



Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 12:25 PM EST

PDB ID : 7T4Q
EMDB ID : EMD-25685
Title : CryoEM structure of the HCMV Pentamer gH/gL/UL128/UL130/UL131A in complex with neutralizing fabs 2C12, 7I13 and 13H11
Authors : Kschonsak, M.; Johnson, M.C.; Schelling, R.; Green, E.M.; Rouge, L.; Ho, H.; Patel, N.; Kilic, C.; Kraft, E.; Arthur, C.P.; Rohou, A.L.; Comps-Agrar, L.; Martinez-Martin, N.; Perez, L.; Payandeh, J.; Ciferri, C.
Deposited on : 2021-12-10
Resolution : 2.90 Å(reported)
Based on initial model : 5VOB

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
Mogul : 2022.3.0, CSD as543be (2022)
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

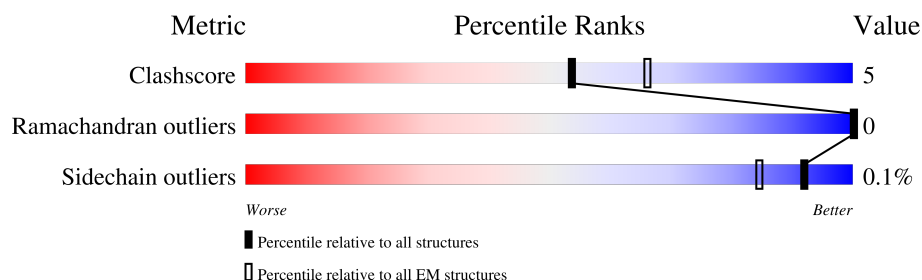
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	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	A	767	
2	B	278	
3	C	171	
4	D	254	
5	E	129	
6	F	252	
7	G	240	
8	H	237	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	251	<div><div></div><div>42%6%51%</div></div>
10	J	250	<div><div></div><div>44%.52%</div></div>
11	K	237	<div><div></div><div>41%.56%</div></div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 15473 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 Envelope glycoprotein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	623	Total	C	N	O	S	0	0
			5018	3218	848	928	24		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	716	GLY	-	expression tag	UNP F5H9T3
A	717	THR	-	expression tag	UNP F5H9T3
A	718	LYS	-	expression tag	UNP F5H9T3
A	719	LEU	-	expression tag	UNP F5H9T3
A	720	GLY	-	expression tag	UNP F5H9T3
A	721	PRO	-	expression tag	UNP F5H9T3
A	722	GLU	-	expression tag	UNP F5H9T3
A	723	GLN	-	expression tag	UNP F5H9T3
A	724	LYS	-	expression tag	UNP F5H9T3
A	725	LEU	-	expression tag	UNP F5H9T3
A	726	ILE	-	expression tag	UNP F5H9T3
A	727	SER	-	expression tag	UNP F5H9T3
A	728	GLU	-	expression tag	UNP F5H9T3
A	729	GLU	-	expression tag	UNP F5H9T3
A	730	ASP	-	expression tag	UNP F5H9T3
A	731	LEU	-	expression tag	UNP F5H9T3
A	732	ASN	-	expression tag	UNP F5H9T3
A	733	SER	-	expression tag	UNP F5H9T3
A	734	ALA	-	expression tag	UNP F5H9T3
A	735	VAL	-	expression tag	UNP F5H9T3
A	736	ASP	-	expression tag	UNP F5H9T3
A	737	GLY	-	expression tag	UNP F5H9T3
A	738	SER	-	expression tag	UNP F5H9T3
A	739	GLY	-	expression tag	UNP F5H9T3
A	740	LEU	-	expression tag	UNP F5H9T3
A	741	ASN	-	expression tag	UNP F5H9T3
A	742	ASP	-	expression tag	UNP F5H9T3
A	743	ILE	-	expression tag	UNP F5H9T3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	744	PHE	-	expression tag	UNP F5H9T3
A	745	GLU	-	expression tag	UNP F5H9T3
A	746	ALA	-	expression tag	UNP F5H9T3
A	747	GLN	-	expression tag	UNP F5H9T3
A	748	LYS	-	expression tag	UNP F5H9T3
A	749	ILE	-	expression tag	UNP F5H9T3
A	750	GLU	-	expression tag	UNP F5H9T3
A	751	TRP	-	expression tag	UNP F5H9T3
A	752	HIS	-	expression tag	UNP F5H9T3
A	753	GLU	-	expression tag	UNP F5H9T3
A	754	ASN	-	expression tag	UNP F5H9T3
A	755	LEU	-	expression tag	UNP F5H9T3
A	756	TYR	-	expression tag	UNP F5H9T3
A	757	PHE	-	expression tag	UNP F5H9T3
A	758	GLN	-	expression tag	UNP F5H9T3
A	759	GLY	-	expression tag	UNP F5H9T3
A	760	HIS	-	expression tag	UNP F5H9T3
A	761	HIS	-	expression tag	UNP F5H9T3
A	762	HIS	-	expression tag	UNP F5H9T3
A	763	HIS	-	expression tag	UNP F5H9T3
A	764	HIS	-	expression tag	UNP F5H9T3
A	765	HIS	-	expression tag	UNP F5H9T3
A	766	HIS	-	expression tag	UNP F5H9T3
A	767	HIS	-	expression tag	UNP F5H9T3

- Molecule 2 is a protein called Envelope glycoprotein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	233	Total	C	N	O	S	0	0
			1843	1173	322	340	8		

- Molecule 3 is a protein called Envelope protein UL128.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	124	Total	C	N	O	S	0	0
			999	626	182	182	9		

- Molecule 4 is a protein called Envelope glycoprotein UL130.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	164	Total	C	N	O	S	0	0
			1335	851	234	242	8		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	215	GLY	-	expression tag	UNP Q38M07
D	216	SER	-	expression tag	UNP Q38M07
D	217	GLU	-	expression tag	UNP Q38M07
D	218	ASN	-	expression tag	UNP Q38M07
D	219	LEU	-	expression tag	UNP Q38M07
D	220	TYR	-	expression tag	UNP Q38M07
D	221	PHE	-	expression tag	UNP Q38M07
D	222	GLN	-	expression tag	UNP Q38M07
D	223	GLY	-	expression tag	UNP Q38M07
D	224	SER	-	expression tag	UNP Q38M07
D	225	ALA	-	expression tag	UNP Q38M07
D	226	TRP	-	expression tag	UNP Q38M07
D	227	SER	-	expression tag	UNP Q38M07
D	228	HIS	-	expression tag	UNP Q38M07
D	229	PRO	-	expression tag	UNP Q38M07
D	230	GLN	-	expression tag	UNP Q38M07
D	231	PHE	-	expression tag	UNP Q38M07
D	232	GLU	-	expression tag	UNP Q38M07
D	233	LYS	-	expression tag	UNP Q38M07
D	234	GLY	-	expression tag	UNP Q38M07
D	235	GLY	-	expression tag	UNP Q38M07
D	236	GLY	-	expression tag	UNP Q38M07
D	237	SER	-	expression tag	UNP Q38M07
D	238	GLY	-	expression tag	UNP Q38M07
D	239	GLY	-	expression tag	UNP Q38M07
D	240	GLY	-	expression tag	UNP Q38M07
D	241	SER	-	expression tag	UNP Q38M07
D	242	GLY	-	expression tag	UNP Q38M07
D	243	GLY	-	expression tag	UNP Q38M07
D	244	GLY	-	expression tag	UNP Q38M07
D	245	SER	-	expression tag	UNP Q38M07
D	246	ALA	-	expression tag	UNP Q38M07
D	247	TRP	-	expression tag	UNP Q38M07
D	248	SER	-	expression tag	UNP Q38M07
D	249	HIS	-	expression tag	UNP Q38M07
D	250	PRO	-	expression tag	UNP Q38M07
D	251	GLN	-	expression tag	UNP Q38M07
D	252	PHE	-	expression tag	UNP Q38M07
D	253	GLU	-	expression tag	UNP Q38M07
D	254	LYS	-	expression tag	UNP Q38M07

- Molecule 5 is a protein called Envelope protein UL131A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	111	Total	C	N	O	S	0	0
			917	571	173	171	2		

