



## Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 02:37 AM UTC

PDB ID : 9K12 / pdb\_00009k12  
EMDB ID : EMD-61962  
Title : A cryo-EM structure of *B. oleracea* RNA polymerase V in complex with 1U scaffold at 3.5 Angstrom  
Authors : Xie, G.; Du, X.; Du, J.  
Deposited on : 2024-10-16  
Resolution : 3.46 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](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:

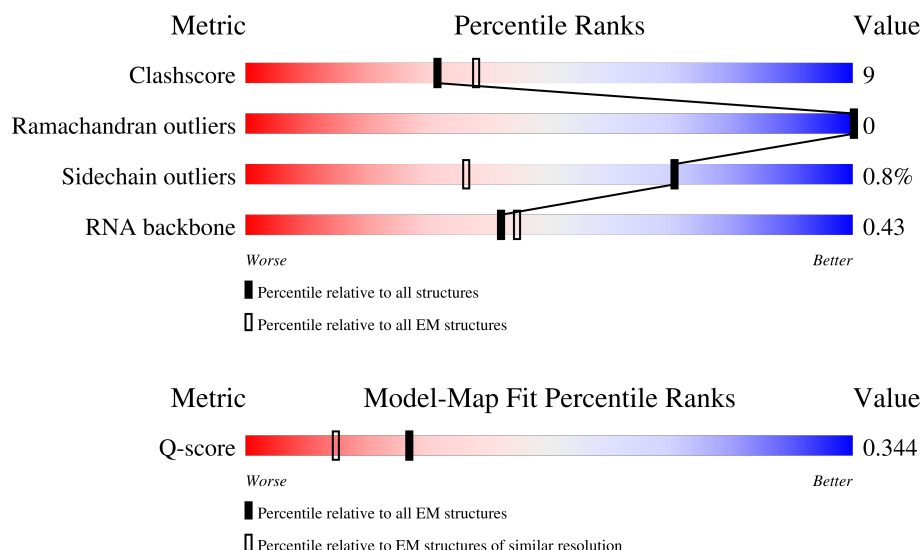
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 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 3.46 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.





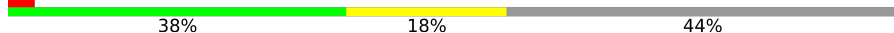







Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13788 ( 2.96 - 3.96 )

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	T	34	<div> <div>62%</div> <div>15% 53% 32%</div> </div>
2	N	34	<div> <div>59%</div> <div>29% 47% 24%</div> </div>
3	P	20	<div> <div>40%</div> <div>10% 20% 20% 5% 45%</div> </div>

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Mol	Chain	Length	Quality of chain
4	A	2032	
5	C	319	
6	F	144	
7	J	71	
8	K	116	
9	L	51	
10	H	146	
11	I	114	
12	E	230	
13	B	1169	

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 23813 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 (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	23	Total	C	N	O	P	0	0
			465	223	80	139	23		

- Molecule 2 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	26	Total	C	N	O	P	0	0
			537	255	102	154	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	11	Total	C	N	O	P	0	0
			237	106	46	74	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	845	Total	C	N	O	S	0	0
			6615	4180	1137	1254	44		

- Molecule 5 is a protein called DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	287	Total	C	N	O	S	0	0
			2256	1418	380	445	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	THR	SER	conflict	UNP A0A0D3D418

- Molecule 6 is a protein called DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	80	Total	C	N	O	S	0	0
			660	420	114	122	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	51	GLU	ASP	conflict	UNP A0A0D3BZZ8

- Molecule 7 is a protein called DNA-directed RNA polymerase II, IV and V subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	63	Total	C	N	O	S	0	0
			507	324	85	91	7		

- Molecule 8 is a protein called DNA-directed RNA polymerase RBP11-like dimerisation domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	108	Total	C	N	O	S	0	0
			890	565	156	167	2		

- Molecule 9 is a protein called DNA-directed RNA polymerase II, IV and V subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	45	Total	C	N	O	S	0	0
			365	224	70	67	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	18	GLU	LYS	conflict	UNP A0A0D2ZPP3
L	32	CYS	ARG	conflict	UNP A0A0D2ZPP3

- Molecule 10 is a protein called DNA-directed RNA polymerase II, IV and V subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	141	Total	C	N	O	S	0	0
			1129	729	183	208	9		

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	97	Total	C	N	O	S	0	0
			787	482	150	143	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	20	ARG	LYS	conflict	UNP A0A0D3A7P5
I	40	ASP	ASN	conflict	UNP A0A0D3A7P5

- Molecule 12 is a protein called RNA polymerase subunit H/Rpb5 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	209	Total	C	N	O	S	0	0
			1706	1085	303	316	2		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	101	GLY	SER	conflict	UNP A0A0D3DTU3
E	182	GLN	HIS	conflict	UNP A0A0D3DTU3
E	210	ILE	VAL	conflict	UNP A0A0D3DTU3

- Molecule 13 is a protein called DNA-directed RNA polymerase IV and V subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	966	Total	C	N	O	S	0	0
			7652	4821	1356	1431	44		

- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
14	A	1	Total	Mg	0
			1	1	

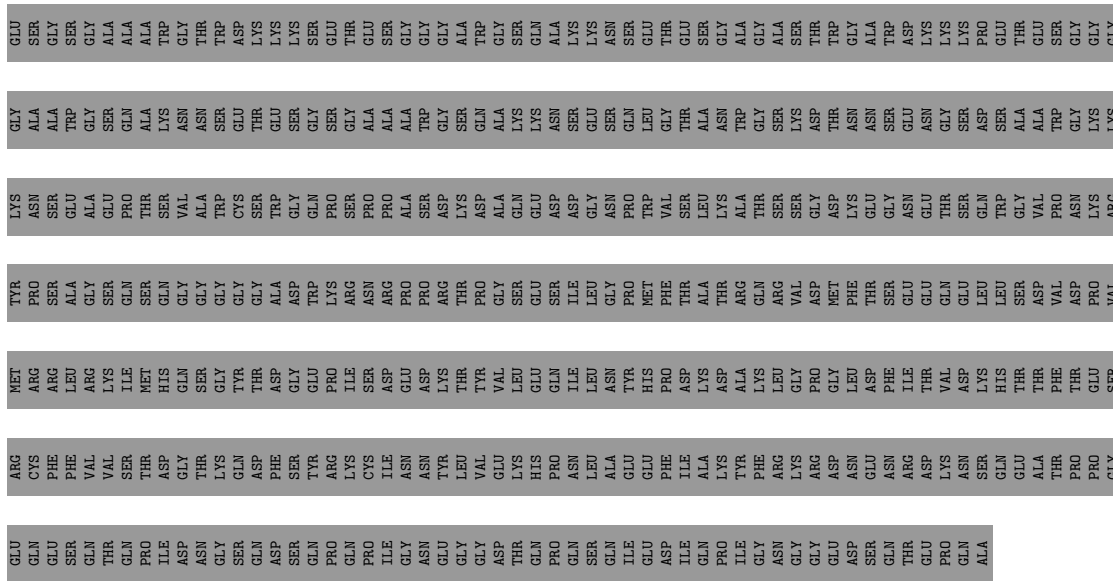
- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total 1	Zn 1	0
15	C	1	Total 1	Zn 1	0
15	J	1	Total 1	Zn 1	0
15	L	1	Total 1	Zn 1	0
15	I	2	Total 2	Zn 2	0

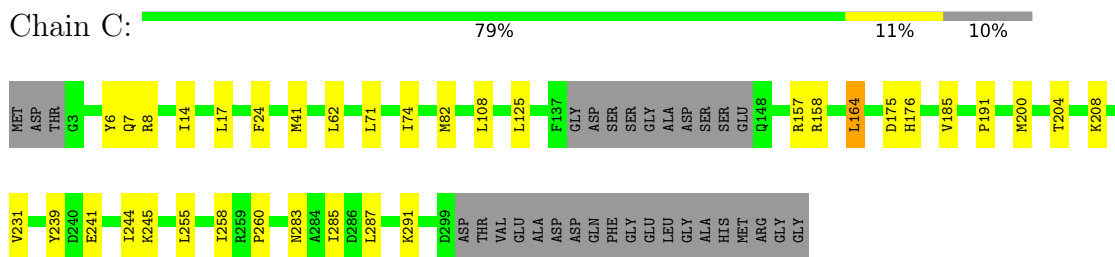




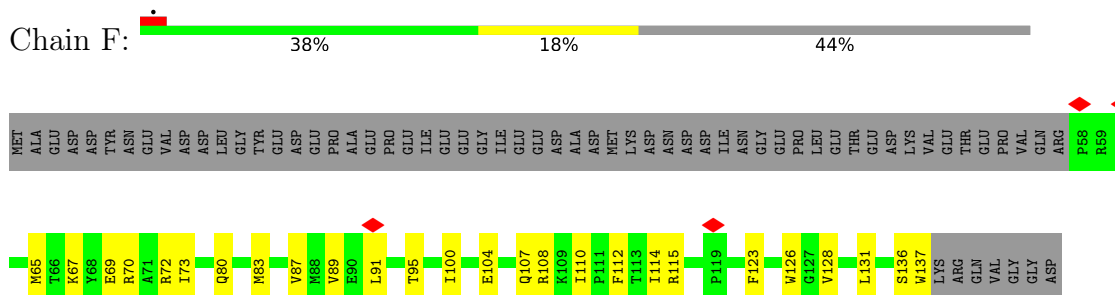




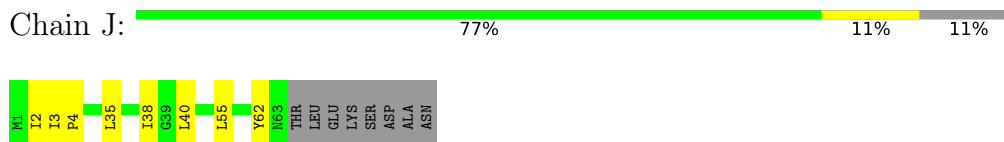
- Molecule 5: DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein



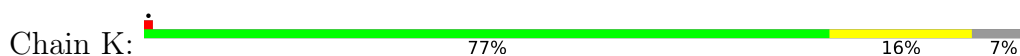
- Molecule 6: DNA-directed RNA polymerase RpoA/D/Rpb3-type domain-containing protein



- Molecule 7: DNA-directed RNA polymerase II, IV and V subunit 10

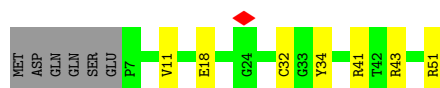
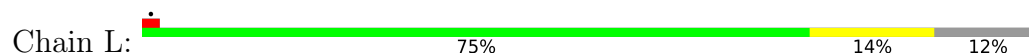


- Molecule 8: DNA-directed RNA polymerase RBP11-like dimerisation domain-containing protein

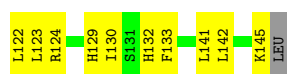




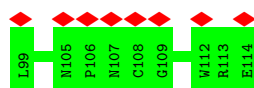
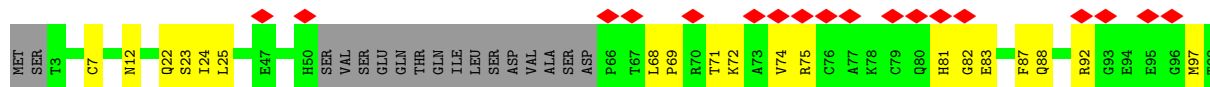
- Molecule 9: DNA-directed RNA polymerase II, IV and V subunit 12



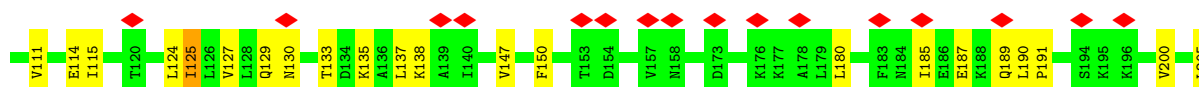
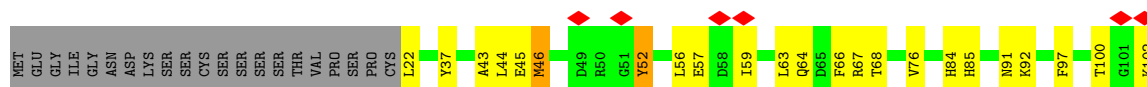
- Molecule 10: DNA-directed RNA polymerase II, IV and V subunit 8



