



Full wwPDB EM Validation Report ⓘ

Jul 14, 2026 – 07:06 AM JST

PDB ID : 9WQ7 / pdb_00009wq7
EMDB ID : EMD-66161
Title : Structure of yeast Pol II-Elf1 complex containing a cisplatin-ICL lesion at +7 position.
Authors : Xu, J.; Zhu, L.
Deposited on : 2025-09-10
Resolution : 2.72 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

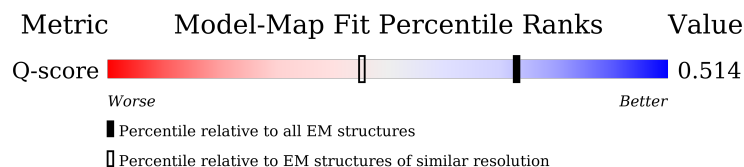
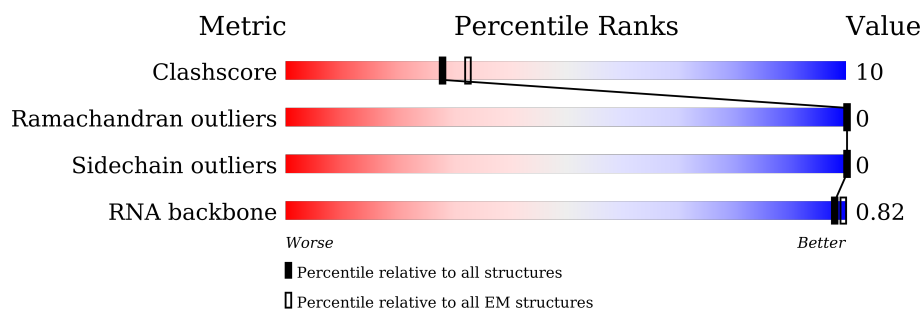
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 2.72 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.



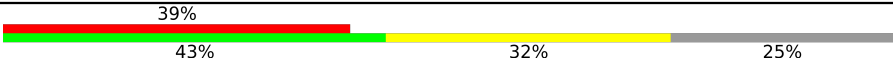
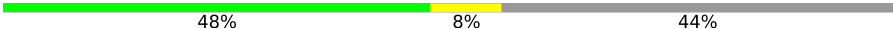
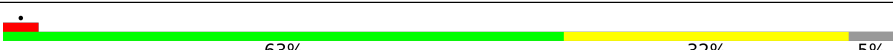
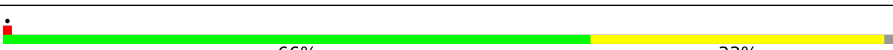
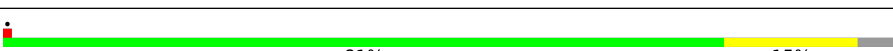
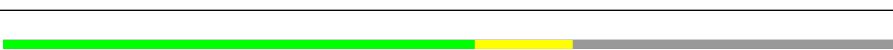
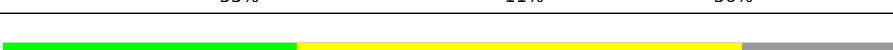
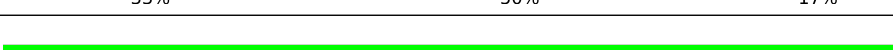
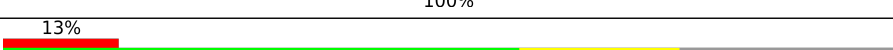
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10355 (2.22 - 3.22)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	5% 64% 18% 18%
2	B	1224	5% 77% 20% •
3	C	318	65% 19% 17%

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Mol	Chain	Length	Quality of chain
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	18	
14	P	6	
15	Q	85	
16	T	25	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	ZN	Q	101	-	-	X	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 33146 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1424	Total	C	N	O	S	0	0
			11205	7060	1958	2125	62		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1183	Total	C	N	O	S	0	0
			9421	5955	1648	1762	56		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	265	Total	C	N	O	S	0	0
			2086	1312	347	414	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	165	Total	C	N	O	S	0	0
			1326	820	237	267	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	87	Total	C	N	O	S	0	0
			705	451	119	132	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1339	861	222	248	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	139	Total	C	N	O	S	0	0
			1113	699	187	223	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			924	593	157	172	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			359	221	71	63	4		

- Molecule 13 is a DNA chain called DNA (NTS, non-template strand).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	15	Total	C	N	O	P	0	0
			321	149	73	84	15		

- Molecule 14 is a RNA chain called RNA (5'-R(P*GP*GP*GP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	6	Total	C	N	O	P	0	0
			135	60	30	39	6		

- Molecule 15 is a protein called Transcription elongation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	64	Total	C	N	O	S	0	0
			504	316	84	99	5		

- Molecule 16 is a DNA chain called DNA (TS, template strand).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	22	Total	C	N	O	P	0	0
			430	208	59	141	22		

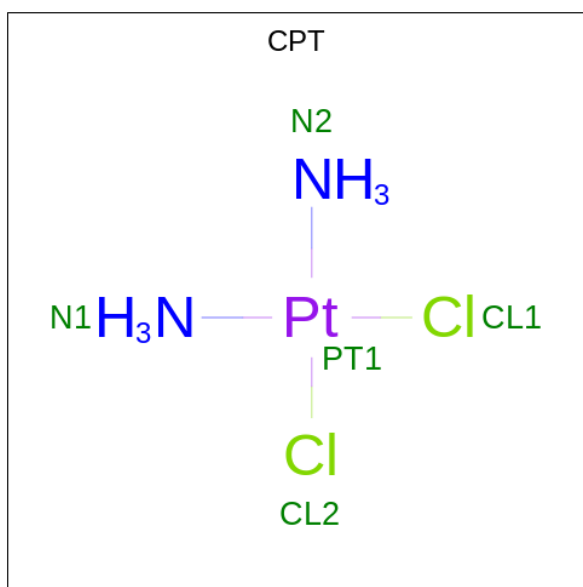
- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 19 is Cisplatin (CCD ID: CPT) (formula: $\text{Cl}_2\text{H}_6\text{N}_2\text{Pt}$) (labeled as "Ligand of Interest" by depositor).

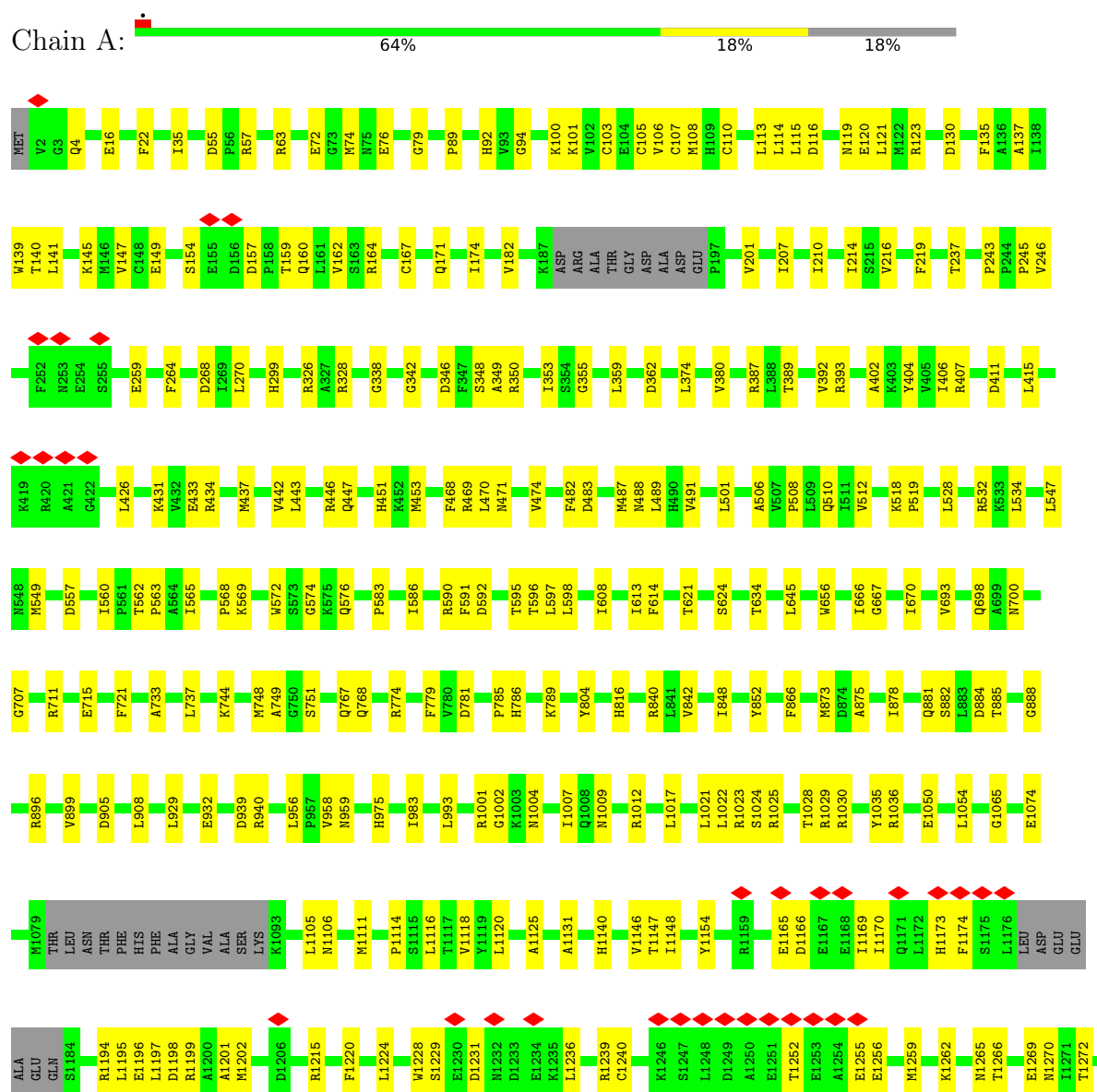


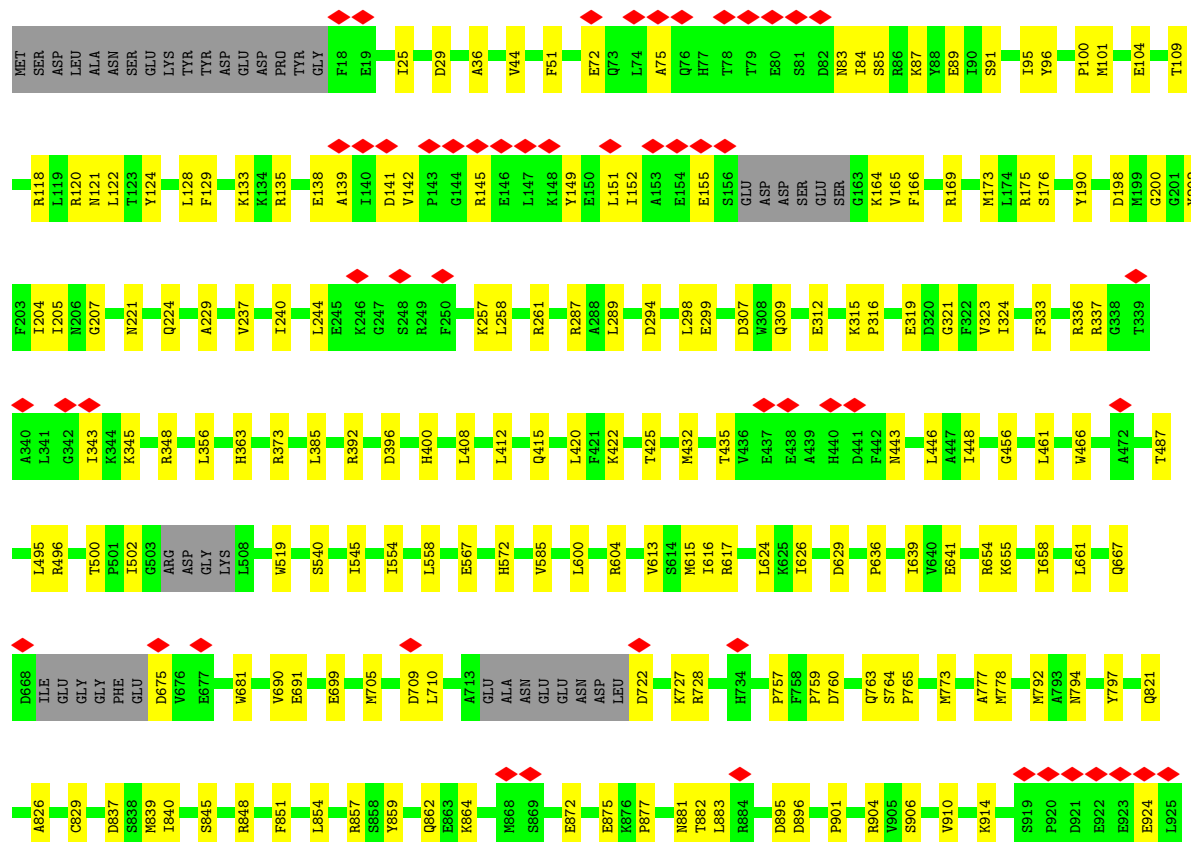
Mol	Chain	Residues	Atoms			AltConf
19	T	1	Total	N	Pt	0
			3	2	1	

3 Residue-property plots

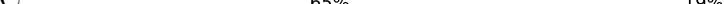
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

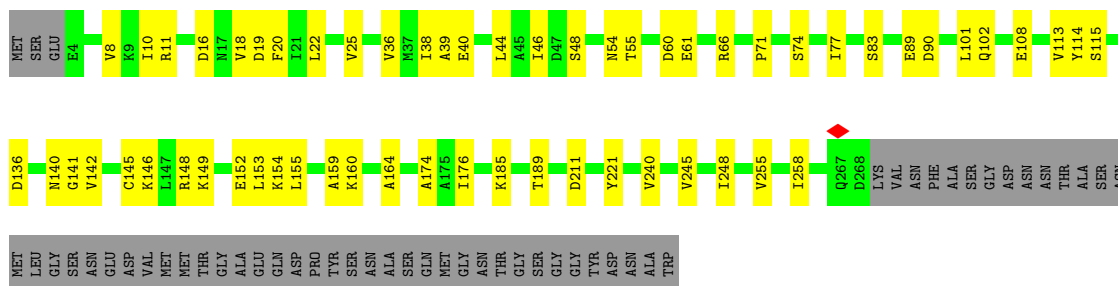
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



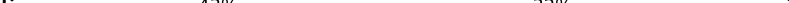


- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:  65% 19% 17%



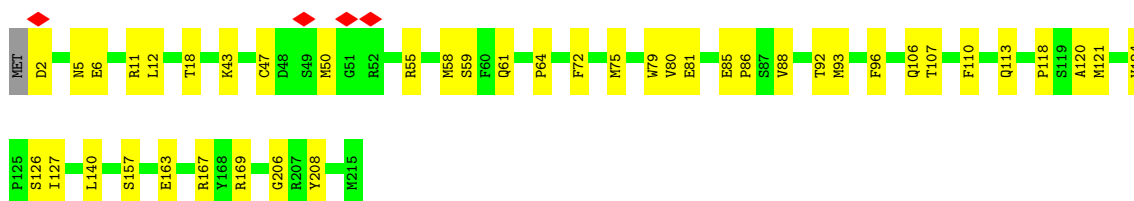
- Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D: 

