Full wwPDB EM Validation Report ⓘ

Mar 3, 2024 – 03:32 PM EST

PDB ID	:	5VVS
EMDB ID	:	EMD-8737
Title	:	RNA pol II elongation complex
Authors	:	Lahiri, I.; Leschziner, A.E.
Deposited on	:	2017-05-20
Resolution	:	6.40 Å(reported)

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

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

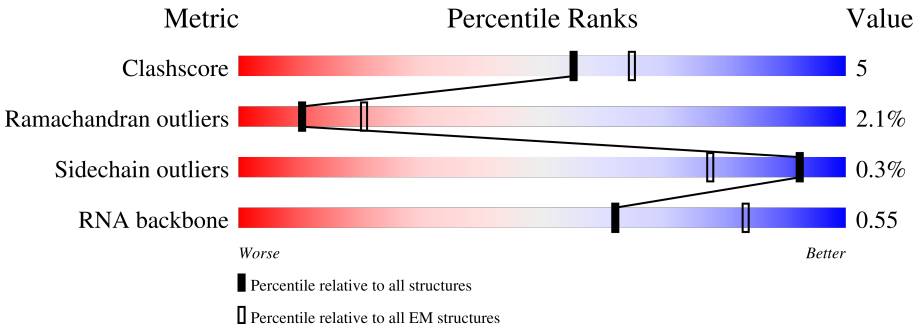
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 6.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	76% 8% 16%
2	B	1224	5% 87% 10%
3	C	318	74% 10% 15%
4	D	221	9% 73% 6% 21%
5	E	215	87% 12%
6	F	155	46% 6% 48%
7	G	171	16% 92% 8%

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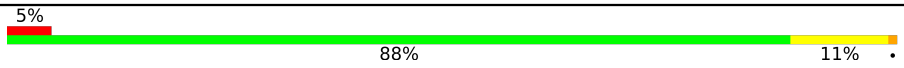
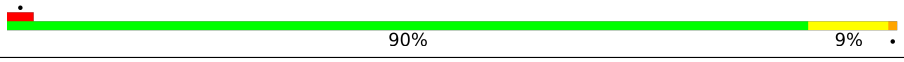
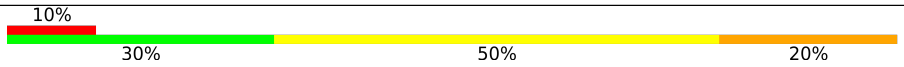
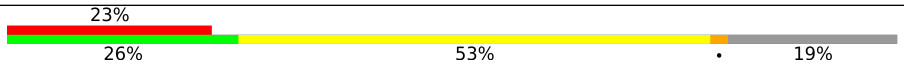
Mol	Chain	Length	Quality of chain
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	R	10	
14	N	47	
15	T	47	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 33790 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	1455	11444	7205	1997	2180	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	1207	9608	6062	1678	1812	56	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	270	2125	1336	353	422	14	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	175	1409	870	251	286	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	215	1760	1116	310	322	12	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	81	657	419	111	124	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	146	Total	C	N	O	S	0	0
			1161	726	195	235	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	122	Total	C	N	O	S	0	0
			997	613	182	191	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	70	Total	C	N	O	S	0	0
			578	366	102	104	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	111	Total	C	N	O	S	0	0
			895	575	152	166	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	46	Total	C	N	O	S	0	0
			364	224	72	64	4		

- Molecule 13 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	10	Total	C	N	O	P	0	0
			220	98	45	67	10		

- Molecule 14 is a DNA chain called DNA (NTS).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	22	Total	C	N	O	P	0	0
			460	216	96	126	22		

- Molecule 15 is a DNA chain called DNA (TS).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	38	Total	C	N	O	P	0	0
			763	365	124	236	38		

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

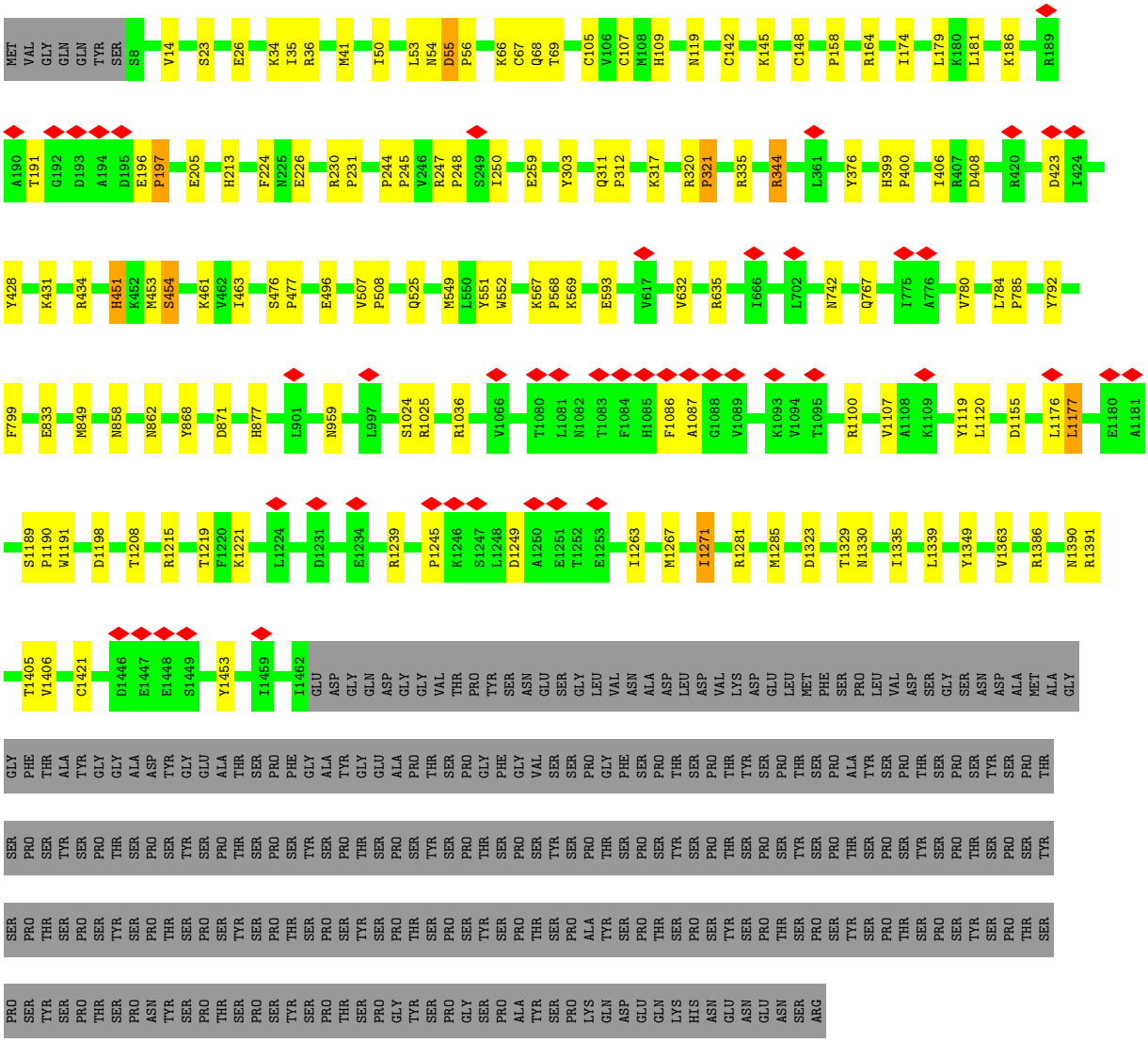
Mol	Chain	Residues	Atoms		AltConf
17	R	1	Total	Mg	0
			1	1	

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.

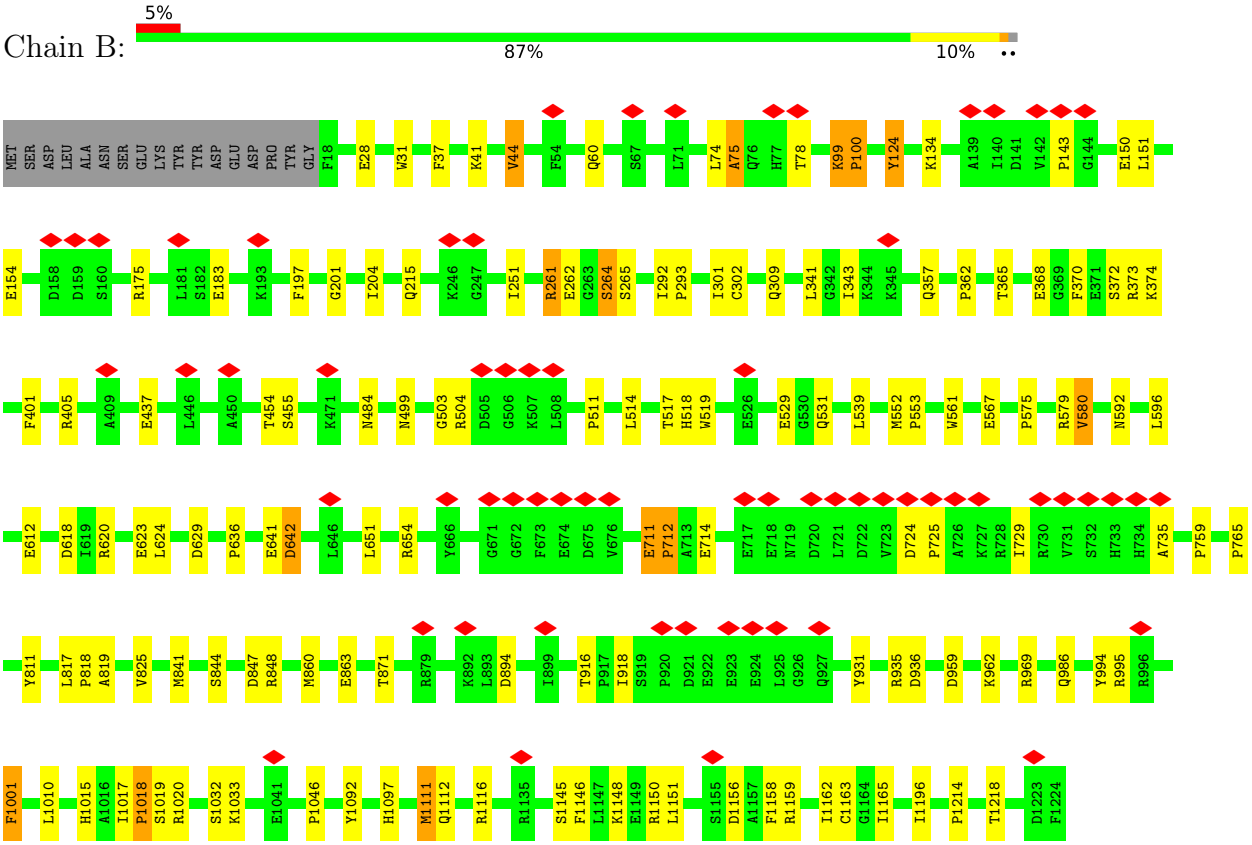
• Molecule 1: DNA-directed RNA polymerase II subunit RPB1

Chain A:



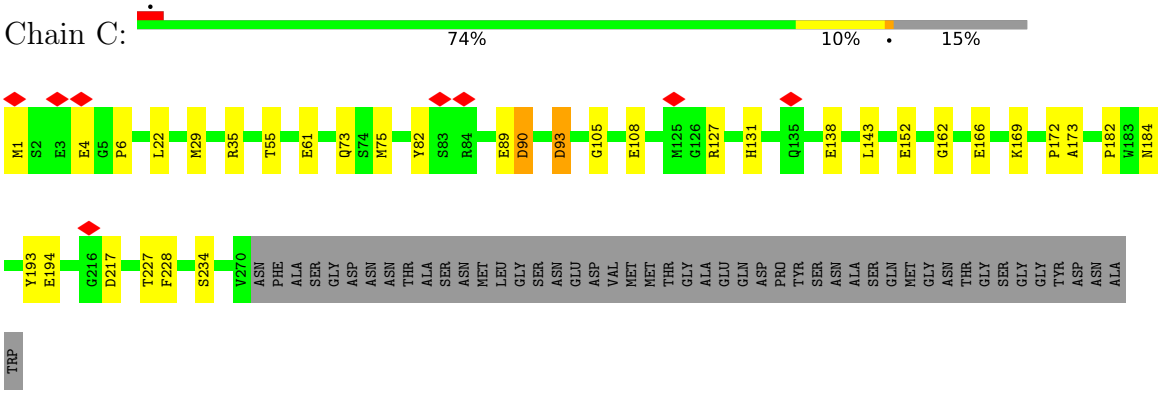
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:



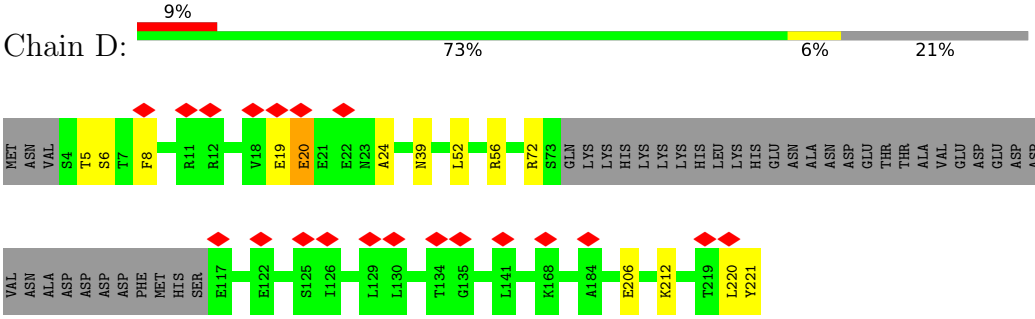
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



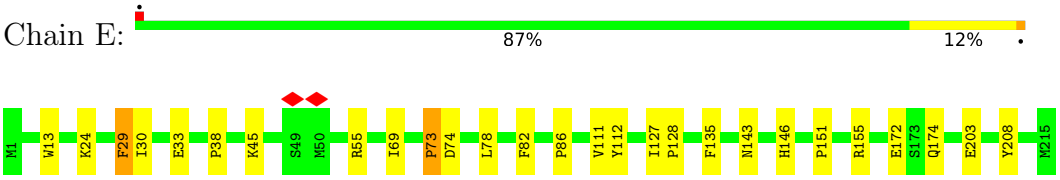
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D:



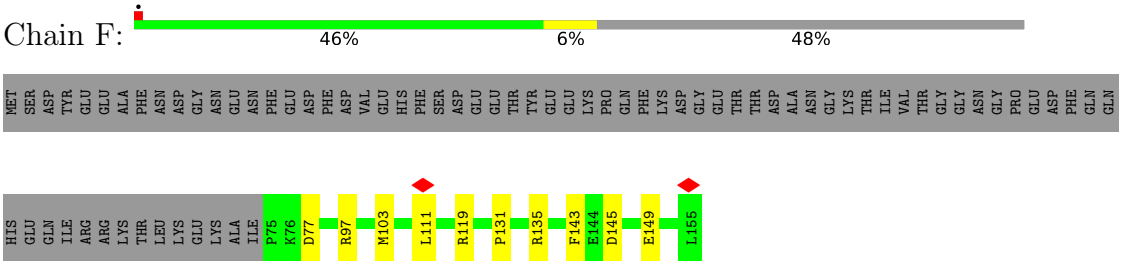
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



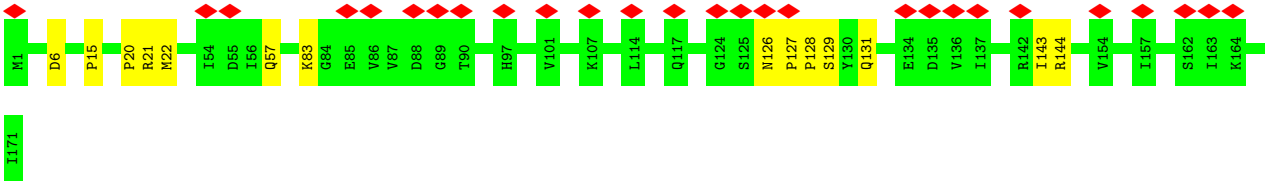
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



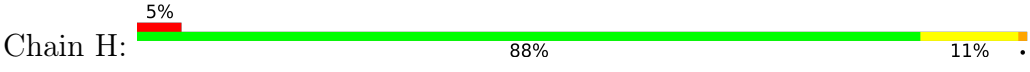
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

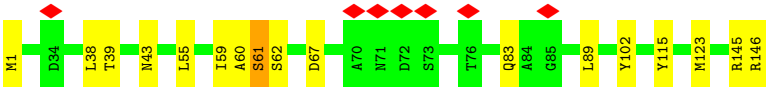
Chain G:



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

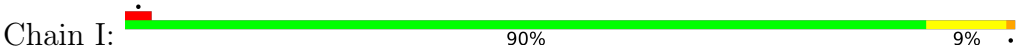
Chain H:

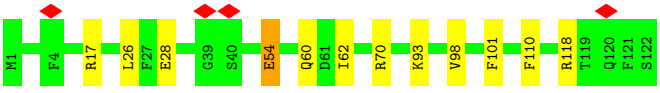




• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

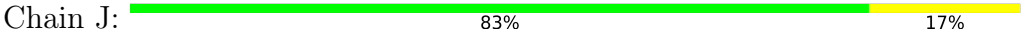
Chain I:

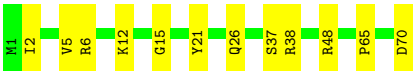




• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

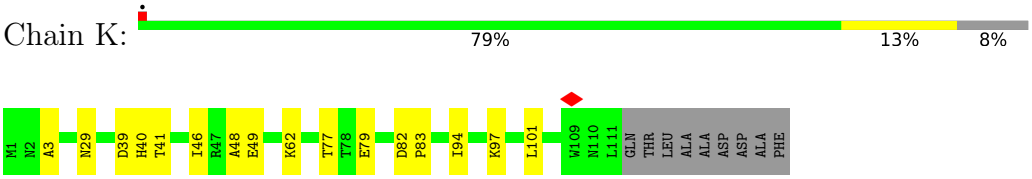
Chain J:





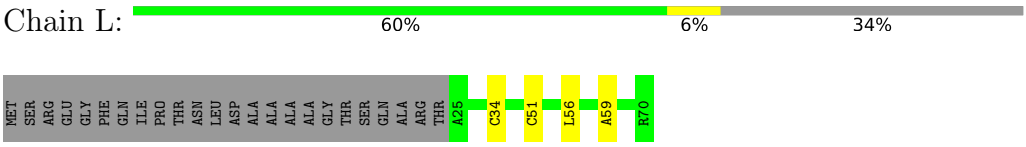
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K:



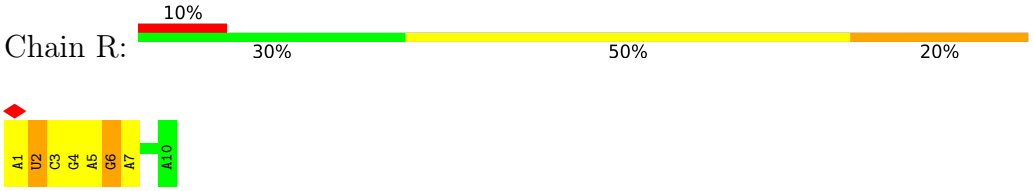
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



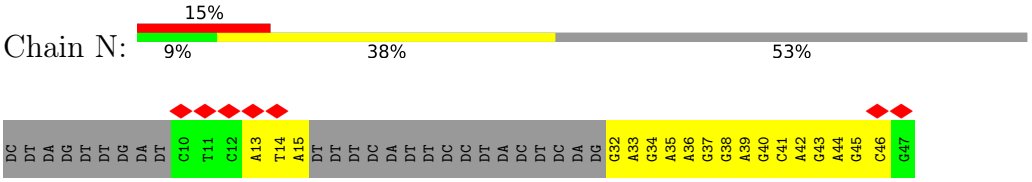
• Molecule 13: RNA

Chain R:



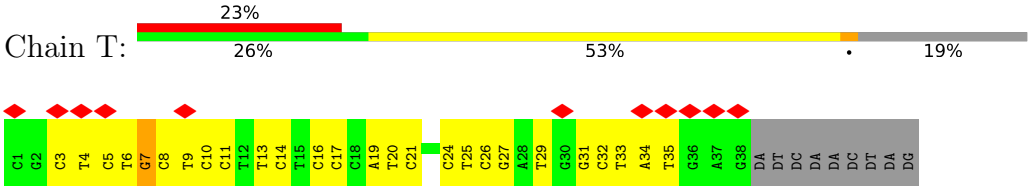
• Molecule 14: DNA (NTS)

Chain N:



• Molecule 15: DNA (TS)

Chain T:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19331	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	7.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.069	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0256	Depositor
Map size (Å)	460.80002, 460.80002, 460.80002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	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	0.84	0/11651	0.76	8/15761 (0.1%)
2	B	0.85	0/9799	0.79	8/13221 (0.1%)
3	C	0.88	0/2163	0.75	0/2930
4	D	0.92	0/1419	0.66	1/1903 (0.1%)
5	E	0.88	0/1796	0.82	3/2416 (0.1%)
6	F	0.90	0/669	0.79	0/903
7	G	0.76	0/1368	0.80	2/1844 (0.1%)
8	H	0.82	0/1181	0.83	2/1602 (0.1%)
9	I	0.86	0/1016	0.80	0/1365
10	J	0.87	0/587	0.82	2/786 (0.3%)
11	K	0.88	0/913	0.76	0/1232
12	L	0.76	0/366	0.86	0/485
13	R	0.65	1/247 (0.4%)	0.79	0/384
14	N	0.37	0/518	0.65	0/796
15	T	0.42	1/849 (0.1%)	0.73	0/1305
All	All	0.83	2/34542 (0.0%)	0.77	26/46933 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	R	6	G	C1'-N9	-6.36	1.38	1.46
15	T	7	DG	C1'-N9	-5.66	1.39	1.47

