expression tag	UNP P01552
A	-2	PHE	-	expression tag	UNP P01552
A	-1	GLY	-	expression tag	UNP P01552
A	0	SER	-	expression tag	UNP P01552
S	-5	GLY	-	expression tag	UNP P01552
S	-4	SER	-	expression tag	UNP P01552
S	-3	GLU	-	expression tag	UNP P01552
S	-2	PHE	-	expression tag	UNP P01552
S	-1	GLY	-	expression tag	UNP P01552
S	0	SER	-	expression tag	UNP P01552

- Molecule 2 is a protein called 14G8 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1615	1031	265	313	6			
2	H	213	Total	C	N	O	S	0	0	0
			1615	1031	265	313	6			

- Molecule 3 is a protein called 14G8 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	213	Total	C	N	O	S	0	0	0
			1651	1025	282	338	6			
3	L	213	Total	C	N	O	S	0	0	0
			1651	1025	282	338	6			

- Molecule 4 is a protein called 6D3 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	210	Total	C	N	O	S	0	0	0
			1583	1008	254	314	7			
4	F	210	Total	C	N	O	S	0	0	0
			1583	1008	254	314	7			

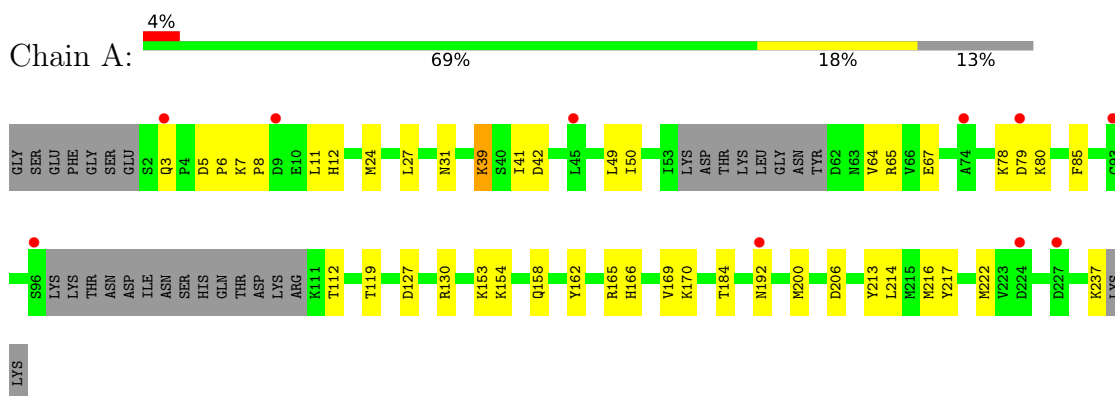
- Molecule 5 is a protein called 6D3 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	220	Total	C	N	O	S	0	0	0
			1710	1069	280	353	8			
5	G	220	Total	C	N	O	S	0	0	0
			1710	1069	280	353	8			

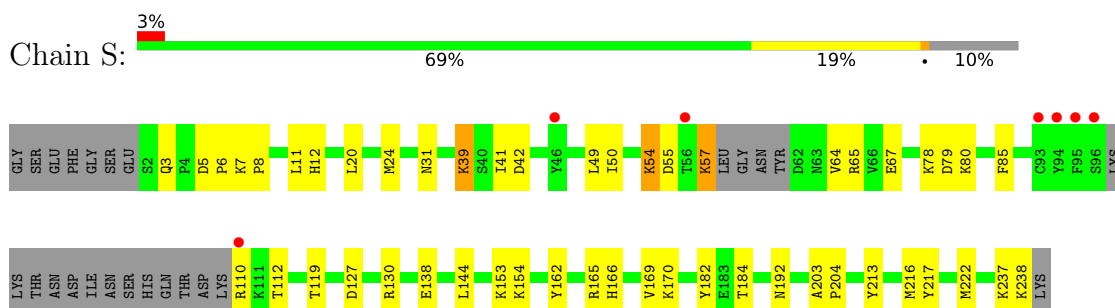
3 Residue-property plots [i](#)

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.

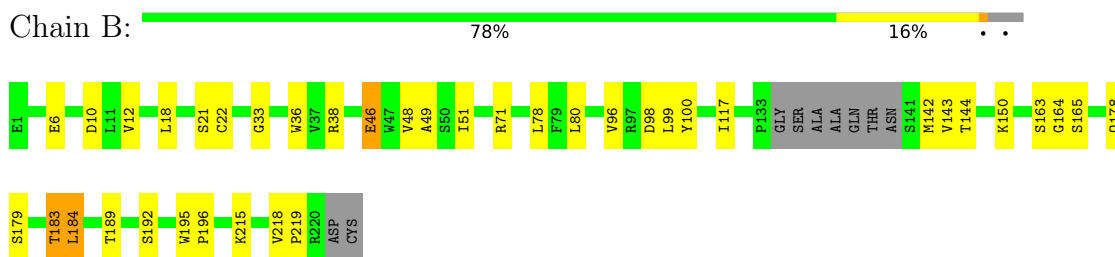
- Molecule 1: Enterotoxin type B



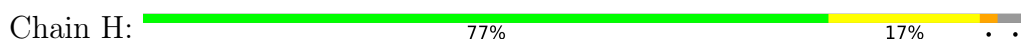
- Molecule 1: Enterotoxin type B

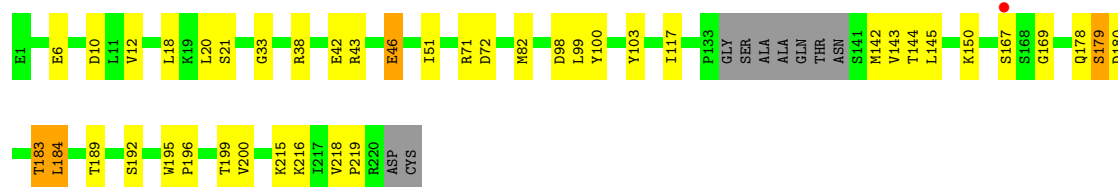


- Molecule 2: 14G8 heavy chain

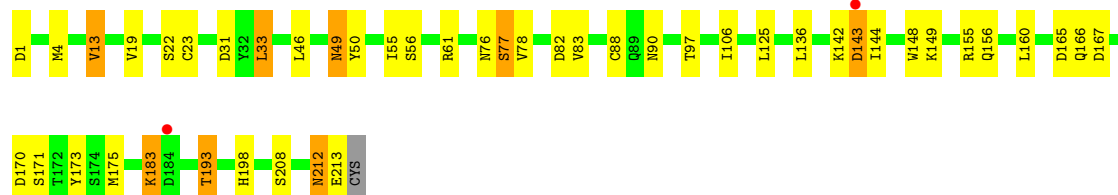
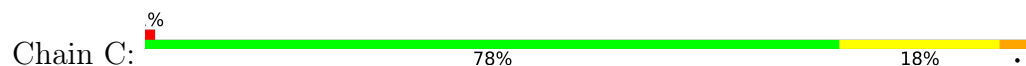