- Molecule 6 is a protein called Fab 2C12 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	124	Total	C	N	O	S	0	0
			962	615	160	182	5		

- Molecule 7 is a protein called Fab 2C12 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	112	Total	C	N	O	S	0	0
			828	519	140	165	4		

- Molecule 8 is a protein called Fab 7I13 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	107	Total	C	N	O	S	0	0
			813	511	139	161	2		

- Molecule 9 is a protein called Fab 7I13 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	122	Total	C	N	O	S	0	0
			960	612	163	181	4		

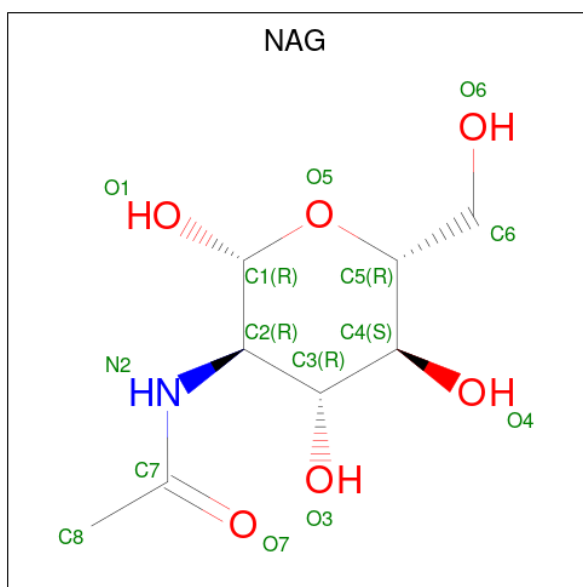
- Molecule 10 is a protein called Fab 13H11 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	121	Total	C	N	O	S	0	0
			924	581	160	178	5		

- Molecule 11 is a protein called Fab 13H11 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	105	Total	C	N	O	S	0	0
			790	500	131	156	3		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

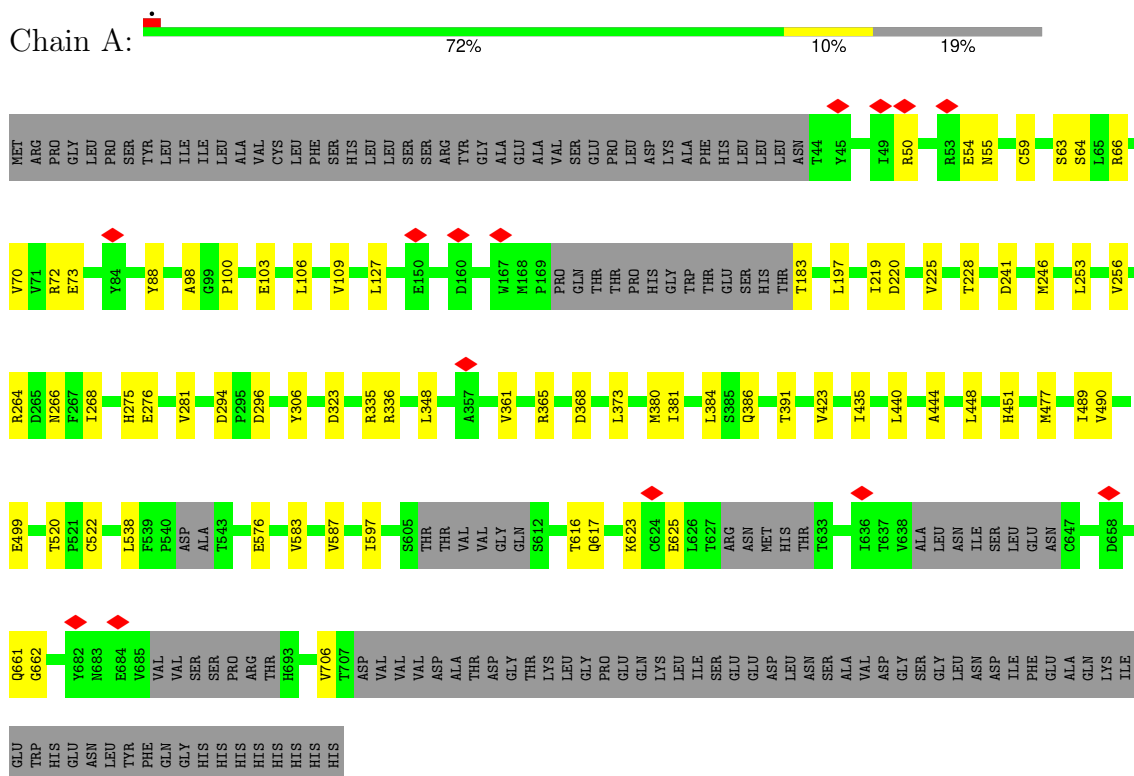


Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total	C	N	O	0
			14	8	1	5	
12	A	1	Total	C	N	O	0
			14	8	1	5	
12	A	1	Total	C	N	O	0
			14	8	1	5	
12	B	1	Total	C	N	O	0
			14	8	1	5	
12	D	1	Total	C	N	O	0
			14	8	1	5	
12	E	1	Total	C	N	O	0
			14	8	1	5	

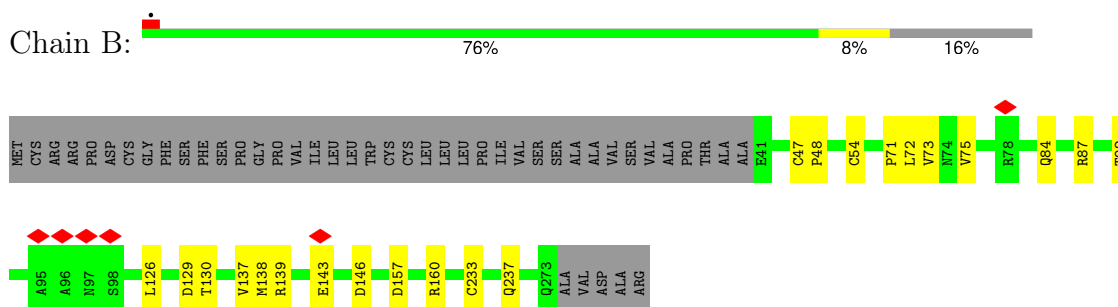
3 Residue-property plots

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

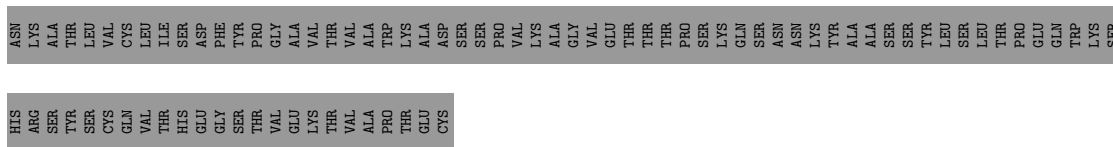
• Molecule 1: Envelope glycoprotein H



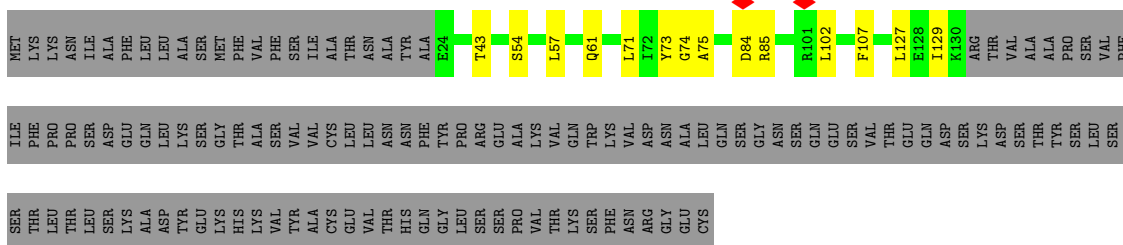
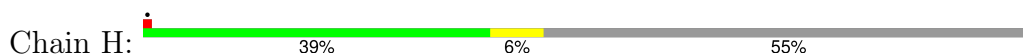
• Molecule 2: Envelope glycoprotein L