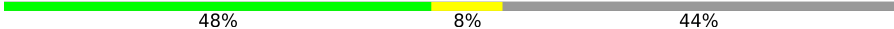


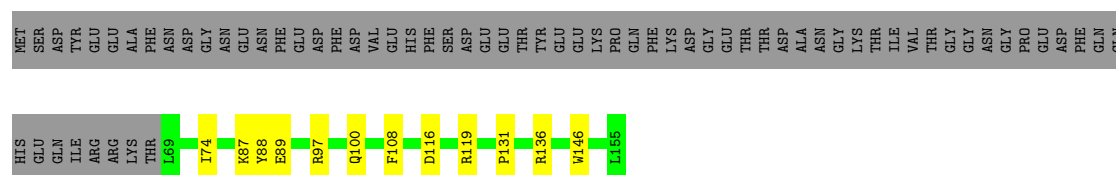
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 80% 20%



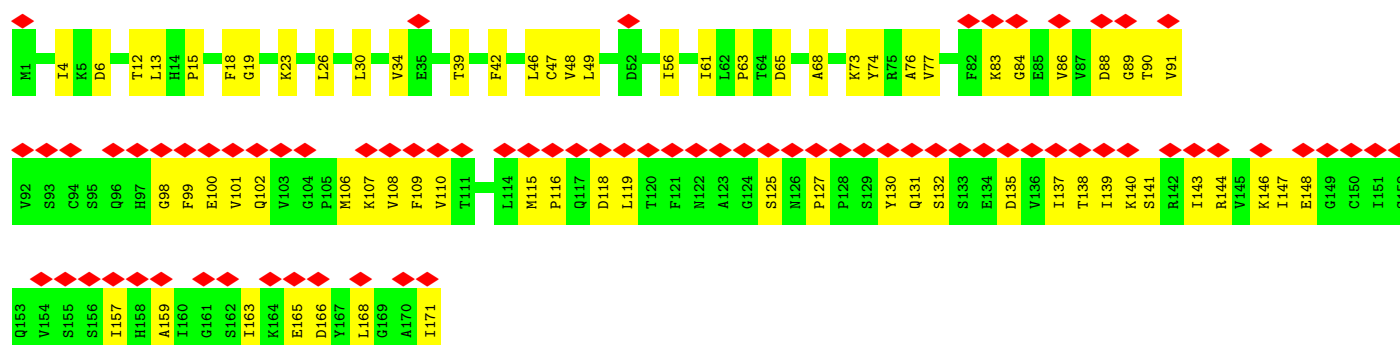
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 



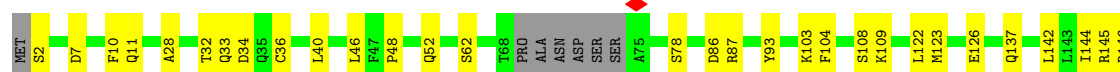
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G: 



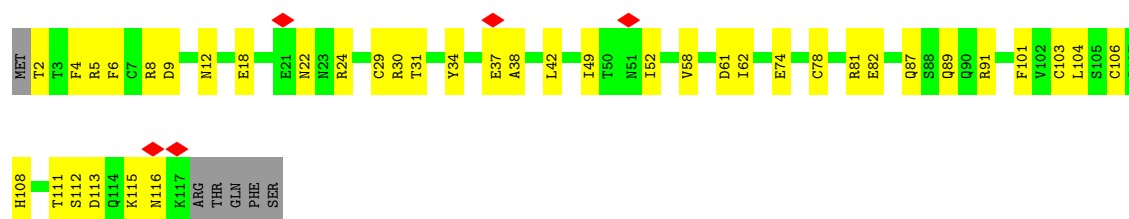
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 



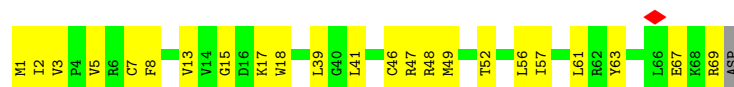
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I: 

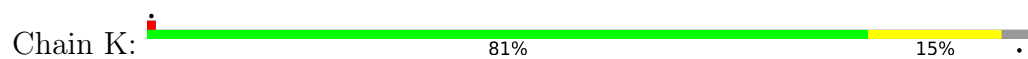


- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

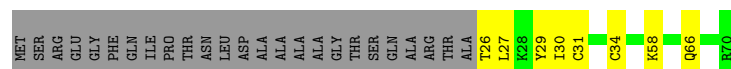
Chain J: 



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



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



- Molecule 13: DNA (NTS, non-template strand)



- Molecule 14: RNA (5'-R(P*GP*GP*GP*AP*AP*A)-3')



There are no outlier residues recorded for this chain.

- Molecule 15: Transcription elongation factor 1



- Molecule 16: DNA (TS, template strand)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	147292	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.817	Depositor
Minimum map value	-0.401	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	297.6, 297.6, 297.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

5 Model quality

5.1 Standard geometry

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

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	0/11406	0.33	0/15423
2	B	0.26	0/9607	0.33	0/12958
3	C	0.26	0/2124	0.32	0/2879
4	D	0.14	0/1334	0.36	0/1789
5	E	0.23	0/1788	0.34	0/2406
6	F	0.26	0/717	0.33	0/967
7	G	0.16	0/1367	0.36	0/1844
8	H	0.22	0/1131	0.26	0/1532
9	I	0.18	0/962	0.31	0/1295
10	J	0.28	0/578	0.32	0/775
11	K	0.25	0/942	0.28	0/1272
12	L	0.21	0/361	0.32	0/478
13	N	0.56	0/364	0.84	0/562
14	P	0.68	0/152	0.86	0/236
15	Q	0.14	0/512	0.32	0/690
16	T	0.63	0/474	1.04	0/725
All	All	0.26	0/33819	0.36	0/45831

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	11205	0	11277	213	0
2	B	9421	0	9421	186	0
3	C	2086	0	2045	46	0
4	D	1326	0	1348	61	0
5	E	1752	0	1776	26	0
6	F	705	0	731	7	0
7	G	1339	0	1357	56	0
8	H	1113	0	1079	20	0
9	I	944	0	899	31	0
10	J	569	0	585	18	0
11	K	924	0	934	16	0
12	L	359	0	381	8	0
13	N	321	0	166	7	0
14	P	135	0	66	0	0
15	Q	504	0	493	15	0
16	T	430	0	252	15	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
17	Q	1	0	0	2	0
18	A	1	0	0	0	0
19	T	3	0	0	2	0
All	All	33146	0	32810	632	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 10.

