Full wwPDB EM Validation Report (i)

Nov 9, 2022 – 01:27 AM JST

PDB ID	:	6ACD
EMDB ID	:	EMD-9589
Title	:	Trypsin-cleaved and low pH-treated SARS-CoV spike glycoprotein and ACE2 complex, ACE2-free conformation with one RBD in up conformation
Authors	:	Gui, M.; Song, W.
Deposited on	:	2018-07-26
Resolution	:	3.90 Å(reported)

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 (i) 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 (i)) were used in the production of this report:

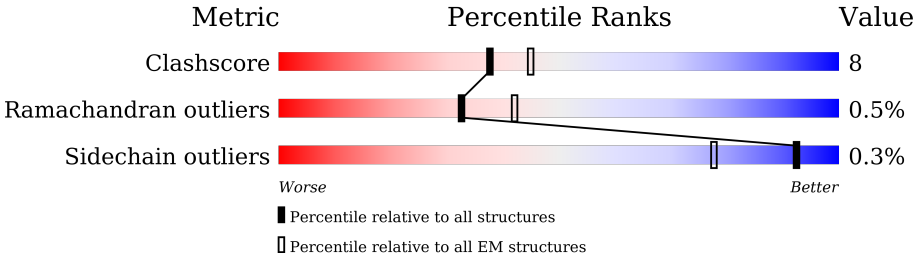
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	1203	25% 71% 17% • 11%
1	B	1203	25% 69% 19% 11%
1	C	1203	33% 69% 18% • 12%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 24845 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
			Total	C	N	O	S		
1	A	1065	8302	5304	1374	1579	45	0	0
1	B	1065	8302	5304	1374	1579	45	0	0
1	C	1057	8241	5264	1364	1568	45	0	0

There are 21 discrepancies between the modelled and reference sequences:

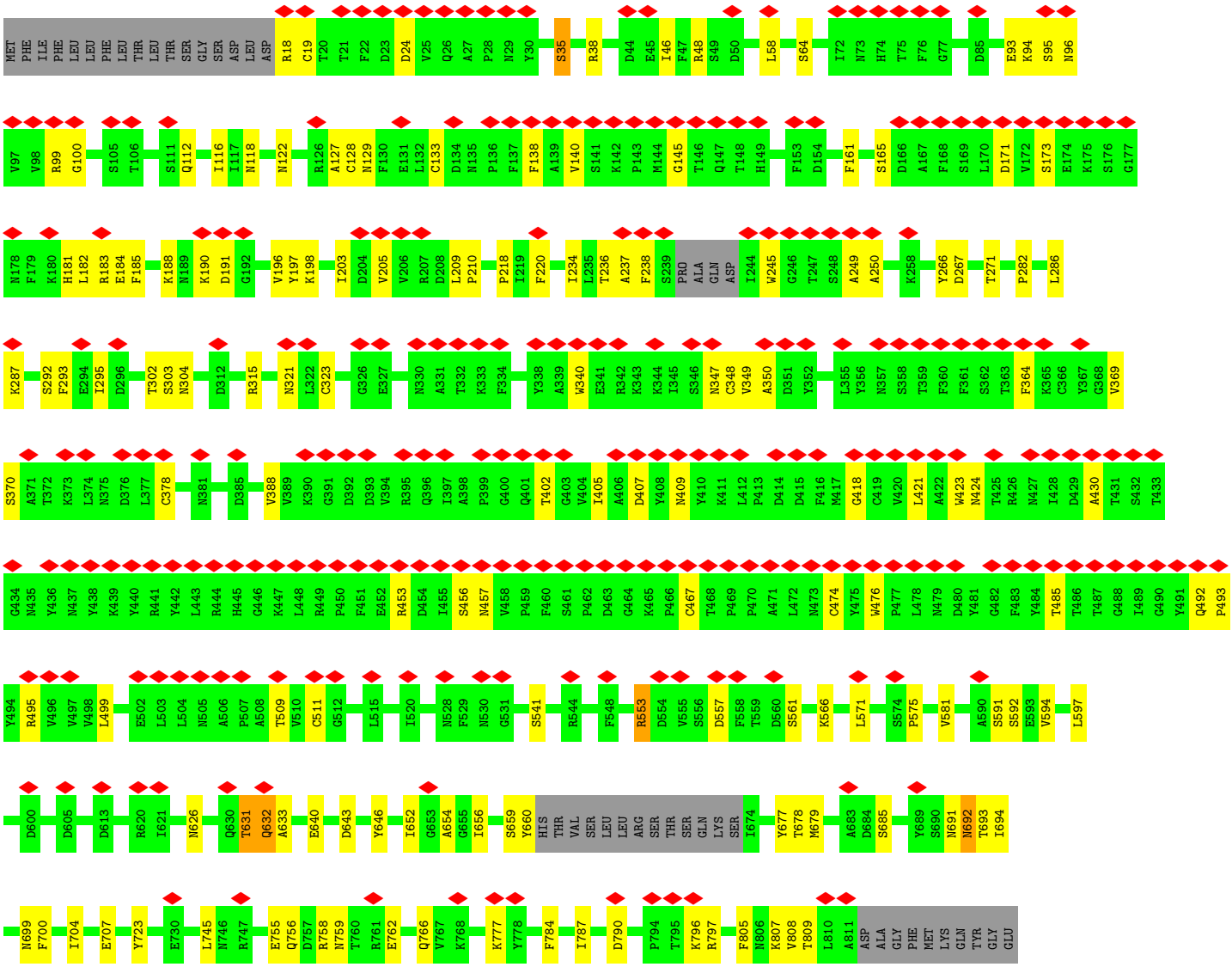
Chain	Residue	Modelled	Actual	Comment	Reference
A	1197	SER	-	expression tag	UNP P59594
A	1198	HIS	-	expression tag	UNP P59594
A	1199	PRO	-	expression tag	UNP P59594
A	1200	GLN	-	expression tag	UNP P59594
A	1201	PHE	-	expression tag	UNP P59594
A	1202	GLU	-	expression tag	UNP P59594
A	1203	LYS	-	expression tag	UNP P59594
B	1197	SER	-	expression tag	UNP P59594
B	1198	HIS	-	expression tag	UNP P59594
B	1199	PRO	-	expression tag	UNP P59594
B	1200	GLN	-	expression tag	UNP P59594
B	1201	PHE	-	expression tag	UNP P59594
B	1202	GLU	-	expression tag	UNP P59594
B	1203	LYS	-	expression tag	UNP P59594
C	1197	SER	-	expression tag	UNP P59594
C	1198	HIS	-	expression tag	UNP P59594
C	1199	PRO	-	expression tag	UNP P59594
C	1200	GLN	-	expression tag	UNP P59594
C	1201	PHE	-	expression tag	UNP P59594
C	1202	GLU	-	expression tag	UNP P59594
C	1203	LYS	-	expression tag	UNP P59594

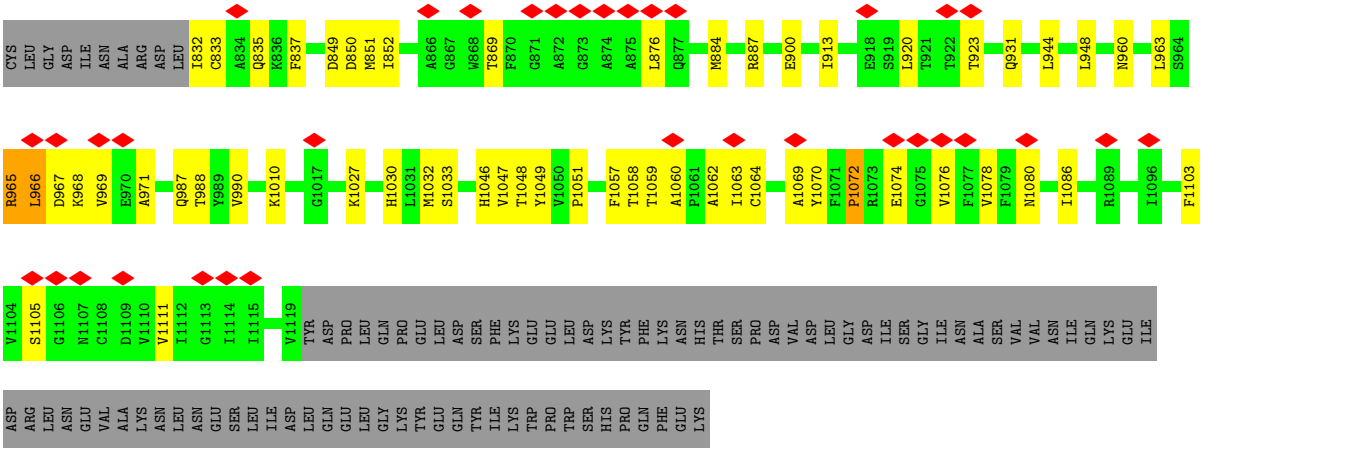
3 Residue-property plots (i)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Spike glycoprotein

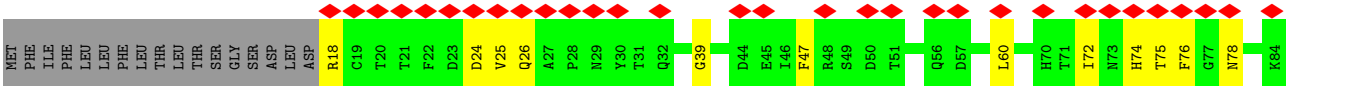
Chain A:

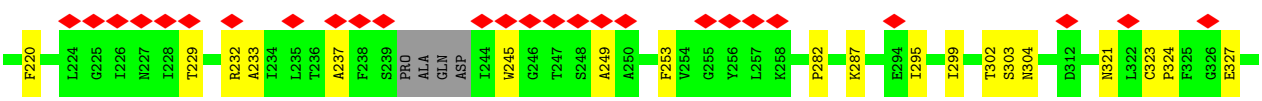


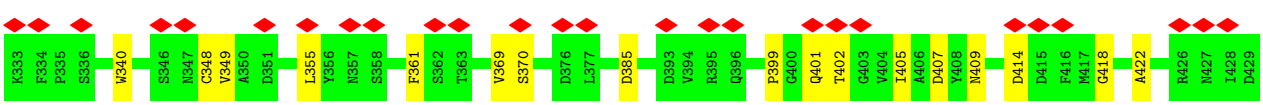


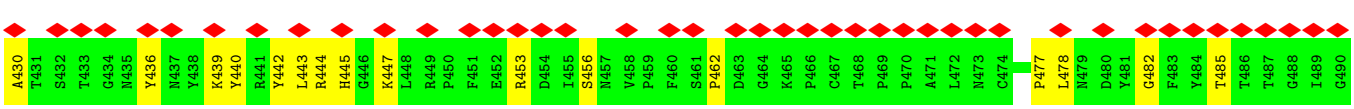
- Molecule 1: Spike glycoprotein

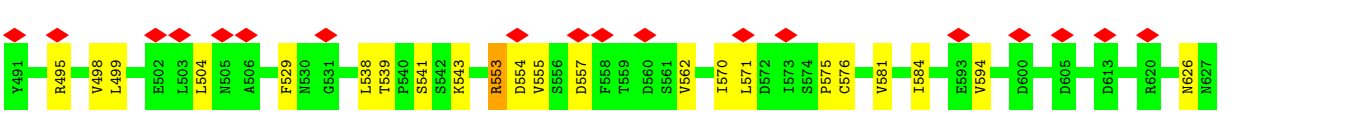
Chain B:

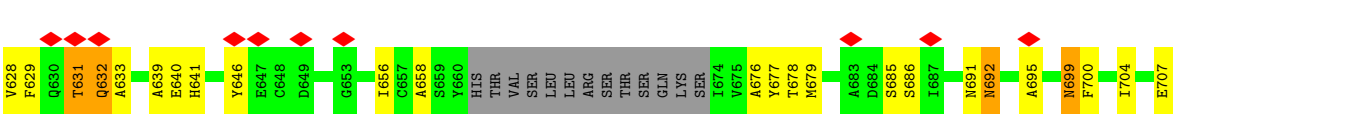


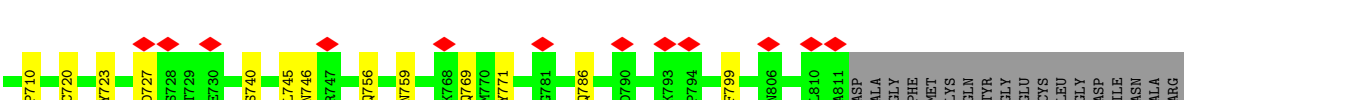


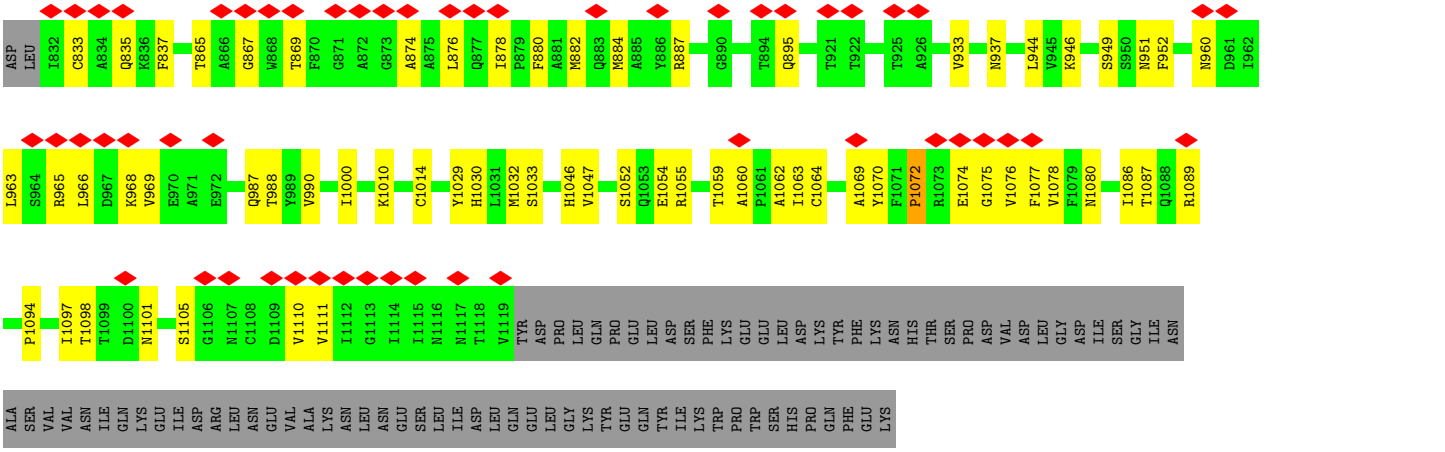






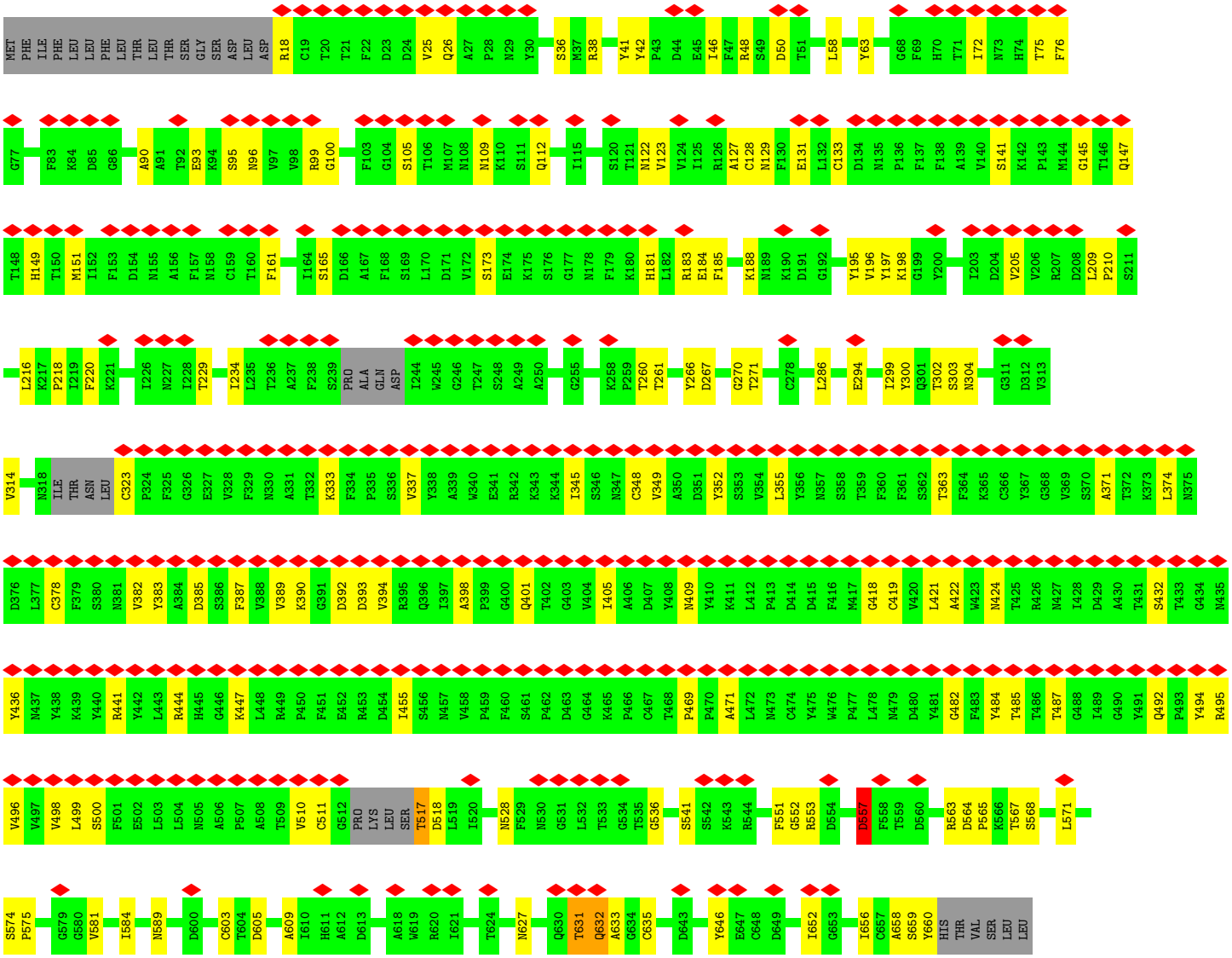


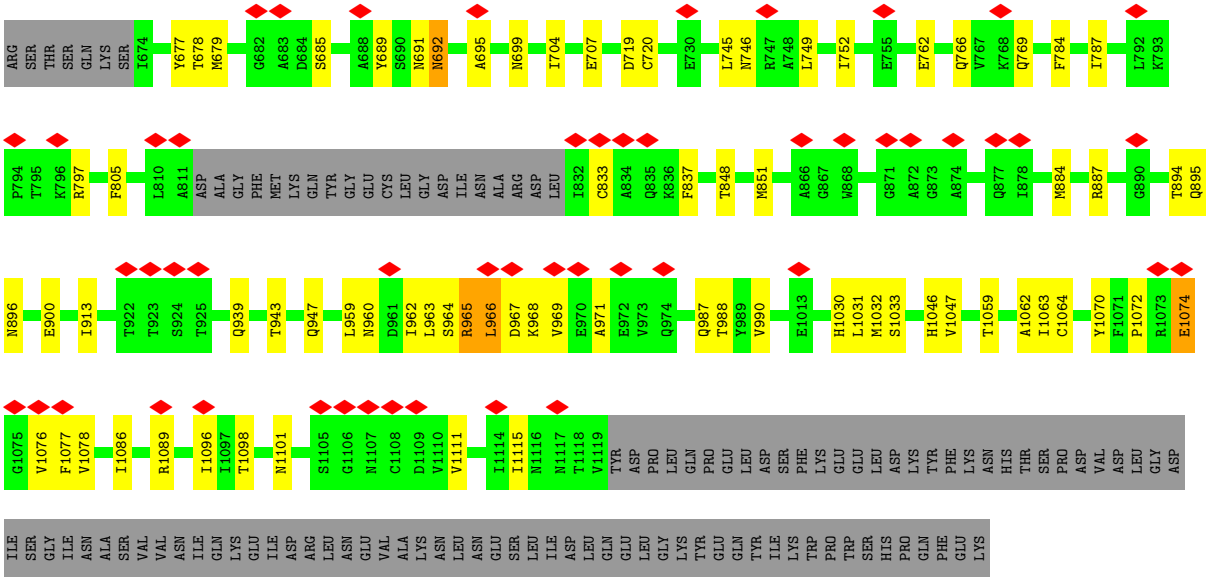




- Molecule 1: Spike glycoprotein

Chain C:




ARG SER THR SER GLN LYS SER I674 Y677 T678 M679 G682 A683 D684 S685 A688 Y689 S690 N691 N692 A695 N699 I704 E707 D719 C720 E730 L745 N746 R747 A748 L749 I752 E755 E762 Q766 V767 K768 Q769 F784 I787 L792 K793
P794 T795 K796 R797 F805 L810 A811 ASP ALA GLY PHE MET LYS GLN TYR GLY GLU CYS LEU GLY ASP ILE ASN ALA ARG ASP LEU I832 C833 A834 Q835 R836 F837 T848 M851 A866 G867 W868 G871 A872 G873 A874 Q877 I878 N884 R887 G890 T894 Q895
N896 E900 I913 T922 T923 S924 T925 Q939 T943 Q947 L959 N960 D961 I962 L963 S964 R965 L966 D967 K968 V969 E970 A971 E972 V973 Q974 Q987 T988 Y989 V990 E1013 H1030 L1031 M1032 S1033 H1046 V1047 T1059 A1062 I1063 C1064 Y1070 F1071 P1072 R1073 E1074
G1075 V1076 F1077 V1078 I1086 R1089 I1096 I1097 T1098 N1101 S1105 G1106 N1107 C1108 D1109 V1110 V1111 I1114 I1115 N1116 N1117 T1118 V1119 TYR ASP PRO LEU GLN PRO GLU LEU ASP SER PHE LYS GLU GLU LEU ASP LYS TYR PHE LYS ASN HIS THR SER PRO ASP VAL ASP LEU GLY ASP
ILE SER GLY ILE ASN ALA SER VAL VAL ASN ILE GLN LYS GLU ILE ASP ARG LEU ASN GLU VAL ALA LYS ASN LEU ASN GLU SER LEU ILE ASP LEU GLN GLU LEU GLY LYS TYR GLU GLN TYR ILE LYS TRP PRO TRP SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	174489	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 ($e^-/Å^2$)	50	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	39.640	Depositor
Minimum map value	-15.664	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.873	Depositor
Recommended contour level	8.0	Depositor
Map size (Å)	380.16, 380.16, 380.16	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.38	0/8499	0.60	2/11568 (0.0%)
1	B	0.38	0/8499	0.60	3/11568 (0.0%)
1	C	0.38	0/8435	0.61	5/11477 (0.0%)
All	All	0.38	0/25433	0.60	10/34613 (0.0%)

