Full wwPDB EM Validation Report ⓘ

Oct 21, 2024 – 01:36 pm BST

PDB ID	:	8RAM
EMDB ID	:	EMD-19019
Title	:	Structure of Sen1 bound RNA Polymerase II pre-termination complex
Authors	:	Rengachari, S.; Lidscreiber, M.; Cramer, P.
Deposited on	:	2023-12-01
Resolution	:	2.80 Å(reported)
Based on initial models	:	2XZO, ?, 6I59, 7NKX

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

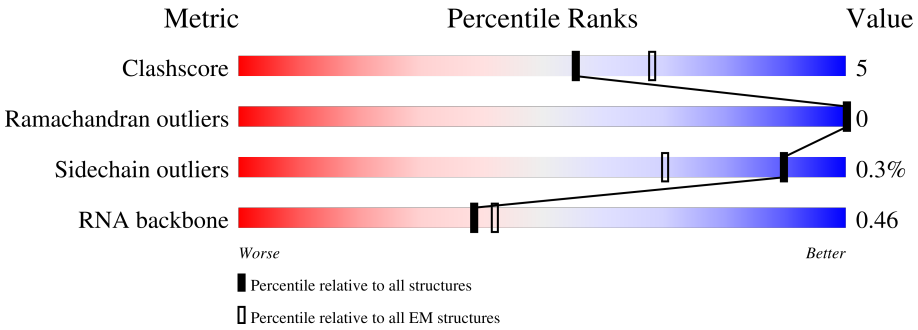
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1733	69% 12% 19%
2	B	1224	77% 14% 9%
3	C	318	72% 11% 17%
4	D	221	64% 8% 28%
5	E	215	85% 14%
6	F	155	47% 8% 45%
7	G	171	89% 11%

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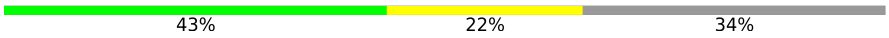
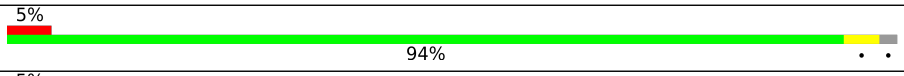
Mol	Chain	Length	Quality of chain
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	145	
14	N	58	
15	O	2231	
16	P	35	
17	T	58	
18	Y	102	
19	Z	1063	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 42965 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1400	11020	6948	1929	2081	62	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1113	8839	5596	1553	1635	55	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	264	2078	1308	346	411	13	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	159	1270	788	223	257	2	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	214	1752	1111	309	321	11	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	85	688	439	116	130	3	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1068	673	180	211	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	118	Total	C	N	O	S	0	0
			964	592	178	184	10		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	1
			920	590	157	171	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	43	Total	C	N	O	S	0	0
			343	211	69	59	4		

- Molecule 13 is a protein called Transcription elongation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	65	Total	C	N	O	S	0	0
			504	311	87	101	5		

- Molecule 14 is a DNA chain called Non-template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	27	Total	C	N	O	P	0	0
			547	262	98	160	27		

- Molecule 15 is a protein called Helicase SEN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	690	Total	C	N	O	S	0	0
			5523	3491	963	1038	31		

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	29	Total	C	N	O	P	0	0
			624	278	116	201	29		

- Molecule 17 is a DNA chain called Template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	38	Total	C	N	O	P	0	0
			786	374	142	232	38		

- Molecule 18 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	100	Total	C	N	O	S	0	0
			760	474	129	147	10		

- Molecule 19 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	429	Total	C	N	O	S	0	0
			3397	2150	605	633	9		

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
20	A	2	Total	Zn	0
			2	2	
20	B	1	Total	Zn	0
			1	1	

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

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

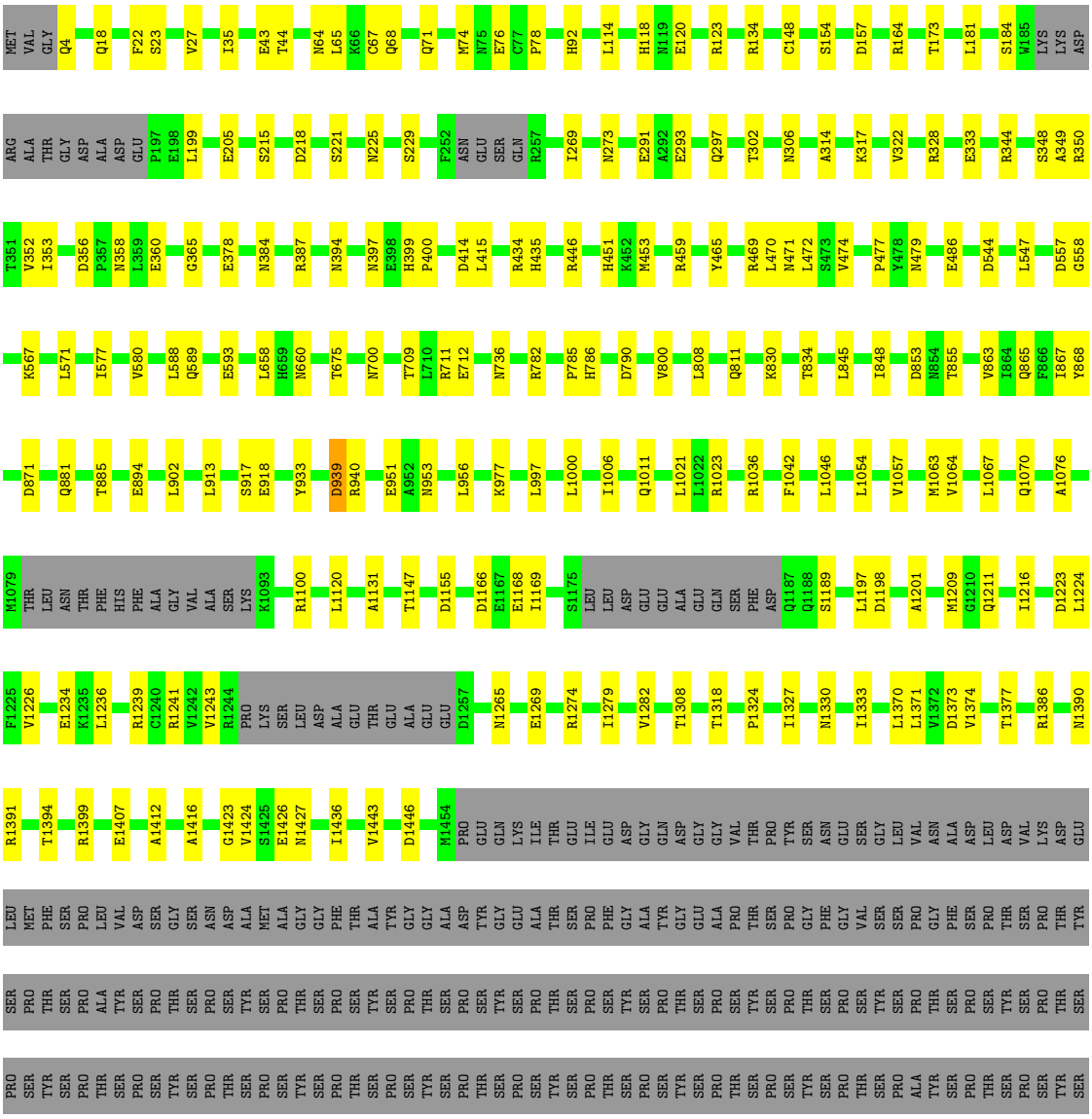
Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total Mg 1 1	0

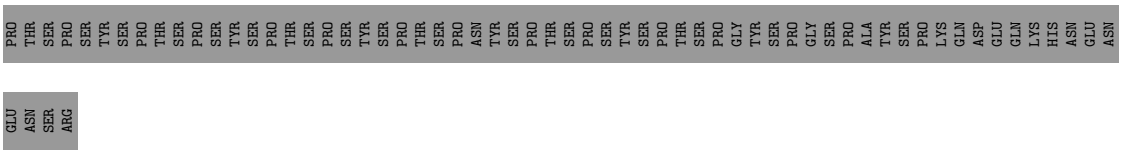
3 Residue-property plots (i)

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 II subunit RPB1

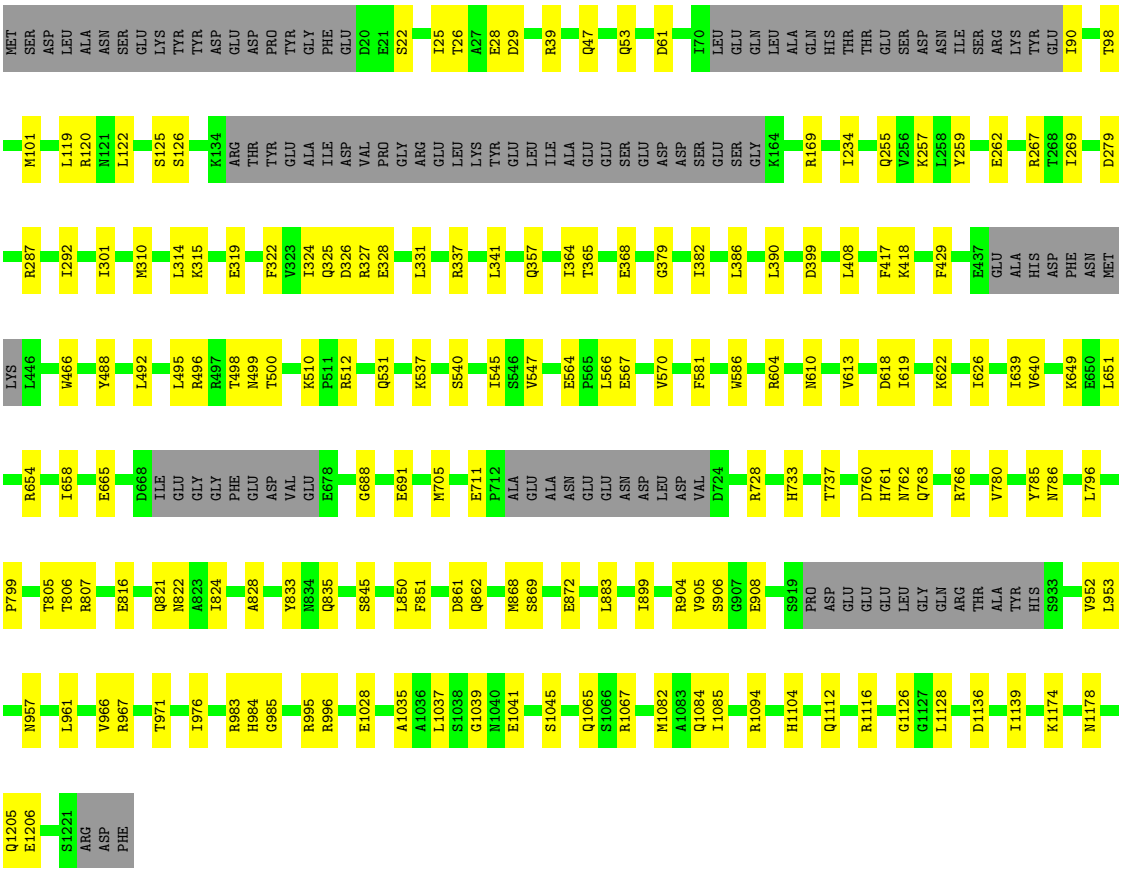
Chain A:





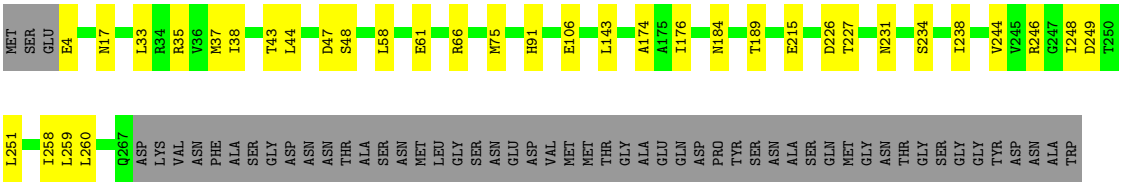
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:



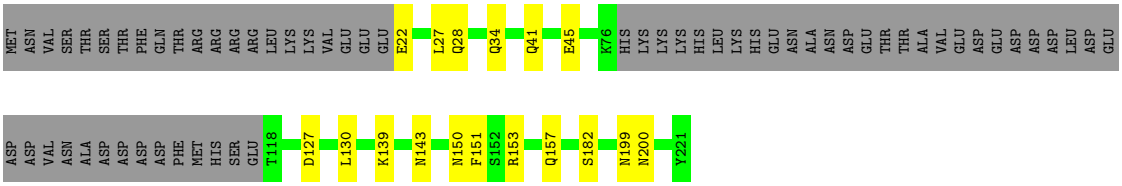
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D:

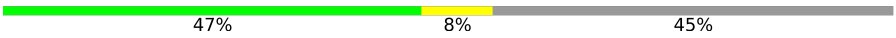


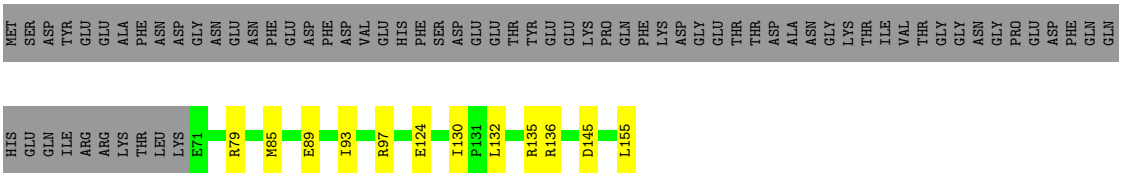
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:

• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:





• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

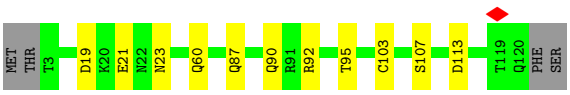
Chain G:

• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:

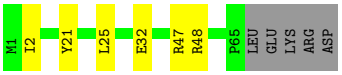
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:



• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:

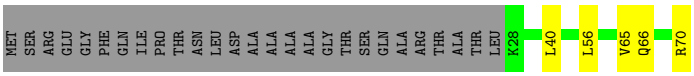


• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K:

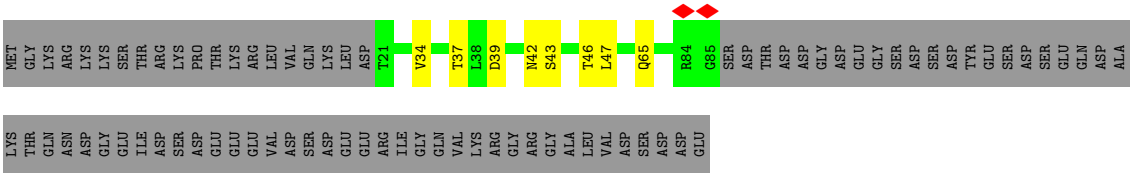
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



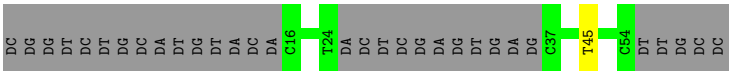
• Molecule 13: Transcription elongation factor 1

Chain M:



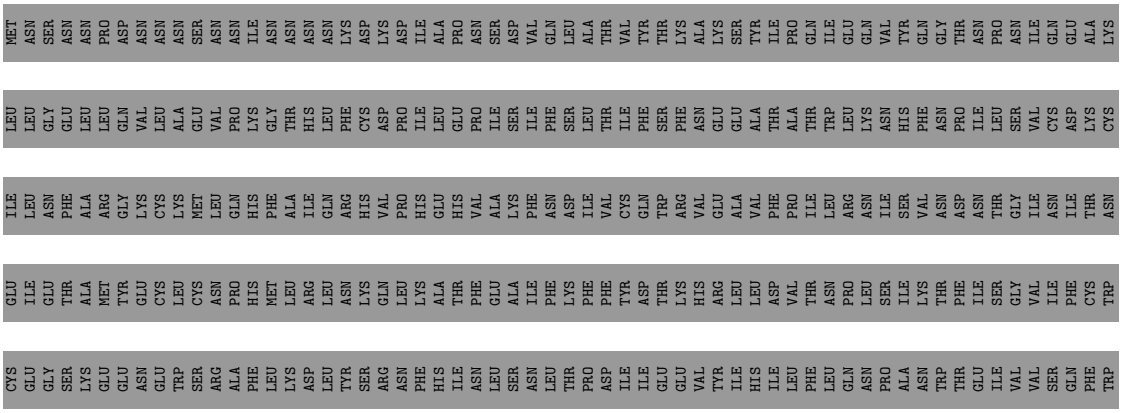
• Molecule 14: Non-template strand

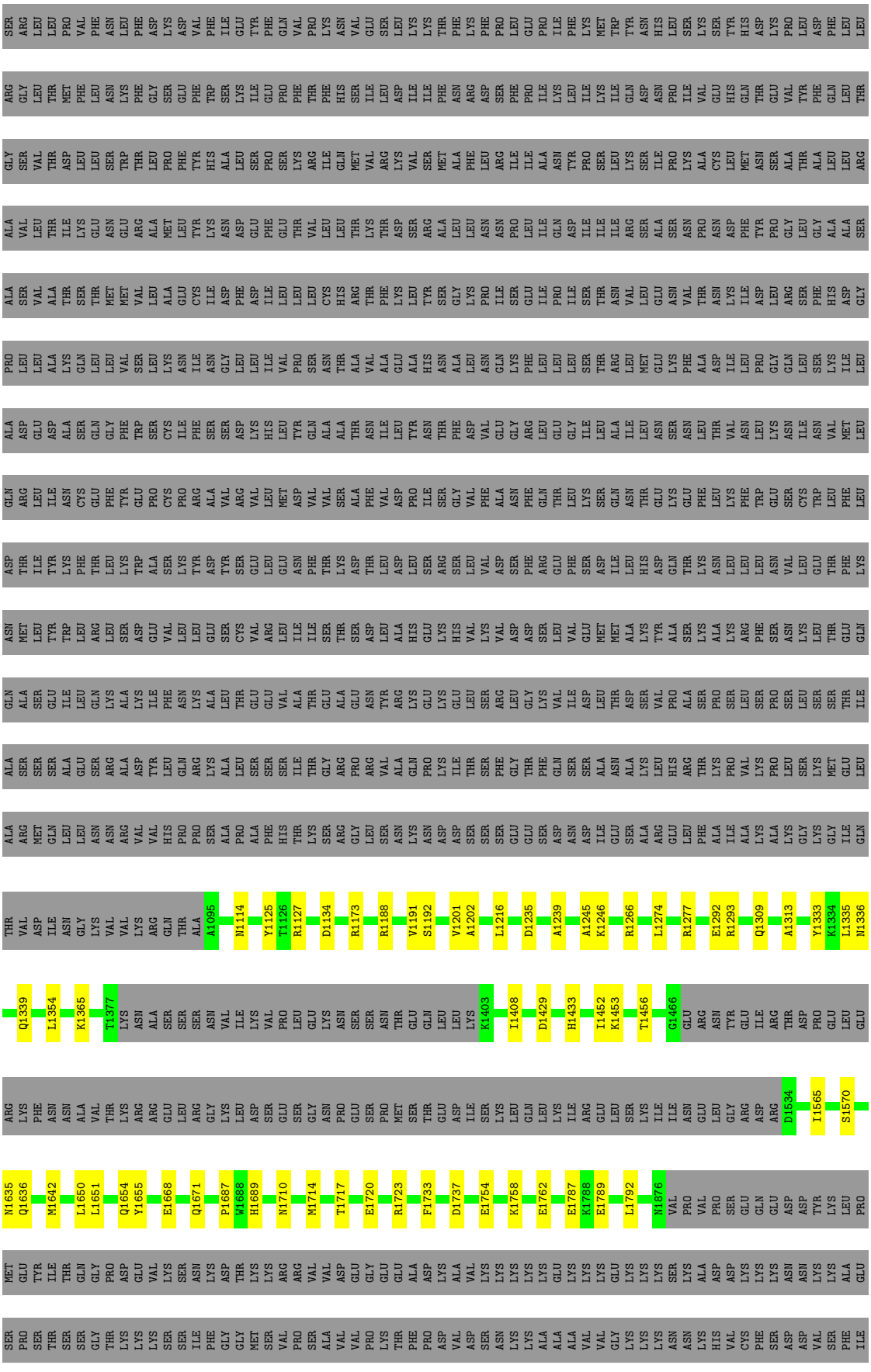
Chain N:



• Molecule 15: Helicase SEN1

Chain O:




A1095
N1114
Y1125
T1126
R1127
D1134
R1173
R1188
V1191
S1192
V1201
A1202
L1216
D1235
A1239
A1245
K1246
R1266
L1274
R1277
E1292
R1293
Q1309
A1313
Y1333
K1334
L1335
N1336
Q1339
L1354
K1365
T1377
K1403
I1408
D1429
H1433
I1452
K1453
T1456
G1466
D1534
I1565
S1570
N1635
Q1636
M1642
L1650
L1651
Q1654
Y1665
E1668
Q1671
P1687
W1688
H1689
N1710
M1714
T1717
E1720
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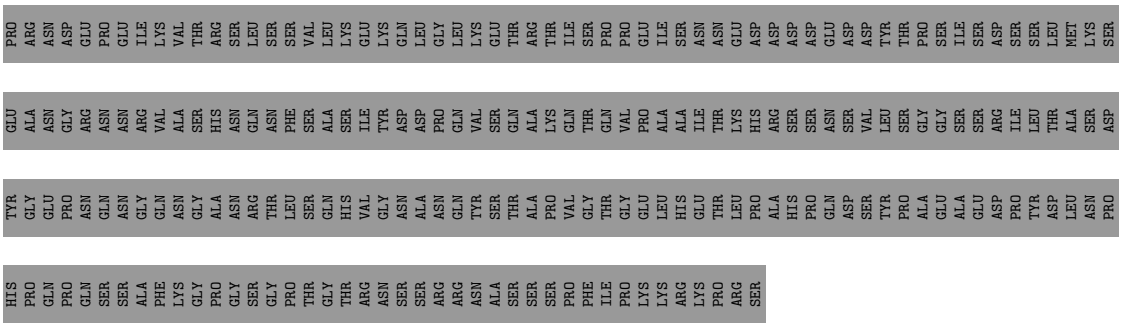
E1762
E1787
K1788
E1789
L1792
N1876

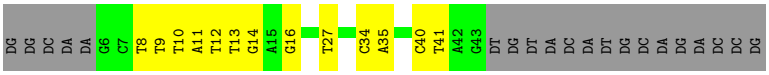


• Molecule 16: RNA

Chain P:

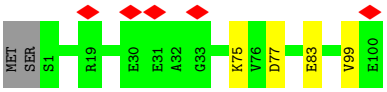
• Molecule 17: Template strand

Chain T:



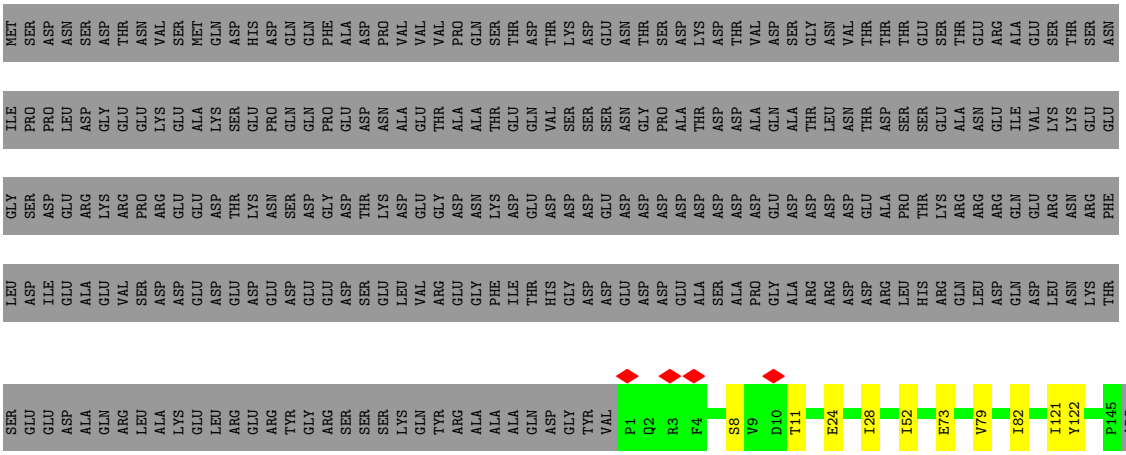
• Molecule 18: Transcription elongation factor SPT4

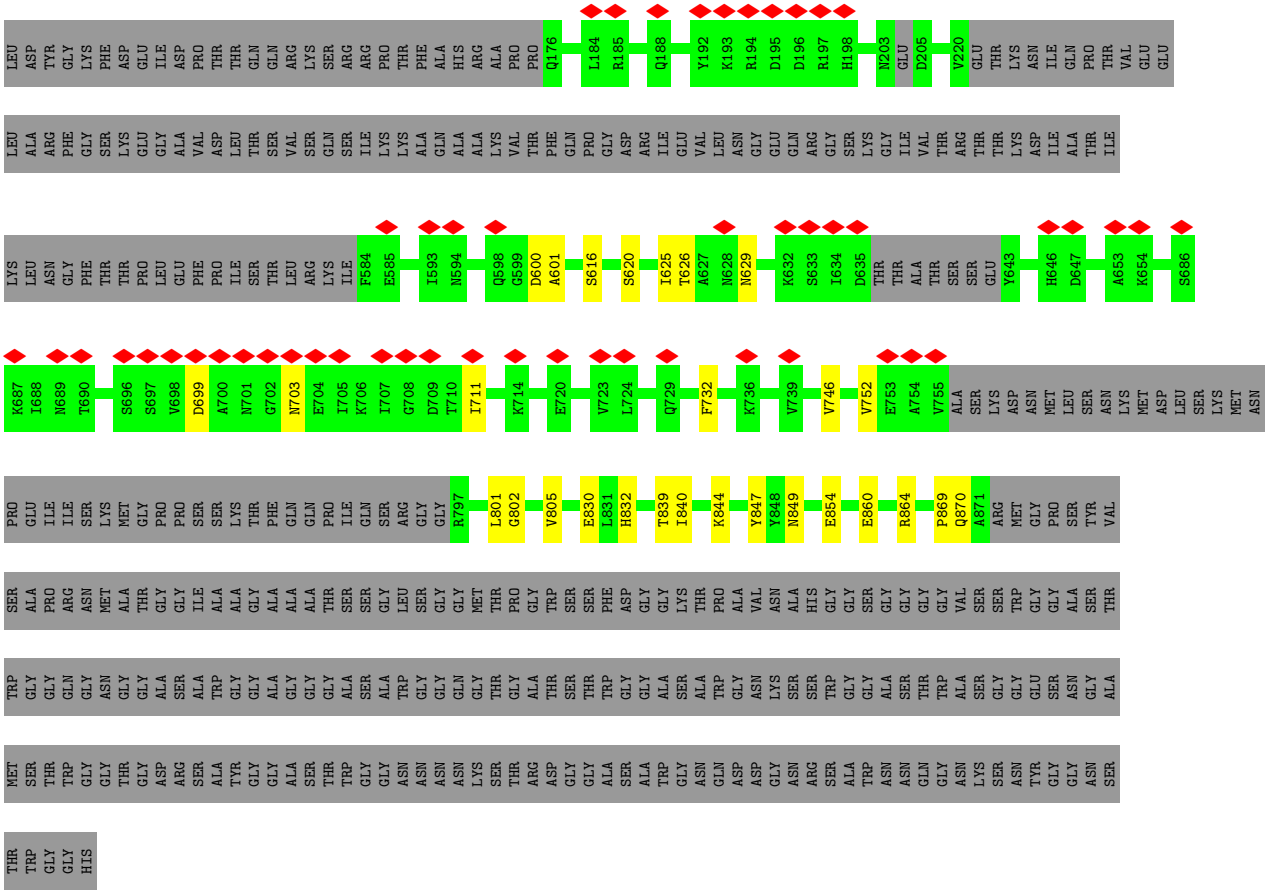
Chain Y:



• Molecule 19: Transcription elongation factor SPT5

Chain Z:




LEU ASP TYR GLY LYS PHE ASP GLU ILE ASP PRO THR THR GLN GLN ARG LYS SER ARG ARG PRO THR PHE ALA HIS ARG ALA PRO PRO Q176 L184 R185 Q188 Y192 K193 R194 D195 D196 R197 H198 N203 GLU D205 V220 GLU THR LYS ASN ILE GLN PRO THR VAL GLU GLU
LEU ALA ARG PHE GLY SER LYS GLU GLY ALA VAL ASP LEU THR SER VAL SER GLN SER ILE LYS LYS ALA GLN ALA ALA LYS VAL THR PHE GLN PRO GLY ASP ARG ILE GLU VAL LEU ASN GLY GLU GLN ARG GLY SER LYS GLY ILE VAL THR ARG THR THR LYS ASP ILE ALA THR ILE
LYS LEU ASN GLY PHE THR THR PRO LEU GLU PHE PRO ILE SER THR LEU ARG LYS ILE F584 E585 I593 N594 Q598 G599 D600 A601 S616 S620 I625 T626 A627 N628 N629 K632 S633 I634 D635 THR THR ALA THR SER SER GLU Y643 H646 D647 A653 K654 S686
K687 I688 N689 T690 S696 S697 V698 D699 A700 N701 G702 N703 E704 I705 K706 I707 G708 D709 T710 I711 K714 E720 V723 L724 Q729 F732 K736 V739 V746 V752 E753 A754 V755 ALA SER LYS ASP ASN MET LEU SER ASN LYS MET ASP LEU SER LYS MET ASN
PRO GLU ILE ILE SER LYS MET GLY PRO PRO SER SER LYS THR PHE GLN GLN PRO ILE GLN SER ARG GLY GLY R797 L801 G802 V805 E830 L831 H832 T839 I840 K844 Y847 Y848 N849 E854 E860 R864 P869 Q870 A871 ARG MET GLY PRO SER TYR VAL
SER ALA PRO ARG ASN MET ALA THR GLY GLY ILE ALA ALA GLY ALA ALA ALA THR SER SER GLY LEU SER GLY GLY MET THR PRO GLY TRP SER SER PHE ASP GLY GLY LYS THR PRO ALA VAL ASN ALA HIS GLY GLY SER GLY GLY GLY GLY VAL SER SER TRP GLY GLY ALA SER THR
TRP GLY GLY GLN GLY ASN GLY GLY ALA SER ALA TRP GLY GLY ALA GLY GLY GLY ALA SER ALA TRP GLY GLY GLN GLY THR GLY ALA THR SER SER THR TRP GLY GLY ALA SER ALA TRP GLY ASN LYS SER SER TRP GLY GLY ALA SER THR TRP GLY GLU SER ASN GLY ALA
MET SER THR TRP GLY GLY THR GLY ASP ARG SER ALA TYR GLY GLY ALA SER THR TRP GLY GLY ASN ASN ASN ASN LYS SER THR ARG ASP GLY GLY ALA SER ALA TRP GLY ASN GLN ASP ASP GLY ASN ARG SER ALA TRP ASN ASN GLN GLY ASN LYS SER ASN TYR GLY GLY ASN SER
THR TRP GLY GLY HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95644	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.02	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.166	Depositor
Minimum map value	-0.057	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.006	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: MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.23	0/11217	0.39	0/15166
2	B	0.24	0/9011	0.40	0/12149
3	C	0.23	0/2116	0.40	0/2868
4	D	0.24	0/1279	0.38	0/1716
5	E	0.24	0/1788	0.38	0/2406
6	F	0.23	0/700	0.38	0/945
7	G	0.25	0/1368	0.41	0/1844
8	H	0.24	0/1086	0.43	0/1470
9	I	0.24	0/982	0.42	0/1321
10	J	0.24	0/541	0.38	0/727
11	K	0.24	0/938	0.38	0/1267
12	L	0.22	0/345	0.41	0/457
13	M	0.24	0/512	0.39	0/689
14	N	0.51	0/611	0.89	0/936
15	O	0.24	0/5625	0.37	0/7580
16	P	0.11	0/697	0.65	0/1083
17	T	0.52	0/881	0.94	0/1360
18	Y	0.23	0/776	0.39	0/1050
19	Z	0.23	0/3443	0.40	0/4632
All	All	0.25	0/43916	0.43	0/59666

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11020	0	11104	144	0
2	B	8839	0	8896	112	0
3	C	2078	0	2041	25	0
4	D	1270	0	1287	11	0
5	E	1752	0	1776	20	0
6	F	688	0	707	7	0
7	G	1340	0	1357	12	0
8	H	1068	0	1040	14	0
9	I	964	0	922	9	0
10	J	532	0	542	5	0
11	K	920	0	929	15	0
12	L	343	0	363	4	0
13	M	504	0	480	5	0
14	N	547	0	306	1	0
15	O	5523	0	5555	34	0
16	P	624	0	315	1	0
17	T	786	0	431	11	0
18	Y	760	0	741	3	0
19	Z	3397	0	3506	28	0
20	A	2	0	0	0	0
20	B	1	0	0	0	0
20	C	1	0	0	0	0
20	I	2	0	0	0	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0
20	M	1	0	0	0	0
21	A	1	0	0	0	0
All	All	42965	0	42298	410	0