All (632) 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)
9:I:78:CYS:SG	9:I:106:CYS:HB3	2.07	0.94
4:D:214:LEU:O	4:D:218:GLU:N	2.03	0.90
4:D:210:ILE:O	4:D:214:LEU:N	2.06	0.88
16:T:12:DC:C5	19:T:101:CPT:N1	2.41	0.87
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.54	0.87
1:A:469:ARG:NH2	2:B:991:GLY:O	2.10	0.85
2:B:312:GLU:OE1	2:B:315:LYS:NZ	2.14	0.81
4:D:211:LEU:HA	4:D:214:LEU:HB2	1.63	0.80
1:A:1286:LYS:HD2	1:A:1302:PRO:HB2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:ARG:NH2	2:B:294:ASP:OD1	2.18	0.77
2:B:337:ARG:HH21	15:Q:65:GLN:HE21	1.29	0.77
7:G:125:SER:HB3	7:G:131:GLN:HB2	1.66	0.77
3:C:102:GLN:HG2	3:C:154:LYS:HG2	1.68	0.76
1:A:597:LEU:HD21	8:H:103:LYS:HG2	1.70	0.73
9:I:74:GLU:OE1	9:I:81:ARG:NH2	2.21	0.73
2:B:229:ALA:O	2:B:261:ARG:NH1	2.21	0.72
1:A:107:CYS:SG	1:A:171:GLN:NE2	2.63	0.72
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.71	0.72
5:E:2:ASP:HB2	5:E:5:ASN:HB3	1.70	0.71
4:D:206:GLU:HA	4:D:209:ARG:HG2	1.72	0.71
2:B:837:ASP:OD1	2:B:1020:ARG:NH2	2.23	0.71
6:F:97:ARG:NH1	6:F:100:GLN:OE1	2.24	0.70
2:B:135:ARG:HD2	2:B:155:GLU:HG3	1.72	0.70
1:A:562:THR:O	1:A:576:GLN:NE2	2.24	0.70
2:B:85:SER:N	2:B:139:ALA:O	2.24	0.70
2:B:928:ARG:NH1	2:B:929:THR:O	2.25	0.70
2:B:996:ARG:NH1	3:C:174:ALA:O	2.24	0.69
16:T:12:DC:H5	19:T:101:CPT:N1	1.90	0.69
1:A:1166:ASP:OD2	1:A:1239:ARG:NH1	2.24	0.69
1:A:1256:GLU:HA	1:A:1259:MET:HB3	1.73	0.69
2:B:999:MET:HE3	2:B:1008:PRO:HG2	1.74	0.69
1:A:929:LEU:HD21	1:A:983:ILE:HG21	1.73	0.69
10:J:48:ARG:NH1	10:J:49:MET:SD	2.65	0.69
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.74	0.69
2:B:307:ASP:OD2	2:B:392:ARG:NH1	2.26	0.68
2:B:728:ARG:NH1	2:B:760:ASP:OD2	2.25	0.68
1:A:1173:HIS:NE2	1:A:1228:TRP:O	2.26	0.67
2:B:901:PRO:HA	2:B:949:VAL:HG13	1.75	0.67
7:G:108:VAL:HG22	7:G:159:ALA:HB3	1.77	0.67
1:A:896:ARG:HD2	1:A:1030:ARG:HH11	1.59	0.67
4:D:14:ARG:HH12	4:D:18:VAL:H	1.43	0.67
1:A:767:GLN:NE2	1:A:768:GLN:O	2.27	0.66
15:Q:52:CYS:HG	17:Q:101:ZN:ZN	1.07	0.66
1:A:1397:LEU:HB2	1:A:1426:GLU:HG3	1.78	0.66
5:E:106:GLN:HG2	5:E:107:THR:HG23	1.77	0.66
4:D:209:ARG:O	4:D:213:GLU:N	2.25	0.66
1:A:596:THR:OG1	1:A:598:LEU:O	2.13	0.66
1:A:707:GLY:HA2	1:A:1281:ARG:HD3	1.78	0.66
1:A:1215:ARG:NH2	1:A:1272:THR:O	2.29	0.65
11:K:24:ASP:OD2	11:K:74:ARG:NE	2.23	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1111:MET:HE3	1:A:1114:PRO:HA	1.79	0.65
3:C:10:ILE:HA	3:C:20:PHE:HA	1.79	0.65
2:B:1219:ASP:OD1	4:D:13:ARG:NH2	2.30	0.65
4:D:185:CYS:SG	4:D:186:ASP:N	2.70	0.64
9:I:5:ARG:HH12	9:I:38:ALA:HA	1.63	0.64
1:A:1147:THR:HG21	1:A:1195:LEU:HD23	1.80	0.63
2:B:337:ARG:NH1	15:Q:68:ASP:OD1	2.30	0.63
4:D:152:SER:O	4:D:155:ARG:NH2	2.30	0.63
7:G:39:THR:HG23	7:G:42:PHE:H	1.64	0.63
2:B:309:GLN:HE22	9:I:52:ILE:HD11	1.64	0.63
7:G:15:PRO:HA	7:G:18:PHE:CE2	2.33	0.63
8:H:10:PHE:HB3	8:H:28:ALA:HB1	1.80	0.63
1:A:1116:LEU:HD21	1:A:1327:ILE:HD11	1.80	0.63
4:D:59:ILE:HD11	7:G:77:VAL:HG21	1.80	0.63
8:H:2:SER:HA	8:H:62:SER:HB3	1.81	0.63
2:B:319:GLU:OE1	9:I:30:ARG:NH1	2.31	0.63
4:D:208:GLU:O	4:D:212:LYS:N	2.32	0.62
1:A:1445:ILE:HG13	7:G:61:ILE:HD11	1.80	0.62
2:B:487:THR:OG1	2:B:777:ALA:O	2.17	0.62
3:C:258:ILE:HG13	11:K:42:LEU:HD21	1.81	0.62
3:C:71:PRO:HG3	10:J:13:VAL:HG21	1.82	0.62
1:A:1329:THR:HG22	1:A:1331:SER:H	1.64	0.62
15:Q:52:CYS:SG	17:Q:101:ZN:ZN	1.87	0.62
4:D:62:ALA:HB2	7:G:49:LEU:HD13	1.81	0.62
2:B:85:SER:HB2	2:B:139:ALA:HB3	1.82	0.61
1:A:483:ASP:HB2	2:B:987:LYS:HG3	1.82	0.61
1:A:568:PRO:HD2	8:H:46:LEU:HG	1.81	0.61
4:D:174:PRO:HA	4:D:177:VAL:HG22	1.81	0.61
6:F:136:ARG:HD2	6:F:146:TRP:CD1	2.35	0.61
2:B:101:MET:HE2	2:B:109:THR:HG22	1.82	0.61
2:B:400:HIS:NE2	2:B:699:GLU:OE2	2.25	0.61
4:D:30:GLY:O	4:D:34:GLN:NE2	2.29	0.61
4:D:141:LEU:HA	7:G:46:LEU:HD12	1.83	0.61
4:D:166:LEU:O	4:D:169:SER:OG	2.14	0.61
1:A:1199:ARG:NH1	1:A:1231:ASP:OD1	2.34	0.61
2:B:896:ASP:OD2	12:L:58:LYS:NZ	2.32	0.61
2:B:952:VAL:HG12	2:B:966:VAL:HG13	1.83	0.61
1:A:1423:GLY:O	1:A:1427:ASN:ND2	2.34	0.60
2:B:91:SER:HB3	2:B:133:LYS:HB3	1.83	0.60
1:A:1279:ILE:HD12	1:A:1308:THR:HG21	1.82	0.60
4:D:69:ALA:HA	4:D:72:ARG:HG2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:792:MET:SD	2:B:857:ARG:NH2	2.75	0.60
3:C:83:SER:HB3	3:C:160:LYS:HG2	1.84	0.60
10:J:7:CYS:HA	10:J:49:MET:HG3	1.84	0.60
1:A:1154:TYR:OH	9:I:18:GLU:OE2	2.20	0.60
1:A:346:ASP:OD1	2:B:1106:ARG:NE	2.35	0.59
4:D:118:THR:HG23	4:D:121:LYS:H	1.67	0.59
2:B:604:ARG:NH2	2:B:691:GLU:OE2	2.34	0.59
1:A:359:LEU:O	1:A:471:ASN:ND2	2.34	0.59
8:H:123:MET:HE2	8:H:142:LEU:HD13	1.84	0.59
2:B:901:PRO:HD3	2:B:952:VAL:HG22	1.84	0.59
2:B:881:ASN:O	2:B:934:LYS:NZ	2.34	0.59
1:A:715:GLU:OE2	1:A:774:ARG:NH1	2.36	0.59
1:A:881:GLN:NE2	1:A:958:VAL:O	2.34	0.59
7:G:106:MET:HE3	7:G:157:ILE:HG23	1.84	0.59
1:A:693:VAL:HG21	1:A:721:PHE:HE2	1.66	0.59
1:A:1148:ILE:N	1:A:1196:GLU:O	2.34	0.59
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.85	0.58
1:A:1165:GLU:OE1	1:A:1194:ARG:NH2	2.36	0.58
2:B:778:MET:HE1	2:B:1098:MET:HE2	1.86	0.58
7:G:47:CYS:SG	7:G:48:VAL:N	2.75	0.58
7:G:127:PRO:HD2	7:G:138:THR:HB	1.84	0.58
2:B:129:PHE:HB3	2:B:164:LYS:HB2	1.83	0.58
16:T:10:DC:H2"	16:T:11:DT:H5"	1.85	0.58
1:A:120:GLU:OE1	1:A:123:ARG:NH2	2.37	0.58
1:A:534:LEU:O	1:A:574:GLY:HA3	2.04	0.57
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.85	0.57
15:Q:33:SER:HA	15:Q:50:LYS:HE2	1.85	0.57
1:A:182:VAL:HG12	1:A:201:VAL:HG22	1.86	0.57
2:B:896:ASP:OD2	12:L:29:TYR:OH	2.14	0.57
5:E:12:LEU:HG	5:E:58:MET:HE1	1.86	0.57
7:G:137:ILE:HD13	7:G:143:ILE:HD12	1.86	0.57
1:A:1009:ASN:OD1	1:A:1012:ARG:NH2	2.37	0.57
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.40	0.57
2:B:91:SER:HB3	2:B:133:LYS:HD2	1.85	0.57
7:G:116:PRO:HD2	7:G:119:LEU:HB3	1.86	0.57
2:B:839:MET:HE1	2:B:980:PHE:HB2	1.86	0.56
7:G:90:THR:O	7:G:102:GLN:N	2.31	0.56
1:A:528:LEU:HD23	1:A:751:SER:HA	1.86	0.56
1:A:840:ARG:NH1	1:A:1106:ASN:OD1	2.38	0.56
1:A:1265:ASN:ND2	1:A:1269:GLU:OE2	2.37	0.56
2:B:422:LYS:HA	2:B:425:THR:HG22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:32:THR:OG1	8:H:33:GLN:OE1	2.23	0.56
1:A:63:ARG:NE	1:A:63:ARG:O	2.37	0.56
1:A:882:SER:O	1:A:1025:ARG:NH2	2.36	0.56
1:A:1030:ARG:NH2	1:A:1035:TYR:OH	2.34	0.56
7:G:143:ILE:HD11	7:G:163:ILE:HD13	1.87	0.56
2:B:709:ASP:HB3	2:B:710:LEU:HD12	1.87	0.56
1:A:147:VAL:HG13	1:A:149:GLU:HG2	1.87	0.55
1:A:1220:PHE:HD2	1:A:1224:LEU:HD22	1.70	0.55
1:A:1443:VAL:HG12	7:G:61:ILE:HD13	1.87	0.55
4:D:141:LEU:HD13	7:G:46:LEU:HB3	1.87	0.55
2:B:1163:CYS:HB2	2:B:1187:ASN:HD21	1.71	0.55
5:E:85:GLU:OE2	5:E:92:THR:HG21	2.06	0.55
7:G:86:VAL:HA	7:G:146:LYS:HA	1.87	0.55
1:A:700:ASN:O	9:I:115:LYS:NZ	2.38	0.55
1:A:1105:LEU:HB3	1:A:1384:VAL:CG2	2.36	0.55
13:N:14:DG:H2''	13:N:15:DA:C8	2.41	0.55
16:T:17:DT:H2'	16:T:18:DC:C6	2.41	0.55
1:A:560:ILE:H	8:H:78:SER:HB2	1.70	0.55
1:A:1173:HIS:CE1	1:A:1229:SER:HA	2.41	0.55
1:A:1288:ASP:HA	1:A:1302:PRO:HA	1.88	0.55
2:B:151:LEU:HD21	2:B:155:GLU:OE1	2.06	0.55
16:T:11:DT:H2''	16:T:12:DC:C6	2.42	0.55
1:A:114:LEU:O	1:A:164:ARG:NH2	2.39	0.55
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.39	0.55
1:A:157:ASP:OD1	1:A:160:GLN:NE2	2.40	0.54
1:A:666:ILE:HG21	2:B:1030:LEU:HD22	1.89	0.54
7:G:84:GLY:N	7:G:147:ILE:O	2.38	0.54
3:C:55:THR:HG1	3:C:152:GLU:H	1.52	0.54
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.88	0.54
8:H:108:SER:OG	8:H:109:LYS:N	2.40	0.54
5:E:118:PRO:HA	5:E:121:MET:HB2	1.90	0.54
2:B:51:PHE:HB2	2:B:173:MET:HE3	1.90	0.54
2:B:89:GLU:HG3	2:B:135:ARG:HB2	1.89	0.54
1:A:446:ARG:HB2	1:A:487:MET:HE3	1.88	0.54
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.88	0.54
3:C:22:LEU:HG	3:C:25:VAL:HG11	1.89	0.54
2:B:759:PRO:HG2	2:B:1046:PRO:HB3	1.90	0.54
2:B:862:GLN:O	2:B:914:LYS:NZ	2.39	0.54
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.41	0.54
2:B:1165:ILE:HG23	4:D:17:LYS:HD3	1.90	0.54
1:A:711:ARG:NH2	9:I:87:GLN:OE1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:119:LEU:HD13	7:G:132:SER:HB3	1.89	0.53
4:D:165:GLN:HA	4:D:168:LYS:HB3	1.90	0.53
7:G:143:ILE:HD11	7:G:163:ILE:HG21	1.90	0.53
12:L:26:THR:OG1	12:L:27:LEU:N	2.39	0.53
4:D:16:LYS:HG3	4:D:18:VAL:HG23	1.90	0.53
3:C:38:ILE:HG12	3:C:176:ILE:HD12	1.89	0.53
3:C:142:VAL:HG13	10:J:15:GLY:HA3	1.91	0.53
6:F:116:ASP:HB3	6:F:119:ARG:HG2	1.91	0.53
2:B:1041:GLU:N	2:B:1041:GLU:OE1	2.42	0.53
3:C:185:LYS:NZ	3:C:211:ASP:O	2.36	0.53
1:A:1255:GLU:O	1:A:1259:MET:N	2.31	0.53
2:B:500:THR:HG22	2:B:502:ILE:HG12	1.90	0.53
1:A:1170:ILE:O	1:A:1174:PHE:N	2.42	0.53
1:A:1384:VAL:HA	1:A:1389:PHE:HD1	1.73	0.53
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.91	0.53
2:B:287:ARG:NH1	2:B:321:GLY:O	2.42	0.53
2:B:298:LEU:HD12	9:I:6:PHE:HZ	1.73	0.53
2:B:941:LEU:HD21	2:B:946:ASN:HA	1.90	0.52
2:B:1135:ARG:HG3	2:B:1147:LEU:HD11	1.91	0.52
4:D:178:ALA:O	4:D:182:SER:N	2.32	0.52
11:K:102:LYS:NZ	11:K:106:GLU:OE2	2.34	0.52
1:A:884:ASP:HB3	1:A:896:ARG:HH12	1.74	0.52
5:E:79:TRP:NE1	5:E:81:GLU:OE1	2.35	0.52
1:A:1120:LEU:HD11	1:A:1131:ALA:HB2	1.92	0.52
2:B:173:MET:O	2:B:176:SER:OG	2.22	0.52
1:A:387:ARG:HH21	1:A:437:MET:HE1	1.75	0.52
10:J:2:ILE:HD12	10:J:57:ILE:HD13	1.91	0.52
1:A:852:TYR:OH	6:F:89:GLU:OE2	2.16	0.52
2:B:895:ASP:HB2	12:L:27:LEU:HD11	1.92	0.52
16:T:24:DC:H2'	16:T:25:DC:C6	2.45	0.52
3:C:10:ILE:HG22	3:C:20:PHE:HB3	1.92	0.52
1:A:744:LYS:HG3	1:A:748:MET:HE2	1.92	0.52
4:D:160:VAL:HA	4:D:163:VAL:HB	1.91	0.52
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.92	0.52
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.10	0.52
9:I:111:THR:HG23	9:I:113:ASP:H	1.75	0.52
1:A:451:HIS:ND1	1:A:453:MET:HE2	2.26	0.51
1:A:1318:THR:OG1	5:E:11:ARG:NH1	2.42	0.51
4:D:56:ARG:HB2	4:D:148:LEU:HD22	1.93	0.51
16:T:23:DC:H2'	16:T:24:DC:C6	2.46	0.51
1:A:908:LEU:HA	1:A:1029:ARG:HH12	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.92	0.51
2:B:415:GLN:HE21	2:B:466:TRP:CD1	2.29	0.51
4:D:63:LEU:HB3	4:D:129:LEU:HD22	1.92	0.51
5:E:126:SER:OG	5:E:127:ILE:N	2.44	0.51
1:A:512:VAL:HA	1:A:519:PRO:HA	1.93	0.50
1:A:975:HIS:CD2	1:A:1036:ARG:HD2	2.46	0.50
1:A:406:ILE:HB	1:A:431:LYS:HB2	1.93	0.50
4:D:155:ARG:H	4:D:159:THR:HG21	1.77	0.50
9:I:103:CYS:HB3	9:I:106:CYS:SG	2.52	0.50
11:K:77:THR:OG1	11:K:81:TYR:O	2.30	0.50
1:A:583:PRO:HG2	1:A:586:ILE:HG13	1.93	0.50
1:A:939:ASP:OD2	1:A:1023:ARG:NE	2.39	0.50
2:B:95:ILE:HD11	2:B:128:LEU:HD22	1.94	0.50
2:B:323:VAL:HG11	15:Q:61:ASN:HB2	1.93	0.50
5:E:79:TRP:HD1	5:E:96:PHE:HE1	1.60	0.50
2:B:138:GLU:N	2:B:138:GLU:OE1	2.44	0.50
1:A:349:ALA:HB2	1:A:374:LEU:HD11	1.92	0.50
3:C:10:ILE:HD11	11:K:112:GLN:CG	2.42	0.50
3:C:153:LEU:HD11	3:C:155:LEU:HD23	1.93	0.50
7:G:115:MET:HB3	7:G:119:LEU:O	2.12	0.50
1:A:1454:MET:SD	1:A:1454:MET:N	2.84	0.50
1:A:140:THR:HG23	1:A:141:LEU:HD12	1.94	0.50
1:A:451:HIS:CE1	1:A:453:MET:HB2	2.47	0.50
1:A:583:PRO:HD3	1:A:645:LEU:HD13	1.93	0.50
2:B:83:ASN:O	2:B:141:ASP:N	2.45	0.50
4:D:195:ILE:HB	4:D:198:LEU:HG	1.94	0.50
4:D:202:ILE:HG23	4:D:207:LEU:HB2	1.93	0.50
2:B:166:PHE:CZ	2:B:169:ARG:HG3	2.47	0.49
2:B:821:GLN:OE1	2:B:851:PHE:N	2.43	0.49
9:I:101:PHE:HE1	9:I:112:SER:HB3	1.76	0.49
4:D:205:ASP:OD1	4:D:206:GLU:N	2.45	0.49
1:A:346:ASP:HB3	2:B:1107:ALA:O	2.12	0.49
1:A:402:ALA:HA	1:A:434:ARG:HA	1.93	0.49
2:B:315:LYS:HE3	9:I:4:PHE:CE1	2.48	0.49
13:N:10:DG:H2''	13:N:11:DA:H5'	1.95	0.49
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.95	0.49
2:B:722:ASP:OD1	2:B:722:ASP:N	2.44	0.49
2:B:83:ASN:HB2	2:B:141:ASP:O	2.12	0.49
2:B:138:GLU:HB3	2:B:152:ILE:HD12	1.94	0.49
2:B:87:LYS:HB2	2:B:149:TYR:CE1	2.48	0.49
4:D:164:ILE:O	4:D:168:LYS:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:214:LEU:HA	4:D:217:LEU:HB2	1.94	0.49
5:E:169:ARG:HH12	6:F:74:ILE:HD11	1.78	0.49
2:B:299:GLU:OE2	2:B:572:HIS:ND1	2.46	0.49
1:A:1252:THR:O	1:A:1256:GLU:HG3	2.12	0.49
1:A:1288:ASP:OD2	1:A:1300:LYS:HB3	2.13	0.49
4:D:167:LEU:O	4:D:170:THR:OG1	2.21	0.49
2:B:25:ILE:HA	2:B:655:LYS:HD3	1.93	0.49
2:B:298:LEU:HD12	9:I:6:PHE:CZ	2.48	0.49
2:B:600:LEU:HB3	2:B:615:MET:SD	2.53	0.49
11:K:114:LEU:H	11:K:114:LEU:HD23	1.78	0.49
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.95	0.48
1:A:157:ASP:OD2	1:A:159:THR:OG1	2.31	0.48
1:A:888:GLY:O	1:A:940:ARG:NH2	2.46	0.48
2:B:44:VAL:HG11	2:B:495:LEU:HD13	1.95	0.48
3:C:89:GLU:HG2	3:C:90:ASP:N	2.27	0.48
1:A:1114:PRO:HB2	1:A:1311:VAL:HG23	1.95	0.48
3:C:255:VAL:HG21	11:K:94:ILE:HG21	1.95	0.48
9:I:106:CYS:SG	9:I:108:HIS:HB3	2.53	0.48
4:D:50:LEU:HD13	4:D:55:ALA:HA	1.95	0.48
7:G:132:SER:OG	7:G:135:ASP:OD1	2.29	0.48
12:L:31:CYS:SG	12:L:34:CYS:N	2.77	0.48
1:A:130:ASP:OD1	1:A:130:ASP:N	2.47	0.48
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.95	0.48
2:B:420:LEU:HD21	2:B:456:GLY:HA3	1.95	0.48
2:B:1056:SER:HB2	2:B:1066:SER:HB2	1.95	0.48
2:B:85:SER:O	2:B:139:ALA:N	2.47	0.48
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.49	0.48
1:A:149:GLU:HB2	1:A:164:ARG:HH21	1.77	0.47
2:B:345:LYS:HG2	15:Q:74:PHE:HD2	1.78	0.47
1:A:1001:ARG:HH22	1:A:1054:LEU:HD22	1.79	0.47
2:B:244:LEU:HD23	2:B:244:LEU:H	1.79	0.47
2:B:1081:LEU:O	3:C:189:THR:HG22	2.14	0.47
3:C:101:LEU:HD21	3:C:113:VAL:HG11	1.96	0.47
2:B:84:ILE:HG13	2:B:84:ILE:O	2.14	0.47
1:A:362:ASP:HB3	1:A:508:PRO:HD3	1.95	0.47
2:B:554:ILE:HD11	2:B:613:VAL:HG21	1.95	0.47
1:A:470:LEU:HD21	1:A:482:PHE:HE1	1.79	0.47
1:A:518:LYS:NZ	1:A:624:SER:O	2.41	0.47
2:B:773:MET:CE	2:B:987:LYS:HE3	2.44	0.47
3:C:18:VAL:HG12	3:C:240:VAL:HG22	1.96	0.47
9:I:2:THR:HG22	9:I:42:LEU:HG	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:LEU:HD23	1:A:145:LYS:HG3	1.97	0.47
1:A:1252:THR:HA	1:A:1255:GLU:HG2	1.96	0.47
2:B:705:MET:H	2:B:710:LEU:HD22	1.79	0.47
3:C:66:ARG:NH2	10:J:3:VAL:O	2.44	0.47
1:A:491:VAL:O	2:B:1150:ARG:NH2	2.47	0.47
1:A:905:ASP:OD1	1:A:905:ASP:N	2.46	0.47
1:A:1220:PHE:CD2	1:A:1224:LEU:HD22	2.49	0.47
3:C:36:VAL:HG13	3:C:40:GLU:HB2	1.97	0.47
3:C:46:ILE:HA	3:C:159:ALA:HA	1.97	0.47
5:E:18:THR:OG1	5:E:140:LEU:O	2.25	0.47
10:J:41:LEU:HD22	10:J:46:CYS:HB3	1.96	0.47
10:J:67:GLU:HG2	12:L:30:ILE:HG12	1.97	0.47
2:B:883:LEU:HD21	2:B:928:ARG:HD3	1.97	0.47
5:E:64:PRO:HB3	5:E:75:MET:SD	2.55	0.47
13:N:5:DG:H1	16:T:14:DC:H5	1.62	0.47
1:A:1017:LEU:HB2	5:E:206:GLY:N	2.30	0.47
2:B:135:ARG:HD2	2:B:155:GLU:CG	2.43	0.47
1:A:1422:ARG:HD3	2:B:1224:PHE:HD2	1.80	0.47
2:B:198:ASP:OD2	2:B:202:TYR:OH	2.29	0.47
3:C:48:SER:OG	12:L:66:GLN:OE1	2.33	0.47
1:A:1345:ARG:NE	1:A:1373:ASP:OD1	2.34	0.46
2:B:412:LEU:O	2:B:466:TRP:NE1	2.42	0.46
7:G:30:LEU:O	7:G:34:VAL:HG12	2.15	0.46
7:G:83:LYS:NZ	7:G:148:GLU:O	2.32	0.46
7:G:88:ASP:HA	7:G:144:ARG:HA	1.96	0.46
1:A:121:LEU:HB3	1:A:141:LEU:HD21	1.97	0.46
1:A:355:GLY:O	1:A:469:ARG:NH1	2.48	0.46
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	1.97	0.46
2:B:165:VAL:HB	2:B:448:ILE:HD13	1.98	0.46
16:T:6:DT:H2''	16:T:7:DC:OP2	2.15	0.46
1:A:105:CYS:SG	1:A:139:TRP:HA	2.55	0.46
2:B:373:ARG:HD2	2:B:567:GLU:OE2	2.16	0.46
5:E:121:MET:HE2	5:E:124:VAL:HG21	1.98	0.46
