



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 11:45 AM UTC

PDB ID : 7B7U / pdb_00007b7u
EMDB ID : EMD-12087
Title : Cryo-EM structure of mammalian RNA polymerase II in complex with human RPAP2
Authors : Fianu, I.; Dienemann, C.; Aibara, S.; Schilbach, S.; Cramer, P.
Deposited on : 2020-12-11
Resolution : 2.80 Å(reported)
Based on initial model : 5FLM

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.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

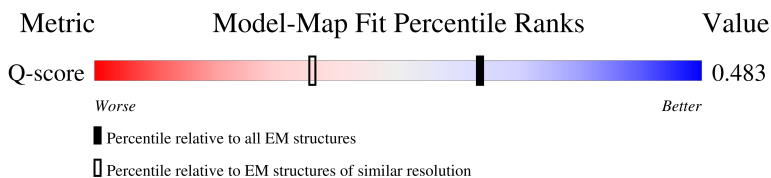
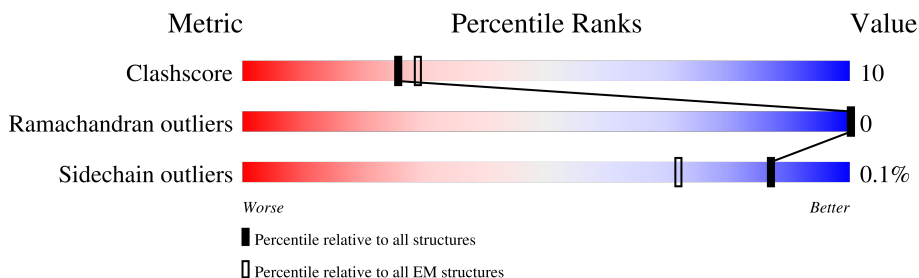
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	-
Q-score	-	25397	11806 (2.30 - 3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1970	 6% 37% 13% 50%
2	B	1174	 6% 62% 21% 17%
3	C	271	 6% 68% 26% 5%
4	E	210	 81% 19%

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Mol	Chain	Length	Quality of chain
5	F	127	
6	H	150	
7	I	125	
8	J	67	
9	K	117	
10	L	58	
11	M	612	
12	N	30	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 25091 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	986	Total	C	N	O	S	0	0
			7861	4957	1388	1478	38		

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	487	SER	-	insertion	UNP I3LJR4
A	488	VAL	ARG	conflict	UNP I3LJR4
A	489	THR	SER	conflict	UNP I3LJR4
A	490	THR	VAL	conflict	UNP I3LJR4
A	491	PRO	HIS	conflict	UNP I3LJR4
A	492	TYR	TRP	conflict	UNP I3LJR4
A	493	ASN	LEU	conflict	UNP I3LJR4
A	494	ALA	ARG	conflict	UNP I3LJR4
A	495	ASP	GLU	conflict	UNP I3LJR4
A	496	PHE	ALA	conflict	UNP I3LJR4
A	497	ASP	ALA	conflict	UNP I3LJR4
A	499	ASP	-	insertion	UNP I3LJR4
A	500	GLU	-	insertion	UNP I3LJR4
A	501	MET	ALA	conflict	UNP I3LJR4
A	502	ASN	GLY	conflict	UNP I3LJR4
A	504	HIS	-	insertion	UNP I3LJR4
A	507	GLN	-	insertion	UNP I3LJR4
A	508	SER	-	insertion	UNP I3LJR4
A	509	LEU	GLY	conflict	UNP I3LJR4
A	510	GLU	ASP	conflict	UNP I3LJR4
A	512	ARG	-	insertion	UNP I3LJR4
A	513	ALA	-	insertion	UNP I3LJR4
A	514	GLU	-	insertion	UNP I3LJR4
A	515	ILE	-	insertion	UNP I3LJR4
A	516	GLN	-	insertion	UNP I3LJR4
A	517	GLU	-	insertion	UNP I3LJR4
A	518	LEU	-	insertion	UNP I3LJR4
A	519	ALA	-	insertion	UNP I3LJR4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	520	MET	-	insertion	UNP I3LJR4
A	521	VAL	-	insertion	UNP I3LJR4
A	522	PRO	-	insertion	UNP I3LJR4
A	523	ARG	-	insertion	UNP I3LJR4
A	524	MET	-	insertion	UNP I3LJR4
A	525	ILE	GLY	conflict	UNP I3LJR4
A	526	VAL	GLY	conflict	UNP I3LJR4
A	527	THR	ASP	conflict	UNP I3LJR4
A	529	GLN	GLY	conflict	UNP I3LJR4
A	1301	ILE	-	insertion	UNP I3LJR4
A	1302	GLU	-	insertion	UNP I3LJR4
A	1303	GLN	-	insertion	UNP I3LJR4
A	1304	ILE	-	insertion	UNP I3LJR4
A	1306	LYS	-	insertion	UNP I3LJR4
A	1307	VAL	-	insertion	UNP I3LJR4
A	1308	TYR	-	insertion	UNP I3LJR4
A	1309	MET	-	insertion	UNP I3LJR4
A	1310	HIS	-	insertion	UNP I3LJR4
A	1311	LEU	SER	conflict	UNP I3LJR4
A	1312	PRO	ARG	conflict	UNP I3LJR4
A	1313	GLN	SER	conflict	UNP I3LJR4

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	979	Total	C	N	O	S	0	0
			7842	4990	1350	1454	48		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	257	Total	C	N	O	S	0	0
			2059	1294	351	408	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	78	Total	C	N	O	S	0	0
			626	401	106	114	5		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	148	Total	C	N	O	S	0	0
			1184	748	194	237	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	115	Total	C	N	O	S	0	0
			938	580	167	180	11		

- Molecule 8 is a protein called Uncharacterized Protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 9 is a protein called RNA_pol_L_2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 10 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 11 is a protein called Putative RNA polymerase II subunit B1 CTD phosphatase RPAP2.

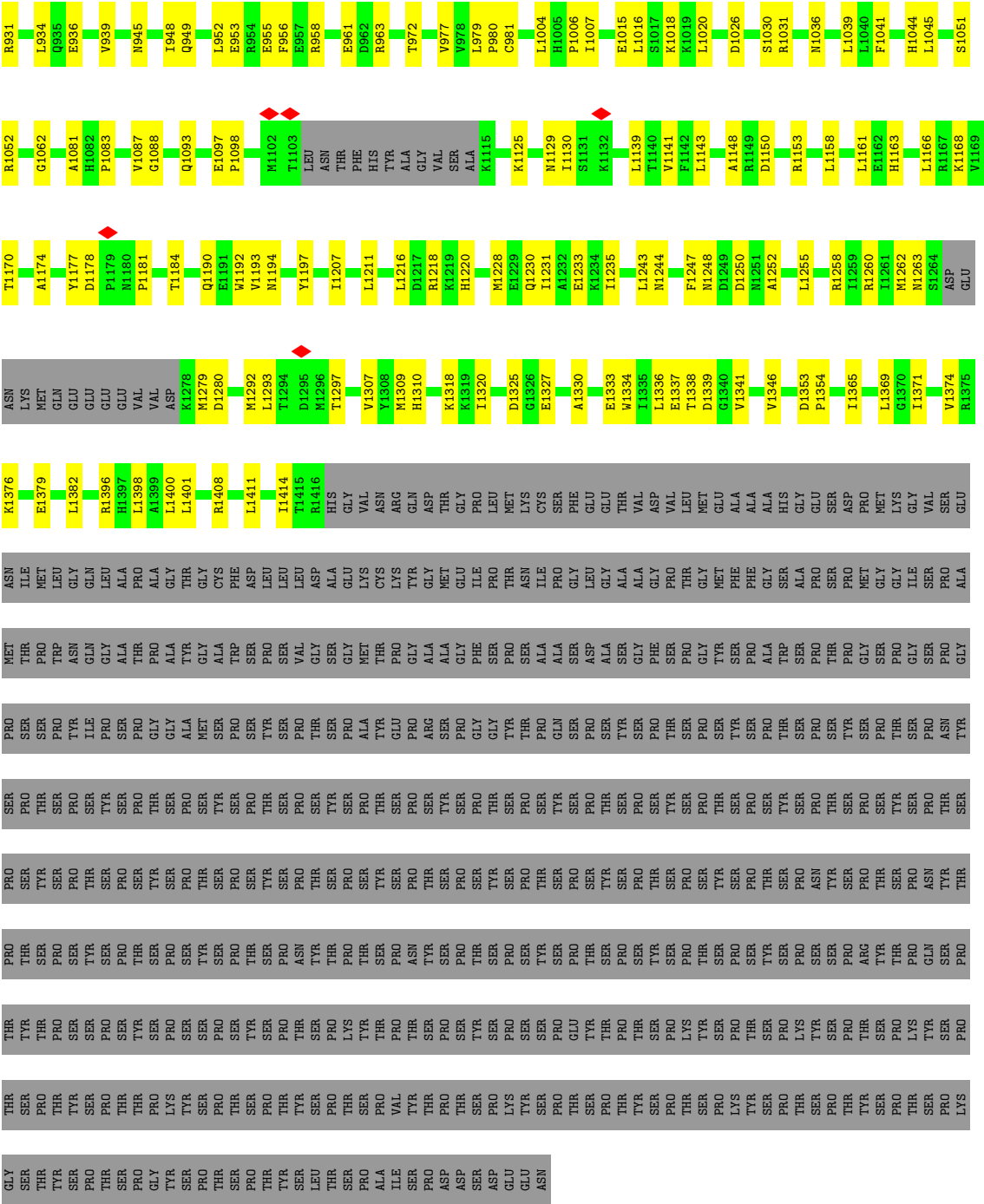
Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	108	Total	C	N	O	S	0	0
			880	566	148	160	6		

- Molecule 12 is a protein called Unknown.

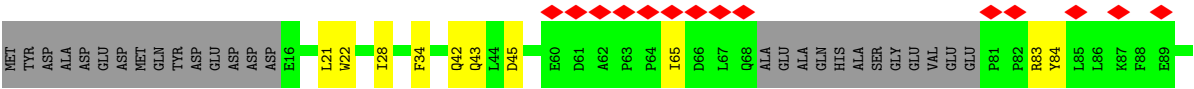
Mol	Chain	Residues	Atoms				AltConf	Trace
12	N	30	Total	C	N	O	0	0
			150	90	30	30		

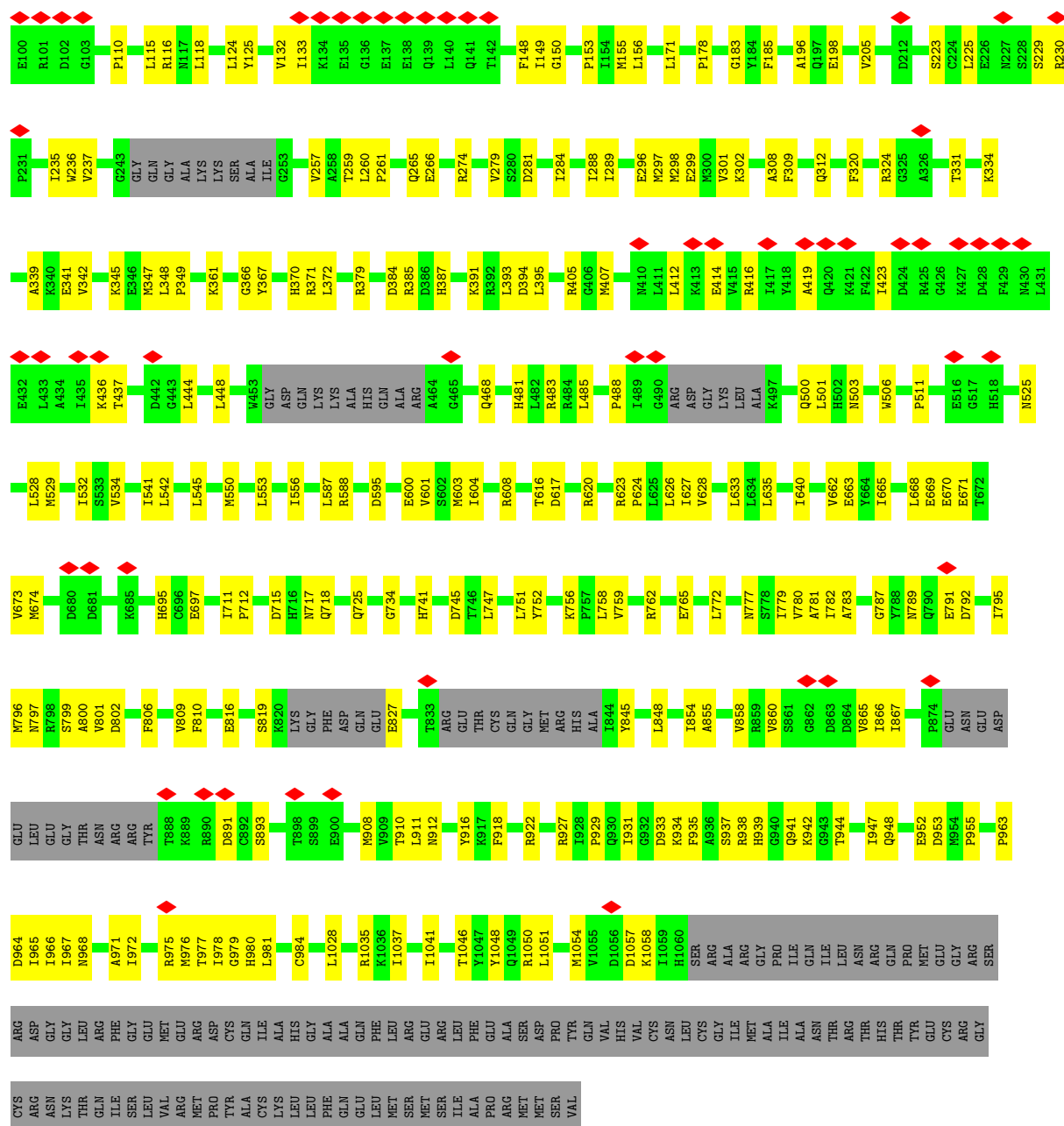
- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
13	C	1	Total	Zn	0
			1	1	
13	I	2	Total	Zn	0
			2	2	
13	J	1	Total	Zn	0
			1	1	
13	L	1	Total	Zn	0
			1	1	
13	M	1	Total	Zn	0
			1	1	