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	124	TYR	CB-CG-CD1	-7.10	116.74	121.00
8	H	102	TYR	CB-CG-CD2	-6.47	117.12	121.00
7	G	144	ARG	NE-CZ-NH2	-6.09	117.26	120.30
5	E	112	TYR	CB-CG-CD1	-6.08	117.35	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1156	ASP	CB-CG-OD2	6.05	123.74	118.30
8	H	145	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	A	434	ARG	NE-CZ-NH1	5.55	123.08	120.30
10	J	21	TYR	CB-CG-CD2	-5.55	117.67	121.00
4	D	56	ARG	NE-CZ-NH2	-5.50	117.55	120.30
7	G	21	ARG	NE-CZ-NH2	-5.44	117.58	120.30
5	E	127	ILE	C-N-CD	-5.40	108.73	120.60
2	B	1156	ASP	CB-CG-OD1	-5.38	113.45	118.30
1	A	792	TYR	CB-CG-CD2	-5.36	117.78	121.00
2	B	405	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	335	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	428	TYR	CB-CG-CD1	-5.26	117.84	121.00
1	A	303	TYR	CB-CG-CD1	-5.25	117.85	121.00
2	B	1092	TYR	CB-CG-CD2	-5.21	117.88	121.00
2	B	994	TYR	CB-CG-CD2	-5.19	117.89	121.00
1	A	1100	ARG	NE-CZ-NH2	-5.18	117.71	120.30
2	B	99	LYS	C-N-CD	-5.17	109.23	120.60
10	J	48	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	1239	ARG	NE-CZ-NH2	-5.09	117.76	120.30
2	B	969	ARG	NE-CZ-NH1	-5.05	117.77	120.30
5	E	155	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	A	1349	TYR	CB-CG-CD1	-5.01	117.99	121.00

