



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:58 PM UTC

PDB ID : 5X58 / pdb_00005x58
EMDB ID : EMD-6703
Title : Prefusion structure of SARS-CoV spike glycoprotein, conformation 1
Authors : Yuan, Y.; Cao, D.; Zhang, Y.; Ma, J.; Qi, J.; Wang, Q.; Lu, G.; Wu, Y.; Yan, J.; Shi, Y.; Zhang, X.; Gao, G.F.
Deposited on : 2017-02-15
Resolution : 3.20 Å (reported)
Based on initial models : 2AJF, 5X4S

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

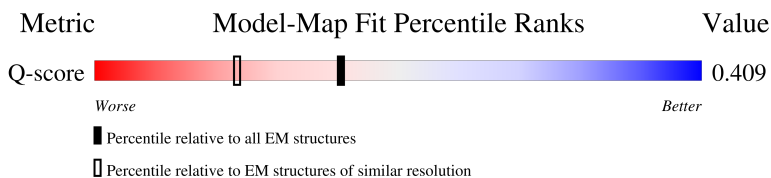
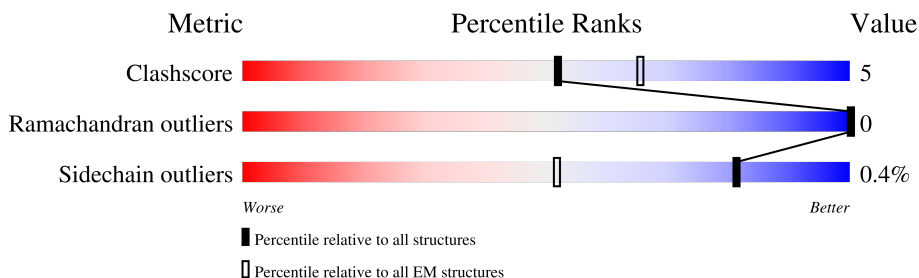
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1228	22% 72% 13% 14%
1	B	1228	22% 72% 14% 14%
1	C	1228	22% 72% 14% 14%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 25265 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1054	Total	C	N	O	S	0	0
			8234	5260	1363	1567	44		
1	B	1053	Total	C	N	O	S	0	0
			8226	5256	1362	1564	44		
1	C	1052	Total	C	N	O	S	0	0
			8217	5250	1360	1563	44		

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	

Continued on next page...

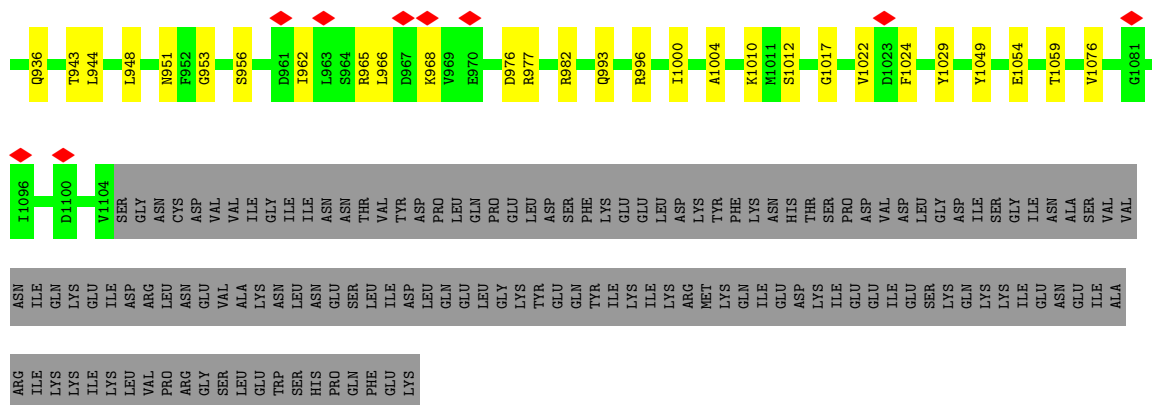
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	

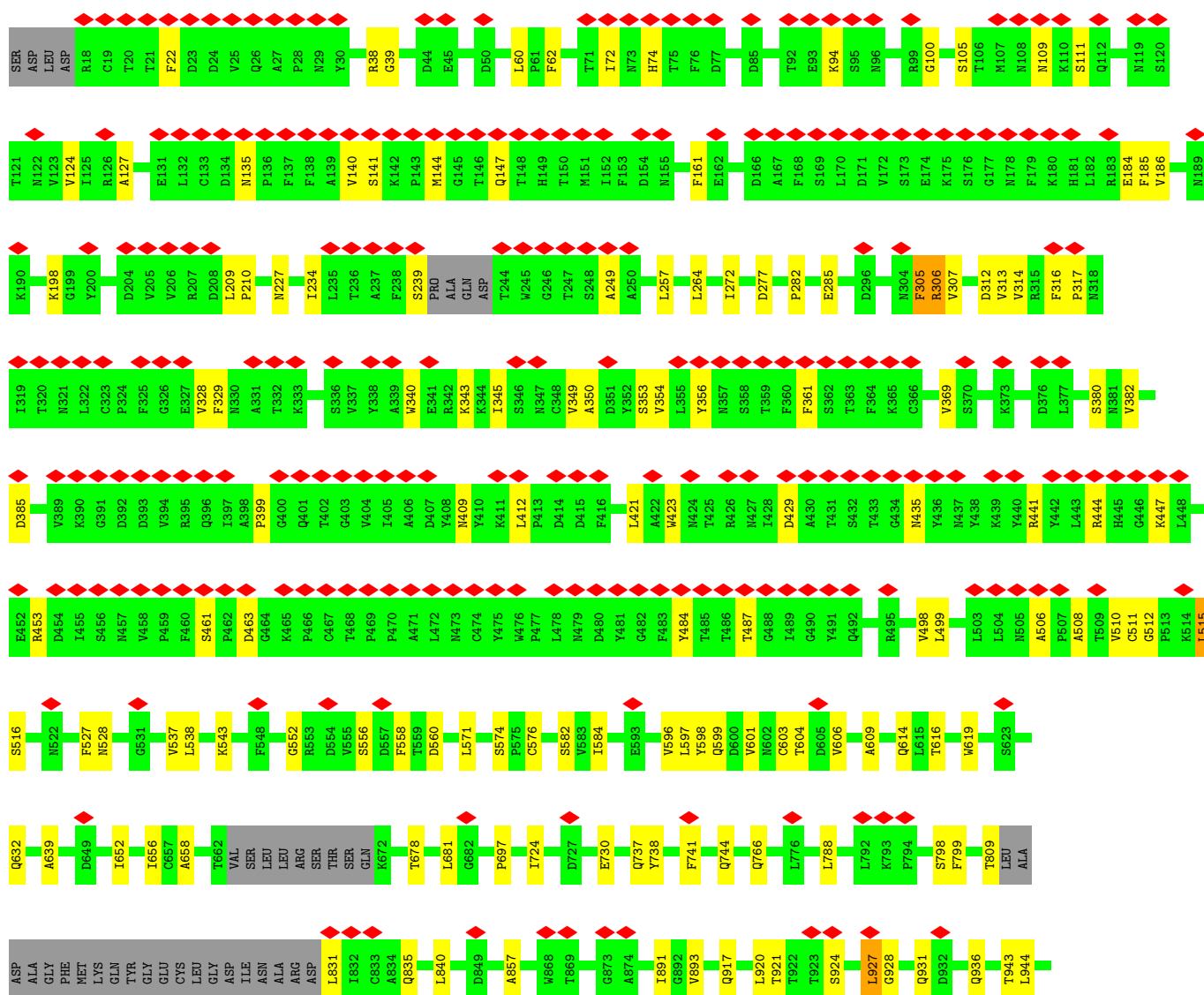
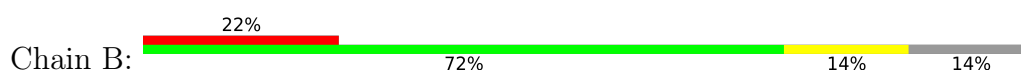
Continued on next page...

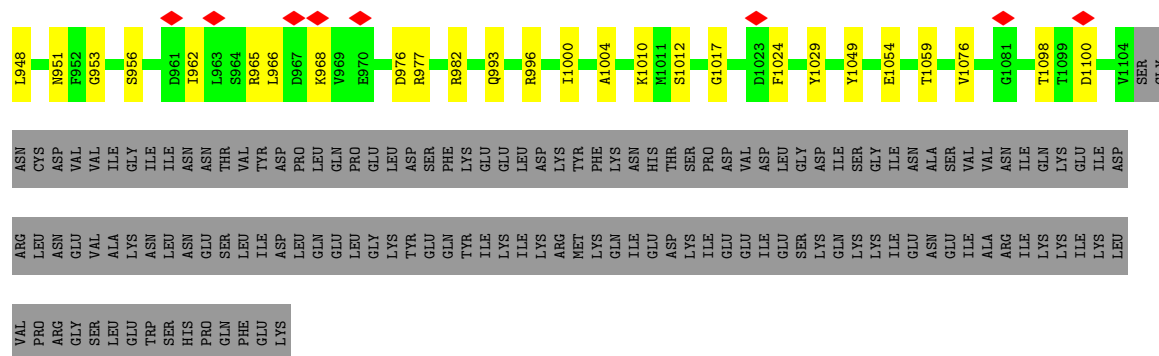
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	

