



## Full wwPDB EM Validation Report ⓘ

May 6, 2025 – 04:05 AM EDT

PDB ID : 8TUG / pdb\_00008tug  
EMDB ID : EMD-41623  
Title : Cryo-EM structure of CPD-stalled Pol II in complex with Rad26 (engaged state)  
Authors : Sarsam, R.D.; Lahiri, I.; Leschziner, A.E.  
Deposited on : 2023-08-16  
Resolution : 3.50 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

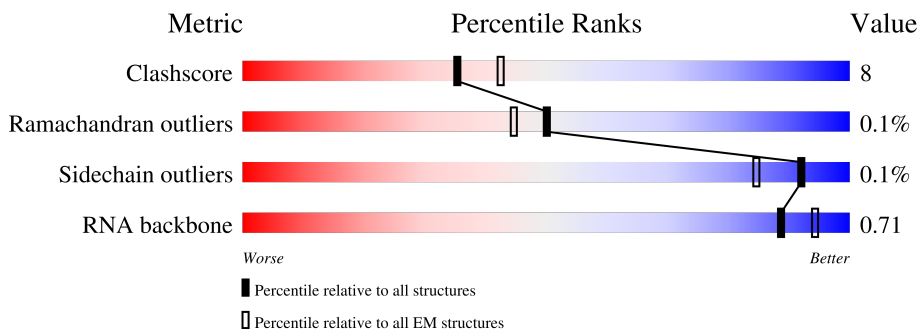
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 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.





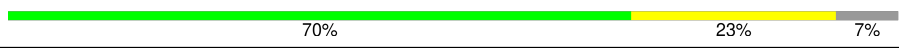


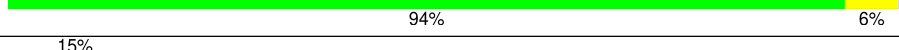


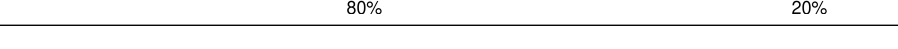
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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	
2	B	1224	
3	C	318	
4	D	221	
5	E	215	
6	F	155	
7	G	171	

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Mol	Chain	Length	Quality of chain
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	503	
14	N	47	
15	T	46	
16	R	10	

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 65461 atoms, of which 31025 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	1367	Total	C	H	N	O	S	0	0
			21594	6779	10845	1885	2024	61		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	1041	Total	C	H	N	O	S	0	0
			16596	5266	8295	1443	1538	54		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	266	Total	C	H	N	O	S	0	0
			4146	1317	2051	348	417	13		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	142	Total	C	H	N	O	S	0	0
			2276	702	1142	198	232	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	215	Total	C	H	N	O	S	0	0
			3548	1116	1788	310	322	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	81	Total	C	H	N	O	S	0	0
			1330	419	673	111	124	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	H	N	O	S	0	0
			2687	861	1347	222	249	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	133	Total	C	H	N	O	S	0	0
			2090	668	1030	174	213	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	117	Total	C	H	N	O	S	0	0
			1862	585	909	174	184	10		

- Molecule 10 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	65	Total	C	H	N	O	S	0	0
			1075	339	543	93	94	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	104	Total	C	H	N	O	S	0	0
			1674	534	840	142	157	1		

- Molecule 12 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	46	Total	C	H	N	O	S	0	0
			751	224	387	72	64	4		

- Molecule 13 is a protein called DNA repair and recombination protein RAD26.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	503	Total	C	N	O	0	0
			2516	1509	503	504		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	47	Total	C	H	N	O	P	0	0
			1496	460	531	176	282	47		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
15	T	46	Total	C	H	N	O	P	0	0
			1481	454	534	155	291	47		

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	R	10	Total	C	H	N	O	P	0	0
			330	98	110	45	67	10		

- 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	

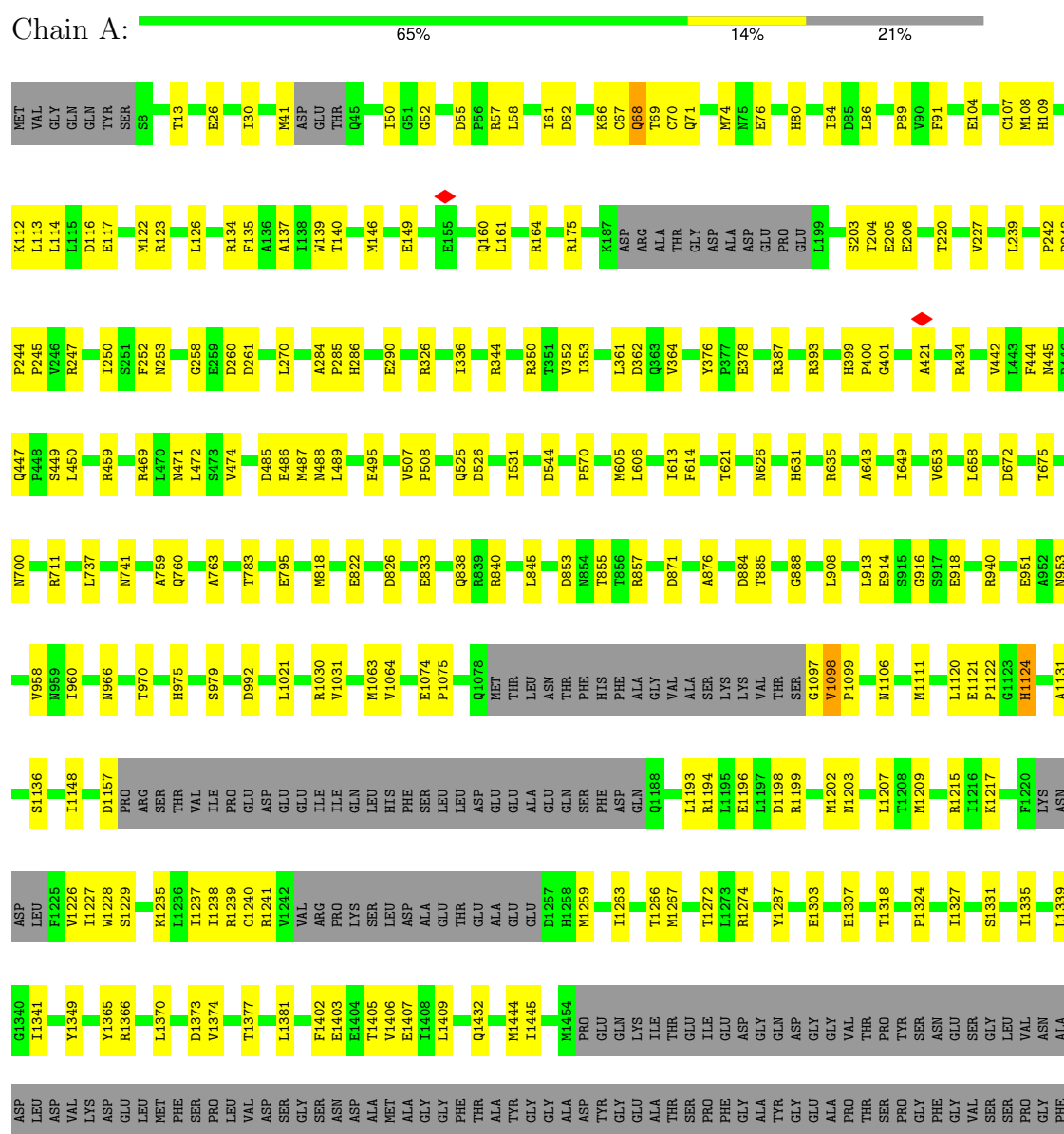
- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

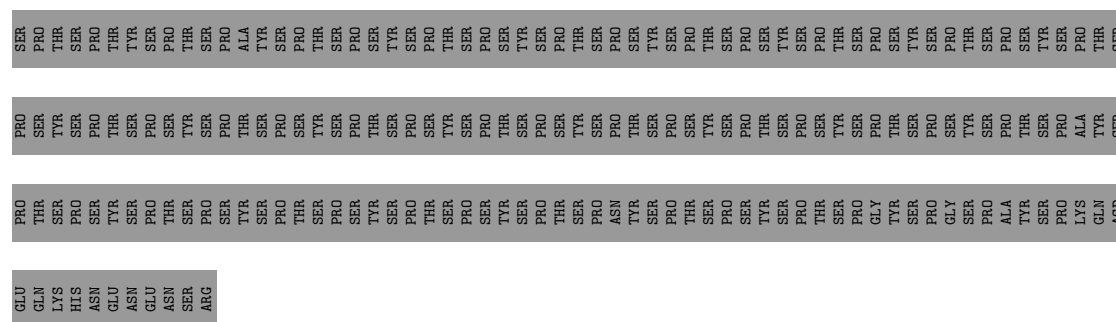
Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Mg	0
			1	1	

### 3 Residue-property plots

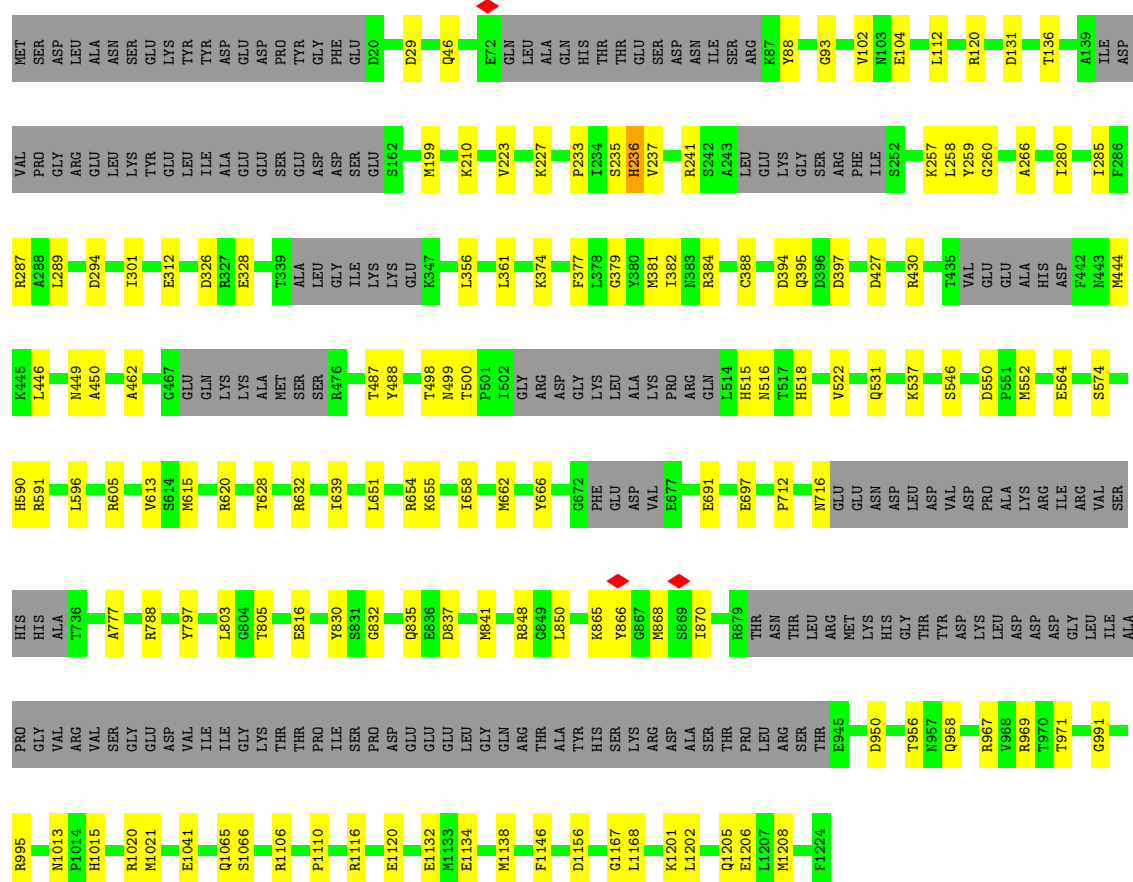
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

