



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:15 PM UTC

PDB ID : 6HLQ / pdb_00006hlq
EMDB ID : EMD-0239
Title : Yeast RNA polymerase I* elongation complex bound to nucleotide analog GM-PCPP
Authors : Tafur, L.; Sadian, Y.; Weis, F.; Muller, C.W.
Deposited on : 2018-09-11
Resolution : 3.18 Å (reported)
Based on initial models : 4C3I, 5M5X, 2E2J, 4C2M, 4A3J

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:

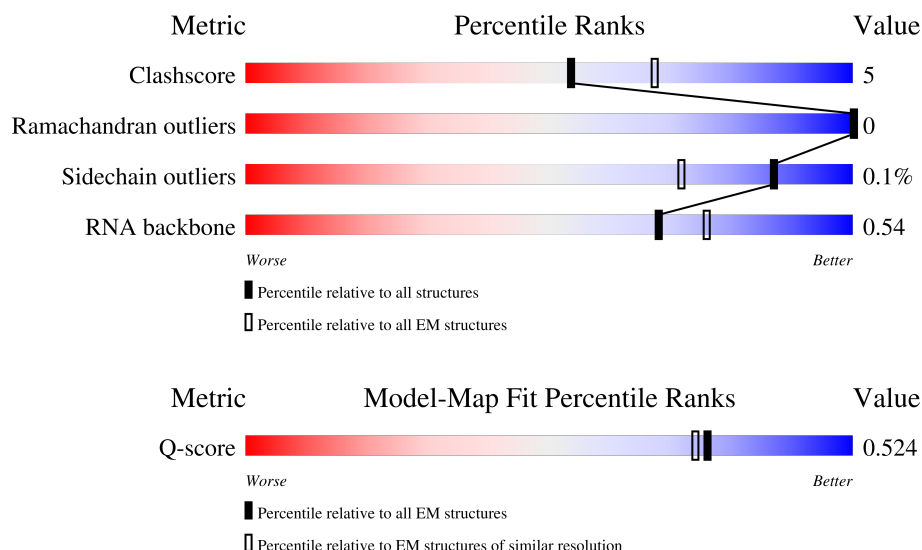
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 3.18 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	14470 (2.68 - 3.68)

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	1664	
2	B	1203	
3	C	335	

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Mol	Chain	Length	Quality of chain
4	D	137	
5	E	215	
6	F	155	
7	G	326	
8	H	146	
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	R	20	
14	S	38	
15	T	38	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 32731 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 I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1456	Total	C	N	O	S	0	0
			11498	7259	2000	2177	62		

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1167	Total	C	N	O	S	0	0
			9279	5867	1630	1731	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	304	Total	C	N	O	S	0	0
			2415	1535	414	458	8		

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	57	Total	C	N	O	0	0
			452	285	77	90		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1747	1109	308	319	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	100	Total	C	N	O	S	0	0
			823	522	144	154	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	176	Total	C	N	O	S	0	0
			1386	897	232	252	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	131	Total	C	N	O	S	0	0
			1052	664	176	208	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	111	Total	C	N	O	S	0	0
			844	523	143	169	9		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	98	Total	C	N	O	S	0	0
			766	481	124	156	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 13 is a RNA chain called RNA.

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

- Molecule 14 is a DNA chain called Non-template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	28	Total	C	N	O	P	0	0
			581	276	114	163	28		

- Molecule 15 is a DNA chain called Template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	36	Total	C	N	O	P	0	0
			732	350	127	219	36		

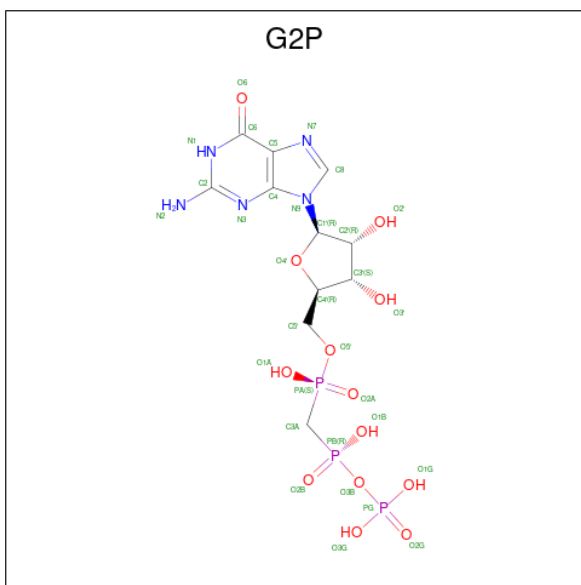
- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 18 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: G2P) (formula: C₁₁H₁₈N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
18	T	1	Total	C	N	O	P	0
			32	11	5	13	3	

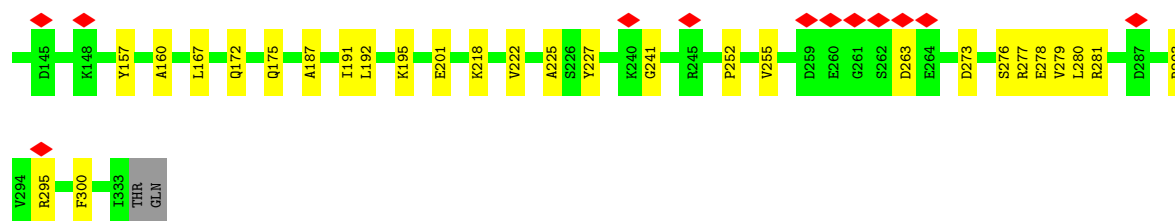


Frequency	Percentage
Daily	80%
Weekly	17%
Monthly	3%

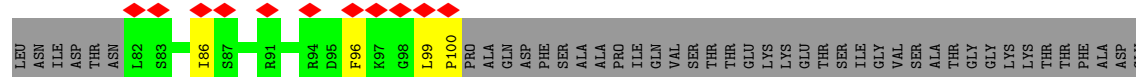
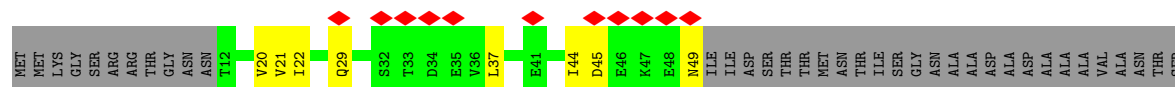
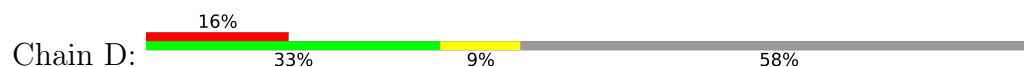


Category	Percentage
Very bad	5%
Bad	79%
Good	12%
Very good	9%

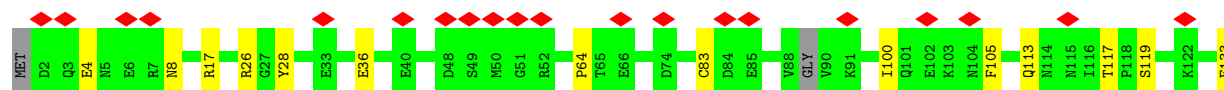
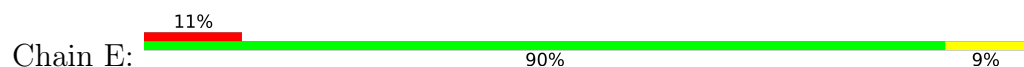




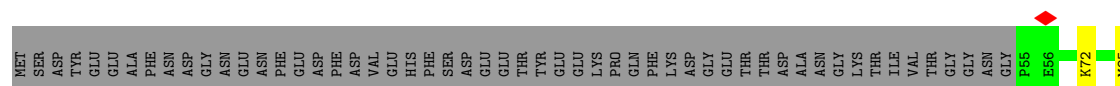
- Molecule 4: DNA-directed RNA polymerase I subunit RPA14



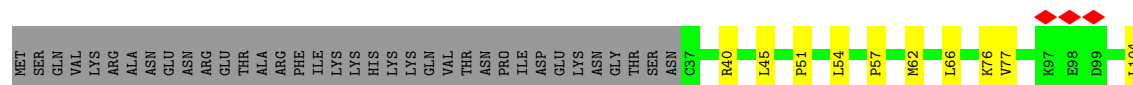
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

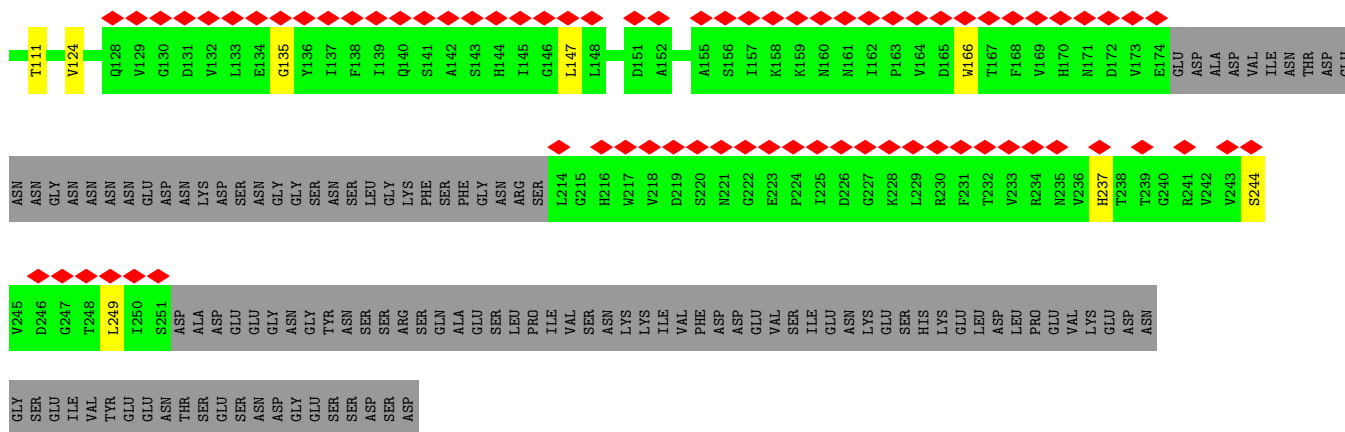


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

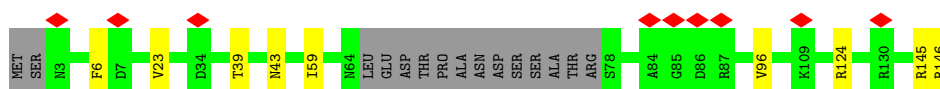
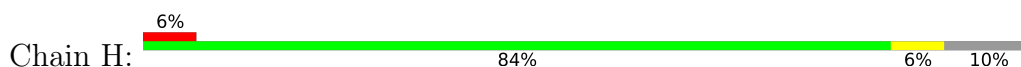


