Full wwPDB EM Validation Report

Sep 10, 2022 – 07:31 am BST

PDB ID	:	7Z1L
EMDB ID	:	EMD-14447
Title	:	Structure of yeast RNA Polymerase III Pre-Termination Complex (PTC)
Authors	:	Girbig, M.; Mueller, C.W.
Deposited on	:	2022-02-24
Resolution	:	2.80 Å(reported)
Based on initial model	:	6TUT

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 (i)) were used in the production of this report:

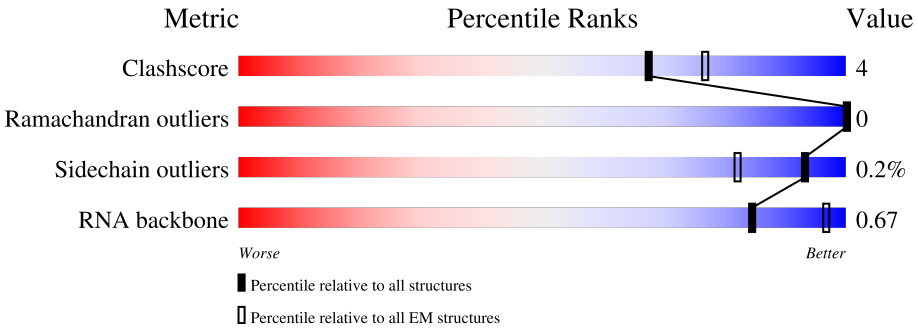
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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	A	1460	87% 11%
2	B	1149	84% 11%
3	C	335	90% 10%
4	D	161	34% 75% 16% 10%
5	E	215	9% 93% 7%
6	F	155	48% 5% 46%
7	G	212	19% 83% 11% 6%

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Mol	Chain	Length	Quality of chain
8	H	146	82% 11% 8%
9	I	110	50% 85% 15%
10	J	70	89% 10%
11	K	142	60% 12% 28%
12	L	70	6% 57% 7% 36%
13	M	282	12% 64% 5% 30%
14	N	422	6% 31% 5% 64%
15	O	654	7% 78% 9% 13%
16	P	317	9% 38% 6% 56%
17	Q	251	13% 45% 51%
18	R	24	29% 8% 63%
19	S	44	52% 5% 43%
20	T	44	59% 7% 34%

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 42330 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	1436	11228	7080	1981	2106	61	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	1101	8693	5503	1499	1631	60	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	334	2647	1676	453	510	8	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	145	1185	755	200	224	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	215	1759	1116	310	321	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	83	671	429	114	125	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	199	Total	C	N	O	S	0	0
			1594	1038	258	291	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	135	Total	C	N	O	S	0	0
			1084	683	183	214	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	110	Total	C	N	O	S	0	0
			873	546	145	171	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	102	Total	C	N	O	S	0	0
			801	501	131	164	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	196	Total	C	N	O	S	0	0
			1594	1012	272	309	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	153	Total	C	N	O	S	0	0
			1196	754	220	219	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	570	Total	C	N	O	S	0	0
			4577	2908	787	863	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	140	Total	C	N	O	S	0	0
			1159	756	179	220	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	123	Total	C	N	O	S	0	0
			981	633	163	182	3		

- Molecule 18 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	9	Total	C	N	O	P	0	0
			195	87	39	60	9		

- Molecule 19 is a DNA chain called NT-DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	25	Total	C	N	O	P	0	0
			507	246	78	158	25		

- Molecule 20 is a DNA chain called T-DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	29	Total	C	N	O	P	0	0
			597	284	109	175	29		

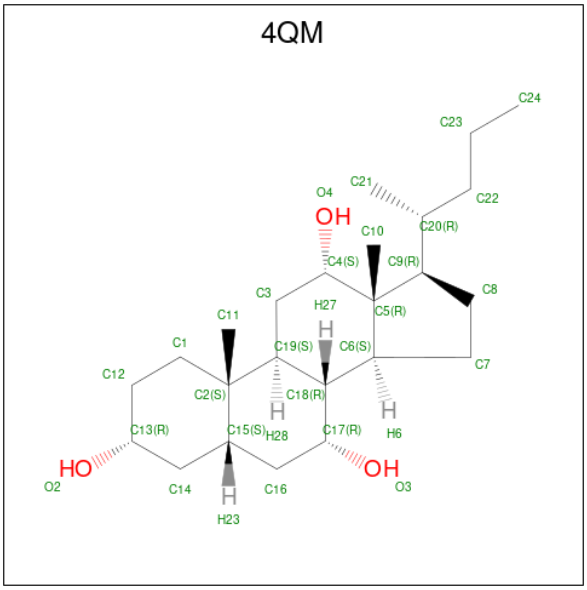
- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 23 is (3R,5S,7R,8R,9S,10S,12S,13R,14S,17R)-10,13-dimethyl-17-[(2R)-pentan-2-yl]-2,3,4,5,6,7,8,9,11,12,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthrene-3,7,12-triol (three-letter code: 4QM) (formula: $C_{24}H_{42}O_3$).



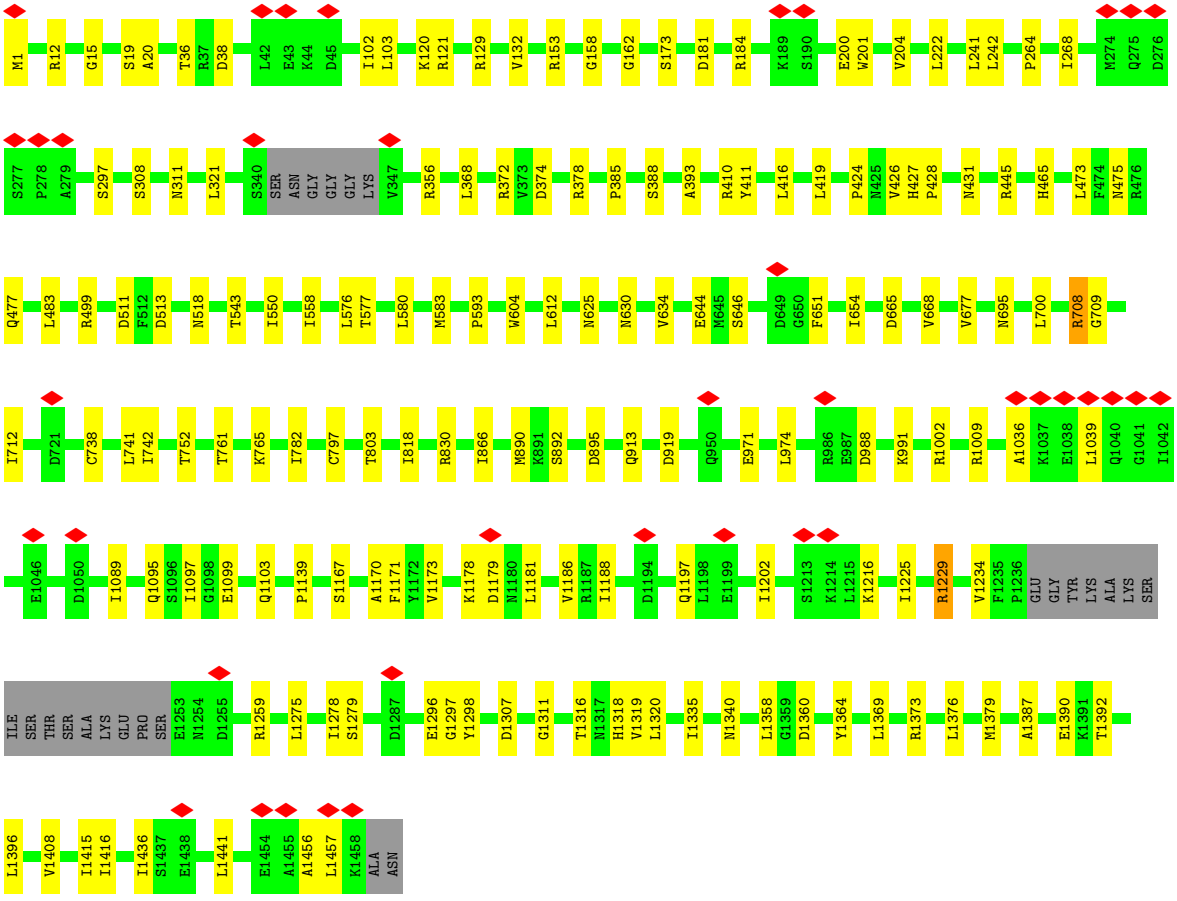
Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C O 27 24 3	0
23	C	1	Total C O 27 24 3	0

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.

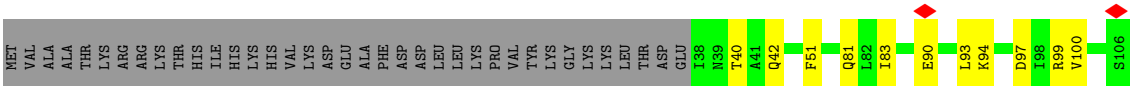
• Molecule 1: DNA-directed RNA polymerase III subunit RPC1

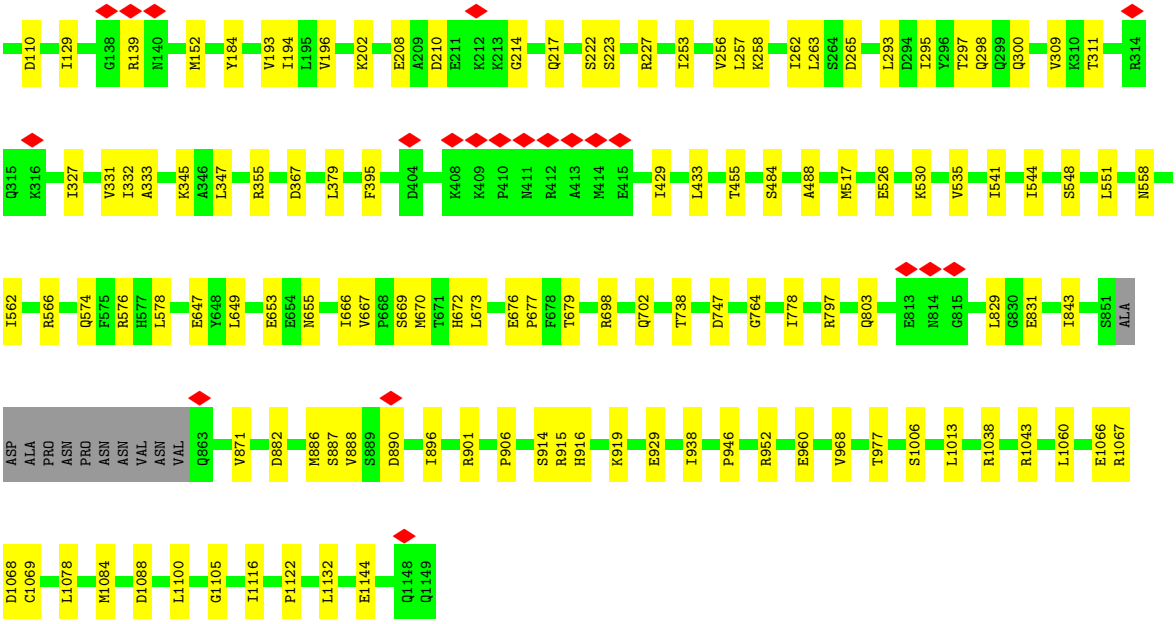
Chain A:



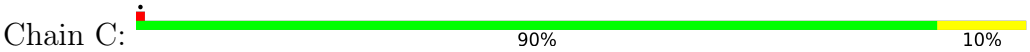
• Molecule 2: DNA-directed RNA polymerase III subunit RPC2

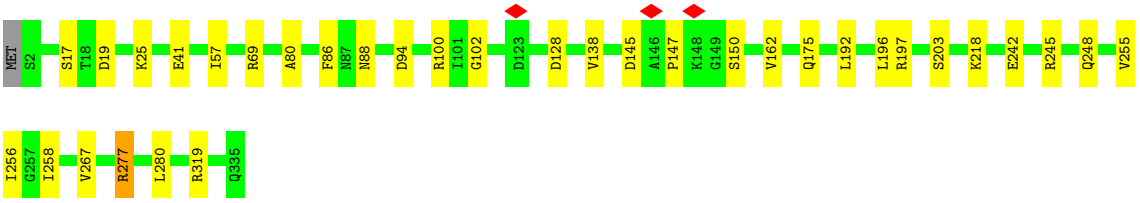
Chain B:



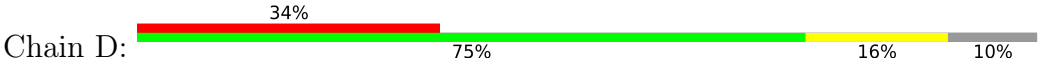


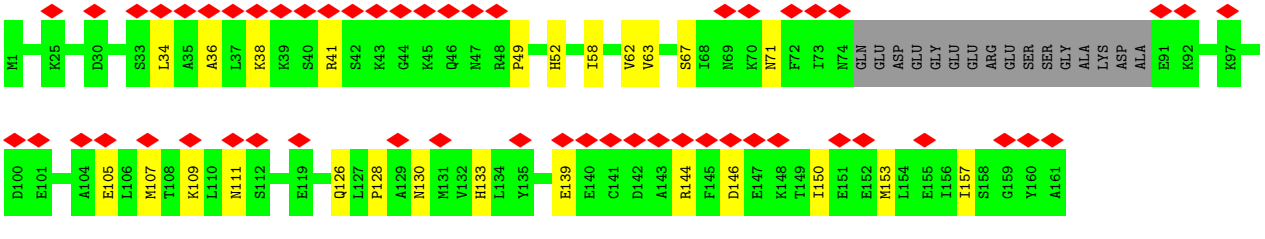
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