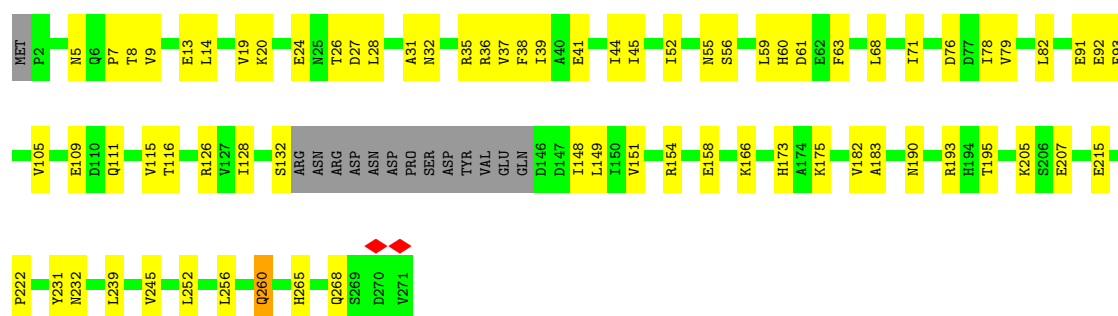
● Molecule 2: DNA-directed RNA polymerase subunit beta



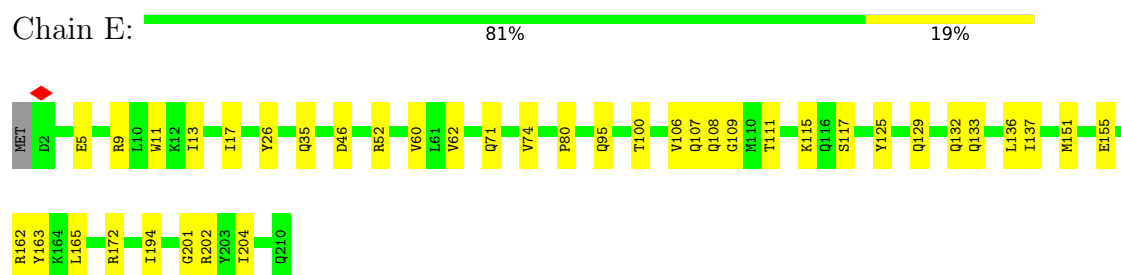


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

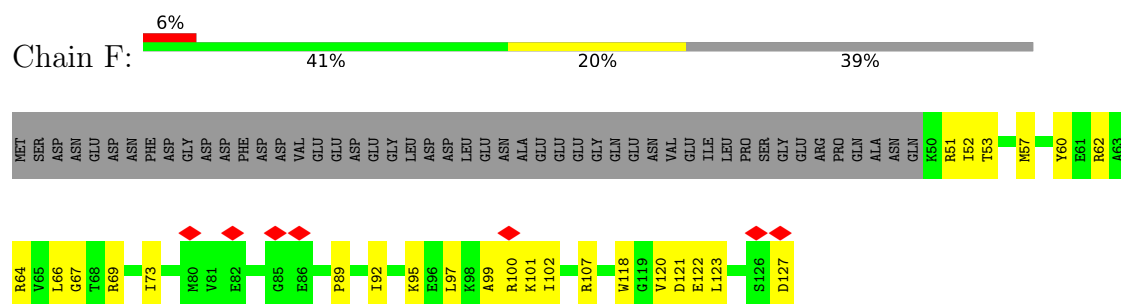
Chain C: 68% 26% 5%



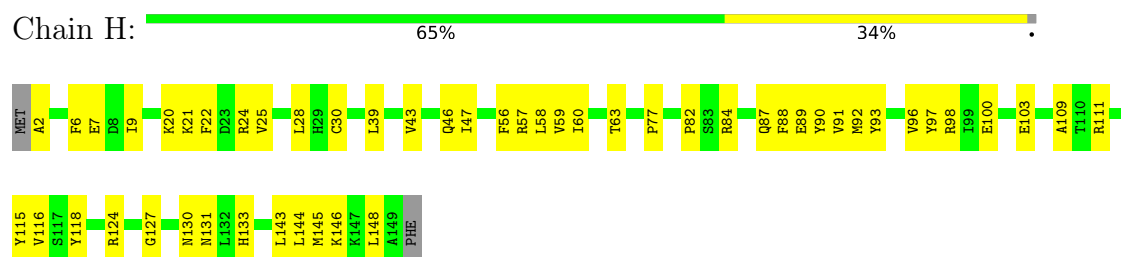
- Molecule 4: DNA-directed RNA polymerase II subunit E



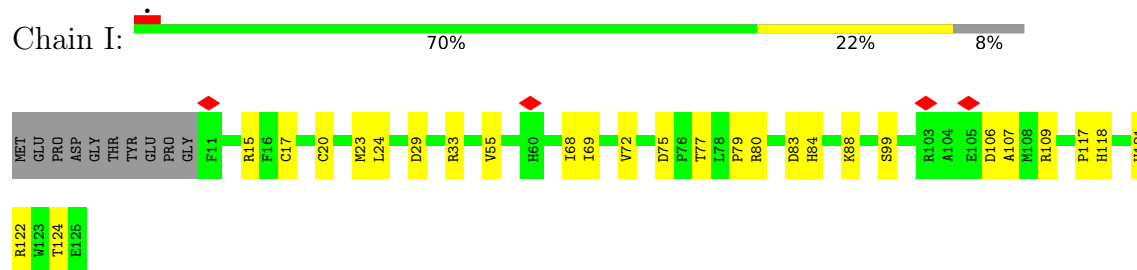
- Molecule 5: DNA-directed RNA polymerase II subunit F



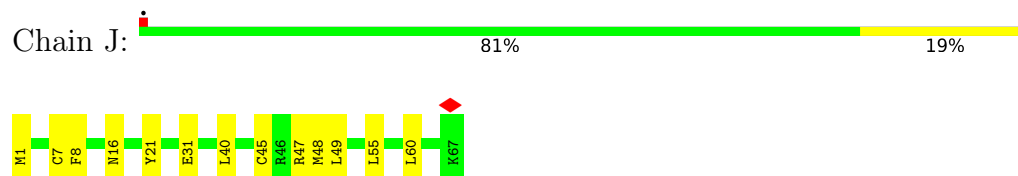
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 7: DNA-directed RNA polymerase II subunit RPB9

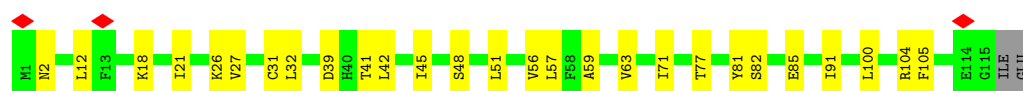


- Molecule 8: Uncharacterized Protein



- Molecule 9: RNA_pol_L_2 domain-containing protein

Chain K:  75% 23%



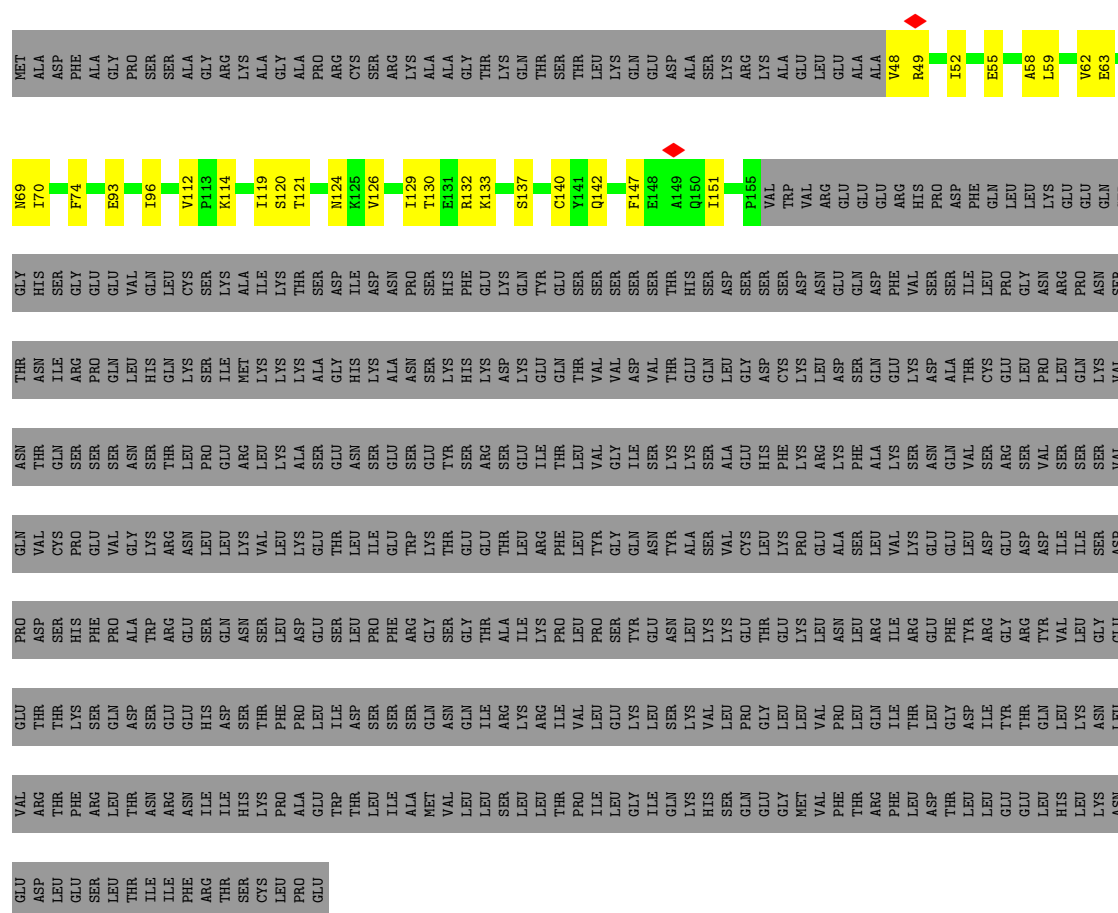
- Molecule 10: RNA polymerase II subunit K

Chain L:  7% 50% 26% 24%

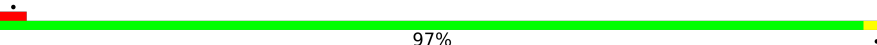


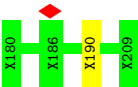
- Molecule 11: Putative RNA polymerase II subunit B1 CTD phosphatase RPAP2

Chain M:  13% 5% 82%



- Molecule 12: Unknown

Chain N:  97%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	364771	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.150	Depositor
Minimum map value	-0.055	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	377.99997, 377.99997, 377.99997	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.05, 1.05, 1.05	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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.12	0/7997	0.36	0/10805
2	B	0.12	0/7999	0.34	0/10808
3	C	0.12	0/2102	0.32	0/2857
4	E	0.13	0/1751	0.36	0/2366
5	F	0.14	0/636	0.43	0/859
6	H	0.13	0/1204	0.41	1/1623 (0.1%)
7	I	0.12	0/960	0.36	0/1300
8	J	0.13	0/542	0.31	0/730
9	K	0.12	0/939	0.31	0/1271
10	L	0.16	0/377	0.52	0/500
11	M	0.15	0/897	0.45	0/1204
All	All	0.12	0/25404	0.36	1/34323 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	82	PRO	N-CA-CB	5.94	109.86	103.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	724	GLU	Peptide

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	A	7861	0	7914	175	0
2	B	7842	0	7881	178	0
3	C	2059	0	2007	52	0
4	E	1720	0	1737	28	0
5	F	626	0	657	18	0
6	H	1184	0	1141	39	0
7	I	938	0	872	17	0
8	J	533	0	553	10	0
9	K	920	0	942	21	0
10	L	372	0	378	13	0
11	M	880	0	896	20	0
12	N	150	0	40	1	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
13	M	1	0	0	0	0
All	All	25091	0	25018	515	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 10.