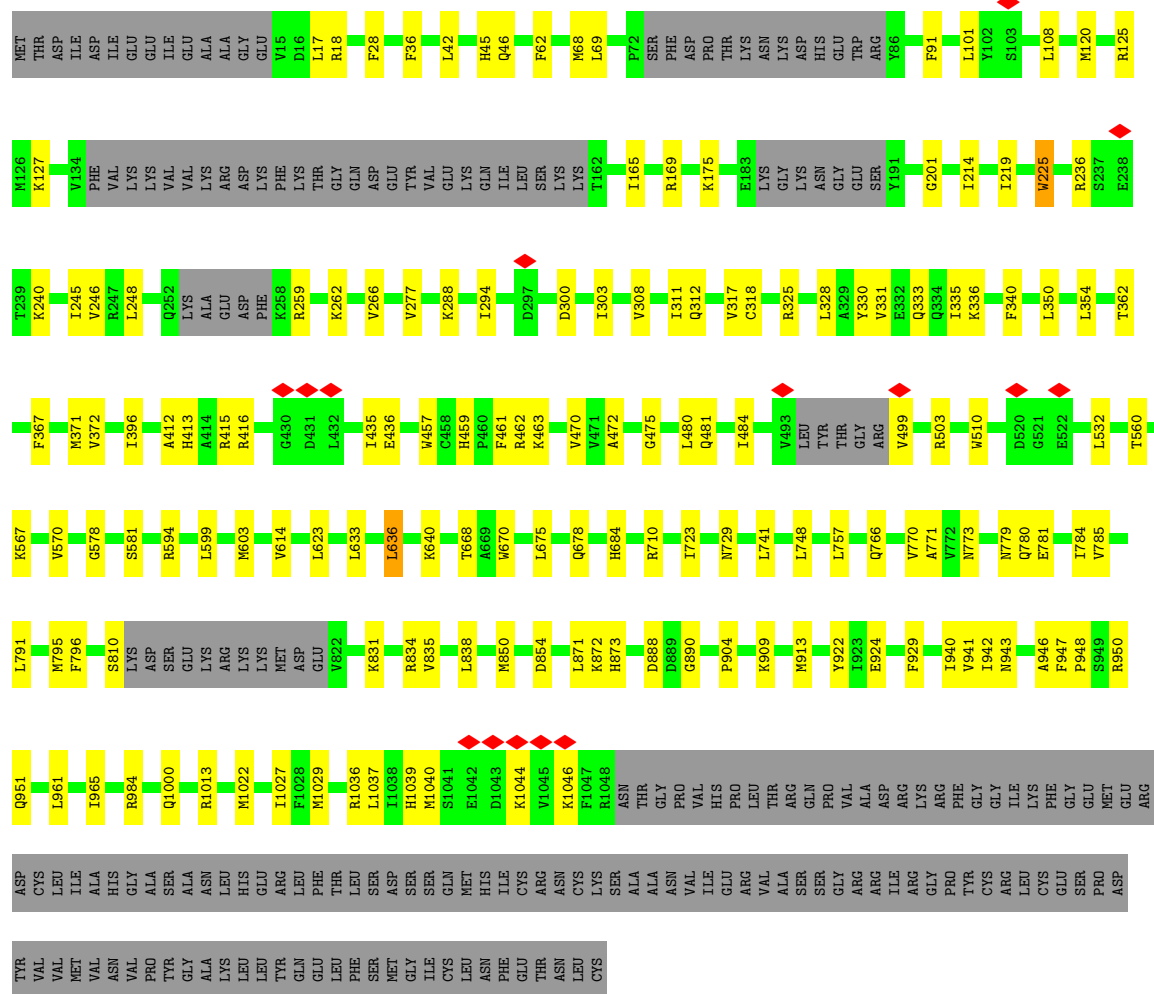
- Molecule 11: DNA-directed RNA polymerase subunit



- Molecule 12: RNA polymerase subunit H/Rpb5 C-terminal domain-containing protein



- Molecule 13: DNA-directed RNA polymerase IV and V subunit 2



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79987	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.5625	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0118	Depositor
Map size (Å)	328.5, 328.5, 328.5	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.095, 1.095, 1.095	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	T	0.37	0/518	0.44	0/793
2	N	0.37	0/603	0.43	0/929
3	P	0.79	4/265 (1.5%)	0.21	0/411
4	A	0.14	0/6729	0.42	1/9086 (0.0%)
5	C	0.14	0/2286	0.39	0/3087
6	F	0.17	0/673	0.49	0/905
7	J	0.15	0/515	0.41	0/696
8	K	0.15	0/908	0.35	0/1224
9	L	0.13	0/369	0.34	0/493
10	H	0.16	0/1155	0.49	0/1557
11	I	0.14	0/804	0.36	0/1081
12	E	0.12	0/1732	0.36	0/2332
13	B	0.13	0/7801	0.37	0/10513
All	All	0.18	4/24358 (0.0%)	0.40	1/33107 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	15	G	C1'-N9	-6.07	1.38	1.48
3	P	14	C	C1'-N1	6.03	1.57	1.48
3	P	17	C	C1'-N1	5.69	1.56	1.48
3	P	19	C	C1'-N1	5.33	1.56	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	MET	CB-CA-C	5.23	115.81	109.85

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	T	465	0	262	39	0
2	N	537	0	293	25	0
3	P	237	0	121	10	0
4	A	6615	0	6668	130	0
5	C	2256	0	2269	25	0
6	F	660	0	669	20	0
7	J	507	0	512	6	0
8	K	890	0	883	15	0
9	L	365	0	364	5	0
10	H	1129	0	1128	30	0
11	I	787	0	736	14	0
12	E	1706	0	1759	27	0
13	B	7652	0	7589	105	0
14	A	1	0	0	0	0
15	A	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
All	All	23813	0	23253	407	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 9.

