Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 11:13 pm GMT

PDB ID	:	7B7U
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:

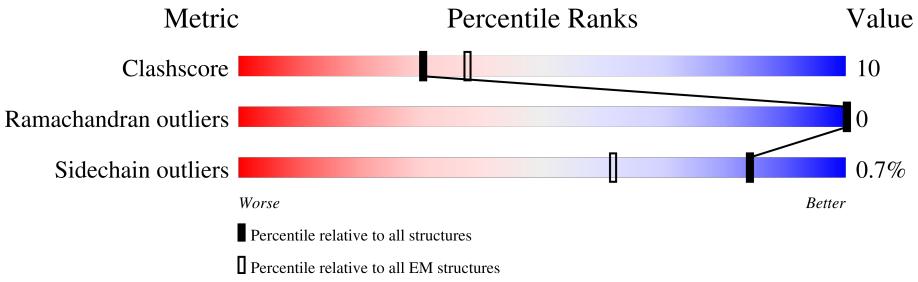
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	37% 13% 50%
2	B	1174	6% 63% 20% 17%
3	C	271	68% 27% 5%
4	E	210	81% 17%
5	F	127	6% 42% 19% 39%
6	H	150	65% 33%
7	I	125	70% 20% 8%
8	J	67	85% 15%

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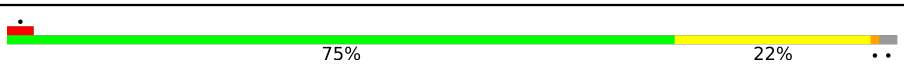
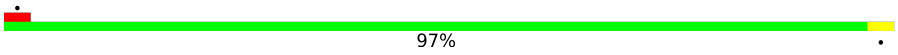
Mol	Chain	Length	Quality of chain
9	K	117	
10	L	58	
11	M	612	
12	N	30	

2 Entry composition (i)

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
			Total	C	N	O	S		
1	A	986	7861	4957	1388	1478	38	0	0

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 (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

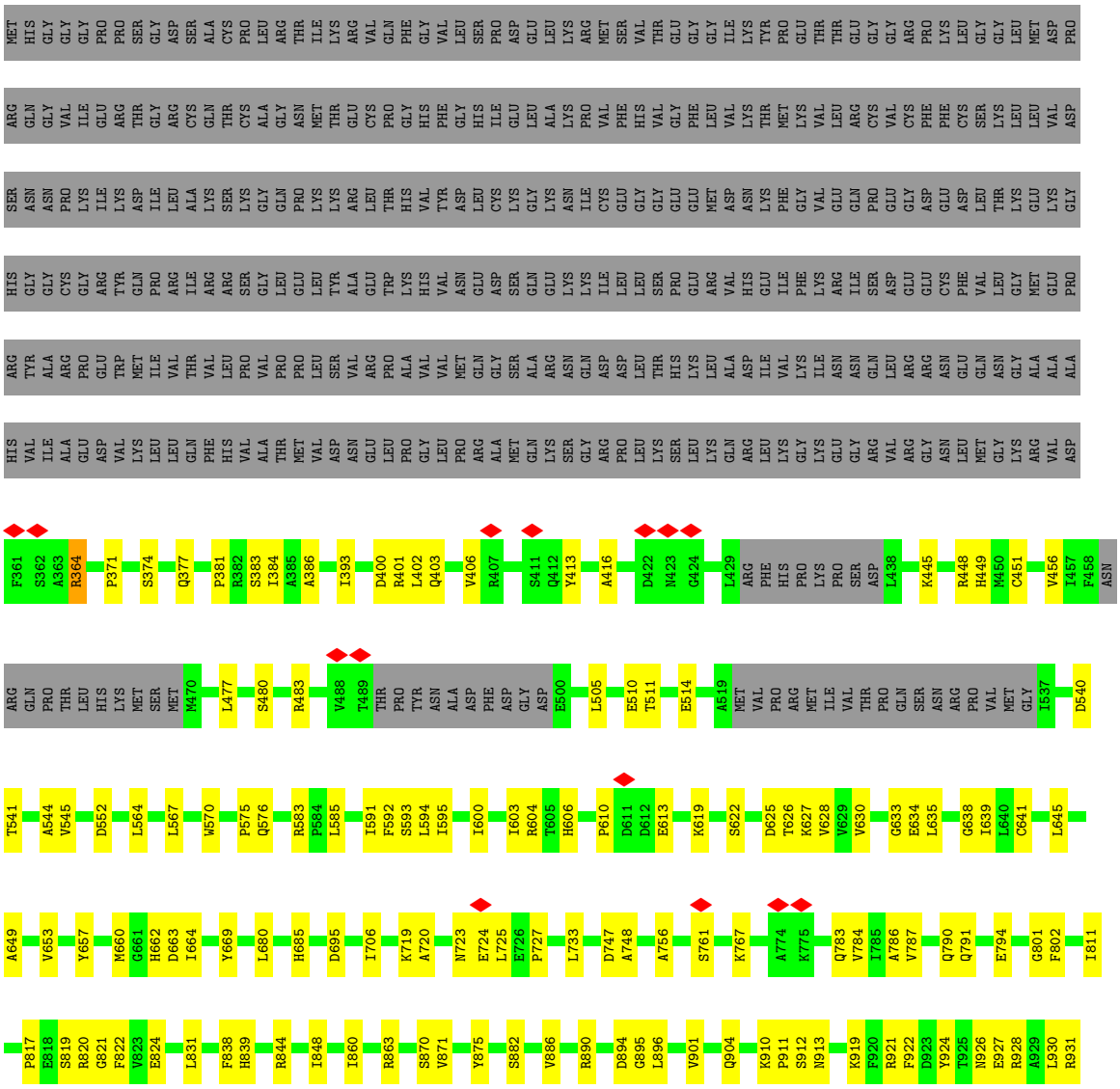
Mol	Chain	Residues	Atoms		AltConf
13	C	1	Total	Zn	0
			1	1	
13	I	2	Total	Zn	0
			2	2	
13	J	1	Total	Zn	0
			1	1	
13	L	1	Total	Zn	0
			1	1	
13	M	1	Total	Zn	0
			1	1	

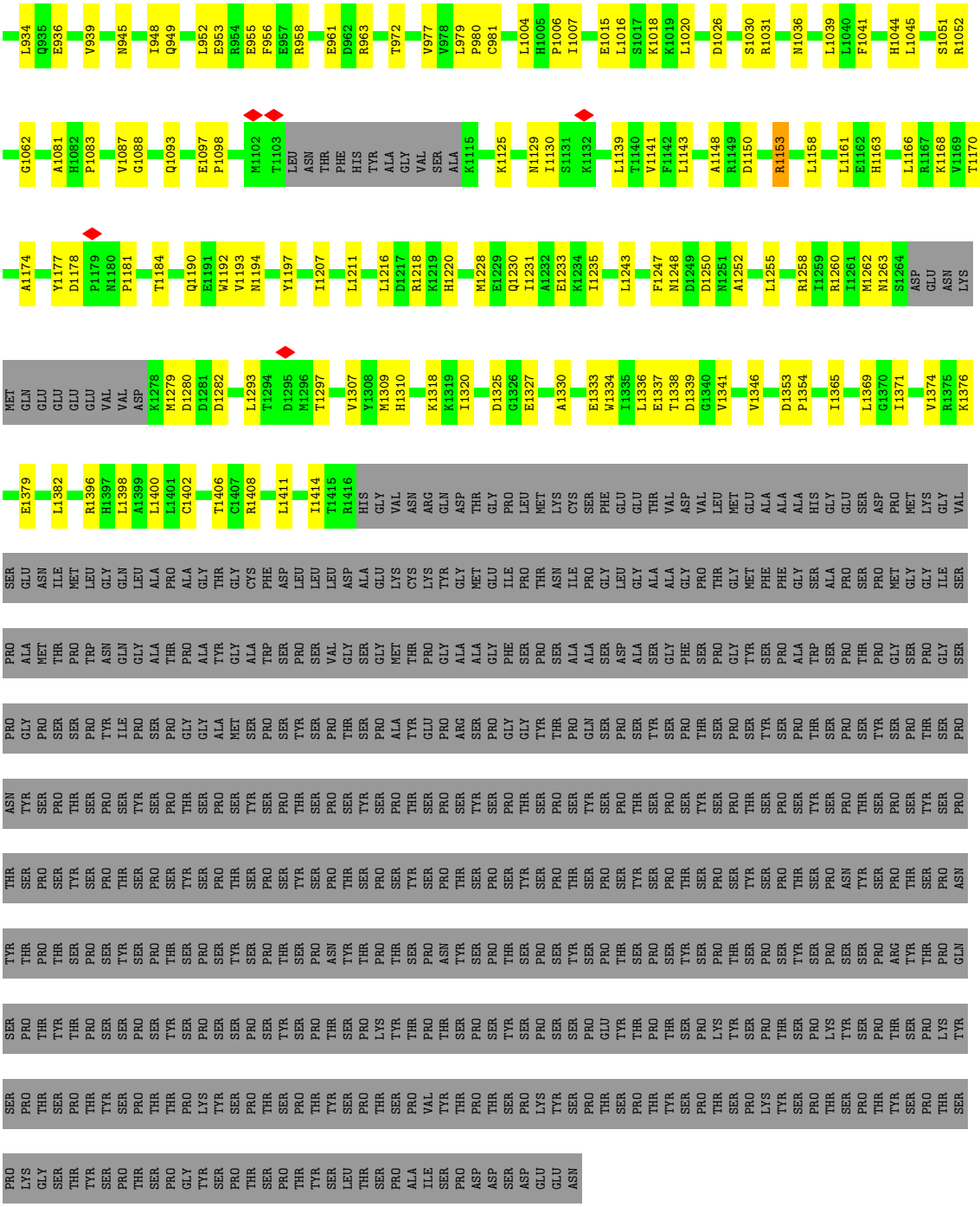
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-directed RNA polymerase subunit

