Full wwPDB EM Validation Report (i)

Nov 29, 2022 – 12:09 PM JST

PDB ID	:	7WD0
EMDB ID	:	EMD-32431
Title	:	SARS-CoV-2 Beta spike in complex with two S5D2 Fabs
Authors	:	Wang, Y.F.; Cong, Y.
Deposited on	:	2021-12-20
Resolution	:	3.30 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:

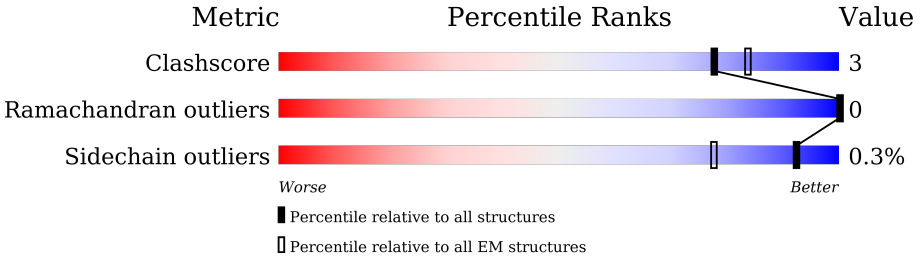
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.30 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	1258	. 79% 7% 14%
1	B	1258	6% 78% 8% 14%
1	C	1258	6% 77% 8% 14%
2	a	214	26% 99% .
2	c	214	55% 100%
3	b	217	29% 99% .
3	d	217	67% 100%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 31996 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	1079	8454	5399	1410	1606	39	0	0
1	B	1079	8454	5399	1410	1606	39	0	0
1	C	1079	8454	5399	1410	1606	39	0	0

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	PHE	LEU	variant	UNP P0DTC2
A	80	ALA	ASP	variant	UNP P0DTC2
A	215	GLY	ASP	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	246	ILE	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	484	LYS	GLU	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	682	GLY	ARG	variant	UNP P0DTC2
A	683	SER	ARG	variant	UNP P0DTC2
A	685	SER	ARG	variant	UNP P0DTC2
A	701	VAL	ALA	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1207	GLU	-	expression tag	UNP P0DTC2
A	1208	GLN	-	expression tag	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLU	-	expression tag	UNP P0DTC2
A	1239	ASN	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	TYR	-	expression tag	UNP P0DTC2
A	1242	PHE	-	expression tag	UNP P0DTC2
A	1243	GLN	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	ASP	-	expression tag	UNP P0DTC2
A	1246	TYR	-	expression tag	UNP P0DTC2
A	1247	LYS	-	expression tag	UNP P0DTC2
A	1248	ASP	-	expression tag	UNP P0DTC2
A	1249	ASP	-	expression tag	UNP P0DTC2
A	1250	ASP	-	expression tag	UNP P0DTC2
A	1251	ASP	-	expression tag	UNP P0DTC2
A	1252	LYS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2
A	1261	HIS	-	expression tag	UNP P0DTC2
B	18	PHE	LEU	variant	UNP P0DTC2
B	80	ALA	ASP	variant	UNP P0DTC2
B	215	GLY	ASP	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	246	ILE	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	484	LYS	GLU	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	682	GLY	ARG	variant	UNP P0DTC2
B	683	SER	ARG	variant	UNP P0DTC2
B	685	SER	ARG	variant	UNP P0DTC2
B	701	VAL	ALA	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1207	GLU	-	expression tag	UNP P0DTC2
B	1208	GLN	-	expression tag	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLU	-	expression tag	UNP P0DTC2
B	1239	ASN	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	TYR	-	expression tag	UNP P0DTC2
B	1242	PHE	-	expression tag	UNP P0DTC2
B	1243	GLN	-	expression tag	UNP P0DTC2
B	1244	GLY	-	expression tag	UNP P0DTC2
B	1245	ASP	-	expression tag	UNP P0DTC2
B	1246	TYR	-	expression tag	UNP P0DTC2
B	1247	LYS	-	expression tag	UNP P0DTC2
B	1248	ASP	-	expression tag	UNP P0DTC2
B	1249	ASP	-	expression tag	UNP P0DTC2
B	1250	ASP	-	expression tag	UNP P0DTC2
B	1251	ASP	-	expression tag	UNP P0DTC2
B	1252	LYS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
B	1261	HIS	-	expression tag	UNP P0DTC2
C	18	PHE	LEU	variant	UNP P0DTC2
C	80	ALA	ASP	variant	UNP P0DTC2
C	215	GLY	ASP	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	246	ILE	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	484	LYS	GLU	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	682	GLY	ARG	variant	UNP P0DTC2
C	683	SER	ARG	variant	UNP P0DTC2
C	685	SER	ARG	variant	UNP P0DTC2
C	701	VAL	ALA	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1207	GLU	-	expression tag	UNP P0DTC2
C	1208	GLN	-	expression tag	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1238	GLU	-	expression tag	UNP P0DTC2
C	1239	ASN	-	expression tag	UNP P0DTC2
C	1240	LEU	-	expression tag	UNP P0DTC2
C	1241	TYR	-	expression tag	UNP P0DTC2
C	1242	PHE	-	expression tag	UNP P0DTC2
C	1243	GLN	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2
C	1245	ASP	-	expression tag	UNP P0DTC2
C	1246	TYR	-	expression tag	UNP P0DTC2
C	1247	LYS	-	expression tag	UNP P0DTC2
C	1248	ASP	-	expression tag	UNP P0DTC2
C	1249	ASP	-	expression tag	UNP P0DTC2
C	1250	ASP	-	expression tag	UNP P0DTC2
C	1251	ASP	-	expression tag	UNP P0DTC2
C	1252	LYS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2
C	1260	HIS	-	expression tag	UNP P0DTC2
C	1261	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Heavy chain of S5D2 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	a	214	1627	1031	260	329	7	0	0
			Total	C	N	O	S		
2	c	214	1627	1031	260	329	7	0	0

- Molecule 3 is a protein called Light chain of S5D2 Fab.

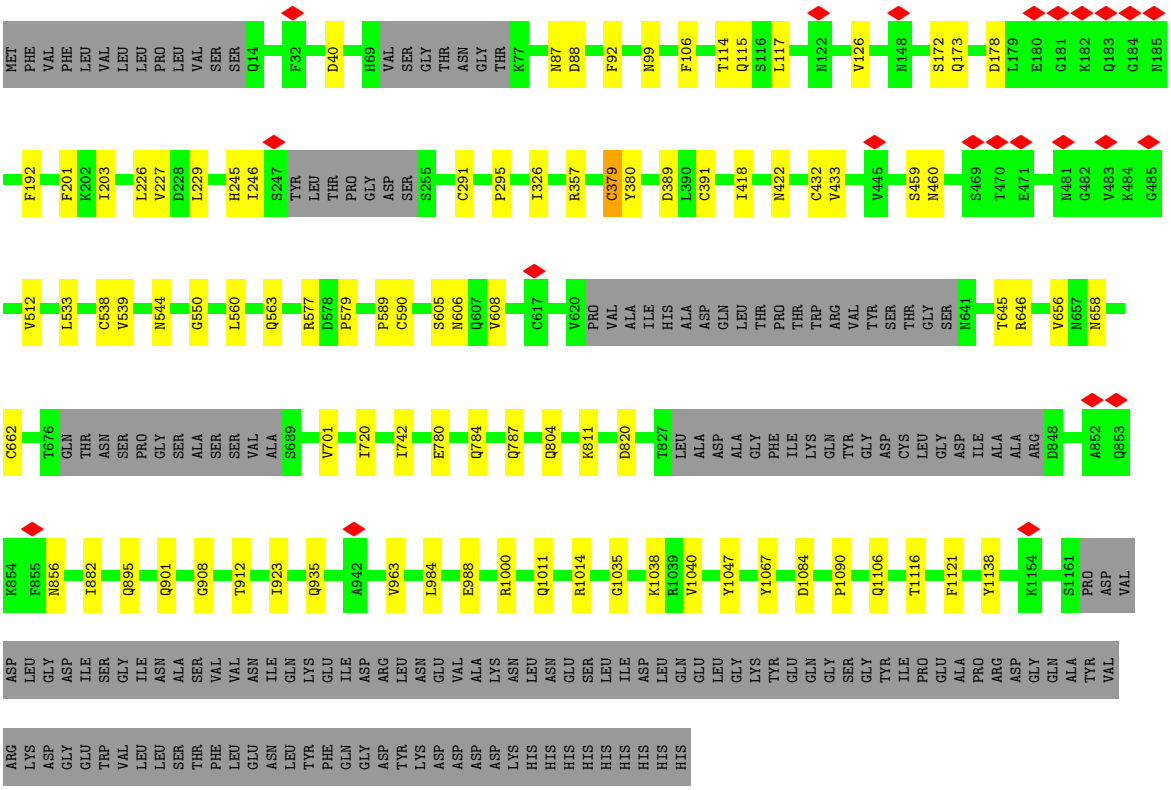
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	b	217	1690	1058	280	346	6	0	0
			Total	C	N	O	S		
3	d	217	1690	1058	280	346	6	0	0

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.