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	5
1	B	0	7
1	C	0	3
All	All	0	15

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	557	ASP	CB-CG-OD1	7.57	125.12	118.30
1	C	517	THR	N-CA-C	7.50	131.24	111.00
1	A	966	LEU	CA-CB-CG	6.75	130.83	115.30
1	B	557	ASP	CB-CG-OD1	6.70	124.33	118.30
1	B	966	LEU	CA-CB-CG	6.18	129.52	115.30
1	C	557	ASP	CB-CG-OD1	5.64	123.37	118.30
1	C	966	LEU	CA-CB-CG	5.38	127.67	115.30
1	C	517	THR	C-N-CA	-5.29	108.48	121.70
1	B	504	LEU	CA-CB-CG	5.07	126.95	115.30
1	C	517	THR	CB-CA-C	-5.02	98.06	111.60

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1074	GLU	Peptide
1	A	35	SER	Peptide
1	A	553	ARG	Peptide
1	A	631	THR	Peptide
1	A	923	THR	Peptide
1	B	1052	SER	Peptide
1	B	1074	GLU	Peptide
1	B	1077	PHE	Peptide
1	B	553	ARG	Peptide
1	B	629	PHE	Peptide
1	B	631	THR	Peptide
1	B	727	ASP	Peptide
1	C	1074	GLU	Peptide
1	C	1077	PHE	Peptide
1	C	631	THR	Peptide

