



Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 02:37 AM JST

PDB ID : 7DD2
EMDB ID : EMD-30642
Title : S-3C1-F2 structure, two RBDs are up and one RBD is down, the two up RBD bind with a 3C1 fab.
Authors : Cong, Y.; Liu, C.X.
Deposited on : 2020-10-27
Resolution : 5.60 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 ⓘ 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

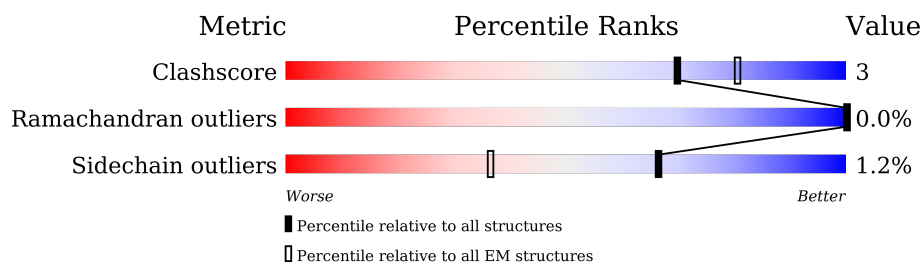
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.60 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	C	1261	<div> <div>11%</div> <div>74%</div> <div>9%</div> <div>16%</div> </div>
1	D	1261	<div> <div>10%</div> <div>76%</div> <div>8%</div> <div>16%</div> </div>
1	K	1261	<div> <div>12%</div> <div>76%</div> <div>8%</div> <div>16%</div> </div>
2	A	222	<div> <div>42%</div> <div>87%</div> <div>12%</div> </div>
2	E	222	<div> <div>59%</div> <div>92%</div> <div>8%</div> </div>
3	B	214	<div> <div>37%</div> <div>91%</div> <div>9%</div> </div>
3	H	214	<div> <div>47%</div> <div>85%</div> <div>14%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 31623 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	C	1061	Total	C	N	O	S	0	0
			8304	5296	1388	1582	38		
1	D	1059	Total	C	N	O	S	0	0
			8289	5287	1385	1579	38		
1	K	1061	Total	C	N	O	S	0	0
			8304	5296	1388	1582	38		

There are 174 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
D	682	GLY	ARG	engineered mutation	UNP P0DTC2
D	683	SER	ARG	engineered mutation	UNP P0DTC2
D	685	SER	ARG	engineered mutation	UNP P0DTC2
D	986	PRO	LYS	engineered mutation	UNP P0DTC2
D	987	PRO	VAL	engineered mutation	UNP P0DTC2
D	1209	GLY	-	expression tag	UNP P0DTC2
D	1210	SER	-	expression tag	UNP P0DTC2
D	1211	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1212	TYR	-	expression tag	UNP P0DTC2
D	1213	ILE	-	expression tag	UNP P0DTC2
D	1214	PRO	-	expression tag	UNP P0DTC2
D	1215	GLU	-	expression tag	UNP P0DTC2
D	1216	ALA	-	expression tag	UNP P0DTC2
D	1217	PRO	-	expression tag	UNP P0DTC2
D	1218	ARG	-	expression tag	UNP P0DTC2
D	1219	ASP	-	expression tag	UNP P0DTC2
D	1220	GLY	-	expression tag	UNP P0DTC2
D	1221	GLN	-	expression tag	UNP P0DTC2
D	1222	ALA	-	expression tag	UNP P0DTC2
D	1223	TYR	-	expression tag	UNP P0DTC2
D	1224	VAL	-	expression tag	UNP P0DTC2
D	1225	ARG	-	expression tag	UNP P0DTC2
D	1226	LYS	-	expression tag	UNP P0DTC2
D	1227	ASP	-	expression tag	UNP P0DTC2
D	1228	GLY	-	expression tag	UNP P0DTC2
D	1229	GLU	-	expression tag	UNP P0DTC2
D	1230	TRP	-	expression tag	UNP P0DTC2
D	1231	VAL	-	expression tag	UNP P0DTC2
D	1232	LEU	-	expression tag	UNP P0DTC2
D	1233	LEU	-	expression tag	UNP P0DTC2
D	1234	SER	-	expression tag	UNP P0DTC2
D	1235	THR	-	expression tag	UNP P0DTC2
D	1236	PHE	-	expression tag	UNP P0DTC2
D	1237	LEU	-	expression tag	UNP P0DTC2
D	1238	GLU	-	expression tag	UNP P0DTC2
D	1239	ASN	-	expression tag	UNP P0DTC2
D	1240	LEU	-	expression tag	UNP P0DTC2
D	1241	TYR	-	expression tag	UNP P0DTC2
D	1242	PHE	-	expression tag	UNP P0DTC2
D	1243	GLN	-	expression tag	UNP P0DTC2
D	1244	GLY	-	expression tag	UNP P0DTC2
D	1245	ASP	-	expression tag	UNP P0DTC2
D	1246	TYR	-	expression tag	UNP P0DTC2
D	1247	LYS	-	expression tag	UNP P0DTC2
D	1248	ASP	-	expression tag	UNP P0DTC2
D	1249	ASP	-	expression tag	UNP P0DTC2
D	1250	ASP	-	expression tag	UNP P0DTC2
D	1251	ASP	-	expression tag	UNP P0DTC2
D	1252	LYS	-	expression tag	UNP P0DTC2
D	1253	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1254	HIS	-	expression tag	UNP P0DTC2
D	1255	HIS	-	expression tag	UNP P0DTC2
D	1256	HIS	-	expression tag	UNP P0DTC2
D	1257	HIS	-	expression tag	UNP P0DTC2
D	1258	HIS	-	expression tag	UNP P0DTC2
D	1259	HIS	-	expression tag	UNP P0DTC2
D	1260	HIS	-	expression tag	UNP P0DTC2
D	1261	HIS	-	expression tag	UNP P0DTC2
K	682	GLY	ARG	engineered mutation	UNP P0DTC2
K	683	SER	ARG	engineered mutation	UNP P0DTC2
K	685	SER	ARG	engineered mutation	UNP P0DTC2
K	986	PRO	LYS	engineered mutation	UNP P0DTC2
K	987	PRO	VAL	engineered mutation	UNP P0DTC2
K	1209	GLY	-	expression tag	UNP P0DTC2
K	1210	SER	-	expression tag	UNP P0DTC2
K	1211	GLY	-	expression tag	UNP P0DTC2
K	1212	TYR	-	expression tag	UNP P0DTC2
K	1213	ILE	-	expression tag	UNP P0DTC2
K	1214	PRO	-	expression tag	UNP P0DTC2
K	1215	GLU	-	expression tag	UNP P0DTC2
K	1216	ALA	-	expression tag	UNP P0DTC2
K	1217	PRO	-	expression tag	UNP P0DTC2
K	1218	ARG	-	expression tag	UNP P0DTC2
K	1219	ASP	-	expression tag	UNP P0DTC2
K	1220	GLY	-	expression tag	UNP P0DTC2
K	1221	GLN	-	expression tag	UNP P0DTC2
K	1222	ALA	-	expression tag	UNP P0DTC2
K	1223	TYR	-	expression tag	UNP P0DTC2
K	1224	VAL	-	expression tag	UNP P0DTC2
K	1225	ARG	-	expression tag	UNP P0DTC2
K	1226	LYS	-	expression tag	UNP P0DTC2
K	1227	ASP	-	expression tag	UNP P0DTC2
K	1228	GLY	-	expression tag	UNP P0DTC2
K	1229	GLU	-	expression tag	UNP P0DTC2
K	1230	TRP	-	expression tag	UNP P0DTC2
K	1231	VAL	-	expression tag	UNP P0DTC2
K	1232	LEU	-	expression tag	UNP P0DTC2
K	1233	LEU	-	expression tag	UNP P0DTC2
K	1234	SER	-	expression tag	UNP P0DTC2
K	1235	THR	-	expression tag	UNP P0DTC2
K	1236	PHE	-	expression tag	UNP P0DTC2
K	1237	LEU	-	expression tag	UNP P0DTC2

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

- Molecule 2 is a protein called The heavy chain of 3C1 fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	221	Total	C	N	O	S	0	0
			1691	1069	273	342	7		
2	A	221	Total	C	N	O	S	0	0
			1691	1069	273	342	7		