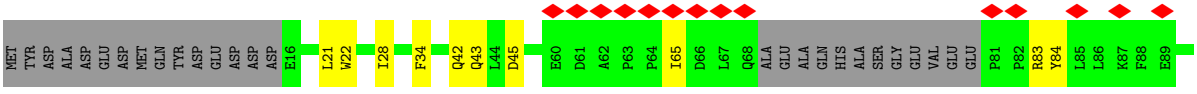
Chain A:

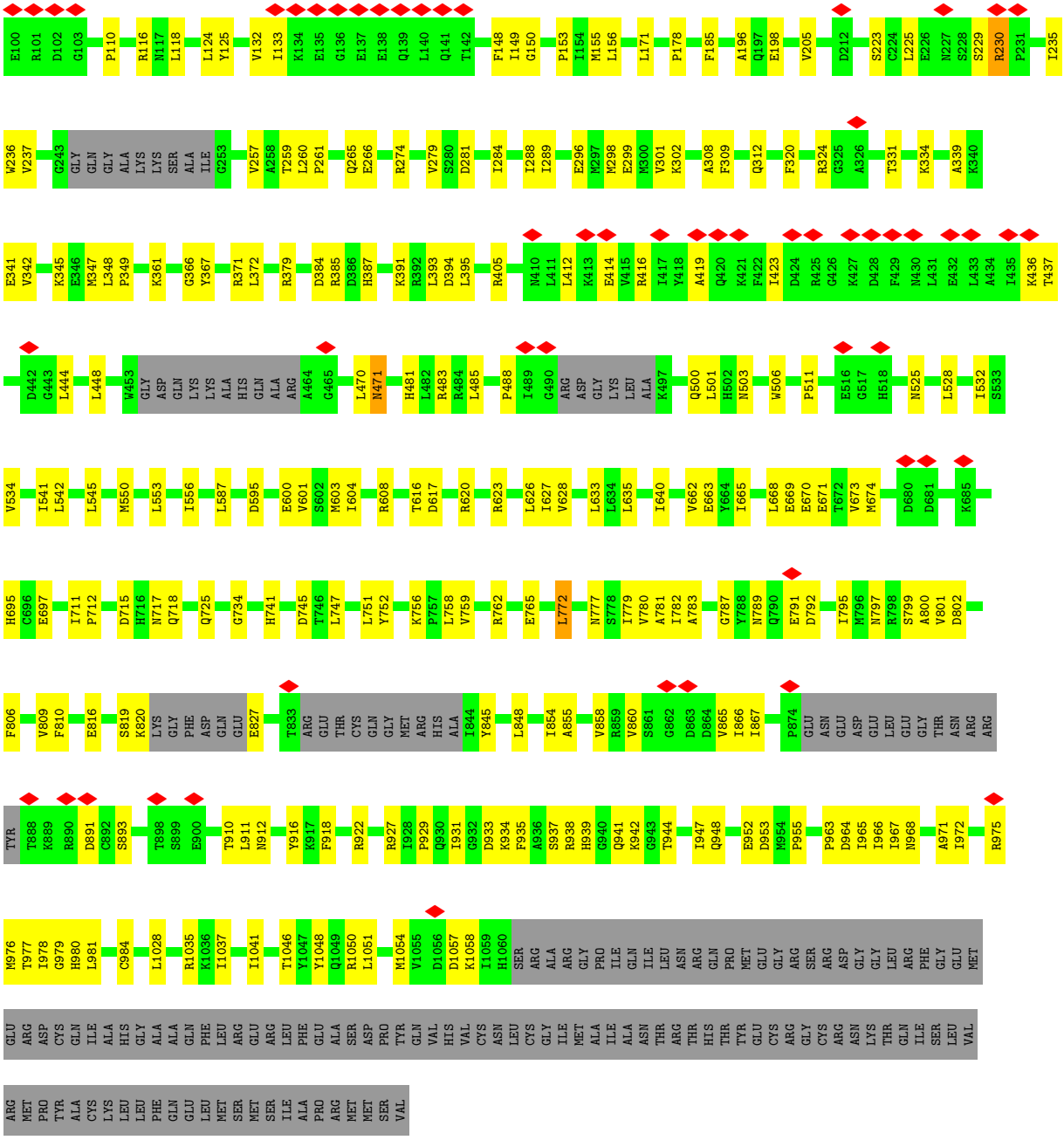




• Molecule 2: DNA-directed RNA polymerase subunit beta

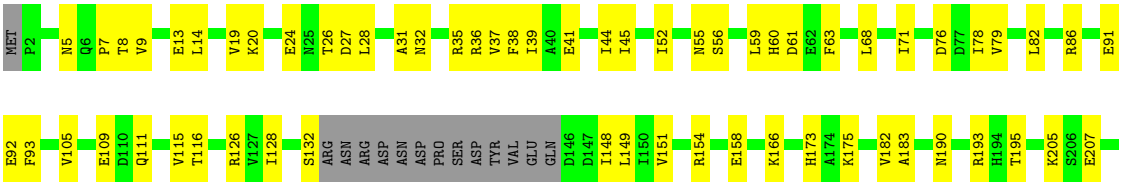
Chain B:

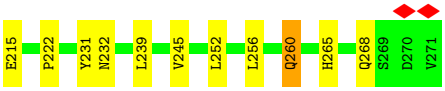




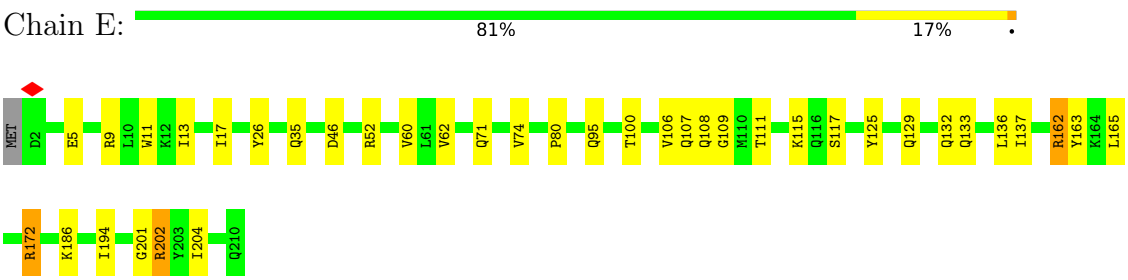
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:

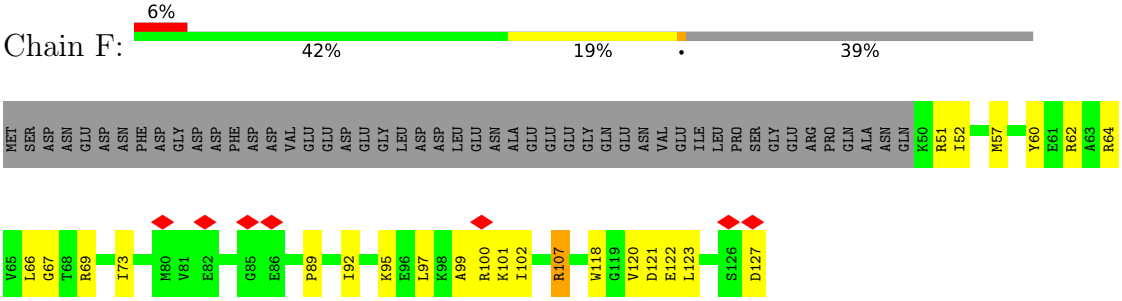




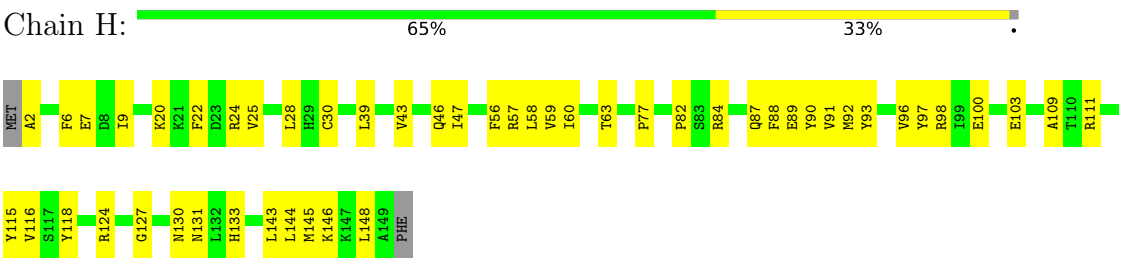
• Molecule 4: DNA-directed RNA polymerase II subunit E



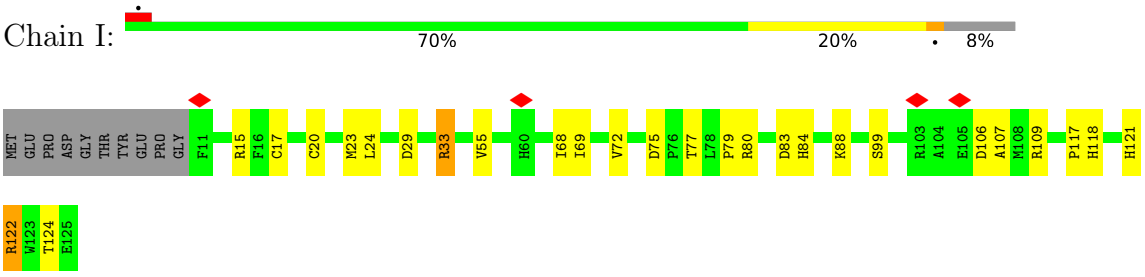
• Molecule 5: DNA-directed RNA polymerase II subunit F



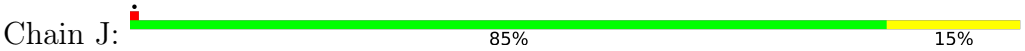
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

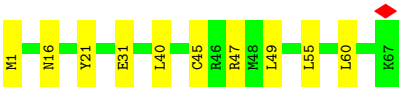


• Molecule 7: DNA-directed RNA polymerase II subunit RPB9

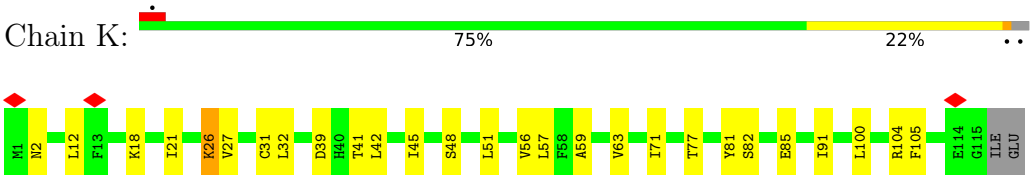


• Molecule 8: Uncharacterized Protein

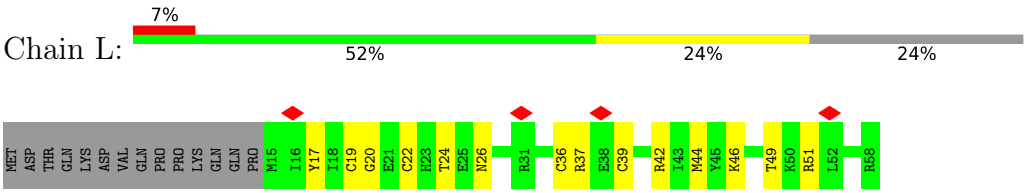




• Molecule 9: RNA_pol_L_2 domain-containing protein



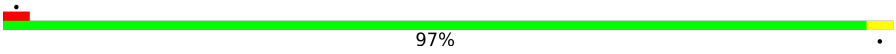
• Molecule 10: RNA polymerase II subunit K

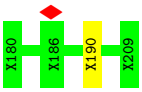


• Molecule 11: Putative RNA polymerase II subunit B1 CTD phosphatase RPAP2

• Molecule 12: Unknown

Chain N:





4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	377.99997, 377.99997, 377.99997	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	0.24	0/7997	0.43	0/10805
2	B	0.25	0/7999	0.43	1/10808 (0.0%)
3	C	0.24	0/2102	0.42	0/2857
4	E	0.24	0/1751	0.44	0/2366
5	F	0.24	0/636	0.47	0/859
6	H	0.25	0/1204	0.47	1/1623 (0.1%)
7	I	0.25	0/960	0.46	0/1300
8	J	0.27	0/542	0.42	0/730
9	K	0.25	0/939	0.41	0/1271
10	L	0.27	0/377	0.53	0/500
11	M	0.27	0/897	0.48	0/1204
All	All	0.25	0/25404	0.44	2/34323 (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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	82	PRO	N-CA-CB	5.47	109.86	103.30
2	B	772	LEU	CA-CB-CG	5.15	127.14	115.30

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7861	0	7914	171	0
2	B	7842	0	7881	171	0
3	C	2059	0	2007	52	0
4	E	1720	0	1737	27	0
5	F	626	0	657	16	0
6	H	1184	0	1141	36	0
7	I	938	0	872	17	0
8	J	533	0	553	8	0
9	K	920	0	942	21	0
10	L	372	0	378	12	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	497	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 (497) 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
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
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
1:A:1207:ILE:HA	1:A:1262:MET:HE1	1.78	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
3:C:190:ASN:O	3:C:193:ARG:NH1	2.30	0.64
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
10:L:22:CYS:SG	10:L:24:THR:OG1	2.53	0.60
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
2:B:309:PHE:O	2:B:312:GLN:NE2	2.35	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1307:VAL:HG13	1:A:1338:THR:HG22	1.87	0.55
2:B:471:ASN:H	2:B:481:HIS:HD1	1.54	0.55
1:A:794:GLU:OE2	2:B:500:GLN:NE2	2.40	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
3:C:91:GLU:CD	3:C:92:GLU:H	2.11	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
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
1:A:761:SER:O	1:A:767:LYS:NZ	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:56:SER:HB2	3:C:158:GLU:H	1.74	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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:867:ILE:O	2:B:893:SER:OG	2.21	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
3:C:45:ILE:HG13	3:C:79:VAL:HG12	1.96	0.47
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
2:B:595:ASP:OD1	2:B:595:ASP:N	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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: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
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
1:A:886:VAL:HG21	4:E:165:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
2:B:229:SER:C	2:B:230:ARG:HD3	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:1282:ASP:N	1:A:1282:ASP:OD1	2.52	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
2:B:470:LEU:HD12	2:B:481:HIS:HD1	1.85	0.41
1:A:1143:LEU:HD12	1:A:1148:ALA:HA	2.01	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:HG13	5:F:52:ILE:O	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:924:TYR:OH	1:A:953:GLU:OE2	2.22	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
2:B:820:LYS:HZ1	2:B:827:GLU:N	2.19	0.41
3:C:8:THR:OG1	3:C:24:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:111:THR:OG1	11:M:93:GLU:OE2	2.27	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
1:A:1402:CYS:O	1:A:1406:THR:OG1	2.34	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
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
11:M:69:ASN:OD1	11:M:69:ASN:N	2.52	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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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
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%)	870 (99%)	5 (1%)	86	96
2	B	866/1027 (84%)	864 (100%)	2 (0%)	93	98
3	C	234/248 (94%)	232 (99%)	2 (1%)	78	94