All (515) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1211:LEU:HD11	1:A:1258:ARG:HB3	1.61	0.82
4:E:62:VAL:O	4:E:71:GLN:HA	1.79	0.81
9:K:26:LYS:HD2	9:K:27:VAL:HG23	1.66	0.78
1:A:948:ILE:HD12	1:A:1007:ILE:HG13	1.66	0.77
1:A:603:ILE:HG23	1:A:627:LYS:HD3	1.69	0.74
1:A:567:LEU:HD21	1:A:595:ILE:HG12	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:ARG:HG2	2:B:918:PHE:HZ	1.51	0.74
8:J:21:TYR:OH	8:J:31:GLU:OE2	2.05	0.74
2:B:717:ASN:ND2	2:B:977:THR:OG1	2.22	0.73
2:B:941:GLN:H	2:B:975:ARG:HB2	1.54	0.72
7:I:17:CYS:HB3	7:I:20:CYS:SG	2.28	0.72
10:L:19:CYS:SG	10:L:20:GLY:N	2.61	0.72
2:B:971:ALA:HB1	2:B:975:ARG:HG2	1.70	0.71
5:F:66:LEU:HD21	5:F:97:LEU:HD22	1.72	0.71
1:A:622:SER:OG	1:A:626:THR:N	2.24	0.71
2:B:115:LEU:HB3	2:B:908:MET:HE1	1.74	0.70
7:I:68:ILE:O	7:I:122:ARG:NH1	2.23	0.70
2:B:617:ASP:O	2:B:620:ARG:NH1	2.25	0.69
2:B:198:GLU:HB3	2:B:488:PRO:HD3	1.73	0.69
2:B:296:GLU:OE2	2:B:379:ARG:NH2	2.25	0.69
1:A:719:LYS:HB3	1:A:725:LEU:HD11	1.73	0.69
1:A:593:SER:HB3	1:A:634:GLU:HB2	1.74	0.69
3:C:205:LYS:NZ	3:C:215:GLU:O	2.26	0.69
9:K:82:SER:OG	9:K:85:GLU:OE1	2.11	0.69
1:A:393:ILE:HG22	1:A:445:LYS:HG2	1.76	0.68
5:F:92:ILE:HA	5:F:95:LYS:HG2	1.75	0.67
1:A:660:MET:HG2	1:A:664:ILE:HD11	1.77	0.67
3:C:173:HIS:HB3	3:C:175:LYS:HG2	1.75	0.67
6:H:2:ALA:O	6:H:84:ARG:NH1	2.28	0.67
6:H:59:VAL:HB	6:H:144:LEU:HB2	1.77	0.66
6:H:58:LEU:HD11	6:H:143:LEU:HD11	1.77	0.66
2:B:806:PHE:O	2:B:1050:ARG:NH1	2.26	0.66
2:B:407:MET:HE1	2:B:444:LEU:HG	1.76	0.66
4:E:80:PRO:HB2	4:E:108:GLN:HE22	1.61	0.66
11:M:142:GLN:NE2	12:N:190:UNK:O	2.29	0.65
4:E:163:TYR:HB3	4:E:165:LEU:HD13	1.79	0.65
6:H:90:TYR:HB3	6:H:145:MET:HB2	1.79	0.65
2:B:908:MET:HE3	10:L:43:ILE:HG23	1.77	0.65
11:M:93:GLU:HA	11:M:96:ILE:HD12	1.78	0.65
2:B:866:ILE:HG13	2:B:867:ILE:HG13	1.78	0.65
6:H:115:TYR:OH	6:H:124:ARG:NH1	2.30	0.65
8:J:1:MET:HA	8:J:55:LEU:HB2	1.78	0.65
1:A:1150:ASP:OD2	1:A:1153:ARG:NH2	2.30	0.64
2:B:601:VAL:HG22	2:B:616:THR:HG22	1.79	0.64
1:A:1178:ASP:OD2	1:A:1260:ARG:NH2	2.31	0.64
1:A:1207:ILE:HG22	1:A:1262:MET:HE1	1.79	0.64
3:C:190:ASN:O	3:C:193:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1026:ASP:O	1:A:1031:ARG:NH1	2.31	0.63
2:B:196:ALA:HA	2:B:394:ASP:O	1.98	0.63
4:E:115:LYS:NZ	4:E:129:GLN:OE1	2.31	0.63
1:A:1166:LEU:HB3	1:A:1293:LEU:HD12	1.80	0.63
1:A:413:TYR:O	1:A:449:HIS:ND1	2.30	0.63
6:H:130:ASN:O	6:H:133:HIS:ND1	2.32	0.63
2:B:783:ALA:O	2:B:789:ASN:ND2	2.31	0.63
1:A:604:ARG:NH2	1:A:649:ALA:O	2.30	0.63
2:B:553:LEU:HD12	2:B:556:ILE:HD11	1.81	0.62
2:B:779:ILE:O	2:B:964:ASP:N	2.32	0.62
10:L:17:TYR:O	10:L:26:ASN:N	2.26	0.62
1:A:921:ARG:HH21	1:A:956:PHE:HB3	1.64	0.62
7:I:117:PRO:O	7:I:118:HIS:ND1	2.32	0.62
1:A:1036:ASN:OD1	4:E:202:ARG:NH1	2.28	0.62
6:H:20:LYS:NZ	6:H:22:PHE:O	2.31	0.62
9:K:77:THR:OG1	9:K:81:TYR:O	2.12	0.62
4:E:60:VAL:HB	4:E:74:VAL:HB	1.81	0.61
6:H:77:PRO:HB3	9:K:57:LEU:HD21	1.82	0.61
1:A:1143:LEU:HB2	1:A:1148:ALA:HB2	1.83	0.61
2:B:952:GLU:HB2	3:C:36:ARG:HG3	1.82	0.61
2:B:65:ILE:HD11	2:B:412:LEU:HD22	1.83	0.61
3:C:20:LYS:NZ	3:C:207:GLU:OE2	2.33	0.61
6:H:98:ARG:NH2	6:H:100:GLU:OE2	2.34	0.61
2:B:758:LEU:HD21	8:J:47:ARG:HG2	1.82	0.60
2:B:933:ASP:OD2	2:B:1050:ARG:NH2	2.35	0.60
9:K:56:VAL:HG12	9:K:77:THR:HG22	1.84	0.60
2:B:663:GLU:OE1	2:B:695:HIS:NE2	2.33	0.59
3:C:116:THR:HG22	3:C:149:LEU:HA	1.84	0.59
2:B:751:LEU:HD11	2:B:806:PHE:HA	1.83	0.59
2:B:483:ARG:O	2:B:525:ASN:ND2	2.34	0.59
1:A:761:SER:O	1:A:767:LYS:NZ	2.32	0.59
2:B:309:PHE:O	2:B:312:GLN:NE2	2.35	0.59
3:C:91:GLU:CD	3:C:92:GLU:H	2.11	0.59
1:A:1279:MET:SD	1:A:1280:ASP:N	2.76	0.59
1:A:931:ARG:NH1	1:A:936:GLU:OE1	2.36	0.59
1:A:1141:VAL:HB	1:A:1336:LEU:HB2	1.85	0.59
3:C:148:ILE:HD13	8:J:16:ASN:HB3	1.85	0.59
10:L:22:CYS:SG	10:L:24:THR:OG1	2.53	0.59
1:A:945:ASN:O	1:A:949:GLN:NE2	2.36	0.59
2:B:171:LEU:HD13	2:B:178:PRO:HA	1.83	0.59
11:M:137:SER:OG	11:M:140:CYS:SG	2.60	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:LEU:HD22	2:B:485:LEU:HD22	1.84	0.59
1:A:1097:GLU:HG3	1:A:1098:PRO:HD3	1.85	0.58
2:B:600:GLU:O	2:B:620:ARG:NH2	2.35	0.58
4:E:95:GLN:OE1	4:E:125:TYR:OH	2.22	0.58
1:A:1139:LEU:HD12	1:A:1341:VAL:HG23	1.85	0.58
11:M:120:SER:O	11:M:124:ASN:N	2.36	0.58
1:A:381:PRO:HB3	1:A:480:SER:HA	1.85	0.58
1:A:790:GLN:NE2	1:A:791:GLN:O	2.33	0.58
2:B:984:CYS:SG	2:B:1046:THR:OG1	2.49	0.58
1:A:575:PRO:HG3	1:A:594:LEU:HD11	1.83	0.58
1:A:1365:ILE:HG23	1:A:1369:LEU:HD12	1.85	0.58
1:A:811:ILE:HD12	7:I:79:PRO:HB3	1.86	0.58
1:A:913:ASN:OD1	1:A:963:ARG:NH2	2.37	0.58
11:M:112:VAL:HG12	11:M:114:LYS:H	1.67	0.58
1:A:706:ILE:HG21	1:A:824:GLU:HG3	1.86	0.58
6:H:63:THR:O	6:H:84:ARG:NH2	2.37	0.58
1:A:456:VAL:HG12	1:A:505:LEU:HB3	1.86	0.57
2:B:419:ALA:O	2:B:423:ILE:HB	2.03	0.57
2:B:741:HIS:O	2:B:922:ARG:NH2	2.37	0.57
2:B:28:ILE:HD11	2:B:640:ILE:HG23	1.85	0.57
1:A:483:ARG:HH21	2:B:931:ILE:HD11	1.70	0.57
4:E:117:SER:HB2	11:M:59:LEU:HD21	1.85	0.57
2:B:320:PHE:O	2:B:324:ARG:NH2	2.38	0.57
3:C:7:PRO:O	9:K:104:ARG:NH1	2.32	0.57
1:A:364:ARG:HH12	2:B:1058:LYS:HB2	1.69	0.57
1:A:583:ARG:NH1	3:C:222:PRO:O	2.38	0.57
1:A:747:ASP:OD1	1:A:748:ALA:N	2.37	0.57
1:A:1148:ALA:HB1	1:A:1333:GLU:HB3	1.85	0.57
1:A:863:ARG:NH2	1:A:1129:ASN:OD1	2.36	0.57
2:B:274:ARG:NH2	2:B:281:ASP:OD1	2.37	0.57
5:F:118:TRP:HB3	5:F:123:LEU:HD11	1.87	0.57
6:H:7:GLU:OE2	6:H:57:ARG:NH2	2.37	0.57
2:B:978:ILE:HA	2:B:981:LEU:HG	1.87	0.57
1:A:416:ALA:HA	1:A:448:ARG:HA	1.86	0.56
2:B:34:PHE:HZ	2:B:528:LEU:HB3	1.70	0.56
1:A:979:LEU:HD12	1:A:1041:PHE:HD1	1.70	0.56
1:A:540:ASP:OD1	1:A:541:THR:N	2.39	0.56
1:A:1181:PRO:O	1:A:1184:THR:OG1	2.23	0.56
3:C:60:HIS:CE1	3:C:63:PHE:HB2	2.41	0.56
1:A:1130:ILE:HD12	1:A:1411:LEU:HB3	1.88	0.56
2:B:792:ASP:O	2:B:975:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:PHE:H	1:A:1052:ARG:HD2	1.71	0.56
2:B:626:LEU:HD23	2:B:662:VAL:HG12	1.87	0.56
6:H:130:ASN:OD1	6:H:131:ASN:N	2.39	0.56
1:A:1168:LYS:O	1:A:1220:HIS:ND1	2.38	0.56
2:B:858:VAL:HG13	10:L:49:THR:HG21	1.88	0.56
2:B:912:ASN:OD1	2:B:916:TYR:N	2.39	0.56
1:A:1218:ARG:NH1	1:A:1250:ASP:O	2.39	0.56
2:B:155:MET:HE3	2:B:183:GLY:HA2	1.86	0.56
2:B:867:ILE:O	2:B:893:SER:OG	2.21	0.55
1:A:1307:VAL:HG13	1:A:1338:THR:HG22	1.87	0.55
1:A:794:GLU:OE2	2:B:500:GLN:NE2	2.40	0.55
1:A:924:TYR:OH	1:A:953:GLU:OE2	2.22	0.55
2:B:385:ARG:O	2:B:391:LYS:NZ	2.29	0.55
3:C:31:ALA:O	3:C:231:TYR:OH	2.23	0.55
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.88	0.55
1:A:1030:SER:OG	4:E:162:ARG:NE	2.40	0.55
2:B:734:GLY:HA2	2:B:751:LEU:HB2	1.89	0.55
2:B:348:LEU:O	2:B:361:LYS:NZ	2.40	0.55
3:C:78:ILE:HD11	3:C:126:ARG:HB3	1.89	0.55
2:B:752:TYR:HE1	2:B:809:VAL:HG13	1.72	0.55
1:A:839:HIS:HE1	2:B:718:GLN:HB2	1.71	0.55
10:L:36:CYS:SG	10:L:39:CYS:HB3	2.46	0.55
1:A:448:ARG:NH2	1:A:451:CYS:SG	2.80	0.54
2:B:274:ARG:NH1	2:B:308:ALA:O	2.40	0.54
9:K:63:VAL:HG22	9:K:71:ILE:HG22	1.88	0.54
1:A:719:LYS:O	1:A:723:ASN:N	2.39	0.54
1:A:1408:ARG:CZ	4:E:172:ARG:HH12	2.20	0.54
4:E:100:THR:HA	4:E:125:TYR:HD1	1.71	0.54
3:C:52:ILE:HD12	3:C:61:ASP:HB3	1.89	0.54
6:H:6:PHE:HB3	6:H:60:ILE:HB	1.89	0.54
1:A:1193:VAL:HG13	1:A:1197:TYR:CD2	2.43	0.54
7:I:109:ARG:HD3	7:I:124:THR:HG21	1.89	0.54
1:A:628:VAL:HG22	1:A:638:GLY:HA3	1.88	0.54
1:A:1039:LEU:HD22	4:E:201:GLY:HA3	1.89	0.54
4:E:9:ARG:HG3	4:E:136:LEU:HD21	1.88	0.54
1:A:1190:GLN:NE2	1:A:1194:ASN:OD1	2.41	0.54
1:A:545:VAL:HG11	1:A:645:LEU:HD22	1.89	0.54
5:F:60:TYR:O	5:F:64:ARG:HG2	2.07	0.54
2:B:628:VAL:HG22	2:B:633:LEU:HD23	1.88	0.53
6:H:103:GLU:HB3	6:H:109:ALA:HB2	1.90	0.53
1:A:860:ILE:HD11	1:A:1125:LYS:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:912:SER:OG	1:A:1325:ASP:O	2.25	0.53
1:A:1004:LEU:HD13	1:A:1062:GLY:HA2	1.91	0.53
9:K:42:LEU:HD23	9:K:45:ILE:HD11	1.89	0.53
4:E:107:GLN:HA	4:E:132:GLN:HB2	1.90	0.53
2:B:288:ILE:HD13	2:B:366:GLY:HA2	1.89	0.53
7:I:83:ASP:OD1	7:I:84:HIS:N	2.42	0.53
9:K:21:ILE:HG23	9:K:31:CYS:SG	2.49	0.53
1:A:1244:ASN:HB3	1:A:1262:MET:HE3	1.89	0.53
3:C:56:SER:HB2	3:C:158:GLU:H	1.74	0.53
1:A:623:PRO:O	6:H:21:LYS:NZ	2.27	0.53
2:B:298:MET:O	2:B:302:LYS:HG2	2.09	0.53
2:B:341:GLU:OE1	2:B:345:LYS:NZ	2.41	0.53
2:B:780:VAL:HA	2:B:965:ILE:O	2.09	0.53
2:B:806:PHE:HB3	2:B:1050:ARG:HD2	1.91	0.53