- Molecule 7: DNA-directed RNA polymerase I subunit RPA43

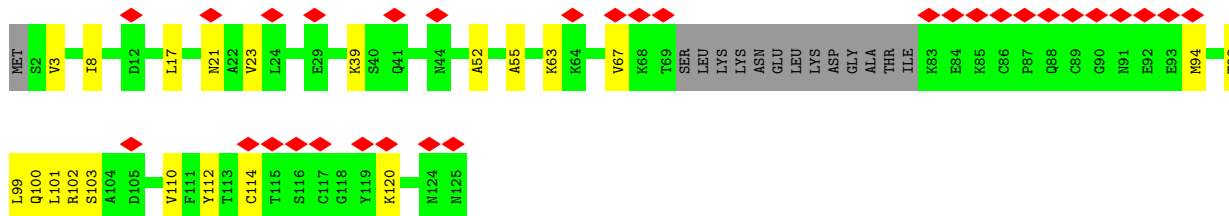




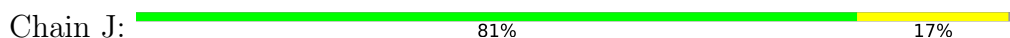
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



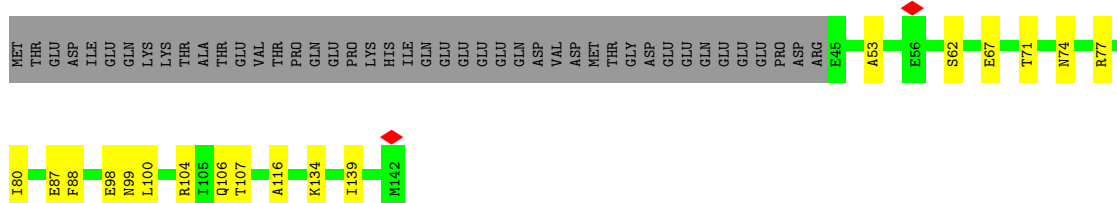
- Molecule 9: DNA-directed RNA polymerase I subunit RPA12



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

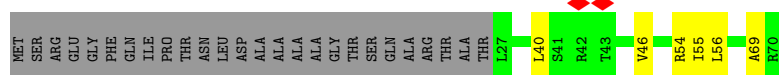


- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2



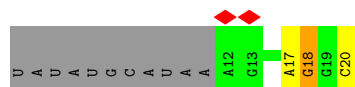
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 



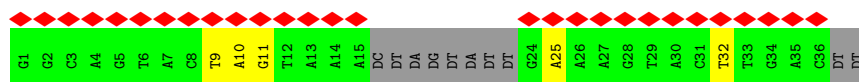
- Molecule 13: RNA

Chain R: 



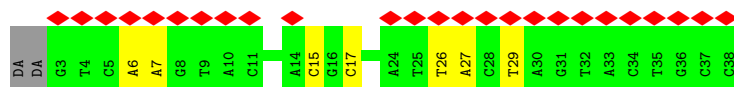
- Molecule 14: Non-template strand

Chain S: 



- Molecule 15: Template strand

Chain T: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	182488	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	39	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.449	Depositor
Minimum map value	-0.306	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.066	Depositor
Map size (Å)	270.4, 270.4, 270.4	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, G2P, 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	0.23	0/11706	0.50	1/15809 (0.0%)
2	B	0.24	0/9484	0.54	0/12819
3	C	0.19	0/2467	0.43	0/3344
4	D	0.15	0/458	0.48	0/620
5	E	0.21	0/1782	0.47	0/2398
6	F	0.20	0/838	0.45	0/1129
7	G	0.17	0/1421	0.40	0/1938
8	H	0.19	0/1070	0.45	0/1449
9	I	0.19	0/856	0.50	0/1155
10	J	0.25	0/578	0.54	0/775
11	K	0.22	0/776	0.53	0/1047
12	L	0.23	0/354	0.57	0/468
13	R	0.12	0/218	0.22	0/338
14	S	0.21	0/653	0.41	0/1004
15	T	0.24	0/818	0.41	0/1259
All	All	0.22	0/33479	0.50	1/45552 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1641	ILE	N-CA-C	-5.31	107.65	112.96