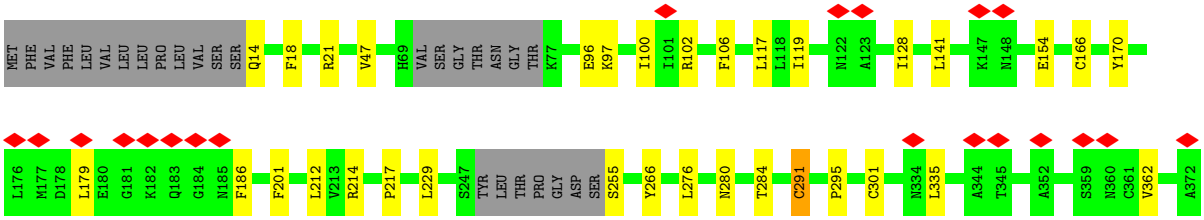
• Molecule 1: Spike glycoprotein

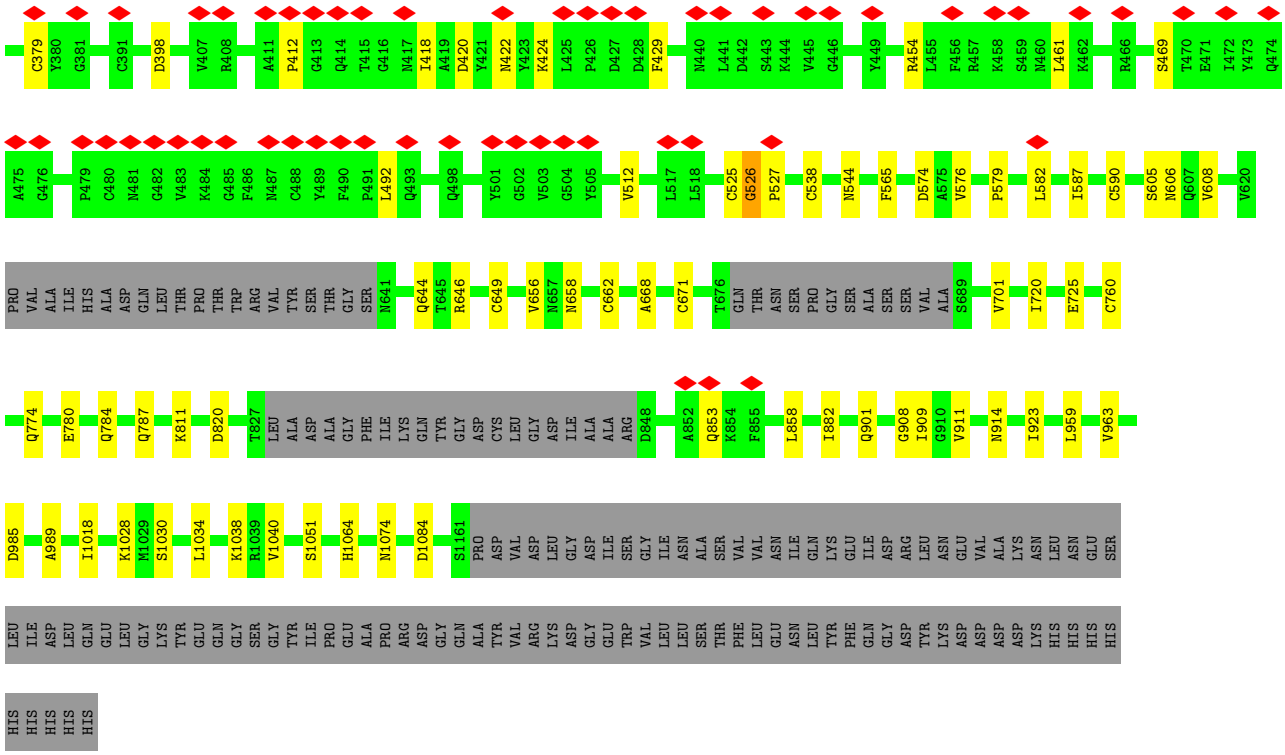
Chain A:



• Molecule 1: Spike glycoprotein

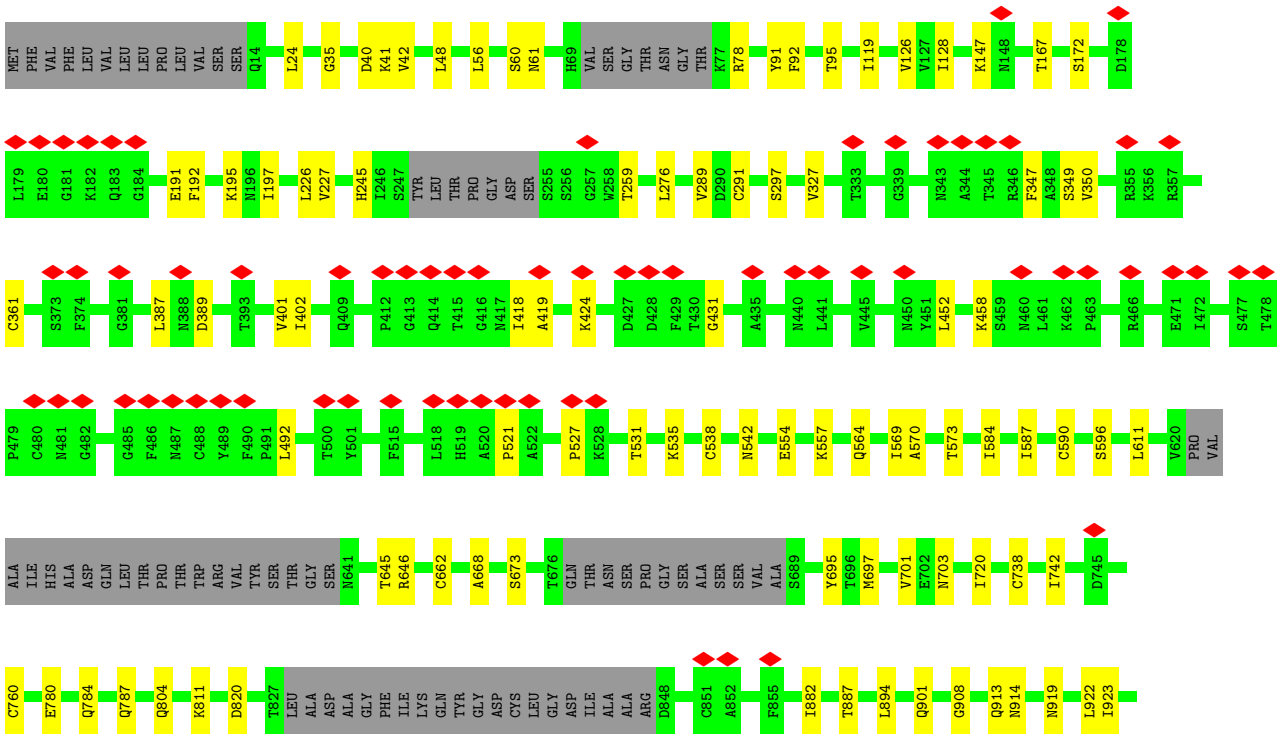
Chain B:

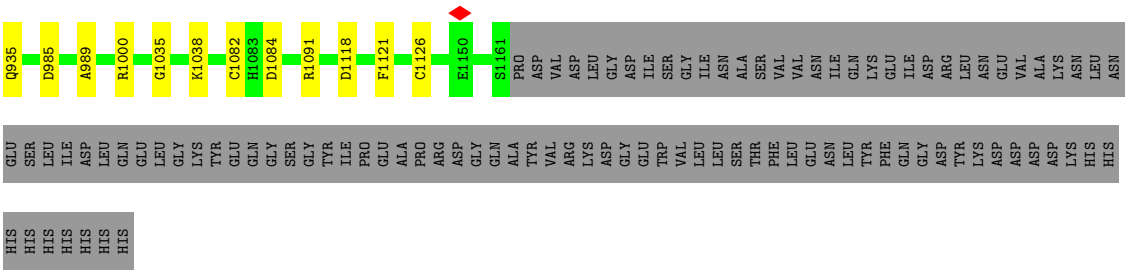




- Molecule 1: Spike glycoprotein

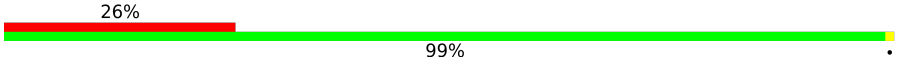
Chain C:

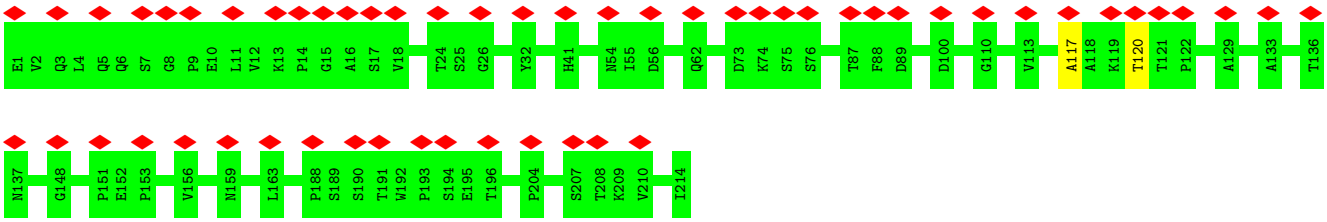




• Molecule 2: Heavy chain of S5D2 Fab

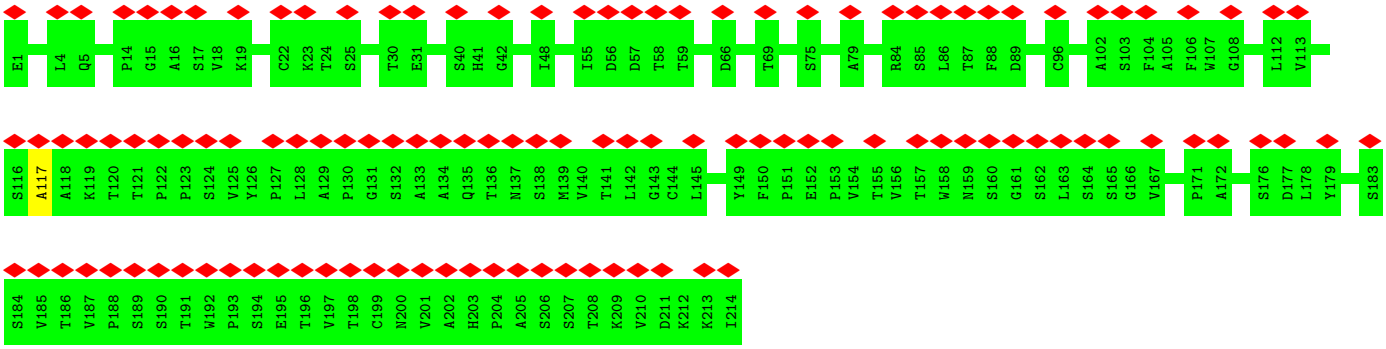
Chain a:





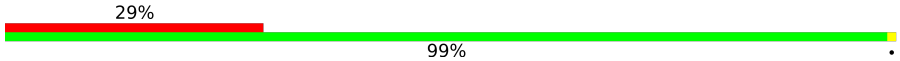
• Molecule 2: Heavy chain of S5D2 Fab

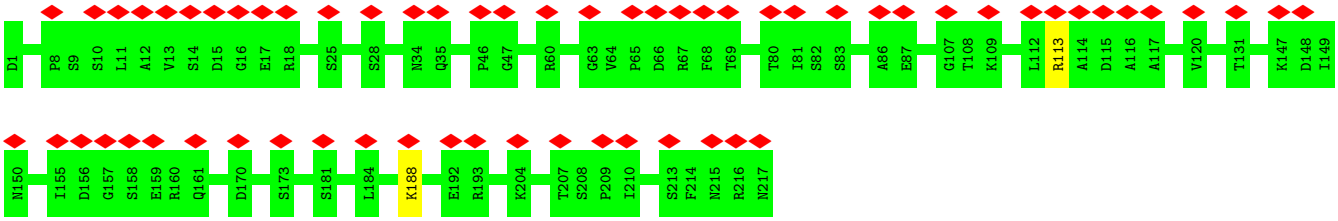
Chain c:



• Molecule 3: Light chain of S5D2 Fab

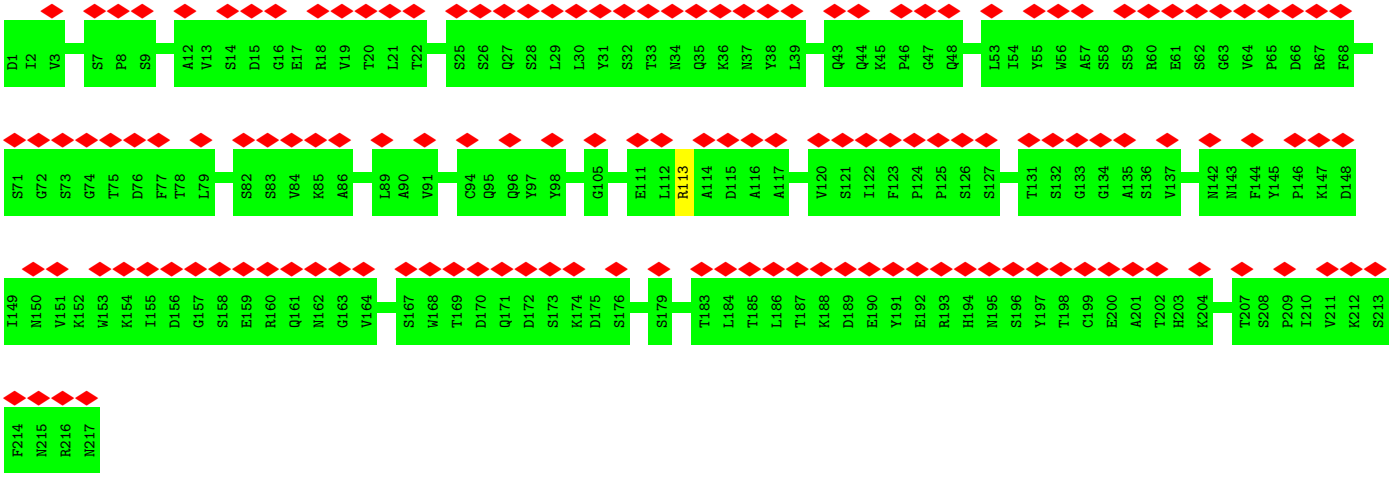
Chain b:





• Molecule 3: Light chain of S5D2 Fab

Chain d:


D1 I2 V3
S7 P8 S9
A12 V13 S14 D15 G16 E17 R18 V19 T20 L21 T22
S25 S26 Q27 S28 L29 L30 Y31 S32 T33 N34 Q35 K36 N37 Y38 L39
Q43 Q44 K45 P46 G47 Q48
L53 I54 Y55 W56 A57 S58 S59 R60 E61 S62 G63 V64 P65 D66 R67 F68
S71 G72 S73 G74 T75 D76 F77 T78 L79
S82 S83 V84 K85 A86
L89 A90 V91
C94 Q95 Q96 Y97 Y98
G105
E111 I112 R113 A114 D115 A116 A117
V120 S121 I122 F123 P124 P125 S126 S127
T131 S132 G133 G134 A135 S136 V137
N142 N143 F144 Y145 P146 K147 D148
I149 N150 V151 K152 W153 K154 I155 D156 G157 S158 E159 R160 Q161 N162 G163 V164
S167 W168 T169 D170 Q171 D172 S173 K174 D175 S176
S179
T183 L184 T185 L186 T187 K188 D189 E190 Y191 E192 R193 H194 N195 S196 Y197 T198 C199 E200 A201 T202 H203 K204
T207 S208 P209 I210 V211 K212 S213
F214 N215 R216 N217