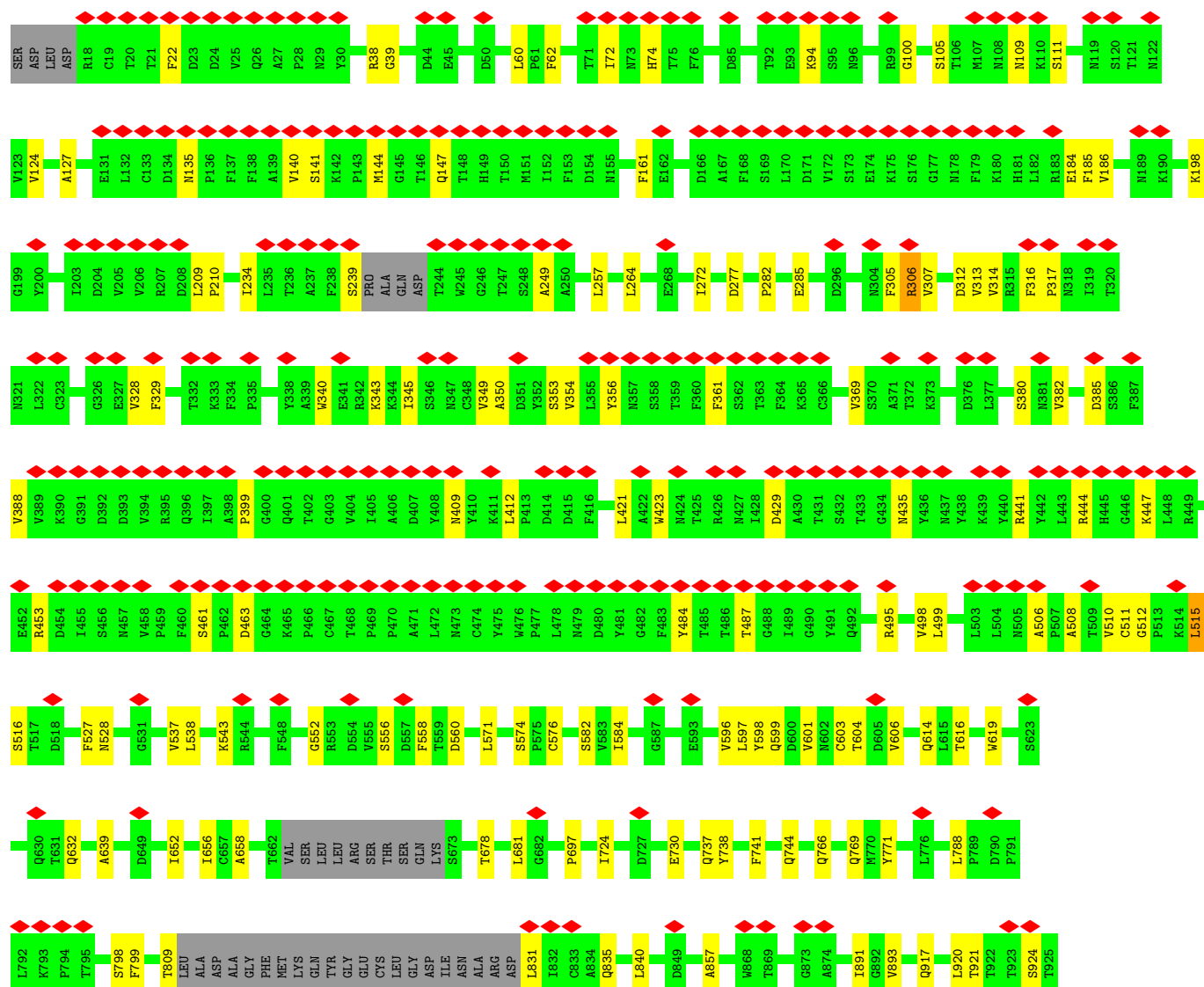


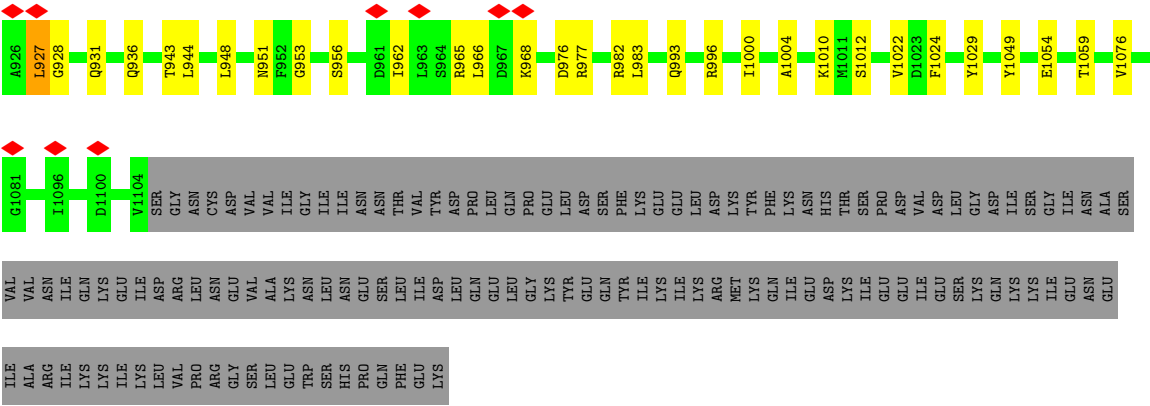
• Molecule 1: Spike glycoprotein





• Molecule 1: Spike glycoprotein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.309	Depositor
Minimum map value	-0.182	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.0456	Depositor
Map size (Å)	260.0, 260.0, 260.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.31	0/8432	0.70	8/11475 (0.1%)
1	B	0.31	0/8424	0.70	8/11464 (0.1%)
1	C	0.31	0/8415	0.70	8/11453 (0.1%)
All	All	0.31	0/25271	0.70	24/34392 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
1	C	0	4
All	All	0	12

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	ARG	N-CA-C	7.92	120.17	110.91
1	C	306	ARG	N-CA-C	7.88	120.13	110.91
1	B	306	ARG	N-CA-C	7.87	120.12	110.91
1	B	354	VAL	N-CA-C	-6.73	103.92	110.72
1	C	354	VAL	N-CA-C	-6.72	103.94	110.72
1	A	354	VAL	N-CA-C	-6.71	103.94	110.72
1	B	928	GLY	N-CA-C	5.85	119.72	112.64
1	C	928	GLY	N-CA-C	5.83	119.70	112.64
1	A	928	GLY	N-CA-C	5.83	119.69	112.64
1	A	556	SER	CA-C-N	5.40	127.78	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	556	SER	C-N-CA	5.40	127.78	120.38
1	B	556	SER	CA-C-N	5.38	127.75	120.38
1	B	556	SER	C-N-CA	5.38	127.75	120.38
1	C	556	SER	CA-C-N	5.37	127.74	120.38
1	C	556	SER	C-N-CA	5.37	127.74	120.38
1	C	927	LEU	CA-C-N	5.19	125.85	119.99
1	C	927	LEU	C-N-CA	5.19	125.85	119.99
1	A	927	LEU	CA-C-N	5.19	125.85	119.99
1	A	927	LEU	C-N-CA	5.19	125.85	119.99
1	A	515	LEU	CA-CB-CG	5.18	134.43	116.30
1	C	515	LEU	CA-CB-CG	5.18	134.42	116.30
1	B	515	LEU	CA-CB-CG	5.17	134.40	116.30
1	B	927	LEU	CA-C-N	5.12	125.78	119.99
1	B	927	LEU	C-N-CA	5.12	125.78	119.99

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	316	PHE	Peptide
1	A	512	GLY	Peptide
1	A	616	THR	Peptide
1	A	741	PHE	Peptide
1	B	316	PHE	Peptide
1	B	512	GLY	Peptide
1	B	616	THR	Peptide
1	B	741	PHE	Peptide
1	C	316	PHE	Peptide
1	C	512	GLY	Peptide
1	C	616	THR	Peptide
1	C	741	PHE	Peptide

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	8234	0	8002	95	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	8226	0	7997	97	0
1	C	8217	0	7984	95	0
2	A	196	0	180	3	0
2	B	196	0	180	3	0
2	C	196	0	180	3	0
All	All	25265	0	24523	267	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 5.