All (407) 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:T:15:DA:C2	2:N:21:DA:C2	2.32	1.17
1:T:12:DC:C2'	1:T:13:DT:H72	1.94	0.98
1:T:15:DA:H2	2:N:21:DA:C2	1.76	0.95
1:T:12:DC:H2'	1:T:13:DT:H72	1.52	0.91
1:T:12:DC:H2'	1:T:13:DT:C7	2.04	0.88
1:T:15:DA:C2	2:N:21:DA:H2	1.87	0.88
1:T:12:DC:C2'	1:T:13:DT:C7	2.52	0.86
1:T:15:DA:N1	2:N:21:DA:N1	2.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:748:LEU:HB3	13:B:965:ILE:HD11	1.65	0.78
4:A:916:LEU:HB2	4:A:940:HIS:HE1	1.48	0.77
4:A:674:MET:HG3	4:A:695:LEU:HD21	1.67	0.76
13:B:165:ILE:HD12	13:B:435:ILE:HG23	1.68	0.75
1:T:15:DA:N1	2:N:21:DA:C2	2.56	0.73
12:E:180:LEU:HD21	12:E:187:GLU:HG2	1.71	0.73
12:E:100:THR:HA	12:E:129:GLN:HG2	1.72	0.71
1:T:13:DT:C2	2:N:23:DG:N2	2.58	0.71
12:E:76:VAL:HB	12:E:97:PHE:HB2	1.73	0.70
13:B:834:ARG:HB3	13:B:854:ASP:HA	1.72	0.70
13:B:475:GLY:HA3	13:B:481:GLN:HE21	1.56	0.70
2:N:17:DG:C2	13:B:461:PHE:CE2	2.80	0.69
10:H:40:PHE:HB3	10:H:124:ARG:HB2	1.75	0.69
13:B:965:ILE:HG22	13:B:1000:GLN:HE22	1.57	0.69
12:E:63:LEU:HD21	12:E:67:ARG:HH21	1.58	0.68
13:B:246:VAL:HG22	13:B:266:VAL:HG22	1.75	0.68
12:E:133:THR:HG22	12:E:135:LYS:H	1.60	0.66
1:T:12:DC:N1	1:T:13:DT:H72	2.11	0.66
5:C:41:MET:HE3	5:C:185:VAL:HG11	1.77	0.66
8:K:48:MET:HE3	8:K:48:MET:O	1.95	0.66
3:P:16:A:H2'	3:P:17:C:C6	2.30	0.66
13:B:350:LEU:HD22	13:B:354:LEU:HD22	1.77	0.66
12:E:217:GLY:H	12:E:221:GLU:HG3	1.60	0.65
13:B:791:LEU:HD21	13:B:904:PRO:HD2	1.77	0.65
4:A:626:MET:HG2	4:A:631:MET:HG2	1.78	0.64
1:T:12:DC:H2''	1:T:13:DT:C7	2.28	0.64
13:B:396:ILE:HD12	13:B:623:LEU:HD21	1.80	0.63
2:N:21:DA:C6	2:N:22:DA:N6	2.66	0.63
4:A:529:VAL:HG22	10:H:93:MET:HE1	1.81	0.62
4:A:1040:ASP:HB3	4:A:1043:ILE:HG12	1.81	0.62
6:F:80:GLN:HA	6:F:83:MET:HG3	1.82	0.62
13:B:872:LYS:HG3	13:B:873:HIS:H	1.65	0.62
4:A:591:GLU:O	4:A:591:GLU:HG2	1.99	0.62
1:T:20:DG:C8	1:T:21:DT:H71	2.34	0.61
10:H:92:VAL:HG12	10:H:142:LEU:HA	1.82	0.61
13:B:277:VAL:HG11	13:B:330:TYR:HD2	1.65	0.61
4:A:1049:ILE:HG22	4:A:1051:ASN:H	1.64	0.61
4:A:1023:VAL:HG13	4:A:1024:LEU:HD12	1.82	0.61
13:B:946:ALA:HA	13:B:950:ARG:HH21	1.66	0.61
10:H:37:LEU:HD21	10:H:129:HIS:CD2	2.37	0.60
13:B:300:ASP:O	13:B:303:ILE:HG12	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:544:ILE:HD12	4:A:544:ILE:H	1.67	0.60
10:H:130:ILE:HG23	10:H:133:PHE:HD2	1.66	0.59
4:A:1111:SER:HB3	4:A:1114:GLN:HG2	1.83	0.59
4:A:465:ALA:O	4:A:469:VAL:HG12	2.02	0.59
1:T:25:DA:H2''	1:T:26:DT:H5''	1.84	0.59
3:P:16:A:H2'	3:P:17:C:H6	1.66	0.58
5:C:7:GLN:HG2	8:K:97:GLU:OE2	2.03	0.58
4:A:804:SER:HA	12:E:189:GLN:HB3	1.83	0.58
1:T:12:DC:H2'	1:T:13:DT:H73	1.84	0.58
4:A:626:MET:HE3	4:A:630:ASP:HB3	1.84	0.58
1:T:8:DA:H2''	1:T:9:DG:C8	2.38	0.58
4:A:605:GLN:HG2	4:A:609:MET:HE2	1.85	0.58
1:T:14:DT:C2	1:T:15:DA:C6	2.92	0.57
13:B:367:PHE:O	13:B:371:MET:HG3	2.04	0.57
2:N:14:DC:H5	13:B:340:PHE:HB2	1.69	0.57
10:H:111:GLU:HB2	10:H:122:LEU:HD11	1.86	0.57
13:B:457:TRP:HB2	13:B:470:VAL:HG21	1.85	0.57
13:B:770:VAL:HG12	13:B:940:ILE:HB	1.85	0.57
10:H:34:SER:HB3	10:H:39:MET:HB2	1.87	0.57
6:F:69:GLU:O	6:F:73:ILE:HG22	2.05	0.57
5:C:108:LEU:HB2	5:C:125:LEU:HD23	1.86	0.57
7:J:3:ILE:HD12	7:J:4:PRO:HD2	1.87	0.57
13:B:773:ASN:HD22	13:B:1027:ILE:HD12	1.69	0.57
10:H:39:MET:HE3	10:H:39:MET:HA	1.87	0.57
2:N:17:DG:C5	13:B:219:ILE:HD11	2.40	0.56
12:E:185:ILE:HD13	12:E:190:LEU:HG	1.87	0.56
13:B:831:LYS:HG3	13:B:835:VAL:H	1.70	0.56
1:T:21:DT:H2'	1:T:22:DC:C6	2.41	0.56
2:N:12:DG:C8	2:N:13:DC:C5	2.93	0.56
11:I:23:SER:C	11:I:24:ILE:HD13	2.30	0.56
1:T:12:DC:C2'	1:T:13:DT:H73	2.36	0.56
12:E:124:LEU:H	12:E:147:VAL:HG12	1.70	0.56
3:P:17:C:H2'	3:P:18:G:C8	2.41	0.56
4:A:1058:TRP:CD1	4:A:1058:TRP:H	2.22	0.56
8:K:105:PHE:O	8:K:109:VAL:HG12	2.06	0.56
11:I:75:ARG:HH21	11:I:82:GLY:HA3	1.71	0.56
13:B:594:ARG:HA	13:B:599:LEU:HB2	1.87	0.56
2:N:17:DG:C2	13:B:461:PHE:HE2	2.23	0.55
13:B:570:VAL:HG12	13:B:614:VAL:HB	1.89	0.55
13:B:835:VAL:HG13	13:B:838:LEU:HB2	1.88	0.55
4:A:342:PRO:HG2	4:A:345:ILE:HB	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:593:GLY:HA2	6:F:136:SER:HB2	1.88	0.55
13:B:325:ARG:HE	13:B:328:LEU:HD23	1.72	0.55
4:A:1050:TRP:CD1	11:I:72:LYS:HZ3	2.25	0.55
4:A:577:LEU:HD12	4:A:578:ALA:N	2.21	0.54
1:T:20:DG:N7	1:T:21:DT:H73	2.23	0.54
1:T:8:DA:H2''	1:T:9:DG:N7	2.22	0.54
1:T:7:DA:C8	1:T:7:DA:H5'	2.42	0.54
2:N:14:DC:C5	13:B:340:PHE:HB2	2.43	0.54
3:P:13:G:H2'	3:P:14:C:C6	2.43	0.54
5:C:8:ARG:HG2	8:K:52:ARG:HH22	1.73	0.54
4:A:941:LEU:HB2	4:A:1003:PRO:HB2	1.89	0.54
5:C:157:ARG:HG3	5:C:158:ARG:H	1.72	0.53
10:H:14:VAL:HG13	10:H:55:GLY:H	1.72	0.53
4:A:592:LYS:H	6:F:137:TRP:HB2	1.73	0.53
1:T:20:DG:C6	1:T:21:DT:C4	2.97	0.53
4:A:331:ASP:HB2	4:A:437:LYS:HB3	1.90	0.53
4:A:375:TYR:HB3	4:A:382:TYR:CZ	2.43	0.53
12:E:125:ILE:HG23	12:E:150:PHE:CE1	2.44	0.53
4:A:613:ASP:HB3	4:A:614:PRO:HD3	1.91	0.53
13:B:165:ILE:HG13	13:B:436:GLU:HG2	1.90	0.53
4:A:698:GLN:HG3	13:B:951:GLN:HG2	1.90	0.53
11:I:68:LEU:HD21	11:I:87:PHE:HB3	1.90	0.53
13:B:214:ILE:HD11	13:B:472:ALA:HB2	1.91	0.53
13:B:741:LEU:HD13	13:B:766:GLN:HE21	1.74	0.53
4:A:885:ARG:NH1	4:A:886:CYS:HB2	2.24	0.53
1:T:12:DC:C1'	1:T:13:DT:H72	2.39	0.53
4:A:372:CYS:HA	4:A:402:ARG:HA	1.91	0.53
5:C:14:ILE:HG12	5:C:24:PHE:HB3	1.92	0.53
12:E:44:LEU:HG	12:E:59:ILE:HG13	1.90	0.52
4:A:605:GLN:HB3	4:A:606:PRO:HD3	1.91	0.52
1:T:20:DG:C8	1:T:21:DT:C7	2.92	0.52
4:A:858:MET:HA	4:A:858:MET:HE3	1.92	0.52
10:H:93:MET:HE2	10:H:93:MET:HA	1.91	0.52
4:A:1029:TYR:HD2	13:B:259:ARG:HH22	1.57	0.52
5:C:241:GLU:HB2	5:C:245:LYS:HE2	1.91	0.52
6:F:91:LEU:HG	6:F:100:ILE:HD11	1.92	0.52
13:B:909:LYS:HD3	13:B:1039:HIS:HB2	1.92	0.52
12:E:200:VAL:HG13	12:E:205:LEU:HB2	1.91	0.52
1:T:23:DG:H2'	1:T:24:DC:C6	2.46	0.51
3:P:13:G:H2'	3:P:14:C:H6	1.75	0.51
5:C:17:LEU:HB3	8:K:112:PHE:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:784:ILE:HG22	13:B:942:ILE:HG22	1.92	0.51
2:N:21:DA:H2"	2:N:22:DA:C8	2.45	0.51
4:A:1155:MET:HG3	4:A:1156:THR:HG23	1.91	0.51
4:A:885:ARG:HH11	4:A:886:CYS:HB2	1.75	0.51
13:B:308:VAL:HA	13:B:311:ILE:HG22	1.91	0.51
1:T:6:DC:H2"	1:T:7:DA:C8	2.46	0.51
4:A:441:LEU:C	4:A:442:MET:HE2	2.35	0.51
5:C:71:LEU:HD11	5:C:164:LEU:HD11	1.91	0.51
7:J:38:ILE:HG23	7:J:40:LEU:HD23	1.91	0.51
13:B:961:LEU:O	13:B:965:ILE:HG23	2.10	0.51
1:T:20:DG:C5	1:T:21:DT:C5	2.99	0.51
2:N:29:DG:H2"	2:N:30:DA:C8	2.46	0.51
4:A:900:ARG:HD2	4:A:1048:ILE:HG13	1.93	0.51
10:H:42:HIS:NE2	10:H:122:LEU:HB3	2.26	0.51
5:C:6:TYR:HB3	8:K:52:ARG:HG3	1.92	0.51
13:B:175:LYS:HB2	13:B:201:GLY:HA3	1.93	0.51
1:T:20:DG:N7	1:T:21:DT:C7	2.74	0.51
13:B:17:LEU:HD13	13:B:633:LEU:HD23	1.93	0.51
4:A:414:ARG:HD2	4:A:415:PRO:HD2	1.93	0.50
4:A:938:HIS:HB3	4:A:940:HIS:CE1	2.46	0.50
4:A:797:VAL:HB	4:A:807:GLN:HB3	1.93	0.50
11:I:7:CYS:HB3	11:I:12:ASN:H	1.77	0.50
13:B:330:TYR:O	13:B:333:GLN:HG3	2.11	0.50
4:A:875:ARG:HD3	4:A:1076:VAL:O	2.12	0.50
4:A:940:HIS:CD2	4:A:1002:MET:HE1	2.46	0.50
4:A:980:LYS:HG3	4:A:1010:TYR:HB3	1.93	0.50
13:B:42:LEU:HD11	13:B:757:LEU:HD21	1.92	0.50
4:A:940:HIS:CG	4:A:1002:MET:HE1	2.47	0.50
4:A:553:LEU:HD23	4:A:562:VAL:HG21	1.93	0.50
4:A:885:ARG:HE	12:E:22:LEU:N	2.09	0.50
4:A:947:GLU:HB3	11:I:92:ARG:HD2	1.94	0.50
9:L:41:ARG:HH22	9:L:43:ARG:HD3	1.77	0.50
5:C:285:ILE:HG21	8:K:102:LYS:HB2	1.93	0.49
4:A:522:ARG:HH22	4:A:546:GLN:HG3	1.77	0.49
4:A:751:PRO:HB2	13:B:510:TRP:HH2	1.77	0.49
12:E:85:HIS:HB2	12:E:91:ASN:HD22	1.77	0.49
13:B:45:HIS:CD2	13:B:46:GLN:HG2	2.48	0.49
13:B:277:VAL:HG11	13:B:330:TYR:CD2	2.45	0.49
4:A:323:SER:HA	4:A:457:LEU:O	2.12	0.49
8:K:67:LEU:HD21	13:B:922:TYR:HE1	1.77	0.49
4:A:783:MET:HE1	4:A:830:VAL:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:760:ALA:HA	4:A:763:GLU:HG2	1.95	0.49
10:H:97:LEU:HA	10:H:114:VAL:HG12	1.94	0.49
13:B:120:MET:HE1	13:B:888:ASP:HB2	1.95	0.49
4:A:465:ALA:HA	4:A:468:GLU:OE1	2.12	0.49
4:A:1112:ILE:HG13	4:A:1161:MET:HE1	1.94	0.48
6:F:114:ILE:HG13	6:F:126:TRP:HB3	1.95	0.48
10:H:98:TYR:CZ	10:H:113:TYR:HB3	2.48	0.48
13:B:413:HIS:CD2	13:B:416:ARG:HH12	2.31	0.48
1:T:15:DA:H61	2:N:20:DC:H42	1.60	0.48
4:A:783:MET:HG3	4:A:787:ARG:NH2	2.28	0.48
13:B:1013:ARG:HD2	13:B:1022:MET:HG2	1.95	0.48
7:J:62:TYR:HB3	13:B:729:ASN:HD21	1.79	0.48
4:A:1083:GLN:HE22	4:A:1089:ARG:NH1	2.12	0.48
4:A:527:PRO:HG3	4:A:539:TRP:CH2	2.48	0.48
4:A:586:THR:HA	4:A:589:MET:HG3	1.96	0.48
9:L:11:VAL:HG12	9:L:18:GLU:HG2	1.96	0.48
13:B:779:ASN:HB3	13:B:785:VAL:HG23	1.95	0.48
4:A:442:MET:HE2	4:A:442:MET:N	2.29	0.48
4:A:855:TRP:CZ2	4:A:859:LYS:HE3	2.48	0.48
6:F:65:MET:HG3	6:F:131:LEU:HD13	1.95	0.48
4:A:360:ILE:HD11	4:A:396:PRO:HG3	1.95	0.47
7:J:55:LEU:HD23	7:J:55:LEU:O	2.14	0.47
13:B:499:VAL:HG21	13:B:503:ARG:HG3	1.96	0.47
5:C:71:LEU:HA	5:C:74:ILE:HD12	1.97	0.47
3:P:13:G:C4	3:P:14:C:C5	3.03	0.47
12:E:37:TYR:HB2	12:E:66:PHE:CD2	2.49	0.47
12:E:43:ALA:O	12:E:46:MET:HG3	2.15	0.47
13:B:225:TRP:HB2	13:B:236:ARG:HH12	1.79	0.47
1:T:27:DT:H2"	1:T:28:DA:C8	2.49	0.47
5:C:175:ASP:HA	8:K:10:PHE:CZ	2.50	0.47
11:I:97:MET:HE3	11:I:97:MET:HB2	1.82	0.47
12:E:115:ILE:HG21	12:E:124:LEU:HD22	1.97	0.47
4:A:512:SER:O	4:A:516:LEU:HG	2.14	0.47
4:A:543:GLN:O	4:A:546:GLN:HG2	2.14	0.47
1:T:12:DC:C6	1:T:13:DT:H72	2.50	0.47
5:C:191:PRO:HB3	5:C:239:TYR:HE2	1.80	0.47
13:B:723:ILE:HG22	13:B:741:LEU:HG	1.97	0.47
4:A:506:VAL:HG13	4:A:541:PHE:HE1	1.80	0.46
6:F:112:PHE:HB2	6:F:128:VAL:HG11	1.98	0.46
4:A:675:LEU:HD22	4:A:681:ARG:HB3	1.98	0.46
13:B:68:MET:HE3	13:B:415:ARG:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:459:HIS:HB3	13:B:462:ARG:O	2.15	0.46
13:B:567:LYS:HD2	13:B:581:SER:HA	1.95	0.46