- Molecule 2: 14G8 heavy chain

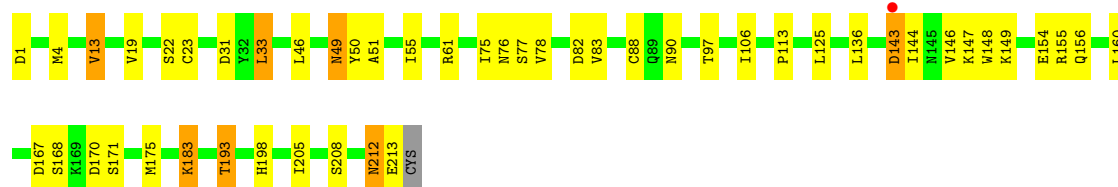
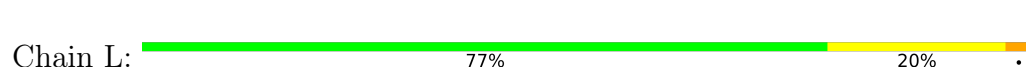




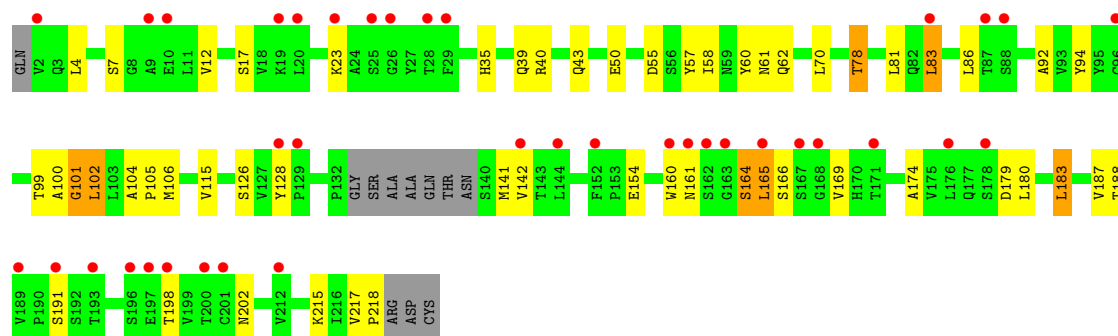
• Molecule 3: 14G8 light chain



• Molecule 3: 14G8 light chain

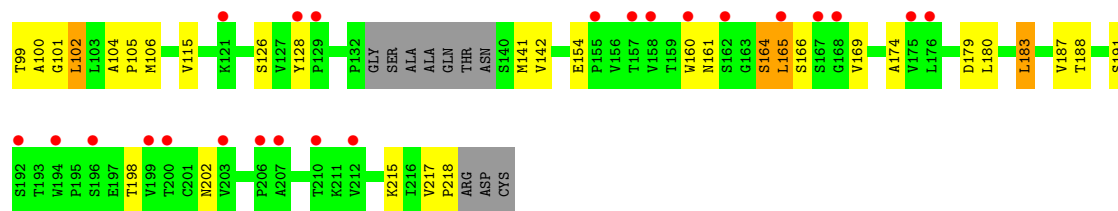


• Molecule 4: 6D3 heavy chain

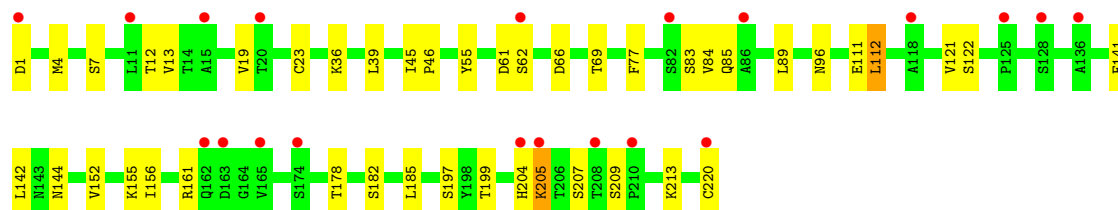
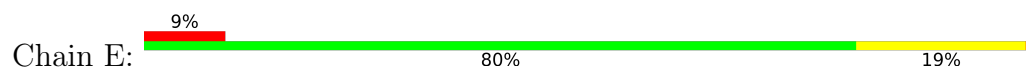


• Molecule 4: 6D3 heavy chain

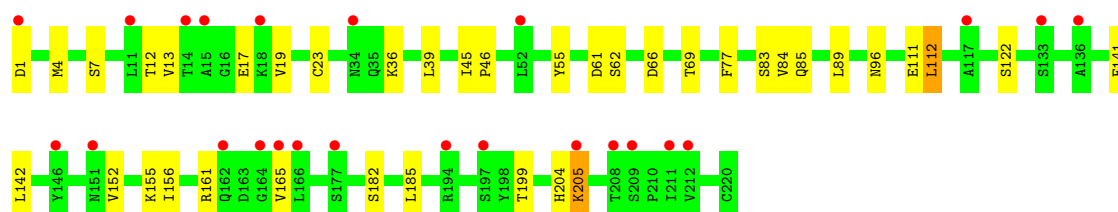
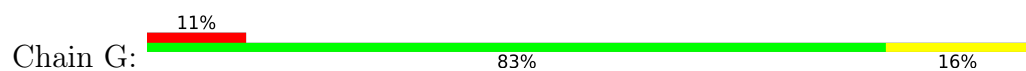




