Full wwPDB EM Validation Report ⓘ

Mar 28, 2023 – 12:17 PM JST

PDB ID	:	8HIM
EMDB ID	:	EMD-34821
Title	:	A cryo-EM structure of B. oleracea RNA polymerase V elongation complex at 2.73 Angstrom
Authors	:	Hu, H.; Xie, G.; Du, X.; Du, J.
Deposited on	:	2022-11-21
Resolution	:	2.80 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:

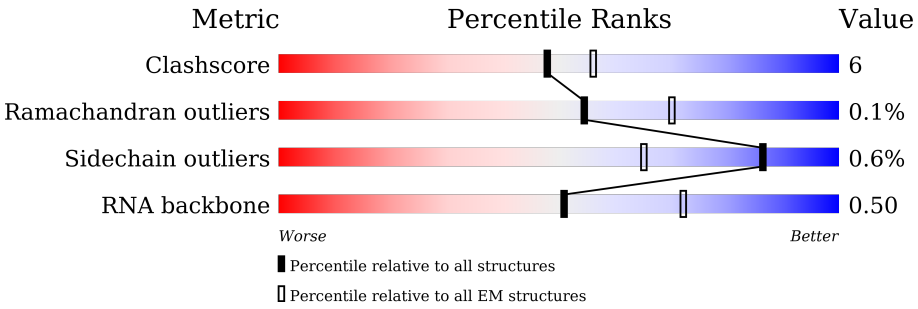
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
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	T	34	35% 15% 59% · 24%
2	N	34	50% 18% 59% 24%
3	P	20	5% 35% 20% 45%
4	A	2032	5% 37% · 58%
5	C	319	· 82% 8% · 10%
6	F	144	6% 48% 8% 44%
7	J	69	90% · 9%

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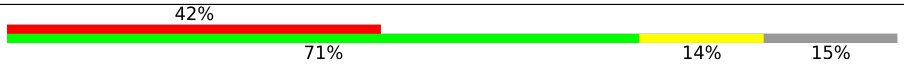
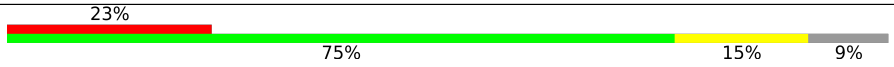
Mol	Chain	Length	Quality of chain
8	K	116	
9	L	51	
10	H	146	
11	I	114	
12	E	230	
13	B	1169	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 23948 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	T	26	529	253	92	158	26	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	N	26	539	257	100	156	26	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	P	11	239	107	49	72	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	848	6640	4195	1143	1258	44	0	0

- Molecule 5 is a protein called RPOLD domain-containing protein.

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 8 is a protein called RNA_pol_L_2 domain-containing protein.

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

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

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

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	971	Total	C	N	O	S	0	0
			7694	4848	1364	1438	44		

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

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

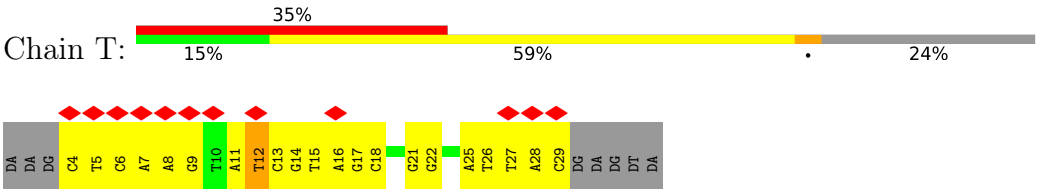
- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

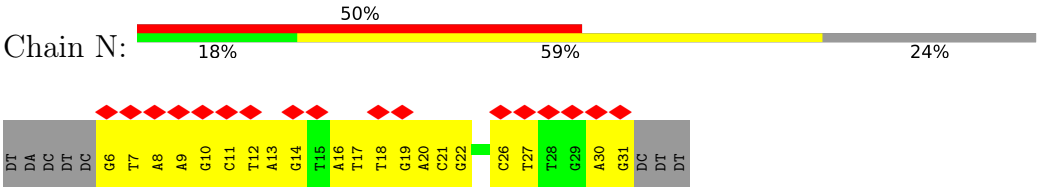
3 Residue-property plots (i)

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.

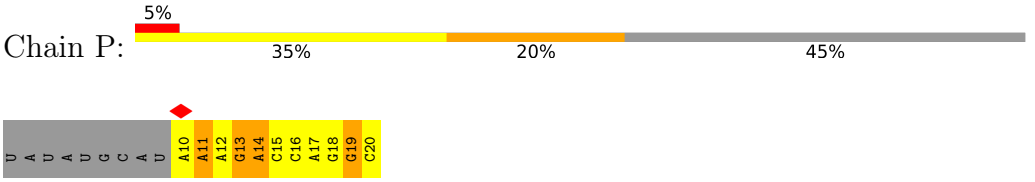
• Molecule 1: DNA (34-MER)



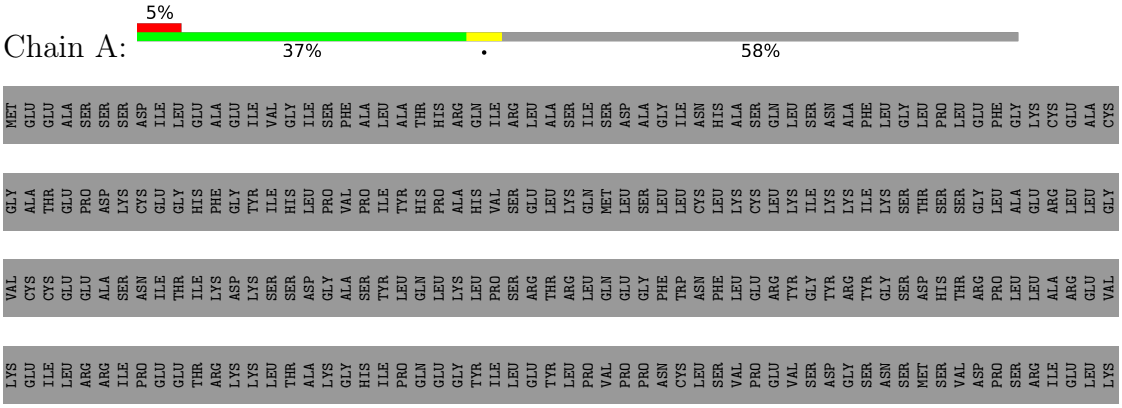
• Molecule 2: DNA (34-MER)

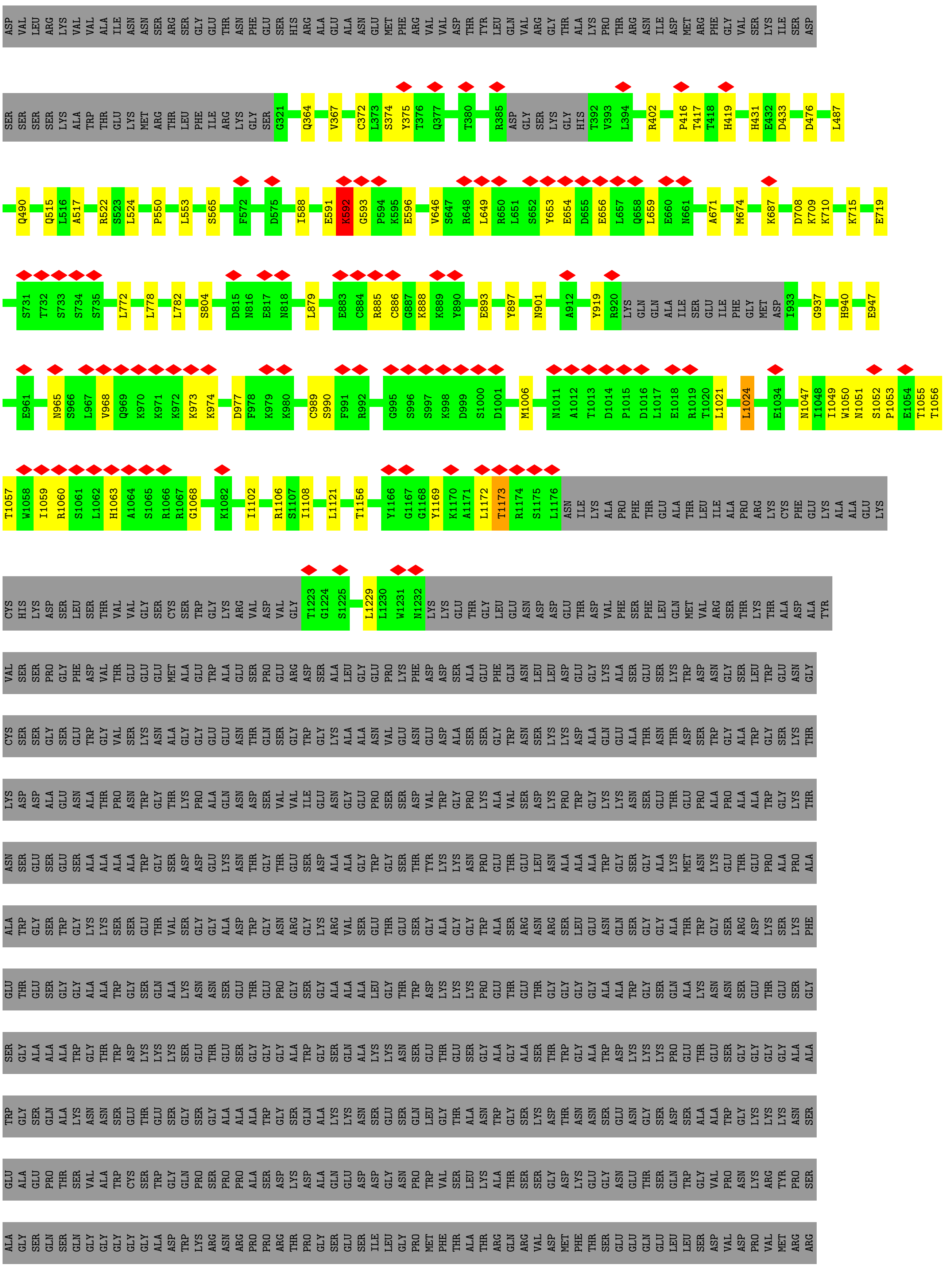


• Molecule 3: RNA (5'-R(*UP*AP*UP*AP*UP*GP*CP*AP*UP*AP*AP*AP*GP*AP*CP*CP *AP*GP*GP*C)-3')