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	11444	0	11502	93	0
2	B	9608	0	9578	107	0
3	C	2125	0	2094	26	0
4	D	1409	0	1423	10	0
5	E	1760	0	1788	16	0
6	F	657	0	673	10	0
7	G	1340	0	1357	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1161	0	1124	11	0
9	I	997	0	959	8	0
10	J	578	0	590	4	0
11	K	895	0	903	11	0
12	L	364	0	389	1	0
13	R	220	0	110	13	0
14	N	460	0	246	14	0
15	T	763	0	431	35	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	R	1	0	0	0	0
All	All	33790	0	33167	353	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 (353) 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)
15:T:3:DC:H2”	15:T:4:DT:H72	1.50	0.94
2:B:343:ILE:HG22	2:B:343:ILE:O	1.74	0.88
15:T:19:DA:C8	15:T:20:DT:H72	2.11	0.85
5:E:208:TYR:CD2	5:E:208:TYR:O	2.32	0.83
2:B:580:VAL:HG12	2:B:580:VAL:O	1.77	0.82
2:B:251:ILE:HG22	2:B:251:ILE:O	1.81	0.80
10:J:70:ASP:OXT	10:J:70:ASP:OD1	2.05	0.74
2:B:519:TRP:O	2:B:519:TRP:CE3	2.42	0.73
7:G:131:GLN:OE1	7:G:131:GLN:O	2.07	0.73
1:A:69:THR:O	1:A:69:THR:HG22	1.86	0.73
2:B:44:VAL:HG12	2:B:44:VAL:O	1.88	0.73
14:N:34:DG:H2’	14:N:35:DA:C8	2.24	0.72
15:T:9:DT:H2”	15:T:10:DC:C5	2.25	0.71
1:A:1363:VAL:HG12	1:A:1363:VAL:O	1.91	0.70
1:A:1191:TRP:HA	1:A:1191:TRP:CE3	2.24	0.70
1:A:145:LYS:O	1:A:145:LYS:HG2	1.91	0.69
2:B:539:LEU:HD12	2:B:539:LEU:O	1.95	0.67
15:T:3:DC:H2”	15:T:4:DT:C7	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:108:GLU:OE1	3:C:108:GLU:N	2.26	0.67
2:B:60:GLN:N	2:B:60:GLN:OE1	2.28	0.67
15:T:10:DC:H2'	15:T:11:DC:C6	2.28	0.67
2:B:518:HIS:HD2	2:B:518:HIS:O	1.79	0.66
13:R:5:A:O5'	13:R:5:A:H8	1.79	0.66
15:T:5:DC:C5	15:T:6:DT:H73	2.30	0.66
6:F:149:GLU:OE1	6:F:149:GLU:N	2.24	0.66
1:A:868:TYR:C	1:A:868:TYR:CD2	2.70	0.65
15:T:16:DC:N3	15:T:17:DC:N4	2.45	0.65
2:B:175:ARG:O	2:B:175:ARG:HG2	1.96	0.64
13:R:4:G:O5'	13:R:4:G:H8	1.80	0.64
14:N:42:DA:C2	15:T:7:DG:C2	2.86	0.64
1:A:1191:TRP:HA	1:A:1191:TRP:HE3	1.62	0.64
15:T:3:DC:C2'	15:T:4:DT:H72	2.25	0.64
1:A:247:ARG:O	1:A:247:ARG:HG3	1.96	0.64
2:B:341:LEU:O	2:B:341:LEU:HD23	1.98	0.64
2:B:518:HIS:C	2:B:518:HIS:CD2	2.69	0.64
1:A:226:GLU:N	1:A:226:GLU:OE1	2.32	0.63
15:T:26:DC:H2"	15:T:27:DG:H5'	1.80	0.63
2:B:37:PHE:O	2:B:37:PHE:CD1	2.52	0.63
2:B:261:ARG:N	2:B:261:ARG:HD2	2.15	0.62
1:A:1271:ILE:O	1:A:1271:ILE:HG22	1.98	0.62
14:N:40:DG:H2"	14:N:41:DC:C6	2.35	0.61
1:A:551:TYR:C	1:A:551:TYR:CD2	2.74	0.60
2:B:1015:HIS:ND1	2:B:1015:HIS:C	2.54	0.60
14:N:34:DG:C6	14:N:35:DA:C6	2.90	0.60
1:A:453:MET:SD	1:A:453:MET:N	2.75	0.60
8:H:61:SER:OG	8:H:62:SER:N	2.35	0.60
11:K:29:ASN:ND2	11:K:77:THR:OG1	2.35	0.60
1:A:742:ASN:OD1	1:A:742:ASN:N	2.34	0.60
15:T:9:DT:H2"	15:T:10:DC:C6	2.37	0.59
2:B:183:GLU:N	2:B:183:GLU:OE1	2.35	0.59
15:T:4:DT:H2"	15:T:5:DC:C6	2.38	0.59
2:B:343:ILE:O	2:B:343:ILE:CG2	2.47	0.59
2:B:529:GLU:N	2:B:529:GLU:OE1	2.36	0.59
15:T:5:DC:C6	15:T:6:DT:H71	2.38	0.58
15:T:34:DA:H2"	15:T:35:DT:C7	2.34	0.58
15:T:5:DC:C6	15:T:6:DT:C7	2.87	0.58
2:B:518:HIS:O	2:B:518:HIS:CD2	2.58	0.57
2:B:714:GLU:OE1	2:B:714:GLU:N	2.35	0.57
1:A:1086:PHE:O	1:A:1086:PHE:CD1	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:R:1:A:C2'	13:R:2:U:H5'	2.33	0.57
2:B:871:THR:HG23	2:B:871:THR:O	2.05	0.57
1:A:551:TYR:CD2	1:A:551:TYR:O	2.58	0.56
3:C:169:LYS:HD2	3:C:169:LYS:N	2.20	0.56
1:A:191:THR:HG22	1:A:191:THR:O	2.05	0.56
3:C:227:THR:HG22	3:C:227:THR:O	2.06	0.56
2:B:251:ILE:O	2:B:251:ILE:CG2	2.52	0.56
3:C:127:ARG:O	3:C:127:ARG:HG2	2.06	0.56
3:C:55:THR:OG1	3:C:152:GLU:N	2.39	0.56
13:R:1:A:H3'	13:R:2:U:C6	2.40	0.56
2:B:44:VAL:O	2:B:44:VAL:CG1	2.54	0.55
2:B:624:LEU:C	2:B:624:LEU:HD23	2.27	0.55
9:I:54:GLU:N	9:I:54:GLU:OE1	2.39	0.55
1:A:68:GLN:O	1:A:68:GLN:HG2	2.07	0.55
1:A:549:MET:SD	1:A:549:MET:C	2.85	0.55
1:A:1024:SER:OG	1:A:1025:ARG:N	2.39	0.55
1:A:1421:CYS:O	1:A:1421:CYS:SG	2.65	0.55
14:N:13:DA:H1'	14:N:14:DT:H5'	1.88	0.54
1:A:463:ILE:O	1:A:463:ILE:HG13	2.07	0.54
15:T:25:DT:H2"	15:T:26:DC:C6	2.42	0.54
13:R:1:A:OP2	13:R:1:A:H8	1.90	0.54
2:B:651:LEU:O	2:B:654:ARG:NH1	2.41	0.54
3:C:166:GLU:HA	3:C:166:GLU:OE1	2.07	0.54
1:A:461:LYS:HD3	1:A:461:LYS:C	2.27	0.54
1:A:868:TYR:CD2	1:A:868:TYR:O	2.61	0.54
1:A:431:LYS:HD2	1:A:431:LYS:N	2.23	0.54
14:N:40:DG:H2"	14:N:41:DC:H6	1.71	0.54
10:J:37:SER:OG	10:J:38:ARG:NH1	2.41	0.54
2:B:918:ILE:HG23	2:B:918:ILE:O	2.09	0.53
2:B:372:SER:OG	2:B:373:ARG:N	2.41	0.53
15:T:34:DA:H2"	15:T:35:DT:H71	1.90	0.53
2:B:341:LEU:HD23	2:B:341:LEU:C	2.29	0.53
1:A:525:GLN:OE1	1:A:525:GLN:N	2.39	0.53
2:B:78:THR:O	2:B:78:THR:HG22	2.08	0.53
1:A:1215:ARG:NH1	1:A:1219:THR:OG1	2.42	0.53
15:T:19:DA:N9	15:T:20:DT:H72	2.23	0.53
2:B:357:GLN:O	2:B:365:THR:OG1	2.28	0.52
6:F:111:LEU:HD23	6:F:111:LEU:O	2.08	0.52
1:A:1120:LEU:HD12	1:A:1120:LEU:C	2.30	0.52
2:B:531:GLN:OE1	2:B:531:GLN:N	2.32	0.52
14:N:42:DA:H2"	14:N:43:DG:O5'	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:N	1:A:56:PRO:CD	2.73	0.52
3:C:22:LEU:HB2	3:C:228:PHE:HB2	1.91	0.52
6:F:119:ARG:HA	6:F:119:ARG:NE	2.25	0.52
2:B:561:TRP:HA	2:B:561:TRP:CE3	2.45	0.52
2:B:1150:ARG:HA	2:B:1150:ARG:NE	2.25	0.52
9:I:60:GLN:OE1	9:I:60:GLN:N	2.36	0.51
2:B:580:VAL:O	2:B:580:VAL:CG1	2.50	0.51
1:A:53:LEU:O	1:A:54:ASN:HB2	2.10	0.51
3:C:194:GLU:OE1	3:C:194:GLU:HA	2.10	0.51
13:R:1:A:H3'	13:R:2:U:C5	2.46	0.51
2:B:341:LEU:O	2:B:341:LEU:CD2	2.58	0.51
6:F:145:ASP:OD1	6:F:145:ASP:C	2.49	0.50
1:A:461:LYS:HD3	1:A:461:LYS:O	2.11	0.50
2:B:261:ARG:HD2	2:B:261:ARG:H	1.76	0.50
2:B:1019:SER:OG	2:B:1020:ARG:NH2	2.44	0.50
14:N:36:DA:C2	14:N:37:DG:C4	2.99	0.50
2:B:592:ASN:OD1	2:B:592:ASN:C	2.50	0.50
9:I:26:LEU:C	9:I:26:LEU:HD12	2.31	0.50
14:N:45:DG:H2"	14:N:46:DC:C5	2.47	0.50
1:A:496:GLU:CD	1:A:496:GLU:H	2.15	0.50
2:B:711:GLU:HB3	2:B:712:PRO:HD2	1.94	0.50
15:T:20:DT:H2'	15:T:21:DC:C6	2.46	0.50
1:A:569:LYS:HE2	1:A:569:LYS:HA	1.93	0.50
1:A:959:ASN:C	1:A:959:ASN:OD1	2.50	0.50
1:A:1386:ARG:HA	1:A:1390:ASN:HB3	1.94	0.50
2:B:28:GLU:OE1	2:B:28:GLU:N	2.37	0.50
2:B:519:TRP:O	2:B:519:TRP:CD2	2.64	0.50
1:A:567:LYS:O	1:A:569:LYS:N	2.45	0.49
15:T:7:DG:H2'	15:T:8:DC:C6	2.47	0.49
8:H:43:ASN:OD1	8:H:43:ASN:C	2.50	0.49
2:B:368:GLU:OE1	2:B:368:GLU:N	2.35	0.49
8:H:89:LEU:C	8:H:89:LEU:HD12	2.33	0.49
14:N:38:DG:H2"	14:N:39:DA:C8	2.47	0.49
9:I:98:VAL:O	9:I:98:VAL:HG13	2.12	0.49
8:H:43:ASN:OD1	8:H:43:ASN:O	2.30	0.49
1:A:1335:ILE:O	1:A:1339:LEU:N	2.46	0.49
2:B:894:ASP:OD1	2:B:894:ASP:C	2.49	0.49
2:B:215:GLN:HG2	2:B:499:ASN:HB2	1.95	0.48
1:A:1221:LYS:N	1:A:1221:LYS:HD2	2.28	0.48
2:B:454:THR:OG1	2:B:455:SER:N	2.47	0.48
2:B:1112:GLN:O	2:B:1116:ARG:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:19:DA:H2"	15:T:20:DT:H73	1.95	0.48
1:A:69:THR:O	1:A:69:THR:CG2	2.59	0.48
7:G:127:PRO:O	7:G:129:SER:N	2.46	0.48
13:R:5:A:O2'	13:R:6:G:H5'	2.13	0.48
2:B:1162:ILE:HG23	2:B:1162:ILE:O	2.13	0.48
1:A:1176:LEU:O	1:A:1177:LEU:CB	2.61	0.48
5:E:13:TRP:O	5:E:13:TRP:HD1	1.97	0.48
2:B:309:GLN:OE1	2:B:309:GLN:N	2.40	0.48
1:A:1405:THR:OG1	1:A:1406:VAL:N	2.47	0.48
2:B:529:GLU:CD	2:B:529:GLU:H	2.17	0.48
2:B:31:TRP:O	2:B:811:TYR:OH	2.31	0.47
5:E:33:GLU:OE1	5:E:33:GLU:N	2.33	0.47
2:B:1163:CYS:SG	2:B:1165:ILE:HG22	2.53	0.47
9:I:101:PHE:HB2	9:I:110:PHE:HB2	1.95	0.47
1:A:320:ARG:O	1:A:321:PRO:C	2.52	0.47
2:B:1001:PHE:HD1	2:B:1001:PHE:O	1.97	0.47
2:B:514:LEU:C	2:B:514:LEU:HD23	2.35	0.47
1:A:552:TRP:HA	11:K:62:LYS:HD2	1.96	0.47
3:C:93:ASP:OD1	3:C:93:ASP:N	2.48	0.47
1:A:453:MET:O	1:A:454:SER:CB	2.63	0.47
1:A:259:GLU:OE1	1:A:259:GLU:N	2.40	0.46
2:B:620:ARG:HB3	2:B:620:ARG:CZ	2.45	0.46
15:T:5:DC:C5	15:T:6:DT:C7	2.97	0.46
1:A:1329:THR:OG1	1:A:1330:ASN:N	2.48	0.46
13:R:4:G:H2'	13:R:5:A:C8	2.49	0.46
2:B:518:HIS:HD2	2:B:518:HIS:C	2.13	0.46
3:C:35:ARG:NH1	11:K:40:HIS:NE2	2.62	0.46
2:B:641:GLU:O	2:B:642:ASP:CB	2.64	0.46
5:E:208:TYR:O	5:E:208:TYR:HD2	1.93	0.46
2:B:1001:PHE:O	2:B:1001:PHE:CD1	2.69	0.46
15:T:31:DG:H2"	15:T:32:DC:OP2	2.14	0.46
2:B:484:ASN:OD1	2:B:484:ASN:C	2.54	0.46
2:B:629:ASP:C	2:B:629:ASP:OD1	2.50	0.46
1:A:767:GLN:HA	1:A:799:PHE:HA	1.97	0.46
1:A:376:TYR:C	1:A:376:TYR:CD2	2.89	0.46
5:E:13:TRP:O	5:E:13:TRP:CD1	2.68	0.46
3:C:29:MET:SD	3:C:29:MET:C	2.94	0.46
3:C:217:ASP:OD1	3:C:217:ASP:C	2.55	0.46
1:A:344:ARG:HD3	1:A:344:ARG:N	2.30	0.45
2:B:1017:ILE:N	2:B:1018:PRO:CD	2.79	0.45
8:H:39:THR:O	8:H:123:MET:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:580:VAL:HA	2:B:624:LEU:HB3	1.99	0.45
2:B:592:ASN:OD1	2:B:592:ASN:O	2.34	0.45
11:K:101:LEU:C	11:K:101:LEU:HD23	2.36	0.45
3:C:89:GLU:O	3:C:90:ASP:CB	2.64	0.45
15:T:5:DC:C2	15:T:6:DT:C5	3.05	0.45
1:A:406:ILE:HB	1:A:431:LYS:HB2	1.98	0.45
2:B:1032:SER:OG	2:B:1033:LYS:N	2.50	0.45
5:E:69:ILE:HB	5:E:73:PRO:HA	1.98	0.45
9:I:17:ARG:HG3	9:I:28:GLU:HB3	1.98	0.45
15:T:24:DC:H5"	15:T:24:DC:H6	1.82	0.45
15:T:29:DT:OP2	15:T:29:DT:H3'	2.16	0.45
1:A:107:CYS:SG	1:A:148:CYS:SG	3.11	0.45
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.99	0.45
3:C:61:GLU:OE1	3:C:61:GLU:N	2.35	0.45
3:C:73:GLN:N	3:C:131:HIS:O	2.44	0.45
1:A:311:GLN:HB3	1:A:312:PRO:HD3	1.97	0.45
1:A:635:ARG:NH1	1:A:877:HIS:ND1	2.63	0.45
1:A:1119:TYR:CD1	1:A:1119:TYR:N	2.85	0.45
2:B:150:GLU:OE1	2:B:150:GLU:N	2.36	0.45
2:B:596:LEU:HD23	2:B:596:LEU:C	2.37	0.45
5:E:172:GLU:C	5:E:172:GLU:OE1	2.55	0.45
7:G:126:ASN:HA	7:G:127:PRO:C	2.37	0.45
1:A:453:MET:O	1:A:454:SER:HB3	2.16	0.45
15:T:13:DT:H2"	15:T:14:DC:H6	1.81	0.45
2:B:302:CYS:O	2:B:302:CYS:SG	2.75	0.45
2:B:1111:MET:SD	2:B:1111:MET:C	2.95	0.45
3:C:143:LEU:HD23	3:C:143:LEU:C	2.37	0.45
1:A:230:ARG:HB3	1:A:231:PRO:HD2	1.99	0.44
3:C:4:GLU:HA	11:K:97:LYS:HG3	1.99	0.44
3:C:169:LYS:N	3:C:169:LYS:CD	2.80	0.44
1:A:1198:ASP:C	1:A:1198:ASP:OD1	2.56	0.44
2:B:552:MET:HB3	2:B:553:PRO:HD3	1.99	0.44
4:D:206:GLU:OE1	4:D:206:GLU:HA	2.17	0.44
3:C:22:LEU:N	3:C:22:LEU:HD12	2.32	0.44
5:E:29:PHE:CD2	5:E:29:PHE:O	2.70	0.44
11:K:79:GLU:H	11:K:79:GLU:CD	2.20	0.44
1:A:67:CYS:SG	1:A:67:CYS:O	2.74	0.44
2:B:197:PHE:CD2	2:B:197:PHE:C	2.91	0.44
2:B:959:ASP:C	2:B:959:ASP:OD1	2.56	0.44
1:A:1263:ILE:O	1:A:1267:MET:N	2.49	0.44
2:B:264:SER:OG	2:B:265:SER:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:19:DA:C2'	15:T:20:DT:C7	2.95	0.44
1:A:109:HIS:H	1:A:213:HIS:HE2	1.65	0.44
1:A:205:GLU:CD	1:A:205:GLU:H	2.19	0.44
1:A:196:GLU:O	1:A:197:PRO:C	2.56	0.44
1:A:1391:ARG:O	1:A:1391:ARG:HG2	2.17	0.44
13:R:1:A:H2'	13:R:2:U:H5'	1.99	0.44
1:A:423:ASP:C	1:A:423:ASP:OD1	2.55	0.44
8:H:146:ARG:OXT	8:H:146:ARG:HG3	2.18	0.44
1:A:451:HIS:N	1:A:451:HIS:CD2	2.84	0.44
2:B:37:PHE:CD1	2:B:37:PHE:C	2.82	0.44
10:J:5:VAL:O	10:J:6:ARG:HB2	2.18	0.44
1:A:1155:ASP:OD1	1:A:1155:ASP:C	2.55	0.43
2:B:1001:PHE:CD1	2:B:1001:PHE:C	2.89	0.43
13:R:2:U:C5	13:R:2:U:OP2	2.71	0.43
1:A:849:MET:SD	1:A:849:MET:C	2.97	0.43
4:D:39:ASN:OD1	4:D:39:ASN:C	2.56	0.43
15:T:16:DC:C4	15:T:17:DC:N4	2.85	0.43
15:T:34:DA:H2"	15:T:35:DT:C5	2.52	0.43
1:A:34:LYS:O	1:A:36:ARG:NH1	2.52	0.43
1:A:1189:SER:HB2	1:A:1190:PRO:HD2	1.99	0.43
2:B:134:LYS:N	2:B:134:LYS:HD3	2.32	0.43
2:B:539:LEU:HD12	2:B:539:LEU:C	2.38	0.43
4:D:19:GLU:O	4:D:20:GLU:HB2	2.18	0.43
2:B:292:ILE:HB	2:B:293:PRO:HD3	2.01	0.43
5:E:24:LYS:HB3	5:E:30:ILE:HB	1.99	0.43
2:B:74:LEU:O	2:B:75:ALA:C	2.57	0.43
5:E:143:ASN:O	5:E:146:HIS:ND1	2.51	0.43
13:R:6:G:H2'	13:R:7:A:C8	2.53	0.43
15:T:16:DC:C2	15:T:17:DC:C4	3.07	0.43
1:A:105:CYS:HB3	1:A:142:CYS:SG	2.58	0.43
1:A:399:HIS:N	1:A:400:PRO:HD2	2.33	0.43
1:A:551:TYR:C	1:A:551:TYR:HD2	2.19	0.43
2:B:567:GLU:OE1	2:B:567:GLU:N	2.46	0.43
2:B:1145:SER:OG	2:B:1146:PHE:N	2.51	0.43
2:B:124:TYR:HB2	2:B:204:ILE:HB	2.01	0.43
2:B:729:ILE:O	2:B:729:ILE:HG23	2.17	0.43
2:B:99:LYS:O	2:B:100:PRO:C	2.56	0.43
2:B:1111:MET:SD	2:B:1116:ARG:HA	2.59	0.43
3:C:82:TYR:CE1	3:C:162:GLY:HA2	2.53	0.43
5:E:55:ARG:HD3	5:E:82:PHE:CE2	2.54	0.43
8:H:115:TYR:N	8:H:115:TYR:CD1	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:R:1:A:OP2	13:R:1:A:C8	2.71	0.43
2:B:995:ARG:HD3	2:B:995:ARG:HA	1.86	0.43
5:E:111:VAL:HA	5:E:135:PHE:O	2.18	0.43
1:A:868:TYR:O	1:A:868:TYR:HD2	2.01	0.42
2:B:37:PHE:O	2:B:41:LYS:N	2.51	0.42
2:B:1158:PHE:N	2:B:1196:ILE:O	2.51	0.42
3:C:1:MET:SD	11:K:48:ALA:O	2.77	0.42
7:G:143:ILE:HG23	7:G:143:ILE:O	2.19	0.42
2:B:844:SER:O	2:B:848:ARG:HG2	2.19	0.42
2:B:863:GLU:HB2	2:B:962:LYS:HB3	2.01	0.42
3:C:173:ALA:HA	3:C:234:SER:HA	2.01	0.42
3:C:193:TYR:CD1	3:C:193:TYR:C	2.92	0.42
1:A:23:SER:O	1:A:26:GLU:N	2.52	0.42
1:A:1285:MET:O	1:A:1285:MET:SD	2.77	0.42
2:B:618:ASP:OD1	2:B:618:ASP:C	2.58	0.42
15:T:13:DT:H2"	15:T:14:DC:C6	2.54	0.42
1:A:50:ILE:HB	1:A:53:LEU:O	2.18	0.42
1:A:632:VAL:O	1:A:635:ARG:HB3	2.18	0.42
1:A:862:ASN:HA	5:E:174:GLN:HA	2.01	0.42
9:I:118:ARG:HA	9:I:118:ARG:NE	2.34	0.42
11:K:39:ASP:OD1	11:K:39:ASP:C	2.57	0.42
12:L:34:CYS:SG	12:L:51:CYS:SG	3.17	0.42
1:A:1086:PHE:O	1:A:1086:PHE:HD1	2.02	0.42
1:A:1245:PRO:HA	1:A:1249:ASP:HB3	2.01	0.42
2:B:841:MET:SD	2:B:1010:LEU:HD13	2.59	0.42
5:E:203:GLU:OE1	5:E:203:GLU:HA	2.19	0.42
15:T:16:DC:C2	15:T:17:DC:N4	2.87	0.42
1:A:567:LYS:HB2	1:A:567:LYS:HE2	1.84	0.42
2:B:503:GLY:O	2:B:504:ARG:HB2	2.20	0.42
2:B:847:ASP:O	3:C:169:LYS:NZ	2.53	0.42
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.83	0.42
1:A:1107:VAL:HG12	1:A:1107:VAL:O	2.20	0.42
2:B:817:LEU:N	2:B:818:PRO:HD3	2.35	0.42
2:B:936:ASP:C	2:B:936:ASP:OD1	2.58	0.42
4:D:24:ALA:HA	7:G:83:LYS:HB3	2.02	0.42
4:D:212:LYS:HA	4:D:212:LYS:HD3	1.78	0.42
14:N:44:DA:H2"	14:N:45:DG:C8	2.55	0.42
2:B:262:GLU:OE1	2:B:262:GLU:N	2.44	0.41
2:B:579:ARG:N	2:B:579:ARG:HD2	2.35	0.41
4:D:39:ASN:HB2	7:G:6:ASP:HB3	2.02	0.41
8:H:1:MET:HB3	8:H:62:SER:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:101:PHE:CD1	9:I:101:PHE:N	2.88	0.41
1:A:507:VAL:HB	1:A:508:PRO:HD3	2.01	0.41
1:A:1281:ARG:CZ	1:A:1281:ARG:HB2	2.50	0.41
2:B:860:MET:SD	2:B:860:MET:N	2.93	0.41
4:D:72:ARG:HA	4:D:72:ARG:NE	2.35	0.41
14:N:32:DG:H2"	14:N:33:DA:OP2	2.19	0.41
5:E:78:LEU:C	5:E:78:LEU:HD23	2.40	0.41
10:J:6:ARG:HA	10:J:12:LYS:O	2.20	0.41
1:A:1323:ASP:OD1	1:A:1323:ASP:C	2.59	0.41
2:B:825:VAL:HG12	2:B:1010:LEU:HB3	2.02	0.41
3:C:75:MET:SD	3:C:75:MET:N	2.87	0.41
6:F:103:MET:SD	7:G:15:PRO:HB3	2.60	0.41
14:N:39:DA:H2"	14:N:40:DG:H8	1.85	0.41
3:C:127:ARG:O	3:C:127:ARG:CG	2.69	0.41
15:T:19:DA:C2'	15:T:20:DT:H72	2.51	0.41
1:A:496:GLU:CD	1:A:496:GLU:N	2.74	0.41
8:H:59:ILE:O	8:H:60:ALA:C	2.59	0.41
13:R:6:G:H2'	13:R:7:A:H8	1.85	0.41
1:A:179:LEU:HD13	1:A:179:LEU:HA	1.91	0.41
1:A:858:ASN:C	1:A:858:ASN:OD1	2.59	0.41
2:B:370:PHE:HA	2:B:374:LYS:HB2	2.02	0.41
2:B:401:PHE:HB3	2:B:517:THR:HB	2.03	0.41
2:B:916:THR:O	2:B:935:ARG:N	2.54	0.41
14:N:15:DA:H61	15:T:33:DT:H3	1.69	0.41
1:A:14:VAL:HA	2:B:1218:THR:HA	2.03	0.41
1:A:1453:TYR:CE1	6:F:131:PRO:HA	2.56	0.41
2:B:918:ILE:O	2:B:918:ILE:CG2	2.68	0.41
5:E:208:TYR:O	5:E:208:TYR:CG	2.69	0.41
6:F:111:LEU:HD23	6:F:111:LEU:C	2.41	0.41
6:F:135:ARG:HG3	6:F:143:PHE:HB2	2.01	0.41
8:H:38:LEU:C	8:H:38:LEU:HD23	2.41	0.41
2:B:759:PRO:HD2	2:B:1046:PRO:HB3	2.03	0.41
2:B:931:TYR:O	2:B:931:TYR:CD1	2.74	0.41
4:D:220:LEU:O	4:D:221:TYR:C	2.59	0.40
11:K:46:ILE:O	11:K:49:GLU:HG2	2.22	0.40
11:K:82:ASP:HA	11:K:83:PRO:HD3	1.93	0.40
1:A:174:ILE:HG23	1:A:181:LEU:HB3	2.03	0.40
1:A:476:SER:HB3	1:A:477:PRO:CD	2.51	0.40
1:A:784:LEU:HB3	1:A:785:PRO:HD2	2.02	0.40
2:B:151:LEU:O	2:B:154:GLU:HB3	2.21	0.40
6:F:77:ASP:C	6:F:77:ASP:OD1	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:55:LEU:C	8:H:55:LEU:HD12	2.41	0.40
11:K:94:ILE:O	11:K:97:LYS:HB3	2.21	0.40
2:B:618:ASP:HB3	2:B:623:GLU:HB2	2.04	0.40
1:A:1208:THR:O	1:A:1208:THR:HG23	2.21	0.40
2:B:1148:LYS:HA	2:B:1151:LEU:HB3	2.04	0.40
4:D:5:THR:OG1	4:D:6:SER:N	2.53	0.40
4:D:52:LEU:C	4:D:52:LEU:HD23	2.42	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	1453/1733 (84%)	1292 (89%)	137 (9%)	24 (2%)	9 42
2	B	1205/1224 (98%)	1089 (90%)	90 (8%)	26 (2%)	6 35
3	C	268/318 (84%)	232 (87%)	28 (10%)	8 (3%)	4 28
4	D	171/221 (77%)	157 (92%)	12 (7%)	2 (1%)	13 50
5	E	213/215 (99%)	190 (89%)	15 (7%)	8 (4%)	3 24
6	F	79/155 (51%)	73 (92%)	6 (8%)	0	100 100
7	G	169/171 (99%)	153 (90%)	12 (7%)	4 (2%)	6 33
8	H	144/146 (99%)	118 (82%)	23 (16%)	3 (2%)	7 36
9	I	120/122 (98%)	102 (85%)	16 (13%)	2 (2%)	9 42
10	J	68/70 (97%)	59 (87%)	5 (7%)	4 (6%)	1 17
11	K	109/120 (91%)	103 (94%)	4 (4%)	2 (2%)	8 40
12	L	44/70 (63%)	35 (80%)	7 (16%)	2 (4%)	2 22
All	All	4043/4565 (89%)	3603 (89%)	355 (9%)	85 (2%)	10 36