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	E	191/192 (100%)	187 (98%)	4 (2%)	53 84
5	F	68/111 (61%)	67 (98%)	1 (2%)	65 89
6	H	128/131 (98%)	128 (100%)	0	100 100
7	I	104/112 (93%)	102 (98%)	2 (2%)	57 85
8	J	56/56 (100%)	56 (100%)	0	100 100
9	K	104/106 (98%)	103 (99%)	1 (1%)	76 93
10	L	41/55 (74%)	41 (100%)	0	100 100
11	M	99/561 (18%)	98 (99%)	1 (1%)	76 93
All	All	2766/4348 (64%)	2748 (99%)	18 (1%)	84 95

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	364	ARG
1	A	619	LYS
1	A	928	ARG
1	A	1093	GLN
1	A	1153	ARG
2	B	230	ARG
2	B	471	ASN
3	C	86	ARG
3	C	260	GLN
4	E	162	ARG
4	E	172	ARG
4	E	186	LYS
4	E	202	ARG
5	F	107	ARG
7	I	33	ARG
7	I	122	ARG
9	K	26	LYS
11	M	56	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	468	GLN
2	B	582	GLN
2	B	717	ASN

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Mol	Chain	Res	Type
3	C	60	HIS
4	E	108	GLN
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 monosaccharides 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.

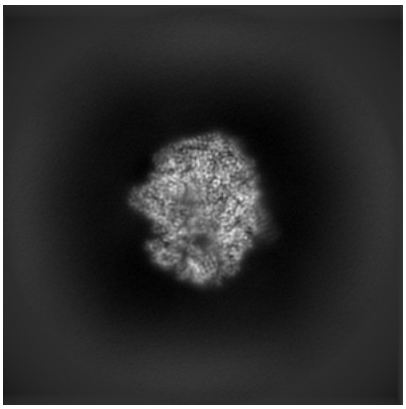
6 Map visualisation

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.

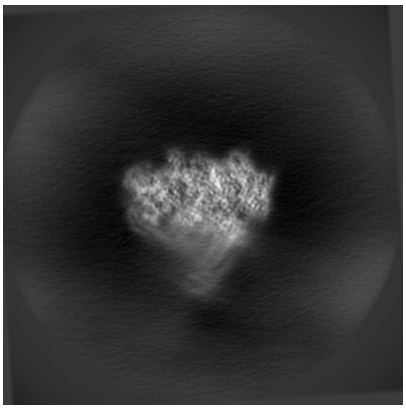
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

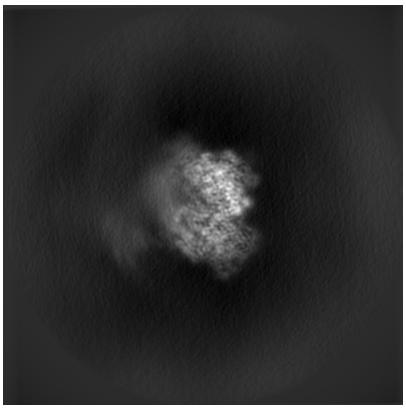
6.1.1 Primary map



X

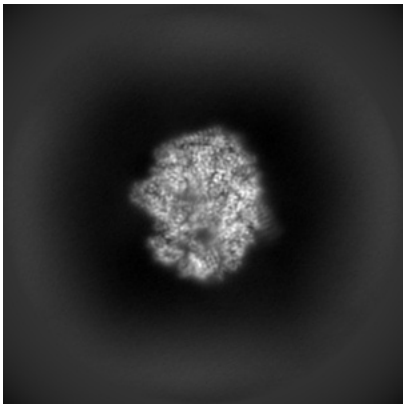


Y

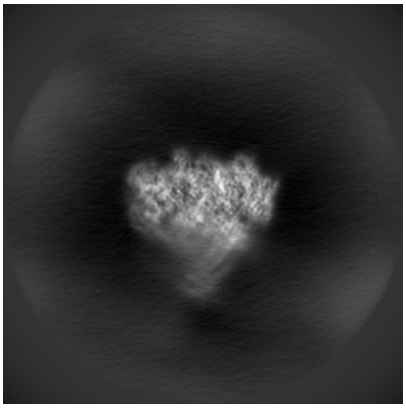


Z

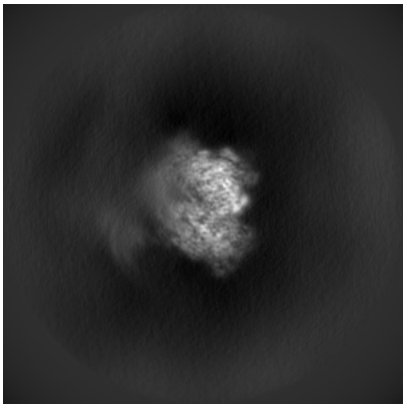
6.1.2 Raw map



X



Y

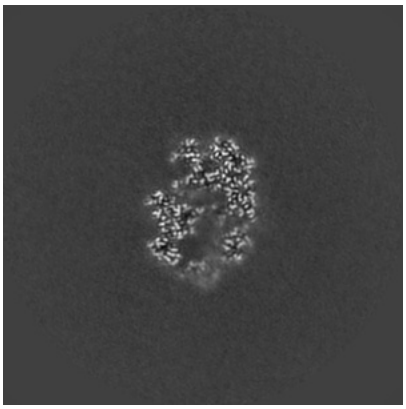


Z

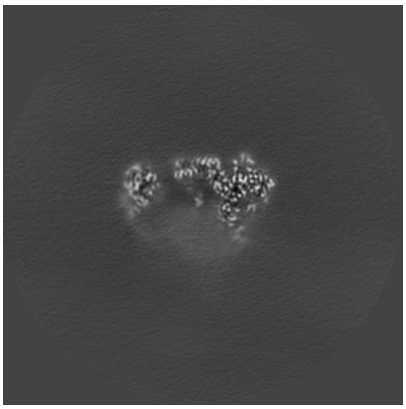
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