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	11498	0	11570	121	0
2	B	9279	0	9169	135	0
3	C	2415	0	2403	27	0
4	D	452	0	455	7	0
5	E	1747	0	1772	10	0
6	F	823	0	841	7	0
7	G	1386	0	1386	12	0
8	H	1052	0	1021	5	0
9	I	844	0	823	14	0
10	J	569	0	585	9	0
11	K	766	0	765	15	0
12	L	352	0	374	7	0
13	R	195	0	99	4	0
14	S	581	0	316	10	0
15	T	732	0	408	7	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	R	1	0	0	0	0
18	T	32	0	14	4	0
All	All	32731	0	32001	330	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (330) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:ILE:H	11:K:106:GLN:HE22	1.35	0.73
1:A:672:ASP:H	2:B:783:MET:HE3	1.56	0.71
2:B:817:ARG:CZ	14:S:9:DT:OP2	2.39	0.70
1:A:590:ASN:HD21	2:B:1075:GLU:HG2	1.57	0.69
2:B:675:ALA:HB3	2:B:689:VAL:HG12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:898:LEU:HB3	12:L:46:VAL:HG21	1.78	0.66
2:B:750:PRO:HG2	2:B:753:LYS:HB3	1.78	0.64
1:A:464:GLU:HA	1:A:469:LYS:HD2	1.79	0.63
1:A:120:CYS:HB2	1:A:189:VAL:HG21	1.80	0.63
1:A:438:ILE:HA	1:A:456:VAL:HG12	1.81	0.61
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.83	0.61
1:A:363:PRO:O	1:A:368:ARG:NH1	2.33	0.61
1:A:716:PRO:O	1:A:730:GLN:NE2	2.33	0.60
11:K:67:GLU:HA	11:K:99:ASN:HB3	1.82	0.60
1:A:1274:GLU:OE2	1:A:1288:ARG:NH2	2.34	0.60
2:B:817:ARG:NH1	14:S:9:DT:OP2	2.34	0.60
6:F:101:ILE:HD12	6:F:107:VAL:HG22	1.83	0.59
1:A:325:ASP:O	1:A:329:ARG:NH1	2.36	0.59
2:B:234:ILE:HG22	2:B:250:LEU:HB2	1.84	0.59
1:A:110:LEU:HD23	1:A:227:LEU:HD23	1.83	0.59
3:C:37:LYS:O	11:K:134:LYS:NZ	2.31	0.59
2:B:1045:GLN:HB3	2:B:1063:ARG:HG3	1.85	0.59
2:B:252:TYR:OH	2:B:305:ARG:NH1	2.36	0.58
1:A:1273:THR:HB	1:A:1291:VAL:HB	1.86	0.58
1:A:843:ARG:NH1	2:B:988:GLU:OE2	2.37	0.58
9:I:98:THR:HG22	9:I:110:VAL:HG22	1.85	0.58
2:B:143:TRP:HB3	2:B:152:LEU:HB2	1.85	0.58
1:A:1038:ILE:HD12	1:A:1584:LEU:HD12	1.87	0.57
2:B:296:ASP:OD2	2:B:379:ARG:NH1	2.36	0.57
10:J:8:PHE:H	10:J:49:MET:HE3	1.70	0.57
2:B:394:PRO:O	2:B:400:GLN:NE2	2.38	0.57
2:B:770:ASN:O	10:J:48:ARG:NH1	2.38	0.57
1:A:1322:ILE:HG21	1:A:1457:ILE:HD11	1.85	0.57
1:A:1478:ALA:HB1	9:I:21:ASN:HB3	1.87	0.57
1:A:621:THR:HG21	1:A:670:ILE:HD13	1.87	0.56
2:B:186:GLU:HB3	2:B:189:GLU:HB2	1.86	0.56
1:A:1089:LEU:HD21	1:A:1175:MET:HE1	1.86	0.56
1:A:29:ALA:HA	2:B:1129:ARG:HH12	1.70	0.56
2:B:292:ILE:O	2:B:379:ARG:NH2	2.38	0.56
1:A:843:ARG:NH2	1:A:983:LYS:O	2.39	0.56
1:A:621:THR:OG1	1:A:626:ALA:O	2.23	0.56
2:B:612:LYS:NZ	2:B:662:ASP:OD1	2.39	0.56
2:B:1006:ASN:HD21	2:B:1010:ASN:HB2	1.70	0.56
2:B:320:LEU:HB3	2:B:326:VAL:HG22	1.87	0.56
2:B:674:ILE:HG22	2:B:688:HIS:HB2	1.88	0.56
9:I:8:ILE:HG13	9:I:17:LEU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:465:LEU:HA	2:B:485:THR:HG21	1.87	0.56
3:C:40:PHE:O	11:K:134:LYS:NZ	2.37	0.56
2:B:52:LEU:HB2	2:B:61:LEU:HG	1.88	0.56
2:B:711:GLN:HG2	2:B:713:PRO:HD2	1.87	0.55
2:B:743:ARG:NH2	2:B:804:TYR:OH	2.39	0.55
1:A:1487:ASN:OD1	2:B:305:ARG:NH2	2.38	0.55
7:G:237:HIS:HB2	7:G:244:SER:HB3	1.88	0.55
1:A:1657:LEU:HD12	7:G:104:LEU:HB3	1.88	0.55
2:B:203:ILE:HD11	2:B:408:LEU:HD23	1.88	0.55
1:A:24:ILE:HG22	1:A:27:LEU:HD23	1.89	0.55
2:B:12:ARG:NH2	2:B:990:ASP:OD2	2.40	0.55
2:B:934:ILE:O	3:C:69:ARG:NH1	2.40	0.54
2:B:145:VAL:HG21	2:B:441:LYS:HG2	1.89	0.54
1:A:546:LEU:HD22	1:A:554:ARG:HG3	1.89	0.54
2:B:137:LEU:HD13	2:B:161:LEU:HD22	1.87	0.54
1:A:49:LEU:O	1:A:368:ARG:NH2	2.40	0.54
3:C:91:VAL:HG11	10:J:60:PHE:HB3	1.88	0.54
1:A:1332:GLU:HA	1:A:1335:LYS:HG2	1.90	0.54
5:E:26:ARG:NH2	5:E:133:GLU:OE1	2.41	0.54
3:C:293:ARG:O	3:C:295:ARG:NH2	2.41	0.54
2:B:963:PHE:O	2:B:1027:TYR:OH	2.26	0.53
5:E:4:GLU:OE1	5:E:8:ASN:ND2	2.41	0.53
2:B:516:THR:HA	2:B:519:LYS:HE2	1.90	0.53
2:B:626:ILE:HG22	2:B:642:LEU:HG	1.90	0.53
3:C:87:ASN:ND2	3:C:201:GLU:OE2	2.41	0.53
8:H:23:VAL:HA	8:H:43:ASN:HA	1.90	0.53
2:B:237:ARG:NH2	2:B:245:SER:OG	2.41	0.53
1:A:549:MET:O	1:A:554:ARG:NH2	2.42	0.53
1:A:590:ASN:HB3	1:A:634:ASN:HB2	1.89	0.53
14:S:32:DT:H3	15:T:7:DA:H61	1.55	0.53
2:B:931:TRP:HD1	2:B:936:MET:HG2	1.74	0.53
1:A:1221:ARG:NH2	1:A:1544:ASN:OD1	2.42	0.53
3:C:252:PRO:HG2	3:C:273:ASP:HA	1.90	0.53
1:A:1239:THR:HG23	1:A:1518:VAL:HG13	1.91	0.53
3:C:218:LYS:NZ	12:L:69:ALA:O	2.39	0.53
14:S:11:DG:O6	15:T:27:DA:N6	2.41	0.53
1:A:673:HIS:HD2	1:A:817:PHE:HB2	1.73	0.52
2:B:1025:ASP:OD2	3:C:277:ARG:NH1	2.42	0.52
3:C:172:GLN:H	3:C:175:GLN:HE21	1.55	0.52
6:F:85:MET:HB2	6:F:151:LEU:HB3	1.92	0.52
1:A:857:ALA:HB2	1:A:899:LYS:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1135:PHE:HB2	2:B:1167:PHE:HA	1.91	0.52
2:B:1061:LYS:O	2:B:1065:ARG:NH1	2.42	0.52
1:A:847:LEU:HD21	1:A:946:LEU:HD22	1.92	0.52
6:F:72:LYS:NZ	6:F:140:ASP:OD2	2.40	0.52
1:A:15:ASP:N	1:A:15:ASP:OD1	2.40	0.52
1:A:1053:ASP:OD2	1:A:1580:ARG:NH1	2.43	0.52
5:E:83:CYS:O	5:E:113:GLN:NE2	2.37	0.52
11:K:80:ILE:HD11	11:K:116:ALA:HB1	1.92	0.52
2:B:524:SER:HB3	2:B:528:LEU:HB2	1.91	0.52
2:B:73:ILE:HD13	2:B:428:VAL:HG23	1.92	0.51
2:B:210:ARG:HA	2:B:401:GLU:HB2	1.91	0.51
10:J:41:LEU:HD22	10:J:46:CYS:HB3	1.92	0.51
2:B:252:TYR:HB2	2:B:381:LEU:HD21	1.92	0.51
9:I:94:MET:HE3	9:I:114:CYS:HB2	1.93	0.51
1:A:24:ILE:HA	1:A:27:LEU:HB3	1.93	0.51
1:A:1269:LYS:HE3	1:A:1271:ILE:HD11	1.92	0.51
2:B:1043:LYS:O	2:B:1063:ARG:NE	2.44	0.51
1:A:79:ILE:HG12	1:A:360:LEU:HB2	1.92	0.51
12:L:40:LEU:HD21	12:L:46:VAL:HG22	1.93	0.51
11:K:104:ARG:HE	11:K:106:GLN:HE21	1.59	0.51
1:A:483:VAL:O	1:A:613:THR:OG1	2.25	0.51
2:B:858:ILE:HD11	2:B:903:ILE:HG21	1.92	0.51
1:A:1562:ILE:HD12	1:A:1595:TYR:HE1	1.75	0.51
2:B:208:VAL:O	2:B:401:GLU:N	2.44	0.50
9:I:101:LEU:HB3	9:I:102:ARG:HD3	1.93	0.50
1:A:1091:VAL:HG13	1:A:1133:LEU:HD23	1.94	0.50
2:B:495:ARG:NH2	13:R:17:A:O3'	2.43	0.50
2:B:790:ASN:HB2	2:B:946:ASP:HA	1.94	0.50
2:B:217:ILE:HD12	2:B:235:GLN:HB3	1.93	0.50
2:B:852:VAL:HG13	2:B:856:ASP:HB2	1.94	0.50
11:K:62:SER:OG	11:K:104:ARG:NH1	2.38	0.50
1:A:581:ILE:HD11	1:A:605:VAL:HG11	1.93	0.50
2:B:1070:ARG:NH2	15:T:17:DC:OP1	2.45	0.50
1:A:1443:GLN:NE2	1:A:1464:ASP:OD2	2.44	0.50
1:A:1662:ASN:HB2	7:G:57:PRO:HD2	1.93	0.50
1:A:660:PRO:O	1:A:1581:HIS:NE2	2.40	0.50
1:A:1216:THR:HG23	1:A:1221:ARG:HD3	1.94	0.50
2:B:202:LEU:HD23	2:B:488:ALA:HB2	1.94	0.49
3:C:192:LEU:HD21	3:C:195:LYS:HE3	1.94	0.49
1:A:402:ASP:HB3	1:A:419:ILE:HG12	1.93	0.49
2:B:1055:LEU:HD12	2:B:1056:THR:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ARG:NH1	1:A:558:ALA:O	2.45	0.49
2:B:72:VAL:HG12	2:B:96:SER:HA	1.94	0.49
2:B:773:VAL:HG22	2:B:947:ILE:HB	1.93	0.49
1:A:98:LEU:HD13	1:A:320:VAL:HG13	1.94	0.49
7:G:135:GLY:HA3	7:G:147:LEU:HD13	1.93	0.49
10:J:36:LEU:HD11	10:J:51:LEU:HB2	1.95	0.49
2:B:346:ASP:HA	2:B:349:VAL:HG12	1.93	0.49
2:B:753:LYS:NZ	2:B:758:ASP:OD2	2.41	0.49
2:B:1132:SER:HA	2:B:1169:GLY:HA3	1.95	0.49
1:A:1055:ILE:HD11	1:A:1580:ARG:HH12	1.78	0.49
7:G:77:VAL:HG11	7:G:124:VAL:HG11	1.94	0.49
1:A:593:PRO:HG3	18:T:3000:G2P:H2N2	1.76	0.49
2:B:817:ARG:HG2	14:S:10:DA:P	2.53	0.49
14:S:11:DG:N2	15:T:29:DT:O2	2.46	0.49
2:B:1105:ARG:HD3	2:B:1203:LYS:HA	1.93	0.49
8:H:39:THR:HB	8:H:124:ARG:HB3	1.95	0.49
1:A:747:ILE:HG22	1:A:774:GLY:HA2	1.94	0.48
1:A:115:VAL:HG12	1:A:334:VAL:HG21	1.95	0.48
1:A:1654:PHE:O	6:F:92:ARG:NH1	2.46	0.48
2:B:526:GLY:H	2:B:696:ILE:HG23	1.77	0.48
2:B:545:PHE:HE1	2:B:649:MET:HE3	1.78	0.48
2:B:913:ILE:HA	2:B:927:CYS:HB2	1.95	0.48
2:B:1016:GLY:O	3:C:69:ARG:NH1	2.45	0.48
3:C:279:VAL:HG23	3:C:280:LEU:HD12	1.95	0.48
2:B:216:ALA:HB1	2:B:384:LEU:HD22	1.95	0.48
2:B:656:LEU:HD11	2:B:689:VAL:HG13	1.95	0.48
5:E:113:GLN:HA	5:E:137:GLU:HG2	1.94	0.48
2:B:817:ARG:HD2	14:S:9:DT:OP1	2.13	0.48
2:B:132:SER:OG	2:B:134:ARG:NH1	2.42	0.48
10:J:48:ARG:O	10:J:52:THR:OG1	2.25	0.48
2:B:518:ARG:NH1	2:B:539:CYS:O	2.44	0.48
1:A:1317:ILE:HA	1:A:1321:PHE:HB3	1.95	0.48
2:B:135:GLY:O	2:B:161:LEU:N	2.45	0.48
2:B:658:LEU:HD12	9:I:120:LYS:HZ1	1.79	0.48
1:A:826:PHE:HB3	2:B:777:SER:HB2	1.96	0.48
1:A:1634:LEU:HD13	1:A:1643:VAL:HG11	1.94	0.48
2:B:70:GLU:HG2	2:B:98:SER:HB2	1.96	0.48
1:A:325:ASP:HB3	1:A:329:ARG:HH12	1.79	0.47
2:B:130:LEU:HD12	2:B:808:LYS:HD3	1.96	0.47
1:A:520:ARG:HH12	1:A:559:ASN:HA	1.79	0.47
1:A:597:LYS:O	2:B:1082:HIS:NE2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:489:GLU:HG3	2:B:495:ARG:HE	1.79	0.47
5:E:28:TYR:HA	5:E:64:PRO:HA	1.96	0.47
11:K:88:PHE:HB3	11:K:106:GLN:HB2	1.94	0.47
7:G:51:PRO:HA	7:G:54:LEU:HG	1.96	0.47
1:A:389:VAL:HG22	1:A:433:ASP:HB3	1.95	0.47
2:B:991:THR:HG22	2:B:993:ALA:H	1.79	0.47
4:D:37:LEU:HD21	4:D:96:PHE:HB2	1.96	0.47