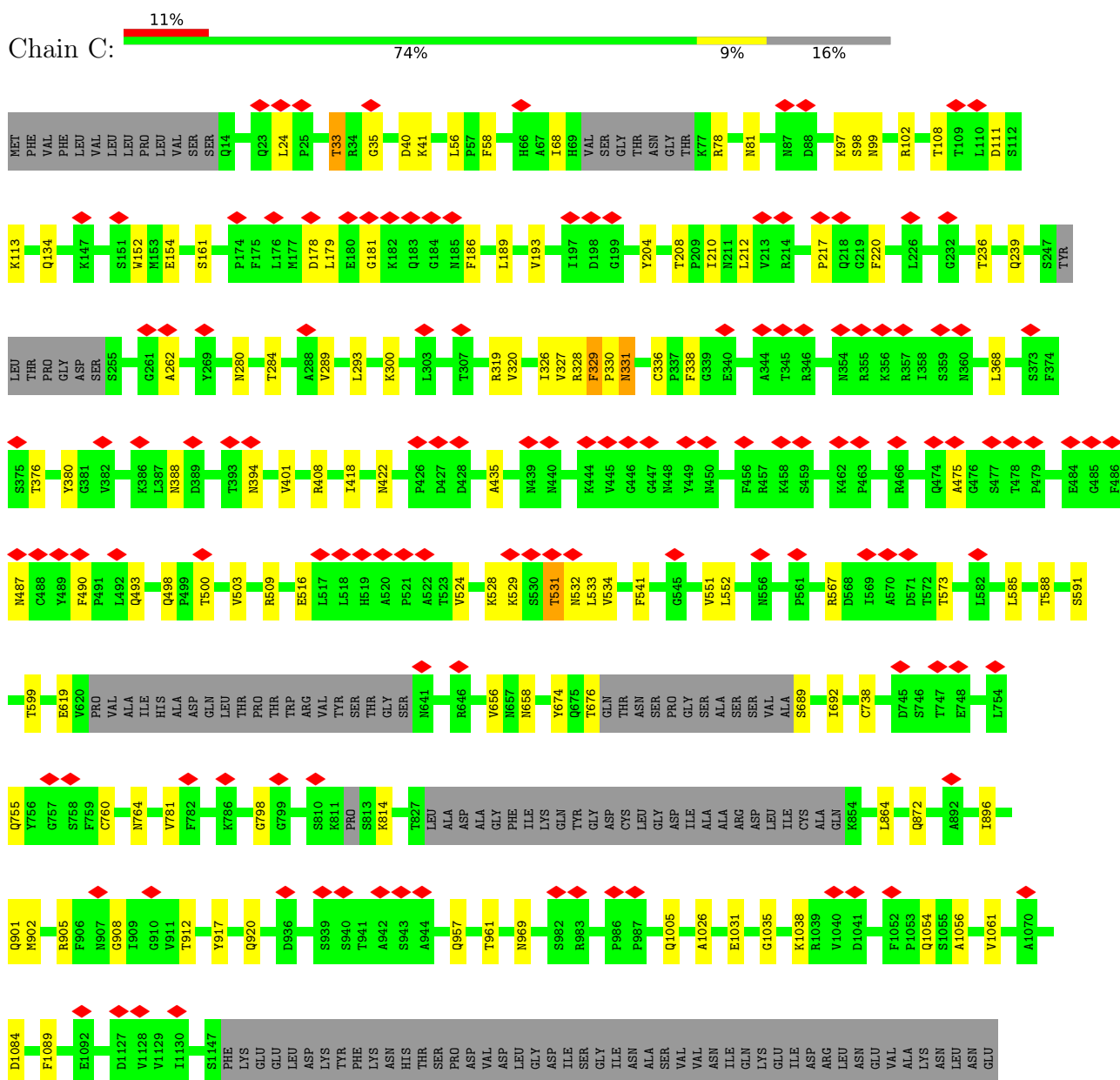
- Molecule 3 is a protein called The light chain of 3C1 fab.

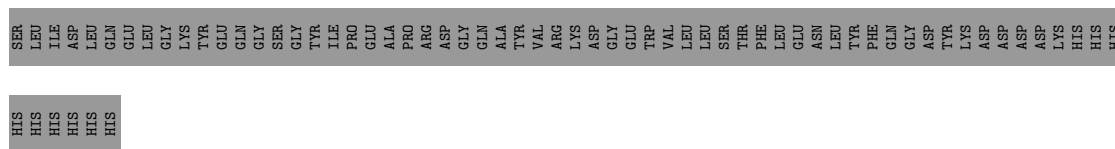
Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	213	Total	C	N	O	S	0	0
			1672	1041	286	338	7		
3	B	213	Total	C	N	O	S	0	0
			1672	1041	286	338	7		

3 Residue-property plots [i](#)

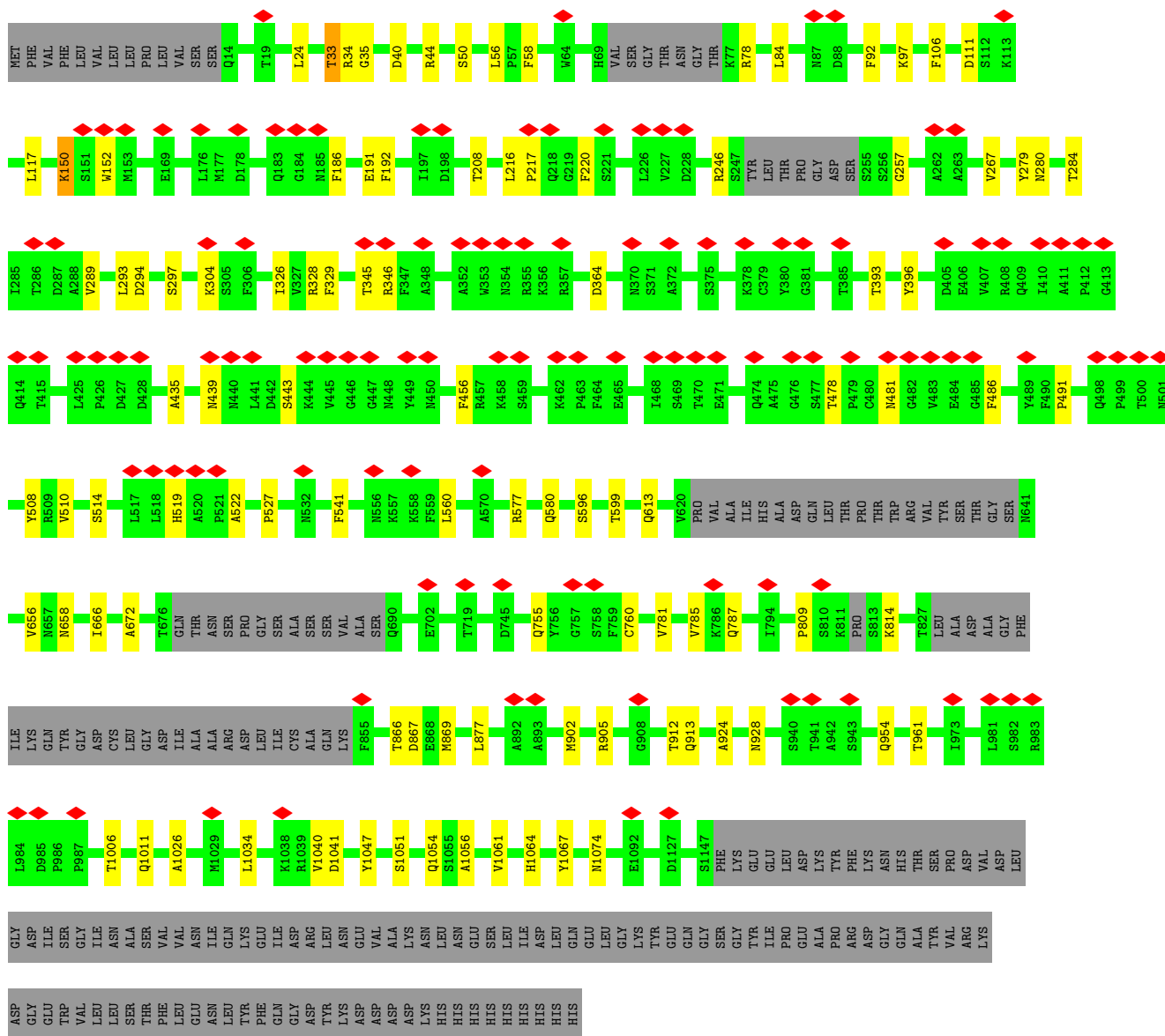
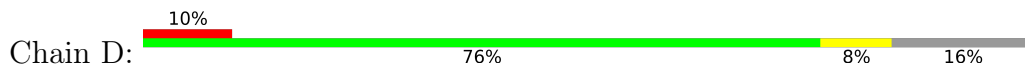
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

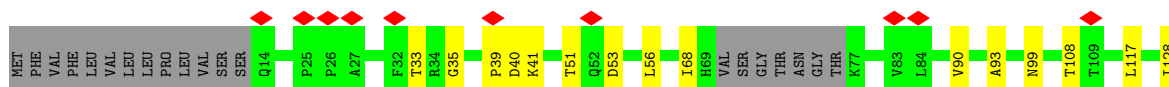
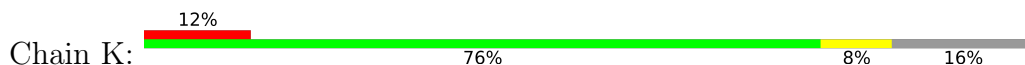