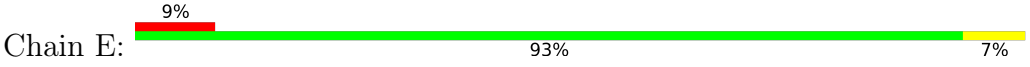


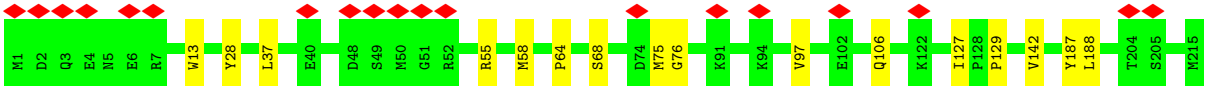
• Molecule 4: DNA-directed RNA polymerase III subunit RPC9





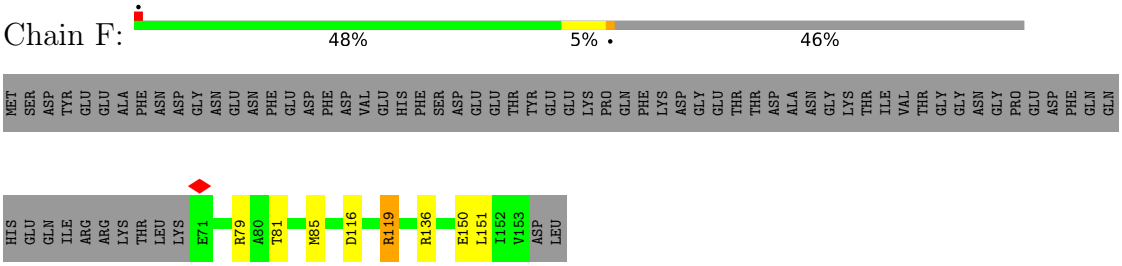
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1





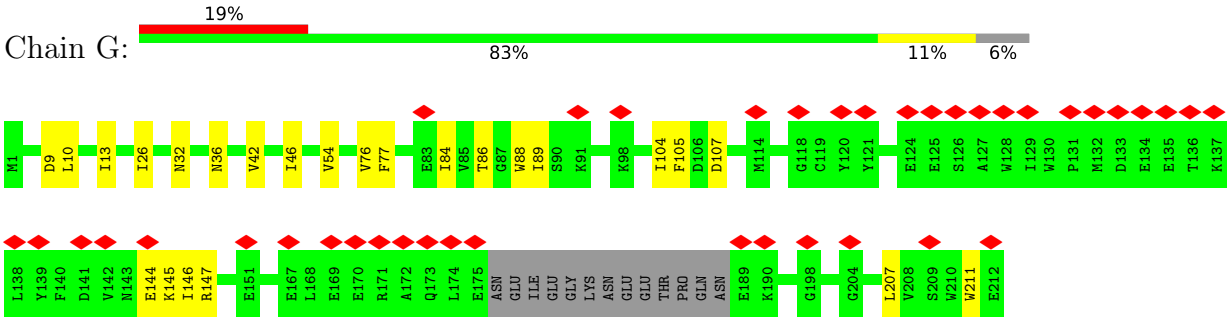
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



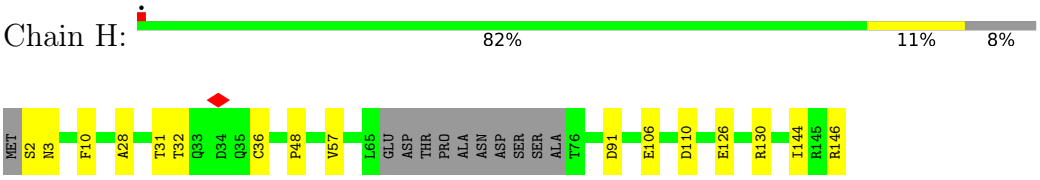
• Molecule 7: DNA-directed RNA polymerase III subunit RPC8

Chain G:



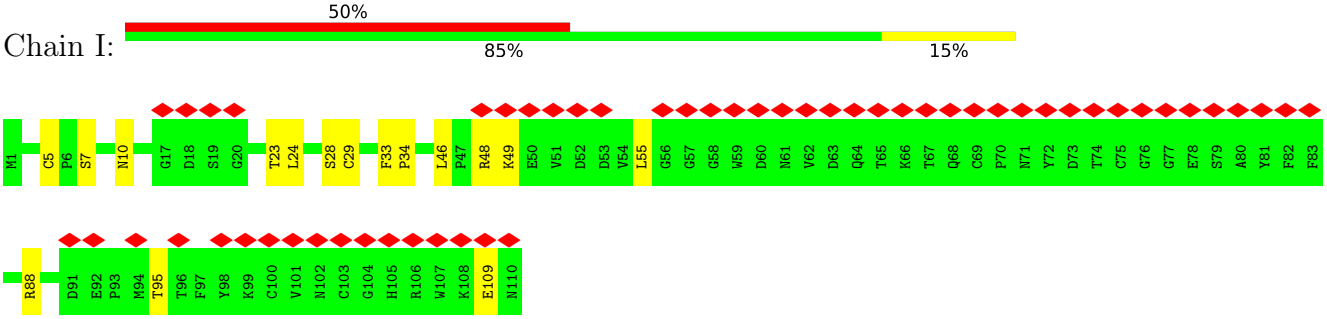
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



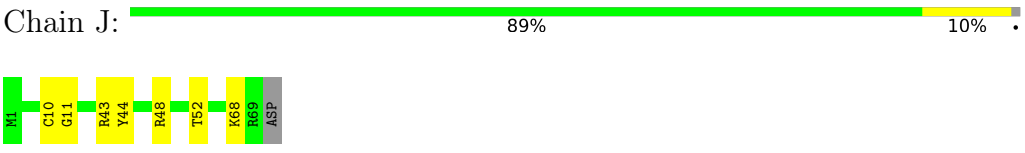
• Molecule 9: DNA-directed RNA polymerase III subunit RPC10

Chain I:



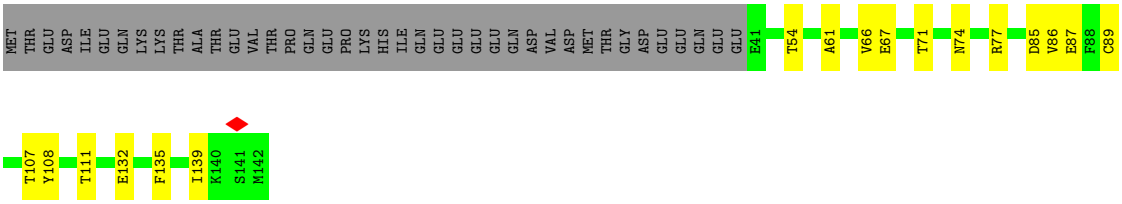
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:

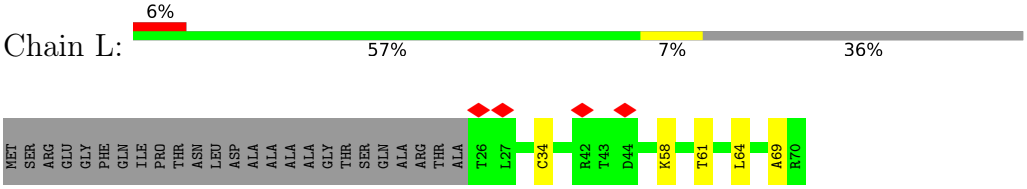


• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

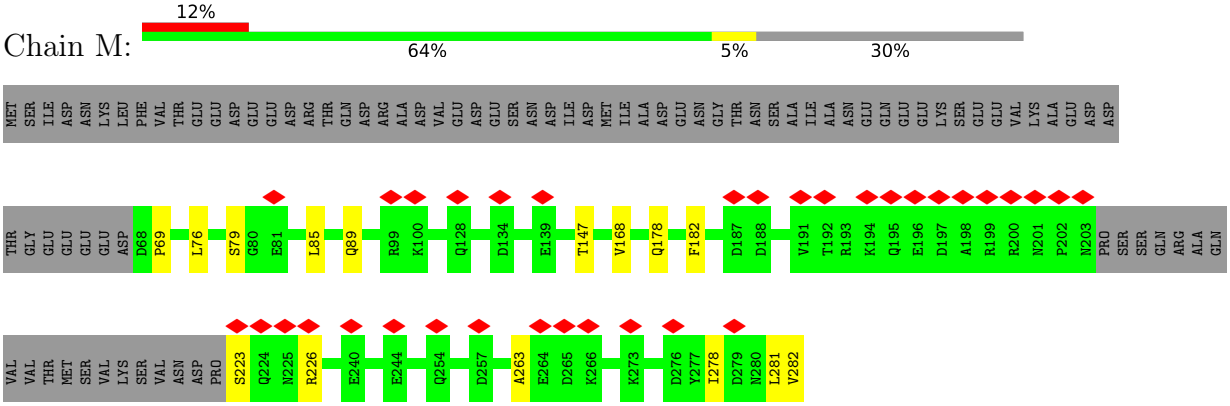
Chain K:



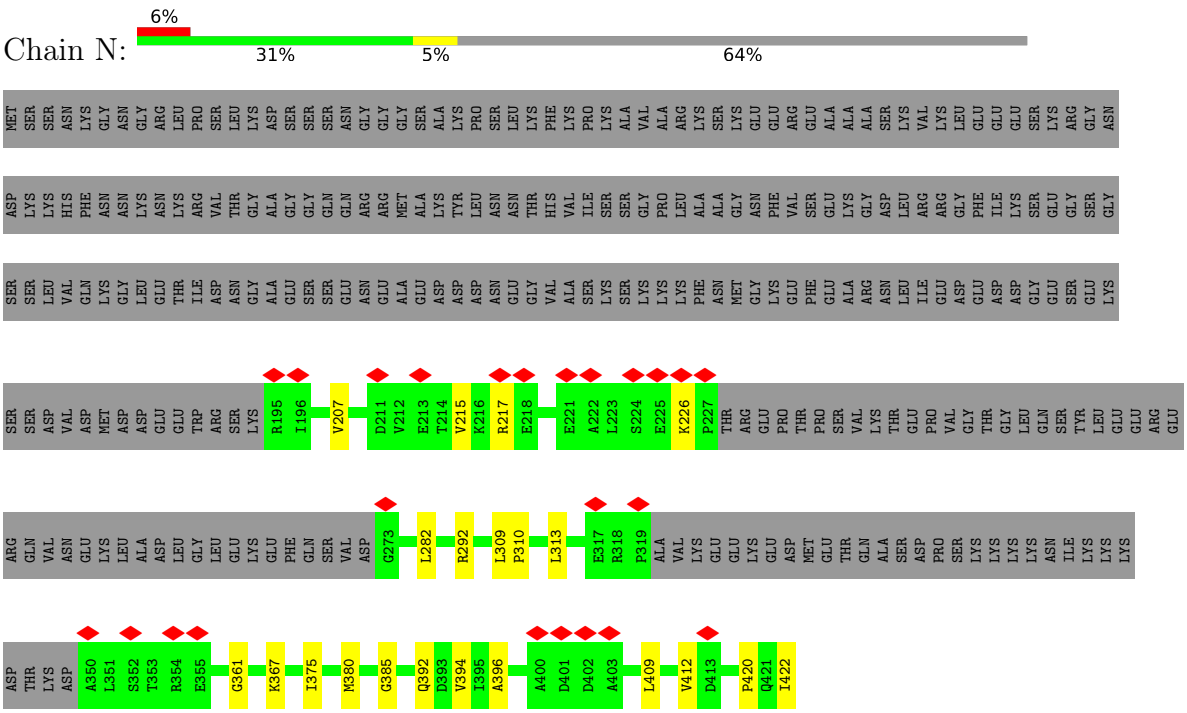
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