1:A:400:ASP:OD1	1:A:401:ARG:N	2.42	0.53
1:A:926:ASN:O	1:A:927:GLU:HG3	2.08	0.52
2:B:116:ARG:HD2	2:B:118:LEU:HD23	1.92	0.52
1:A:801:GLY:HA3	2:B:503:ASN:HB2	1.91	0.52
2:B:972:ILE:HD13	2:B:976:MET:HG3	1.91	0.52
2:B:225:LEU:HD12	2:B:230:ARG:NH2	2.24	0.52
2:B:468:GLN:HE21	2:B:481:HIS:HE2	1.58	0.52
2:B:635:LEU:HD21	2:B:640:ILE:HD11	1.92	0.52
1:A:695:ASP:N	1:A:695:ASP:OD1	2.41	0.52
2:B:929:PRO:HB3	2:B:935:PHE:HZ	1.73	0.52
3:C:32:ASN:OD1	3:C:35:ARG:NH2	2.39	0.52
1:A:680:LEU:HD11	1:A:685:HIS:HB2	1.91	0.51
3:C:7:PRO:HD2	9:K:100:LEU:HD23	1.91	0.51
3:C:27:ASP:OD2	9:K:48:SER:OG	2.22	0.51
4:E:11:TRP:NE1	4:E:35:GLN:O	2.38	0.51
4:E:46:ASP:OD1	4:E:52:ARG:NH2	2.42	0.51
2:B:384:ASP:HB3	2:B:387:HIS:HB2	1.93	0.51
6:H:97:TYR:CZ	6:H:115:TYR:HB3	2.45	0.51
2:B:297:MET:HE1	2:B:370:HIS:CD2	2.46	0.51
1:A:1374:VAL:HG21	1:A:1411:LEU:HD11	1.93	0.51
1:A:901:VAL:HA	1:A:980:PRO:HA	1.93	0.51
2:B:623:ARG:NH2	2:B:697:GLU:OE2	2.40	0.51
3:C:105:VAL:HG11	3:C:115:VAL:HG22	1.92	0.51
3:C:154:ARG:HB2	8:J:60:LEU:HD22	1.92	0.51
6:H:24:ARG:HB2	6:H:46:GLN:HB2	1.92	0.51
8:J:40:LEU:HB3	8:J:45:CYS:HB2	1.93	0.51
2:B:759:VAL:O	2:B:938:ARG:NH2	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:PHE:HA	1:A:595:ILE:HD12	1.93	0.51
2:B:670:GLU:HA	2:B:673:VAL:HG12	1.93	0.50
2:B:845:TYR:HA	2:B:848:LEU:HD23	1.92	0.50
2:B:939:HIS:HB2	2:B:980:HIS:HB2	1.92	0.50
1:A:1170:THR:HA	1:A:1216:LEU:HD13	1.92	0.50
3:C:256:LEU:HD22	9:K:91:ILE:HG13	1.93	0.50
1:A:904:GLN:NE2	1:A:981:CYS:O	2.41	0.50
2:B:929:PRO:O	2:B:948:GLN:NE2	2.36	0.50
11:M:119:ILE:HG22	11:M:126:VAL:HG22	1.94	0.50
2:B:288:ILE:HG22	2:B:289:ILE:HG13	1.94	0.50
1:A:1015:GLU:HG3	1:A:1018:LYS:HE3	1.93	0.50
1:A:1218:ARG:NH2	1:A:1252:ALA:O	2.44	0.50
2:B:529:MET:HE3	2:B:624:PRO:HG2	1.94	0.50
4:E:5:GLU:OE1	4:E:9:ARG:NH1	2.45	0.50
1:A:819:SER:OG	1:A:820:ARG:N	2.45	0.50
3:C:78:ILE:HG22	3:C:82:LEU:HD13	1.94	0.50
2:B:296:GLU:HA	2:B:299:GLU:HG2	1.92	0.50
2:B:379:ARG:O	2:B:608:ARG:NH2	2.41	0.50
2:B:797:ASN:HB3	2:B:800:ALA:HB3	1.94	0.50
3:C:37:VAL:HG13	3:C:41:GLU:HB2	1.94	0.50
1:A:625:ASP:OD2	1:A:639:ILE:HG13	2.12	0.49
1:A:868:MET:HE1	1:A:1401:LEU:HA	1.94	0.49
9:K:41:THR:O	9:K:45:ILE:HG12	2.12	0.49
1:A:663:ASP:N	1:A:663:ASP:OD1	2.45	0.49
1:A:783:GLN:HA	1:A:787:VAL:O	2.12	0.49
2:B:780:VAL:HG22	2:B:965:ILE:HB	1.94	0.49
1:A:733:LEU:HD12	7:I:106:ASP:HA	1.93	0.49
2:B:795:ILE:HG22	2:B:947:ILE:H	1.76	0.49
3:C:260:GLN:CA	3:C:260:GLN:HE21	2.24	0.49
5:F:89:PRO:HA	5:F:92:ILE:HG12	1.94	0.49
1:A:383:SER:HB3	9:K:2:ASN:HD22	1.77	0.49
2:B:762:ARG:O	2:B:765:GLU:HB3	2.13	0.49
2:B:797:ASN:OD1	2:B:799:SER:OG	2.24	0.49
2:B:955:PRO:O	2:B:963:PRO:HD2	2.12	0.49
2:B:367:TYR:OH	2:B:371:ARG:NH1	2.45	0.49
2:B:927:ARG:NH1	2:B:1057:ASP:OD1	2.35	0.49
2:B:235:ILE:HG22	2:B:261:PRO:HD3	1.95	0.49
2:B:545:LEU:HB3	2:B:550:MET:SD	2.53	0.49
3:C:36:ARG:HH21	9:K:39:ASP:HB2	1.78	0.49
3:C:52:ILE:HG21	3:C:55:ASN:HB2	1.94	0.49
3:C:128:ILE:HD12	3:C:132:SER:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:25:VAL:HA	6:H:43:VAL:O	2.13	0.49
2:B:414:GLU:OE2	2:B:436:LYS:NZ	2.37	0.48
2:B:717:ASN:HD21	2:B:979:GLY:HA3	1.78	0.48
5:F:102:ILE:HB	5:F:120:VAL:HG11	1.95	0.48
1:A:720:ALA:O	1:A:723:ASN:HB3	2.13	0.48
1:A:1163:HIS:CE1	1:A:1297:THR:HG23	2.48	0.48
2:B:387:HIS:NE2	2:B:671:GLU:OE2	2.45	0.48
5:F:51:ARG:NH1	5:F:122:GLU:OE2	2.45	0.48
1:A:958:ARG:O	1:A:961:GLU:HG3	2.13	0.48
2:B:795:ILE:HG13	2:B:966:ILE:HB	1.95	0.48
2:B:845:TYR:OH	2:B:891:ASP:OD2	2.26	0.48
1:A:610:PRO:HG2	1:A:613:GLU:HG2	1.95	0.48
2:B:1050:ARG:NH2	2:B:1054:MET:SD	2.87	0.48
3:C:13:GLU:HB2	3:C:20:LYS:HB2	1.95	0.48
4:E:151:MET:HE3	4:E:155:GLU:HB3	1.95	0.48
1:A:1318:LYS:HD2	1:A:1330:ALA:HB1	1.96	0.48
2:B:848:LEU:HA	2:B:854:ILE:HG22	1.95	0.48
9:K:51:LEU:HD12	9:K:59:ALA:HB3	1.96	0.48
2:B:665:ILE:HG23	2:B:669:GLU:HB3	1.96	0.48
1:A:364:ARG:NH1	2:B:1058:LYS:O	2.46	0.48
2:B:298:MET:HA	2:B:301:VAL:HG12	1.96	0.48
5:F:57:MET:HB2	5:F:123:LEU:HD23	1.95	0.48
1:A:374:SER:HB3	1:A:377:GLN:HB2	1.96	0.48
1:A:1016:LEU:O	1:A:1020:LEU:HG	2.14	0.47
2:B:265:GLN:OE1	2:B:324:ARG:NE	2.46	0.47
2:B:855:ALA:HB3	10:L:49:THR:HG22	1.96	0.47
2:B:302:LYS:NZ	7:I:23:MET:SD	2.71	0.47
2:B:501:LEU:HD11	2:B:511:PRO:HA	1.96	0.47
2:B:782:ILE:HG12	2:B:967:ILE:HD11	1.96	0.47
9:K:12:LEU:HD21	9:K:18:LYS:HD3	1.96	0.47
1:A:381:PRO:HG2	1:A:384:ILE:HB	1.97	0.47
1:A:1174:ALA:HB2	7:I:55:VAL:HG23	1.97	0.47
2:B:205:VAL:O	2:B:371:ARG:NH2	2.48	0.47
1:A:863:ARG:HE	1:A:1414:ILE:HB	1.80	0.47
2:B:796:MET:HE1	2:B:935:PHE:CE1	2.50	0.47
3:C:93:PHE:HE1	3:C:166:LYS:HD3	1.80	0.47
2:B:223:SER:OG	2:B:349:PRO:HD2	2.15	0.47
7:I:29:ASP:OD1	7:I:29:ASP:N	2.47	0.47
10:L:19:CYS:HA	10:L:44:MET:HB2	1.95	0.47
2:B:229:SER:C	2:B:230:ARG:HD3	2.40	0.47
3:C:45:ILE:HG13	3:C:79:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:LEU:HD12	2:B:230:ARG:HH22	1.79	0.47
2:B:937:SER:HB3	2:B:1048:TYR:CE1	2.49	0.47
7:I:88:LYS:HE3	7:I:121:HIS:HB2	1.97	0.47
1:A:1354:PRO:HB3	4:E:137:ILE:HG12	1.95	0.47
2:B:674:MET:HB2	7:I:77:THR:HG22	1.97	0.47
1:A:977:VAL:HG13	1:A:979:LEU:HD23	1.96	0.47
2:B:848:LEU:HD21	2:B:865:VAL:HG12	1.95	0.47
4:E:111:THR:OG1	11:M:93:GLU:OE2	2.27	0.47
6:H:56:PHE:HE2	6:H:58:LEU:HD13	1.79	0.47
11:M:58:ALA:O	11:M:62:VAL:HG23	2.15	0.47
1:A:477:LEU:HD13	1:A:483:ARG:HD2	1.96	0.46
1:A:510:GLU:HG3	5:F:67:GLY:HA3	1.97	0.46
1:A:606:HIS:CE1	1:A:641:CYS:HB3	2.50	0.46
2:B:772:LEU:O	2:B:772:LEU:HD12	2.16	0.46
2:B:942:LYS:HG3	2:B:1051:LEU:HD12	1.97	0.46
2:B:953:ASP:OD1	3:C:36:ARG:NH2	2.34	0.46
3:C:35:ARG:HD2	3:C:39:ILE:HD12	1.97	0.46
2:B:802:ASP:HB3	3:C:173:HIS:CE1	2.51	0.46
11:M:70:ILE:HG23	11:M:74:PHE:HD2	1.81	0.46
6:H:87:GLN:N	6:H:87:GLN:OE1	2.49	0.46
1:A:386:ALA:HB2	1:A:413:TYR:HD1	1.81	0.46
1:A:955:GLU:HA	1:A:958:ARG:HG2	1.97	0.46
3:C:38:PHE:HE1	3:C:245:VAL:HA	1.80	0.46
1:A:727:PRO:HB3	1:A:733:LEU:HD23	1.97	0.46
1:A:1087:VAL:HG22	1:A:1400:LEU:HD22	1.96	0.46
2:B:229:SER:HB2	2:B:230:ARG:HH11	1.81	0.46
2:B:257:VAL:HG21	2:B:266:GLU:HB2	1.96	0.46
5:F:69:ARG:O	5:F:73:ILE:HG12	2.16	0.46
5:F:127:ASP:OD1	5:F:127:ASP:N	2.49	0.46
10:L:26:ASN:HA	10:L:37:ARG:HH12	1.81	0.46
1:A:912:SER:HB2	1:A:1327:GLU:HG3	1.98	0.46
6:H:145:MET:HB3	6:H:145:MET:HE2	1.81	0.46
2:B:791:GLU:HA	2:B:968:ASN:HD22	1.81	0.46
11:M:52:ILE:HA	11:M:55:GLU:OE2	2.15	0.46
2:B:587:LEU:HB3	2:B:603:MET:SD	2.56	0.45
1:A:511:THR:HA	1:A:514:GLU:HG3	1.99	0.45
1:A:930:LEU:O	1:A:934:LEU:N	2.47	0.45
1:A:1243:LEU:HD21	1:A:1292:MET:HE1	1.98	0.45
2:B:747:LEU:HA	2:B:810:PHE:HE1	1.82	0.45
8:J:40:LEU:HD22	8:J:45:CYS:HB3	1.99	0.45
1:A:863:ARG:HG2	1:A:1414:ILE:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1161:LEU:HD22	1:A:1346:VAL:HG22	1.98	0.45
2:B:84:TYR:HD2	2:B:132:VAL:HG12	1.80	0.45
2:B:110:PRO:HB3	2:B:156:LEU:HD11	1.99	0.45
4:E:17:ILE:HG21	4:E:74:VAL:HG11	1.99	0.45
5:F:99:ALA:HB1	5:F:101:LYS:NZ	2.32	0.45
5:F:100:ARG:NH2	5:F:121:ASP:O	2.48	0.45
1:A:1376:LYS:O	1:A:1379:GLU:HG3	2.16	0.45
2:B:21:LEU:O	2:B:21:LEU:HD23	2.17	0.45
2:B:395:LEU:HD21	2:B:532:ILE:HG13	1.98	0.45
2:B:541:ILE:HD12	2:B:541:ILE:H	1.81	0.45
2:B:781:ALA:O	2:B:966:ILE:HA	2.17	0.45
1:A:576:GLN:HB3	6:H:93:TYR:CD2	2.51	0.45
1:A:630:VAL:HG22	1:A:635:LEU:HA	1.99	0.45
2:B:22:TRP:HH2	2:B:626:LEU:HD11	1.81	0.45
6:H:96:VAL:HG23	6:H:116:VAL:HG22	1.98	0.45
1:A:585:LEU:HD12	6:H:47:ILE:HD13	1.98	0.45
1:A:1371:ILE:HA	1:A:1374:VAL:HG12	1.98	0.45
3:C:14:LEU:HD12	3:C:19:VAL:HG22	1.99	0.45
3:C:38:PHE:CE1	3:C:245:VAL:HA	2.52	0.45
7:I:15:ARG:HB3	7:I:24:LEU:HD12	1.99	0.45
2:B:284:ILE:O	2:B:288:ILE:HG12	2.17	0.45
2:B:588:ARG:HA	2:B:603:MET:HE1	1.99	0.45
1:A:1228:MET:HE1	1:A:1255:LEU:HD13	1.99	0.45
1:A:1230:GLN:O	1:A:1233:GLU:HG3	2.17	0.45
2:B:339:ALA:HA	2:B:342:VAL:HG12	1.97	0.45
2:B:934:LYS:HA	2:B:944:THR:HA	1.99	0.45
3:C:9:VAL:HG11	9:K:105:PHE:HD1	1.81	0.45
9:K:82:SER:N	9:K:85:GLU:OE2	2.50	0.45
2:B:260:LEU:HD23	2:B:347:MET:HG2	1.97	0.45
2:B:858:VAL:HG12	10:L:51:ARG:HD2	1.99	0.45
3:C:59:LEU:HD12	3:C:151:VAL:HG23	1.98	0.45
1:A:896:LEU:HA	1:A:1081:ALA:H	1.82	0.44
1:A:972:THR:HA	1:A:1320:ILE:HG21	1.99	0.44
1:A:1006:PRO:HB3	1:A:1051:SER:HB2	1.99	0.44
2:B:153:PRO:HD3	2:B:444:LEU:HD13	1.98	0.44