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	129238	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)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.037	Depositor
Minimum map value	-1.612	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.095	Depositor
Recommended contour level	0.66	Depositor
Map size (Å)	437.2, 437.2, 437.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.093, 1.093, 1.093	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	0.26	0/8651	0.45	1/11765 (0.0%)
1	B	0.27	0/8651	0.47	2/11765 (0.0%)
1	C	0.26	0/8649	0.47	0/11759
2	a	0.26	0/1670	0.48	0/2283
2	c	0.26	0/1670	0.48	0/2283
3	b	0.27	0/1729	0.48	0/2349
3	d	0.28	0/1729	0.50	0/2349
All	All	0.26	0/32749	0.47	3/44553 (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	2
1	B	0	5
1	C	0	4
2	a	0	2
2	c	0	2
3	b	0	2
3	d	0	2
All	All	0	19

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	492	LEU	CA-CB-CG	8.57	135.00	115.30
1	B	582	LEU	CA-CB-CG	6.45	130.12	115.30
1	A	379	CYS	CA-CB-SG	6.12	125.02	114.00

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	CYS	Mainchain,Peptide
1	B	291	CYS	Mainchain,Peptide
1	B	335	LEU	Mainchain,Peptide
1	B	526	GLY	Mainchain
1	C	291	CYS	Mainchain,Peptide
1	C	361	CYS	Peptide
1	C	531	THR	Peptide
2	a	117	ALA	Mainchain,Peptide
3	b	113	ARG	Mainchain,Peptide
2	c	117	ALA	Mainchain,Peptide
3	d	113	ARG	Mainchain,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	8454	0	8243	50	0
1	B	8454	0	8249	56	0
1	C	8454	0	8245	58	0
2	a	1627	0	1572	0	0
2	c	1627	0	1572	0	0
3	b	1690	0	1621	0	0
3	d	1690	0	1621	0	0
All	All	31996	0	31123	150	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 3.