1:T:14:DT:N3	1:T:15:DA:C6	2.83	0.46
4:A:660:GLU:HA	4:A:663:ILE:HG12	1.96	0.46
13:B:412:ALA:HA	13:B:415:ARG:HD3	1.98	0.46
13:B:785:VAL:HB	13:B:941:VAL:HB	1.96	0.46
13:B:850:MET:HE2	13:B:850:MET:HA	1.97	0.46
4:A:329:THR:O	4:A:437:LYS:HA	2.16	0.46
4:A:479:LEU:HD23	4:A:487:LEU:HD22	1.98	0.46
4:A:725:TYR:HB2	4:A:752:TYR:OH	2.15	0.46
4:A:772:LEU:HD11	4:A:845:LEU:HD21	1.97	0.46
13:B:68:MET:HE1	13:B:91:PHE:CE2	2.51	0.46
13:B:603:MET:HE2	13:B:603:MET:HB3	1.86	0.46
13:B:924:GLU:HB3	13:B:929:PHE:CE2	2.51	0.46
2:N:19:DA:C8	2:N:19:DA:H5'	2.50	0.46
4:A:938:HIS:CE1	4:A:1004:CYS:SG	3.05	0.46
5:C:287:LEU:O	5:C:291:LYS:HG2	2.16	0.46
13:B:459:HIS:CG	13:B:462:ARG:HB2	2.51	0.46
13:B:640:LYS:HA	13:B:640:LYS:HD3	1.71	0.46
4:A:938:HIS:HB3	4:A:940:HIS:NE2	2.31	0.46
6:F:87:VAL:HG12	6:F:89:VAL:H	1.81	0.46
8:K:33:PHE:HD1	8:K:73:VAL:HG13	1.81	0.46
12:E:56:LEU:HD23	12:E:57:GLU:HG2	1.97	0.46
4:A:411:PHE:CZ	4:A:458:PHE:HB2	2.51	0.45
4:A:1228:GLU:HB3	6:F:115:ARG:NH2	2.30	0.45
10:H:50:TYR:O	10:H:52:MET:HE2	2.15	0.45
4:A:530:VAL:HB	10:H:92:VAL:HG23	1.98	0.45
6:F:104:GLU:C	6:F:110:ILE:HD11	2.41	0.45
4:A:935:LEU:HD21	4:A:1017:LEU:HD11	1.99	0.45
13:B:125:ARG:HD2	13:B:169:ARG:HH21	1.81	0.45
4:A:915:PHE:HB2	4:A:1029:TYR:OH	2.16	0.45
10:H:42:HIS:CD2	10:H:122:LEU:HB3	2.51	0.45
12:E:64:GLN:O	12:E:68:THR:HG23	2.17	0.45
10:H:93:MET:HB2	10:H:141:LEU:HB3	1.97	0.45
13:B:1040:MET:O	13:B:1044:LYS:HG2	2.17	0.45
4:A:375:TYR:CZ	4:A:400:VAL:HG13	2.52	0.45
4:A:638:ILE:HD11	4:A:701:PHE:CG	2.52	0.45
5:C:62:LEU:HD11	7:J:2:ILE:HD11	1.99	0.45
5:C:157:ARG:HG3	5:C:158:ARG:N	2.32	0.45
9:L:32:CYS:HB3	9:L:34:TYR:HD2	1.82	0.45
6:F:67:LYS:HD2	6:F:67:LYS:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:670:TRP:HB2	13:B:675:LEU:HD22	1.99	0.45
1:T:21:DT:H2'	1:T:22:DC:H6	1.81	0.44
11:I:88:GLN:CG	11:I:97:MET:HE2	2.46	0.44
10:H:106:GLN:HE22	10:H:109:LYS:HG2	1.81	0.44
1:T:28:DA:H2'	1:T:29:DC:O4'	2.18	0.44
4:A:1229:LEU:HD12	6:F:72:ARG:HG2	1.99	0.44
8:K:23:ARG:HG3	8:K:30:ALA:O	2.17	0.44
4:A:356:SER:HA	4:A:396:PRO:HB3	1.98	0.44
13:B:68:MET:O	13:B:69:LEU:HD23	2.18	0.44
13:B:462:ARG:C	13:B:463:LYS:HD2	2.42	0.44
6:F:107:GLN:O	6:F:108:ARG:HG2	2.18	0.44
6:F:137:TRP:CE3	6:F:137:TRP:HA	2.52	0.44
11:I:22:GLN:HB3	11:I:24:ILE:HD11	2.00	0.44
11:I:71:THR:HG21	11:I:74:VAL:HB	1.99	0.44
1:T:14:DT:C4	1:T:15:DA:N6	2.86	0.44
3:P:17:C:H2'	3:P:18:G:H8	1.83	0.44
4:A:377:GLN:HG3	4:A:382:TYR:CE1	2.53	0.44
13:B:532:LEU:HD23	13:B:532:LEU:HA	1.82	0.44
13:B:780:GLN:HA	13:B:943:ASN:ND2	2.32	0.44
13:B:909:LYS:HG2	13:B:1037:LEU:HD12	2.00	0.44
2:N:13:DC:H5''	13:B:240:LYS:HE2	2.00	0.44
4:A:1053:PRO:HD2	4:A:1055:THR:HG22	1.99	0.44
13:B:248:LEU:HD23	13:B:262:LYS:HD3	2.00	0.44
2:N:10:DG:O6	2:N:11:DT:H73	2.17	0.43
4:A:344:GLU:HG2	4:A:345:ILE:N	2.33	0.43
4:A:547:LEU:HD23	4:A:547:LEU:HA	1.86	0.43
4:A:943:LYS:O	4:A:947:GLU:HG2	2.18	0.43
5:C:244:ILE:HD11	5:C:258:ILE:HG22	1.99	0.43
11:I:68:LEU:HD12	11:I:69:PRO:HD2	1.99	0.43
13:B:362:THR:HG23	13:B:560:THR:HB	2.00	0.43
13:B:810:SER:HB3	13:B:890:GLY:C	2.43	0.43
13:B:871:LEU:H	13:B:871:LEU:HD12	1.83	0.43
10:H:30:ILE:O	10:H:42:HIS:HA	2.18	0.43
11:I:81:HIS:CE1	11:I:83:GLU:HB3	2.53	0.43
12:E:137:LEU:HD12	12:E:138:LYS:N	2.32	0.43
13:B:1036:ARG:HH21	13:B:1040:MET:HE2	1.83	0.43
4:A:332:ALA:HB1	4:A:609:MET:HE1	2.01	0.43
4:A:1024:LEU:HG	4:A:1028:ILE:HD12	2.00	0.43
13:B:18:ARG:NH2	13:B:678:GLN:HA	2.34	0.43
13:B:336:LYS:HD2	13:B:336:LYS:HA	1.88	0.43
4:A:643:SER:OG	4:A:644:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1060:ARG:CZ	4:A:1061:SER:H	2.31	0.43
4:A:810:TYR:HE1	4:A:1150:LEU:HD22	1.83	0.43
4:A:352:GLU:HG3	4:A:399:ILE:HG23	2.00	0.43
10:H:90:GLU:H	10:H:90:GLU:HG3	1.64	0.43
12:E:191:PRO:HB2	12:E:227:ARG:HG2	2.01	0.43
13:B:779:ASN:HD22	13:B:941:VAL:HG12	1.83	0.43
4:A:846:ASP:OD1	4:A:848:SER:HB3	2.18	0.43
6:F:83:MET:HE2	6:F:83:MET:O	2.19	0.43
10:H:8:PHE:HB3	10:H:62:MET:HB3	2.00	0.43
10:H:48:GLU:OE2	10:H:49:VAL:HG13	2.18	0.43
12:E:111:VAL:O	12:E:114:GLU:HG3	2.18	0.43
4:A:358:HIS:O	6:F:95:THR:HG23	2.18	0.43
4:A:474:SER:HB3	4:A:477:LYS:HG2	2.01	0.43
4:A:1108:ILE:HD12	4:A:1108:ILE:HA	1.89	0.43
5:C:291:LYS:HB3	5:C:291:LYS:HE2	1.79	0.43
3:P:11:A:H2'	3:P:12:A:C8	2.53	0.43
5:C:204:THR:O	5:C:208:LYS:HG3	2.19	0.43
13:B:781:GLU:CD	13:B:781:GLU:O	2.62	0.43
4:A:913:VAL:HG23	4:A:914:GLU:HG2	1.99	0.42
4:A:1164:PHE:HA	4:A:1169:TYR:CE1	2.54	0.42
1:T:6:DC:C4	1:T:7:DA:N6	2.87	0.42
3:P:13:G:C6	3:P:14:C:C4	3.07	0.42
4:A:706:LEU:HD11	4:A:721:MET:HE2	2.01	0.42
4:A:954:GLN:HE22	4:A:957:LEU:HD23	1.84	0.42
4:A:1118:LEU:HG	4:A:1119:LEU:HG	2.02	0.42
13:B:28:PHE:CD2	13:B:636:LEU:HD11	2.55	0.42
13:B:259:ARG:HD2	13:B:259:ARG:O	2.20	0.42
2:N:22:DA:H2''	2:N:23:DG:H5'	2.00	0.42
5:C:17:LEU:HB3	8:K:112:PHE:HD2	1.84	0.42
7:J:35:LEU:HD23	7:J:35:LEU:HA	1.86	0.42
8:K:51:HIS:CD2	8:K:59:ALA:HB3	2.53	0.42
10:H:92:VAL:O	10:H:93:MET:HE2	2.20	0.42
12:E:45:GLU:OE2	12:E:45:GLU:HA	2.19	0.42
13:B:36:PHE:CD1	13:B:36:PHE:C	2.97	0.42
13:B:1046:LYS:HB3	13:B:1046:LYS:HE2	1.61	0.42
4:A:529:VAL:HB	4:A:538:ALA:HB3	2.02	0.42
4:A:1116:GLN:HB2	4:A:1124:ALA:HB2	2.01	0.42
8:K:14:GLU:HG3	8:K:15:GLY:H	1.85	0.42
10:H:107:THR:N	10:H:108:PRO:HD2	2.35	0.42
4:A:549:PHE:HE2	4:A:567:LEU:HG	1.83	0.42
4:A:335:ASN:HB2	4:A:338:GLU:CD	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:585:VAL:O	4:A:589:MET:HG3	2.20	0.42
6:F:67:LYS:NZ	6:F:70:ARG:HH22	2.18	0.42
4:A:592:LYS:HB3	4:A:596:GLU:HG3	2.02	0.42
4:A:649:LEU:HD11	4:A:656:GLU:HB3	2.02	0.42
4:A:916:LEU:HD23	4:A:991:PHE:CD2	2.54	0.42
4:A:920:ARG:HB2	4:A:936:HIS:NE2	2.35	0.42
13:B:317:VAL:HG23	13:B:318:CYS:SG	2.60	0.42
1:T:13:DT:H5'	1:T:13:DT:C6	2.55	0.42
13:B:675:LEU:HA	13:B:678:GLN:HG2	2.02	0.42
4:A:449:ASP:HB2	13:B:781:GLU:OE1	2.20	0.41
13:B:288:LYS:HB2	13:B:288:LYS:HE2	1.75	0.41
13:B:636:LEU:HD23	13:B:636:LEU:HA	1.87	0.41
4:A:809:LYS:HB3	4:A:809:LYS:HE2	1.93	0.41
10:H:45:VAL:HG13	10:H:52:MET:HE1	2.02	0.41
8:K:36:GLU:HA	8:K:70:LYS:HG3	2.01	0.41
1:T:21:DT:C2	1:T:22:DC:C5	3.08	0.41
4:A:589:MET:C	6:F:137:TRP:HB3	2.45	0.41
13:B:480:LEU:O	13:B:484:ILE:HG23	2.20	0.41
13:B:947:PHE:N	13:B:948:PRO:HD2	2.36	0.41
4:A:555:CYS:H	4:A:562:VAL:HG13	1.85	0.41
5:C:82:MET:HE2	5:C:283:ASN:OD1	2.21	0.41
12:E:52:TYR:N	12:E:52:TYR:CD1	2.88	0.41
13:B:294:ILE:HG23	13:B:372:VAL:HG23	2.01	0.41
2:N:10:DG:N2	2:N:12:DG:H5'	2.36	0.41
5:C:239:TYR:HE1	5:C:260:PRO:HG3	1.86	0.41
9:L:43:ARG:HD3	9:L:43:ARG:HA	1.90	0.41
12:E:84:HIS:HA	12:E:92:LYS:HA	2.02	0.41
13:B:125:ARG:HH12	13:B:127:LYS:HE2	1.86	0.41
13:B:570:VAL:HG22	13:B:578:GLY:O	2.20	0.41
4:A:980:LYS:HG3	4:A:980:LYS:O	2.20	0.41
10:H:112:MET:O	10:H:122:LEU:HD12	2.20	0.41
13:B:510:TRP:HZ2	13:B:670:TRP:HZ3	1.68	0.41
2:N:18:DC:H4'	2:N:19:DA:OP1	2.21	0.41
13:B:668:THR:HG23	13:B:684:HIS:HB2	2.03	0.41
2:N:12:DG:C8	2:N:13:DC:C4	3.09	0.41
4:A:340:GLY:O	4:A:341:ILE:HD13	2.20	0.41
4:A:340:GLY:C	4:A:341:ILE:HD13	2.46	0.41
4:A:577:LEU:O	4:A:581:ILE:HG12	2.21	0.41
4:A:792:THR:HG23	4:A:794:ASP:OD1	2.20	0.41
4:A:1048:ILE:HB	11:I:69:PRO:HG3	2.03	0.41
5:C:200:MET:SD	5:C:255:LEU:HD11	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:82:LYS:HZ1	10:H:85:LEU:N	2.19	0.41
13:B:331:VAL:O	13:B:335:ILE:HG23	2.21	0.41
13:B:771:ALA:HB2	13:B:1029:MET:HE3	2.03	0.41
13:B:795:MET:HG2	13:B:796:PHE:CD2	2.56	0.41
13:B:965:ILE:HG21	13:B:984:ARG:HB3	2.03	0.41
4:A:784:ALA:HA	4:A:787:ARG:HH21	1.86	0.41
4:A:798:ARG:HG2	4:A:805:ILE:HG12	2.03	0.41
4:A:919:TYR:CG	11:I:25:LEU:HD13	2.55	0.41
13:B:101:LEU:HB3	13:B:108:LEU:HB2	2.02	0.41
4:A:662:SER:O	4:A:666:VAL:HG22	2.21	0.40
10:H:145:LYS:HD3	10:H:145:LYS:HA	1.77	0.40
4:A:544:ILE:HG22	4:A:607:LEU:HD11	2.03	0.40
4:A:582:ASN:HA	4:A:585:VAL:HG12	2.03	0.40
4:A:657:LEU:O	4:A:660:GLU:HG3	2.21	0.40
4:A:659:LEU:HD23	4:A:659:LEU:HA	1.96	0.40
4:A:708:ASP:HB3	4:A:718:VAL:HG21	2.02	0.40
4:A:1227:PHE:CE1	6:F:114:ILE:HB	2.56	0.40
5:C:176:HIS:CD2	9:L:51:ARG:HG3	2.56	0.40
12:E:37:TYR:HB2	12:E:66:PHE:CE2	2.57	0.40
12:E:102:LYS:HA	12:E:130:ASN:HD21	1.85	0.40
2:N:8:DA:H4'	2:N:9:DA:OP1	2.20	0.40
3:P:14:C:H2'	3:P:15:G:H8	1.87	0.40
4:A:631:MET:HE3	4:A:631:MET:HA	2.03	0.40
13:B:18:ARG:HH22	13:B:678:GLN:HA	1.87	0.40
2:N:17:DG:N1	13:B:461:PHE:CE2	2.90	0.40
10:H:40:PHE:O	10:H:123:LEU:HD12	2.22	0.40
13:B:710:ARG:NH2	13:B:950:ARG:HG2	2.36	0.40
4:A:405:MET:C	4:A:405:MET:HE2	2.47	0.40
4:A:836:MET:O	4:A:839:PRO:HD2	2.21	0.40
10:H:14:VAL:HG12	10:H:56:ASP:H	1.87	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	
4	A	837/2032 (41%)	798 (95%)	39 (5%)	0	100	100
5	C	283/319 (89%)	276 (98%)	7 (2%)	0	100	100
6	F	78/144 (54%)	71 (91%)	7 (9%)	0	100	100
7	J	61/71 (86%)	60 (98%)	1 (2%)	0	100	100
8	K	106/116 (91%)	102 (96%)	4 (4%)	0	100	100
9	L	43/51 (84%)	40 (93%)	3 (7%)	0	100	100
10	H	139/146 (95%)	124 (89%)	15 (11%)	0	100	100
11	I	93/114 (82%)	88 (95%)	5 (5%)	0	100	100
12	E	207/230 (90%)	198 (96%)	9 (4%)	0	100	100
13	B	952/1169 (81%)	921 (97%)	31 (3%)	0	100	100
All	All	2799/4392 (64%)	2678 (96%)	121 (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	
4	A	750/1709 (44%)	744 (99%)	6 (1%)	73	77
5	C	253/276 (92%)	251 (99%)	2 (1%)	73	77
6	F	72/128 (56%)	71 (99%)	1 (1%)	59	72
7	J	56/63 (89%)	56 (100%)	0	100	100
8	K	98/105 (93%)	98 (100%)	0	100	100
9	L	40/46 (87%)	40 (100%)	0	100	100
10	H	123/127 (97%)	121 (98%)	2 (2%)	55	71
11	I	85/101 (84%)	85 (100%)	0	100	100
12	E	190/209 (91%)	186 (98%)	4 (2%)	47	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	B	845/1026 (82%)	839 (99%)	6 (1%)	76	78
All	All	2512/3790 (66%)	2491 (99%)	21 (1%)	70	77

