



## Full wwPDB EM Validation Report ⓘ

Jun 1, 2024 – 10:29 AM EDT

PDB ID : 7UBM  
EMDB ID : EMD-26438  
Title : Transcription antitermination complex: "pre-engaged" Qlambda-loading complex  
Authors : Yin, Z.; Ebright, R.H.  
Deposited on : 2022-03-15  
Resolution : 3.13 Å (reported)  
Based on initial models : 4YLN, 6P18

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

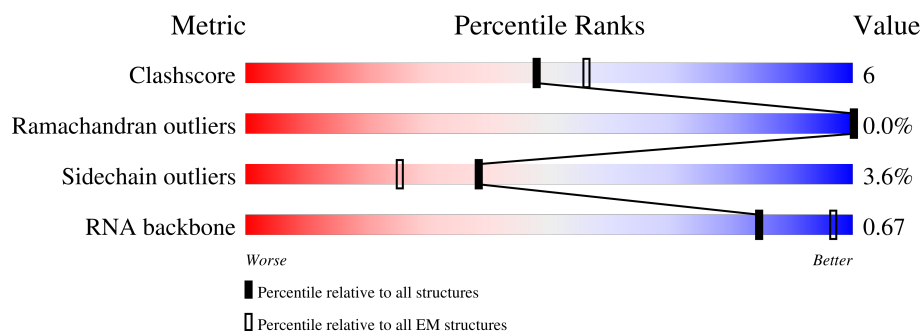
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.13 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
RNA backbone	4643	859

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  $\geq 3$ , 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	1	61	
2	2	61	
3	A	329	
3	B	329	
4	C	1342	
5	D	1430	
6	E	91	

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Mol	Chain	Length	Quality of chain
7	F	627	<p>27% 42% 13% 44%</p>
8	Q	207	<p>13% 63% 21%</p>
9	R	11	<p>91% 9%</p>

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 31583 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 DNA chain called DNA (53-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	53	Total	C	N	O	P	0	0
			1096	525	195	323	53		

- Molecule 2 is a DNA chain called DNA (52-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	52	Total	C	N	O	P	0	0
			1052	506	184	310	52		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	230	Total	C	N	O	S	0	0
			1786	1112	317	351	6		
3	B	228	Total	C	N	O	S	0	0
			1767	1100	312	349	6		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	1340	Total	C	N	O	S	0	0
			10568	6629	1841	2055	43		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	1327	Total	C	N	O	S	0	0
			10319	6484	1839	1947	49		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1408	LEU	-	expression tag	UNP P0A8T7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1409	GLU	-	expression tag	UNP P0A8T7
D	1410	ARG	-	expression tag	UNP P0A8T7
D	1411	ARG	-	expression tag	UNP P0A8T7
D	1412	ALA	-	expression tag	UNP P0A8T7
D	1413	SER	-	expression tag	UNP P0A8T7
D	1414	GLU	-	expression tag	UNP P0A8T7
D	1415	ASN	-	expression tag	UNP P0A8T7
D	1416	LEU	-	expression tag	UNP P0A8T7
D	1417	TYR	-	expression tag	UNP P0A8T7
D	1418	PHE	-	expression tag	UNP P0A8T7
D	1419	GLN	-	expression tag	UNP P0A8T7
D	1420	GLY	-	expression tag	UNP P0A8T7
D	1421	HIS	-	expression tag	UNP P0A8T7
D	1422	HIS	-	expression tag	UNP P0A8T7
D	1423	HIS	-	expression tag	UNP P0A8T7
D	1424	HIS	-	expression tag	UNP P0A8T7
D	1425	HIS	-	expression tag	UNP P0A8T7
D	1426	HIS	-	expression tag	UNP P0A8T7
D	1427	HIS	-	expression tag	UNP P0A8T7
D	1428	HIS	-	expression tag	UNP P0A8T7
D	1429	HIS	-	expression tag	UNP P0A8T7
D	1430	HIS	-	expression tag	UNP P0A8T7

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	75	Total	C	N	O	S	0	0
			600	365	114	120	1		

- Molecule 7 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	353	Total	C	N	O	S	0	0
			2900	1823	521	539	17		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-13	MET	-	expression tag	UNP Q0P6L9
F	-12	GLY	-	expression tag	UNP Q0P6L9
F	-11	SER	-	expression tag	UNP Q0P6L9
F	-10	SER	-	expression tag	UNP Q0P6L9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-9	HIS	-	expression tag	UNP Q0P6L9
F	-8	HIS	-	expression tag	UNP Q0P6L9
F	-7	HIS	-	expression tag	UNP Q0P6L9
F	-6	HIS	-	expression tag	UNP Q0P6L9
F	-5	HIS	-	expression tag	UNP Q0P6L9
F	-4	HIS	-	expression tag	UNP Q0P6L9
F	-3	SER	-	expression tag	UNP Q0P6L9
F	-2	SER	-	expression tag	UNP Q0P6L9
F	-1	GLY	-	expression tag	UNP Q0P6L9
F	0	HIS	-	expression tag	UNP Q0P6L9

- Molecule 8 is a protein called Antitermination protein Q.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	163	Total	C	N	O	S	0	0
			1250	782	231	226	11		

- Molecule 9 is a RNA chain called RNA (5'-R(\*UP\*GP\*GP\*GP\*AP\*GP\*AP\*GP\*GP\*UP\*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	11	Total	C	N	O	P	0	0
			241	108	49	74	10		

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
10	D	2	Total	Zn	0
			2	2	
10	Q	1	Total	Zn	0
			1	1	

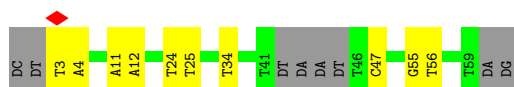
- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
11	D	1	Total	Mg	0
			1	1	

### 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.

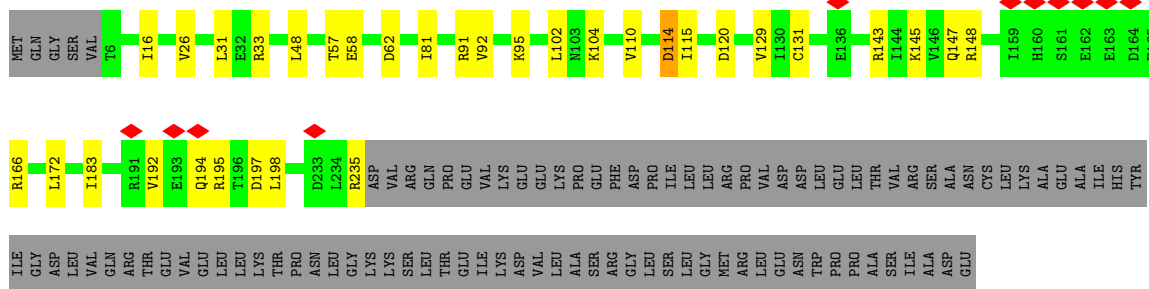
- Molecule 1: DNA (53-MER)



- Molecule 2: DNA (52-MER)

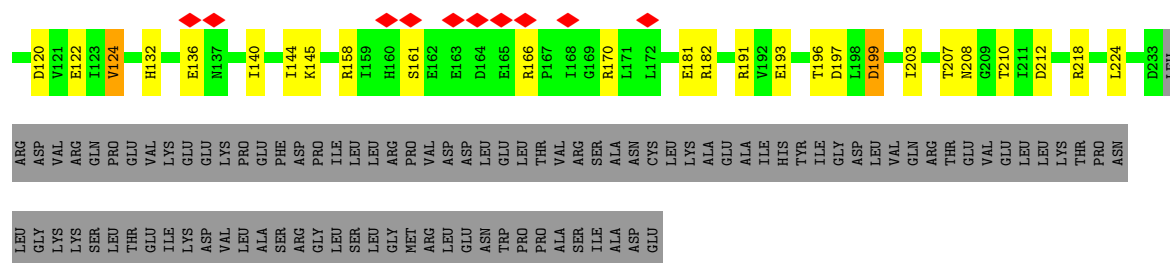


- Molecule 3: DNA-directed RNA polymerase subunit alpha

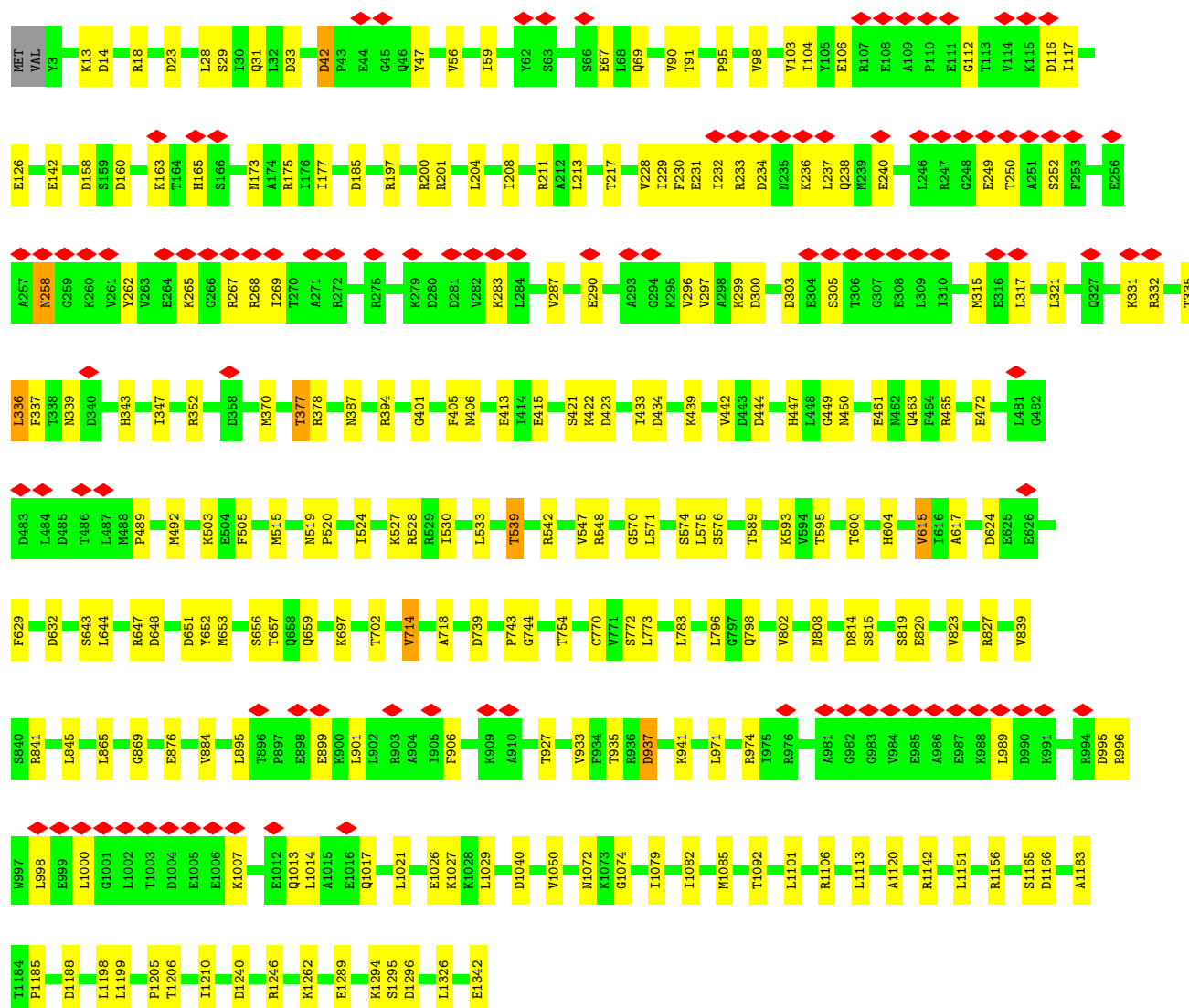
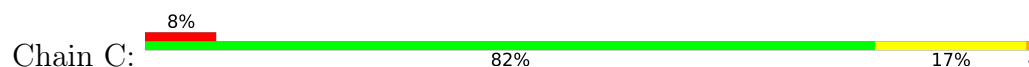


- Molecule 3: DNA-directed RNA polymerase subunit alpha

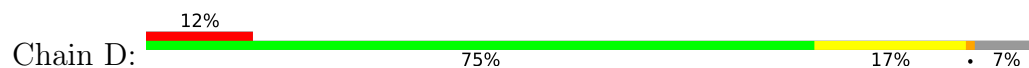




• Molecule 4: DNA-directed RNA polymerase subunit beta



• Molecule 5: DNA-directed RNA polymerase subunit beta'