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	MET
1	A	66	LYS
1	A	119	ASN
1	A	186	LYS
1	A	250	ILE
1	A	321	PRO
1	A	568	PRO
1	A	593	GLU
1	A	1177	LEU
2	B	100	PRO
2	B	642	ASP
2	B	711	GLU
2	B	725	PRO
2	B	1018	PRO
2	B	1214	PRO
3	C	90	ASP
3	C	172	PRO
5	E	128	PRO
7	G	22	MET
9	I	62	ILE
11	K	41	THR
1	A	164	ARG
1	A	317	LYS
1	A	408	ASP
1	A	454	SER
1	A	871	ASP
2	B	44	VAL
2	B	75	ALA
2	B	201	GLY
2	B	712	PRO
2	B	735	ALA
3	C	105	GLY
3	C	184	ASN
7	G	128	PRO
8	H	67	ASP
8	H	83	GLN
9	I	93	LYS
10	J	65	PRO
1	A	197	PRO
1	A	224	PHE
1	A	833	GLU
2	B	575	PRO
2	B	986	GLN

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Mol	Chain	Res	Type
3	C	93	ASP
4	D	8	PHE
5	E	29	PHE
5	E	45	LYS
7	G	20	PRO
7	G	57	GLN
8	H	61	SER
10	J	26	GLN
11	K	3	ALA
1	A	1087	ALA
2	B	143	PRO
2	B	264	SER
2	B	362	PRO
2	B	511	PRO
2	B	636	PRO
2	B	819	ALA
5	E	38	PRO
5	E	151	PRO
12	L	59	ALA
1	A	35	ILE
1	A	248	PRO
1	A	1271	ILE
2	B	437	GLU
2	B	612	GLU
2	B	1097	HIS
3	C	138	GLU
4	D	20	GLU
5	E	74	ASP
5	E	86	PRO
10	J	2	ILE
12	L	56	LEU
2	B	580	VAL
2	B	724	ASP
2	B	301	ILE
10	J	15	GLY
1	A	55	ASP
1	A	158	PRO
1	A	780	VAL
2	B	765	PRO
3	C	6	PRO
3	C	182	PRO
5	E	73	PRO