● Molecule 5: 6D3 light chain



● Molecule 5: 6D3 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	301.33Å 109.82Å 82.78Å 90.00° 94.53° 90.00°	Depositor
Resolution (Å)	45.71 – 2.70 45.71 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (45.71-2.70) 97.7 (45.71-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.240 , 0.278 0.236 , 0.269	Depositor DCC
R_{free} test set	3614 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16749	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.44% 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	0.96	0/1830	0.96	2/2462 (0.1%)
1	S	0.89	0/1883	0.92	2/2530 (0.1%)
2	B	1.01	0/1657	0.97	2/2264 (0.1%)
2	H	1.05	2/1657 (0.1%)	1.00	1/2264 (0.0%)
3	C	1.02	0/1690	0.95	0/2296
3	L	1.05	0/1690	0.95	0/2296
4	D	0.66	1/1626 (0.1%)	0.77	0/2228
4	F	0.63	0/1626	0.78	1/2228 (0.0%)
5	E	0.64	0/1749	0.82	1/2380 (0.0%)
5	G	0.62	0/1749	0.81	1/2380 (0.0%)
All	All	0.87	3/17157 (0.0%)	0.90	10/23328 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	101	GLY	C-O	-5.93	1.16	1.23
2	H	103	TYR	CA-C	-5.89	1.45	1.52
2	H	169	GLY	C-O	-5.80	1.17	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	7	SER	N-CA-C	7.31	114.71	108.13
5	E	7	SER	N-CA-C	6.90	114.34	108.13
1	A	3	GLN	CA-C-N	-6.14	114.22	120.85
1	A	3	GLN	C-N-CA	-6.14	114.22	120.85
1	S	3	GLN	CA-C-N	-5.69	114.89	120.52
1	S	3	GLN	C-N-CA	-5.69	114.89	120.52
2	B	33	GLY	N-CA-C	-5.64	102.17	110.97
2	H	33	GLY	N-CA-C	-5.62	103.16	111.03
2	B	96	VAL	N-CA-C	5.35	117.47	108.81
4	F	12	VAL	N-CA-C	5.05	115.54	108.17

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	1789	0	1724	28	0
1	S	1842	0	1787	29	0
2	B	1615	0	1589	22	0
2	H	1615	0	1589	25	0
3	C	1651	0	1566	34	0
3	L	1651	0	1566	34	0
4	D	1583	0	1547	40	0
4	F	1583	0	1547	40	0
5	E	1710	0	1635	23	0
5	G	1710	0	1635	23	0
All	All	16749	0	16185	288	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 9.

