Full wwPDB EM Validation Report (i)

Apr 23, 2024 – 12:19 am BST

PDB ID	:	7AEA
EMDB ID	:	EMD-11742
Title	:	Cryo-EM structure of human RNA Polymerase III elongation complex 2
Authors	:	Girbig, M.; Misiaszek, A.D.; Vorlaender, M.K.; Mueller, C.W.
Deposited on	:	2020-09-17
Resolution	:	3.40 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 (i) 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 (1)) were used in the production of this report:

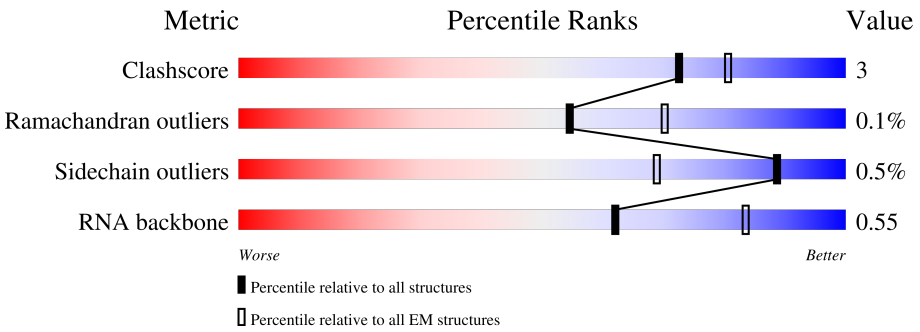
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.40 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	1390	7%, 89%, 10%, •
2	B	1133	•, 87%, 10%, •
3	C	346	•, 90%, 9%, •
4	D	148	30%, 66%, 18%, 16%
5	E	210	•, 94%, 5%
6	F	127	•, 57%, 5%, 39%
7	G	204	24%, 82%, 11%, 7%

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Mol	Chain	Length	Quality of chain
8	H	150	7% 87% 11%
9	I	108	51% 86% 13%
10	J	67	82% 16%
11	K	133	78% 20%
12	L	58	74% 5% 21%
13	M	708	15% 46% 6% 47%
14	N	398	12% 42% 53%
15	O	534	28% 88% 8%
16	P	316	23% 42% 54%
17	Q	223	23% 43% 53%
18	R	19	32% 11% 16% 5% 68%
19	S	46	26% 15% 17% 67%
20	T	46	48% 35% 15% 50%

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 42422 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 III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1381	10848	6876	1891	2008	73	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1097	8680	5499	1516	1597	68	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	343	2736	1723	488	514	11	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	124	1001	626	174	198	3	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	209	1715	1083	300	324	8	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	78	627	402	106	114	5	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	189	1509	979	237	286	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	148	1186	750	194	237	5	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	107	849	525	157	154	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	66	524	339	88	91	6	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	107	856	531	153	165	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	46	388	241	75	66	6	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	375	3025	1921	525	559	20	0	0

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	186	1448	907	251	281	9	0	0

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	512	4075	2565	712	774	24	0	0

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	146	1147	727	185	224	11	0	0

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	104	883	572	146	159	6	0	0

- Molecule 18 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
18	R	6	132	59	28	39	6	0	0

- Molecule 19 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
19	S	15	300	144	51	90	15	0	0

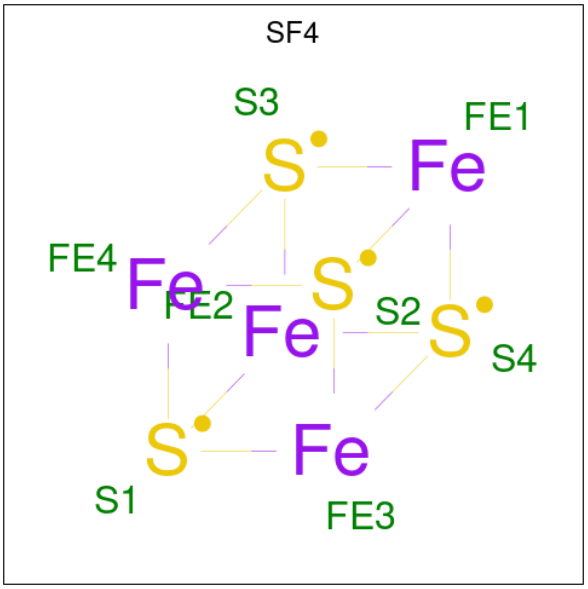
- Molecule 20 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
20	T	23	477	227	85	142	23	0	0

- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 22 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
22	P	1	8	4	4	0

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

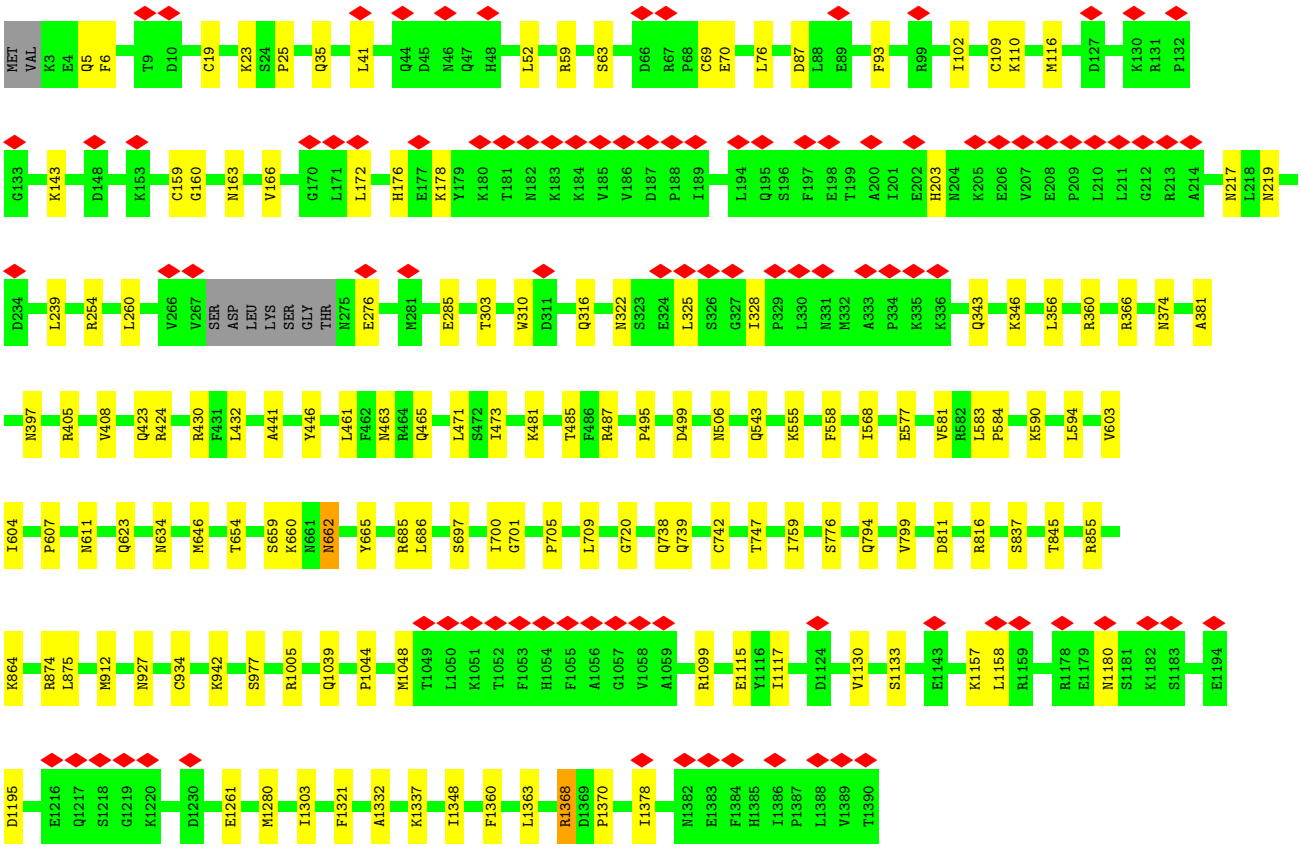
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
23	R	1	1	1	0

3 Residue-property plots (i)

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

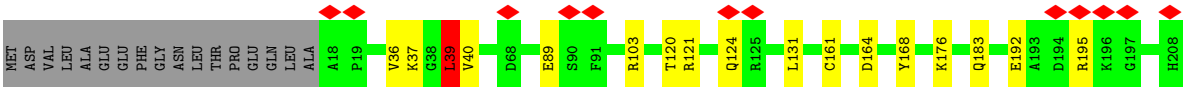
• Molecule 1: DNA-directed RNA polymerase III subunit RPC1

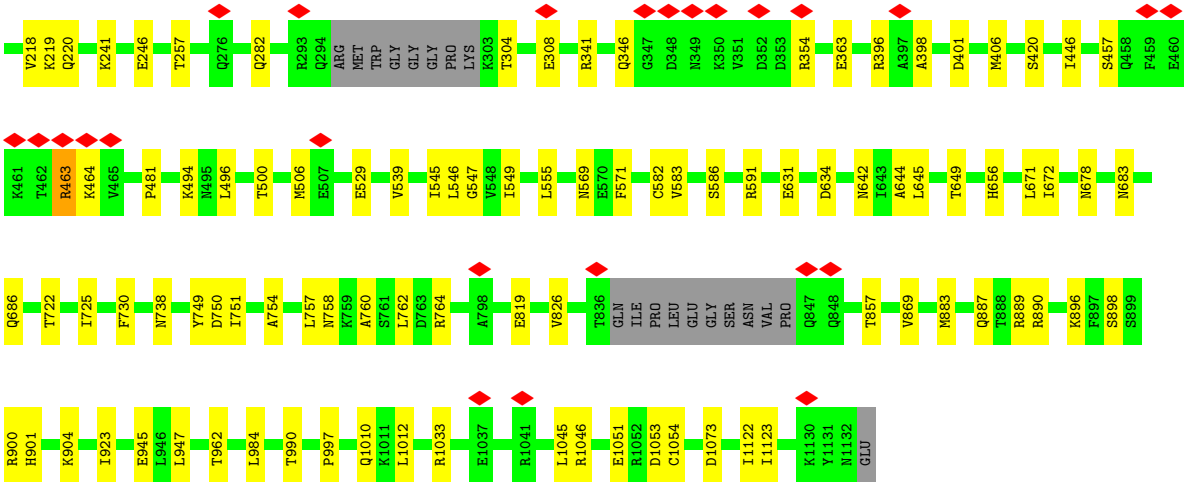
Chain A:



• Molecule 2: DNA-directed RNA polymerase III subunit RPC2

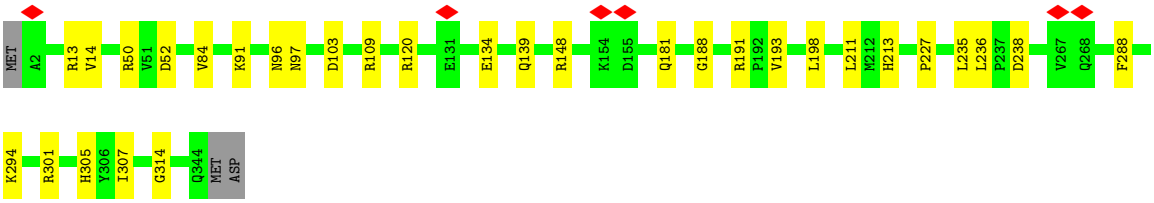
Chain B:





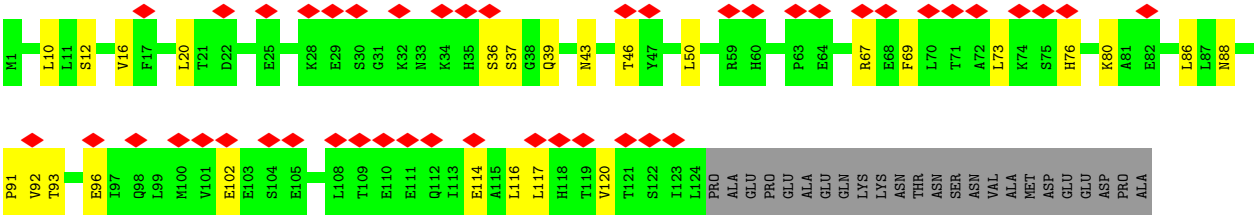
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C:



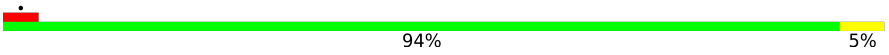
• Molecule 4: DNA-directed RNA polymerase III subunit RPC9

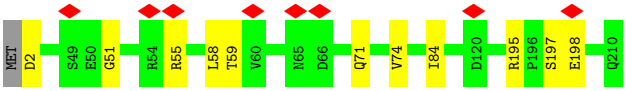
Chain D:



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

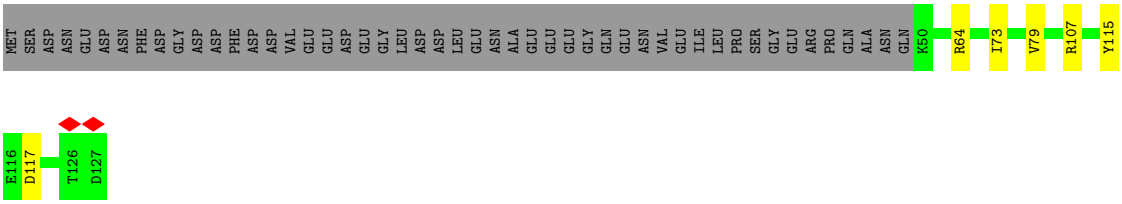
Chain E:





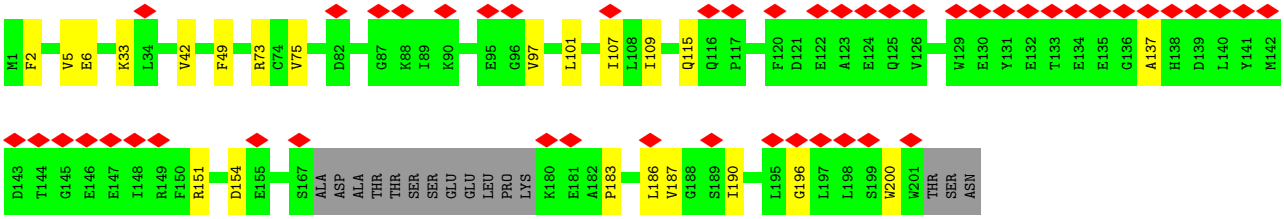
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



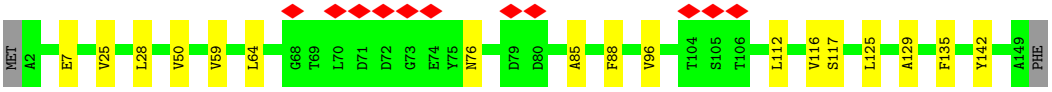
• Molecule 7: DNA-directed RNA polymerase III subunit RPC8

Chain G:



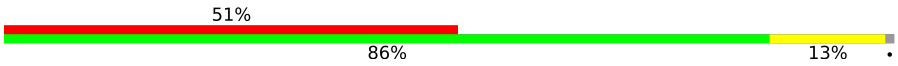
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

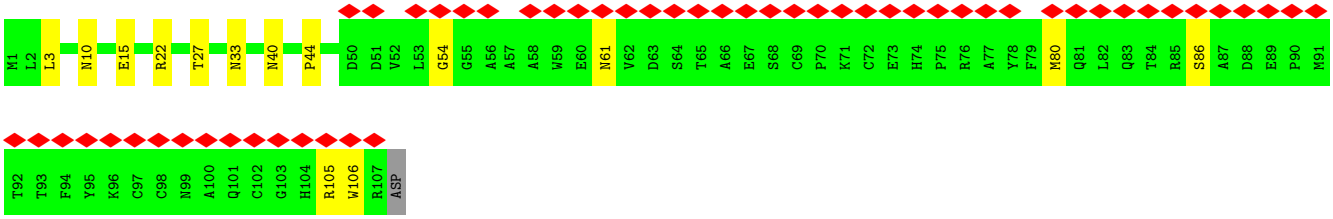
Chain H:



• Molecule 9: DNA-directed RNA polymerase III subunit RPC10

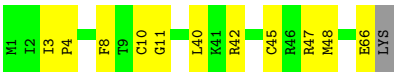
Chain I:





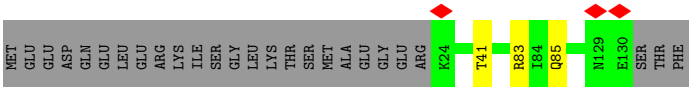
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K:

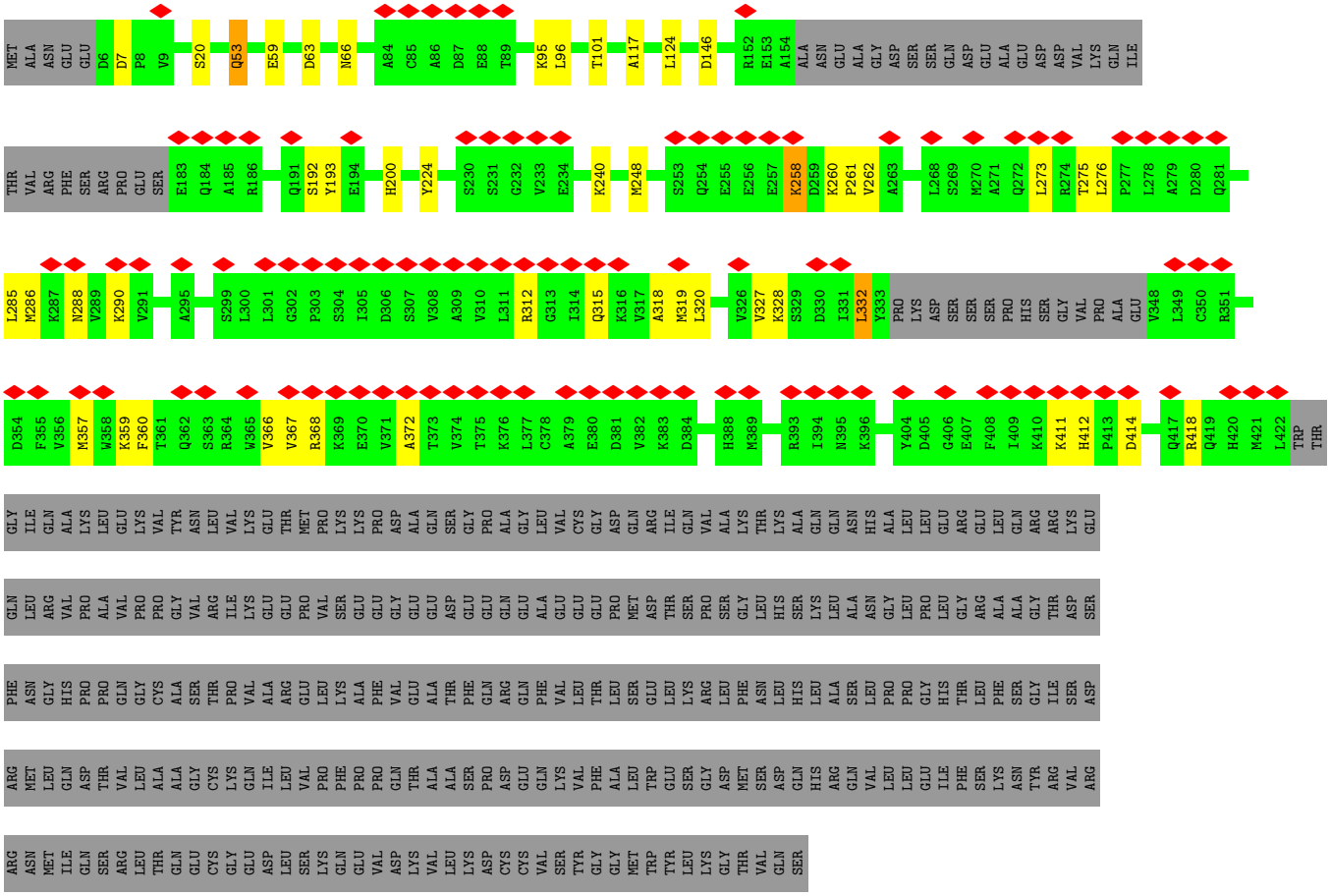


• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 74% 5% 21%

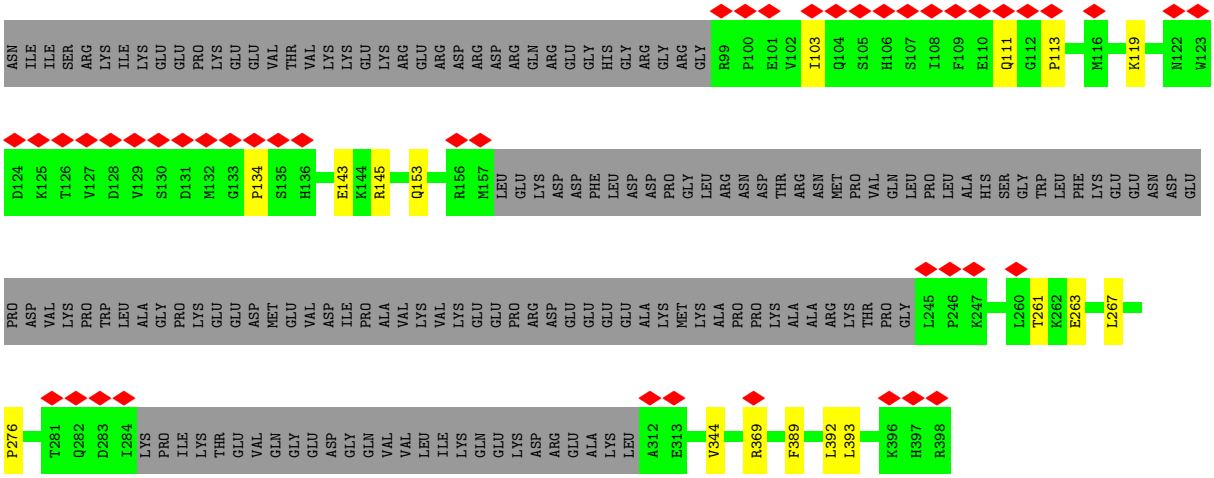
• Molecule 13: DNA-directed RNA polymerase III subunit RPC5

Chain M: 15% 46% 6% 47%



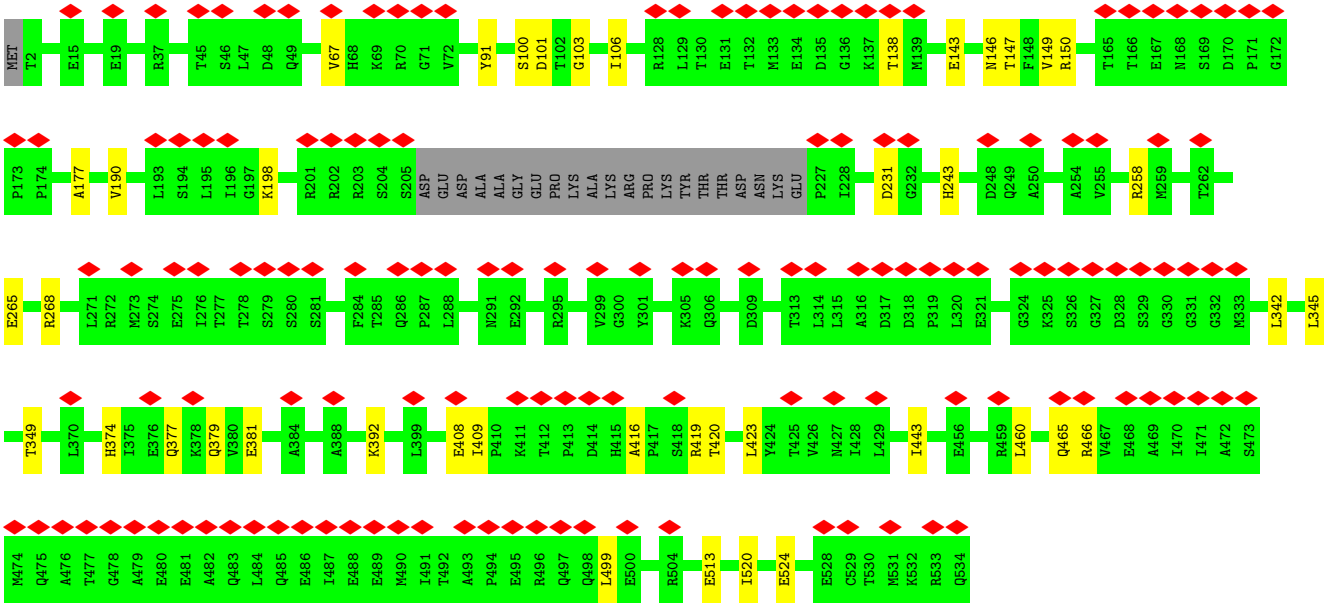
• Molecule 14: DNA-directed RNA polymerase III subunit RPC4

Chain N: 12% 42% • 53%



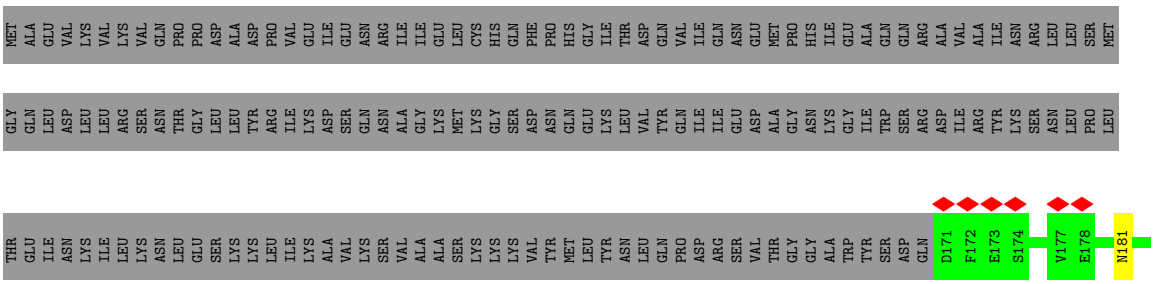
- Molecule 15: DNA-directed RNA polymerase III subunit RPC3

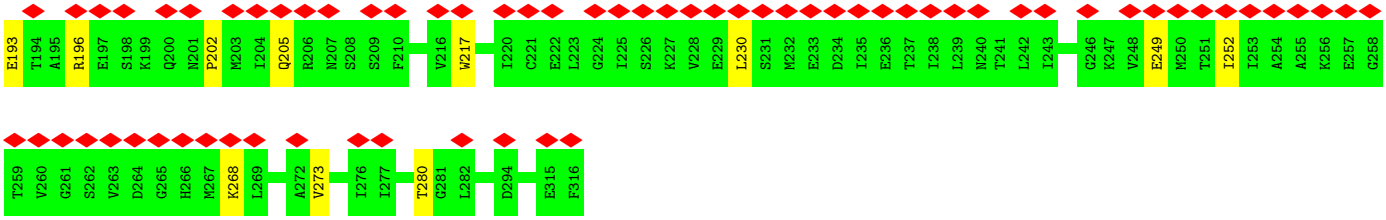
Chain O:



- Molecule 16: DNA-directed RNA polymerase III subunit RPC6

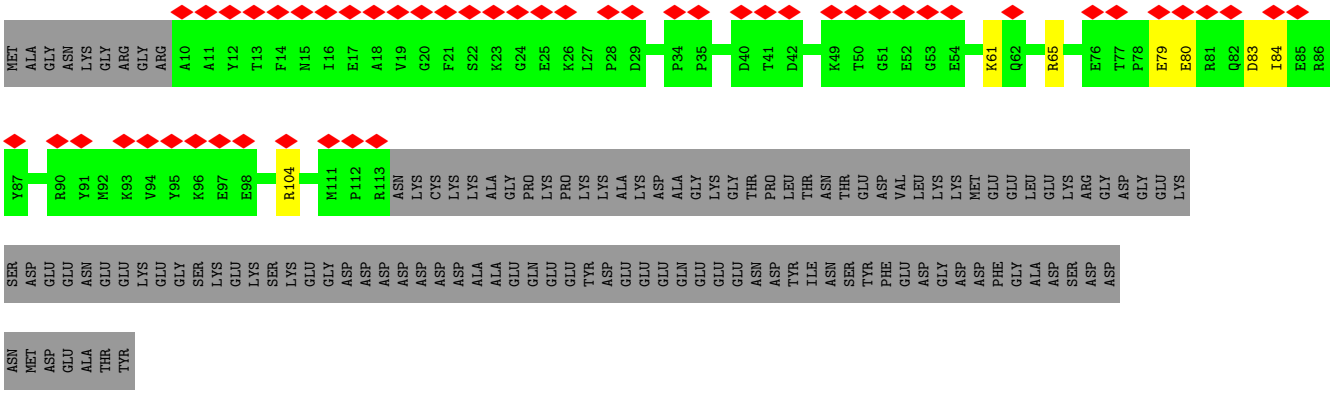
Chain P:





- Molecule 17: DNA-directed RNA polymerase III subunit RPC7

Chain Q:

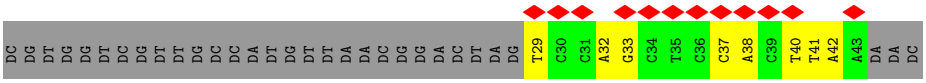


- Molecule 18: RNA

Chain R:

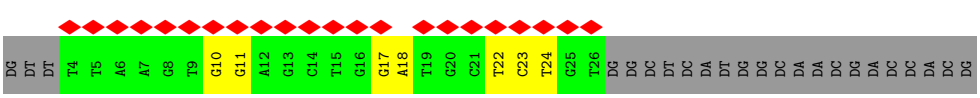
- Molecule 19: Non-template DNA

Chain S:



- Molecule 20: Template DNA

Chain T:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	31737	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.4	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.377	Depositor
Minimum map value	-0.477	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	352.8, 352.8, 352.8	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SF4, 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	0.31	0/11044	0.53	1/14893 (0.0%)
2	B	0.34	0/8845	0.54	1/11930 (0.0%)
3	C	0.32	0/2790	0.54	0/3782
4	D	0.25	0/1013	0.50	0/1365
5	E	0.28	0/1745	0.50	0/2358
6	F	0.31	0/637	0.53	0/861
7	G	0.30	0/1551	0.54	0/2110
8	H	0.33	0/1207	0.53	0/1628
9	I	0.32	0/870	0.61	0/1175
10	J	0.35	0/533	0.54	0/719
11	K	0.33	0/871	0.52	0/1174
12	L	0.33	0/394	0.51	0/524
13	M	0.27	0/3088	0.55	0/4171
14	N	0.30	0/1466	0.59	0/1972
15	O	0.25	0/4141	0.49	0/5592
16	P	0.26	0/1171	0.43	0/1584
17	Q	0.26	0/909	0.52	0/1227
18	R	0.28	0/148	1.00	1/229 (0.4%)
19	S	0.54	0/334	0.97	0/511
20	T	0.60	0/534	1.02	0/824
All	All	0.31	0/43291	0.55	3/58629 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
13	M	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	39	LEU	C-N-CA	6.13	137.02	121.70
1	A	1158	LEU	CA-CB-CG	5.36	127.63	115.30
18	R	14	A	P-O3'-C3'	5.07	125.78	119.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	39	LEU	Peptide
13	M	366	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10848	0	11090	92	0
2	B	8680	0	8806	72	0
3	C	2736	0	2712	17	0
4	D	1001	0	1028	17	0
5	E	1715	0	1733	7	0
6	F	627	0	659	6	0
7	G	1509	0	1461	13	0
8	H	1186	0	1147	10	0
9	I	849	0	812	8	0
10	J	524	0	540	8	0
11	K	856	0	840	3	0
12	L	388	0	394	3	0
13	M	3025	0	3041	25	0
14	N	1448	0	1489	10	0
15	O	4075	0	4149	25	0
16	P	1147	0	1118	7	0
17	Q	883	0	883	5	0
18	R	132	0	66	1	0
19	S	300	0	170	5	0
20	T	477	0	262	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	A	2	0	0	0	0
21	B	1	0	0	0	0
21	I	2	0	0	0	0
21	J	1	0	0	0	0
21	L	1	0	0	0	0
22	P	8	0	0	0	0
23	R	1	0	0	0	0
All	All	42422	0	42400	285	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 3.