• Molecule 4: DNA-directed RNA polymerase V largest subunit

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SER SER SER SER LYS ALA TRP THR GLU LYS MET ARG THR LEU PHE ILE ARG LYS GLY SER G321 Q364 V367 C372 L373 S374 Y375 T376 Q377 T380 R385 ASP GLY SER LYS GLY HIS T392 V393 L394 R402 P416 T417 T418 H419 H431 E432 D433 D476 L487
Q490 Q515 L516 A517 R522 S523 L524 P550 L553 S565 F572 D575 I588 E591 K592 G593 P594 K595 E596 V646 S647 R648 L649 R650 L651 S652 Y653 E654 D655 E656 L657 Q658 L659 E660 N661 A671 M674 K687 D708 K709 K710 K715 E719
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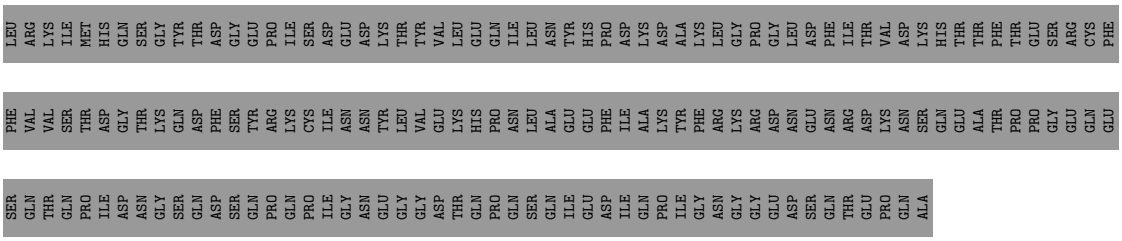
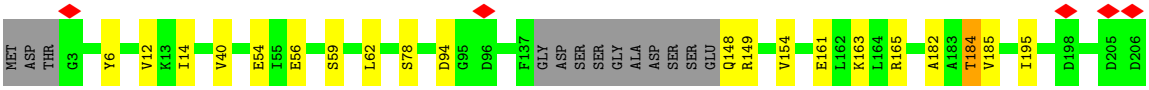
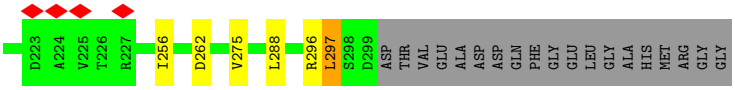
E961 N965 S966 L967 V968 Q969 K970 K971 K972 K973 K974 D977 F978 K979 K980 G989 S990 F991 R992 G995 S996 S997 K998 D999 S1000 D1001 M1006 N1011 A1012 T1013 D1014 P1015 D1016 L1017 E1018 R1019 T1020 L1021 L1024 E1034 N1047 I1048 I1049 W1050 N1051 S1052 P1053 E1054 T1055 T1056
T1057 W1058 I1059 R1060 S1061 L1062 H1063 A1064 S1065 R1066 R1067 G1068 K1082 I1102 R1106 S1107 I1108 L1121 T1156 Y1166 G1167 G1168 Y1169 K1170 A1171 L1172 T1173 R1174 S1175 L1176 ASN ILE LYS ALA PRO PHE THR GLU ALA THR LEU ILE ALA PRO ARG LYS CYS PHE GLU LYS ALA ALA GLU LYS
CYS HIS LYS ASP SER LEU SER THR VAL VAL GLY SER CYS SER TRP GLY LYS ARG VAL ASP VAL GLY T1223 G1224 S1225 L1229 L1230 W1231 N1232 LYS LYS GLU THR GLY LEU GLU ASN ASP ASP GLU THR ASP VAL PHE SER PHE LEU GLN MET VAL ARG SER THR LYS THR ALA ASP ALA TYR
VAL SER SER PRO GLY PHE ASP VAL THR GLU GLU GLU MET ALA GLU TRP ALA GLU SER PRO GLU ARG ASP SER ALA LEU GLY GLU PRO LYS PHE ASP SER ALA GLU PHE GLN ASN LEU LEU ASP GLU GLY LYS ALA SER GLU SER LYS TRP ASP ASN GLY SER LEU TRP GLU ASN GLY
CYS SER SER GLY SER GLU TRP GLY VAL SER LYS ASN ALA GLY GLY GLU ASN THR GLN SER GLY TRP GLY LYS ALA ALA ASN VAL GLU ASN GLU ASP ALA SER SER GLY TRP ASN SER LYS LYS ASP ALA GLN GLU ALA THR ASN THR ASP SER TRP GLY ALA TRP GLY SER LYS THR
LYS ASP ASP ALA GLU ASN ALA THR PRO ASN TRP GLY THR LYS PRO ALA GLN ASN ASP SER VAL VAL ILE GLU ASN GLY GLU PRO SER SER ASP VAL TRP GLY PRO LYS ALA VAL SER ASP LYS PRO TRP GLY LYS LYS ASN SER GLU THR GLU PRO ALA PRO ALA ALA TRP GLY LYS THR
ASN SER GLU SER GLU SER ALA ALA ALA ALA TRP GLY SER ASP ASP GLU LYS ASN THR GLY THR GLU SER ASP ALA ALA GLY TRP GLY SER THR TYR LYS LYS ASN PRO GLU THR GLU LEU ASN ALA ALA ALA TRP GLY SER GLY ALA LYS MET ASN LYS GLU THR GLU PRO ALA PRO ALA
ALA TRP GLY SER TRP GLY LYS LYS SER SER GLU THR VAL SER GLY GLY ALA ASP TRP GLY ASN ARG GLY LYS ARG VAL SER GLU THR GLU SER GLY ALA GLY GLY TRP ALA SER ARG ASN ARG SER LEU GLU ASN GLN SER GLY ALA THR TRP GLY SER ARG ASP LYS SER LYS PHE
GLU THR GLU SER GLY GLY ALA ALA TRP GLY SER GLN ALA LYS ASN ASN SER GLU THR GLU PRO GLY SER GLY ALA ALA ALA LEU GLY THR TRP ASP LYS LYS LYS PRO GLU THR GLU THR GLY GLY GLY ALA ALA TRP GLY SER GLN ALA LYS ASN ASN SER GLU THR GLU SER GLY
SER GLY ALA ALA ALA TRP GLY THR TRP ASP LYS LYS LYS SER GLU THR GLU SER GLY GLY GLY ALA TRP GLY SER GLN ALA LYS LYS ASN SER GLU THR GLU SER GLY ALA GLY ALA SER THR TRP GLY ALA TRP ASP LYS LYS LYS PRO GLU THR GLU SER GLY GLY GLY ALA ALA
TRP GLY SER GLN ALA LYS ASN ASN SER GLU THR GLU SER GLY SER GLY ALA ALA ALA TRP GLY SER GLN ALA LYS LYS ASN SER GLU SER GLN LEU GLY THR ALA ASN TRP GLY SER LYS ASP THR ASN ASN SER GLU ASN GLY SER ASP SER ALA ALA TRP GLY LYS LYS ASN SER
GLU ALA GLU PRO THR SER VAL ALA TRP CYS SER TRP GLY GLN PRO SER PRO PRO ALA SER ASP LYS ASP ALA GLN GLU ASP ASP GLY ASN PRO TRP VAL SER LEU LYS ALA THR SER SER GLY ASP LYS GLU GLY ASN GLU THR SER GLN TRP GLY VAL PRO ASN LYS ARG TYR PRO SER
ALA GLY SER GLN SER GLN GLY GLY GLY GLY ALA ASP TRP LYS ARG ASN ARG PRO PRO ARG THR PRO GLY SER GLU SER ILE LEU GLY PRO MET PHE THR ALA THR ARG GLN ARG VAL ASP MET PHE THR SER GLU GLU GLN GLN LEU LEU SER ASP VAL ASP PRO VAL MET ARG ARG



• Molecule 5: RPOLD domain-containing protein

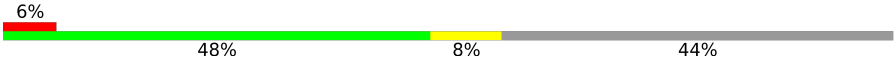
Chain C:

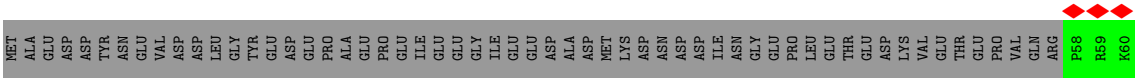


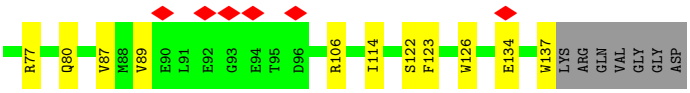


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:

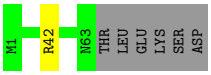






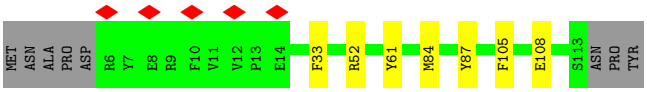
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



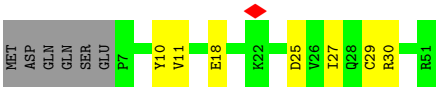
• Molecule 8: RNA_pol_L_2 domain-containing protein

Chain K:



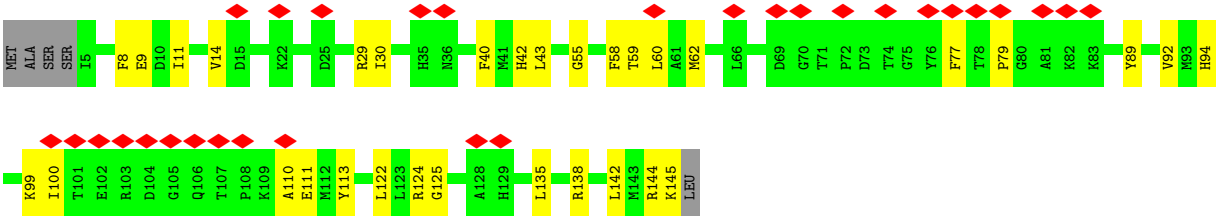
• Molecule 9: DNA-directed RNA polymerases II, IV and V subunit 12

Chain L:



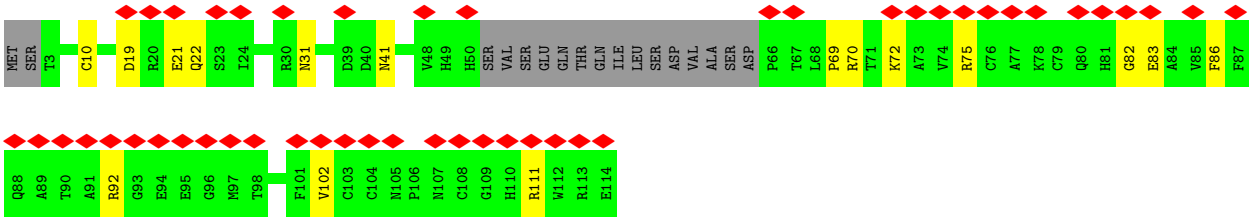
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



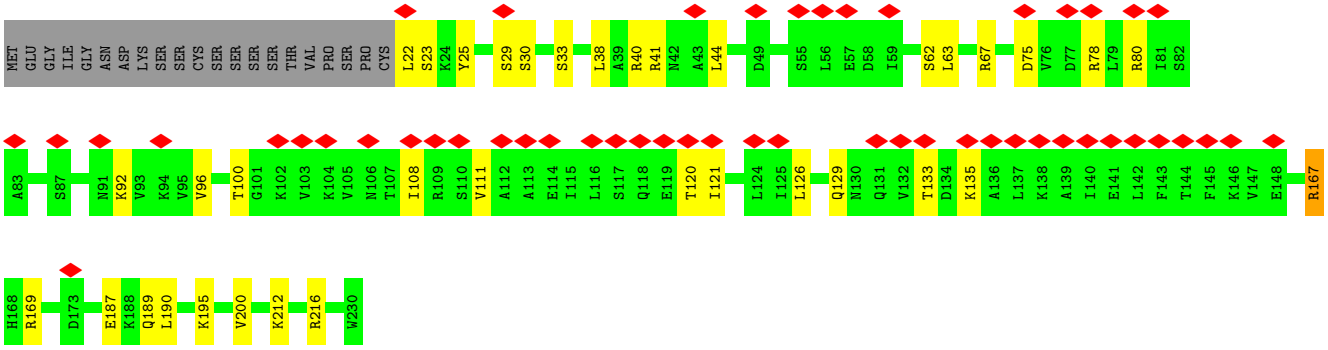
• Molecule 11: DNA-directed RNA polymerase subunit

Chain I:



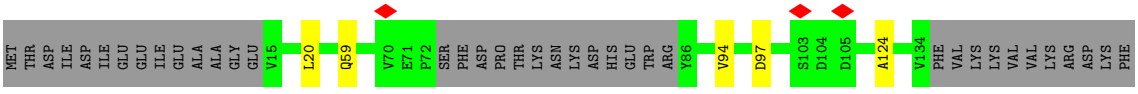
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC1

