



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:31 AM UTC

PDB ID : 8TMY / pdb_00008tmy
Title : Crystal structure of SARS-CoV-2 spike stem helix peptide in complex with neutralizing antibody CHM-16
Authors : Feng, Z.; Wilson, I.A.
Deposited on : 2023-07-31
Resolution : 3.07 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

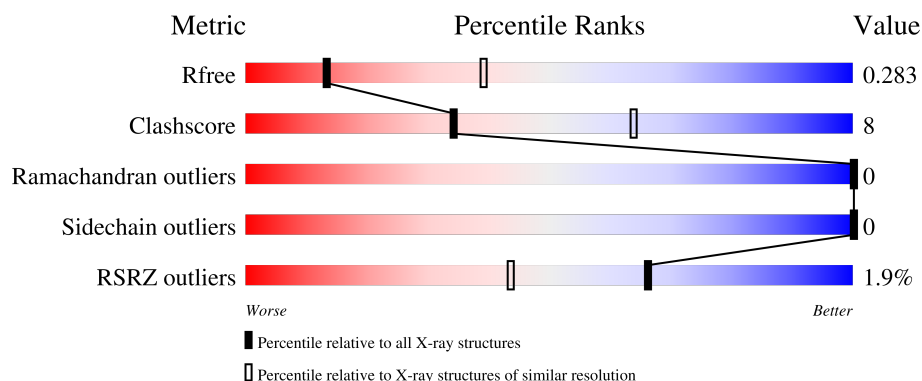
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.07 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	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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	M	25	48% 52%
1	N	25	56% 8% 36%
1	S	25	4% 44% 52%
2	A	221	3% 86% 14%
2	C	221	4% 77% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	221	% 81% 15%
3	B	212	83% 17%
3	D	212	3% 75% 25%
3	L	212	81% 19%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10123 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 Stem helix peptide of Spike protein S2'.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	M	12	Total	C	N	O	2	1	0
			104	71	15	18			
1	N	16	Total	C	N	O	2	1	0
			137	91	21	25			
1	S	12	Total	C	N	O	0	0	0
			106	71	15	20			

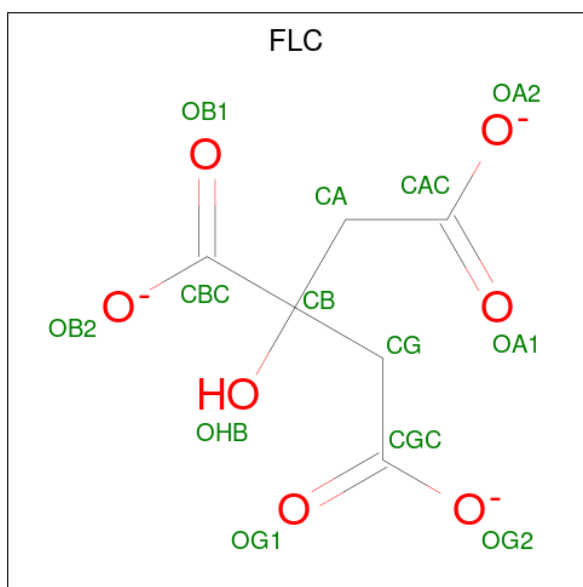
- Molecule 2 is a protein called Neutralizing antibody CHM-16 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	213	Total	C	N	O	S	0	0	0
			1601	1011	274	310	6			
2	A	220	Total	C	N	O	S	0	0	0
			1647	1036	282	323	6			
2	C	214	Total	C	N	O	S	0	0	0
			1607	1014	275	312	6			

- Molecule 3 is a protein called Neutralizing antibody CHM-16 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	212	Total	C	N	O	S	0	0	0
			1636	1022	279	329	6			
3	B	212	Total	C	N	O	S	0	0	0
			1636	1022	279	329	6			
3	D	212	Total	C	N	O	S	0	0	0
			1636	1022	279	329	6			

- Molecule 4 is CITRATE ANION (CCD ID: FLC) (formula: C₆H₅O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	6	7		

3 Residue-property plots

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.