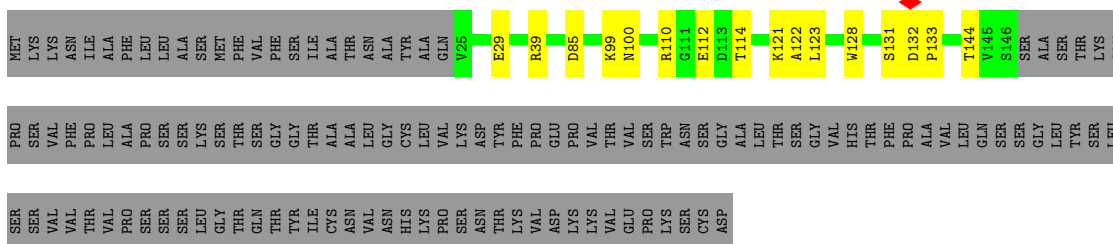
• Molecule 3: Envelope protein UL128



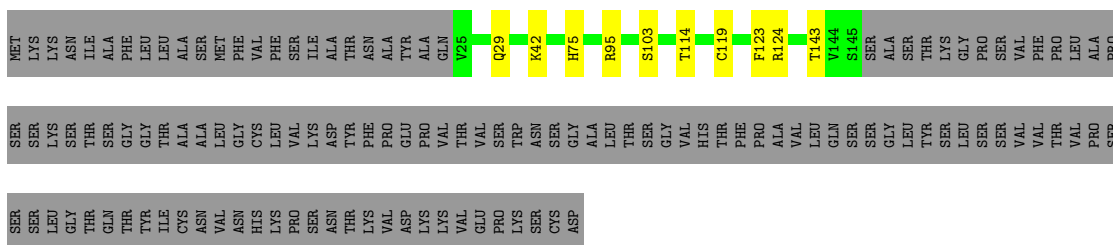
- Molecule 8: Fab 7I13 light chain



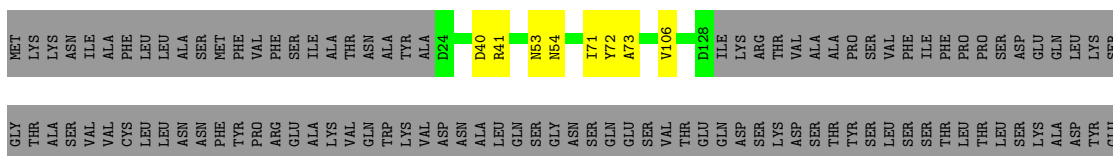
- Molecule 9: Fab 7I13 heavy chain



- Molecule 10: Fab 13H11 heavy chain



- Molecule 11: Fab 13H11 light chain



LYS
HIS
LYS
VAL
TYR
ALA
CYS
GLU
VAL
THR
HIS
GLN
GLY
LEU
SER
PRO
VAL
THR
LYS
SER
PHE
ASN
ARG
GLY
GLU
CYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	4792984	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 ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	30.294	Depositor
Minimum map value	-15.369	Depositor
Average map value	-0.025	Depositor
Map value standard deviation	0.591	Depositor
Recommended contour level	4.9	Depositor
Map size (Å)	382.336, 382.336, 382.336	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1948, 1.1948, 1.1948	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/5133	0.52	0/6983
2	B	0.27	0/1888	0.53	0/2577
3	C	0.26	0/1017	0.57	0/1372
4	D	0.27	0/1371	0.54	0/1862
5	E	0.27	0/937	0.57	0/1268
6	F	0.25	0/986	0.50	0/1351
7	G	0.27	0/848	0.51	0/1151
8	H	0.26	0/832	0.54	0/1130
9	I	0.27	0/985	0.55	0/1336
10	J	0.27	0/944	0.52	0/1280
11	K	0.27	0/808	0.49	0/1100
All	All	0.26	0/15749	0.53	0/21410