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

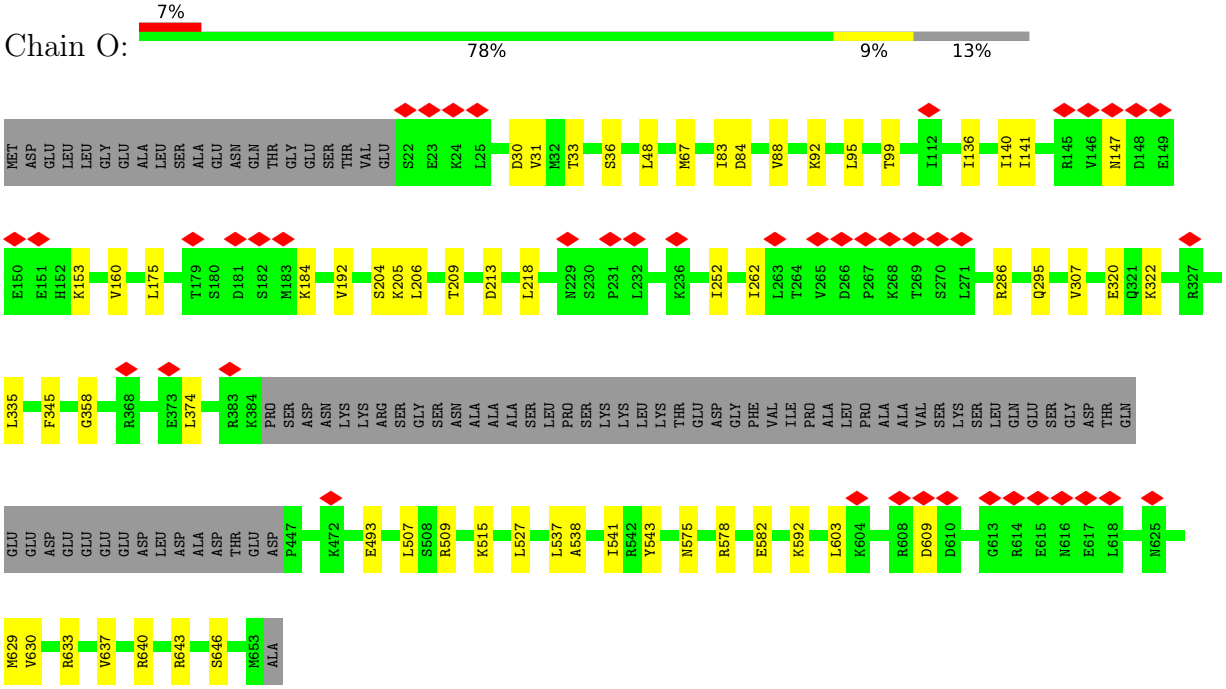


• Molecule 14: DNA-directed RNA polymerase III subunit RPC4



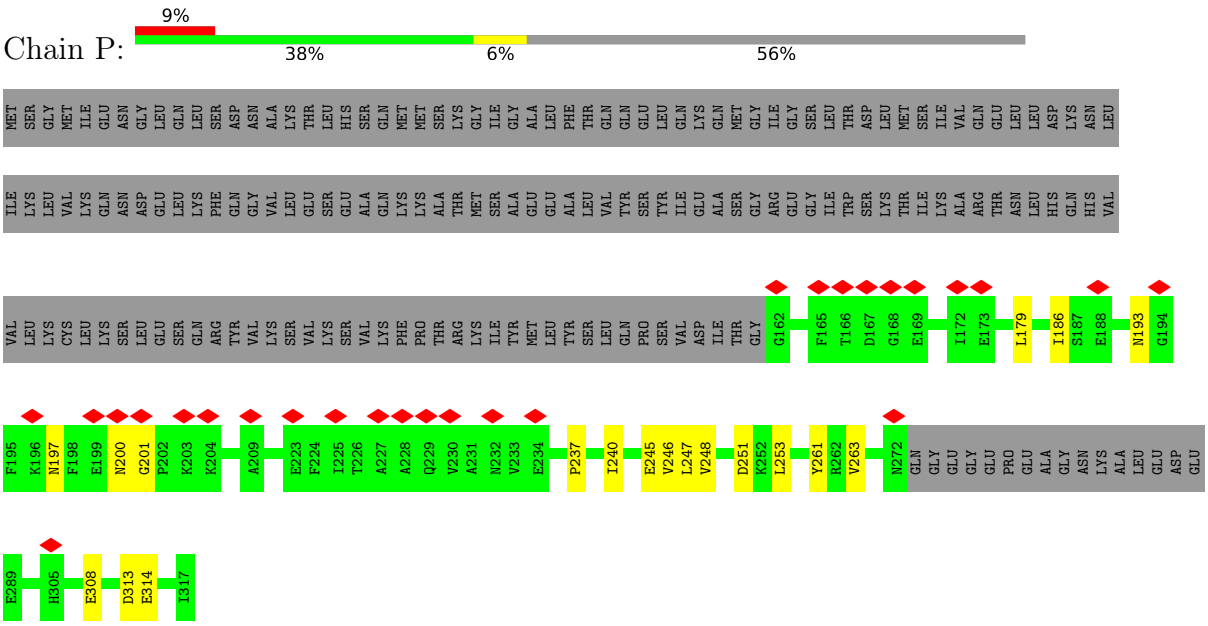
• Molecule 15: DNA-directed RNA polymerase III subunit RPC3

Chain O:



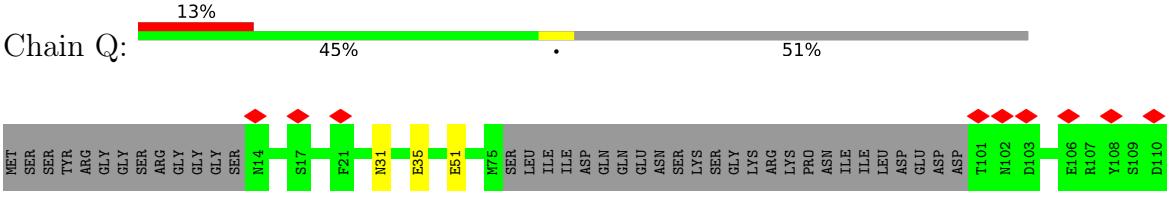
• Molecule 16: DNA-directed RNA polymerase III subunit RPC6

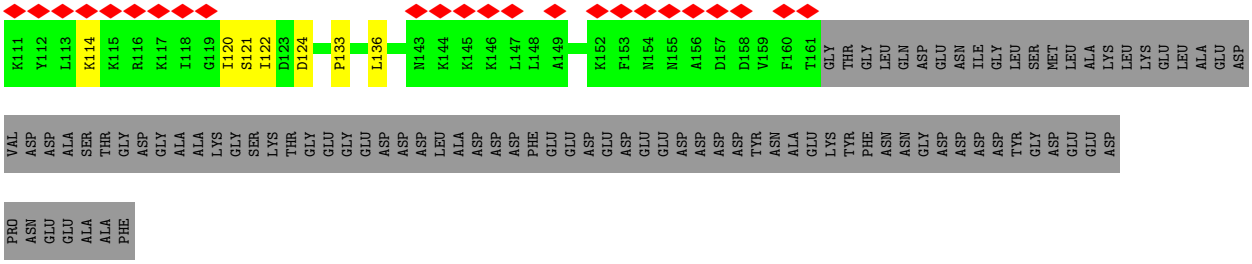
Chain P:



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

Chain Q:



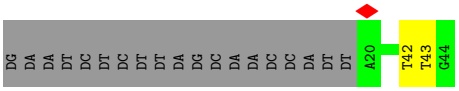


• Molecule 18: RNA

Chain R:

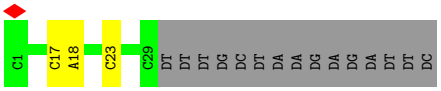
• Molecule 19: NT-DNA

Chain S:



• Molecule 20: T-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	47279	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.9	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2250	Depositor
Magnification	Not provided	
Image detector	GATAN K2 IS (4k x 4k)	Depositor
Maximum map value	0.251	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	364.35, 364.35, 364.35	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.041, 1.041, 1.041	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4QM, 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	A	0.26	0/11429	0.52	0/15440
2	B	0.27	0/8845	0.51	0/11929
3	C	0.26	0/2703	0.50	0/3666
4	D	0.26	0/1203	0.47	0/1610
5	E	0.27	0/1795	0.53	0/2416
6	F	0.26	0/683	0.52	0/923
7	G	0.26	0/1634	0.51	0/2217
8	H	0.27	0/1102	0.57	0/1492
9	I	0.26	0/894	0.51	0/1208
10	J	0.26	0/577	0.54	0/772
11	K	0.26	0/812	0.52	0/1096
12	L	0.25	0/360	0.65	0/478
13	M	0.25	0/1628	0.49	0/2204
14	N	0.24	0/1210	0.53	0/1625
15	O	0.25	0/4646	0.49	0/6267
16	P	0.27	0/1190	0.48	1/1616 (0.1%)
17	Q	0.27	0/1004	0.48	0/1354
18	R	0.18	0/218	0.71	0/338
19	S	0.53	0/564	1.06	0/868
20	T	0.49	0/669	0.89	0/1031
All	All	0.27	0/43166	0.53	1/58550 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	P	251	ASP	CB-CG-OD1	5.45	123.21	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11228	0	11362	104	0
2	B	8693	0	8820	87	0
3	C	2647	0	2616	25	0
4	D	1185	0	1206	18	0
5	E	1759	0	1788	9	0
6	F	671	0	692	4	0
7	G	1594	0	1580	18	0
8	H	1084	0	1057	9	0
9	I	873	0	818	10	0
10	J	569	0	584	7	0
11	K	801	0	795	11	0
12	L	358	0	381	5	0
13	M	1594	0	1552	10	0
14	N	1196	0	1257	17	0
15	O	4577	0	4754	36	0
16	P	1159	0	1109	11	0
17	Q	981	0	979	6	0
18	R	195	0	99	0	0
19	S	507	0	289	1	0
20	T	597	0	328	3	0
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	A	1	0	0	0	0
23	A	27	0	0	0	0
23	C	27	0	0	0	0
All	All	42330	0	42066	330	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 4.