All (150) 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:B:14:GLN:N	1:B:255:SER:HG	1.89	0.69
1:A:1035:GLY:HA3	1:B:1040:VAL:HG21	1.84	0.60
1:B:1051:SER:HG	1:B:1064:HIS:HD1	1.50	0.58
1:A:720:ILE:HG13	1:A:923:ILE:HG23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:HG	1:A:227:VAL:HG23	1.85	0.57
1:A:563:GLN:HE21	1:C:41:LYS:HA	1.71	0.56
1:A:912:THR:OG1	1:A:1106:GLN:NE2	2.39	0.56
1:C:662:CYS:HB2	1:C:697:MET:HG3	1.87	0.56
1:C:720:ILE:HG13	1:C:923:ILE:HG23	1.88	0.55
1:B:720:ILE:HG13	1:B:923:ILE:HG23	1.88	0.54
1:A:787:GLN:NE2	1:B:701:VAL:O	2.39	0.54
1:C:119:ILE:HG12	1:C:128:ILE:HG12	1.90	0.54
1:A:203:ILE:HD11	1:A:229:LEU:HD11	1.91	0.53
1:A:560:LEU:O	1:A:577:ARG:NH2	2.42	0.52
1:A:1040:VAL:HG21	1:C:1035:GLY:HA3	1.91	0.52
1:B:853:GLN:HB3	1:B:858:LEU:HB2	1.91	0.52
1:C:347:PHE:HB2	1:C:401:VAL:HG23	1.90	0.52
1:A:295:PRO:HB2	1:A:608:VAL:HG11	1.91	0.52
1:A:895:GLN:NE2	1:B:1074:ASN:OD1	2.43	0.52
1:B:787:GLN:NE2	1:C:701:VAL:O	2.43	0.52
1:A:1121:PHE:HE1	1:C:914:ASN:HD21	1.58	0.51
1:A:433:VAL:HG22	1:A:512:VAL:HG13	1.91	0.51
1:B:398:ASP:HB2	1:B:512:VAL:HB	1.92	0.51
1:A:780:GLU:O	1:A:784:GLN:NE2	2.43	0.51
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.44	0.51
1:B:276:LEU:HD11	1:B:301:CYS:HA	1.93	0.51
1:B:420:ASP:OD1	1:B:424:LYS:NZ	2.44	0.51
1:A:357:ARG:HH12	1:C:167:THR:HG22	1.75	0.50
1:B:212:LEU:HB3	1:B:217:PRO:HB3	1.92	0.50
1:C:389:ASP:HA	1:C:527:PRO:HD3	1.92	0.50
1:A:172:SER:OG	1:A:173:GLN:N	2.44	0.50
1:B:908:GLY:O	1:B:1038:LYS:NZ	2.44	0.50
1:C:327:VAL:HG13	1:C:542:ASN:HB3	1.92	0.50
1:B:201:PHE:HB2	1:B:229:LEU:HB2	1.93	0.50
1:B:787:GLN:HE22	1:C:701:VAL:HG13	1.75	0.50
1:C:780:GLU:O	1:C:784:GLN:NE2	2.45	0.50
1:B:422:ASN:HA	1:B:461:LEU:HD12	1.94	0.50
1:A:418:ILE:HA	1:A:422:ASN:HD22	1.76	0.50
1:A:701:VAL:O	1:C:787:GLN:NE2	2.41	0.50
1:B:780:GLU:O	1:B:784:GLN:NE2	2.44	0.49
1:C:92:PHE:HB2	1:C:192:PHE:HB2	1.93	0.49
1:C:452:LEU:HD13	1:C:492:LEU:HD21	1.94	0.49
1:A:804:GLN:OE1	1:A:935:GLN:NE2	2.46	0.49
1:C:804:GLN:OE1	1:C:935:GLN:NE2	2.46	0.49
1:A:984:LEU:HD13	1:A:988:GLU:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:908:GLY:O	1:A:1038:LYS:NZ	2.46	0.49
1:C:908:GLY:O	1:C:1038:LYS:NZ	2.46	0.49
1:C:573:THR:HG22	1:C:587:ILE:HG13	1.95	0.48
1:B:295:PRO:HB2	1:B:608:VAL:HG11	1.94	0.48
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.96	0.48
1:C:557:LYS:HB2	1:C:584:ILE:HG21	1.96	0.48
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.96	0.48
1:C:60:SER:OG	1:C:61:ASN:N	2.46	0.48
1:C:1084:ASP:N	1:C:1084:ASP:OD1	2.47	0.48
1:A:645:THR:OG1	1:A:646:ARG:N	2.46	0.48
1:B:214:ARG:NH2	1:B:266:TYR:OH	2.45	0.48
1:C:919:ASN:HB3	1:C:922:LEU:HB3	1.94	0.48
1:B:47:VAL:HG12	1:C:569:ILE:HG22	1.96	0.47
1:B:646:ARG:NH2	1:B:668:ALA:O	2.47	0.47
1:A:1090:PRO:O	1:C:913:GLN:NE2	2.47	0.47
1:A:40:ASP:N	1:A:40:ASP:OD1	2.46	0.47
1:A:87:ASN:ND2	1:A:88:ASP:OD1	2.48	0.47
1:A:379:CYS:HB3	1:A:432:CYS:HA	1.96	0.47
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.45	0.47
1:C:226:LEU:HG	1:C:227:VAL:HG13	1.97	0.47
1:B:538:CYS:HB2	1:B:590:CYS:HB3	1.55	0.46
1:B:963:VAL:HG11	1:C:570:ALA:HB1	1.96	0.46
1:A:544:ASN:HD21	1:A:579:PRO:HB3	1.79	0.46
1:C:738:CYS:HB2	1:C:760:CYS:HB2	1.42	0.46
1:A:1084:ASP:OD1	1:A:1084:ASP:N	2.48	0.46
1:A:550:GLY:HA2	1:A:589:PRO:HA	1.96	0.46
1:B:574:ASP:HA	1:B:587:ILE:HB	1.96	0.46
1:C:1082:CYS:HB2	1:C:1126:CYS:HB3	1.65	0.46
1:C:538:CYS:HB2	1:C:590:CYS:HB3	1.80	0.46
1:B:725:GLU:OE2	1:B:1028:LYS:NZ	2.48	0.46
1:C:40:ASP:HB3	1:C:42:VAL:HG23	1.98	0.46
1:C:535:LYS:NZ	1:C:554:GLU:OE2	2.44	0.46
1:A:92:PHE:HB2	1:A:192:PHE:HB2	1.98	0.46
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.42	0.46
1:B:1084:ASP:N	1:B:1084:ASP:OD1	2.48	0.45
1:B:102:ARG:HH12	1:B:179:LEU:HD11	1.81	0.45
1:B:280:ASN:OD1	1:B:284:THR:N	2.49	0.45
1:A:126:VAL:HB	1:A:172:SER:HB3	1.97	0.45
1:A:605:SER:OG	1:A:606:ASN:N	2.50	0.45
1:A:326:ILE:HD13	1:A:533:LEU:HD12	1.99	0.45
1:A:882:ILE:O	1:A:901:GLN:NE2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1030:SER:HA	1:B:1034:LEU:HD12	1.97	0.45
1:C:195:LYS:HE2	1:C:197:ILE:HD11	1.99	0.45
1:B:811:LYS:NZ	1:B:820:ASP:OD2	2.45	0.45
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.41	0.44
1:B:18:PHE:HB2	1:B:21:ARG:HB2	1.99	0.44
1:B:141:LEU:HD11	1:B:154:GLU:HG3	1.99	0.44
1:B:412:PRO:HG3	1:B:429:PHE:HB3	1.99	0.44
1:B:565:PHE:HD2	1:B:576:VAL:HG22	1.83	0.44
1:B:914:ASN:HD21	1:C:1121:PHE:HE1	1.65	0.44
1:A:201:PHE:HB2	1:A:229:LEU:HB2	2.00	0.44
1:C:387:LEU:HD11	1:C:431:GLY:HA2	1.98	0.44
1:C:245:HIS:N	1:C:259:THR:O	2.51	0.44
1:C:646:ARG:NH2	1:C:668:ALA:O	2.50	0.44
1:B:882:ILE:O	1:B:901:GLN:NE2	2.50	0.44
1:B:985:ASP:O	1:B:989:ALA:N	2.51	0.44
1:C:35:GLY:HA3	1:C:56:LEU:HB3	2.00	0.44
1:B:96:GLU:OE1	1:B:100:ILE:N	2.46	0.44
1:C:48:LEU:HD11	1:C:276:LEU:HB3	2.00	0.44
1:A:459:SER:OG	1:A:460:ASN:N	2.51	0.44
1:A:1047:TYR:HB2	1:A:1067:TYR:HB3	2.00	0.44
1:C:673:SER:OG	1:C:695:TYR:OH	2.35	0.43
1:B:97:LYS:HG3	1:B:186:PHE:HA	2.00	0.43
1:B:119:ILE:HG12	1:B:128:ILE:HG12	2.01	0.43
1:B:454:ARG:NH2	1:B:469:SER:O	2.51	0.43
1:B:605:SER:OG	1:B:606:ASN:N	2.52	0.43
1:C:521:PRO:HG3	1:C:564:GLN:HG3	1.99	0.43
1:B:544:ASN:HD21	1:B:579:PRO:HB3	1.83	0.43
1:B:774:GLN:HE22	1:B:1018:ILE:HG21	1.84	0.43
1:C:419:ALA:HB1	1:C:424:LYS:HG2	2.00	0.43
1:A:538:CYS:HB2	1:A:590:CYS:HB3	1.58	0.43
1:B:418:ILE:HA	1:B:422:ASN:HD22	1.84	0.43
1:C:985:ASP:O	1:C:989:ALA:N	2.49	0.43
1:C:349:SER:OG	1:C:350:VAL:N	2.52	0.43
1:B:662:CYS:HB2	1:B:671:CYS:HB3	1.71	0.43
1:C:703:ASN:OD1	1:C:703:ASN:N	2.52	0.42
1:C:882:ILE:O	1:C:901:GLN:NE2	2.47	0.42
1:A:1011:GLN:OE1	1:A:1014:ARG:NH1	2.52	0.42
1:B:526:GLY:HA3	1:B:527:PRO:HD3	1.90	0.42
1:C:91:TYR:OH	1:C:191:GLU:OE1	2.35	0.42
1:A:326:ILE:HD12	1:A:539:VAL:HG21	2.01	0.42
1:B:291:CYS:HB3	1:B:301:CYS:HB2	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:645:THR:OG1	1:C:646:ARG:N	2.52	0.42
1:A:245:HIS:HA	1:A:246:ILE:HA	1.76	0.42
1:C:24:LEU:HD11	1:C:78:ARG:HB3	2.02	0.42
1:C:147:LYS:HE2	1:C:147:LYS:HB3	1.83	0.41
1:A:114:THR:OG1	1:A:115:GLN:N	2.54	0.41
1:C:402:ILE:HG21	1:C:418:ILE:HD13	2.03	0.41
1:C:289:VAL:HG13	1:C:297:SER:HB3	2.02	0.41
1:C:887:THR:HB	1:C:894:LEU:HD12	2.02	0.41
1:A:99:ASN:ND2	1:A:178:ASP:O	2.47	0.41
1:B:644:GLN:HA	1:B:649:CYS:HA	2.02	0.41
1:A:656:VAL:HG12	1:A:658:ASN:H	1.86	0.41
1:A:856:ASN:HD22	1:A:963:VAL:HG13	1.86	0.41
1:B:212:LEU:HD22	1:B:217:PRO:HD3	2.03	0.41
1:C:1091:ARG:NH1	1:C:1118:ASP:O	2.53	0.41
1:A:389:ASP:OD1	1:A:389:ASP:N	2.52	0.40
1:B:362:VAL:HG13	1:B:525:CYS:HB2	2.04	0.40
1:B:853:GLN:HG2	1:B:959:LEU:HB3	2.03	0.40
1:C:126:VAL:HB	1:C:172:SER:HB3	2.03	0.40
1:C:596:SER:HB3	1:C:611:LEU:HB3	2.04	0.40
1:B:909:ILE:HG13	1:B:911:VAL:HG23	2.02	0.40
1:B:128:ILE:HB	1:B:170:TYR:HB3	2.02	0.40
1:B:656:VAL:HG12	1:B:658:ASN:H	1.86	0.40
1:A:1116:THR:HG22	1:A:1138:TYR:HB3	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	1065/1258 (85%)	1037 (97%)	28 (3%)	0	100	100
1	B	1065/1258 (85%)	1015 (95%)	50 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1064/1258 (85%)	1019 (96%)	45 (4%)	0	100	100
2	a	212/214 (99%)	208 (98%)	4 (2%)	0	100	100
2	c	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
3	b	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
3	d	215/217 (99%)	205 (95%)	10 (5%)	0	100	100
All	All	4048/4636 (87%)	3899 (96%)	149 (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 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	944/1095 (86%)	941 (100%)	3 (0%)	92	96
1	B	944/1095 (86%)	941 (100%)	3 (0%)	92	96
1	C	944/1095 (86%)	942 (100%)	2 (0%)	93	97
2	a	186/186 (100%)	185 (100%)	1 (0%)	88	93
2	c	186/186 (100%)	186 (100%)	0	100	100
3	b	193/194 (100%)	192 (100%)	1 (0%)	88	93
3	d	193/194 (100%)	193 (100%)	0	100	100
All	All	3590/4045 (89%)	3580 (100%)	10 (0%)	92	96

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	380	TYR
1	A	391	CYS
1	A	662	CYS
1	B	166	CYS
1	B	379	CYS
1	B	760	CYS

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Mol	Chain	Res	Type
1	C	95	THR
1	C	458	LYS
2	a	120	THR
3	b	188	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	ASN
1	A	563	GLN
1	A	613	GLN
1	A	804	GLN
1	A	913	GLN
1	A	935	GLN
1	A	1106	GLN
1	A	1159	HIS
1	B	422	ASN
1	B	787	GLN
1	B	914	ASN
1	B	1010	GLN
1	B	1106	GLN
1	B	1159	HIS
1	C	188	ASN
1	C	334	ASN
1	C	414	GLN
1	C	644	GLN
1	C	804	GLN
1	C	914	ASN
1	C	935	GLN
1	C	1048	HIS
1	C	1083	HIS
1	C	1106	GLN
3	b	171	GLN
3	b	195	ASN
3	b	217	ASN
2	c	6	GLN
2	c	39	GLN
2	c	52	ASN
3	d	43	GLN
3	d	44	GLN

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	3
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	241:LEU	C	245:HIS	N	14.41
1	B	241:LEU	C	245:HIS	N	11.03
1	C	241:LEU	C	245:HIS	N	10.19
1	C	246:ILE	C	247:SER	N	6.70
1	C	245:HIS	C	246:ILE	N	3.75

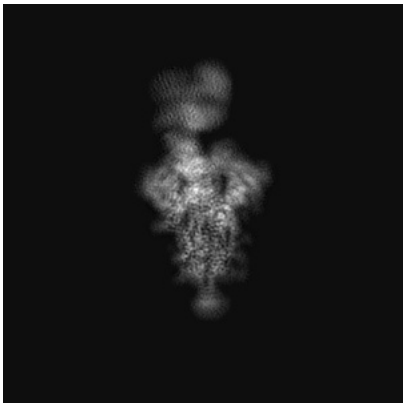
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-32431. These allow visual inspection of the internal detail of the map and identification of artifacts.