2:B:636:PRO:HA	2:B:691:GLU:O	2.14	0.46
3:C:16:ASP:OD1	3:C:16:ASP:N	2.47	0.46
13:N:7:DG:H4'	13:N:8:DA:OP1	2.15	0.46
1:A:443:LEU:HD13	1:A:501:LEU:HD11	1.98	0.46
2:B:133:LYS:HD3	2:B:135:ARG:HH21	1.81	0.46
2:B:904:ARG:CZ	2:B:948:ILE:HD11	2.45	0.46
8:H:86:ASP:O	8:H:87:ARG:NH1	2.48	0.46
9:I:89:GLN:HA	9:I:91:ARG:HH12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:866:PHE:N	5:E:208:TYR:OH	2.45	0.46
2:B:133:LYS:HD3	2:B:135:ARG:NH2	2.30	0.46
2:B:237:VAL:HG13	2:B:257:LYS:HG2	1.98	0.46
3:C:8:VAL:HG11	11:K:105:PHE:HA	1.97	0.46
4:D:48:ILE:HG13	4:D:48:ILE:O	2.16	0.46
4:D:176:GLU:HA	4:D:179:GLN:HB2	1.97	0.46
2:B:875:GLU:O	2:B:877:PRO:HD3	2.15	0.46
5:E:93:MET:HG2	5:E:120:ALA:HB1	1.98	0.46
15:Q:30:HIS:CG	15:Q:51:ILE:HG13	2.51	0.46
2:B:343:ILE:HB	2:B:348:ARG:HE	1.81	0.46
2:B:641:GLU:OE2	2:B:654:ARG:NH2	2.49	0.46
2:B:864:LYS:HG2	2:B:872:GLU:OE1	2.16	0.46
1:A:848:ILE:HB	1:A:1065:GLY:HA3	1.98	0.46
2:B:773:MET:HE1	2:B:987:LYS:HE3	1.97	0.46
3:C:108:GLU:HA	3:C:149:LYS:HD2	1.98	0.46
4:D:213:GLU:O	4:D:217:LEU:N	2.49	0.46
7:G:100:GLU:HG3	7:G:109:PHE:HD1	1.80	0.46
11:K:18:LYS:NZ	11:K:38:GLU:OE2	2.40	0.46
2:B:617:ARG:NH2	9:I:61:ASP:OD2	2.43	0.45
3:C:142:VAL:HG11	10:J:5:VAL:HG13	1.98	0.45
1:A:389:THR:O	1:A:393:ARG:HG2	2.15	0.45
4:D:66:ARG:HH22	4:D:134:THR:HB	1.81	0.45
9:I:24:ARG:NH2	9:I:37:GLU:OE2	2.45	0.45
1:A:781:ASP:HB2	1:A:789:LYS:HD3	1.99	0.45
1:A:446:ARG:HB2	1:A:487:MET:HG2	1.99	0.45
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.97	0.45
2:B:337:ARG:NH2	15:Q:65:GLN:HE21	2.05	0.45
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.81	0.45
7:G:74:TYR:CE2	7:G:76:ALA:HB2	2.51	0.45
7:G:101:VAL:HG13	7:G:108:VAL:HB	1.97	0.45
7:G:116:PRO:HD2	7:G:119:LEU:HD23	1.98	0.45
2:B:336:ARG:HH11	15:Q:68:ASP:HA	1.80	0.45
2:B:408:LEU:HD23	2:B:545:ILE:HG21	1.98	0.45
4:D:53:SER:OG	4:D:154:PHE:N	2.47	0.45
7:G:86:VAL:HG22	7:G:146:LYS:HB2	1.97	0.45
1:A:848:ILE:HG21	1:A:1370:LEU:HD11	1.99	0.45
1:A:932:GLU:CD	1:A:1028:THR:HG1	2.24	0.45
2:B:118:ARG:HG3	2:B:204:ILE:HD13	1.99	0.45
2:B:862:GLN:HA	2:B:963:PHE:HB2	1.97	0.45
4:D:204:ASP:O	4:D:208:GLU:N	2.37	0.45
1:A:119:ASN:O	1:A:123:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:GLY:O	2:B:1129:ARG:NH1	2.50	0.45
1:A:1428:VAL:HG13	2:B:1151:LEU:HD13	1.99	0.45
2:B:104:GLU:OE2	2:B:120:ARG:NH2	2.33	0.45
1:A:4:GLN:OE1	2:B:1159:ARG:HB3	2.16	0.45
1:A:342:GLY:O	2:B:1129:ARG:NH1	2.49	0.45
2:B:1169:MET:SD	2:B:1201:LYS:HG2	2.57	0.45
3:C:245:VAL:HG13	11:K:102:LYS:HE2	1.98	0.45
7:G:144:ARG:HH12	7:G:171:ILE:N	2.15	0.45
3:C:148:ARG:NH1	10:J:61:LEU:O	2.46	0.45
7:G:102:GLN:HB2	7:G:107:LYS:HZ3	1.81	0.45
1:A:74:MET:O	2:B:1116:ARG:NH2	2.50	0.45
1:A:442:VAL:HG21	1:A:489:LEU:HD11	1.99	0.45
2:B:859:TYR:OH	2:B:942:ARG:HG2	2.17	0.45
1:A:786:HIS:HE1	2:B:519:TRP:CE2	2.36	0.44
1:A:1289:ARG:HG3	1:A:1291:VAL:HG23	1.98	0.44
1:A:1450:LEU:HD21	7:G:19:GLY:O	2.18	0.44
2:B:75:ALA:HB3	2:B:141:ASP:OD2	2.17	0.44
2:B:315:LYS:N	2:B:316:PRO:HD2	2.33	0.44
7:G:15:PRO:HA	7:G:18:PHE:CD2	2.53	0.44
7:G:91:VAL:HA	7:G:101:VAL:HA	1.99	0.44
1:A:885:THR:HG23	1:A:1024:SER:HB2	1.99	0.44
2:B:727:LYS:HE3	2:B:1049:ASP:HB2	1.98	0.44
3:C:258:ILE:CG1	11:K:42:LEU:HD21	2.45	0.44
4:D:161:GLY:HA2	4:D:164:ILE:HG22	1.99	0.44
13:N:3:DG:H2''	13:N:4:DA:C8	2.53	0.44
1:A:350:ARG:NH1	1:A:488:ASN:OD1	2.50	0.44
1:A:1422:ARG:HD3	2:B:1224:PHE:CD2	2.53	0.44
2:B:173:MET:HG3	2:B:176:SER:HB3	1.99	0.44
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.99	0.44
7:G:88:ASP:OD1	7:G:89:GLY:N	2.44	0.44
13:N:14:DG:H1	16:T:5:DC:H42	1.66	0.44
1:A:569:LYS:HD2	3:C:221:TYR:HB2	1.99	0.44
1:A:1196:GLU:N	1:A:1196:GLU:OE1	2.51	0.44
2:B:138:GLU:O	2:B:149:TYR:HA	2.17	0.44
2:B:667:GLN:HE22	2:B:675:ASP:HA	1.83	0.44
3:C:115:SER:OG	3:C:141:GLY:HA3	2.17	0.44
5:E:2:ASP:O	5:E:6:GLU:N	2.38	0.44
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.18	0.44
1:A:110:CYS:HB3	1:A:167:CYS:SG	2.58	0.44
1:A:1198:ASP:HB3	1:A:1201:ALA:HB3	1.99	0.44
7:G:138:THR:O	7:G:141:SER:OG	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:34:ASP:OD1	8:H:34:ASP:N	2.50	0.44
9:I:113:ASP:HB3	9:I:116:ASN:HB3	2.00	0.44
16:T:19:DC:H2'	16:T:20:DT:C6	2.53	0.44
1:A:35:ILE:HG22	1:A:270:LEU:HD11	2.00	0.44
1:A:72:GLU:HB3	1:A:76:GLU:HB2	1.99	0.44
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.99	0.44
1:A:404:TYR:HB2	1:A:433:GLU:HB3	1.99	0.44
1:A:1120:LEU:HB2	1:A:1125:ALA:HA	2.00	0.44
1:A:1146:VAL:HG11	1:A:1202:MET:HE2	1.98	0.44
2:B:910:VAL:HA	2:B:940:PRO:HA	1.99	0.44
4:D:159:THR:O	4:D:163:VAL:N	2.46	0.44
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.99	0.44
11:K:27:ALA:HB3	11:K:74:ARG:HH22	1.82	0.44
11:K:49:GLU:HB2	11:K:94:ILE:HD11	1.99	0.44
15:Q:65:GLN:N	15:Q:68:ASP:OD2	2.38	0.44
1:A:259:GLU:HB2	1:A:264:PHE:CE2	2.53	0.44
1:A:443:LEU:HD22	2:B:1146:PHE:CE2	2.53	0.44
5:E:88:VAL:HG21	5:E:110:PHE:HE2	1.82	0.44
1:A:79:GLY:HA3	1:A:245:PRO:HG2	2.00	0.44
2:B:629:ASP:OD1	2:B:629:ASP:N	2.51	0.44
2:B:1133:MET:SD	16:T:20:DT:H4'	2.58	0.44
3:C:114:TYR:CG	3:C:140:ASN:HB3	2.52	0.44
1:A:55:ASP:OD2	1:A:57:ARG:NH2	2.45	0.43
1:A:92:HIS:CD2	1:A:94:GLY:H	2.36	0.43
1:A:159:THR:OG1	1:A:160:GLN:OE1	2.34	0.43
2:B:363:HIS:CD2	2:B:585:VAL:HG22	2.53	0.43
3:C:11:ARG:N	3:C:19:ASP:O	2.47	0.43
4:D:63:LEU:HB3	4:D:129:LEU:CD2	2.48	0.43
1:A:106:VAL:HG11	1:A:214:ILE:HG12	1.99	0.43
1:A:407:ARG:HH21	1:A:411:ASP:HB3	1.83	0.43
1:A:471:ASN:O	1:A:474:VAL:HG12	2.18	0.43
8:H:48:PRO:O	8:H:146:ARG:NH2	2.47	0.43
1:A:113:LEU:HD23	1:A:115:LEU:H	1.83	0.43
2:B:312:GLU:HA	2:B:315:LYS:NZ	2.34	0.43
1:A:667:GLY:HA2	1:A:670:ILE:HD12	2.01	0.43
2:B:36:ALA:HB2	2:B:661:LEU:HD22	2.00	0.43
2:B:258:LEU:HB2	2:B:385:LEU:HD21	2.00	0.43
1:A:103:CYS:HB2	1:A:108:MET:SD	2.59	0.43
2:B:773:MET:HE3	2:B:773:MET:HB2	1.93	0.43
2:B:1156:ASP:OD1	2:B:1156:ASP:N	2.50	0.43
7:G:98:GLY:HA2	7:G:130:TYR:OH	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:VAL:HG21	1:A:426:LEU:HD12	2.01	0.43
4:D:209:ARG:HA	4:D:212:LYS:HB2	2.01	0.43
13:N:11:DA:H5'	13:N:11:DA:C8	2.54	0.43
1:A:1004:ASN:OD1	1:A:1007:ILE:HG12	2.18	0.43
1:A:1224:LEU:HD21	1:A:1240:CYS:HB3	2.00	0.43
2:B:72:GLU:HA	2:B:87:LYS:HG3	2.01	0.43
2:B:904:ARG:NH1	12:L:66:GLN:O	2.52	0.43
8:H:40:LEU:HD21	8:H:144:ILE:HD11	2.01	0.43
1:A:101:LYS:HD3	1:A:135:PHE:HE2	1.84	0.43
4:D:50:LEU:HD22	4:D:54:GLU:HG2	2.00	0.43
7:G:119:LEU:HB2	7:G:132:SER:HB3	2.01	0.43
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.54	0.43
2:B:778:MET:HG3	2:B:794:ASN:HB3	2.00	0.43
4:D:151:PHE:HB3	4:D:153:ARG:CZ	2.48	0.43
5:E:163:GLU:O	5:E:167:ARG:HG2	2.18	0.43
8:H:11:GLN:NE2	8:H:52:GLN:OE1	2.52	0.43
1:A:608:ILE:HD12	1:A:613:ILE:HG13	1.99	0.42
1:A:884:ASP:HB2	1:A:1024:SER:OG	2.19	0.42
2:B:845:SER:OG	2:B:1009:ASP:OD1	2.33	0.42
4:D:39:ASN:HA	7:G:6:ASP:OD2	2.19	0.42
1:A:100:LYS:HE3	1:A:174:ILE:O	2.20	0.42
1:A:137:ALA:HA	1:A:140:THR:HG22	2.00	0.42
6:F:87:LYS:HG3	6:F:88:TYR:N	2.35	0.42
9:I:8:ARG:NH1	9:I:9:ASP:HB2	2.34	0.42
9:I:58:VAL:HA	9:I:62:ILE:HD12	2.01	0.42
1:A:92:HIS:HD2	1:A:94:GLY:H	1.67	0.42
1:A:549:MET:HE3	1:A:656:TRP:HB2	1.99	0.42
1:A:1336:MET:HG2	1:A:1341:ILE:HA	2.01	0.42
7:G:139:ILE:HG22	7:G:140:LYS:HG3	2.01	0.42
1:A:154:SER:HA	1:A:162:VAL:HG22	2.02	0.42
2:B:96:TYR:HD2	2:B:164:LYS:HE3	1.84	0.42
4:D:206:GLU:OE1	4:D:209:ARG:HD3	2.20	0.42
1:A:506:ALA:O	1:A:510:GLN:HG2	2.20	0.42
1:A:804:TYR:OH	1:A:816:HIS:NE2	2.41	0.42
2:B:100:PRO:HG2	2:B:124:TYR:CZ	2.55	0.42
4:D:40:HIS:CE1	7:G:73:LYS:HB3	2.55	0.42
1:A:216:VAL:HA	1:A:219:PHE:CE2	2.54	0.42
1:A:698:GLN:O	9:I:112:SER:OG	2.33	0.42
1:A:1262:LYS:O	1:A:1266:THR:HG22	2.19	0.42
2:B:415:GLN:HE21	2:B:466:TRP:HD1	1.66	0.42
2:B:1129:ARG:HB3	16:T:22:DT:P	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:54:ASN:ND2	3:C:60:ASP:OD1	2.23	0.42
4:D:117:GLU:HA	4:D:121:LYS:HE3	2.01	0.42
4:D:213:GLU:O	4:D:217:LEU:HG	2.20	0.42
7:G:63:PRO:C	7:G:65:ASP:H	2.28	0.42
8:H:7:ASP:OD1	8:H:7:ASP:N	2.52	0.42
1:A:207:ILE:HA	1:A:210:ILE:HG22	2.02	0.42
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.84	0.42
2:B:924:GLU:O	2:B:928:ARG:HB3	2.20	0.42
3:C:152:GLU:OE1	10:J:69:ARG:NH1	2.52	0.42
4:D:214:LEU:C	4:D:217:LEU:H	2.28	0.42
5:E:12:LEU:HD22	5:E:55:ARG:HE	1.84	0.42
5:E:43:LYS:O	5:E:47:CYS:HB3	2.19	0.42
7:G:34:VAL:HG21	7:G:74:TYR:OH	2.20	0.42
8:H:36:CYS:HA	8:H:126:GLU:O	2.20	0.42
1:A:116:ASP:H	1:A:164:ARG:NH1	2.18	0.42
1:A:348:SER:HA	1:A:489:LEU:O	2.20	0.42
1:A:447:GLN:HG2	2:B:1134:GLU:OE2	2.19	0.42
1:A:993:LEU:HD11	1:A:1050:GLU:HB2	2.02	0.42
2:B:221:ASN:HA	2:B:240:ILE:HD11	2.01	0.42
2:B:224:GLN:HA	2:B:396:ASP:OD2	2.20	0.42
2:B:315:LYS:HB3	9:I:4:PHE:CZ	2.55	0.42
2:B:877:PRO:HB3	2:B:882:THR:HG21	2.01	0.42
8:H:104:PHE:CE1	8:H:137:GLN:HG2	2.54	0.42
1:A:16:GLU:OE1	4:D:13:ARG:NH1	2.48	0.42
1:A:557:ASP:N	1:A:557:ASP:OD1	2.47	0.42
1:A:842:VAL:HG11	2:B:1136:ASP:CG	2.45	0.42
7:G:23:LYS:HD2	7:G:56:ILE:HD12	2.01	0.42
16:T:14:DC:H6	16:T:14:DC:H2'	1.62	0.42
1:A:899:VAL:HB	1:A:929:LEU:HD12	2.02	0.42
2:B:432:MET:HA	2:B:435:THR:HG22	2.01	0.42
2:B:1074:ASN:OD1	2:B:1076:HIS:N	2.51	0.42
4:D:31:GLN:OE1	4:D:31:GLN:N	2.53	0.42
4:D:214:LEU:O	4:D:217:LEU:N	2.53	0.42
7:G:13:LEU:HD11	7:G:26:LEU:HG	2.00	0.42
10:J:17:LYS:HB3	10:J:39:LEU:HD13	2.02	0.42
15:Q:61:ASN:OD1	15:Q:64:SER:N	2.53	0.42
2:B:415:GLN:NE2	2:B:466:TRP:HD1	2.18	0.41
2:B:681:TRP:CH2	2:B:690:VAL:HG21	2.54	0.41
2:B:826:ALA:O	2:B:1011:ILE:HA	2.19	0.41
2:B:986:GLN:NE2	2:B:1022:THR:OG1	2.53	0.41
7:G:137:ILE:HG21	7:G:143:ILE:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:VAL:O	1:A:328:ARG:NH2	2.37	0.41
1:A:840:ARG:HG2	1:A:1402:PHE:CZ	2.55	0.41
2:B:333:PHE:O	2:B:336:ARG:HB3	2.21	0.41
2:B:558:LEU:HD11	2:B:626:ILE:HD12	2.02	0.41
5:E:61:GLN:HB2	5:E:79:TRP:CZ3	2.55	0.41
7:G:90:THR:C	7:G:101:VAL:HG23	2.45	0.41
9:I:29:CYS:HB2	9:I:34:TYR:HB3	2.02	0.41
10:J:48:ARG:O	10:J:52:THR:OG1	2.33	0.41
1:A:1148:ILE:HA	9:I:49:ILE:HD13	2.02	0.41
1:A:1169:ILE:HD13	1:A:1229:SER:HB3	2.01	0.41
1:A:1434:ALA:HB3	1:A:1436:ILE:HG12	2.03	0.41
2:B:848:ARG:NH1	10:J:8:PHE:O	2.50	0.41
4:D:172:LEU:HG	4:D:176:GLU:OE1	2.19	0.41
15:Q:23:PHE:HB3	15:Q:70:TYR:CE1	2.56	0.41
15:Q:72:ASP:HA	15:Q:75:ASP:OD2	2.20	0.41
1:A:614:PHE:HB3	8:H:122:LEU:HD21	2.02	0.41
1:A:1197:LEU:HB2	1:A:1236:LEU:HB2	2.02	0.41
2:B:175:ARG:HG3	2:B:200:GLY:HA3	2.02	0.41
7:G:99:PHE:CE1	7:G:110:VAL:HB	2.55	0.41
7:G:118:ASP:OD1	7:G:119:LEU:N	2.52	0.41
10:J:1:MET:HA	10:J:56:LEU:HB2	2.02	0.41
2:B:315:LYS:HB3	9:I:4:PHE:HZ	1.85	0.41
2:B:906:SER:O	2:B:941:LEU:HD23	2.19	0.41
7:G:166:ASP:OD1	7:G:166:ASP:N	2.53	0.41
1:A:597:LEU:CD2	8:H:103:LYS:HG2	2.42	0.41
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.56	0.41
2:B:89:GLU:CG	2:B:135:ARG:HB2	2.50	0.41
2:B:829:CYS:SG	2:B:1014:PRO:HD2	2.60	0.41
3:C:145:CYS:SG	3:C:146:LYS:N	2.94	0.41
5:E:59:SER:OG	5:E:80:VAL:O	2.35	0.41
8:H:93:TYR:HA	8:H:145:ARG:HB3	2.02	0.41
10:J:41:LEU:O	10:J:47:ARG:NH1	2.52	0.41
11:K:63:VAL:HG22	11:K:71:PHE:HB3	2.03	0.41
1:A:547:LEU:HD12	11:K:51:LEU:HD21	2.02	0.41
1:A:1266:THR:O	1:A:1270:ASN:HB3	2.20	0.41
2:B:616:ILE:O	2:B:624:LEU:HD12	2.20	0.41
16:T:20:DT:H2'	16:T:21:DT:C6	2.55	0.41
1:A:1341:ILE:HD11	1:A:1376:THR:HB	2.03	0.41
2:B:142:VAL:HG21	2:B:145:ARG:NH2	2.36	0.41
2:B:315:LYS:HE3	9:I:4:PHE:CZ	2.56	0.41
1:A:353:ILE:HG22	1:A:468:PHE:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:ILE:HG21	8:H:46:LEU:HD23	2.02	0.41
1:A:591:PHE:HA	1:A:595:THR:HG21	2.03	0.41
1:A:592:ASP:O	1:A:595:THR:HG22	2.20	0.41
1:A:733:ALA:O	1:A:737:LEU:HG	2.20	0.41
1:A:1349:TYR:HA	1:A:1372:VAL:HG11	2.02	0.41
1:A:1420:ASP:OD1	1:A:1420:ASP:N	2.46	0.41
2:B:190:TYR:HD1	10:J:63:TYR:CE1	2.39	0.41
2:B:289:LEU:HD22	2:B:356:LEU:HD13	2.02	0.41
2:B:496:ARG:NH1	2:B:540:SER:O	2.30	0.41
2:B:764:SER:OG	2:B:765:PRO:HD3	2.21	0.41
2:B:954:VAL:HG12	2:B:964:VAL:HG12	2.03	0.41
2:B:1080:LYS:HB3	3:C:189:THR:HG23	2.02	0.41
5:E:72:PHE:CE1	5:E:157:SER:HB3	2.56	0.41
9:I:82:GLU:OE1	9:I:104:LEU:HB2	2.21	0.41
1:A:881:GLN:CD	1:A:959:ASN:HA	2.46	0.41
1:A:1140:HIS:NE2	1:A:1272:THR:OG1	2.33	0.41
2:B:29:ASP:HB3	2:B:658:ILE:HG13	2.03	0.41
2:B:443:ASN:HB3	2:B:446:LEU:HD13	2.03	0.41
4:D:206:GLU:O	4:D:210:ILE:HG12	2.21	0.41
1:A:89:PRO:HB3	1:A:237:THR:HG22	2.01	0.40
1:A:512:VAL:HG23	1:A:634:THR:HG21	2.02	0.40
3:C:11:ARG:NH2	3:C:19:ASP:OD1	2.49	0.40
3:C:74:SER:HB3	3:C:77:ILE:HB	2.04	0.40
9:I:12:ASN:ND2	9:I:31:THR:HG21	2.37	0.40
15:Q:60:ILE:HB	15:Q:64:SER:OG	2.21	0.40
1:A:114:LEU:HD23	1:A:145:LYS:CG	2.51	0.40
1:A:956:LEU:HD13	1:A:1021:LEU:HD22	2.02	0.40
2:B:287:ARG:NH1	2:B:324:ILE:O	2.54	0.40
2:B:797:TYR:CE1	2:B:854:LEU:HG	2.56	0.40
3:C:136:ASP:OD1	3:C:136:ASP:N	2.52	0.40
7:G:165:GLU:HB2	7:G:168:LEU:HG	2.03	0.40
1:A:975:HIS:HA	1:A:1036:ARG:HD3	2.02	0.40
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.57	0.40
4:D:56:ARG:HA	4:D:148:LEU:HD13	2.03	0.40
9:I:22:ASN:HB2	9:I:24:ARG:HH11	1.87	0.40
1:A:875:ALA:HB1	1:A:1364:ASN:HD22	1.86	0.40
1:A:1383:SER:O	1:A:1388:GLY:HA3	2.21	0.40
2:B:122:LEU:O	2:B:207:GLY:N	2.54	0.40
3:C:10:ILE:HD13	3:C:10:ILE:HG21	1.78	0.40
4:D:59:ILE:HD11	7:G:77:VAL:HG11	2.02	0.40
4:D:208:GLU:O	4:D:212:LYS:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:209:ARG:HG3	4:D:210:ILE:N	2.36	0.40
1:A:532:ARG:HD3	1:A:749:ALA:HB2	2.03	0.40
1:A:1315:GLU:O	1:A:1318:THR:HG22	2.21	0.40
3:C:248:ILE:HG21	11:K:102:LYS:HB2	2.02	0.40
5:E:50:MET:SD	5:E:50:MET:N	2.95	0.40
6:F:108:PHE:CZ	6:F:131:PRO:HG3	2.56	0.40
7:G:4:ILE:HA	7:G:77:VAL:HA	2.04	0.40
7:G:12:THR:HA	7:G:68:ALA:O	2.21	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	1416/1733 (82%)	1374 (97%)	42 (3%)	0	100	100
2	B	1173/1224 (96%)	1120 (96%)	53 (4%)	0	100	100
3	C	263/318 (83%)	253 (96%)	10 (4%)	0	100	100
4	D	161/221 (73%)	157 (98%)	4 (2%)	0	100	100
5	E	212/215 (99%)	204 (96%)	8 (4%)	0	100	100
6	F	85/155 (55%)	82 (96%)	3 (4%)	0	100	100
7	G	169/171 (99%)	156 (92%)	13 (8%)	0	100	100
8	H	135/146 (92%)	133 (98%)	2 (2%)	0	100	100
9	I	114/122 (93%)	109 (96%)	5 (4%)	0	100	100
10	J	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
11	K	113/120 (94%)	111 (98%)	2 (2%)	0	100	100
12	L	43/70 (61%)	42 (98%)	1 (2%)	0	100	100
15	Q	62/85 (73%)	61 (98%)	1 (2%)	0	100	100
All	All	4013/4650 (86%)	3868 (96%)	145 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	1246/1520 (82%)	1246 (100%)	0	100	100
2	B	1026/1061 (97%)	1026 (100%)	0	100	100
3	C	233/274 (85%)	233 (100%)	0	100	100
4	D	147/200 (74%)	147 (100%)	0	100	100
5	E	196/197 (100%)	196 (100%)	0	100	100
6	F	77/137 (56%)	77 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	122/128 (95%)	122 (100%)	0	100	100
9	I	110/116 (95%)	110 (100%)	0	100	100
10	J	64/65 (98%)	64 (100%)	0	100	100
11	K	99/102 (97%)	99 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
15	Q	61/79 (77%)	61 (100%)	0	100	100
All	All	3573/4088 (87%)	3573 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	45	GLN
1	A	64	ASN
1	A	92	HIS
1	A	169	ASN
1	A	171	GLN
1	A	253	ASN
1	A	256	GLN