1:A:1634:LEU:O	1:A:1640:ARG:NH2	2.43	0.47
2:B:1082:HIS:HB2	2:B:1084:THR:HG22	1.96	0.47
9:I:3:VAL:HG22	9:I:8:ILE:HG22	1.96	0.47
1:A:729:LYS:HG3	1:A:776:LEU:HG	1.95	0.47
2:B:664:VAL:HG11	2:B:672:MET:HE1	1.96	0.47
9:I:52:ALA:HB3	9:I:55:ALA:HB2	1.97	0.47
3:C:255:VAL:HG21	3:C:273:ASP:HB3	1.95	0.47
1:A:1559:ARG:NH1	1:A:1583:ASP:OD1	2.38	0.47
2:B:525:TRP:NE1	2:B:690:GLU:OE2	2.38	0.47
1:A:1240:LEU:HB3	1:A:1536:ILE:HD12	1.97	0.47
2:B:887:LEU:HB2	12:L:56:LEU:HB2	1.97	0.47
2:B:1102:SER:HA	2:B:1175:THR:HA	1.97	0.46
1:A:1316:VAL:HG11	1:A:1498:ILE:HD13	1.96	0.46
2:B:12:ARG:NE	2:B:985:ILE:O	2.45	0.46
3:C:278:GLU:OE2	3:C:281:ARG:NH1	2.48	0.46
5:E:145:THR:HA	5:E:150:VAL:HG21	1.98	0.46
1:A:481:ARG:HH21	1:A:634:ASN:HD21	1.61	0.46
11:K:87:GLU:H	11:K:107:THR:HA	1.79	0.46
1:A:1568:ASN:HA	1:A:1571:SER:HB2	1.96	0.46
4:D:99:LEU:HD12	4:D:100:PRO:HD2	1.98	0.46
1:A:589:MET:HB3	1:A:633:MET:HE2	1.98	0.46
2:B:129:ARG:HG2	12:L:55:ILE:HD11	1.97	0.46
2:B:417:ILE:HG22	2:B:457:ILE:HD13	1.98	0.46
18:T:3000:G2P:H8	18:T:3000:G2P:H5'1	1.97	0.46
2:B:204:ARG:HG2	2:B:502:MET:HE3	1.98	0.46
7:G:166:TRP:HZ3	7:G:249:LEU:HD13	1.81	0.46
2:B:731:VAL:HG21	10:J:59:LYS:HG2	1.98	0.46
2:B:1090:ASP:HA	2:B:1094:ASN:HB2	1.98	0.46
1:A:1175:MET:HA	1:A:1178:LEU:HD23	1.97	0.46
2:B:1004:GLY:O	3:C:276:SER:OG	2.30	0.46
1:A:579:ARG:NH1	1:A:580:HIS:O	2.48	0.45
1:A:1603:MET:HE2	1:A:1612:LYS:HG2	1.97	0.45
4:D:29:GLN:HE21	7:G:40:ARG:HH21	1.64	0.45
1:A:229:SER:O	1:A:230:ARG:NE	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:GLU:OE1	2:B:1084:THR:OG1	2.33	0.45
1:A:992:PRO:HB2	2:B:676:VAL:HG21	1.99	0.45
1:A:1550:LEU:HD13	1:A:1595:TYR:HB2	1.98	0.45
1:A:399:LEU:HD11	1:A:422:ARG:HE	1.80	0.45
1:A:1094:ALA:HB2	1:A:1132:TYR:HB3	1.99	0.45
1:A:1459:LYS:NZ	1:A:1471:GLU:OE1	2.40	0.45
4:D:20:VAL:HG12	4:D:21:VAL:HG23	1.99	0.45
1:A:36:THR:HG23	1:A:45:VAL:HG11	1.99	0.45
1:A:1295:ARG:HD2	1:A:1468:LYS:HE3	1.98	0.45
2:B:16:PHE:HZ	2:B:751:ILE:HD13	1.82	0.45
2:B:916:LYS:NZ	13:R:20:C:OP1	2.50	0.45
4:D:45:ASP:O	4:D:49:ASN:ND2	2.49	0.45
1:A:134:TYR:OH	1:A:215:GLU:OE1	2.35	0.45
2:B:327:LEU:HD21	2:B:351:GLN:HG3	1.99	0.45
1:A:986:PHE:HB3	2:B:960:ILE:HD12	1.99	0.45
3:C:65:ASN:HD21	3:C:68:ARG:HH21	1.65	0.45
1:A:1240:LEU:HD23	1:A:1536:ILE:HG13	1.98	0.45
2:B:215:MET:HE3	2:B:217:ILE:HD11	1.99	0.45
1:A:1022:CYS:SG	1:A:1615:TYR:OH	2.65	0.44
9:I:100:GLN:NE2	9:I:103:SER:O	2.47	0.44
14:S:9:DT:H2''	14:S:10:DA:C8	2.51	0.44
1:A:496:GLY:HA3	1:A:615:ARG:HB2	1.99	0.44
2:B:609:ARG:NH1	2:B:668:GLU:OE2	2.49	0.44
2:B:752:VAL:O	2:B:920:ARG:NH1	2.43	0.44
3:C:157:TYR:HB2	3:C:160:ALA:HB2	1.99	0.44
3:C:227:TYR:HB3	3:C:300:PHE:CD1	2.53	0.44
8:H:6:PHE:HB3	8:H:59:ILE:HB	1.99	0.44
4:D:44:ILE:HD12	4:D:86:ILE:HG23	1.99	0.44
1:A:1626:VAL:HG21	2:B:1194:ILE:HD12	1.99	0.44
2:B:26:ILE:O	10:J:62:ARG:NH1	2.50	0.44
2:B:547:HIS:CE1	2:B:695:ASN:HA	2.53	0.44
2:B:218:ILE:HD12	2:B:391:PRO:HG3	1.99	0.44
2:B:404:LEU:HD11	2:B:551:ILE:HG21	2.00	0.44
3:C:100:ARG:NH2	3:C:192:LEU:O	2.49	0.44
3:C:136:LEU:HB2	3:C:167:LEU:HD23	2.00	0.44
5:E:154:ILE:O	5:E:197:LYS:N	2.45	0.44
2:B:892:SER:OG	2:B:894:LYS:O	2.35	0.44
2:B:886:ASN:HB2	2:B:902:SER:HB3	2.00	0.43
1:A:3:ILE:HA	7:G:111:THR:HG22	2.00	0.43
1:A:1023:LEU:HB3	1:A:1190:SER:HB2	1.99	0.43
1:A:1447:GLN:HE21	1:A:1459:LYS:HA	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:LEU:HA	2:B:60:LEU:H	1.82	0.43
3:C:47:LEU:HD11	11:K:139:ILE:HD11	2.00	0.43
1:A:1046:VAL:HG12	1:A:1047:GLN:HG3	2.00	0.43
1:A:1437:ASN:O	1:A:1444:ARG:NH1	2.51	0.43
1:A:1543:SER:OG	1:A:1544:ASN:N	2.49	0.43
3:C:241:GLY:N	3:C:263:ASP:OD2	2.49	0.43
9:I:23:VAL:O	9:I:39:LYS:NZ	2.52	0.43
1:A:943:ILE:HG12	2:B:960:ILE:HD11	2.00	0.43
5:E:117:THR:HG22	5:E:119:SER:H	1.84	0.43
2:B:724:GLN:NE2	13:R:18:G:O3'	2.51	0.43
3:C:104:VAL:HG23	3:C:191:ILE:HD12	2.00	0.43
1:A:130:ILE:HB	1:A:212:VAL:HG12	2.00	0.43
9:I:94:MET:HE2	9:I:112:TYR:HB3	2.00	0.43
2:B:398:GLN:HG3	2:B:667:PHE:HA	2.00	0.43
11:K:74:ASN:OD1	11:K:77:ARG:NH1	2.51	0.43
1:A:721:LYS:HB2	8:H:96:VAL:HG22	2.00	0.42
2:B:127:ARG:NH2	2:B:193:TYR:OH	2.52	0.42
18:T:3000:G2P:O2B	18:T:3000:G2P:O1A	2.37	0.42
2:B:606:ASP:HB3	9:I:99:LEU:HD21	2.01	0.42
11:K:53:ALA:HB1	11:K:104:ARG:HH12	1.84	0.42
1:A:101:SER:HA	1:A:108:PHE:HA	2.02	0.42
1:A:732:ILE:HA	1:A:735:VAL:HB	2.00	0.42
1:A:121:LYS:NZ	1:A:133:SER:O	2.53	0.42
1:A:1140:PHE:HZ	1:A:1170:MET:HB3	1.85	0.42
1:A:119:ALA:HB2	1:A:334:VAL:HG22	2.01	0.42
1:A:1643:VAL:HG13	1:A:1645:LYS:HG2	2.01	0.42
11:K:98:GLU:HB3	11:K:100:LEU:HD13	2.01	0.42
1:A:31:GLN:HB3	1:A:78:HIS:CE1	2.55	0.42
1:A:100:ALA:HB1	1:A:227:LEU:HB3	2.02	0.42
2:B:420:TYR:HE1	2:B:455:GLU:HG2	1.85	0.42
2:B:1047:ARG:NH1	2:B:1066:HIS:O	2.52	0.42
3:C:222:VAL:HG11	3:C:225:ALA:HB2	2.02	0.42
1:A:504:LYS:HG3	2:B:1046:VAL:HG11	2.02	0.41
2:B:921:HIS:NE2	2:B:965:GLU:OE1	2.38	0.41
5:E:17:ARG:NH2	5:E:36:GLU:OE2	2.53	0.41
1:A:110:LEU:HD13	1:A:230:ARG:HD2	2.02	0.41
1:A:1242:ILE:HD11	1:A:1519:LEU:HD22	2.02	0.41
2:B:50:ASN:OD1	2:B:167:SER:OG	2.31	0.41
2:B:527:PHE:HB3	2:B:649:MET:HE2	2.02	0.41
11:K:104:ARG:HH21	11:K:106:GLN:HE21	1.68	0.41
2:B:656:LEU:HD21	2:B:681:ILE:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:658:LEU:HA	9:I:120:LYS:HZ2	1.85	0.41
14:S:32:DT:O4	15:T:6:DA:N6	2.53	0.41
1:A:591:ARG:NH1	13:R:20:C:O2'	2.53	0.41
1:A:1050:TYR:CZ	1:A:1580:ARG:HB3	2.56	0.41
1:A:1187:ILE:HD12	2:B:1077:ASP:HB2	2.02	0.41
1:A:1613:MET:HE3	1:A:1622:LEU:HD12	2.03	0.41
3:C:107:LYS:HE3	3:C:187:ALA:HA	2.02	0.41
6:F:107:VAL:HG12	6:F:109:VAL:H	1.86	0.41
2:B:920:ARG:HE	2:B:1032:TYR:HB3	1.84	0.41
7:G:62:MET:HA	7:G:66:LEU:HB2	2.03	0.41
1:A:509:GLU:HG3	1:A:579:ARG:HE	1.85	0.41
1:A:568:VAL:O	1:A:571:HIS:ND1	2.49	0.41
2:B:157:ASP:N	2:B:157:ASP:OD1	2.53	0.41
9:I:63:LYS:O	9:I:67:VAL:HG23	2.21	0.41
2:B:718:GLN:O	2:B:722:GLY:N	2.43	0.41
1:A:90:PHE:HB3	1:A:355:PHE:HD1	1.86	0.41
1:A:1181:PRO:HD2	6:F:86:THR:HG21	2.03	0.41
2:B:19:LEU:HD11	10:J:25:LEU:HB3	2.02	0.41
1:A:1129:PRO:HG2	1:A:1178:LEU:HD11	2.02	0.41
6:F:107:VAL:HG11	6:F:111:LEU:HD21	2.03	0.41
15:T:15:DC:H42	18:T:3000:G2P:H1	1.69	0.41
1:A:833:LEU:HD22	1:A:943:ILE:HG21	2.03	0.40
2:B:651:ARG:HH12	2:B:690:GLU:HG2	1.86	0.40
3:C:69:ARG:HE	11:K:71:THR:HG22	1.86	0.40
4:D:22:ILE:HG23	7:G:76:LYS:HG3	2.03	0.40
15:T:26:DT:H6	15:T:26:DT:H2'	1.70	0.40
2:B:221:SER:OG	14:S:25:DA:OP2	2.28	0.40
2:B:891:GLU:HG2	12:L:54:ARG:HG3	2.03	0.40
2:B:895:PHE:HE1	12:L:54:ARG:HH12	1.68	0.40
8:H:145:ARG:HG2	8:H:146:ARG:HG3	2.03	0.40
1:A:372:LYS:HG3	1:A:377:VAL:HG22	2.03	0.40
1:A:588:LEU:HD21	2:B:1079:LEU:HD21	2.03	0.40
2:B:138:LEU:HD12	2:B:155:VAL:HG12	2.03	0.40
2:B:214:PRO:O	2:B:380:LYS:NZ	2.42	0.40
2:B:1110:ILE:HD12	2:B:1178:ILE:HD13	2.02	0.40
2:B:58:GLY:O	2:B:62:ASN:ND2	2.50	0.40
2:B:614:GLU:HG2	2:B:616:LYS:HD3	2.03	0.40
1:A:1660:VAL:HB	7:G:57:PRO:HG3	2.03	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	1438/1664 (86%)	1365 (95%)	73 (5%)	0	100	100
2	B	1159/1203 (96%)	1097 (95%)	62 (5%)	0	100	100
3	C	302/335 (90%)	298 (99%)	4 (1%)	0	100	100
4	D	53/137 (39%)	51 (96%)	2 (4%)	0	100	100
5	E	209/215 (97%)	202 (97%)	7 (3%)	0	100	100
6	F	98/155 (63%)	98 (100%)	0	0	100	100
7	G	172/326 (53%)	167 (97%)	5 (3%)	0	100	100
8	H	127/146 (87%)	124 (98%)	3 (2%)	0	100	100
9	I	107/125 (86%)	99 (92%)	8 (8%)	0	100	100
10	J	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
11	K	96/142 (68%)	91 (95%)	5 (5%)	0	100	100
12	L	42/70 (60%)	37 (88%)	5 (12%)	0	100	100
All	All	3870/4588 (84%)	3692 (95%)	178 (5%)	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	1285/1465 (88%)	1283 (100%)	2 (0%)	87	88
2	B	1020/1053 (97%)	1020 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	268/296 (90%)	268 (100%)	0	100	100
4	D	54/116 (47%)	54 (100%)	0	100	100
5	E	196/197 (100%)	196 (100%)	0	100	100
6	F	90/137 (66%)	90 (100%)	0	100	100
7	G	156/291 (54%)	155 (99%)	1 (1%)	78	82
8	H	115/128 (90%)	115 (100%)	0	100	100
9	I	98/110 (89%)	98 (100%)	0	100	100
10	J	64/65 (98%)	64 (100%)	0	100	100
11	K	88/130 (68%)	88 (100%)	0	100	100
12	L	39/57 (68%)	39 (100%)	0	100	100
All	All	3473/4045 (86%)	3470 (100%)	3 (0%)	87	90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	586	VAL
1	A	587	VAL
7	G	45	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	470	HIS
1	A	521	GLN
1	A	590	ASN
1	A	620	ASN
1	A	691	GLN
1	A	694	GLN
1	A	767	ASN
1	A	901	ASN
1	A	923	ASN
1	A	1088	HIS
1	A	1108	HIS
1	A	1141	GLN
1	A	1293	HIS
1	A	1314	GLN