2:B:627:ILE:HD11	2:B:663:GLU:HB3	1.98	0.44
2:B:756:LYS:O	2:B:777:ASN:ND2	2.47	0.44
2:B:1028:LEU:HD13	2:B:1041:ILE:HB	1.99	0.44
6:H:92:MET:HB2	6:H:143:LEU:HB3	1.99	0.44
1:A:1158:LEU:HD12	1:A:1336:LEU:HD22	1.98	0.44
6:H:9:ILE:HD12	6:H:57:ARG:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:930:LEU:HB3	1:A:939:VAL:HG22	2.00	0.44
6:H:39:LEU:HD22	6:H:58:LEU:HD22	1.99	0.44
6:H:56:PHE:CD2	6:H:145:MET:HE3	2.52	0.44
1:A:544:ALA:HB2	1:A:680:LEU:HD22	2.00	0.44
2:B:712:PRO:HD3	2:B:938:ARG:HD2	1.99	0.44
6:H:88:PHE:HB2	6:H:144:LEU:HD12	1.99	0.44
1:A:458:PHE:HB3	1:A:501:MET:HE2	1.99	0.44
1:A:591:ILE:O	1:A:595:ILE:HG13	2.17	0.44
1:A:894:ASP:OD2	1:A:1396:ARG:NH2	2.51	0.44
2:B:819:SER:H	2:B:827:GLU:HB2	1.82	0.44
1:A:552:ASP:OD1	6:H:22:PHE:HB3	2.18	0.44
1:A:817:PRO:O	1:A:822:PHE:HB3	2.18	0.44
5:F:52:ILE:O	5:F:53:THR:OG1	2.32	0.44
11:M:129:ILE:HB	11:M:132:ARG:HB3	1.98	0.44
1:A:821:GLY:HA2	1:A:838:PHE:CD2	2.53	0.44
1:A:839:HIS:CE1	2:B:718:GLN:HB2	2.53	0.44
1:A:1310:HIS:NE2	1:A:1337:GLU:OE2	2.51	0.44
2:B:229:SER:HA	2:B:405:ARG:NH2	2.33	0.44
3:C:76:ASP:HA	3:C:239:LEU:HD12	2.00	0.44
8:J:7:CYS:HA	8:J:48:MET:HE3	2.00	0.44
1:A:886:VAL:HG21	4:E:165:LEU:HD21	2.00	0.43
1:A:1382:LEU:HB3	1:A:1398:LEU:HD11	1.99	0.43
2:B:45:ASP:HB3	2:B:534:VAL:HG11	2.00	0.43
2:B:83:ARG:HE	2:B:133:ILE:HD12	1.83	0.43
2:B:274:ARG:HG2	2:B:279:VAL:HA	2.00	0.43
11:M:130:THR:HA	11:M:133:LYS:HD2	2.00	0.43
1:A:871:VAL:HB	1:A:1088:GLY:HA3	2.00	0.43
1:A:1263:ASN:HA	11:M:121:THR:HG21	1.99	0.43
2:B:42:GLN:HG2	2:B:43:GLN:N	2.33	0.43
4:E:9:ARG:O	4:E:13:ILE:HG12	2.19	0.43
5:F:57:MET:HE3	5:F:62:ARG:HB2	2.00	0.43
7:I:75:ASP:O	7:I:80:ARG:NH1	2.37	0.43
9:K:31:CYS:SG	9:K:32:LEU:N	2.91	0.43
11:M:120:SER:O	11:M:124:ASN:CA	2.66	0.43
2:B:43:GLN:HG2	2:B:395:LEU:HD12	2.01	0.43
1:A:910:LYS:N	1:A:911:PRO:HD2	2.34	0.43
2:B:801:VAL:HG13	2:B:929:PRO:HG2	2.01	0.43
10:L:17:TYR:CE2	10:L:44:MET:HG3	2.53	0.43
1:A:600:ILE:H	1:A:633:GLY:CA	2.31	0.43
3:C:265:HIS:O	3:C:268:GLN:HG3	2.19	0.43
2:B:125:TYR:HD1	2:B:148:PHE:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:260:GLN:HE21	3:C:260:GLN:HA	1.83	0.43
2:B:542:LEU:O	2:B:545:LEU:N	2.51	0.43
2:B:416:ARG:HA	2:B:416:ARG:CZ	2.49	0.43
3:C:5:ASN:HD21	3:C:26:THR:HA	1.84	0.43
2:B:124:LEU:O	2:B:149:ILE:HG22	2.19	0.42
2:B:236:TRP:HB2	2:B:259:THR:HB	2.01	0.42
2:B:595:ASP:OD1	2:B:595:ASP:N	2.50	0.42
3:C:68:LEU:HA	3:C:71:ILE:HD12	2.00	0.42
4:E:194:ILE:HG13	4:E:204:ILE:HG12	2.01	0.42
1:A:919:LYS:O	1:A:1052:ARG:HD3	2.19	0.42
6:H:57:ARG:HG3	6:H:148:LEU:HD21	2.01	0.42
6:H:77:PRO:HG3	9:K:57:LEU:HD11	2.01	0.42
6:H:91:VAL:HG22	6:H:144:LEU:HD13	2.01	0.42
1:A:371:PRO:HG3	2:B:787:GLY:HA3	2.01	0.42
2:B:150:GLY:HA2	2:B:437:THR:HB	2.00	0.42
3:C:109:GLU:HB2	3:C:111:GLN:OE1	2.19	0.42
4:E:133:GLN:HA	4:E:136:LEU:HD12	2.02	0.42
1:A:364:ARG:NH1	2:B:1058:LYS:HB2	2.34	0.42
2:B:745:ASP:OD1	2:B:745:ASP:N	2.48	0.42
1:A:1193:VAL:HG13	1:A:1197:TYR:CE2	2.54	0.42
1:A:1231:ILE:O	1:A:1235:ILE:HG12	2.19	0.42
3:C:76:ASP:OD1	3:C:76:ASP:N	2.51	0.42
1:A:1036:ASN:HD21	4:E:204:ILE:HD12	1.83	0.42
5:F:107:ARG:H	5:F:107:ARG:HD3	1.85	0.42
8:J:8:PHE:CD2	8:J:48:MET:HE1	2.54	0.42
2:B:1035:ARG:HA	3:C:28:LEU:HD21	2.01	0.42
6:H:111:ARG:HH21	6:H:127:GLY:HA2	1.85	0.42
1:A:1243:LEU:HD12	1:A:1243:LEU:HA	1.84	0.42
1:A:1339:ASP:OD1	1:A:1339:ASP:N	2.52	0.42
1:A:401:ARG:HG3	1:A:402:LEU:HD22	2.01	0.42
1:A:1192:TRP:CE2	1:A:1248:ASN:HA	2.54	0.42
3:C:44:ILE:HA	3:C:79:VAL:HG11	2.01	0.42
1:A:606:HIS:HE1	1:A:641:CYS:HB3	1.85	0.41
1:A:904:GLN:OE1	1:A:1044:HIS:NE2	2.46	0.41
2:B:789:ASN:ND2	2:B:966:ILE:HG22	2.35	0.41
5:F:62:ARG:O	5:F:66:LEU:HD23	2.20	0.41
7:I:99:SER:OG	7:I:107:ALA:HB1	2.20	0.41
1:A:756:ALA:HB2	1:A:786:ALA:HB2	2.02	0.41
1:A:844:ARG:O	1:A:848:ILE:HG12	2.20	0.41
1:A:1309:MET:HG2	1:A:1334:TRP:CE3	2.55	0.41
2:B:331:THR:HG23	2:B:334:LYS:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1143:LEU:HD12	1:A:1148:ALA:HA	2.01	0.41
2:B:967:ILE:HD12	2:B:976:MET:HE1	2.02	0.41
6:H:89:GLU:HG3	6:H:146:LYS:HD2	2.02	0.41
11:M:147:PHE:CZ	11:M:151:ILE:HD11	2.55	0.41
1:A:653:VAL:HG11	1:A:669:TYR:OH	2.20	0.41
2:B:84:TYR:CZ	2:B:423:ILE:HD11	2.55	0.41
2:B:711:ILE:HG13	2:B:725:GLN:HG2	2.01	0.41
5:F:52:ILE:O	5:F:52:ILE:HG13	2.20	0.41
7:I:69:ILE:O	7:I:72:VAL:HG12	2.20	0.41
1:A:657:TYR:CE1	1:A:662:HIS:HB3	2.55	0.41
1:A:1177:TYR:OH	7:I:33:ARG:NH1	2.51	0.41
1:A:1353:ASP:HA	1:A:1354:PRO:HD3	1.91	0.41
2:B:816:GLU:N	2:B:816:GLU:OE1	2.53	0.41
2:B:860:VAL:HG11	2:B:866:ILE:HG22	2.01	0.41
2:B:1037:ILE:O	3:C:195:THR:HG22	2.20	0.41
3:C:37:VAL:HG21	3:C:252:LEU:HD13	2.03	0.41
6:H:30:CYS:HB2	6:H:39:LEU:HD23	2.02	0.41
6:H:96:VAL:HA	6:H:116:VAL:HA	2.01	0.41
2:B:237:VAL:HG12	2:B:372:LEU:HD22	2.01	0.41
3:C:8:THR:OG1	3:C:24:GLU:HB2	2.21	0.41
6:H:118:TYR:CZ	6:H:143:LEU:HB2	2.55	0.41
1:A:1228:MET:HB3	1:A:1247:PHE:HB2	2.01	0.41
2:B:347:MET:SD	2:B:361:LYS:HD3	2.60	0.41
2:B:819:SER:N	2:B:827:GLU:OE1	2.53	0.41
1:A:564:LEU:HD22	1:A:570:TRP:CE2	2.55	0.41
1:A:952:LEU:O	1:A:955:GLU:HG3	2.21	0.41
10:L:17:TYR:CE1	10:L:46:LYS:HB3	2.56	0.41
11:M:48:VAL:O	11:M:49:ARG:HG3	2.21	0.41
1:A:660:MET:CG	1:A:664:ILE:HD11	2.49	0.41
1:A:790:GLN:HA	1:A:822:PHE:HA	2.03	0.41
1:A:948:ILE:HG23	1:A:1007:ILE:CG1	2.51	0.41
1:A:1016:LEU:HD23	1:A:1045:LEU:HD21	2.01	0.41
1:A:1325:ASP:HB3	1:A:1327:GLU:OE1	2.21	0.41
2:B:116:ARG:CZ	10:L:42:ARG:NH1	2.83	0.41
2:B:506:TRP:NE1	2:B:697:GLU:OE2	2.43	0.41
2:B:604:ILE:HG12	2:B:668:LEU:HB3	2.02	0.41
2:B:782:ILE:HG23	2:B:967:ILE:HG13	2.03	0.41
4:E:26:TYR:HB3	4:E:62:VAL:HB	2.03	0.41
11:M:59:LEU:O	11:M:63:GLU:OE1	2.39	0.41
1:A:802:PHE:HB3	2:B:671:GLU:HG3	2.03	0.41
6:H:28:LEU:HD22	6:H:43:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:49:LEU:HD12	8:J:49:LEU:HA	1.85	0.41
1:A:870:SER:HB2	1:A:882:SER:HB3	2.03	0.40
1:A:875:TYR:HA	1:A:1083:PRO:HB3	2.02	0.40
2:B:910:THR:HG22	2:B:911:LEU:N	2.36	0.40
1:A:583:ARG:HG3	1:A:585:LEU:HG	2.03	0.40
1:A:784:VAL:HG13	2:B:978:ILE:HD13	2.04	0.40
1:A:1216:LEU:HB2	1:A:1255:LEU:CD1	2.51	0.40
2:B:153:PRO:HG2	2:B:448:LEU:HD12	2.04	0.40
2:B:155:MET:HB2	2:B:185:PHE:CE2	2.55	0.40
3:C:35:ARG:HG2	3:C:182:VAL:HG11	2.02	0.40
1:A:403:GLN:HA	1:A:406:VAL:HG12	2.03	0.40
1:A:890:ARG:HB3	1:A:895:GLY:N	2.35	0.40
4:E:106:VAL:HG21	4:E:109:GLY:HA2	2.03	0.40
1:A:831:LEU:HG	2:B:715:ASP:O	2.21	0.40
2:B:747:LEU:HD13	2:B:810:PHE:CE1	2.56	0.40
11:M:59:LEU:O	11:M:62:VAL:HB	2.20	0.40
11:M:69:ASN:OD1	11:M:69:ASN:N	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	972/1970 (49%)	921 (95%)	51 (5%)	0	100	100
2	B	963/1174 (82%)	912 (95%)	51 (5%)	0	100	100
3	C	253/271 (93%)	244 (96%)	9 (4%)	0	100	100
4	E	207/210 (99%)	201 (97%)	6 (3%)	0	100	100
5	F	76/127 (60%)	73 (96%)	3 (4%)	0	100	100
6	H	146/150 (97%)	138 (94%)	8 (6%)	0	100	100
7	I	113/125 (90%)	106 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	J	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
9	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
10	L	42/58 (72%)	41 (98%)	1 (2%)	0	100	100
11	M	106/612 (17%)	100 (94%)	6 (6%)	0	100	100
All	All	3056/4881 (63%)	2908 (95%)	148 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	875/1749 (50%)	874 (100%)	1 (0%)	88	97
2	B	866/1027 (84%)	866 (100%)	0	100	100
3	C	234/248 (94%)	233 (100%)	1 (0%)	84	94
4	E	191/192 (100%)	191 (100%)	0	100	100
5	F	68/111 (61%)	68 (100%)	0	100	100
6	H	128/131 (98%)	128 (100%)	0	100	100
7	I	104/112 (93%)	104 (100%)	0	100	100
8	J	56/56 (100%)	56 (100%)	0	100	100
9	K	104/106 (98%)	104 (100%)	0	100	100
10	L	41/55 (74%)	41 (100%)	0	100	100
11	M	99/561 (18%)	99 (100%)	0	100	100
All	All	2766/4348 (64%)	2764 (100%)	2 (0%)	87	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1093	GLN
3	C	260	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	792	ASN
1	A	947	HIS
1	A	982	ASN
1	A	1093	GLN
1	A	1190	GLN
1	A	1248	ASN
1	A	1291	ASN
1	A	1299	GLN
1	A	1303	GLN
1	A	1394	ASN
2	B	98	HIS
2	B	370	HIS
2	B	468	GLN
2	B	717	ASN
2	B	755	GLN
2	B	986	GLN
2	B	992	ASN
3	C	25	ASN
3	C	60	HIS
4	E	30	GLN
4	E	108	GLN
4	E	132	GLN
4	E	210	GLN
9	K	2	ASN
11	M	138	ASN
11	M	142	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