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	1271/1520 (84%)	1268 (100%)	3 (0%)	93 96
2	B	1046/1061 (99%)	1042 (100%)	4 (0%)	91 94
3	C	238/274 (87%)	238 (100%)	0	100 100
4	D	157/200 (78%)	157 (100%)	0	100 100
5	E	197/197 (100%)	197 (100%)	0	100 100
6	F	72/137 (53%)	72 (100%)	0	100 100
7	G	152/152 (100%)	152 (100%)	0	100 100
8	H	128/128 (100%)	128 (100%)	0	100 100
9	I	116/116 (100%)	114 (98%)	2 (2%)	60 78
10	J	65/65 (100%)	65 (100%)	0	100 100
11	K	96/102 (94%)	96 (100%)	0	100 100
12	L	40/57 (70%)	40 (100%)	0	100 100
All	All	3578/4009 (89%)	3569 (100%)	9 (0%)	92 95

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	344	ARG
1	A	451	HIS
1	A	1036	ARG
2	B	261	ARG
2	B	1001	PHE
2	B	1111	MET
2	B	1159	ARG
9	I	54	GLU
9	I	70	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1128	GLN
1	A	1188	GLN
2	B	518	HIS
2	B	1178	ASN
11	K	29	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	R	9/10 (90%)	2 (22%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	R	2	U
13	R	3	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 9 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.

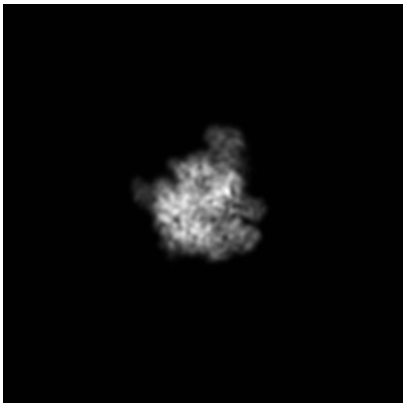
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8737. These allow visual inspection of the internal detail of the map and identification of artifacts.

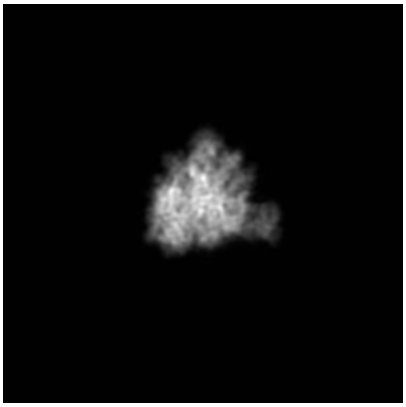
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

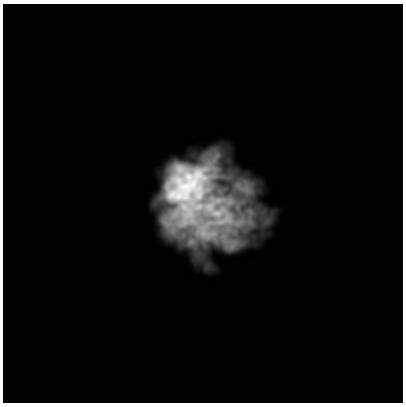
6.1.1 Primary map



X



Y

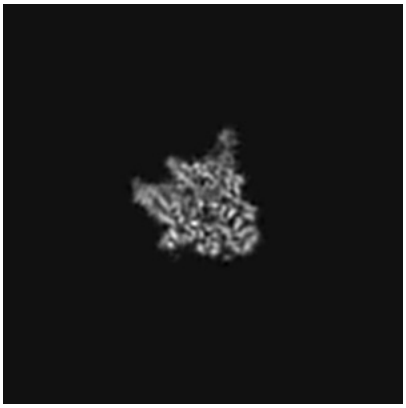


Z

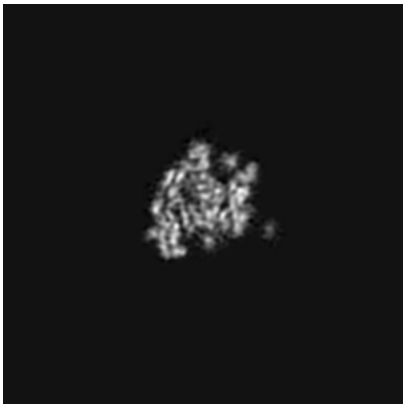
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 192



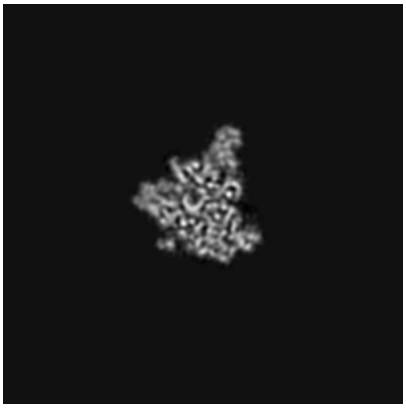
Y Index: 192

Z Index: 192

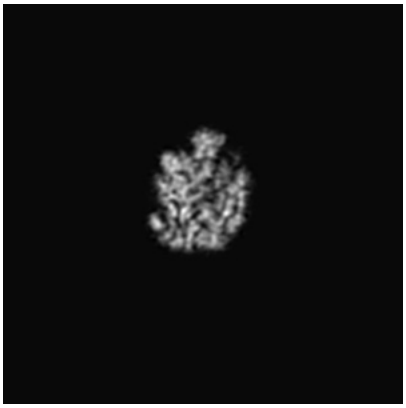
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 185



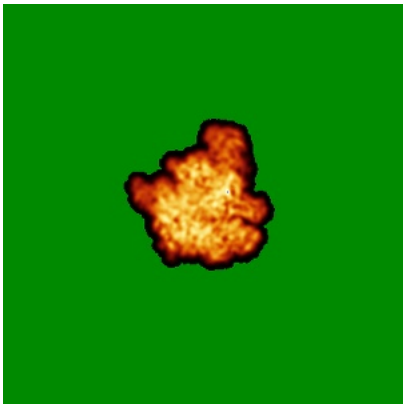
Y Index: 173

Z Index: 191

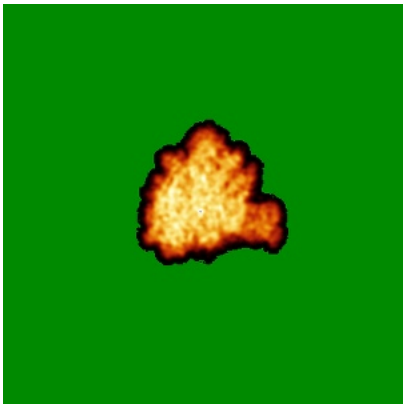
The images above show the largest variance slices of the map in three orthogonal directions.

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

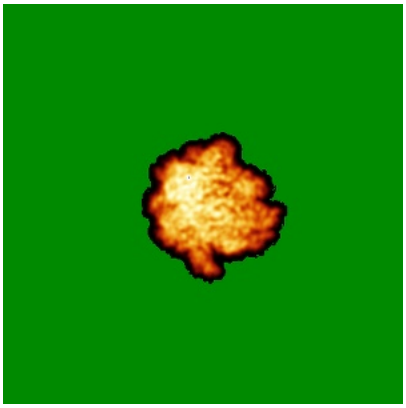
6.4.1 Primary map



X



Y

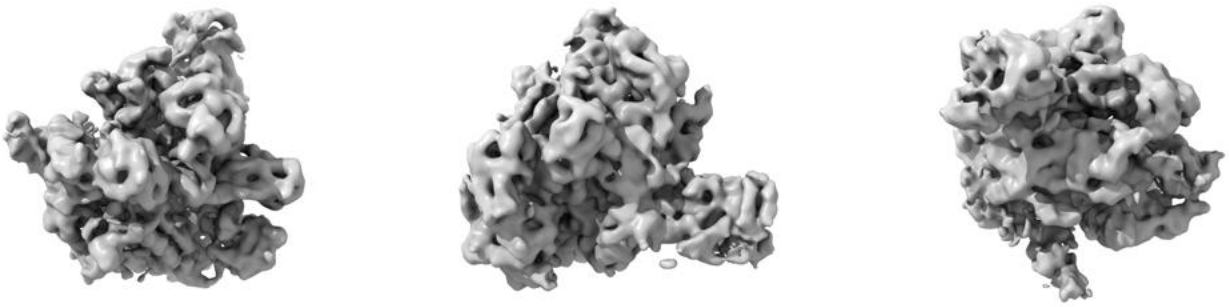


Z

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 0.0256. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

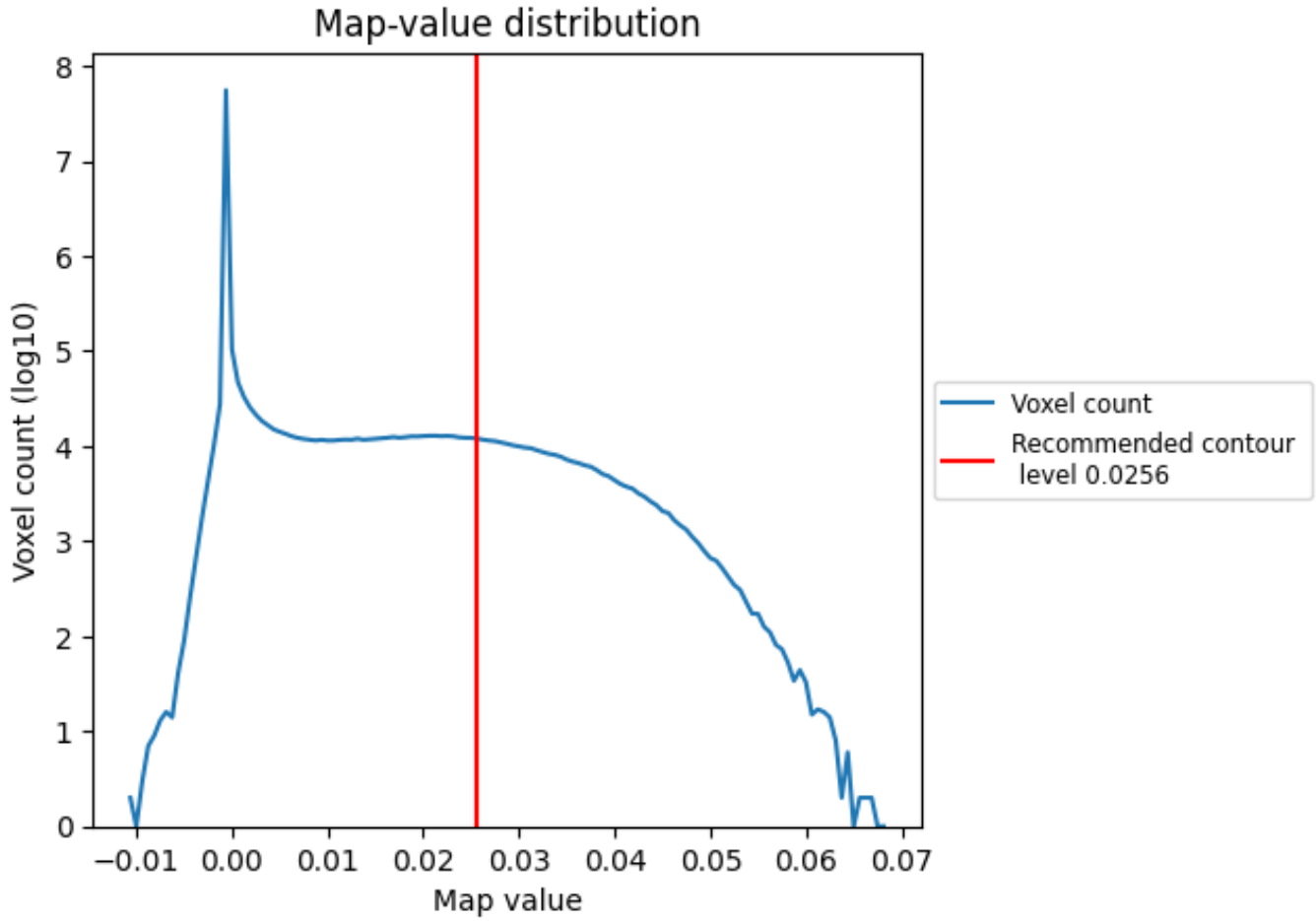
6.6 Mask visualisation (i)