All (267) 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:A:953:GLY:HA3	1:A:977:ARG:HH11	1.61	0.66
1:C:953:GLY:HA3	1:C:977:ARG:HH11	1.61	0.66
1:B:891:ILE:HD12	1:B:1029:TYR:HB3	1.78	0.65
1:C:891:ILE:HD12	1:C:1029:TYR:HB3	1.78	0.65
1:A:891:ILE:HD12	1:A:1029:TYR:HB3	1.78	0.63
1:B:953:GLY:HA3	1:B:977:ARG:HH11	1.61	0.63
1:A:831:LEU:HB3	1:C:632:GLN:HE22	1.64	0.63
1:A:632:GLN:HE22	1:B:831:LEU:HB3	1.64	0.61
1:B:385:ASP:HB2	1:B:498:VAL:HB	1.83	0.60
1:B:632:GLN:HE22	1:C:831:LEU:HB3	1.64	0.60
1:C:385:ASP:HB2	1:C:498:VAL:HB	1.83	0.59
1:A:385:ASP:HB2	1:A:498:VAL:HB	1.83	0.59
1:B:38:ARG:NH1	1:B:184:GLU:OE2	2.36	0.59
1:A:349:VAL:HG13	1:A:511:CYS:HB3	1.85	0.59
1:A:38:ARG:NH1	1:A:184:GLU:OE2	2.36	0.59
1:C:317:PRO:HG2	1:C:511:CYS:HB2	1.85	0.58
1:B:349:VAL:HG13	1:B:511:CYS:HB3	1.85	0.58
1:C:38:ARG:NH1	1:C:184:GLU:OE2	2.36	0.58
1:A:317:PRO:HG2	1:A:511:CYS:HB2	1.85	0.58
1:C:349:VAL:HG13	1:C:511:CYS:HB3	1.85	0.58
1:B:317:PRO:HG2	1:B:511:CYS:HB2	1.85	0.57
1:C:62:PHE:HD2	1:C:277:ASP:HB2	1.69	0.57
1:B:62:PHE:HD2	1:B:277:ASP:HB2	1.69	0.57
1:A:62:PHE:HD2	1:A:277:ASP:HB2	1.69	0.56
1:C:421:LEU:HD13	1:C:499:LEU:HD13	1.88	0.56
1:C:599:GLN:HG3	1:C:606:VAL:HG11	1.87	0.56
1:C:380:SER:HA	1:C:508:ALA:HA	1.88	0.56
1:B:340:TRP:O	1:B:453:ARG:NH1	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:LEU:HD13	1:B:499:LEU:HD13	1.87	0.56
1:A:599:GLN:HG3	1:A:606:VAL:HG11	1.87	0.56
1:A:380:SER:HA	1:A:508:ALA:HA	1.88	0.55
1:A:409:ASN:HD21	1:A:441:ARG:HB2	1.71	0.55
1:B:599:GLN:HG3	1:B:606:VAL:HG11	1.87	0.55
1:C:314:VAL:HA	1:C:516:SER:HB2	1.88	0.55
1:A:340:TRP:O	1:A:453:ARG:NH1	2.39	0.55
1:B:380:SER:HA	1:B:508:ALA:HA	1.88	0.55
1:B:314:VAL:HA	1:B:516:SER:HB2	1.88	0.55
1:C:340:TRP:O	1:C:453:ARG:NH1	2.39	0.55
1:C:409:ASN:HD21	1:C:441:ARG:HB2	1.71	0.55
1:A:421:LEU:HD13	1:A:499:LEU:HD13	1.88	0.54
1:B:409:ASN:HD21	1:B:441:ARG:HB2	1.72	0.54
1:C:936:GLN:HG2	1:C:996:ARG:HE	1.72	0.54
1:A:282:PRO:HG2	1:A:597:LEU:HD11	1.89	0.54
1:A:314:VAL:HA	1:A:516:SER:HB2	1.88	0.54
1:A:285:GLU:HB2	1:A:619:TRP:HE1	1.73	0.54
1:B:766:GLN:NE2	1:B:1012:SER:OG	2.41	0.54
1:A:766:GLN:NE2	1:A:1012:SER:OG	2.41	0.53
1:B:282:PRO:HG2	1:B:597:LEU:HD11	1.89	0.53
1:A:936:GLN:HG2	1:A:996:ARG:HE	1.72	0.53
1:C:282:PRO:HG2	1:C:597:LEU:HD11	1.89	0.53
1:B:936:GLN:HG2	1:B:996:ARG:HE	1.72	0.53
1:C:766:GLN:NE2	1:C:1012:SER:OG	2.41	0.53
1:A:798:SER:OG	1:A:799:PHE:N	2.42	0.53
1:B:285:GLU:HB2	1:B:619:TRP:HE1	1.73	0.53
1:A:329:PHE:HZ	1:A:499:LEU:HD11	1.74	0.53
1:B:329:PHE:HZ	1:B:499:LEU:HD11	1.74	0.53
1:A:109:ASN:ND2	2:A:1314:NAG:O3	2.42	0.53
1:B:798:SER:OG	1:B:799:PHE:N	2.42	0.52
1:C:798:SER:OG	1:C:799:PHE:N	2.42	0.52
1:C:329:PHE:HZ	1:C:499:LEU:HD11	1.74	0.52
1:C:285:GLU:HB2	1:C:619:TRP:HE1	1.73	0.52
1:A:948:LEU:HD13	1:C:558:PHE:HE2	1.75	0.52
1:B:558:PHE:HE2	1:C:948:LEU:HD13	1.75	0.52
1:A:965:ARG:HB2	1:C:369:VAL:HA	1.93	0.51
1:B:109:ASN:ND2	2:B:1314:NAG:O3	2.43	0.51
1:A:558:PHE:HE2	1:B:948:LEU:HD13	1.75	0.51
1:C:127:ALA:HB3	1:C:161:PHE:HB3	1.93	0.51
1:C:353:SER:HA	1:C:356:TYR:HB3	1.92	0.51
1:A:369:VAL:HA	1:B:965:ARG:HB2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:VAL:HG13	1:A:257:LEU:HD11	1.93	0.51
1:B:353:SER:HA	1:B:356:TYR:HB3	1.92	0.51
1:B:543:LYS:NZ	1:B:560:ASP:OD2	2.44	0.51
1:C:543:LYS:NZ	1:C:560:ASP:OD2	2.44	0.51
1:A:538:LEU:HD12	1:A:571:LEU:HD13	1.93	0.51
1:A:543:LYS:NZ	1:A:560:ASP:OD2	2.44	0.50
1:C:186:VAL:HG13	1:C:257:LEU:HD11	1.93	0.50
1:A:39:GLY:HA3	1:A:60:LEU:HB3	1.93	0.50
1:A:185:PHE:HE1	1:A:198:LYS:HG3	1.75	0.50
1:A:353:SER:HA	1:A:356:TYR:HB3	1.92	0.50
1:C:39:GLY:HA3	1:C:60:LEU:HB3	1.93	0.50
1:B:127:ALA:HB3	1:B:161:PHE:HB3	1.93	0.50
1:B:185:PHE:HE1	1:B:198:LYS:HG3	1.75	0.50
1:A:312:ASP:O	1:A:528:ASN:N	2.41	0.50
1:B:186:VAL:HG13	1:B:257:LEU:HD11	1.93	0.50
1:C:1000:ILE:O	1:C:1004:ALA:N	2.45	0.50
1:B:312:ASP:O	1:B:528:ASN:N	2.41	0.50
1:A:127:ALA:HB3	1:A:161:PHE:HB3	1.93	0.50
1:B:39:GLY:HA3	1:B:60:LEU:HB3	1.93	0.50
1:C:185:PHE:HE1	1:C:198:LYS:HG3	1.75	0.50
1:B:1000:ILE:O	1:B:1004:ALA:N	2.45	0.49
1:B:369:VAL:HA	1:C:965:ARG:HB2	1.93	0.49
1:C:109:ASN:ND2	2:C:1314:NAG:O3	2.44	0.49
1:C:788:LEU:HD13	1:C:857:ALA:HB2	1.95	0.49
1:A:788:LEU:HD13	1:A:857:ALA:HB2	1.95	0.49
1:A:1010:LYS:NZ	1:A:1024:PHE:O	2.46	0.49
1:C:538:LEU:HD12	1:C:571:LEU:HD13	1.93	0.49
1:B:788:LEU:HD13	1:B:857:ALA:HB2	1.95	0.49
1:B:1010:LYS:NZ	1:B:1024:PHE:O	2.46	0.49
1:C:1010:LYS:NZ	1:C:1024:PHE:O	2.46	0.49
1:A:484:TYR:HB2	1:A:487:THR:HG23	1.95	0.49
1:B:100:GLY:HA3	1:B:234:ILE:HB	1.95	0.49
1:B:538:LEU:HD12	1:B:571:LEU:HD13	1.93	0.49
1:A:603:CYS:SG	1:A:604:THR:N	2.85	0.48
1:B:484:TYR:HB2	1:B:487:THR:HG23	1.95	0.48
1:C:603:CYS:SG	1:C:604:THR:N	2.85	0.48
1:A:100:GLY:HA3	1:A:234:ILE:HB	1.95	0.48
1:B:603:CYS:SG	1:B:604:THR:N	2.85	0.48
1:C:840:LEU:HD11	1:C:944:LEU:HD23	1.96	0.48
1:C:312:ASP:O	1:C:528:ASN:N	2.41	0.48
1:C:724:ILE:O	1:C:982:ARG:NH1	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:GLY:HA3	1:C:234:ILE:HB	1.95	0.48
1:B:140:VAL:HG22	1:B:147:GLN:HA	1.96	0.48
1:C:345:ILE:HD13	1:C:382:VAL:HG23	1.96	0.48
1:B:313:VAL:HA	1:B:528:ASN:HB3	1.96	0.48
1:C:313:VAL:HA	1:C:528:ASN:HB3	1.96	0.48
1:C:484:TYR:HB2	1:C:487:THR:HG23	1.95	0.48
1:A:313:VAL:HA	1:A:528:ASN:HB3	1.96	0.48
1:C:527:PHE:HB3	1:C:538:LEU:HD21	1.95	0.48
1:B:345:ILE:HD13	1:B:382:VAL:HG23	1.96	0.47
1:B:891:ILE:HB	1:B:893:VAL:HG12	1.96	0.47
1:C:140:VAL:HG22	1:C:147:GLN:HA	1.96	0.47
1:A:328:VAL:HG22	1:A:343:LYS:HD3	1.96	0.47
1:A:94:LYS:NZ	1:A:249:ALA:O	2.48	0.47
1:A:361:PHE:HA	1:A:423:TRP:HB3	1.96	0.47
1:B:527:PHE:HB3	1:B:538:LEU:HD21	1.95	0.47
1:C:105:SER:HB2	1:C:111:SER:HB2	1.97	0.47
1:C:328:VAL:HG22	1:C:343:LYS:HD3	1.96	0.47
1:A:527:PHE:HB3	1:A:538:LEU:HD21	1.95	0.47
1:B:141:SER:HB3	1:B:144:MET:HB2	1.95	0.47
1:A:724:ILE:O	1:A:982:ARG:NH1	2.45	0.47
1:A:1000:ILE:O	1:A:1004:ALA:N	2.45	0.47
1:A:141:SER:HB3	1:A:144:MET:HB2	1.96	0.47
1:B:105:SER:HB2	1:B:111:SER:HB2	1.97	0.47
1:B:840:LEU:HD11	1:B:944:LEU:HD23	1.96	0.47
1:B:1059:THR:OG1	1:B:1076:VAL:O	2.32	0.47
1:C:141:SER:HB3	1:C:144:MET:HB2	1.95	0.47
1:A:140:VAL:HG22	1:A:147:GLN:HA	1.96	0.47
1:B:94:LYS:NZ	1:B:249:ALA:O	2.48	0.47
1:A:380:SER:HB3	1:A:506:ALA:HB3	1.97	0.47
1:A:738:TYR:OH	1:A:976:ASP:OD1	2.31	0.47
1:B:361:PHE:HA	1:B:423:TRP:HB3	1.96	0.47
1:C:965:ARG:HG3	1:C:966:LEU:HD12	1.97	0.47
1:A:105:SER:HB2	1:A:111:SER:HB2	1.97	0.47
1:A:744:GLN:HG3	1:C:943:THR:HG21	1.97	0.47
1:A:965:ARG:HG3	1:A:966:LEU:HD12	1.97	0.47
1:C:584:ILE:HB	1:C:596:VAL:HG22	1.97	0.47
1:A:345:ILE:HD13	1:A:382:VAL:HG23	1.96	0.46
1:A:840:LEU:HD11	1:A:944:LEU:HD23	1.96	0.46
1:B:724:ILE:O	1:B:982:ARG:NH1	2.45	0.46
1:B:965:ARG:HG3	1:B:966:LEU:HD12	1.97	0.46
1:C:94:LYS:NZ	1:C:249:ALA:O	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:ARG:HB3	1:C:576:CYS:HB3	1.97	0.46
1:C:1059:THR:OG1	1:C:1076:VAL:O	2.32	0.46
1:A:943:THR:HG21	1:B:744:GLN:HG3	1.97	0.46
1:A:1059:THR:OG1	1:A:1076:VAL:O	2.32	0.46
1:B:461:SER:OG	1:B:463:ASP:OD1	2.32	0.46
1:A:891:ILE:HB	1:A:893:VAL:HG12	1.96	0.46
1:B:328:VAL:HG22	1:B:343:LYS:HD3	1.96	0.46
1:C:891:ILE:HB	1:C:893:VAL:HG12	1.96	0.46
1:C:917:GLN:O	1:C:921:THR:OG1	2.34	0.46
1:A:993:GLN:OE1	1:A:996:ARG:NH1	2.49	0.46
1:C:361:PHE:HA	1:C:423:TRP:HB3	1.96	0.45
1:A:306:ARG:HB3	1:A:576:CYS:HB3	1.97	0.45
1:A:596:VAL:HG21	1:A:639:ALA:HB2	1.98	0.45
1:B:306:ARG:HB3	1:B:576:CYS:HB3	1.97	0.45
1:B:444:ARG:NH2	2:C:1310:NAG:O7	2.45	0.45
1:C:380:SER:HB3	1:C:506:ALA:HB3	1.97	0.45
1:B:584:ILE:HB	1:B:596:VAL:HG22	1.97	0.45
1:B:917:GLN:O	1:B:921:THR:OG1	2.34	0.45
1:C:993:GLN:OE1	1:C:996:ARG:NH1	2.49	0.45
1:A:584:ILE:HB	1:A:596:VAL:HG22	1.97	0.45
1:B:596:VAL:HG21	1:B:639:ALA:HB2	1.98	0.45
1:B:943:THR:HG21	1:C:744:GLN:HG3	1.97	0.45
1:B:993:GLN:OE1	1:B:996:ARG:NH1	2.49	0.45
1:B:380:SER:HB3	1:B:506:ALA:HB3	1.97	0.45
1:C:596:VAL:HG21	1:C:639:ALA:HB2	1.98	0.44
1:C:738:TYR:OH	1:C:976:ASP:OD1	2.31	0.44
1:B:582:SER:O	1:B:598:TYR:N	2.50	0.44
1:B:956:SER:H	1:B:962:ILE:HD11	1.83	0.44
1:B:738:TYR:OH	1:B:976:ASP:OD1	2.31	0.44
1:A:582:SER:O	1:A:598:TYR:N	2.51	0.44
1:A:956:SER:H	1:A:962:ILE:HD11	1.83	0.44
1:B:124:VAL:HG21	2:B:1312:NAG:H82	2.00	0.44
1:C:399:PRO:HD3	1:C:412:LEU:HD23	2.00	0.44
1:A:737:GLN:HB2	1:C:951:ASN:HB3	2.00	0.44
1:A:917:GLN:O	1:A:921:THR:OG1	2.33	0.44
1:C:956:SER:H	1:C:962:ILE:HD11	1.83	0.44
1:A:264:LEU:HD22	1:A:272:ILE:HD13	2.00	0.44
1:B:399:PRO:HD3	1:B:412:LEU:HD23	2.00	0.44
1:C:582:SER:O	1:C:598:TYR:N	2.50	0.44
1:B:951:ASN:HB3	1:C:737:GLN:HB2	2.00	0.43
1:C:1029:TYR:HB2	1:C:1049:TYR:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:VAL:HG21	2:A:1312:NAG:H82	1.99	0.43
1:A:601:VAL:HG22	1:B:835:GLN:HE22	1.82	0.43
1:A:835:GLN:HE22	1:C:601:VAL:HG22	1.82	0.43
1:B:264:LEU:HD22	1:B:272:ILE:HD13	2.00	0.43
1:B:601:VAL:HG22	1:C:835:GLN:HE22	1.82	0.43
1:B:656:ILE:HA	1:B:678:THR:HA	2.01	0.43
1:A:444:ARG:NH2	2:B:1310:NAG:O7	2.45	0.43
1:A:951:ASN:HB3	1:B:737:GLN:HB2	2.00	0.43
1:B:652:ILE:HD11	1:B:658:ALA:HB2	2.01	0.43
1:C:769:GLN:NE2	1:C:771:TYR:OH	2.48	0.43
1:A:399:PRO:HD3	1:A:412:LEU:HD23	2.00	0.43
1:A:730:GLU:HG3	1:A:968:LYS:HD3	2.01	0.43
1:B:1029:TYR:HB2	1:B:1049:TYR:HB3	2.01	0.43
1:C:264:LEU:HD22	1:C:272:ILE:HD13	2.00	0.43
1:A:1029:TYR:HB2	1:A:1049:TYR:HB3	2.00	0.43
2:A:1310:NAG:O7	1:C:444:ARG:NH2	2.45	0.43
1:C:652:ILE:HD11	1:C:658:ALA:HB2	2.01	0.43
1:A:209:LEU:HD12	1:A:210:PRO:HD2	2.01	0.43
1:B:305:PHE:HD1	1:B:305:PHE:HA	1.76	0.43
1:A:552:GLY:O	1:A:560:ASP:N	2.50	0.42
1:C:124:VAL:HG21	2:C:1312:NAG:H82	2.00	0.42
1:A:652:ILE:HD11	1:A:658:ALA:HB2	2.01	0.42
1:C:656:ILE:HA	1:C:678:THR:HA	2.01	0.42
1:B:22:PHE:H	1:B:135:ASN:HD22	1.68	0.42
1:B:209:LEU:HD12	1:B:210:PRO:HD2	2.01	0.42
1:B:1098:THR:OG1	1:B:1100:ASP:OD1	2.34	0.42
1:C:350:ALA:HB3	1:C:510:VAL:HG13	2.02	0.42
1:A:22:PHE:H	1:A:135:ASN:HD22	1.67	0.42
1:B:537:VAL:N	1:B:574:SER:O	2.44	0.42
1:A:444:ARG:NH1	1:A:447:LYS:O	2.53	0.42
1:B:730:GLU:HG3	1:B:968:LYS:HD3	2.01	0.42
1:A:656:ILE:HA	1:A:678:THR:HA	2.01	0.42
1:B:444:ARG:NH1	1:B:447:LYS:O	2.53	0.42
1:C:209:LEU:HD12	1:C:210:PRO:HD2	2.01	0.42
1:C:444:ARG:NH1	1:C:447:LYS:O	2.53	0.42
1:C:552:GLY:O	1:C:560:ASP:N	2.50	0.42
1:C:730:GLU:HG3	1:C:968:LYS:HD3	2.01	0.42
1:A:140:VAL:O	1:A:239:SER:N	2.53	0.42
1:A:307:VAL:N	1:A:614:GLN:O	2.53	0.42
1:C:22:PHE:H	1:C:135:ASN:HD22	1.68	0.42
1:A:350:ALA:HB3	1:A:510:VAL:HG13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:924:SER:HB2	1:A:927:LEU:HG	2.02	0.41
1:B:72:ILE:HG23	1:B:74:HIS:H	1.85	0.41
1:C:307:VAL:N	1:C:614:GLN:O	2.53	0.41
1:B:140:VAL:O	1:B:239:SER:N	2.53	0.41
1:C:72:ILE:HG23	1:C:74:HIS:H	1.86	0.41
1:A:1022:VAL:HG21	1:B:1017:GLY:HA3	2.02	0.41
1:B:924:SER:HB2	1:B:927:LEU:HG	2.02	0.41
1:C:697:PRO:HA	1:C:1054:GLU:HA	2.03	0.41
1:C:924:SER:HB2	1:C:927:LEU:HG	2.03	0.41
1:A:697:PRO:HA	1:A:1054:GLU:HA	2.03	0.41
1:B:609:ALA:HB1	1:B:614:GLN:HB2	2.03	0.41
1:C:461:SER:OG	1:C:463:ASP:OD1	2.32	0.41
1:A:72:ILE:HG23	1:A:74:HIS:H	1.86	0.41
1:A:429:ASP:O	1:A:435:ASN:ND2	2.54	0.41
1:B:552:GLY:O	1:B:560:ASP:N	2.50	0.41
1:B:697:PRO:HA	1:B:1054:GLU:HA	2.03	0.41
1:A:609:ALA:HB1	1:A:614:GLN:HB2	2.03	0.41
1:B:307:VAL:N	1:B:614:GLN:O	2.53	0.41
1:B:429:ASP:O	1:B:435:ASN:ND2	2.54	0.41
1:C:429:ASP:O	1:C:435:ASN:ND2	2.54	0.41
1:A:809:THR:H	1:A:931:GLN:HE22	1.69	0.40
1:C:809:THR:H	1:C:931:GLN:HE22	1.69	0.40
1:C:983:LEU:HD13	1:C:983:LEU:HA	1.95	0.40
1:A:582:SER:H	1:A:598:TYR:HB2	1.86	0.40
1:B:809:THR:H	1:B:931:GLN:HE22	1.69	0.40
1:C:388:VAL:HG22	1:C:495:ARG:HG2	2.03	0.40
1:A:91:ALA:HA	1:A:252:TYR:HA	2.03	0.40
1:A:388:VAL:HG22	1:A:495:ARG:HG2	2.03	0.40
1:B:350:ALA:HB3	1:B:510:VAL:HG13	2.02	0.40
1:C:140:VAL:O	1:C:239:SER:N	2.53	0.40
1:C:537:VAL:N	1:C:574:SER:O	2.44	0.40
1:A:1017:GLY:HA3	1:C:1022:VAL:HG21	2.02	0.40
1:B:105:SER:OG	1:B:227:ASN:O	2.34	0.40
1:B:582:SER:H	1:B:598:TYR:HB2	1.86	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 PDB entries followed by that with respect to all EM entries.