All (288) 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)
5:E:4:MET:HE3	5:E:23:CYS:SG	1.93	1.08
4:D:169:VAL:HG22	4:D:187:VAL:HG22	1.34	1.07
4:F:169:VAL:HG22	4:F:187:VAL:HG22	1.38	1.01
5:G:4:MET:HE3	5:G:23:CYS:SG	2.00	1.00
3:L:148:TRP:H	3:L:156:GLN:HE22	1.05	0.95
3:C:148:TRP:H	3:C:156:GLN:HE22	1.07	0.93
4:D:161:ASN:HB2	4:D:164:SER:OG	1.73	0.88
4:F:161:ASN:HB2	4:F:164:SER:OG	1.74	0.88
4:D:161:ASN:HB2	4:D:164:SER:HG	1.43	0.83
2:B:142:MET:HE3	2:B:189:THR:HG22	1.61	0.82
3:C:83:VAL:CG1	3:C:106:ILE:HG12	2.13	0.79
4:D:217:VAL:HG13	4:D:218:PRO:HD2	1.64	0.79
3:L:83:VAL:CG1	3:L:106:ILE:HG12	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:217:VAL:HG13	4:F:218:PRO:HD2	1.66	0.78
3:C:83:VAL:HG13	3:C:106:ILE:HG12	1.66	0.76
4:D:142:VAL:HG23	4:D:191:SER:HB3	1.68	0.73
4:D:141:MET:HE3	4:D:188:THR:HG22	1.71	0.73
3:L:125:LEU:O	3:L:183:LYS:HE3	1.88	0.72
4:F:101:GLY:O	4:F:102:LEU:HB2	1.89	0.72
4:D:169:VAL:HG22	4:D:187:VAL:CG2	2.17	0.71
4:F:142:VAL:HG23	4:F:191:SER:HB3	1.71	0.71
4:F:141:MET:HE3	4:F:188:THR:HG22	1.73	0.70
2:H:142:MET:HE3	2:H:189:THR:HG22	1.74	0.70
3:C:148:TRP:H	3:C:156:GLN:NE2	1.89	0.67
5:G:156:ILE:HD12	5:G:161:ARG:HD2	1.77	0.67
3:L:136:LEU:N	3:L:136:LEU:HD12	2.09	0.67
4:F:169:VAL:HG22	4:F:187:VAL:CG2	2.21	0.67
3:L:83:VAL:HG13	3:L:106:ILE:HG12	1.76	0.66
2:H:150:LYS:HA	2:H:183:THR:HG23	1.77	0.66
4:F:183:LEU:C	4:F:183:LEU:HD12	2.21	0.66
5:E:156:ILE:HD12	5:E:161:ARG:HD2	1.79	0.65
3:C:136:LEU:HD12	3:C:136:LEU:N	2.11	0.65
4:D:183:LEU:HD12	4:D:183:LEU:C	2.21	0.65
2:B:150:LYS:HA	2:B:183:THR:HG23	1.78	0.64
3:L:148:TRP:N	3:L:156:GLN:HE22	1.87	0.64
2:B:184:LEU:C	2:B:184:LEU:HD12	2.24	0.62
1:A:165:ARG:O	1:A:169:VAL:HG23	1.99	0.62
1:A:216:MET:HE3	1:A:217:TYR:CZ	2.35	0.61
1:S:165:ARG:O	1:S:169:VAL:HG23	2.00	0.61
3:C:144:ILE:HD12	3:C:198:HIS:HD2	1.64	0.61
5:E:39:LEU:HD13	5:E:77:PHE:CG	2.36	0.60
3:C:33:LEU:HD13	3:C:33:LEU:C	2.27	0.59
4:F:39:GLN:O	4:F:92:ALA:HB1	2.02	0.59
1:S:153:LYS:NZ	4:F:55:ASP:OD2	2.35	0.59
3:L:4:MET:HE3	3:L:23:CYS:SG	2.42	0.59
2:H:143:VAL:HG23	2:H:192:SER:HB3	1.83	0.59
3:L:148:TRP:H	3:L:156:GLN:NE2	1.89	0.59
3:C:125:LEU:O	3:C:183:LYS:HE3	2.02	0.59
5:G:12:THR:HA	5:G:111:GLU:O	2.03	0.58
5:G:39:LEU:HD13	5:G:77:PHE:CG	2.36	0.58
1:S:127:ASP:OD1	4:F:50:GLU:OE2	2.21	0.58
5:E:12:THR:HA	5:E:111:GLU:O	2.04	0.58
5:E:89:LEU:HD12	5:E:89:LEU:O	2.04	0.58
4:D:58:ILE:HG21	4:D:60:TYR:CZ	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:12:VAL:HG11	4:F:86:LEU:CD1	2.34	0.58
2:H:143:VAL:HG23	2:H:192:SER:CB	2.32	0.58
4:F:23:LYS:HG3	4:F:78:THR:HG23	1.86	0.58
4:D:23:LYS:HG3	4:D:78:THR:HG23	1.86	0.57
2:B:143:VAL:HG23	2:B:192:SER:HB3	1.87	0.57
3:C:49:ASN:H	3:C:49:ASN:HD22	1.53	0.57
1:S:119:THR:HG22	1:S:222:MET:HE2	1.86	0.57
2:H:142:MET:HB3	2:H:189:THR:CG2	2.35	0.57
1:S:41:ILE:HD12	1:S:42:ASP:HB2	1.87	0.56
4:D:12:VAL:HG11	4:D:86:LEU:CD1	2.35	0.56
1:S:166:HIS:CE1	1:S:170:LYS:HE2	2.40	0.56
1:A:166:HIS:CE1	1:A:170:LYS:HE2	2.40	0.56
2:H:38:ARG:NE	2:H:46:GLU:OE1	2.34	0.56
4:D:179:ASP:O	4:D:180:LEU:HD23	2.06	0.56
5:E:204:HIS:CG	5:E:205:LYS:H	2.24	0.56
4:F:198:THR:HG23	4:F:215:LYS:HD2	1.88	0.55
5:G:156:ILE:CD1	5:G:161:ARG:HD2	2.35	0.55
4:D:198:THR:HG23	4:D:215:LYS:HD2	1.88	0.55
4:F:58:ILE:HG21	4:F:60:TYR:CZ	2.41	0.55
5:G:89:LEU:HD12	5:G:89:LEU:O	2.06	0.55
1:A:153:LYS:NZ	4:D:55:ASP:OD2	2.40	0.55
4:D:141:MET:HE3	4:D:188:THR:CG2	2.35	0.55
3:C:46:LEU:HG	3:C:55:ILE:CD1	2.37	0.55
2:B:99:LEU:HD23	2:B:100:TYR:CE2	2.41	0.55
3:C:77:SER:O	3:C:77:SER:OG	2.21	0.55
3:L:144:ILE:HD12	3:L:198:HIS:HD2	1.72	0.55
1:A:65:ARG:NH1	1:A:67:GLU:CD	2.65	0.55
4:D:101:GLY:O	4:D:102:LEU:CD1	2.55	0.54
5:E:4:MET:CE	5:E:23:CYS:SG	2.84	0.54
2:B:143:VAL:HG23	2:B:192:SER:CB	2.37	0.54
3:L:46:LEU:HG	3:L:55:ILE:CD1	2.37	0.54
1:A:64:VAL:HG22	1:A:112:THR:HG23	1.90	0.54
3:C:4:MET:HE3	3:C:23:CYS:SG	2.47	0.54
4:F:141:MET:HE3	4:F:188:THR:CG2	2.37	0.54
3:L:46:LEU:HG	3:L:55:ILE:HD13	1.89	0.54
5:G:204:HIS:CG	5:G:205:LYS:H	2.25	0.54
1:A:41:ILE:HD12	1:A:42:ASP:HB2	1.89	0.53
3:C:144:ILE:HD12	3:C:198:HIS:CD2	2.42	0.53
4:D:39:GLN:O	4:D:92:ALA:HB1	2.08	0.53
2:H:99:LEU:HD23	2:H:100:TYR:CE2	2.44	0.53
4:F:160:TRP:CE2	4:F:187:VAL:HG23	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:65:ARG:NH1	1:S:67:GLU:CD	2.67	0.53
3:L:49:ASN:H	3:L:49:ASN:HD22	1.55	0.53
4:F:101:GLY:O	4:F:102:LEU:CB	2.55	0.53