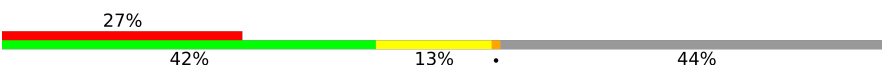


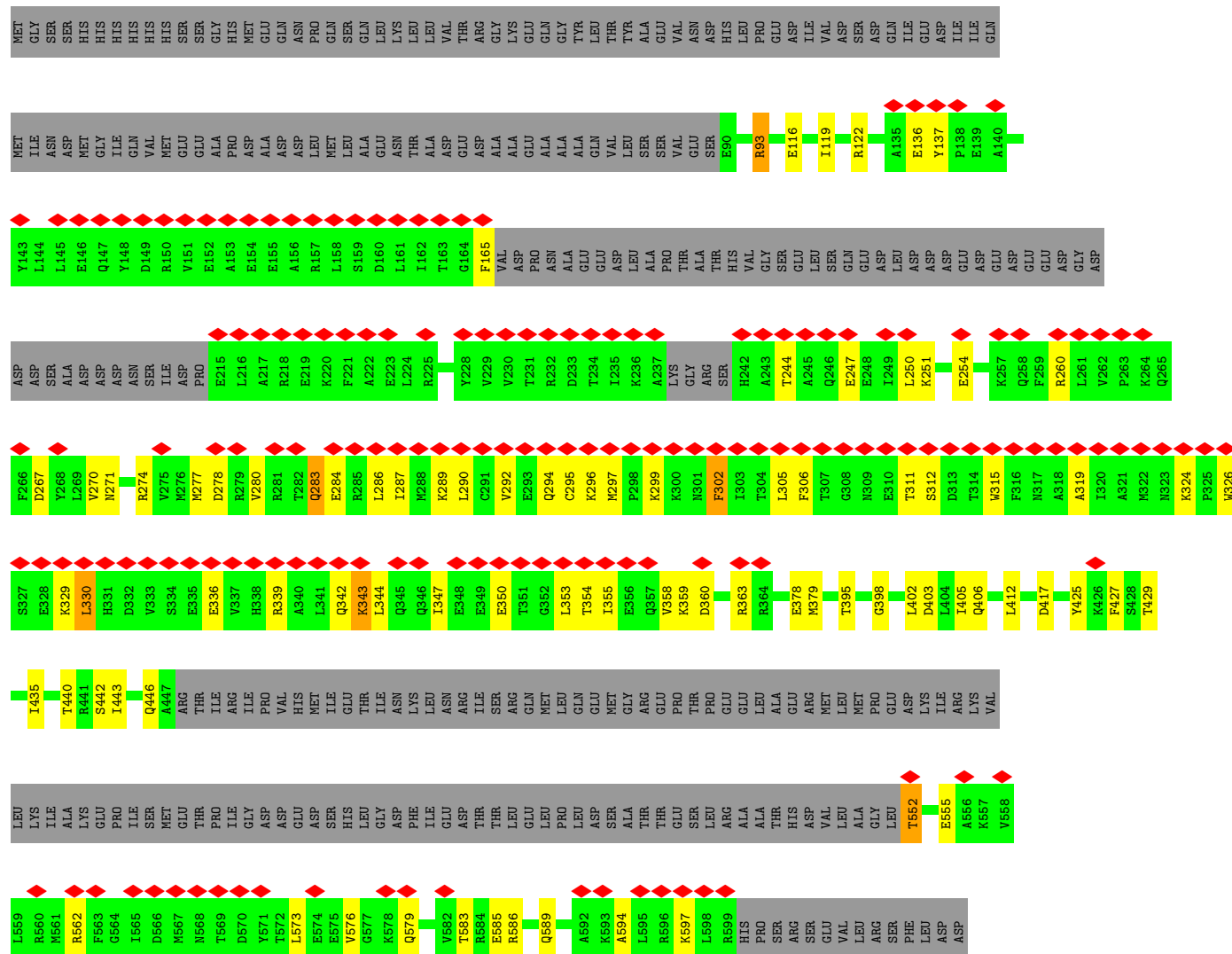




ALA  
GLU  
GLY  
ARG  
ARG

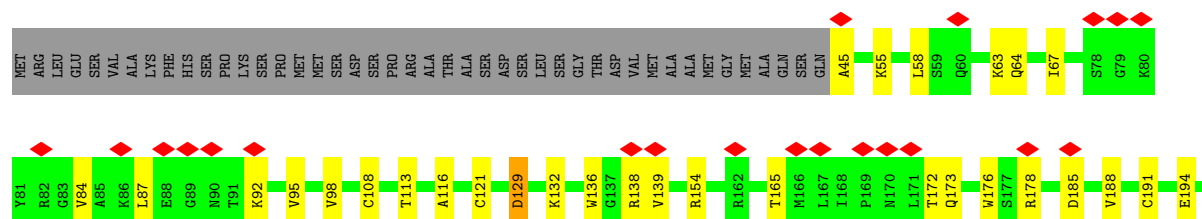
• Molecule 7: RNA polymerase sigma factor RpoD

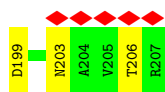
Chain F: 



• Molecule 8: Antitermination protein Q

Chain Q: 





- Molecule 9: RNA (5'-R(\*UP\*GP\*GP\*GP\*AP\*GP\*AP\*GP\*GP\*UP\*A)-3')

Chain R:  91% 9%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	11913	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 ( $e^-/\text{\AA}^2$ )	1.41	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.258	Depositor
Minimum map value	-0.151	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0306	Depositor
Map size (Å)	272.896, 272.896, 272.896	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.066, 1.066, 1.066	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	1	0.58	0/1228	1.01	0/1894
2	2	0.61	0/1176	1.01	0/1806
3	A	0.29	0/1808	0.49	0/2450
3	B	0.31	0/1789	0.52	0/2425
4	C	0.33	0/10737	0.52	0/14486
5	D	0.31	0/10476	0.52	0/14146
6	E	0.27	0/602	0.48	0/810
7	F	0.27	0/2936	0.58	0/3935
8	Q	0.27	0/1273	0.54	0/1715
9	R	0.66	0/271	1.09	0/423
All	All	0.35	0/32296	0.59	0/44090

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

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	1	1096	0	605	7	0
2	2	1052	0	590	7	0
3	A	1786	0	1813	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1767	0	1789	29	0
4	C	10568	0	10575	124	0
5	D	10319	0	10527	137	0
6	E	600	0	607	7	0
7	F	2900	0	2956	69	0
8	Q	1250	0	1257	16	0
9	R	241	0	120	0	0
10	D	2	0	0	0	0
10	Q	1	0	0	0	0
11	D	1	0	0	0	0
All	All	31583	0	30839	394	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 6.