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	468	GLU
4	A	472	LEU
4	A	590	VAL
4	A	789	ILE
4	A	848	SER
4	A	1102	ILE
5	C	164	LEU
5	C	231	VAL
6	F	123	PHE
10	H	52	MET
10	H	132	HIS
12	E	46	MET
12	E	52	TYR
12	E	125	ILE
12	E	127	VAL
13	B	62	PHE
13	B	225	TRP
13	B	245	ILE
13	B	312	GLN
13	B	636	LEU
13	B	913	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	419	HIS
4	A	486	GLN
4	A	582	ASN
4	A	940	HIS
4	A	965	ASN
4	A	1047	ASN
4	A	1083	GLN
4	A	1100	HIS
4	A	1114	GLN
8	K	51	HIS

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Mol	Chain	Res	Type
8	K	89	GLN
10	H	94	HIS
11	I	81	HIS
12	E	91	ASN
12	E	182	GLN
13	B	334	GLN
13	B	473	ASN
13	B	481	GLN
13	B	634	HIS
13	B	678	GLN
13	B	720	GLN
13	B	745	GLN
13	B	766	GLN
13	B	767	ASN
13	B	773	ASN
13	B	824	GLN
13	B	849	ASN
13	B	873	HIS
13	B	926	GLN
13	B	951	GLN
13	B	1000	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	P	10/20 (50%)	3 (30%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	P	11	A
3	P	13	G
3	P	14	C

There are no RNA pucker outliers to report.

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

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](#)

Of 7 ligands modelled in this entry, 7 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 [i](#)

There are no chain breaks in this entry.

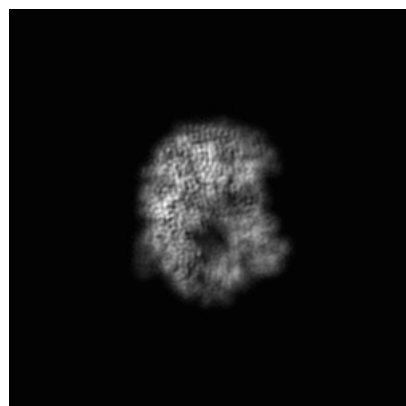
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61962. These allow visual inspection of the internal detail of the map and identification of artifacts.

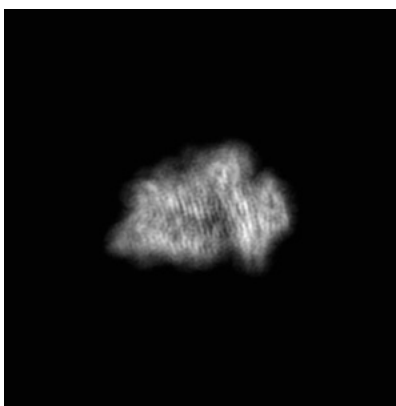
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

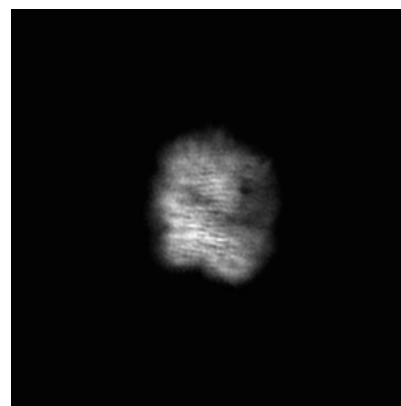
#### 6.1.1 Primary map



X

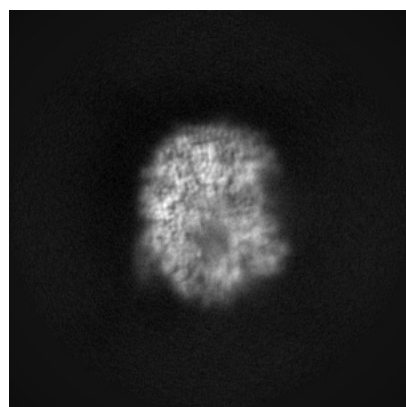


Y

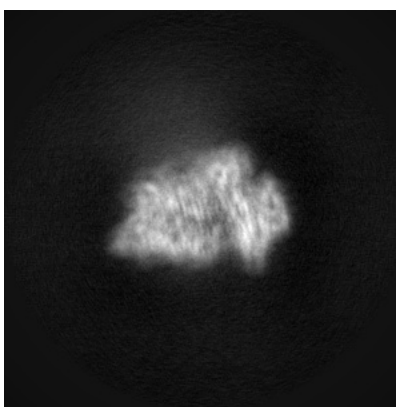


Z

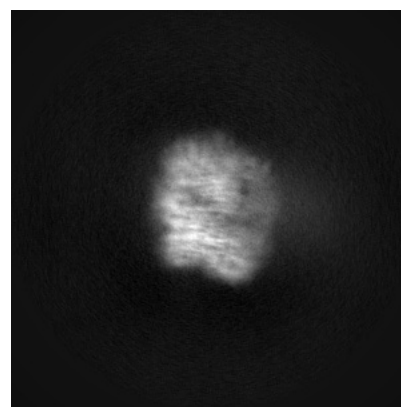
#### 6.1.2 Raw map



X



Y

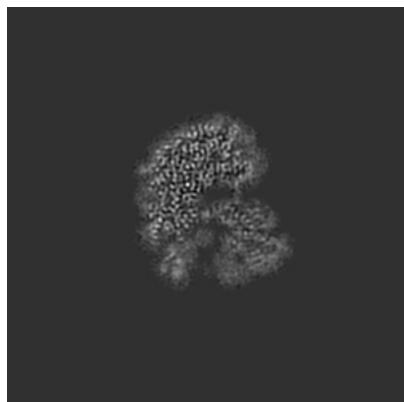


Z

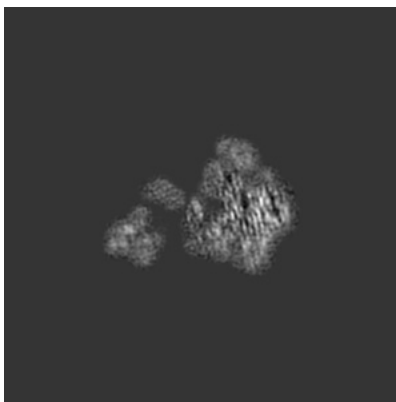
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