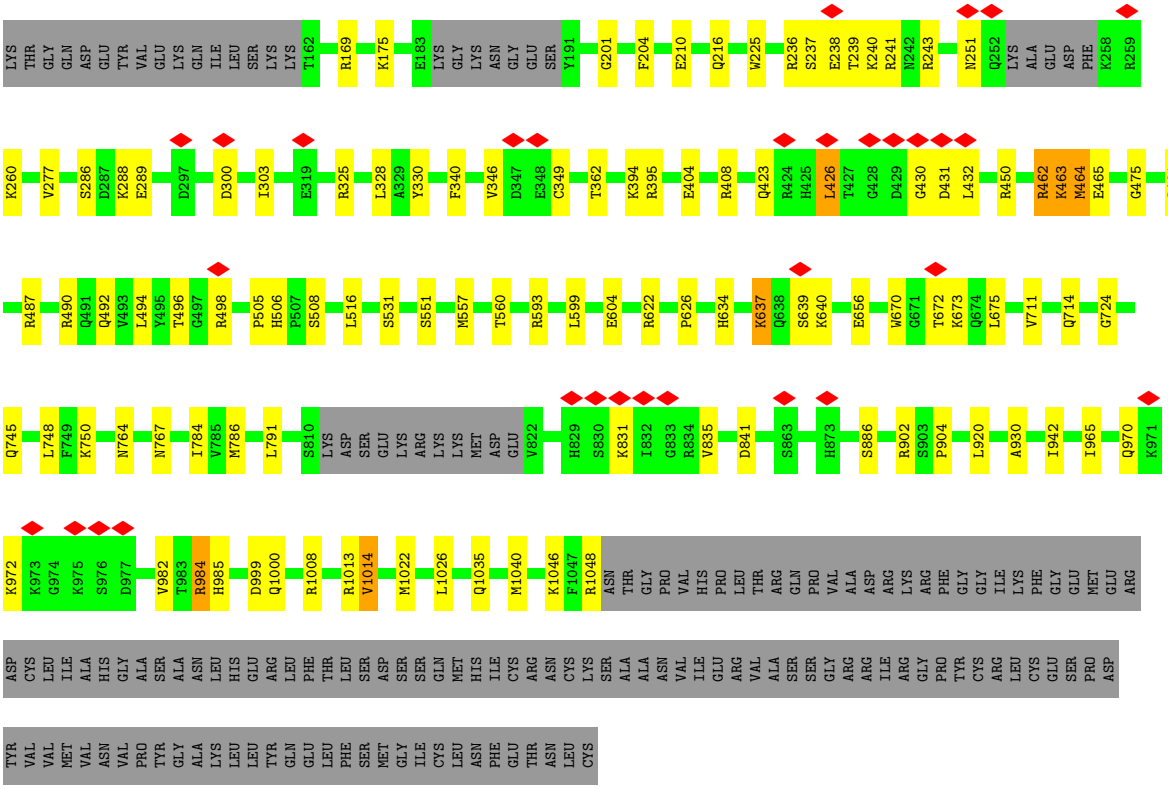
Chain E:



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

Chain B:

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K260 V277 S286 D287 K288 E289 D297 D300 I303 E319 R325 L328 A329 Y330 F340 V346 D347 E348 C349 T362 K394 R395 E404 R408 Q423 R424 H425 L426 T427 G428 D429 G430 D431 L432 R450 R462 K463 M464 E465 G475 Q481
R487 R490 Q491 Q492 V493 L494 Y495 T496 G497 R498 P505 H506 P507 S508 L516 S531 S551 M557 T560 R593 L599 E604 R622 P626 H634 K637 Q638 S639 K640 E656 W670 G671 T672 K673 Q674 L675 V711 Q714 G724
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K972 K973 G974 K975 S976 D977 V982 T983 R984 H985 D999 Q1000 R1008 R1013 V1014 M1022 L1026 Q1035 M1040 K1046 F1047 R1048 ASN THR GLY PRO VAL HIS PRO LEU THR ARG GLN PRO VAL ALA ASP ARG LYS ARG PHE GLY GLY ILE LYS PHE GLY GLU MET GLU ARG
ASP CYS LEU ILE ALA HIS GLY ALA SER ALA ASN LEU HIS GLU ARG LEU PHE THR LEU SER ASP SER SER GLN MET HIS ILE CYS ARG ASN CYS LYS SER ALA ALA ASN VAL ILE GLU ARG VAL ALA SER SER GLY ARG ARG ILE ARG GLY PRO TYR CYS ARG LEU CYS GLU SER PRO ASP
TYR VAL VAL MET VAL ASN VAL PRO TYR GLY ALA ALA LYS LEU LEU TYR GLN GLU LEU PHE SER MET GLY ILE CYS LEU ASN PHE GLU THR ASN LEU CYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	503124	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 ($e^-/Å^2$)	1.5625	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.154	Depositor
Minimum map value	-0.069	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0245	Depositor
Map size (Å)	328.5, 328.5, 328.5	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.095, 1.095, 1.095	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	T	0.69	0/591	0.96	2/909 (0.2%)
2	N	0.41	0/605	0.81	0/933
3	P	0.14	0/268	0.65	0/416
4	A	0.38	0/6754	0.58	0/9119
5	C	0.41	0/2286	0.58	0/3087
6	F	0.35	0/673	0.52	0/905
7	J	0.47	0/515	0.60	0/696
8	K	0.39	0/908	0.54	0/1224
9	L	0.44	0/369	0.57	0/493
10	H	0.32	0/1155	0.63	0/1557
11	I	0.31	0/804	0.53	0/1081
12	E	0.31	0/1732	0.62	0/2332
13	B	0.44	1/7845 (0.0%)	0.56	0/10574
All	All	0.41	1/24505 (0.0%)	0.60	2/33326 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	505	PRO	C-N	-5.04	1.22	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	11	DA	P-O3'-C3'	-5.30	113.34	119.70
1	T	12	DT	P-O3'-C3'	-5.10	113.58	119.70

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	T	529	0	295	19	0
2	N	539	0	295	37	0
3	P	239	0	122	13	0
4	A	6640	0	6697	82	0
5	C	2256	0	2269	23	0
6	F	660	0	669	11	0
7	J	507	0	512	2	0
8	K	890	0	883	10	0
9	L	365	0	365	5	0
10	H	1129	0	1128	18	0
11	I	787	0	737	17	0
12	E	1706	0	1759	23	0
13	B	7694	0	7632	79	0
14	A	1	0	0	0	0
15	A	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
All	All	23948	0	23363	292	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 6.