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	A	5018	0	4976	47	0
2	B	1843	0	1833	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	999	0	1000	25	0
4	D	1335	0	1307	19	0
5	E	917	0	878	12	0
6	F	962	0	959	7	0
7	G	828	0	792	5	0
8	H	813	0	788	11	0
9	I	960	0	915	13	0
10	J	924	0	900	5	0
11	K	790	0	777	5	0
12	A	42	0	39	2	0
12	B	14	0	13	0	0
12	D	14	0	13	0	0
12	E	14	0	13	0	0
All	All	15473	0	15203	152	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (152) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:VAL:HG22	1:A:435:ILE:HD11	1.65	0.79
1:A:72:ARG:NH1	1:A:73:GLU:O	2.18	0.76
3:C:97:ASN:ND2	5:E:32:ARG:O	2.24	0.70
3:C:152:SER:HB3	3:C:161:VAL:HG11	1.74	0.69
9:I:123:LEU:N	9:I:132:ASP:OD2	2.26	0.69
1:A:365:ARG:NH2	1:A:368:ASP:OD2	2.26	0.68
1:A:256:VAL:O	1:A:264:ARG:NH2	2.30	0.65
1:A:423:VAL:HG13	1:A:435:ILE:CD1	2.27	0.64
3:C:161:VAL:HG12	3:C:161:VAL:O	1.98	0.62
3:C:51:ARG:NH2	6:F:125:GLN:OE1	2.32	0.62
1:A:275:HIS:ND1	1:A:306:TYR:OH	2.24	0.62
3:C:159:LEU:O	3:C:159:LEU:HD23	1.98	0.62
3:C:156:HIS:CE1	3:C:161:VAL:HG13	2.34	0.62
3:C:143:ILE:N	4:D:97:GLN:OE1	2.32	0.61
7:G:51:ASP:OD1	7:G:52:VAL:N	2.33	0.60
1:A:538:LEU:HD23	1:A:538:LEU:O	2.02	0.59
3:C:144:VAL:HG13	3:C:144:VAL:O	2.03	0.59
5:E:27:LYS:NZ	6:F:82:GLU:O	2.33	0.59
3:C:59:PRO:O	9:I:110:ARG:NH2	2.36	0.58
1:A:296:ASP:OD1	1:A:335:ARG:NH2	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:GLN:O	2:B:87:ARG:NH1	2.37	0.57
8:H:43:THR:O	8:H:43:THR:HG23	2.05	0.57
2:B:137:VAL:HG22	3:C:159:LEU:HD11	1.87	0.56
11:K:106:VAL:HG13	11:K:106:VAL:O	2.06	0.56
2:B:75:VAL:O	2:B:75:VAL:HG13	2.06	0.56
3:C:156:HIS:HE1	3:C:161:VAL:HG13	1.68	0.56
2:B:233:CYS:O	2:B:237:GLN:N	2.39	0.56
5:E:102:ASN:OD1	5:E:103:LYS:N	2.40	0.56
4:D:59:PHE:HE2	4:D:88:LEU:HD21	1.72	0.55
2:B:92:THR:HG23	2:B:92:THR:O	2.08	0.54
1:A:64:SER:O	1:A:66:ARG:HG3	2.08	0.54
1:A:106:LEU:O	1:A:109:VAL:HG22	2.08	0.54
6:F:111:ASP:OD1	6:F:112:PRO:HD2	2.07	0.53
9:I:39:ARG:HG3	9:I:39:ARG:HH11	1.73	0.53
1:A:59:CYS:N	2:B:54:CYS:SG	2.83	0.52
8:H:102:LEU:HD21	8:H:127:LEU:HD21	1.90	0.52
4:D:121:ILE:HD11	4:D:147:PHE:HB2	1.92	0.51
8:H:57:LEU:O	8:H:74:GLY:O	2.28	0.51
1:A:661:GLN:HG2	1:A:662:GLY:N	2.25	0.51
9:I:128:TRP:O	9:I:132:ASP:HB2	2.11	0.51
1:A:197:LEU:HD11	1:A:228:THR:HG21	1.94	0.50
3:C:75:GLY:O	3:C:79:THR:HG23	2.11	0.50
9:I:110:ARG:HD2	9:I:112:GLU:OE2	2.11	0.50
1:A:294:ASP:OD2	1:A:335:ARG:NH1	2.45	0.50
3:C:77:VAL:O	3:C:81:THR:HG23	2.12	0.50
1:A:348:LEU:HD23	1:A:373:LEU:HD11	1.94	0.49
1:A:323:ASP:OD2	1:A:336:ARG:NH1	2.44	0.49
3:C:73:ILE:H	3:C:73:ILE:HD12	1.77	0.49
9:I:123:LEU:HB3	9:I:132:ASP:OD2	2.13	0.49
5:E:44:LEU:HD12	5:E:91:ASP:OD2	2.11	0.49
9:I:121:LYS:NZ	9:I:122:ALA:O	2.40	0.49
1:A:597:ILE:HG23	1:A:616:THR:HG21	1.95	0.49
1:A:253:LEU:O	1:A:253:LEU:HD12	2.13	0.49
8:H:54:SER:OG	8:H:75:ALA:HB2	2.13	0.49
3:C:129:PRO:HD2	4:D:206:PHE:CE2	2.48	0.49
4:D:152:VAL:HG22	4:D:153:PRO:HD2	1.94	0.49
4:D:177:GLU:OE2	4:D:193:ARG:NH2	2.43	0.49
3:C:150:LEU:O	3:C:153:VAL:HG12	2.13	0.48
9:I:29:GLU:OE1	9:I:29:GLU:N	2.44	0.48
1:A:183:THR:N	1:A:361:VAL:O	2.46	0.47
2:B:71:PRO:HG2	2:B:75:VAL:HG12	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:115:THR:HG22	6:F:146:VAL:H	1.79	0.47
1:A:66:ARG:HD2	1:A:70:VAL:HG21	1.96	0.47
1:A:706:VAL:HG12	1:A:706:VAL:O	2.14	0.47
8:H:107:PHE:CZ	8:H:129:ILE:HD13	2.49	0.47
1:A:100:PRO:HA	1:A:103:GLU:CD	2.35	0.47
4:D:105:THR:HG23	4:D:106:TRP:N	2.30	0.47
1:A:268:ILE:HD12	1:A:276:GLU:OE1	2.15	0.47
7:G:58:VAL:HG12	7:G:59:SER:N	2.30	0.46
3:C:45:ASP:O	3:C:57:ARG:N	2.43	0.46
4:D:171:MET:CE	9:I:131:SER:HB3	2.46	0.46
4:D:79:THR:HG21	4:D:83:CYS:CB	2.45	0.46
2:B:72:LEU:H	2:B:72:LEU:HD23	1.80	0.46
2:B:73:VAL:O	2:B:73:VAL:HG12	2.16	0.46
5:E:36:TYR:CE1	5:E:40:CYS:SG	3.09	0.46
5:E:101:THR:HG22	5:E:102:ASN:N	2.32	0.45
1:A:225:VAL:O	1:A:225:VAL:HG13	2.16	0.45
2:B:129:ASP:OD1	2:B:130:THR:N	2.50	0.45
2:B:139:ARG:O	2:B:143:GLU:HG3	2.16	0.45
11:K:40:ASP:OD1	11:K:41:ARG:N	2.50	0.45
11:K:72:TYR:CD1	11:K:73:ALA:N	2.85	0.45
1:A:55:ASN:ND2	12:A:801:NAG:N2	2.65	0.45
4:D:128:THR:HA	4:D:134:ASP:OD2	2.17	0.45
5:E:28:ASN:O	5:E:32:ARG:NH1	2.50	0.45
10:J:29:GLN:NE2	10:J:119:CYS:H	2.15	0.45
6:F:27:LEU:HD23	6:F:47:PHE:HB3	1.98	0.44
2:B:157:ASP:O	2:B:157:ASP:OD1	2.35	0.44
3:C:54:VAL:O	3:C:54:VAL:HG13	2.17	0.44
3:C:150:LEU:HA	3:C:153:VAL:HG12	1.98	0.44
1:A:241:ASP:O	10:J:75:HIS:NE2	2.47	0.44
5:E:89:ILE:HD13	5:E:118:ARG:HG2	1.99	0.44
1:A:451:HIS:HB2	1:A:490:VAL:HG13	1.99	0.44
1:A:576:GLU:HA	1:A:576:GLU:OE1	2.18	0.44
6:F:39:GLN:N	6:F:39:GLN:OE1	2.50	0.44
10:J:42:LYS:HZ1	10:J:103:SER:CB	2.31	0.44
3:C:56:LEU:HD12	3:C:65:TYR:CE1	2.52	0.44
1:A:444:ALA:O	1:A:448:LEU:HD23	2.17	0.44
1:A:587:VAL:HG13	1:A:617:GLN:HE21	1.83	0.44
1:A:499:GLU:OE2	1:A:520:THR:HG23	2.17	0.43
7:G:36:SER:OG	7:G:37:PRO:HD2	2.17	0.43
1:A:98:ALA:HB2	2:B:72:LEU:HD12	1.99	0.43
1:A:246:MET:HG3	1:A:281:VAL:HG12	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:ILE:HD12	1:A:391:THR:OG1	2.19	0.43
9:I:85:ASP:N	9:I:85:ASP:OD1	2.52	0.43
1:A:63:SER:HB2	1:A:88:TYR:HD1	1.84	0.43
8:H:43:THR:O	8:H:43:THR:CG2	2.66	0.43
7:G:36:SER:HB3	7:G:39:GLN:OE1	2.19	0.43
8:H:61:GLN:HB2	8:H:71:LEU:HD11	1.99	0.43
4:D:93:ASN:OD1	4:D:93:ASN:C	2.57	0.43
5:E:73:ASN:O	5:E:76:VAL:HG12	2.18	0.42
1:A:54:GLU:OE1	1:A:54:GLU:N	2.44	0.42
5:E:105:THR:O	5:E:105:THR:HG23	2.19	0.42
11:K:53:ASN:O	11:K:54:ASN:CG	2.58	0.42
3:C:162:CYS:O	3:C:163:ARG:HB2	2.19	0.42
1:A:63:SER:HB2	1:A:88:TYR:CD1	2.55	0.42
1:A:219:ILE:O	1:A:219:ILE:HG22	2.19	0.42
4:D:79:THR:HG21	4:D:83:CYS:HB3	2.01	0.42
10:J:123:PHE:CD2	10:J:124:ARG:HD2	2.55	0.42
1:A:55:ASN:ND2	12:A:801:NAG:C1	2.83	0.42
2:B:146:ASP:O	2:B:146:ASP:OD1	2.38	0.42
3:C:70:THR:HA	3:C:73:ILE:CD1	2.50	0.42
3:C:73:ILE:O	3:C:77:VAL:HG23	2.20	0.42
8:H:73:TYR:HB2	9:I:133:PRO:HG3	2.01	0.42
8:H:84:ASP:OD1	8:H:85:ARG:N	2.53	0.42
1:A:220:ASP:OD1	1:A:386:GLN:NE2	2.43	0.42
9:I:114:THR:HG23	9:I:144:THR:HA	2.01	0.42
1:A:623:LYS:O	1:A:625:GLU:HG3	2.20	0.42
2:B:47:CYS:N	2:B:48:PRO:CD	2.83	0.42
1:A:50:ARG:HD2	1:A:70:VAL:HG22	2.01	0.41
1:A:520:THR:HG22	1:A:522:CYS:H	1.85	0.41
2:B:126:LEU:HD12	2:B:138:MET:HG3	2.01	0.41
2:B:160:ARG:NE	4:D:56:TYR:CD1	2.88	0.41
4:D:73:GLY:HA2	4:D:114:LEU:HD13	2.02	0.41
9:I:99:LYS:O	9:I:100:ASN:HB2	2.20	0.41
2:B:157:ASP:OD1	4:D:97:GLN:HA	2.21	0.41
4:D:79:THR:HG22	4:D:80:GLY:N	2.36	0.41
1:A:489:ILE:HG12	1:A:583:VAL:HA	2.02	0.41
1:A:440:LEU:HD11	1:A:477:MET:HE1	2.01	0.41
1:A:127:LEU:HD22	1:A:266:ASN:HB3	2.02	0.41
5:E:25:ALA:HB1	5:E:36:TYR:HE1	1.86	0.41
6:F:121:VAL:CG1	6:F:135:PHE:HB2	2.51	0.41
10:J:114:THR:HG23	10:J:143:THR:HA	2.02	0.41
4:D:125:MET:HG3	5:E:124:VAL:HG11	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:76:VAL:O	7:G:76:VAL:HG12	2.21	0.41
8:H:107:PHE:CE2	8:H:129:ILE:HD13	2.56	0.41
3:C:93:LEU:HD23	3:C:96:CYS:SG	2.62	0.40
4:D:163:VAL:HG21	4:D:206:PHE:CE2	2.57	0.40
2:B:87:ARG:HH11	2:B:87:ARG:HG3	1.85	0.40
11:K:71:ILE:HG22	11:K:73:ALA:O	2.22	0.40
1:A:380:MET:SD	1:A:384:LEU:HD12	2.62	0.40
8:H:84:ASP:OD1	8:H:84:ASP:C	2.60	0.40
3:C:143:ILE:HD13	4:D:66:ARG:CZ	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	609/767 (79%)	585 (96%)	24 (4%)	0	100	100
2	B	231/278 (83%)	218 (94%)	13 (6%)	0	100	100
3	C	122/171 (71%)	118 (97%)	4 (3%)	0	100	100
4	D	162/254 (64%)	157 (97%)	5 (3%)	0	100	100
5	E	109/129 (84%)	108 (99%)	1 (1%)	0	100	100
6	F	122/252 (48%)	117 (96%)	5 (4%)	0	100	100
7	G	110/240 (46%)	103 (94%)	7 (6%)	0	100	100
8	H	105/237 (44%)	103 (98%)	2 (2%)	0	100	100
9	I	120/251 (48%)	116 (97%)	4 (3%)	0	100	100
10	J	119/250 (48%)	112 (94%)	7 (6%)	0	100	100
11	K	103/237 (44%)	100 (97%)	3 (3%)	0	100	100
All	All	1912/3066 (62%)	1837 (96%)	75 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	566/692 (82%)	566 (100%)	0	100	100
2	B	202/238 (85%)	202 (100%)	0	100	100
3	C	110/153 (72%)	110 (100%)	0	100	100
4	D	150/223 (67%)	150 (100%)	0	100	100
5	E	98/114 (86%)	98 (100%)	0	100	100
6	F	109/218 (50%)	109 (100%)	0	100	100
7	G	92/201 (46%)	92 (100%)	0	100	100
8	H	88/202 (44%)	88 (100%)	0	100	100
9	I	102/212 (48%)	102 (100%)	0	100	100
10	J	101/211 (48%)	100 (99%)	1 (1%)	73	91
11	K	88/204 (43%)	88 (100%)	0	100	100
All	All	1706/2668 (64%)	1705 (100%)	1 (0%)	92	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	95	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	NAG	E	201	5	14,14,15	0.17	0	17,19,21	0.65	0
12	NAG	B	301	2	14,14,15	0.27	0	17,19,21	0.48	0
12	NAG	A	801	-	14,14,15	0.25	0	17,19,21	0.47	0
12	NAG	D	301	4	14,14,15	0.16	0	17,19,21	0.69	0
12	NAG	A	803	1	14,14,15	0.20	0	17,19,21	0.51	0
12	NAG	A	802	-	14,14,15	0.19	0	17,19,21	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	E	201	5	-	2/6/23/26	0/1/1/1
12	NAG	B	301	2	-	0/6/23/26	0/1/1/1
12	NAG	A	801	-	-	0/6/23/26	0/1/1/1
12	NAG	D	301	4	-	0/6/23/26	0/1/1/1
12	NAG	A	803	1	-	0/6/23/26	0/1/1/1
12	NAG	A	802	-	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	E	201	NAG	O5-C5-C6-O6
12	E	201	NAG	C4-C5-C6-O6
12	A	802	NAG	O5-C5-C6-O6
12	A	802	NAG	C1-C2-N2-C7
12	A	802	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	801	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