All (394) 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)
7:F:247:GLU:HA	7:F:250:LEU:CD2	1.50	1.40
7:F:283:GLN:HA	7:F:286:LEU:CD2	1.55	1.33
7:F:283:GLN:O	7:F:286:LEU:HG	1.48	1.10
7:F:247:GLU:O	7:F:250:LEU:HG	1.57	1.03
7:F:283:GLN:CD	7:F:286:LEU:HD21	1.77	1.02
7:F:247:GLU:HA	7:F:250:LEU:HD23	1.04	1.01
7:F:283:GLN:HA	7:F:286:LEU:HD23	1.02	1.00
7:F:283:GLN:CA	7:F:286:LEU:HD23	1.93	0.98
7:F:247:GLU:CA	7:F:250:LEU:CD2	2.45	0.95
7:F:247:GLU:CA	7:F:250:LEU:HD23	1.97	0.94
7:F:247:GLU:HA	7:F:250:LEU:HD21	1.50	0.92
7:F:283:GLN:HA	7:F:286:LEU:HD21	1.54	0.87
7:F:302:PHE:O	7:F:306:PHE:HB2	1.75	0.86
7:F:283:GLN:CA	7:F:286:LEU:CD2	2.49	0.82
7:F:283:GLN:NE2	7:F:286:LEU:HD21	2.00	0.76
7:F:324:LYS:HE3	7:F:326:TRP:HE1	1.56	0.69
5:D:674:THR:O	5:D:678:ARG:HB2	1.95	0.66
4:C:604:HIS:HD1	4:C:652:TYR:HH	1.45	0.65
4:C:104:ILE:HD12	4:C:116:ASP:HB3	1.79	0.64
7:F:283:GLN:O	7:F:286:LEU:CG	2.38	0.64
1:1:24:DT:H2"	1:1:25:DT:H71	1.79	0.64
4:C:1101:LEU:HD13	5:D:504:GLN:HG3	1.81	0.63
5:D:123:ARG:O	5:D:127:LEU:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:87:LEU:HB2	8:Q:92:LYS:HB2	1.80	0.62
5:D:281:ARG:O	5:D:285:LEU:HB2	2.00	0.62
5:D:824:PRO:HG3	5:D:835:LEU:HB2	1.82	0.61
4:C:1185:PRO:HB2	4:C:1188:ASP:HB3	1.83	0.61
4:C:213:LEU:HD22	4:C:422:LYS:HG3	1.81	0.60
5:D:968:ASN:HD21	5:D:972:LYS:HB3	1.67	0.60
4:C:702:THR:HG23	4:C:1185:PRO:HA	1.83	0.60
7:F:247:GLU:CA	7:F:250:LEU:HD21	2.23	0.60
4:C:401:GLY:O	4:C:405:PHE:HB2	2.02	0.59
7:F:267:ASP:HA	7:F:270:VAL:HG12	1.84	0.59
4:C:204:LEU:HB3	4:C:208:ILE:HD12	1.83	0.59
7:F:353:LEU:HD22	7:F:358:VAL:HG13	1.85	0.59
4:C:528:ARG:NH2	4:C:576:SER:O	2.35	0.58
7:F:283:GLN:CG	7:F:286:LEU:HD21	2.32	0.58
4:C:743:PRO:HA	4:C:974:ARG:HH22	1.67	0.58
5:D:1327:GLU:OE1	5:D:1330:ARG:NH1	2.36	0.58
5:D:156:ARG:HH21	5:D:191:SER:HB2	1.68	0.58
8:Q:203:ASN:HA	8:Q:206:THR:HG22	1.86	0.58
3:A:48:LEU:HG	3:A:183:ILE:HD12	1.85	0.58
4:C:444:ASP:O	4:C:450:ASN:ND2	2.37	0.57
4:C:657:THR:HG21	4:C:1188:ASP:HB2	1.84	0.57
6:E:44:ASP:OD2	6:E:52:ARG:NH1	2.37	0.57
8:Q:185:ASP:HA	8:Q:188:VAL:HG22	1.87	0.57
3:A:192:VAL:HG21	3:A:198:LEU:HD12	1.87	0.57
3:A:235:ARG:HE	3:B:218:ARG:HE	1.52	0.57
7:F:311:THR:HA	7:F:344:LEU:HD13	1.87	0.57
1:1:47:DC:H2'	4:C:200:ARG:HG3	1.86	0.56
3:A:57:THR:HG22	3:A:58:GLU:HG3	1.87	0.56
4:C:106:GLU:HB2	4:C:112:GLY:HA3	1.88	0.56
5:D:151:MET:HG2	5:D:153:ASN:H	1.68	0.56
4:C:935:THR:HG21	4:C:941:LYS:HB3	1.86	0.56
5:D:1046:ILE:HD12	5:D:1059:LEU:HD21	1.87	0.56
3:B:111:THR:HG23	3:B:113:ALA:H	1.71	0.56
4:C:228:VAL:HG23	4:C:335:THR:HG23	1.88	0.56
5:D:495:ASN:ND2	5:D:1247:LYS:O	2.39	0.56
4:C:937:ASP:OD1	4:C:937:ASP:N	2.37	0.56
2:2:18:DC:H2'	2:2:19:DT:C6	2.41	0.56
3:A:145:LYS:HD3	3:A:147:GLN:HE21	1.71	0.55
4:C:819:SER:OG	4:C:820:GLU:N	2.39	0.55
5:D:886:VAL:HG21	5:D:1230:THR:HG21	1.88	0.55
4:C:317:LEU:HA	4:C:321:LEU:HD23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:814:ASP:OD1	4:C:1106:ARG:NH2	2.40	0.55
4:C:1142:ARG:NH2	4:C:1166:ASP:OD1	2.40	0.55
5:D:245:LEU:HD23	5:D:250:ARG:HG2	1.88	0.55
4:C:158:ASP:O	4:C:173:ASN:ND2	2.40	0.55
4:C:743:PRO:O	4:C:1013:GLN:NE2	2.40	0.55
5:D:141:PHE:HB3	5:D:293:ARG:HD2	1.88	0.54
7:F:585:GLU:OE1	7:F:589:GLN:NE2	2.40	0.54
3:B:80:GLU:O	3:B:84:ASN:ND2	2.41	0.54
1:1:34:DT:H3'	7:F:429:THR:HG21	1.89	0.54
5:D:71:LEU:HB2	5:D:90:VAL:HG21	1.91	0.53
7:F:562:ARG:HE	7:F:573:LEU:HG	1.73	0.53
5:D:93:THR:OG1	5:D:94:GLN:N	2.42	0.53
3:A:92:VAL:O	3:A:148:ARG:NH2	2.40	0.53
5:D:74:LYS:NZ	5:D:75:TYR:OH	2.42	0.53
5:D:1034:PHE:HB2	5:D:1083:ALA:HA	1.89	0.53
5:D:1265:THR:HG22	5:D:1279:GLN:HG3	1.91	0.53
5:D:802:ASP:OD2	5:D:1348:LYS:NZ	2.35	0.53
5:D:822:MET:SD	5:D:838:ARG:NH2	2.80	0.53
5:D:24:LEU:HD12	5:D:232:ASN:HD22	1.73	0.53
5:D:1041:ILE:HB	5:D:1044:GLN:HE21	1.73	0.53
2:2:17:DC:H2'	2:2:18:DC:C6	2.44	0.53
4:C:461:GLU:OE2	4:C:465:ARG:NH2	2.42	0.53
5:D:105:ILE:HD12	5:D:242:LEU:HD23	1.91	0.53
3:A:33:ARG:HH21	3:A:197:ASP:HA	1.74	0.52
3:B:199:ASP:OD1	3:B:199:ASP:N	2.42	0.52
4:C:42:ASP:N	4:C:42:ASP:OD1	2.41	0.52
5:D:873:GLU:O	5:D:990:ARG:NH2	2.42	0.52
5:D:482:ALA:O	6:E:16:ARG:NH1	2.42	0.52
8:Q:199:ASP:O	8:Q:203:ASN:ND2	2.43	0.52
7:F:295:CYS:HA	7:F:330:LEU:HD21	1.90	0.52
5:D:294:ASN:ND2	7:F:406:GLN:OE1	2.39	0.52
5:D:1146:GLU:HA	5:D:1309:ILE:HG22	1.90	0.52
5:D:1281:GLU:HB3	5:D:1284:ARG:HG2	1.92	0.52
7:F:347:ILE:HA	7:F:350:GLU:HG2	1.92	0.52
5:D:816:THR:HG22	5:D:883:ARG:HH21	1.74	0.52
4:C:339:ASN:HB2	4:C:343:HIS:H	1.75	0.52
4:C:1342:GLU:HA	5:D:18:ASP:HB2	1.91	0.52
7:F:398:GLY:O	7:F:446:GLN:NE2	2.42	0.52
3:A:114:ASP:OD1	3:A:114:ASP:N	2.43	0.51
5:D:460:ASP:OD1	5:D:460:ASP:N	2.43	0.51
3:A:104:LYS:HG2	3:A:110:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:230:PHE:HE1	4:C:287:VAL:HG21	1.74	0.51
4:C:533:LEU:HD21	4:C:571:LEU:HD13	1.91	0.51
5:D:554:GLU:OE2	5:D:570:LYS:NZ	2.39	0.51
4:C:519:ASN:OD1	4:C:519:ASN:N	2.43	0.51
5:D:1047:THR:HG23	5:D:1060:VAL:HB	1.93	0.51
4:C:539:THR:HG23	4:C:542:ARG:HB2	1.92	0.51
4:C:1026:GLU:OE2	4:C:1027:LYS:NZ	2.44	0.51
7:F:326:TRP:O	7:F:330:LEU:HB2	2.10	0.51
5:D:475:GLU:OE2	6:E:28:ARG:NH1	2.43	0.51
4:C:236:LYS:O	4:C:238:GLN:NE2	2.44	0.51
4:C:995:ASP:OD1	4:C:996:ARG:NH1	2.44	0.51
5:D:836:ARG:NH1	5:D:870:ASP:OD1	2.44	0.51
5:D:1031:VAL:HG11	5:D:1088:VAL:HG21	1.91	0.51
8:Q:84:VAL:HG22	8:Q:92:LYS:HE3	1.92	0.51
4:C:718:ALA:HB2	4:C:783:LEU:HD21	1.93	0.51
7:F:165:PHE:O	7:F:260:ARG:NH1	2.44	0.51
4:C:1074:GLY:HA2	5:D:462:ASP:HA	1.92	0.50
4:C:406:ASN:ND2	4:C:413:GLU:O	2.45	0.50
5:D:169:LEU:HD12	5:D:173:GLY:HA2	1.92	0.50
5:D:478:LEU:HG	6:E:47:THR:HG23	1.94	0.50
7:F:295:CYS:SG	7:F:299:LYS:NZ	2.84	0.50
5:D:1143:ASP:OD1	5:D:1148:ARG:NH1	2.40	0.50
5:D:1261:LEU:O	5:D:1304:ARG:NH2	2.41	0.50
7:F:295:CYS:HB3	7:F:297:MET:HG2	1.94	0.50
7:F:312:SER:O	7:F:315:TRP:NE1	2.45	0.50
4:C:629:PHE:O	4:C:647:ARG:NH2	2.45	0.50
4:C:1151:LEU:HD13	4:C:1198:LEU:HD12	1.93	0.50
5:D:830:ASP:OD1	5:D:832:LYS:NZ	2.44	0.50
5:D:1064:SER:OG	5:D:1075:ARG:NH1	2.44	0.50
4:C:489:PRO:HA	4:C:492:MET:HG2	1.93	0.49
5:D:527:LEU:HB2	5:D:550:VAL:HG12	1.94	0.49
5:D:830:ASP:OD1	5:D:830:ASP:N	2.44	0.49
4:C:262:TYR:O	4:C:267:ARG:NH2	2.46	0.49
5:D:1119:ASP:OD1	5:D:1119:ASP:N	2.45	0.49
4:C:520:PRO:HG3	4:C:714:VAL:HG11	1.95	0.49
5:D:1212:ASP:N	5:D:1212:ASP:OD1	2.37	0.49
7:F:277:MET:HA	7:F:280:VAL:HG12	1.93	0.49
5:D:1249:ASN:HD22	5:D:1251:LYS:HG2	1.78	0.49
5:D:416:ILE:HG13	5:D:441:LEU:HD21	1.94	0.49
4:C:211:ARG:NH2	4:C:217:THR:OG1	2.44	0.49
5:D:826:ILE:HG22	5:D:831:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:271:ASN:HA	7:F:274:ARG:HB2	1.94	0.49
5:D:202:ARG:HH21	5:D:1275:LEU:HD21	1.78	0.49
5:D:208:THR:O	5:D:214:ARG:NH2	2.39	0.48
5:D:1033:GLY:HA3	5:D:1082:ASP:HA	1.94	0.48
8:Q:55:LYS:HG3	8:Q:108:CYS:HA	1.96	0.48
3:B:124:VAL:HG11	3:B:210:THR:H	1.79	0.48
4:C:29:SER:O	4:C:33:ASP:HB2	2.13	0.48
5:D:115:TRP:O	5:D:119:SER:HB3	2.13	0.48
7:F:311:THR:HG23	7:F:344:LEU:HD22	1.96	0.48
8:Q:132:LYS:O	8:Q:136:TRP:HB2	2.13	0.48
4:C:103:VAL:HG12	4:C:117:ILE:HD12	1.96	0.48
4:C:300:ASP:OD1	4:C:300:ASP:N	2.44	0.48
7:F:116:GLU:HG2	7:F:427:PHE:HB2	1.95	0.48
7:F:119:ILE:HG21	7:F:379:MET:HB2	1.95	0.48
1:1:3:DT:O4	1:1:4:DA:N6	2.46	0.48
4:C:841:ARG:NH1	5:D:256:ASP:O	2.46	0.48
7:F:283:GLN:CA	7:F:286:LEU:HD21	2.32	0.48
8:Q:129:ASP:OD1	8:Q:129:ASP:N	2.45	0.48
5:D:218:THR:HA	5:D:221:ILE:HG22	1.95	0.48
5:D:762:ASN:OD1	5:D:762:ASN:N	2.46	0.48
3:B:95:LYS:NZ	3:B:120:ASP:OD2	2.46	0.48
4:C:234:ASP:OD1	4:C:236:LYS:NZ	2.42	0.48
4:C:530:ILE:HD11	4:C:575:LEU:HD12	1.95	0.48
5:D:452:LEU:HB3	5:D:500:ILE:HG23	1.95	0.48
5:D:572:THR:OG1	5:D:573:THR:N	2.47	0.48
4:C:95:PRO:HA	4:C:126:GLU:HG2	1.95	0.48
7:F:343:LYS:HE3	7:F:343:LYS:HB3	1.70	0.48
3:B:166:ARG:HB2	3:B:170:ARG:HD2	1.95	0.48
4:C:67:GLU:OE2	4:C:69:GLN:NE2	2.47	0.48
4:C:624:ASP:N	4:C:624:ASP:OD1	2.46	0.48
5:D:644:MET:O	5:D:764:ARG:NH1	2.44	0.48
7:F:319:ALA:HB1	7:F:326:TRP:HH2	1.79	0.48
4:C:989:LEU:HD11	4:C:1000:LEU:HD21	1.95	0.47
4:C:1165:SER:OG	4:C:1166:ASP:N	2.48	0.47
5:D:708:ASN:ND2	5:D:714:GLU:O	2.47	0.47
4:C:422:LYS:HE2	4:C:422:LYS:HB2	1.70	0.47
4:C:772:SER:OG	4:C:773:LEU:N	2.47	0.47
5:D:533:ALA:HB1	5:D:574:VAL:HG13	1.95	0.47
1:1:55:DG:H2"	1:1:56:DT:H5"	1.95	0.47
4:C:14:ASP:HA	4:C:1183:ALA:HB3	1.96	0.47
5:D:264:ASP:OD1	5:D:264:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:1163:VAL:HG13	5:D:1200:GLU:HA	1.96	0.47
4:C:865:LEU:HD23	4:C:869:GLY:HA2	1.96	0.47
5:D:355:ILE:HG22	5:D:447:ILE:HB	1.97	0.47
3:A:81:ILE:HG12	3:A:131:CYS:HB3	1.96	0.47
3:B:197:ASP:OD1	3:B:197:ASP:N	2.48	0.47
4:C:1296:ASP:OD1	5:D:345:LYS:NZ	2.43	0.47
5:D:1058:SER:OG	5:D:1108:GLN:NE2	2.48	0.47
4:C:160:ASP:HB2	4:C:163:LYS:HG2	1.97	0.47
4:C:377:THR:OG1	4:C:378:ARG:N	2.48	0.47
5:D:959:LYS:NZ	5:D:961:SER:OG	2.48	0.47
5:D:977:SER:HG	5:D:980:THR:HG1	1.62	0.47
5:D:1174:ARG:HD3	5:D:1187:GLU:HG2	1.96	0.47
6:E:40:PRO:O	6:E:52:ARG:NH2	2.48	0.47
7:F:359:LYS:HD3	7:F:359:LYS:HA	1.72	0.47
2:2:19:DT:H2'	2:2:20:DC:C6	2.50	0.47