All (330) 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)
14:N:217:ARG:HH12	14:N:282:LEU:HD13	1.50	0.76
1:A:36:THR:HG22	1:A:38:ASP:H	1.58	0.69
15:O:603:LEU:HD21	15:O:630:VAL:HG11	1.74	0.69
1:A:120:LYS:HG3	1:A:241:LEU:HD11	1.75	0.68
1:A:162:GLY:HA3	1:A:181:ASP:O	1.93	0.68
1:A:513:ASP:HB2	2:B:919:LYS:HG3	1.76	0.68
5:E:127:ILE:HG22	5:E:129:PRO:HD2	1.78	0.66
15:O:322:LYS:HD2	15:O:358:GLY:HA3	1.78	0.66
2:B:566:ARG:NH1	14:N:385:GLY:O	2.30	0.65
1:A:1197:GLN:HG3	9:I:55:LEU:HD23	1.79	0.65
1:A:393:ALA:HB3	1:A:499:ARG:HB2	1.78	0.64
13:M:147:THR:HG23	13:M:182:PHE:HB3	1.79	0.64
16:P:193:ASN:HB2	16:P:197:ASN:HB2	1.80	0.64
1:A:1415:ILE:HD13	2:B:1067:ARG:HD3	1.79	0.63
2:B:916:HIS:NE2	2:B:960:GLU:OE1	2.29	0.63
2:B:395:PHE:HB2	2:B:429:ILE:HD11	1.79	0.62
4:D:58:ILE:HB	7:G:36:ASN:HD22	1.65	0.62
1:A:473:LEU:HD11	2:B:1078:LEU:HD21	1.82	0.62
4:D:105:GLU:OE1	4:D:109:LYS:NZ	2.30	0.61
2:B:517:MET:H	2:B:679:THR:HG23	1.64	0.61
4:D:130:ASN:ND2	7:G:211:TRP:O	2.34	0.61
2:B:1105:GLY:HA2	2:B:1116:ILE:HG21	1.83	0.60
3:C:100:ARG:NH2	3:C:192:LEU:O	2.34	0.60
2:B:698:ARG:HD2	2:B:952:ARG:HB3	1.83	0.60
14:N:309:LEU:HD23	14:N:313:LEU:HD21	1.83	0.60
6:F:79:ARG:NH2	6:F:150:GLU:OE2	2.35	0.60
2:B:738:THR:HG23	2:B:977:THR:HA	1.83	0.60
2:B:566:ARG:HH21	14:N:282:LEU:HD11	1.67	0.59
1:A:475:ASN:HD21	2:B:1066:GLU:HG2	1.68	0.59
3:C:196:LEU:O	3:C:197:ARG:NH1	2.34	0.59
1:A:153:ARG:NH1	1:A:158:GLY:O	2.35	0.59
14:N:380:MET:HG2	14:N:420:PRO:HA	1.85	0.58
3:C:256:ILE:HG22	3:C:267:VAL:HA	1.85	0.58
1:A:1099:GLU:OE2	1:A:1103:GLN:NE2	2.37	0.58
8:H:110:ASP:OD2	8:H:130:ARG:NH1	2.37	0.58
1:A:583:MET:HB3	1:A:700:LEU:HB2	1.85	0.58
15:O:286:ARG:NH1	15:O:320:GLU:OE2	2.37	0.58
5:E:76:GLY:N	5:E:106:GLN:OE1	2.37	0.57
7:G:9:ASP:OD1	7:G:10:LEU:N	2.36	0.57
15:O:592:LYS:HB2	15:O:637:VAL:HG11	1.85	0.57
2:B:327:ILE:O	2:B:345:LYS:NZ	2.38	0.57
13:M:79:SER:HB2	13:M:263:ALA:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:42:DT:H2"	19:S:43:DT:H5"	1.87	0.57
2:B:526:GLU:OE1	2:B:558:ASN:ND2	2.37	0.57
14:N:226:LYS:HD2	14:N:292:ARG:HH22	1.70	0.57
1:A:1307:ASP:OD2	9:I:88:ARG:NH1	2.37	0.56
13:M:69:PRO:O	14:N:367:LYS:NZ	2.39	0.56
1:A:782:ILE:HG13	1:A:803:THR:HG23	1.87	0.56
1:A:974:LEU:O	1:A:1002:ARG:NH1	2.37	0.56
1:A:1225:ILE:O	1:A:1229:ARG:HB2	2.05	0.56
2:B:676:GLU:OE2	2:B:679:THR:OG1	2.17	0.56
2:B:484:SER:HA	2:B:488:ALA:HB2	1.88	0.56
1:A:830:ARG:NH2	2:B:655:ASN:O	2.37	0.56
2:B:829:LEU:O	12:L:58:LYS:NZ	2.39	0.56
1:A:483:LEU:HD13	1:A:550:ILE:HG21	1.88	0.55
2:B:355:ARG:NH2	2:B:367:ASP:OD2	2.40	0.55
3:C:218:LYS:NZ	12:L:69:ALA:O	2.34	0.55
1:A:1373:ARG:NH1	1:A:1390:GLU:OE2	2.39	0.55
3:C:86:PHE:O	3:C:203:SER:OG	2.22	0.55
4:D:63:VAL:O	4:D:67:SER:HB3	2.06	0.55
2:B:331:VAL:HG12	2:B:332:ILE:HG12	1.88	0.55
13:M:89:GLN:OE1	13:M:178:GLN:NE2	2.36	0.55
16:P:253:LEU:HD13	16:P:261:TYR:HB3	1.89	0.55
1:A:200:GLU:HG2	15:O:515:LYS:HB3	1.89	0.55
3:C:69:ARG:HE	11:K:71:THR:HB	1.71	0.55
2:B:535:VAL:HG13	14:N:310:PRO:HB3	1.88	0.55
4:D:126:GLN:HE22	7:G:84:ILE:HG13	1.72	0.55
2:B:541:ILE:HD12	2:B:544:ILE:HD11	1.88	0.54
15:O:307:VAL:HG13	15:O:374:LEU:HD11	1.89	0.54
2:B:208:GLU:OE2	2:B:217:GLN:NE2	2.36	0.54
1:A:577:THR:HG21	11:K:89:CYS:H	1.73	0.54
1:A:625:ASN:HA	1:A:654:ILE:O	2.08	0.54
2:B:227:ARG:HG3	2:B:333:ALA:HB1	1.90	0.54
1:A:201:TRP:HA	1:A:204:VAL:HG12	1.90	0.54
15:O:88:VAL:HG22	15:O:92:LYS:HE2	1.89	0.54
1:A:426:VAL:HG12	1:A:428:PRO:HD2	1.90	0.54
2:B:831:GLU:HB3	12:L:61:THR:HB	1.90	0.53
4:D:71:ASN:O	7:G:147:ARG:NH2	2.39	0.53
1:A:129:ARG:HB2	1:A:132:VAL:HG23	1.90	0.53
14:N:392:GLN:HB2	14:N:412:VAL:HB	1.89	0.53
1:A:1095:GLN:HE22	2:B:1069:CYS:HA	1.74	0.53
4:D:139:GLU:O	4:D:144:ARG:NH2	2.42	0.53
8:H:48:PRO:O	8:H:146:ARG:NH2	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:62:VAL:HG22	7:G:104:ILE:HD12	1.91	0.53
8:H:10:PHE:HB3	8:H:28:ALA:HB1	1.90	0.53
15:O:295:GLN:NE2	15:O:646:SER:O	2.41	0.53
2:B:702:GLN:HE21	2:B:915:ARG:HA	1.74	0.52
5:E:187:TYR:HD1	5:E:188:LEU:HD12	1.73	0.52
9:I:7:SER:OG	9:I:29:CYS:SG	2.64	0.52
13:M:76:LEU:HD12	13:M:168:VAL:HB	1.91	0.52
15:O:640:ARG:NH1	16:P:308:GLU:O	2.41	0.52
9:I:24:LEU:HB2	9:I:33:PHE:HB3	1.90	0.52
1:A:752:THR:HA	1:A:761:THR:HG21	1.92	0.52
2:B:578:LEU:HD21	13:M:282:VAL:HG11	1.92	0.52
1:A:708:ARG:NH1	1:A:709:GLY:O	2.42	0.52
1:A:19:SER:OG	1:A:20:ALA:N	2.43	0.52
15:O:140:ILE:HG21	15:O:160:VAL:HG21	1.92	0.52
1:A:12:ARG:NH1	2:B:1144:GLU:OE2	2.42	0.52
2:B:184:TYR:HB3	2:B:193:VAL:HG22	1.92	0.52
9:I:5:CYS:SG	9:I:7:SER:OG	2.68	0.52
13:M:278:ILE:HD12	14:N:422:ILE:HG22	1.92	0.52
17:Q:133:PRO:HD2	17:Q:136:LEU:HD12	1.92	0.52
2:B:309:VAL:HG12	2:B:311:THR:H	1.75	0.51
1:A:1097:ILE:HD13	1:A:1358:LEU:HD22	1.91	0.51
1:A:1316:THR:HG22	1:A:1318:HIS:H	1.74	0.51
3:C:255:VAL:HG12	3:C:256:ILE:HG23	1.92	0.51
3:C:128:ASP:O	3:C:175:GLN:NE2	2.38	0.51
7:G:144:GLU:HB3	7:G:207:LEU:HD11	1.91	0.51
2:B:574:GLN:HB3	14:N:422:ILE:HD11	1.91	0.51
3:C:17:SER:OG	3:C:19:ASP:OD1	2.28	0.51
1:A:477:GLN:OE1	1:A:518:ASN:ND2	2.43	0.51
1:A:892:SER:HA	1:A:1376:LEU:HD11	1.91	0.51
2:B:548:SER:HB2	2:B:551:LEU:HD12	1.91	0.51
6:F:116:ASP:HB3	6:F:119:ARG:HE	1.76	0.51
16:P:200:ASN:OD1	16:P:201:GLY:N	2.44	0.51
15:O:136:ILE:O	15:O:140:ILE:HG12	2.11	0.51
1:A:1396:LEU:HD13	2:B:1132:LEU:HD21	1.93	0.51
3:C:248:GLN:HA	3:C:256:ILE:HD11	1.93	0.51
9:I:10:ASN:ND2	9:I:28:SER:OG	2.44	0.50
2:B:263:LEU:HD21	2:B:298:GLN:HB2	1.93	0.50
4:D:52:HIS:HE2	7:G:32:ASN:HA	1.76	0.50
14:N:207:VAL:HG11	14:N:215:VAL:HG11	1.93	0.50
1:A:630:ASN:ND2	1:A:665:ASP:OD1	2.45	0.50
2:B:666:ILE:HD11	2:B:673:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:95:THR:OG1	9:I:109:GLU:O	2.24	0.50
1:A:1179:ASP:OD1	1:A:1179:ASP:N	2.44	0.50
1:A:15:GLY:HA2	1:A:1408:VAL:HG23	1.92	0.50
15:O:609:ASP:OD1	15:O:609:ASP:N	2.45	0.50
8:H:31:THR:HG22	8:H:32:THR:HG23	1.93	0.49
20:T:17:DC:H2'	20:T:18:DA:C8	2.47	0.49
14:N:361:GLY:HA3	14:N:375:ILE:HD13	1.94	0.49
16:P:245:GLU:HA	16:P:248:VAL:HG12	1.94	0.49
1:A:971:GLU:OE2	1:A:1009:ARG:NH2	2.41	0.49
13:M:223:SER:O	13:M:226:ARG:NH1	2.45	0.49
1:A:102:ILE:HG13	1:A:242:LEU:HD22	1.95	0.49
1:A:388:SER:OG	1:A:695:ASN:ND2	2.45	0.49
2:B:194:ILE:HG12	2:B:455:THR:HG22	1.95	0.49
2:B:1084:MET:HG3	2:B:1122:PRO:HD3	1.94	0.48
4:D:36:ALA:O	4:D:41:ARG:NE	2.46	0.48
15:O:175:LEU:HD22	15:O:184:LYS:HG2	1.93	0.48
1:A:1436:ILE:HD12	7:G:54:VAL:HG21	1.96	0.48
15:O:575:ASN:OD1	15:O:578:ARG:NH2	2.46	0.48
1:A:374:ASP:OD2	2:B:1043:ARG:NH2	2.46	0.48
1:A:1167:SER:HA	9:I:46:LEU:HD13	1.96	0.48
2:B:97:ASP:OD2	2:B:99:ARG:NH2	2.46	0.48
6:F:85:MET:HB2	6:F:151:LEU:HB3	1.96	0.48
1:A:1234:VAL:HG13	1:A:1259:ARG:HH11	1.78	0.48
1:A:1369:LEU:HG	1:A:1379:MET:HG3	1.94	0.48
2:B:647:GLU:OE2	2:B:672:HIS:NE2	2.34	0.48
8:H:2:SER:OG	8:H:3:ASN:N	2.46	0.48
3:C:19:ASP:OD1	3:C:19:ASP:N	2.46	0.48
1:A:1036:ALA:HB3	1:A:1039:LEU:HB2	1.95	0.48
1:A:297:SER:HB3	17:Q:31:ASN:HB2	1.95	0.48
1:A:580:LEU:HD23	1:A:583:MET:HE3	1.95	0.47
15:O:84:ASP:N	15:O:84:ASP:OD1	2.47	0.47
1:A:1170:ALA:HA	1:A:1188:ILE:HA	1.95	0.47
1:A:1387:ALA:HB1	1:A:1392:THR:HG23	1.95	0.47
1:A:368:LEU:HD22	1:A:1416:ILE:HG23	1.97	0.47
1:A:580:LEU:HD11	1:A:612:LEU:HD13	1.95	0.47
2:B:886:MET:HG2	2:B:896:ILE:HG12	1.96	0.47
1:A:385:PRO:HG3	2:B:764:GLY:HA3	1.95	0.47
1:A:1139:PRO:HG3	1:A:1298:TYR:CZ	2.50	0.47
16:P:237:PRO:HA	16:P:240:ILE:HG22	1.95	0.47
1:A:558:ILE:HG22	1:A:797:CYS:HB3	1.96	0.47
1:A:1:MET:N	7:G:36:ASN:OD1	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:145:ASP:OD1	3:C:145:ASP:N	2.48	0.47
15:O:48:LEU:HD22	15:O:582:GLU:HG3	1.96	0.47
1:A:1278:ILE:HD13	1:A:1297:GLY:HA3	1.96	0.47
3:C:138:VAL:HG11	3:C:162:VAL:HG22	1.96	0.47
1:A:378:ARG:HB2	2:B:1060:LEU:HD11	1.96	0.47
5:E:55:ARG:HA	5:E:58:MET:HG2	1.97	0.47
11:K:85:ASP:OD2	11:K:111:THR:OG1	2.29	0.47
3:C:80:ALA:HB3	3:C:102:GLY:HA2	1.97	0.46
4:D:128:PRO:HD2	4:D:157:ILE:HG21	1.97	0.46
2:B:83:ILE:HD12	2:B:93:LEU:HD22	1.96	0.46
2:B:667:VAL:HG22	2:B:670:MET:HG2	1.97	0.46
10:J:10:CYS:SG	10:J:43:ARG:NH2	2.80	0.46
1:A:741:LEU:HD21	1:A:765:LYS:HE3	1.97	0.46
1:A:919:ASP:N	1:A:919:ASP:OD1	2.48	0.46
2:B:914:SER:O	2:B:914:SER:OG	2.31	0.46
15:O:538:ALA:HA	15:O:541:ILE:HD12	1.97	0.46
7:G:42:VAL:HG12	7:G:76:VAL:HG21	1.97	0.46
15:O:95:LEU:O	15:O:99:THR:OG1	2.27	0.46
1:A:988:ASP:HB2	1:A:991:LYS:HD3	1.98	0.46
2:B:40:THR:HG23	2:B:42:GLN:HG3	1.98	0.46
4:D:34:LEU:HA	4:D:38:LYS:HE2	1.97	0.46
1:A:372:ARG:NH1	20:T:23:DC:OP1	2.42	0.46
1:A:577:THR:HG21	11:K:89:CYS:N	2.31	0.46
13:M:85:LEU:HD11	14:N:394:VAL:HB	1.97	0.46
1:A:424:PRO:HG2	1:A:445:ARG:HB3	1.98	0.46
1:A:738:CYS:O	1:A:742:ILE:HG12	2.16	0.46
2:B:882:ASP:OD1	2:B:901:ARG:NE	2.41	0.46
11:K:66:VAL:HG12	11:K:67:GLU:HG3	1.98	0.46
1:A:1311:GLY:HA3	5:E:142:VAL:HG21	1.98	0.45
2:B:576:ARG:NH1	2:B:653:GLU:OE2	2.49	0.45
2:B:938:ILE:HG12	10:J:43:ARG:HD2	1.97	0.45
1:A:1173:VAL:HG12	1:A:1186:VAL:HG22	1.97	0.45
6:F:81:THR:HG21	6:F:136:ARG:HD3	1.99	0.45
15:O:643:ARG:NH2	17:Q:51:GLU:OE1	2.50	0.45
3:C:277:ARG:HB2	3:C:280:LEU:HD12	1.98	0.45
3:C:86:PHE:HE1	12:L:64:LEU:HD12	1.82	0.45
11:K:54:THR:HG22	11:K:61:ALA:HA	1.99	0.45
15:O:335:LEU:HD23	15:O:345:PHE:HZ	1.82	0.45
1:A:121:ARG:NH1	15:O:213:ASP:OD1	2.38	0.45
1:A:268:ILE:O	1:A:356:ARG:NH2	2.44	0.45
1:A:892:SER:HB2	1:A:1376:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:36:SER:OG	16:P:314:GLU:OE2	2.25	0.45
15:O:218:LEU:HD11	15:O:252:ILE:HD12	1.98	0.45
1:A:1319:VAL:HG13	1:A:1320:LEU:HD12	1.98	0.45
5:E:68:SER:OG	5:E:75:MET:SD	2.74	0.45
15:O:31:VAL:HG13	17:Q:35:GLU:HG2	1.99	0.45
2:B:210:ASP:O	2:B:214:GLY:N	2.49	0.45
2:B:929:GLU:HB2	3:C:69:ARG:HG2	1.98	0.45
1:A:173:SER:HB3	1:A:321:LEU:HD11	1.99	0.44
11:K:87:GLU:HB3	11:K:108:TYR:CZ	2.52	0.44
1:A:1456:ALA:O	1:A:1457:LEU:N	2.50	0.44
15:O:206:LEU:HA	15:O:209:THR:HG22	1.98	0.44
1:A:712:ILE:HG22	2:B:946:PRO:HB3	2.00	0.44
2:B:887:SER:OG	2:B:888:VAL:N	2.50	0.44
1:A:913:GLN:NE2	1:A:1360:ASP:OD2	2.50	0.44
1:A:1319:VAL:HG21	1:A:1335:ILE:HG13	1.99	0.44
2:B:110:ASP:OD1	2:B:110:ASP:N	2.49	0.44
16:P:186:ILE:HG22	16:P:263:VAL:HG23	2.00	0.44
1:A:634:VAL:O	1:A:646:SER:HB2	2.17	0.44
2:B:257:LEU:HD22	2:B:262:ILE:HD12	1.99	0.44
7:G:13:ILE:HD11	7:G:26:ILE:HG13	1.99	0.44
1:A:511:ASP:OD1	1:A:511:ASP:N	2.50	0.44
4:D:150:ILE:HA	4:D:153:MET:HG2	1.99	0.44
1:A:593:PRO:HD3	1:A:612:LEU:HD21	1.99	0.44
2:B:797:ARG:HG2	2:B:803:GLN:HB3	1.99	0.44
2:B:81:GLN:OE1	2:B:94:LYS:HG3	2.18	0.44
7:G:105:PHE:CE2	7:G:107:ASP:HB2	2.53	0.44
1:A:427:HIS:O	1:A:465:HIS:ND1	2.50	0.44
1:A:1178:LYS:HD2	1:A:1181:LEU:HD11	1.98	0.44
1:A:1275:LEU:HB2	1:A:1278:ILE:HG12	1.99	0.44
1:A:644:GLU:HA	1:A:651:PHE:HB3	2.00	0.43
2:B:51:PHE:CD2	2:B:517:MET:HG3	2.53	0.43
10:J:10:CYS:SG	10:J:11:GLY:N	2.91	0.43
2:B:222:SER:HB2	2:B:333:ALA:HB3	2.00	0.43
2:B:843:ILE:HB	2:B:871:VAL:HB	2.01	0.43
4:D:126:GLN:OE1	4:D:133:HIS:NE2	2.45	0.43
15:O:192:VAL:HG13	15:O:262:ILE:HD11	1.98	0.43
9:I:23:THR:HG22	9:I:34:PRO:HA	2.00	0.43
1:A:103:LEU:HD13	1:A:222:LEU:HD13	1.99	0.43
1:A:890:MET:HG2	2:B:1068:ASP:CG	2.38	0.43
4:D:107:MET:O	4:D:111:ASN:ND2	2.51	0.43
15:O:507:LEU:HD21	15:O:537:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:120:ILE:HG13	17:Q:124:ASP:HB2	2.00	0.43
1:A:483:LEU:HD11	1:A:543:THR:HA	1.99	0.43
1:A:1279:SER:N	1:A:1296:GLU:O	2.47	0.43
2:B:530:LYS:HG3	2:B:562:ILE:HD11	2.01	0.43
15:O:67:MET:HG3	15:O:83:ILE:HG12	2.00	0.43
3:C:88:ASN:ND2	3:C:94:ASP:OD1	2.52	0.43
2:B:747:ASP:OD1	2:B:747:ASP:N	2.51	0.43
15:O:527:LEU:HD23	16:P:246:VAL:HG21	2.01	0.43
5:E:13:TRP:NE1	5:E:37:LEU:O	2.47	0.43
10:J:48:ARG:O	10:J:52:THR:OG1	2.33	0.42
15:O:30:ASP:HA	15:O:33:THR:HG22	2.00	0.42
16:P:179:LEU:HB3	16:P:247:LEU:HD21	2.01	0.42
13:M:281:LEU:HD12	13:M:281:LEU:HA	1.84	0.42
2:B:253:ILE:HA	2:B:256:VAL:HG12	2.01	0.42
2:B:968:VAL:HG13	10:J:44:TYR:HB2	2.00	0.42
17:Q:121:SER:OG	17:Q:122:ILE:N	2.53	0.42
20:T:17:DC:H2'	20:T:18:DA:H8	1.84	0.42
1:A:308:SER:OG	1:A:311:ASN:OD1	2.37	0.42
3:C:319:ARG:NH2	11:K:132:GLU:OE2	2.49	0.42
5:E:97:VAL:HG13	5:E:127:ILE:HD11	2.01	0.42
10:J:68:LYS:HE3	12:L:34:CYS:HB2	2.02	0.42
11:K:135:PHE:CE2	11:K:139:ILE:HD11	2.54	0.42
2:B:890:ASP:OD1	2:B:890:ASP:N	2.51	0.42
2:B:1088:ASP:OD1	2:B:1088:ASP:N	2.53	0.42
2:B:347:LEU:HG	2:B:541:ILE:HD11	2.01	0.42
1:A:410:ARG:NH1	1:A:411:TYR:OH	2.52	0.42
1:A:668:VAL:HG12	1:A:677:VAL:HG23	2.01	0.42
2:B:1006:SER:HB3	2:B:1013:LEU:HD21	2.01	0.42
5:E:28:TYR:HA	5:E:64:PRO:HA	2.02	0.42
11:K:86:VAL:HG22	11:K:107:THR:HG22	2.01	0.42
2:B:293:LEU:O	2:B:295:ILE:HG13	2.20	0.42
2:B:202:LYS:HD2	2:B:223:SER:HB3	2.02	0.42
2:B:649:LEU:HD11	2:B:672:HIS:CE1	2.55	0.42
15:O:204:SER:OG	15:O:205:LYS:N	2.52	0.42
15:O:543:TYR:OH	16:P:313:ASP:OD1	2.31	0.42
2:B:100:VAL:HG22	2:B:129:ILE:HG12	2.02	0.42
1:A:895:ASP:OD1	1:A:895:ASP:N	2.53	0.41
1:A:1360:ASP:O	1:A:1364:TYR:HB3	2.20	0.41
4:D:38:LYS:HD2	4:D:49:PRO:HD3	2.02	0.41
8:H:106:GLU:OE1	8:H:106:GLU:N	2.53	0.41
1:A:1216:LYS:O	1:A:1259:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:396:ALA:HB2	14:N:409:LEU:HD11	2.01	0.41
1:A:1171:PHE:HE1	9:I:48:ARG:HH11	1.68	0.41
2:B:90:GLU:OE2	2:B:139:ARG:NH2	2.54	0.41
2:B:258:LYS:NZ	2:B:265:ASP:OD1	2.40	0.41
2:B:667:VAL:HG23	2:B:669:SER:H	1.85	0.41
4:D:71:ASN:HB2	7:G:86:THR:HG21	2.02	0.41
2:B:702:GLN:NE2	2:B:915:ARG:HG3	2.35	0.41
1:A:264:PRO:HB3	1:A:268:ILE:HD11	2.02	0.41
3:C:25:LYS:NZ	8:H:91:ASP:OD1	2.54	0.41
1:A:818:ILE:HG12	1:A:866:ILE:HG22	2.01	0.41
14:N:394:VAL:HG23	14:N:409:LEU:HB2	2.03	0.41
1:A:576:LEU:HD22	1:A:604:TRP:CG	2.55	0.41
2:B:196:VAL:HG13	2:B:379:LEU:HD23	2.03	0.41
7:G:88:TRP:CZ2	7:G:145:LYS:HD3	2.56	0.41
11:K:74:ASN:OD1	11:K:77:ARG:NH2	2.54	0.41
14:N:226:LYS:HD2	14:N:292:ARG:HH12	1.86	0.41
1:A:1089:ILE:HD12	1:A:1089:ILE:HA	1.98	0.40
2:B:676:GLU:HA	2:B:677:PRO:HD3	1.88	0.40
2:B:1100:LEU:HD23	2:B:1100:LEU:HA	1.92	0.40
3:C:245:ARG:HH12	3:C:258:ILE:HG21	1.86	0.40
7:G:46:ILE:HD11	7:G:77:PHE:HB2	2.03	0.40
7:G:89:ILE:HD11	7:G:146:ILE:HD12	2.03	0.40
8:H:57:VAL:HG22	8:H:144:ILE:HG12	2.03	0.40
15:O:493:GLU:OE1	15:O:509:ARG:NH1	2.45	0.40
15:O:629:MET:SD	15:O:633:ARG:NE	2.89	0.40
1:A:374:ASP:OD1	2:B:1038:ARG:NE	2.42	0.40
2:B:297:THR:HG23	2:B:300:GLN:H	1.86	0.40
2:B:778:ILE:HG23	2:B:906:PRO:HD2	2.04	0.40
3:C:147:PRO:HB2	3:C:150:SER:HB2	2.03	0.40
4:D:146:ASP:O	4:D:150:ILE:HG13	2.22	0.40
8:H:36:CYS:HA	8:H:126:GLU:O	2.21	0.40
1:A:416:LEU:HD23	1:A:419:LEU:HD12	2.03	0.40
2:B:152:MET:SD	2:B:433:LEU:HD21	2.62	0.40
3:C:242:GLU:HA	3:C:245:ARG:HD3	2.03	0.40
3:C:319:ARG:HD3	3:C:319:ARG:HA	1.90	0.40
15:O:147:ASN:HA	15:O:153:LYS:HD3	2.03	0.40
1:A:431:ASN:OD1	1:A:465:HIS:NE2	2.52	0.40
1:A:1441:LEU:HD11	7:G:54:VAL:HG22	2.03	0.40
3:C:41:GLU:HB3	3:C:57:ILE:HB	2.03	0.40
1:A:1188:ILE:HD11	1:A:1202:ILE:HG13	2.04	0.40
2:B:968:VAL:HG21	10:J:48:ARG:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:141:ILE:HD12	15:O:153:LYS:HG3	2.03	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	1428/1460 (98%)	1391 (97%)	37 (3%)	0	100	100
2	B	1097/1149 (96%)	1068 (97%)	29 (3%)	0	100	100
3	C	332/335 (99%)	323 (97%)	9 (3%)	0	100	100
4	D	141/161 (88%)	136 (96%)	5 (4%)	0	100	100
5	E	213/215 (99%)	202 (95%)	11 (5%)	0	100	100
6	F	81/155 (52%)	79 (98%)	2 (2%)	0	100	100
7	G	195/212 (92%)	186 (95%)	9 (5%)	0	100	100
8	H	131/146 (90%)	129 (98%)	2 (2%)	0	100	100
9	I	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
10	J	65/70 (93%)	64 (98%)	1 (2%)	0	100	100
11	K	100/142 (70%)	98 (98%)	2 (2%)	0	100	100
12	L	43/70 (61%)	41 (95%)	2 (5%)	0	100	100
13	M	192/282 (68%)	186 (97%)	6 (3%)	0	100	100
14	N	147/422 (35%)	143 (97%)	4 (3%)	0	100	100
15	O	566/654 (86%)	557 (98%)	9 (2%)	0	100	100
16	P	136/317 (43%)	133 (98%)	3 (2%)	0	100	100
17	Q	119/251 (47%)	112 (94%)	7 (6%)	0	100	100
All	All	5094/6151 (83%)	4953 (97%)	141 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1239/1257 (99%)	1235 (100%)	4 (0%)	92 98
2	B	964/1006 (96%)	964 (100%)	0	100 100
3	C	295/296 (100%)	294 (100%)	1 (0%)	92 98
4	D	133/145 (92%)	133 (100%)	0	100 100
5	E	197/197 (100%)	197 (100%)	0	100 100
6	F	73/137 (53%)	72 (99%)	1 (1%)	67 90
7	G	173/190 (91%)	173 (100%)	0	100 100
8	H	119/128 (93%)	119 (100%)	0	100 100
9	I	98/98 (100%)	97 (99%)	1 (1%)	76 93
10	J	64/65 (98%)	64 (100%)	0	100 100
11	K	92/130 (71%)	92 (100%)	0	100 100
12	L	40/57 (70%)	40 (100%)	0	100 100
13	M	171/249 (69%)	171 (100%)	0	100 100
14	N	131/360 (36%)	131 (100%)	0	100 100
15	O	524/593 (88%)	524 (100%)	0	100 100
16	P	130/285 (46%)	130 (100%)	0	100 100
17	Q	109/212 (51%)	108 (99%)	1 (1%)	78 94
All	All	4552/5405 (84%)	4544 (100%)	8 (0%)	93 98