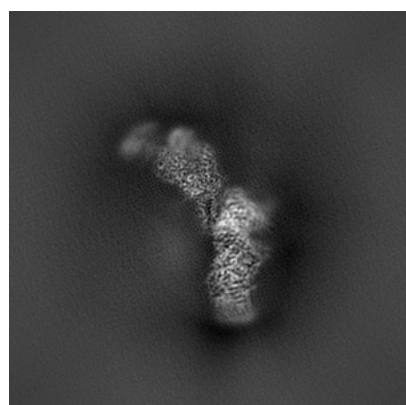
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25685. These allow visual inspection of the internal detail of the map and identification of artifacts.

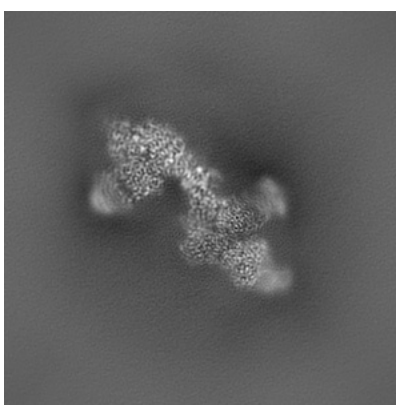
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

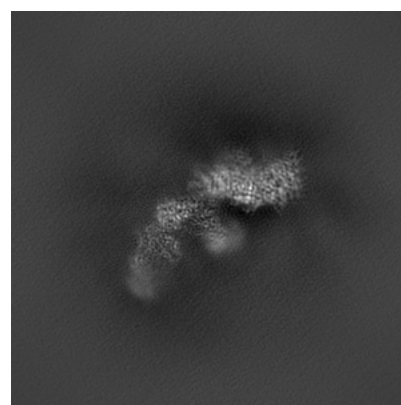
6.1.1 Primary map



X



Y

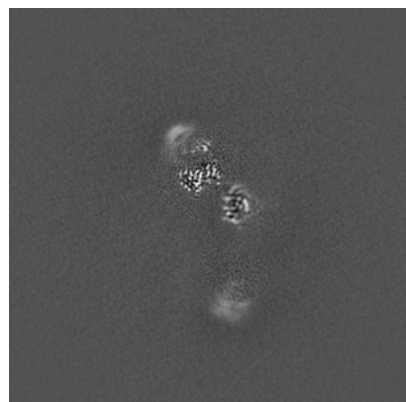


Z

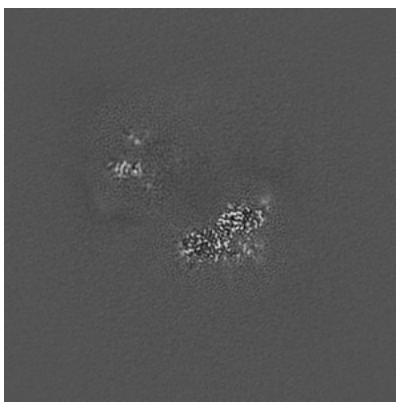
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

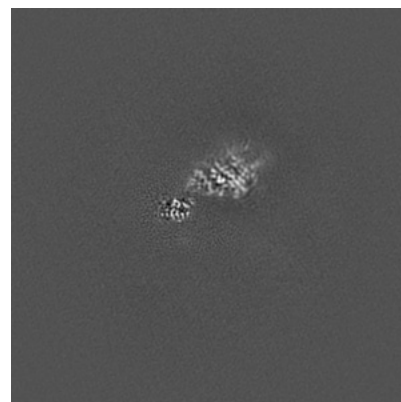
6.2.1 Primary map



X Index: 160



Y Index: 160

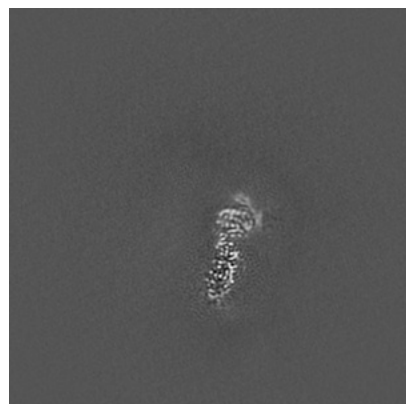


Z Index: 160

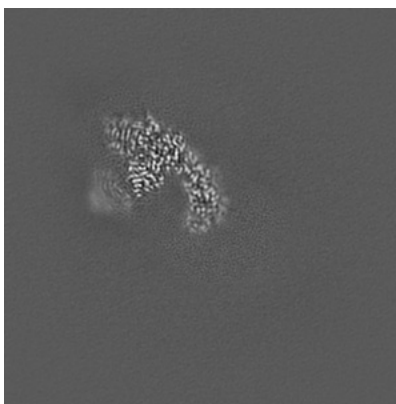
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