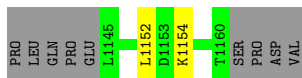
- Molecule 1: Stem helix peptide of Spike protein S2'

Chain M: 



- Molecule 1: Stem helix peptide of Spike protein S2'

Chain N: 



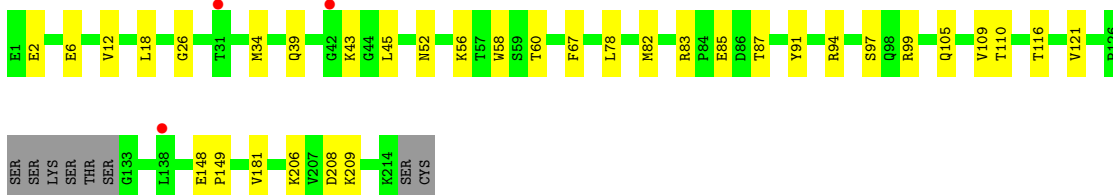
- Molecule 1: Stem helix peptide of Spike protein S2'

Chain S: 



- Molecule 2: Neutralizing antibody CHM-16 Heavy Chain

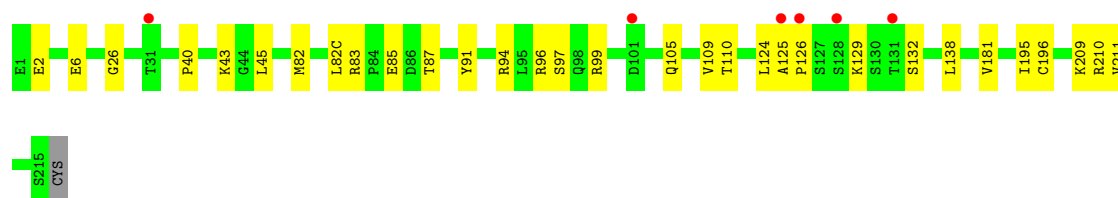
Chain H: 



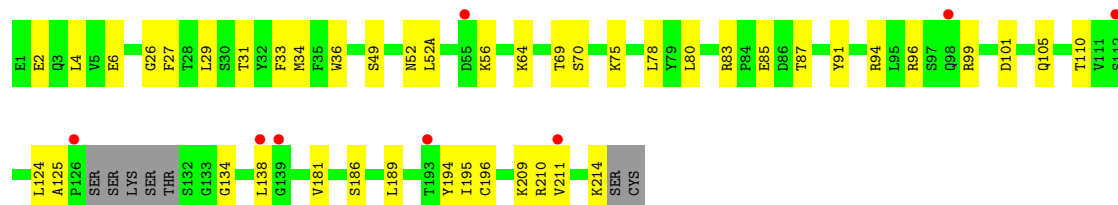
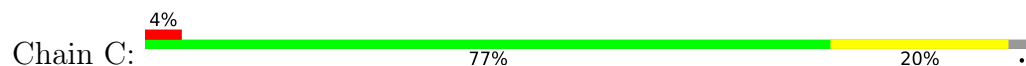
- Molecule 2: Neutralizing antibody CHM-16 Heavy Chain

Chain A: 

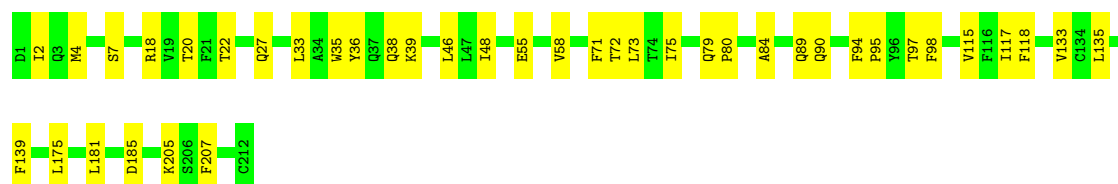
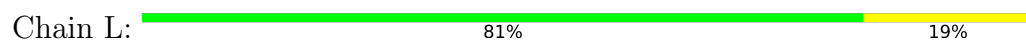