5.2 Too-close contacts (i)

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	8302	0	8082	136	0
1	B	8302	0	8082	143	0
1	C	8241	0	8009	154	0
All	All	24845	0	24173	395	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 (395) 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:C:418:GLY:HA3	1:C:499:LEU:O	1.61	1.00
1:C:314:VAL:H	1:C:517:THR:HG21	1.29	0.96
1:A:100:GLY:HA2	1:A:116:ILE:O	1.68	0.92
1:B:18:ARG:N	1:B:133:CYS:HG	1.66	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:GLU:O	1:C:181:HIS:HB2	1.77	0.84
1:B:1069:ALA:HB3	1:B:1105:SER:O	1.77	0.84
1:A:418:GLY:HA3	1:A:499:LEU:O	1.83	0.79
1:A:1069:ALA:HB3	1:A:1105:SER:O	1.87	0.74
1:C:18:ARG:N	1:C:133:CYS:HG	1.86	0.73
1:C:692:ASN:HB3	1:C:1059:THR:H	1.53	0.73
1:A:18:ARG:N	1:A:133:CYS:HG	1.87	0.71
1:B:740:SER:H	1:C:947:GLN:HE22	1.39	0.71
1:C:419:CYS:O	1:C:498:VAL:HA	1.91	0.71
1:B:692:ASN:HB3	1:B:1059:THR:H	1.56	0.70
1:C:383:TYR:HB2	1:C:500:SER:HB2	1.73	0.70
1:C:314:VAL:N	1:C:517:THR:HG21	1.95	0.69
1:A:405:ILE:HG23	1:A:409:ASN:HD22	1.55	0.69
1:C:405:ILE:HG23	1:C:409:ASN:HD22	1.58	0.68
1:C:536:GLY:HA3	1:C:574:SER:HA	1.75	0.67
1:C:390:LYS:HE3	1:C:392:ASP:HB2	1.75	0.67
1:A:685:SER:HB2	1:C:769:GLN:HE21	1.60	0.65
1:B:348:CYS:SG	1:B:349:VAL:N	2.70	0.65
1:C:960:ASN:H	1:C:963:LEU:HD13	1.62	0.64
1:B:405:ILE:HG23	1:B:409:ASN:HD22	1.60	0.64
1:A:745:LEU:HD22	1:A:990:VAL:HG21	1.80	0.63
1:A:1072:PRO:HB3	1:A:1086:ILE:HD13	1.80	0.63
1:B:340:TRP:O	1:B:453:ARG:NH1	2.30	0.63
1:B:987:GLN:NE2	1:C:988:THR:OG1	2.31	0.63
1:B:385:ASP:HB2	1:B:498:VAL:HB	1.79	0.63
1:C:314:VAL:HG13	1:C:528:ASN:HB3	1.81	0.62
1:A:960:ASN:H	1:A:963:LEU:HD13	1.65	0.62
1:B:302:THR:HG23	1:B:581:VAL:HG23	1.82	0.62
1:C:1078:VAL:HA	1:C:1086:ILE:HG12	1.80	0.62
1:A:58:LEU:HB2	1:A:188:LYS:HE3	1.81	0.62
1:A:347:ASN:H	1:A:509:THR:HB	1.65	0.62
1:A:369:VAL:HA	1:C:965:ARG:HB2	1.81	0.61
1:C:99:ARG:HD2	1:C:147:GLN:HE22	1.65	0.61
1:B:626:ASN:ND2	1:B:639:ALA:O	2.33	0.61
1:A:140:VAL:HG13	1:A:145:GLY:HA2	1.81	0.61
1:A:707:GLU:OE1	1:A:1046:HIS:NE2	2.33	0.61
1:B:869:THR:OG1	1:C:1089:ARG:NH1	2.33	0.61
1:C:887:ARG:NH1	1:C:1032:MET:SD	2.74	0.61
1:B:887:ARG:NH1	1:B:1032:MET:SD	2.73	0.61
1:A:128:CYS:SG	1:A:129:ASN:N	2.74	0.61
1:A:348:CYS:SG	1:A:349:VAL:N	2.74	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:ARG:NH1	1:B:447:LYS:O	2.34	0.60
1:C:127:ALA:HB3	1:C:161:PHE:HB3	1.82	0.60
1:B:745:LEU:HD22	1:B:990:VAL:HG21	1.84	0.60
1:C:652:ILE:HD11	1:C:658:ALA:HB2	1.83	0.60
1:A:692:ASN:HB3	1:A:1059:THR:H	1.67	0.60
1:A:887:ARG:NH1	1:A:1032:MET:SD	2.75	0.60
1:C:196:VAL:HB	1:C:220:PHE:HB2	1.83	0.60
1:B:91:ALA:HB3	1:B:183:ARG:HB2	1.83	0.60
1:B:94:LYS:HB3	1:B:175:LYS:HB2	1.82	0.60
1:B:418:GLY:HA3	1:B:499:LEU:O	2.02	0.59
1:B:833:CYS:SG	1:C:632:GLN:NE2	2.75	0.59
1:C:50:ASP:HA	1:C:266:TYR:O	2.03	0.59
1:C:128:CYS:SG	1:C:129:ASN:N	2.75	0.59
1:A:988:THR:OG1	1:C:987:GLN:NE2	2.35	0.59
1:B:769:GLN:HE21	1:C:685:SER:HB2	1.67	0.59
1:C:149:HIS:NE2	1:C:151:MET:SD	2.76	0.59
1:C:564:ASP:HB3	1:C:568:SER:HB3	1.84	0.59
1:A:869:THR:OG1	1:B:1089:ARG:NH1	2.36	0.59
1:A:851:MET:SD	1:A:851:MET:N	2.76	0.58
1:B:47:PHE:HB3	1:C:552:GLY:HA2	1.85	0.58
1:B:1064:CYS:HB2	1:B:1111:VAL:HG11	1.83	0.58
1:A:632:GLN:NE2	1:C:833:CYS:SG	2.76	0.58
1:B:707:GLU:OE2	1:B:1010:LYS:NZ	2.36	0.58
1:C:1096:ILE:O	1:C:1101:ASN:ND2	2.37	0.58
1:B:188:LYS:HB3	1:B:195:TYR:HB2	1.85	0.58
1:B:707:GLU:OE1	1:B:1046:HIS:NE2	2.37	0.58
1:B:99:ARG:NH2	1:B:171:ASP:O	2.36	0.57
1:B:835:GLN:HG2	1:C:575:PRO:HG2	1.87	0.57
1:C:302:THR:HG23	1:C:581:VAL:HG23	1.85	0.57
1:A:302:THR:HG23	1:A:581:VAL:HG23	1.87	0.57
1:B:25:VAL:HA	1:B:76:PHE:HB3	1.86	0.57
1:A:1078:VAL:HA	1:A:1086:ILE:HG12	1.87	0.57
1:A:700:PHE:HA	1:A:1051:PRO:HA	1.87	0.57
1:B:1063:ILE:HB	1:B:1070:TYR:HB2	1.86	0.57
1:B:324:PRO:O	1:B:327:GLU:HB3	2.04	0.56
1:C:141:SER:HB3	1:C:145:GLY:H	1.70	0.56
1:A:138:PHE:HB2	1:A:236:THR:HA	1.87	0.56
1:C:1063:ILE:HB	1:C:1070:TYR:HB2	1.87	0.56
1:C:1064:CYS:HB2	1:C:1111:VAL:HG11	1.87	0.56
1:A:575:PRO:HD3	1:C:837:PHE:HB3	1.87	0.56
1:B:867:GLY:HA3	1:B:876:LEU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:960:ASN:H	1:B:963:LEU:HD13	1.70	0.56
1:B:72:ILE:H	1:B:75:THR:HB	1.70	0.56
1:C:784:PHE:HA	1:C:787:ILE:HD12	1.86	0.56
1:C:707:GLU:OE1	1:C:1046:HIS:NE2	2.39	0.56
1:C:1030:HIS:HE1	1:C:1033:SER:HB2	1.70	0.56
1:B:120:SER:HA	1:B:170:LEU:HD23	1.87	0.56
1:A:38:ARG:NH1	1:A:184:GLU:OE2	2.38	0.55
1:C:422:ALA:HA	1:C:495:ARG:O	2.06	0.55
1:B:439:LYS:HD3	1:B:478:LEU:HB3	1.87	0.55
1:C:517:THR:OG1	1:C:518:ASP:N	2.39	0.55
1:B:710:PRO:HB2	1:B:1000:ILE:HD11	1.89	0.55
1:A:96:ASN:HA	1:A:183:ARG:HH12	1.71	0.55
1:A:837:PHE:HB3	1:B:575:PRO:HD3	1.88	0.55
1:C:631:THR:O	1:C:633:ALA:N	2.40	0.55
1:A:99:ARG:HD3	1:A:118:ASN:HB2	1.89	0.55
1:B:90:ALA:HB3	1:B:253:PHE:HB2	1.88	0.55
1:A:99:ARG:NH2	1:A:171:ASP:O	2.38	0.54
1:A:24:ASP:HB3	1:A:245:TRP:HE1	1.72	0.54
1:B:72:ILE:HG13	1:B:74:HIS:H	1.72	0.54
1:B:445:HIS:HE1	1:B:462:PRO:HA	1.72	0.54
1:A:456:SER:HB2	1:C:112:GLN:HE22	1.72	0.54
1:A:631:THR:HB	1:A:654:ALA:HB3	1.90	0.54
1:A:707:GLU:OE2	1:A:1010:LYS:NZ	2.33	0.54
1:A:900:GLU:HA	1:B:1110:VAL:HG11	1.89	0.54
1:C:260:THR:OG1	1:C:261:THR:N	2.41	0.54
1:A:755:GLU:OE2	1:A:758:ARG:NH1	2.40	0.54
1:B:1078:VAL:HA	1:B:1086:ILE:HG12	1.88	0.54
1:A:424:ASN:ND2	1:A:492:GLN:OE1	2.40	0.54
1:C:42:TYR:HB2	1:C:218:PRO:HD3	1.90	0.54
1:C:1062:ALA:HB3	1:C:1111:VAL:HG13	1.90	0.53
1:A:777:LYS:NZ	1:A:790:ASP:OD1	2.41	0.53
1:B:116:ILE:HG12	1:B:125:ILE:HG12	1.90	0.53
1:B:402:THR:HB	1:B:407:ASP:HB2	1.91	0.53
1:C:517:THR:HG23	1:C:517:THR:O	2.07	0.53
1:B:99:ARG:HD3	1:B:118:ASN:HB2	1.91	0.52
1:C:960:ASN:HA	1:C:963:LEU:HB2	1.92	0.52
1:A:315:ARG:HH22	1:A:566:LYS:HD2	1.74	0.52
1:C:48:ARG:HB2	1:C:266:TYR:HD2	1.74	0.52
1:A:196:VAL:HB	1:A:220:PHE:HB2	1.90	0.52
1:C:299:ILE:HG12	1:C:584:ILE:HG13	1.90	0.52
1:C:424:ASN:ND2	1:C:492:GLN:OE1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:TRP:O	1:A:453:ARG:NH1	2.43	0.52
1:C:966:LEU:HB2	1:C:971:ALA:HB2	1.90	0.52
1:C:36:SER:HA	1:C:63:TYR:H	1.75	0.52
1:C:96:ASN:HA	1:C:183:ARG:HH12	1.75	0.52
1:C:209:LEU:HD12	1:C:210:PRO:HD2	1.92	0.52
1:A:808:VAL:HA	1:A:931:GLN:HE21	1.73	0.52
1:A:1060:ALA:HB2	1:A:1080:ASN:HD22	1.74	0.52
1:B:756:GLN:HA	1:B:759:ASN:HD22	1.75	0.52
1:A:190:LYS:NZ	1:A:191:ASP:OD2	2.42	0.52
1:A:704:ILE:HG12	1:A:1047:VAL:HG22	1.92	0.52
1:C:100:GLY:HA3	1:C:234:ILE:HB	1.90	0.52
1:B:100:GLY:HA2	1:B:117:ILE:HG22	1.92	0.52
1:C:541:SER:HA	1:C:571:LEU:HG	1.92	0.52
1:A:631:THR:O	1:A:633:ALA:N	2.42	0.51
1:C:887:ARG:NH1	1:C:1031:LEU:O	2.40	0.51
1:C:968:LYS:HG3	1:C:969:VAL:HG23	1.92	0.51
1:A:1062:ALA:HB3	1:A:1111:VAL:HG13	1.92	0.51
1:A:35:SER:OG	1:A:64:SER:N	2.42	0.51
1:B:47:PHE:N	1:C:551:PHE:O	2.40	0.51
1:C:38:ARG:NH1	1:C:184:GLU:OE2	2.43	0.51
1:C:385:ASP:HB2	1:C:498:VAL:HB	1.92	0.51
1:A:323:CYS:N	1:A:348:CYS:SG	2.84	0.51
1:B:24:ASP:HB3	1:B:245:TRP:HE1	1.76	0.51
1:B:95:SER:OG	1:B:173:SER:O	2.28	0.50
1:B:190:LYS:O	1:B:193:PHE:HB2	2.11	0.50
1:A:553:ARG:HD2	1:C:46:ILE:HG21	1.92	0.50
1:A:835:GLN:NE2	1:B:575:PRO:O	2.43	0.50
1:A:1103:PHE:HE2	1:C:896:ASN:HD21	1.60	0.50
1:B:78:ASN:O	1:B:232:ARG:NH2	2.44	0.50
1:C:432:SER:HA	1:C:485:THR:H	1.75	0.50
1:A:1063:ILE:HB	1:A:1070:TYR:HB2	1.94	0.50
1:B:678:THR:OG1	1:B:679:MET:N	2.43	0.50
1:B:1087:THR:HG22	1:B:1094:PRO:HA	1.94	0.50
1:C:363:THR:O	1:C:421:LEU:HA	2.12	0.50
1:C:441:ARG:NH2	1:C:455:ILE:O	2.45	0.50
1:B:127:ALA:HB3	1:B:161:PHE:HB3	1.94	0.50
1:C:185:PHE:HE1	1:C:198:LYS:HG3	1.77	0.50
1:B:538:LEU:HD22	1:B:570:ILE:HD12	1.93	0.50
1:A:94:LYS:NZ	1:A:249:ALA:O	2.39	0.50
1:B:302:THR:OG1	1:B:303:SER:N	2.43	0.50
1:A:321:ASN:HB3	1:A:348:CYS:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:762:GLU:O	1:C:766:GLN:NE2	2.38	0.50
1:C:896:ASN:O	1:C:900:GLU:HB2	2.12	0.50
1:B:631:THR:O	1:B:633:ALA:N	2.40	0.49
1:B:884:MET:HA	1:B:887:ARG:HB2	1.94	0.49
1:A:282:PRO:HB2	1:A:594:VAL:HG21	1.94	0.49
1:B:529:PHE:HE2	1:B:562:VAL:HG21	1.77	0.49
1:B:539:THR:HG23	1:B:571:LEU:HB2	1.94	0.49
1:C:1098:THR:H	1:C:1101:ASN:HB2	1.77	0.49
1:B:626:ASN:ND2	1:B:640:GLU:OE2	2.45	0.49
1:B:1030:HIS:HE1	1:B:1033:SER:HB2	1.76	0.49
1:C:337:VAL:HG22	1:C:387:PHE:HB2	1.95	0.49
1:B:282:PRO:HB2	1:B:594:VAL:HG21	1.94	0.49
1:C:745:LEU:HD22	1:C:990:VAL:HG21	1.93	0.49
1:C:968:LYS:HG3	1:C:969:VAL:H	1.77	0.49
1:B:436:TYR:HE1	1:B:482:GLY:HA2	1.77	0.49
1:B:115:ILE:O	1:B:125:ILE:HA	2.13	0.48
1:B:133:CYS:HB2	1:B:136:PRO:HD3	1.94	0.48
1:A:304:ASN:ND2	1:C:719:ASP:OD1	2.46	0.48
1:A:678:THR:OG1	1:A:679:MET:N	2.40	0.48
1:B:78:ASN:ND2	1:B:233:ALA:O	2.45	0.48
1:B:141:SER:HB3	1:B:144:MET:HB2	1.93	0.48
1:A:185:PHE:HE1	1:A:198:LYS:HG3	1.79	0.48
1:B:105:SER:O	1:B:229:THR:OG1	2.30	0.48
1:A:966:LEU:HB2	1:A:971:ALA:HB2	1.94	0.48
1:B:835:GLN:NE2	1:C:575:PRO:O	2.39	0.48
1:C:95:SER:H	1:C:181:HIS:CD2	2.32	0.48
1:C:323:CYS:SG	1:C:349:VAL:N	2.86	0.48
1:A:626:ASN:ND2	1:A:640:GLU:OE2	2.38	0.48
1:A:659:SER:OG	1:A:660:TYR:N	2.47	0.48
1:C:720:CYS:SG	1:C:746:ASN:ND2	2.87	0.48