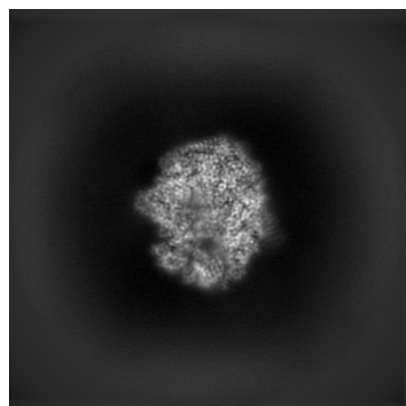
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12087. These allow visual inspection of the internal detail of the map and identification of artifacts.

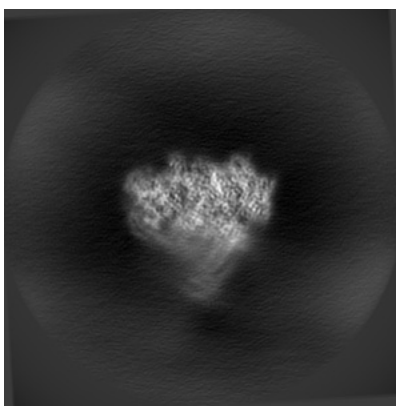
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

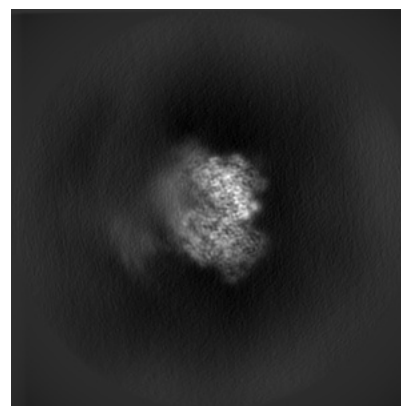
6.1.1 Primary map



X

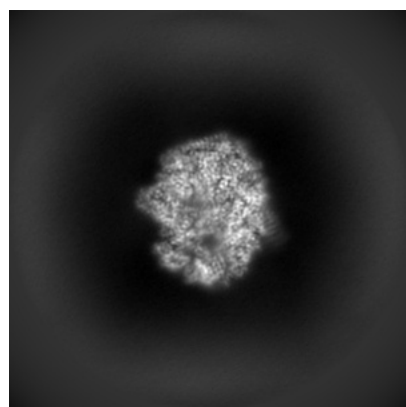


Y

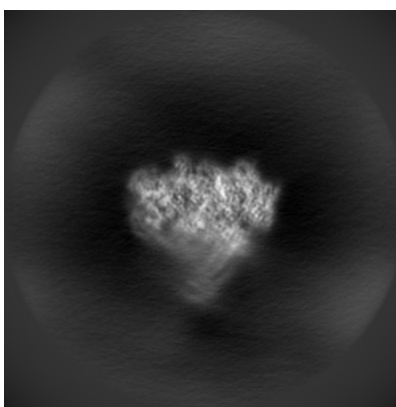


Z

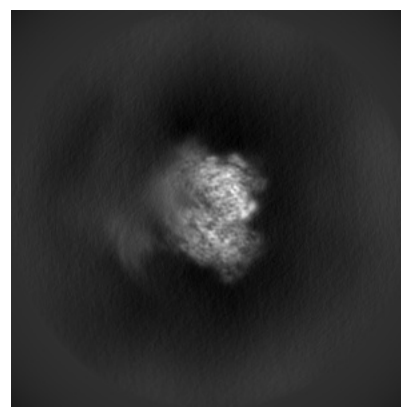
6.1.2 Raw map



X



Y

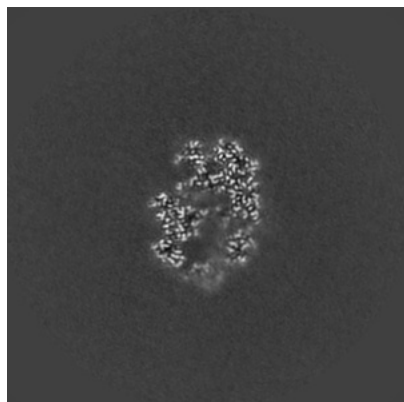


Z

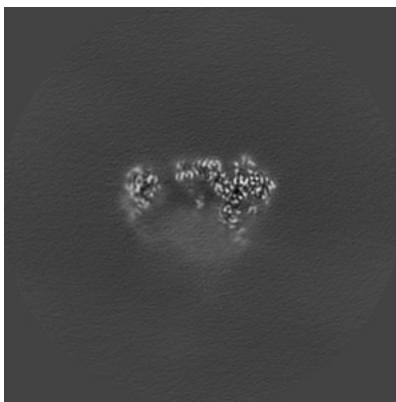
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

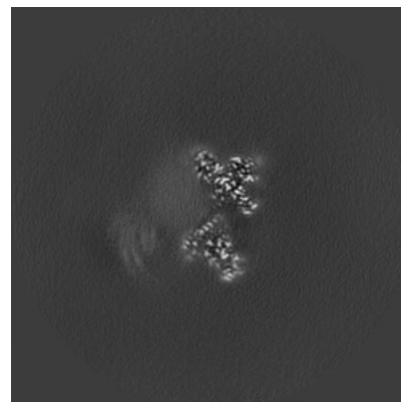
6.2.1 Primary map



X Index: 180

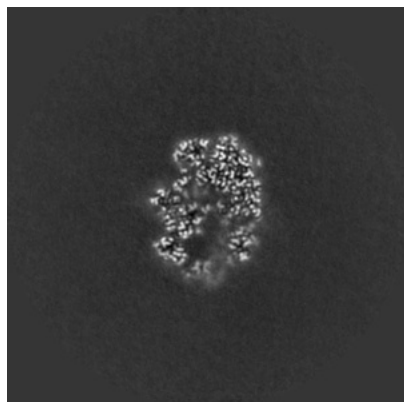


Y Index: 180

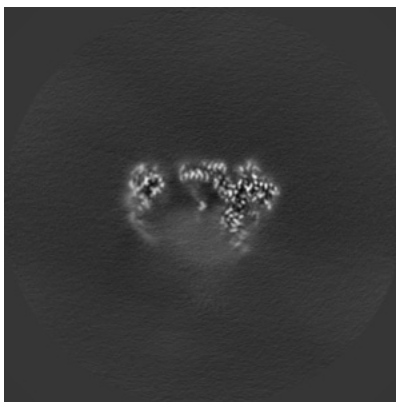


Z Index: 180

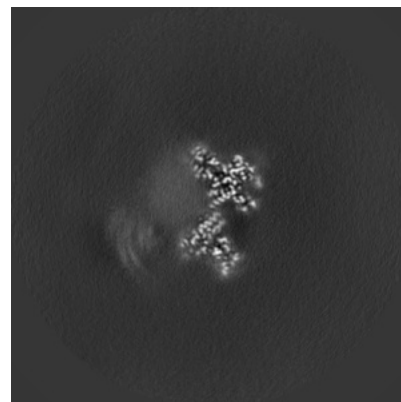
6.2.2 Raw map



X Index: 180



Y Index: 180

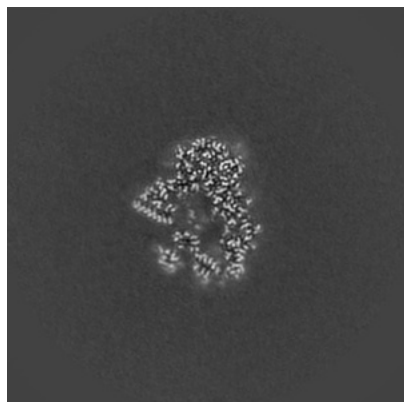


Z Index: 180

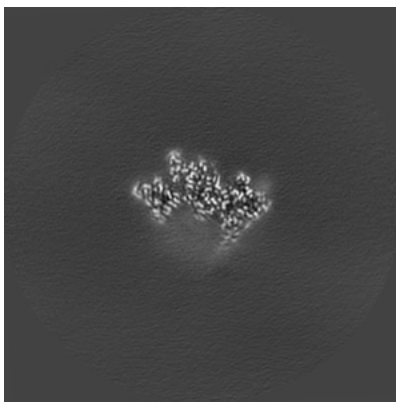
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

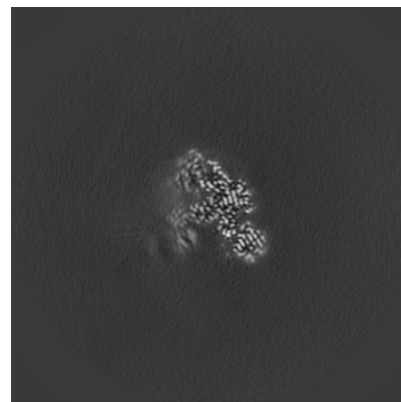
6.3.1 Primary map



X Index: 194

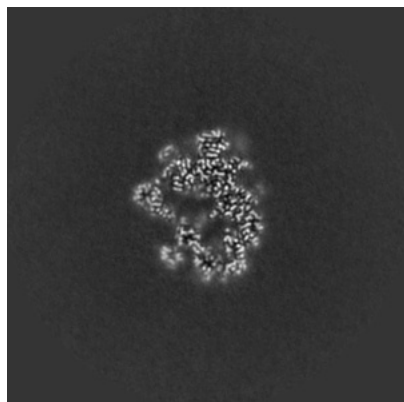


Y Index: 206

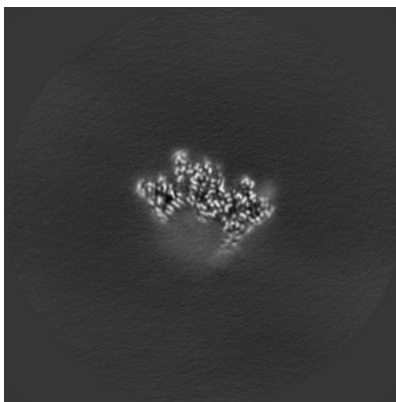


Z Index: 206

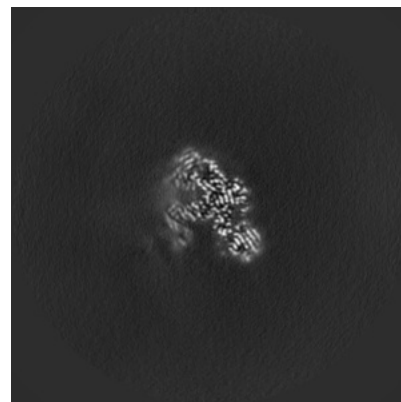
6.3.2 Raw map



X Index: 197



Y Index: 207

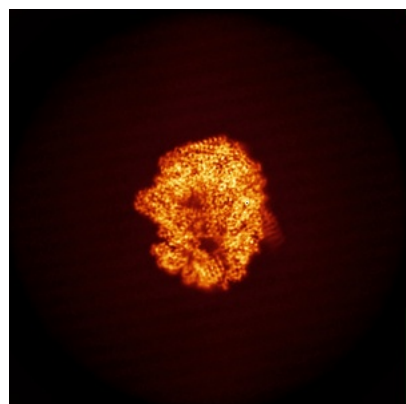


Z Index: 209

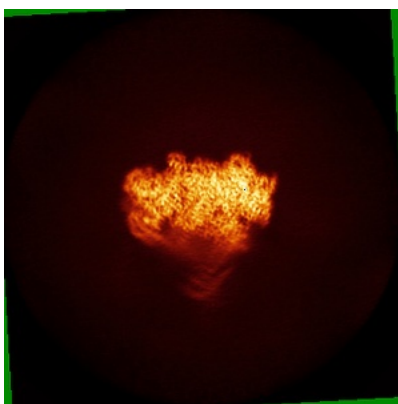
The images above show the largest variance slices of the map in three orthogonal directions.

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

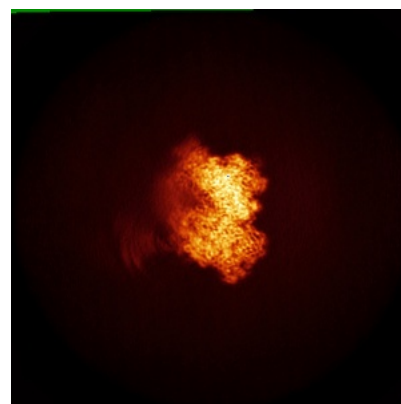
6.4.1 Primary map



X

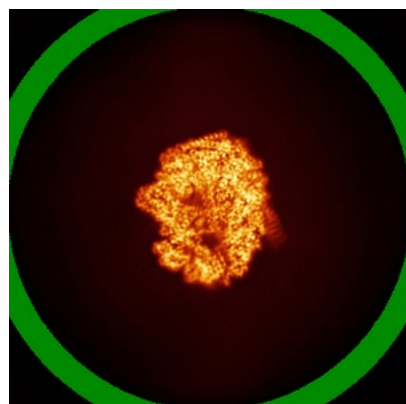


Y

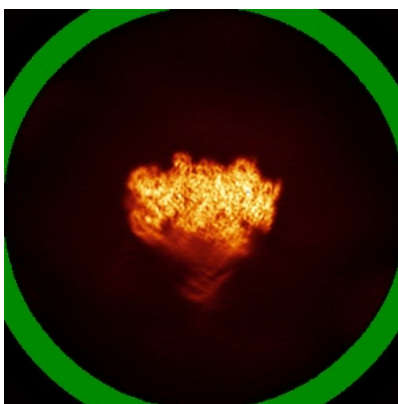


Z

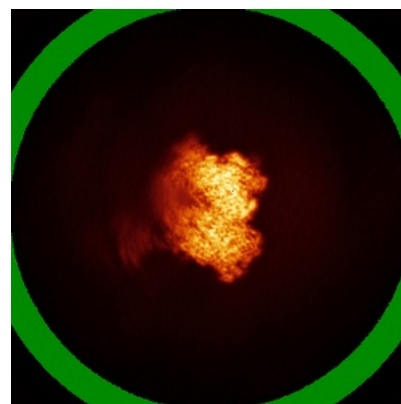
6.4.2 Raw map



X



Y

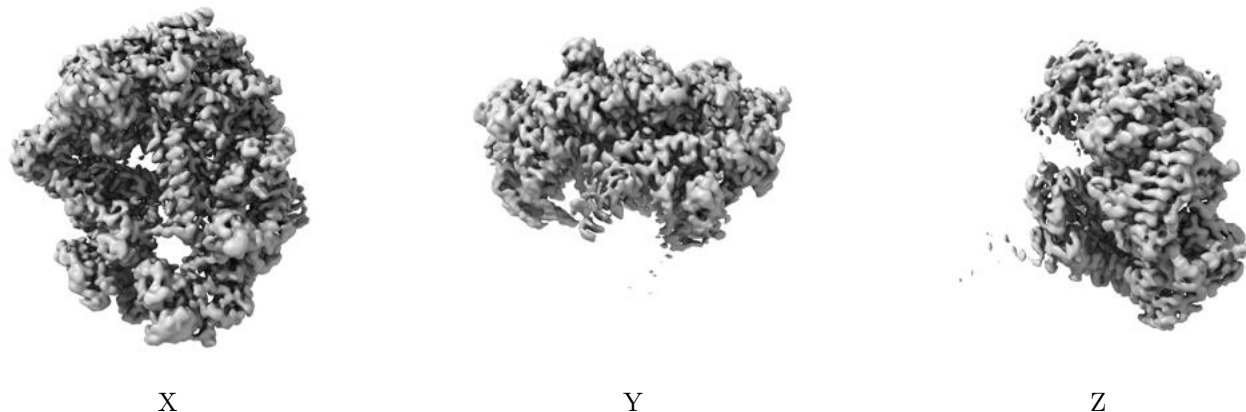


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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



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.