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Mol	Chain	Res	Type
1	A	1315	ASN
1	A	1447	GLN
2	B	43	GLN
2	B	171	HIS
2	B	173	ASN
2	B	212	ASN
2	B	246	GLN
2	B	368	GLN
2	B	427	GLN
2	B	433	ASN
2	B	555	GLN
2	B	720	GLN
2	B	724	GLN
2	B	745	GLN
2	B	896	GLN
2	B	899	GLN
2	B	1038	HIS
3	C	53	ASN
3	C	65	ASN
3	C	175	GLN
4	D	29	GLN
5	E	8	ASN
5	E	153	HIS
5	E	179	GLN
6	F	59	GLN
6	F	60	GLN
7	G	126	GLN
8	H	11	GLN
8	H	131	ASN
9	I	95	ASN
11	K	106	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	R	8/20 (40%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	R	18	G

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	G2P	T	3000	-	30,34,34	1.84	8 (26%)	46,54,54	1.82	9 (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
18	G2P	T	3000	-	-	3/19/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	T	3000	G2P	PA-O2A	4.25	1.61	1.51
18	T	3000	G2P	PB-O2B	4.16	1.61	1.51
18	T	3000	G2P	PB-O1B	-3.29	1.48	1.56
18	T	3000	G2P	PA-O1A	-3.25	1.48	1.56
18	T	3000	G2P	C5-C4	3.17	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	T	3000	G2P	PB-O3B	2.85	1.61	1.58
18	T	3000	G2P	C6-N1	-2.56	1.34	1.38
18	T	3000	G2P	C5-N7	-2.18	1.34	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	T	3000	G2P	C5-C4-N3	-6.26	118.43	128.39
18	T	3000	G2P	C2-N3-C4	4.89	120.73	112.30
18	T	3000	G2P	N9-C4-N3	4.67	135.29	125.95
18	T	3000	G2P	PB-O3B-PG	-3.28	120.68	132.45
18	T	3000	G2P	C6-C5-N7	2.97	135.70	130.29
18	T	3000	G2P	C3'-C2'-C1'	2.61	106.39	101.46
18	T	3000	G2P	C4-C5-N7	-2.46	106.78	110.67
18	T	3000	G2P	O6-C6-C5	-2.06	121.10	126.53
18	T	3000	G2P	C2'-C3'-C4'	2.04	106.56	102.61

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	T	3000	G2P	O4'-C4'-C5'-O5'
18	T	3000	G2P	PA-C3A-PB-O1B
18	T	3000	G2P	PB-C3A-PA-O2A

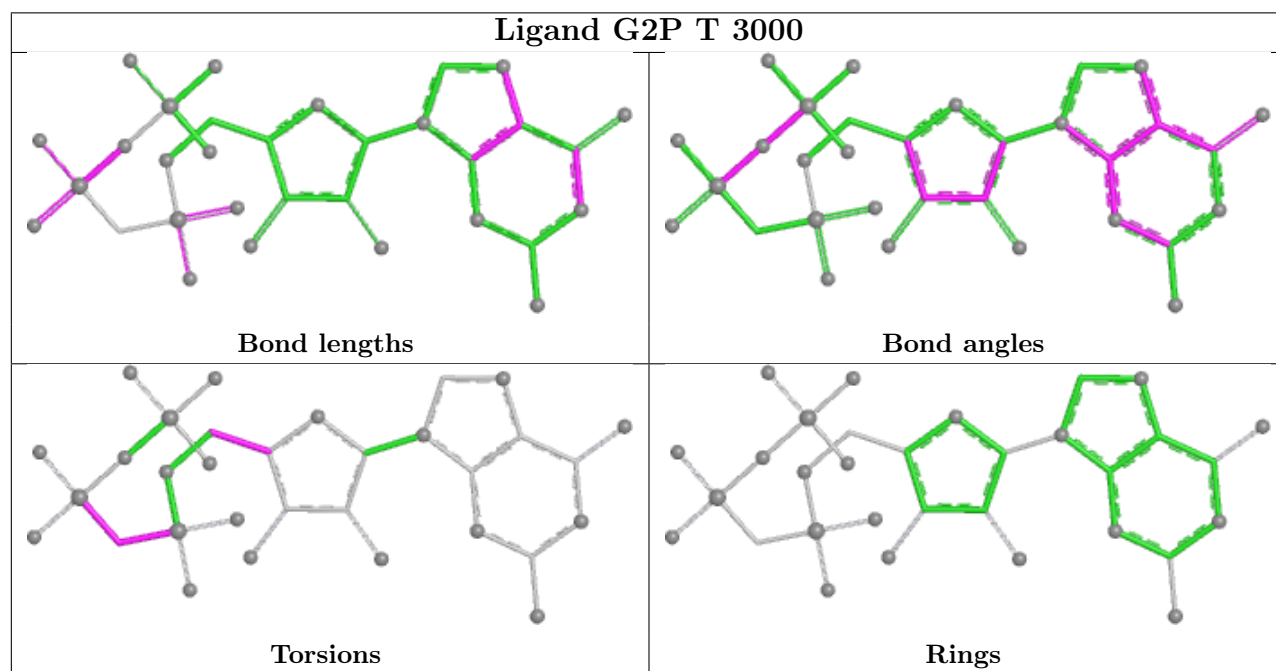
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	T	3000	G2P	4	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.

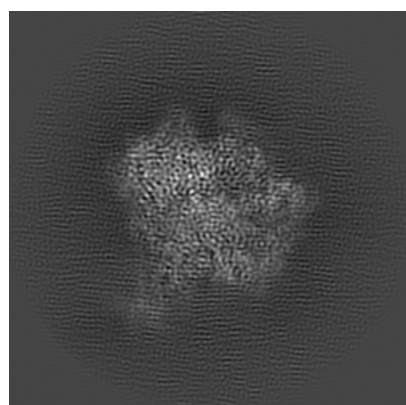
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0239. These allow visual inspection of the internal detail of the map and identification of artifacts.