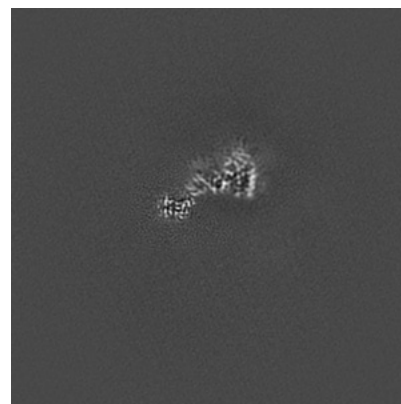
6.3.1 Primary map



X Index: 191



Y Index: 178

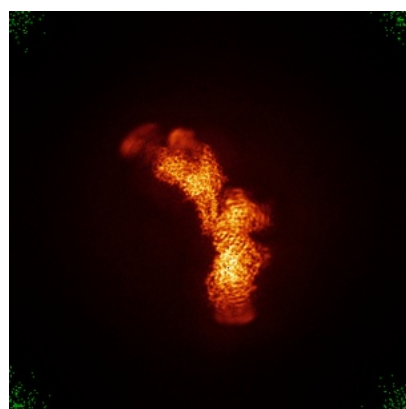


Z Index: 156

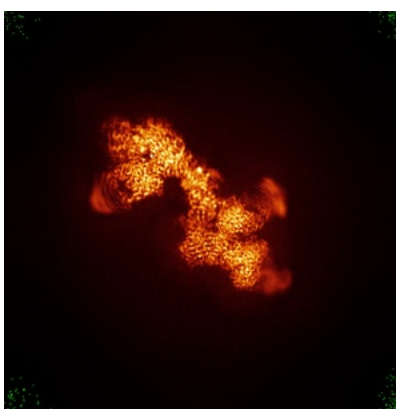
The images above show the largest variance slices of the map in three orthogonal directions.

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

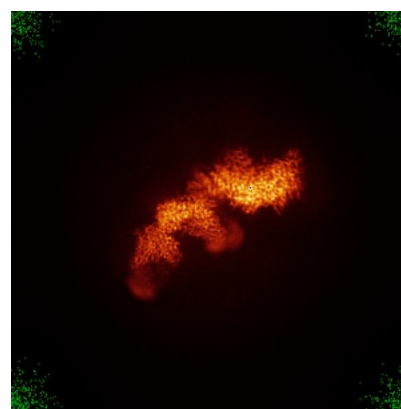
6.4.1 Primary map



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

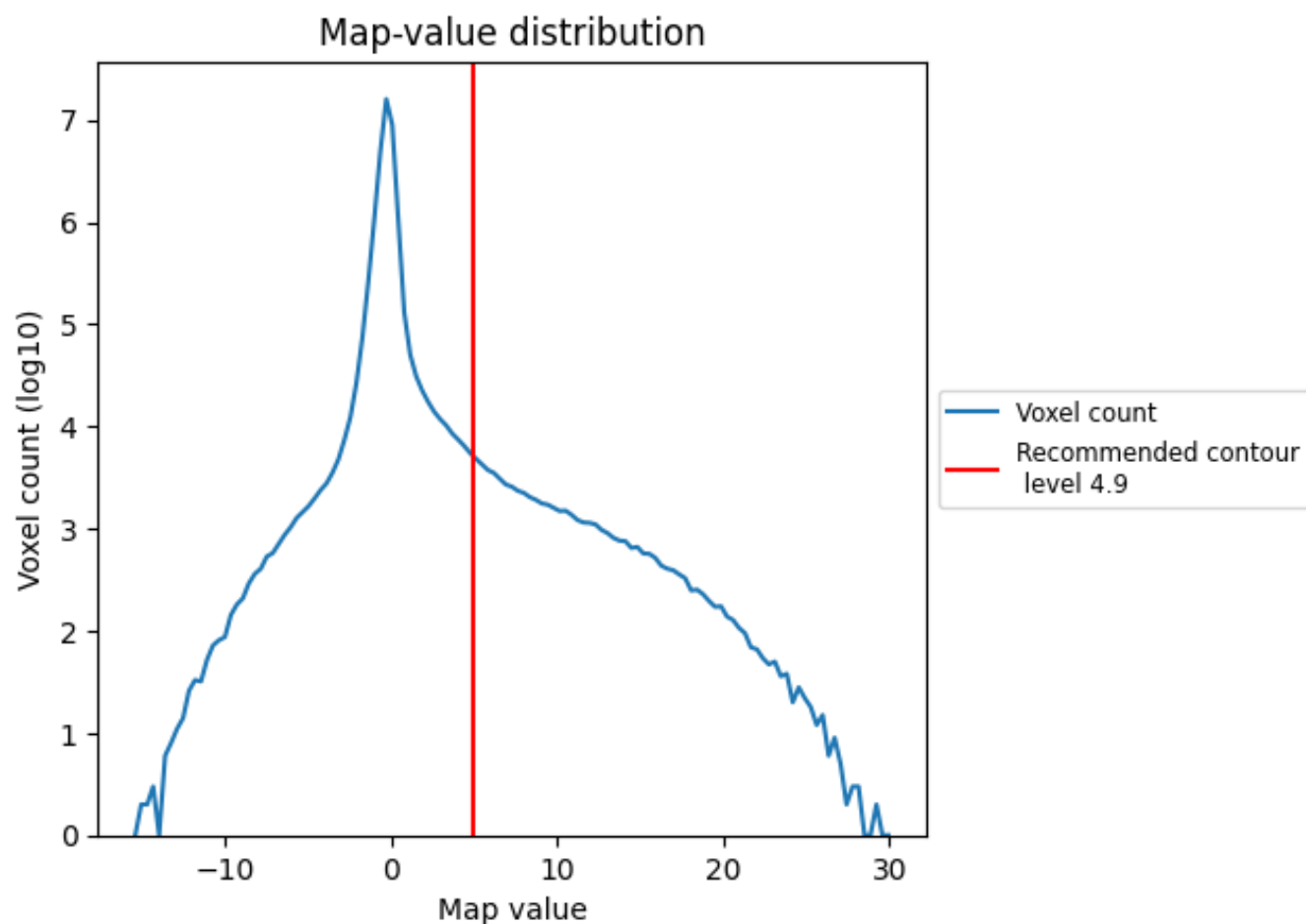
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