3:B:26:VAL:HG22	3:B:203:ILE:HB	1.97	0.47
5:D:161:THR:HG23	5:D:164:GLN:H	1.80	0.47
3:B:158:ARG:HD2	3:B:158:ARG:HA	1.73	0.46
4:C:233:ARG:NH1	4:C:331:LYS:O	2.45	0.46
4:C:820:GLU:HB3	4:C:1082:ILE:HG23	1.97	0.46
5:D:416:ILE:HG23	5:D:439:PRO:HG2	1.97	0.46
3:B:100:LEU:O	3:B:144:ILE:N	2.48	0.46
5:D:1173:ARG:HH12	5:D:1192:LYS:HA	1.81	0.46
7:F:284:GLU:HA	7:F:287:ILE:HG12	1.97	0.46
3:B:93:GLN:NE2	3:B:122:GLU:OE1	2.45	0.46
4:C:250:THR:HA	4:C:268:ARG:HA	1.98	0.46
5:D:848:VAL:HG22	5:D:858:VAL:HG22	1.97	0.46
5:D:1071:GLY:O	5:D:1075:ARG:NH2	2.49	0.46
7:F:251:LYS:HA	7:F:254:GLU:HG3	1.96	0.46
2:2:19:DT:H2'	2:2:20:DC:H6	1.80	0.46
3:A:58:GLU:HG2	3:A:172:LEU:HD23	1.96	0.46
4:C:231:GLU:OE2	4:C:233:ARG:NH2	2.46	0.46
4:C:632:ASP:HA	4:C:647:ARG:HD2	1.97	0.46
5:D:806:ASP:OD1	5:D:806:ASP:N	2.44	0.46
5:D:960:LEU:HB3	5:D:963:VAL:HG21	1.96	0.46
5:D:481:ARG:NH1	6:E:3:ARG:O	2.49	0.46
7:F:360:ASP:HB2	7:F:363:ARG:HH21	1.81	0.46
3:B:104:LYS:HG2	3:B:110:VAL:HB	1.98	0.46
2:2:54:DT:O4	8:Q:178:ARG:NH2	2.48	0.46
4:C:423:ASP:N	4:C:423:ASP:OD1	2.49	0.46
3:A:16:ILE:HG12	3:A:26:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:64:VAL:HG11	3:B:78:ILE:HD13	1.97	0.46
4:C:158:ASP:HA	4:C:442:VAL:HB	1.98	0.46
4:C:421:SER:OG	4:C:422:LYS:N	2.49	0.46
4:C:823:VAL:HG21	4:C:1079:ILE:HD13	1.98	0.46
5:D:674:THR:OG1	5:D:675:ALA:N	2.49	0.46
8:Q:64:GLN:HA	8:Q:67:ILE:HD12	1.98	0.46
4:C:519:ASN:HD22	4:C:796:LEU:HD22	1.80	0.46
4:C:819:SER:HB2	4:C:1085:MET:HG3	1.97	0.46
5:D:1079:LYS:HA	5:D:1098:GLN:HA	1.98	0.46
3:B:207:THR:OG1	3:B:208:ASN:N	2.50	0.45
5:D:576:ARG:HD3	5:D:593:ASN:HA	1.97	0.45
4:C:18:ARG:O	4:C:1156:ARG:NH1	2.46	0.45
4:C:59:ILE:HD13	4:C:472:GLU:HG2	1.97	0.45
4:C:228:VAL:HG13	4:C:337:PHE:HB2	1.97	0.45
4:C:739:ASP:OD1	4:C:739:ASP:N	2.48	0.45
7:F:247:GLU:CB	7:F:250:LEU:HD21	2.45	0.45
3:B:11:PRO:O	3:B:12:ARG:NH1	2.49	0.45
4:C:23:ASP:N	4:C:23:ASP:OD1	2.48	0.45
4:C:303:ASP:OD2	4:C:305:SER:OG	2.32	0.45
4:C:643:SER:OG	4:C:644:LEU:N	2.49	0.45
5:D:678:ARG:HE	5:D:678:ARG:HB3	1.53	0.45
5:D:926:PRO:HG2	5:D:1248:ILE:HD11	1.99	0.45
7:F:402:LEU:HD23	7:F:405:ILE:HD11	1.97	0.45
8:Q:113:THR:HB	8:Q:116:ALA:HB3	1.98	0.45
3:A:95:LYS:NZ	3:A:120:ASP:OD2	2.49	0.45
4:C:971:LEU:HD11	4:C:1014:LEU:HD22	1.98	0.45
4:C:1205:PRO:HG2	4:C:1210:ILE:HG22	1.98	0.45
5:D:515:ARG:NH2	5:D:718:SER:O	2.46	0.45
3:A:62:ASP:OD1	3:A:143:ARG:NH2	2.44	0.45
3:B:106:GLY:HA2	3:B:136:GLU:HA	1.99	0.45
4:C:615:VAL:H	4:C:651:ASP:HB2	1.81	0.45
5:D:1084:GLN:NE2	5:D:1086:ASN:OD1	2.50	0.45
5:D:110:PRO:HB3	5:D:240:THR:HG22	1.99	0.45
4:C:268:ARG:NH1	4:C:269:ILE:O	2.50	0.45
4:C:744:GLY:HA2	4:C:1013:GLN:HE22	1.82	0.45
4:C:1017:GLN:O	4:C:1021:LEU:HB2	2.17	0.45
5:D:216:LYS:HE3	5:D:216:LYS:HB2	1.83	0.45
3:B:158:ARG:NH1	3:B:161:SER:OG	2.49	0.45
4:C:31:GLN:NE2	4:C:527:LYS:O	2.45	0.45
4:C:895:LEU:HD11	4:C:899:GLU:HG3	1.99	0.45
5:D:992:LYS:HE3	5:D:992:LYS:HB3	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:278:ARG:NH2	7:F:403:ASP:OD1	2.39	0.44
7:F:594:ALA:HA	7:F:597:LYS:HG2	1.98	0.44
4:C:163:LYS:HA	4:C:163:LYS:HD3	1.86	0.44
5:D:26:SER:H	5:D:29:MET:HE3	1.83	0.44
7:F:247:GLU:C	7:F:250:LEU:HG	2.35	0.44
7:F:292:VAL:HG22	7:F:299:LYS:HE2	1.99	0.44
7:F:339:ARG:HG2	7:F:342:GLN:HE21	1.80	0.44
7:F:412:LEU:HD13	7:F:435:ILE:HD11	2.00	0.44
3:A:166:ARG:HH22	4:C:876:GLU:HG2	1.81	0.44
4:C:315:MET:HA	4:C:352:ARG:HH12	1.82	0.44
4:C:1289:GLU:HG3	4:C:1294:LYS:HE3	1.98	0.44
7:F:290:LEU:HD13	7:F:336:GLU:HB2	1.99	0.44
4:C:798:GLN:OE1	4:C:827:ARG:NH2	2.49	0.44
5:D:820:ILE:HD13	5:D:820:ILE:HA	1.90	0.44
7:F:122:ARG:NH2	7:F:378:GLU:OE1	2.47	0.44
3:B:67:GLU:HA	3:B:78:ILE:HD11	2.00	0.44
3:B:75:GLN:HE21	3:B:132:HIS:HB2	1.83	0.44
5:D:1107:VAL:HG22	5:D:1122:ALA:HB2	1.99	0.44
7:F:583:THR:HB	7:F:586:ARG:HB3	1.99	0.44
6:E:3:ARG:HG2	6:E:48:VAL:HG11	1.99	0.43
8:Q:95:VAL:HA	8:Q:98:VAL:HG22	1.99	0.43
1:1:24:DT:H3'	7:F:583:THR:HG22	2.00	0.43
2:2:20:DC:H2'	2:2:21:DT:C6	2.53	0.43
5:D:109:SER:HB2	5:D:296:LYS:HE2	2.00	0.43
5:D:353:SER:HB3	5:D:447:ILE:HG13	2.01	0.43
5:D:709:ARG:HD2	5:D:709:ARG:HA	1.85	0.43
3:B:20:SER:H	3:B:23:HIS:HB3	1.83	0.43
3:B:46:ILE:HD11	3:B:224:LEU:HD13	2.00	0.43
5:D:45:ASN:HD21	5:D:47:ARG:HB3	1.82	0.43
7:F:576:VAL:HA	7:F:579:GLN:HG3	2.01	0.43
4:C:142:GLU:HB3	4:C:515:MET:HE2	2.01	0.43
4:C:185:ASP:HB2	4:C:197:ARG:HB2	2.01	0.43
5:D:646:ILE:HD11	5:D:764:ARG:HD3	2.01	0.43
4:C:1120:ALA:HB2	4:C:1199:LEU:HG	2.01	0.43
4:C:28:LEU:HD21	4:C:524:ILE:HG13	1.99	0.43
3:A:194:GLN:HG2	3:A:195:ARG:HG2	1.99	0.43
3:B:76:GLU:HB2	3:B:80:GLU:HG3	2.01	0.43
4:C:229:ILE:HG23	4:C:240:GLU:HB3	2.00	0.43
4:C:656:SER:OG	4:C:657:THR:N	2.51	0.43
5:D:641:ILE:HD12	5:D:641:ILE:HA	1.91	0.43
5:D:1021:ASP:OD2	5:D:1021:ASP:N	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:296:VAL:HB	4:C:336:LEU:HD11	2.00	0.43
4:C:933:VAL:HG13	4:C:1050:VAL:HG22	2.00	0.43
5:D:930:LEU:HA	5:D:1244:GLN:HG3	2.01	0.43
7:F:250:LEU:HD12	7:F:250:LEU:C	2.40	0.43
4:C:42:ASP:OD2	4:C:47:TYR:N	2.45	0.42
4:C:548:ARG:HA	4:C:570:GLY:HA3	2.01	0.42
4:C:593:LYS:O	4:C:600:THR:OG1	2.37	0.42
5:D:393:THR:OG1	5:D:394:ILE:N	2.52	0.42
5:D:511:TYR:CG	5:D:728:SER:HB3	2.54	0.42
5:D:885:VAL:HG12	5:D:1258:ARG:HD2	2.01	0.42
5:D:972:LYS:HA	5:D:972:LYS:HD2	1.88	0.42
7:F:93:ARG:HE	7:F:93:ARG:HB2	1.74	0.42
7:F:294:GLN:HE21	7:F:330:LEU:HD11	1.84	0.42
4:C:434:ASP:HB3	4:C:439:LYS:HG3	2.00	0.42
4:C:1072:ASN:OD1	4:C:1072:ASN:N	2.49	0.42
4:C:299:LYS:NZ	4:C:300:ASP:O	2.53	0.42
4:C:1240:ASP:O	4:C:1262:LYS:NZ	2.51	0.42
5:D:399:LYS:HE3	5:D:400:MET:HG3	2.02	0.42
5:D:1311:LYS:HB3	5:D:1311:LYS:HE2	1.85	0.42
5:D:395:LYS:HA	5:D:395:LYS:HD2	1.88	0.42
7:F:247:GLU:O	7:F:250:LEU:CG	2.48	0.42
8:Q:136:TRP:HB3	8:Q:138:ARG:HG2	2.02	0.42
4:C:249:GLU:H	4:C:269:ILE:HG22	1.85	0.42
4:C:290:GLU:H	4:C:290:GLU:HG3	1.71	0.42
4:C:413:GLU:HG3	4:C:415:GLU:H	1.84	0.42
5:D:123:ARG:HA	5:D:126:LEU:HB3	2.01	0.42
5:D:709:ARG:NE	5:D:710:ASP:H	2.17	0.42
5:D:1318:SER:HB2	5:D:1321:SER:HB3	2.02	0.42
4:C:808:ASN:H	5:D:633:ALA:HB2	1.83	0.42
5:D:836:ARG:HG3	5:D:869:CYS:HB3	2.01	0.42
4:C:229:ILE:HD11	4:C:332:ARG:HG2	2.02	0.42
5:D:982:LEU:O	5:D:983:LYS:NZ	2.44	0.42
7:F:302:PHE:HA	7:F:305:LEU:HG	2.02	0.42
3:B:191:ARG:HH22	5:D:370:LYS:HE3	1.84	0.42
4:C:617:ALA:HB3	4:C:653:MET:HG3	2.01	0.42
5:D:325:LYS:HA	5:D:325:LYS:HD3	1.86	0.42
5:D:1087:ASP:OD2	5:D:1097:ALA:N	2.53	0.42
4:C:589:THR:HG1	4:C:659:GLN:HE21	1.61	0.42
5:D:660:GLU:HB3	5:D:685:ILE:HD13	2.00	0.42
5:D:846:GLU:HA	5:D:860:ARG:HG3	2.01	0.42
7:F:296:LYS:HA	7:F:296:LYS:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:173:GLN:HA	8:Q:176:TRP:HB3	2.01	0.42
4:C:201:ARG:NH2	4:C:370:MET:O	2.41	0.41
5:D:141:PHE:HA	5:D:180:MET:HG2	2.02	0.41
1:1:11:DA:H2''	1:1:12:DA:H2'	2.03	0.41
4:C:175:ARG:HG2	4:C:177:ILE:HG13	2.02	0.41
4:C:252:SER:O	4:C:265:LYS:NZ	2.48	0.41
4:C:503:LYS:HD2	4:C:503:LYS:HA	1.76	0.41
7:F:440:THR:HA	7:F:443:ILE:HG22	2.02	0.41
8:Q:45:ALA:N	8:Q:194:GLU:OE2	2.52	0.41
5:D:87:LYS:HB2	5:D:87:LYS:HE2	1.94	0.41
7:F:247:GLU:HA	7:F:250:LEU:CG	2.39	0.41
7:F:552:THR:OG1	7:F:555:GLU:OE1	2.36	0.41
5:D:663:GLU:OE2	5:D:667:GLN:NE2	2.54	0.41
5:D:807:LEU:HD22	5:D:1259:GLN:HE21	1.86	0.41
5:D:825:VAL:HG23	5:D:832:LYS:HB2	2.02	0.41
7:F:354:THR:OG1	7:F:355:ILE:N	2.52	0.41
3:A:102:LEU:HB2	3:A:115:ILE:HG12	2.03	0.41
4:C:447:HIS:HD2	4:C:449:GLY:H	1.68	0.41
5:D:807:LEU:HD12	5:D:807:LEU:HA	1.92	0.41
3:B:166:ARG:NE	3:B:170:ARG:O	2.45	0.41
5:D:984:LEU:HD13	5:D:993:GLU:HB3	2.02	0.41
2:2:15:DT:H1'	5:D:427:PRO:HB3	2.03	0.41
3:B:11:PRO:HB2	3:B:28:LEU:HG	2.03	0.41
4:C:347:ILE:HD11	4:C:433:ILE:HD11	2.03	0.41
3:A:31:LEU:HD23	3:A:31:LEU:HA	1.89	0.41
3:B:58:GLU:HB3	3:B:145:LYS:HB3	2.02	0.41
4:C:297:VAL:HB	4:C:317:LEU:HD11	2.03	0.41
5:D:964:LYS:HB3	5:D:977:SER:HB3	2.01	0.41
5:D:1026:PRO:HB2	5:D:1028:ILE:HG23	2.02	0.41
5:D:538:ARG:HA	5:D:538:ARG:HD3	1.83	0.41
5:D:836:ARG:O	5:D:840:LEU:HB2	2.21	0.41
5:D:868:TRP:HA	5:D:871:LEU:HD12	2.03	0.41
5:D:1040:MET:HB2	5:D:1046:ILE:HD13	2.03	0.41
5:D:66:LYS:HB2	5:D:69:GLU:HB3	2.03	0.40
5:D:252:LEU:HD12	5:D:252:LEU:HA	1.86	0.40
5:D:807:LEU:HD23	5:D:1255:VAL:HG13	2.02	0.40
8:Q:172:THR:OG1	8:Q:173:GLN:N	2.54	0.40
3:B:71:LYS:HZ3	3:B:140:ILE:HD12	1.87	0.40
3:B:181:GLU:H	3:B:207:THR:HA	1.87	0.40
4:C:258:ASN:OD1	4:C:258:ASN:N	2.51	0.40
4:C:463:GLN:HG3	4:C:505:PHE:HB2	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:85:CYS:O	5:D:89:GLY:N	2.44	0.40
4:C:387:ASN:HB3	4:C:394:ARG:HE	1.87	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	
3	A	228/329 (69%)	224 (98%)	4 (2%)	0	100	100
3	B	226/329 (69%)	215 (95%)	10 (4%)	1 (0%)	34	67
4	C	1338/1342 (100%)	1277 (95%)	61 (5%)	0	100	100
5	D	1321/1430 (92%)	1265 (96%)	56 (4%)	0	100	100
6	E	73/91 (80%)	71 (97%)	2 (3%)	0	100	100
7	F	345/627 (55%)	328 (95%)	17 (5%)	0	100	100
8	Q	161/207 (78%)	155 (96%)	6 (4%)	0	100	100
All	All	3692/4355 (85%)	3535 (96%)	156 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	193	GLU