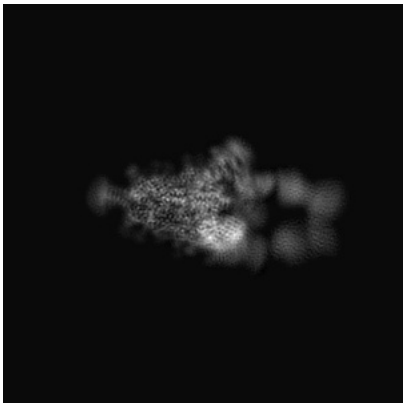
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

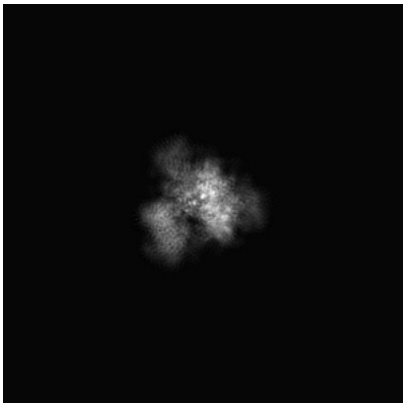
6.1.1 Primary map



X



Y



Z

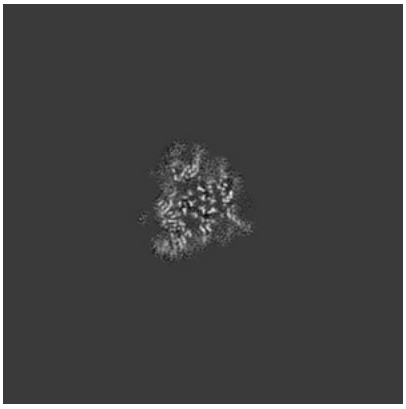
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

X Index: 200

Y Index: 200

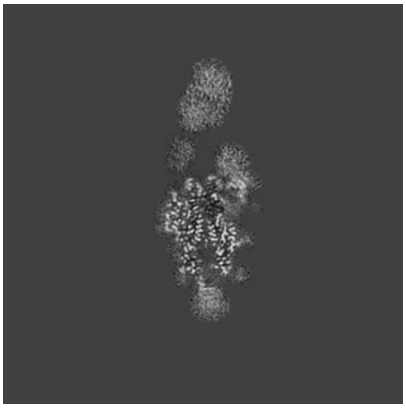


Z Index: 200

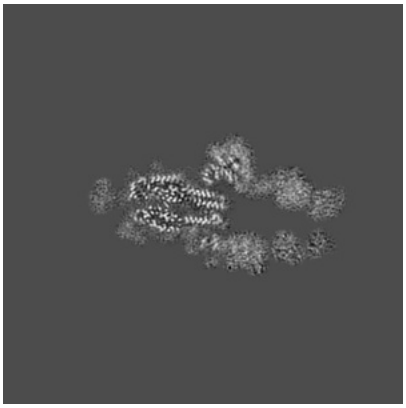
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

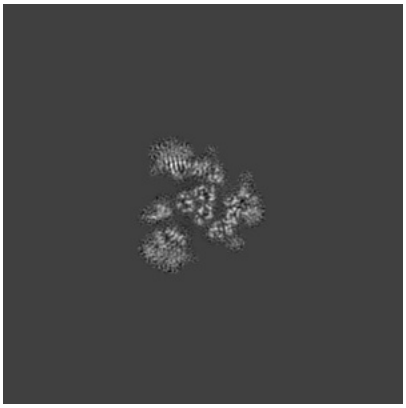
6.3.1 Primary map



X Index: 204



Y Index: 193



Z Index: 214

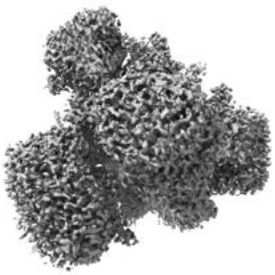
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.66. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

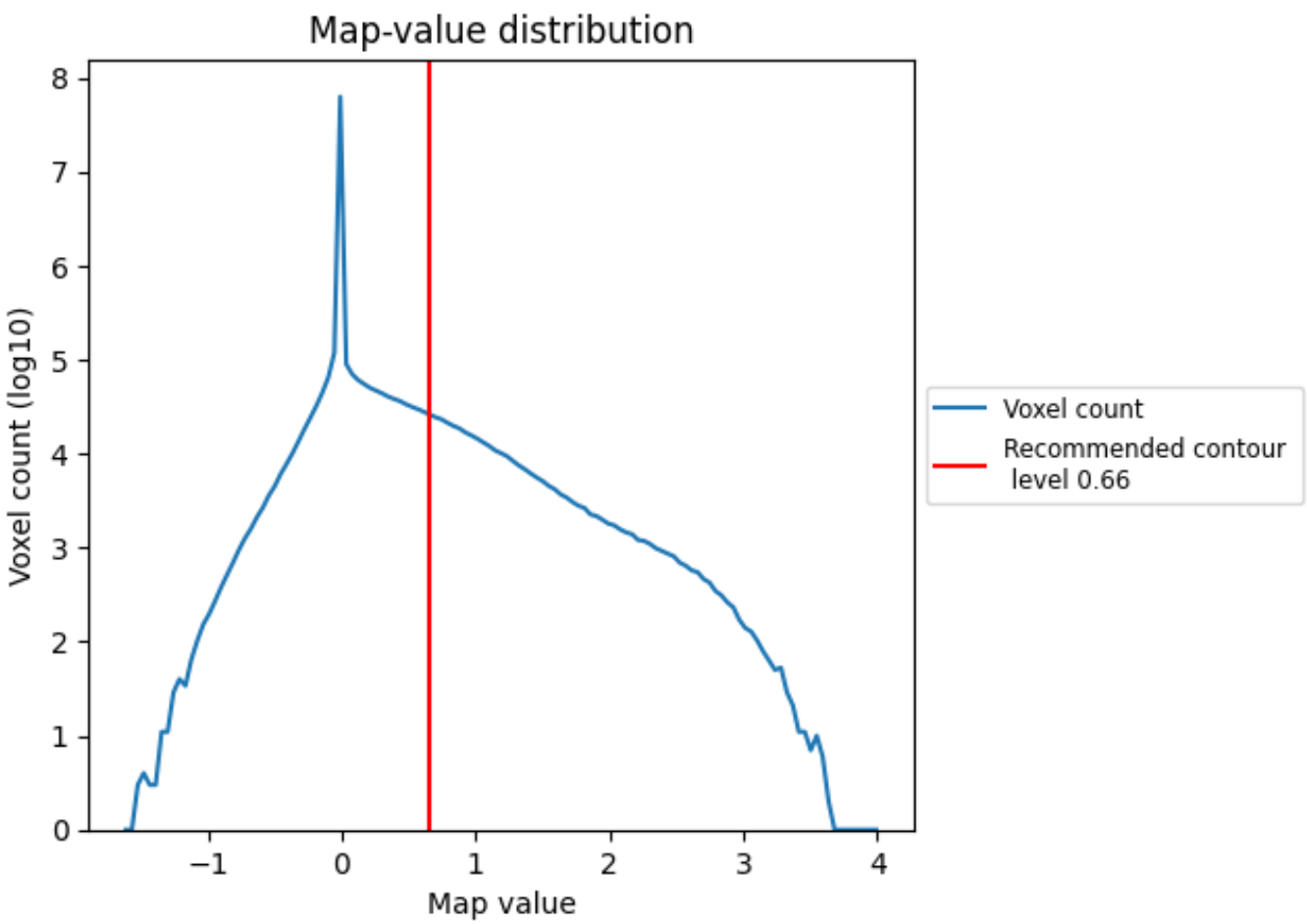
6.5 Mask visualisation (i)