All (285) 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:O:91:TYR:HH	15:O:243:HIS:HE2	1.42	0.65
7:G:107:ILE:HG12	7:G:186:LEU:HD23	1.79	0.64
2:B:131:LEU:HD21	2:B:406:MET:HG3	1.80	0.64
2:B:121:ARG:HD3	2:B:401:ASP:HB3	1.78	0.64
1:A:934:CYS:O	1:A:1005:ARG:NH2	2.31	0.63
2:B:1046:ARG:HD3	20:T:22:DT:H5'	1.79	0.63
14:N:111:GLN:HE21	14:N:113:PRO:HD2	1.64	0.62
13:M:286:MET:HG3	13:M:327:VAL:HG23	1.82	0.62
1:A:381:ALA:HB3	1:A:487:ARG:HB2	1.83	0.61
1:A:720:GLY:HA3	1:A:759:ILE:HD11	1.83	0.61
1:A:23:LYS:HG3	2:B:1123:ILE:HG13	1.83	0.61
1:A:52:LEU:O	1:A:59:ARG:NH1	2.33	0.61
2:B:396:ARG:HE	2:B:398:ALA:HB3	1.65	0.61
1:A:607:PRO:HD2	1:A:611:ASN:HD22	1.65	0.61
1:A:303:THR:OG1	15:O:377:GLN:NE2	2.34	0.60
2:B:506:MET:SD	2:B:569:ASN:ND2	2.74	0.60
7:G:97:VAL:HB	7:G:109:ILE:HB	1.83	0.60
3:C:50:ARG:NH1	3:C:52:ASP:OD2	2.34	0.60
17:Q:61:LYS:HE3	17:Q:65:ARG:HH22	1.65	0.60
4:D:20:LEU:HD22	4:D:46:THR:HG23	1.83	0.60
15:O:349:THR:HG23	16:P:280:THR:HG21	1.84	0.60
2:B:725:ILE:HG23	2:B:730:PHE:HB3	1.85	0.59
13:M:315:GLN:HG2	13:M:418:ARG:HH11	1.66	0.59
1:A:285:GLU:OE1	1:A:316:GLN:NE2	2.36	0.59
1:A:855:ARG:NH2	2:B:481:PRO:O	2.36	0.59
15:O:465:GLN:OE1	15:O:466:ARG:NH1	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:PRO:O	1:A:254:ARG:NH2	2.37	0.58
1:A:463:ASN:HD21	2:B:1051:GLU:HG2	1.69	0.58
2:B:672:ILE:HD13	2:B:683:ASN:HD22	1.68	0.58
15:O:374:HIS:HB3	15:O:423:LEU:HD23	1.86	0.58
7:G:6:GLU:HG2	7:G:73:ARG:HG2	1.86	0.57
1:A:1378:ILE:HA	4:D:67:ARG:HH21	1.69	0.57
2:B:722:THR:HG23	2:B:962:THR:HA	1.86	0.57
7:G:154:ASP:HB3	7:G:187:VAL:HB	1.87	0.56
1:A:217:ASN:HD22	15:O:408:GLU:HB3	1.71	0.56
3:C:14:VAL:HB	3:C:301:ARG:HB2	1.87	0.56
1:A:581:VAL:H	11:K:85:GLN:HE22	1.51	0.56
9:I:105:ARG:NH2	9:I:106:TRP:O	2.39	0.56
13:M:414:ASP:OD2	13:M:418:ARG:NH2	2.39	0.56
1:A:1044:PRO:HB3	1:A:1280:MET:HG3	1.89	0.55
8:H:112:LEU:HD13	8:H:129:ALA:HB2	1.89	0.55
13:M:318:ALA:HA	13:M:328:LYS:HB2	1.88	0.55
2:B:591:ARG:NH2	2:B:634:ASP:OD2	2.38	0.55
1:A:1099:ARG:NH1	9:I:54:GLY:O	2.39	0.55
1:A:543:GLN:NE2	2:B:751:ILE:O	2.40	0.55
1:A:360:ARG:NH1	20:T:23:DC:OP1	2.40	0.55
1:A:590:LYS:NZ	8:H:88:PHE:O	2.39	0.55
1:A:738:GLN:NE2	1:A:742:CYS:O	2.38	0.55
2:B:923:ILE:HD11	10:J:42:ARG:HB3	1.89	0.55
2:B:869:VAL:HG22	2:B:883:MET:HG3	1.88	0.55
9:I:33:ASN:ND2	14:N:134:PRO:O	2.39	0.55
15:O:265:GLU:OE1	15:O:268:ARG:NH1	2.39	0.55
1:A:374:ASN:ND2	2:B:749:TYR:OH	2.40	0.54
15:O:231:ASP:OD1	17:Q:104:ARG:NH2	2.38	0.54
2:B:904:LYS:NZ	18:R:19:G:OP1	2.36	0.54
1:A:76:LEU:O	2:B:1033:ARG:NH2	2.40	0.54
2:B:571:PHE:O	2:B:591:ARG:NH1	2.36	0.54
5:E:2:ASP:N	14:N:103:ILE:O	2.41	0.54
4:D:91:PRO:HD2	4:D:120:VAL:HG11	1.90	0.54
1:A:397:ASN:ND2	6:F:73:ILE:O	2.39	0.54
1:A:405:ARG:NH2	1:A:441:ALA:O	2.40	0.54
1:A:568:ILE:HG23	1:A:603:VAL:HG11	1.89	0.54
2:B:686:GLN:HE22	2:B:1010:GLN:HE22	1.54	0.54
1:A:356:LEU:HD22	1:A:1348:ILE:HG23	1.90	0.54
1:A:794:GLN:HE21	1:A:799:VAL:HG13	1.73	0.54
2:B:282:GLN:NE2	13:M:146:ASP:OD2	2.39	0.54
2:B:304:THR:O	2:B:308:GLU:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:463:ARG:NH2	2:B:464:LYS:O	2.41	0.54
16:P:252:ILE:HG12	16:P:268:LYS:HG2	1.89	0.53
2:B:218:VAL:HG11	2:B:346:GLN:HE22	1.73	0.53
8:H:96:VAL:HG22	8:H:116:VAL:HG22	1.89	0.53
1:A:35:GLN:NE2	1:A:87:ASP:OD2	2.42	0.53
1:A:485:THR:OG1	1:A:487:ARG:NH1	2.42	0.53
2:B:176:LYS:NZ	2:B:420:SER:O	2.41	0.53
1:A:19:CYS:HA	1:A:1337:LYS:HA	1.91	0.53
1:A:374:ASN:OD1	1:A:685:ARG:NH2	2.41	0.53
2:B:120:THR:HG23	2:B:124:GLN:HA	1.90	0.53
13:M:262:VAL:HB	13:M:275:THR:HB	1.89	0.53
2:B:760:ALA:O	2:B:764:ARG:NH1	2.42	0.53
9:I:44:PRO:O	9:I:86:SER:OG	2.27	0.53
1:A:604:ILE:HD11	1:A:686:LEU:HD22	1.91	0.53
2:B:103:ARG:NH2	2:B:168:TYR:OH	2.40	0.52
19:S:40:DT:H2"	19:S:41:DT:H5"	1.89	0.52
10:J:8:PHE:H	10:J:48:MET:HE3	1.74	0.52
15:O:258:ARG:NH2	16:P:249:GLU:OE2	2.42	0.52
1:A:794:GLN:HG3	1:A:799:VAL:HA	1.92	0.52
13:M:357:MET:HA	13:M:360:PHE:HD2	1.75	0.52
3:C:91:LYS:HB2	3:C:213:HIS:HB2	1.91	0.52
13:M:59:GLU:HG2	13:M:101:THR:HG22	1.91	0.52
1:A:1039:GLN:HE22	2:B:1054:CYS:HA	1.74	0.52
1:A:1368:ARG:HD2	1:A:1370:PRO:HD3	1.92	0.52
2:B:586:SER:O	2:B:591:ARG:NH1	2.43	0.52
3:C:97:ASN:ND2	3:C:103:ASP:OD1	2.42	0.52
13:M:117:ALA:HB1	13:M:124:LEU:HD11	1.92	0.52
1:A:41:LEU:HD13	1:A:276:GLU:HG3	1.93	0.51
1:A:701:GLY:HA3	2:B:984:LEU:HD13	1.91	0.51
14:N:145:ARG:HD3	14:N:153:GLN:HB2	1.90	0.51
3:C:109:ARG:NH2	3:C:198:LEU:O	2.39	0.51
2:B:631:GLU:OE2	2:B:656:HIS:NE2	2.38	0.51
13:M:240:LYS:NZ	13:M:248:MET:SD	2.77	0.51
13:M:117:ALA:HB3	14:N:267:LEU:HB2	1.92	0.51
1:A:700:ILE:HG21	2:B:947:LEU:HD22	1.92	0.51
16:P:193:GLU:OE1	16:P:196:ARG:NH2	2.44	0.51
2:B:896:LYS:HG2	2:B:1012:LEU:HD12	1.93	0.51
5:E:59:THR:O	5:E:71:GLN:NE2	2.35	0.51
13:M:327:VAL:HG21	13:M:332:LEU:HD23	1.93	0.51
3:C:139:GLN:HE21	3:C:211:LEU:HD11	1.76	0.51
14:N:389:PHE:O	14:N:393:LEU:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:202:PRO:HA	16:P:205:GLN:HB3	1.91	0.51
1:A:1157:LYS:NZ	1:A:1195:ASP:OD2	2.44	0.50
3:C:236:LEU:HD12	3:C:307:ILE:HD11	1.92	0.50
4:D:10:LEU:HD11	17:Q:84:ILE:HG21	1.93	0.50
1:A:219:ASN:HB2	1:A:310:TRP:HH2	1.76	0.50
1:A:799:VAL:HG23	1:A:837:SER:HA	1.94	0.50
10:J:10:CYS:SG	10:J:11:GLY:N	2.85	0.50
1:A:6:PHE:HE1	7:G:33:LYS:HG2	1.76	0.50
1:A:63:SER:HB3	1:A:260:LEU:HB3	1.94	0.50
5:E:84:ILE:HD13	19:S:42:DA:H5"	1.93	0.50
1:A:461:LEU:HD23	1:A:473:ILE:HD11	1.93	0.50
1:A:1332:ALA:HB2	2:B:1122:ILE:HG23	1.93	0.50
2:B:195:ARG:NH2	19:S:29:DT:O5'	2.45	0.49
1:A:424:ARG:NH2	1:A:446:TYR:O	2.45	0.49
2:B:89:GLU:OE1	12:L:35:ARG:NH2	2.38	0.49
2:B:678:ASN:HD22	2:B:683:ASN:HD21	1.60	0.49
13:M:261:PRO:HD2	13:M:276:LEU:HD12	1.94	0.49
1:A:654:THR:O	1:A:662:ASN:ND2	2.46	0.49
4:D:114:GLU:HA	4:D:117:LEU:HD13	1.94	0.49
7:G:49:PHE:HB2	7:G:75:VAL:HG13	1.94	0.49
8:H:7:GLU:HG3	8:H:59:VAL:HG22	1.94	0.49
14:N:261:THR:HG22	14:N:263:GLU:H	1.77	0.49
1:A:864:LYS:NZ	1:A:1048:MET:O	2.34	0.49
2:B:36:VAL:HG12	2:B:37:LYS:HG3	1.93	0.49
5:E:58:LEU:HB2	5:E:74:VAL:HB	1.94	0.49
10:J:40:LEU:HD22	10:J:45:CYS:HB3	1.94	0.49
15:O:342:LEU:HD23	15:O:345:LEU:HD12	1.95	0.49
4:D:10:LEU:HD12	4:D:80:LYS:HE3	1.94	0.49
1:A:109:CYS:SG	1:A:110:LYS:N	2.86	0.48
14:N:276:PRO:HG3	14:N:344:VAL:HG11	1.95	0.48
9:I:61:ASN:HD22	9:I:80:MET:HA	1.78	0.48
1:A:481:LYS:HB2	1:A:487:ARG:HH21	1.78	0.48
2:B:722:THR:H	2:B:725:ILE:HD12	1.79	0.48
3:C:148:ARG:NH2	10:J:66:GLU:O	2.43	0.48
9:I:15:GLU:OE2	9:I:22:ARG:NH2	2.43	0.48
1:A:875:LEU:HD23	1:A:1303:ILE:HG21	1.95	0.48
1:A:558:PHE:HB3	1:A:594:LEU:HD13	1.96	0.48
2:B:750:ASP:HA	2:B:754:ALA:HB3	1.96	0.48
11:K:41:THR:OG1	11:K:83:ARG:NE	2.45	0.48
2:B:161:CYS:HB3	2:B:164:ASP:HB2	1.96	0.48
2:B:396:ARG:HG2	2:B:398:ALA:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:826:VAL:HG12	2:B:857:THR:HG22	1.96	0.47
13:M:258:LYS:HZ3	13:M:276:LEU:HD21	1.80	0.47
14:N:344:VAL:HG23	14:N:392:LEU:HD21	1.96	0.47
1:A:69:CYS:SG	1:A:70:GLU:N	2.87	0.47
1:A:623:GLN:O	1:A:634:ASN:ND2	2.46	0.47
1:A:665:TYR:OH	1:A:912:MET:O	2.32	0.47
2:B:183:GLN:NE2	2:B:363:GLU:OE1	2.43	0.47
8:H:28:LEU:HD21	8:H:50:VAL:HG11	1.96	0.47
2:B:539:VAL:HG12	2:B:583:VAL:HB	1.95	0.47
15:O:149:VAL:HG12	15:O:190:VAL:HG21	1.96	0.47
20:T:10:DG:H2'	20:T:11:DG:C8	2.50	0.47
2:B:887:GLN:OE1	2:B:889:ARG:NH2	2.44	0.47
1:A:423:GLN:OE1	1:A:430:ARG:NH2	2.47	0.47
10:J:3:ILE:HD12	10:J:4:PRO:HD2	1.97	0.47
3:C:188:GLY:O	3:C:191:ARG:NH1	2.48	0.47
3:C:236:LEU:HD13	3:C:305:HIS:CE1	2.49	0.47
2:B:457:SER:OG	2:B:494:LYS:NZ	2.48	0.46
3:C:84:VAL:HB	3:C:227:PRO:HG3	1.97	0.46
15:O:520:ILE:O	15:O:524:GLU:N	2.43	0.46
1:A:203:HIS:HB2	15:O:379:GLN:HE21	1.79	0.46
1:A:811:ASP:OD1	1:A:811:ASP:N	2.47	0.46
2:B:341:ARG:NH2	2:B:582:CYS:SG	2.88	0.46
4:D:20:LEU:HB2	4:D:50:LEU:HD13	1.97	0.46
2:B:257:THR:HG21	2:B:529:GLU:HG3	1.97	0.46
1:A:583:LEU:HD12	1:A:584:PRO:HD2	1.97	0.46
15:O:409:ILE:O	15:O:420:THR:OG1	2.31	0.46
1:A:1363:LEU:HD11	6:F:107:ARG:HH21	1.80	0.46
2:B:738:ASN:O	10:J:47:ARG:NH1	2.49	0.46
1:A:1261:GLU:OE2	5:E:195:ARG:NE	2.48	0.46
6:F:107:ARG:HD2	6:F:115:TYR:HB2	1.98	0.46
15:O:138:THR:HG21	15:O:198:LYS:HD3	1.98	0.46
1:A:93:PHE:HB2	1:A:172:LEU:HD23	1.97	0.46
5:E:51:GLY:HA3	5:E:55:ARG:HD3	1.96	0.46
6:F:73:ILE:HD12	6:F:79:VAL:HG22	1.97	0.46
4:D:92:VAL:HG13	4:D:93:THR:HG23	1.98	0.46
13:M:63:ASP:OD1	13:M:66:ASN:ND2	2.49	0.46
1:A:659:SER:OG	1:A:660:LYS:N	2.48	0.45
1:A:577:GLU:O	11:K:83:ARG:NH2	2.49	0.45
1:A:1360:PHE:O	6:F:64:ARG:NH1	2.49	0.45
15:O:258:ARG:HH21	16:P:273:VAL:HG11	1.82	0.45
2:B:678:ASN:HD21	2:B:901:HIS:HD2	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:102:GLU:OE2	7:G:151:ARG:NH2	2.40	0.45
15:O:443:ILE:HG23	15:O:513:GLU:HG3	1.99	0.45
2:B:900:ARG:NH2	2:B:945:GLU:OE2	2.49	0.45
3:C:13:ARG:NE	3:C:238:ASP:OD2	2.50	0.45
4:D:86:LEU:HD13	4:D:116:LEU:HD11	1.98	0.45
15:O:103:GLY:HA2	15:O:106:ILE:HD12	1.99	0.45
1:A:942:LYS:HG2	1:A:977:SER:HB2	1.99	0.45
13:M:312:ARG:HH22	13:M:412:HIS:CE1	2.35	0.45
1:A:1117:ILE:HG23	1:A:1130:VAL:HG22	1.99	0.45
15:O:416:ALA:HB3	15:O:419:ARG:HG2	1.98	0.45
2:B:990:THR:HA	2:B:997:PRO:HA	1.98	0.44
1:A:845:THR:HG23	2:B:645:LEU:HD11	1.98	0.44
4:D:16:VAL:HG21	7:G:2:PHE:HD2	1.83	0.44
7:G:190:ILE:HD11	7:G:196:GLY:HA2	1.98	0.44
1:A:159:CYS:SG	1:A:160:GLY:N	2.90	0.44
1:A:555:LYS:HD3	8:H:25:VAL:HG11	1.99	0.44
1:A:874:ARG:HG2	1:A:1321:PHE:HZ	1.82	0.44
4:D:39:GLN:O	4:D:43:ASN:ND2	2.51	0.44
13:M:95:LYS:HG3	13:M:96:LEU:HG	1.99	0.44
17:Q:83:ASP:OD1	17:Q:83:ASP:N	2.46	0.44
2:B:446:ILE:HG13	2:B:671:LEU:HD11	1.98	0.44
13:M:359:LYS:HG2	13:M:367:VAL:HG12	1.99	0.44
20:T:17:DG:H2'	20:T:18:DA:C8	2.52	0.44
13:M:273:LEU:HD13	13:M:275:THR:H	1.83	0.44
1:A:325:LEU:HB2	1:A:328:ILE:HD11	1.99	0.44
1:A:646:MET:O	8:H:117:SER:OG	2.27	0.44
17:Q:79:GLU:O	17:Q:80:GLU:HG3	2.18	0.44
7:G:101:LEU:HB2	7:G:107:ILE:HD11	2.00	0.44
1:A:465:GLN:HG2	20:T:22:DT:H1'	2.00	0.43
13:M:20:SER:OG	13:M:224:TYR:O	2.34	0.43
2:B:192:GLU:OE1	2:B:354:ARG:NH2	2.51	0.43
2:B:923:ILE:HG13	10:J:42:ARG:HD2	2.00	0.43
4:D:12:SER:HB2	4:D:88:ASN:HD21	1.83	0.43
3:C:193:VAL:HG11	3:C:314:GLY:HA3	2.01	0.43
13:M:192:SER:OG	13:M:193:TYR:N	2.51	0.43
3:C:134:GLU:O	3:C:181:GLN:NE2	2.47	0.43
13:M:7:ASP:OD1	13:M:7:ASP:N	2.52	0.43
15:O:381:GLU:OE2	15:O:392:LYS:NZ	2.41	0.43
1:A:366:ARG:HD2	2:B:1045:LEU:HD11	2.00	0.43
1:A:408:VAL:HG13	1:A:432:LEU:HD21	2.00	0.43
2:B:898:SER:HB2	2:B:1012:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:147:THR:HG22	15:O:150:ARG:HH22	1.83	0.43
1:A:463:ASN:HB3	1:A:506:ASN:HB2	1.99	0.43
2:B:496:LEU:HD22	2:B:500:THR:HG21	2.01	0.43
2:B:644:ALA:HB1	2:B:649:THR:HB	2.01	0.43
15:O:100:SER:OG	15:O:101:ASP:N	2.52	0.43
4:D:93:THR:OG1	4:D:96:GLU:OE1	2.34	0.43
13:M:53:GLN:HG3	13:M:200:HIS:CE1	2.54	0.43
1:A:1115:GLU:HB3	1:A:1133:SER:HB2	2.01	0.42
2:B:757:LEU:HD13	2:B:762:LEU:HD11	2.02	0.42
1:A:471:LEU:HB3	1:A:495:PRO:HB3	2.01	0.42
8:H:64:LEU:HB2	8:H:142:TYR:CE2	2.55	0.42
1:A:176:HIS:CD2	1:A:178:LYS:HB2	2.55	0.42
3:C:235:LEU:HB2	3:C:301:ARG:HH11	1.82	0.42
15:O:460:LEU:HB3	15:O:499:LEU:HD21	2.01	0.42
1:A:1039:GLN:NE2	2:B:1053:ASP:O	2.52	0.42
2:B:549:ILE:HD13	2:B:555:LEU:HD22	2.01	0.42
1:A:739:GLN:HG3	1:A:747:THR:HG23	2.02	0.42
1:A:705:PRO:HB3	1:A:709:LEU:HD23	2.01	0.42
2:B:539:VAL:HG23	2:B:546:LEU:HB2	2.02	0.42
13:M:368:ARG:O	13:M:372:ALA:N	2.46	0.42
4:D:69:PHE:HE1	4:D:120:VAL:HA	1.85	0.41
1:A:102:ILE:HG23	1:A:166:VAL:HG12	2.02	0.41
1:A:322:ASN:OD1	1:A:343:GLN:NE2	2.53	0.41
3:C:288:PHE:HA	3:C:294:LYS:HG2	2.01	0.41
19:S:32:DA:H2"	19:S:33:DG:H5"	2.01	0.41
1:A:697:SER:O	1:A:776:SER:OG	2.27	0.41
2:B:219:LYS:HG3	2:B:220:GLN:HG2	2.02	0.41
9:I:10:ASN:ND2	9:I:27:THR:OG1	2.53	0.41
1:A:499:ASP:OD1	1:A:499:ASP:N	2.53	0.41
8:H:64:LEU:HD11	8:H:85:ALA:HB2	2.02	0.41
15:O:143:GLU:HA	15:O:146:ASN:HD22	1.85	0.41
16:P:217:TRP:NE1	16:P:230:LEU:O	2.38	0.41
2:B:545:ILE:HG22	2:B:547:GLY:H	1.86	0.41
7:G:5:VAL:HG21	7:G:42:VAL:HB	2.02	0.41
15:O:67:VAL:HG22	15:O:177:ALA:HB3	2.03	0.41
9:I:3:LEU:HD13	14:N:143:GLU:HG3	2.02	0.41
1:A:5:GLN:HB2	7:G:183:PRO:HG3	2.03	0.41
8:H:125:LEU:HD23	8:H:135:PHE:HE2	1.86	0.41
1:A:816:ARG:NH1	2:B:642:ASN:OD1	2.40	0.41
2:B:241:LYS:NZ	2:B:246:GLU:O	2.54	0.41
6:F:107:ARG:NE	6:F:117:ASP:OD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:37:DC:H2"	19:S:38:DA:C8	2.56	0.41
20:T:23:DC:H2'	20:T:24:DT:H71	2.02	0.41
1:A:343:GLN:HA	1:A:346:LYS:HG2	2.03	0.41
4:D:36:SER:OG	4:D:37:SER:N	2.54	0.40
4:D:73:LEU:HA	4:D:76:HIS:HD2	1.86	0.40
1:A:143:LYS:HB2	1:A:239:LEU:HG	2.03	0.40
2:B:1073:ASP:OD1	2:B:1073:ASP:N	2.54	0.40
1:A:116:MET:SD	1:A:163:ASN:ND2	2.95	0.40
2:B:819:GLU:HG3	12:L:49:THR:HG21	2.04	0.40
3:C:96:ASN:HA	12:L:48:ARG:HD3	2.03	0.40
5:E:197:SER:OG	5:E:198:GLU:N	2.54	0.40
7:G:115:GLN:HE22	7:G:200:TRP:HZ3	1.68	0.40
13:M:315:GLN:HE22	13:M:320:LEU:HD22	1.85	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	1377/1390 (99%)	1321 (96%)	56 (4%)	0	100	100
2	B	1091/1133 (96%)	1034 (95%)	55 (5%)	2 (0%)	47	78
3	C	341/346 (99%)	331 (97%)	10 (3%)	0	100	100
4	D	122/148 (82%)	118 (97%)	4 (3%)	0	100	100
5	E	207/210 (99%)	202 (98%)	5 (2%)	0	100	100
6	F	76/127 (60%)	75 (99%)	1 (1%)	0	100	100
7	G	185/204 (91%)	175 (95%)	9 (5%)	1 (0%)	29	61
8	H	146/150 (97%)	144 (99%)	2 (1%)	0	100	100
9	I	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
10	J	64/67 (96%)	62 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	105/133 (79%)	103 (98%)	2 (2%)	0	100	100
12	L	44/58 (76%)	43 (98%)	1 (2%)	0	100	100
13	M	367/708 (52%)	338 (92%)	29 (8%)	0	100	100
14	N	180/398 (45%)	172 (96%)	8 (4%)	0	100	100
15	O	508/534 (95%)	487 (96%)	21 (4%)	0	100	100
16	P	144/316 (46%)	140 (97%)	4 (3%)	0	100	100
17	Q	102/223 (46%)	97 (95%)	5 (5%)	0	100	100
All	All	5164/6253 (83%)	4939 (96%)	222 (4%)	3 (0%)	54	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	40	VAL
7	G	137	ALA
2	B	39	LEU