### 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	
3	A	198/286 (69%)	195 (98%)	3 (2%)	65	84
3	B	196/286 (68%)	191 (97%)	5 (3%)	46	73
4	C	1154/1157 (100%)	1112 (96%)	42 (4%)	35	66
5	D	1110/1189 (93%)	1069 (96%)	41 (4%)	34	65
6	E	65/75 (87%)	65 (100%)	0	100	100
7	F	310/552 (56%)	294 (95%)	16 (5%)	23	53
8	Q	128/164 (78%)	120 (94%)	8 (6%)	18	46
All	All	3161/3709 (85%)	3046 (96%)	115 (4%)	38	66

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	91	ARG
3	A	114	ASP
3	A	129	VAL
3	B	124	VAL
3	B	182	ARG
3	B	196	THR
3	B	199	ASP
3	B	212	ASP
4	C	13	LYS
4	C	42	ASP
4	C	56	VAL
4	C	90	VAL
4	C	91	THR
4	C	98	VAL
4	C	165	HIS
4	C	232	ILE
4	C	237	LEU
4	C	258	ASN
4	C	283	LYS
4	C	336	LEU
4	C	377	THR
4	C	539	THR
4	C	547	VAL
4	C	574	SER
4	C	595	THR
4	C	615	VAL
4	C	648	ASP

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Mol	Chain	Res	Type
4	C	697	LYS
4	C	714	VAL
4	C	754	THR
4	C	770	CYS
4	C	802	VAL
4	C	815	SER
4	C	839	VAL
4	C	845	LEU
4	C	884	VAL
4	C	901	LEU
4	C	906	PHE
4	C	927	THR
4	C	937	ASP
4	C	998	LEU
4	C	1007	LYS
4	C	1029	LEU
4	C	1040	ASP
4	C	1092	THR
4	C	1113	LEU
4	C	1206	THR
4	C	1246	ARG
4	C	1295	SER
4	C	1326	LEU
5	D	18	ASP
5	D	24	LEU
5	D	48	THR
5	D	49	PHE
5	D	70	CYS
5	D	77	ARG
5	D	78	LEU
5	D	151	MET
5	D	227	PHE
5	D	264	ASP
5	D	284	ASP
5	D	329	ASP
5	D	357	VAL
5	D	399	LYS
5	D	424	ASN
5	D	489	ASN
5	D	504	GLN
5	D	505	ASP
5	D	553	THR

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Mol	Chain	Res	Type
5	D	569	LEU
5	D	579	LEU
5	D	638	SER
5	D	645	VAL
5	D	674	THR
5	D	678	ARG
5	D	691	ASP
5	D	697	MET
5	D	703	THR
5	D	709	ARG
5	D	751	ASP
5	D	823	THR
5	D	889	ASP
5	D	978	ARG
5	D	1021	ASP
5	D	1116	SER
5	D	1121	LEU
5	D	1169	THR
5	D	1313	SER
5	D	1321	SER
5	D	1366	HIS
5	D	1368	ASP
7	F	93	ARG
7	F	136	GLU
7	F	137	TYR
7	F	244	THR
7	F	278	ASP
7	F	283	GLN
7	F	289	LYS
7	F	302	PHE
7	F	329	LYS
7	F	330	LEU
7	F	343	LYS
7	F	395	THR
7	F	417	ASP
7	F	425	TYR
7	F	442	SER
7	F	552	THR
8	Q	58	LEU
8	Q	63	LYS
8	Q	121	CYS
8	Q	129	ASP

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Mol	Chain	Res	Type
8	Q	139	VAL
8	Q	154	ARG
8	Q	165	THR
8	Q	191	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	147	GLN
3	A	186	ASN
4	C	173	ASN
4	C	219	GLN
4	C	238	GLN
4	C	357	ASN
4	C	447	HIS
4	C	518	ASN
4	C	799	ASN
4	C	1008	GLN
4	C	1009	ASN
4	C	1017	GLN
5	D	80	HIS
5	D	196	GLN
5	D	364	HIS
5	D	450	HIS
5	D	792	ASN
5	D	897	HIS
5	D	1044	GLN
5	D	1108	GLN
5	D	1249	ASN
5	D	1259	GLN
6	E	61	ASN
6	E	70	GLN
7	F	129	GLN
7	F	147	GLN
7	F	271	ASN
7	F	283	GLN
7	F	294	GLN
7	F	309	ASN
7	F	323	ASN
7	F	342	GLN
7	F	409	ASN
7	F	589	GLN

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Mol	Chain	Res	Type
8	Q	203	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	R	10/11 (90%)	1 (10%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	R	2	G

There are no RNA pucker outliers to report.

## 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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

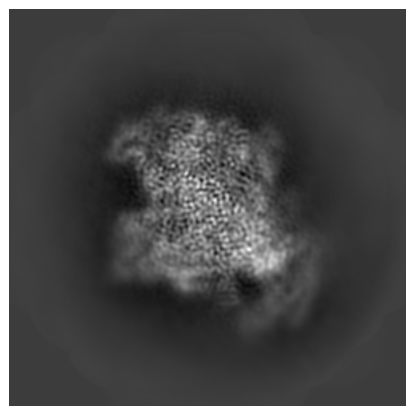
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26438. These allow visual inspection of the internal detail of the map and identification of artifacts.

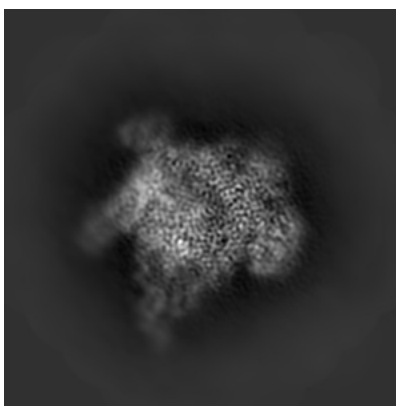
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

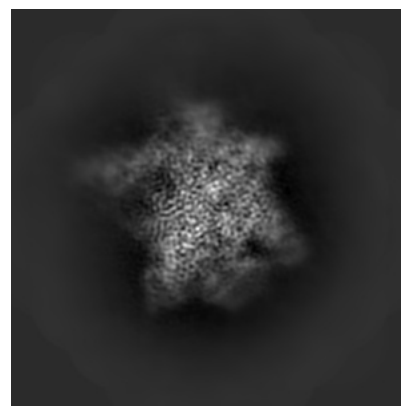
#### 6.1.1 Primary map



X

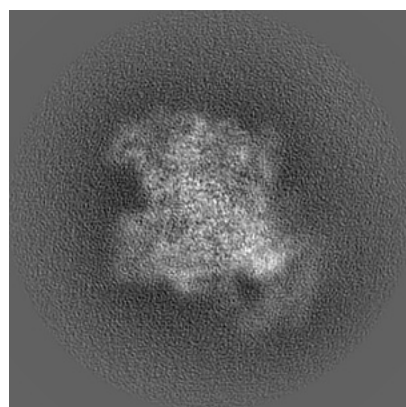


Y

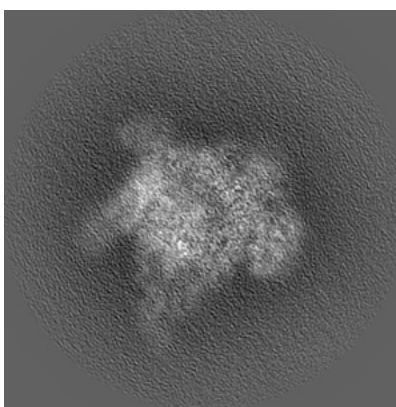


Z

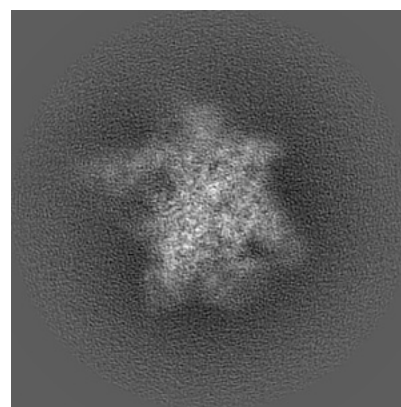
#### 6.1.2 Raw map



X



Y

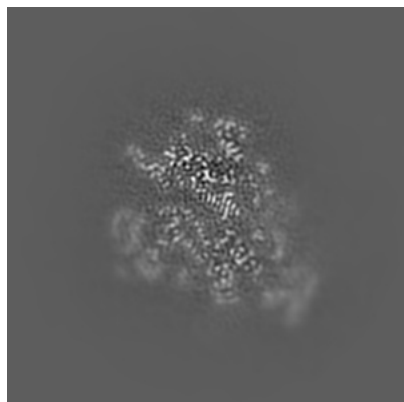


Z

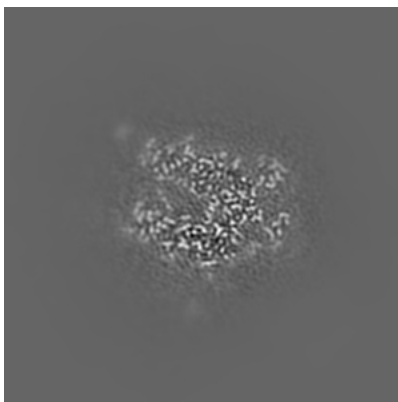
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