1:B:771:TYR:OH	1:B:874:ALA:O	2.31	0.48
1:C:363:THR:HB	1:C:422:ALA:HB3	1.95	0.48
1:A:960:ASN:HA	1:A:963:LEU:HB2	1.95	0.48
1:A:402:THR:HB	1:A:407:ASP:HB2	1.95	0.48
1:A:182:LEU:HD22	1:A:203:ILE:HD13	1.95	0.48
1:A:1064:CYS:HB2	1:A:1111:VAL:HG21	1.96	0.48
1:B:443:LEU:HB2	1:B:477:PRO:HB3	1.96	0.48
1:C:848:THR:HB	1:C:851:MET:HG2	1.96	0.47
1:B:704:ILE:HG12	1:B:1047:VAL:HG22	1.96	0.47
1:B:541:SER:HB3	1:B:543:LYS:HG2	1.97	0.47
1:A:140:VAL:O	1:A:238:PHE:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:659:SER:OG	1:C:660:TYR:N	2.47	0.47
1:C:48:ARG:HB2	1:C:266:TYR:CD2	2.50	0.47
1:A:99:ARG:HG3	1:A:138:PHE:HE2	1.80	0.47
1:A:267:ASP:OD1	1:A:271:THR:N	2.44	0.47
1:C:787:ILE:HD11	1:C:913:ILE:HD13	1.97	0.47
1:C:41:TYR:HB3	1:C:216:LEU:HB2	1.97	0.47
1:C:704:ILE:HG12	1:C:1047:VAL:HG22	1.96	0.47
1:A:693:THR:HA	1:A:1058:THR:HA	1.97	0.47
1:A:138:PHE:HB3	1:A:140:VAL:HG23	1.97	0.47
1:C:58:LEU:HB2	1:C:188:LYS:HE3	1.97	0.47
1:A:370:SER:HB3	1:C:967:ASP:HB2	1.97	0.46
1:B:399:PRO:HB3	1:B:414:ASP:HA	1.98	0.46
1:C:95:SER:OG	1:C:173:SER:O	2.26	0.46
1:A:797:ARG:HD2	1:A:805:PHE:HE2	1.79	0.46
1:B:95:SER:H	1:B:181:HIS:CD2	2.33	0.46
1:A:38:ARG:HD2	1:A:209:LEU:HD21	1.98	0.46
1:A:46:ILE:HG21	1:B:553:ARG:HD2	1.98	0.46
1:A:796:LYS:HD2	1:A:850:ASP:HB3	1.96	0.46
1:A:876:LEU:HA	1:B:695:ALA:HB3	1.96	0.46
1:C:72:ILE:HG13	1:C:75:THR:H	1.80	0.46
1:A:19:CYS:HA	1:A:133:CYS:HB3	1.98	0.46
1:A:209:LEU:HD12	1:A:210:PRO:HD2	1.97	0.46
1:B:321:ASN:HB3	1:B:348:CYS:HA	1.98	0.46
1:A:968:LYS:HG3	1:A:969:VAL:HG23	1.97	0.46
1:B:554:ASP:OD1	1:B:555:VAL:N	2.49	0.46
1:C:294:GLU:OE2	1:C:589:ASN:ND2	2.42	0.46
1:A:388:VAL:HG22	1:A:495:ARG:HG2	1.98	0.46
1:B:128:CYS:SG	1:B:129:ASN:N	2.88	0.46
1:A:127:ALA:HB3	1:A:161:PHE:HB3	1.98	0.46
1:B:968:LYS:HG3	1:B:969:VAL:H	1.80	0.46
1:A:378:CYS:HA	1:A:511:CYS:HA	1.98	0.46
1:A:787:ILE:HD11	1:A:913:ILE:HD13	1.98	0.46
1:A:561:SER:HA	1:A:571:LEU:HA	1.97	0.45
1:A:835:GLN:NE2	1:B:576:CYS:O	2.49	0.45
1:B:209:LEU:HD12	1:B:210:PRO:HD2	1.97	0.45
1:B:878:ILE:HG23	1:B:882:MET:HB2	1.97	0.45
1:B:1060:ALA:HB2	1:B:1080:ASN:HD22	1.80	0.45
1:C:383:TYR:O	1:C:499:LEU:HA	2.16	0.45
1:C:563:ARG:HH21	1:C:567:THR:HG23	1.81	0.45
1:C:959:LEU:HD23	1:C:962:ILE:HD11	1.96	0.45
1:A:694:ILE:N	1:A:1057:PHE:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:CYS:HA	1:C:511:CYS:HA	1.98	0.45
1:A:95:SER:OG	1:A:173:SER:O	2.24	0.45
1:A:430:ALA:O	1:A:485:THR:OG1	2.31	0.45
1:C:749:LEU:HD23	1:C:752:ILE:HD12	1.98	0.45
1:B:96:ASN:HA	1:B:183:ARG:HH12	1.81	0.45
1:A:832:ILE:O	1:B:632:GLN:NE2	2.49	0.45
1:C:603:CYS:SG	1:C:627:ASN:ND2	2.82	0.45
1:C:26:GLN:HB2	1:C:75:THR:HA	1.99	0.45
1:C:348:CYS:HB3	1:C:510:VAL:HB	1.99	0.45
1:A:1027:LYS:H	1:A:1048:THR:HG21	1.82	0.45
1:A:597:LEU:HD22	1:A:652:ILE:HG23	1.97	0.45
1:B:401:GLN:HE21	1:C:968:LYS:HG2	1.82	0.45
1:B:837:PHE:HB3	1:C:575:PRO:HD3	1.98	0.45
1:C:25:VAL:HA	1:C:76:PHE:HB3	1.98	0.45
1:C:95:SER:H	1:C:181:HIS:HD2	1.63	0.45
1:C:345:ILE:HB	1:C:382:VAL:HG23	1.98	0.44
1:B:699:ASN:HD22	1:B:700:PHE:H	1.64	0.44
1:C:444:ARG:NH1	1:C:447:LYS:O	2.50	0.44
1:C:894:THR:OG1	1:C:895:GLN:N	2.51	0.44
1:C:371:ALA:HA	1:C:374:LEU:HB2	2.00	0.44
1:A:95:SER:H	1:A:181:HIS:CD2	2.35	0.44
1:C:267:ASP:OD1	1:C:271:THR:N	2.40	0.44
1:A:112:GLN:HE22	1:B:456:SER:HB2	1.82	0.44
1:B:968:LYS:HG3	1:B:969:VAL:HG23	2.00	0.44
1:C:939:GLN:O	1:C:943:THR:OG1	2.25	0.44
1:A:205:VAL:HG21	1:A:210:PRO:HD3	2.00	0.44
1:A:292:SER:OG	1:A:293:PHE:N	2.51	0.44
1:A:122:ASN:ND2	1:A:165:SER:O	2.39	0.44
1:B:723:TYR:OH	1:B:944:LEU:O	2.31	0.44
1:C:1063:ILE:HG23	1:C:1115:ILE:HB	1.99	0.44
1:A:364:PHE:HD1	1:A:421:LEU:HD13	1.83	0.43
1:B:1029:TYR:HE2	1:B:1089:ARG:HH22	1.66	0.43
1:C:421:LEU:O	1:C:496:VAL:HA	2.18	0.43
1:B:1062:ALA:HB3	1:B:1111:VAL:HG13	1.99	0.43
1:C:422:ALA:HB2	1:C:496:VAL:HG22	2.00	0.43
1:C:436:TYR:HE1	1:C:482:GLY:HA2	1.83	0.43
1:A:884:MET:HA	1:A:887:ARG:HB2	1.99	0.43
1:B:355:LEU:HA	1:B:361:PHE:HE2	1.84	0.43
1:C:90:ALA:HA	1:C:183:ARG:O	2.18	0.43
1:B:25:VAL:HG13	1:B:76:PHE:HD2	1.84	0.43
1:B:876:LEU:HA	1:C:695:ALA:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:951:ASN:OD1	1:B:952:PHE:N	2.52	0.43
1:C:603:CYS:N	1:C:635:CYS:SG	2.91	0.43
1:A:656:ILE:HA	1:A:678:THR:HA	2.00	0.43
1:A:809:THR:H	1:A:931:GLN:HE21	1.67	0.43
1:B:1014:CYS:HB3	1:B:1030:HIS:CE1	2.53	0.43
1:C:484:TYR:HB2	1:C:487:THR:HG23	2.01	0.43
1:A:467:CYS:HB2	1:A:474:CYS:HB3	1.83	0.43
1:A:833:CYS:SG	1:B:632:GLN:NE2	2.90	0.43
1:A:965:ARG:HB2	1:B:369:VAL:HA	2.01	0.43
1:B:658:ALA:HA	1:B:676:ALA:HA	2.01	0.43
1:C:267:ASP:OD1	1:C:270:GLY:N	2.52	0.43
1:C:286:LEU:HD21	1:C:300:TYR:HD2	1.83	0.43
1:A:430:ALA:HB2	1:A:493:PRO:HG3	1.99	0.43
1:C:50:ASP:CA	1:C:266:TYR:O	2.67	0.43
1:C:389:VAL:HB	1:C:393:ASP:HB2	2.00	0.43
1:C:605:ASP:O	1:C:609:ALA:CB	2.66	0.43
1:A:457:ASN:HD21	1:A:476:TRP:HD1	1.67	0.43
1:A:784:PHE:HA	1:A:787:ILE:HD12	1.99	0.43
1:B:880:PHE:HB2	1:C:689:TYR:OH	2.19	0.43
1:C:469:PRO:HA	1:C:471:ALA:H	1.83	0.43
1:B:94:LYS:NZ	1:B:249:ALA:O	2.36	0.42
1:C:398:ALA:HB3	1:C:401:GLN:HG3	2.00	0.42
1:C:797:ARG:HD2	1:C:805:PHE:HE2	1.82	0.42
1:C:884:MET:HA	1:C:887:ARG:HB2	2.01	0.42
1:A:541:SER:HA	1:A:571:LEU:HG	2.01	0.42
1:A:762:GLU:O	1:A:766:GLN:NE2	2.43	0.42
1:B:946:LYS:O	1:B:949:SER:OG	2.30	0.42
1:C:652:ILE:HD12	1:C:656:ILE:HG22	2.01	0.42
1:A:756:GLN:HA	1:A:759:ASN:HD22	1.84	0.42
1:B:299:ILE:HG12	1:B:584:ILE:HG13	2.01	0.42
1:C:109:ASN:HA	1:C:131:GLU:HA	2.02	0.42
1:C:564:ASP:N	1:C:568:SER:O	2.41	0.42
1:A:967:ASP:HB2	1:B:370:SER:HB3	2.01	0.42
1:B:720:CYS:SG	1:B:746:ASN:ND2	2.92	0.42
1:C:352:TYR:HD1	1:C:355:LEU:HD12	1.83	0.42
1:B:91:ALA:HB1	1:B:93:GLU:HG2	2.02	0.42
1:A:93:GLU:HA	1:A:250:ALA:HB1	2.02	0.42
1:B:1097:ILE:HA	1:B:1101:ASN:HD22	1.84	0.42
1:A:100:GLY:HA3	1:A:234:ILE:HB	2.02	0.42
1:A:287:LYS:HA	1:A:295:ILE:HD11	2.01	0.42
1:B:138:PHE:HE1	1:B:152:ILE:HD11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:VAL:HB	1:B:220:PHE:HB2	2.02	0.42
1:B:287:LYS:HA	1:B:295:ILE:HD11	2.01	0.42
1:B:786:GLN:HB3	1:B:799:PHE:HB3	2.02	0.42
1:B:933:VAL:O	1:B:937:ASN:ND2	2.52	0.42
1:C:105:SER:O	1:C:229:THR:OG1	2.38	0.42
1:C:302:THR:OG1	1:C:303:SER:N	2.52	0.42
1:A:423:TRP:HE1	1:A:495:ARG:HD2	1.85	0.42
1:B:422:ALA:HA	1:B:495:ARG:O	2.20	0.42
1:B:656:ILE:HA	1:B:678:THR:HA	2.01	0.41
1:C:394:VAL:HG21	1:C:494:TYR:HD2	1.84	0.41
1:A:303:SER:OG	1:A:304:ASN:N	2.54	0.41
1:C:188:LYS:HB3	1:C:195:TYR:HB2	2.01	0.41
1:C:1031:LEU:HD12	1:C:1031:LEU:HA	1.92	0.41
1:A:237:ALA:HB1	1:A:245:TRP:HA	2.03	0.41
1:A:1030:HIS:HE1	1:A:1033:SER:HB2	1.86	0.41
1:B:1098:THR:H	1:B:1101:ASN:HD22	1.69	0.41
1:A:643:ASP:OD1	1:A:643:ASP:N	2.54	0.41
1:A:1032:MET:HB2	1:A:1047:VAL:HB	2.02	0.41
1:A:1049:TYR:CE2	1:A:1051:PRO:HG3	2.56	0.41
1:A:48:ARG:HB2	1:A:266:TYR:CE2	2.55	0.41
1:B:303:SER:OG	1:B:304:ASN:N	2.54	0.41
1:B:646:TYR:HB2	1:B:677:TYR:CZ	2.56	0.41
1:B:26:GLN:HB2	1:B:75:THR:HA	2.02	0.41
1:B:122:ASN:OD1	1:B:123:VAL:N	2.53	0.41
1:C:41:TYR:OH	1:C:188:LYS:NZ	2.48	0.41
1:C:964:SER:OG	1:C:965:ARG:N	2.54	0.41
1:A:96:ASN:HD22	1:A:171:ASP:H	1.69	0.41
1:A:286:LEU:HG	1:A:295:ILE:HD13	2.03	0.41
1:A:807:LYS:NZ	1:A:920:LEU:O	2.42	0.41
1:A:849:ASP:HA	1:A:852:ILE:HD12	2.03	0.41
1:B:187:PHE:HE1	1:B:196:VAL:HG13	1.86	0.41
1:B:1072:PRO:HB3	1:B:1086:ILE:HD13	2.01	0.41
1:C:122:ASN:OD1	1:C:123:VAL:N	2.54	0.41
1:C:678:THR:OG1	1:C:679:MET:N	2.51	0.41
1:A:302:THR:OG1	1:A:303:SER:N	2.51	0.41
1:B:39:GLY:HA3	1:B:60:LEU:HB3	2.03	0.41
1:B:430:ALA:O	1:B:485:THR:OG1	2.36	0.41
1:B:440:TYR:HE2	1:B:442:TYR:HB3	1.86	0.41
1:C:205:VAL:HG21	1:C:210:PRO:HD3	2.03	0.41
1:C:303:SER:OG	1:C:304:ASN:N	2.54	0.40
1:C:564:ASP:HA	1:C:565:PRO:HD3	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:TYR:CD1	1:A:218:PRO:HA	2.55	0.40
1:A:350:ALA:N	1:A:511:CYS:O	2.52	0.40
1:A:646:TYR:HB2	1:A:677:TYR:CZ	2.56	0.40
1:B:237:ALA:HB1	1:B:245:TRP:HA	2.03	0.40
1:B:1054:GLU:O	1:B:1055:ARG:NH1	2.53	0.40
1:C:197:TYR:CD1	1:C:218:PRO:HA	2.56	0.40
1:C:553:ARG:HD2	1:C:557:ASP:HA	2.02	0.40
1:A:591:SER:OG	1:A:592:SER:N	2.55	0.40
1:B:323:CYS:N	1:B:348:CYS:SG	2.94	0.40
1:B:628:VAL:HG13	1:B:641:HIS:CE1	2.56	0.40
1:C:646:TYR:HB2	1:C:677:TYR:CZ	2.57	0.40
1:A:723:TYR:OH	1:A:944:LEU:O	2.36	0.40
1:A:723:TYR:CZ	1:A:948:LEU:HG	2.56	0.40
1:B:180:LYS:HG3	1:B:202:PRO:HB3	2.02	0.40
1:B:685:SER:OG	1:B:686:SER:N	2.54	0.40
1:B:960:ASN:HA	1:B:963:LEU:HB2	2.03	0.40
1:C:122:ASN:ND2	1:C:165:SER:O	2.42	0.40
1:C:1031:LEU:N	1:C:1047:VAL:O	2.52	0.40
1:A:987:GLN:NE2	1:B:988:THR:OG1	2.55	0.40
1:B:123:VAL:HB	1:B:165:SER:HB3	2.02	0.40
1:B:865:THR:HA	1:C:689:TYR:CE1	2.56	0.40
1:B:895:GLN:HG3	1:C:1074:GLU:HG2	2.04	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 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	1057/1203 (88%)	892 (84%)	160 (15%)	5 (0%)	29	67
1	B	1057/1203 (88%)	900 (85%)	151 (14%)	6 (1%)	25	63
1	C	1045/1203 (87%)	897 (86%)	142 (14%)	6 (1%)	25	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3159/3609 (88%)	2689 (85%)	453 (14%)	17 (0%)	32 67