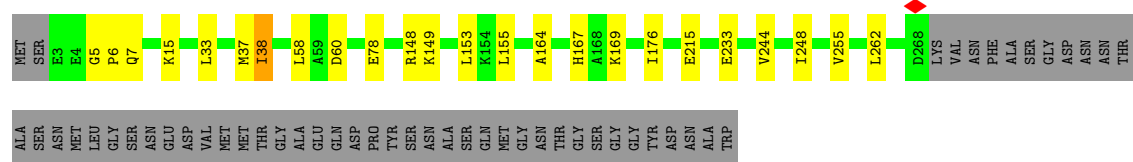




- Molecule 2: DNA-directed RNA polymerase subunit beta

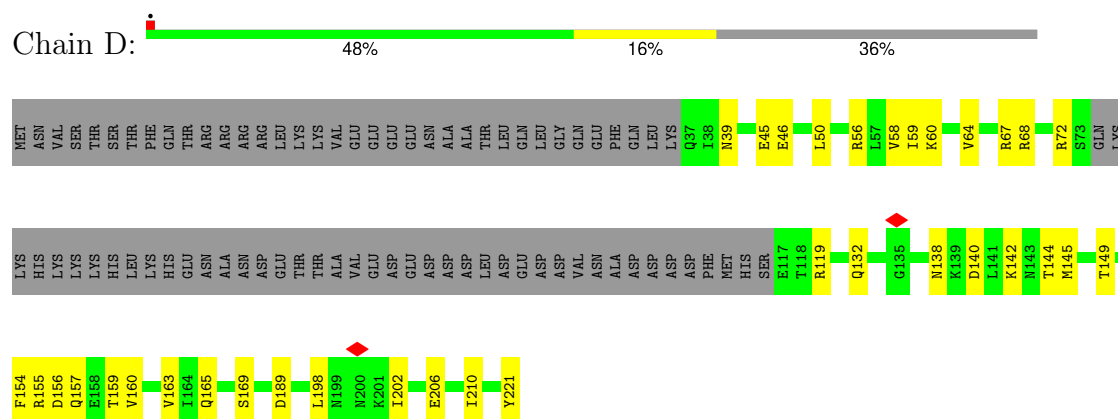


- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

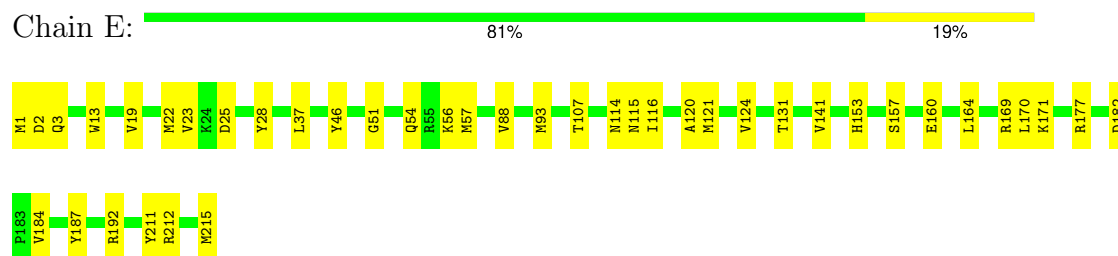




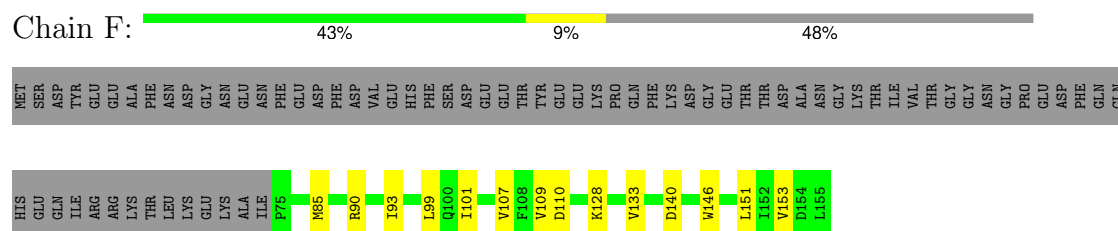
- Molecule 4: DNA-directed RNA polymerase II subunit RPB4



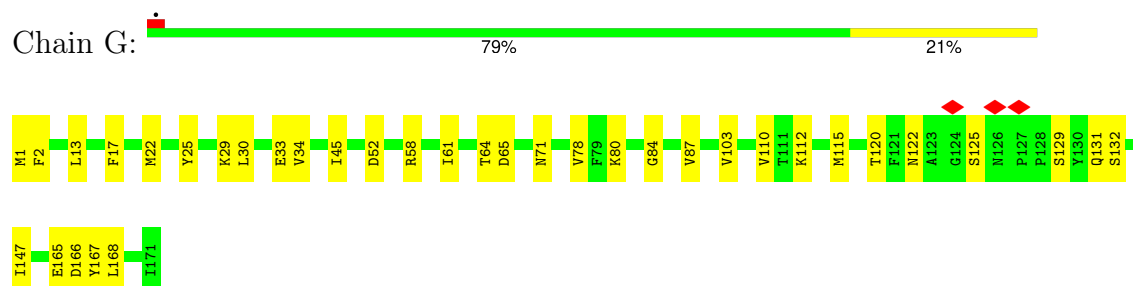
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



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

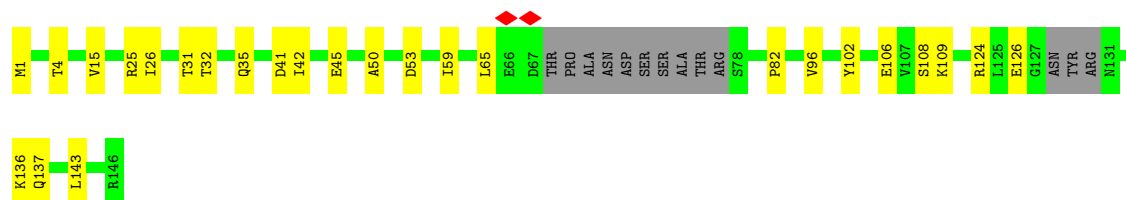


- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

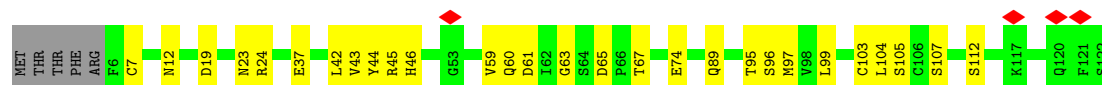


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

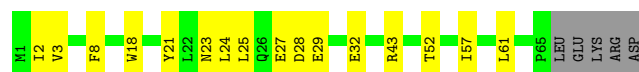




- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



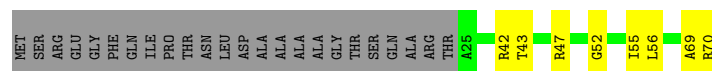
- Molecule 10: DNA-directed RNA polymerases II subunit RPABC5



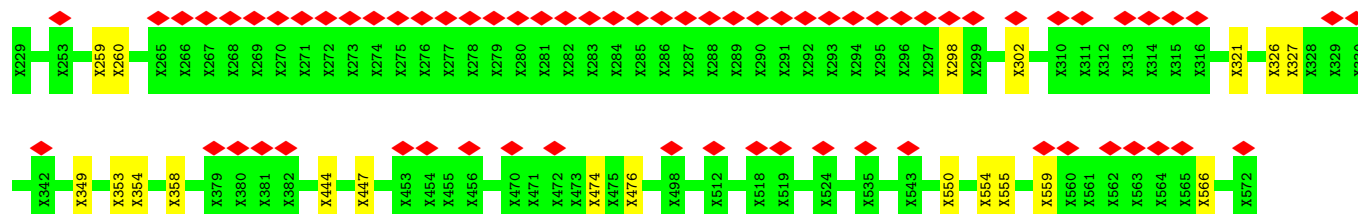
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



- Molecule 12: DNA-directed RNA polymerases II subunit RPABC4

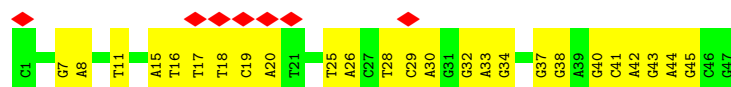


- Molecule 13: DNA repair and recombination protein RAD26

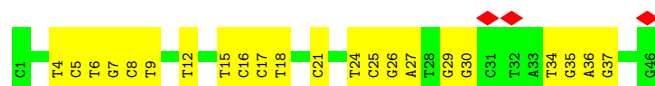




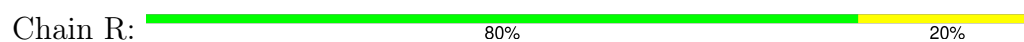
- Molecule 14: DNA (NTS)



- Molecule 15: DNA (TS)



- Molecule 16: RNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	59	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	6.298	Depositor
Minimum map value	-2.307	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.138	Depositor
Recommended contour level	0.647	Depositor
Map size ( $\text{\AA}$ )	445.44, 445.44, 445.44	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.16, 1.16, 1.16	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.09	0/10939	0.26	1/14785 (0.0%)
2	B	0.08	0/8463	0.22	0/11406
3	C	0.09	0/2133	0.23	0/2891
4	D	0.11	0/1142	0.27	0/1534
5	E	0.10	0/1796	0.26	0/2416
6	F	0.09	0/669	0.24	0/903
7	G	0.11	0/1368	0.29	0/1844
8	H	0.11	0/1076	0.32	0/1455
9	I	0.09	0/971	0.23	0/1305
10	J	0.12	0/541	0.30	0/727
11	K	0.12	0/850	0.27	0/1148
12	L	0.09	0/366	0.28	0/485
14	N	0.21	0/1082	0.44	0/1668
15	T	0.21	0/1010	0.47	0/1551
16	R	0.13	0/247	0.31	0/384
All	All	0.10	0/32653	0.27	1/44502 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	68	GLN	CA-CB-CG	5.39	124.87	114.10

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	10749	10845	10845	190	0
2	B	8301	8295	8295	92	0
3	C	2095	2051	2051	20	0
4	D	1134	1142	1142	26	0
5	E	1760	1788	1788	33	0
6	F	657	673	673	11	0
7	G	1340	1347	1357	44	0
8	H	1060	1030	1030	21	0
9	I	953	909	907	18	0
10	J	532	543	543	18	0
11	K	834	840	839	22	0
12	L	364	387	387	7	0
13	M	2516	0	527	16	0
14	N	965	531	531	22	0
15	T	947	534	534	21	0
16	R	220	110	110	1	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
18	A	1	0	0	0	0
All	All	34436	31025	31559	505	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 8.