All (292) 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)
4:A:885:ARG:HG2	12:E:23:SER:OG	1.62	0.98
4:A:1052:SER:OG	4:A:1068:GLY:HA2	1.72	0.89
4:A:897:TYR:OH	11:I:69:PRO:HG2	1.76	0.84
4:A:1052:SER:HG	4:A:1068:GLY:HA2	1.43	0.81
4:A:1050:TRP:CE3	4:A:1052:SER:HB2	2.18	0.78
2:N:11:DC:H1'	2:N:12:DT:C5	2.18	0.78
4:A:550:PRO:HG3	4:A:592:LYS:HG3	1.66	0.77
4:A:1050:TRP:CZ3	4:A:1052:SER:HB2	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:297:LEU:HD12	8:K:84:MET:HE3	1.67	0.77
4:A:588:ILE:O	4:A:592:LYS:HB2	1.83	0.76
2:N:21:DC:H2"	2:N:22:DG:C8	2.22	0.73
13:B:1013:ARG:HD2	13:B:1022:MET:HG2	1.69	0.73
1:T:27:DT:H2"	1:T:28:DA:C8	2.24	0.72
3:P:15:C:H2'	3:P:16:C:C6	2.24	0.72
4:A:885:ARG:NH1	4:A:886:CYS:HB2	2.04	0.72
1:T:12:DT:H2"	1:T:13:DC:H5'	1.70	0.72
12:E:40:ARG:HD3	12:E:80:ARG:HD3	1.73	0.71
4:A:1057:THR:HB	4:A:1060:ARG:HB2	1.75	0.68
2:N:16:DA:H5"	13:B:243:ARG:HH22	1.58	0.68
2:N:12:DT:H1'	2:N:13:DA:O4'	1.93	0.67
3:P:17:A:H2'	3:P:18:G:C8	2.30	0.67
2:N:8:DA:H4'	2:N:9:DA:H4'	1.76	0.66
2:N:30:DA:H1'	2:N:31:DG:C4	2.31	0.65
3:P:12:A:H2'	3:P:13:G:H8	1.60	0.65
13:B:430:GLY:O	13:B:432:LEU:N	2.29	0.65
2:N:10:DG:N2	2:N:12:DT:H5'	2.11	0.64
4:A:1049:ILE:HG22	4:A:1051:ASN:H	1.61	0.64
4:A:893:GLU:O	4:A:897:TYR:HD2	1.80	0.64
1:T:13:DC:H1'	1:T:14:DG:H5'	1.80	0.63
4:A:1021:LEU:HA	4:A:1024:LEU:HD23	1.80	0.63
2:N:8:DA:H4'	2:N:9:DA:OP1	1.97	0.63
13:B:1013:ARG:HD3	13:B:1014:VAL:H	1.64	0.63
3:P:20:C:H4'	4:A:417:THR:OG1	1.99	0.62
1:T:28:DA:H2'	1:T:29:DC:O4'	2.00	0.62
5:C:297:LEU:HG	8:K:87:TYR:CD2	2.34	0.62
4:A:550:PRO:CG	4:A:592:LYS:HG3	2.31	0.61
2:N:6:DG:H1'	2:N:7:DT:O4'	2.00	0.61
11:I:10:CYS:SG	11:I:31:ASN:ND2	2.74	0.61
1:T:4:DC:H1'	1:T:5:DT:C4	2.36	0.60
4:A:940:HIS:NE2	4:A:989:CYS:SG	2.74	0.60
4:A:885:ARG:CG	12:E:23:SER:OG	2.42	0.60
13:B:496:THR:O	13:B:496:THR:HG23	2.02	0.60
4:A:649:LEU:HD12	4:A:656:GLU:HB3	1.84	0.59
12:E:133:THR:HG22	12:E:135:LYS:H	1.66	0.59
9:L:11:VAL:HG12	9:L:18:GLU:HG2	1.85	0.59
5:C:297:LEU:HD12	8:K:84:MET:CE	2.32	0.59
4:A:885:ARG:HH11	4:A:886:CYS:HB2	1.67	0.59
5:C:184:THR:HG21	7:J:42:ARG:NH1	2.18	0.59
13:B:1013:ARG:HD3	13:B:1014:VAL:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:16:DA:H5"	13:B:243:ARG:NH2	2.18	0.58
3:P:12:A:H2'	3:P:13:G:C8	2.39	0.58
1:T:17:DG:H1'	1:T:18:DC:H5'	1.84	0.57
4:A:593:GLY:O	6:F:137:TRP:N	2.37	0.57
9:L:25:ASP:OD1	9:L:25:ASP:N	2.37	0.57
13:B:423:GLN:HA	13:B:426:LEU:HD23	1.87	0.57
13:B:750:LYS:O	13:B:985:HIS:HA	2.05	0.57
4:A:1057:THR:HG21	4:A:1063:HIS:NE2	2.20	0.57
2:N:17:DT:H72	13:B:243:ARG:HH11	1.70	0.56
4:A:1021:LEU:HD12	4:A:1024:LEU:HD21	1.85	0.56
12:E:100:THR:HA	12:E:129:GLN:HG2	1.87	0.56
4:A:715:LYS:NZ	4:A:719:GLU:OE2	2.37	0.56
6:F:77:ARG:NH1	6:F:80:GLN:OE1	2.39	0.56
3:P:16:C:H2'	3:P:17:A:H8	1.70	0.56
12:E:187:GLU:HA	12:E:190:LEU:HD12	1.88	0.56
10:H:40:PHE:HB3	10:H:124:ARG:HB2	1.88	0.56
13:B:430:GLY:C	13:B:432:LEU:N	2.57	0.56
11:I:70:ARG:NH1	11:I:83:GLU:OE2	2.39	0.55
1:T:18:DC:H42	3:P:19:G:H1	1.53	0.55
6:F:106:ARG:NH2	6:F:134:GLU:OE2	2.39	0.55
12:E:92:LYS:HG3	12:E:121:ILE:HA	1.86	0.55
3:P:11:A:H2'	3:P:12:A:C8	2.41	0.55
5:C:6:TYR:HB3	8:K:52:ARG:HG3	1.87	0.55
12:E:22:LEU:HA	12:E:25:TYR:HB3	1.87	0.55
4:A:897:TYR:HE2	11:I:86:PHE:HE2	1.55	0.55
4:A:1050:TRP:CE3	11:I:72:LYS:HD3	2.41	0.55
13:B:20:LEU:HD21	13:B:637:LYS:HB3	1.89	0.55
13:B:750:LYS:HE2	13:B:984:ARG:HH12	1.72	0.55
4:A:973:LYS:HG3	4:A:974:LYS:HD3	1.89	0.55
5:C:297:LEU:HG	8:K:87:TYR:CE2	2.42	0.55
13:B:239:THR:HG22	13:B:241:ARG:H	1.71	0.55
13:B:557:MET:SD	13:B:557:MET:N	2.78	0.55
2:N:18:DT:H4'	2:N:19:DG:OP1	2.06	0.54
4:A:372:CYS:HA	4:A:402:ARG:HA	1.89	0.54
2:N:21:DC:H2"	2:N:22:DG:H8	1.70	0.54
12:E:167:ARG:HH12	12:E:216:ARG:HH12	1.55	0.54
4:A:879:LEU:HD22	4:A:1102:ILE:HD11	1.90	0.54
2:N:13:DA:H5"	13:B:240:LYS:HE2	1.89	0.54
4:A:1050:TRP:HE3	11:I:72:LYS:HZ2	1.55	0.54
12:E:33:SER:OG	12:E:67:ARG:NH2	2.40	0.54
13:B:965:ILE:HD12	13:B:984:ARG:HE	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:714:GLN:HE22	13:B:1035:GLN:HE22	1.54	0.53
2:N:9:DA:H3'	13:B:464:MET:SD	2.48	0.53
4:A:897:TYR:O	4:A:901:ASN:ND2	2.42	0.53
2:N:13:DA:H2"	2:N:14:DG:C5'	2.38	0.53
4:A:1053:PRO:O	4:A:1055:THR:HG23	2.08	0.53
11:I:102:VAL:HB	11:I:111:ARG:HG2	1.90	0.53
4:A:476:ASP:OD1	4:A:476:ASP:N	2.39	0.53
4:A:654:GLU:OE2	4:A:710:LYS:NZ	2.41	0.53
2:N:10:DG:H5'	2:N:10:DG:N3	2.24	0.53
13:B:634:HIS:O	13:B:637:LYS:HG2	2.08	0.53
3:P:16:C:H2'	3:P:17:A:C8	2.44	0.52
2:N:19:DG:H1'	2:N:20:DA:H5'	1.91	0.52
4:A:1057:THR:CB	4:A:1060:ARG:HB2	2.39	0.52
13:B:999:ASP:OD1	13:B:1008:ARG:NH1	2.41	0.52
13:B:430:GLY:C	13:B:432:LEU:H	2.12	0.52
1:T:25:DA:H2"	1:T:26:DT:H5"	1.92	0.52
5:C:62:LEU:HD12	5:C:154:VAL:HG23	1.92	0.52
12:E:29:SER:OG	12:E:30:SER:N	2.43	0.52
2:N:26:DC:H2"	2:N:27:DT:C4	2.45	0.51
4:A:778:LEU:O	4:A:782:LEU:HB2	2.09	0.51
9:L:27:ILE:HB	13:B:886:SER:HB3	1.93	0.51
1:T:15:DT:H2"	1:T:16:DA:C4	2.46	0.51
10:H:111:GLU:HA	10:H:124:ARG:HA	1.93	0.51
13:B:325:ARG:HE	13:B:328:LEU:HD23	1.76	0.51
4:A:374:SER:OG	4:A:375:TYR:N	2.43	0.51
4:A:593:GLY:H	6:F:137:TRP:HB2	1.76	0.51
12:E:38:LEU:HD23	12:E:41:ARG:HD3	1.93	0.51
5:C:59:SER:HB2	5:C:161:GLU:H	1.76	0.50
4:A:487:LEU:O	4:A:490:GLN:NE2	2.43	0.50
5:C:195:ILE:HG22	5:C:256:ILE:HG22	1.94	0.50
5:C:94:ASP:N	5:C:94:ASP:OD1	2.40	0.50
13:B:982:VAL:HG12	13:B:984:ARG:HG2	1.93	0.50
13:B:748:LEU:HB3	13:B:965:ILE:HD11	1.93	0.50
13:B:902:ARG:NH1	13:B:1040:MET:SD	2.84	0.50
1:T:15:DT:C2	1:T:16:DA:C8	2.99	0.50
13:B:487:ARG:NH1	13:B:531:SER:O	2.44	0.50
6:F:122:SER:OG	6:F:123:PHE:N	2.45	0.50
13:B:506:HIS:HD2	13:B:508:SER:H	1.59	0.50
4:A:517:ALA:HB2	4:A:524:LEU:HD13	1.94	0.49
13:B:124:ALA:O	13:B:169:ARG:HA	2.11	0.49
11:I:75:ARG:HA	11:I:82:GLY:HA2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:54:GLU:OE1	5:C:165:ARG:NH2	2.37	0.49
13:B:831:LYS:HG3	13:B:835:VAL:H	1.78	0.49
13:B:59:GLN:HE22	13:B:94:VAL:H	1.61	0.48
11:I:21:GLU:HG2	11:I:22:GLN:HG3	1.95	0.48
13:B:670:TRP:HB2	13:B:675:LEU:HD22	1.95	0.48
10:H:8:PHE:HB3	10:H:62:MET:HB2	1.95	0.48
13:B:475:GLY:HA3	13:B:481:GLN:HE21	1.79	0.48
10:H:11:ILE:HG13	10:H:59:THR:HB	1.94	0.48
12:E:62:SER:OG	12:E:63:LEU:N	2.46	0.48
13:B:930:ALA:HB1	13:B:1014:VAL:CG1	2.44	0.48
13:B:1013:ARG:NH2	13:B:1013:ARG:HA	2.28	0.48
11:I:75:ARG:HE	11:I:82:GLY:HA3	1.79	0.48
4:A:653:TYR:OH	4:A:1047:ASN:ND2	2.38	0.48
10:H:94:HIS:HE1	10:H:138:ARG:HB3	1.79	0.48
4:A:1021:LEU:HD12	4:A:1024:LEU:CD2	2.44	0.48
1:T:5:DT:H2"	1:T:6:DC:C5	2.49	0.47
4:A:1057:THR:HG21	4:A:1063:HIS:CE1	2.50	0.47
10:H:14:VAL:HG23	10:H:55:GLY:H	1.79	0.47
3:P:10:A:H2'	3:P:11:A:H8	1.80	0.47
4:A:1060:ARG:HG3	4:A:1106:ARG:HH11	1.79	0.47
12:E:195:LYS:HA	12:E:200:VAL:HG11	1.97	0.47
13:B:216:GLN:HE22	13:B:492:GLN:CD	2.18	0.47
4:A:919:TYR:O	11:I:41:ASN:ND2	2.47	0.47
4:A:977:ASP:OD1	4:A:977:ASP:N	2.42	0.47
4:A:1050:TRP:CZ3	4:A:1052:SER:CB	2.95	0.47
10:H:9:GLU:HA	10:H:60:LEU:O	2.15	0.47
4:A:885:ARG:O	4:A:888:LYS:HG2	2.14	0.47
13:B:639:SER:OG	13:B:640:LYS:N	2.48	0.47
5:C:78:SER:O	5:C:275:VAL:HG12	2.15	0.47
13:B:362:THR:HG23	13:B:560:THR:HB	1.96	0.47
1:T:14:DG:H1	2:N:21:DC:H42	1.63	0.46
4:A:671:ALA:HA	4:A:674:MET:HG2	1.98	0.46
13:B:462:ARG:HG2	13:B:465:GLU:OE2	2.15	0.46
13:B:516:LEU:HD13	13:B:711:VAL:HG11	1.97	0.46
10:H:92:VAL:HG12	10:H:142:LEU:HA	1.98	0.46
1:T:14:DG:H2"	1:T:15:DT:OP2	2.16	0.46
2:N:10:DG:H1	2:N:12:DT:H3'	1.79	0.46
2:N:12:DT:C6	2:N:13:DA:C5	3.03	0.46
5:C:182:ALA:HB1	5:C:185:VAL:HG23	1.96	0.46
5:C:184:THR:HG21	7:J:42:ARG:CZ	2.46	0.46
4:A:1057:THR:HB	4:A:1060:ARG:CB	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:10:TYR:OH	13:B:841:ASP:OD2	2.34	0.46
12:E:92:LYS:HD2	12:E:120:THR:HG23	1.96	0.46
4:A:416:PRO:HA	4:A:419:HIS:HB2	1.97	0.46
4:A:592:LYS:HD2	4:A:592:LYS:HA	1.46	0.46
2:N:7:DT:H5'	2:N:8:DA:O5'	2.16	0.45
4:A:1053:PRO:HB2	4:A:1055:THR:HG23	1.98	0.45
4:A:1172:LEU:HD12	4:A:1173:THR:N	2.31	0.45
13:B:551:SER:OG	13:B:593:ARG:NH1	2.48	0.45
2:N:10:DG:H3'	2:N:12:DT:OP2	2.16	0.45
13:B:404:GLU:OE2	13:B:408:ARG:NH1	2.50	0.45
10:H:29:ARG:HA	10:H:43:LEU:O	2.17	0.45
2:N:26:DC:H2"	2:N:27:DT:C5	2.52	0.45
2:N:18:DT:H2"	2:N:19:DG:H5"	1.98	0.45
4:A:1056:THR:O	4:A:1057:THR:OG1	2.29	0.45
6:F:114:ILE:HG12	6:F:126:TRP:HB3	1.98	0.45
11:I:19:ASP:OD1	11:I:19:ASP:N	2.42	0.45
4:A:893:GLU:O	4:A:897:TYR:CD2	2.67	0.44
12:E:75:ASP:OD1	12:E:78:ARG:NH1	2.50	0.44
13:B:175:LYS:HB2	13:B:201:GLY:HA3	1.99	0.44
2:N:13:DA:H2"	2:N:14:DG:O5'	2.17	0.44
2:N:14:DG:C8	13:B:340:PHE:HB2	2.52	0.44
13:B:286:SER:HB2	13:B:289:GLU:HG2	2.00	0.44
13:B:626:PRO:HA	13:B:656:GLU:O	2.16	0.44
5:C:297:LEU:HG	8:K:87:TYR:HD2	1.79	0.44
10:H:99:LYS:HB3	10:H:113:TYR:HD2	1.83	0.44
10:H:145:LYS:HA	10:H:145:LYS:HD3	1.78	0.44
5:C:14:ILE:HD12	8:K:108:GLU:HB3	1.98	0.44
4:A:897:TYR:OH	11:I:86:PHE:CE2	2.65	0.44
4:A:1059:ILE:HB	4:A:1108:ILE:HD11	2.00	0.44
4:A:1121:LEU:HD11	4:A:1156:THR:HB	2.00	0.44
4:A:989:CYS:SG	4:A:990:SER:N	2.91	0.44
13:B:791:LEU:HD22	13:B:904:PRO:HD2	2.00	0.44
13:B:1046:LYS:HB3	13:B:1046:LYS:HE2	1.76	0.44
3:P:10:A:H2'	3:P:11:A:C8	2.52	0.43
13:B:288:LYS:HE2	13:B:288:LYS:HB2	1.81	0.43
4:A:708:ASP:OD1	4:A:708:ASP:N	2.49	0.43
13:B:599:LEU:HD23	13:B:599:LEU:HA	1.91	0.43
4:A:596:GLU:N	6:F:137:TRP:HE1	2.16	0.43
4:A:885:ARG:HG2	12:E:23:SER:HG	1.76	0.43
10:H:14:VAL:HG13	10:H:58:PHE:HE1	1.83	0.43
4:A:897:TYR:CE2	11:I:86:PHE:HE2	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1169:TYR:O	4:A:1173:THR:HB	2.17	0.43
13:B:97:ASP:OD1	13:B:97:ASP:N	2.52	0.43
10:H:89:TYR:HA	10:H:144:ARG:HB3	2.01	0.43
1:T:25:DA:C6	1:T:26:DT:C4	3.07	0.43
2:N:7:DT:H3'	2:N:8:DA:N3	2.34	0.43
4:A:804:SER:HA	12:E:189:GLN:HB3	2.01	0.43
13:B:640:LYS:HA	13:B:640:LYS:HD3	1.74	0.43
13:B:490:ARG:HD3	13:B:492:GLN:CG	2.49	0.43
13:B:670:TRP:O	13:B:672:THR:N	2.49	0.43
13:B:724:GLY:HA3	13:B:764:ASN:HD22	1.84	0.43
4:A:515:GLN:NE2	8:K:61:TYR:O	2.52	0.43
6:F:77:ARG:HA	6:F:77:ARG:HD2	1.81	0.43
13:B:784:ILE:HG22	13:B:942:ILE:HG22	2.00	0.43
10:H:30:ILE:O	10:H:42:HIS:HA	2.19	0.43
13:B:300:ASP:HB3	13:B:303:ILE:HG12	2.01	0.43
4:A:553:LEU:HD13	4:A:592:LYS:HG2	2.01	0.42
5:C:262:ASP:N	5:C:262:ASP:OD1	2.47	0.42
13:B:745:GLN:NE2	13:B:767:ASN:H	2.17	0.42
5:C:56:GLU:OE1	5:C:163:LYS:NZ	2.42	0.42
5:C:296:ARG:C	5:C:297:LEU:HD23	2.39	0.42
12:E:96:VAL:HB	12:E:126:LEU:HD23	2.01	0.42
2:N:10:DG:H22	13:B:463:LYS:HD2	1.83	0.42
12:E:169:ARG:HH21	12:E:212:LYS:HD3	1.84	0.42
4:A:522:ARG:NH1	4:A:565:SER:O	2.53	0.42
6:F:87:VAL:HG12	6:F:89:VAL:H	1.85	0.42
13:B:346:VAL:HA	13:B:349:CYS:HB2	2.01	0.42
13:B:965:ILE:HG22	13:B:1000:GLN:HE22	1.84	0.42
3:P:14:A:H2'	3:P:15:C:C6	2.54	0.42
5:C:12:VAL:HG11	8:K:105:PHE:HD1	1.85	0.42
13:B:204:PHE:O	13:B:210:GLU:HA	2.20	0.42
13:B:237:SER:OG	13:B:238:GLU:N	2.51	0.42
2:N:10:DG:N7	2:N:11:DC:C6	2.87	0.42
2:N:12:DT:H72	2:N:13:DA:H62	1.85	0.42
1:T:8:DA:H2"	1:T:9:DG:C8	2.55	0.42
2:N:6:DG:O3'	2:N:7:DT:H4'	2.20	0.42
10:H:100:ILE:HG22	10:H:135:LEU:HD13	2.01	0.42
13:B:498:ARG:HA	13:B:498:ARG:HD2	1.76	0.42
2:N:19:DG:OP2	13:B:494:LEU:HD22	2.19	0.42
4:A:596:GLU:H	6:F:137:TRP:HE1	1.66	0.42
1:T:6:DC:H2"	1:T:7:DA:C8	2.54	0.41
4:A:947:GLU:O	11:I:92:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:13:DA:H2'	2:N:14:DG:C2	2.55	0.41
13:B:673:LYS:HA	13:B:673:LYS:HD3	1.81	0.41
13:B:496:THR:O	13:B:496:THR:CG2	2.68	0.41
3:P:15:C:H2'	3:P:16:C:H6	1.82	0.41
4:A:772:LEU:HD23	4:A:772:LEU:HA	1.94	0.41
4:A:431:HIS:HD2	4:A:433:ASP:H	1.67	0.41
4:A:897:TYR:CE2	11:I:86:PHE:CE2	3.09	0.41
13:B:277:VAL:HG11	13:B:330:TYR:HD2	1.85	0.41
4:A:885:ARG:CB	12:E:23:SER:OG	2.69	0.41
5:C:40:VAL:HG21	5:C:288:LEU:HD13	2.01	0.41
12:E:108:ILE:HA	12:E:111:VAL:HG12	2.02	0.41
4:A:937:GLY:O	4:A:1006:MET:HA	2.20	0.41
5:C:297:LEU:HD11	8:K:33:PHE:CE2	2.56	0.41
2:N:12:DT:H72	13:B:340:PHE:CE1	2.56	0.41
4:A:709:LYS:HA	4:A:709:LYS:HD3	1.82	0.41
5:C:148:GLN:HB3	5:C:149:ARG:H	1.66	0.41
10:H:77:PHE:O	10:H:79:PRO:HD3	2.21	0.41
10:H:110:ALA:N	10:H:125:GLY:O	2.51	0.41
11:I:75:ARG:HH11	11:I:82:GLY:HA3	1.85	0.41
13:B:786:MET:HG3	13:B:920:LEU:HD13	2.02	0.41
1:T:6:DC:H1'	1:T:7:DA:H5'	2.03	0.41
1:T:27:DT:H5"	13:B:450:ARG:NH1	2.35	0.40
4:A:687:LYS:HE3	4:A:687:LYS:HB2	1.89	0.40
4:A:1229:LEU:HD23	6:F:114:ILE:HG22	2.04	0.40
13:B:251:ASN:OD1	13:B:260:LYS:NZ	2.52	0.40
4:A:364:GLN:HA	4:A:367:VAL:HG12	2.04	0.40
13:B:394:LYS:O	13:B:395:ARG:NH1	2.49	0.40
13:B:1013:ARG:HH22	13:B:1026:LEU:HA	1.87	0.40
4:A:885:ARG:HE	12:E:22:LEU:N	2.20	0.40
9:L:29:CYS:SG	9:L:30:ARG:N	2.94	0.40
10:H:42:HIS:CD2	10:H:122:LEU:HB3	2.57	0.40
1:T:21:DG:H2'	1:T:22:DG:C8	2.56	0.40
2:N:11:DC:H1'	2:N:12:DT:C6	2.55	0.40
4:A:646:VAL:HG23	4:A:659:LEU:HD11	2.03	0.40
4:A:965:ASN:HA	4:A:968:VAL:HG12	2.03	0.40
13:B:225:TRP:HB2	13:B:236:ARG:HH12	1.87	0.40
13:B:604:GLU:OE1	13:B:622:ARG:NH1	2.47	0.40
13:B:970:GLN:HE21	13:B:972:LYS:HE2	1.87	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
4	A	840/2032 (41%)	795 (95%)	44 (5%)	1 (0%)	51 81
5	C	283/319 (89%)	272 (96%)	10 (4%)	1 (0%)	34 66
6	F	78/144 (54%)	71 (91%)	7 (9%)	0	100 100
7	J	61/69 (88%)	60 (98%)	1 (2%)	0	100 100
8	K	106/116 (91%)	102 (96%)	4 (4%)	0	100 100
9	L	43/51 (84%)	37 (86%)	6 (14%)	0	100 100
10	H	139/146 (95%)	119 (86%)	20 (14%)	0	100 100
11	I	93/114 (82%)	86 (92%)	7 (8%)	0	100 100
12	E	207/230 (90%)	198 (96%)	9 (4%)	0	100 100
13	B	959/1169 (82%)	907 (95%)	51 (5%)	1 (0%)	51 81
All	All	2809/4390 (64%)	2647 (94%)	159 (6%)	3 (0%)	54 81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	B	431	ASP
4	A	592	LYS
5	C	184	THR