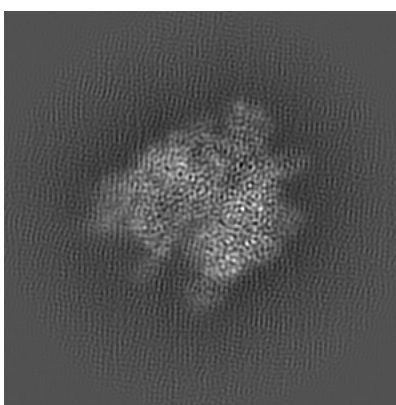
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

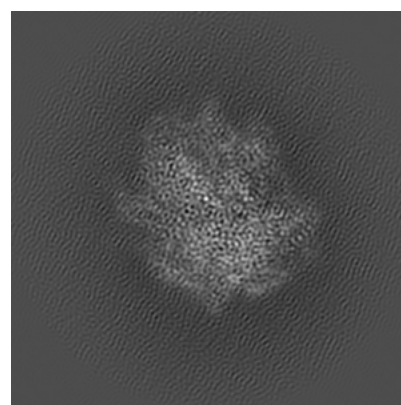
6.1.1 Primary map



X



Y

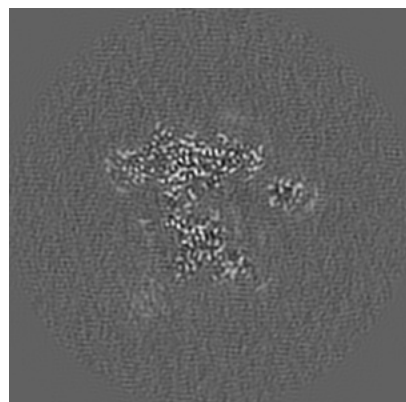


Z

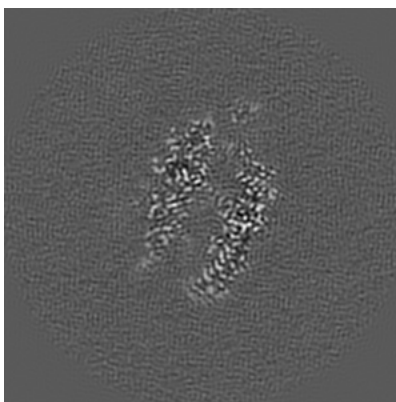
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

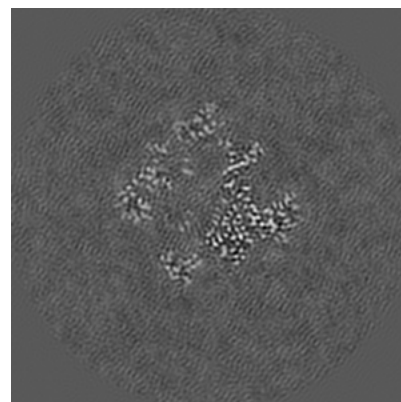
6.2.1 Primary map



X Index: 130



Y Index: 130

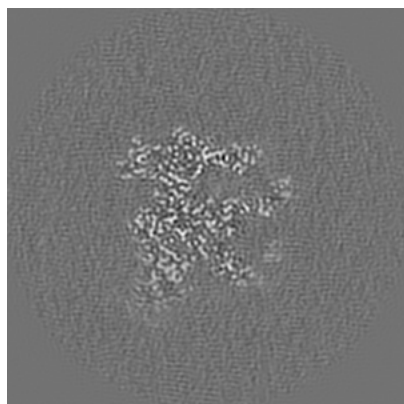


Z Index: 130

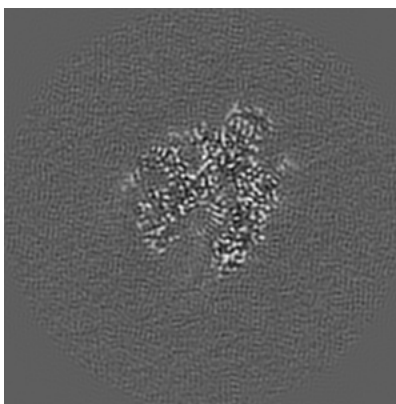
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

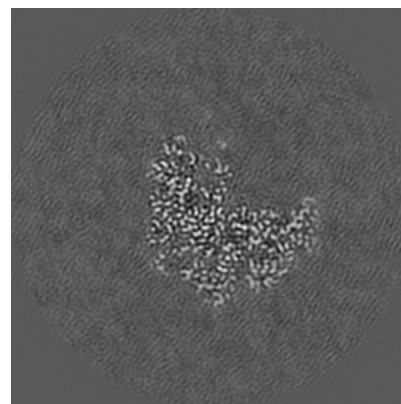
6.3.1 Primary map



X Index: 142



Y Index: 119

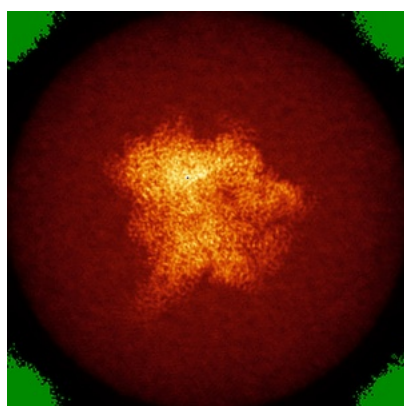


Z Index: 152

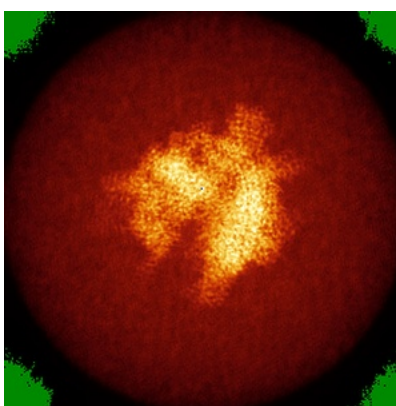
The images above show the largest variance slices of the map in three orthogonal directions.

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

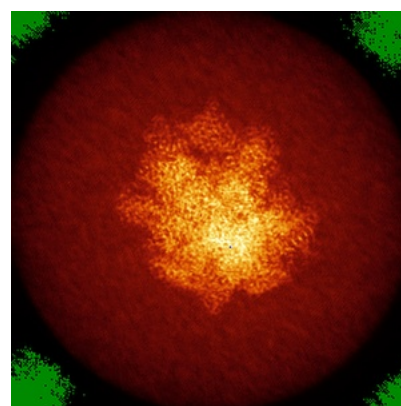
6.4.1 Primary map



X



Y

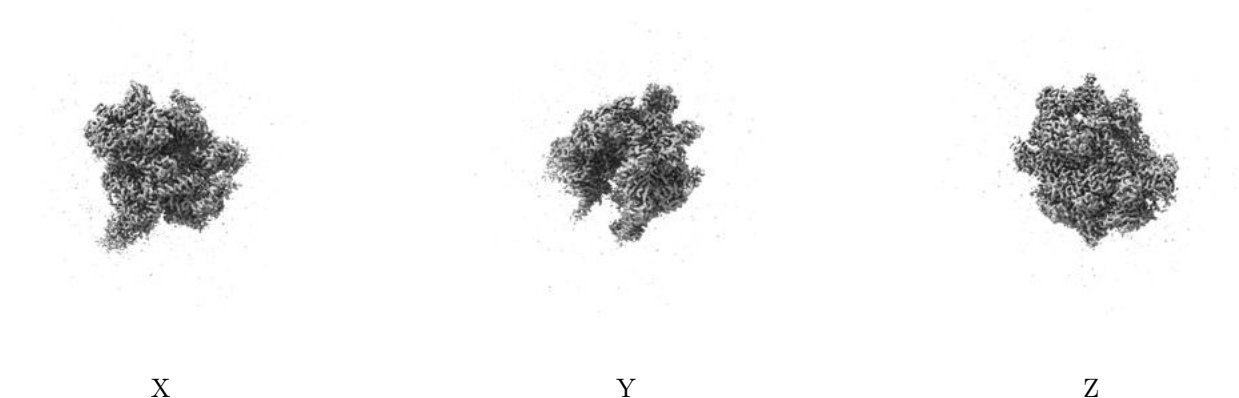


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.066. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

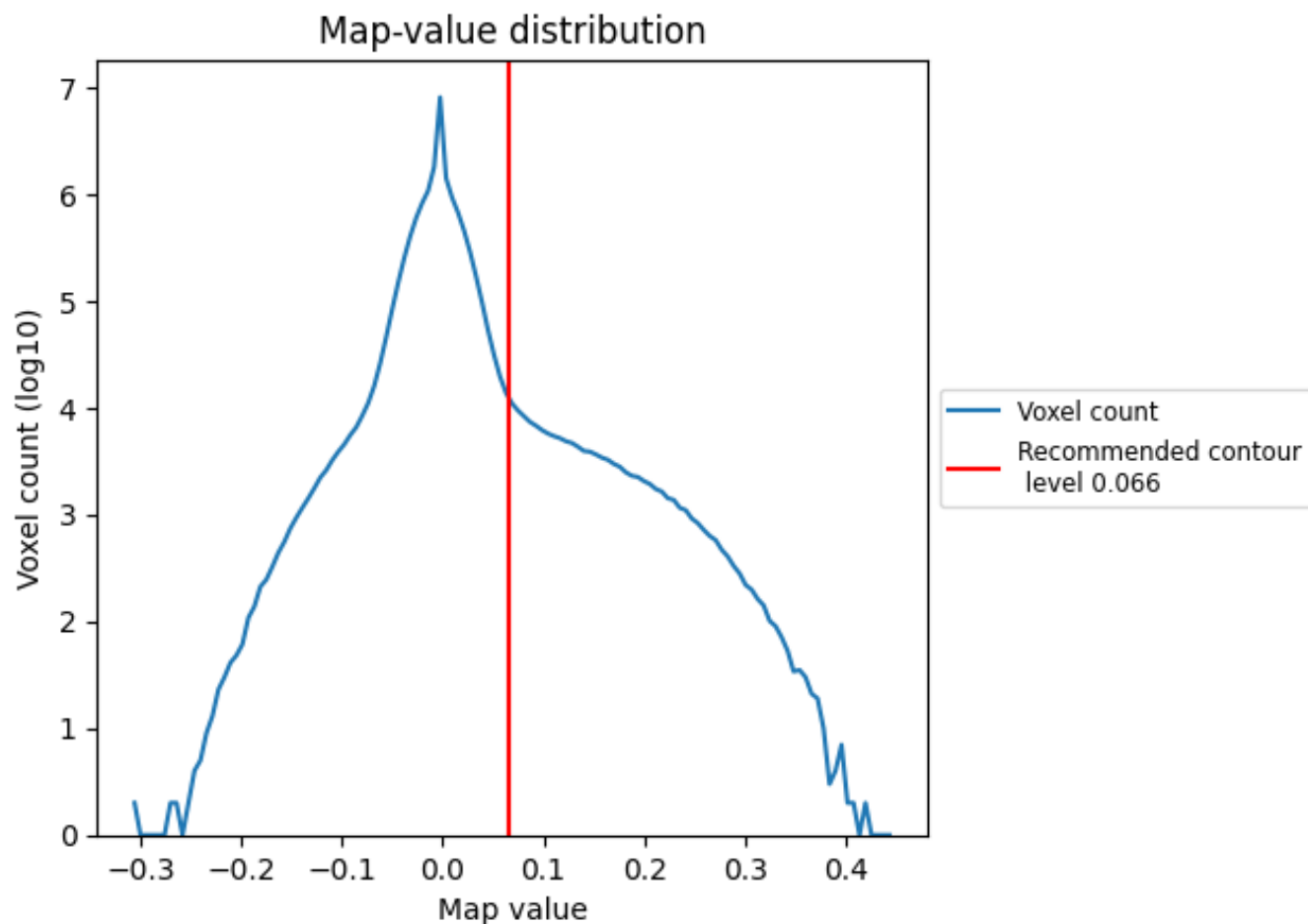
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