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

7 Map analysis (i)

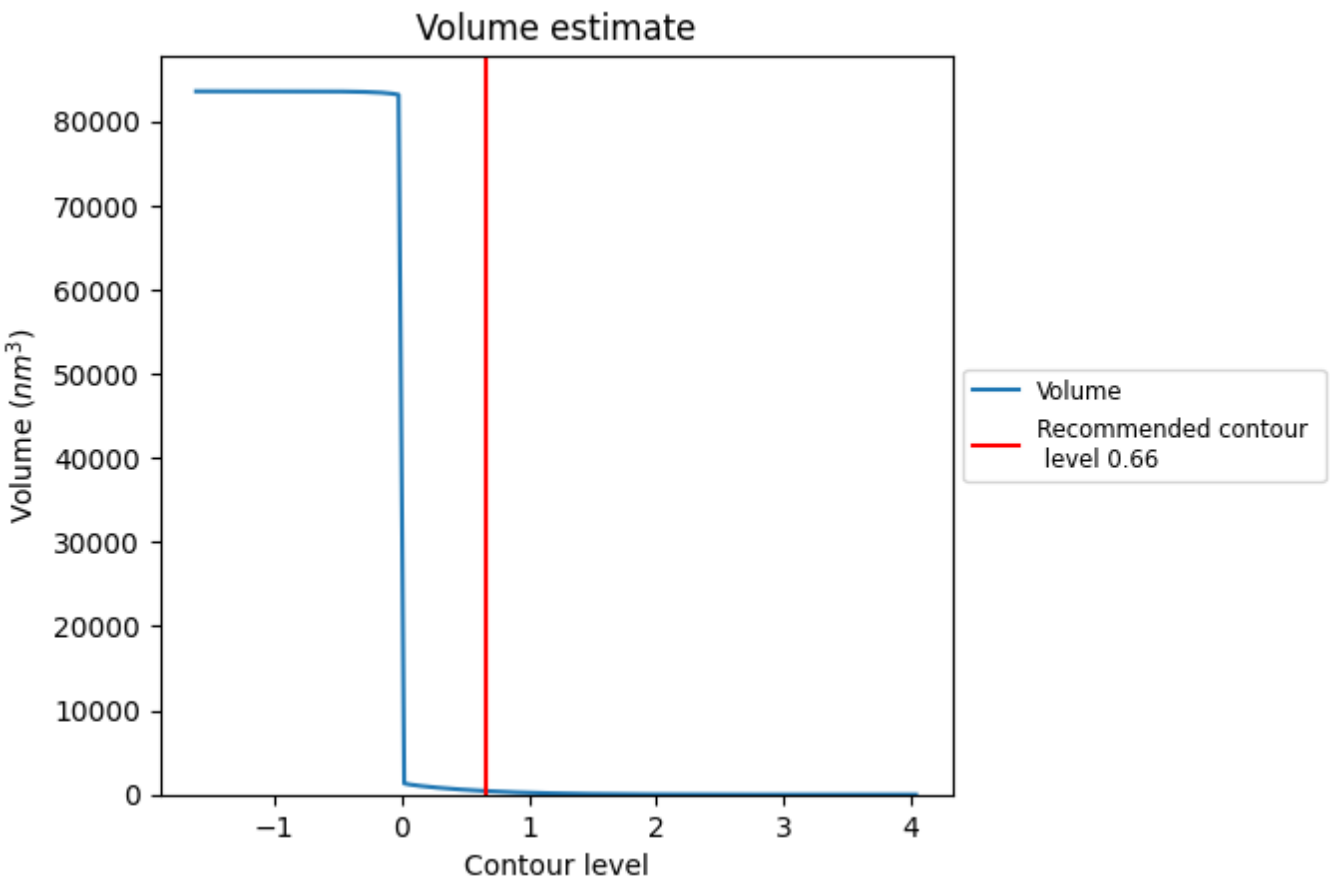
This section contains the results of statistical analysis of the map.

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.

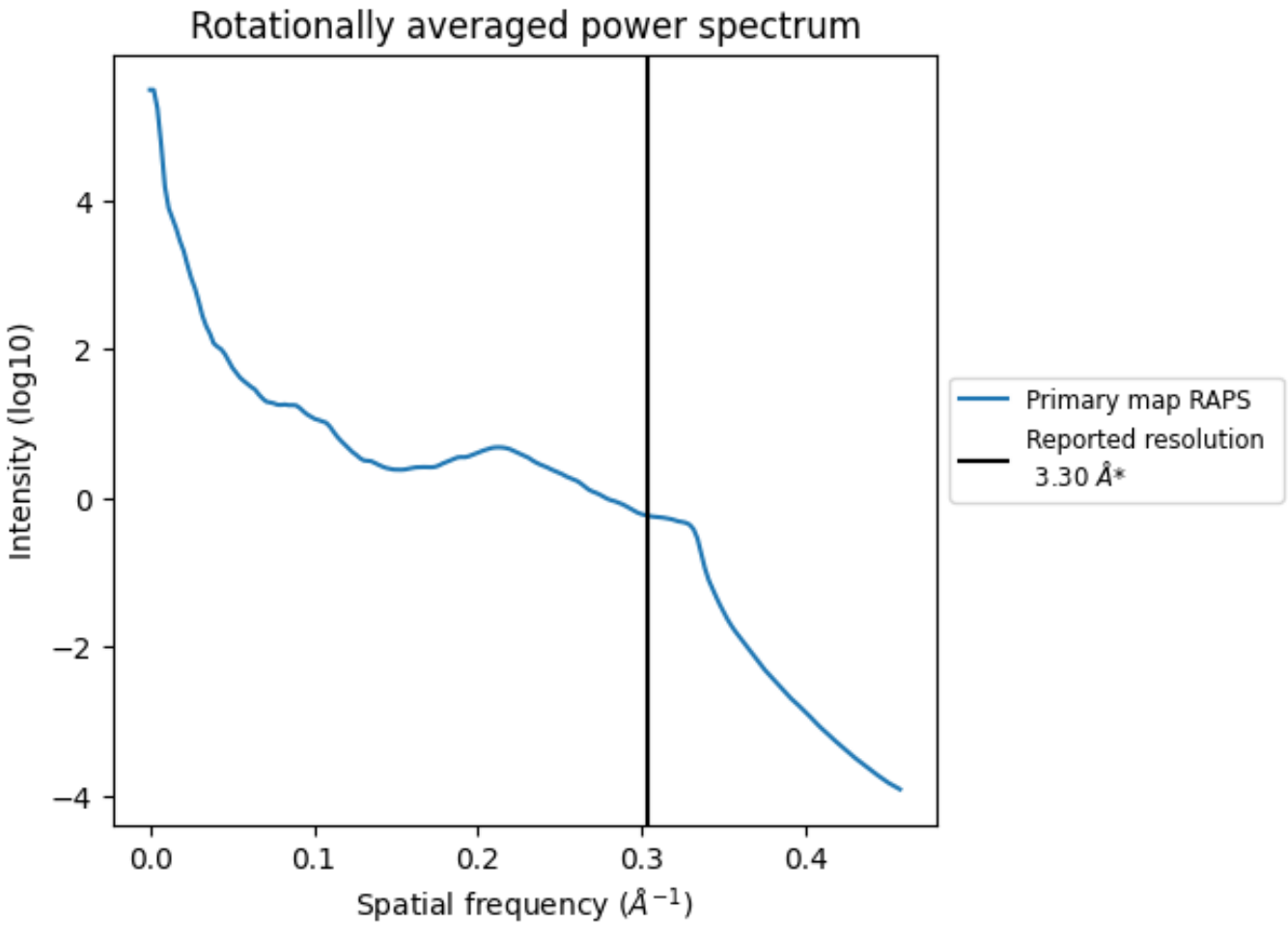
7.2 Volume estimate (i)



The volume at the recommended contour level is 424 nm^3; this corresponds to an approximate mass of 383 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 0.303 Å^{-1}

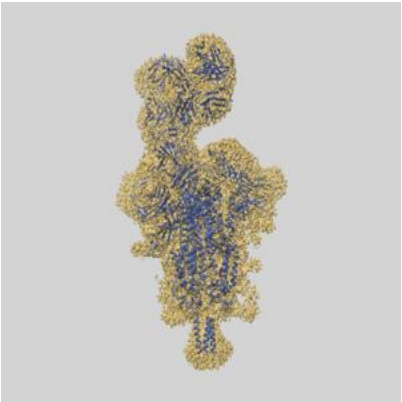
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

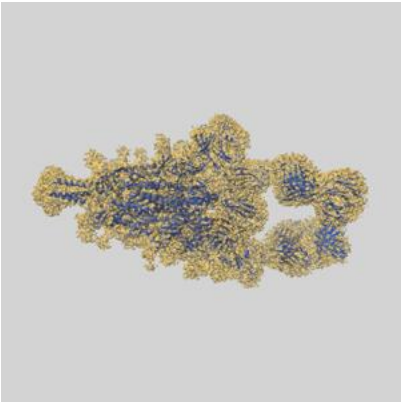
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-32431 and PDB model 7WD0. Per-residue inclusion information can be found in section 3 on page 9.