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	ARG
1	A	708	ARG
1	A	1229	ARG
1	A	1340	ASN

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Mol	Chain	Res	Type
3	C	277	ARG
6	F	119	ARG
9	I	49	LYS
17	Q	114	LYS

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

Mol	Chain	Res	Type
2	B	702	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	R	8/24 (33%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
18	R	15	C
18	R	17	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 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
23	4QM	C	401	-	30,30,30	1.87	11 (36%)	47,48,48	3.43	26 (55%)
23	4QM	A	2003	-	30,30,30	1.87	11 (36%)	47,48,48	3.38	26 (55%)

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
23	4QM	C	401	-	-	1/7/72/72	0/4/4/4
23	4QM	A	2003	-	-	1/7/72/72	0/4/4/4

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	2003	4QM	C16-C17	3.80	1.59	1.52
23	C	401	4QM	C16-C17	3.79	1.59	1.52
23	C	401	4QM	C16-C15	3.71	1.59	1.53
23	A	2003	4QM	C16-C15	3.69	1.59	1.53
23	A	2003	4QM	C7-C6	-3.25	1.47	1.54
23	C	401	4QM	C7-C6	-3.11	1.47	1.54
23	C	401	4QM	C2-C19	2.99	1.61	1.56
23	C	401	4QM	C14-C13	2.92	1.57	1.51
23	A	2003	4QM	C14-C13	2.80	1.57	1.51
23	A	2003	4QM	C5-C6	-2.65	1.51	1.55
23	A	2003	4QM	C2-C19	2.61	1.60	1.56
23	C	401	4QM	C1-C2	2.58	1.58	1.54
23	C	401	4QM	C5-C6	-2.52	1.51	1.55
23	A	2003	4QM	C1-C2	2.51	1.58	1.54
23	C	401	4QM	C3-C4	-2.38	1.49	1.53
23	A	2003	4QM	C18-C6	-2.36	1.49	1.53
23	A	2003	4QM	O4-C4	-2.35	1.39	1.43
23	A	2003	4QM	C3-C4	-2.35	1.49	1.53
23	C	401	4QM	O4-C4	-2.34	1.39	1.43
23	A	2003	4QM	O3-C17	-2.25	1.38	1.43
23	C	401	4QM	O3-C17	-2.23	1.38	1.43
23	C	401	4QM	C18-C6	-2.21	1.49	1.53