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	632	GLN
1	C	632	GLN
1	A	632	GLN
1	A	692	ASN
1	A	1072	PRO
1	B	692	ASN
1	B	1072	PRO
1	C	692	ASN
1	C	1072	PRO
1	A	691	ASN
1	C	557	ASP
1	C	691	ASN
1	B	691	ASN
1	C	1076	VAL
1	B	1075	GLY
1	A	1076	VAL
1	B	1076	VAL

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 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	922/1048 (88%)	920 (100%)	2 (0%)	93 96
1	B	922/1048 (88%)	920 (100%)	2 (0%)	93 96
1	C	914/1048 (87%)	911 (100%)	3 (0%)	92 95
All	All	2758/3144 (88%)	2751 (100%)	7 (0%)	92 95

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	699	ASN
1	A	965	ARG
1	B	699	ASN
1	B	965	ARG
1	C	333	LYS
1	C	699	ASN
1	C	965	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	147	GLN
1	A	149	HIS
1	A	181	HIS
1	A	479	ASN
1	A	632	GLN
1	A	699	ASN
1	A	733	ASN
1	A	759	ASN
1	A	931	GLN
1	A	935	ASN
1	A	942	ASN
1	A	987	GLN
1	A	1030	HIS
1	B	129	ASN
1	B	181	HIS
1	B	304	ASN
1	B	401	GLN
1	B	409	ASN
1	B	445	HIS
1	B	632	GLN
1	B	699	ASN
1	B	759	ASN
1	B	769	GLN
1	B	937	ASN
1	B	984	GLN
1	B	987	GLN
1	B	1030	HIS
1	B	1101	ASN
1	C	147	GLN
1	C	181	HIS
1	C	304	ASN

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Mol	Chain	Res	Type
1	C	632	GLN
1	C	692	ASN
1	C	699	ASN
1	C	769	GLN
1	C	835	GLN
1	C	947	GLN
1	C	984	GLN
1	C	987	GLN
1	C	993	GLN
1	C	1101	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

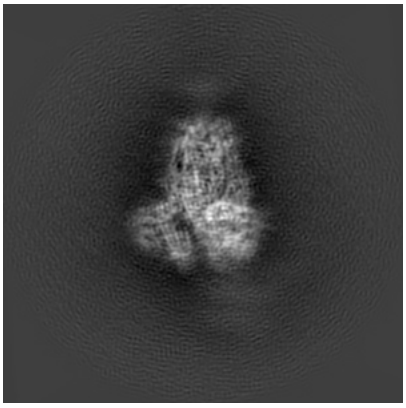
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9589. These allow visual inspection of the internal detail of the map and identification of artifacts.

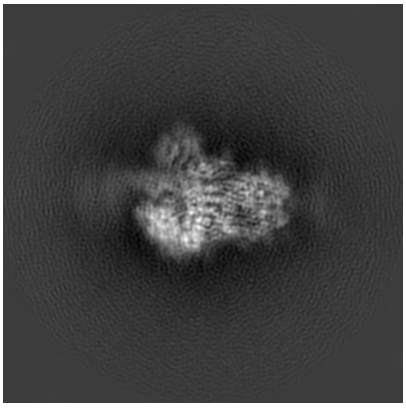
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

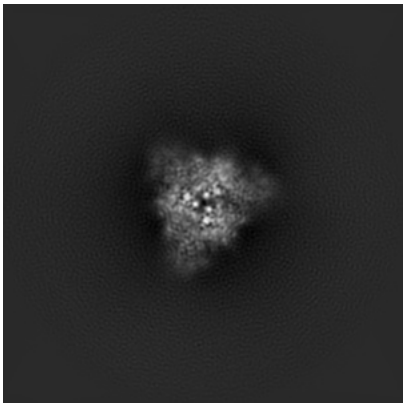
6.1.1 Primary map



X



Y

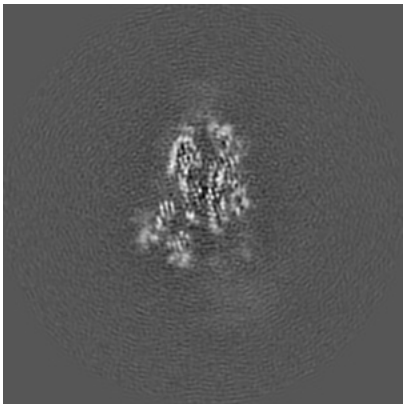


Z

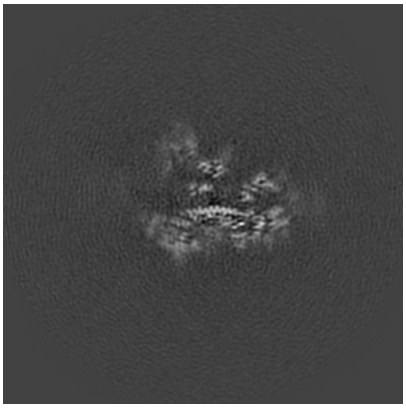
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

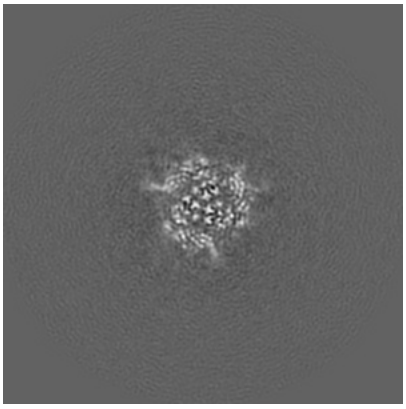
6.2.1 Primary map



X Index: 144



Y Index: 144

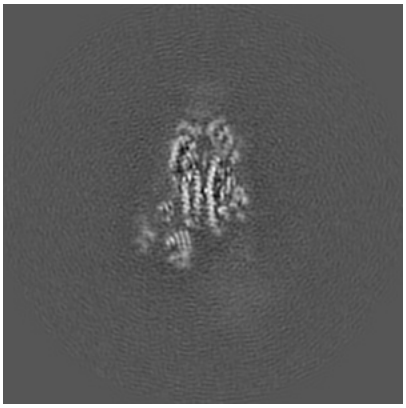


Z Index: 144

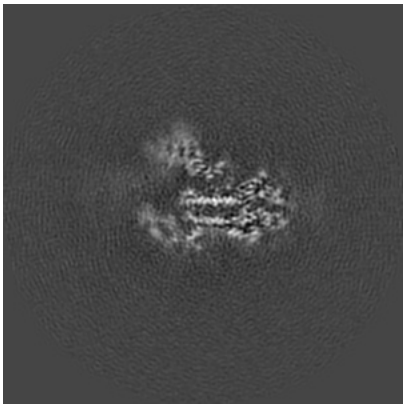
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

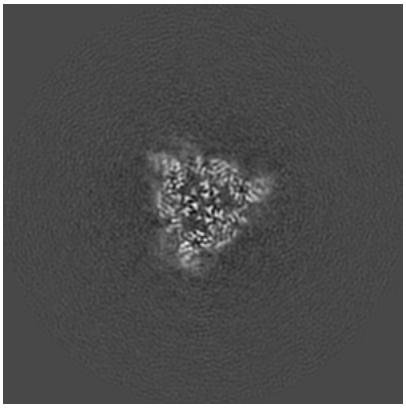
6.3.1 Primary map



X Index: 146



Y Index: 149

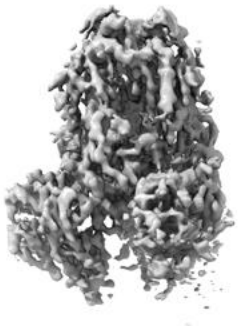


Z Index: 140

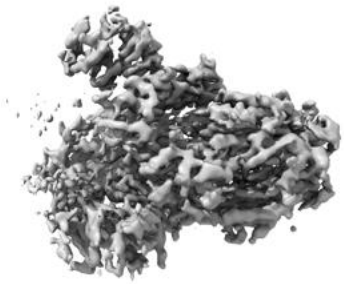
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

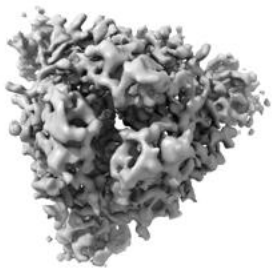
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

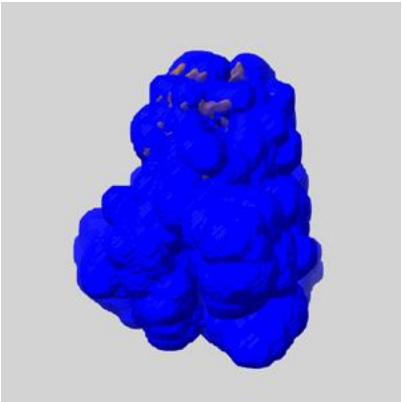
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

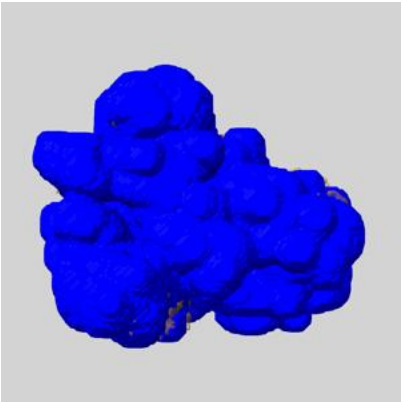
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

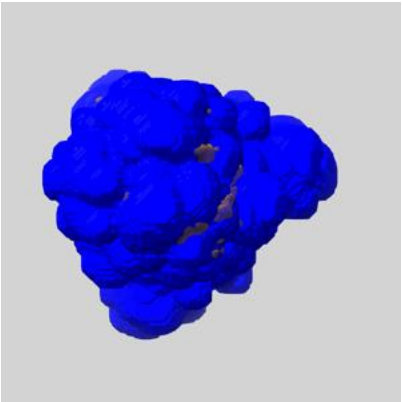
6.5.1 emd_9589_msk_1.map (i)