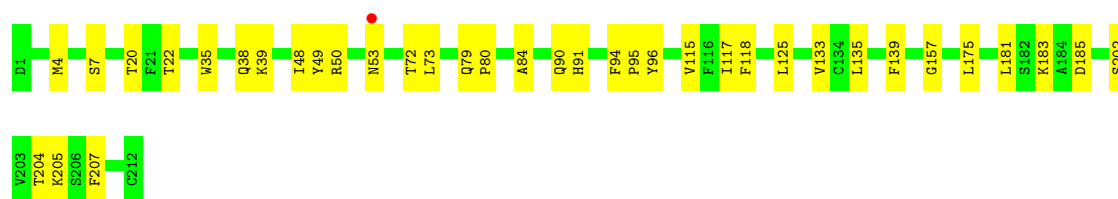
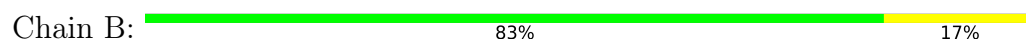
• Molecule 2: Neutralizing antibody CHM-16 Heavy Chain



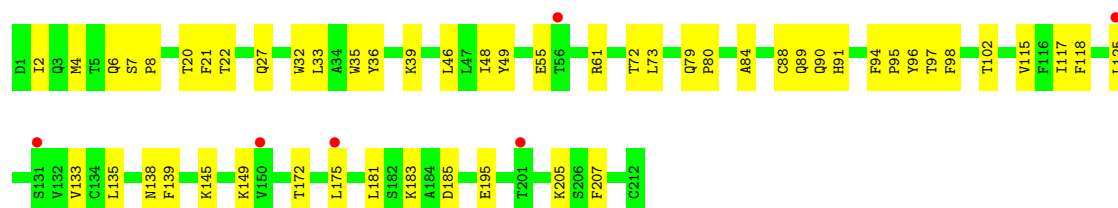
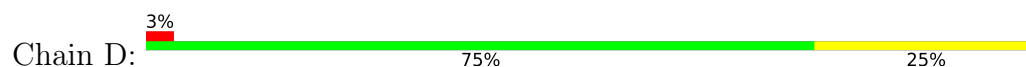
• Molecule 3: Neutralizing antibody CHM-16 Light Chain



• Molecule 3: Neutralizing antibody CHM-16 Light Chain



• Molecule 3: Neutralizing antibody CHM-16 Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.46Å 73.68Å 330.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.06 – 3.07 33.06 – 3.07	Depositor EDS
% Data completeness (in resolution range)	93.0 (33.06-3.07) 93.2 (33.06-3.07)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.06Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.243 , 0.286 0.244 , 0.283	Depositor DCC
R_{free} test set	2018 reflections (5.82%)	wwPDB-VP
Wilson B-factor (Å ²)	59.2	Xtriage
Anisotropy	0.703	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.055 for k,h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	10123	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.87% 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

Bond lengths and bond angles in the following residue types are not validated in this section: FLC

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	M	0.07	0/109	0.15	0/143
1	N	0.08	0/143	0.26	0/190
1	S	0.08	0/108	0.19	0/141
2	A	0.11	0/1687	0.34	0/2295
2	C	0.10	0/1646	0.32	0/2239
2	H	0.10	0/1640	0.32	0/2231
3	B	0.10	0/1671	0.32	0/2270
3	D	0.09	0/1671	0.29	0/2270
3	L	0.09	0/1671	0.31	0/2270
All	All	0.10	0/10346	0.31	0/14049