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	401	4QM	C10-C5-C4	8.00	117.21	109.07
23	A	2003	4QM	C10-C5-C4	7.74	116.95	109.07
23	C	401	4QM	C10-C5-C6	-6.61	100.87	111.21
23	A	2003	4QM	C10-C5-C6	-6.31	101.34	111.21
23	C	401	4QM	C2-C19-C18	5.99	118.25	111.82
23	C	401	4QM	C1-C2-C15	5.98	116.61	107.77
23	A	2003	4QM	C1-C2-C15	5.86	116.44	107.77
23	C	401	4QM	C5-C6-C18	-5.75	107.40	114.74
23	C	401	4QM	C5-C9-C20	-5.61	112.79	119.50
23	C	401	4QM	C11-C2-C1	-5.61	99.22	108.26
23	A	2003	4QM	C5-C6-C18	-5.50	107.72	114.74
23	A	2003	4QM	C5-C9-C20	-5.49	112.94	119.50
23	A	2003	4QM	C11-C2-C1	-5.44	99.50	108.26
23	A	2003	4QM	C6-C18-C17	-5.35	104.71	111.81
23	A	2003	4QM	C19-C2-C15	-5.03	101.51	108.58
23	C	401	4QM	C6-C18-C17	-5.00	105.18	111.81
23	A	2003	4QM	C2-C19-C18	4.83	117.00	111.82
23	A	2003	4QM	C9-C5-C6	-4.76	95.29	100.09
23	C	401	4QM	C19-C2-C15	-4.63	102.07	108.58
23	C	401	4QM	C9-C5-C4	-4.50	113.56	117.67
23	C	401	4QM	C9-C5-C6	-4.44	95.61	100.09
23	C	401	4QM	C16-C15-C14	4.39	116.25	111.19
23	A	2003	4QM	C9-C5-C4	-4.35	113.69	117.67
23	A	2003	4QM	C7-C6-C5	4.33	107.80	103.55
23	C	401	4QM	C7-C6-C5	4.21	107.69	103.55
23	A	2003	4QM	C16-C15-C14	4.21	116.04	111.19
23	A	2003	4QM	C14-C15-C2	-4.01	108.40	112.66
23	A	2003	4QM	C8-C7-C6	-4.00	97.19	105.13
23	C	401	4QM	C8-C7-C6	-3.98	97.25	105.13
23	C	401	4QM	C11-C2-C19	3.97	116.65	111.18
23	A	2003	4QM	C19-C18-C6	3.91	115.07	109.71
23	C	401	4QM	C14-C15-C2	-3.78	108.64	112.66
23	C	401	4QM	C3-C19-C2	-3.65	109.96	113.73
23	A	2003	4QM	C11-C2-C19	3.63	116.19	111.18
23	A	2003	4QM	C10-C5-C9	3.49	116.67	111.21
23	A	2003	4QM	C3-C19-C2	-3.47	110.15	113.73
23	C	401	4QM	C19-C18-C6	3.45	114.44	109.71
23	A	2003	4QM	C16-C17-C18	-3.35	107.91	111.48
23	C	401	4QM	C16-C17-C18	-3.33	107.93	111.48
23	C	401	4QM	C10-C5-C9	3.28	116.35	111.21
23	C	401	4QM	C21-C20-C9	3.18	117.80	112.92
23	A	2003	4QM	C21-C20-C9	3.14	117.74	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	2003	4QM	O3-C17-C18	-2.95	102.84	109.43
23	C	401	4QM	O3-C17-C18	-2.86	103.04	109.43
23	C	401	4QM	C15-C14-C13	2.63	116.63	112.76
23	A	2003	4QM	C15-C14-C13	2.58	116.55	112.76
23	C	401	4QM	C6-C5-C4	2.45	109.68	107.40
23	A	2003	4QM	C16-C15-C2	2.26	115.06	112.66
23	A	2003	4QM	C8-C9-C20	-2.22	108.72	112.15
23	C	401	4QM	C16-C15-C2	2.14	114.93	112.66
23	C	401	4QM	C8-C9-C20	-2.09	108.91	112.15
23	A	2003	4QM	C6-C5-C4	2.01	109.27	107.40

There are no chirality outliers.

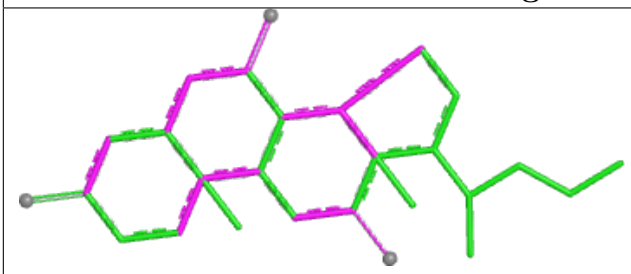
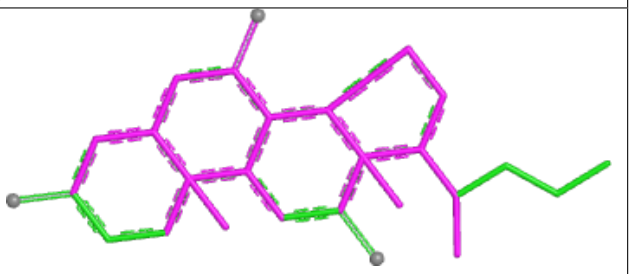
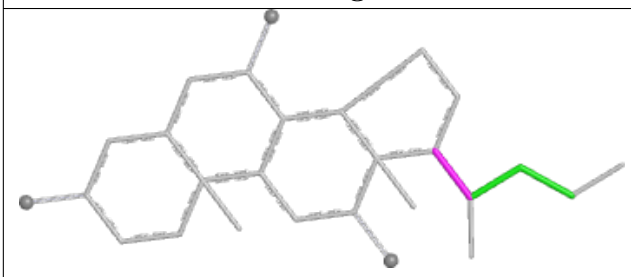
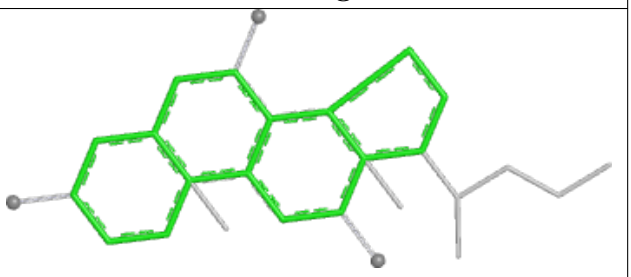
All (2) torsion outliers are listed below:

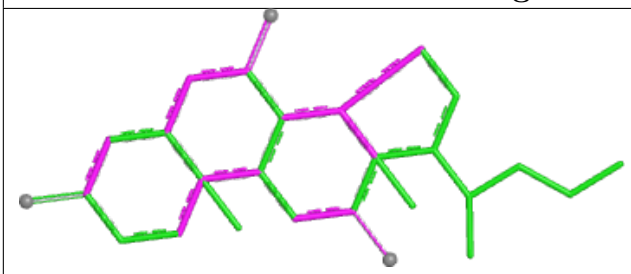
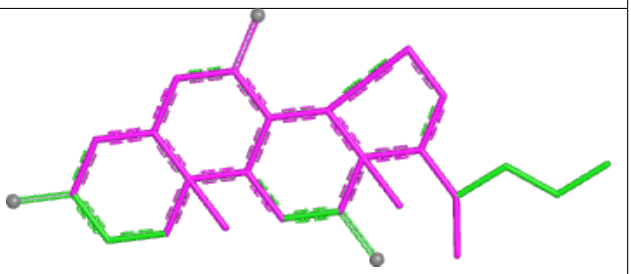
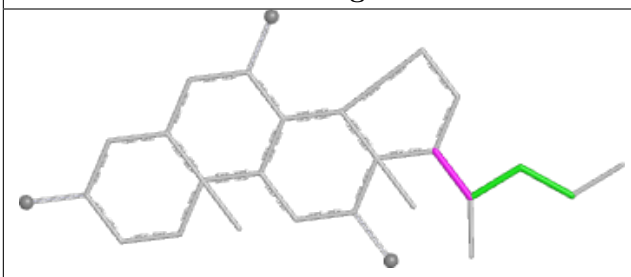
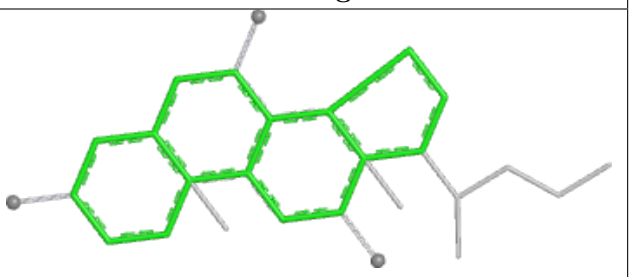
Mol	Chain	Res	Type	Atoms
23	C	401	4QM	C22-C20-C9-C5
23	A	2003	4QM	C22-C20-C9-C5

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 4QM C 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 4QM A 2003	
 Bond lengths	 Bond angles
 Torsions	 Rings

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
1	A	1
10	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1456:ALA	C	1457:LEU	N	3.23
1	J	67:GLU	C	68:LYS	N	3.12

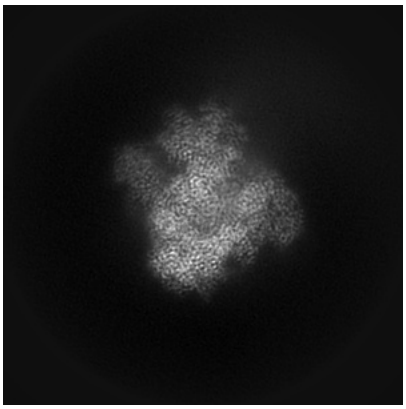
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14447. These allow visual inspection of the internal detail of the map and identification of artifacts.

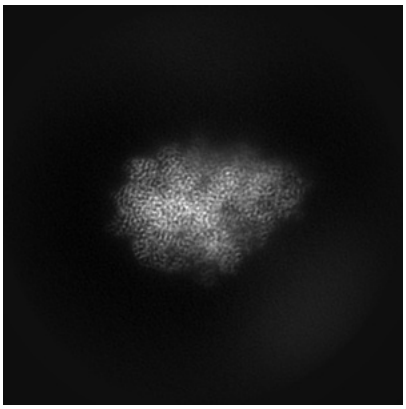
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

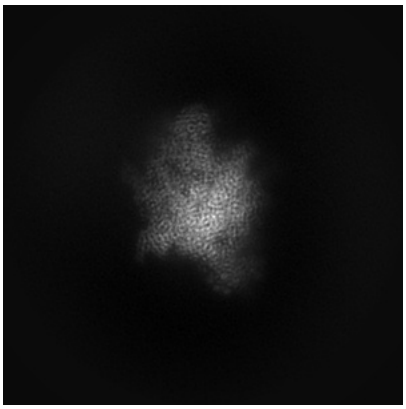
6.1.1 Primary map



X

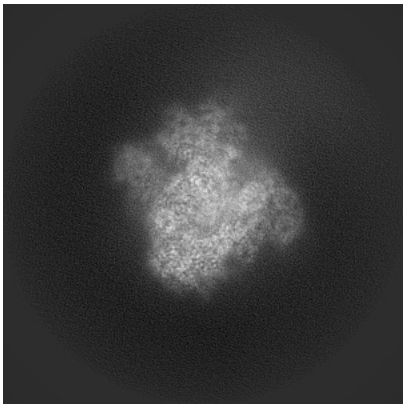


Y

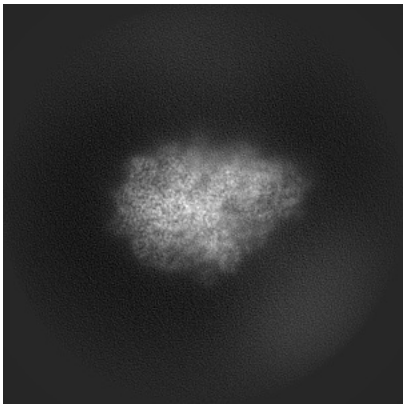


Z

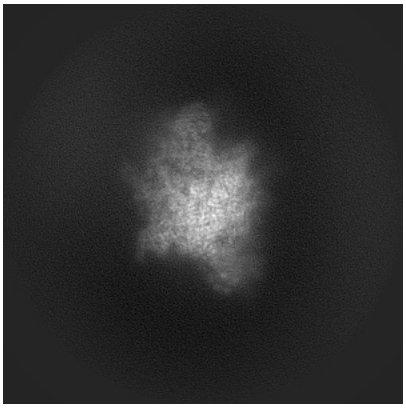
6.1.2 Raw map



X



Y

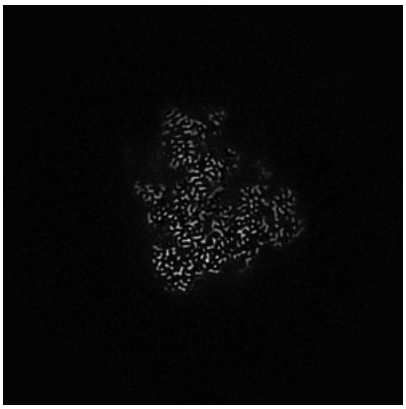


Z

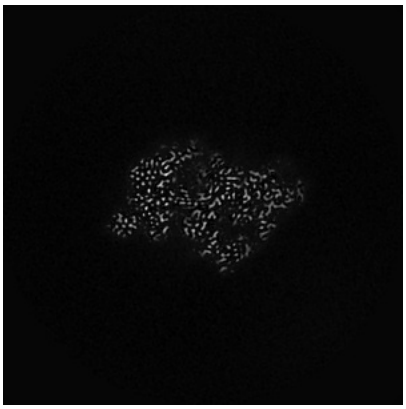
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