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	1046/1228 (85%)	950 (91%)	96 (9%)	0	100	100
1	B	1045/1228 (85%)	950 (91%)	95 (9%)	0	100	100
1	C	1044/1228 (85%)	948 (91%)	96 (9%)	0	100	100
All	All	3135/3684 (85%)	2848 (91%)	287 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	914/1073 (85%)	910 (100%)	4 (0%)	84	86
1	B	913/1073 (85%)	909 (100%)	4 (0%)	84	86
1	C	912/1073 (85%)	908 (100%)	4 (0%)	84	86
All	All	2739/3219 (85%)	2727 (100%)	12 (0%)	81	86

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305	PHE
1	A	515	LEU
1	A	681	LEU
1	A	920	LEU
1	B	305	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	515	LEU
1	B	681	LEU
1	B	920	LEU
1	C	305	PHE
1	C	515	LEU
1	C	681	LEU
1	C	920	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	135	ASN
1	A	149	HIS
1	A	409	ASN
1	A	505	ASN
1	A	522	ASN
1	A	526	ASN
1	A	528	ASN
1	A	549	GLN
1	A	599	GLN
1	A	614	GLN
1	A	632	GLN
1	A	641	HIS
1	A	661	HIS
1	A	721	ASN
1	A	733	ASN
1	A	744	GLN
1	A	766	GLN
1	A	806	ASN
1	A	835	GLN
1	A	904	GLN
1	A	917	GLN
1	A	931	GLN
1	A	937	ASN
1	A	987	GLN
1	A	1090	ASN
1	B	70	HIS
1	B	135	ASN
1	B	149	HIS
1	B	201	GLN
1	B	409	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	457	ASN
1	B	505	ASN
1	B	522	ASN
1	B	526	ASN
1	B	528	ASN
1	B	549	GLN
1	B	611	HIS
1	B	614	GLN
1	B	632	GLN
1	B	641	HIS
1	B	661	HIS
1	B	721	ASN
1	B	733	ASN
1	B	744	GLN
1	B	766	GLN
1	B	806	ASN
1	B	835	GLN
1	B	904	GLN
1	B	917	GLN
1	B	931	GLN
1	B	937	ASN
1	B	987	GLN
1	B	1090	ASN
1	C	70	HIS
1	C	135	ASN
1	C	149	HIS
1	C	201	GLN
1	C	409	ASN
1	C	505	ASN
1	C	522	ASN
1	C	528	ASN
1	C	549	GLN
1	C	599	GLN
1	C	614	GLN
1	C	632	GLN
1	C	641	HIS
1	C	661	HIS
1	C	721	ASN
1	C	733	ASN
1	C	766	GLN
1	C	806	ASN
1	C	835	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	904	GLN
1	C	917	GLN
1	C	931	GLN
1	C	937	ASN
1	C	1090	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 ⓘ