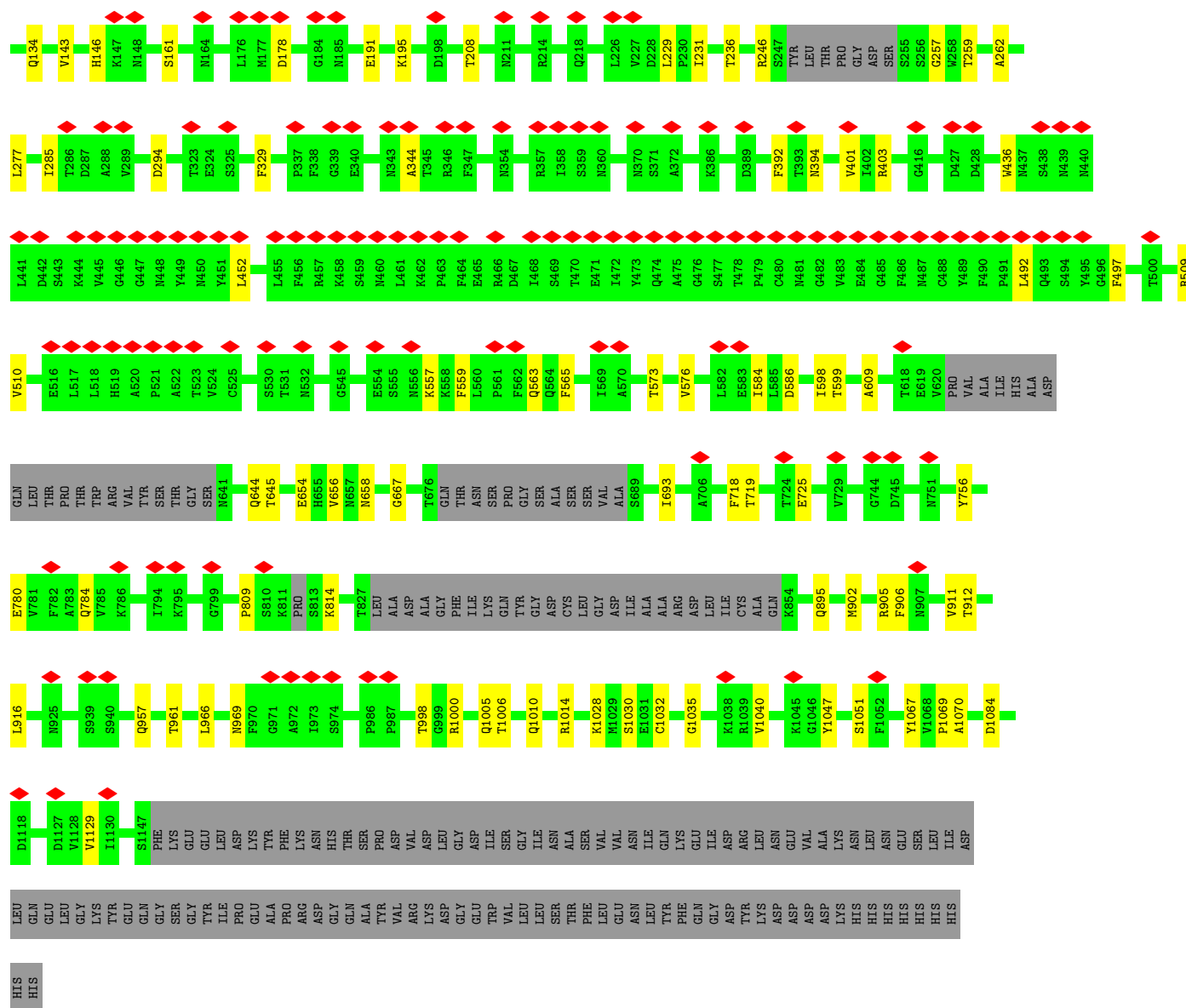


- Molecule 1: Spike glycoprotein

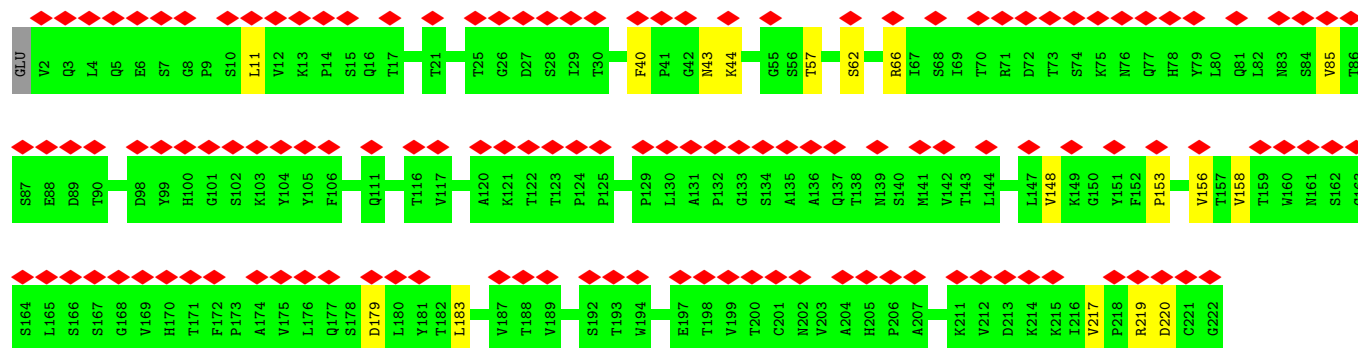
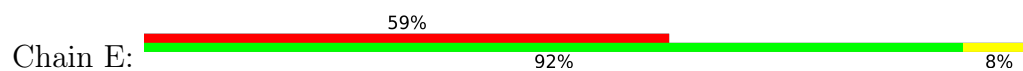


- Molecule 1: Spike glycoprotein

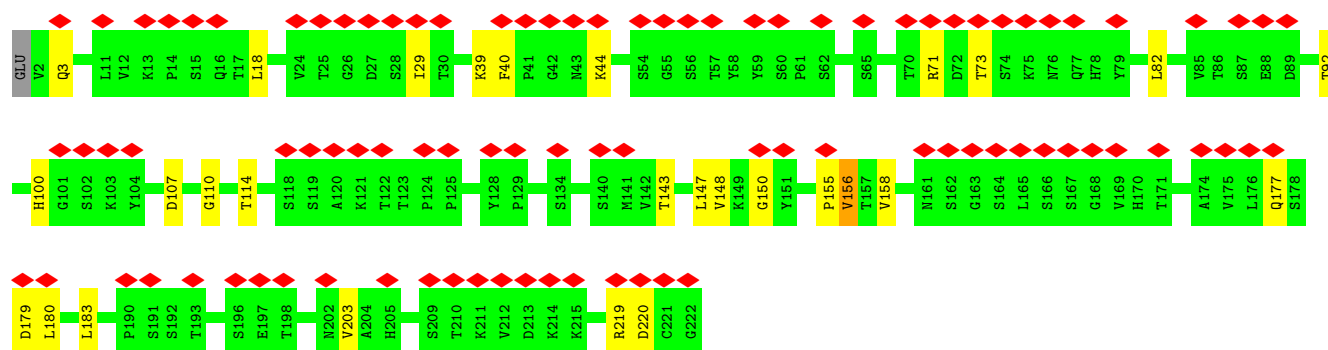
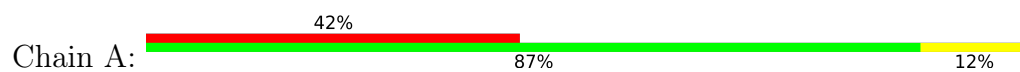




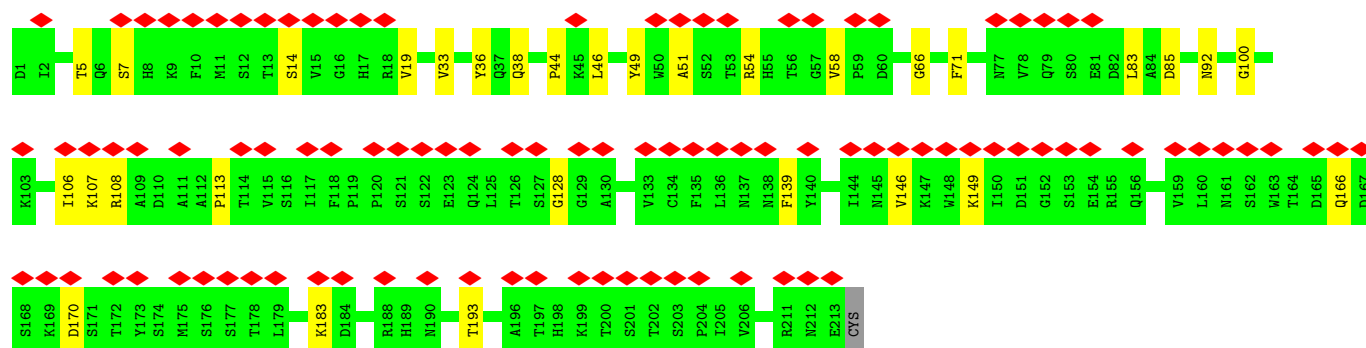
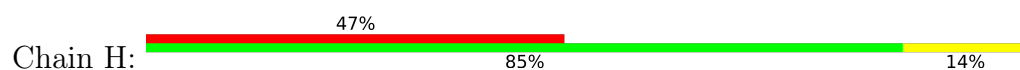
- Molecule 2: The heavy chain of 3C1 fab



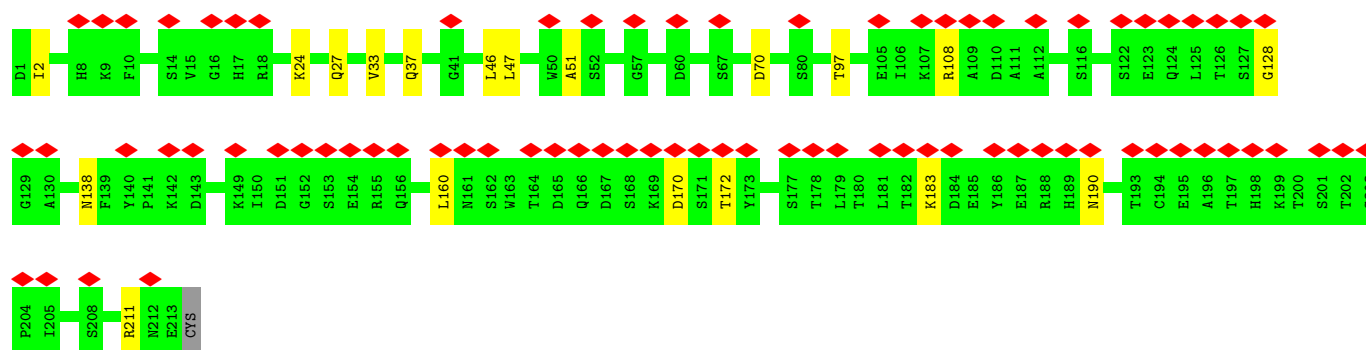
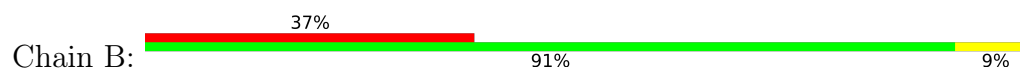
- Molecule 2: The heavy chain of 3C1 fab



- Molecule 3: The light chain of 3C1 fab



- Molecule 3: The light chain of 3C1 fab



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31143	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 ($e^-/\text{\AA}^2$)	49.6	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	2.631	Depositor
Minimum map value	-1.434	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.094	Depositor
Recommended contour level	0.9	Depositor
Map size (Å)	489.59998, 489.59998, 489.59998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	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	C	0.25	0/8494	0.43	0/11554
1	D	0.25	0/8479	0.43	0/11535
1	K	0.25	0/8494	0.43	0/11554
2	A	0.24	0/1739	0.45	0/2381
2	E	0.24	0/1739	0.45	0/2381
3	B	0.24	0/1712	0.44	0/2324
3	H	0.25	0/1712	0.45	0/2324
All	All	0.25	0/32369	0.43	0/44053