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
4	A	753/1709 (44%)	749 (100%)	4 (0%)	88 96
5	C	253/276 (92%)	252 (100%)	1 (0%)	91 97
6	F	72/128 (56%)	72 (100%)	0	100 100
7	J	56/62 (90%)	56 (100%)	0	100 100
8	K	98/105 (93%)	98 (100%)	0	100 100
9	L	40/46 (87%)	40 (100%)	0	100 100
10	H	123/127 (97%)	123 (100%)	0	100 100
11	I	85/101 (84%)	85 (100%)	0	100 100
12	E	190/209 (91%)	188 (99%)	2 (1%)	73 92
13	B	849/1026 (83%)	841 (99%)	8 (1%)	78 94
All	All	2519/3789 (66%)	2504 (99%)	15 (1%)	86 96

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	591	GLU
4	A	592	LYS
4	A	1024	LEU
4	A	1173	THR
5	C	297	LEU
12	E	44	LEU
12	E	167	ARG
13	B	426	LEU
13	B	462	ARG
13	B	463	LYS
13	B	464	MET
13	B	637	LYS
13	B	984	ARG
13	B	1014	VAL
13	B	1048	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	358	HIS
4	A	401	HIS
4	A	421	HIS
4	A	424	GLN

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Mol	Chain	Res	Type
4	A	431	HIS
4	A	611	HIS
4	A	693	ASN
4	A	781	ASN
4	A	942	ASN
4	A	1011	ASN
4	A	1083	GLN
4	A	1114	GLN
4	A	1147	HIS
5	C	279	GLN
8	K	29	ASN
8	K	89	GLN
10	H	94	HIS
11	I	31	ASN
13	B	59	GLN
13	B	216	GLN
13	B	506	HIS
13	B	596	GLN
13	B	679	GLN
13	B	684	HIS
13	B	705	HIS
13	B	714	GLN
13	B	720	GLN
13	B	721	GLN
13	B	745	GLN
13	B	758	GLN
13	B	764	ASN
13	B	767	ASN
13	B	780	GLN
13	B	970	GLN
13	B	1000	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	P	10/20 (50%)	4 (40%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	P	11	A

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Mol	Chain	Res	Type
3	P	13	G
3	P	14	A
3	P	19	G

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

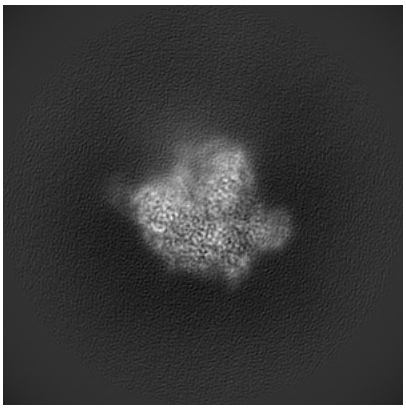
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34821. These allow visual inspection of the internal detail of the map and identification of artifacts.

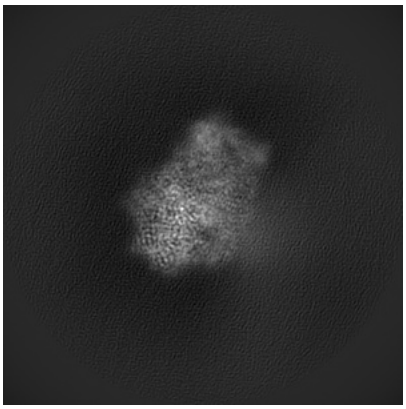
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

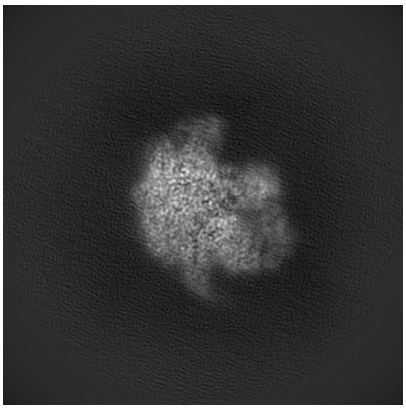
6.1.1 Primary map



X

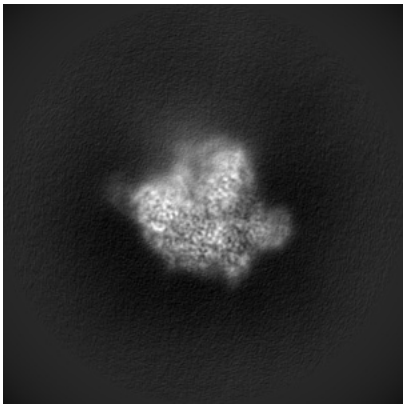


Y

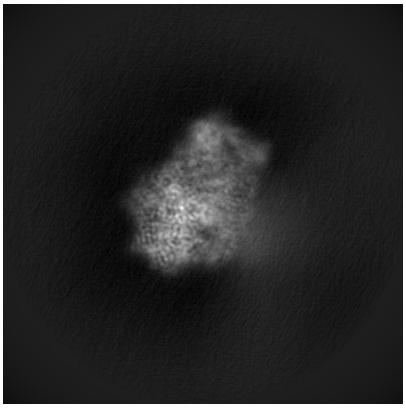


Z

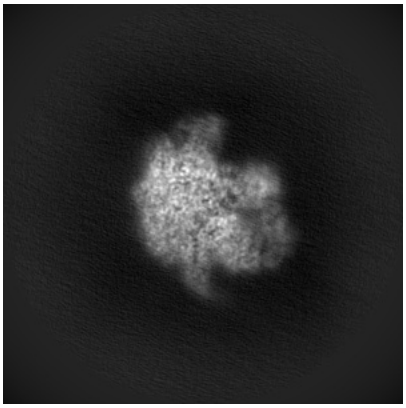
6.1.2 Raw map



X



Y

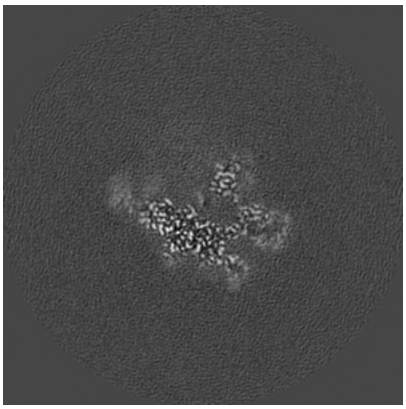


Z

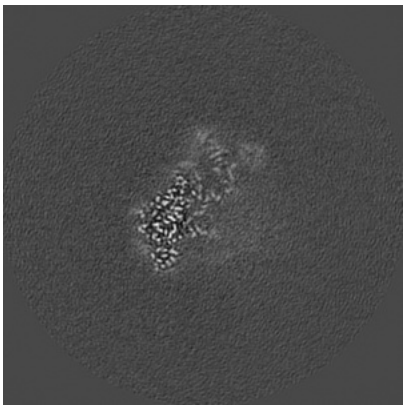
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