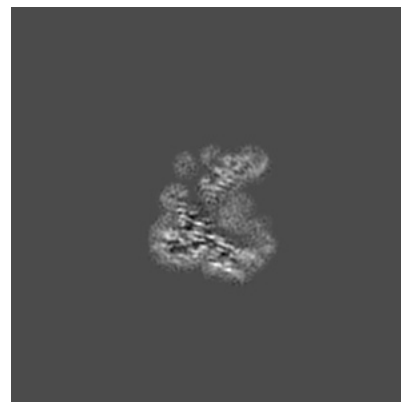
### 6.2.1 Primary map



X Index: 150

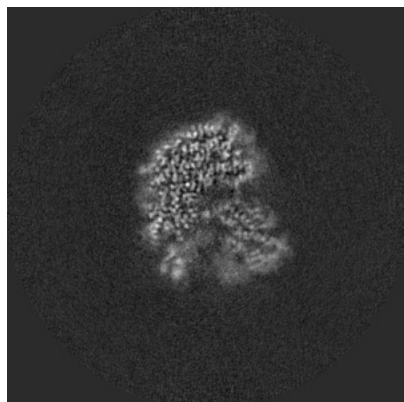


Y Index: 150

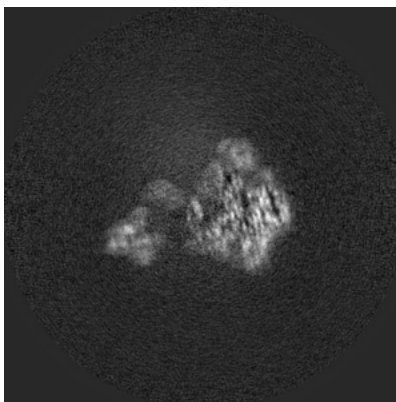


Z Index: 150

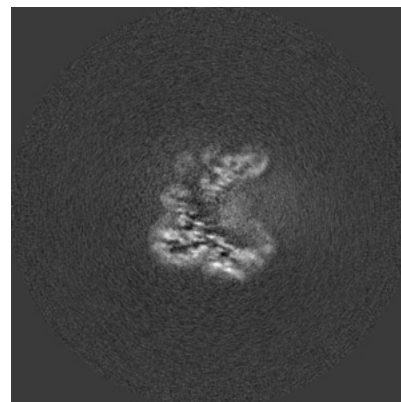
### 6.2.2 Raw map



X Index: 150



Y Index: 150

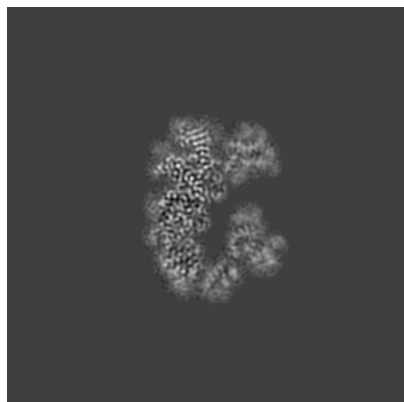


Z Index: 150

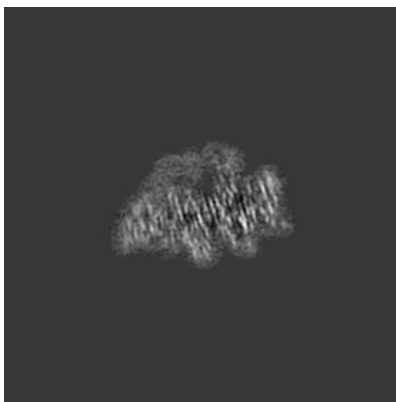
The images above show central slices of the map in three orthogonal directions.

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

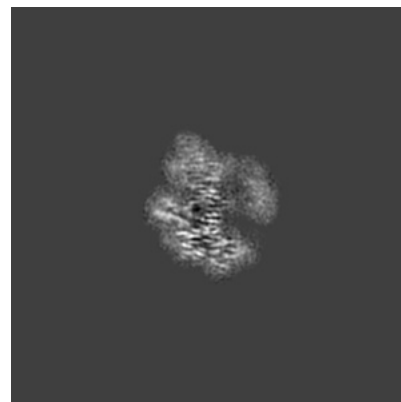
### 6.3.1 Primary map



X Index: 135

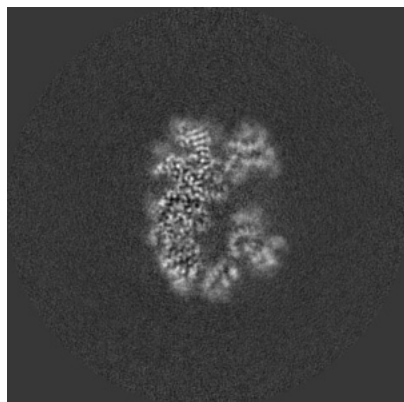


Y Index: 128

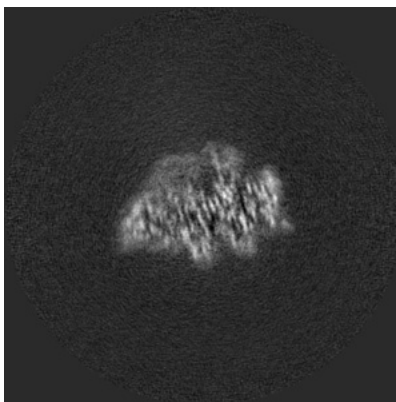


Z Index: 181

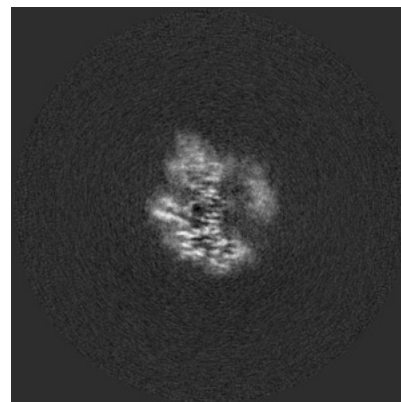
### 6.3.2 Raw map



X Index: 135



Y Index: 127



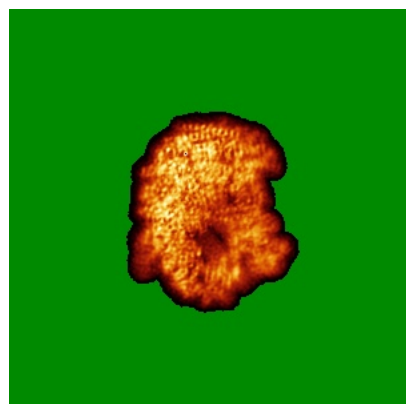
Z Index: 181

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

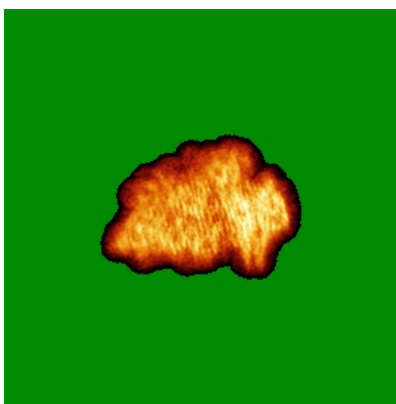


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

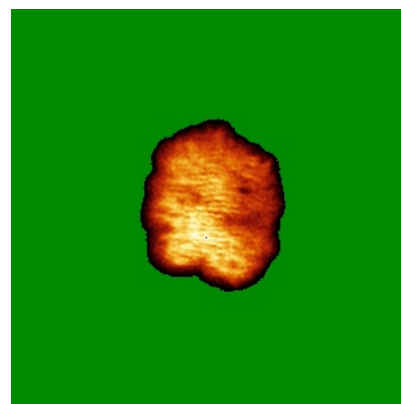
### 6.4.1 Primary map



X

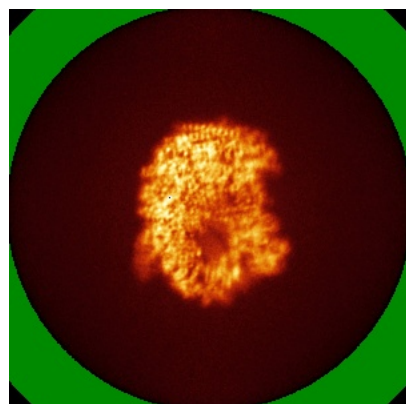


Y

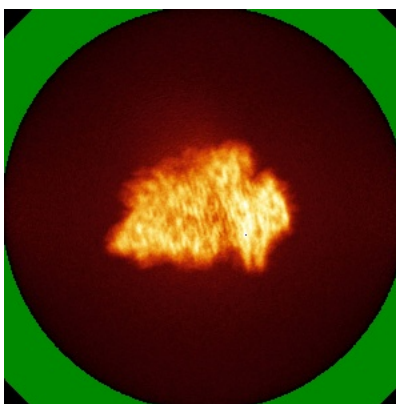


Z

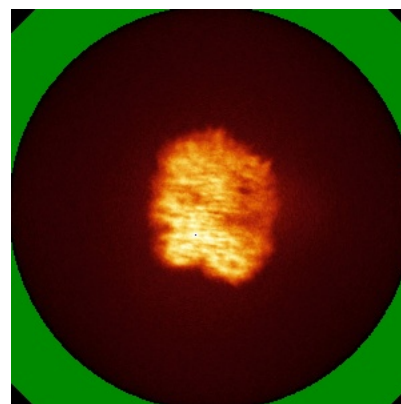
### 6.4.2 Raw map



X



Y

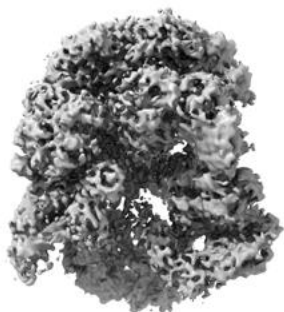


Z

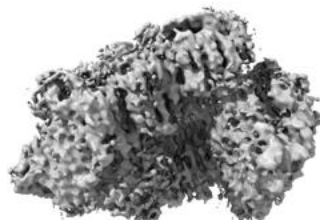
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

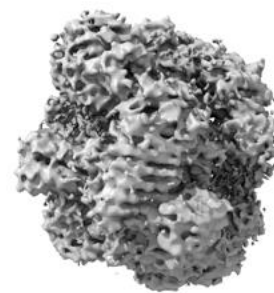
### 6.5.1 Primary map



X



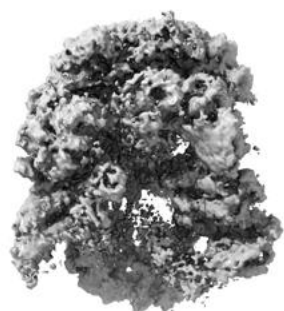
Y



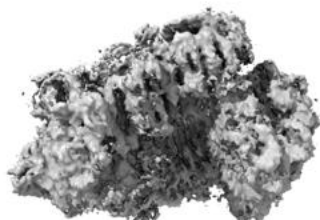
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0118. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

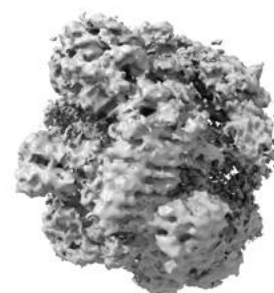
### 6.5.2 Raw map



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.

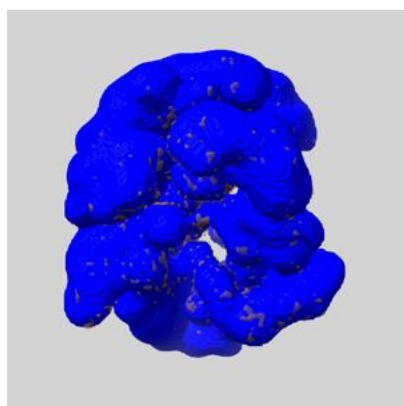
## 6.6 Mask visualisation [i](#)

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

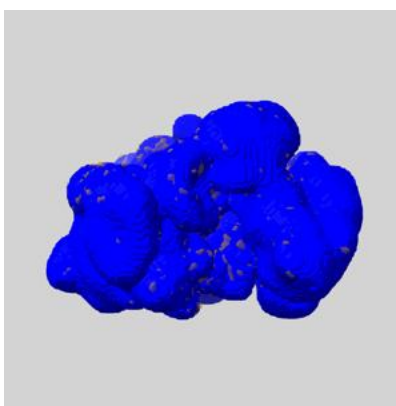
A mask typically either:

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

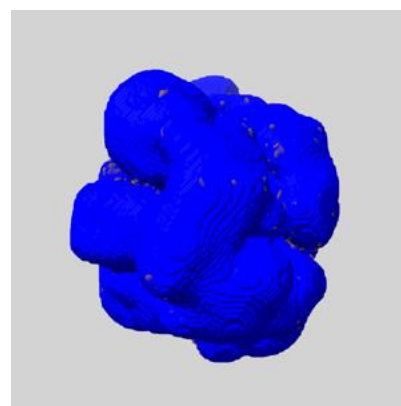
### 6.6.1 emd\_61962\_msk\_1.map [i](#)