4:D:126:SER:HB3	4:D:128:TYR:CZ	2.44	0.53
4:F:126:SER:HB3	4:F:128:TYR:CZ	2.44	0.52
5:G:141:PHE:C	5:G:142:LEU:HD12	2.33	0.52
5:E:155:LYS:HB2	5:E:199:THR:HB	1.92	0.52
2:B:142:MET:HB3	2:B:189:THR:CG2	2.40	0.52
4:D:160:TRP:CE2	4:D:187:VAL:HG23	2.44	0.52
3:L:33:LEU:HD13	3:L:33:LEU:C	2.35	0.52
4:D:100:ALA:HB3	4:D:104:ALA:HB1	1.92	0.52
4:F:100:ALA:HB3	4:F:104:ALA:HB1	1.92	0.51
4:F:179:ASP:O	4:F:180:LEU:HD23	2.09	0.51
1:A:65:ARG:HH12	1:A:67:GLU:CD	2.19	0.51
5:E:121:VAL:O	5:E:213:LYS:NZ	2.40	0.51
1:S:39:LYS:HD3	1:S:79:ASP:HA	1.93	0.51
1:S:64:VAL:HG22	1:S:112:THR:HG23	1.92	0.51
5:E:141:PHE:C	5:E:142:LEU:HD12	2.36	0.51
1:A:64:VAL:HG22	1:A:112:THR:CG2	2.40	0.51
5:G:155:LYS:HB2	5:G:199:THR:HB	1.92	0.51
2:H:184:LEU:HD12	2:H:184:LEU:C	2.36	0.51
1:S:216:MET:HE3	1:S:217:TYR:CZ	2.46	0.50
1:S:64:VAL:HG22	1:S:112:THR:CG2	2.42	0.50
5:E:39:LEU:HD13	5:E:77:PHE:CD1	2.47	0.50
3:L:149:LYS:HB2	3:L:193:THR:HB	1.92	0.50
2:H:20:LEU:HG	2:H:82:MET:HE2	1.93	0.50
5:G:39:LEU:HD13	5:G:77:PHE:CD1	2.47	0.50
1:A:39:LYS:HD3	1:A:79:ASP:HA	1.93	0.50
5:E:156:ILE:CD1	5:E:161:ARG:HD2	2.40	0.50
1:S:138:GLU:OE1	1:S:182:TYR:HE1	1.95	0.49
4:F:160:TRP:CE2	4:F:187:VAL:CG2	2.95	0.49
3:C:13:VAL:HG21	3:C:78:VAL:HG11	1.94	0.49
3:C:46:LEU:HG	3:C:55:ILE:HD13	1.95	0.49
4:D:58:ILE:HG21	4:D:60:TYR:CE2	2.47	0.49
3:C:167:ASP:CG	3:C:170:ASP:OD1	2.55	0.49
1:S:130:ARG:NH2	4:F:57:TYR:OH	2.44	0.49
4:D:183:LEU:C	4:D:183:LEU:CD1	2.85	0.49
4:F:164:SER:O	4:F:165:LEU:O	2.31	0.49
1:A:127:ASP:OD1	4:D:50:GLU:OE2	2.30	0.49
3:L:143:ASP:OD2	3:L:143:ASP:N	2.42	0.49
2:H:51:ILE:HD13	2:H:71:ARG:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:GLN:HG3	1:A:217:TYR:CD2	2.48	0.49
4:F:83:LEU:HD21	4:F:94:TYR:CZ	2.48	0.49
2:B:178:GLN:OE1	3:C:160:LEU:HD11	2.13	0.48
1:S:12:HIS:O	1:S:184:THR:HG22	2.13	0.48
1:A:5:ASP:HB3	1:A:6:PRO:CD	2.43	0.48
2:B:143:VAL:HG12	2:B:144:THR:N	2.27	0.48
5:E:13:VAL:HG21	5:E:19:VAL:HG21	1.95	0.48
2:H:42:GLU:O	2:H:43:ARG:HB2	2.14	0.48
5:G:165:VAL:HG22	5:G:185:LEU:HD13	1.95	0.48
4:F:58:ILE:HG21	4:F:60:TYR:CE2	2.48	0.48
1:S:5:ASP:HB3	1:S:6:PRO:CD	2.44	0.48
3:L:75:ILE:CG2	3:L:78:VAL:HG22	2.44	0.48
1:S:65:ARG:HH12	1:S:67:GLU:CD	2.22	0.47
4:D:101:GLY:O	4:D:102:LEU:HD12	2.14	0.47
1:S:31:ASN:HD22	1:S:31:ASN:N	2.12	0.47
4:D:35:HIS:CG	4:D:106:MET:HE2	2.49	0.47
2:H:218:VAL:CG2	2:H:219:PRO:HD2	2.44	0.47
1:A:11:LEU:HD13	1:A:184:THR:HB	1.97	0.47
4:D:105:PRO:HG3	5:E:55:TYR:HB3	1.95	0.47
4:F:105:PRO:HG3	5:G:55:TYR:HB3	1.97	0.47
5:E:13:VAL:HG21	5:E:19:VAL:CG2	2.45	0.47
1:S:237:LYS:O	1:S:238:LYS:C	2.58	0.47
3:L:147:LYS:NZ	3:L:154:GLU:OE2	2.22	0.47
4:F:183:LEU:C	4:F:183:LEU:CD1	2.87	0.47
3:C:61:ARG:HH21	3:C:82:ASP:CG	2.23	0.47
2:H:72:ASP:OD1	2:H:72:ASP:C	2.57	0.47
3:L:155:ARG:O	3:L:156:GLN:NE2	2.48	0.46
2:H:195:TRP:CD1	2:H:196:PRO:HA	2.50	0.46
5:G:142:LEU:HD21	5:G:152:VAL:HG22	1.96	0.46
5:E:142:LEU:HD21	5:E:152:VAL:HG22	1.96	0.46
2:B:218:VAL:CG2	2:B:219:PRO:HD2	2.46	0.46
4:D:160:TRP:CE2	4:D:187:VAL:CG2	2.98	0.46
2:H:218:VAL:HG23	2:H:219:PRO:HD2	1.97	0.46
3:C:149:LYS:HB2	3:C:193:THR:HB	1.98	0.46
5:G:61:ASP:OD1	5:G:62:SER:N	2.49	0.46
1:S:11:LEU:HD13	1:S:184:THR:HB	1.98	0.45
3:L:212:ASN:ND2	3:L:213:GLU:OE2	2.49	0.45
1:A:119:THR:HG22	1:A:222:MET:HE2	1.97	0.45
3:L:61:ARG:HH21	3:L:82:ASP:CG	2.25	0.45
1:A:12:HIS:O	1:A:184:THR:HG22	2.16	0.45
2:H:143:VAL:O	2:H:189:THR:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:167:ASP:CG	3:L:170:ASP:OD1	2.60	0.45
4:D:164:SER:O	4:D:165:LEU:O	2.35	0.45
5:E:61:ASP:OD1	5:E:62:SER:N	2.50	0.45
1:S:162:TYR:CD2	1:S:162:TYR:C	2.95	0.45
3:L:61:ARG:HB2	3:L:76:ASN:O	2.17	0.45
5:G:4:MET:CE	5:G:23:CYS:SG	2.90	0.45
3:L:31:ASP:O	3:L:50:TYR:HA	2.17	0.45
4:F:160:TRP:CD2	4:F:187:VAL:HG21	2.52	0.45
3:C:49:ASN:HD22	3:C:49:ASN:N	2.13	0.44
5:G:13:VAL:HG21	5:G:19:VAL:HG21	1.99	0.44
1:A:130:ARG:NH2	4:D:57:TYR:OH	2.48	0.44
5:E:144:ASN:ND2	5:E:178:THR:OG1	2.49	0.44
4:F:35:HIS:CG	4:F:106:MET:HE2	2.52	0.44
4:F:40:ARG:HB2	4:F:43:GLN:HG3	1.99	0.44
2:B:218:VAL:HG23	2:B:219:PRO:HD2	1.99	0.44
1:S:7:LYS:HB3	1:S:8:PRO:HD2	2.00	0.44
4:D:61:ASN:O	4:D:62:GLN:C	2.60	0.44
2:H:145:LEU:HD12	2:H:200:VAL:HG11	1.99	0.44
1:S:166:HIS:NE2	1:S:170:LYS:HE2	2.33	0.44
3:C:61:ARG:NH2	3:C:82:ASP:OD1	2.51	0.44
1:A:85:PHE:CD1	1:A:85:PHE:C	2.95	0.44
1:A:166:HIS:NE2	1:A:170:LYS:HE2	2.33	0.43
2:B:99:LEU:HD23	2:B:100:TYR:CZ	2.53	0.43