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	C	8304	0	8101	68	0
1	D	8289	0	8081	57	0
1	K	8304	0	8101	55	0
2	A	1691	0	1626	15	0
2	E	1691	0	1626	9	0
3	B	1672	0	1587	12	0
3	H	1672	0	1587	18	0
All	All	31623	0	30709	212	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 (212) 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:329:PHE:CD2	1:C:330:PRO:HD2	1.97	0.98
1:C:329:PHE:CE1	1:C:528:LYS:HG3	2.18	0.78
1:C:329:PHE:CG	1:C:330:PRO:HD2	2.30	0.67
2:E:40:PHE:HB2	2:E:44:LYS:HB2	1.84	0.59
1:K:1047:TYR:HB2	1:K:1067:TYR:HB3	1.83	0.59
2:A:39:LYS:HB3	2:A:92:THR:HB	1.86	0.58
1:C:781:VAL:HG22	1:C:1026:ALA:HB2	1.86	0.57
1:D:902:MET:SD	1:D:905:ARG:NH1	2.78	0.57
1:C:189:LEU:HB2	1:C:210:ILE:HG12	1.85	0.57
1:K:902:MET:SD	1:K:905:ARG:NH1	2.78	0.56
2:A:40:PHE:HB2	2:A:44:LYS:HB3	1.87	0.56
1:C:1035:GLY:HA3	1:K:1040:VAL:HG21	1.86	0.56
1:C:328:ARG:HG3	1:C:533:LEU:HD22	1.86	0.56
1:C:35:GLY:HA3	1:C:56:LEU:HB3	1.88	0.55
1:D:150:LYS:HG2	1:D:152:TRP:H	1.71	0.54
1:C:896:ILE:HG23	1:C:901:GLN:HE21	1.72	0.54
1:C:326:ILE:HB	1:C:541:PHE:HA	1.90	0.54
1:C:212:LEU:HD21	1:C:217:PRO:HG3	1.90	0.53
1:C:902:MET:SD	1:C:905:ARG:NH1	2.82	0.53
3:H:14:SER:HB3	3:H:107:LYS:HB2	1.91	0.53
1:D:1040:VAL:HG21	1:K:1035:GLY:HA3	1.90	0.53
1:C:475:ALA:HB3	1:C:487:ASN:HB3	1.91	0.52
1:D:97:LYS:HB3	1:D:186:PHE:HA	1.90	0.52
1:D:781:VAL:HG22	1:D:1026:ALA:HB2	1.90	0.52
1:K:598:ILE:HB	1:K:609:ALA:HB3	1.91	0.51
1:K:344:ALA:O	1:K:509:ARG:NH1	2.43	0.51
1:D:329:PHE:O	1:D:580:GLN:NE2	2.43	0.51
3:B:108:ARG:NH1	3:B:170:ASP:O	2.43	0.51
1:D:50:SER:OG	1:D:304:LYS:NZ	2.44	0.51
1:C:1089:PHE:HB3	1:D:913:GLN:HE21	1.76	0.51
1:D:1047:TYR:HB2	1:D:1067:TYR:HB3	1.92	0.51
1:K:246:ARG:HB2	1:K:259:THR:H	1.76	0.51
1:D:478:THR:HB	3:H:5:THR:HG21	1.94	0.50
1:K:780:GLU:O	1:K:784:GLN:NE2	2.44	0.50
3:B:2:ILE:HG23	3:B:27:GLN:HB2	1.92	0.50
1:C:394:ASN:HB2	1:C:516:GLU:HB3	1.93	0.50
1:D:481:ASN:ND2	3:H:7:SER:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:THR:HB	1:C:435:ALA:HB3	1.94	0.50
1:D:34:ARG:NH1	1:D:191:GLU:OE2	2.45	0.50
1:K:68:ILE:HG22	1:K:262:ALA:HA	1.93	0.50
1:D:24:LEU:HD22	1:D:78:ARG:HD2	1.92	0.50
1:D:92:PHE:HB3	1:D:192:PHE:HB2	1.94	0.50
1:K:134:GLN:HB3	1:K:161:SER:HB3	1.94	0.50
3:B:128:GLY:HA2	3:B:183:LYS:HD2	1.94	0.50
3:B:33:VAL:HB	3:B:51:ALA:HB2	1.94	0.49
1:D:486:PHE:HB3	3:H:5:THR:HG23	1.94	0.49
1:K:39:PRO:HG3	1:K:51:THR:HG21	1.94	0.49
1:C:24:LEU:HD22	1:C:78:ARG:HD2	1.95	0.49
3:H:54:ARG:NH1	3:H:58:VAL:O	2.46	0.49
1:C:388:ASN:HB3	1:C:529:LYS:HE3	1.93	0.49
1:C:102:ARG:NH1	1:C:154:GLU:OE2	2.45	0.49
1:C:111:ASP:OD2	1:C:113:LYS:NZ	2.45	0.49
1:C:551:VAL:HB	1:C:588:THR:HB	1.94	0.49
1:D:246:ARG:NH1	1:D:257:GLY:O	2.46	0.49
1:D:1056:ALA:HB2	1:D:1061:VAL:HG23	1.95	0.49
3:B:24:LYS:NZ	3:B:70:ASP:OD1	2.45	0.49
2:E:11:LEU:HB2	2:E:153:PRO:HG3	1.95	0.48
2:E:44:LYS:NZ	3:H:100:GLY:O	2.46	0.48
1:C:134:GLN:HB3	1:C:161:SER:HB2	1.94	0.48
1:C:917:TYR:HB3	1:K:1129:VAL:HG22	1.94	0.48
1:D:560:LEU:O	1:D:577:ARG:NH2	2.45	0.48
1:D:809:PRO:HA	1:D:814:LYS:HG2	1.95	0.48
3:H:149:LYS:HB2	3:H:193:THR:HB	1.95	0.48
1:K:246:ARG:NH1	1:K:257:GLY:O	2.46	0.48
3:H:108:ARG:NH1	3:H:170:ASP:O	2.46	0.48
1:C:676:THR:HG23	1:C:689:SER:HB3	1.96	0.48
1:C:319:ARG:NH1	1:C:320:VAL:O	2.47	0.48
3:H:106:ILE:HB	3:H:166:GLN:HE22	1.79	0.48
1:D:954:GLN:O	1:D:1011:GLN:NE2	2.46	0.47
1:K:436:TRP:HE1	1:K:509:ARG:HD2	1.79	0.47
3:B:37:GLN:HB2	3:B:47:LEU:HB2	1.96	0.47
1:D:869:MET:SD	1:D:869:MET:N	2.88	0.47
1:D:866:THR:OG1	1:D:869:MET:SD	2.73	0.47
1:K:966:LEU:O	1:K:1000:ARG:NH2	2.47	0.47
1:C:41:LYS:HB3	1:K:563:GLN:HA	1.95	0.47
1:D:44:ARG:HB2	1:D:279:TYR:HD2	1.79	0.47
1:D:58:PHE:HB2	1:D:293:LEU:HD22	1.96	0.47
3:H:33:VAL:HB	3:H:51:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3:GLN:NE2	2:A:110:GLY:O	2.48	0.47
3:H:66:GLY:HA3	3:H:71:PHE:HA	1.96	0.47
1:K:644:GLN:NE2	1:K:645:THR:O	2.48	0.47
1:C:289:VAL:HG11	1:C:300:LYS:HB2	1.97	0.47
1:D:84:LEU:HG	1:D:267:VAL:HG11	1.97	0.47
1:K:1032:CYS:SG	1:K:1051:SER:OG	2.71	0.47
1:D:439:ASN:O	1:D:443:SER:OG	2.33	0.47
1:K:725:GLU:OE2	1:K:1028:LYS:NZ	2.41	0.47
2:E:156:VAL:HG21	2:E:183:LEU:HD11	1.96	0.46
1:D:785:VAL:HG12	1:D:787:GLN:H	1.80	0.46
1:C:193:VAL:HB	1:C:204:TYR:HB2	1.97	0.46
1:C:503:VAL:HG11	2:A:100:HIS:HB2	1.97	0.46
3:B:2:ILE:H	3:B:97:THR:HG21	1.80	0.46
1:C:97:LYS:HB3	1:C:186:PHE:HA	1.98	0.46
1:D:666:ILE:HD11	1:D:672:ALA:HB2	1.97	0.46
3:H:113:PRO:HB3	3:H:139:PHE:HB3	1.97	0.46
1:C:280:ASN:OD1	1:C:284:THR:N	2.47	0.46
1:K:756:TYR:HH	1:K:998:THR:HG1	1.61	0.46
1:K:957:GLN:O	1:K:961:THR:OG1	2.32	0.46
2:E:179:ASP:OD1	2:E:179:ASP:N	2.46	0.46
1:K:452:LEU:HD13	1:K:492:LEU:HB3	1.97	0.46
2:A:150:GLY:HA2	2:A:180:LEU:HD13	1.97	0.46
1:C:552:LEU:HB3	1:C:585:LEU:HD13	1.98	0.45
1:C:814:LYS:HZ3	1:C:872:GLN:HG2	1.81	0.45
1:K:401:VAL:HG22	1:K:509:ARG:HG2	1.99	0.45
1:K:559:PHE:HB3	1:K:584:ILE:HB	1.98	0.45
1:C:329:PHE:CG	1:C:330:PRO:CD	2.98	0.45
3:H:128:GLY:HA2	3:H:183:LYS:HB2	1.98	0.45
1:K:117:LEU:HD22	1:K:231:ILE:HD13	1.98	0.45
1:C:99:ASN:ND2	1:C:178:ASP:O	2.46	0.45
1:C:1054:GLN:HB2	1:C:1061:VAL:HB	1.99	0.45
2:A:107:ASP:HB3	3:B:46:LEU:HB2	1.98	0.45
1:C:58:PHE:HB2	1:C:293:LEU:HD22	1.99	0.45
1:K:53:ASP:OD2	1:K:195:LYS:NZ	2.50	0.45
1:K:277:LEU:HD22	1:K:285:ILE:HD13	1.99	0.45
1:K:403:ARG:HG3	1:K:497:PHE:HE1	1.81	0.45
1:D:1006:THR:HG23	1:K:1005:GLN:HE22	1.82	0.45
2:A:148:VAL:HG21	2:A:203:VAL:HG11	1.98	0.45
1:C:498:GLN:NE2	1:C:500:THR:OG1	2.49	0.45
1:K:99:ASN:ND2	1:K:178:ASP:O	2.43	0.45
1:K:108:THR:O	1:K:236:THR:OG1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:656:VAL:HG12	1:D:658:ASN:H	1.82	0.45
2:E:148:VAL:HB	2:E:183:LEU:HB2	1.98	0.45
1:D:294:ASP:N	1:D:294:ASP:OD1	2.49	0.45
1:D:326:ILE:HB	1:D:541:PHE:HA	1.99	0.45
1:C:418:ILE:HA	1:C:422:ASN:HB2	1.98	0.44
1:C:108:THR:O	1:C:236:THR:OG1	2.35	0.44
2:A:177:GLN:HE21	3:B:160:LEU:HD11	1.81	0.44
1:C:969:ASN:HB2	1:D:755:GLN:HB3	2.00	0.44
1:C:1056:ALA:HB2	1:C:1061:VAL:HG23	1.98	0.44
1:D:364:ASP:HA	1:D:527:PRO:HG3	1.98	0.44
1:K:565:PHE:HA	1:K:576:VAL:HA	1.99	0.44
1:K:656:VAL:HG12	1:K:658:ASN:H	1.83	0.44
1:D:328:ARG:NH2	1:D:580:GLN:OE1	2.50	0.44
1:D:393:THR:HA	1:D:522:ALA:HA	1.99	0.44
1:D:1074:ASN:OD1	1:K:895:GLN:NE2	2.50	0.44
3:H:83:LEU:HD22	3:H:166:GLN:HB3	2.00	0.44
2:A:156:VAL:HG21	2:A:183:LEU:HD11	1.99	0.44
1:C:656:VAL:HG12	1:C:658:ASN:H	1.83	0.44
1:C:798:GLY:O	1:C:920:GLN:NE2	2.50	0.44
1:C:338:PHE:HB3	1:C:368:LEU:HD21	1.99	0.43
1:K:557:LYS:HB2	1:K:584:ILE:HD13	2.01	0.43
1:C:908:GLY:O	1:C:1038:LYS:NZ	2.52	0.43
1:K:93:ALA:HA	1:K:191:GLU:HG2	2.00	0.43
1:C:1005:GLN:HE22	1:K:1006:THR:HG23	1.83	0.43
1:D:216:LEU:HA	1:D:217:PRO:HD3	1.91	0.43
1:K:128:ILE:HD13	1:K:229:LEU:HD11	1.99	0.43
1:K:809:PRO:HA	1:K:814:LYS:HG2	1.99	0.43
1:C:152:TRP:HB3	1:C:179:LEU:HB2	1.99	0.43
1:D:396:TYR:HB2	1:D:514:SER:HB2	2.00	0.43
1:D:877:LEU:HD22	1:D:1034:LEU:HD21	2.01	0.43
2:E:62:SER:O	2:E:66:ARG:NH2	2.46	0.43
1:C:68:ILE:HG22	1:C:262:ALA:HA	2.00	0.43
1:C:755:GLN:HB2	1:K:969:ASN:HB2	2.01	0.43
1:D:1054:GLN:HB2	1:D:1061:VAL:HB	2.00	0.43
1:K:654:GLU:HB3	1:K:693:ILE:HG22	2.00	0.43
1:D:456:PHE:H	1:D:491:PRO:HB3	1.84	0.43
1:K:719:THR:HG23	1:K:1070:ALA:HB2	2.01	0.43
1:D:106:PHE:HD2	1:D:117:LEU:HD23	1.84	0.43
2:A:29:ILE:HD12	2:A:73:THR:HA	2.00	0.43
1:D:1051:SER:OG	1:D:1064:HIS:ND1	2.49	0.42
2:E:43:ASN:ND2	3:H:85:ASP:OD2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:179:ASP:OD1	2:A:179:ASP:N	2.53	0.42
1:K:143:VAL:O	1:K:146:HIS:NE2	2.46	0.42
2:A:18:LEU:HB3	2:A:82:LEU:H	1.83	0.42
1:D:289:VAL:HG13	1:D:297:SER:HB2	2.01	0.42
1:K:906:PHE:HB3	1:K:911:VAL:HB	2.02	0.42
1:C:81:ASN:HB3	1:C:239:GLN:HE21	1.83	0.42
1:C:330:PRO:O	1:C:331:ASN:HB3	2.19	0.42
1:C:401:VAL:HG22	1:C:509:ARG:HG2	2.01	0.42
1:D:33:THR:HB	1:D:220:PHE:HD1	1.83	0.42
2:E:219:ARG:HA	2:E:220:ASP:HA	1.75	0.42
1:C:380:TYR:OH	1:C:408:ARG:NH1	2.52	0.42
1:C:738:CYS:SG	1:C:764:ASN:ND2	2.91	0.42
1:D:345:THR:HG22	1:D:346:ARG:HG2	2.02	0.42
1:C:1031:GLU:HA	1:K:1040:VAL:HB	2.02	0.42
1:D:35:GLY:HA3	1:D:56:LEU:HB3	2.02	0.42
1:K:294:ASP:OD1	1:K:294:ASP:N	2.52	0.42
1:C:957:GLN:O	1:C:961:THR:OG1	2.32	0.42
1:D:867:ASP:OD1	1:D:867:ASP:N	2.53	0.42
1:K:718:PHE:HA	1:K:1069:PRO:HA	2.02	0.42
1:C:40:ASP:N	1:C:40:ASP:OD1	2.53	0.41
1:D:111:ASP:N	1:D:111:ASP:OD1	2.52	0.41
3:H:170:ASP:OD1	3:H:170:ASP:N	2.52	0.41
1:K:35:GLY:HA3	1:K:56:LEU:HB3	2.02	0.41
1:D:40:ASP:OD1	1:D:40:ASP:N	2.51	0.41
1:D:519:HIS:O	1:K:41:LYS:NZ	2.45	0.41
1:D:924:ALA:O	1:D:928:ASN:ND2	2.52	0.41
1:C:591:SER:OG	1:C:619:GLU:OE1	2.39	0.41
1:D:1041:ASP:HB2	1:K:1030:SER:HB3	2.02	0.41
1:C:280:ASN:HD21	1:C:284:THR:HB	1.85	0.41
1:C:864:LEU:HA	1:K:667:GLY:HA2	2.03	0.41
3:H:46:LEU:HD21	3:H:49:TYR:HB3	2.01	0.41
1:C:98:SER:HB3	1:C:181:GLY:HA2	2.03	0.41
1:K:1084:ASP:OD1	1:K:1084:ASP:N	2.53	0.41
1:C:567:ARG:HG2	1:C:573:THR:HG22	2.02	0.41
1:D:596:SER:OG	1:D:613:GLN:NE2	2.53	0.41
1:K:40:ASP:OD1	1:K:40:ASP:N	2.52	0.41
1:C:1084:ASP:OD1	1:C:1084:ASP:N	2.54	0.41
1:D:280:ASN:OD1	1:D:284:THR:N	2.54	0.41
3:B:170:ASP:OD1	3:B:170:ASP:N	2.54	0.41
3:B:190:ASN:HA	3:B:211:ARG:HE	1.84	0.41
1:C:33:THR:HB	1:C:220:PHE:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:674:TYR:HE1	1:C:692:ILE:HG12	1.86	0.41
2:A:219:ARG:HA	2:A:220:ASP:HA	1.72	0.41
1:K:1010:GLN:O	1:K:1014:ARG:NH1	2.54	0.40
1:C:531:THR:HB	1:C:532:ASN:H	1.62	0.40
1:K:557:LYS:NZ	1:K:586:ASP:OD2	2.48	0.40
3:B:138:ASN:HA	3:B:172:THR:HB	2.03	0.40
1:C:490:PHE:O	1:C:493:GLN:NE2	2.50	0.40
3:H:38:GLN:HG2	3:H:44:PRO:HB3	2.03	0.40
1:D:435:ALA:HB1	1:D:508:TYR:HB3	2.02	0.40
2:A:114:THR:HB	2:A:155:PRO:HG3	2.03	0.40
2:A:148:VAL:HB	2:A:183:LEU:HD12	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	C	1047/1261 (83%)	1017 (97%)	29 (3%)	1 (0%)	48	83
1	D	1045/1261 (83%)	1024 (98%)	21 (2%)	0	100	100
1	K	1047/1261 (83%)	1017 (97%)	30 (3%)	0	100	100
2	A	219/222 (99%)	214 (98%)	5 (2%)	0	100	100
2	E	219/222 (99%)	217 (99%)	2 (1%)	0	100	100
3	B	211/214 (99%)	206 (98%)	5 (2%)	0	100	100
3	H	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
All	All	3999/4655 (86%)	3902 (98%)	96 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	331	ASN