X



Y

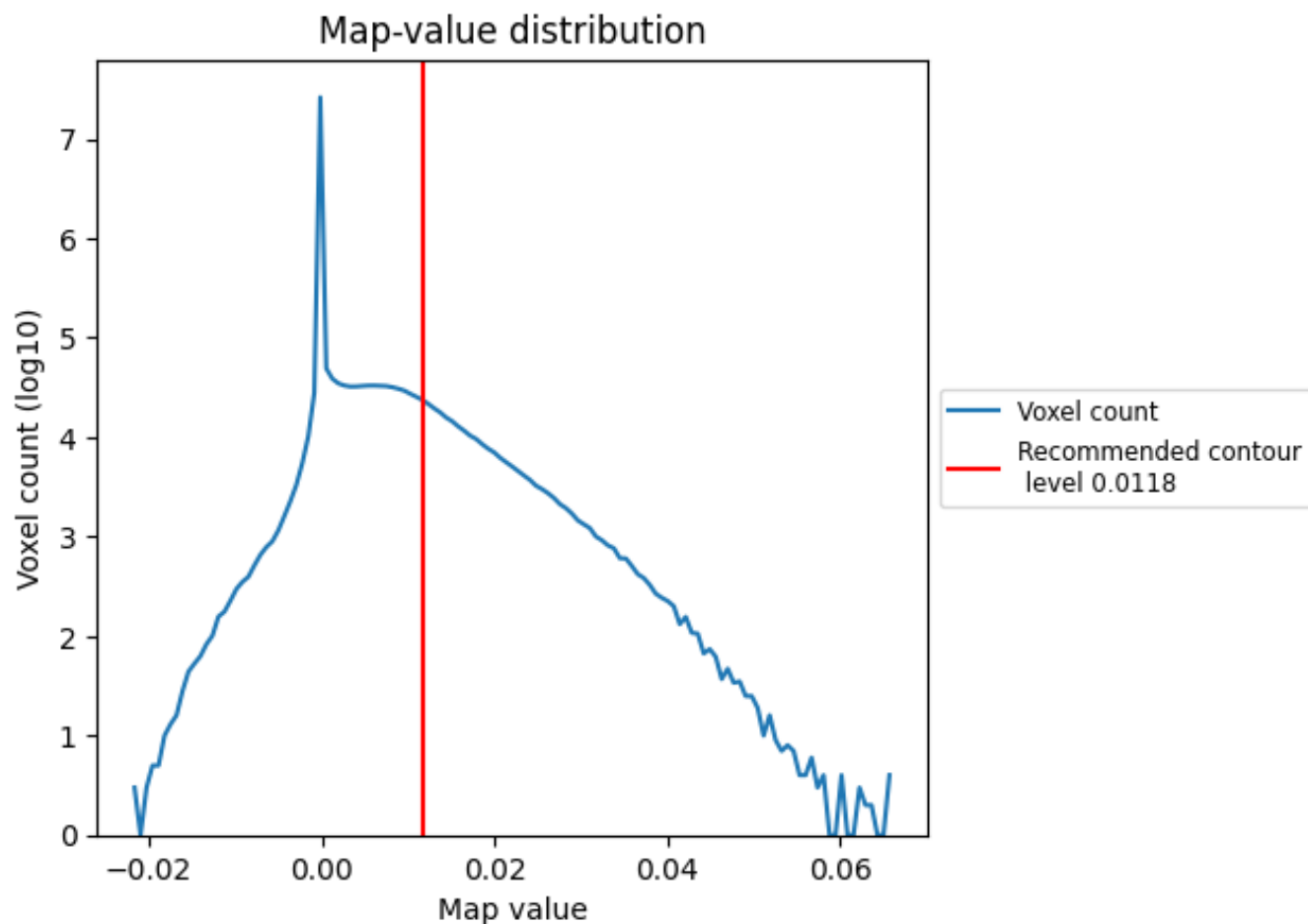


Z

## 7 Map analysis [i](#)

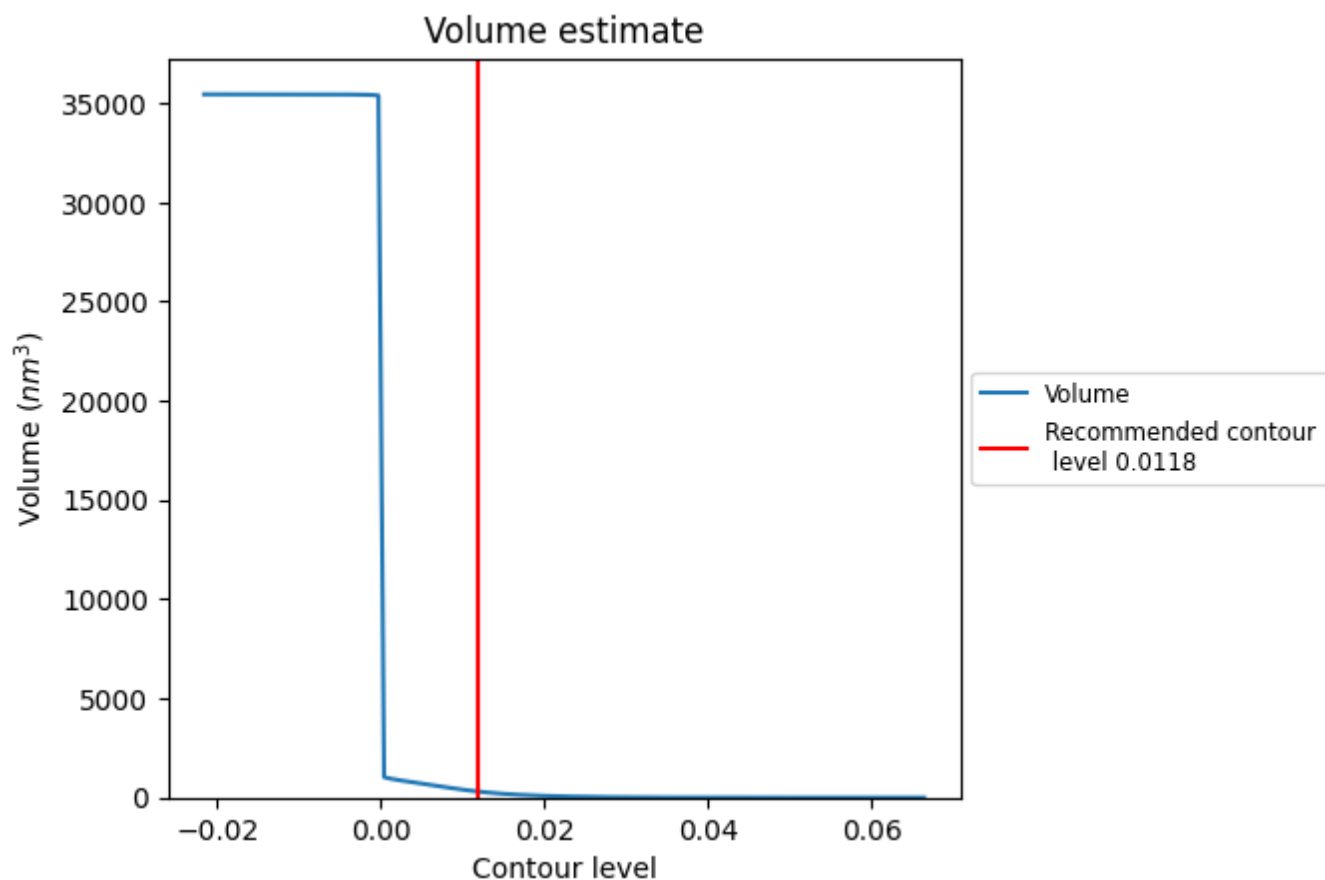
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

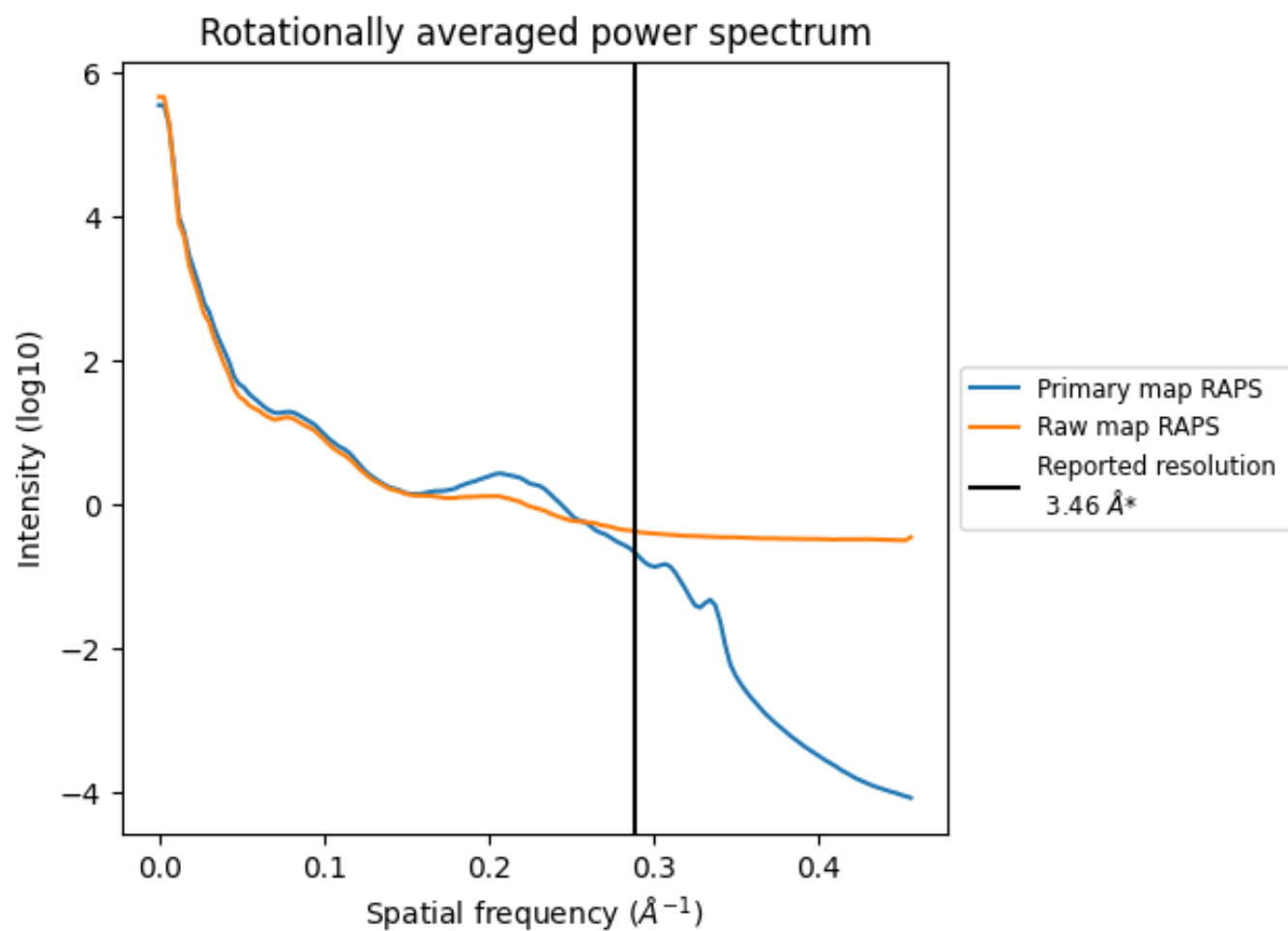
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 308  $\text{nm}^3$ ; this corresponds to an approximate mass of 278 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 ⓘ