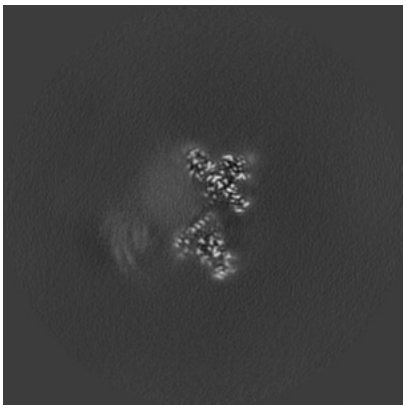
6.2.1 Primary map



X Index: 180

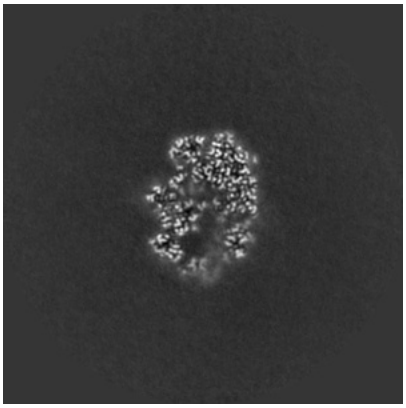


Y Index: 180

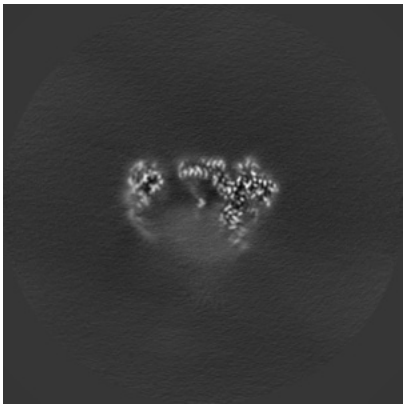


Z Index: 180

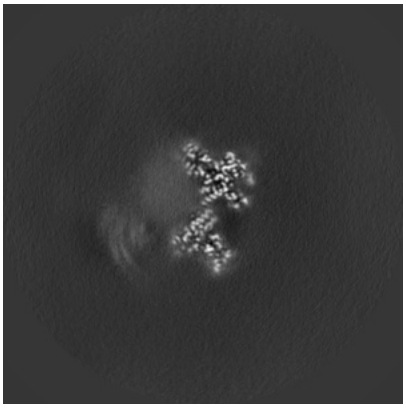
6.2.2 Raw map



X Index: 180



Y Index: 180

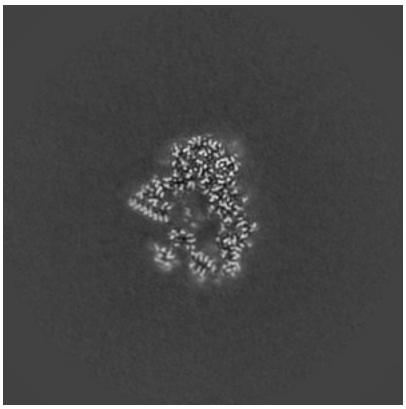


Z Index: 180

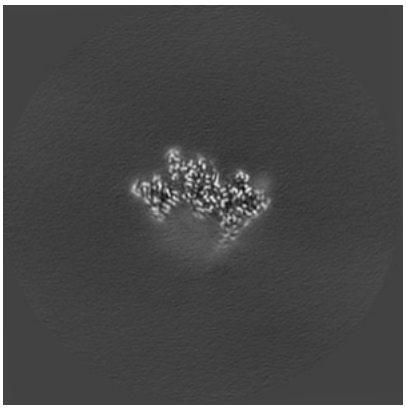
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

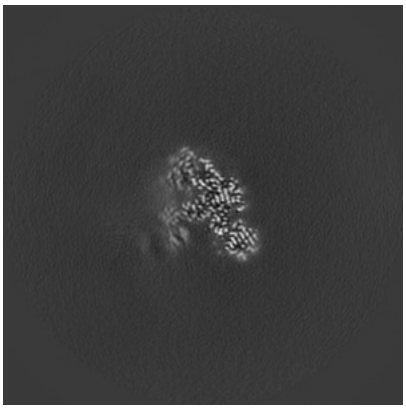
6.3.1 Primary map



X Index: 194

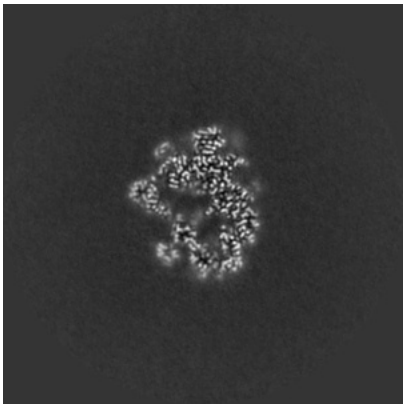


Y Index: 206

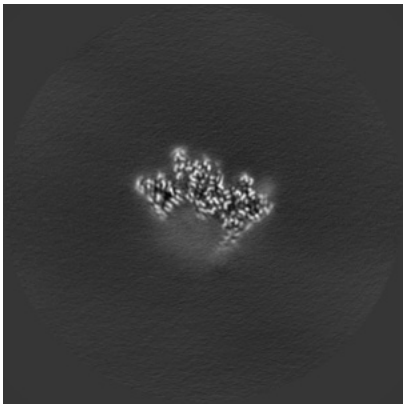


Z Index: 206

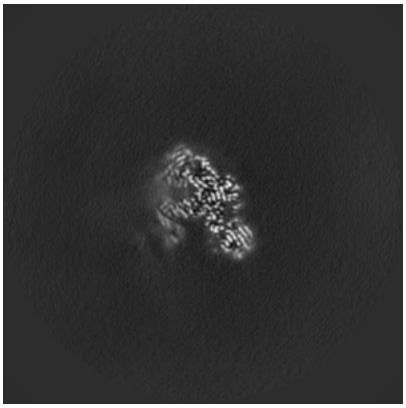
6.3.2 Raw map



X Index: 197



Y Index: 207

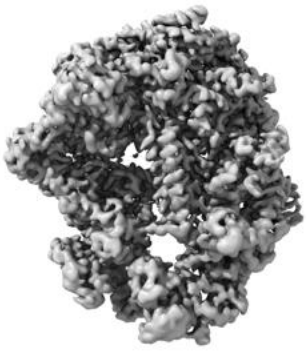


Z Index: 209

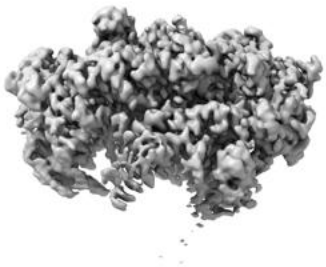
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

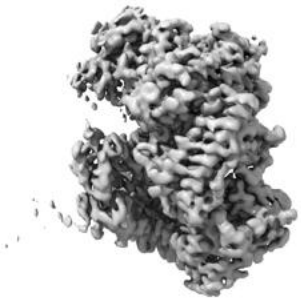
6.4.1 Primary map



X



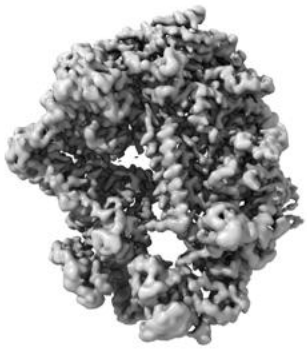
Y



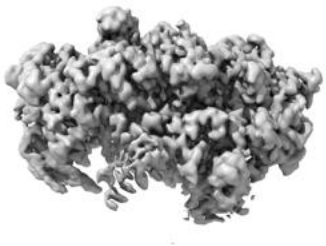
Z

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.

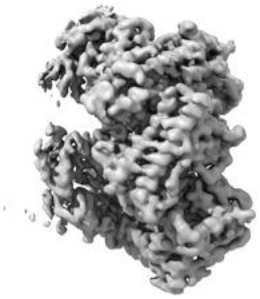
6.4.2 Raw map



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.

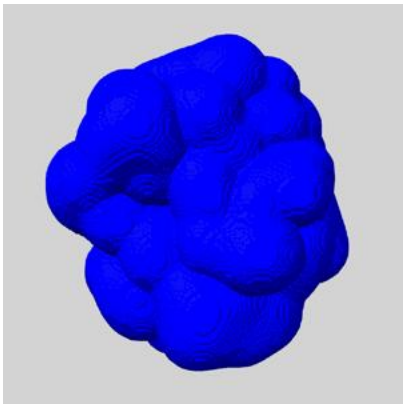
6.5 Mask visualisation (i)

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

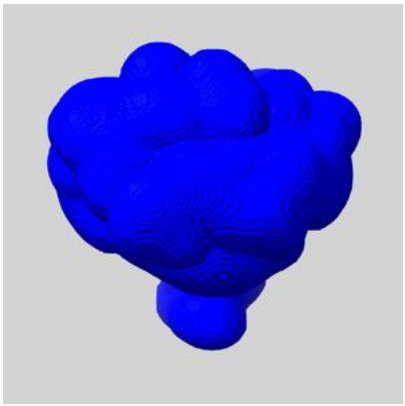
A mask typically either:

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

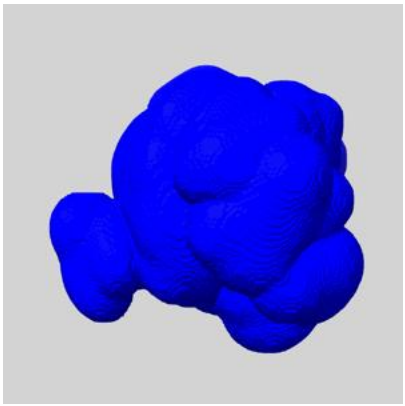
6.5.1 emd_12087_msk_1.map (i)