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	C	928/1099 (84%)	917 (99%)	11 (1%)	67	78
1	D	926/1099 (84%)	918 (99%)	8 (1%)	75	83
1	K	928/1099 (84%)	917 (99%)	11 (1%)	67	78
2	A	197/198 (100%)	192 (98%)	5 (2%)	42	61
2	E	197/198 (100%)	193 (98%)	4 (2%)	50	67
3	B	190/191 (100%)	190 (100%)	0	100	100
3	H	190/191 (100%)	186 (98%)	4 (2%)	48	66
All	All	3556/4075 (87%)	3513 (99%)	43 (1%)	66	78

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	33	THR
1	C	208	THR
1	C	327	VAL
1	C	329	PHE
1	C	336	CYS
1	C	524	VAL
1	C	531	THR
1	C	534	VAL
1	C	599	THR
1	C	760	CYS
1	C	912	THR
1	D	33	THR
1	D	150	LYS
1	D	208	THR
1	D	510	VAL
1	D	599	THR
1	D	760	CYS

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Mol	Chain	Res	Type
1	D	912	THR
1	D	961	THR
2	E	57	THR
2	E	85	VAL
2	E	158	VAL
2	E	217	VAL
3	H	19	VAL
3	H	36	TYR
3	H	92	ASN
3	H	146	VAL
1	K	33	THR
1	K	90	VAL
1	K	208	THR
1	K	329	PHE
1	K	392	PHE
1	K	394	ASN
1	K	510	VAL
1	K	573	THR
1	K	599	THR
1	K	912	THR
1	K	916	LEU
2	A	71	ARG
2	A	143	THR
2	A	147	LEU
2	A	156	VAL
2	A	158	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	239	GLN
1	C	334	ASN
1	C	422	ASN
1	C	564	GLN
1	C	901	GLN
1	C	1005	GLN
1	C	1011	GLN
1	D	437	ASN
1	D	613	GLN
1	D	957	GLN
2	E	76	ASN
3	H	89	GLN

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Mol	Chain	Res	Type
3	H	124	GLN
3	H	166	GLN
1	K	613	GLN
1	K	955	ASN
1	K	965	GLN
1	K	1005	GLN
1	K	1011	GLN
2	A	161	ASN
2	A	177	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 oligosaccharides 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.