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	M	104	0	97	0	0
1	N	137	0	126	2	0
1	S	106	0	99	1	0
2	A	1647	0	1611	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1607	0	1570	33	0
2	H	1601	0	1565	23	0
3	B	1636	0	1578	27	0
3	D	1636	0	1578	36	0
3	L	1636	0	1578	27	0
4	B	13	0	5	0	0
All	All	10123	0	9807	152	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (152) 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)
2:A:96:ARG:HG2	2:A:99:ARG:HG3	1.32	1.10
2:C:96:ARG:HD3	2:C:99:ARG:HG3	1.55	0.89
3:D:4:MET:HE2	3:D:90:GLN:HB3	1.63	0.81
2:A:6:GLU:H	2:A:105:GLN:HE22	1.29	0.80
2:A:2:GLU:HA	2:A:26:GLY:HA3	1.68	0.76
3:B:4:MET:HE2	3:B:90:GLN:HB3	1.67	0.75
3:L:139:PHE:HZ	3:L:175:LEU:HD13	1.53	0.74
3:L:4:MET:HE2	3:L:90:GLN:HB3	1.69	0.73
2:H:6:GLU:H	2:H:105:GLN:HE22	1.37	0.72
2:C:6:GLU:H	2:C:105:GLN:HE22	1.33	0.71
2:A:96:ARG:CG	2:A:99:ARG:HG3	2.17	0.70
2:C:87:THR:HG23	2:C:110:THR:HA	1.73	0.70
3:B:139:PHE:HZ	3:B:175:LEU:HD13	1.57	0.70
2:H:2:GLU:HA	2:H:26:GLY:HA3	1.74	0.68
2:C:124:LEU:HD22	3:D:118:PHE:HB3	1.76	0.67
2:H:148:GLU:HG2	2:H:149:PRO:HA	1.75	0.67
2:A:96:ARG:HE	2:A:97:SER:H	1.42	0.66
3:B:39:LYS:HD3	3:B:84:ALA:HB2	1.77	0.66
2:C:125:ALA:O	2:C:214:LYS:NZ	2.29	0.66
3:D:139:PHE:HZ	3:D:175:LEU:HD13	1.61	0.65
2:H:87:THR:HG23	2:H:110:THR:HA	1.79	0.65
2:A:82:MET:HB3	2:A:82(C):LEU:HD21	1.78	0.65
2:A:87:THR:HG23	2:A:110:THR:HA	1.78	0.65
3:L:39:LYS:HD3	3:L:84:ALA:HB2	1.79	0.65
2:C:134:GLY:O	2:C:186:SER:OG	2.16	0.63
3:L:7:SER:OG	3:L:22:THR:OG1	2.17	0.61
3:D:39:LYS:HD3	3:D:84:ALA:HB2	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2:GLU:OE1	2:H:94:ARG:NH1	2.33	0.61
3:B:7:SER:OG	3:B:22:THR:OG1	2.21	0.59
2:C:2:GLU:HA	2:C:26:GLY:HA3	1.85	0.59
3:D:115:VAL:HG12	3:D:205:LYS:HG3	1.84	0.59
2:H:206:LYS:HB3	3:B:204:THR:HB	1.84	0.58
2:C:29:LEU:HD13	2:C:34:MET:HE3	1.84	0.58
2:H:181:VAL:HG11	3:L:135:LEU:HD22	1.86	0.57
3:L:115:VAL:HG12	3:L:205:LYS:HG3	1.85	0.57
2:A:181:VAL:HG11	3:B:135:LEU:HD22	1.84	0.57
3:D:7:SER:OG	3:D:22:THR:OG1	2.21	0.57
3:L:35:TRP:HB2	3:L:48:ILE:HB	1.85	0.57
2:H:82:MET:HE1	2:H:109:VAL:HG21	1.86	0.57
2:H:99:ARG:NH1	3:L:55:GLU:OE2	2.37	0.56
2:A:124:LEU:HD22	3:B:118:PHE:HB3	1.88	0.56
2:H:39:GLN:OE1	3:L:38:GLN:NE2	2.38	0.56
2:C:83:ARG:NH2	2:C:85:GLU:OE1	2.38	0.56
2:C:181:VAL:HG11	3:D:135:LEU:HD22	1.89	0.55
3:L:89:GLN:HG3	3:L:98:PHE:HB3	1.90	0.54
3:D:35:TRP:HB2	3:D:48:ILE:HB	1.90	0.54
3:B:35:TRP:HB2	3:B:48:ILE:HB	1.89	0.53
3:B:157:GLY:HA2	3:D:32:TRP:HZ2	1.72	0.53
3:D:181:LEU:HD11	3:D:185:ASP:HB3	1.90	0.53
3:L:181:LEU:HD11	3:L:185:ASP:HB3	1.90	0.53
2:C:186:SER:HA	2:C:189:LEU:HD13	1.90	0.53
3:L:46:LEU:HG	3:L:55:GLU:HG3	1.91	0.53
2:H:121:VAL:HG12	2:H:209:LYS:HD2	1.91	0.53