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Mol	Chain	Res	Type
1	A	286	HIS
1	A	287	HIS
1	A	399	HIS
1	A	479	ASN
1	A	786	HIS
1	A	877	HIS
1	A	903	ASN
1	A	975	HIS
1	A	1048	ASN
1	A	1078	GLN
1	A	1265	ASN
1	A	1270	ASN
2	B	115	GLN
2	B	278	GLN
2	B	300	HIS
2	B	383	ASN
2	B	513	GLN
2	B	843	GLN
3	C	73	GLN
3	C	195	GLN
4	D	179	GLN
5	E	115	ASN
8	H	11	GLN
8	H	35	GLN
8	H	137	GLN
9	I	23	ASN
11	K	112	GLN
15	Q	65	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	5/6 (83%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 10 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	$\# Z > 2$
19	CPT	T	101	13,16	0,2,4	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

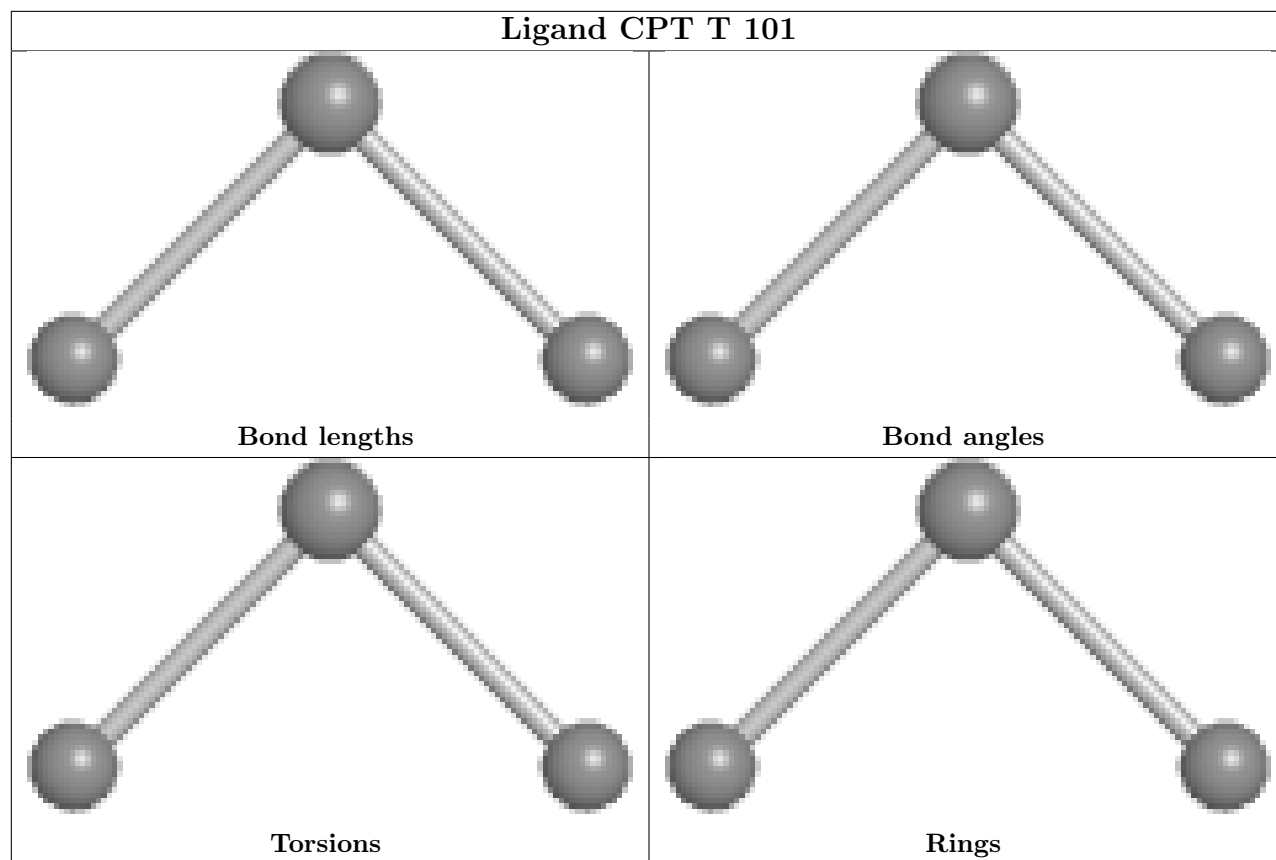
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	T	101	CPT	2	0