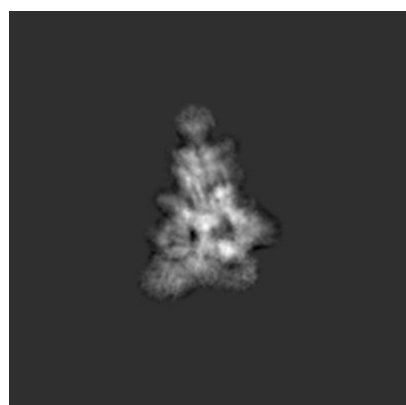
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30642. These allow visual inspection of the internal detail of the map and identification of artifacts.

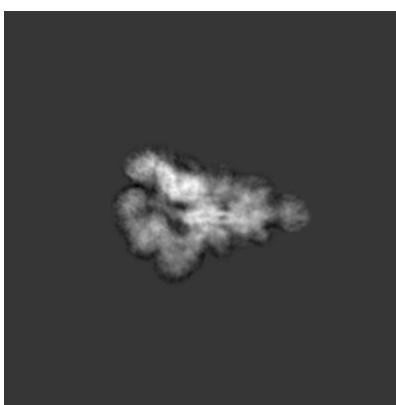
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

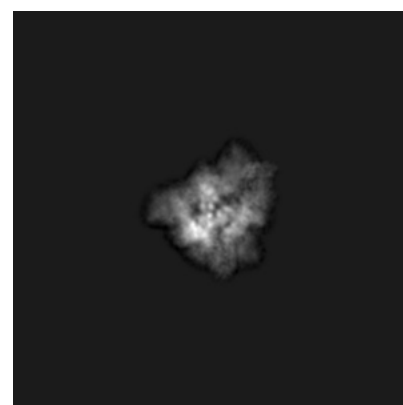
6.1.1 Primary map



X



Y

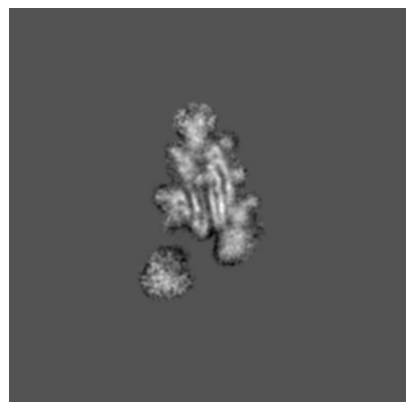


Z

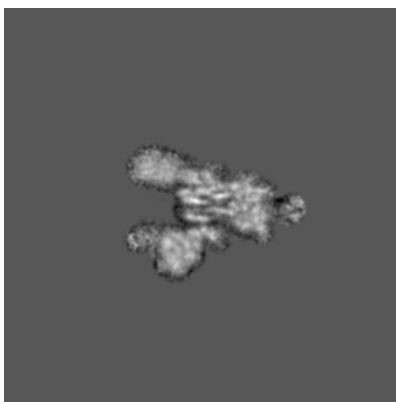
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

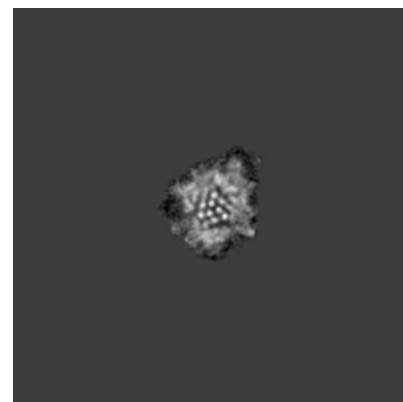
6.2.1 Primary map



X Index: 240



Y Index: 240

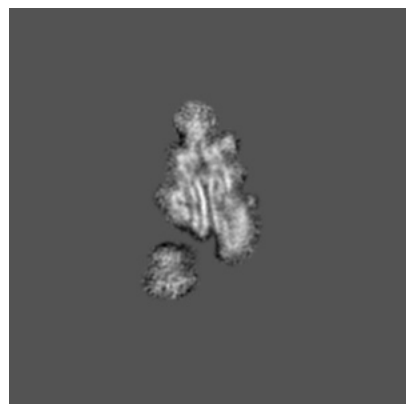


Z Index: 240

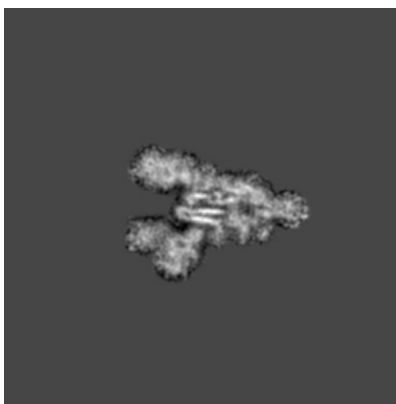
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

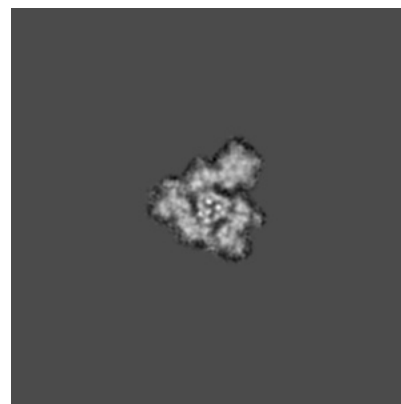
6.3.1 Primary map



X Index: 235



Y Index: 232

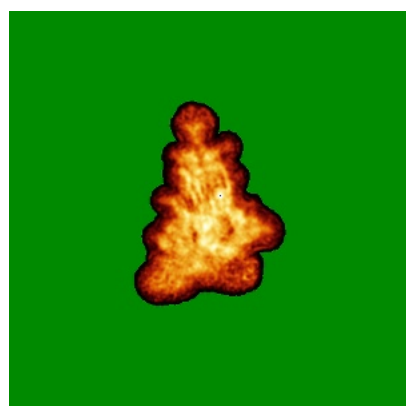


Z Index: 227

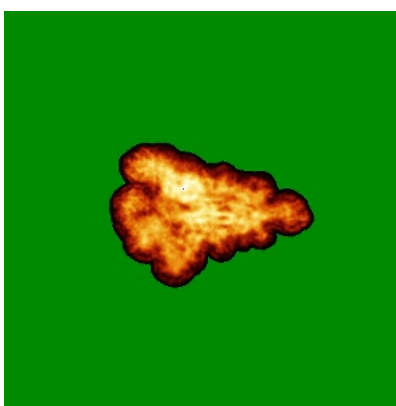
The images above show the largest variance slices of the map in three orthogonal directions.