42 ligands are 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	$\# Z > 2$
2	NAG	A	1308	1	14,14,15	0.50	0	17,19,21	0.65	1 (5%)
2	NAG	B	1304	1	14,14,15	1.50	2 (14%)	17,19,21	1.87	2 (11%)
2	NAG	B	1314	-	14,14,15	0.40	0	17,19,21	0.42	0
2	NAG	C	1311	1	14,14,15	0.37	0	17,19,21	0.63	0
2	NAG	B	1308	1	14,14,15	0.48	0	17,19,21	0.66	1 (5%)
2	NAG	C	1310	1	14,14,15	0.34	0	17,19,21	0.53	0
2	NAG	A	1310	1	14,14,15	0.34	0	17,19,21	0.54	0
2	NAG	C	1314	-	14,14,15	0.39	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1313	1	14,14,15	0.42	0	17,19,21	0.57	0
2	NAG	B	1303	1	14,14,15	0.37	0	17,19,21	1.01	1 (5%)
2	NAG	B	1301	1	14,14,15	0.89	1 (7%)	17,19,21	1.23	2 (11%)
2	NAG	C	1305	1	14,14,15	0.37	0	17,19,21	1.07	1 (5%)
2	NAG	C	1307	1	14,14,15	0.45	0	17,19,21	0.66	0
2	NAG	B	1302	1	14,14,15	0.82	2 (14%)	17,19,21	1.09	2 (11%)
2	NAG	A	1307	1	14,14,15	0.46	0	17,19,21	0.67	0
2	NAG	A	1304	1	14,14,15	1.50	2 (14%)	17,19,21	1.87	2 (11%)
2	NAG	A	1314	-	14,14,15	0.41	0	17,19,21	0.40	0
2	NAG	B	1306	1	14,14,15	0.46	0	17,19,21	0.39	0
2	NAG	C	1304	1	14,14,15	1.50	2 (14%)	17,19,21	1.88	3 (17%)
2	NAG	B	1309	1	14,14,15	0.39	0	17,19,21	0.38	0
2	NAG	B	1311	1	14,14,15	0.38	0	17,19,21	0.64	0
2	NAG	A	1305	1	14,14,15	0.43	0	17,19,21	1.07	1 (5%)
2	NAG	A	1309	1	14,14,15	0.38	0	17,19,21	0.38	0
2	NAG	C	1309	1	14,14,15	0.38	0	17,19,21	0.37	0
2	NAG	B	1305	1	14,14,15	0.36	0	17,19,21	1.06	1 (5%)
2	NAG	A	1313	1	14,14,15	0.43	0	17,19,21	0.57	0
2	NAG	A	1302	1	14,14,15	0.77	0	17,19,21	1.10	2 (11%)
2	NAG	C	1313	1	14,14,15	0.43	0	17,19,21	0.57	0
2	NAG	C	1308	1	14,14,15	0.49	0	17,19,21	0.64	1 (5%)
2	NAG	C	1301	1	14,14,15	0.93	1 (7%)	17,19,21	1.30	2 (11%)
2	NAG	A	1312	1	14,14,15	0.68	1 (7%)	17,19,21	0.63	0
2	NAG	A	1303	1	14,14,15	0.37	0	17,19,21	1.01	1 (5%)
2	NAG	B	1312	1	14,14,15	0.67	1 (7%)	17,19,21	0.62	0
2	NAG	A	1301	-	14,14,15	0.57	0	17,19,21	1.03	1 (5%)
2	NAG	C	1303	1	14,14,15	0.35	0	17,19,21	1.01	1 (5%)
2	NAG	C	1302	1	14,14,15	0.77	0	17,19,21	1.09	2 (11%)
2	NAG	A	1311	1	14,14,15	0.40	0	17,19,21	0.62	0
2	NAG	B	1307	1	14,14,15	0.46	0	17,19,21	0.67	0
2	NAG	A	1306	1	14,14,15	0.47	0	17,19,21	0.40	0
2	NAG	C	1306	1	14,14,15	0.45	0	17,19,21	0.39	0
2	NAG	C	1312	1	14,14,15	0.69	1 (7%)	17,19,21	0.63	0
2	NAG	B	1310	1	14,14,15	0.34	0	17,19,21	0.54	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
2	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1314	-	-	0/6/23/26	0/1/1/1
2	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1314	-	-	0/6/23/26	0/1/1/1
2	NAG	B	1313	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1301	1	-	3/6/23/26	0/1/1/1
2	NAG	C	1305	1	-	4/6/23/26	0/1/1/1
2	NAG	C	1307	1	-	4/6/23/26	0/1/1/1
2	NAG	B	1302	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1307	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1314	-	-	0/6/23/26	0/1/1/1
2	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1309	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1311	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1305	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1309	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1305	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1313	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
2	NAG	C	1313	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1301	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1312	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1312	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1301	-	-	4/6/23/26	0/1/1/1
2	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1302	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1311	1	-	3/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1307	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1312	1	-	4/6/23/26	0/1/1/1
2	NAG	B	1310	1	-	2/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1304	NAG	C1-C2	3.99	1.57	1.52
2	B	1304	NAG	C1-C2	3.97	1.57	1.52
2	C	1304	NAG	C1-C2	3.91	1.57	1.52
2	C	1304	NAG	O5-C1	3.76	1.50	1.43
2	B	1304	NAG	O5-C1	3.69	1.49	1.43
2	A	1304	NAG	O5-C1	3.68	1.49	1.43
2	C	1301	NAG	C1-C2	3.01	1.56	1.52
2	B	1301	NAG	C1-C2	2.84	1.56	1.52
2	A	1312	NAG	C1-C2	2.17	1.55	1.52
2	B	1302	NAG	C1-C2	2.15	1.55	1.52
2	C	1312	NAG	C1-C2	2.09	1.55	1.52
2	B	1312	NAG	C1-C2	2.04	1.55	1.52
2	B	1302	NAG	O5-C1	2.01	1.47	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1304	NAG	C1-O5-C5	6.74	121.21	112.19
2	B	1304	NAG	C1-O5-C5	6.71	121.18	112.19
2	A	1304	NAG	C1-O5-C5	6.69	121.16	112.19
2	C	1301	NAG	C1-O5-C5	3.84	117.34	112.19
2	B	1301	NAG	C1-O5-C5	3.55	116.95	112.19
2	A	1305	NAG	C2-N2-C7	3.40	127.45	122.90
2	B	1305	NAG	C2-N2-C7	3.36	127.40	122.90
2	C	1305	NAG	C2-N2-C7	3.36	127.40	122.90
2	A	1302	NAG	C2-N2-C7	3.32	127.35	122.90
2	C	1302	NAG	C2-N2-C7	3.29	127.31	122.90
2	B	1302	NAG	C2-N2-C7	3.29	127.31	122.90
2	A	1301	NAG	C2-N2-C7	3.26	127.27	122.90
2	A	1303	NAG	C2-N2-C7	3.20	127.19	122.90
2	B	1303	NAG	C2-N2-C7	3.15	127.13	122.90
2	C	1303	NAG	C2-N2-C7	3.15	127.13	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1304	NAG	C4-C3-C2	2.75	115.05	111.02
2	B	1304	NAG	C4-C3-C2	2.75	115.04	111.02
2	C	1304	NAG	C4-C3-C2	2.71	114.99	111.02
2	C	1301	NAG	C2-N2-C7	2.35	126.05	122.90
2	B	1301	NAG	C2-N2-C7	2.32	126.01	122.90
2	B	1308	NAG	C1-O5-C5	2.25	115.20	112.19
2	A	1308	NAG	C1-O5-C5	2.21	115.15	112.19
2	C	1308	NAG	C1-O5-C5	2.15	115.07	112.19
2	C	1302	NAG	C1-O5-C5	2.14	115.05	112.19
2	A	1302	NAG	C1-O5-C5	2.14	115.05	112.19
2	B	1302	NAG	C1-O5-C5	2.13	115.03	112.19
2	C	1304	NAG	C3-C4-C5	2.02	113.89	110.23

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1301	NAG	C4-C5-C6-O6
2	C	1301	NAG	C4-C5-C6-O6
2	A	1310	NAG	O5-C5-C6-O6
2	B	1302	NAG	O5-C5-C6-O6
2	C	1310	NAG	O5-C5-C6-O6
2	A	1305	NAG	O5-C5-C6-O6
2	B	1310	NAG	O5-C5-C6-O6
2	C	1310	NAG	C4-C5-C6-O6
2	A	1302	NAG	O5-C5-C6-O6
2	B	1301	NAG	O5-C5-C6-O6
2	C	1302	NAG	O5-C5-C6-O6
2	A	1310	NAG	C4-C5-C6-O6
2	A	1306	NAG	O5-C5-C6-O6
2	C	1306	NAG	O5-C5-C6-O6
2	B	1310	NAG	C4-C5-C6-O6
2	A	1312	NAG	O5-C5-C6-O6
2	C	1301	NAG	O5-C5-C6-O6
2	B	1312	NAG	O5-C5-C6-O6
2	C	1312	NAG	O5-C5-C6-O6
2	B	1306	NAG	O5-C5-C6-O6
2	A	1305	NAG	C4-C5-C6-O6
2	A	1307	NAG	C8-C7-N2-C2
2	A	1307	NAG	O7-C7-N2-C2
2	A	1311	NAG	C8-C7-N2-C2
2	A	1311	NAG	O7-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1312	NAG	C8-C7-N2-C2
2	A	1312	NAG	O7-C7-N2-C2
2	A	1313	NAG	C8-C7-N2-C2
2	A	1313	NAG	O7-C7-N2-C2
2	B	1307	NAG	C8-C7-N2-C2
2	B	1307	NAG	O7-C7-N2-C2
2	B	1311	NAG	C8-C7-N2-C2
2	B	1311	NAG	O7-C7-N2-C2
2	B	1312	NAG	C8-C7-N2-C2
2	B	1312	NAG	O7-C7-N2-C2
2	B	1313	NAG	C8-C7-N2-C2
2	B	1313	NAG	O7-C7-N2-C2
2	C	1307	NAG	C8-C7-N2-C2
2	C	1307	NAG	O7-C7-N2-C2
2	C	1311	NAG	C8-C7-N2-C2
2	C	1311	NAG	O7-C7-N2-C2
2	C	1312	NAG	C8-C7-N2-C2
2	C	1312	NAG	O7-C7-N2-C2
2	C	1313	NAG	C8-C7-N2-C2
2	C	1313	NAG	O7-C7-N2-C2
2	A	1312	NAG	C4-C5-C6-O6
2	A	1301	NAG	C4-C5-C6-O6
2	B	1312	NAG	C4-C5-C6-O6
2	C	1312	NAG	C4-C5-C6-O6
2	B	1302	NAG	C4-C5-C6-O6
2	B	1305	NAG	O5-C5-C6-O6
2	A	1302	NAG	C4-C5-C6-O6
2	C	1308	NAG	O5-C5-C6-O6
2	C	1302	NAG	C4-C5-C6-O6
2	C	1305	NAG	O5-C5-C6-O6
2	A	1308	NAG	O5-C5-C6-O6
2	A	1306	NAG	C4-C5-C6-O6
2	C	1306	NAG	C4-C5-C6-O6
2	B	1308	NAG	O5-C5-C6-O6
2	A	1301	NAG	O5-C5-C6-O6
2	B	1306	NAG	C4-C5-C6-O6
2	A	1307	NAG	C4-C5-C6-O6
2	C	1307	NAG	C4-C5-C6-O6
2	B	1307	NAG	C4-C5-C6-O6
2	B	1305	NAG	C4-C5-C6-O6
2	A	1303	NAG	C1-C2-N2-C7
2	A	1305	NAG	C1-C2-N2-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	1303	NAG	C1-C2-N2-C7
2	B	1305	NAG	C1-C2-N2-C7
2	C	1303	NAG	C1-C2-N2-C7
2	C	1305	NAG	C1-C2-N2-C7
2	C	1308	NAG	C4-C5-C6-O6
2	A	1307	NAG	O5-C5-C6-O6
2	A	1311	NAG	O5-C5-C6-O6
2	C	1307	NAG	O5-C5-C6-O6
2	B	1307	NAG	O5-C5-C6-O6
2	C	1305	NAG	C4-C5-C6-O6
2	A	1308	NAG	C4-C5-C6-O6
2	C	1301	NAG	C3-C2-N2-C7
2	A	1313	NAG	O5-C5-C6-O6
2	A	1302	NAG	C1-C2-N2-C7
2	A	1309	NAG	C1-C2-N2-C7
2	A	1301	NAG	C1-C2-N2-C7
2	B	1302	NAG	C1-C2-N2-C7
2	B	1309	NAG	C1-C2-N2-C7
2	C	1302	NAG	C1-C2-N2-C7
2	C	1309	NAG	C1-C2-N2-C7
2	B	1311	NAG	O5-C5-C6-O6
2	A	1302	NAG	C3-C2-N2-C7
2	A	1303	NAG	C3-C2-N2-C7
2	A	1305	NAG	C3-C2-N2-C7
2	A	1301	NAG	C3-C2-N2-C7
2	B	1301	NAG	C3-C2-N2-C7
2	B	1302	NAG	C3-C2-N2-C7
2	B	1303	NAG	C3-C2-N2-C7
2	B	1305	NAG	C3-C2-N2-C7
2	C	1302	NAG	C3-C2-N2-C7
2	C	1303	NAG	C3-C2-N2-C7
2	C	1305	NAG	C3-C2-N2-C7
2	B	1308	NAG	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1314	NAG	1	0
2	C	1310	NAG	1	0
2	A	1310	NAG	1	0
2	C	1314	NAG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1314	NAG	1	0
2	A	1312	NAG	1	0
2	B	1312	NAG	1	0
2	C	1312	NAG	1	0
2	B	1310	NAG	1	0

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.