All (505) 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)
7:G:165:GLU:OE2	7:G:168:LEU:CD2	1.64	1.45
7:G:165:GLU:OE2	7:G:168:LEU:CD1	1.73	1.34
7:G:165:GLU:OE2	7:G:168:LEU:CG	1.83	1.25
7:G:168:LEU:HD12	7:G:168:LEU:O	1.13	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:165:GLU:CD	7:G:168:LEU:HD21	1.63	1.22
7:G:165:GLU:OE2	7:G:168:LEU:HD11	1.32	1.20
7:G:165:GLU:OE2	7:G:168:LEU:HD21	1.20	1.17
7:G:168:LEU:CD1	7:G:168:LEU:O	1.98	1.12
7:G:167:TYR:O	7:G:168:LEU:HG	1.64	0.97
7:G:87:VAL:HG11	7:G:103:VAL:HG13	1.53	0.88
4:D:145:MET:HE3	4:D:145:MET:O	1.74	0.88
4:D:72:ARG:O	4:D:72:ARG:NH1	2.09	0.84
7:G:33:GLU:OE2	7:G:33:GLU:N	2.13	0.81
2:B:104:GLU:OE1	12:L:47:ARG:NH2	2.14	0.80
7:G:168:LEU:HD12	7:G:168:LEU:C	2.06	0.80
7:G:1:MET:SD	7:G:2:PHE:N	2.54	0.80
7:G:165:GLU:CD	7:G:168:LEU:HD11	2.06	0.80
4:D:157:GLN:N	4:D:157:GLN:OE1	2.14	0.79
4:D:138:ASN:OD1	4:D:142:LYS:NZ	2.16	0.78
14:N:32:DG:N2	15:T:17:DC:O2	2.16	0.78
3:C:148:ARG:NH1	10:J:61:LEU:O	2.16	0.77
2:B:287:ARG:NH2	2:B:294:ASP:OD1	2.17	0.77
7:G:167:TYR:C	7:G:168:LEU:HG	2.09	0.77
5:E:54:GLN:HB3	5:E:57:MET:HE2	1.68	0.74
1:A:635:ARG:NH2	1:A:876:ALA:O	2.21	0.74
1:A:364:VAL:HG21	1:A:444:PHE:CZ	2.23	0.74
5:E:46:TYR:O	5:E:54:GLN:NE2	2.21	0.73
1:A:66:LYS:O	1:A:69:THR:N	2.20	0.73
1:A:795:GLU:OE1	1:A:795:GLU:N	2.21	0.73
7:G:1:MET:N	7:G:80:LYS:O	2.17	0.73
11:K:79:GLU:OE1	11:K:79:GLU:N	2.21	0.72
2:B:227:LYS:NZ	2:B:388:CYS:SG	2.62	0.72
1:A:1237:ILE:HG22	1:A:1239:ARG:NH1	2.04	0.72
2:B:233:PRO:O	2:B:260:GLY:N	2.23	0.72
3:C:215:GLU:OE1	3:C:215:GLU:N	2.20	0.72
10:J:32:GLU:N	10:J:32:GLU:OE1	2.22	0.71
1:A:250:ILE:HG23	1:A:252:PHE:CE1	2.26	0.71
2:B:605:ARG:NE	2:B:691:GLU:OE2	2.23	0.70
1:A:855:THR:OG1	1:A:857:ARG:NH1	2.24	0.70
9:I:24:ARG:NH1	9:I:37:GLU:OE1	2.24	0.70
1:A:445:ASN:OD1	1:A:449:SER:OG	2.11	0.69
2:B:1134:GLU:OE1	2:B:1134:GLU:N	2.25	0.69
1:A:1238:ILE:O	1:A:1239:ARG:NH1	2.26	0.69
2:B:574:SER:OG	2:B:591:ARG:NH1	2.26	0.69
6:F:128:LYS:NZ	6:F:151:LEU:O	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:155:ARG:NH2	4:D:221:TYR:OXT	2.26	0.68
1:A:1209:MET:HE1	1:A:1228:TRP:CD1	2.29	0.68
2:B:427:ASP:OD1	2:B:430:ARG:NH2	2.26	0.68
1:A:393:ARG:NH1	1:A:421:ALA:O	2.25	0.68
1:A:108:MET:O	1:A:109:HIS:ND1	2.27	0.68
1:A:871:ASP:OD2	1:A:1366:ARG:NH2	2.27	0.67
1:A:1267:MET:HE2	1:A:1267:MET:N	2.08	0.67
13:M:354:UNK:O	13:M:358:UNK:N	2.27	0.67
9:I:65:ASP:OD2	9:I:67:THR:OG1	2.13	0.67
1:A:74:MET:O	2:B:1116:ARG:NH2	2.28	0.66
3:C:169:LYS:NZ	12:L:69:ALA:O	2.28	0.66
1:A:206:GLU:N	1:A:206:GLU:OE1	2.29	0.66
1:A:149:GLU:N	1:A:149:GLU:OE1	2.28	0.66
1:A:1136:SER:O	1:A:1274:ARG:NH1	2.29	0.65
1:A:916:GLY:N	1:A:918:GLU:OE1	2.29	0.65
1:A:50:ILE:HG22	1:A:52:GLY:H	1.61	0.65
1:A:344:ARG:NE	2:B:1120:GLU:OE2	2.30	0.65
9:I:103:CYS:O	9:I:107:SER:N	2.30	0.64
1:A:469:ARG:NH2	2:B:991:GLY:O	2.30	0.64
1:A:1157:ASP:O	1:A:1241:ARG:NH2	2.30	0.64
13:M:550:UNK:O	13:M:554:UNK:N	2.30	0.64
1:A:672:ASP:OD1	1:A:675:THR:OG1	2.15	0.64
2:B:1065:GLN:OE1	2:B:1066:SER:N	2.30	0.64
5:E:177:ARG:O	5:E:212:ARG:NH1	2.30	0.64
7:G:120:THR:N	7:G:132:SER:OG	2.30	0.64
1:A:951:GLU:OE2	1:A:953:ASN:N	2.31	0.64
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.79	0.64
8:H:96:VAL:HG22	8:H:143:LEU:HD22	1.80	0.64
1:A:362:ASP:O	1:A:459:ARG:N	2.30	0.64
1:A:1259:MET:HE3	1:A:1259:MET:H	1.61	0.64
1:A:1111:MET:HE1	1:A:1331:SER:HA	1.80	0.64
1:A:160:GLN:NE2	1:A:161:LEU:O	2.31	0.63
5:E:93:MET:HE3	5:E:93:MET:HA	1.79	0.63
14:N:11:DT:O2	15:T:37:DG:N2	2.31	0.63
1:A:137:ALA:O	1:A:140:THR:OG1	2.16	0.63
11:K:64:GLU:OE1	11:K:64:GLU:N	2.25	0.63
8:H:96:VAL:HG22	8:H:143:LEU:CD2	2.28	0.63
9:I:99:LEU:N	9:I:112:SER:OG	2.31	0.63
2:B:259:TYR:O	2:B:266:ALA:N	2.32	0.63
3:C:5:GLY:O	3:C:7:GLN:NE2	2.31	0.62
1:A:326:ARG:NH2	1:A:1407:GLU:OE2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:THR:O	1:A:69:THR:HG22	1.99	0.62
7:G:165:GLU:OE1	7:G:168:LEU:HD21	1.97	0.62
1:A:250:ILE:HG21	1:A:258:GLY:O	1.99	0.62
1:A:1287:TYR:O	1:A:1303:GLU:N	2.33	0.61
1:A:1209:MET:HE2	1:A:1209:MET:O	2.00	0.61
2:B:564:GLU:N	2:B:564:GLU:OE1	2.33	0.61
3:C:6:PRO:O	11:K:104:ASN:ND2	2.30	0.61
2:B:531:GLN:N	2:B:531:GLN:OE1	2.34	0.61
13:M:474:UNK:O	13:M:476:UNK:N	2.33	0.61
2:B:651:LEU:O	2:B:654:ARG:NH2	2.33	0.61
1:A:908:LEU:HD21	1:A:913:LEU:HD11	1.83	0.61
1:A:531:ILE:HG12	1:A:653:VAL:HG21	1.83	0.60
6:F:85:MET:HE3	6:F:90:ARG:HA	1.84	0.60
5:E:88:VAL:HG11	5:E:116:ILE:HD12	1.83	0.60
13:M:298:UNK:O	13:M:302:UNK:N	2.34	0.60
5:E:121:MET:SD	5:E:121:MET:N	2.75	0.60
1:A:1287:TYR:OH	1:A:1307:GLU:OE2	2.14	0.60
3:C:33:LEU:O	3:C:37:MET:HG3	2.00	0.60
2:B:397:ASP:OD2	2:B:515:HIS:NE2	2.35	0.60
8:H:50:ALA:N	8:H:53:ASP:OD2	2.35	0.60
1:A:442:VAL:HB	1:A:489:LEU:HD11	1.83	0.59
2:B:837:ASP:OD1	2:B:1020:ARG:NH2	2.35	0.59
5:E:3:GLN:NE2	5:E:51:GLY:O	2.36	0.59
7:G:167:TYR:O	7:G:168:LEU:CG	2.47	0.59
13:M:625:UNK:O	13:M:630:UNK:HA	2.02	0.59
1:A:378:GLU:OE2	1:A:387:ARG:NH2	2.36	0.59
1:A:1237:ILE:HG22	1:A:1239:ARG:HH11	1.67	0.59
2:B:1132:GLU:N	2:B:1132:GLU:OE2	2.35	0.59
8:H:106:GLU:OE1	8:H:106:GLU:N	2.35	0.59
1:A:253:ASN:ND2	15:T:29:DG:N3	2.51	0.59
2:B:788:ARG:O	2:B:967:ARG:NH1	2.36	0.59
2:B:356:LEU:O	2:B:374:LYS:NZ	2.35	0.58
2:B:950:ASP:OD1	2:B:969:ARG:NH1	2.36	0.58
8:H:1:MET:SD	8:H:65:LEU:N	2.76	0.58
15:T:25:DC:C2	15:T:26:DG:C8	2.92	0.58
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.03	0.58
1:A:117:GLU:O	1:A:123:ARG:NH1	2.36	0.58
1:A:853:ASP:OD2	1:A:857:ARG:NH1	2.37	0.58
1:A:1215:ARG:NE	1:A:1272:THR:O	2.37	0.58
13:M:615:UNK:O	13:M:619:UNK:N	2.37	0.58
7:G:87:VAL:HG11	7:G:103:VAL:CG1	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:805:THR:OG1	2:B:1041:GLU:OE2	2.09	0.57
2:B:1106:ARG:NH2	2:B:1110:PRO:O	2.37	0.57
1:A:113:LEU:O	1:A:164:ARG:NH1	2.38	0.57
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.87	0.57
2:B:93:GLY:N	2:B:131:ASP:O	2.37	0.57
7:G:110:VAL:HG12	7:G:115:MET:SD	2.45	0.57
1:A:1341:ILE:HG22	5:E:182:ASP:OD2	2.04	0.57
2:B:498:THR:OG1	2:B:537:LYS:O	2.19	0.57
2:B:312:GLU:OE2	9:I:46:HIS:ND1	2.38	0.56
2:B:120:ARG:NE	2:B:956:THR:O	2.37	0.56
1:A:70:CYS:SG	1:A:80:HIS:CE1	2.98	0.56
1:A:175:ARG:NH2	14:N:38:DG:OP1	2.37	0.56
1:A:107:CYS:N	1:A:112:LYS:O	2.37	0.56
1:A:361:LEU:HD12	1:A:643:ALA:HA	1.87	0.56
10:J:29:GLU:N	10:J:29:GLU:OE1	2.38	0.56
2:B:381:MET:HE3	2:B:382:ILE:N	2.19	0.56
4:D:198:LEU:O	4:D:202:ILE:HG22	2.06	0.56
7:G:166:ASP:OD1	7:G:167:TYR:N	2.38	0.56
12:L:42:ARG:O	12:L:43:THR:OG1	2.20	0.56
2:B:46:GLN:N	2:B:46:GLN:OE1	2.38	0.56
14:N:37:DG:N2	15:T:12:DT:O2	2.39	0.56
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.86	0.55
1:A:41:MET:HE3	1:A:41:MET:HA	1.89	0.55
1:A:1444:MET:HB2	6:F:133:VAL:HG13	1.89	0.55
4:D:154:PHE:HB3	4:D:160:VAL:HG22	1.87	0.55
1:A:885:THR:O	1:A:940:ARG:NH1	2.40	0.55
1:A:1209:MET:HE1	1:A:1228:TRP:HD1	1.71	0.55
3:C:233:GLU:OE1	10:J:43:ARG:NH1	2.40	0.55
2:B:289:LEU:HD21	2:B:356:LEU:HD12	1.88	0.55
2:B:394:ASP:OD1	2:B:395:GLN:N	2.38	0.55
2:B:1201:LYS:NZ	2:B:1205:GLN:OE1	2.37	0.55
1:A:108:MET:HE3	1:A:108:MET:HA	1.89	0.54
8:H:31:THR:O	8:H:32:THR:OG1	2.23	0.54
11:K:61:TYR:HB2	11:K:71:PHE:HE1	1.71	0.54
6:F:85:MET:HE1	6:F:93:ILE:HD12	1.89	0.54
14:N:45:DG:N2	15:T:4:DT:O2	2.40	0.54
1:A:68:GLN:O	1:A:68:GLN:CD	2.50	0.54
1:A:1266:THR:HB	1:A:1267:MET:HE2	1.89	0.54
14:N:41:DC:H2"	14:N:42:DA:C8	2.42	0.54
12:L:47:ARG:NH1	12:L:52:GLY:O	2.39	0.54
1:A:26:GLU:O	1:A:30:ILE:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:GLU:OE1	1:A:117:GLU:N	2.38	0.54
1:A:1148:ILE:N	1:A:1196:GLU:O	2.38	0.54
8:H:25:ARG:NE	8:H:41:ASP:OD1	2.35	0.54
14:N:15:DA:N6	14:N:16:DT:O4	2.41	0.54
1:A:966:ASN:O	1:A:970:THR:OG1	2.11	0.53
2:B:241:ARG:NH1	14:N:28:DT:O5'	2.42	0.53
8:H:124:ARG:NH1	8:H:126:GLU:OE2	2.38	0.53
13:M:719:UNK:HA	13:M:741:UNK:CB	2.38	0.53
1:A:250:ILE:HG23	1:A:252:PHE:CD1	2.44	0.53
1:A:783:THR:O	2:B:516:ASN:ND2	2.41	0.53
2:B:381:MET:HE3	2:B:381:MET:C	2.32	0.53
1:A:1405:THR:O	1:A:1409:LEU:HD23	2.08	0.53
2:B:499:ASN:OD1	2:B:500:THR:N	2.41	0.53
1:A:1064:VAL:HG12	1:A:1370:LEU:HD22	1.89	0.53
2:B:615:MET:N	2:B:697:GLU:OE2	2.41	0.53
1:A:116:ASP:OD2	1:A:164:ARG:NE	2.42	0.53
1:A:378:GLU:OE1	1:A:434:ARG:NE	2.42	0.53
4:D:156:ASP:O	4:D:160:VAL:HG23	2.09	0.53
4:D:46:GLU:OE1	4:D:46:GLU:N	2.37	0.53
2:B:816:GLU:N	2:B:816:GLU:OE1	2.42	0.52
3:C:248:ILE:HG21	11:K:102:LYS:HB2	1.91	0.52
11:K:113:THR:HA	11:K:116:ALA:HB3	1.91	0.52
1:A:485:ASP:OD1	16:R:10:A:O3'	2.27	0.52
1:A:606:LEU:HD13	8:H:102:TYR:OH	2.09	0.52
10:J:2:ILE:HD11	10:J:57:ILE:CD1	2.39	0.52
1:A:1238:ILE:C	1:A:1239:ARG:HD2	2.35	0.52
11:K:29:ASN:ND2	11:K:78:THR:O	2.43	0.52
1:A:146:MET:HA	1:A:146:MET:HE3	1.91	0.52
1:A:1148:ILE:HD11	1:A:1198:ASP:HA	1.92	0.52
7:G:71:ASN:OD1	7:G:71:ASN:O	2.27	0.52
15:T:25:DC:C2	15:T:26:DG:N7	2.78	0.52
1:A:626:ASN:O	1:A:631:HIS:ND1	2.38	0.52
3:C:78:GLU:N	3:C:78:GLU:OE1	2.41	0.52
1:A:104:GLU:OE1	1:A:139:TRP:NE1	2.40	0.51
2:B:326:ASP:OD1	2:B:328:GLU:N	2.44	0.51
2:B:848:ARG:NH1	10:J:8:PHE:O	2.44	0.51
1:A:711:ARG:NH1	9:I:97:MET:SD	2.83	0.51
2:B:995:ARG:NH2	3:C:164:ALA:O	2.44	0.51
1:A:1259:MET:H	1:A:1259:MET:CE	2.22	0.51
2:B:444:MET:SD	2:B:444:MET:N	2.84	0.51
5:E:170:LEU:HD23	5:E:171:LYS:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1209:MET:HE2	1:A:1209:MET:C	2.35	0.51
1:A:447:GLN:NE2	2:B:1134:GLU:OE2	2.41	0.51
1:A:114:LEU:O	1:A:164:ARG:NH2	2.44	0.51
10:J:28:ASP:C	10:J:29:GLU:OE1	2.53	0.51
5:E:114:ASN:C	5:E:114:ASN:OD1	2.54	0.51
1:A:84:ILE:HD13	1:A:270:LEU:HD21	1.92	0.50
2:B:550:ASP:OD1	2:B:552:MET:HE2	2.10	0.50
4:D:50:LEU:HD21	4:D:58:VAL:HG21	1.92	0.50
5:E:120:ALA:O	5:E:124:VAL:HG23	2.11	0.50
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.93	0.50
1:A:613:ILE:HG21	8:H:102:TYR:CD1	2.47	0.50
11:K:45:LEU:HD11	11:K:94:ILE:HD12	1.92	0.50
1:A:344:ARG:NH1	15:T:21:DC:OP1	2.45	0.50
4:D:56:ARG:HA	4:D:59:ILE:HG22	1.94	0.50
5:E:157:SER:N	5:E:160:GLU:OE2	2.39	0.50
5:E:1:MET:SD	5:E:2:ASP:N	2.85	0.49
1:A:474:VAL:HG22	1:A:474:VAL:O	2.12	0.49
1:A:1097:GLY:O	1:A:1098:VAL:HB	2.12	0.49
1:A:1263:ILE:HA	1:A:1267:MET:HE3	1.94	0.49
2:B:29:ASP:OD2	2:B:655:LYS:NZ	2.43	0.49
5:E:114:ASN:OD1	5:E:115:ASN:ND2	2.45	0.49
7:G:112:LYS:HA	7:G:115:MET:HE2	1.94	0.49
9:I:60:GLN:HG2	9:I:61:ASP:OD2	2.12	0.49
1:A:362:ASP:N	1:A:362:ASP:OD1	2.45	0.49
1:A:376:TYR:OH	1:A:495:GLU:OE2	2.24	0.49
2:B:102:VAL:HG22	2:B:112:LEU:HD13	1.93	0.49
1:A:1063:MET:HE3	1:A:1063:MET:HA	1.94	0.49
2:B:227:LYS:HA	2:B:236:HIS:HB3	1.94	0.49
4:D:64:VAL:O	4:D:68:ARG:NE	2.46	0.49
13:M:326:UNK:O	13:M:327:UNK:CB	2.60	0.49
1:A:1239:ARG:HD2	1:A:1239:ARG:N	2.28	0.49
5:E:19:VAL:O	5:E:22:MET:HB3	2.13	0.49
1:A:1193:LEU:HD13	1:A:1240:CYS:C	2.38	0.48
10:J:21:TYR:O	10:J:25:LEU:HD23	2.12	0.48
12:L:55:ILE:C	12:L:56:LEU:HD22	2.38	0.48
1:A:818:MET:HE1	2:B:516:ASN:HB3	1.95	0.48
4:D:189:ASP:OD1	4:D:189:ASP:C	2.56	0.48
9:I:19:ASP:O	9:I:23:ASN:N	2.46	0.48
1:A:450:LEU:O	1:A:838:GLN:NE2	2.41	0.48
5:E:157:SER:OG	5:E:160:GLU:OE1	2.30	0.48
7:G:84:GLY:N	7:G:147:ILE:O	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:64:VAL:HG22	4:D:68:ARG:NE	2.29	0.48
5:E:54:GLN:O	5:E:56:LYS:N	2.47	0.48
11:K:77:THR:OG1	11:K:81:TYR:O	2.30	0.48
1:A:445:ASN:ND2	1:A:447:GLN:OE1	2.46	0.48
15:T:24:DT:H2'	15:T:25:DC:H6	1.78	0.48
15:T:34:DT:H2'	15:T:35:DG:O4'	2.13	0.48
1:A:89:PRO:O	1:A:204:THR:HG21	2.12	0.48
1:A:286:HIS:NE2	1:A:290:GLU:OE2	2.46	0.48
2:B:958:GLN:OE1	2:B:958:GLN:N	2.43	0.48
1:A:108:MET:C	1:A:109:HIS:ND1	2.72	0.48
1:A:525:GLN:NE2	2:B:835:GLN:O	2.46	0.48
1:A:1124:HIS:ND1	1:A:1124:HIS:N	2.61	0.48
5:E:169:ARG:NE	6:F:140:ASP:OD2	2.44	0.48
11:K:81:TYR:OH	11:K:89:ASN:OD1	2.31	0.48
1:A:700:ASN:OD1	9:I:96:SER:OG	2.08	0.48
4:D:160:VAL:O	4:D:163:VAL:HG12	2.14	0.48
5:E:164:LEU:HD11	5:E:211:TYR:CE2	2.48	0.48
1:A:91:PHE:HE1	1:A:204:THR:HG23	1.79	0.48
15:T:24:DT:H2'	15:T:25:DC:C6	2.48	0.47
1:A:737:LEU:HD22	1:A:741:ASN:ND2	2.30	0.47
1:A:1381:LEU:N	1:A:1381:LEU:HD12	2.29	0.47
6:F:99:LEU:HD21	7:G:65:ASP:HA	1.97	0.47
1:A:203:SER:OG	1:A:205:GLU:OE1	2.31	0.47
1:A:57:ARG:HA	1:A:68:GLN:HB2	1.96	0.47
1:A:260:ASP:OD1	1:A:261:ASP:N	2.48	0.47
7:G:30:LEU:O	7:G:34:VAL:HG22	2.15	0.47
7:G:165:GLU:CG	7:G:168:LEU:HD11	2.43	0.47
14:N:17:DT:H2''	14:N:18:DT:C5	2.50	0.47
1:A:1445:ILE:HG13	7:G:61:ILE:HD11	1.97	0.47
2:B:29:ASP:O	2:B:658:ILE:HD11	2.14	0.47
4:D:156:ASP:OD1	4:D:159:THR:HG23	2.15	0.47
6:F:133:VAL:HG23	6:F:146:TRP:C	2.39	0.47
2:B:797:TYR:OH	2:B:971:THR:OG1	2.30	0.47
2:B:210:LYS:NZ	2:B:462:ALA:O	2.35	0.47
6:F:101:ILE:HD12	6:F:107:VAL:HG22	1.96	0.47
7:G:165:GLU:CD	7:G:168:LEU:CD2	2.46	0.47
15:T:8:DC:H2'	15:T:9:DT:H71	1.97	0.47
1:A:134:ARG:NH1	1:A:220:THR:O	2.43	0.47
2:B:381:MET:CE	2:B:382:ILE:HD13	2.45	0.47
8:H:31:THR:HG22	8:H:32:THR:HG23	1.96	0.47
14:N:17:DT:H2''	14:N:18:DT:C7	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:35:PHE:CD2	11:K:71:PHE:CE2	3.03	0.46
1:A:86:LEU:HD11	1:A:239:LEU:CD2	2.45	0.46
1:A:914:GLU:N	1:A:979:SER:O	2.46	0.46
8:H:15:VAL:HG22	8:H:26:ILE:HG22	1.96	0.46
4:D:154:PHE:CB	4:D:160:VAL:HG22	2.44	0.46
2:B:223:VAL:HG11	2:B:384:ARG:HD3	1.97	0.46
15:T:35:DG:H2''	15:T:36:DA:C8	2.51	0.46
5:E:107:THR:HG1	5:E:131:THR:HG1	1.54	0.46
10:J:24:LEU:HD23	10:J:28:ASP:OD2	2.15	0.46
1:A:336:ILE:HD13	1:A:1405:THR:HG21	1.96	0.46
1:A:350:ARG:NE	1:A:486:GLU:OE1	2.48	0.46
4:D:206:GLU:O	4:D:210:ILE:HG22	2.15	0.46
5:E:116:ILE:HD11	5:E:120:ALA:CB	2.45	0.46
7:G:165:GLU:CD	7:G:168:LEU:CG	2.78	0.46
1:A:1266:THR:HB	1:A:1267:MET:CE	2.44	0.46
2:B:301:ILE:HD13	2:B:382:ILE:HB	1.98	0.46
3:C:58:LEU:HD11	10:J:2:ILE:CD1	2.46	0.46
3:C:153:LEU:HD11	3:C:155:LEU:HD23	1.97	0.46
7:G:122:ASN:OD1	7:G:131:GLN:N	2.45	0.46
10:J:2:ILE:HG22	10:J:3:VAL:N	2.31	0.46
10:J:23:ASN:HA	10:J:27:GLU:OE1	2.14	0.46
11:K:53:ASP:OD1	11:K:54:ARG:N	2.49	0.46
1:A:822:GLU:O	1:A:826:ASP:OD2	2.34	0.46
1:A:203:SER:OG	1:A:206:GLU:OE1	2.34	0.46
1:A:570:PRO:HG3	8:H:82:PRO:HG3	1.98	0.46
4:D:165:GLN:O	4:D:169:SER:OG	2.27	0.46
5:E:192:ARG:NH1	5:E:215:MET:OXT	2.46	0.46
4:D:140:ASP:O	4:D:144:THR:N	2.40	0.45
1:A:353:ILE:HG21	1:A:487:MET:CG	2.46	0.45
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.98	0.45
1:A:526:ASP:OD2	2:B:1013:ASN:ND2	2.49	0.45
1:A:840:ARG:NH2	1:A:1106:ASN:OD1	2.49	0.45
1:A:544:ASP:OD1	11:K:47:ARG:NH1	2.49	0.45
7:G:52:ASP:OD2	7:G:52:ASP:C	2.60	0.45
14:N:29:DC:H4'	14:N:30:DA:OP1	2.17	0.45
1:A:1194:ARG:NH1	1:A:1237:ILE:HG23	2.31	0.45
1:A:1202:MET:HE3	1:A:1207:LEU:HB2	1.99	0.45
2:B:662:MET:O	2:B:666:TYR:HB3	2.17	0.45
6:F:153:VAL:O	6:F:153:VAL:HG13	2.15	0.45
13:M:555:UNK:O	13:M:559:UNK:N	2.50	0.44
2:B:712:PRO:O	2:B:716:ASN:N	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:60:ASP:OD1	3:C:60:ASP:N	2.50	0.44
1:A:13:THR:OG1	1:A:1432:GLN:OE1	2.30	0.44
1:A:614:PHE:CZ	8:H:102:TYR:CE1	3.06	0.44
1:A:649:ILE:O	1:A:653:VAL:HG23	2.17	0.44
2:B:237:VAL:HG12	2:B:257:LYS:HG2	1.99	0.44
1:A:884:ASP:OD2	1:A:1030:ARG:NH1	2.44	0.44
2:B:427:ASP:OD2	2:B:449:ASN:ND2	2.48	0.44
3:C:167:HIS:NE2	12:L:70:ARG:O	2.49	0.44
13:M:321:UNK:N	13:M:566:UNK:O	2.50	0.44
1:A:833:GLU:OE1	1:A:833:GLU:O	2.35	0.44
2:B:1138:MET:HE2	2:B:1146:PHE:CD2	2.53	0.44
13:M:353:UNK:O	13:M:447:UNK:HA	2.17	0.44
2:B:841:MET:CE	2:B:850:LEU:HD23	2.48	0.44
2:B:1168:LEU:HD12	2:B:1208:MET:HE1	1.99	0.44
11:K:22:ASP:C	11:K:22:ASP:OD2	2.61	0.44
11:K:38:GLU:OE1	11:K:38:GLU:HA	2.17	0.44
1:A:344:ARG:NH2	2:B:1120:GLU:OE1	2.50	0.44
13:M:700:UNK:N	13:M:725:UNK:O	2.51	0.44
1:A:76:GLU:HG3	1:A:76:GLU:O	2.18	0.44
7:G:13:LEU:HD11	7:G:17:PHE:HB2	1.99	0.44
9:I:42:LEU:HD21	9:I:45:ARG:HG2	1.99	0.44
1:A:658:LEU:HD13	2:B:830:TYR:O	2.18	0.44
2:B:620:ARG:NH1	9:I:89:GLN:OE1	2.51	0.44
5:E:153:HIS:CD2	5:E:184:VAL:HG11	2.52	0.44
1:A:1324:PRO:O	1:A:1327:ILE:HG22	2.18	0.43
9:I:103:CYS:SG	9:I:105:SER:OG	2.67	0.43
1:A:68:GLN:O	1:A:68:GLN:OE1	2.36	0.43
1:A:1217:LYS:HA	1:A:1226:VAL:HG21	2.00	0.43
11:K:24:ASP:OD1	11:K:25:THR:N	2.50	0.43
1:A:472:LEU:HD11	2:B:835:GLN:HB2	2.00	0.43
1:A:605:MET:HE3	1:A:621:THR:HG21	2.00	0.43
1:A:1381:LEU:HD12	1:A:1381:LEU:H	1.84	0.43
2:B:1167:GLY:C	2:B:1168:LEU:HD22	2.42	0.43
14:N:25:DT:H4'	14:N:26:DA:OP2	2.17	0.43
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.99	0.43
5:E:164:LEU:HD11	5:E:211:TYR:CD2	2.53	0.43
14:N:19:DC:H1'	14:N:20:DA:C8	2.53	0.43
5:E:13:TRP:NE1	5:E:37:LEU:O	2.49	0.43
5:E:54:GLN:CB	5:E:57:MET:HE2	2.45	0.43
1:A:284:ALA:N	1:A:285:PRO:HD3	2.34	0.43
1:A:1098:VAL:HB	1:A:1099:PRO:CD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:446:LEU:O	2:B:450:ALA:N	2.52	0.43
15:T:5:DC:H2"	15:T:6:DT:C6	2.54	0.43
1:A:444:PHE:CE1	1:A:489:LEU:HD13	2.54	0.43
5:E:25:ASP:OD2	5:E:187:TYR:OH	2.23	0.43
14:N:43:DG:H2"	14:N:44:DA:C8	2.54	0.43
1:A:1349:TYR:HH	1:A:1365:TYR:HD2	1.62	0.43
2:B:546:SER:OG	2:B:632:ARG:N	2.51	0.43
7:G:22:MET:C	7:G:22:MET:SD	3.01	0.43
8:H:35:GLN:H	8:H:35:GLN:CD	2.26	0.43
9:I:7:CYS:N	9:I:12:ASN:O	2.46	0.43
11:K:17:SER:O	11:K:20:LYS:NZ	2.39	0.43
11:K:24:ASP:OD2	11:K:74:ARG:NE	2.42	0.43
1:A:1318:THR:HG22	5:E:141:VAL:HG21	2.01	0.43
13:M:671:UNK:O	13:M:746:UNK:N	2.52	0.43
14:N:40:DG:H2"	14:N:41:DC:C6	2.54	0.43
1:A:66:LYS:O	1:A:67:CYS:C	2.61	0.43
2:B:88:TYR:CE2	2:B:136:THR:HG23	2.54	0.43
2:B:866:TYR:HB3	2:B:868:MET:HE1	2.01	0.43
9:I:63:GLY:HA3	9:I:104:LEU:HD21	2.00	0.43
1:A:1199:ARG:NH2	1:A:1203:ASN:OD1	2.52	0.42
5:E:56:LYS:HG3	5:E:57:MET:SD	2.59	0.42
7:G:1:MET:HE2	7:G:2:PHE:HD2	1.84	0.42
7:G:125:SER:OG	7:G:129:SER:N	2.51	0.42
13:M:629:UNK:N	13:M:630:UNK:HA	2.33	0.42
4:D:67:ARG:NH1	4:D:132:GLN:OE1	2.52	0.42
5:E:23:VAL:HG12	5:E:28:TYR:HB2	2.01	0.42
7:G:45:ILE:HG13	7:G:78:VAL:HG12	2.01	0.42
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.54	0.42
10:J:28:ASP:O	10:J:29:GLU:C	2.62	0.42
14:N:33:DA:H2"	14:N:34:DG:C8	2.54	0.42
1:A:227:VAL:HG22	1:A:227:VAL:O	2.19	0.42
1:A:252:PHE:CD1	1:A:252:PHE:N	2.87	0.42
1:A:352:VAL:HG12	1:A:353:ILE:N	2.34	0.42
1:A:711:ARG:NH2	9:I:95:THR:OG1	2.47	0.42
1:A:888:GLY:O	1:A:940:ARG:NH2	2.46	0.42
1:A:1229:SER:OG	1:A:1237:ILE:O	2.35	0.42
3:C:255:VAL:HG21	11:K:94:ILE:HG21	2.01	0.42
7:G:29:LYS:O	7:G:33:GLU:OE2	2.37	0.42
8:H:4:THR:OG1	8:H:59:ILE:O	2.27	0.42
14:N:11:DT:C2	15:T:37:DG:N2	2.86	0.42
15:T:26:DG:H2"	15:T:27:DA:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:29:DG:H3'	15:T:30:DG:C5'	2.49	0.42
15:T:30:DG:N3	15:T:30:DG:H2'	2.35	0.42
1:A:122:MET:HE1	1:A:126:LEU:HD11	2.01	0.42
2:B:613:VAL:HG22	2:B:628:THR:HG22	2.00	0.42
1:A:526:ASP:OD1	2:B:1015:HIS:ND1	2.53	0.42
2:B:1202:LEU:O	2:B:1206:GLU:HG3	2.19	0.42
8:H:26:ILE:HD13	8:H:42:ILE:HD13	2.01	0.42
1:A:1207:LEU:HD21	1:A:1274:ARG:HE	1.84	0.42
2:B:280:ILE:HG21	2:B:285:ILE:HD11	2.02	0.42
8:H:45:GLU:OE2	8:H:45:GLU:HA	2.20	0.42
8:H:108:SER:O	8:H:109:LYS:HG3	2.19	0.42
1:A:242:PRO:O	1:A:247:ARG:NH2	2.50	0.42
1:A:1120:LEU:HD11	1:A:1131:ALA:HB2	2.02	0.42
1:A:1209:MET:C	1:A:1209:MET:SD	3.03	0.42
4:D:39:ASN:ND2	4:D:45:GLU:OE2	2.53	0.42
5:E:22:MET:CE	5:E:187:TYR:CD1	3.03	0.42
9:I:59:VAL:HG12	9:I:61:ASP:H	1.85	0.42
1:A:759:ALA:O	1:A:763:ALA:N	2.53	0.42
2:B:832:GLY:O	2:B:835:GLN:HG2	2.20	0.42
10:J:27:GLU:CD	10:J:27:GLU:N	2.77	0.42
1:A:69:THR:O	1:A:69:THR:CG2	2.67	0.42
1:A:1074:GLU:HG3	1:A:1075:PRO:HD3	2.01	0.42
4:D:60:LYS:O	4:D:64:VAL:HG12	2.20	0.42
1:A:58:LEU:HD22	1:A:80:HIS:O	2.20	0.42
1:A:61:ILE:HG22	1:A:62:ASP:N	2.34	0.42
2:B:301:ILE:HD12	2:B:379:GLY:O	2.19	0.42
4:D:156:ASP:OD2	4:D:156:ASP:C	2.62	0.41
7:G:64:THR:OG1	7:G:65:ASP:N	2.53	0.41
10:J:2:ILE:HD11	10:J:57:ILE:HD12	2.02	0.41
14:N:7:DG:C2	14:N:8:DA:C4	3.08	0.41
14:N:17:DT:H2"	14:N:18:DT:H73	2.02	0.41
1:A:55:ASP:OD2	1:A:57:ARG:NE	2.52	0.41
1:A:992:ASP:OD2	1:A:992:ASP:C	2.63	0.41
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	2.01	0.41
2:B:235:SER:N	2:B:258:LEU:O	2.45	0.41
2:B:487:THR:HG21	2:B:777:ALA:O	2.20	0.41
3:C:37:MET:HE1	3:C:244:VAL:HG22	2.02	0.41
5:E:88:VAL:CG1	5:E:93:MET:SD	3.08	0.41
14:N:40:DG:N2	15:T:9:DT:O2	2.53	0.41
3:C:15:LYS:N	11:K:120:PHE:O	2.49	0.41
5:E:157:SER:HG	5:E:160:GLU:CD	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:109:VAL:HG12	6:F:110:ASP:N	2.34	0.41
13:M:349:UNK:O	13:M:444:UNK:N	2.54	0.41
1:A:845:LEU:CD2	1:A:1374:VAL:HG21	2.51	0.41
1:A:1199:ARG:NE	1:A:1203:ASN:OD1	2.52	0.41
2:B:199:MET:HE2	2:B:488:TYR:OH	2.18	0.41
7:G:25:TYR:O	7:G:29:LYS:HG2	2.20	0.41
9:I:43:VAL:HG13	9:I:44:TYR:N	2.34	0.41
1:A:447:GLN:OE1	1:A:488:ASN:ND2	2.54	0.41
3:C:262:LEU:HD11	11:K:87:LEU:HD23	2.03	0.41
1:A:69:THR:O	1:A:71:GLN:NE2	2.54	0.41
1:A:362:ASP:OD2	1:A:459:ARG:NE	2.40	0.41
1:A:1227:ILE:HB	1:A:1239:ARG:O	2.20	0.41
1:A:1402:PHE:CE2	1:A:1403:GLU:HG3	2.56	0.41
4:D:119:ARG:HB2	4:D:149:THR:HG22	2.02	0.41
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.03	0.41
1:A:975:HIS:CD2	1:A:975:HIS:O	2.74	0.41
11:K:22:ASP:OD2	11:K:23:PRO:N	2.54	0.41
15:T:15:DT:H2'	15:T:16:DC:C5	2.56	0.41
1:A:507:VAL:N	1:A:508:PRO:HD2	2.36	0.41
1:A:760:GLN:OE1	2:B:1021:MET:HE1	2.20	0.41
13:M:259:UNK:O	13:M:260:UNK:C	2.69	0.41
14:N:32:DG:HI'	14:N:33:DA:C8	2.56	0.41
2:B:803:LEU:HG	10:J:52:THR:HG21	2.03	0.41
4:D:50:LEU:O	7:G:1:MET:HE1	2.20	0.41
1:A:613:ILE:HG21	8:H:102:TYR:CE1	2.56	0.40
1:A:1235:LYS:HB3	1:A:1237:ILE:HD11	2.02	0.40
1:A:1239:ARG:N	1:A:1239:ARG:CD	2.83	0.40
3:C:148:ARG:HG2	3:C:149:LYS:H	1.86	0.40
8:H:136:LYS:C	8:H:137:GLN:OE1	2.64	0.40
1:A:91:PHE:CE1	1:A:204:THR:HG23	2.55	0.40
1:A:1031:VAL:O	1:A:1031:VAL:HG12	2.21	0.40
1:A:1074:GLU:N	1:A:1075:PRO:HD2	2.35	0.40
1:A:1097:GLY:O	1:A:1098:VAL:CB	2.70	0.40
2:B:361:LEU:HD21	2:B:377:PHE:CD1	2.57	0.40
2:B:381:MET:HE1	2:B:382:ILE:HD13	2.01	0.40
2:B:518:HIS:HB3	2:B:522:VAL:HG22	2.02	0.40
2:B:865:LYS:HB2	2:B:870:ILE:HG21	2.03	0.40
6:F:133:VAL:HG11	7:G:58:ARG:NH1	2.36	0.40
1:A:399:HIS:O	1:A:401:GLY:N	2.54	0.40
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	2.03	0.40
2:B:590:HIS:CD2	2:B:596:LEU:HD22	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1156:ASP:N	2:B:1156:ASP:OD1	2.55	0.40
7:G:165:GLU:HG3	7:G:167:TYR:O	2.21	0.40
9:I:74:GLU:OE1	9:I:74:GLU:N	2.54	0.40
15:T:7:DG:C2	15:T:8:DC:C2	3.10	0.40
1:A:244:PRO:N	1:A:245:PRO:CD	2.85	0.40
1:A:471:ASN:O	1:A:474:VAL:HG12	2.21	0.40
12:L:55:ILE:O	12:L:56:LEU:HD22	2.22	0.40
1:A:960:ILE:HD12	1:A:1021:LEU:HG	2.04	0.40
14:N:42:DA:HI'	14:N:43:DG:C8	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	1353/1733 (78%)	1311 (97%)	40 (3%)	2 (0%)	48	79
2	B	1019/1224 (83%)	979 (96%)	40 (4%)	0	100	100
3	C	264/318 (83%)	259 (98%)	5 (2%)	0	100	100
4	D	138/221 (62%)	137 (99%)	1 (1%)	0	100	100
5	E	213/215 (99%)	206 (97%)	7 (3%)	0	100	100
6	F	79/155 (51%)	78 (99%)	1 (1%)	0	100	100
7	G	169/171 (99%)	164 (97%)	5 (3%)	0	100	100
8	H	127/146 (87%)	116 (91%)	11 (9%)	0	100	100
9	I	115/122 (94%)	108 (94%)	7 (6%)	0	100	100
10	J	63/70 (90%)	61 (97%)	2 (3%)	0	100	100
11	K	102/120 (85%)	101 (99%)	1 (1%)	0	100	100
12	L	44/70 (63%)	42 (96%)	2 (4%)	0	100	100
All	All	3686/4565 (81%)	3562 (97%)	122 (3%)	2 (0%)	50	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1098	VAL
1	A	958	VAL