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

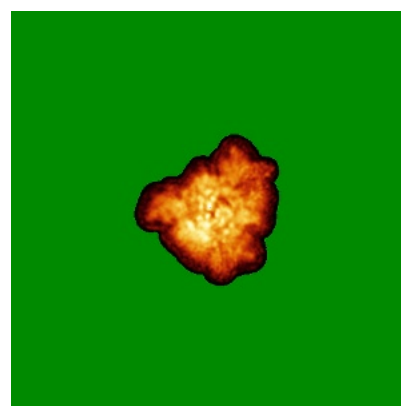
6.4.1 Primary map



X



Y

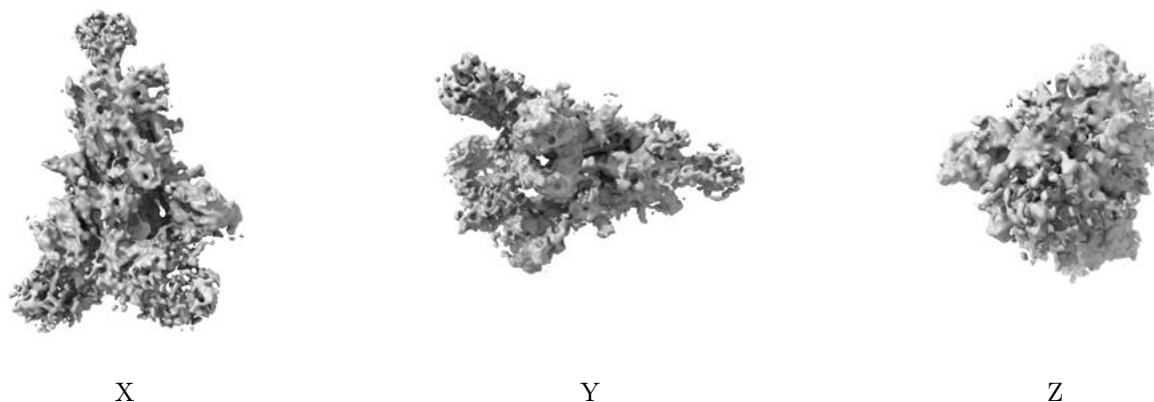


Z

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

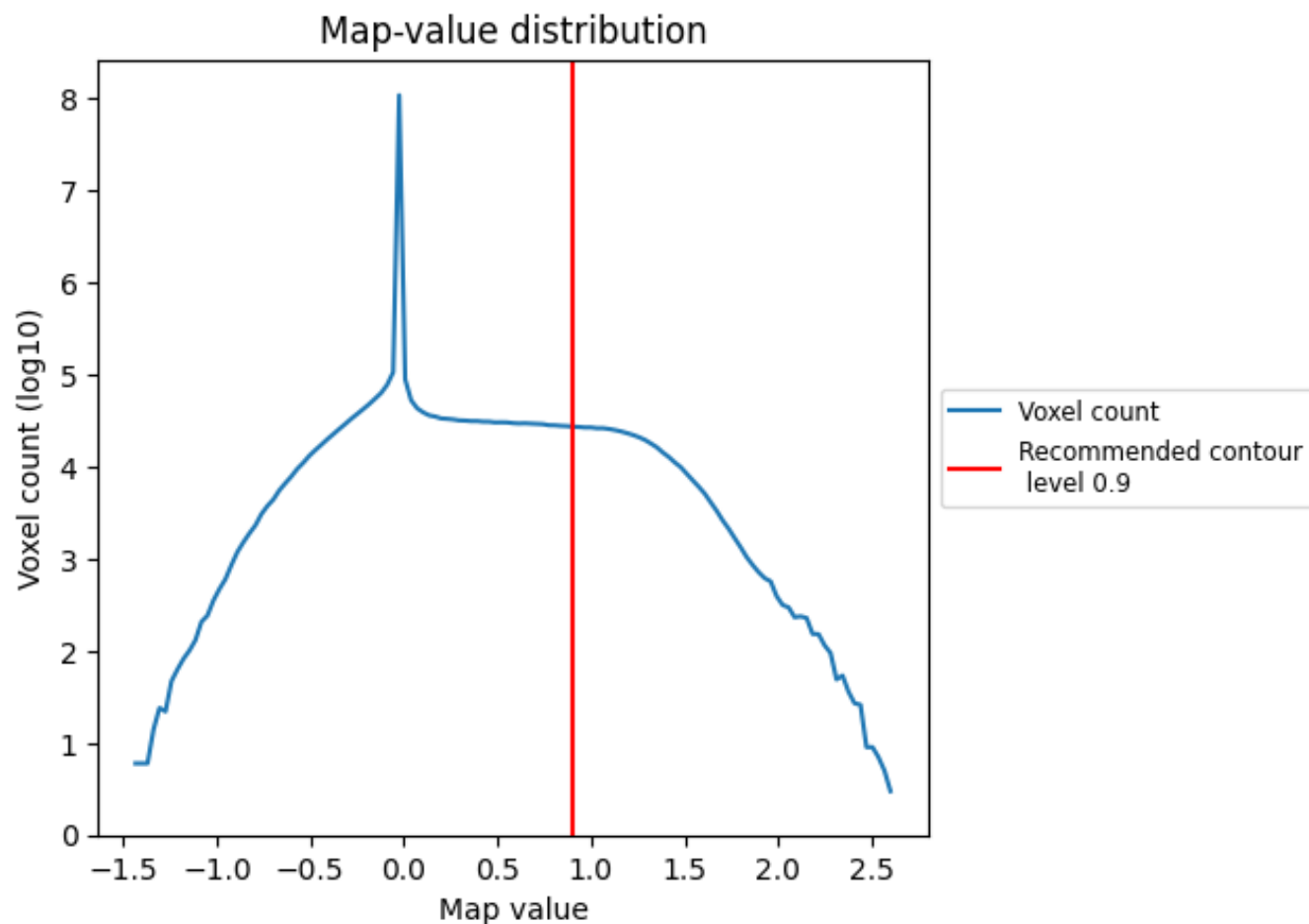
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

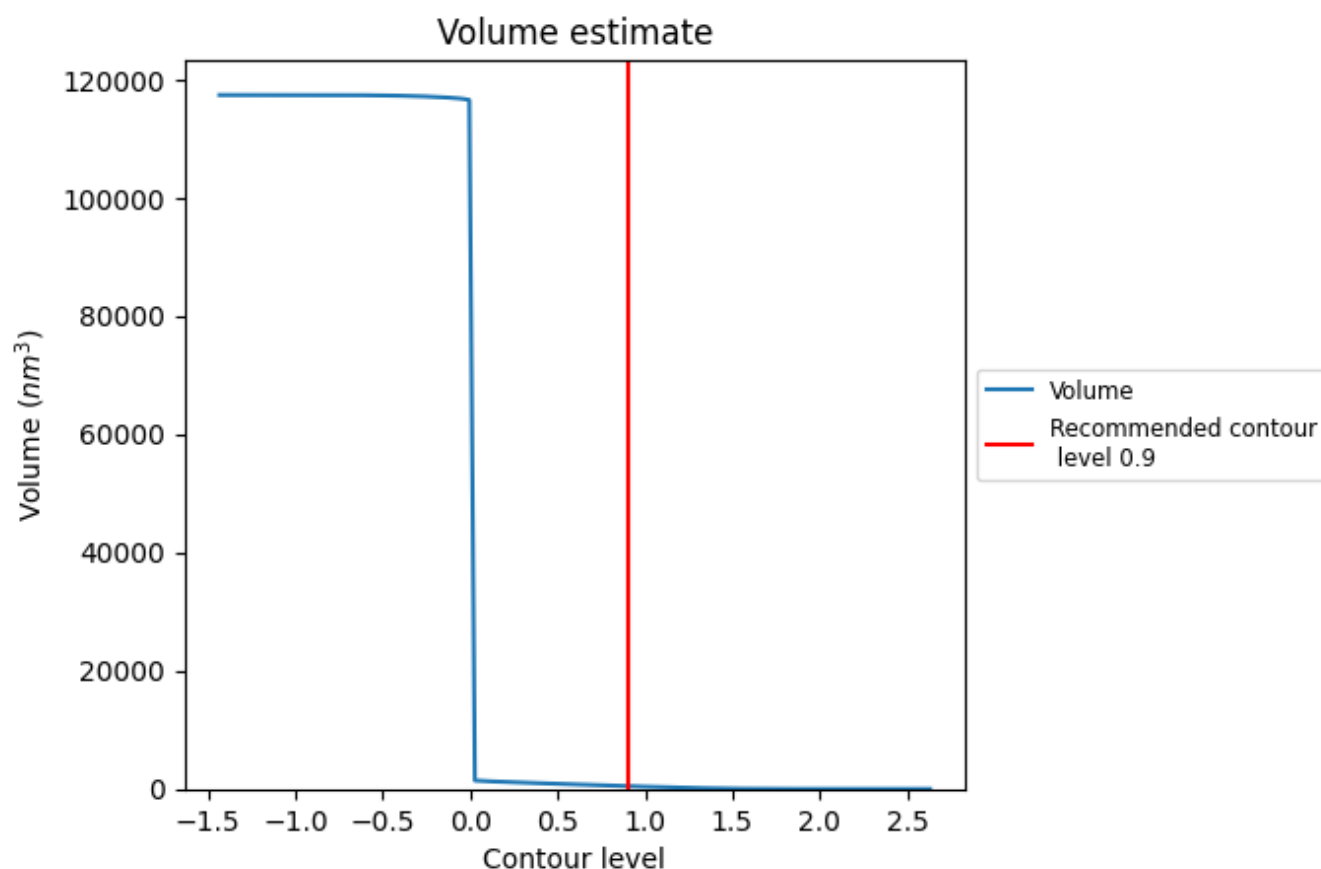
This section contains the results of statistical analysis of the map.

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.

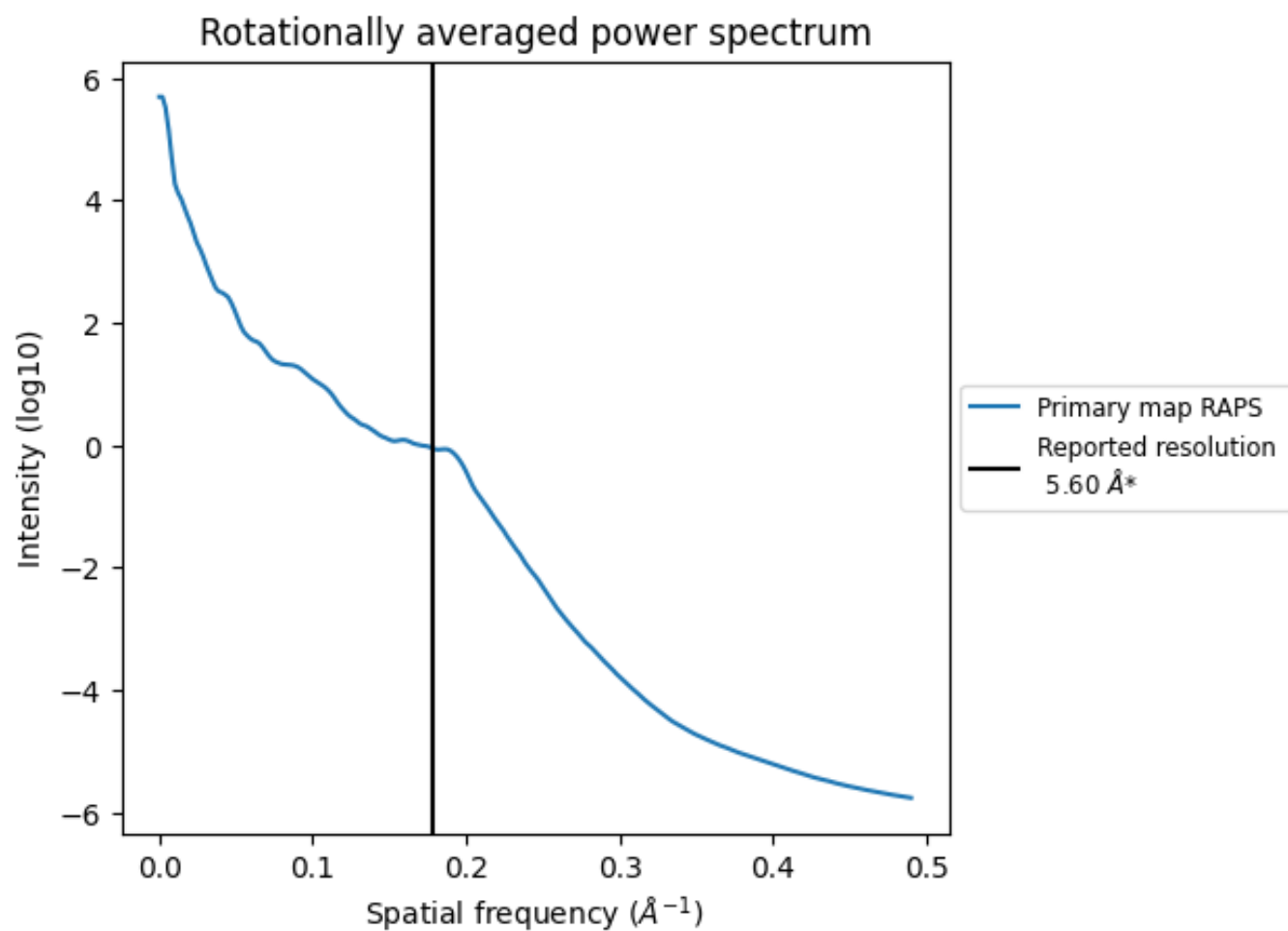
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 481 nm³; this corresponds to an approximate mass of 435 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 0.179 Å⁻¹