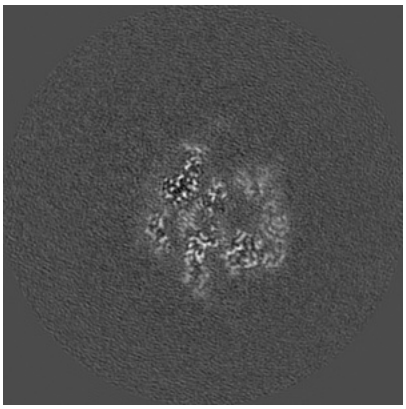
6.2.1 Primary map



X Index: 150

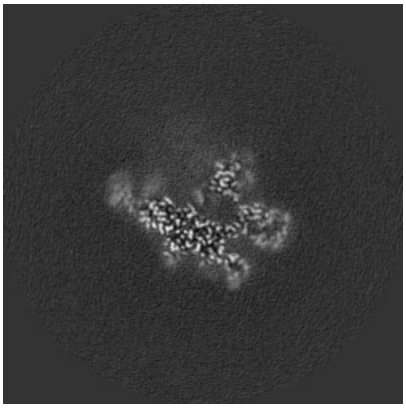


Y Index: 150

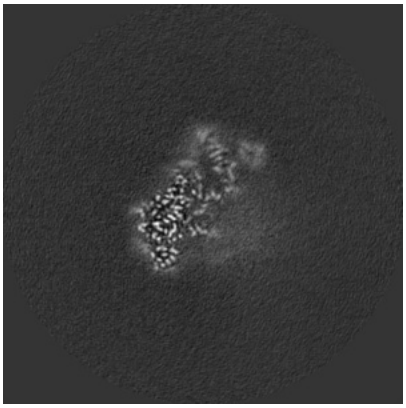


Z Index: 150

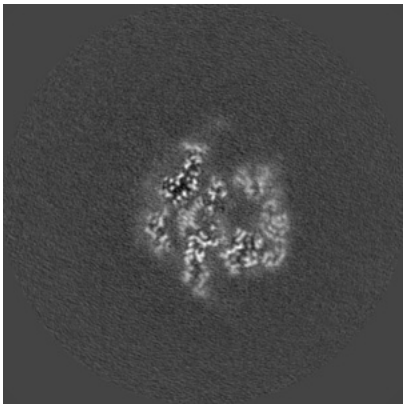
6.2.2 Raw map



X Index: 150



Y Index: 150

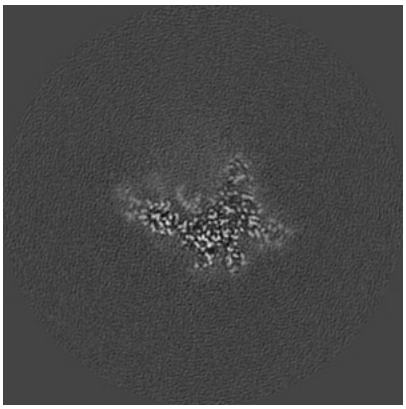


Z Index: 150

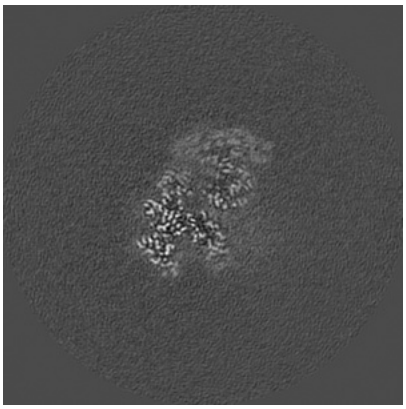
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

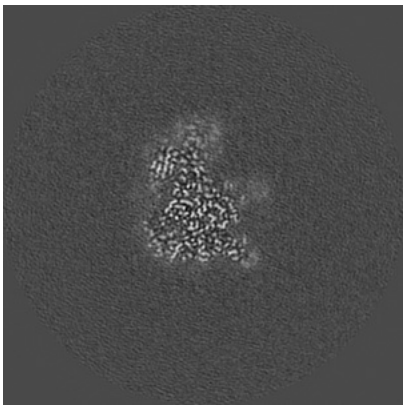
6.3.1 Primary map



X Index: 140

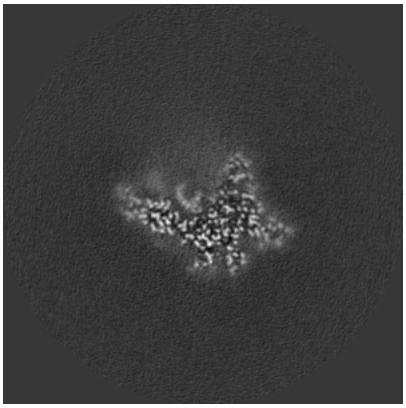


Y Index: 162

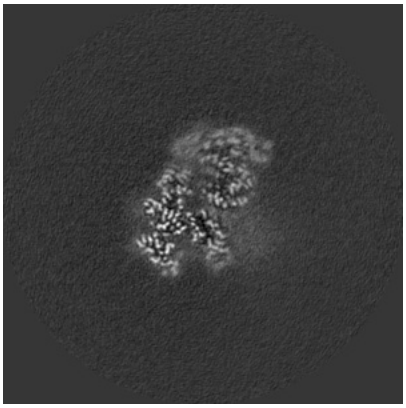


Z Index: 133

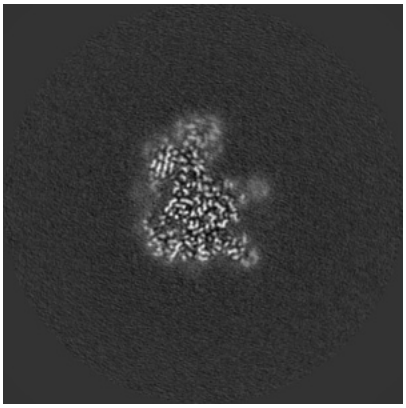
6.3.2 Raw map



X Index: 140



Y Index: 162

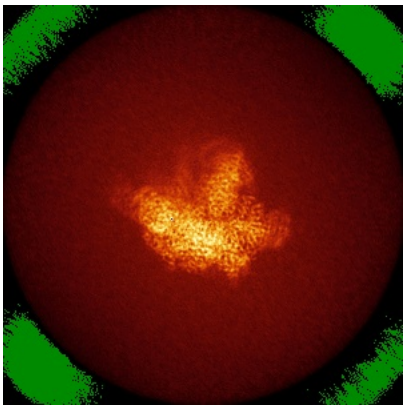


Z Index: 133

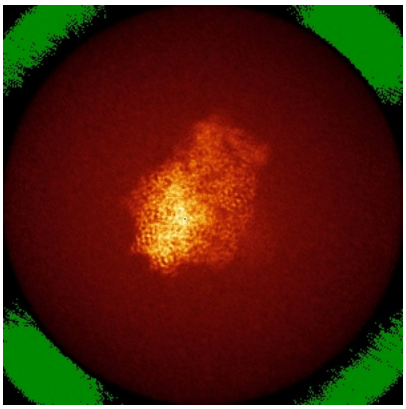
The images above show the largest variance slices of the map in three orthogonal directions.

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

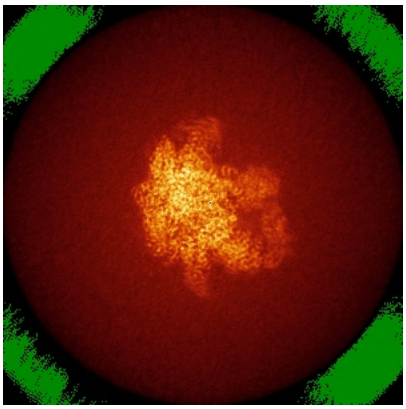
6.4.1 Primary map



X

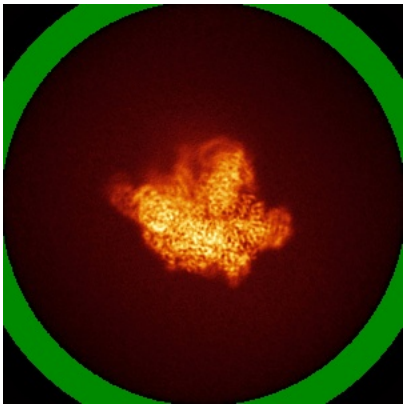


Y

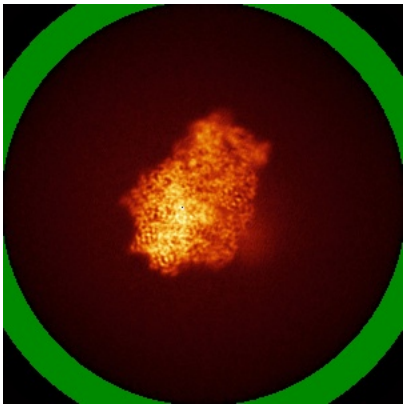


Z

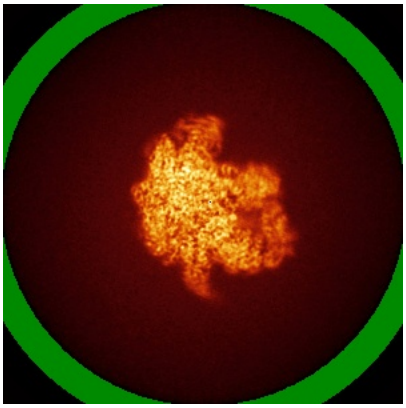
6.4.2 Raw map



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.