### 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	1192/1520 (78%)	1190 (100%)	2 (0%)	92	97
2	B	902/1061 (85%)	901 (100%)	1 (0%)	92	97
3	C	234/274 (85%)	233 (100%)	1 (0%)	89	95
4	D	127/200 (64%)	127 (100%)	0	100	100
5	E	197/197 (100%)	197 (100%)	0	100	100
6	F	72/137 (53%)	72 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	117/128 (91%)	117 (100%)	0	100	100
9	I	111/116 (96%)	111 (100%)	0	100	100
10	J	60/65 (92%)	60 (100%)	0	100	100
11	K	89/102 (87%)	89 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
All	All	3293/4009 (82%)	3289 (100%)	4 (0%)	92	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	PHE
1	A	1124	HIS
2	B	236	HIS
3	C	38	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	363	GLN
1	A	877	HIS
1	A	975	HIS
1	A	1048	ASN
1	A	1390	ASN
2	B	60	GLN
2	B	648	HIS
2	B	1093	GLN
3	C	17	ASN
3	C	65	HIS
3	C	231	ASN
3	C	242	GLN
5	E	101	GLN
7	G	117	GLN
8	H	35	GLN
8	H	134	ASN
9	I	116	ASN
11	K	112	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	R	9/10 (90%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	R	3	C