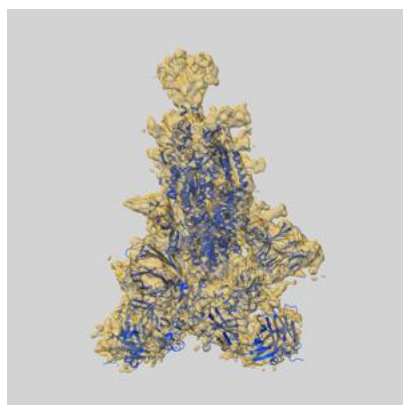
8 Fourier-Shell correlation

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

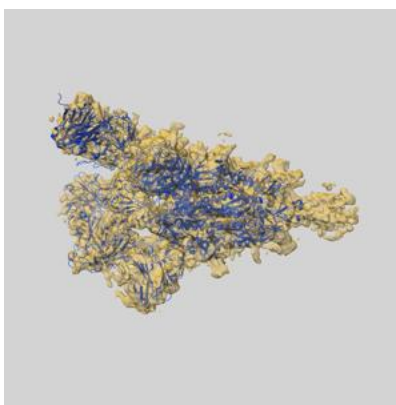
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30642 and PDB model 7DD2. Per-residue inclusion information can be found in section [3](#) on page [8](#).

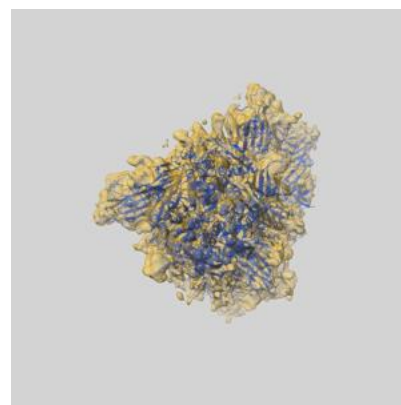
9.1 Map-model overlay [i](#)



X



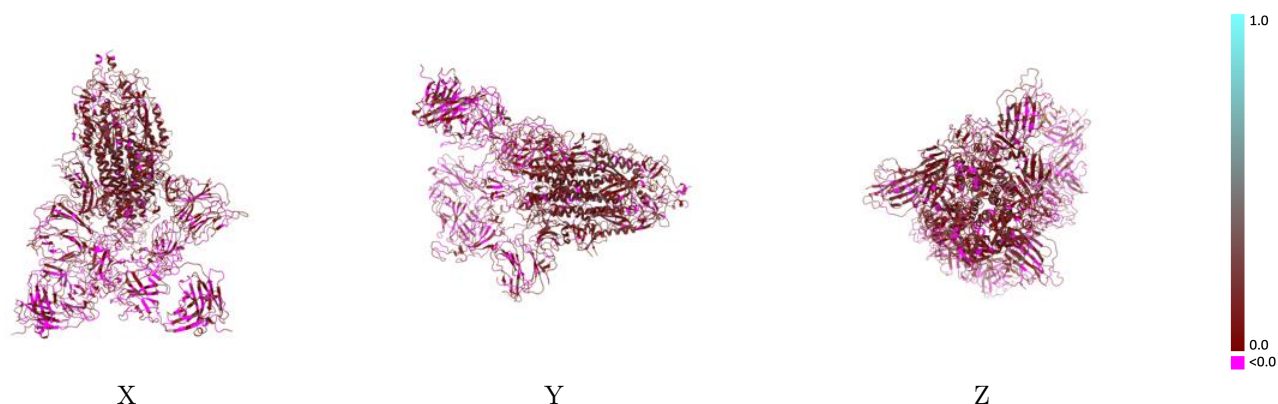
Y



Z

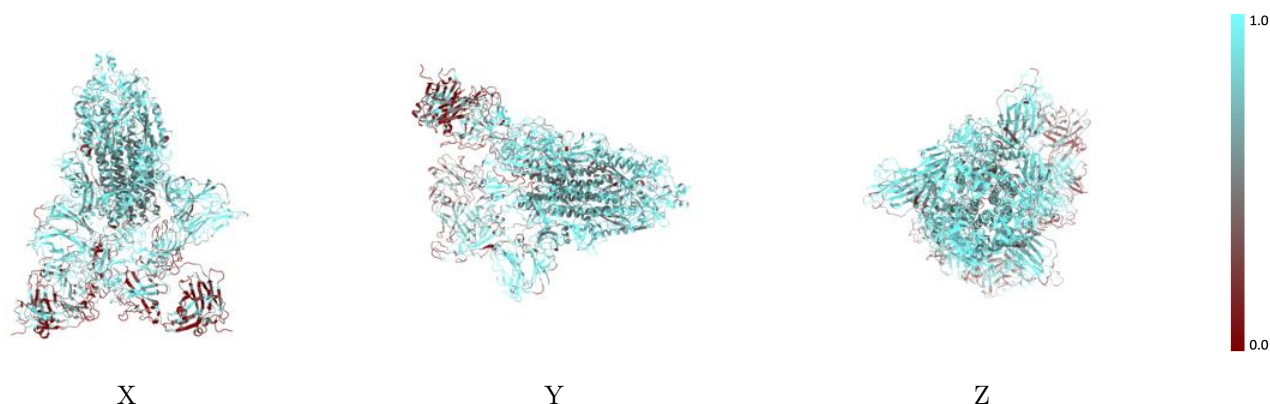
The images above show the 3D surface view of the map at the recommended contour level 0.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



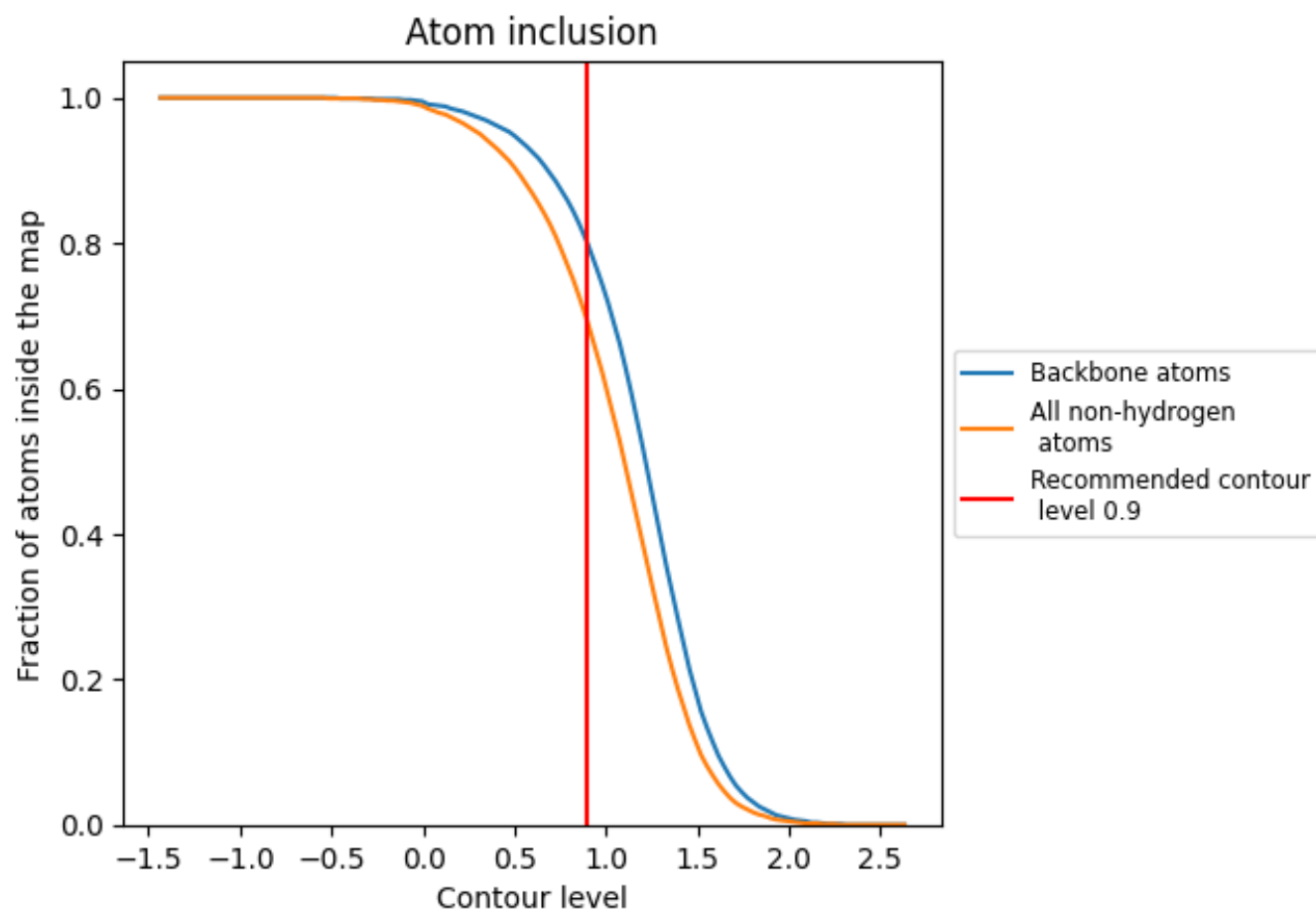
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.9).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 69% 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 (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6910	<div></div> 0.1000
A	<div></div> 0.5250	<div></div> 0.0450
B	<div></div> 0.5640	<div></div> 0.0450
C	<div></div> 0.7450	<div></div> 0.1130
D	<div></div> 0.7590	<div></div> 0.1180
E	<div></div> 0.4000	<div></div> 0.0520
H	<div></div> 0.4780	<div></div> 0.0450
K	<div></div> 0.7300	<div></div> 0.1120

1.0

0.0

<0.0