2:H:83:ARG:NH2	2:H:85:GLU:OE1	2.42	0.52
3:L:2:ILE:HG23	3:L:27:GLN:HG2	1.90	0.52
2:A:6:GLU:OE2	2:A:91:TYR:HA	2.11	0.51
3:D:79:GLN:HG3	3:D:80:PRO:HD2	1.91	0.51
2:A:126:PRO:HB3	2:A:129:LYS:HE3	1.91	0.51
3:B:115:VAL:HG12	3:B:205:LYS:HG3	1.91	0.51
3:D:90:GLN:HE21	3:D:97:THR:H	1.58	0.51
3:B:79:GLN:HG3	3:B:80:PRO:HD2	1.94	0.50
2:C:31:THR:HA	2:C:52(A):LEU:HD23	1.93	0.50
3:B:118:PHE:HB2	3:B:133:VAL:HB	1.92	0.50
3:D:89:GLN:HG3	3:D:98:PHE:HB3	1.92	0.50
2:A:129:LYS:HZ3	3:B:117:ILE:HG23	1.77	0.50
3:L:118:PHE:HB2	3:L:133:VAL:HB	1.94	0.50
3:D:4:MET:HE3	3:D:33:LEU:HD12	1.94	0.49
2:H:208:ASP:HB2	3:B:202:SER:HB2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:83:ARG:NH2	2:A:85:GLU:OE1	2.45	0.49
2:A:129:LYS:NZ	3:B:117:ILE:HG23	2.27	0.49
3:L:117:ILE:HD13	3:L:207:PHE:HD1	1.77	0.49
1:N:1152:LEU:HD13	2:C:33:PHE:CD2	2.48	0.49
2:C:94:ARG:NH2	2:C:101:ASP:OD2	2.45	0.49
2:C:99:ARG:HD3	3:D:49:TYR:CG	2.49	0.48
2:C:138:LEU:HD22	2:C:194:TYR:HD2	1.77	0.48
3:D:94:PHE:CG	3:D:95:PRO:HA	2.49	0.48
2:A:96:ARG:HB3	2:A:99:ARG:HB2	1.95	0.48
3:L:94:PHE:CG	3:L:95:PRO:HA	2.49	0.48
3:B:94:PHE:CG	3:B:95:PRO:HA	2.48	0.48
2:A:40:PRO:HG2	2:A:43:LYS:HE3	1.96	0.48
3:B:181:LEU:HD11	3:B:185:ASP:HB3	1.95	0.47
2:C:6:GLU:OE2	2:C:91:TYR:HA	2.15	0.47
3:D:118:PHE:HB2	3:D:133:VAL:HB	1.96	0.47
2:H:34:MET:HB3	2:H:78:LEU:HD22	1.94	0.47
3:B:49:TYR:CZ	3:B:53:ASN:HB3	2.50	0.47
3:D:21:PHE:HD2	3:D:73:LEU:HD23	1.79	0.46
3:B:49:TYR:HD2	3:B:50:ARG:HG3	1.80	0.46
2:C:196:CYS:SG	2:C:209:LYS:HB3	2.56	0.46
2:H:6:GLU:OE2	2:H:91:TYR:HA	2.16	0.46
2:A:96:ARG:NE	2:A:97:SER:H	2.11	0.46
2:C:99:ARG:HD3	3:D:49:TYR:CD1	2.51	0.46
3:L:20:THR:HG23	3:L:72:THR:HG23	1.98	0.46
1:N:1154:LYS:HB3	1:N:1154:LYS:HE3	1.73	0.45
3:D:149:LYS:NZ	3:D:195:GLU:OE1	2.39	0.45
3:L:18:ARG:HA	3:L:75:ILE:O	2.15	0.45
2:H:12:VAL:HG21	2:H:18:LEU:HB2	1.97	0.45
2:H:58:TRP:CH2	2:H:60:THR:HG22	2.51	0.45
2:C:125:ALA:HB2	2:C:211:VAL:HG13	1.98	0.45
3:B:125:LEU:O	3:B:183:LYS:HD2	2.16	0.45
2:C:69:THR:HG22	2:C:80:LEU:HD12	1.99	0.45
3:D:90:GLN:NE2	3:D:95:PRO:O	2.50	0.45
1:S:1156:PHE:HA	2:H:97:SER:O	2.18	0.44
2:A:125:ALA:HB2	2:A:211:VAL:HG22	2.00	0.44
3:B:35:TRP:CG	3:B:73:LEU:HD13	2.53	0.44
3:L:36:TYR:CE2	3:L:46:LEU:HD13	2.52	0.44
3:D:117:ILE:HD13	3:D:207:PHE:HD1	1.82	0.44
3:L:90:GLN:HE21	3:L:97:THR:H	1.65	0.44
3:D:20:THR:HG23	3:D:72:THR:HG23	2.00	0.44
2:C:52:ASN:HD22	2:C:56:LYS:HB2	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:8:PRO:O	3:D:102:THR:OG1	2.30	0.43
3:L:79:GLN:HG3	3:L:80:PRO:HD2	1.99	0.43
3:L:94:PHE:CD1	3:L:95:PRO:HA	2.52	0.43
2:A:87:THR:HA	2:A:109:VAL:O	2.19	0.43
2:C:36:TRP:HB2	2:C:49:SER:OG	2.19	0.43
2:C:52:ASN:ND2	2:C:56:LYS:HB2	2.33	0.43
2:A:45:LEU:HD21	3:B:38:GLN:HE22	1.83	0.42