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	1204/1212 (99%)	1200 (100%)	4 (0%)	92	97
2	B	959/988 (97%)	956 (100%)	3 (0%)	92	97
3	C	299/302 (99%)	298 (100%)	1 (0%)	92	97
4	D	116/136 (85%)	116 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
6	F	68/111 (61%)	68 (100%)	0	100	100
7	G	168/181 (93%)	168 (100%)	0	100	100
8	H	129/131 (98%)	128 (99%)	1 (1%)	81	91
9	I	93/94 (99%)	92 (99%)	1 (1%)	73	86
10	J	55/56 (98%)	55 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	96/119 (81%)	96 (100%)	0	100	100
12	L	43/55 (78%)	43 (100%)	0	100	100
13	M	337/622 (54%)	328 (97%)	9 (3%)	44	70
14	N	167/347 (48%)	165 (99%)	2 (1%)	71	85
15	O	458/476 (96%)	458 (100%)	0	100	100
16	P	130/280 (46%)	129 (99%)	1 (1%)	81	91
17	Q	96/195 (49%)	96 (100%)	0	100	100
All	All	4609/5497 (84%)	4587 (100%)	22 (0%)	89	94

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	662	ASN
1	A	927	ASN
1	A	1180	ASN
1	A	1368	ARG
2	B	463	ARG
2	B	758	ASN
2	B	890	ARG
3	C	120	ARG
8	H	76	ASN
9	I	40	ASN
13	M	53	GLN
13	M	258	LYS
13	M	260	LYS
13	M	285	LEU
13	M	288	ASN
13	M	290	LYS
13	M	319	MET
13	M	332	LEU
13	M	411	LYS
14	N	119	LYS
14	N	369	ARG
16	P	181	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS

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Mol	Chain	Res	Type
1	A	163	ASN
1	A	176	HIS
1	A	217	ASN
1	A	316	GLN
1	A	374	ASN
1	A	476	HIS
1	A	616	ASN
1	A	662	ASN
1	A	794	GLN
1	A	885	GLN
1	A	927	ASN
1	A	1190	GLN
2	B	320	HIS
2	B	346	GLN
2	B	501	HIS
2	B	683	ASN
2	B	758	ASN
2	B	901	HIS
2	B	1010	GLN
2	B	1093	HIS
2	B	1100	HIS
3	C	305	HIS
4	D	76	HIS
4	D	88	ASN
7	G	115	GLN
8	H	76	ASN
9	I	10	ASN
11	K	74	HIS
11	K	81	ASN
11	K	85	GLN
12	L	23	HIS
13	M	288	ASN
14	N	111	GLN
15	O	113	ASN
15	O	146	ASN
15	O	377	GLN
15	O	445	ASN
16	P	297	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	R	6/19 (31%)	2 (33%)	1 (16%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
18	R	15	C
18	R	18	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
18	R	14	A

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 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	SF4	P	401	-	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	SF4	P	401	-	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

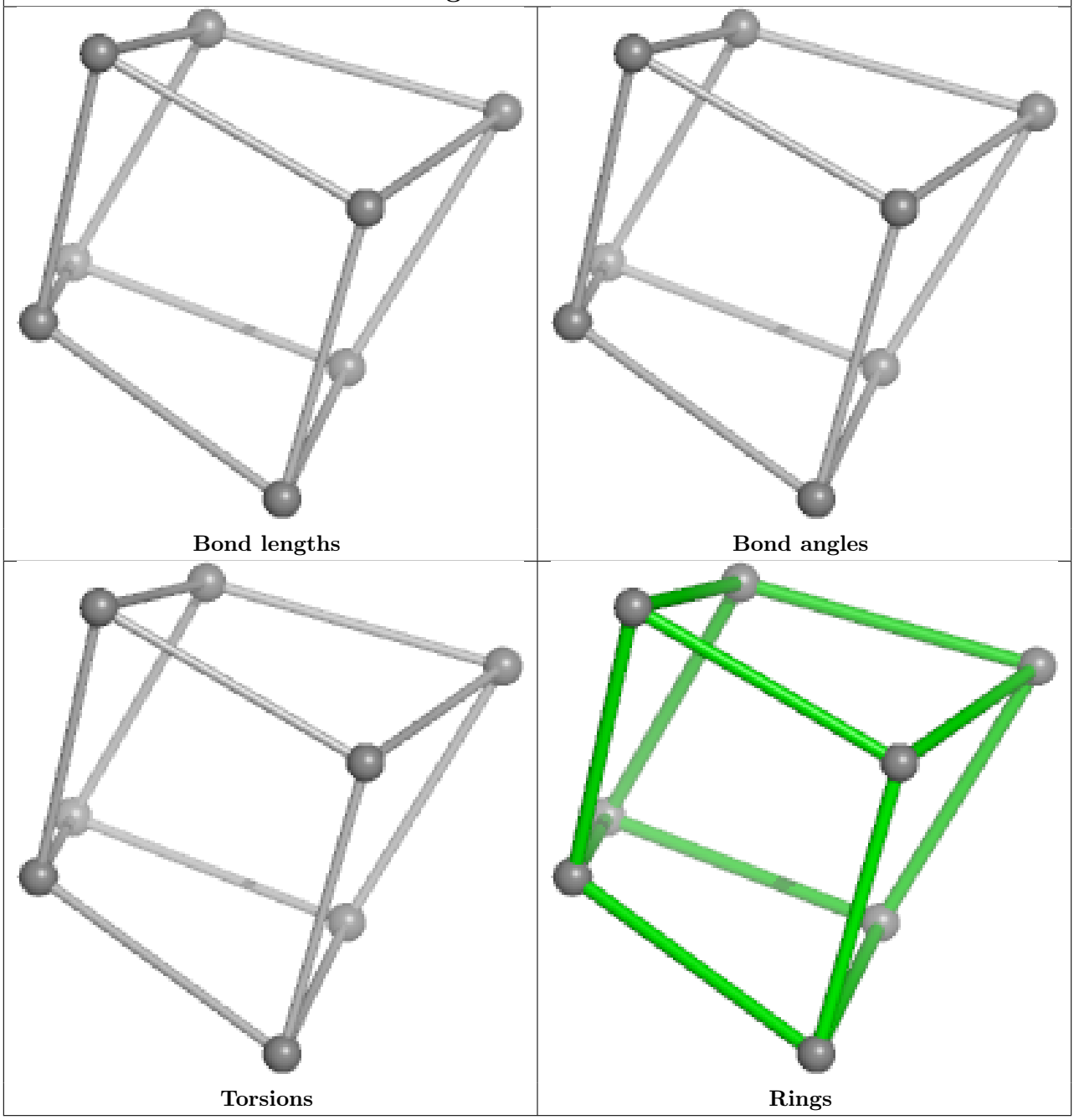
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SF4 P 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	255:GLU	C	256:GLU	N	3.24

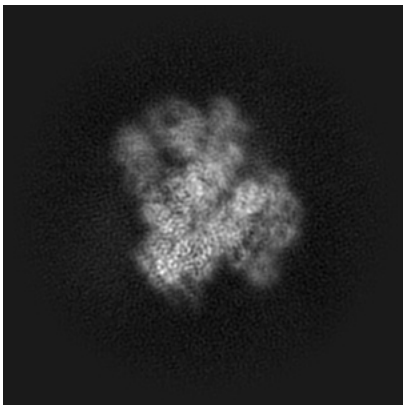
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11742. These allow visual inspection of the internal detail of the map and identification of artifacts.

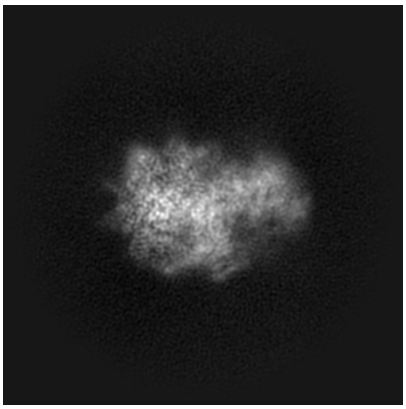
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