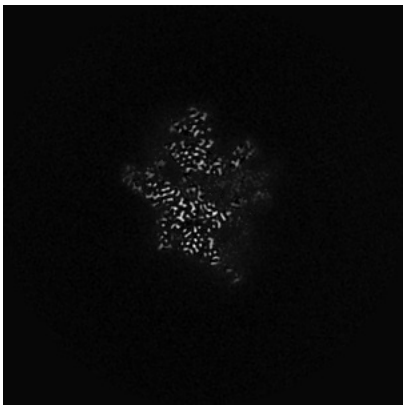
6.2.1 Primary map



X Index: 175

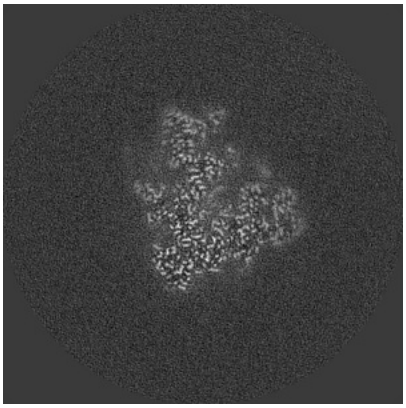


Y Index: 175

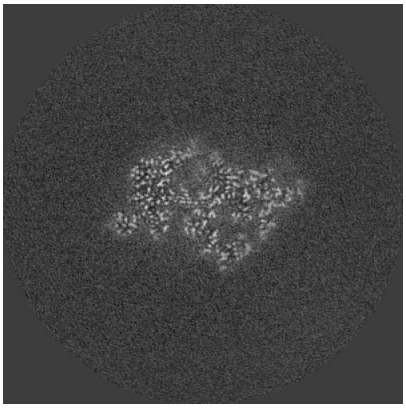


Z Index: 175

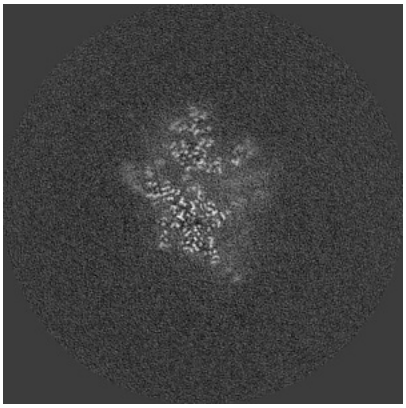
6.2.2 Raw map



X Index: 175



Y Index: 175

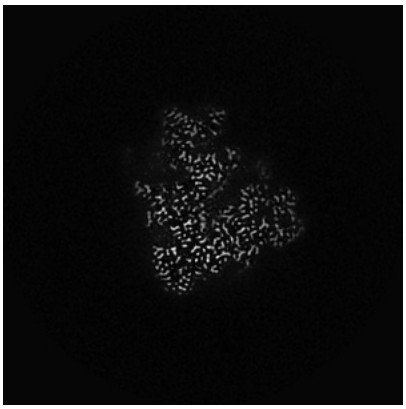


Z Index: 175

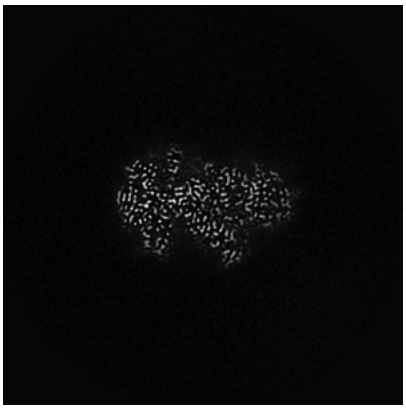
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

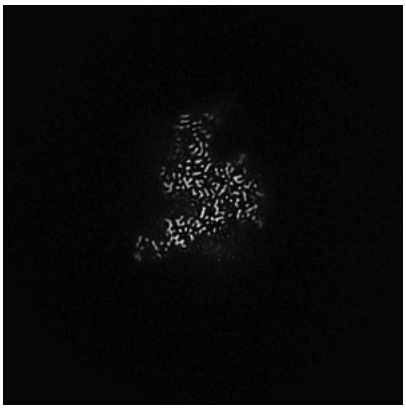
6.3.1 Primary map



X Index: 176

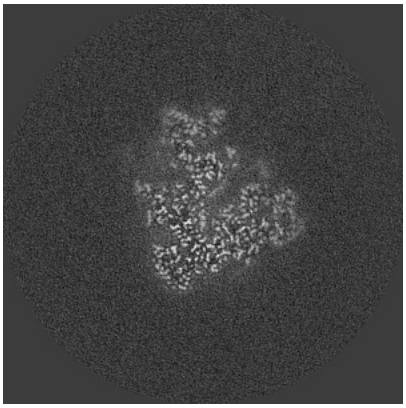


Y Index: 164

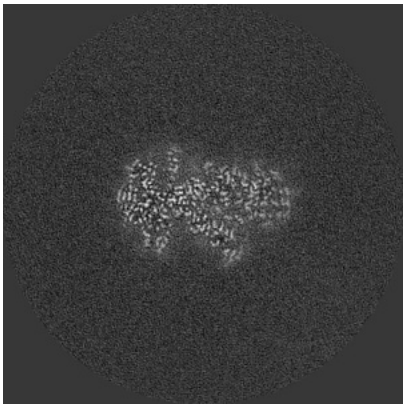


Z Index: 146

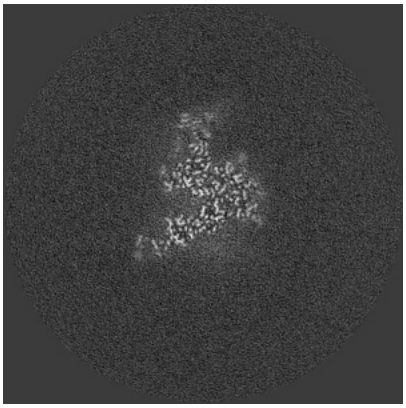
6.3.2 Raw map



X Index: 176



Y Index: 164



Z Index: 146

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

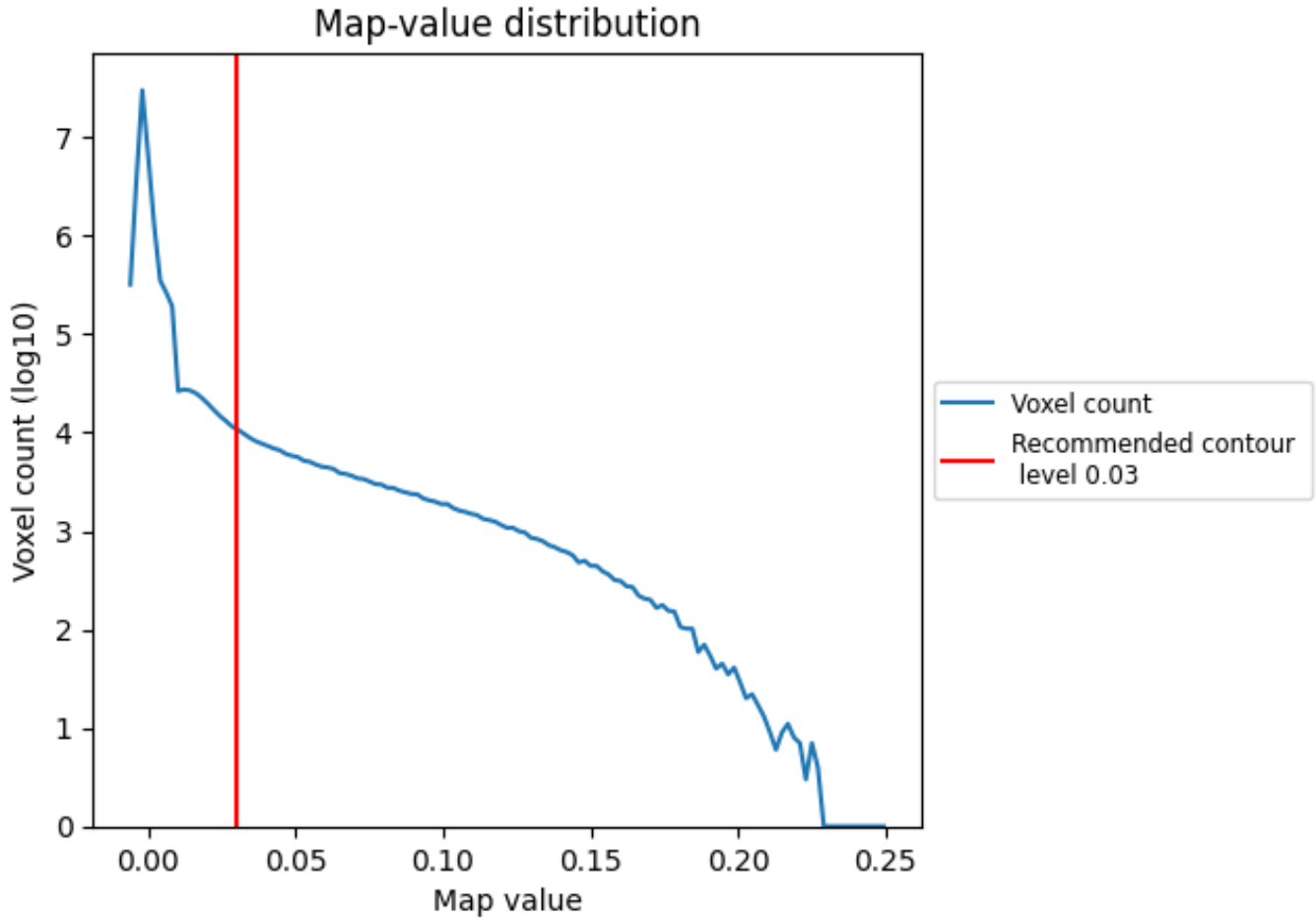
6.5 Mask visualisation (i)

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

7 Map analysis

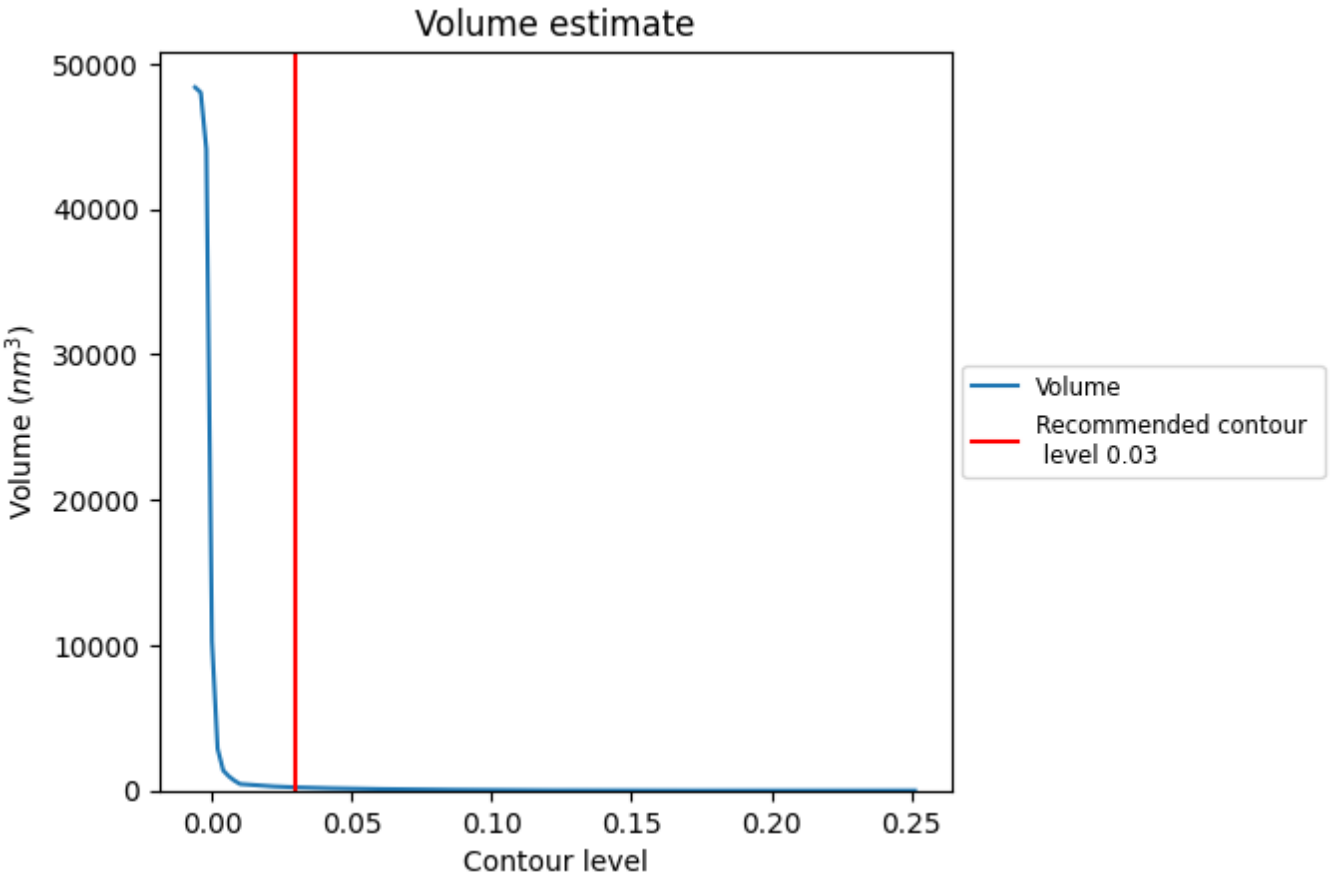
This section contains the results of statistical analysis of the map.