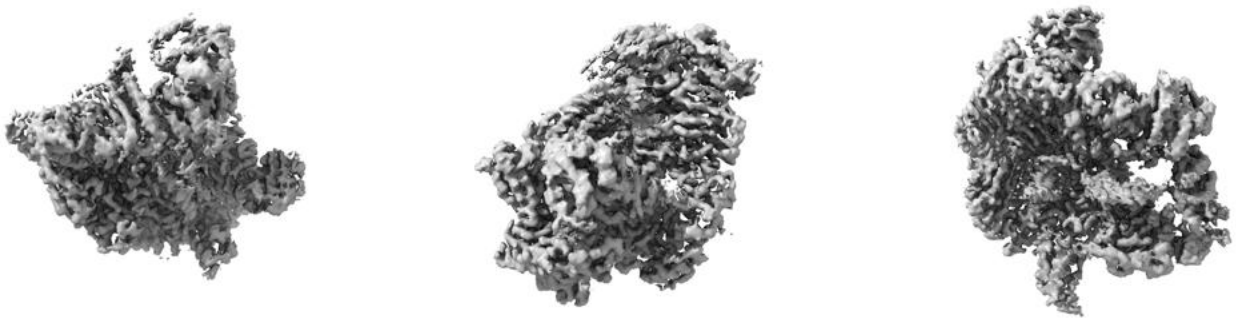
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0245. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

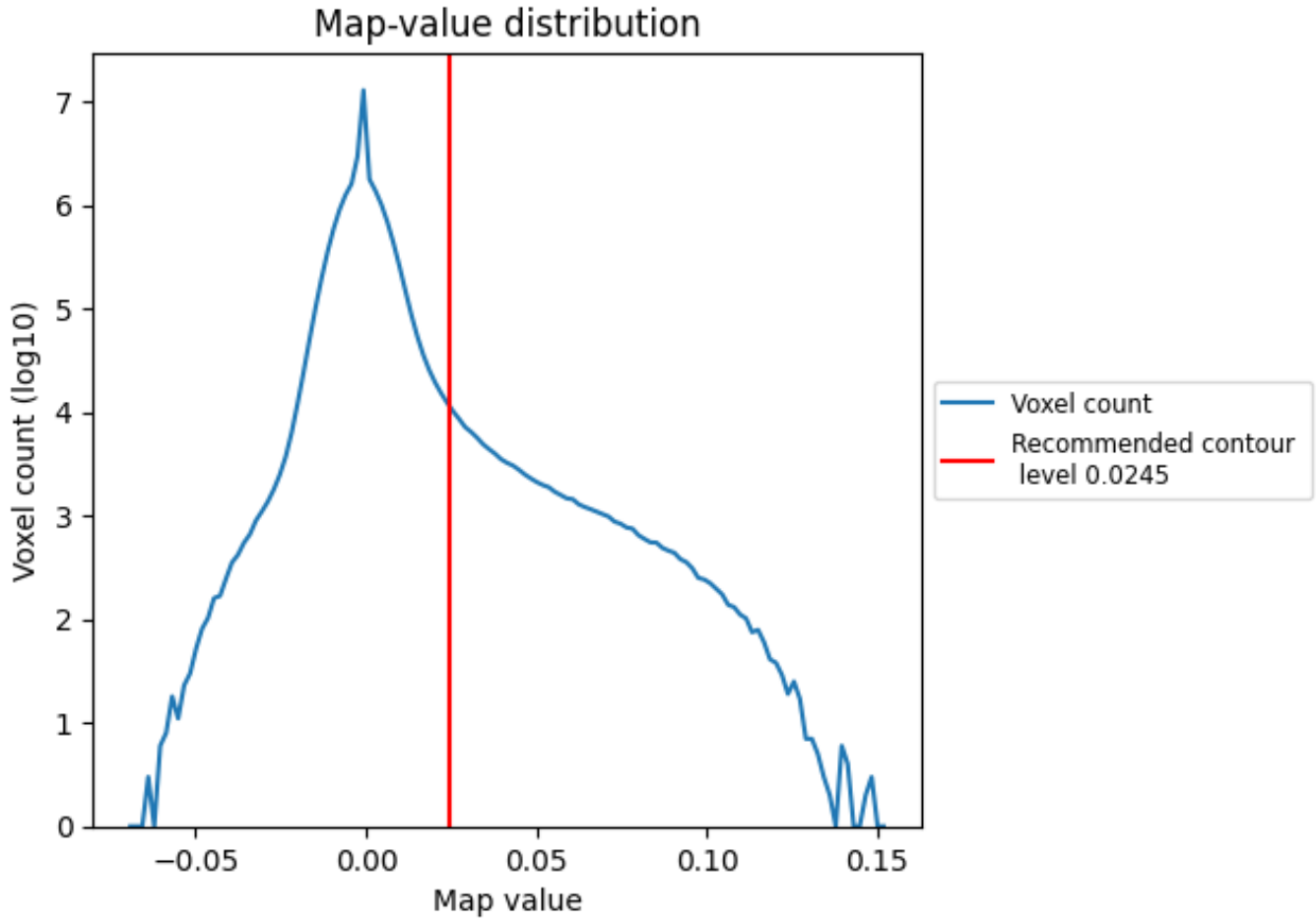
6.6 Mask visualisation (i)

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

7 Map analysis

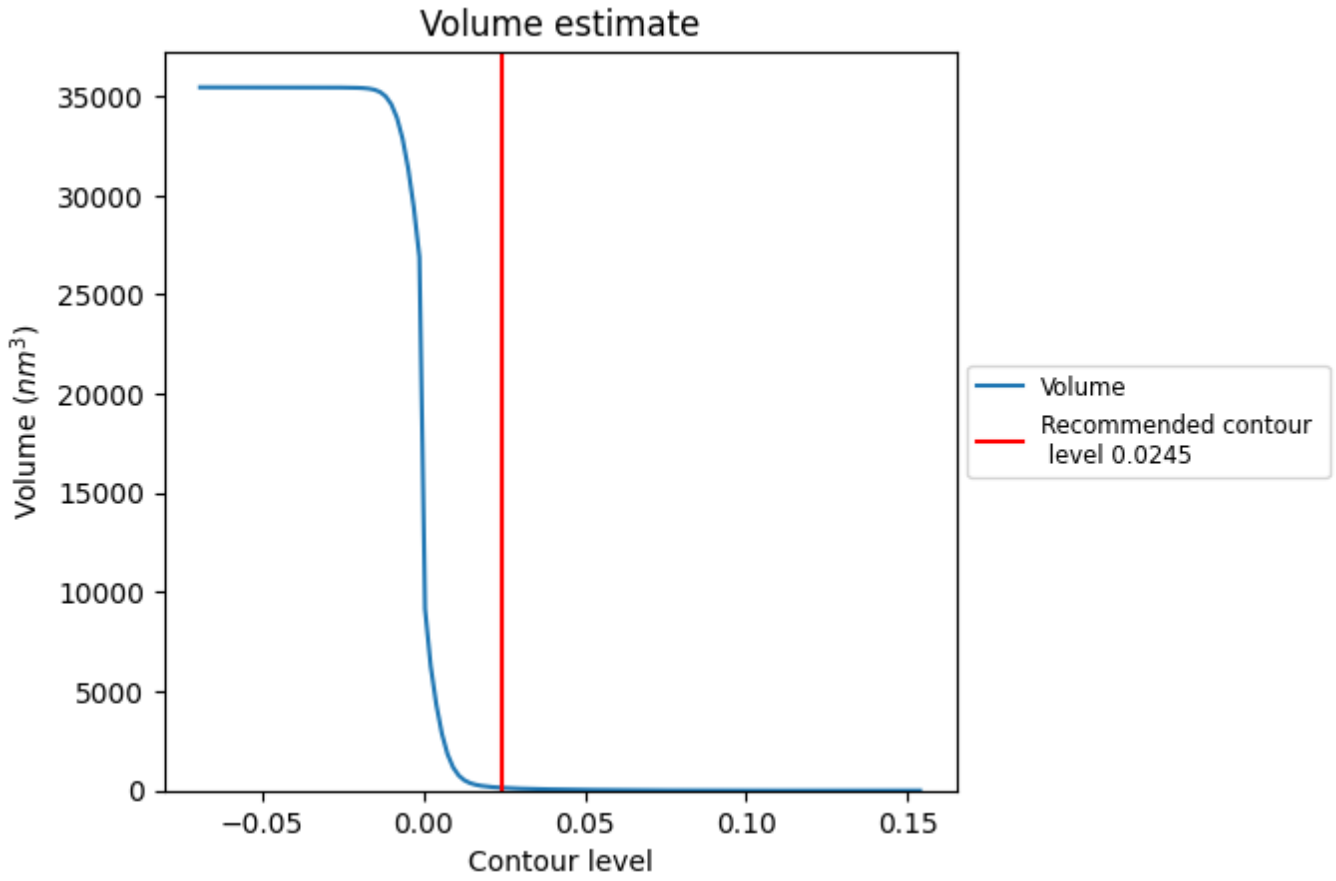
This section contains the results of statistical analysis of the map.

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.

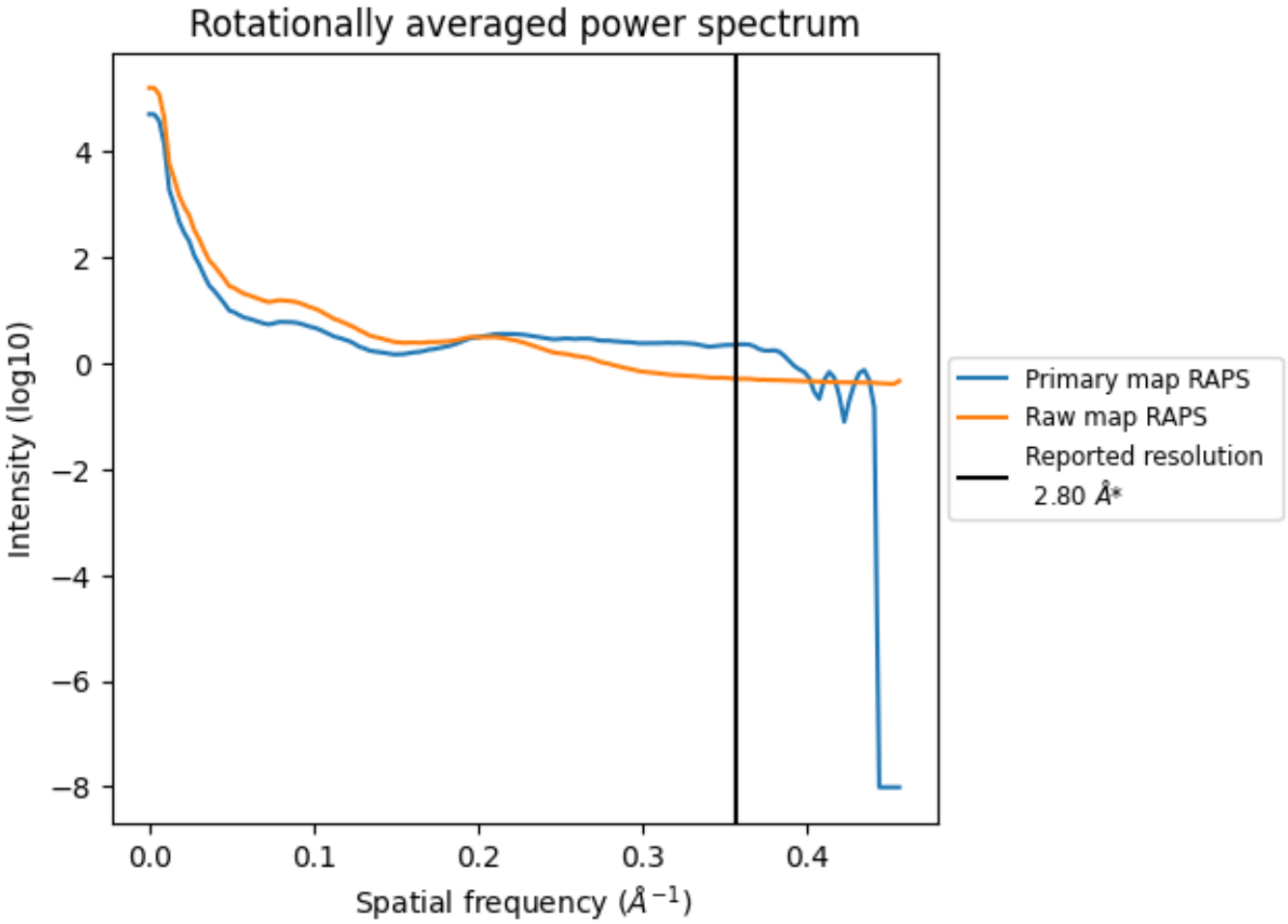
7.2 Volume estimate



The volume at the recommended contour level is 139 nm^3; this corresponds to an approximate mass of 125 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)