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

All (410) 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:956:LEU:HD13	1:A:1021:LEU:HD22	1.46	0.97
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.53	0.90
1:A:853:ASP:OD1	1:A:855:THR:OG1	1.95	0.83
19:Z:8:SER:HG	19:Z:11:THR:HG1	1.27	0.81
2:B:971:THR:OG1	3:C:61:GLU:OE1	2.00	0.80
15:O:1246:LYS:NZ	15:O:1292:GLU:OE2	2.14	0.80
10:J:21:TYR:OH	10:J:32:GLU:OE1	1.99	0.80
4:D:22:GLU:OE1	4:D:28:GLN:NE2	2.15	0.79
2:B:98:THR:O	2:B:126:SER:OG	1.99	0.79
19:Z:849:ASN:ND2	19:Z:869:PRO:O	2.15	0.78
2:B:287:ARG:NH1	2:B:292:ILE:O	2.17	0.78
11:K:11:LEU:O	11:K:37:LYS:NZ	2.17	0.78
2:B:906:SER:OG	19:Z:830:GLU:OE1	2.01	0.77
1:A:811:GLN:NE2	2:B:705:MET:SD	2.58	0.77
1:A:885:THR:O	1:A:940:ARG:NH1	2.18	0.77
2:B:101:MET:O	2:B:169:ARG:NH2	2.17	0.77
3:C:106:GLU:OE1	15:O:1114:ASN:ND2	2.19	0.76
13:M:37:THR:OG1	13:M:46:THR:OG1	2.04	0.76
1:A:134:ARG:NH1	1:A:221:SER:O	2.18	0.76
1:A:306:ASN:ND2	1:A:322:VAL:O	2.19	0.75
1:A:215:SER:OG	1:A:218:ASP:OD1	2.05	0.75
2:B:315:LYS:NZ	2:B:319:GLU:OE2	2.19	0.75
1:A:567:LYS:NZ	8:H:93:TYR:O	2.20	0.74
6:F:97:ARG:NE	6:F:124:GLU:OE1	2.21	0.74
1:A:782:ARG:NH2	1:A:785:PRO:O	2.20	0.73
15:O:1125:TYR:O	15:O:1173:ARG:NH1	2.22	0.73
7:G:129:SER:OG	7:G:137:ILE:O	2.07	0.73
19:Z:626:THR:OG1	19:Z:629:ASN:OD1	2.07	0.73
1:A:1394:THR:O	1:A:1399:ARG:NH1	2.23	0.72
2:B:604:ARG:NH2	2:B:691:GLU:OE2	2.23	0.72
2:B:822:ASN:O	10:J:48:ARG:NH1	2.23	0.72
2:B:862:GLN:OE1	2:B:957:ASN:ND2	2.23	0.71
1:A:1386:ARG:O	1:A:1391:ARG:NH1	2.24	0.71
2:B:26:THR:OG1	2:B:29:ASP:OD1	2.09	0.71
1:A:360:GLU:OE1	1:A:459:ARG:NH2	2.23	0.70
2:B:649:LYS:NZ	2:B:737:THR:O	2.24	0.70
15:O:1717:THR:OG1	15:O:1754:GLU:OE1	2.08	0.70
2:B:399:ASP:OD2	2:B:510:LYS:NZ	2.23	0.70
1:A:350:ARG:NH1	1:A:486:GLU:OE1	2.25	0.70
15:O:1720:GLU:OE1	15:O:1723:ARG:NH2	2.25	0.70
1:A:291:GLU:N	1:A:291:GLU:OE1	2.25	0.70
2:B:766:ARG:NH2	2:B:985:GLY:O	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:8:ASP:OD1	8:H:9:ILE:N	2.24	0.69
1:A:378:GLU:OE2	1:A:384:ASN:ND2	2.26	0.69
1:A:344:ARG:NH1	17:T:27:DT:OP1	2.25	0.69
4:D:153:ARG:NH2	4:D:182:SER:O	2.24	0.69
9:I:19:ASP:O	9:I:23:ASN:N	2.25	0.69
15:O:1758:LYS:NZ	15:O:1762:GLU:OE2	2.26	0.68
1:A:148:CYS:SG	1:A:164:ARG:NH2	2.66	0.68
1:A:317:LYS:O	17:T:35:DA:N6	2.27	0.68
2:B:53:GLN:NE2	2:B:547:VAL:O	2.26	0.68
18:Y:75:LYS:NZ	18:Y:77:ASP:OD1	2.25	0.68
1:A:114:LEU:O	1:A:164:ARG:NH1	2.27	0.68
1:A:881:GLN:HB2	1:A:956:LEU:HD12	1.76	0.68
4:D:139:LYS:O	4:D:143:ASN:ND2	2.27	0.67
15:O:1339:GLN:OE1	15:O:1365:LYS:NZ	2.28	0.67
1:A:378:GLU:OE1	1:A:434:ARG:NE	2.28	0.67
2:B:28:GLU:OE2	2:B:807:ARG:NH1	2.28	0.67
2:B:39:ARG:NH2	2:B:665:GLU:OE1	2.28	0.66
1:A:358:ASN:OD1	2:B:833:TYR:OH	2.12	0.66
1:A:446:ARG:NH1	1:A:479:ASN:O	2.29	0.65
1:A:74:MET:O	2:B:1116:ARG:NH1	2.30	0.65
7:G:85:GLU:N	7:G:85:GLU:OE1	2.29	0.65
1:A:43:GLU:O	1:A:44:THR:OG1	2.14	0.65
3:C:226:ASP:OD1	3:C:227:THR:N	2.29	0.65
1:A:711:ARG:NH1	9:I:95:THR:O	2.30	0.65
2:B:711:GLU:N	2:B:711:GLU:OE1	2.30	0.65
2:B:1065:GLN:OE1	2:B:1067:ARG:N	2.30	0.64
8:H:3:ASN:OD1	8:H:4:THR:N	2.30	0.64
15:O:1336:ASN:ND2	15:O:1655:TYR:OH	2.31	0.64
2:B:328:GLU:N	2:B:328:GLU:OE1	2.30	0.64
19:Z:860:GLU:N	19:Z:860:GLU:OE1	2.30	0.64
2:B:639:ILE:HD12	2:B:688:GLY:O	1.98	0.63
1:A:871:ASP:OD1	5:E:204:THR:OG1	2.10	0.63
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.81	0.63
2:B:908:GLU:N	2:B:908:GLU:OE1	2.32	0.62
15:O:1188:ARG:NH1	15:O:1274:LEU:O	2.32	0.62
7:G:12:THR:OG1	7:G:69:GLU:OE1	2.08	0.62
9:I:90:GLN:OE1	9:I:92:ARG:NH1	2.32	0.62
5:E:24:LYS:NZ	5:E:32:GLN:OE1	2.33	0.62
1:A:951:GLU:OE1	1:A:953:ASN:N	2.33	0.61
19:Z:854:GLU:N	19:Z:854:GLU:OE1	2.33	0.61
4:D:41:GLN:OE1	4:D:41:GLN:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:PHE:CE2	1:A:27:VAL:HG22	2.36	0.60
15:O:1191:VAL:O	15:O:1266:ARG:NH2	2.34	0.60
1:A:68:GLN:N	1:A:68:GLN:OE1	2.33	0.60
1:A:867:ILE:HD11	1:A:1000:LEU:HD11	1.82	0.60
1:A:865:GLN:NE2	1:A:1373:ASP:OD2	2.33	0.60
2:B:816:GLU:N	2:B:816:GLU:OE1	2.35	0.60
4:D:150:ASN:OD1	4:D:151:PHE:N	2.35	0.60
1:A:1318:THR:HG23	5:E:141:VAL:HG11	1.84	0.59
15:O:1654:GLN:N	15:O:1654:GLN:OE1	2.35	0.59
19:Z:870:GLN:OE1	19:Z:870:GLN:N	2.35	0.59
1:A:1168:GLU:N	1:A:1168:GLU:OE1	2.35	0.59
1:A:700:ASN:ND2	9:I:113:ASP:OD2	2.34	0.59
2:B:25:ILE:HD11	2:B:658:ILE:HG13	1.85	0.59
19:Z:28:ILE:CD1	19:Z:52:ILE:HG22	2.32	0.58
19:Z:860:GLU:O	19:Z:864:ARG:N	2.35	0.58
1:A:173:THR:OG1	1:A:184:SER:OG	2.21	0.58
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.38	0.58
2:B:310:MET:HG3	2:B:386:LEU:HD13	1.84	0.58
2:B:733:HIS:O	2:B:733:HIS:ND1	2.37	0.58
2:B:314:LEU:HD21	2:B:386:LEU:HD11	1.85	0.58
3:C:58:LEU:HD11	10:J:2:ILE:HD11	1.86	0.58
1:A:1166:ASP:O	1:A:1169:ILE:HG22	2.03	0.58
15:O:1650:LEU:HD23	15:O:1651:LEU:N	2.19	0.58
19:Z:24:GLU:OE1	19:Z:24:GLU:N	2.37	0.58
1:A:1407:GLU:N	1:A:1407:GLU:OE1	2.37	0.57
2:B:828:ALA:HB2	2:B:1085:ILE:HG23	1.87	0.57
3:C:234:SER:OG	3:C:238:ILE:O	2.08	0.57
1:A:1064:VAL:HG12	1:A:1370:LEU:HD22	1.86	0.57
1:A:348:SER:HB2	2:B:1128:LEU:HD22	1.85	0.57
1:A:1390:ASN:OD1	1:A:1391:ARG:NH2	2.37	0.57
1:A:1100:ARG:NH2	1:A:1330:ASN:OD1	2.38	0.57
2:B:287:ARG:NE	2:B:324:ILE:O	2.38	0.56
2:B:610:ASN:O	2:B:613:VAL:HG12	2.05	0.56
1:A:293:GLU:OE2	1:A:297:GLN:NE2	2.38	0.56
13:M:39:ASP:O	13:M:43:SER:N	2.38	0.56
1:A:43:GLU:OE1	1:A:43:GLU:N	2.38	0.56
1:A:154:SER:OG	1:A:157:ASP:O	2.22	0.56
2:B:899:ILE:O	2:B:952:VAL:HG21	2.05	0.56
7:G:117:GLN:N	7:G:117:GLN:OE1	2.39	0.56
5:E:36:GLU:OE1	5:E:36:GLU:N	2.37	0.56
1:A:269:ILE:O	1:A:273:ASN:ND2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:262:GLU:OE1	2:B:267:ARG:NH2	2.39	0.56
2:B:496:ARG:NH2	2:B:540:SER:O	2.36	0.56
2:B:570:VAL:O	2:B:570:VAL:HG13	2.05	0.56
2:B:499:ASN:OD1	2:B:500:THR:N	2.39	0.56
3:C:91:HIS:O	3:C:91:HIS:ND1	2.39	0.56
5:E:33:GLU:N	5:E:33:GLU:OE1	2.38	0.56
5:E:85:GLU:N	5:E:85:GLU:OE1	2.38	0.56
1:A:845:LEU:HD21	1:A:1374:VAL:HG11	1.87	0.55
2:B:259:TYR:OH	2:B:279:ASP:OD2	2.22	0.55
15:O:1789:GLU:OE1	15:O:1789:GLU:N	2.37	0.55
1:A:1169:ILE:HG21	1:A:1239:ARG:HD3	1.87	0.55
1:A:1426:GLU:OE1	1:A:1426:GLU:N	2.37	0.55
15:O:1453:LYS:O	15:O:1456:THR:HG22	2.06	0.55
1:A:660:ASN:O	2:B:1082:MET:N	2.38	0.55
1:A:1211:GLN:OE1	1:A:1274:ARG:NH1	2.39	0.55
2:B:567:GLU:N	2:B:567:GLU:OE1	2.37	0.55
18:Y:83:GLU:OE1	18:Y:83:GLU:N	2.39	0.55
1:A:365:GLY:N	1:A:469:ARG:O	2.34	0.55
1:A:1063:MET:SD	1:A:1436:ILE:HG23	2.47	0.55
1:A:1155:ASP:OD2	1:A:1239:ARG:NH2	2.40	0.55
8:H:106:GLU:OE1	8:H:106:GLU:N	2.40	0.55
2:B:564:GLU:N	2:B:564:GLU:OE1	2.38	0.55
2:B:868:MET:O	2:B:869:SER:OG	2.19	0.55
4:D:199:ASN:OD1	4:D:200:ASN:N	2.39	0.55
14:N:45:DT:O2	17:T:16:DG:N2	2.39	0.55
15:O:1293:ARG:NH1	15:O:1570:SER:O	2.40	0.54
3:C:258:ILE:HD11	11:K:42:LEU:HD13	1.89	0.54
5:E:40:GLU:OE1	5:E:43:LYS:NZ	2.36	0.54
1:A:67:CYS:O	1:A:71:GLN:N	2.40	0.54
1:A:1070:GLN:NE2	2:B:1136:ASP:OD1	2.40	0.54
18:Y:99:VAL:HG12	18:Y:99:VAL:O	2.08	0.54
1:A:22:PHE:CD2	1:A:27:VAL:HG22	2.42	0.54
11:K:79:GLU:OE1	11:K:79:GLU:N	2.38	0.54
1:A:544:ASP:O	11:K:47:ARG:NH2	2.41	0.54
2:B:322:PHE:O	2:B:325:GLN:NE2	2.39	0.54
4:D:157:GLN:N	4:D:157:GLN:OE1	2.40	0.54
1:A:588:LEU:HD23	1:A:589:GLN:N	2.22	0.54
11:K:38:GLU:OE1	11:K:42:LEU:HD12	2.07	0.54
1:A:1423:GLY:O	1:A:1427:ASN:ND2	2.41	0.54
2:B:512:ARG:NH1	2:B:531:GLN:O	2.41	0.54
2:B:984:HIS:NE2	2:B:1028:GLU:OE1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:GLN:NE2	2:B:495:LEU:O	2.41	0.53
1:A:1120:LEU:HD21	1:A:1131:ALA:HA	1.91	0.53
1:A:1446:ASP:OD1	7:G:58:ARG:NH1	2.41	0.53
15:O:1452:ILE:O	15:O:1452:ILE:HG22	2.09	0.53
5:E:168:TYR:HB3	5:E:170:LEU:HD13	1.90	0.53
2:B:996:ARG:CZ	3:C:38:ILE:HD11	2.38	0.53
3:C:215:GLU:OE1	3:C:215:GLU:N	2.39	0.53
1:A:997:LEU:O	1:A:1011:GLN:NE2	2.42	0.53
1:A:23:SER:O	1:A:27:VAL:HG23	2.08	0.53
1:A:394:ASN:ND2	1:A:400:PRO:O	2.41	0.53
2:B:995:ARG:NH2	11:K:39:ASP:OD2	2.42	0.53
2:B:872:GLU:OE1	2:B:872:GLU:N	2.41	0.52
1:A:863:VAL:O	1:A:863:VAL:HG23	2.10	0.52
2:B:1037:LEU:O	10:J:47:ARG:NH2	2.43	0.52
11:K:36:GLU:OE1	11:K:70:ARG:NE	2.42	0.52
1:A:4:GLN:N	1:A:76:GLU:OE2	2.43	0.52
2:B:357:GLN:NE2	2:B:368:GLU:OE1	2.41	0.52
3:C:17:ASN:OD1	3:C:231:ASN:ND2	2.39	0.52
1:A:593:GLU:N	1:A:593:GLU:OE1	2.40	0.52
3:C:75:MET:O	3:C:246:ARG:NH2	2.39	0.52
5:E:138:ALA:O	5:E:141:VAL:HG12	2.09	0.52
2:B:1104:HIS:NE2	2:B:1126:GLY:O	2.37	0.52
3:C:33:LEU:HD13	3:C:248:ILE:HD13	1.92	0.52
2:B:125:SER:O	2:B:169:ARG:NH2	2.42	0.52
2:B:762:ASN:OD1	2:B:763:GLN:N	2.43	0.52
1:A:577:ILE:O	1:A:580:VAL:HG22	2.09	0.51
1:A:1209:MET:HE3	1:A:1236:LEU:HD13	1.93	0.51
2:B:851:PHE:O	2:B:1094:ARG:NH1	2.44	0.51
19:Z:121:ILE:HD11	19:Z:122:TYR:CZ	2.46	0.51
1:A:120:GLU:OE1	1:A:123:ARG:NH2	2.41	0.51
1:A:977:LYS:O	1:A:1036:ARG:NH2	2.43	0.50
1:A:1279:ILE:HG23	1:A:1308:THR:CG2	2.41	0.50
3:C:259:LEU:HD21	11:K:91:CYS:HB2	1.93	0.50
1:A:1189:SER:O	1:A:1241:ARG:NH1	2.45	0.50
1:A:451:HIS:NE2	1:A:477:PRO:O	2.40	0.50
15:O:1687:PRO:O	15:O:1689:HIS:ND1	2.41	0.50
1:A:1324:PRO:O	1:A:1327:ILE:HG22	2.12	0.50
12:L:65:VAL:HG23	19:Z:832:HIS:NE2	2.26	0.50
2:B:301:ILE:HD13	2:B:379:GLY:HA2	1.94	0.50
2:B:566:LEU:HD22	2:B:586:TRP:O	2.10	0.50
2:B:806:THR:HG23	2:B:1045:SER:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:35:GLN:OE1	8:H:35:GLN:N	2.40	0.50
2:B:1174:LYS:O	2:B:1178:ASN:N	2.44	0.49
1:A:1198:ASP:OD2	1:A:1201:ALA:N	2.44	0.49
2:B:488:TYR:CE2	2:B:492:LEU:HD11	2.47	0.49
2:B:1084:GLN:OE1	2:B:1084:GLN:N	2.42	0.49
5:E:48:ASP:OD1	5:E:51:GLY:N	2.45	0.49
15:O:1429:ASP:OD1	15:O:1433:HIS:N	2.45	0.49
1:A:1234:GLU:OE1	1:A:1234:GLU:N	2.41	0.49
1:A:894:GLU:OE2	1:A:933:TYR:OH	2.30	0.49
1:A:557:ASP:OD1	1:A:558:GLY:N	2.46	0.49
2:B:805:THR:OG1	2:B:1041:GLU:OE2	2.16	0.49
7:G:11:ILE:HD11	7:G:29:LYS:HD3	1.94	0.49
11:K:100:ALA:O	11:K:104:ASN:ND2	2.40	0.49
19:Z:732:PHE:CD1	19:Z:746:VAL:HG22	2.48	0.49
1:A:845:LEU:HD23	1:A:848:ILE:HD12	1.95	0.49
1:A:1265:ASN:ND2	1:A:1269:GLU:OE2	2.43	0.49