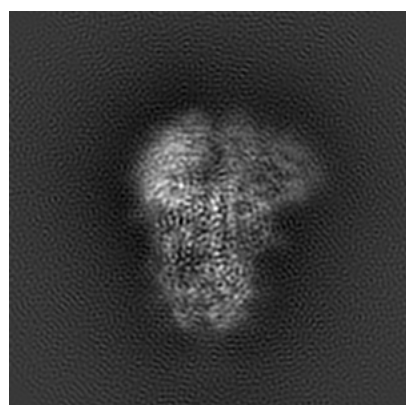
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6703. These allow visual inspection of the internal detail of the map and identification of artifacts.

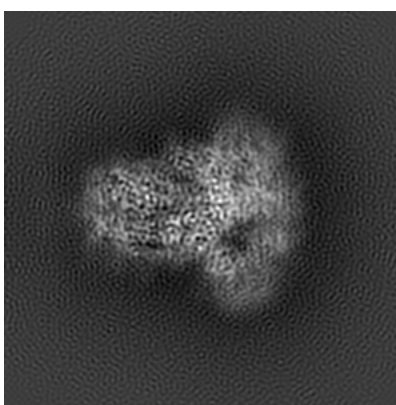
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

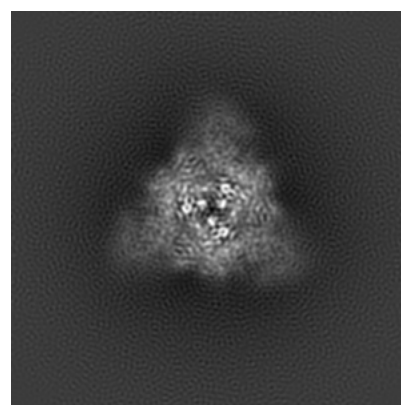
6.1.1 Primary map



X



Y

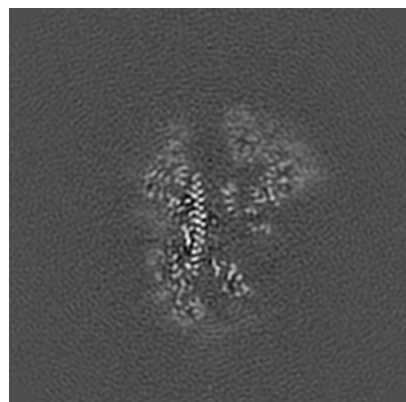


Z

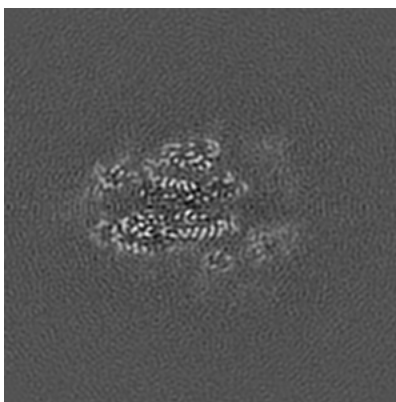
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

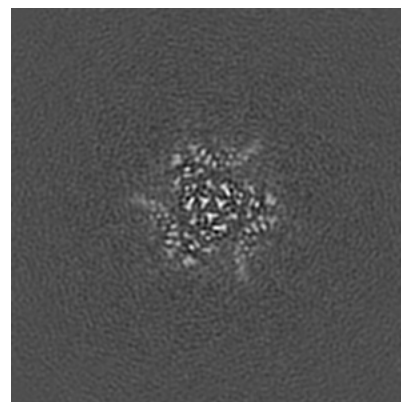
6.2.1 Primary map



X Index: 100



Y Index: 100

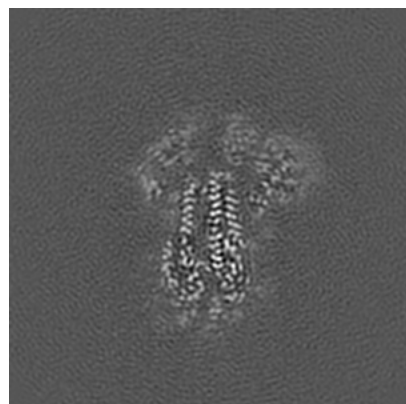


Z Index: 100

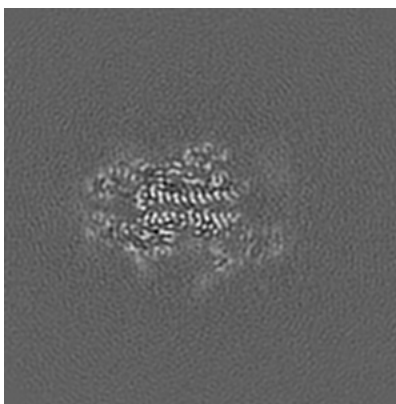
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

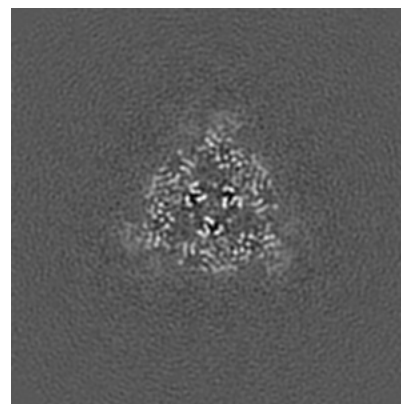
6.3.1 Primary map



X Index: 106



Y Index: 104

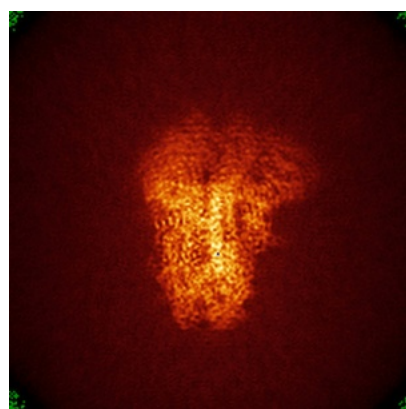


Z Index: 105

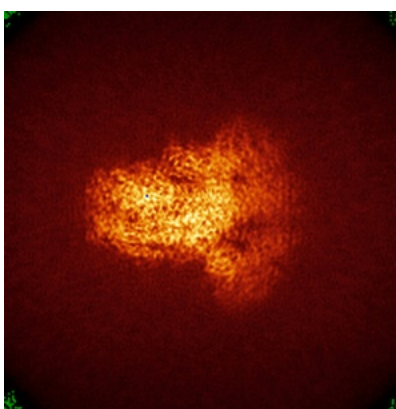
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

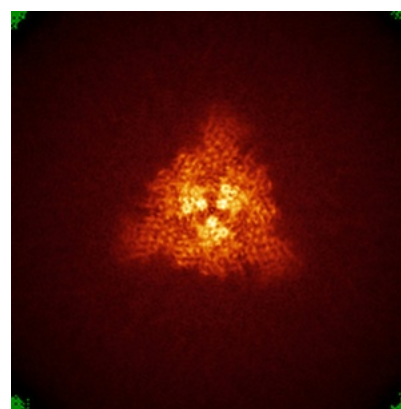
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0456. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

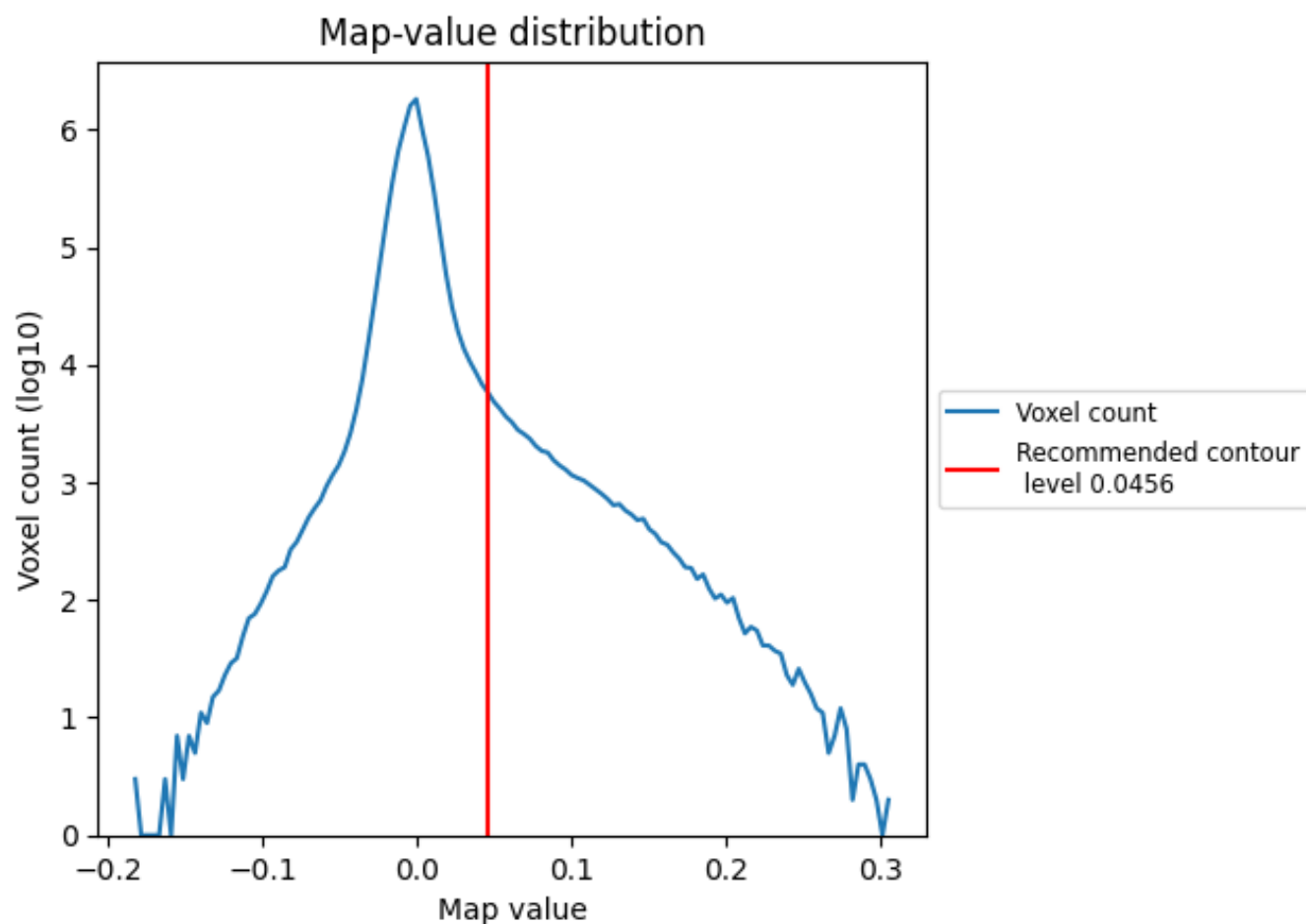
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