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

7 Map analysis

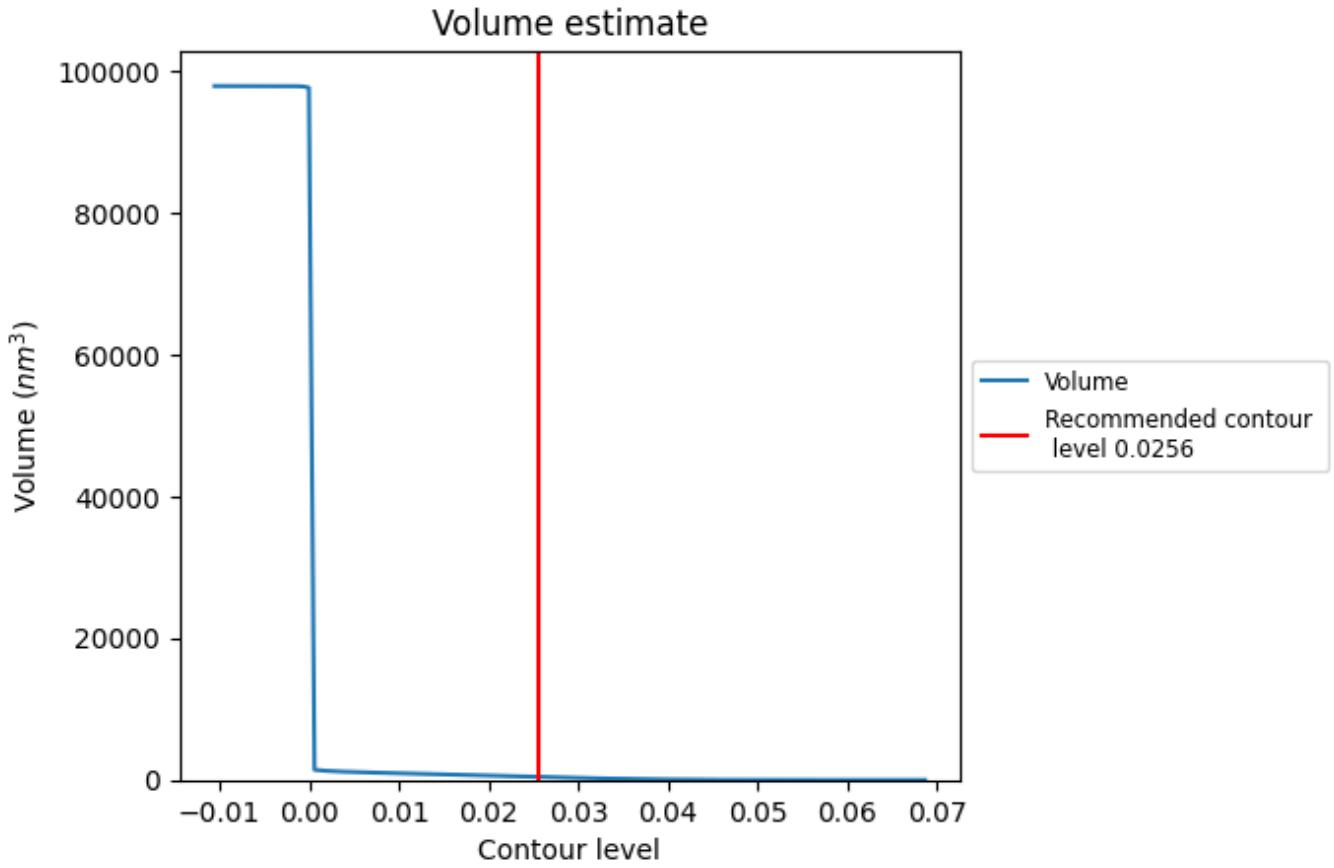
This section contains the results of statistical analysis of the map.

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.

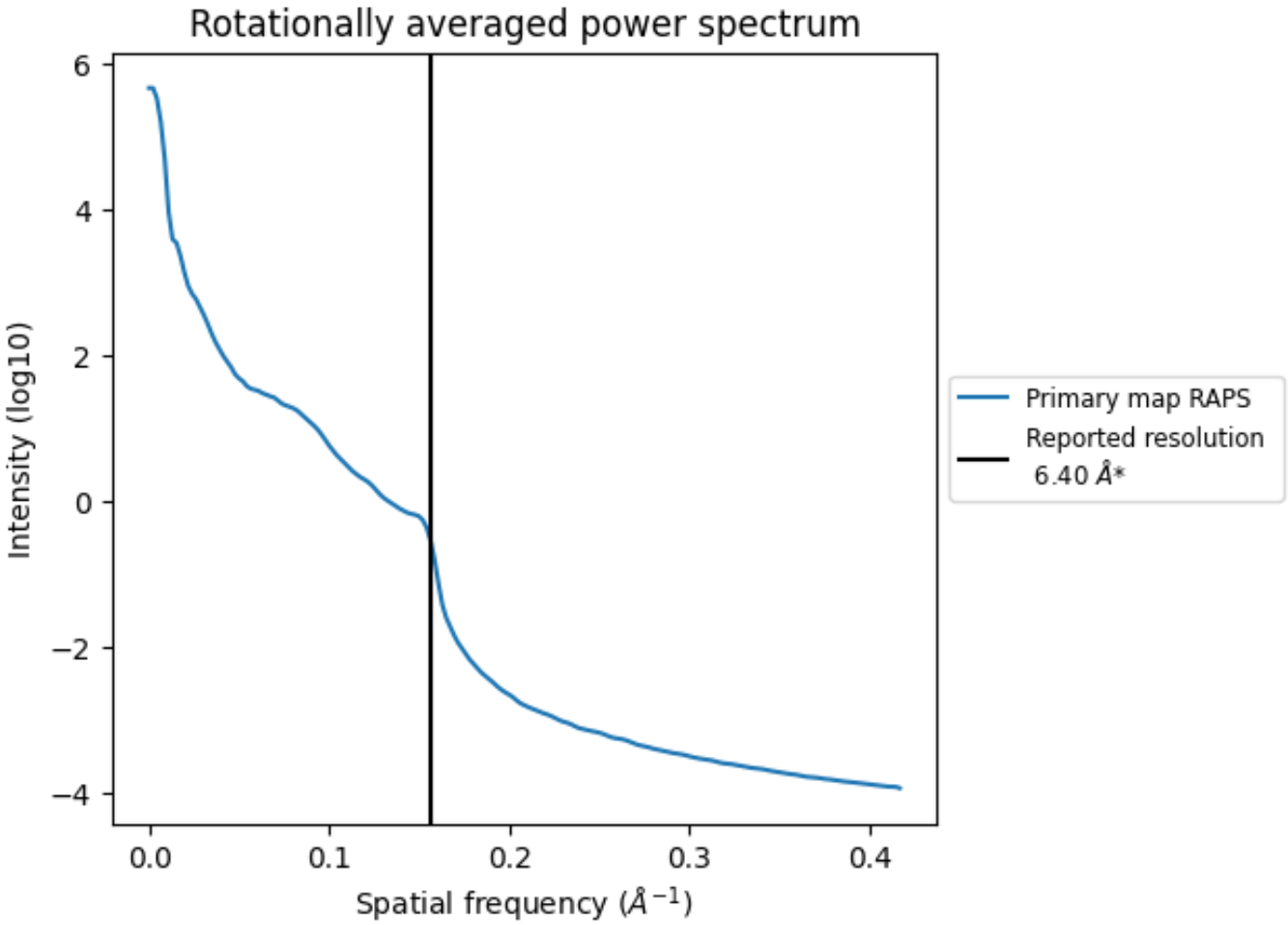
7.2 Volume estimate



The volume at the recommended contour level is 415 nm^3; this corresponds to an approximate mass of 375 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)