X



Y

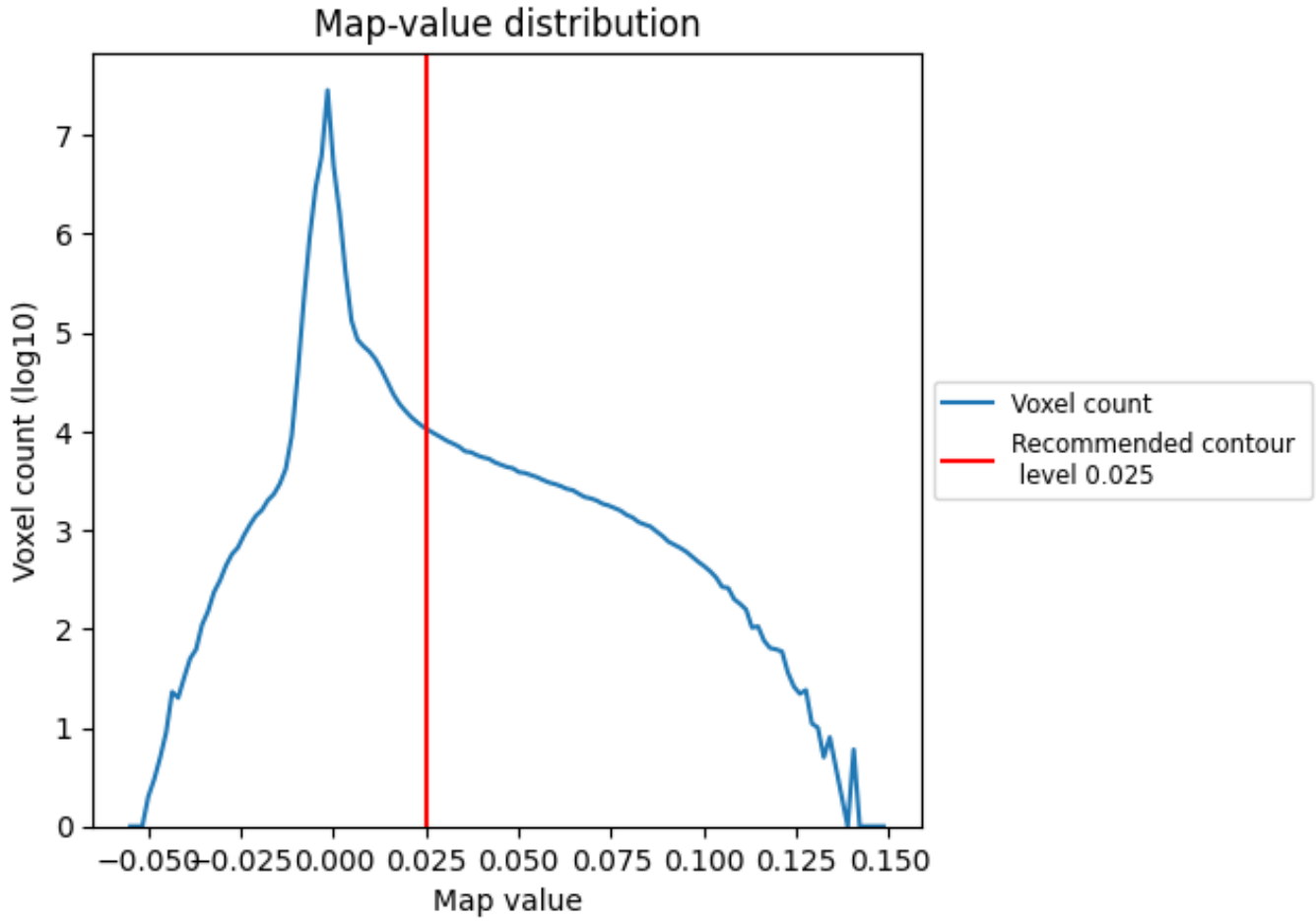


Z

7 Map analysis

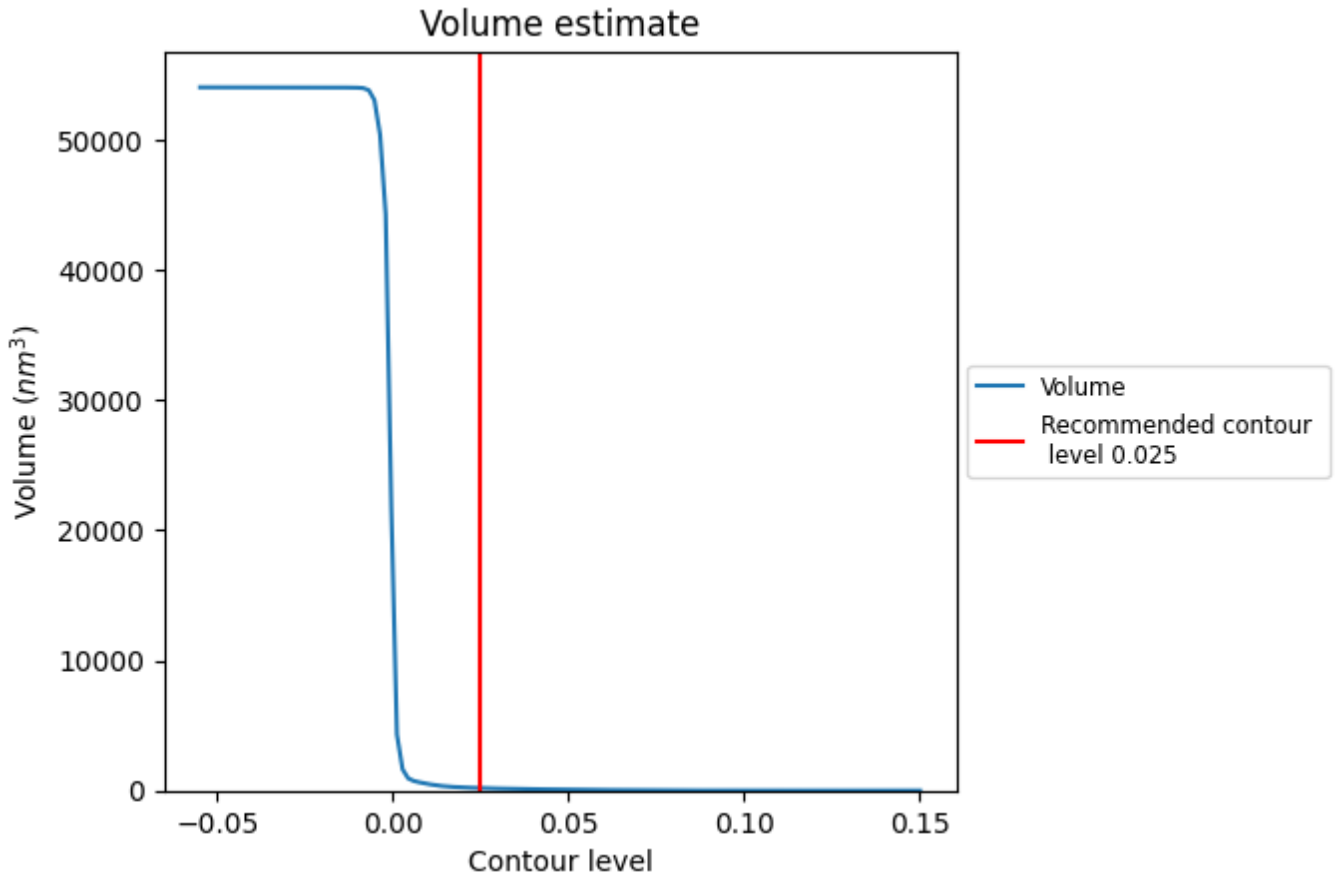
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