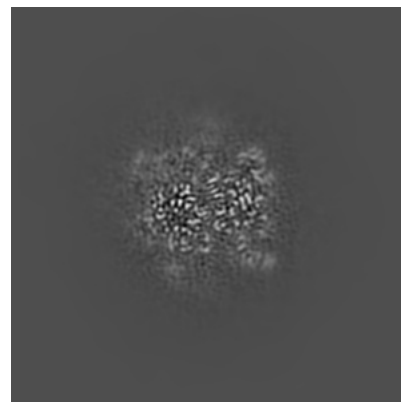
### 6.2.1 Primary map



X Index: 128

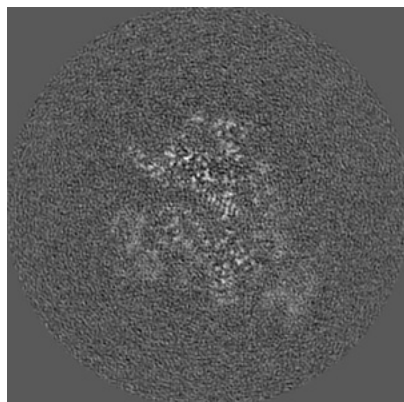


Y Index: 128

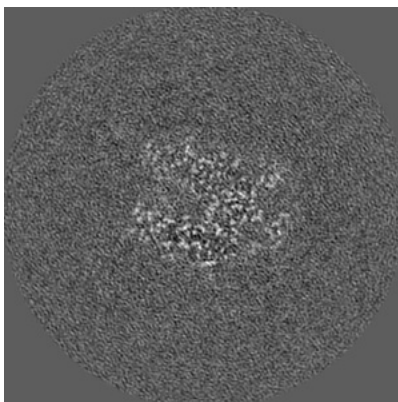


Z Index: 128

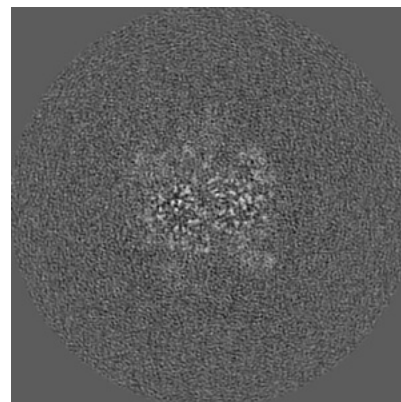
### 6.2.2 Raw map



X Index: 128



Y Index: 128



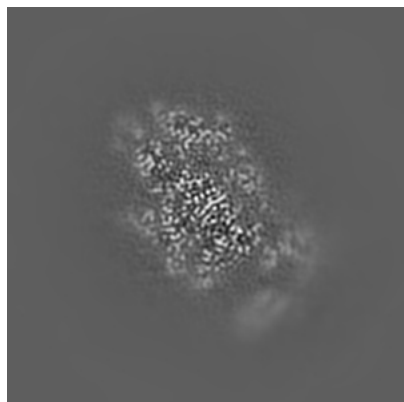
Z Index: 128

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

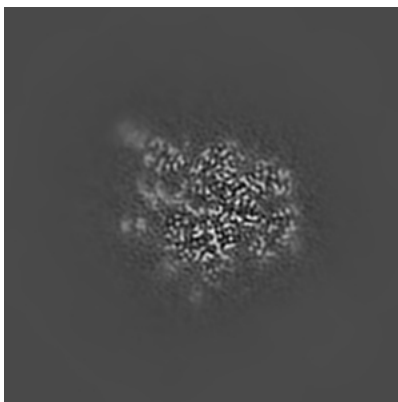


## 6.3 Largest variance slices [i](#)

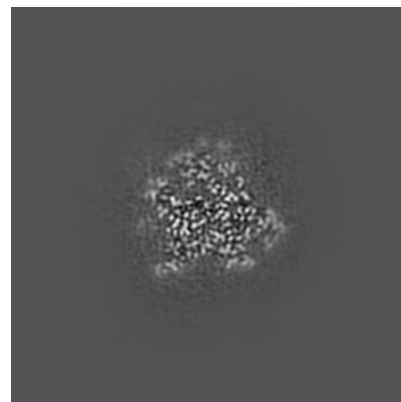
### 6.3.1 Primary map



X Index: 112

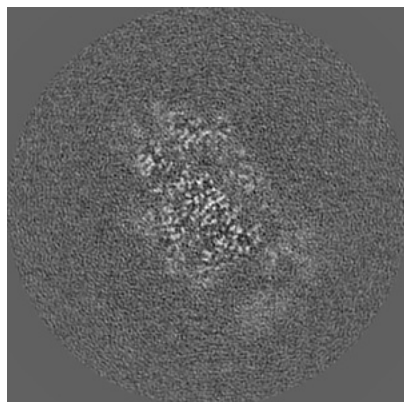


Y Index: 121

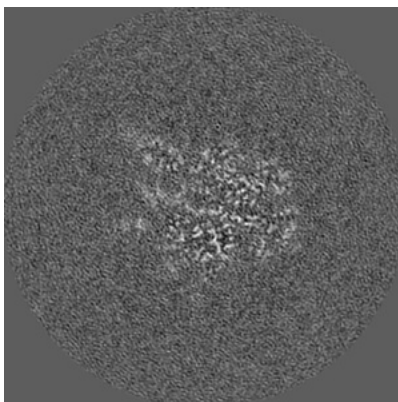


Z Index: 143

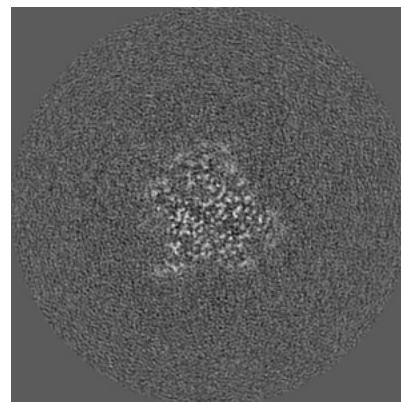
### 6.3.2 Raw map



X Index: 112



Y Index: 121

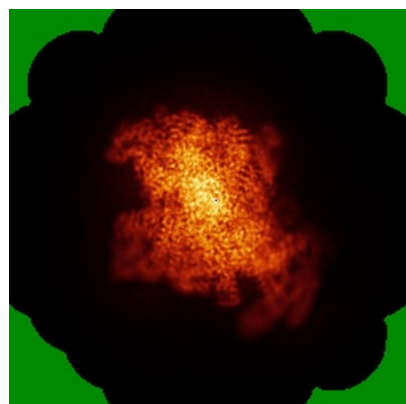


Z Index: 144

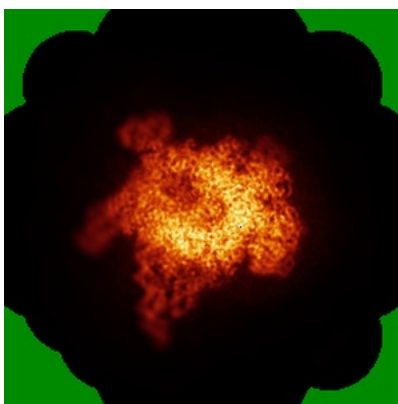
The images above show the largest variance slices of the map in three orthogonal directions.

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

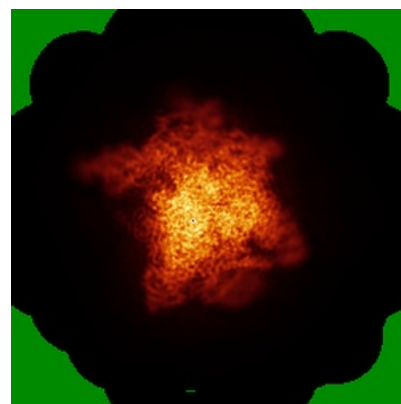
### 6.4.1 Primary map



X

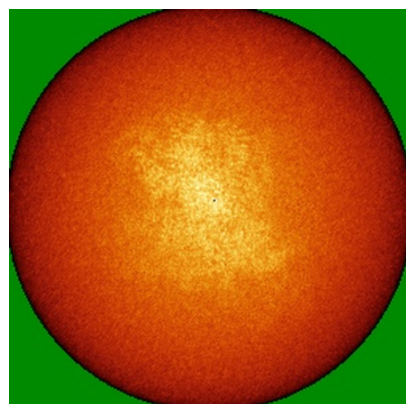


Y

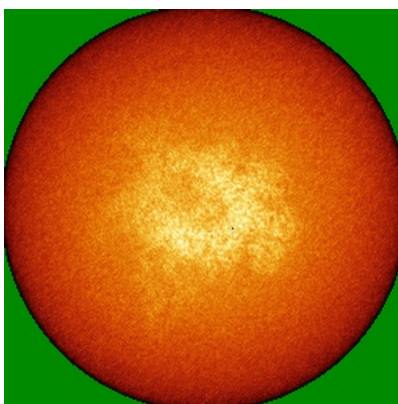


Z

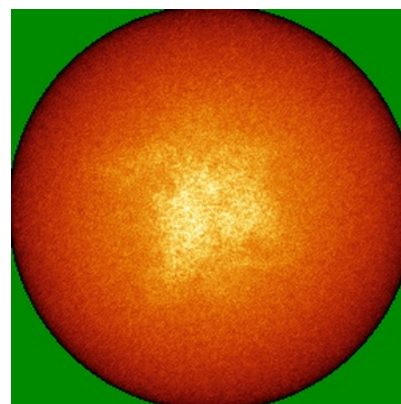
### 6.4.2 Raw map



X



Y

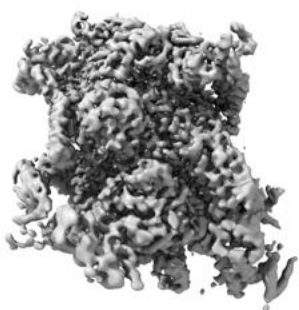


Z

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](#)

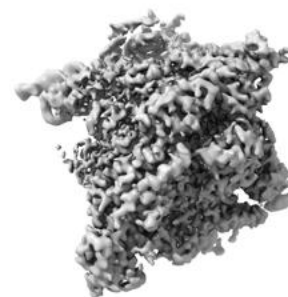
### 6.5.1 Primary map



X



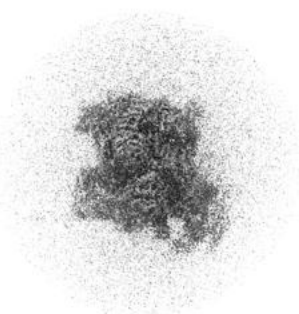
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0306. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

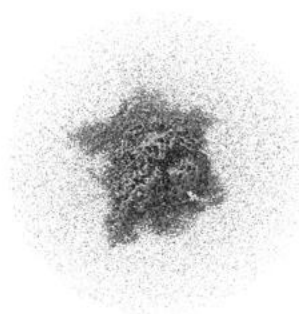
### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