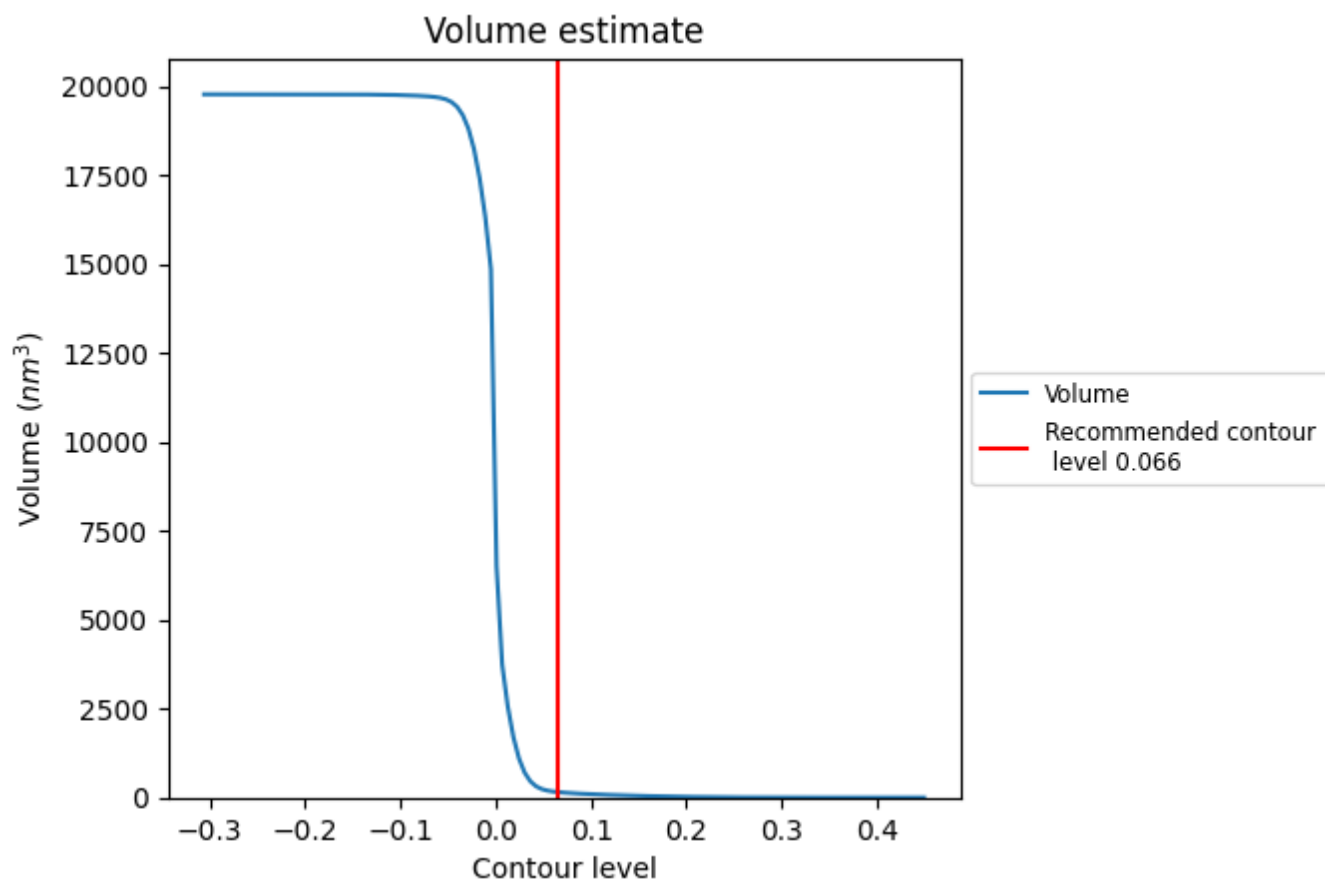
This section contains the results of statistical analysis of the map.

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.

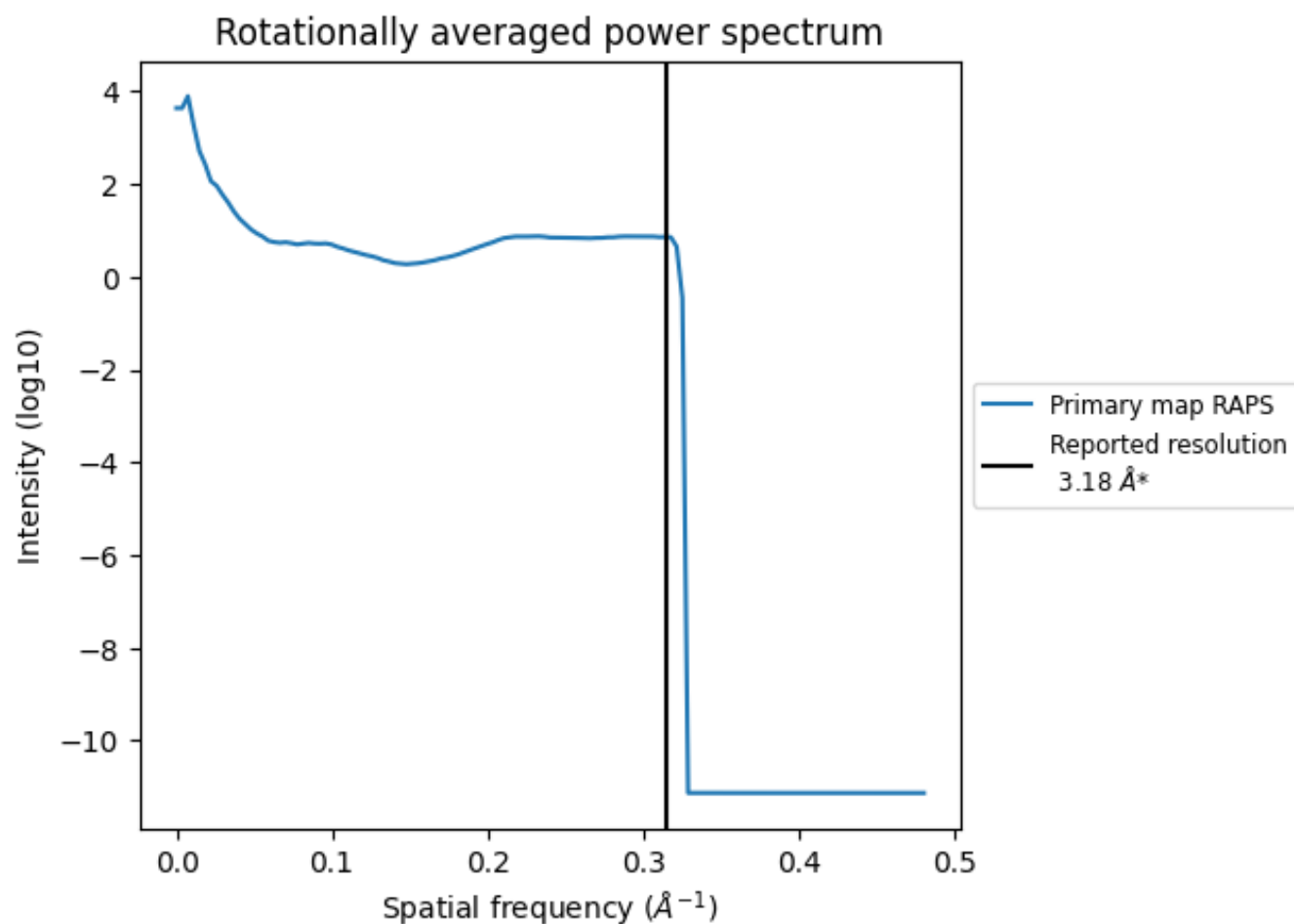
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 152 nm³; this corresponds to an approximate mass of 137 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 ⓘ