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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
15	TTD	T	18	15	42,45,46	1.31	7 (16%)	61,74,77	2.23	12 (19%)

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
15	TTD	T	18	15	-	9/22/109/110	0/5/6/6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	18	TTD	C2T-N1T	3.53	1.43	1.36
15	T	18	TTD	C4T-N3T	-2.78	1.32	1.37
15	T	18	TTD	C1R-N1T	2.77	1.49	1.45
15	T	18	TTD	C5-C6	-2.61	1.52	1.55
15	T	18	TTD	C2T-N3T	-2.60	1.33	1.38
15	T	18	TTD	C2-N3	-2.42	1.33	1.38
15	T	18	TTD	C4-N3	-2.24	1.33	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	18	TTD	N3T-C2T-N1T	7.62	124.76	116.78
15	T	18	TTD	C5-C4-N3	5.31	120.55	116.09
15	T	18	TTD	O4'-C1'-N1	4.98	114.56	108.65
15	T	18	TTD	N3-C2-N1	4.87	121.88	116.78
15	T	18	TTD	C2'-C1'-N1	-4.74	109.18	115.59
15	T	18	TTD	C5T-C4T-N3T	4.59	119.94	116.09
15	T	18	TTD	O4-C4-C5	-4.44	118.58	122.71
15	T	18	TTD	O2T-C2T-N1T	-4.27	117.05	123.44
15	T	18	TTD	O4T-C4T-C5T	-4.22	118.78	122.71
15	T	18	TTD	O4R-C1R-N1T	3.64	112.96	108.65
15	T	18	TTD	O2-C2-N1	-2.59	119.56	123.44
15	T	18	TTD	C6T-C6-N1	-2.03	110.94	118.51

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	18	TTD	O4'-C1'-N1-C2
15	T	18	TTD	O4'-C1'-N1-C6
15	T	18	TTD	O4'-C4R-C5'-O5'
15	T	18	TTD	C2'-C3R-O3R-PB
15	T	18	TTD	C2'-C1'-N1-C6
15	T	18	TTD	O4R-C4'-C5R-O5R
15	T	18	TTD	C2'-C1'-N1-C2
15	T	18	TTD	C3R-O3R-PB-O4P
15	T	18	TTD	C3R-C4R-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	M	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	631:UNK	C	645:UNK	N	4.87
1	M	388:UNK	C	389:UNK	N	3.17
1	M	389:UNK	C	443:UNK	N	3.10



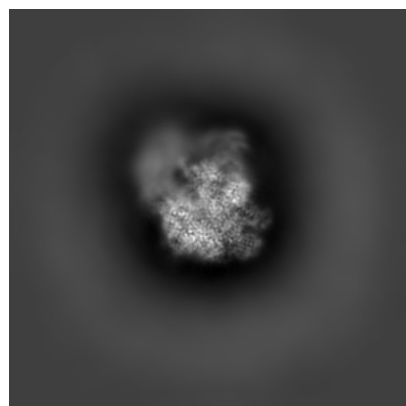
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41623. These allow visual inspection of the internal detail of the map and identification of artifacts.