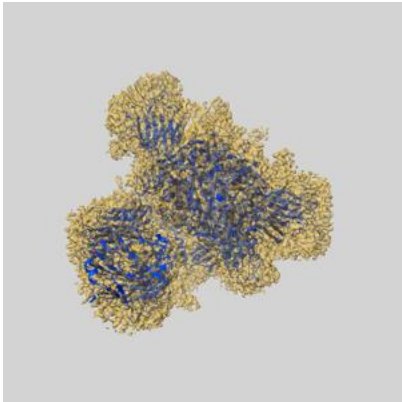
9.1 Map-model overlay (i)



X



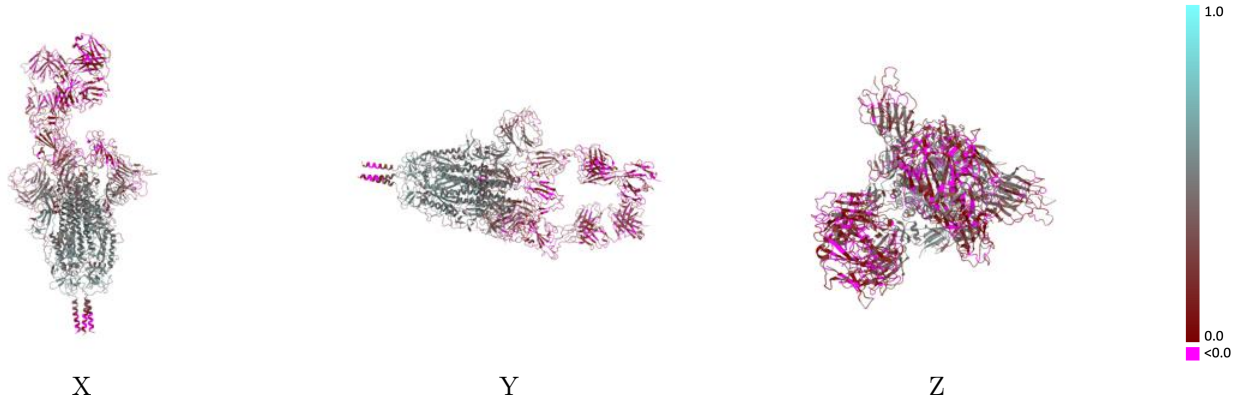
Y



Z

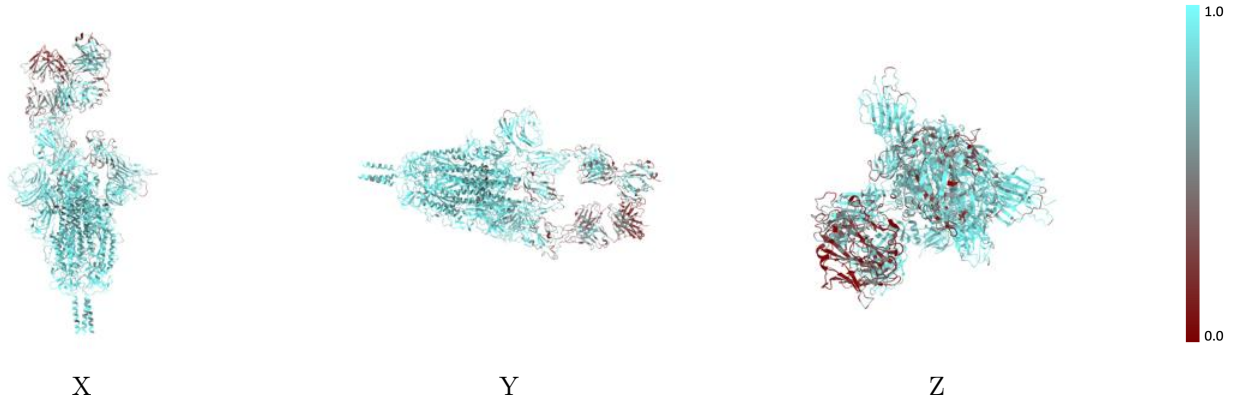
The images above show the 3D surface view of the map at the recommended contour level 0.66 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



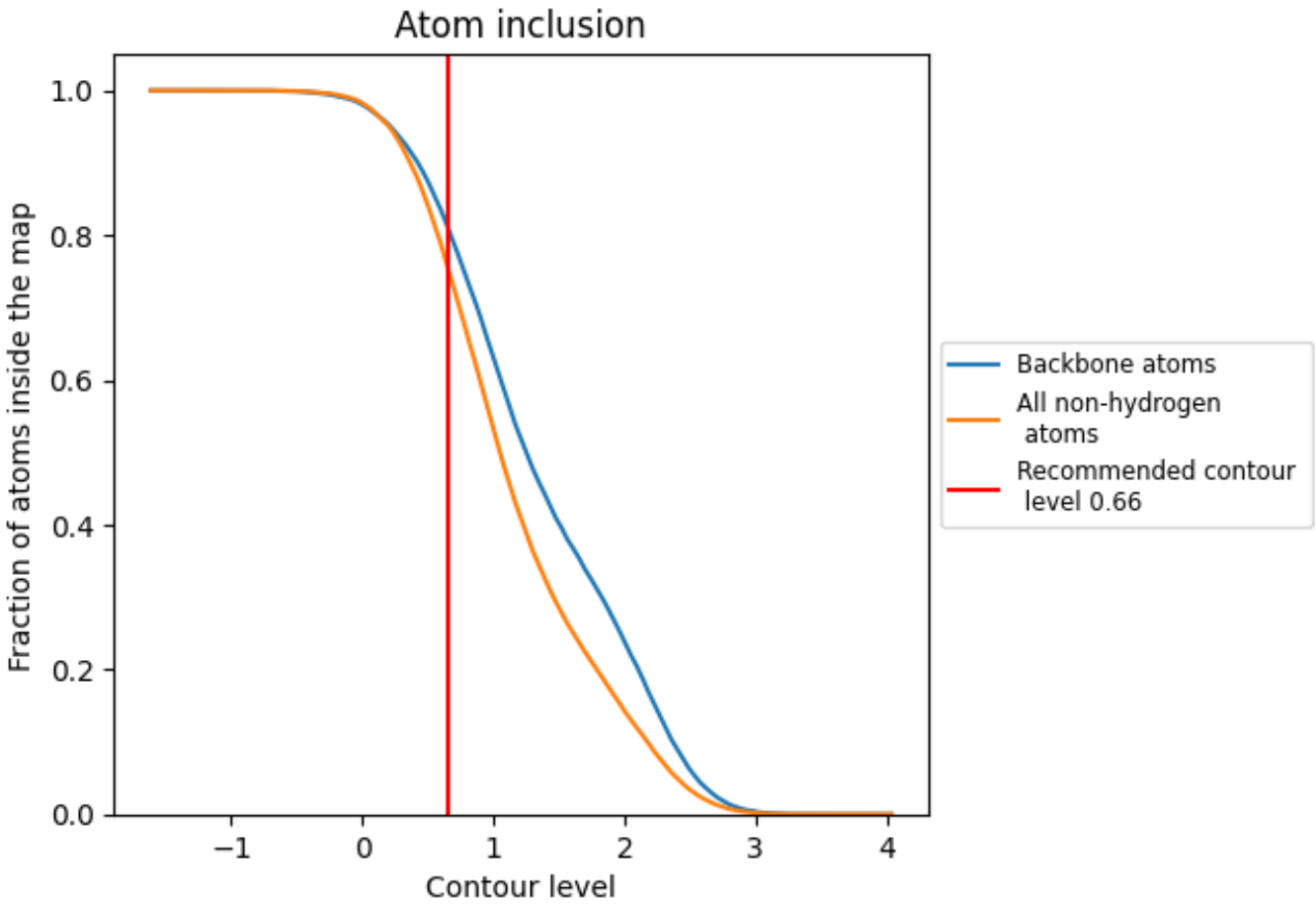
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.66).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 75% 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 (0.66) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7514	0.2910
A	0.8572	0.3620
B	0.8064	0.3360
C	0.8075	0.3380
a	0.6051	0.0750
b	0.5871	0.0670
c	0.3943	0.0970
d	0.3146	0.0950