2:A:195:ILE:HG22	2:A:210:ARG:HA	2.01	0.42
2:C:99:ARG:HD2	3:D:55:GLU:OE2	2.19	0.42
3:D:94:PHE:CD1	3:D:95:PRO:HA	2.55	0.42
2:H:45:LEU:HD21	3:L:38:GLN:HE22	1.84	0.42
3:B:91:HIS:HA	3:B:96:TYR:CD1	2.54	0.42
2:H:43:LYS:HA	2:H:43:LYS:HD2	1.75	0.42
2:A:196:CYS:SG	2:A:209:LYS:HB3	2.59	0.42
3:B:157:GLY:HA2	3:D:32:TRP:CZ2	2.52	0.42
3:L:33:LEU:HD22	3:L:71:PHE:CD2	2.55	0.42
3:L:35:TRP:CG	3:L:73:LEU:HD13	2.55	0.42
2:C:124:LEU:HD11	3:D:133:VAL:HG21	2.00	0.42
3:B:117:ILE:HD13	3:B:207:PHE:HD1	1.85	0.42
2:C:4:LEU:HD21	2:C:27:PHE:CZ	2.55	0.42
2:A:138:LEU:HD12	2:A:211:VAL:HG22	2.02	0.41
2:C:31:THR:O	2:C:31:THR:OG1	2.38	0.41
2:H:67:PHE:CE1	2:H:82:MET:HB3	2.55	0.41
2:H:116:THR:HB	2:A:132:SER:HA	2.03	0.41
3:D:36:TYR:CE2	3:D:46:LEU:HD13	2.55	0.41
2:H:52:ASN:HD21	2:H:56:LYS:H	1.68	0.41
2:A:2:GLU:OE1	2:A:94:ARG:NH1	2.52	0.41
3:D:91:HIS:HA	3:D:96:TYR:CD1	2.55	0.41
3:D:125:LEU:O	3:D:183:LYS:HD2	2.21	0.41
3:B:20:THR:HG23	3:B:72:THR:HG23	2.03	0.41
2:C:96:ARG:HB2	2:C:101:ASP:OD2	2.21	0.41
3:L:55:GLU:O	3:L:58:VAL:HG22	2.21	0.41
3:D:2:ILE:HG23	3:D:27:GLN:HG2	2.02	0.41
3:B:35:TRP:CE2	3:B:73:LEU:HB2	2.56	0.40
2:C:70:SER:O	2:C:78:LEU:HD12	2.22	0.40
3:D:61:ARG:H	3:D:61:ARG:HG2	1.63	0.40
3:D:138:ASN:HA	3:D:172:THR:HB	2.03	0.40
2:C:75:LYS:HE3	2:C:75:LYS:HB3	1.91	0.40
3:D:6:GLN:OE1	3:D:88:CYS:N	2.54	0.40
3:D:145:LYS:HE3	3:D:145:LYS:HB2	1.87	0.40
3:L:90:GLN:NE2	3:L:95:PRO:O	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:195:ILE:HG22	2:C:210:ARG:HA	2.03	0.40
2:C:64:LYS:HA	2:C:64:LYS:HD2	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	11/25 (44%)	11 (100%)	0	0	100	100
1	N	15/25 (60%)	15 (100%)	0	0	100	100
1	S	10/25 (40%)	10 (100%)	0	0	100	100
2	A	218/221 (99%)	205 (94%)	13 (6%)	0	100	100
2	C	210/221 (95%)	200 (95%)	10 (5%)	0	100	100
2	H	209/221 (95%)	199 (95%)	10 (5%)	0	100	100
3	B	210/212 (99%)	202 (96%)	8 (4%)	0	100	100
3	D	210/212 (99%)	202 (96%)	8 (4%)	0	100	100
3	L	210/212 (99%)	202 (96%)	8 (4%)	0	100	100
All	All	1303/1374 (95%)	1246 (96%)	57 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	10/25 (40%)	10 (100%)	0	100	100
1	N	14/25 (56%)	14 (100%)	0	100	100
1	S	11/25 (44%)	11 (100%)	0	100	100
2	A	184/187 (98%)	184 (100%)	0	100	100
2	C	178/187 (95%)	178 (100%)	0	100	100
2	H	177/187 (95%)	177 (100%)	0	100	100
3	B	184/186 (99%)	184 (100%)	0	100	100
3	D	184/186 (99%)	184 (100%)	0	100	100
3	L	184/186 (99%)	184 (100%)	0	100	100
All	All	1126/1194 (94%)	1126 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	76	ASN
2	H	102	HIS
2	H	171	GLN
3	L	138	ASN
2	A	13	GLN
2	A	76	ASN
2	A	98	GLN
2	A	164	HIS
3	B	38	GLN
3	B	138	ASN
2	C	76	ASN
2	C	102	HIS
2	C	199	ASN
3	D	38	GLN
3	D	89	GLN
3	D	90	GLN
3	D	93	ASN