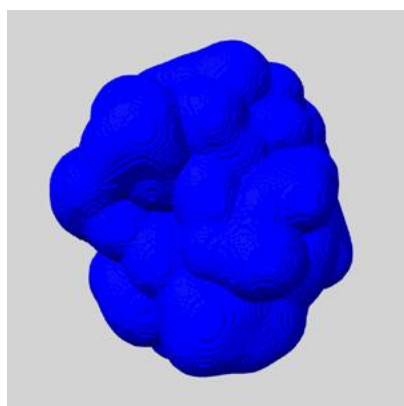
6.6 Mask visualisation [i](#)

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

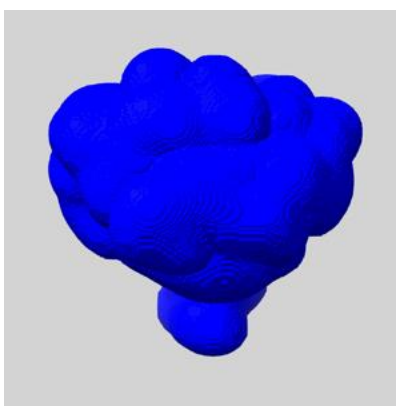
A mask typically either:

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

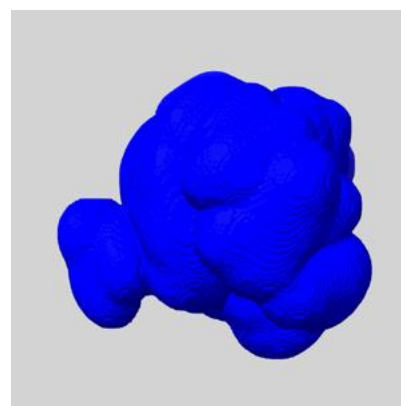
6.6.1 emd_12087_msk_1.map [i](#)



X



Y

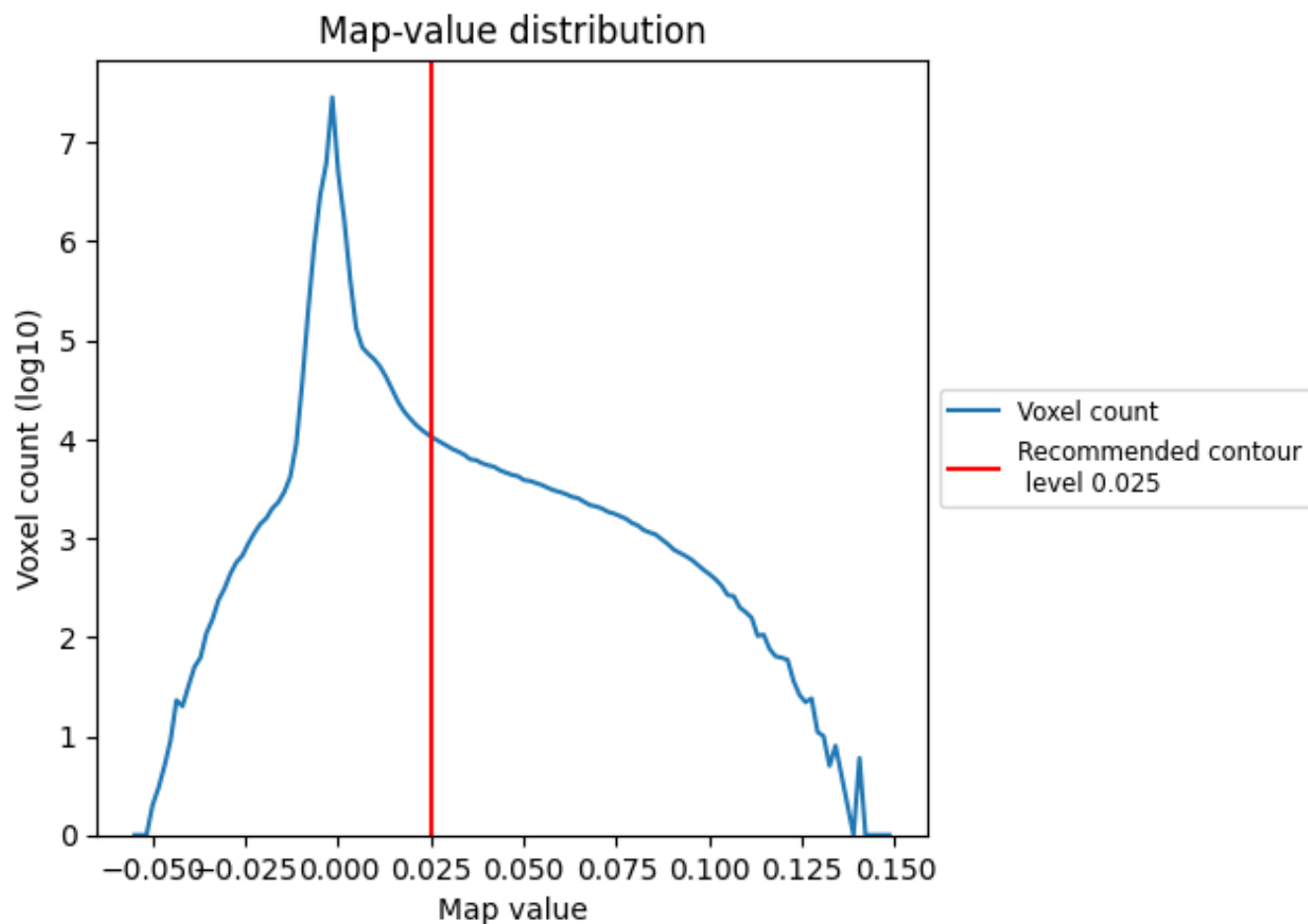


Z

7 Map analysis [i](#)

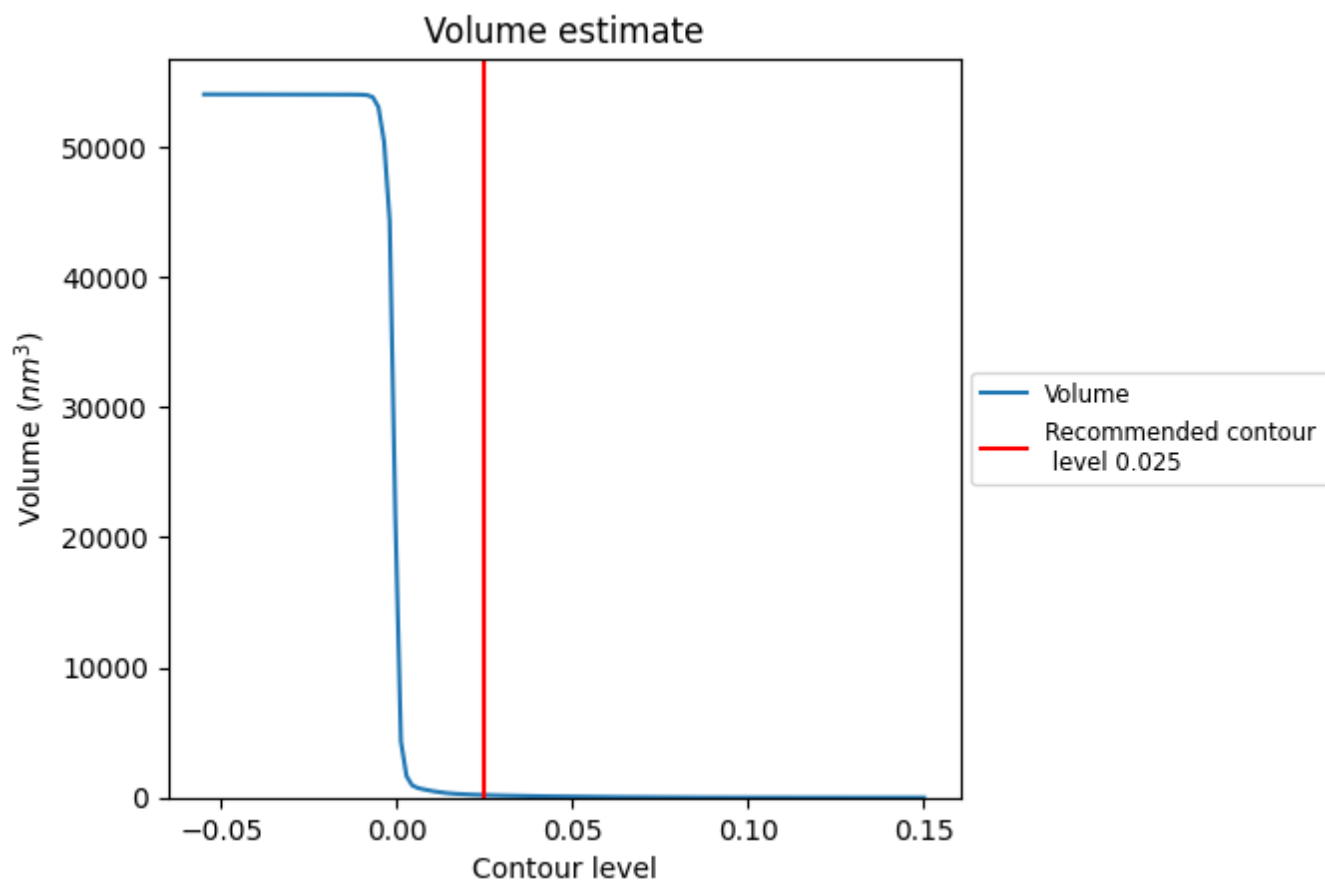
This section contains the results of statistical analysis of the map.

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.

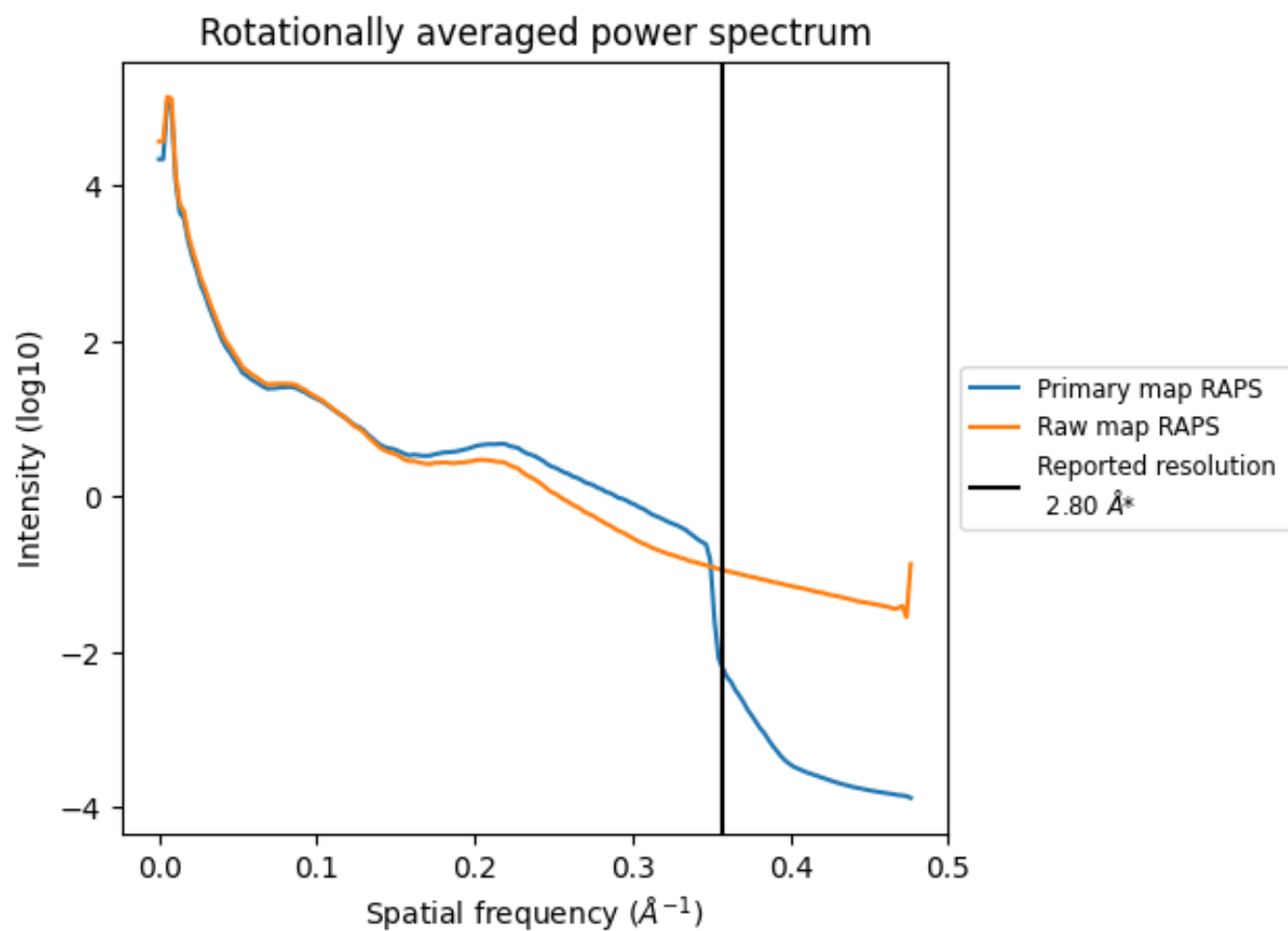
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 192 nm^3 ; this corresponds to an approximate mass of 174 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 ⓘ