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.

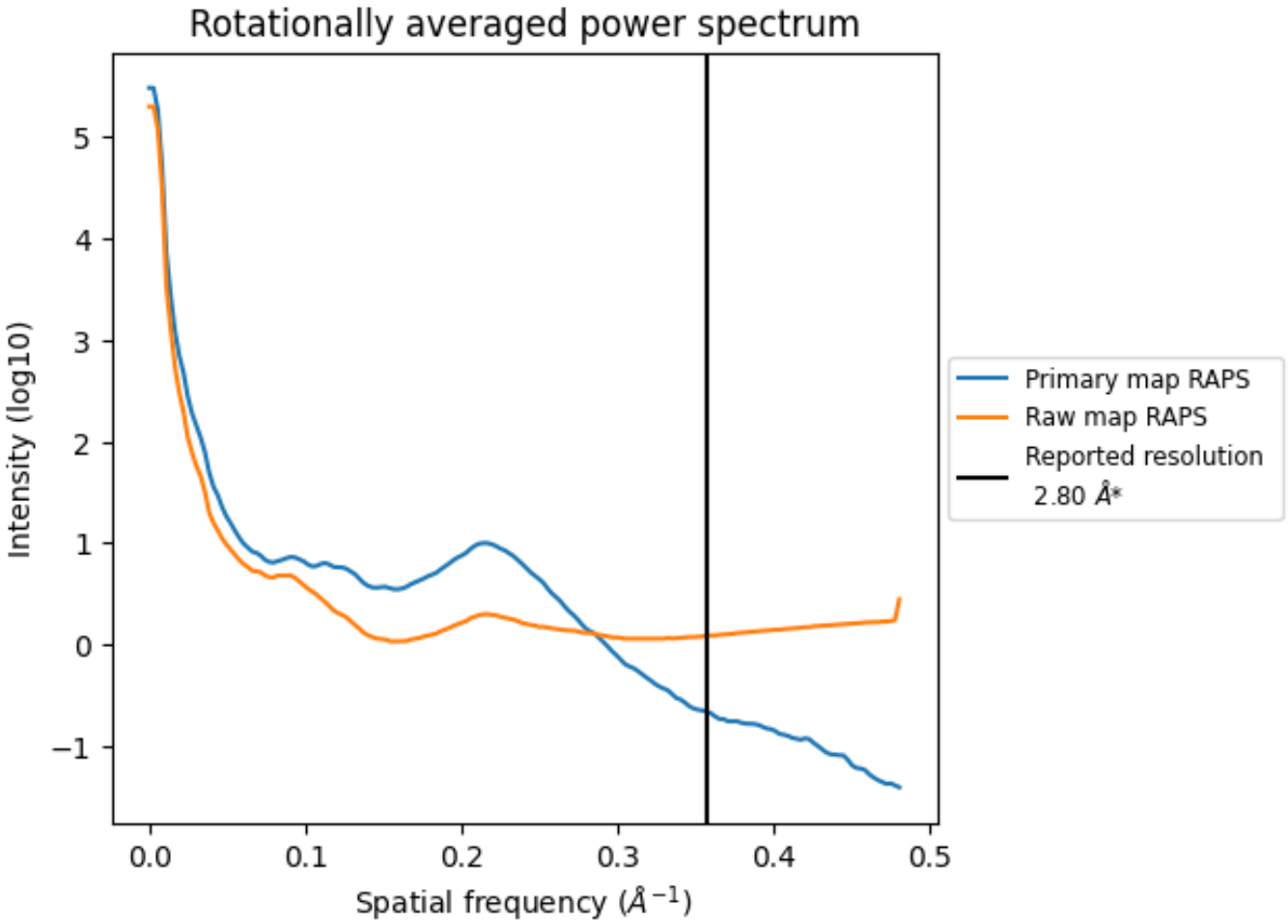
7.2 Volume estimate



The volume at the recommended contour level is 221 nm^3; this corresponds to an approximate mass of 200 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

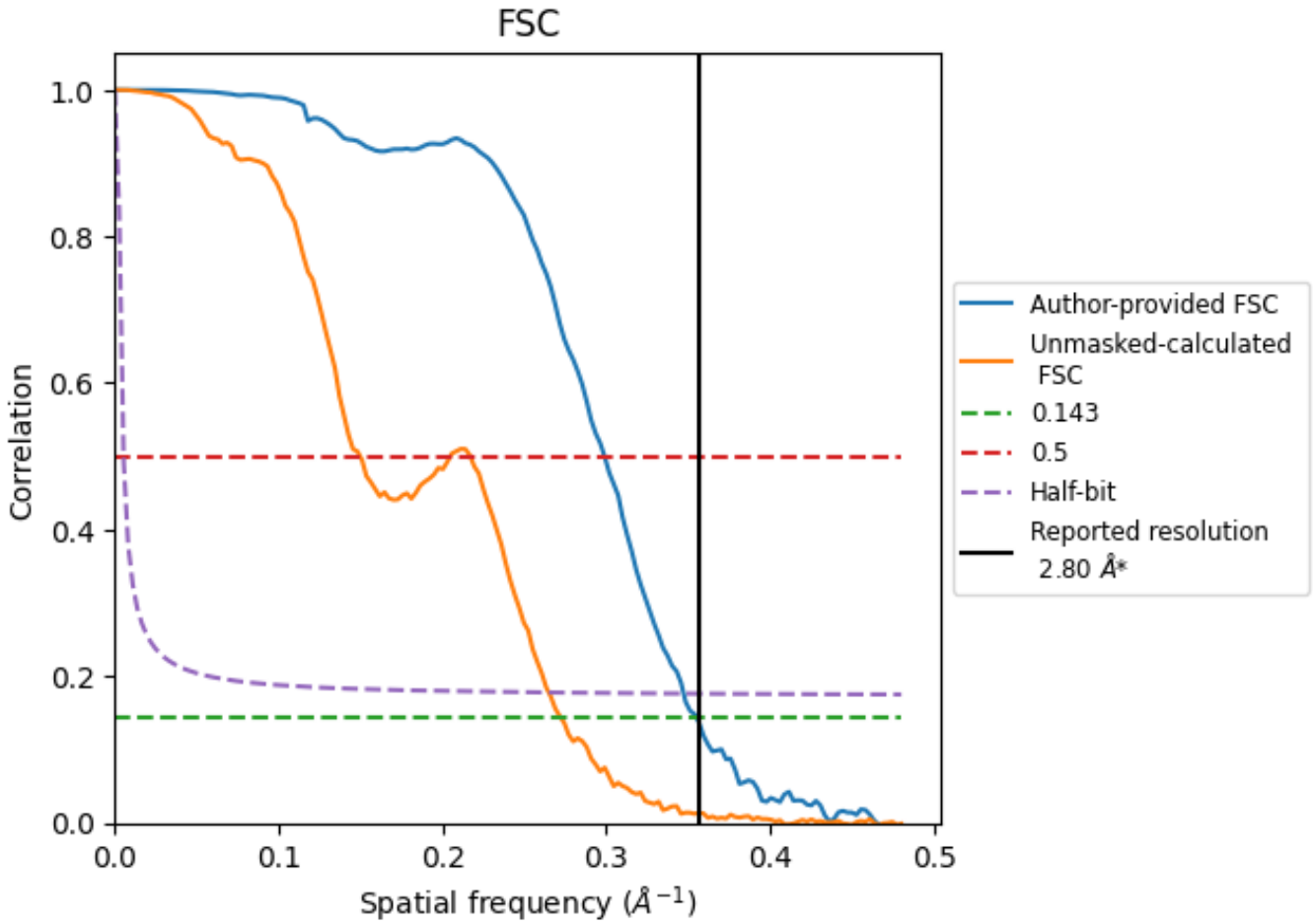


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



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

8.2 Resolution estimates (i)

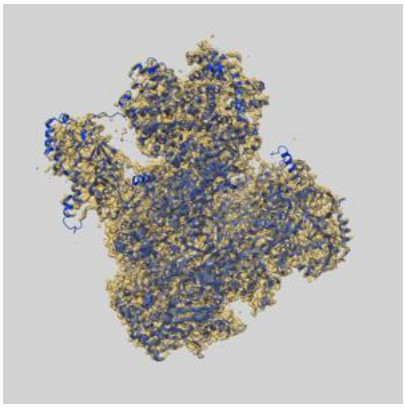
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.82	3.34	2.88
Unmasked-calculated*	3.67	6.68	3.77

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

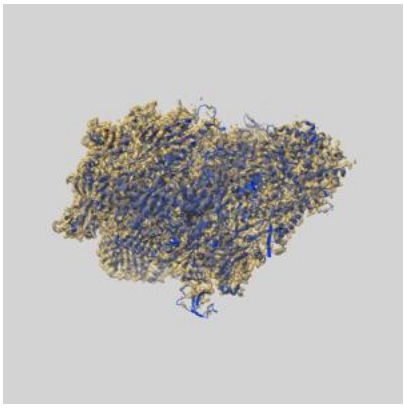
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14447 and PDB model 7Z1L. Per-residue inclusion information can be found in section 3 on page 8.

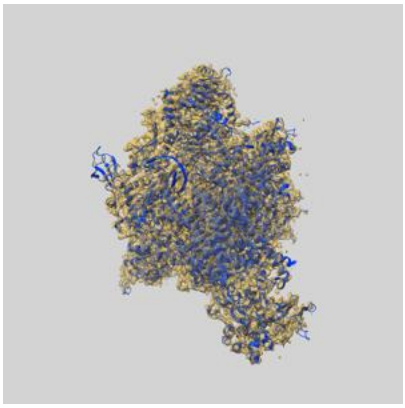
9.1 Map-model overlay



X



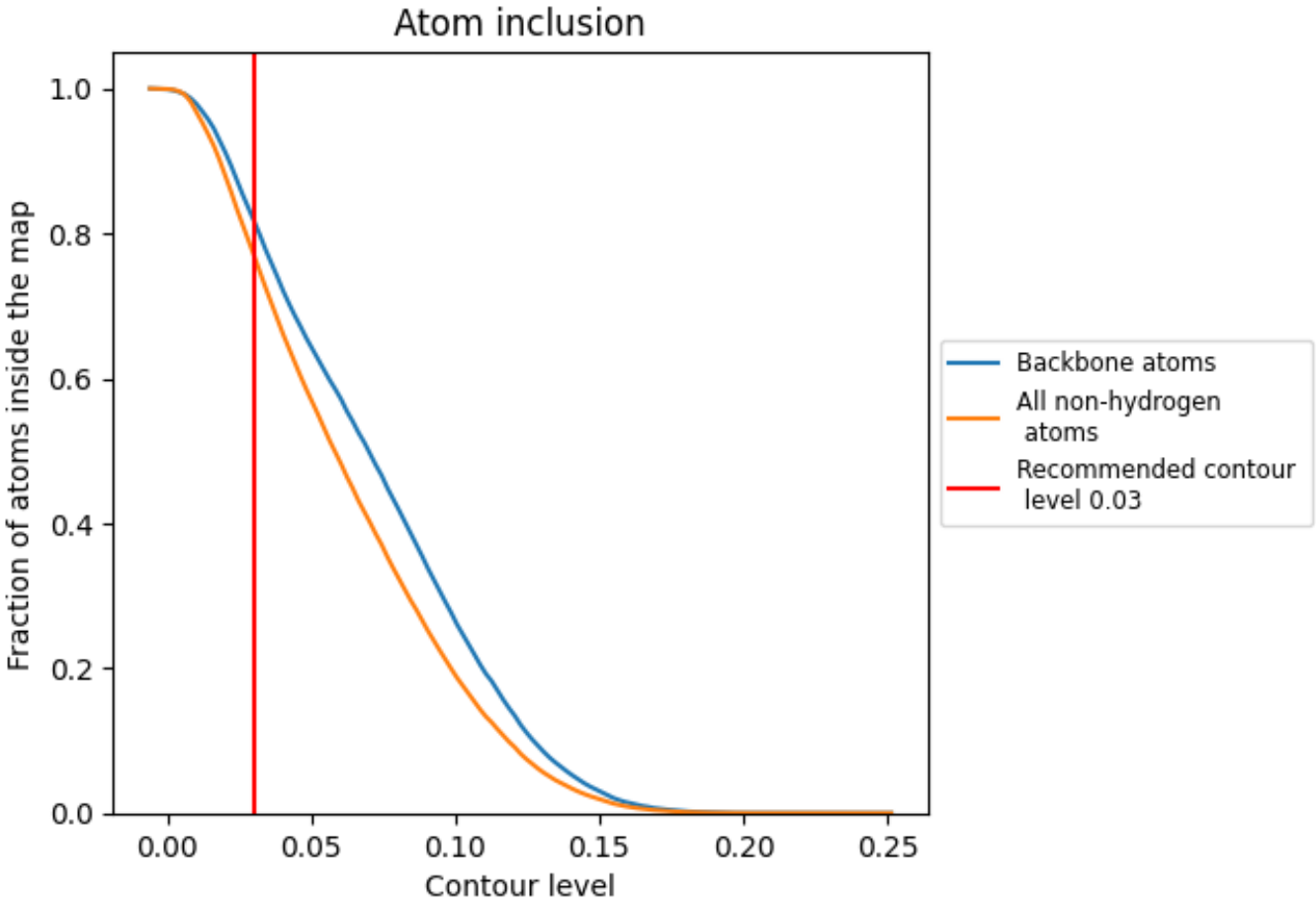
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.