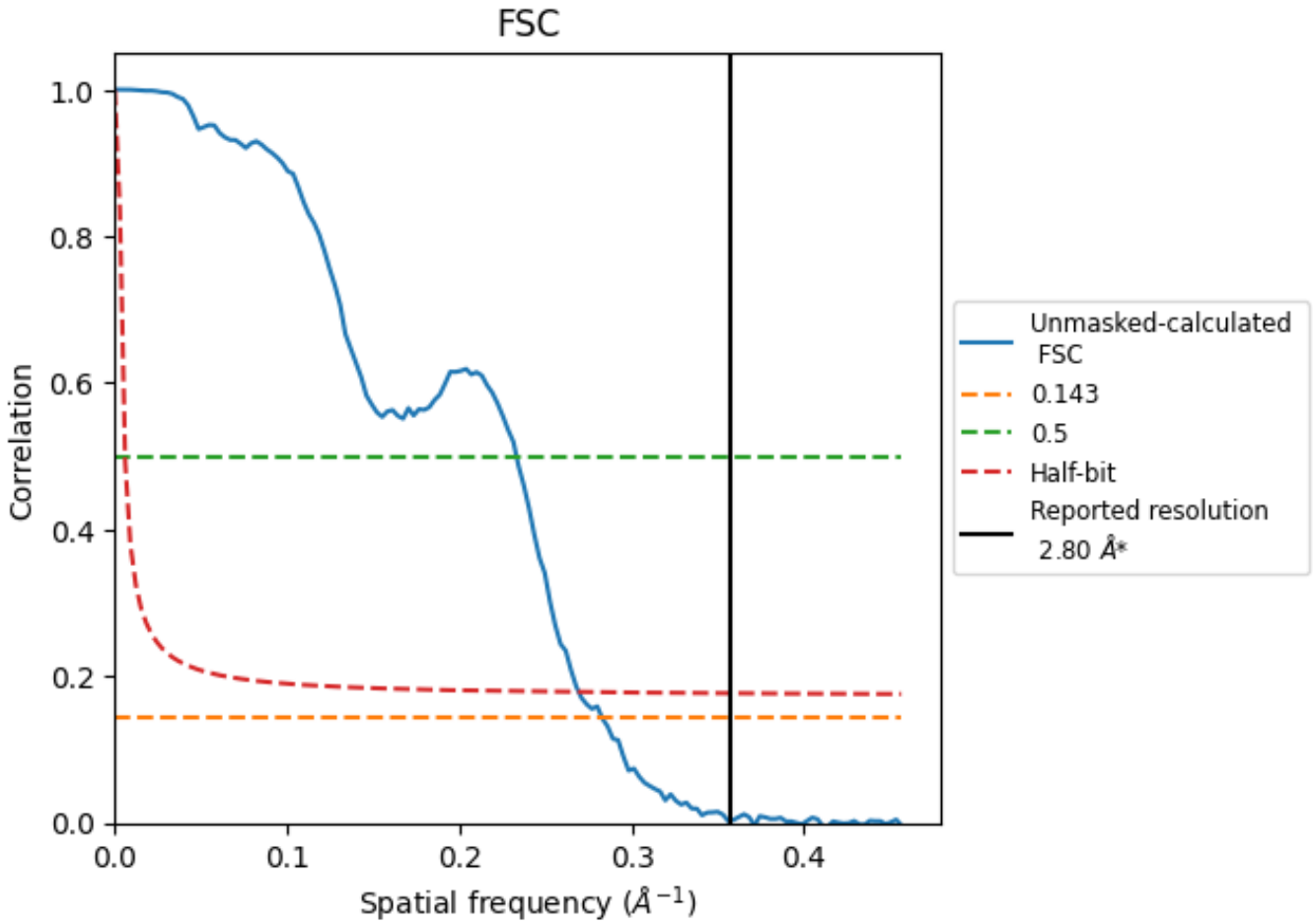


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

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)

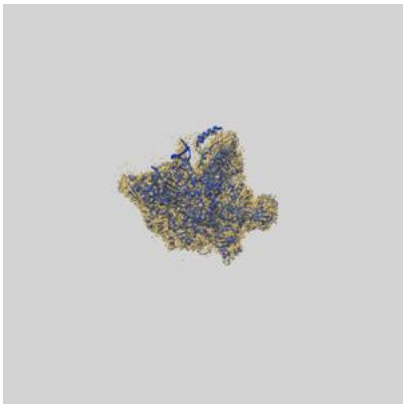
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.53	4.29	3.71

*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 3.53 differs from the reported value 2.8 by more than 10 %

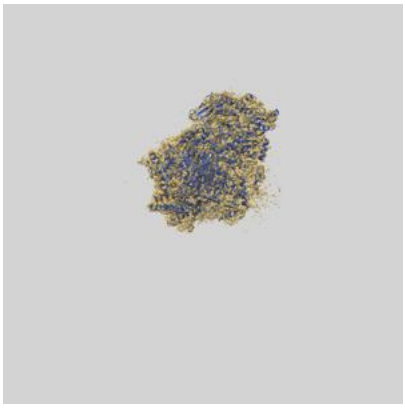
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34821 and PDB model 8HIM. Per-residue inclusion information can be found in section 3 on page 7.

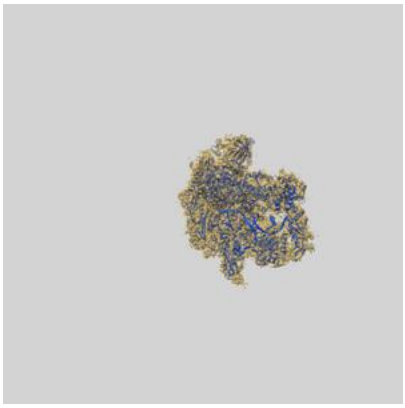
9.1 Map-model overlay



X



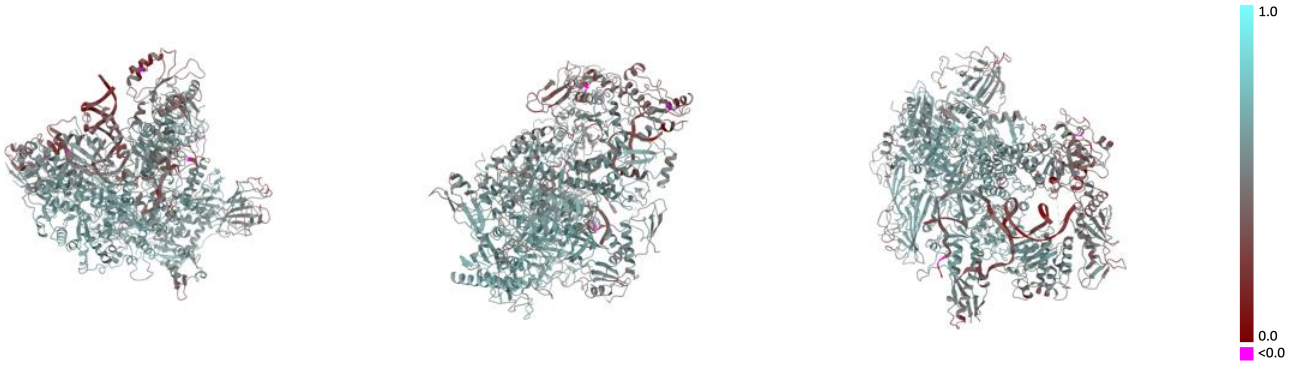
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0245 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.

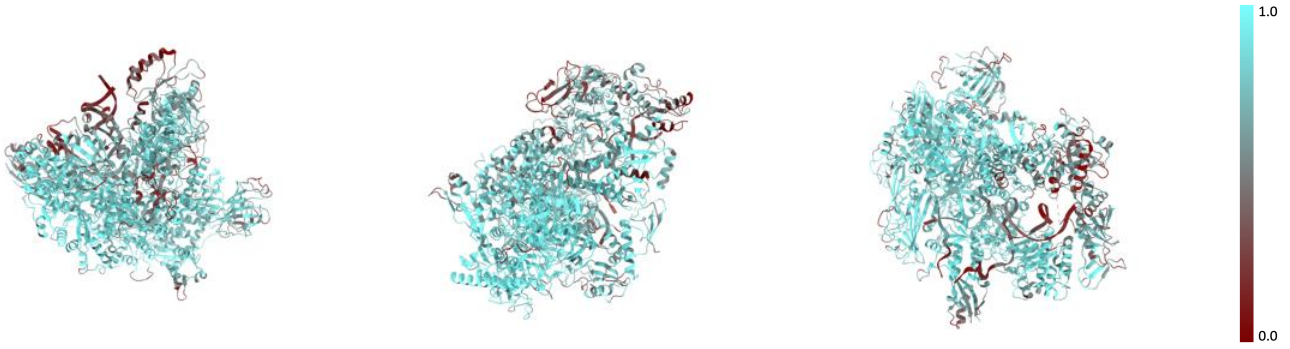
9.2 Q-score mapped to coordinate model (i)



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.

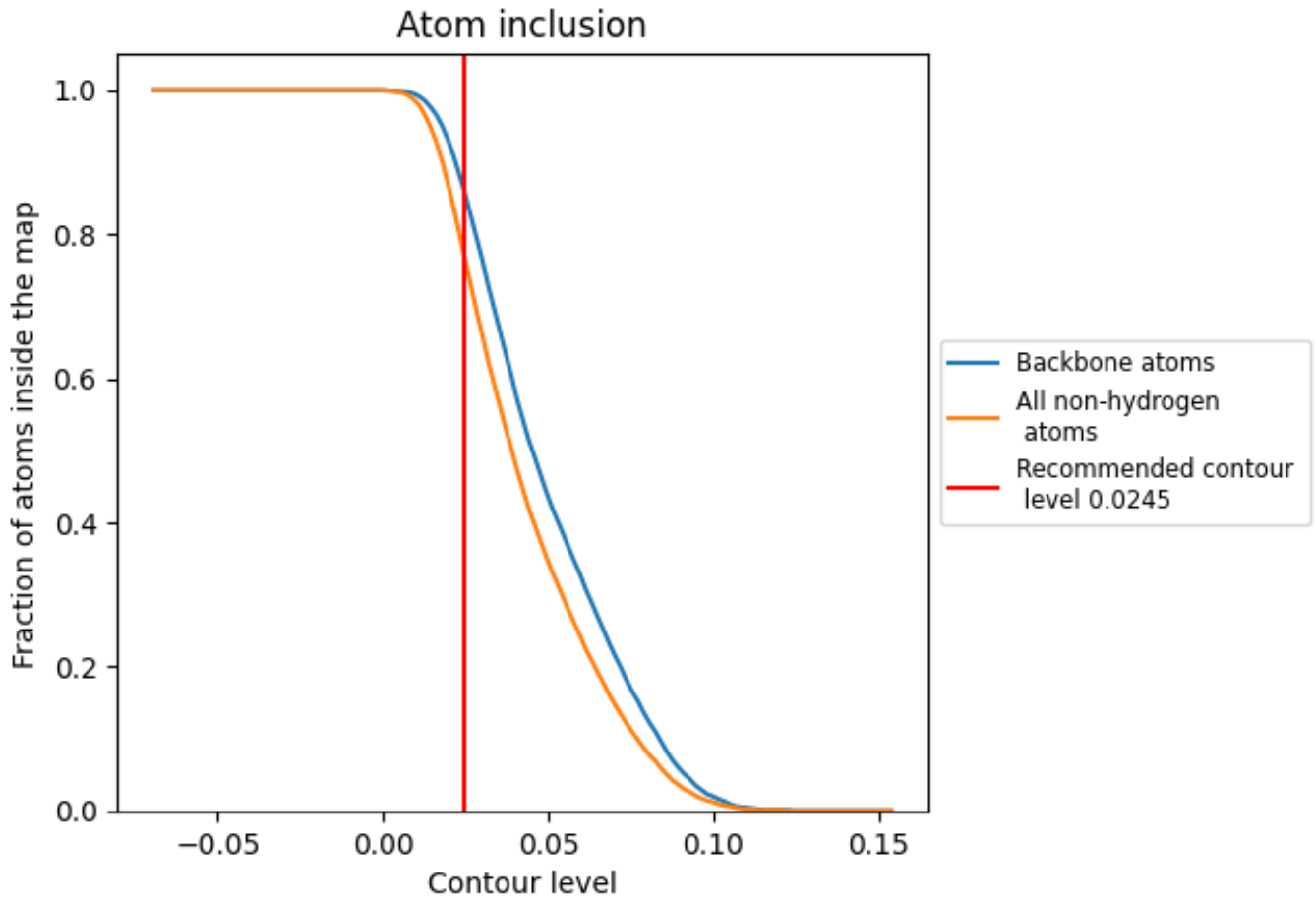
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0245).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 77% 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 (0.0245) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7710	0.5430
A	0.7570	0.5420
B	0.8780	0.5980
C	0.8830	0.6000
E	0.5810	0.4520
F	0.7330	0.5190
H	0.6230	0.4640
I	0.4590	0.4160
J	0.9560	0.6430
K	0.8860	0.6020
L	0.8600	0.5760
N	0.3010	0.2580
P	0.7700	0.4450
T	0.4200	0.3020