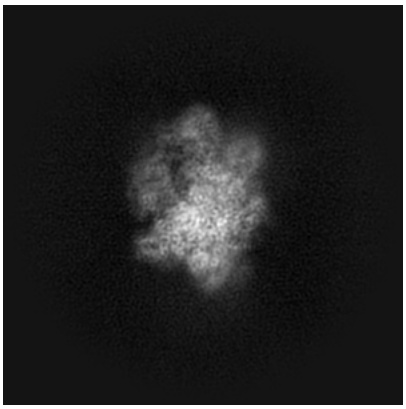
6.1.1 Primary map



X

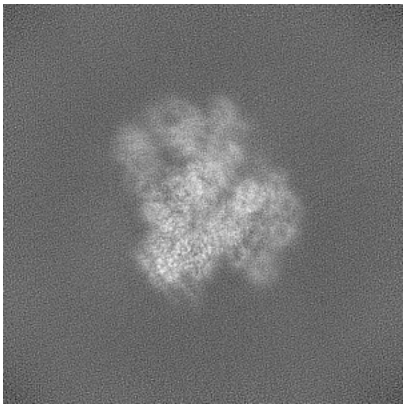


Y

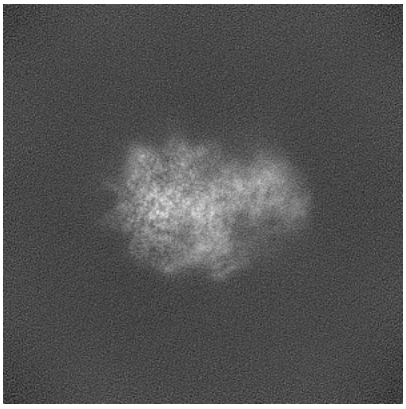


Z

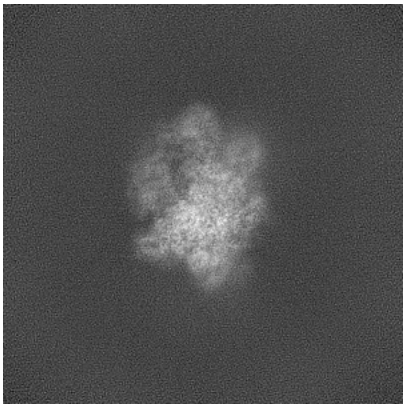
6.1.2 Raw map



X



Y

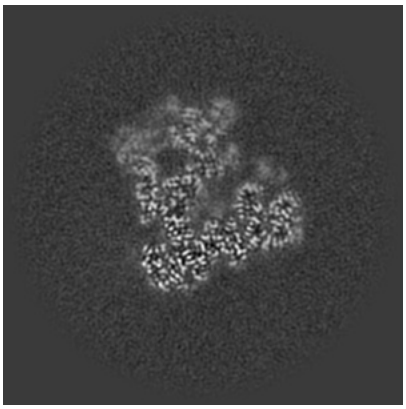


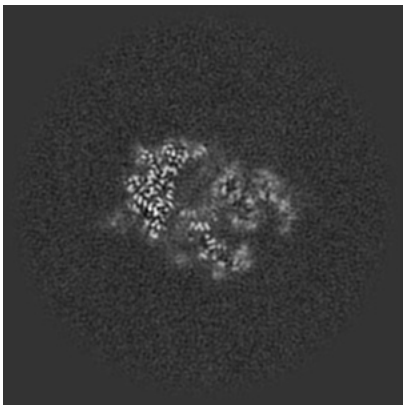
Z

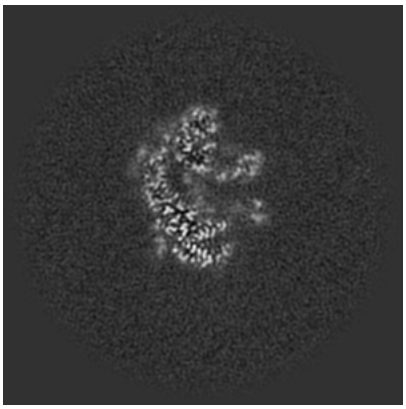
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

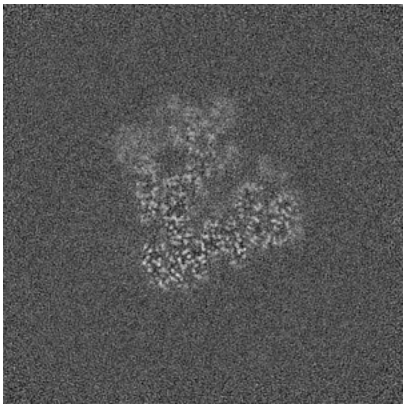
6.2.1 Primary map

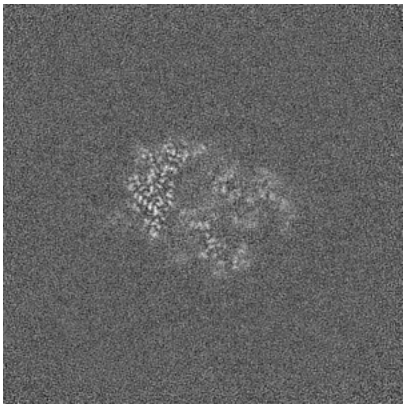

X Index: 168

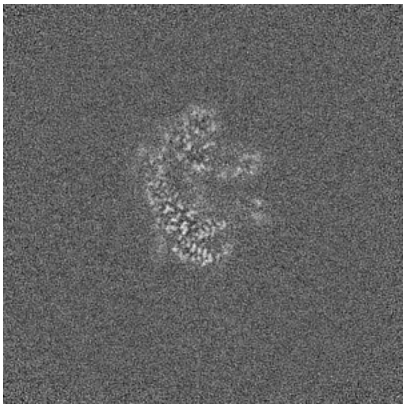

Y Index: 168


Z Index: 168

6.2.2 Raw map


X Index: 168

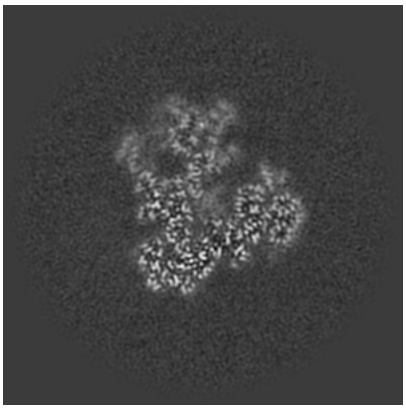

Y Index: 168

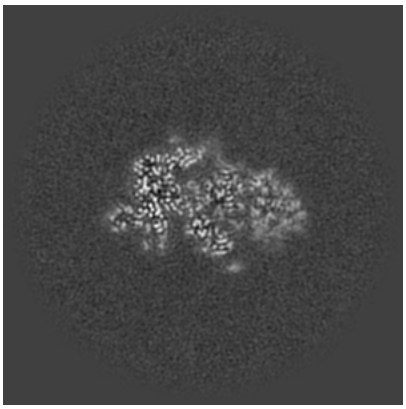

Z Index: 168

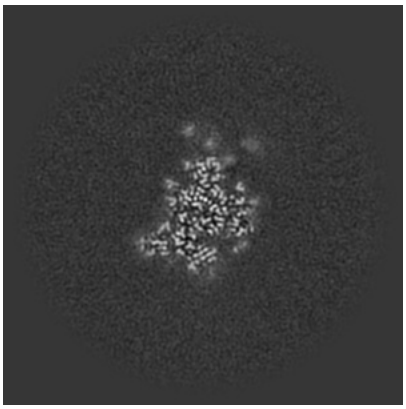
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

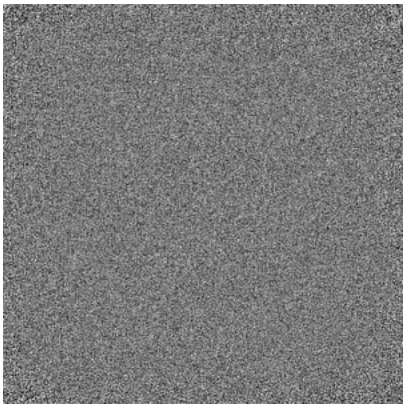
6.3.1 Primary map

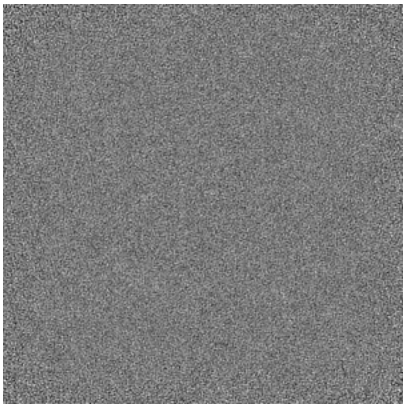

X Index: 164

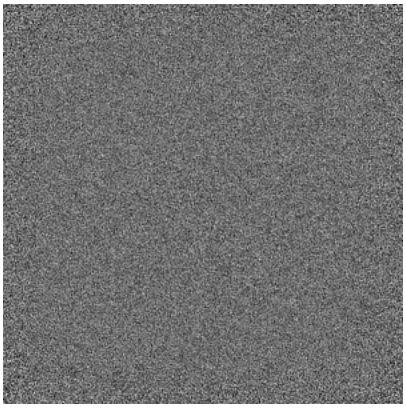

Y Index: 155


Z Index: 128

6.3.2 Raw map


X Index: 0

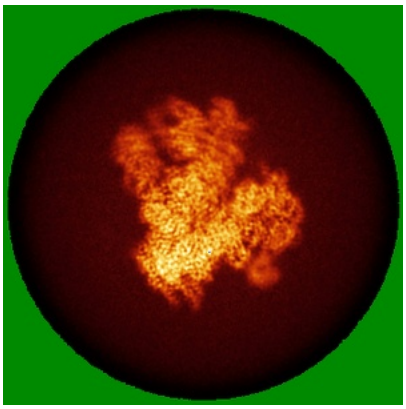

Y Index: 0

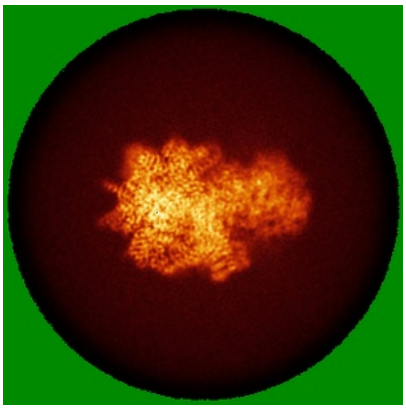

Z Index: 0

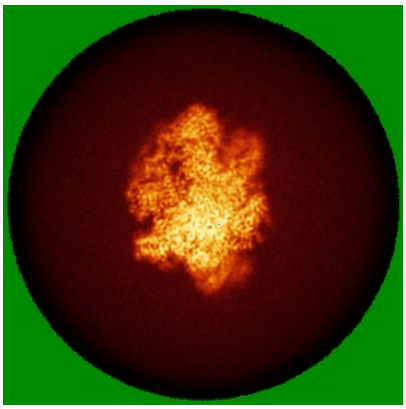
The images above show the largest variance slices of the map in three orthogonal directions.

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

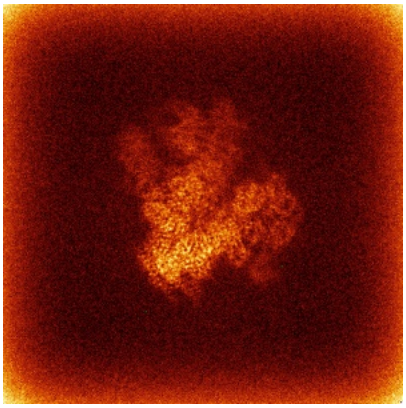
6.4.1 Primary map

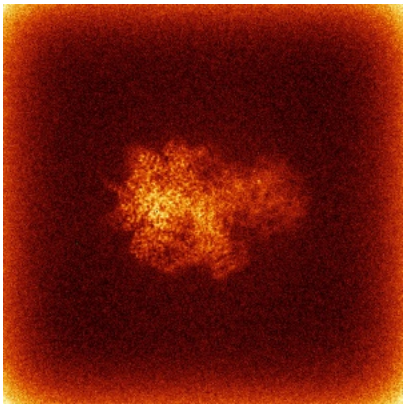

X

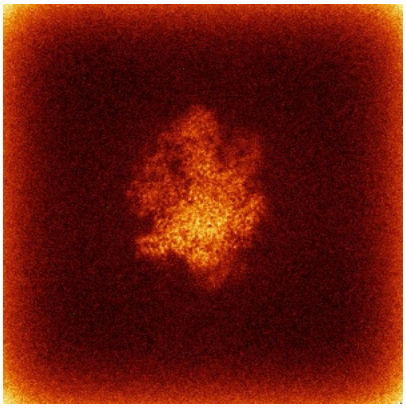

Y


Z

6.4.2 Raw map


X

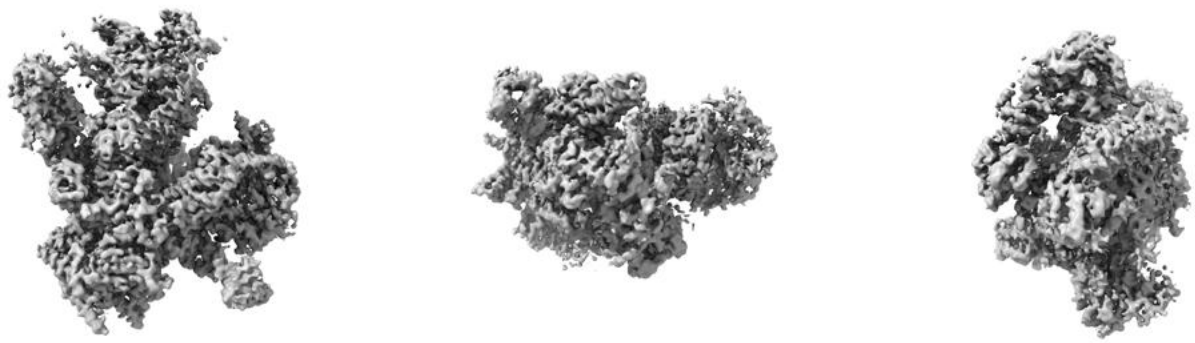

Y


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)

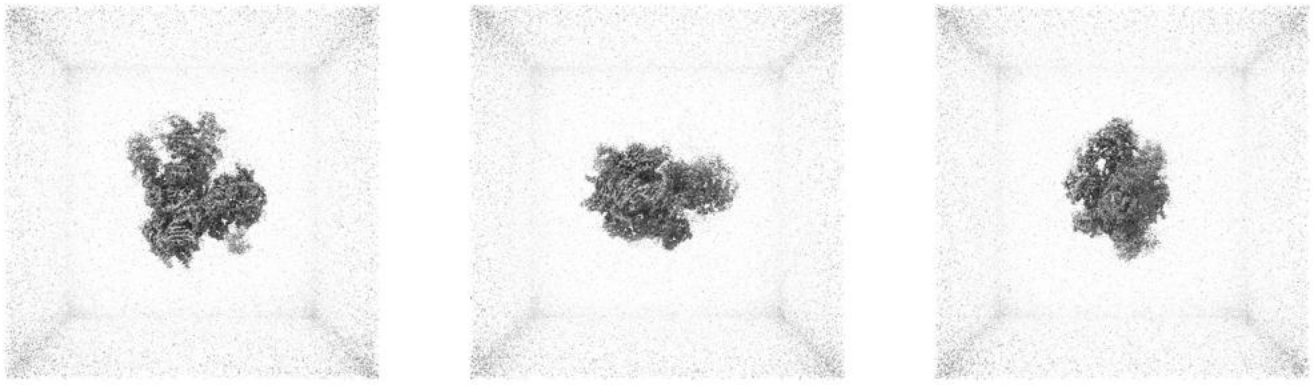
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