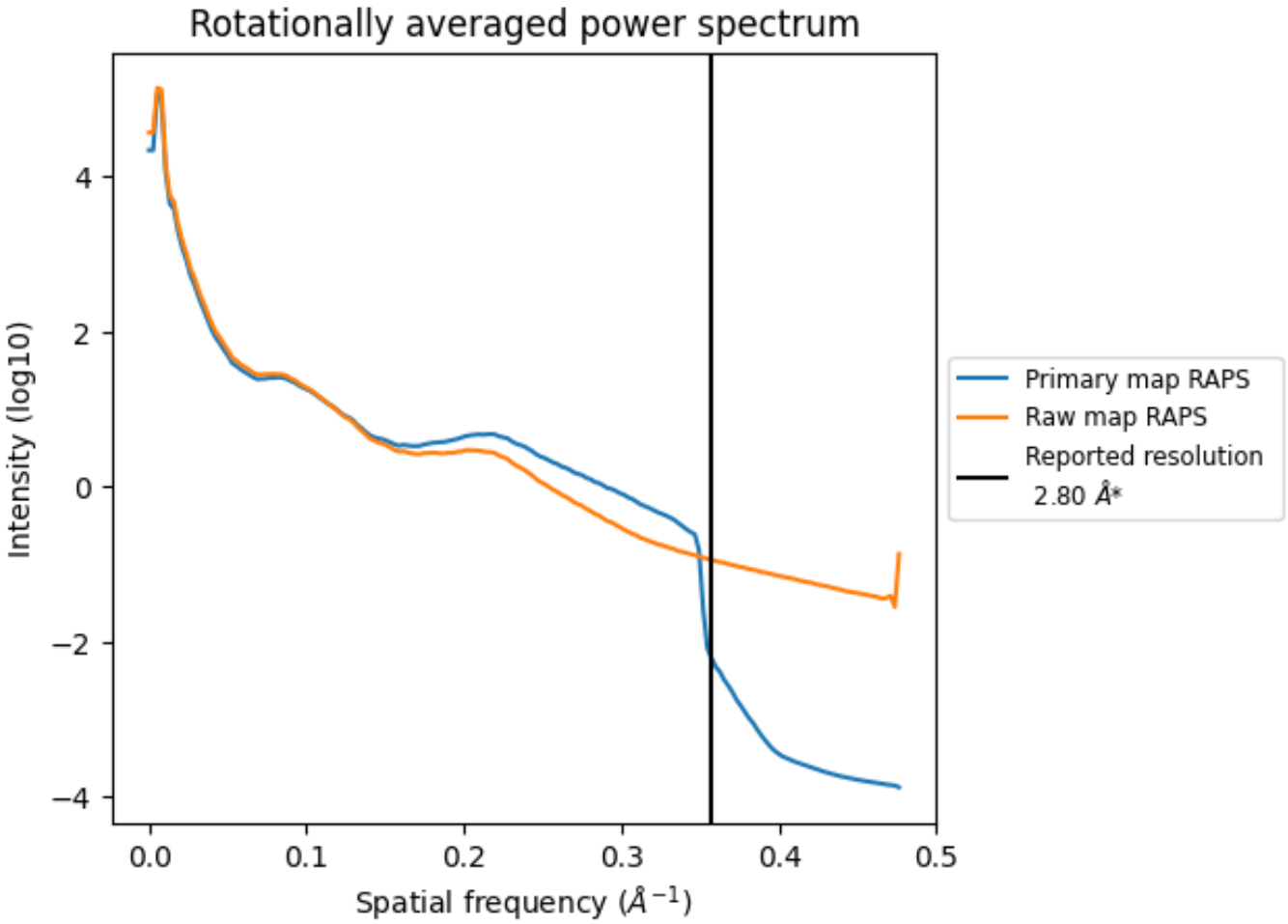
7.2 Volume estimate



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 (i)

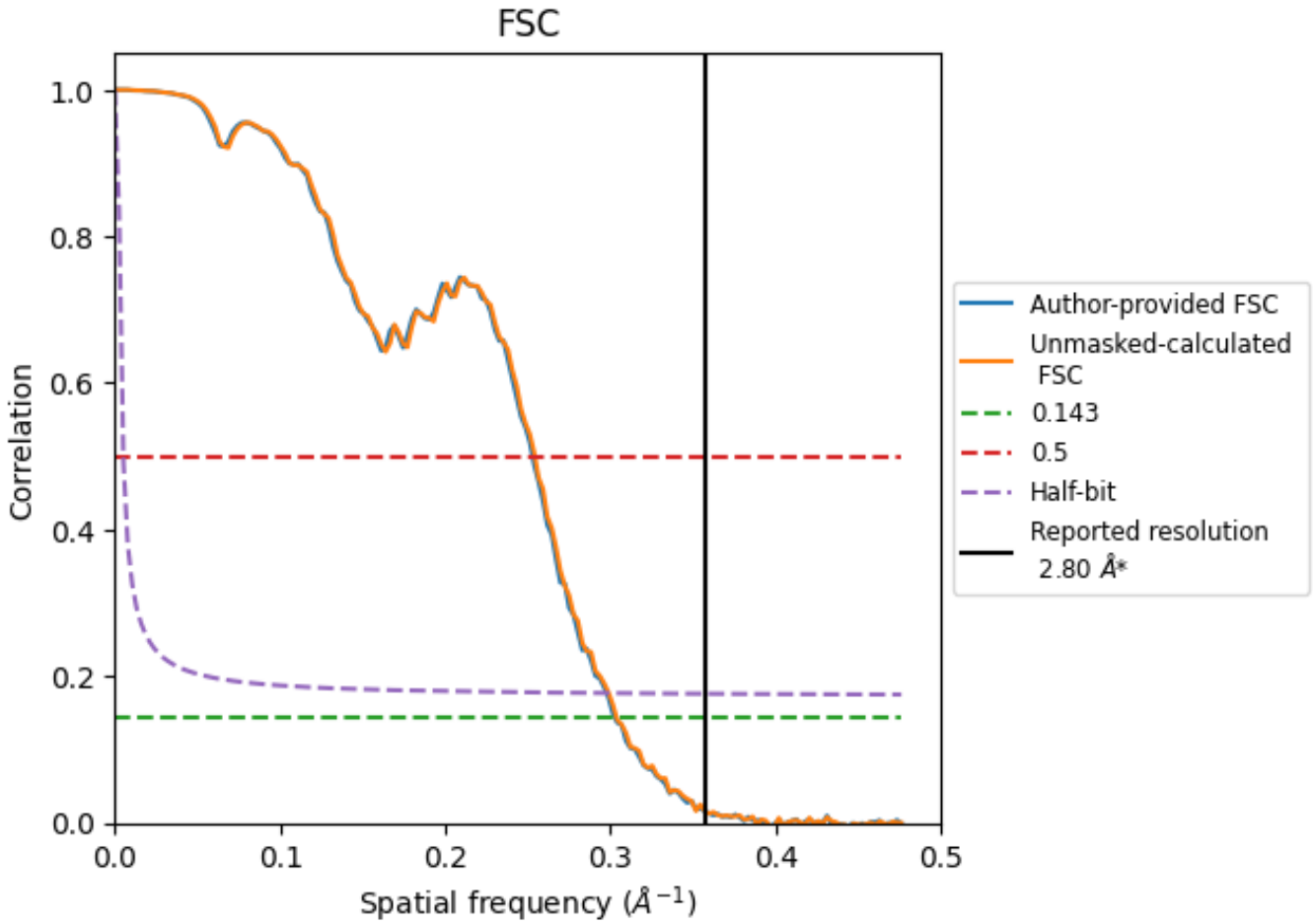


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.357 Å^{-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

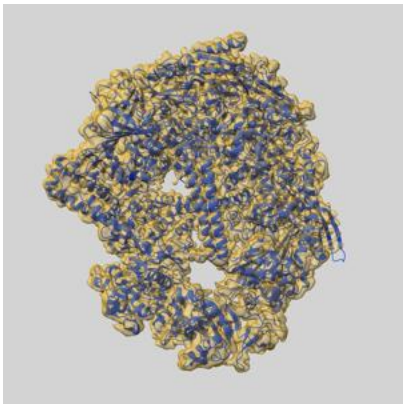
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.30 differs from the reported value 2.8 by more than 10 %

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 %

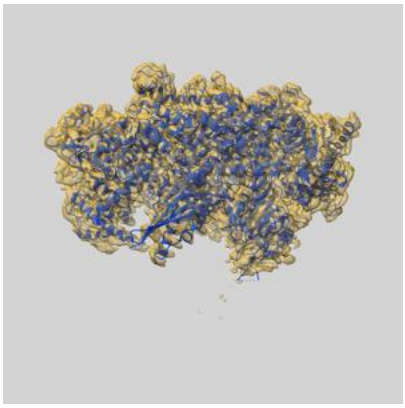
9 Map-model fit

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.