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 than 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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

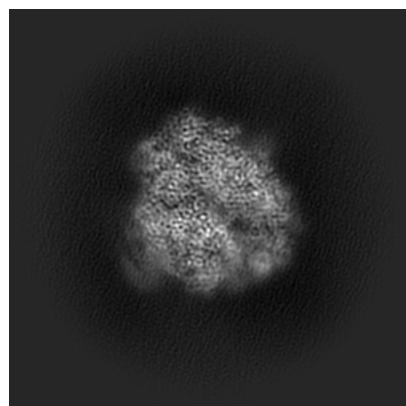
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66161. These allow visual inspection of the internal detail of the map and identification of artifacts.

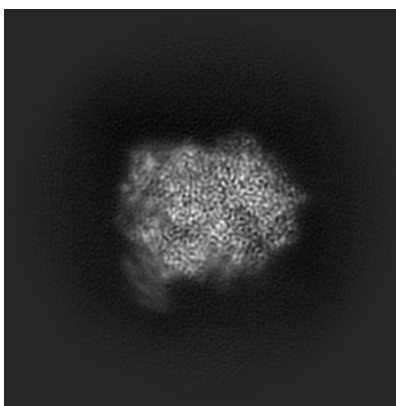
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

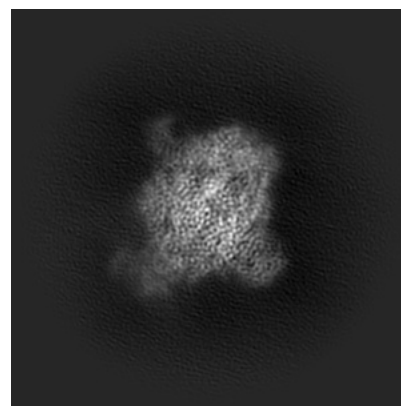
6.1.1 Primary map



X

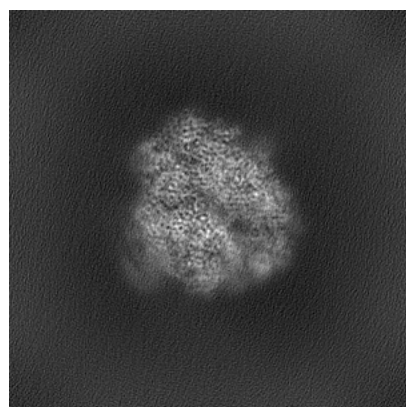


Y

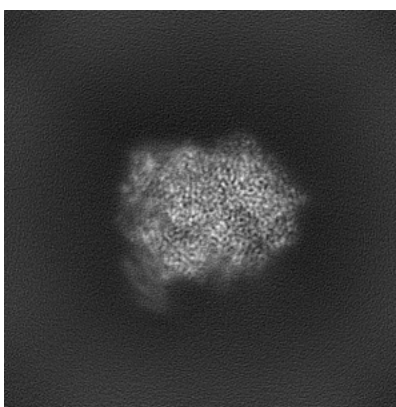


Z

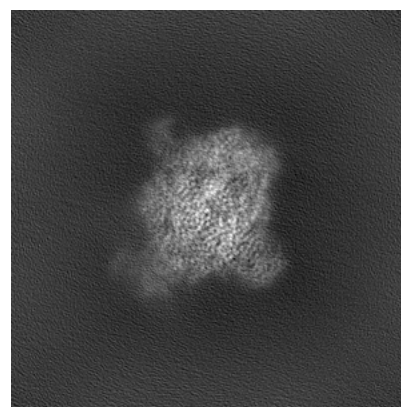
6.1.2 Raw map



X



Y

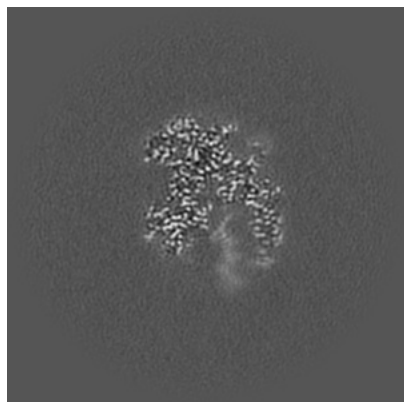


Z

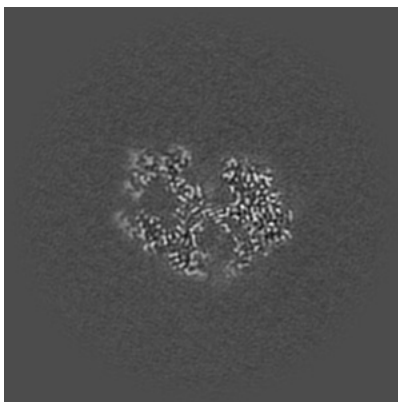
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

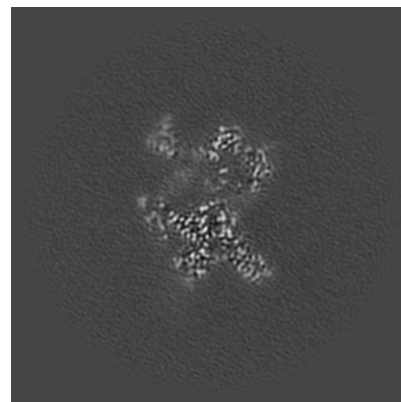
6.2.1 Primary map



X Index: 160

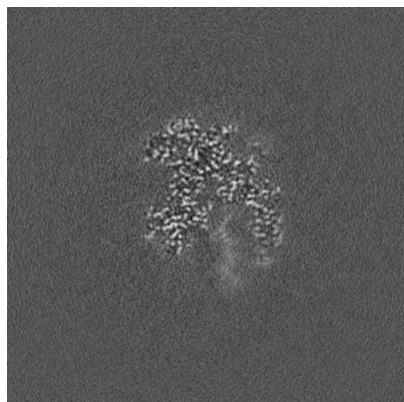


Y Index: 160

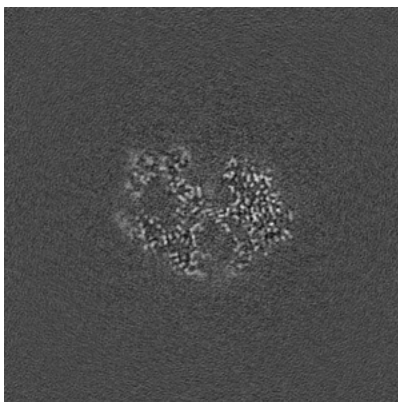


Z Index: 160

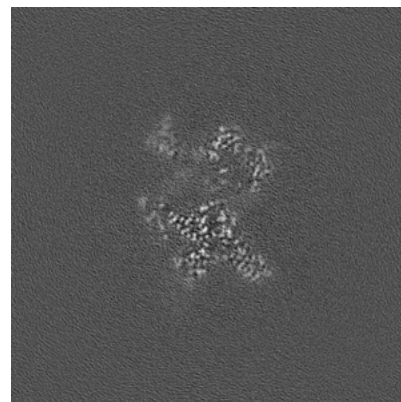
6.2.2 Raw map



X Index: 160



Y Index: 160

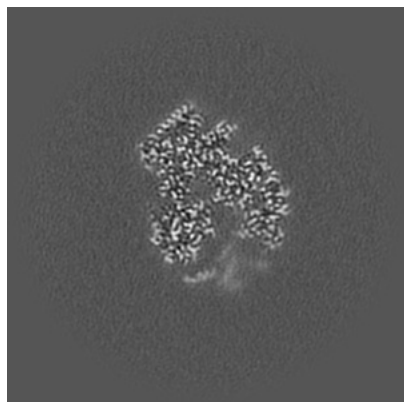


Z Index: 160

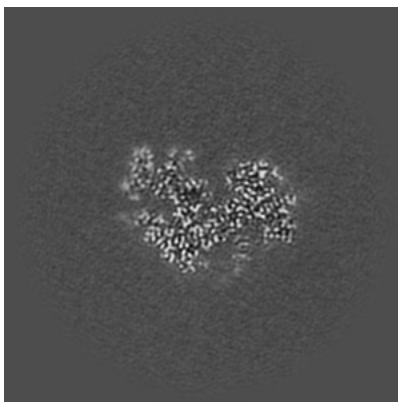
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

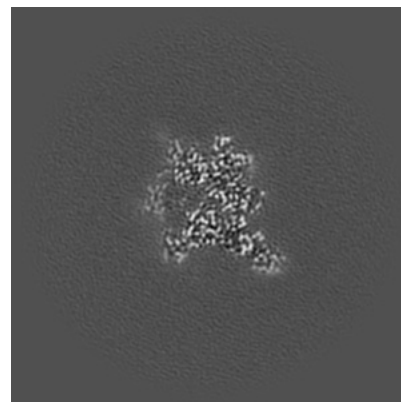
6.3.1 Primary map



X Index: 168

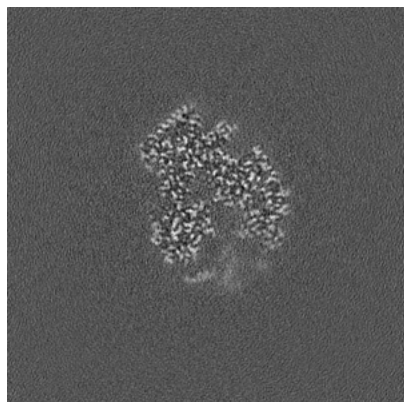


Y Index: 153

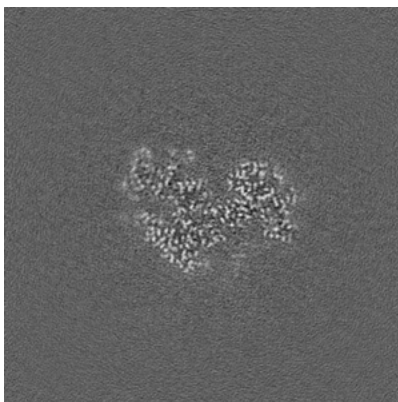


Z Index: 182

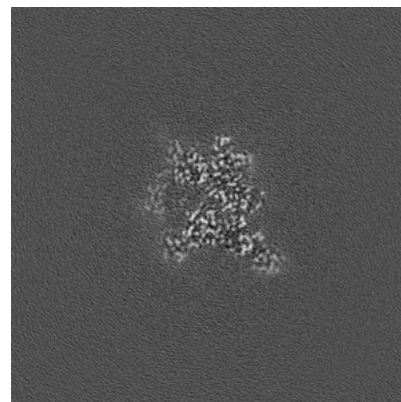
6.3.2 Raw map



X Index: 168



Y Index: 152

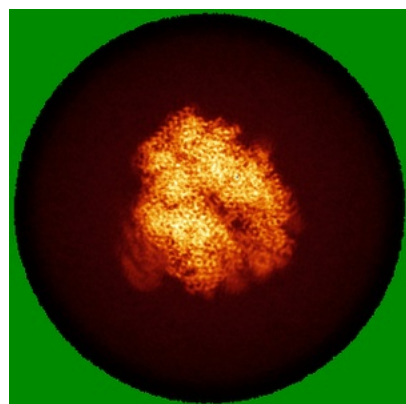


Z Index: 182

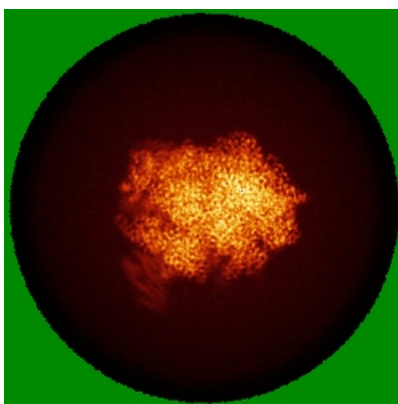
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