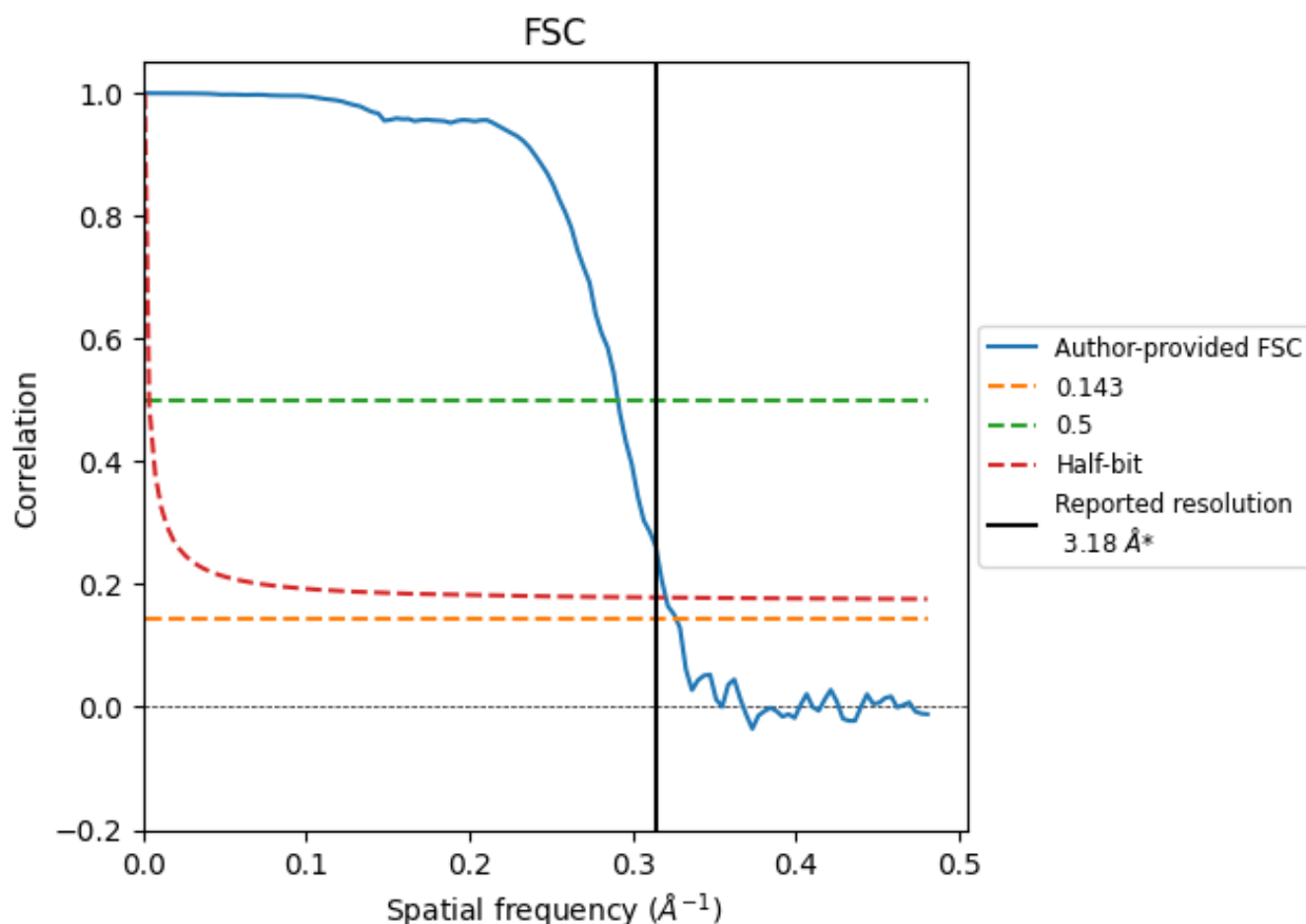


*Reported resolution corresponds to spatial frequency of 0.314 Å⁻¹

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 0.314 Å⁻¹

8.2 Resolution estimates [i](#)

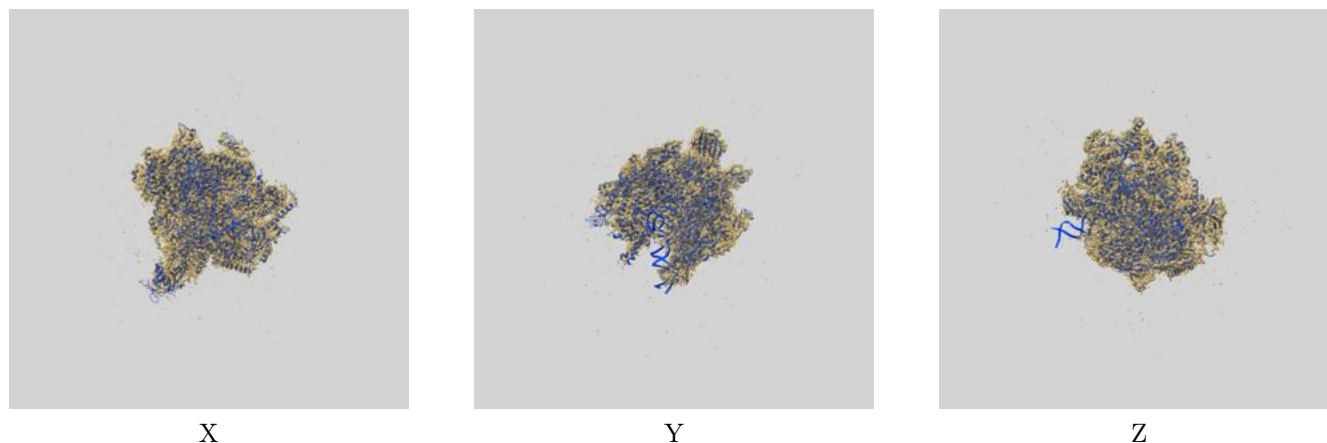
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.18	-	-
Author-provided FSC curve	3.06	3.44	3.12
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

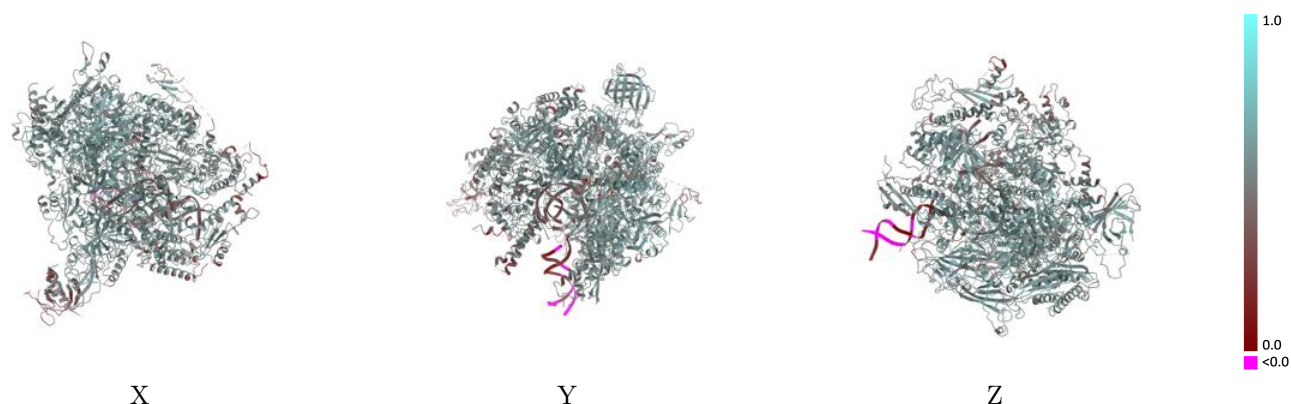
This section contains information regarding the fit between EMDB map EMD-0239 and PDB model 6HLQ. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



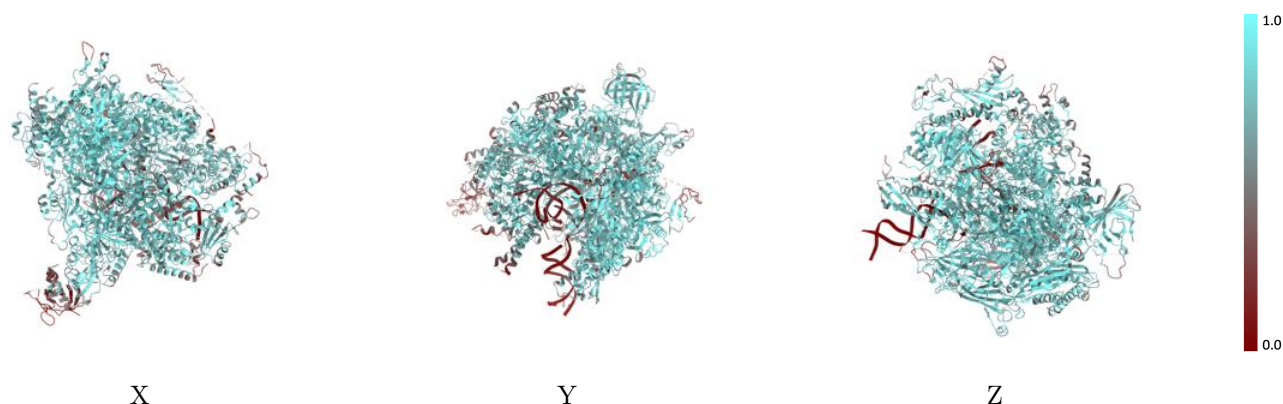
The images above show the 3D surface view of the map at the recommended contour level 0.066 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



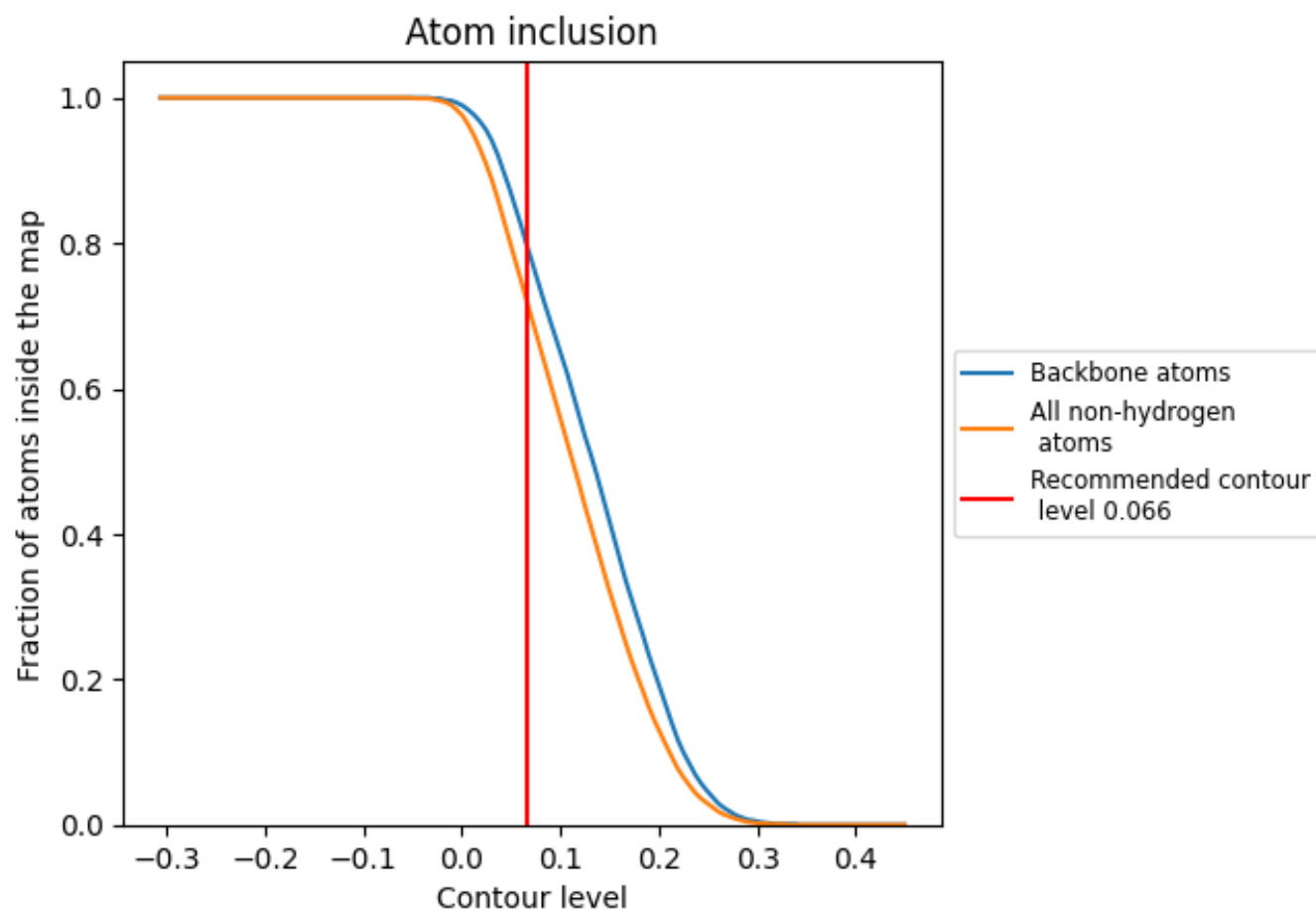
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.066).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 72% 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 (0.066) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7210	 0.5240
A	 0.7550	 0.5360
B	 0.8000	 0.5520
C	 0.7510	 0.5460
D	 0.5070	 0.4430
E	 0.7120	 0.5150
F	 0.8010	 0.5590
G	 0.4580	 0.4350
H	 0.7450	 0.5440
I	 0.5690	 0.4810
J	 0.8370	 0.5780
K	 0.7590	 0.5500
L	 0.7440	 0.5390
R	 0.6330	 0.5290
S	 0.0280	 0.2030
T	 0.2500	 0.3020