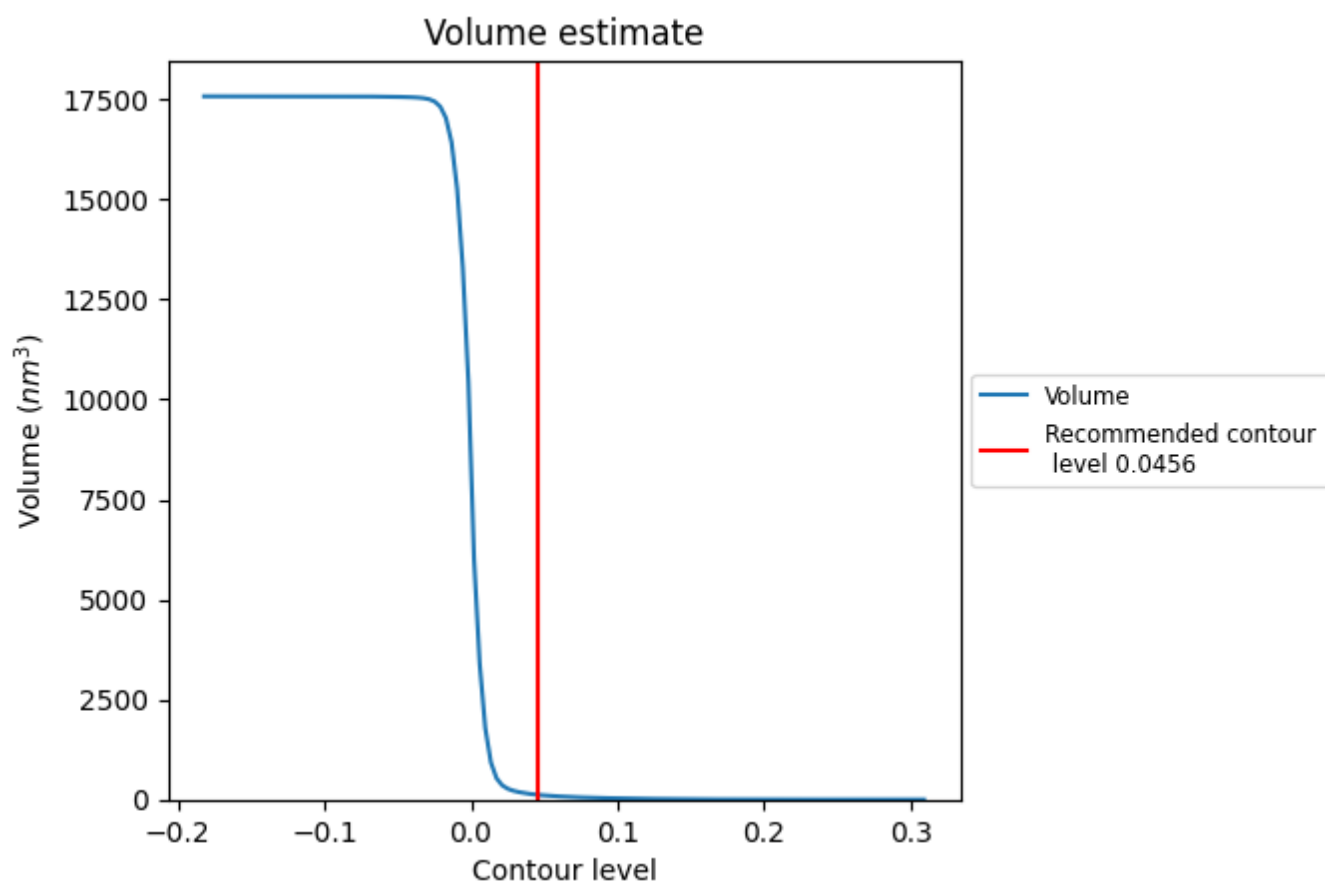
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

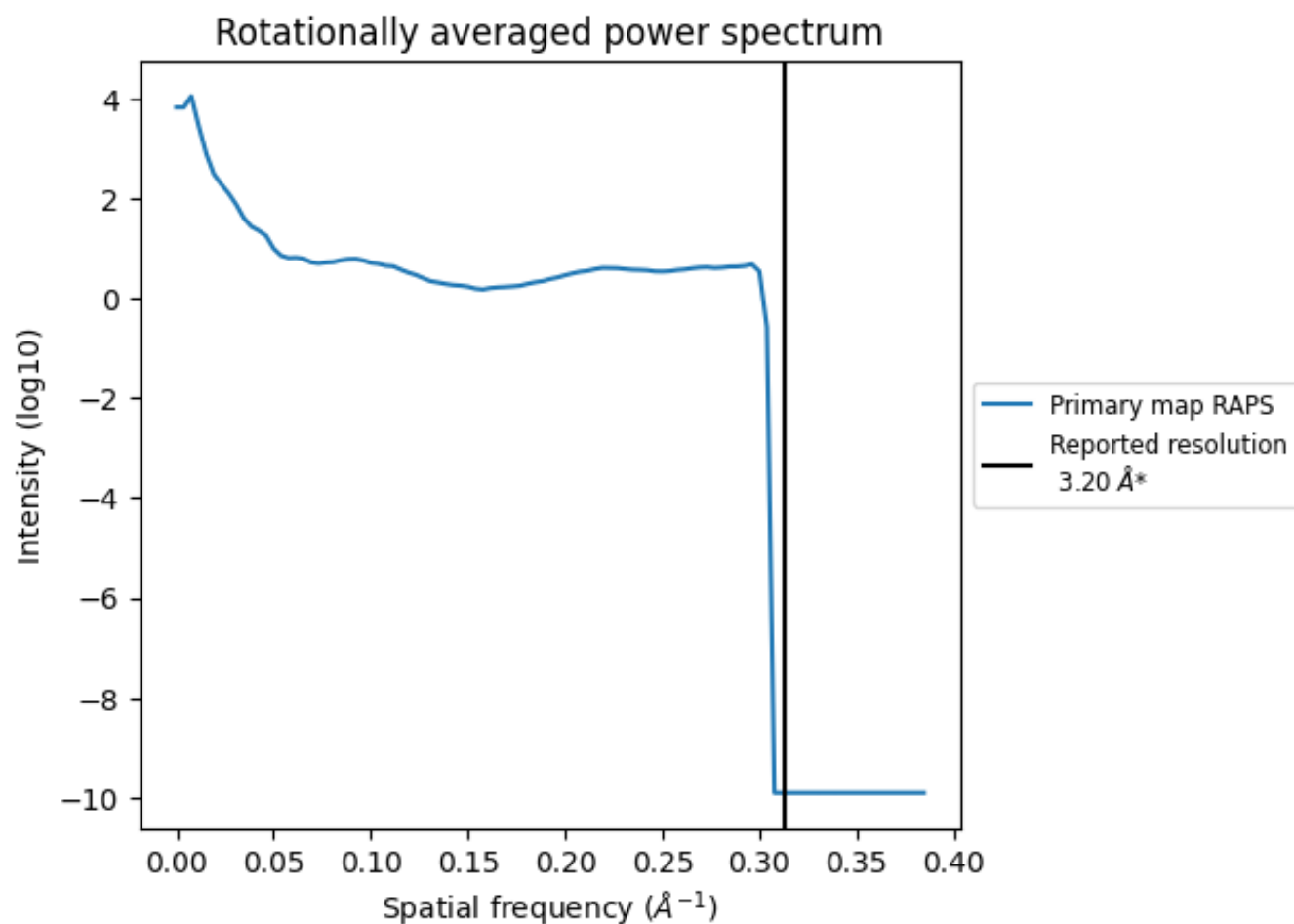
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 118 nm³; this corresponds to an approximate mass of 107 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