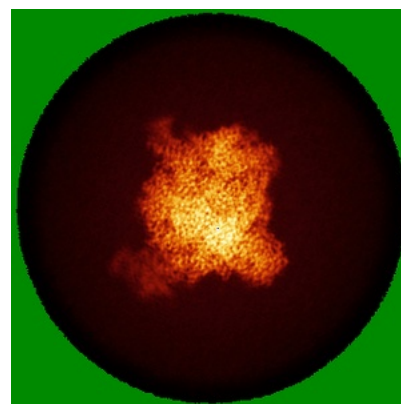
6.4.1 Primary map



X

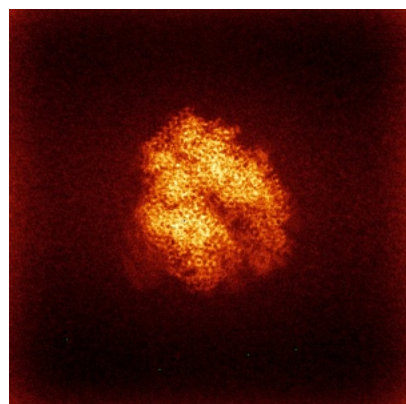


Y

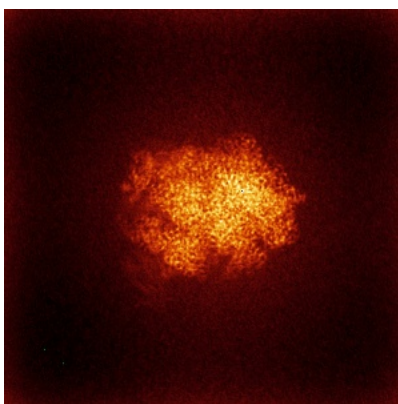


Z

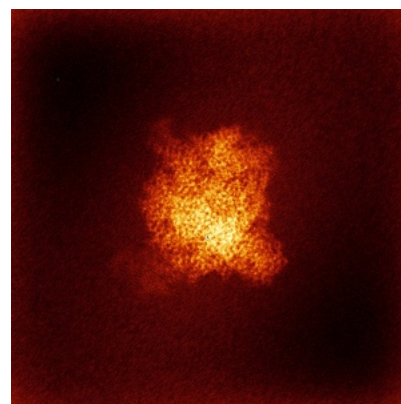
6.4.2 Raw map



X



Y

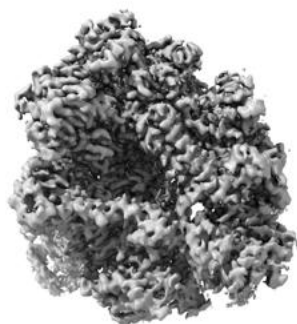


Z

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](#)

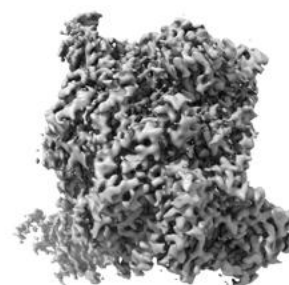
6.5.1 Primary map



X



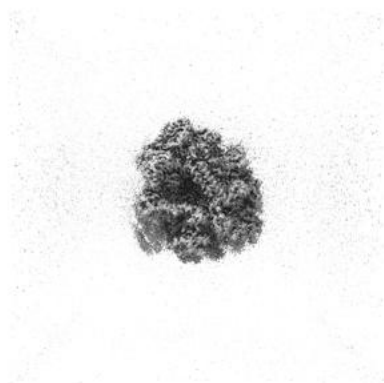
Y



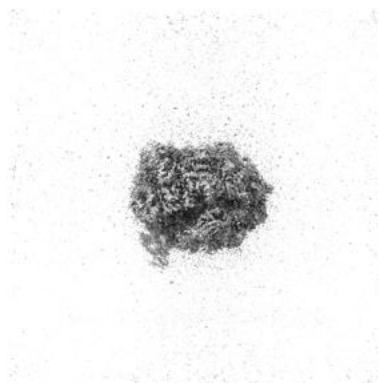
Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

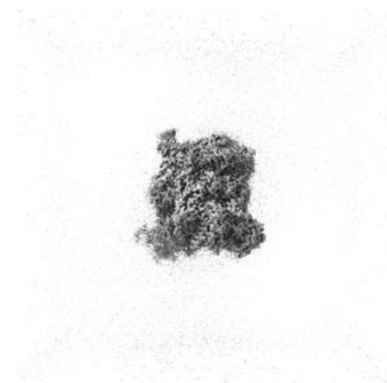
6.5.2 Raw map



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.

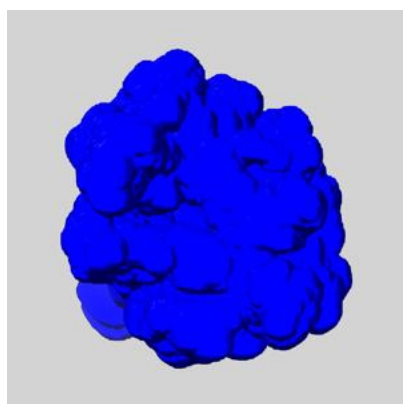
6.6 Mask visualisation [i](#)

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

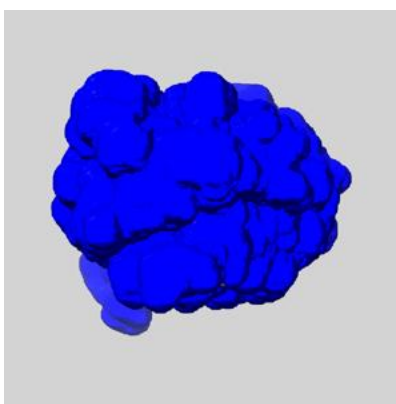
A mask typically either:

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

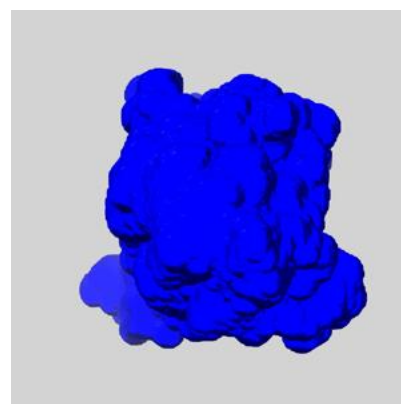
6.6.1 emd_66161_msk_1.map [i](#)



X



Y

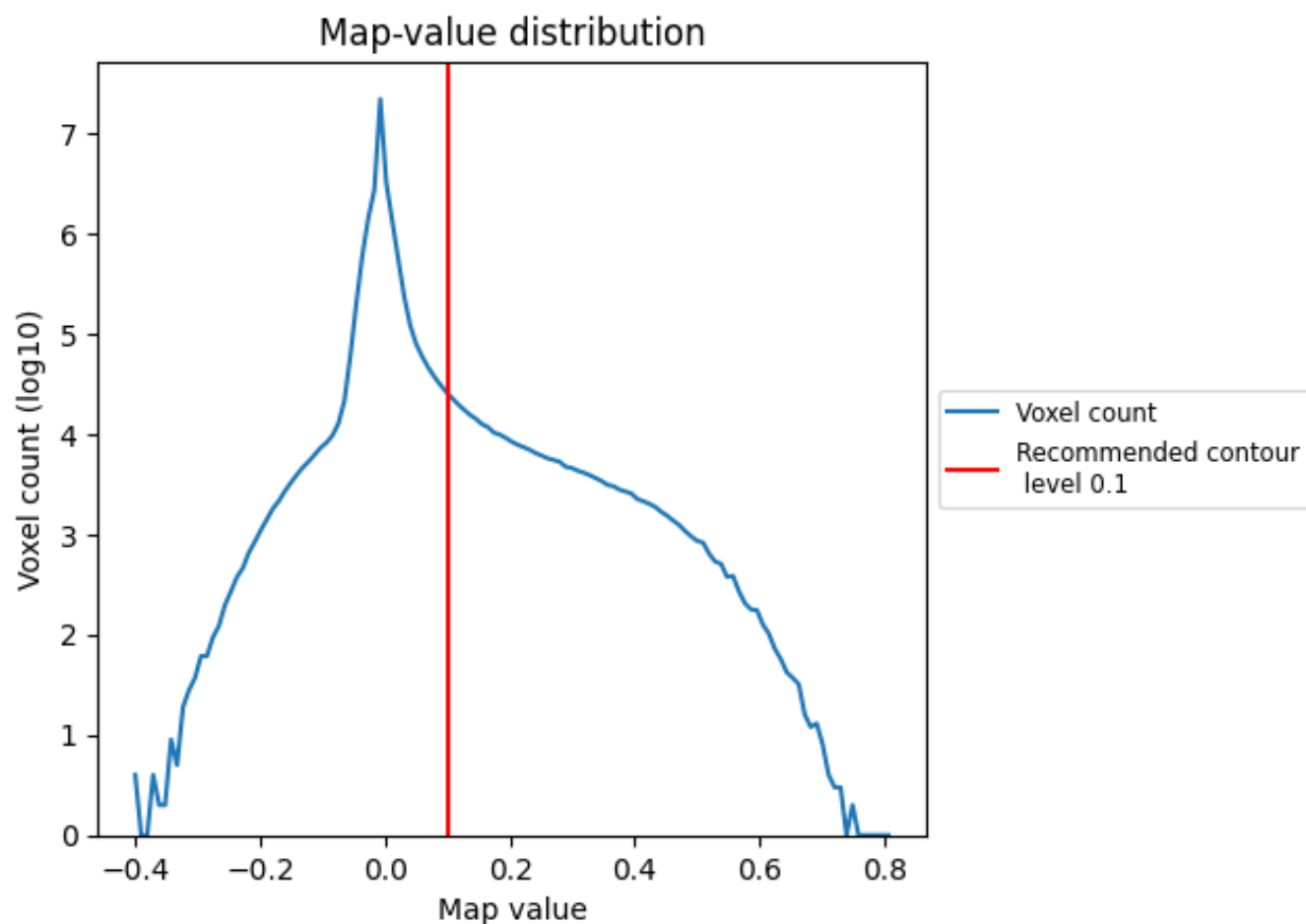


Z

7 Map analysis [i](#)

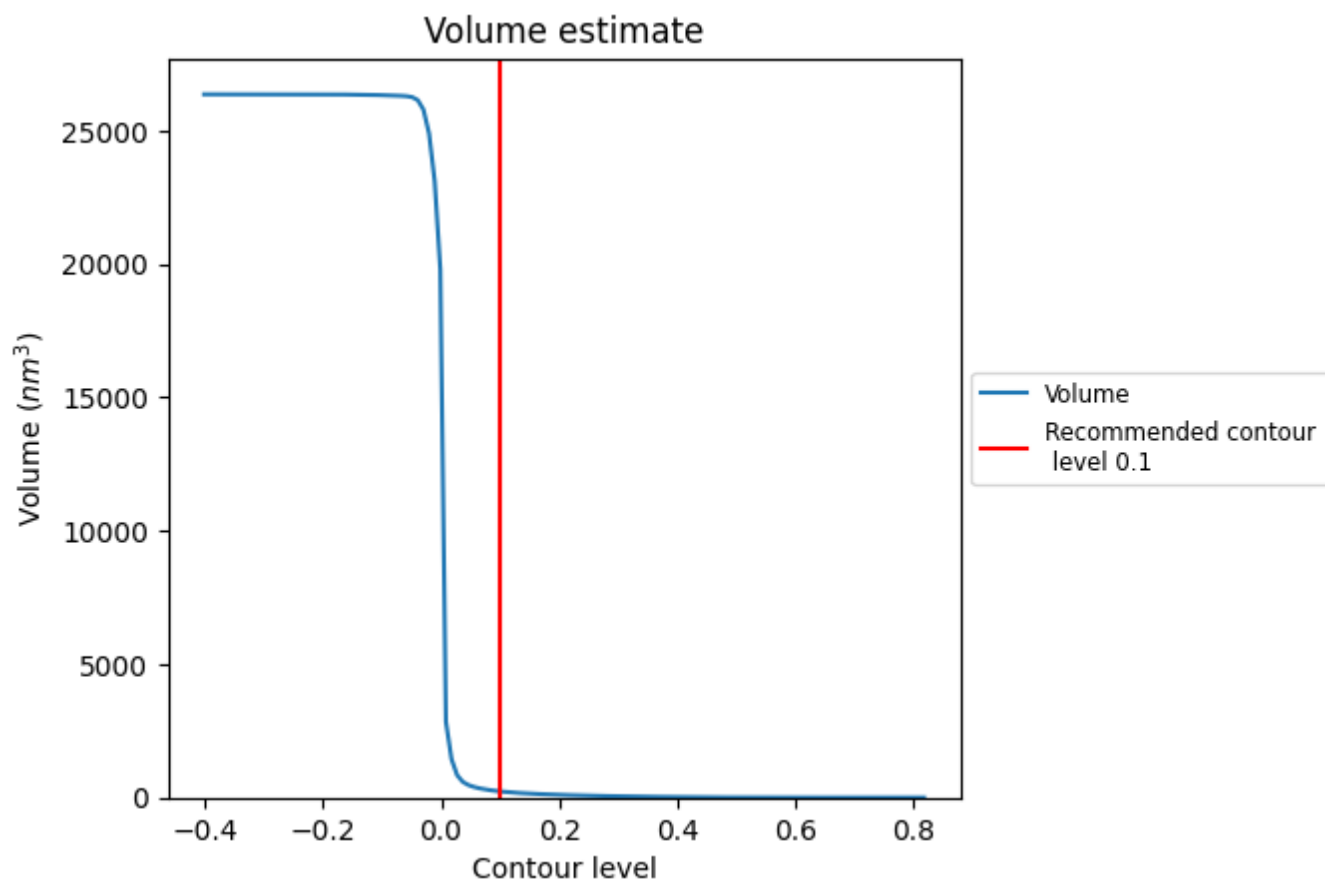
This section contains the results of statistical analysis of the map.

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.