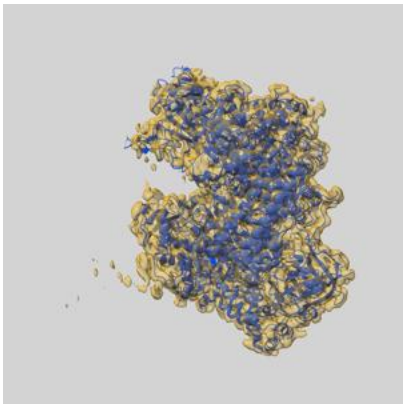
9.1 Map-model overlay



X



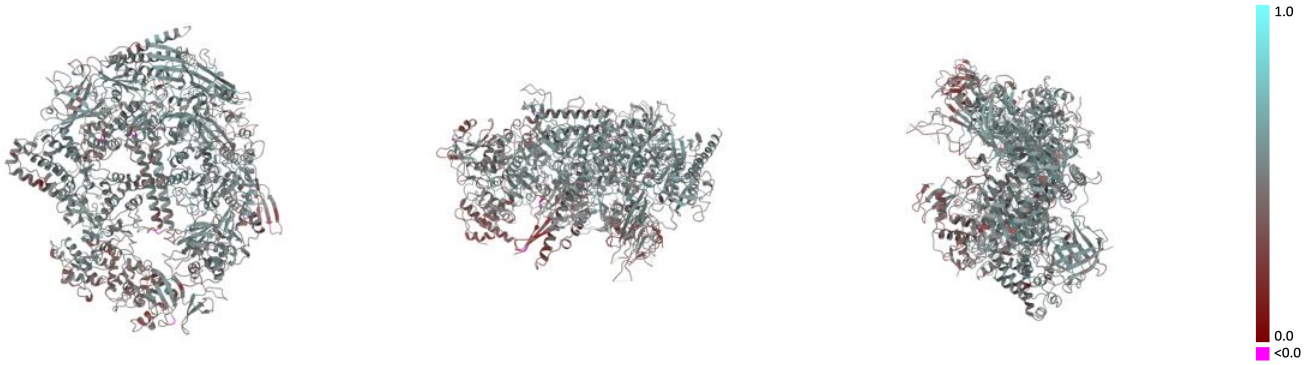
Y



Z

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.

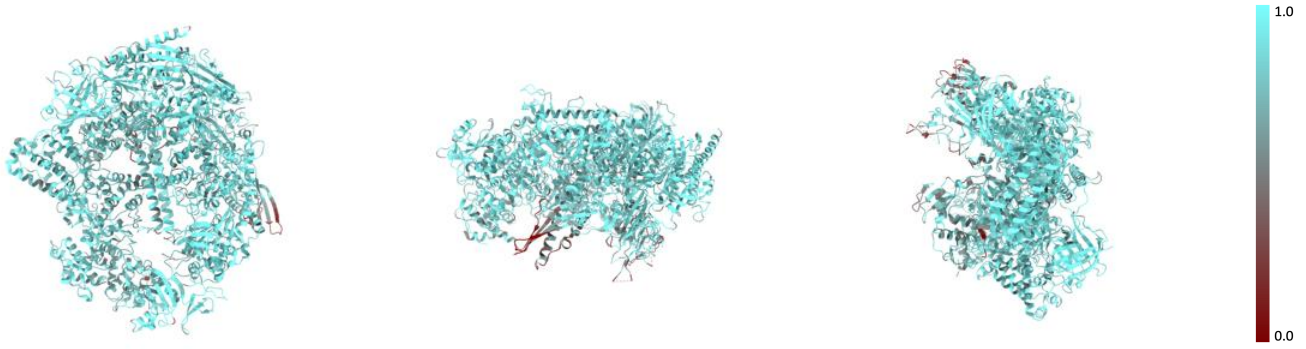
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

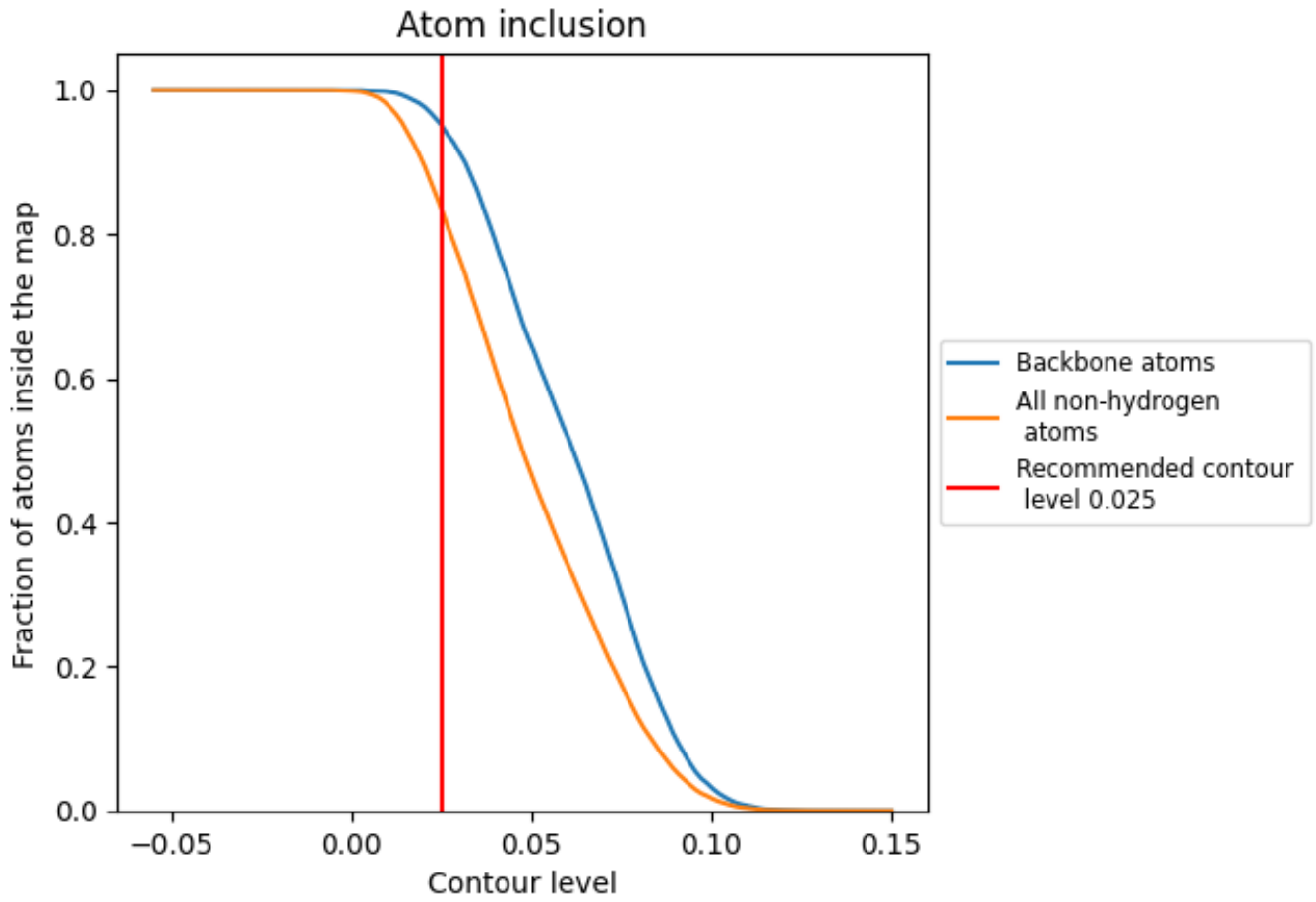
9.3 Atom inclusion mapped to coordinate model



X Y Z

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	0.8359	0.4830
A	0.8271	0.4820
B	0.8184	0.4910
C	0.8999	0.5280
E	0.8708	0.4800
F	0.7199	0.4230
H	0.8868	0.4960
I	0.8498	0.4490
J	0.8906	0.5300
K	0.8695	0.5020
L	0.8062	0.3960
M	0.7875	0.3680
N	0.8867	0.4460