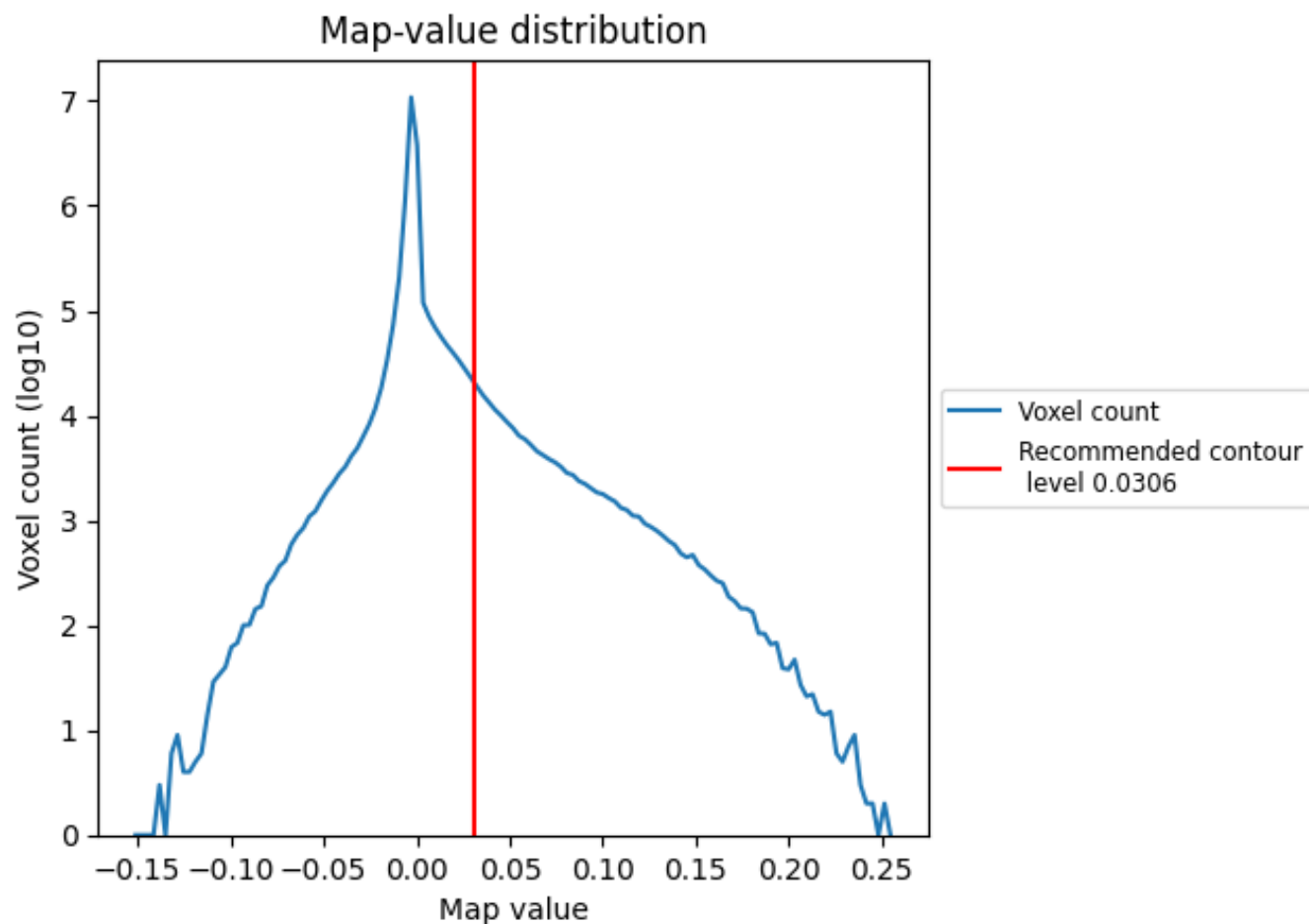
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

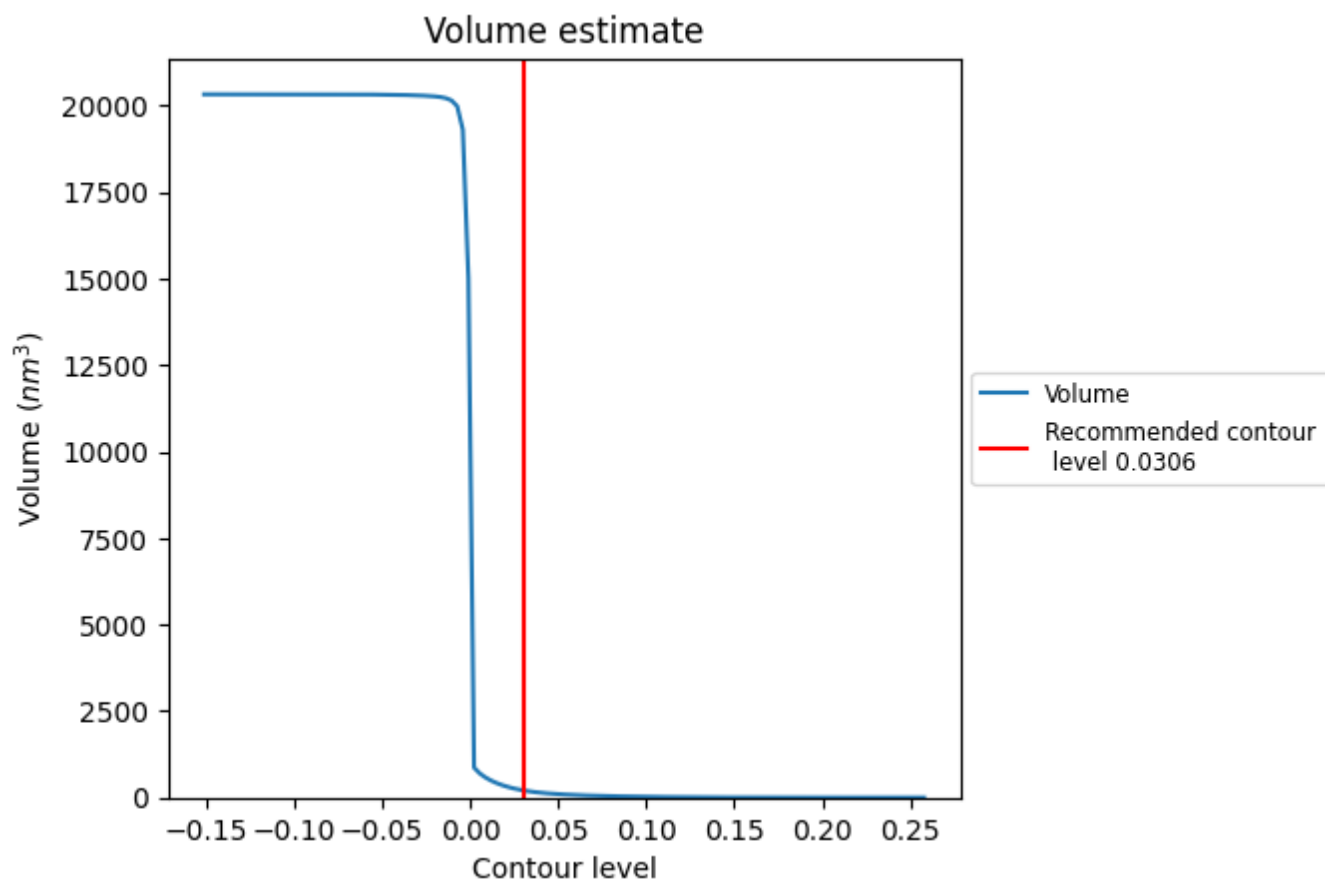
This section contains the results of statistical analysis of the map.

### 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.

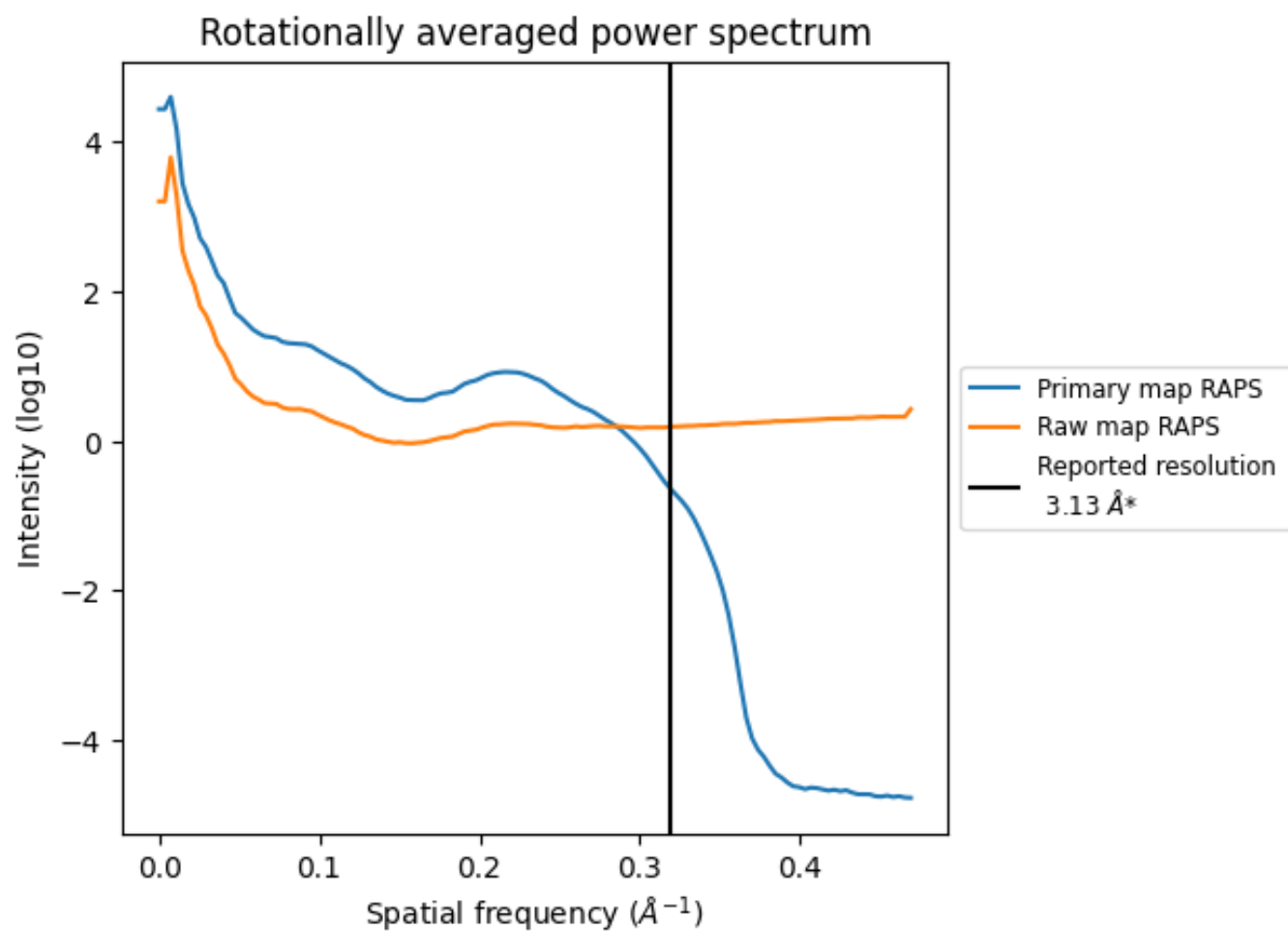
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 203  $\text{nm}^3$ ; this corresponds to an approximate mass of 184 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 ⓘ