X



Y

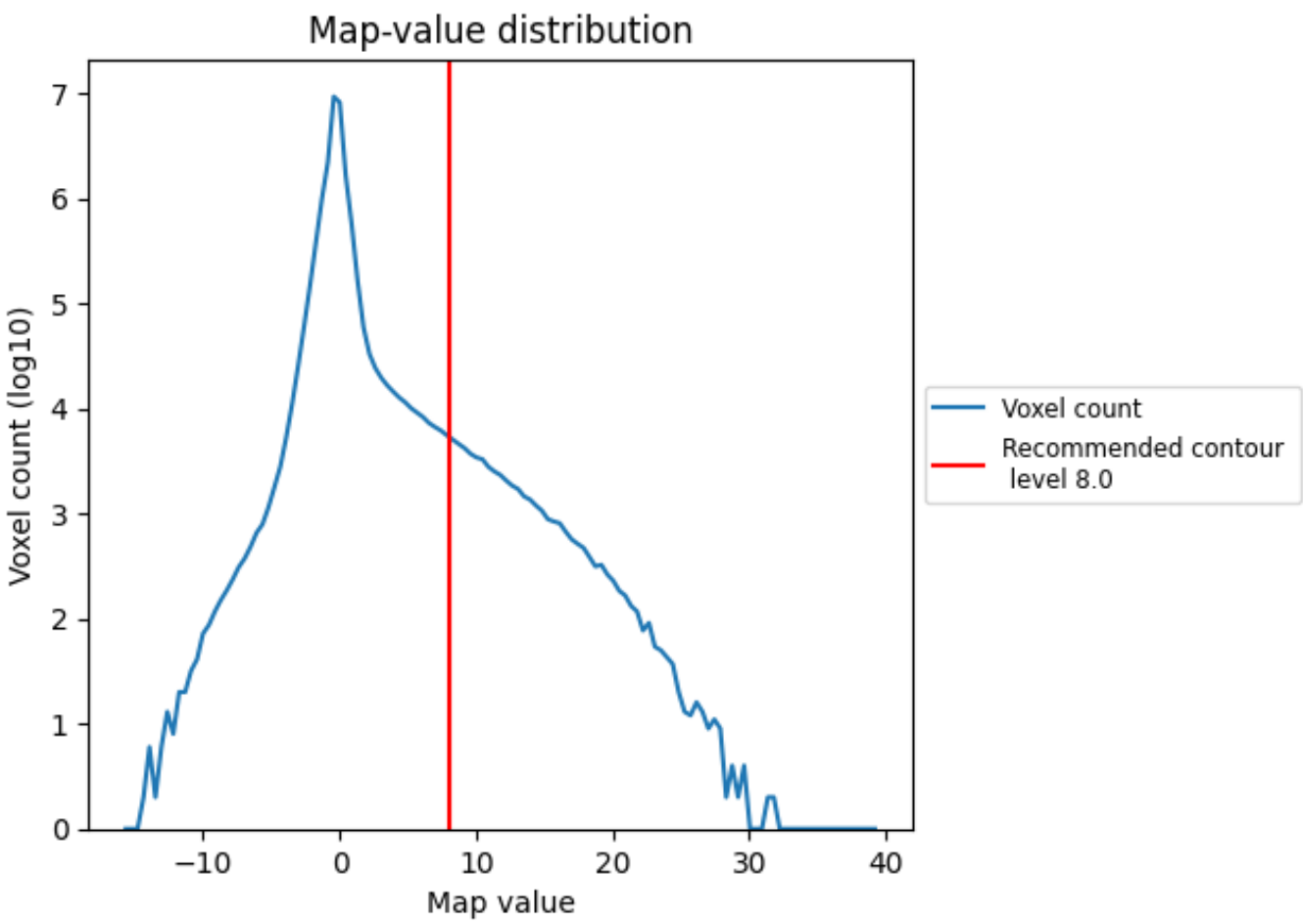


Z

7 Map analysis (i)

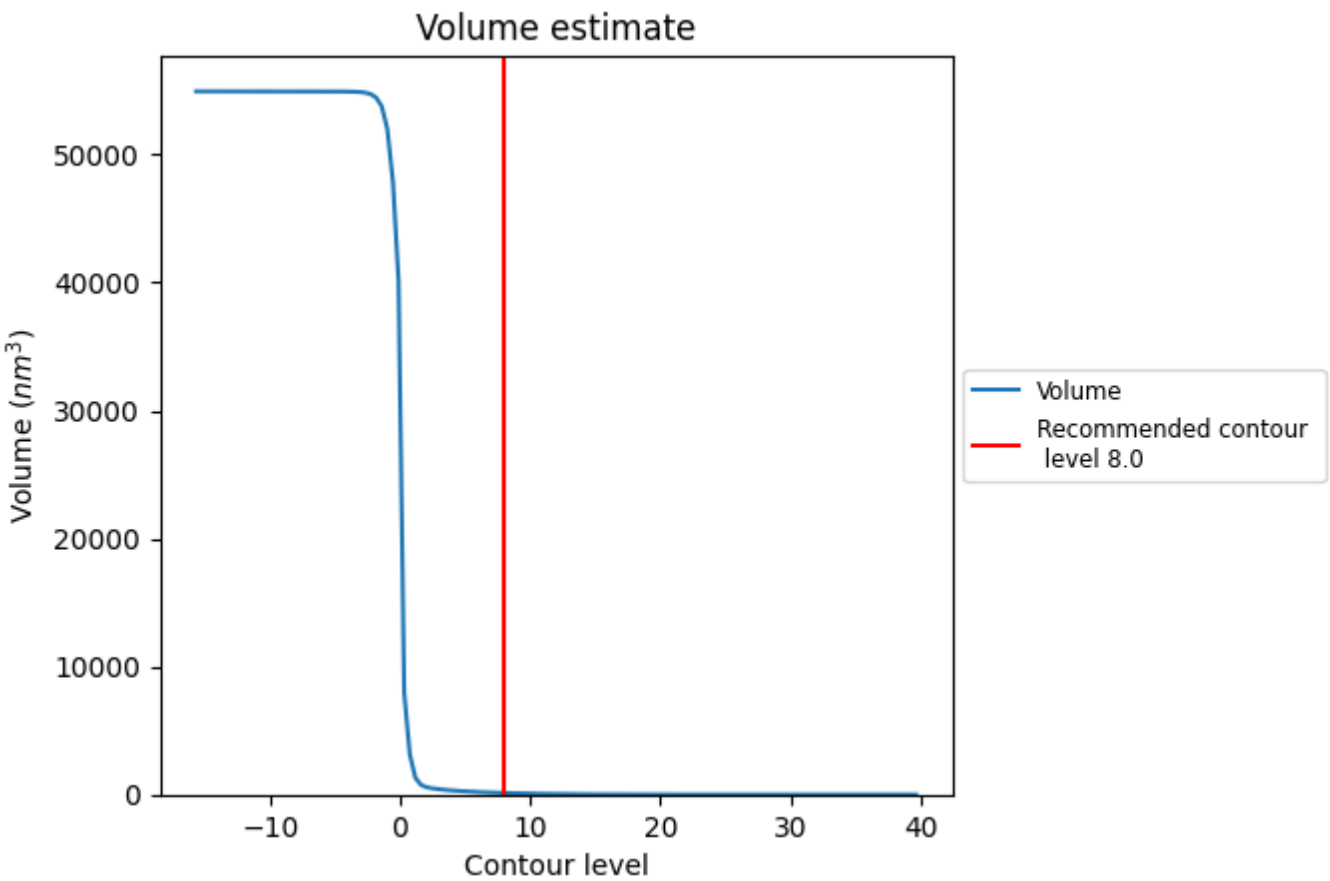
This section contains the results of statistical analysis of the map.

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.

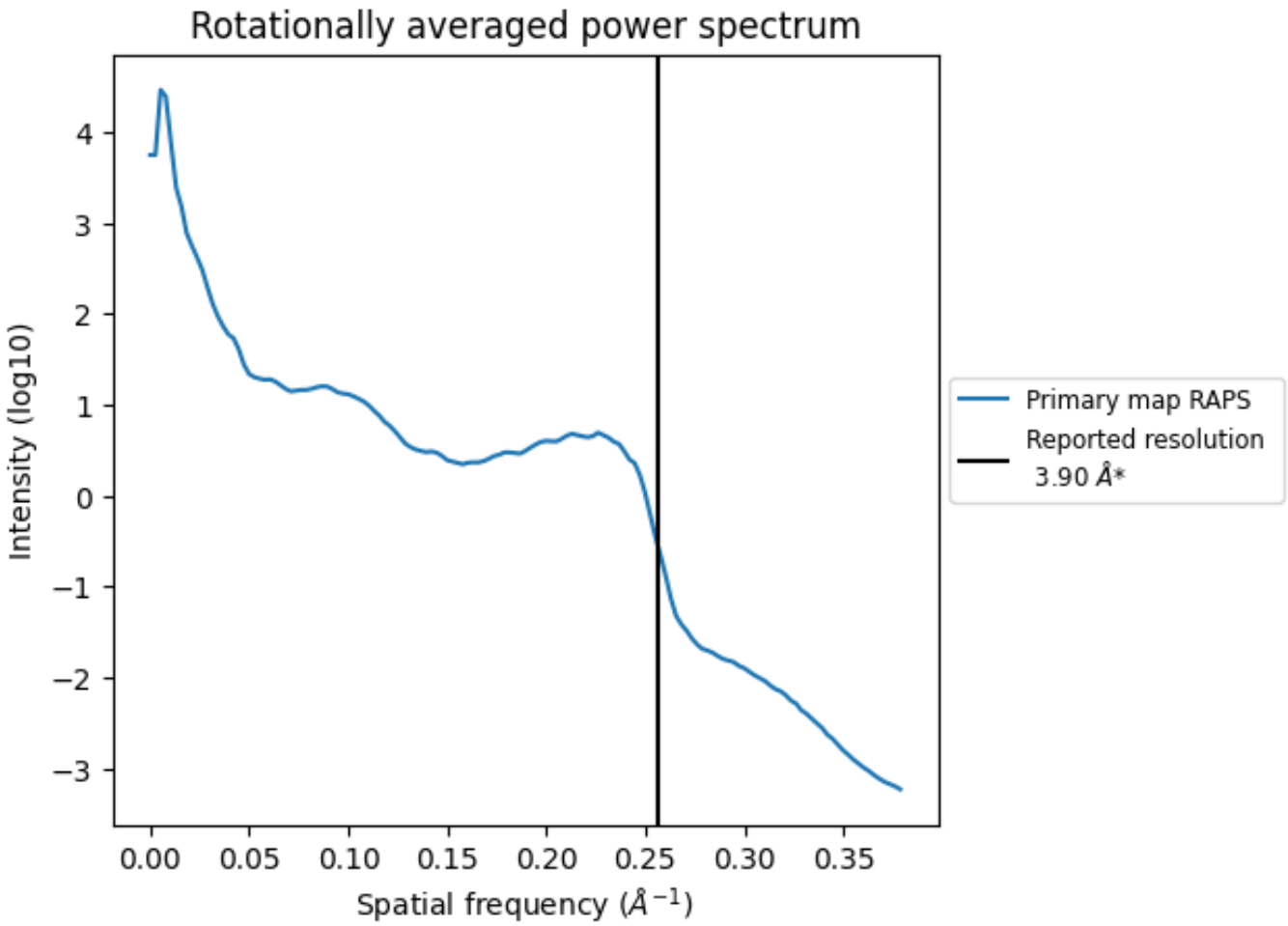
7.2 Volume estimate (i)



The volume at the recommended contour level is 123 nm^3; this corresponds to an approximate mass of 111 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 (i)