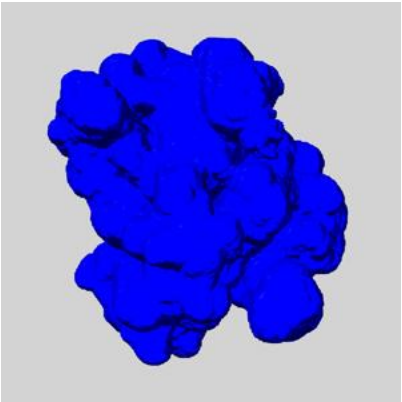
6.6 Mask visualisation (i)

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

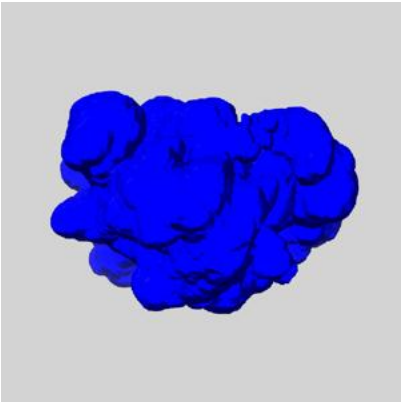
A mask typically either:

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

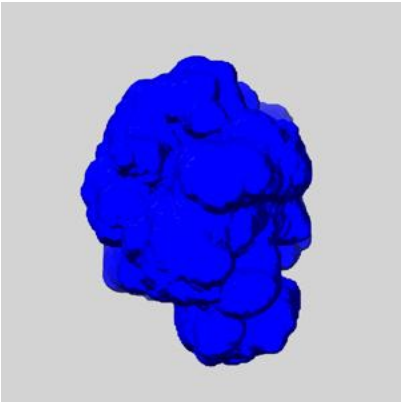
6.6.1 emd_11742_msk_1.map (i)



X



Y

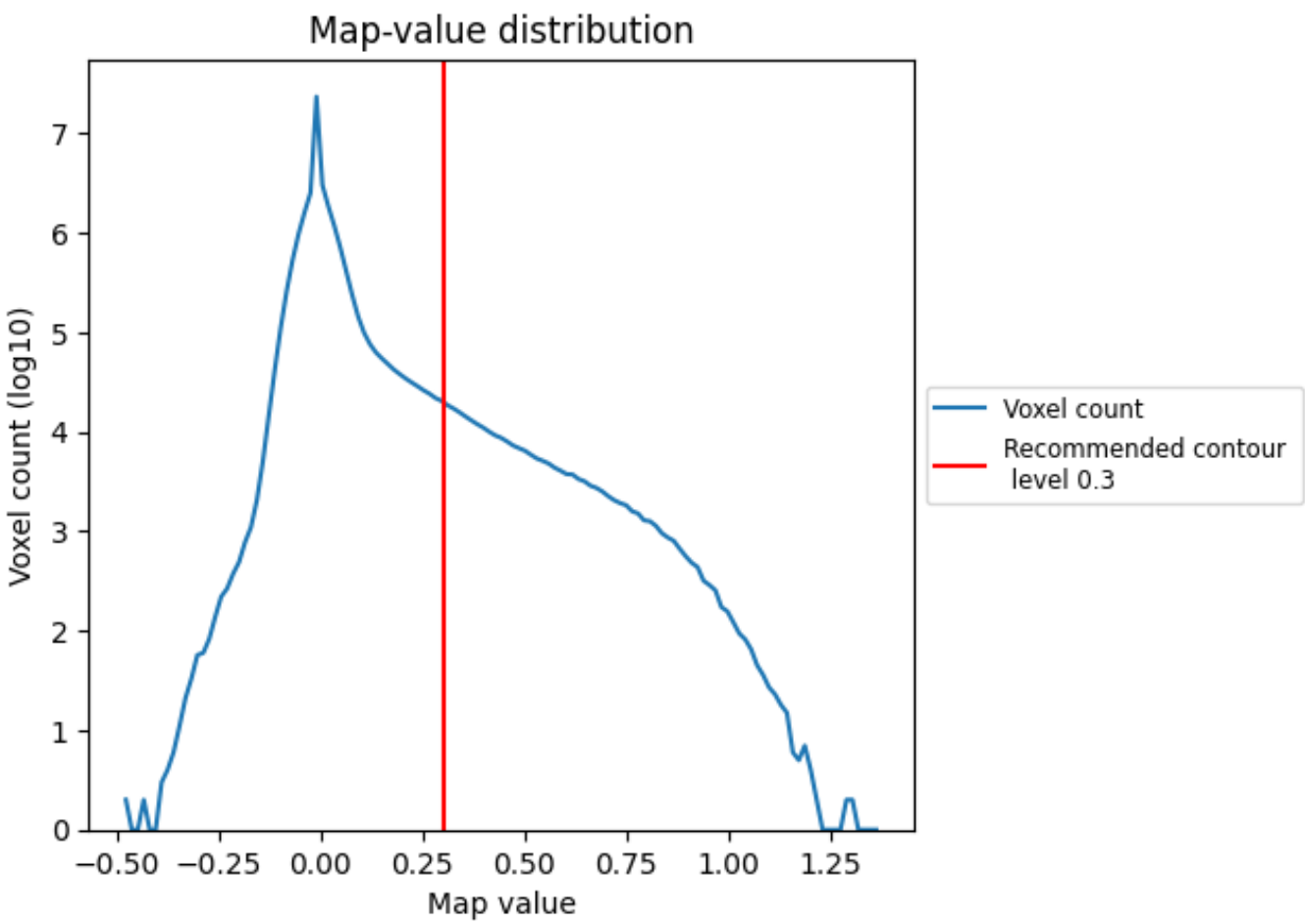


Z

7 Map analysis (i)

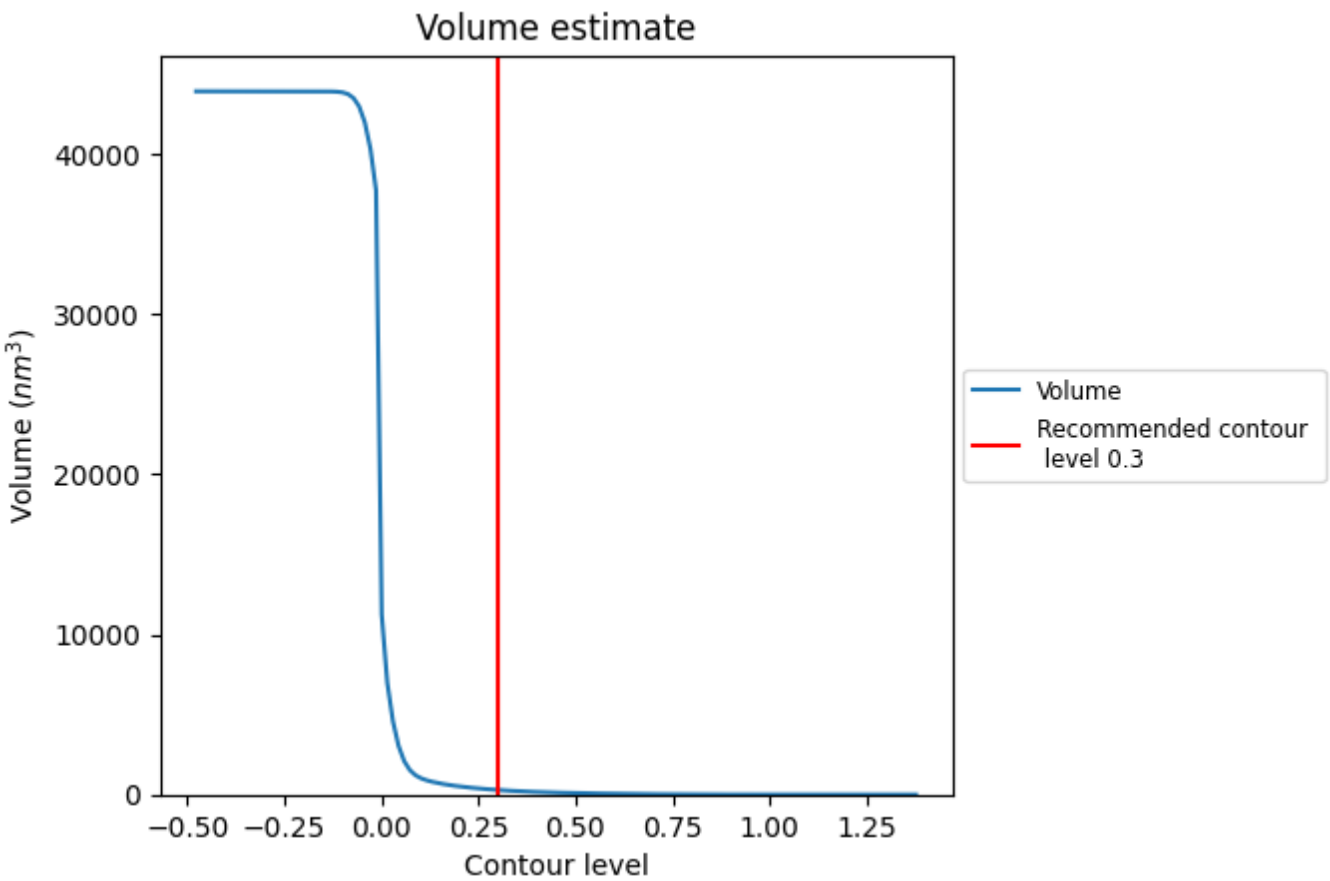
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

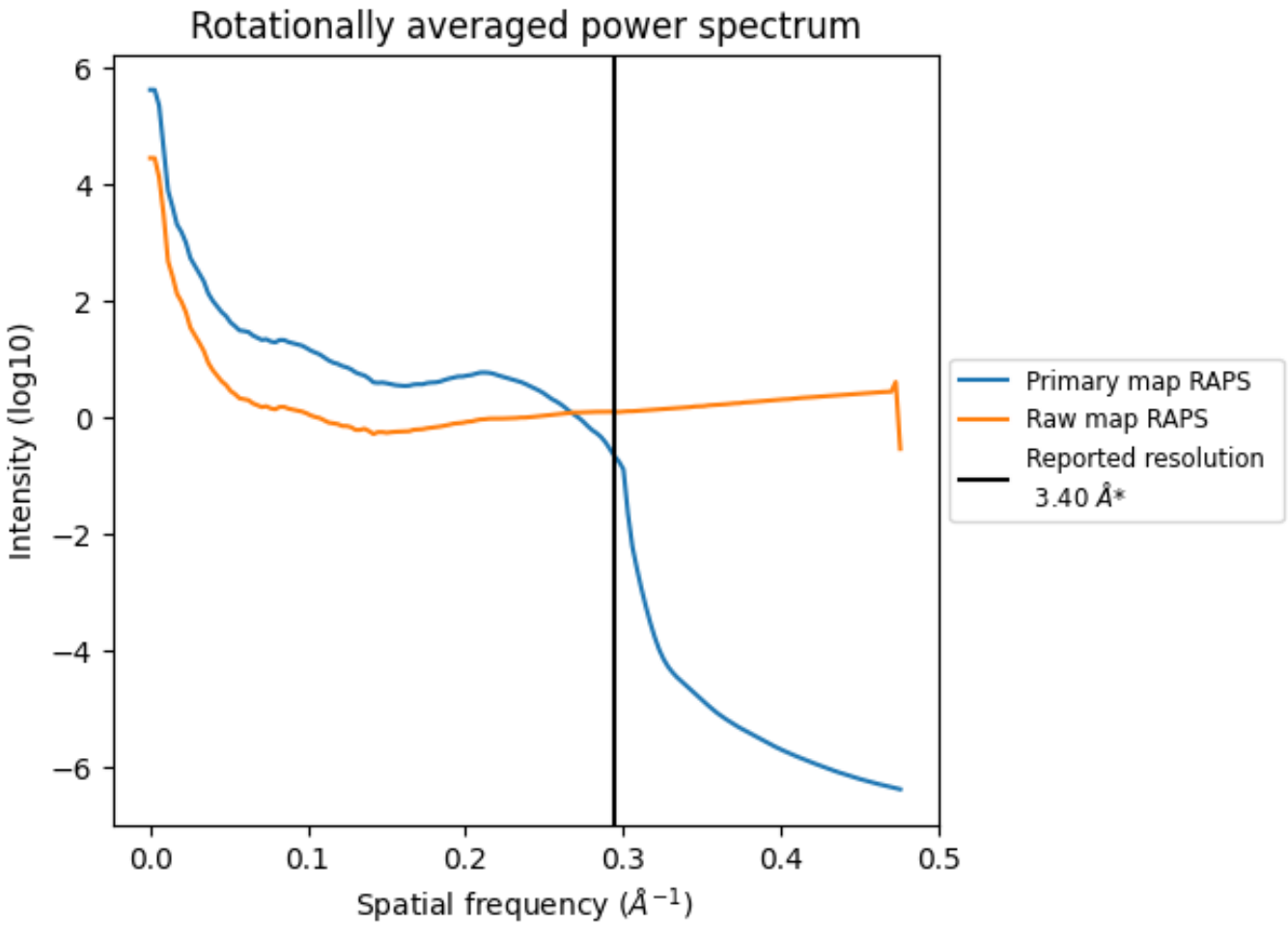
7.2 Volume estimate (i)