4:D:217:VAL:CG1	4:D:218:PRO:HD2	2.41	0.43
1:S:54:LYS:HE3	1:S:54:LYS:HA	2.00	0.43
1:A:27:LEU:HD22	1:A:214:LEU:HD11	1.99	0.43
1:A:49:LEU:HD21	1:A:78:LYS:HB2	2.00	0.43
3:C:33:LEU:HD21	3:C:88:CYS:HB2	1.98	0.43
4:D:83:LEU:HD21	4:D:94:TYR:CZ	2.53	0.43
3:L:144:ILE:HD12	3:L:198:HIS:CD2	2.50	0.43
5:E:45:ILE:HG23	5:E:46:PRO:HD2	2.00	0.43
1:S:203:ALA:HB1	1:S:204:PRO:HD2	1.99	0.43
1:A:162:TYR:CD2	1:A:162:TYR:C	2.96	0.43
4:F:217:VAL:CG1	4:F:218:PRO:HD2	2.42	0.43
5:G:45:ILE:HG23	5:G:46:PRO:HD2	2.00	0.43
5:G:161:ARG:NE	5:G:185:LEU:HD11	2.34	0.43
2:B:22:CYS:HB3	2:B:78:LEU:HB3	1.99	0.43
2:B:18:LEU:HD12	2:B:18:LEU:HA	1.88	0.43
3:C:55:ILE:O	3:C:56:SER:C	2.62	0.43
4:D:183:LEU:HD12	4:D:183:LEU:O	2.19	0.43
3:L:113:PRO:HG2	3:L:205:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:89:LEU:HB3	5:G:112:LEU:HD12	2.01	0.43
2:B:6:GLU:HA	2:B:21:SER:O	2.19	0.42
5:G:13:VAL:HG21	5:G:19:VAL:CG2	2.49	0.42
3:C:61:ARG:HB2	3:C:76:ASN:O	2.19	0.42
5:E:207:SER:OG	5:E:209:SER:O	2.30	0.42
3:C:83:VAL:HG13	3:C:106:ILE:CG1	2.41	0.42
5:G:45:ILE:O	5:G:46:PRO:C	2.63	0.42
5:G:84:VAL:HG12	5:G:85:GLN:N	2.35	0.42
3:C:31:ASP:O	3:C:50:TYR:HA	2.19	0.42
3:C:193:THR:OG1	3:C:208:SER:HB3	2.19	0.42
4:D:70:LEU:HD21	4:D:81:LEU:HD13	2.01	0.42
5:E:84:VAL:HG12	5:E:85:GLN:N	2.34	0.42
5:E:161:ARG:NE	5:E:185:LEU:HD11	2.34	0.42
1:S:24:MET:HE1	1:S:213:TYR:CZ	2.54	0.42
3:C:212:ASN:ND2	3:C:213:GLU:OE2	2.53	0.42
4:F:33:TRP:HE3	4:F:50:GLU:HG2	1.85	0.42
3:C:136:LEU:N	3:C:136:LEU:CD1	2.82	0.42
4:D:160:TRP:CD2	4:D:187:VAL:HG21	2.55	0.42
2:H:18:LEU:HB3	2:H:82:MET:HE3	2.02	0.42
3:L:33:LEU:HD21	3:L:88:CYS:HB2	2.02	0.42
1:A:158:GLN:HG3	1:A:217:TYR:CE2	2.55	0.42
1:S:144:LEU:C	1:S:144:LEU:HD12	2.45	0.42
2:H:98:ASP:CG	2:H:99:LEU:N	2.78	0.42
2:B:36:TRP:CG	2:B:80:LEU:HD22	2.55	0.42
2:B:48:VAL:O	2:B:49:ALA:HB2	2.20	0.42
2:B:51:ILE:HD13	2:B:71:ARG:HG3	2.02	0.41
4:F:91:SER:O	4:F:92:ALA:HB2	2.20	0.41
1:A:206:ASP:OD1	1:A:206:ASP:N	2.45	0.41
4:D:101:GLY:O	4:D:102:LEU:HD13	2.19	0.41
1:S:85:PHE:CD1	1:S:85:PHE:C	2.97	0.41
3:L:50:TYR:O	3:L:51:ALA:HB3	2.20	0.41
3:L:83:VAL:HG12	3:L:106:ILE:HG12	1.98	0.41
4:F:61:ASN:O	4:F:62:GLN:C	2.63	0.41
1:A:165:ARG:HG2	1:A:200:MET:HE3	2.01	0.41
2:B:38:ARG:NE	2:B:46:GLU:OE1	2.42	0.41
1:A:24:MET:HE1	1:A:213:TYR:CZ	2.55	0.41
1:A:31:ASN:N	1:A:31:ASN:HD22	2.16	0.41
2:H:143:VAL:HG12	2:H:144:THR:N	2.36	0.41
3:C:142:LYS:HB3	3:C:173:TYR:CE2	2.55	0.41
4:D:35:HIS:ND1	4:D:106:MET:HE2	2.36	0.41
3:L:146:VAL:O	3:L:146:VAL:HG12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:167:ASP:HB3	3:L:170:ASP:OD1	2.19	0.41
4:F:126:SER:HB3	4:F:128:TYR:CE2	2.55	0.41
3:C:155:ARG:O	3:C:156:GLN:NE2	2.54	0.41
3:C:165:ASP:O	3:C:166:GLN:C	2.61	0.41
4:D:70:LEU:CD2	4:D:81:LEU:HD13	2.51	0.41
1:S:55:ASP:C	1:S:57:LYS:N	2.78	0.41
3:L:13:VAL:HG21	3:L:78:VAL:HG11	2.01	0.41
1:A:7:LYS:HB3	1:A:8:PRO:HD2	2.03	0.41
5:E:89:LEU:HB3	5:E:112:LEU:HD12	2.02	0.41
2:H:178:GLN:OE1	3:L:160:LEU:HD11	2.21	0.41
4:F:5:GLN:HA	4:F:5:GLN:NE2	2.36	0.41
2:B:98:ASP:CG	2:B:99:LEU:N	2.79	0.41
2:B:195:TRP:CD1	2:B:196:PRO:HA	2.56	0.41
3:C:143:ASP:OD2	3:C:143:ASP:N	2.50	0.41
4:D:154:GLU:OE2	4:D:174:ALA:HB3	2.21	0.41
2:H:18:LEU:HD12	2:H:18:LEU:HA	1.86	0.41
4:F:154:GLU:OE2	4:F:174:ALA:HB3	2.21	0.41
3:C:148:TRP:N	3:C:156:GLN:HE22	1.92	0.40
3:L:49:ASN:HD22	3:L:49:ASN:N	2.18	0.40
3:L:193:THR:OG1	3:L:208:SER:HB3	2.21	0.40
4:F:35:HIS:CE1	4:F:50:GLU:HG3	2.56	0.40
1:S:49:LEU:HD21	1:S:78:LYS:HB2	2.03	0.40
2:H:6:GLU:HA	2:H:21:SER:O	2.21	0.40
2:B:164:GLY:O	2:B:165:SER:C	2.64	0.40
4:D:40:ARG:HB2	4:D:43:GLN:HG3	2.02	0.40
2:H:199:THR:CG2	2:H:216:LYS:HG3	2.51	0.40
4:F:70:LEU:HD21	4:F:81:LEU:HD13	2.02	0.40
2:H:179:SER:O	2:H:180:ASP:HB2	2.21	0.40
5:G:17:GLU:O	5:G:84:VAL:HG23	2.22	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	208/245 (85%)	199 (96%)	8 (4%)	1 (0%)	24	48
1	S	214/245 (87%)	203 (95%)	10 (5%)	1 (0%)	24	48
2	B	209/222 (94%)	199 (95%)	10 (5%)	0	100	100
2	H	209/222 (94%)	198 (95%)	10 (5%)	1 (0%)	24	48
3	C	211/214 (99%)	202 (96%)	7 (3%)	2 (1%)	14	35
3	L	211/214 (99%)	204 (97%)	5 (2%)	2 (1%)	14	35
4	D	206/221 (93%)	190 (92%)	15 (7%)	1 (0%)	24	48
4	F	206/221 (93%)	189 (92%)	15 (7%)	2 (1%)	12	32
5	E	218/220 (99%)	204 (94%)	13 (6%)	1 (0%)	24	48
5	G	218/220 (99%)	204 (94%)	13 (6%)	1 (0%)	24	48
All	All	2110/2244 (94%)	1992 (94%)	106 (5%)	12 (1%)	21	44