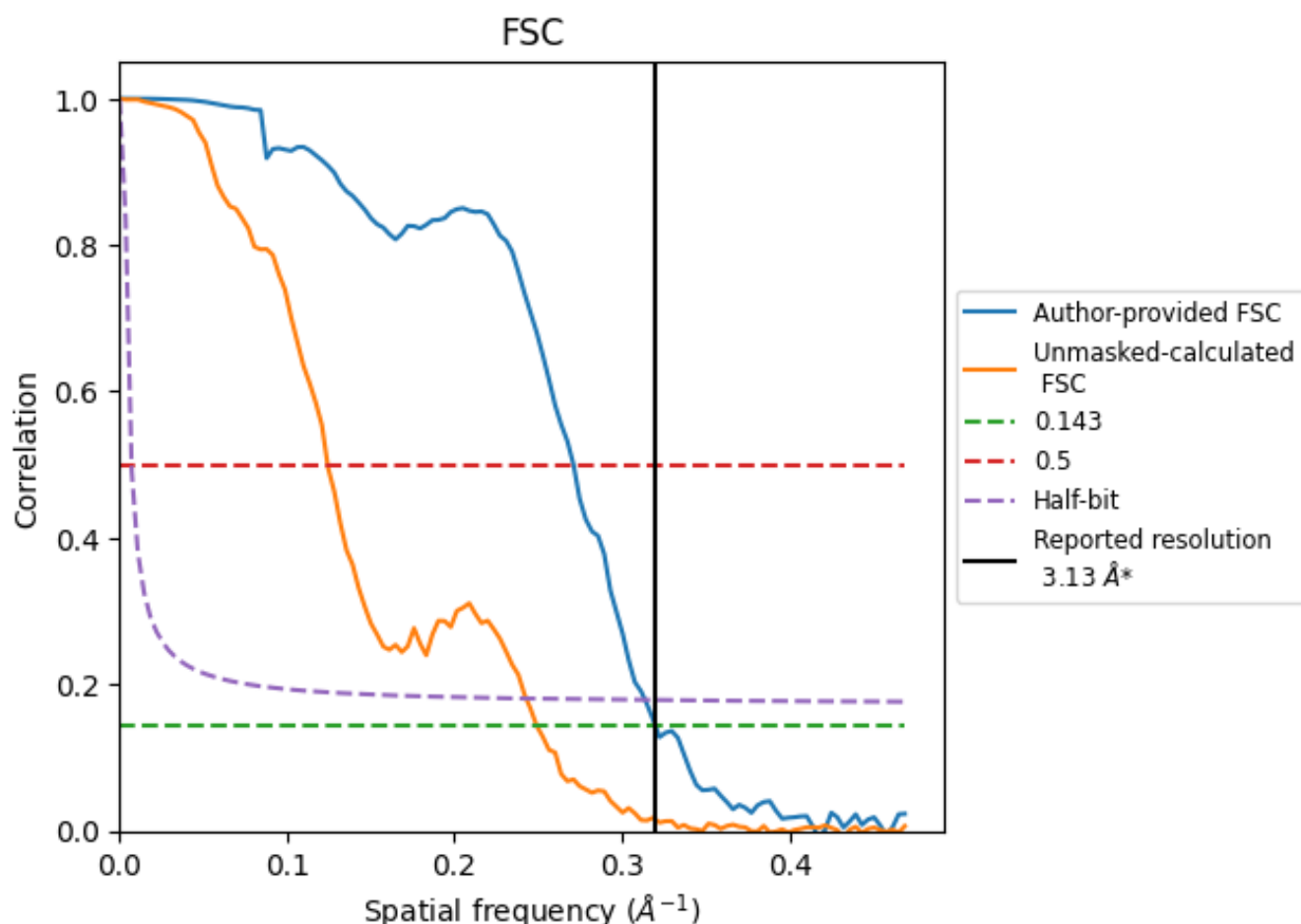


\*Reported resolution corresponds to spatial frequency of 0.319  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.319 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.13	-	-
Author-provided FSC curve	3.12	3.69	3.19
Unmasked-calculated*	4.01	8.05	4.12

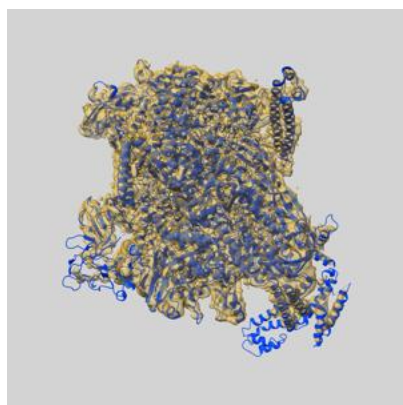
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.01 differs from the reported value 3.13 by more than 10 %



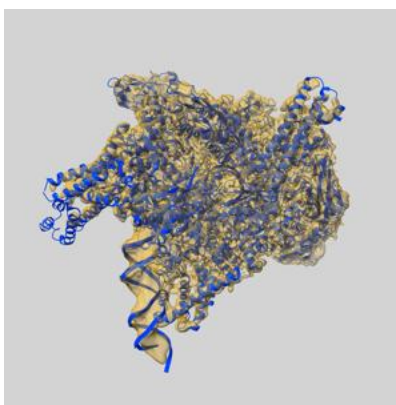
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26438 and PDB model 7UBM. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

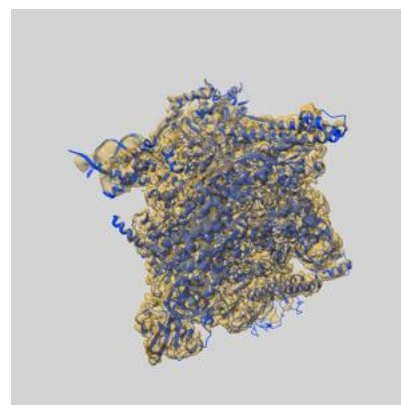
### 9.1 Map-model overlay [i](#)



X



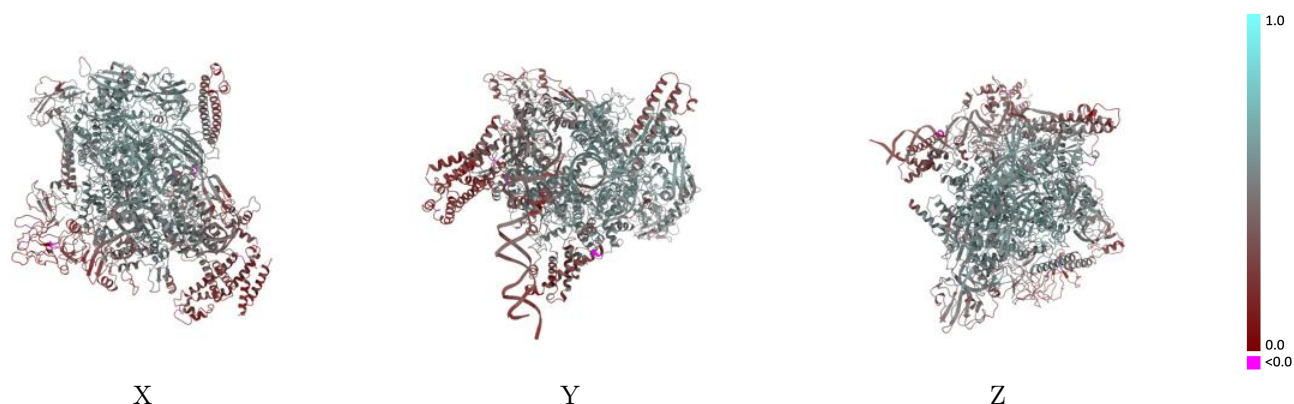
Y



Z

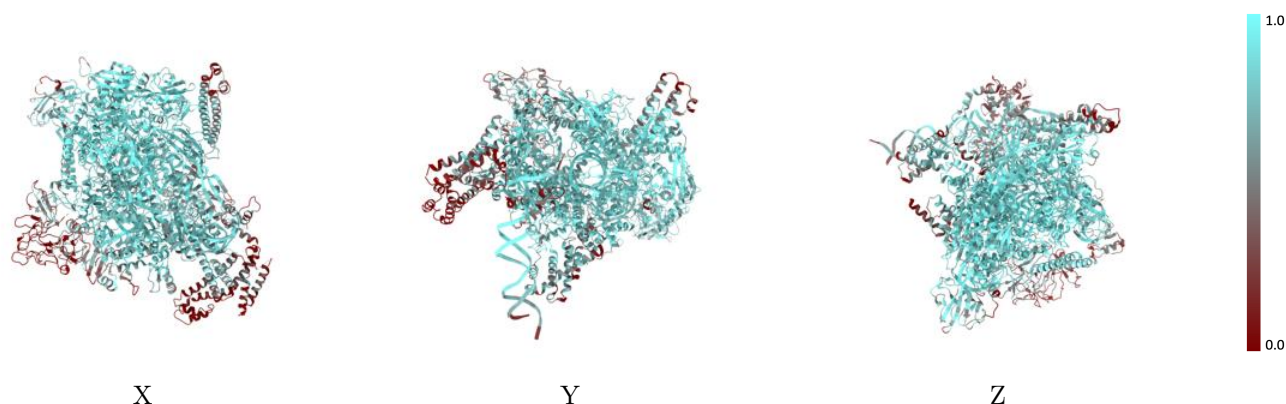
The images above show the 3D surface view of the map at the recommended contour level 0.0306 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



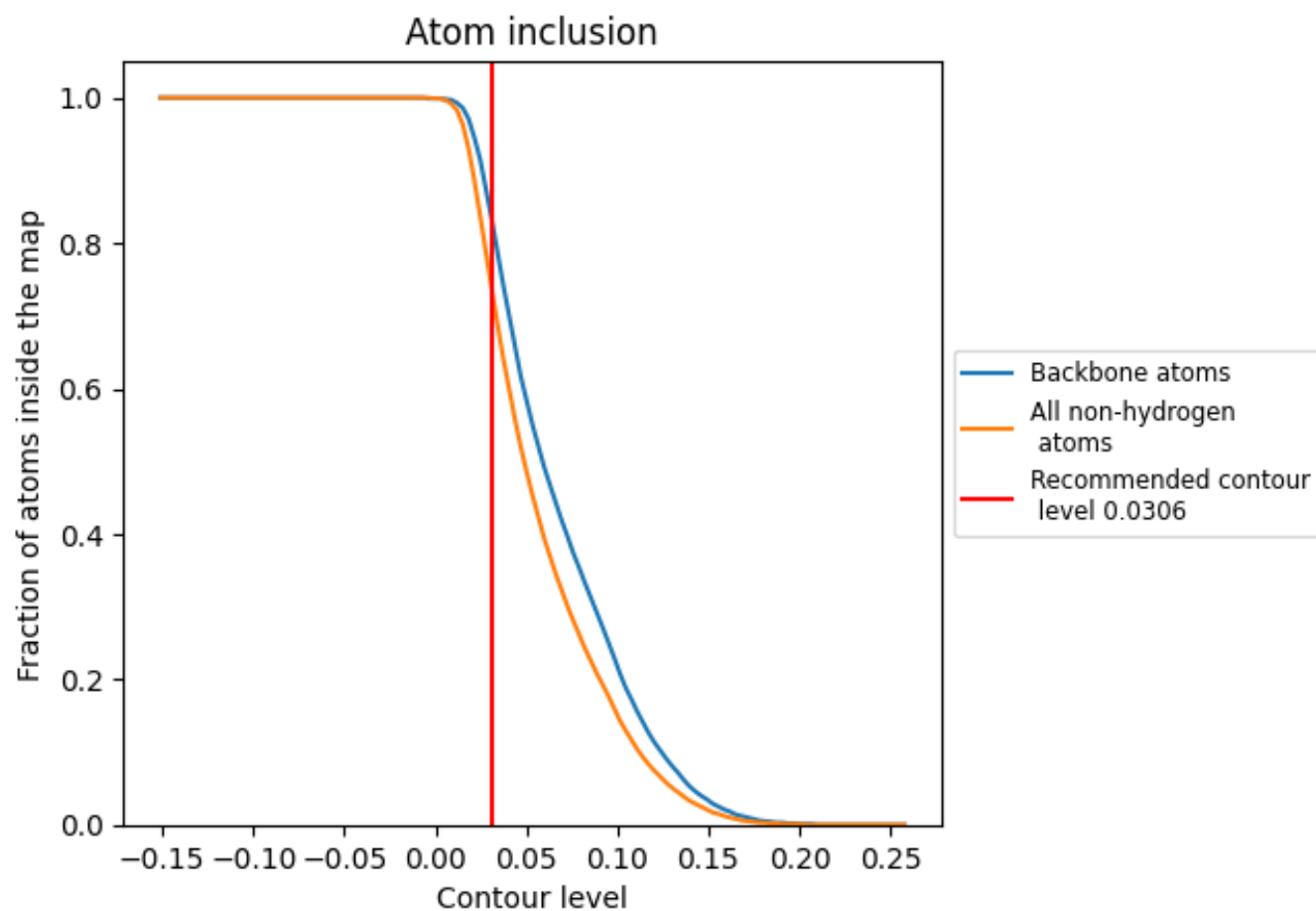
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0306).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 74% 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 (0.0306) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7420	<div></div> 0.4610
1	<div></div> 0.8260	<div></div> 0.3690
2	<div></div> 0.8100	<div></div> 0.3780
A	<div></div> 0.8290	<div></div> 0.5290
B	<div></div> 0.7570	<div></div> 0.4670
C	<div></div> 0.8040	<div></div> 0.5010
D	<div></div> 0.7620	<div></div> 0.4840
E	<div></div> 0.5070	<div></div> 0.4830
F	<div></div> 0.4040	<div></div> 0.2900
Q	<div></div> 0.6360	<div></div> 0.3350
R	<div></div> 0.9250	<div></div> 0.5630

1.0

0.0

<0.0