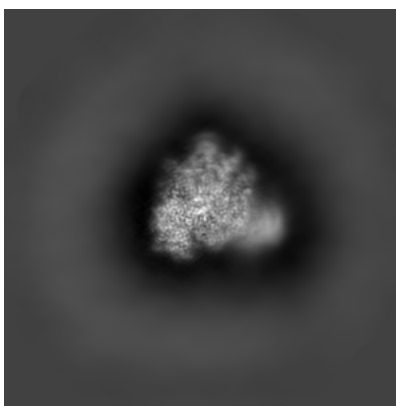
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

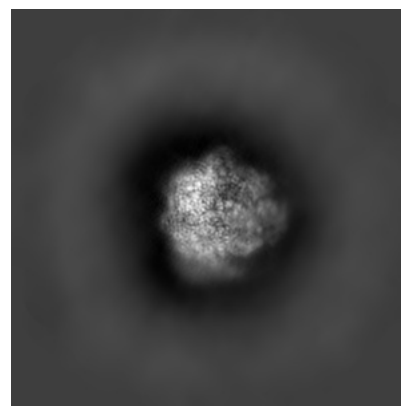
#### 6.1.1 Primary map



X

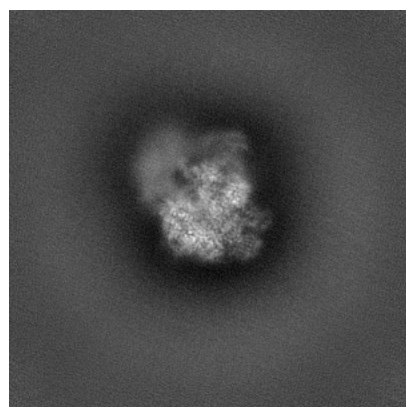


Y

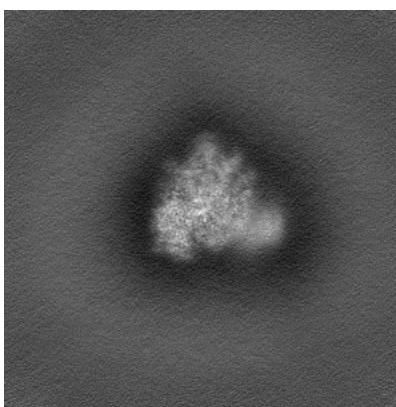


Z

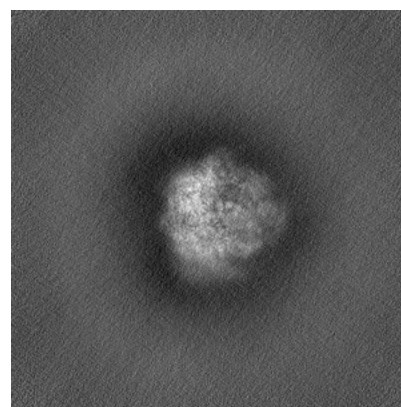
#### 6.1.2 Raw map



X



Y

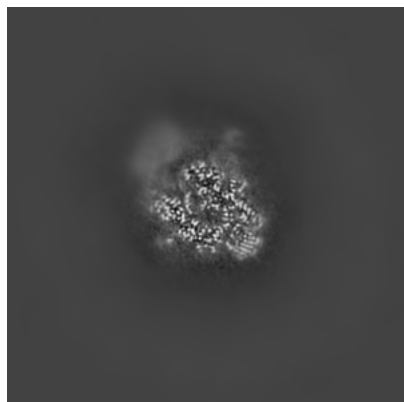


Z

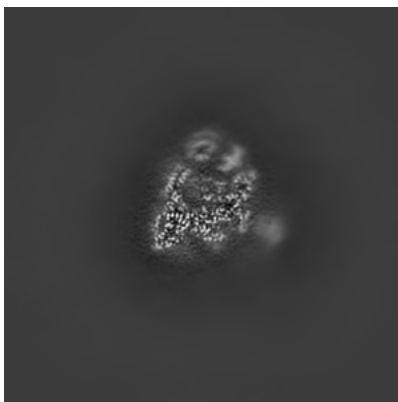
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

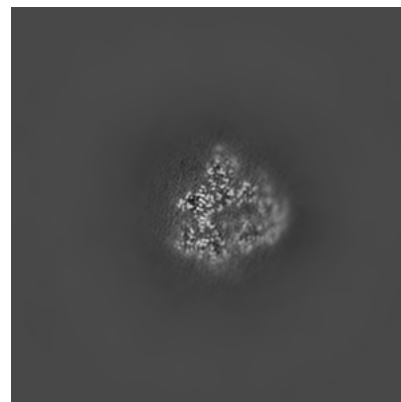
### 6.2.1 Primary map



X Index: 192

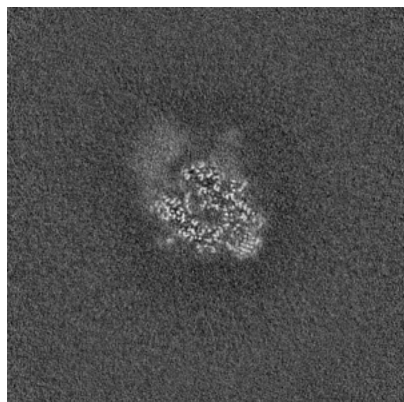


Y Index: 192

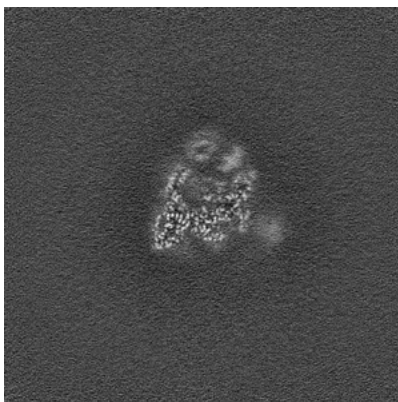


Z Index: 192

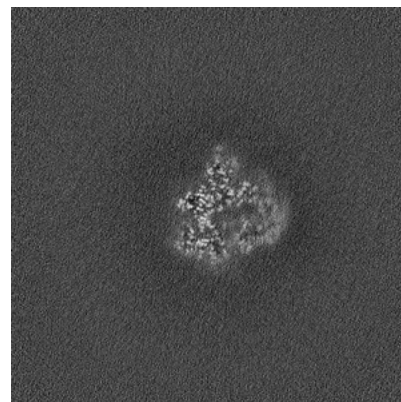
### 6.2.2 Raw map



X Index: 192



Y Index: 192

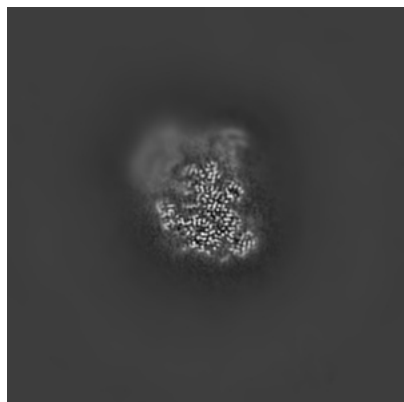


Z Index: 192

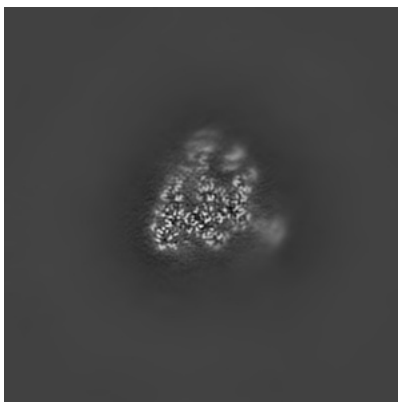
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

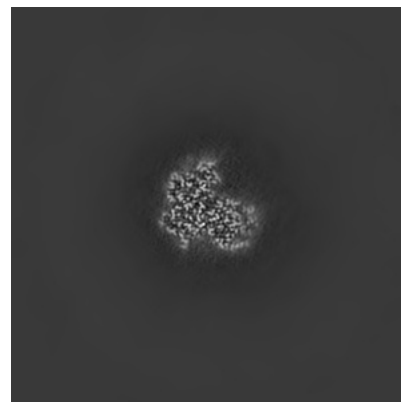
### 6.3.1 Primary map



X Index: 181

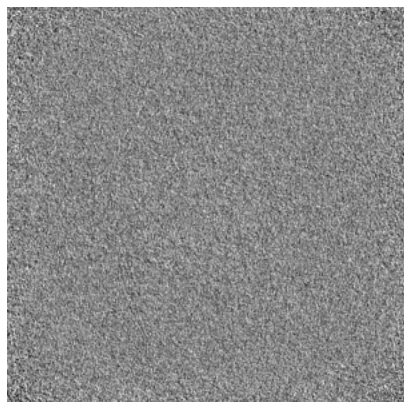


Y Index: 196

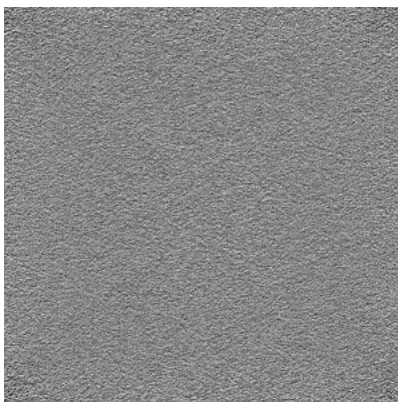


Z Index: 166

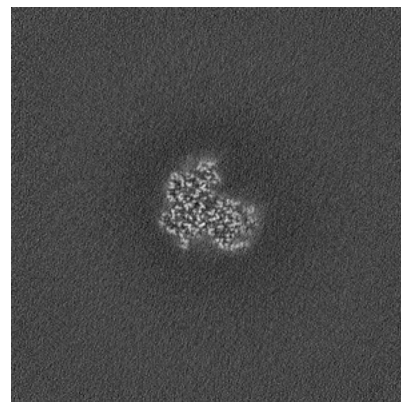
### 6.3.2 Raw map



X Index: 0



Y Index: 0

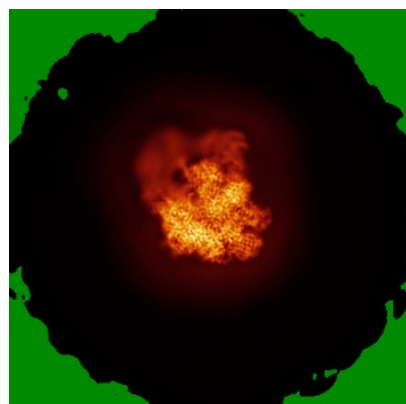


Z Index: 166

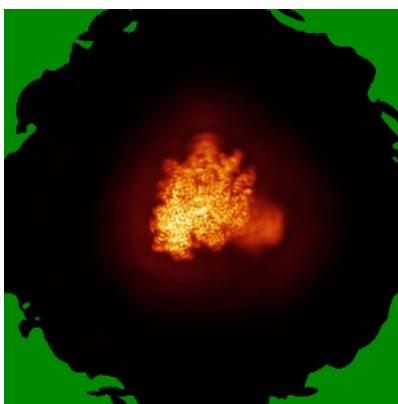
The images above show the largest variance slices of the map in three orthogonal directions.

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

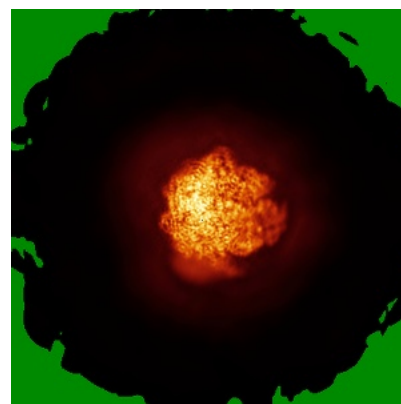
### 6.4.1 Primary map



X

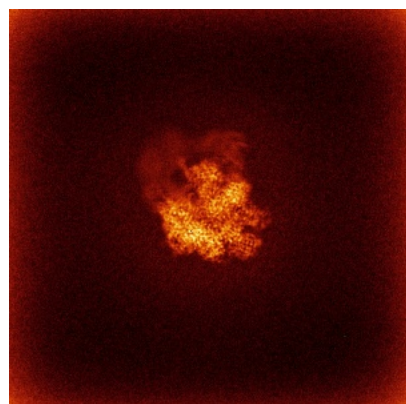


Y

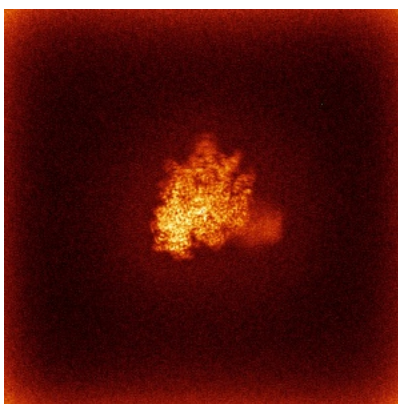


Z

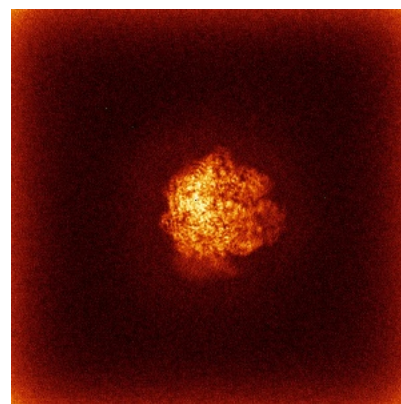
### 6.4.2 Raw map



X



Y



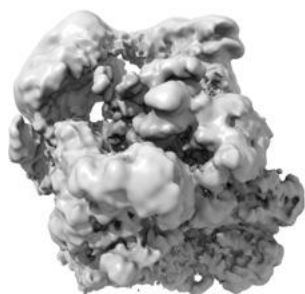
Z

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.