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	165	LEU
4	F	102	LEU
4	F	165	LEU
1	A	192	ASN
3	C	212	ASN
1	S	192	ASN
5	E	83	SER
5	G	83	SER
3	L	77	SER
3	L	212	ASN
3	C	77	SER
2	H	167	SER

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	201/229 (88%)	196 (98%)	5 (2%)	42	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	207/229 (90%)	199 (96%)	8 (4%)	28	57
2	B	182/188 (97%)	173 (95%)	9 (5%)	22	49
2	H	182/188 (97%)	174 (96%)	8 (4%)	25	53
3	C	190/191 (100%)	177 (93%)	13 (7%)	14	35
3	L	190/191 (100%)	176 (93%)	14 (7%)	13	32
4	D	182/190 (96%)	170 (93%)	12 (7%)	15	36
4	F	182/190 (96%)	171 (94%)	11 (6%)	17	41
5	E	198/198 (100%)	187 (94%)	11 (6%)	19	44
5	G	198/198 (100%)	189 (96%)	9 (4%)	24	52
All	All	1912/1992 (96%)	1812 (95%)	100 (5%)	21	47

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	50	ILE
1	A	80	LYS
1	A	154	LYS
1	A	237	LYS
2	B	10	ASP
2	B	12	VAL
2	B	46	GLU
2	B	117	ILE
2	B	163	SER
2	B	179	SER
2	B	183	THR
2	B	184	LEU
2	B	215	LYS
3	C	1	ASP
3	C	13	VAL
3	C	19	VAL
3	C	22	SER
3	C	33	LEU
3	C	49	ASN
3	C	90	ASN
3	C	97	THR
3	C	143	ASP
3	C	171	SER
3	C	175	MET

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Mol	Chain	Res	Type
3	C	183	LYS
3	C	193	THR
4	D	4	LEU
4	D	7	SER
4	D	17	SER
4	D	78	THR
4	D	83	LEU
4	D	99	THR
4	D	102	LEU
4	D	115	VAL
4	D	164	SER
4	D	166	SER
4	D	183	LEU
4	D	202	ASN
5	E	1	ASP
5	E	36	LYS
5	E	66	ASP
5	E	69	THR
5	E	96	ASN
5	E	112	LEU
5	E	122	SER
5	E	182	SER
5	E	197	SER
5	E	205	LYS
5	E	220	CYS
1	S	20	LEU
1	S	39	LYS
1	S	50	ILE
1	S	54	LYS
1	S	57	LYS
1	S	80	LYS
1	S	110	ARG
1	S	154	LYS
2	H	10	ASP
2	H	12	VAL
2	H	46	GLU
2	H	117	ILE
2	H	179	SER
2	H	183	THR
2	H	184	LEU
2	H	215	LYS
3	L	1	ASP

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Mol	Chain	Res	Type
3	L	13	VAL
3	L	19	VAL
3	L	22	SER
3	L	33	LEU
3	L	49	ASN
3	L	90	ASN
3	L	97	THR
3	L	143	ASP
3	L	168	SER
3	L	171	SER
3	L	175	MET
3	L	183	LYS
3	L	193	THR
4	F	4	LEU
4	F	7	SER
4	F	17	SER
4	F	78	THR
4	F	83	LEU
4	F	99	THR
4	F	115	VAL
4	F	164	SER
4	F	166	SER
4	F	183	LEU
4	F	202	ASN
5	G	1	ASP
5	G	36	LYS
5	G	66	ASP
5	G	69	THR
5	G	96	ASN
5	G	112	LEU
5	G	122	SER
5	G	182	SER
5	G	205	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	31	ASN
1	A	171	ASN
1	A	178	ASN
1	A	210	GLN