1:A:78:PRO:O	2:B:1205:GLN:NE2	2.45	0.48
1:A:1042:PHE:CE1	1:A:1046:LEU:HD11	2.48	0.48
19:Z:801:LEU:HD23	19:Z:802:GLY:N	2.28	0.48
2:B:326:ASP:OD1	2:B:327:ARG:N	2.46	0.48
4:D:34:GLN:N	4:D:34:GLN:OE1	2.46	0.48
8:H:109:LYS:O	8:H:129:TYR:OH	2.31	0.48
2:B:119:LEU:HD12	2:B:953:LEU:HD22	1.95	0.48
2:B:364:ILE:CD1	2:B:365:THR:HG22	2.44	0.48
2:B:640:VAL:HG22	2:B:651:LEU:CD2	2.44	0.48
9:I:60:GLN:OE1	9:I:60:GLN:N	2.41	0.48
1:A:1223:ASP:C	1:A:1224:LEU:HD12	2.33	0.48
2:B:786:ASN:O	2:B:967:ARG:NH2	2.46	0.48
2:B:952:VAL:HG22	2:B:966:VAL:HG22	1.95	0.48
15:O:1127:ARG:NH2	15:O:1134:ASP:OD1	2.43	0.48
15:O:1333:TYR:HB3	15:O:1335:LEU:HD13	1.96	0.48
1:A:1373:ASP:O	1:A:1377:THR:N	2.47	0.48
2:B:364:ILE:HD12	2:B:365:THR:HG22	1.95	0.48
2:B:904:ARG:NH1	2:B:905:VAL:O	2.47	0.48
16:P:11:C:O2	16:P:12:U:N3	2.47	0.48
11:K:37:LYS:N	11:K:69:ALA:O	2.46	0.47
3:C:37:MET:SD	3:C:244:VAL:HG12	2.53	0.47
19:Z:28:ILE:HD12	19:Z:52:ILE:HG22	1.96	0.47
1:A:414:ASP:OD1	1:A:415:LEU:N	2.47	0.47
1:A:205:GLU:OE1	1:A:205:GLU:N	2.42	0.47
2:B:824:ILE:N	2:B:824:ILE:HD12	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:9:DT:C6	17:T:10:DT:H72	2.50	0.47
1:A:571:LEU:CD1	8:H:46:LEU:HD11	2.45	0.47
1:A:917:SER:OG	1:A:918:GLU:OE1	2.30	0.47
2:B:640:VAL:HG12	2:B:649:LYS:HG3	1.97	0.47
15:O:1787:GLU:OE1	15:O:1787:GLU:N	2.47	0.47
19:Z:616:SER:O	19:Z:620:SER:N	2.47	0.47
3:C:47:ASP:OD1	12:L:70:ARG:NH1	2.46	0.47
15:O:1668:GLU:O	15:O:1671:GLN:NE2	2.48	0.47
6:F:85:MET:CE	6:F:93:ILE:HD12	2.45	0.47
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.96	0.47
17:T:8:DT:H2'	17:T:9:DT:H72	1.95	0.47
19:Z:699:ASP:OD1	19:Z:703:ASN:N	2.49	0.47
15:O:1408:ILE:HD12	15:O:1408:ILE:N	2.30	0.46
1:A:790:ASP:OD2	9:I:87:GLN:N	2.49	0.46
1:A:1054:LEU:O	1:A:1057:VAL:HG12	2.16	0.46
5:E:26:ARG:NH2	5:E:133:GLU:OE1	2.48	0.46
8:H:92:ASP:O	8:H:145:ARG:NH2	2.47	0.46
1:A:356:ASP:OD1	11:K:65:HIS:NE2	2.48	0.46
1:A:675:THR:OG1	1:A:736:ASN:OD1	2.29	0.46
9:I:21:GLU:OE1	9:I:21:GLU:N	2.45	0.46
2:B:845:SER:HB3	2:B:850:LEU:HD22	1.97	0.46
12:L:40:LEU:HD21	12:L:56:LEU:HD21	1.97	0.46
2:B:234:ILE:HD13	2:B:257:LYS:HD3	1.96	0.46
2:B:785:TYR:O	2:B:967:ARG:NH1	2.48	0.46
3:C:35:ARG:NE	11:K:41:THR:OG1	2.41	0.46
5:E:136:ASN:OD1	5:E:137:GLU:N	2.48	0.46
19:Z:711:ILE:HD12	19:Z:711:ILE:C	2.36	0.46
2:B:301:ILE:HD12	2:B:382:ILE:HG21	1.97	0.46
7:G:86:VAL:HG22	7:G:146:LYS:HG2	1.98	0.45
1:A:349:ALA:O	2:B:1128:LEU:HD21	2.16	0.45
1:A:118:HIS:O	1:A:123:ARG:NH1	2.49	0.45
1:A:1412:ALA:O	1:A:1416:ALA:N	2.49	0.45
1:A:453:MET:SD	1:A:453:MET:N	2.89	0.45
1:A:1318:THR:CG2	5:E:141:VAL:HG11	2.45	0.45
1:A:709:THR:HG23	1:A:712:GLU:H	1.81	0.45
1:A:834:THR:HG21	1:A:1076:ALA:O	2.17	0.45
2:B:619:ILE:N	2:B:619:ILE:HD12	2.32	0.45
3:C:38:ILE:HB	3:C:176:ILE:HD12	1.98	0.45
2:B:1035:ALA:O	2:B:1039:GLY:N	2.42	0.45
15:O:1216:LEU:HD12	15:O:1245:ALA:O	2.17	0.45
1:A:333:GLU:OE1	1:A:333:GLU:N	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:O	1:A:435:HIS:ND1	2.48	0.45
1:A:352:VAL:HG12	1:A:353:ILE:N	2.33	0.44
2:B:618:ASP:O	2:B:622:LYS:N	2.50	0.44
3:C:260:LEU:HD23	3:C:260:LEU:O	2.18	0.44
1:A:68:GLN:O	1:A:71:GLN:NE2	2.50	0.44
7:G:103:VAL:HG13	7:G:103:VAL:O	2.17	0.44
4:D:45:GLU:OE1	4:D:45:GLU:N	2.50	0.44
6:F:79:ARG:NH1	6:F:145:ASP:O	2.49	0.44
1:A:800:VAL:HG11	1:A:808:LEU:HD22	1.99	0.44
1:A:830:LYS:O	1:A:834:THR:HG23	2.17	0.44
2:B:255:GLN:N	2:B:255:GLN:OE1	2.50	0.44
5:E:68:SER:O	5:E:72:PHE:N	2.45	0.44
8:H:143:LEU:N	8:H:143:LEU:HD12	2.32	0.44
1:A:868:TYR:HE1	1:A:1064:VAL:HG13	1.82	0.44
1:A:1216:ILE:HG21	1:A:1226:VAL:HG21	1.99	0.44
2:B:120:ARG:HE	2:B:122:LEU:HD11	1.81	0.44
3:C:184:ASN:ND2	3:C:189:THR:O	2.51	0.44
5:E:185:ALA:O	5:E:189:GLY:N	2.50	0.44
2:B:327:ARG:O	2:B:331:LEU:HD23	2.18	0.44
2:B:337:ARG:NH1	13:M:65:GLN:OE1	2.50	0.44
13:M:39:ASP:OD2	13:M:42:ASN:ND2	2.51	0.44
1:A:571:LEU:HD12	8:H:46:LEU:HD11	2.00	0.44
15:O:1201:VAL:HG22	15:O:1202:ALA:N	2.32	0.44
1:A:225:ASN:O	1:A:229:SER:N	2.51	0.44
1:A:465:TYR:HB3	2:B:976:ILE:HD11	2.00	0.44
1:A:1333:ILE:HD12	1:A:1333:ILE:H	1.83	0.44
2:B:310:MET:CG	2:B:386:LEU:HD13	2.47	0.44
2:B:341:LEU:HD22	19:Z:73:GLU:OE1	2.18	0.44
1:A:472:LEU:HD13	2:B:835:GLN:OE1	2.17	0.43
15:O:1565:ILE:HD12	15:O:1565:ILE:N	2.33	0.43
15:O:1710:ASN:O	15:O:1714:MET:N	2.43	0.43
2:B:581:PHE:O	2:B:626:ILE:N	2.45	0.43
2:B:760:ASP:OD1	2:B:761:HIS:ND1	2.51	0.43
4:D:130:LEU:O	4:D:130:LEU:HD23	2.18	0.43
1:A:471:ASN:O	1:A:474:VAL:HG22	2.18	0.43
1:A:1282:VAL:HG22	1:A:1308:THR:HG23	2.00	0.43
15:O:1309:GLN:O	15:O:1313:ALA:N	2.46	0.43
7:G:39:THR:O	7:G:43:GLY:N	2.51	0.43
15:O:1354:LEU:HD11	15:O:1642:MET:HB3	2.00	0.43
1:A:18:GLN:NE2	1:A:1416:ALA:O	2.51	0.43
2:B:996:ARG:NH1	3:C:174:ALA:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:390:LEU:O	9:I:92:ARG:NH2	2.52	0.43
1:A:1147:THR:HG22	1:A:1197:LEU:CD2	2.49	0.43
1:A:1371:LEU:O	1:A:1374:VAL:HG12	2.19	0.43
2:B:983:ARG:NH2	2:B:1028:GLU:OE2	2.44	0.43
1:A:35:ILE:HD12	1:A:35:ILE:N	2.34	0.42
1:A:181:LEU:HD12	1:A:181:LEU:O	2.19	0.42
1:A:939:ASP:OD2	1:A:1023:ARG:NH2	2.51	0.42
2:B:780:VAL:HG23	2:B:780:VAL:O	2.19	0.42
3:C:251:LEU:HD23	11:K:98:LEU:HD21	2.01	0.42
10:J:21:TYR:CE2	10:J:25:LEU:HD11	2.52	0.42
1:A:1279:ILE:HG23	1:A:1308:THR:HG21	2.00	0.42
1:A:1318:THR:HG22	1:A:1318:THR:O	2.20	0.42
15:O:1635:ASN:OD1	15:O:1636:GLN:N	2.52	0.42
19:Z:121:ILE:HD11	19:Z:122:TYR:CE2	2.54	0.42
2:B:90:ILE:HD12	2:B:90:ILE:N	2.34	0.42
5:E:26:ARG:O	5:E:155:ARG:NH2	2.47	0.42
6:F:130:ILE:HG22	6:F:132:LEU:H	1.84	0.42
8:H:40:LEU:HD21	8:H:42:ILE:HD11	2.00	0.42
17:T:13:DT:H2'	17:T:14:DG:C8	2.54	0.42
19:Z:711:ILE:HD13	19:Z:752:VAL:CG1	2.49	0.42
1:A:786:HIS:ND1	2:B:705:MET:SD	2.93	0.42
1:A:378:GLU:OE2	1:A:387:ARG:NH1	2.52	0.42
2:B:861:ASP:OD1	2:B:862:GLN:N	2.52	0.42
2:B:1112:GLN:O	2:B:1116:ARG:N	2.51	0.42
7:G:119:LEU:HD23	7:G:120:THR:N	2.35	0.42
1:A:1443:VAL:HG23	7:G:61:ILE:HB	2.02	0.42
2:B:269:ILE:HD12	2:B:269:ILE:N	2.34	0.42
15:O:1191:VAL:HG12	15:O:1192:SER:H	1.84	0.42
15:O:1733:PHE:O	15:O:1737:ASP:N	2.52	0.42
1:A:328:ARG:NH2	2:B:1206:GLU:OE2	2.52	0.42
1:A:658:LEU:HD23	1:A:658:LEU:O	2.19	0.42
1:A:808:LEU:O	2:B:728:ARG:NH2	2.53	0.42
2:B:408:LEU:HD11	2:B:545:ILE:HB	2.02	0.42
11:K:111:LEU:HD23	11:K:111:LEU:O	2.20	0.42
13:M:34:VAL:HG13	13:M:47:LEU:HD21	2.02	0.42
19:Z:79:VAL:HG11	19:Z:82:ILE:HD12	2.02	0.42
2:B:417:PHE:O	2:B:418:LYS:C	2.58	0.41
4:D:27:LEU:N	4:D:27:LEU:HD22	2.36	0.41
15:O:1235:ASP:O	15:O:1239:ALA:N	2.53	0.41
3:C:48:SER:OG	12:L:66:GLN:NE2	2.53	0.41
2:B:796:LEU:HD23	2:B:799:PRO:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:LEU:HD13	3:C:248:ILE:CD1	2.50	0.41
5:E:128:PRO:N	5:E:129:PRO:HD2	2.36	0.41
1:A:397:ASN:HB3	19:Z:839:THR:HG21	2.02	0.41
7:G:26:LEU:O	7:G:26:LEU:HD23	2.21	0.41
8:H:38:LEU:HD21	8:H:40:LEU:HB2	2.02	0.41
17:T:40:DC:C6	17:T:41:DT:H72	2.55	0.41
19:Z:805:VAL:HG12	19:Z:847:TYR:CD1	2.55	0.41
1:A:64:ASN:C	1:A:65:LEU:HD12	2.41	0.41
5:E:77:SER:HG	5:E:105:PHE:HD2	1.68	0.41
6:F:155:LEU:N	6:F:155:LEU:HD22	2.36	0.41
3:C:43:THR:HG22	3:C:44:LEU:N	2.36	0.41
1:A:913:LEU:HD23	1:A:913:LEU:N	2.36	0.41
1:A:1006:ILE:N	1:A:1006:ILE:HD12	2.36	0.41
2:B:796:LEU:HD21	2:B:821:GLN:HG3	2.02	0.41
5:E:50:MET:SD	5:E:52:ARG:NH2	2.92	0.41
19:Z:711:ILE:HD13	19:Z:752:VAL:HG11	2.02	0.41
1:A:302:THR:HG21	1:A:314:ALA:HB2	2.03	0.41
1:A:902:LEU:HD23	1:A:902:LEU:O	2.21	0.41
1:A:1436:ILE:HD13	2:B:1139:ILE:HD12	2.01	0.41
3:C:66:ARG:NH2	3:C:143:LEU:O	2.50	0.41
17:T:11:DA:H2'	17:T:12:DT:H6	1.85	0.41
17:T:13:DT:H2'	17:T:14:DG:O4'	2.21	0.41
1:A:1063:MET:O	1:A:1067:LEU:HD13	2.20	0.41
1:A:1223:ASP:O	1:A:1243:VAL:HG22	2.21	0.41
6:F:135:ARG:NH1	6:F:145:ASP:OD2	2.54	0.41
17:T:35:DA:N3	17:T:35:DA:H2'	2.35	0.41
8:H:40:LEU:CD2	8:H:42:ILE:HD11	2.50	0.40
9:I:103:CYS:O	9:I:107:SER:N	2.50	0.40
15:O:1792:LEU:N	15:O:1792:LEU:HD12	2.37	0.40
19:Z:625:ILE:HG22	19:Z:626:THR:N	2.35	0.40
2:B:22:SER:O	2:B:654:ARG:NH1	2.52	0.40
19:Z:840:ILE:HD11	19:Z:844:LYS:HD2	2.04	0.40
1:A:199:LEU:N	1:A:199:LEU:HD12	2.36	0.40
1:A:800:VAL:CG1	1:A:808:LEU:HD22	2.52	0.40
2:B:498:THR:N	2:B:537:LYS:O	2.48	0.40
5:E:165:LEU:O	5:E:169:ARG:N	2.54	0.40
17:T:34:DC:H4'	17:T:35:DA:H5'	2.03	0.40
19:Z:600:ASP:OD1	19:Z:601:ALA:N	2.55	0.40
1:A:956:LEU:HD13	1:A:1021:LEU:CD2	2.34	0.40
6:F:89:GLU:OE2	6:F:136:ARG:NE	2.55	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	1388/1733 (80%)	1350 (97%)	38 (3%)	0	100	100
2	B	1099/1224 (90%)	1070 (97%)	29 (3%)	0	100	100
3	C	262/318 (82%)	255 (97%)	7 (3%)	0	100	100
4	D	155/221 (70%)	152 (98%)	3 (2%)	0	100	100
5	E	212/215 (99%)	210 (99%)	2 (1%)	0	100	100
6	F	83/155 (54%)	81 (98%)	2 (2%)	0	100	100
7	G	169/171 (99%)	169 (100%)	0	0	100	100
8	H	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
9	I	116/122 (95%)	113 (97%)	3 (3%)	0	100	100
10	J	63/70 (90%)	63 (100%)	0	0	100	100
11	K	113/120 (94%)	113 (100%)	0	0	100	100
12	L	41/70 (59%)	40 (98%)	1 (2%)	0	100	100
13	M	63/145 (43%)	63 (100%)	0	0	100	100
15	O	684/2231 (31%)	676 (99%)	8 (1%)	0	100	100
18	Y	98/102 (96%)	98 (100%)	0	0	100	100
19	Z	417/1063 (39%)	412 (99%)	5 (1%)	0	100	100
All	All	5092/8106 (63%)	4990 (98%)	102 (2%)	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	1225/1520 (81%)	1222 (100%)	3 (0%)	92 97
2	B	964/1061 (91%)	959 (100%)	5 (0%)	86 95
3	C	232/274 (85%)	230 (99%)	2 (1%)	75 92
4	D	141/200 (70%)	140 (99%)	1 (1%)	81 94
5	E	196/197 (100%)	196 (100%)	0	100 100
6	F	75/137 (55%)	75 (100%)	0	100 100
7	G	152/152 (100%)	152 (100%)	0	100 100
8	H	117/128 (91%)	117 (100%)	0	100 100
9	I	112/116 (97%)	112 (100%)	0	100 100
10	J	60/65 (92%)	60 (100%)	0	100 100
11	K	99/102 (97%)	99 (100%)	0	100 100
12	L	38/57 (67%)	38 (100%)	0	100 100
13	M	60/131 (46%)	60 (100%)	0	100 100
15	O	615/2010 (31%)	614 (100%)	1 (0%)	92 97
18	Y	85/87 (98%)	85 (100%)	0	100 100
19	Z	376/876 (43%)	376 (100%)	0	100 100
All	All	4547/7113 (64%)	4535 (100%)	12 (0%)	90 97