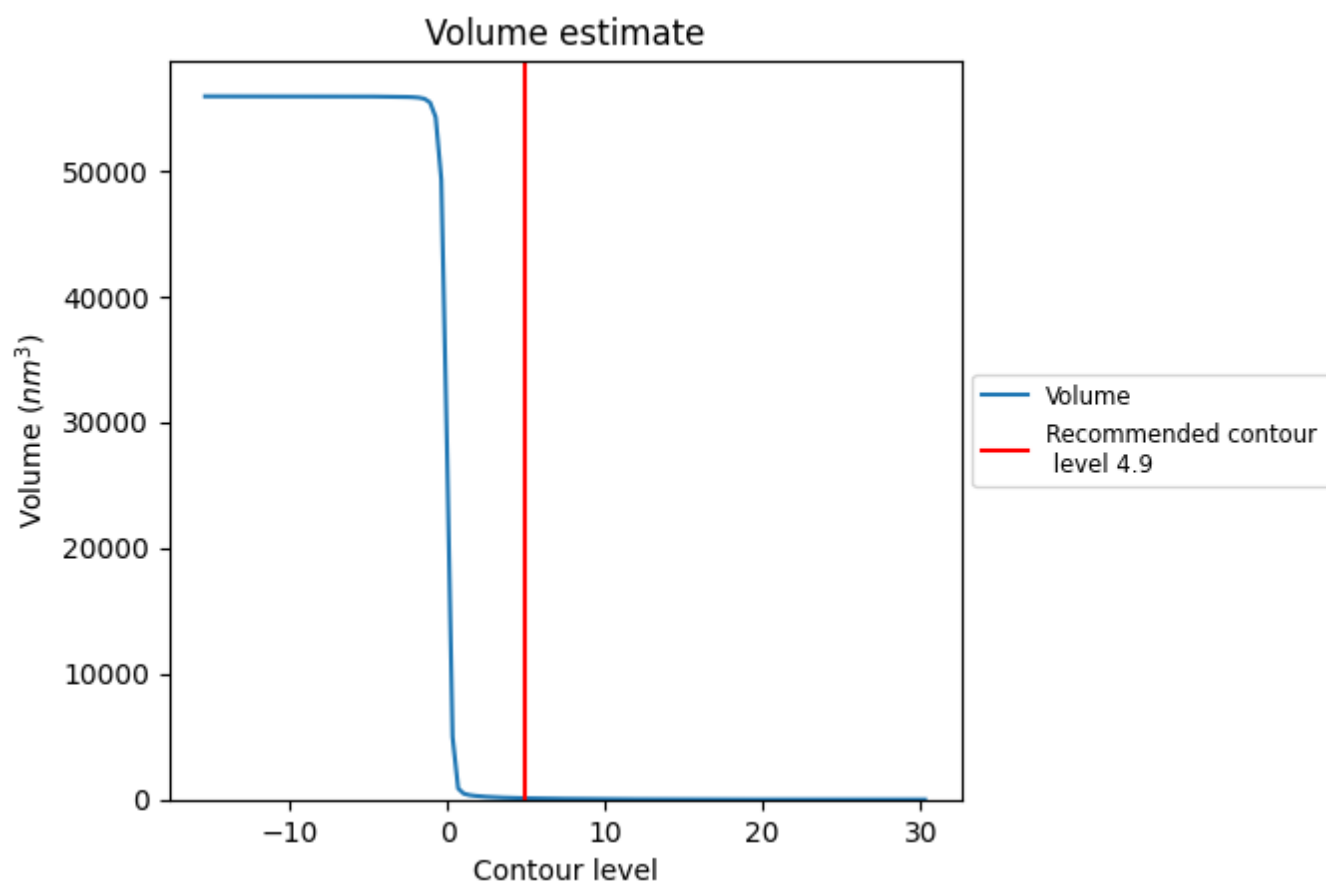
This section contains the results of statistical analysis of the map.

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.

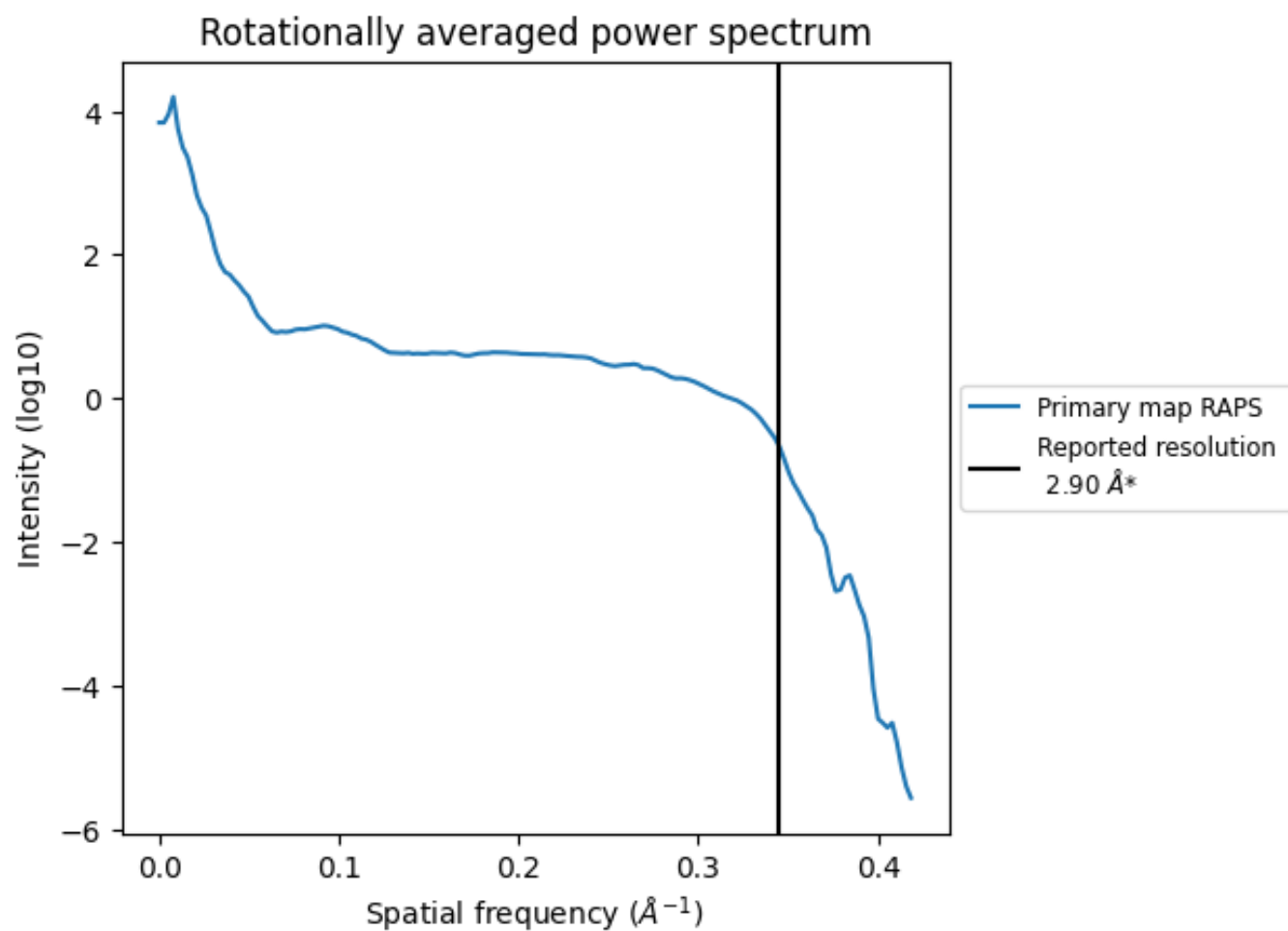
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 106 nm^3 ; this corresponds to an approximate mass of 96 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 0.345 Å⁻¹

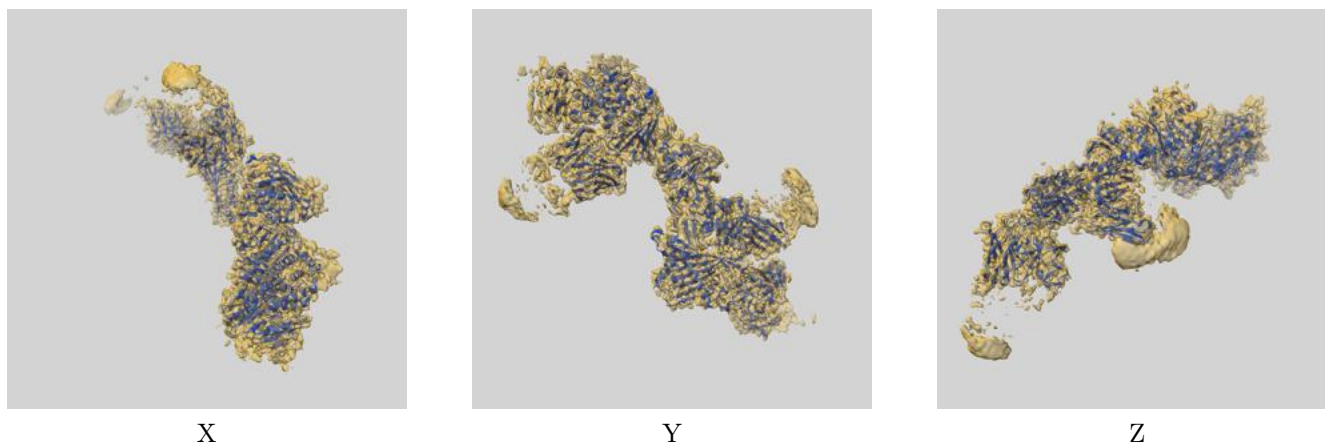
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