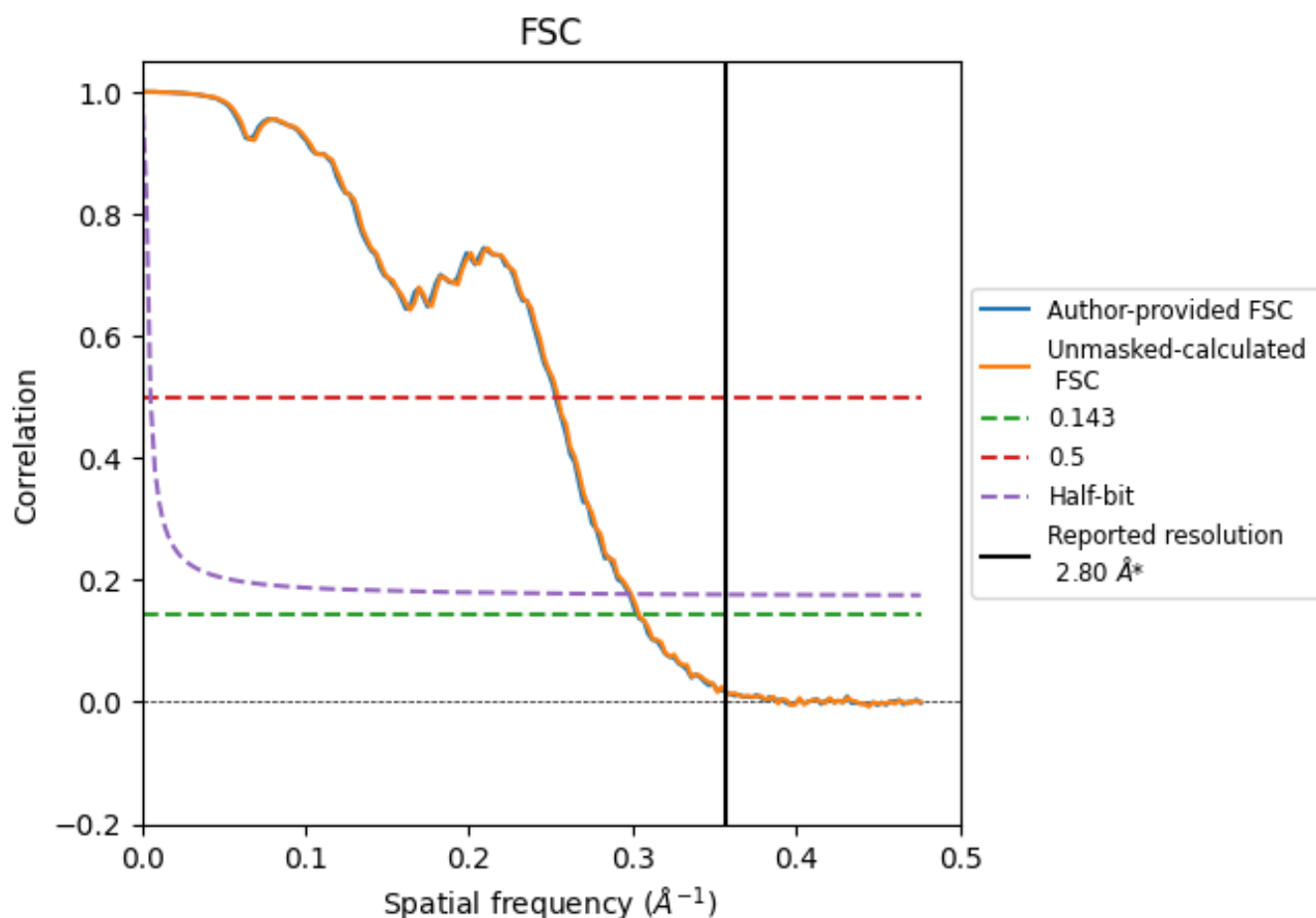


*Reported resolution corresponds to spatial frequency of $0.357 \text{ \AA}^{-1}$

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 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	3.30	3.95	3.36
Unmasked-calculated*	3.29	3.93	3.34

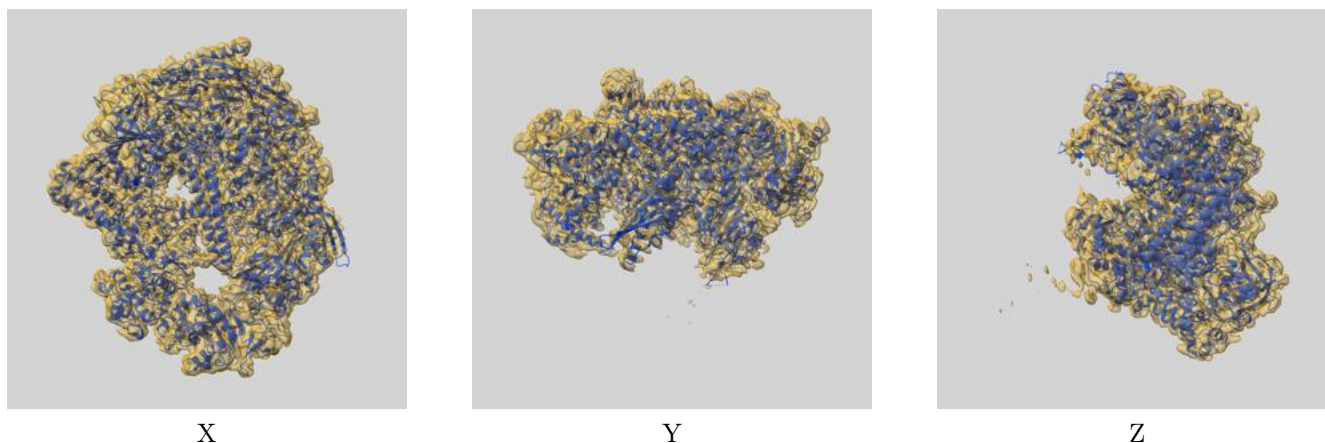
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.30 differs from the reported value 2.8 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.29 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

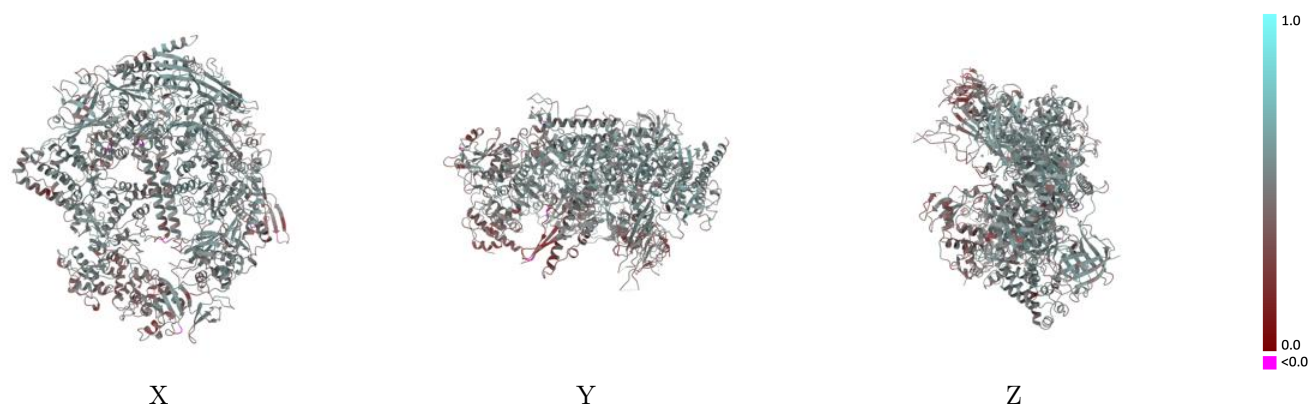
This section contains information regarding the fit between EMDB map EMD-12087 and PDB model 7B7U. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



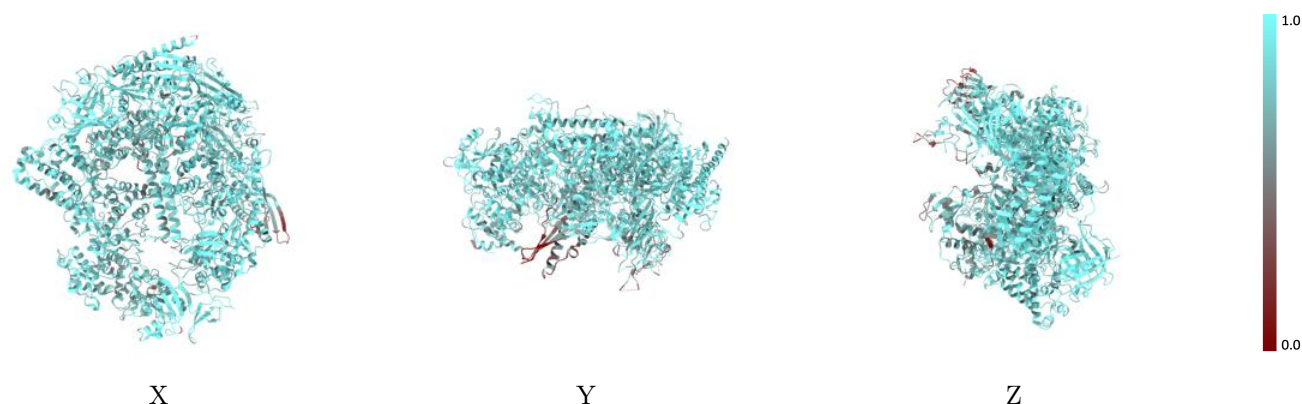
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



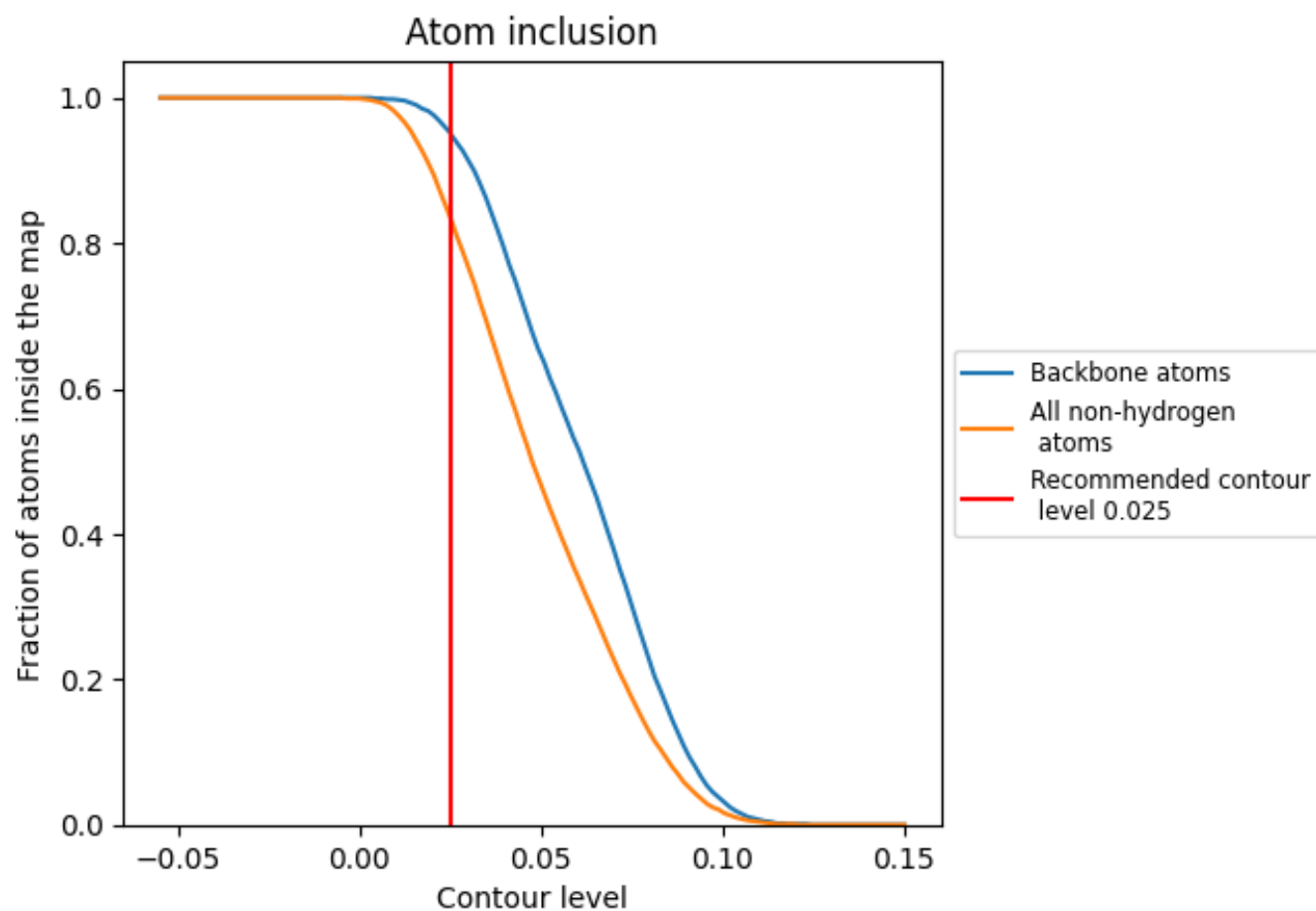
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 84% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8360	0.4830
A	0.8270	0.4820
B	0.8180	0.4910
C	0.9000	0.5280
E	0.8710	0.4800
F	0.7200	0.4230
H	0.8870	0.4960
I	0.8500	0.4490
J	0.8910	0.5300
K	0.8700	0.5020
L	0.8060	0.3960
M	0.7870	0.3680
N	0.8870	0.4460

1.0

0.0

<0.0