5.3.3 RNA ⓘ

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	FLC	B	301	-	12,12,12	0.12	0	17,17,17	0.20	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FLC	B	301	-	-	6/16/16/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	FLC	CA-CB-CBC-OB1
4	B	301	FLC	CA-CB-CBC-OB2
4	B	301	FLC	OHB-CB-CBC-OB1
4	B	301	FLC	OHB-CB-CBC-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	301	FLC	CB-CG-CGC-OG1
4	B	301	FLC	CB-CG-CGC-OG2

There are no ring outliers.

No monomer is involved in short contacts.

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	M	12/25 (48%)	0.27	0 100 100	60, 81, 97, 98	1 (8%)
1	N	16/25 (64%)	0.23	0 100 100	46, 62, 77, 85	1 (6%)
1	S	12/25 (48%)	0.63	1 (8%) 17 9	63, 77, 88, 92	0
2	A	220/221 (99%)	0.25	6 (2%) 56 33	22, 59, 98, 127	0
2	C	214/221 (96%)	0.55	8 (3%) 45 25	33, 66, 96, 115	0
2	H	213/221 (96%)	0.09	3 (1%) 73 51	21, 49, 79, 97	0
3	B	212/212 (100%)	0.11	1 (0%) 87 72	27, 49, 83, 120	0
3	D	212/212 (100%)	0.51	6 (2%) 55 32	35, 65, 111, 121	0
3	L	212/212 (100%)	0.06	0 100 100	25, 46, 88, 109	0
All	All	1323/1374 (96%)	0.26	25 (1%) 66 44	21, 56, 95, 127	2 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	138	LEU	4.6
2	A	31	THR	3.7
3	B	53	ASN	3.3
2	A	126	PRO	2.7
2	A	128	SER	2.6
2	H	42	GLY	2.6
2	H	31	THR	2.5
2	C	55	ASP	2.5
3	D	125	LEU	2.4
2	H	138	LEU	2.4
2	A	131	THR	2.4
2	C	211	VAL	2.4
2	A	101	ASP	2.4
1	S	1157	LYS	2.3
3	D	201	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	126	PRO	2.3
2	C	139	GLY	2.2
3	D	131	SER	2.2
3	D	175	LEU	2.1
2	C	112	SER	2.1
2	C	98	GLN	2.1
2	A	125	ALA	2.1
3	D	150	VAL	2.1
2	C	193	THR	2.1
3	D	56	THR	2.1

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FLC	B	301	13/13	0.74	0.15	68,78,96,104	0

6.5 Other polymers [i](#)

There are no such residues in this entry.