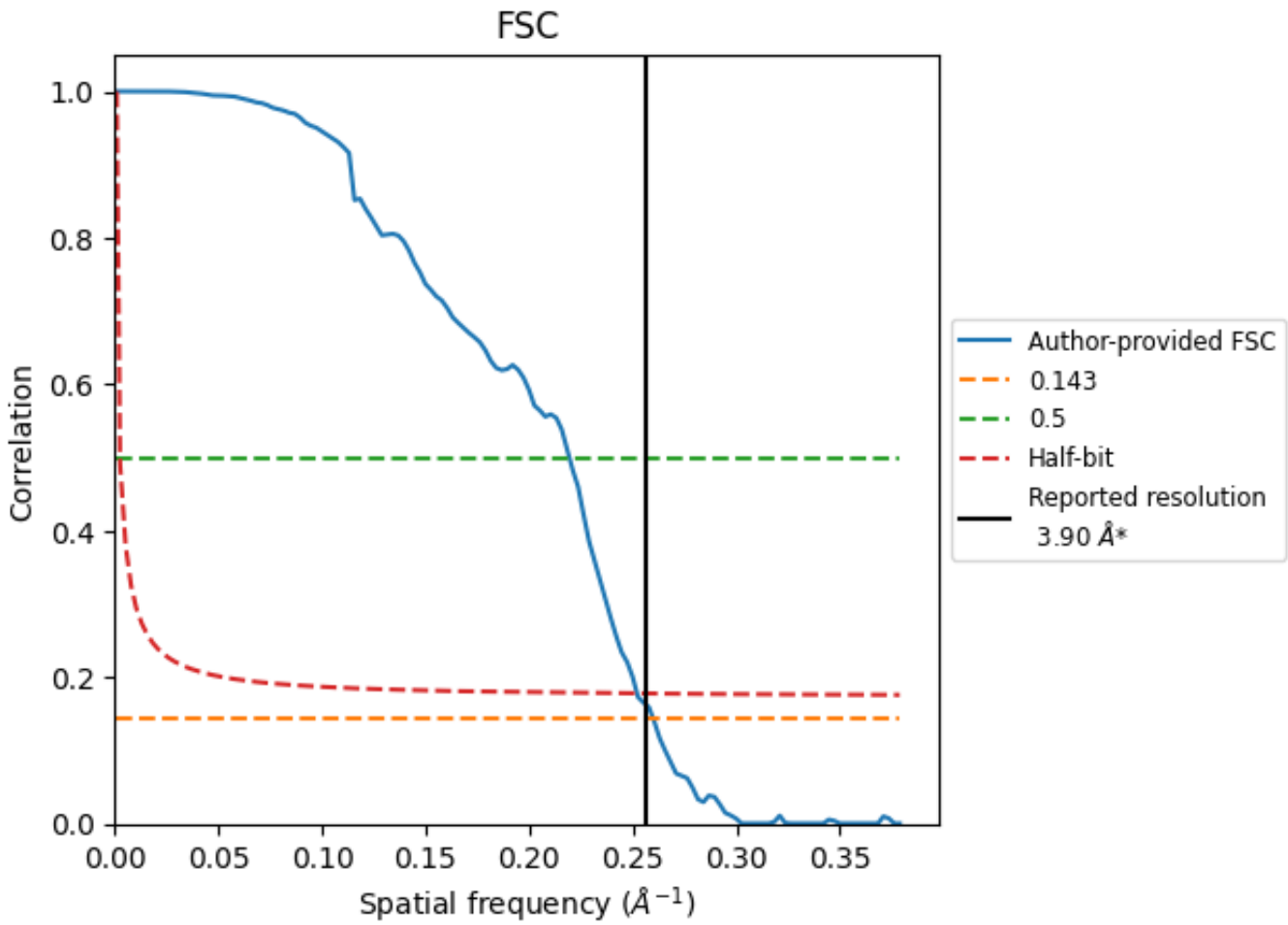


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

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 0.256 Å^{-1}

8.2 Resolution estimates (i)

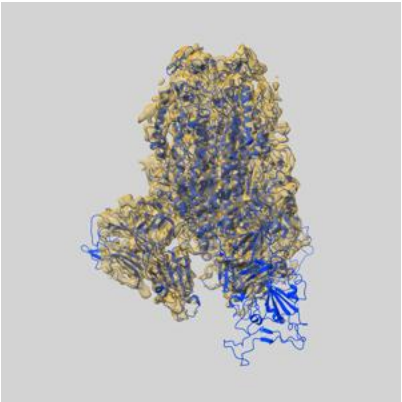
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.85	4.56	3.97
Unmasked-calculated*	-	-	-

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

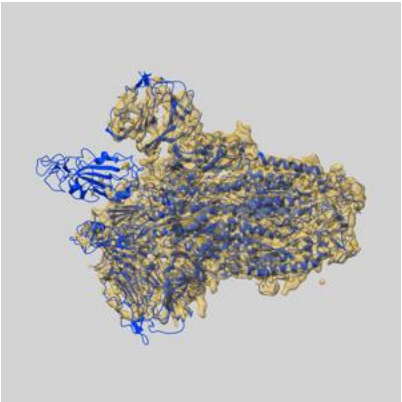
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9589 and PDB model 6ACD. Per-residue inclusion information can be found in section 3 on page 4.

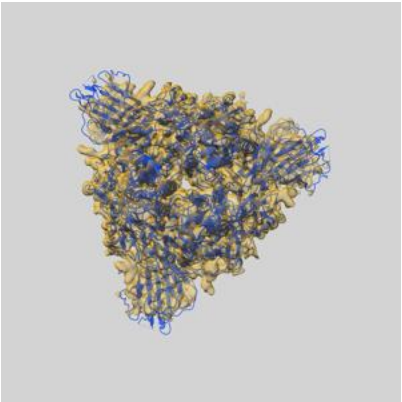
9.1 Map-model overlay (i)



X



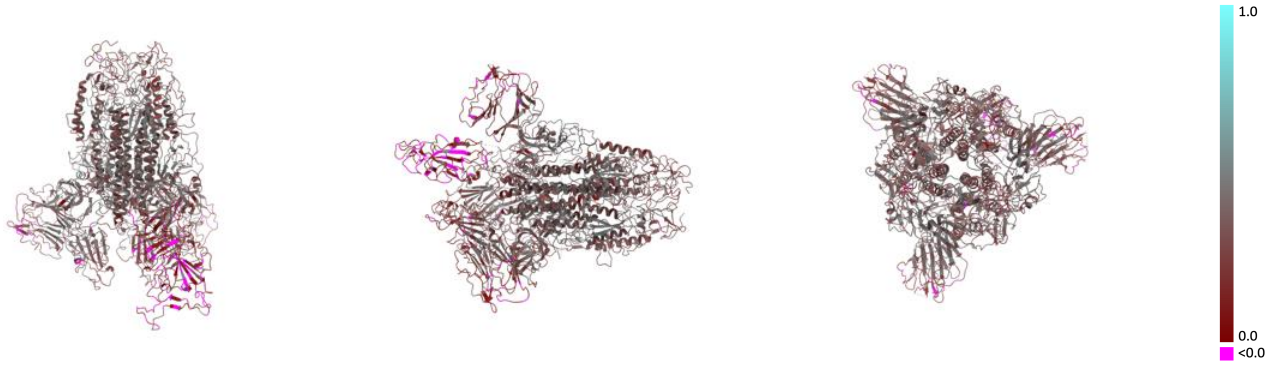
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.0 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.

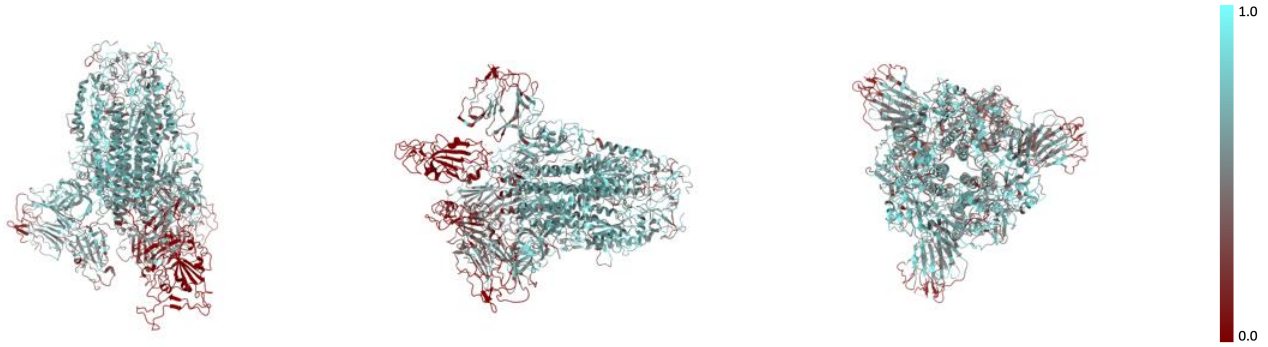
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

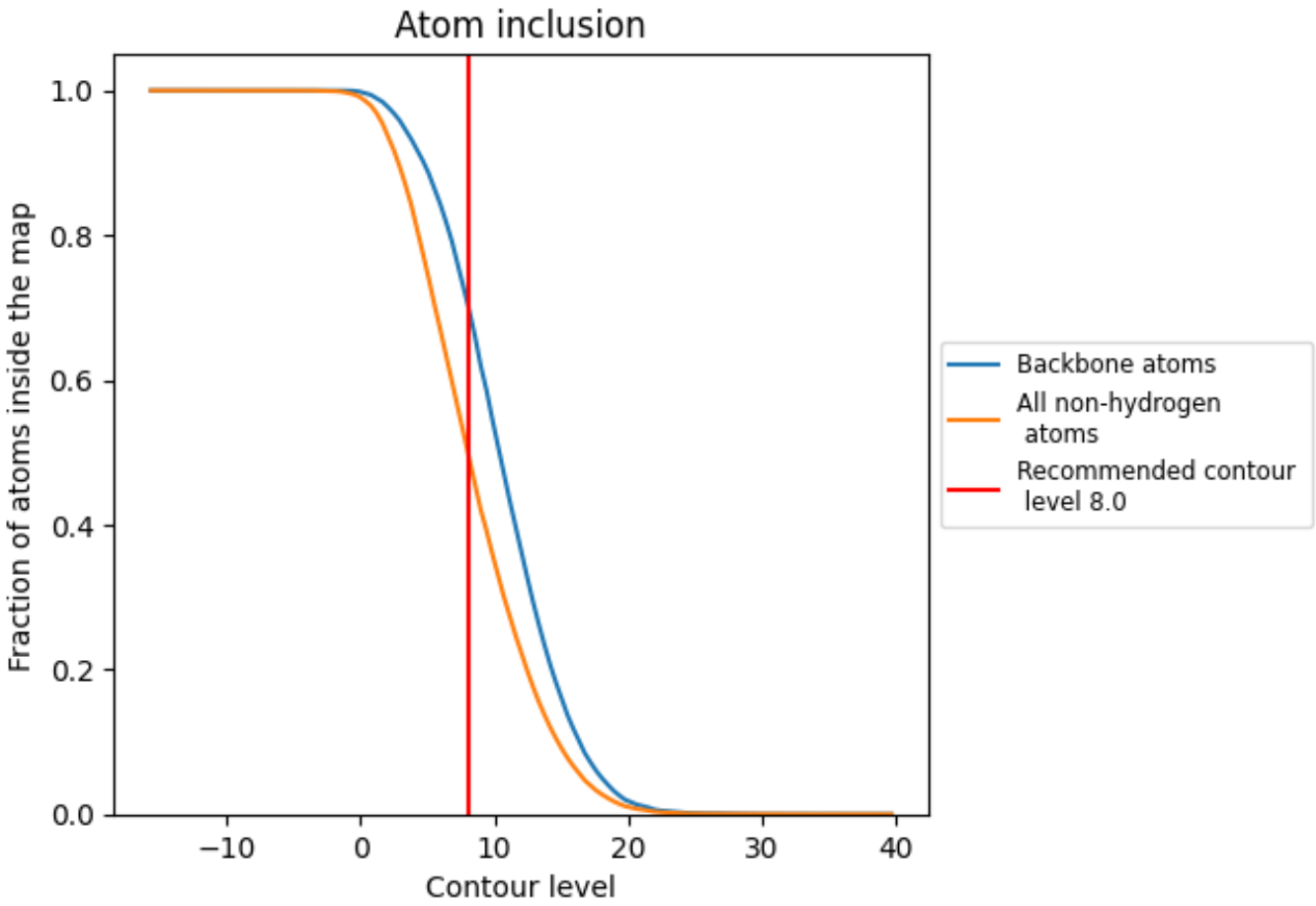
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (8.0).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (8.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5000	0.3240
A	0.5231	0.3400
B	0.5267	0.3320
C	0.4500	0.3000