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Mol	Chain	Res	Type
2	B	39	GLN
2	B	81	GLN
3	C	38	GLN
3	C	49	ASN
3	C	53	GLN
3	C	156	GLN
4	D	5	GLN
4	D	39	GLN
5	E	27	GLN
5	E	31	ASN
5	E	34	ASN
5	E	44	GLN
5	E	85	GLN
5	E	95	GLN
5	E	144	ASN
1	S	31	ASN
1	S	210	GLN
2	H	39	GLN
2	H	81	GLN
3	L	38	GLN
3	L	49	ASN
3	L	53	GLN
3	L	156	GLN
3	L	189	HIS
4	F	5	GLN
5	G	27	GLN
5	G	31	ASN
5	G	85	GLN
5	G	144	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 ⓘ

There are no oligosaccharides 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, 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	214/245 (87%)	0.40	10 (4%) 36 33	29, 46, 74, 82	0
1	S	220/245 (89%)	0.30	7 (3%) 50 46	29, 48, 81, 102	0
2	B	213/222 (95%)	-0.14	0 100 100	22, 34, 46, 56	0
2	H	213/222 (95%)	-0.08	1 (0%) 87 86	23, 34, 46, 53	0
3	C	213/214 (99%)	-0.03	2 (0%) 81 80	24, 37, 60, 88	0
3	L	213/214 (99%)	-0.00	1 (0%) 87 86	24, 37, 55, 80	0
4	D	210/221 (95%)	1.20	38 (18%) 3 3	46, 87, 135, 155	1 (0%)
4	F	210/221 (95%)	1.15	35 (16%) 4 3	49, 89, 142, 162	1 (0%)
5	E	220/220 (100%)	0.83	20 (9%) 15 12	45, 84, 150, 197	0
5	G	220/220 (100%)	0.97	24 (10%) 10 9	47, 87, 160, 199	0
All	All	2146/2244 (95%)	0.46	138 (6%) 25 22	22, 50, 130, 199	2 (0%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	165	LEU	5.3
4	F	23	LYS	5.3
4	D	165	LEU	5.0
5	G	136	ALA	4.9
4	D	83	LEU	4.5
4	D	23	LYS	4.3
4	D	26	GLY	4.0
4	D	160	TRP	4.0
5	G	177	SER	3.9
5	G	165	VAL	3.8
4	F	26	GLY	3.7
4	F	199	VAL	3.6
5	G	34	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
4	F	210	THR	3.5
4	F	168	GLY	3.5
4	D	191	SER	3.4
4	F	29	PHE	3.4
4	F	158	VAL	3.4
4	D	142	VAL	3.4
4	D	129	PRO	3.3
4	F	196	SER	3.2
5	G	208	THR	3.2
5	E	220	CYS	3.2
5	E	136	ALA	3.2
4	F	212	VAL	3.1
5	E	205	LYS	3.1
4	D	167	SER	3.0
5	G	205	LYS	3.0
4	F	24	ALA	3.0
4	D	171	THR	3.0
5	G	52	LEU	2.9
4	D	25	SER	2.8
5	G	117	ALA	2.8
5	G	18	LYS	2.8
4	D	10	GLU	2.7
4	D	196	SER	2.7
5	G	209	SER	2.7
4	D	198	THR	2.7
4	F	83	LEU	2.7
4	F	162	SER	2.7
4	D	152	PHE	2.7
5	E	118	ALA	2.7
4	F	160	TRP	2.7
5	G	166	LEU	2.6
1	S	96	SER	2.6
4	F	192	SER	2.6
5	E	208	THR	2.6
4	D	9	ALA	2.6
5	E	82	SER	2.6
4	D	29	PHE	2.6
4	F	33	TRP	2.6
5	G	15	ALA	2.6
1	A	96	SER	2.5
4	F	75	SER	2.5
5	E	174	SER	2.5

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Mol	Chain	Res	Type	RSRZ
4	D	197	GLU	2.5
4	D	96	CYS	2.5
5	E	128	SER	2.5
1	A	227	ASP	2.5
5	G	1	ASP	2.5
4	D	189	VAL	2.5
4	F	200	THR	2.5
4	F	121	LYS	2.5
4	D	128	TYR	2.5
4	F	128	TYR	2.5
4	D	168	GLY	2.5
4	D	161	ASN	2.5
4	F	194	TRP	2.5
5	E	15	ALA	2.5
4	F	129	PRO	2.4
5	G	197	SER	2.4
5	E	11	LEU	2.4
4	F	2	VAL	2.4
5	E	165	VAL	2.4
1	A	74	ALA	2.4
4	D	162	SER	2.3
4	F	206	PRO	2.3
3	C	184	ASP	2.3
4	F	175	VAL	2.3
4	F	20	LEU	2.3
4	F	207	ALA	2.3
4	D	87	THR	2.3
5	G	14	THR	2.3
5	E	1	ASP	2.3
4	D	212	VAL	2.3
4	F	176	LEU	2.3
4	D	200	THR	2.3
1	A	224	ASP	2.3
5	G	146	TYR	2.2
1	A	79	ASP	2.2
4	F	21	SER	2.2
5	G	133	SER	2.2
5	E	86	ALA	2.2
1	A	93	CYS	2.2
5	E	210	PRO	2.2
3	L	143	ASP	2.2
4	F	203	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
4	D	20	LEU	2.2
4	D	178	SER	2.2
4	F	167	SER	2.2
5	G	151	ASN	2.2
4	D	176	LEU	2.2
5	E	163	ASP	2.2
4	D	88	SER	2.2
1	S	56	THR	2.1
1	S	110	ARG	2.1
4	D	193	THR	2.1
4	F	77	THR	2.1
4	F	155	PRO	2.1
4	D	19	LYS	2.1
5	G	162	GLN	2.1
5	E	62	SER	2.1
5	E	20	THR	2.1
5	E	125	PRO	2.1
4	D	201	CYS	2.1
5	E	204	HIS	2.1
1	A	9	ASP	2.1
4	D	2	VAL	2.1
5	G	212	VAL	2.1
1	A	3	GLN	2.1
4	F	34	MET	2.1
1	S	93	CYS	2.1
5	G	211	ILE	2.1
1	S	95	PHE	2.1
5	G	194	ARG	2.1
4	F	157	THR	2.1
1	A	45	LEU	2.1
4	D	163	GLY	2.1
5	G	164	GLY	2.1
1	S	46	TYR	2.1
1	S	94	TYR	2.1
3	C	143	ASP	2.0
2	H	167	SER	2.0
4	D	28	THR	2.0
4	D	144	LEU	2.0
5	E	162	GLN	2.0
5	G	11	LEU	2.0
1	A	192	ASN	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.