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	470	LEU
1	A	939	ASP
2	B	61	ASP
2	B	429	PHE
2	B	466	TRP
2	B	883	LEU
2	B	961	LEU
3	C	4	GLU
3	C	249	ASP
4	D	127	ASP
15	O	1277	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	47	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	27/35 (77%)	8 (29%)	0

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	2	G
16	P	4	C
16	P	7	G
16	P	10	U
16	P	11	C
16	P	13	A
16	P	21	G
16	P	24	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

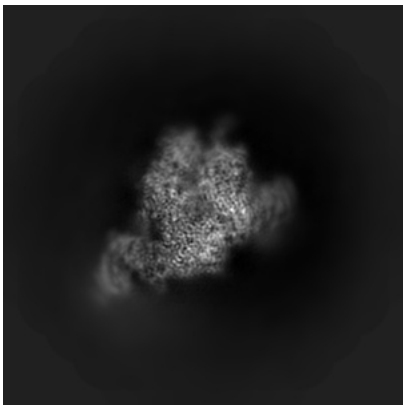
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19019. These allow visual inspection of the internal detail of the map and identification of artifacts.

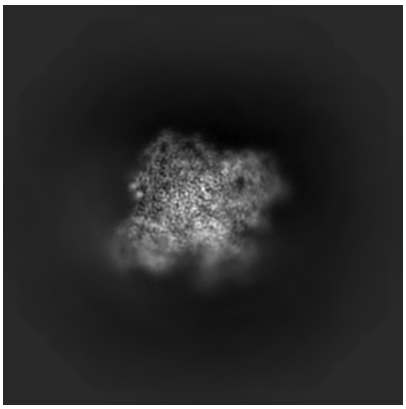
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

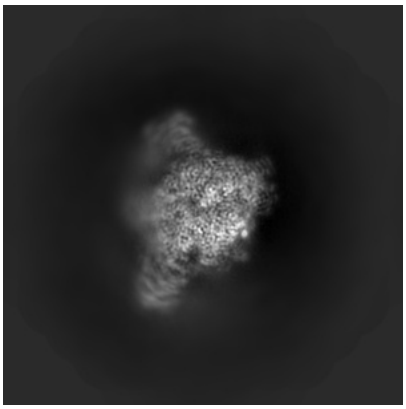
6.1.1 Primary map



X

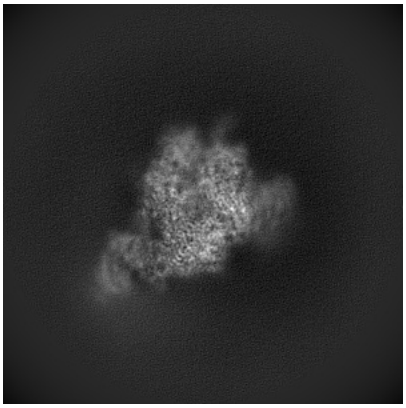


Y

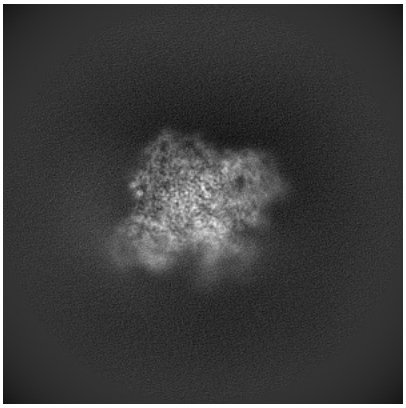


Z

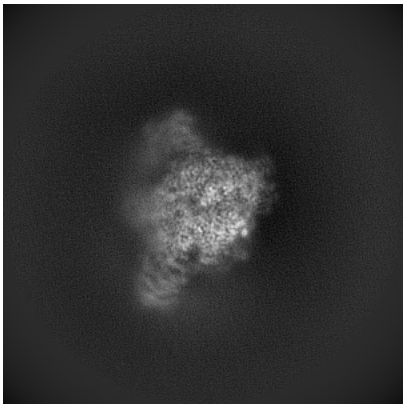
6.1.2 Raw map



X



Y

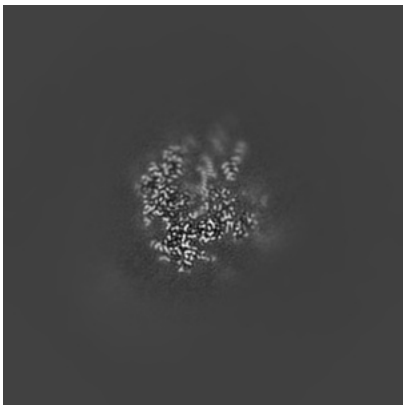


Z

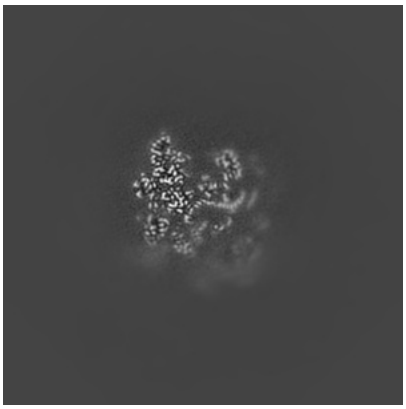
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

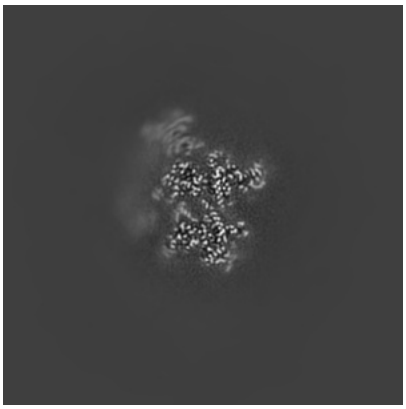
6.2.1 Primary map



X Index: 180

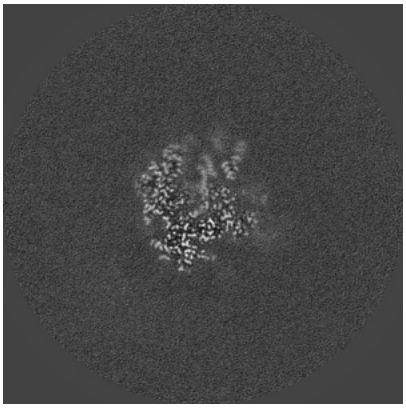


Y Index: 180

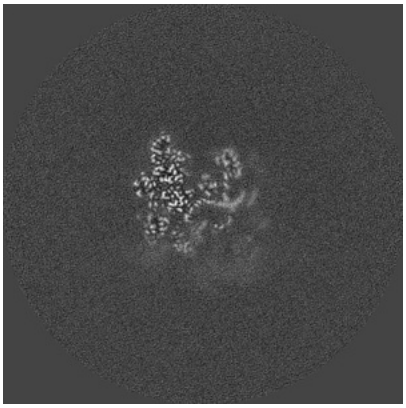


Z Index: 180

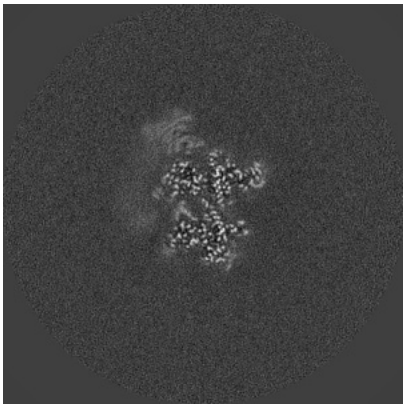
6.2.2 Raw map



X Index: 180



Y Index: 180



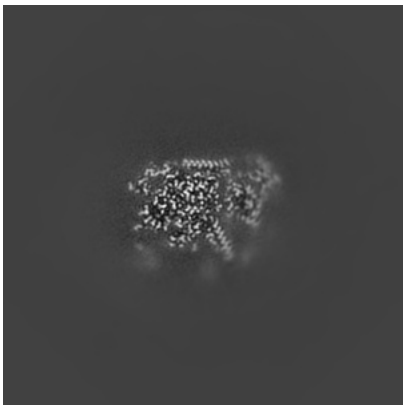
Z Index: 180

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

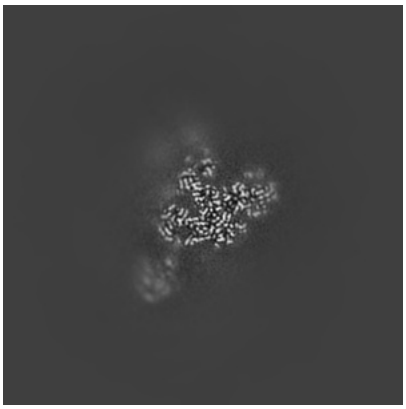
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 189

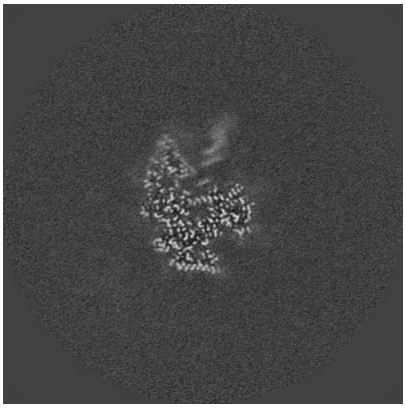


Y Index: 154

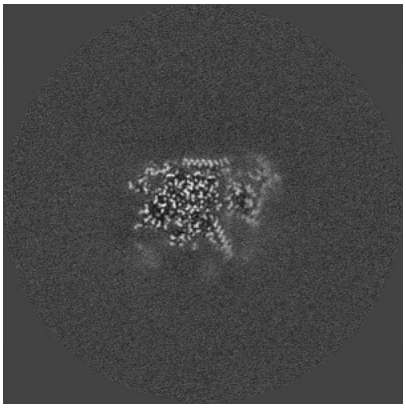


Z Index: 152

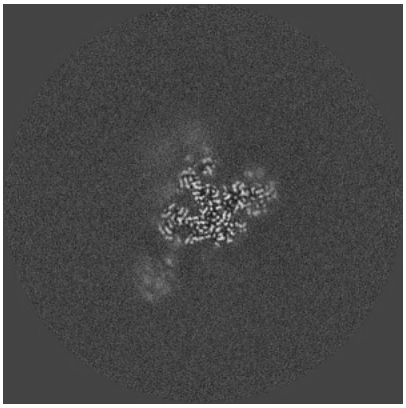
6.3.2 Raw map



X Index: 189



Y Index: 154

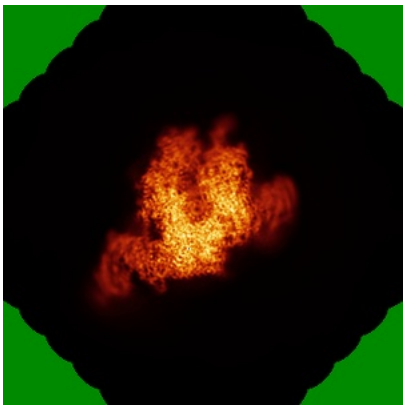


Z Index: 152

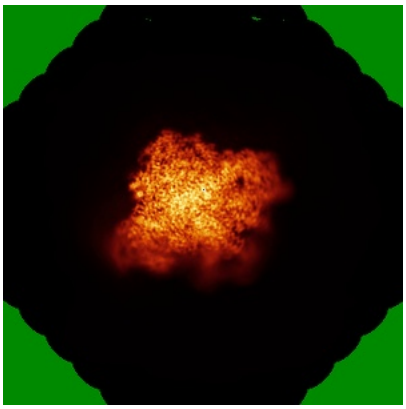
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

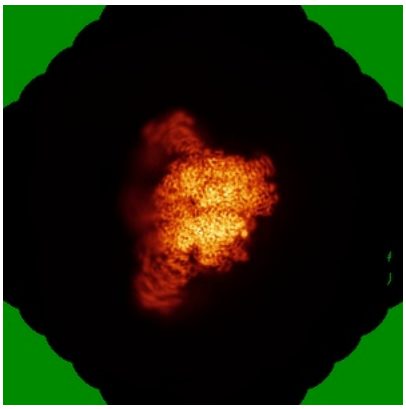
6.4.1 Primary map



X

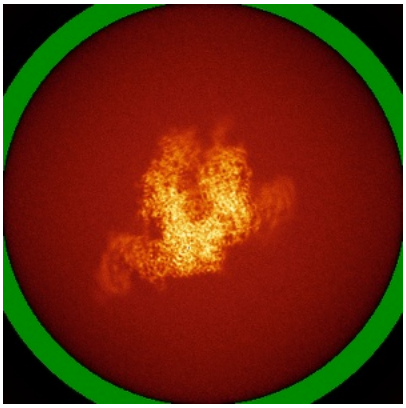


Y

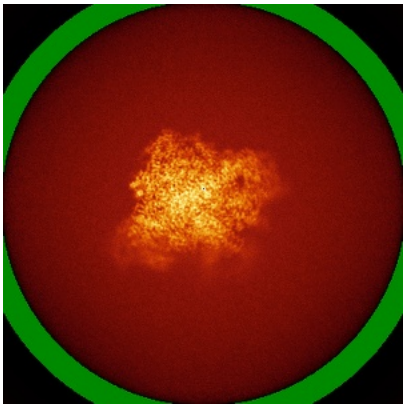


Z

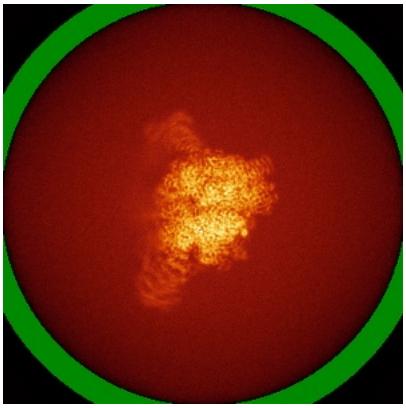
6.4.2 Raw map



X



Y



Z

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

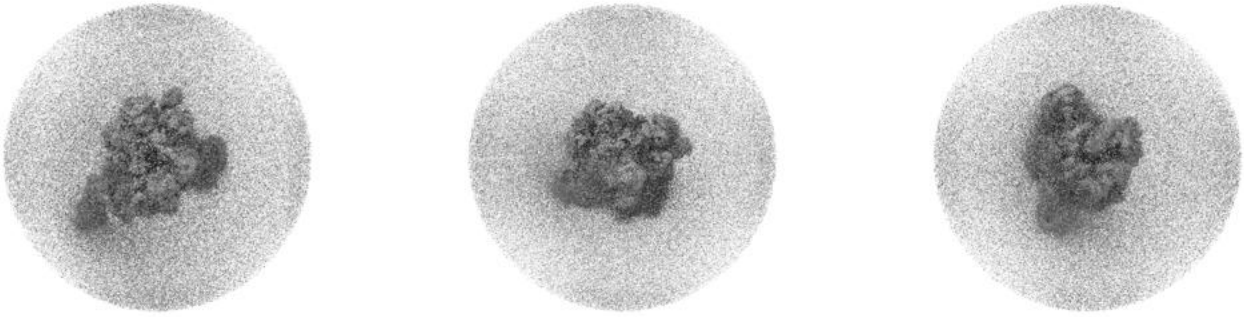
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