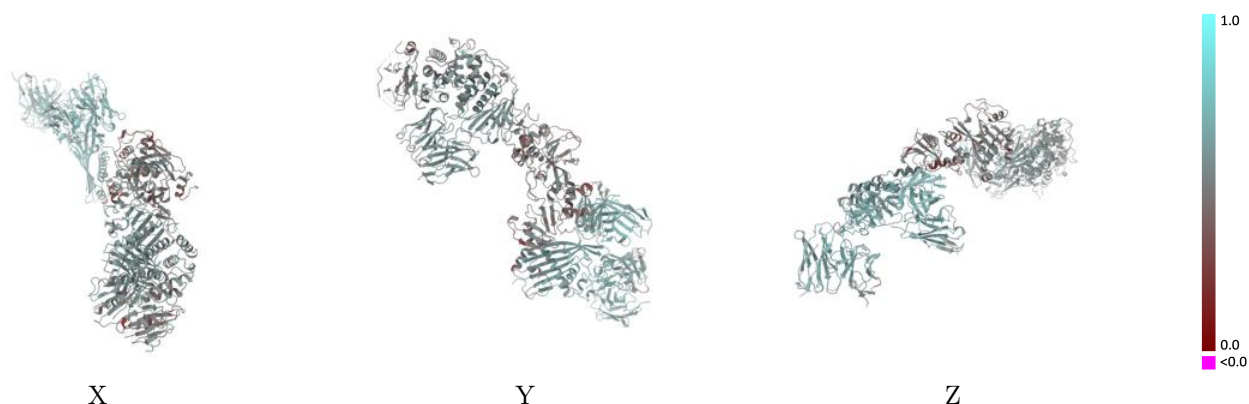
This section contains information regarding the fit between EMDB map EMD-25685 and PDB model 7T4Q. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



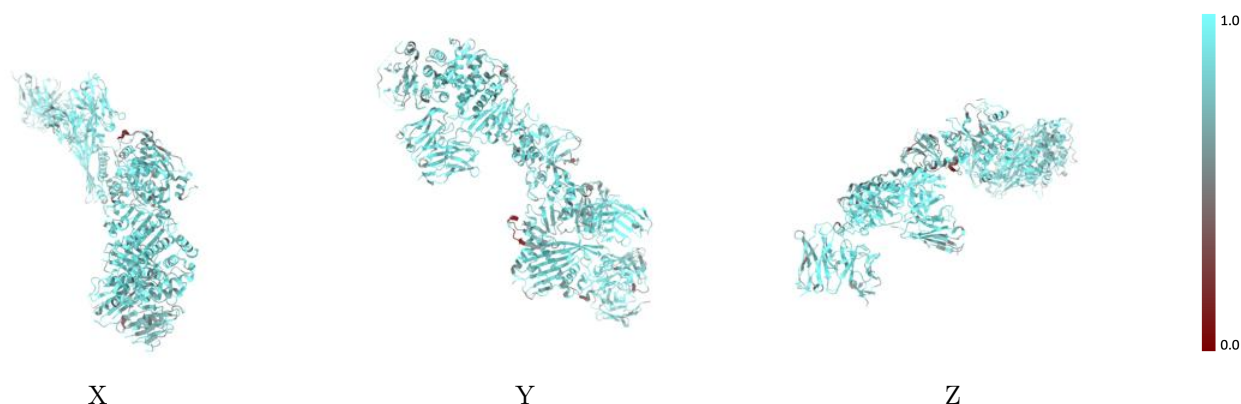
The images above show the 3D surface view of the map at the recommended contour level 4.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



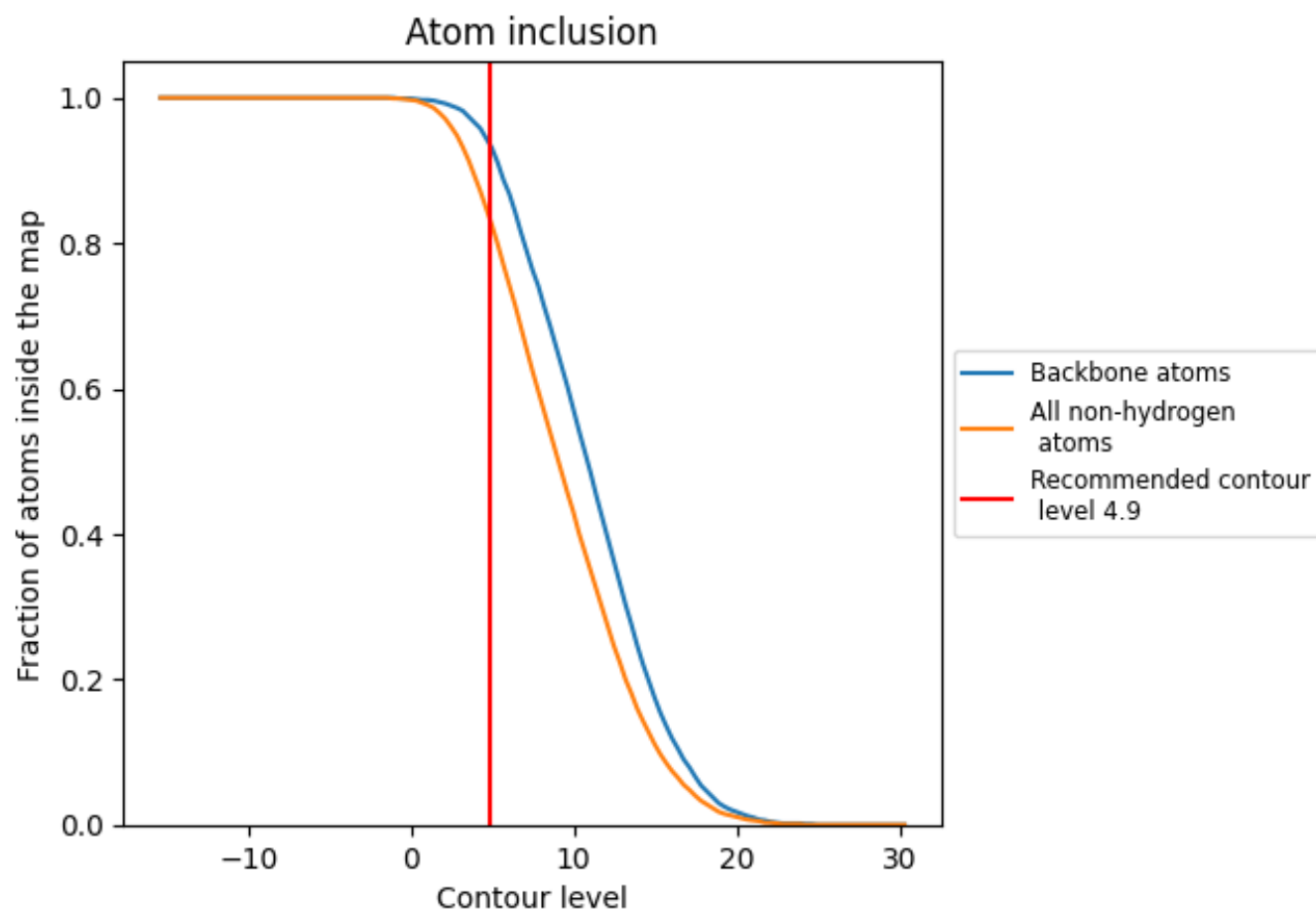
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.9).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 83% 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 (4.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8290	<div><div></div></div> 0.5400
A	<div><div></div></div> 0.8120	<div><div></div></div> 0.5050
B	<div><div></div></div> 0.8200	<div><div></div></div> 0.4600
C	<div><div></div></div> 0.8070	<div><div></div></div> 0.5620
D	<div><div></div></div> 0.7910	<div><div></div></div> 0.5420
E	<div><div></div></div> 0.8580	<div><div></div></div> 0.6010
F	<div><div></div></div> 0.8390	<div><div></div></div> 0.6000
G	<div><div></div></div> 0.8430	<div><div></div></div> 0.5870
H	<div><div></div></div> 0.8320	<div><div></div></div> 0.5990
I	<div><div></div></div> 0.9090	<div><div></div></div> 0.6260
J	<div><div></div></div> 0.8620	<div><div></div></div> 0.5510
K	<div><div></div></div> 0.8600	<div><div></div></div> 0.5430

1.0

0.0

<0.0