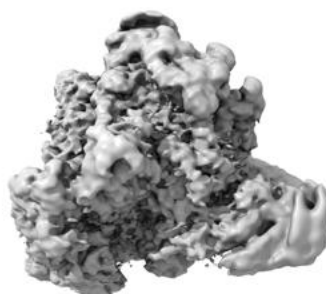


## 6.5 Orthogonal surface views [i](#)

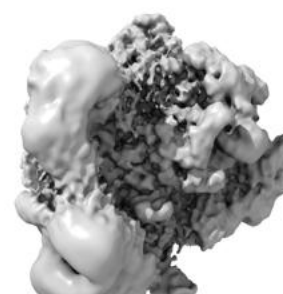
### 6.5.1 Primary map



X



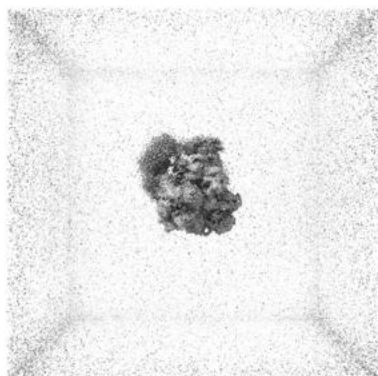
Y



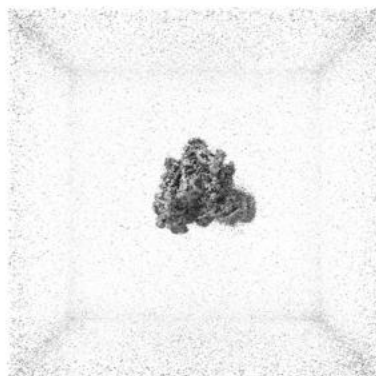
Z

The images above show the 3D surface view of the map at the recommended contour level 0.647. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

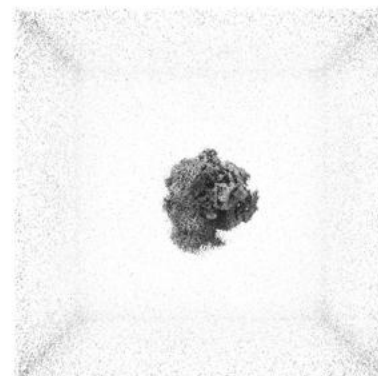
### 6.5.2 Raw map



X



Y



Z

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

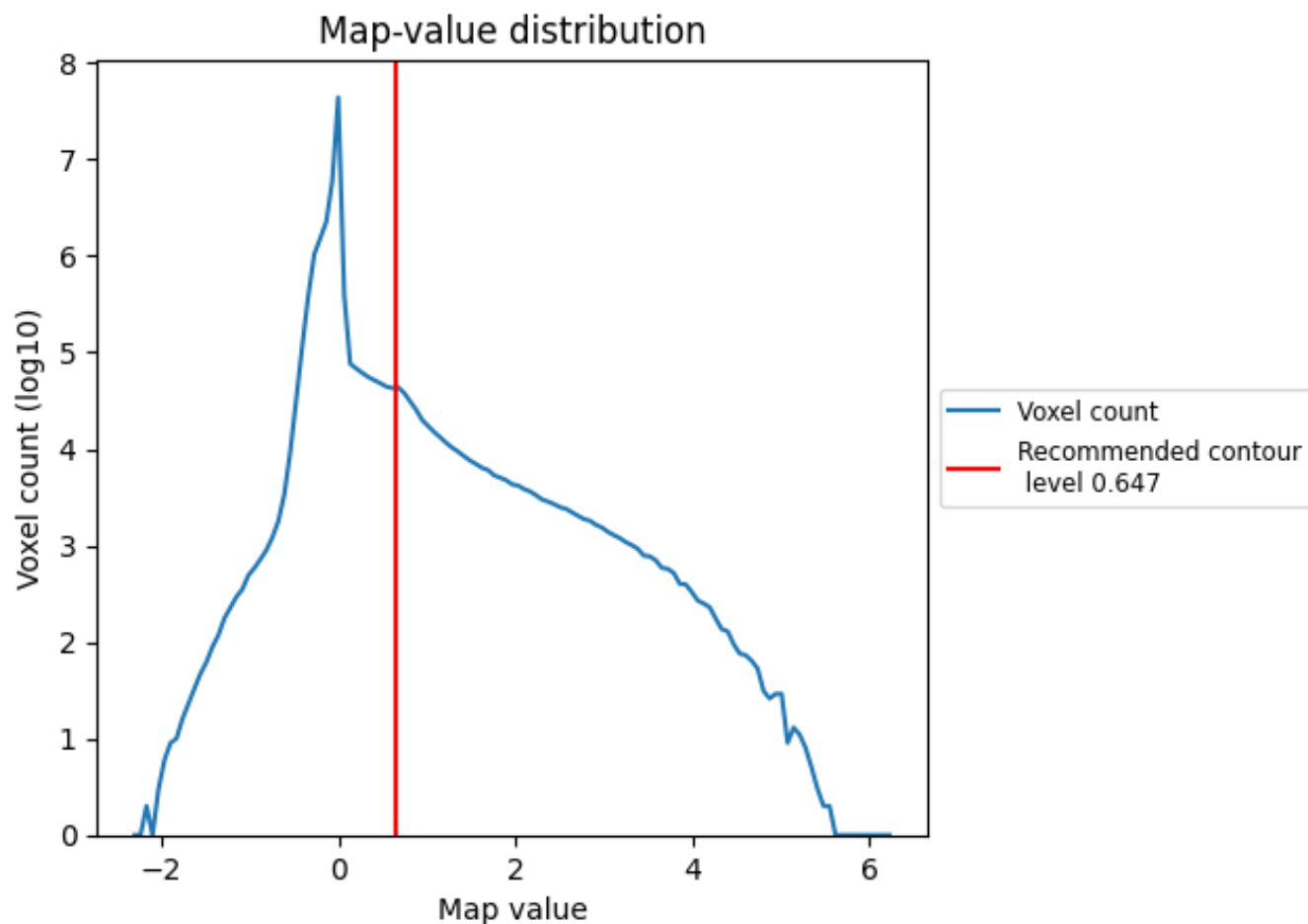
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

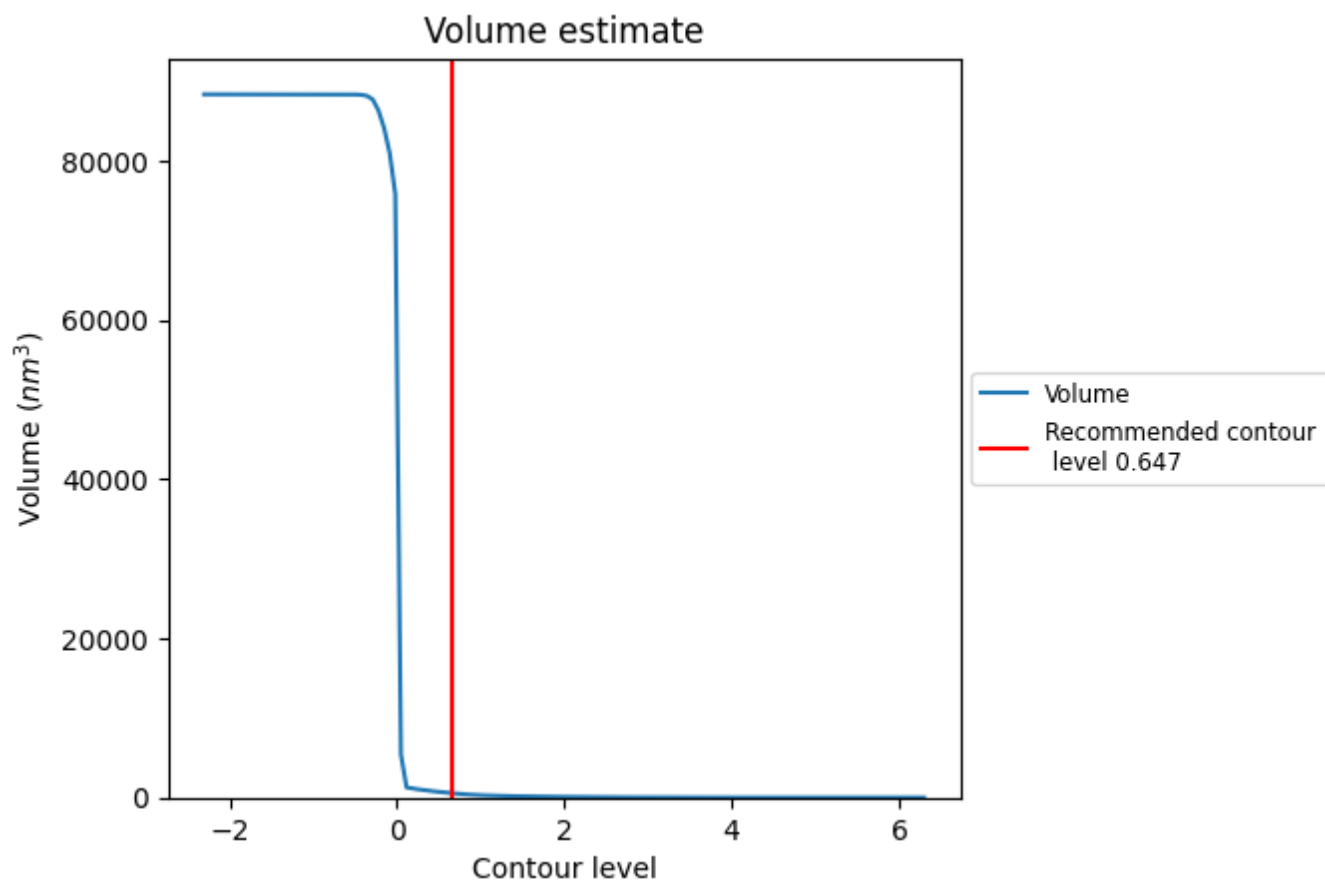
This section contains the results of statistical analysis of the map.

### 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.

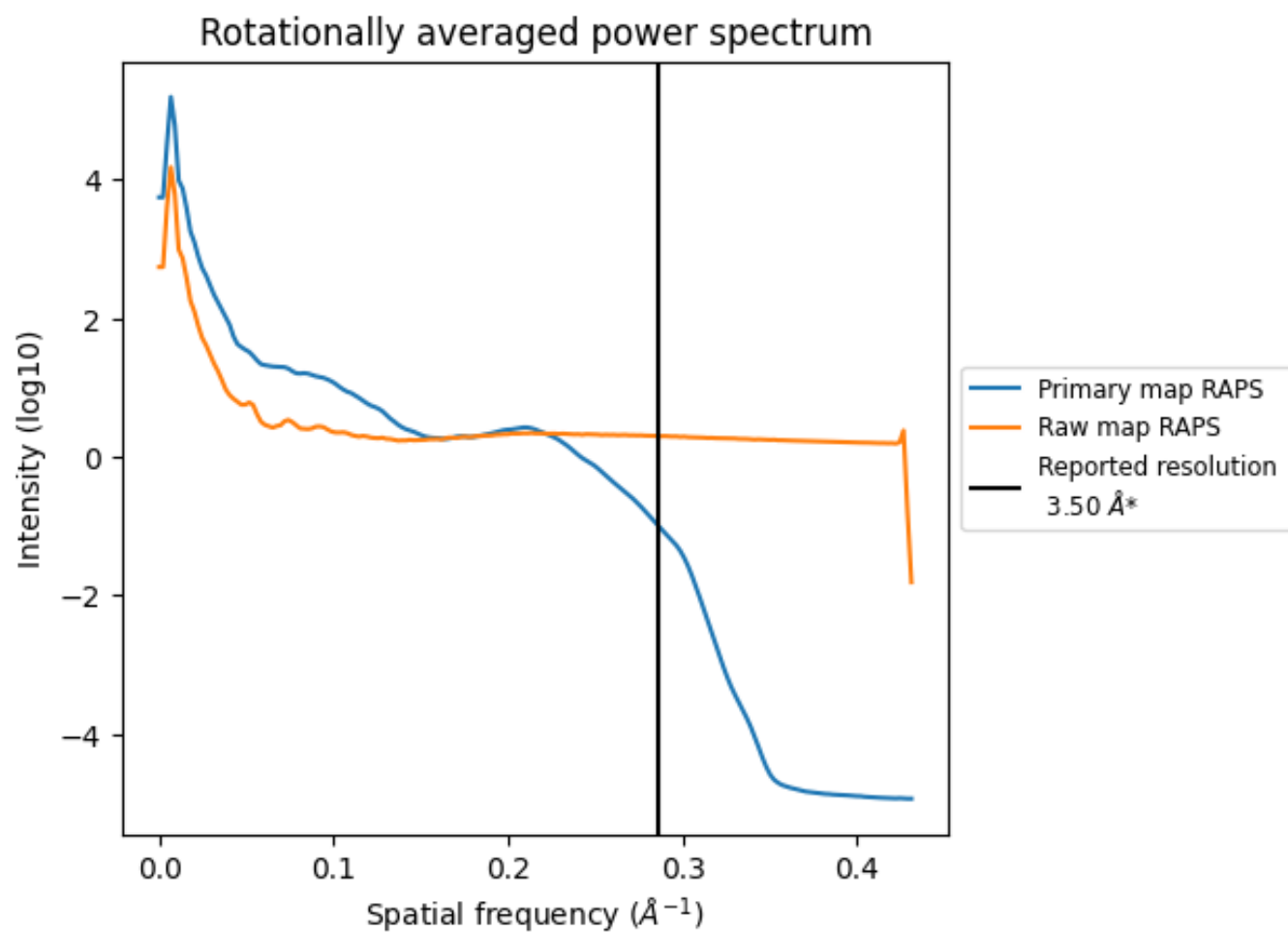
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 563  $\text{nm}^3$ ; this corresponds to an approximate mass of 508 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 ⓘ