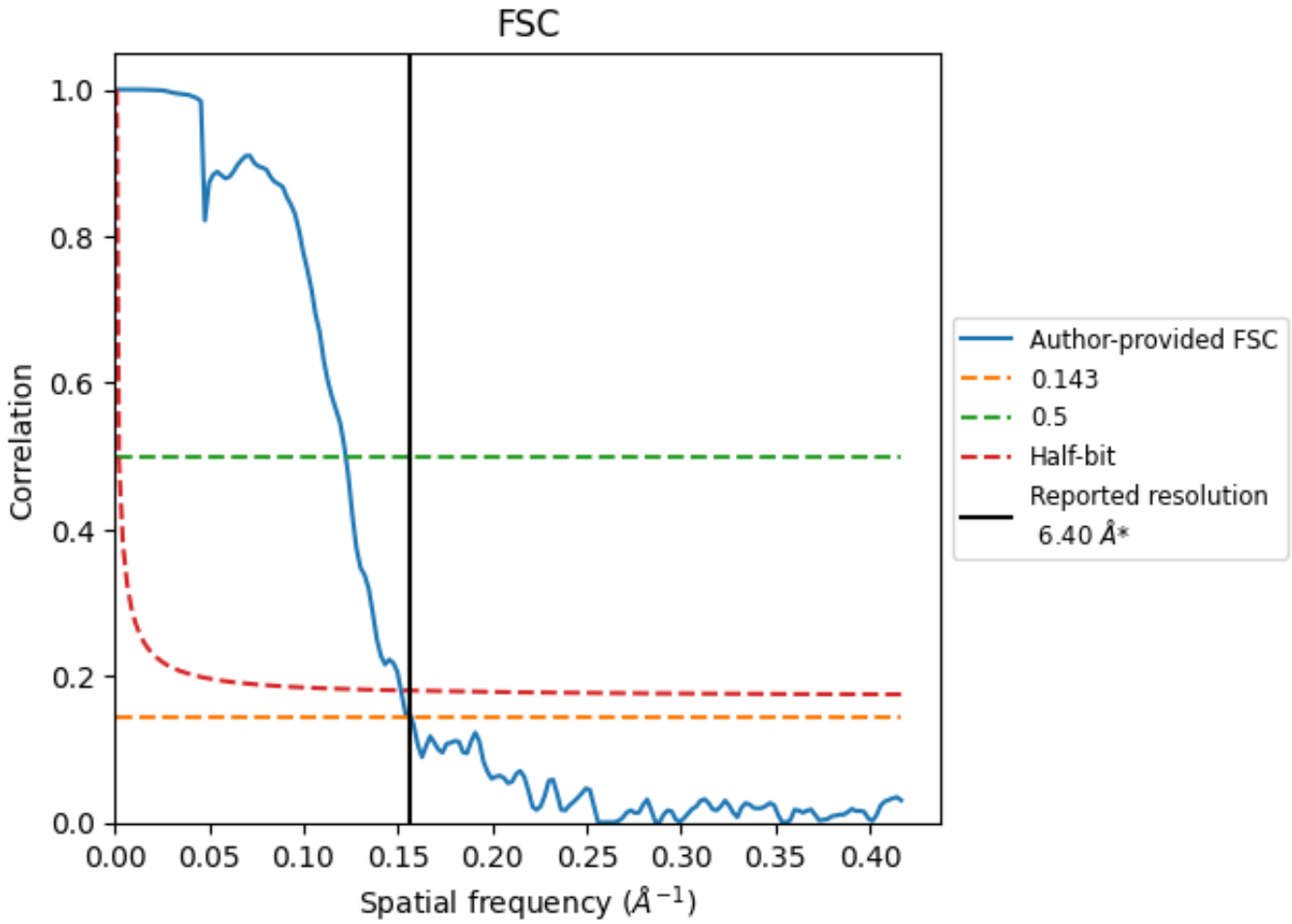


*Reported resolution corresponds to spatial frequency of 0.156 $Å^{-1}$

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 0.156 Å^{-1}

8.2 Resolution estimates (i)

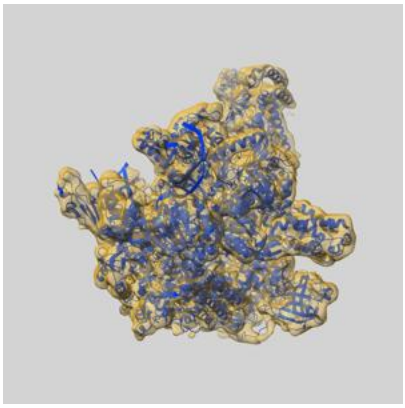
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.40	-	-
Author-provided FSC curve	6.37	8.18	6.60
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

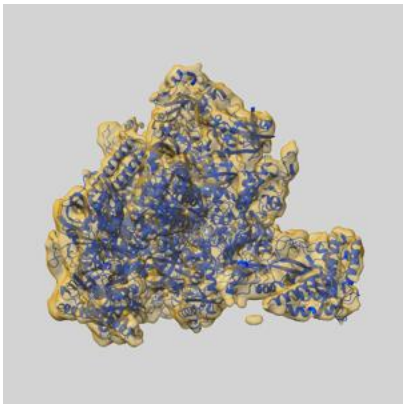
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8737 and PDB model 5VVS. Per-residue inclusion information can be found in section 3 on page 7.

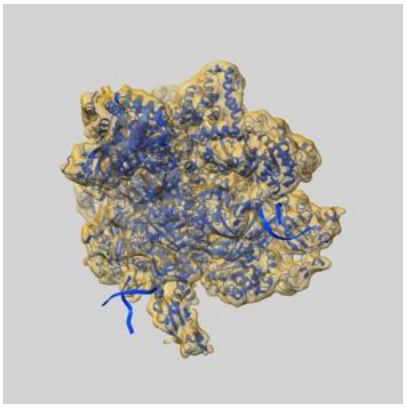
9.1 Map-model overlay



X



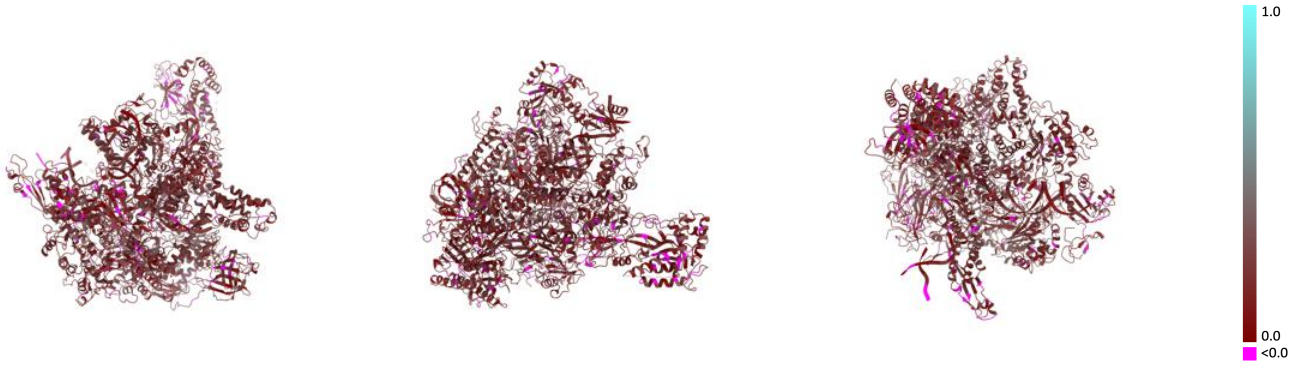
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0256 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.

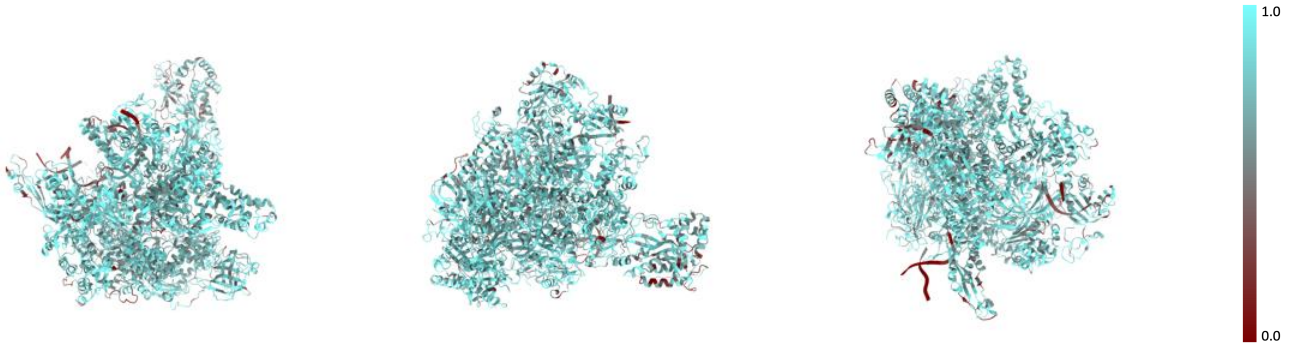
9.2 Q-score mapped to coordinate model (i)



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.

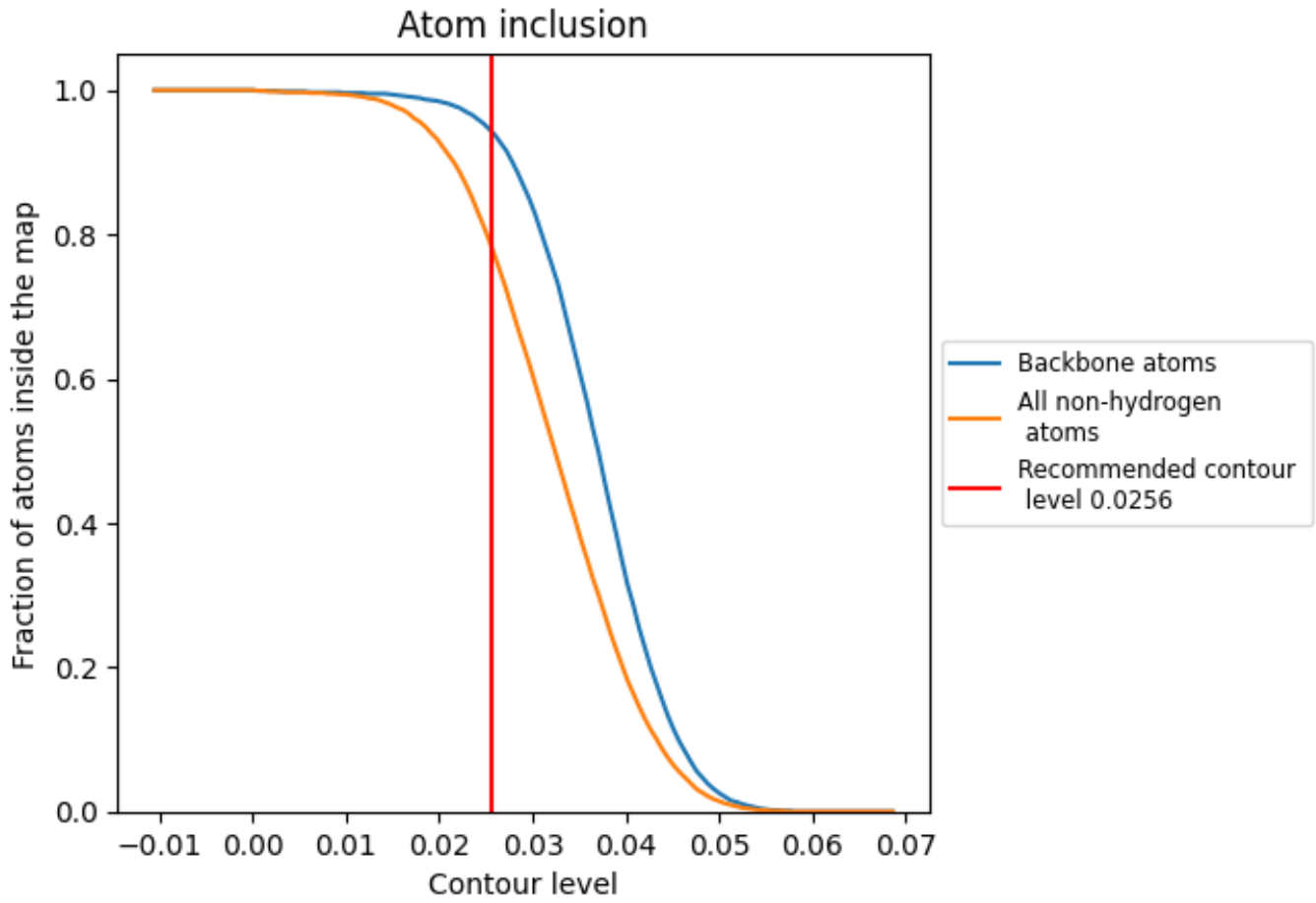
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0256).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 78% 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 (0.0256) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7830	0.1840
A	0.7930	0.1910
B	0.7850	0.1810
C	0.8260	0.1890
D	0.6960	0.1650
E	0.8360	0.1970
F	0.8310	0.1990
G	0.6880	0.1490
H	0.7830	0.1800
I	0.8090	0.1830
J	0.8110	0.1680
K	0.8310	0.1880
L	0.8410	0.1790
N	0.5800	0.1550
R	0.8100	0.2170
T	0.6240	0.1620