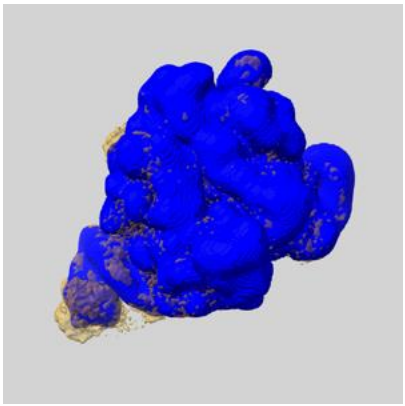
6.6 Mask visualisation

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

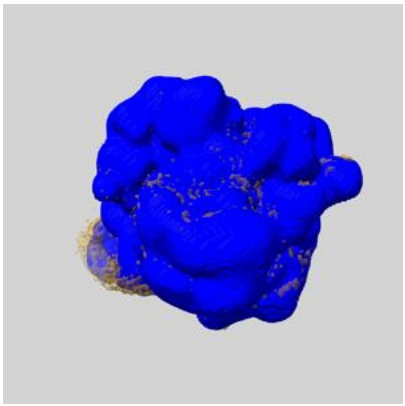
A mask typically either:

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

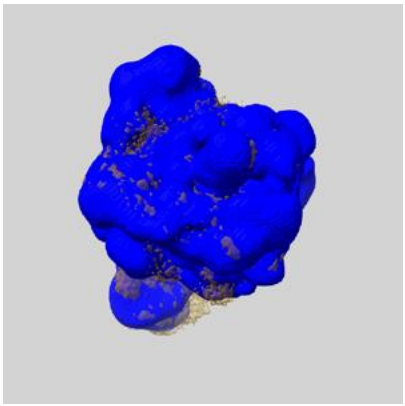
6.6.1 emd_19019_msk_1.map



X



Y

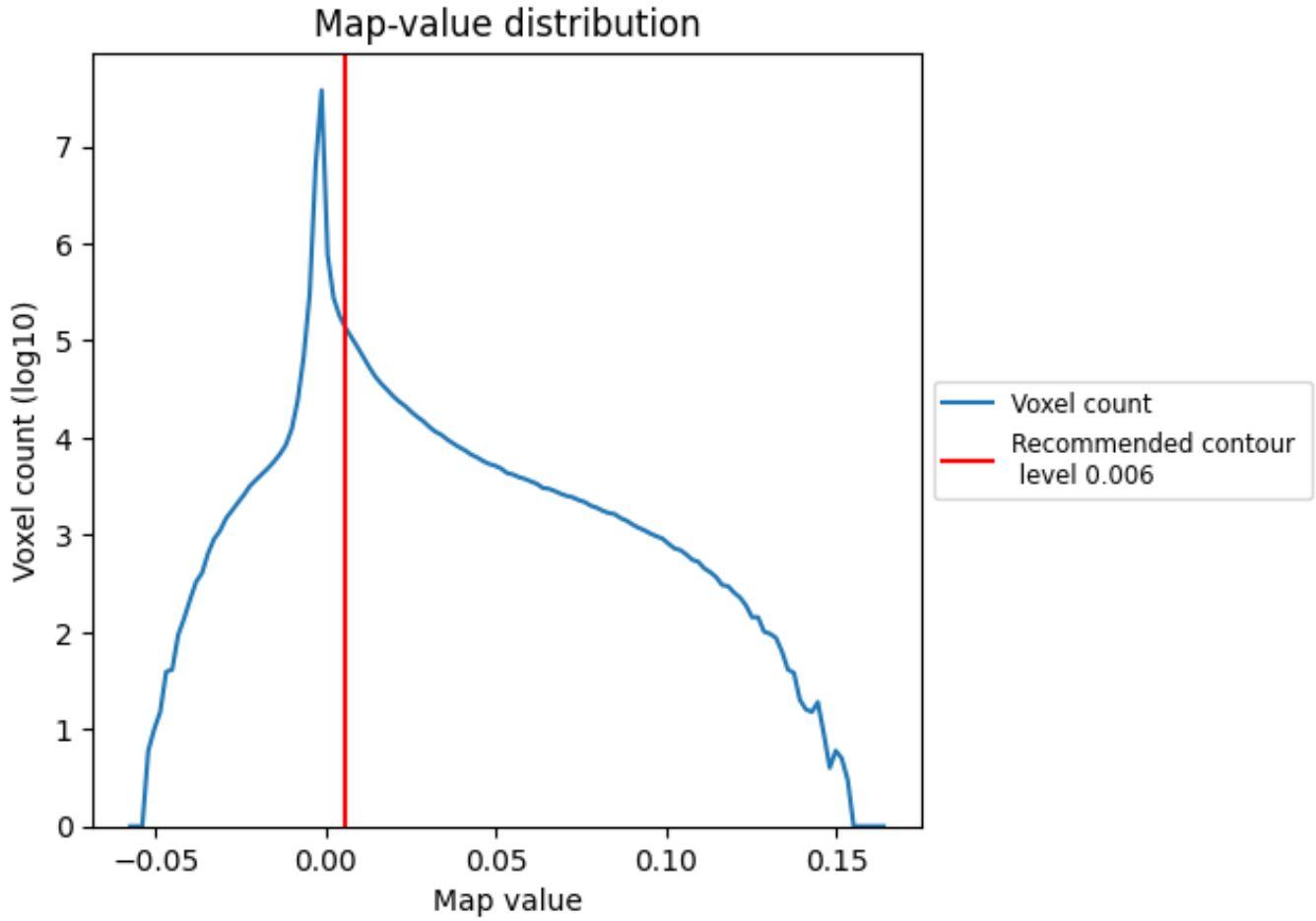


Z

7 Map analysis

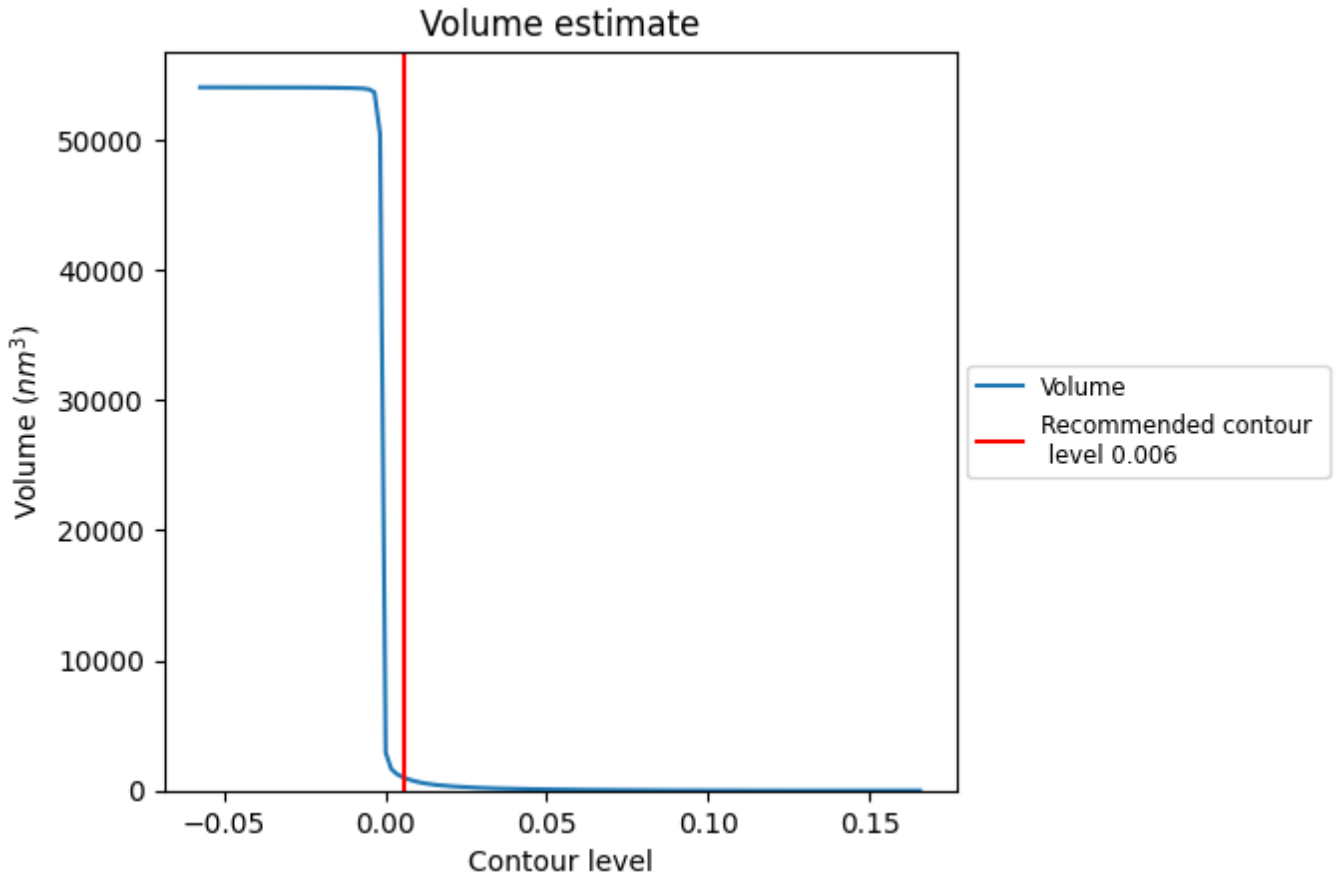
This section contains the results of statistical analysis of the map.

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.

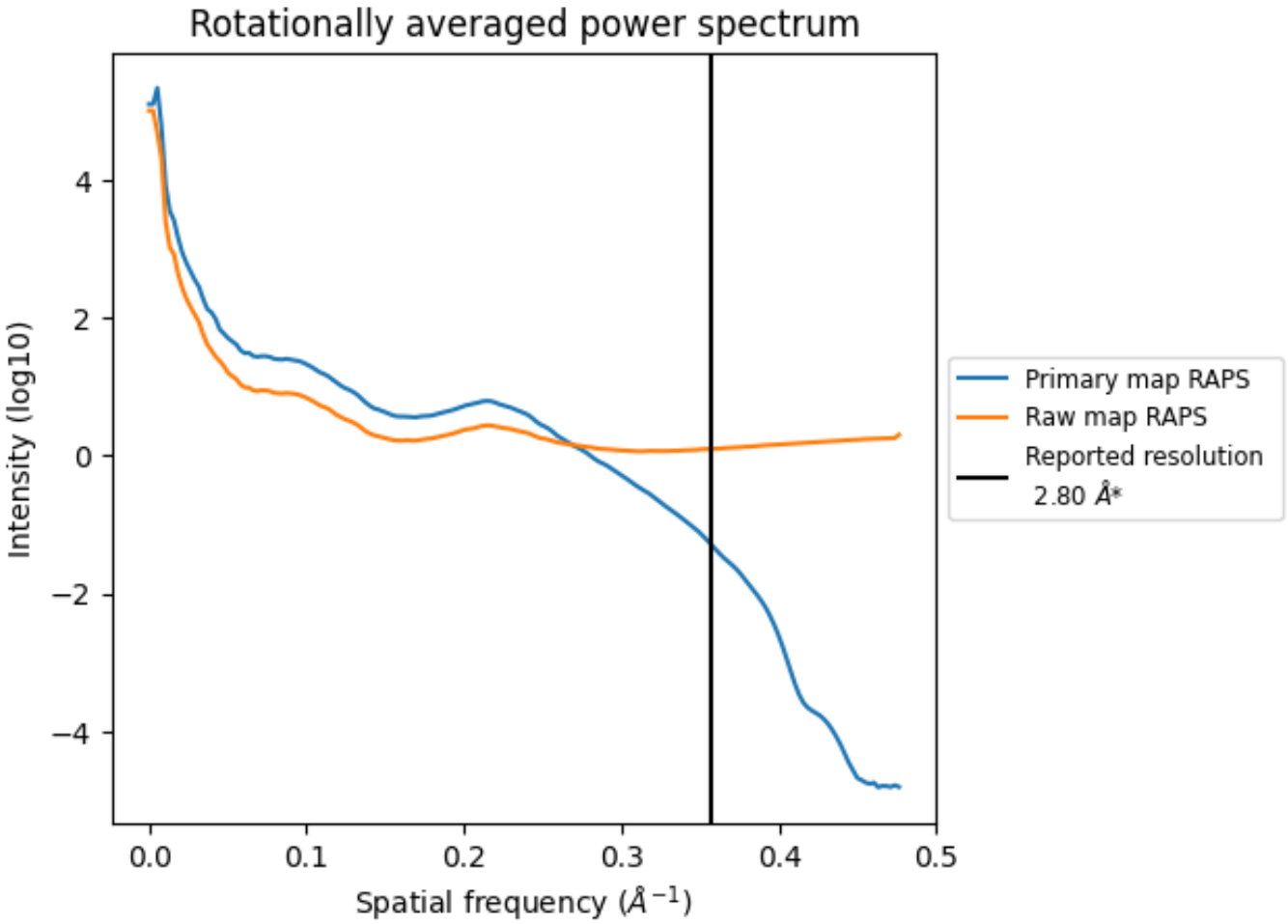
7.2 Volume estimate



The volume at the recommended contour level is 976 nm^3; this corresponds to an approximate mass of 881 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)