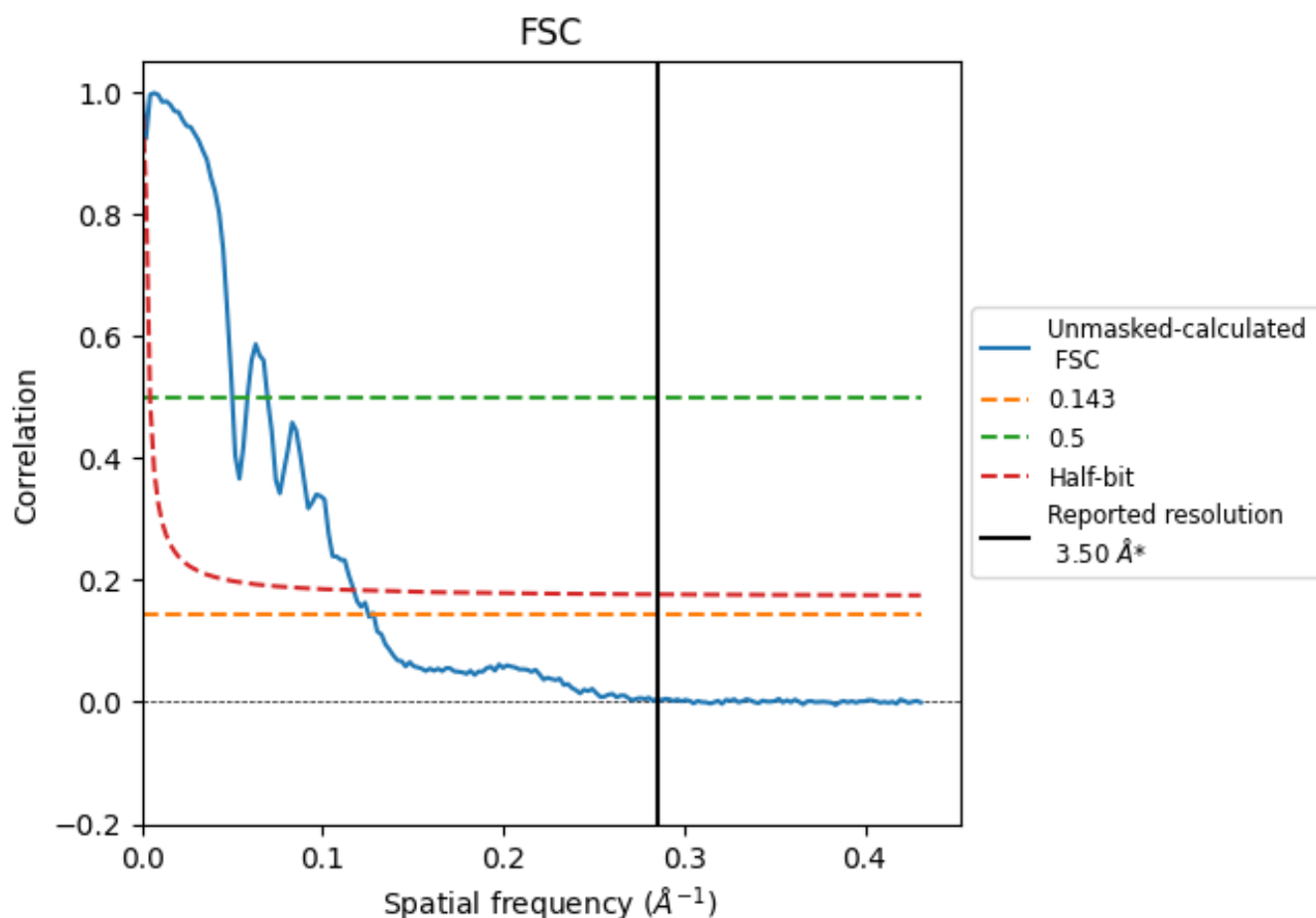
\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>



## 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  $0.286 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

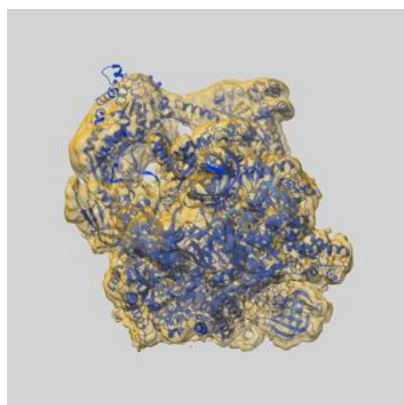
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.97	20.04	8.53

\*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 7.97 differs from the reported value 3.5 by more than 10 %

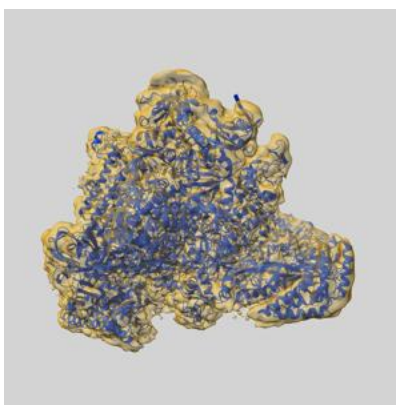
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41623 and PDB model 8TUG. Per-residue inclusion information can be found in section [3](#) on page [7](#).

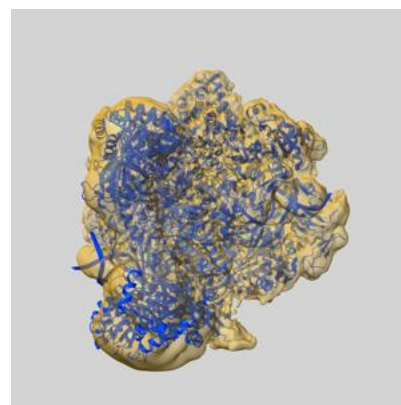
### 9.1 Map-model overlay [i](#)



X



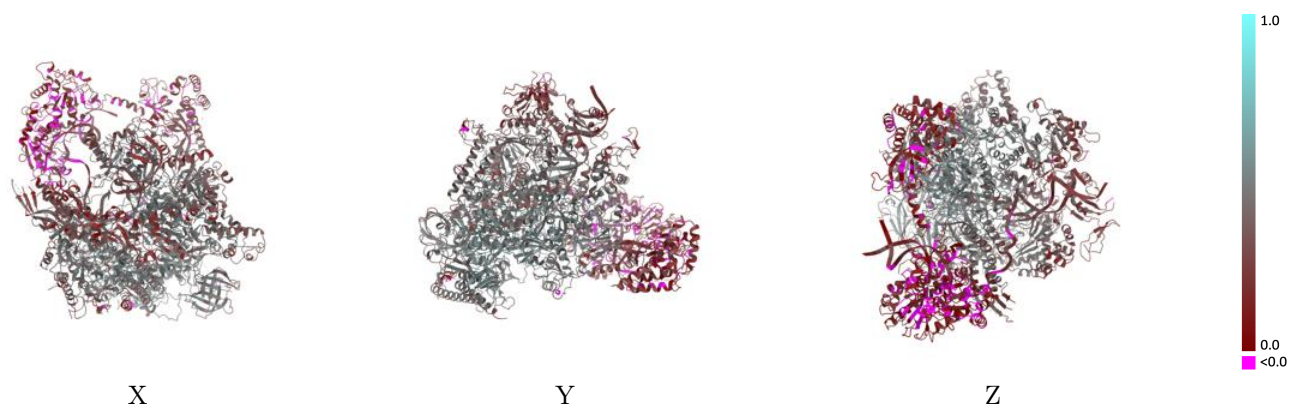
Y



Z

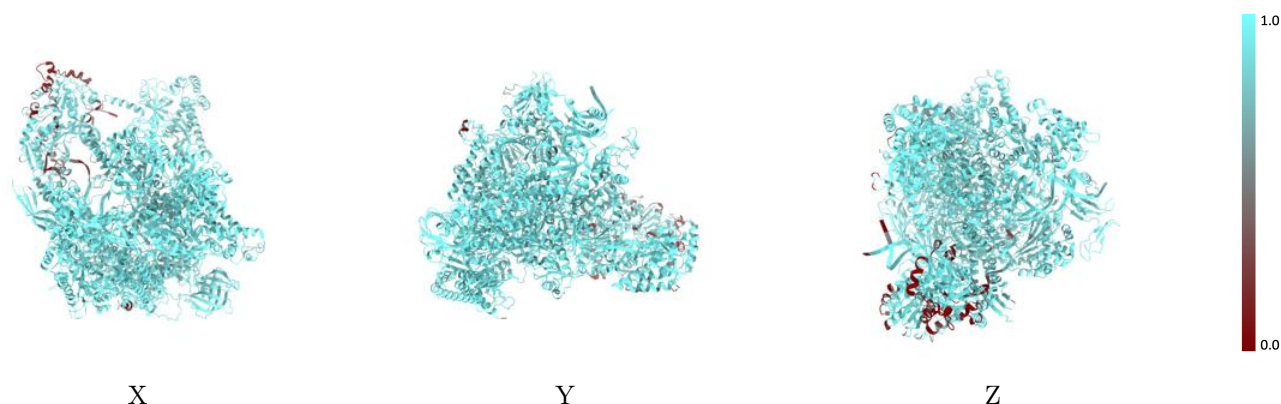
The images above show the 3D surface view of the map at the recommended contour level 0.647 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



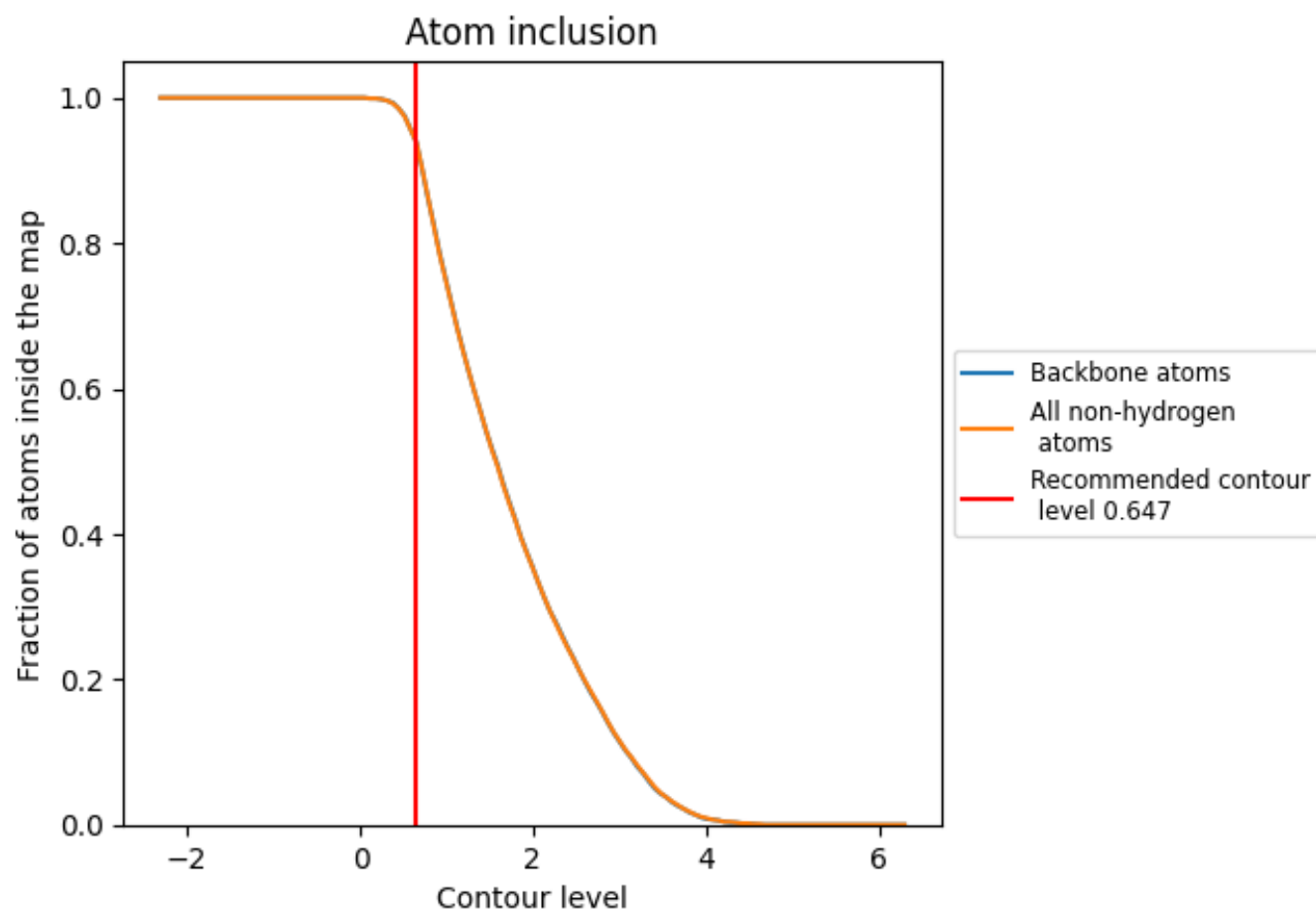
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.647).



































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.647) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9400	 0.3820
A	 0.9560	 0.4390
B	 0.9650	 0.4440
C	 0.9760	 0.4870
D	 0.8920	 0.1690
E	 0.9620	 0.3790
F	 0.9860	 0.4810
G	 0.9550	 0.2240
H	 0.9620	 0.4160
I	 0.9420	 0.2900
J	 0.9900	 0.5020
K	 0.9480	 0.4670
L	 0.9830	 0.3940
M	 0.7930	 0.0840
N	 0.8060	 0.1750
R	 0.9820	 0.4480
T	 0.8950	 0.2700