The volume at the recommended contour level is 286 nm^3; this corresponds to an approximate mass of 258 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)

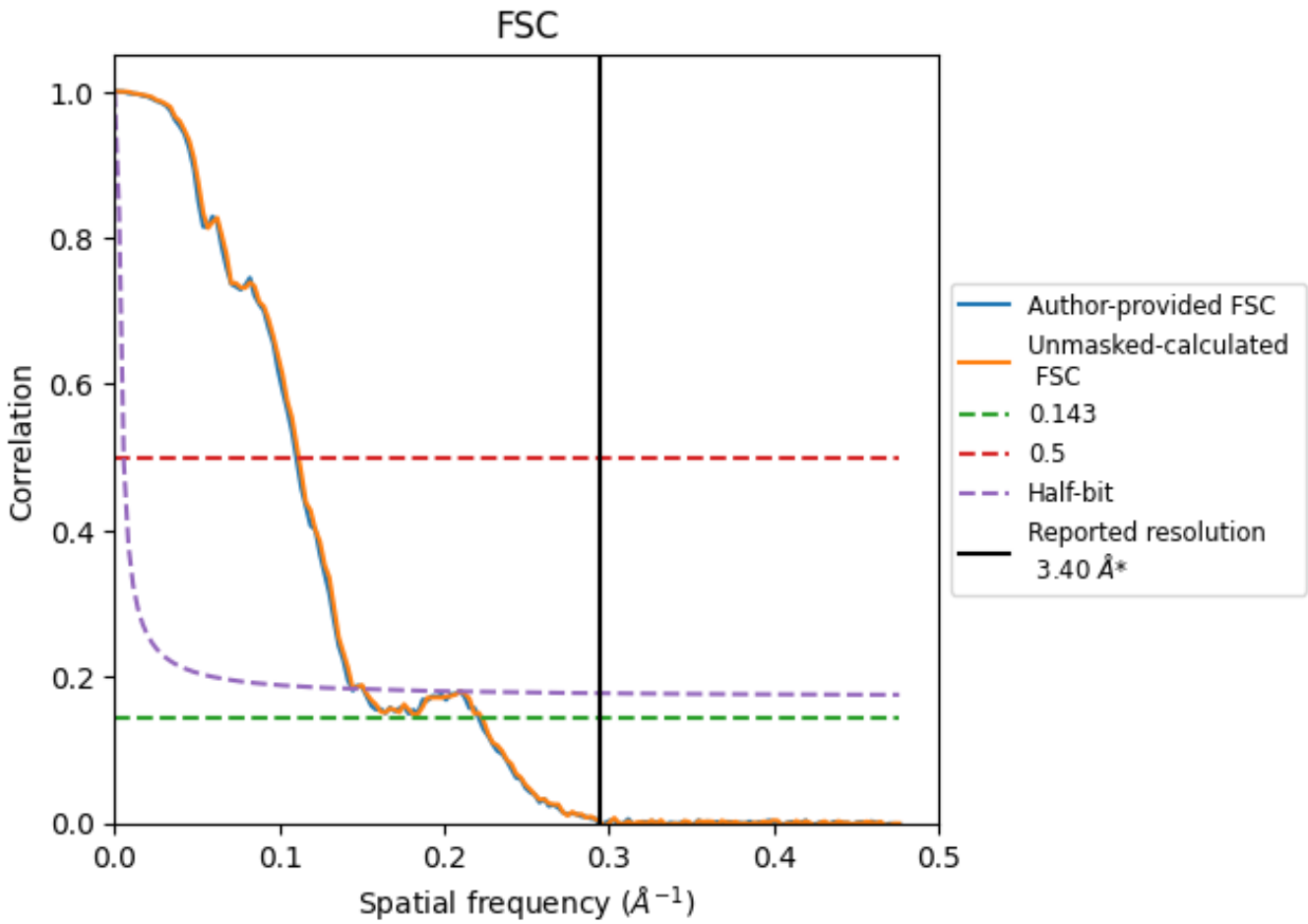


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	4.52	9.07	6.93
Unmasked-calculated*	4.48	8.94	6.60

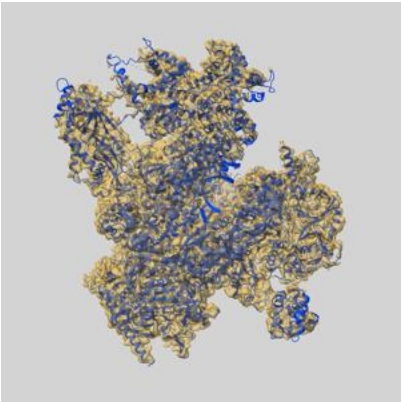
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.52 differs from the reported value 3.4 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.48 differs from the reported value 3.4 by more than 10 %

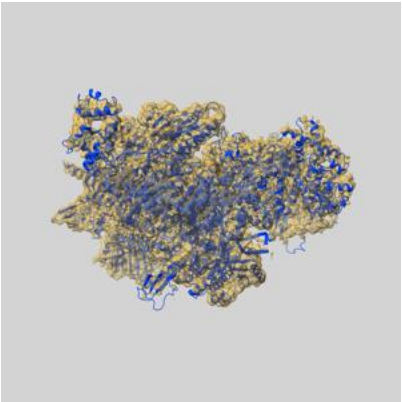
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11742 and PDB model 7AEA. Per-residue inclusion information can be found in section 3 on page 8.

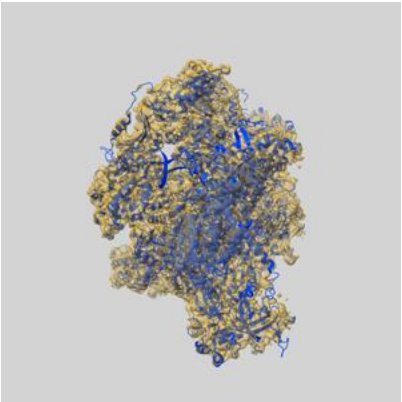
9.1 Map-model overlay (i)



X



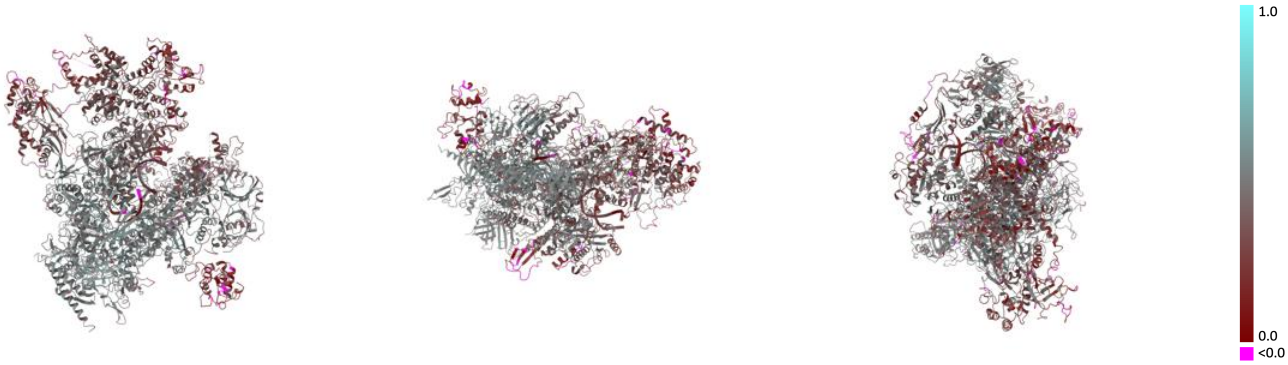
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

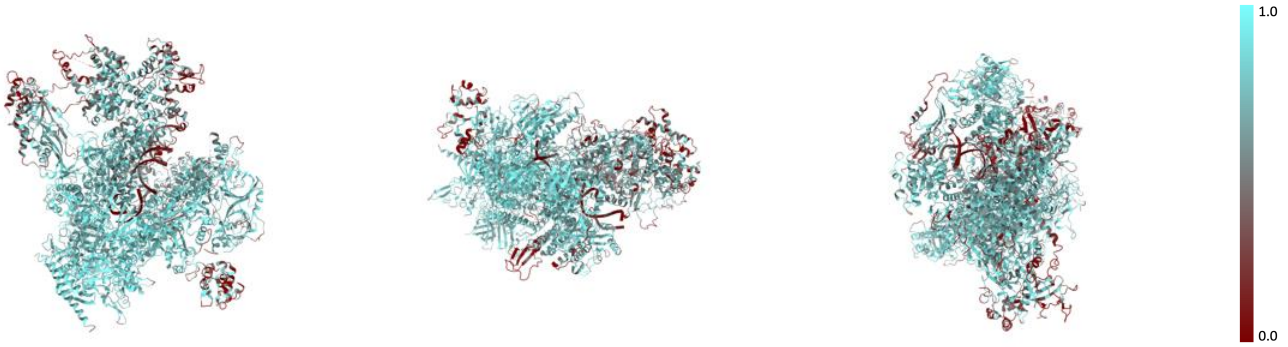
9.2 Q-score mapped to coordinate model (i)



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.

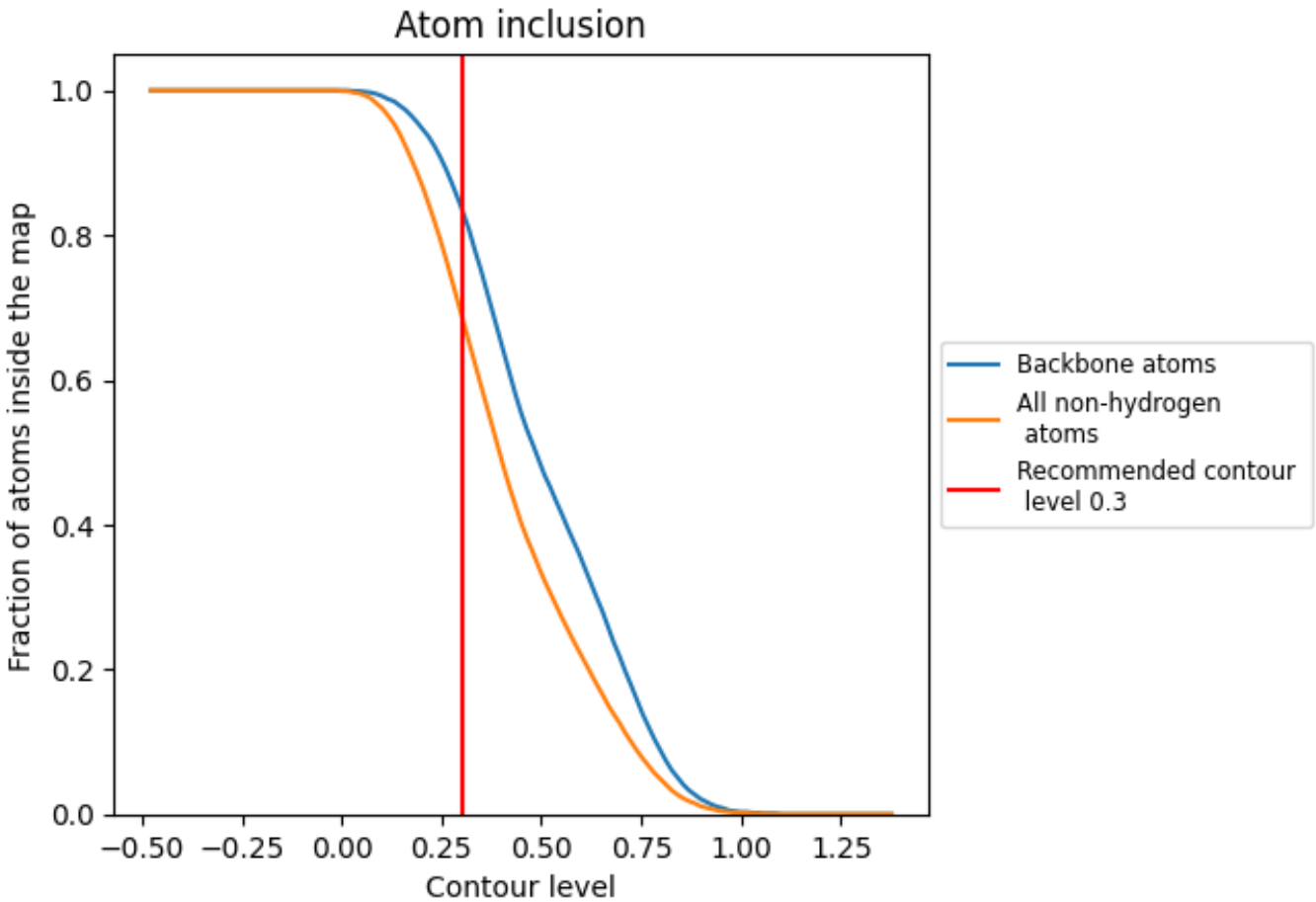
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6910	0.4090
A	0.7540	0.4470
B	0.8110	0.4820
C	0.8400	0.4920
D	0.4920	0.2930
E	0.7740	0.4130
F	0.8290	0.4890
G	0.6030	0.3400
H	0.7810	0.4710
I	0.3970	0.2720
J	0.8520	0.4970
K	0.8100	0.4830
L	0.8230	0.4580
M	0.5840	0.3220
N	0.5670	0.3620
O	0.5550	0.3060
P	0.4070	0.2580
Q	0.4240	0.2850
R	0.0070	0.1080
S	0.2530	0.2970
T	0.1150	0.2430