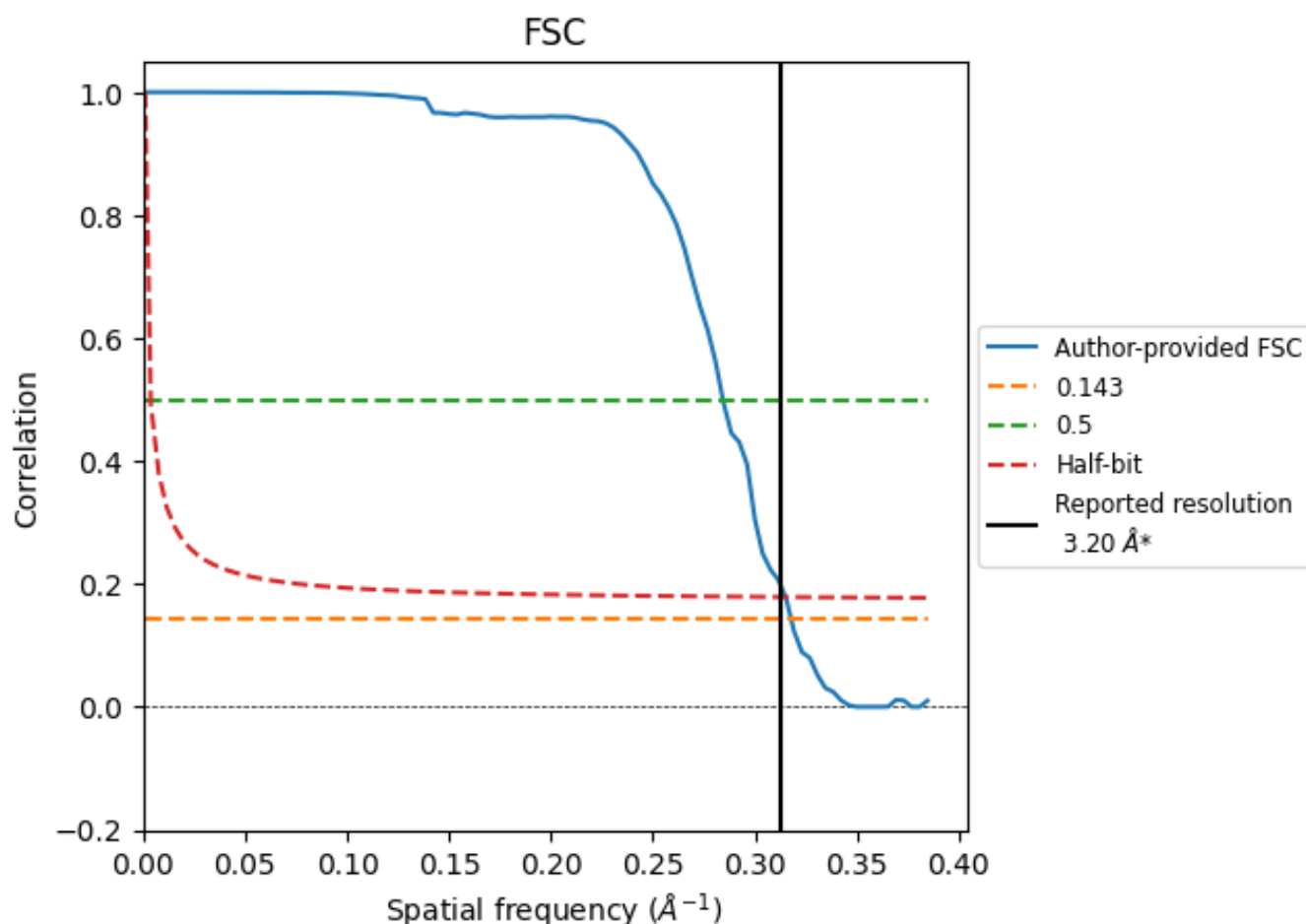


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

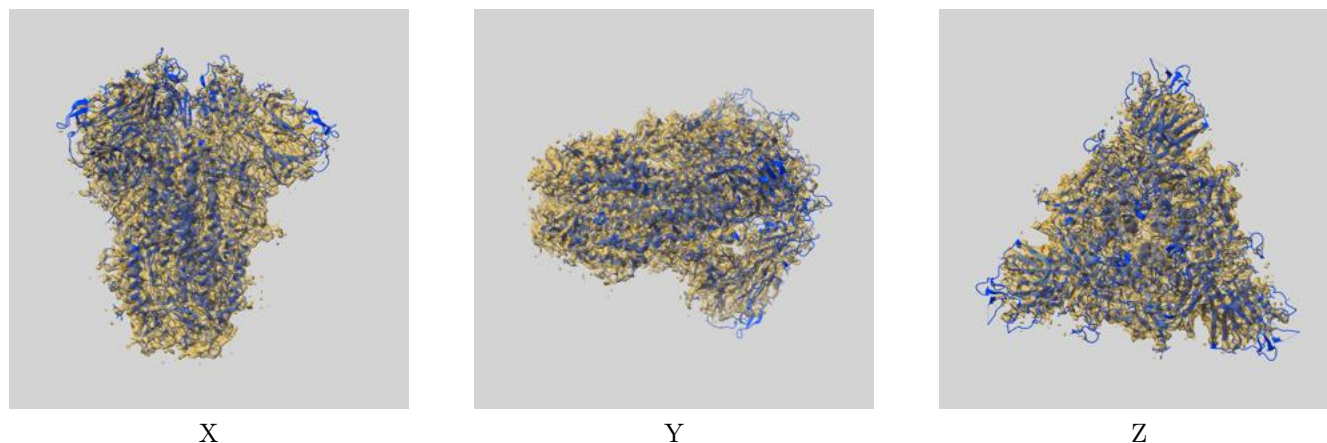
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.15	3.52	3.17
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

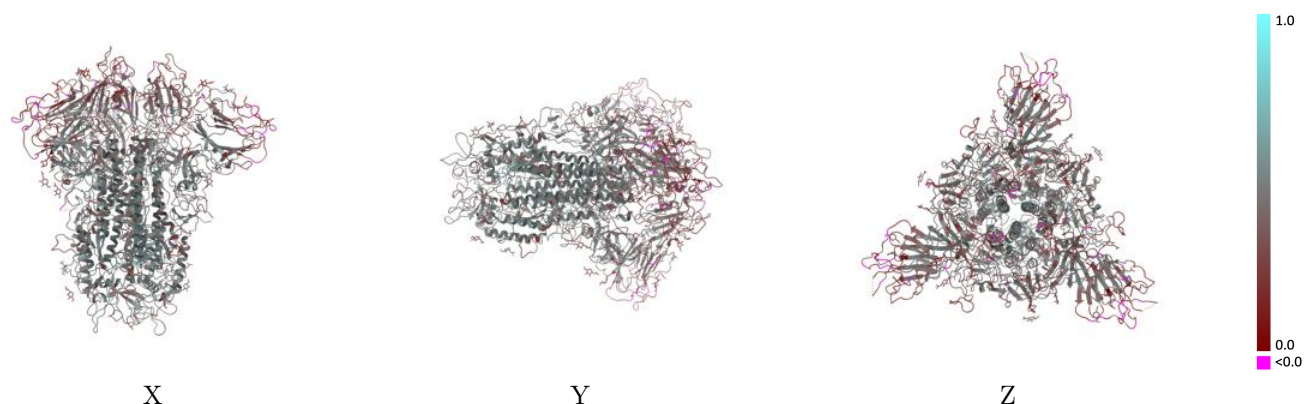
This section contains information regarding the fit between EMDB map EMD-6703 and PDB model 5X58. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



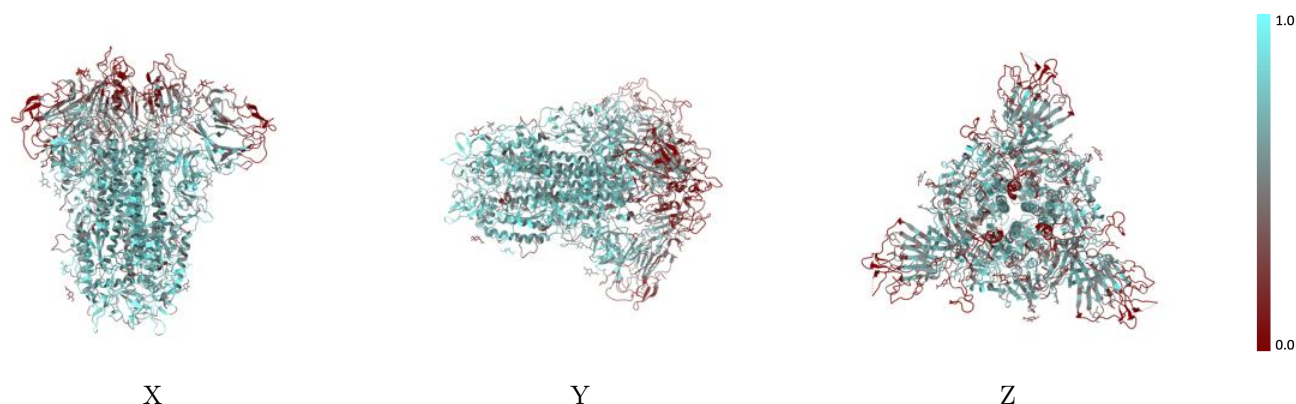
The images above show the 3D surface view of the map at the recommended contour level 0.0456 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



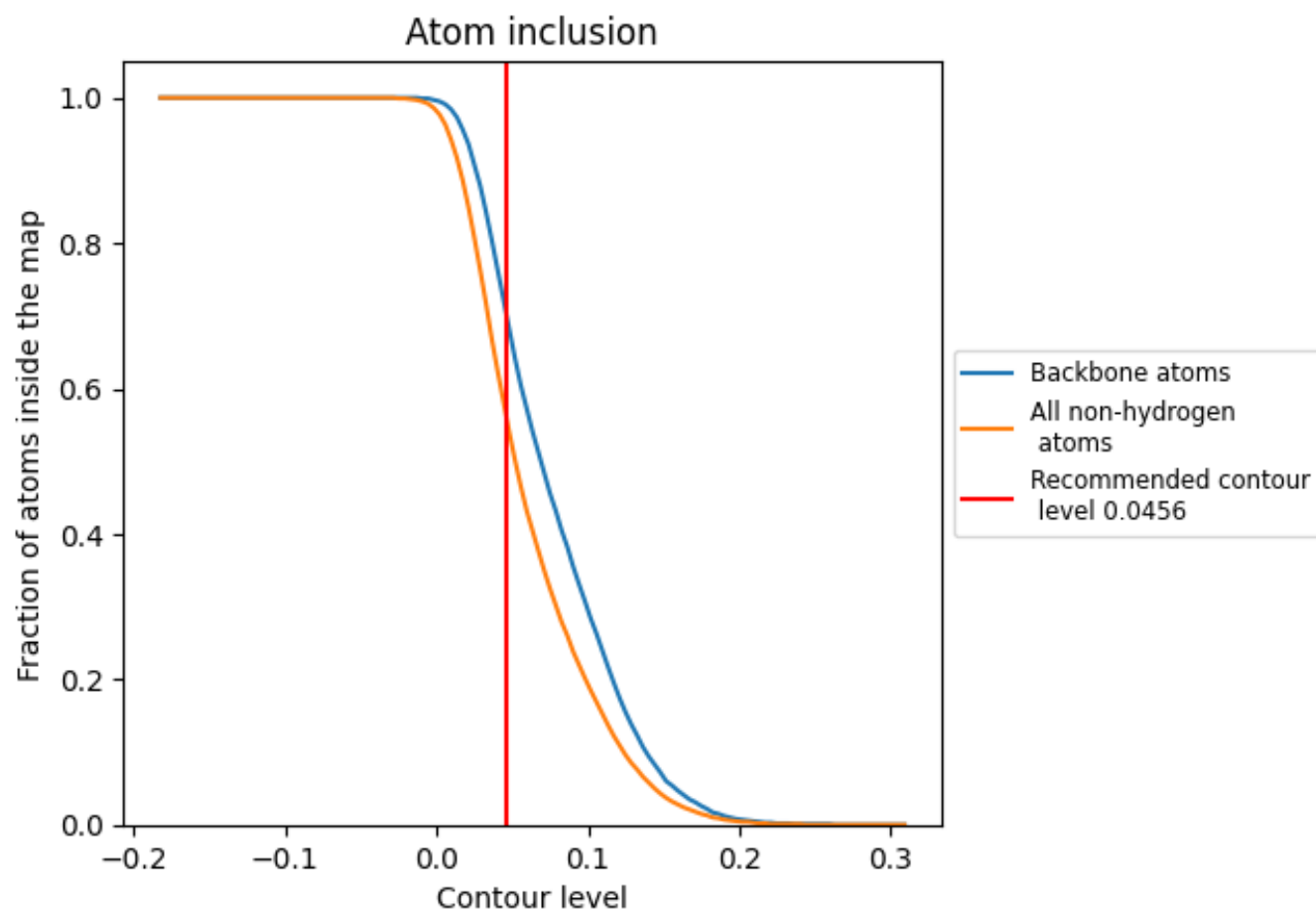
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0456).

9.4 Atom inclusion ⓘ



At the recommended contour level, 71% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0456) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5670	0.4090
A	0.5660	0.4090
B	0.5680	0.4080
C	0.5670	0.4100