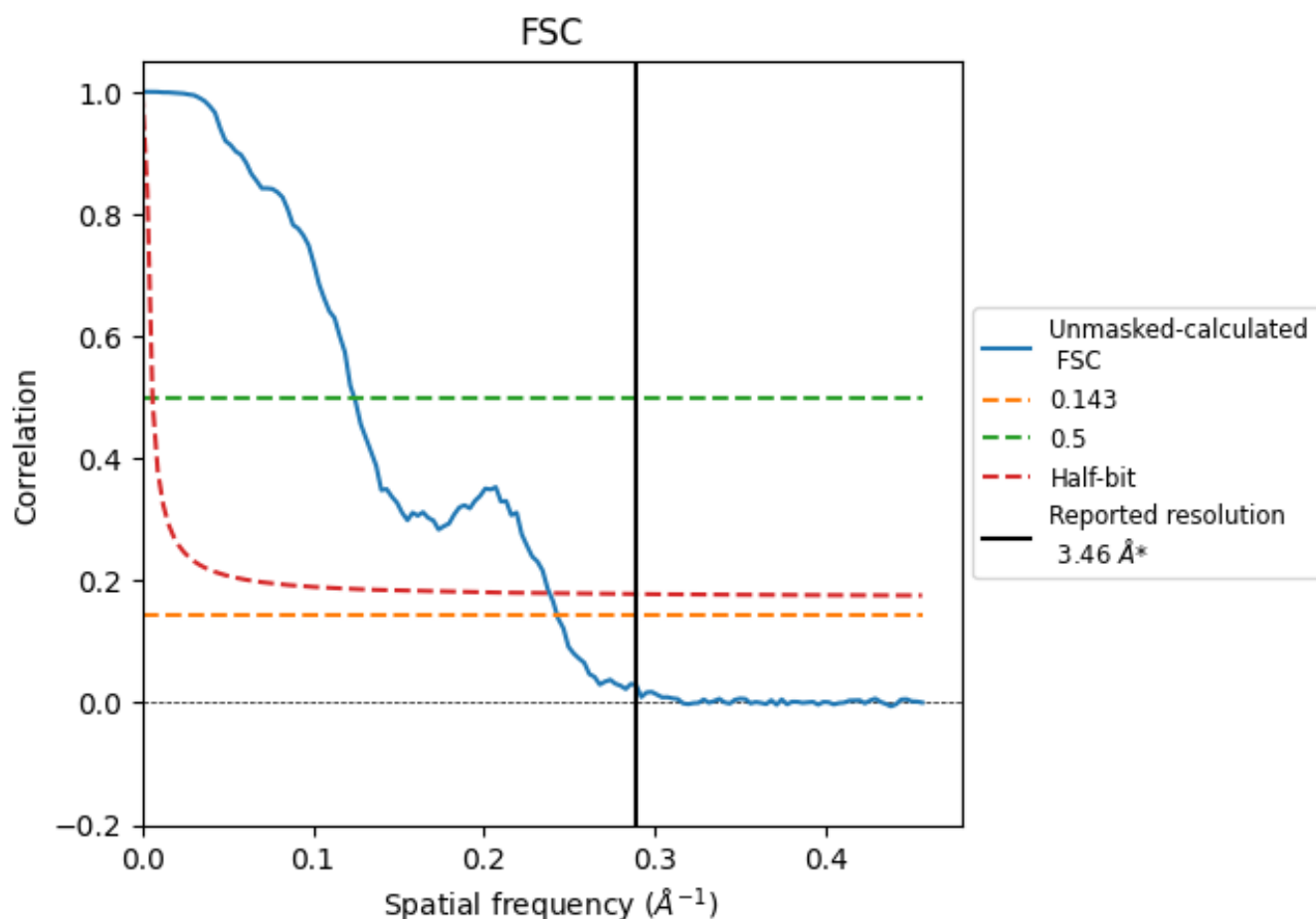


\*Reported resolution corresponds to spatial frequency of 0.289 Å<sup>-1</sup>

## 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 0.289  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.46	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.12	8.06	4.19

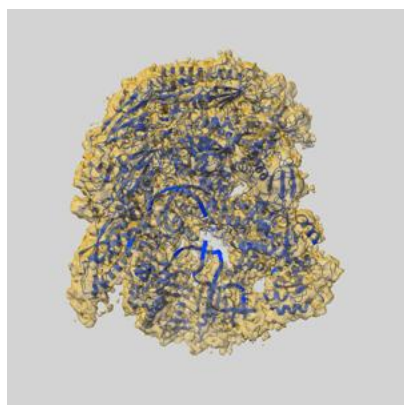
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.12 differs from the reported value 3.46 by more than 10 %



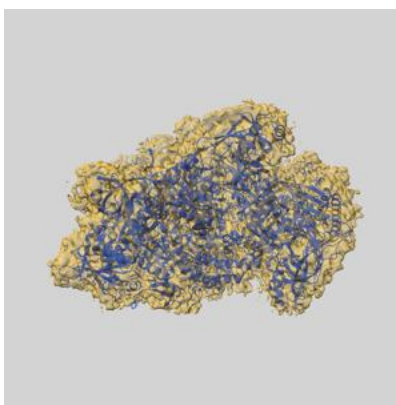
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61962 and PDB model 9K12. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

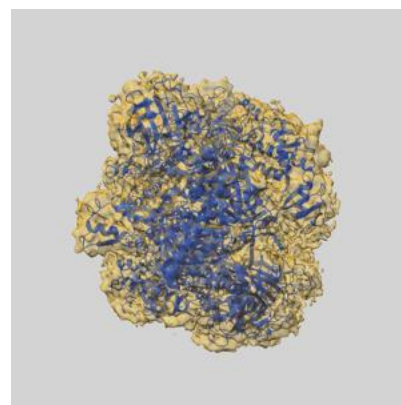
### 9.1 Map-model overlay [i](#)



X



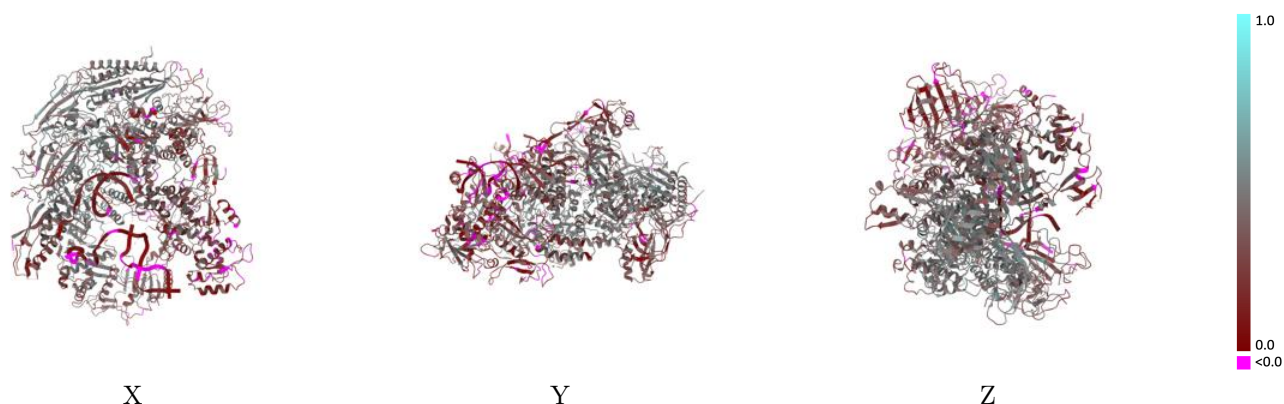
Y



Z

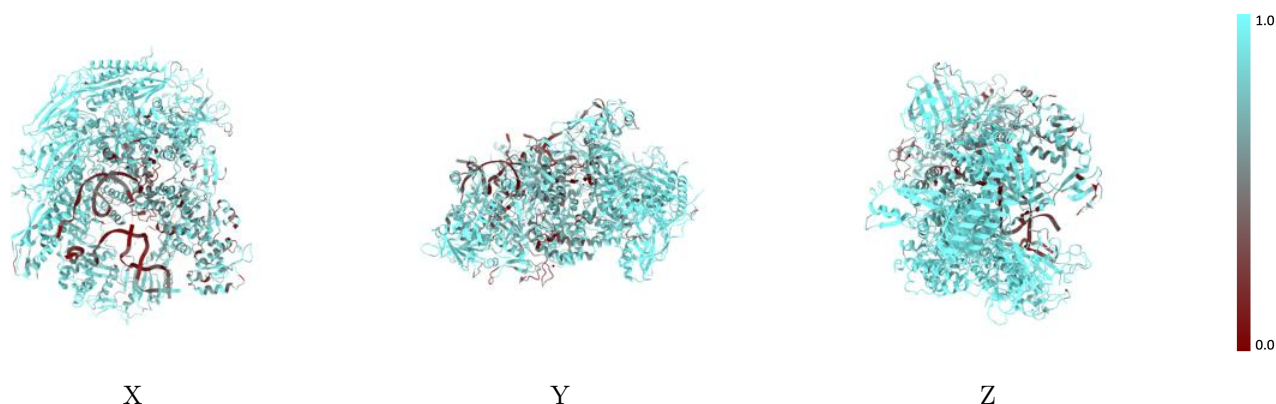
The images above show the 3D surface view of the map at the recommended contour level 0.0118 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



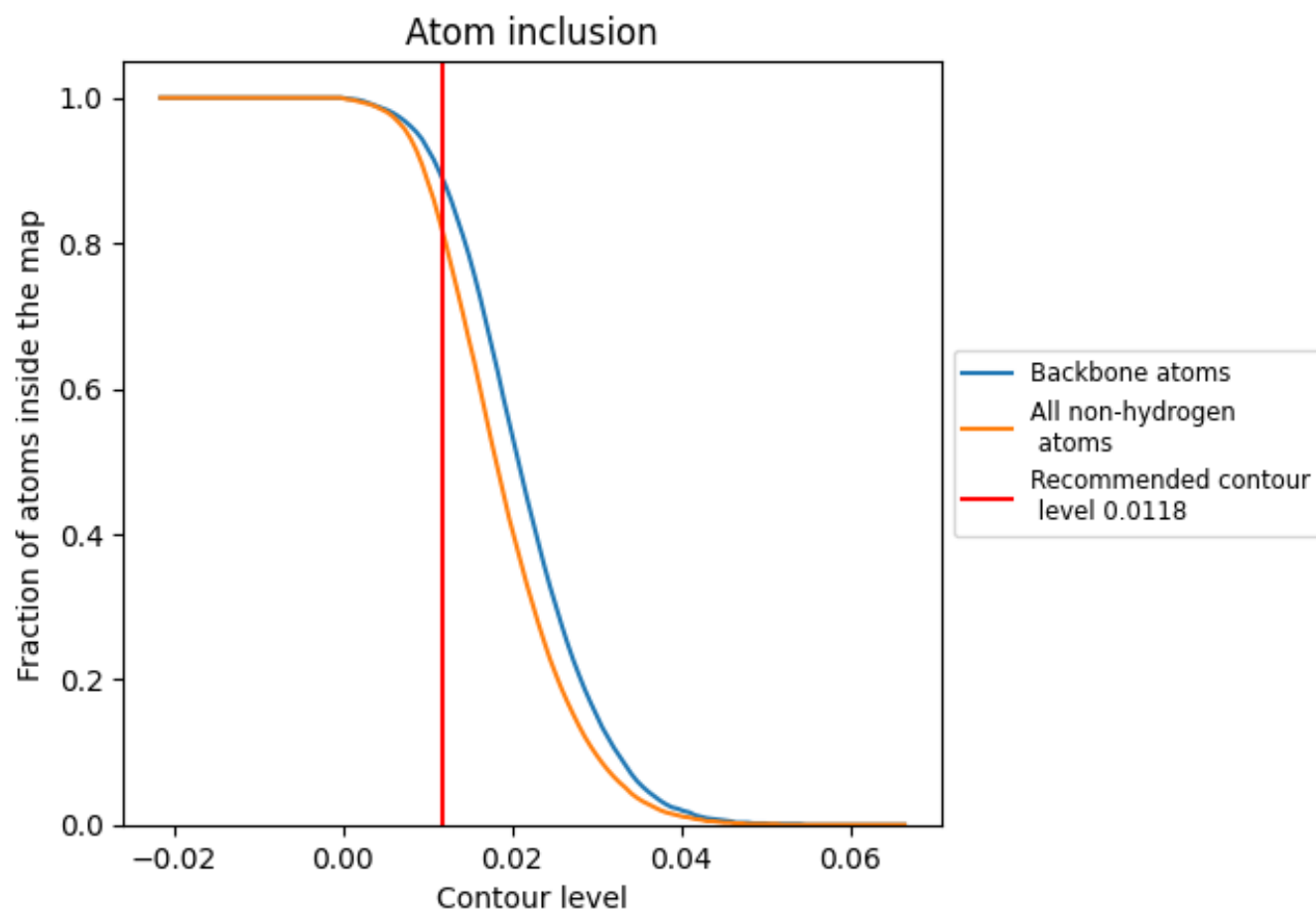
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0118).





























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 81% 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 (0.0118) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8140	 0.3440
A	 0.7590	 0.3200
B	 0.9110	 0.4220
C	 0.9600	 0.4360
E	 0.7160	 0.1940
F	 0.7610	 0.2970
H	 0.8560	 0.2550
I	 0.6700	 0.2350
J	 0.9820	 0.4770
K	 0.9480	 0.4350
L	 0.9200	 0.3700
N	 0.3110	 0.0570
P	 0.2950	 0.0900
T	 0.2020	 0.0750