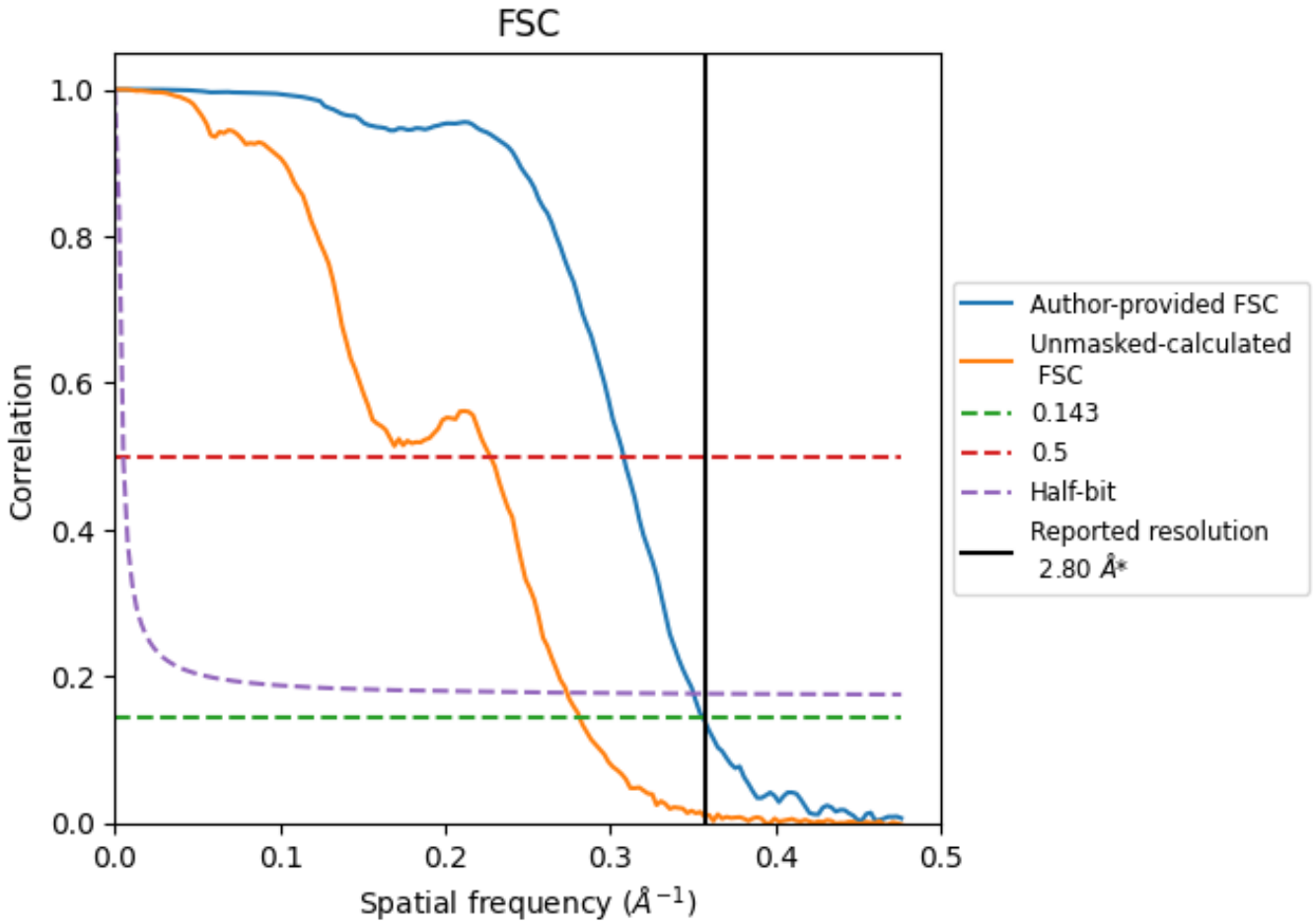


*Reported resolution corresponds to spatial frequency of 0.357 $Å^{-1}$

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)

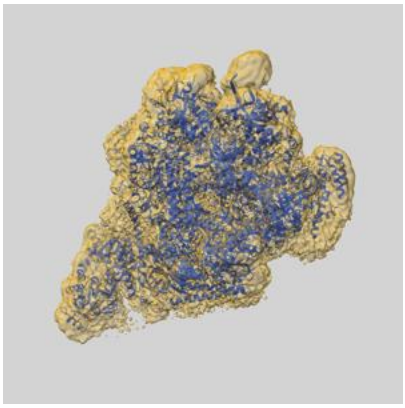
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.81	3.25	2.85
Unmasked-calculated*	3.55	4.40	3.65

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.55 differs from the reported value 2.8 by more than 10 %

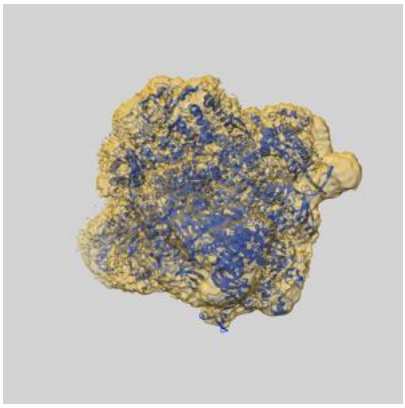
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19019 and PDB model 8RAM. Per-residue inclusion information can be found in section 3 on page 8.

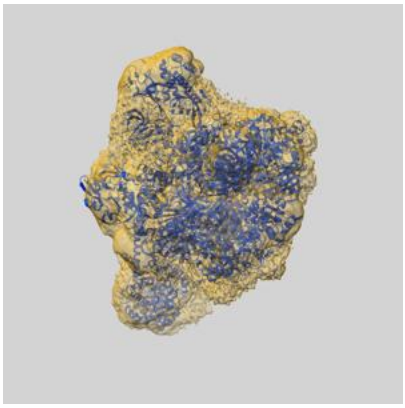
9.1 Map-model overlay



X



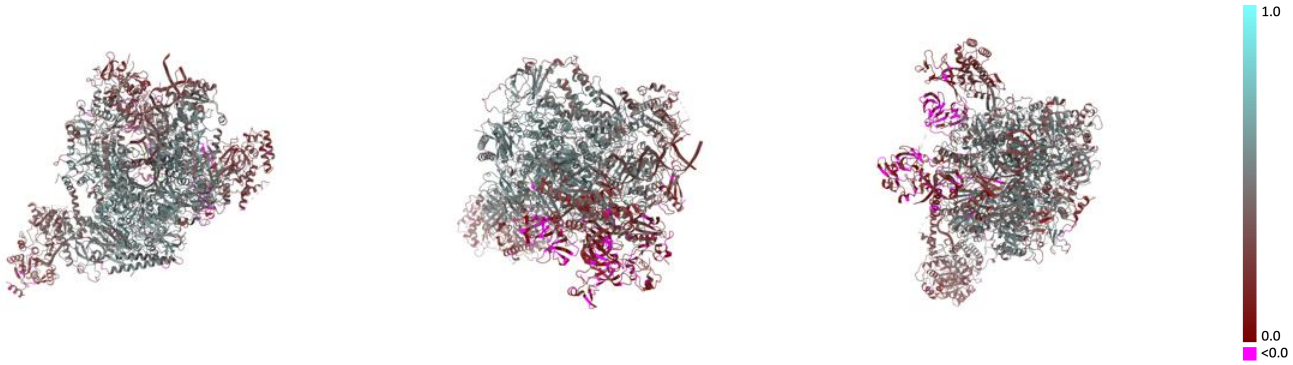
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 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.

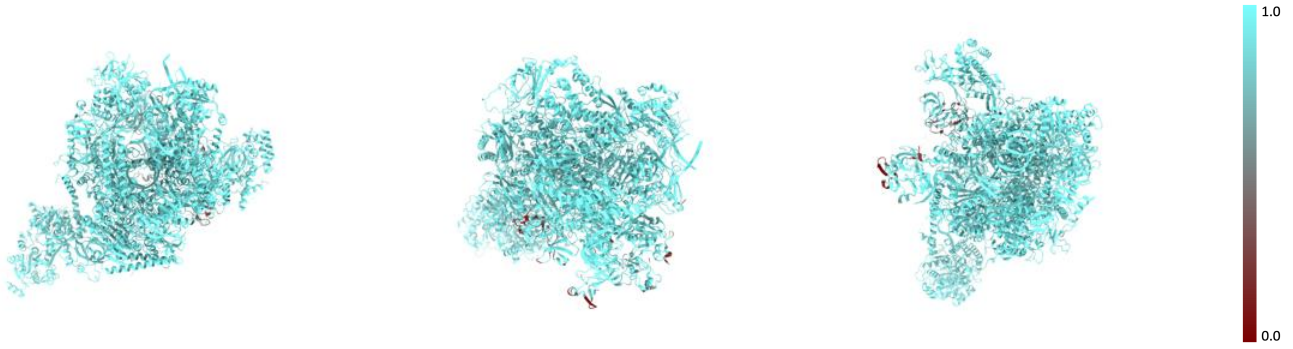
9.2 Q-score mapped to coordinate model (i)



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.

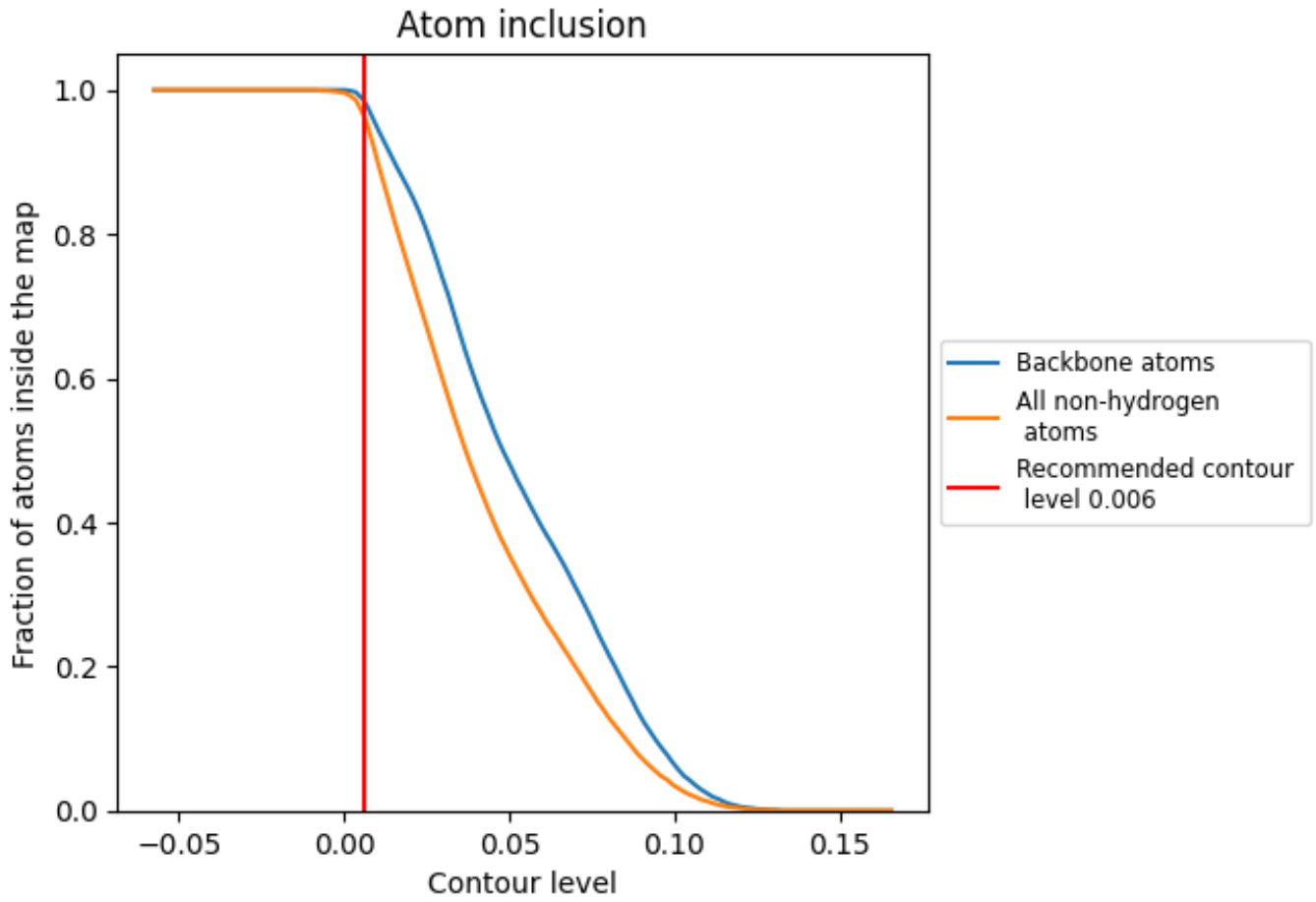
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 96% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9650	0.3940
A	0.9780	0.4730
B	0.9770	0.4930
C	0.9690	0.5160
D	0.9900	0.2080
E	0.9880	0.4370
F	0.9930	0.5020
G	0.9740	0.2550
H	0.9810	0.4610
I	0.9800	0.3300
J	0.9610	0.5270
K	0.9820	0.5200
L	0.9760	0.4450
M	0.9380	0.1650
N	0.9980	0.2320
O	0.9820	0.2960
P	0.9970	0.3000
T	0.9890	0.3230
Y	0.9040	0.1300
Z	0.8170	0.1310