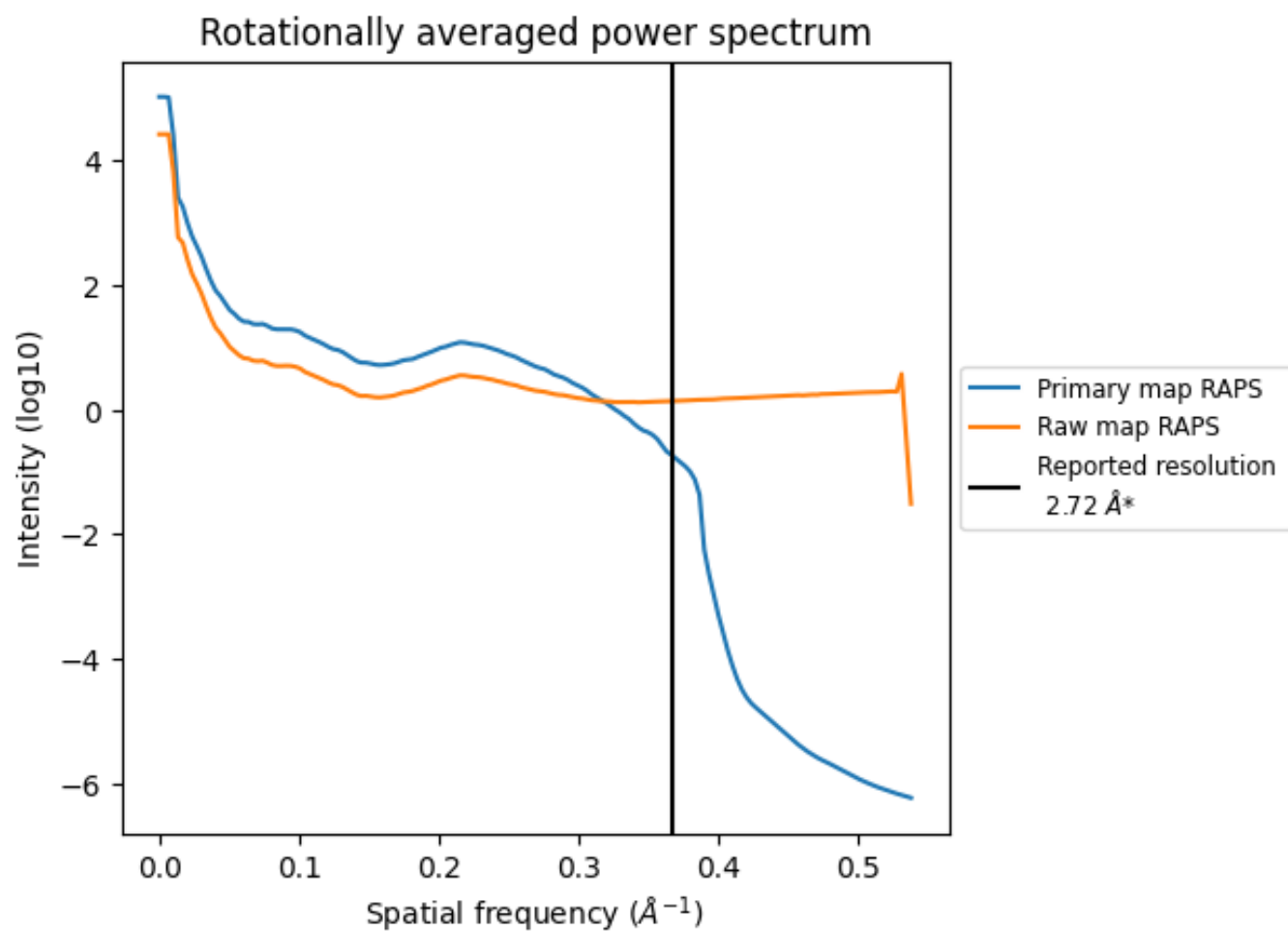
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 231 nm^3 ; this corresponds to an approximate mass of 208 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 ⓘ

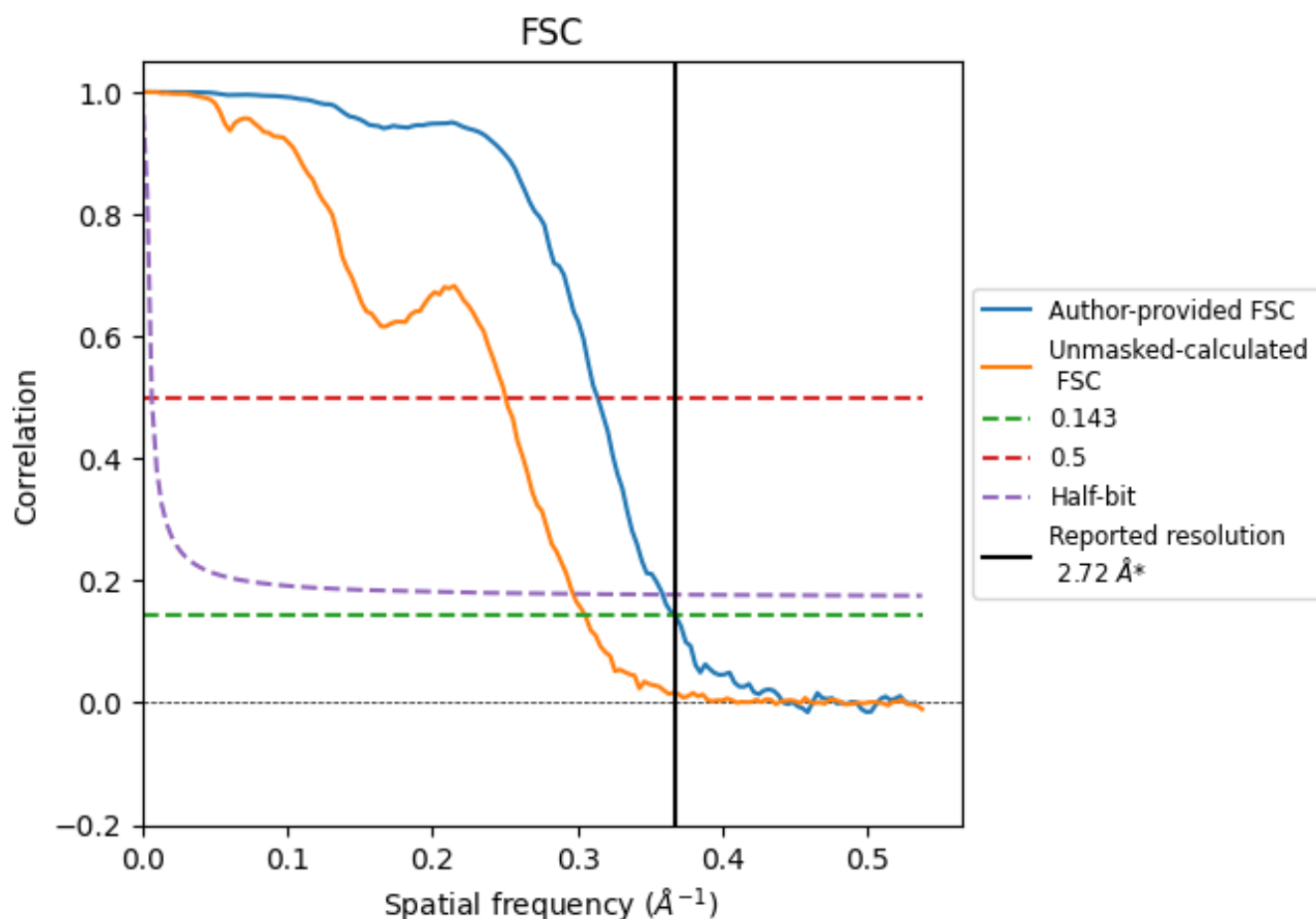


*Reported resolution corresponds to spatial frequency of 0.368 Å⁻¹

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 0.368 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

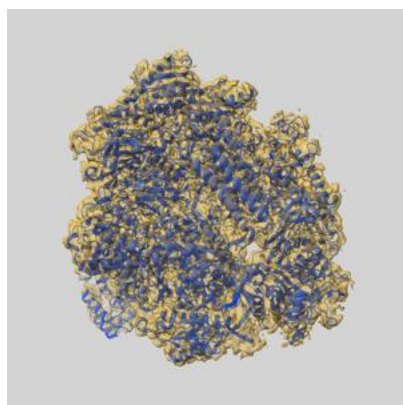
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	2.72	3.19	2.79
Unmasked-calculated*	3.28	3.99	3.37

*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 3.28 differs from the reported value 2.72 by more than 10 %

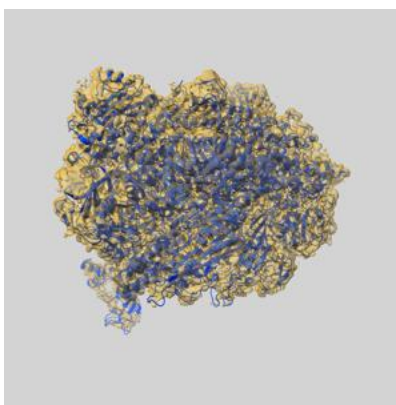
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-66161 and PDB model 9WQ7. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

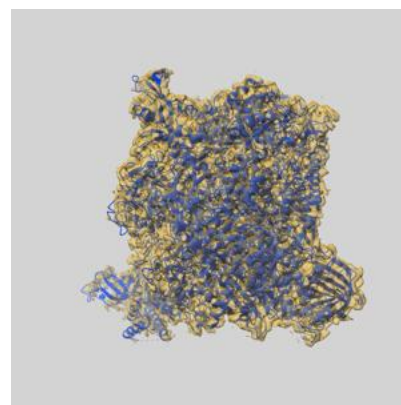
9.1 Map-model overlay [i](#)



X



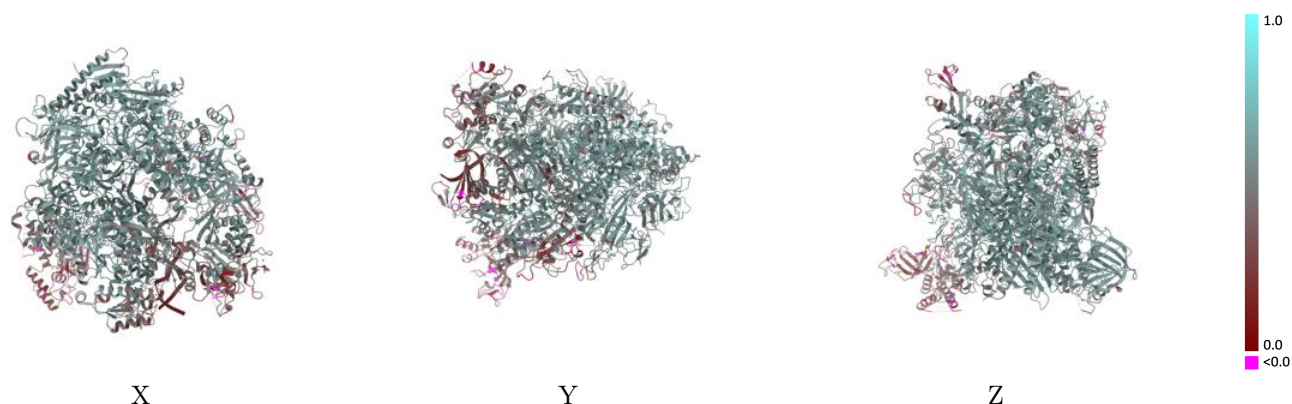
Y



Z

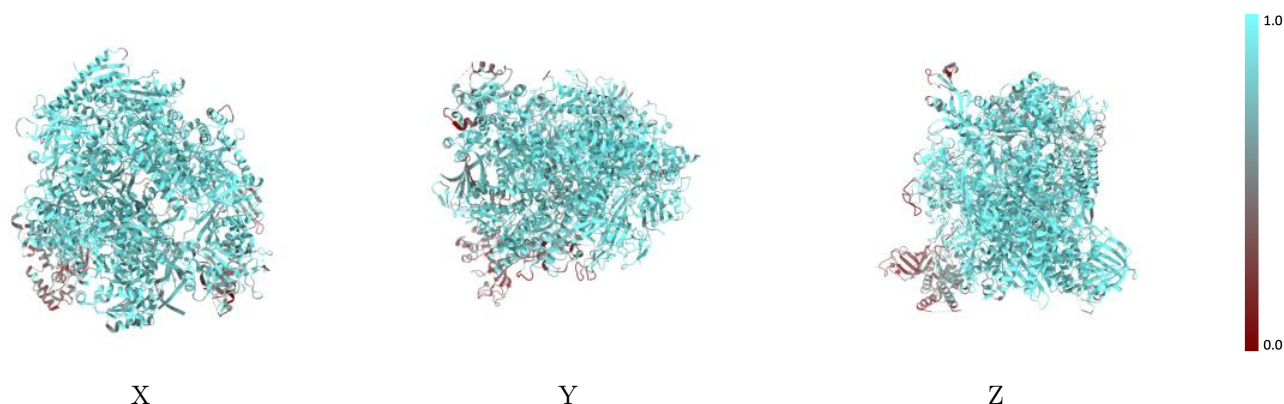
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



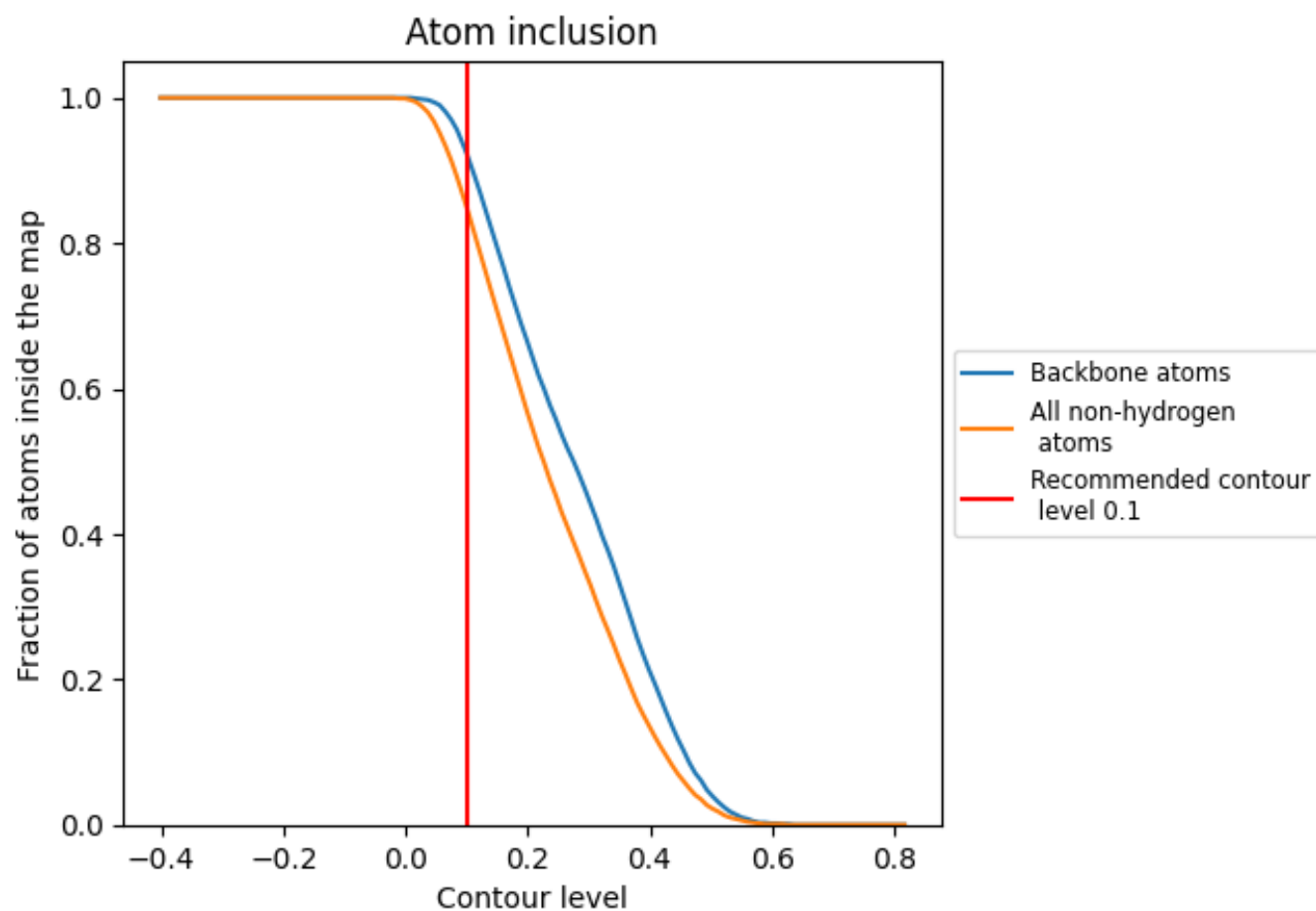
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8500	 0.5140
A	 0.8940	 0.5470
B	 0.8810	 0.5410
C	 0.9180	 0.5680
D	 0.3970	 0.2280
E	 0.8810	 0.4990
F	 0.9260	 0.5750
G	 0.4900	 0.3190
H	 0.8680	 0.5490
I	 0.8240	 0.4690
J	 0.9110	 0.5690
K	 0.9300	 0.5800
L	 0.8760	 0.5060
N	 0.8510	 0.3530
P	 0.9780	 0.5690
Q	 0.6550	 0.2820
T	 0.8660	 0.4220

