



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 03:50 PM UTC

PDB ID : 6FLP / pdb_00006flp
EMDB ID : EMD-4274
Title : CryoEM structure of E.coli RNA polymerase paused elongation complex without RNA hairpin bound to NusA
Authors : Guo, X.; Weixlbaumer, A.
Deposited on : 2018-01-26
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

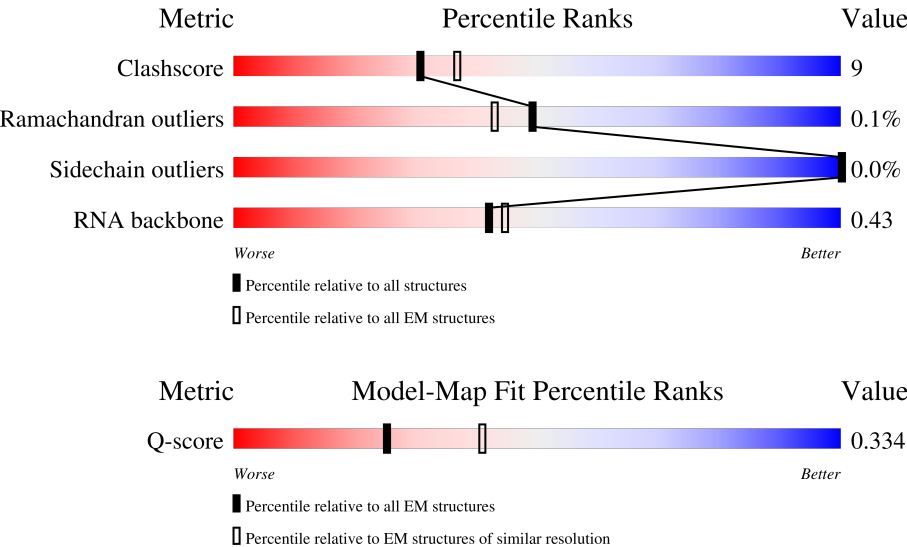
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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	6458 (3.60 - 4.60)

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	329	
1	B	329	
2	C	1342	

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Mol	Chain	Length	Quality of chain
3	D	1407	
4	E	91	
5	N	31	
6	R	10	
7	T	39	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 26512 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 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	229	Total	C	N	O	S	0	0
			1767	1100	313	348	6		
1	B	217	Total	C	N	O	S	0	0
			1667	1041	293	327	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1314	Total	C	N	O	S	0	0
			10363	6502	1806	2012	43		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1334	Total	C	N	O	S	0	0
			10357	6510	1846	1952	49		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	90	Total	C	N	O	S	0	0
			709	430	136	142	1		

- Molecule 5 is a DNA chain called DNA (30-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	31	Total	C	N	O	P	0	0
			647	304	131	181	31		

- Molecule 6 is a RNA chain called RNA (5'-R(P*GP*AP*UP*GP*UP*GP*UP*GP*CP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	10	Total	C	N	O	P	0	0
			214	95	36	73	10		

- Molecule 7 is a DNA chain called DNA (39-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	39	Total	C	N	O	P	0	0
			785	375	135	236	39		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

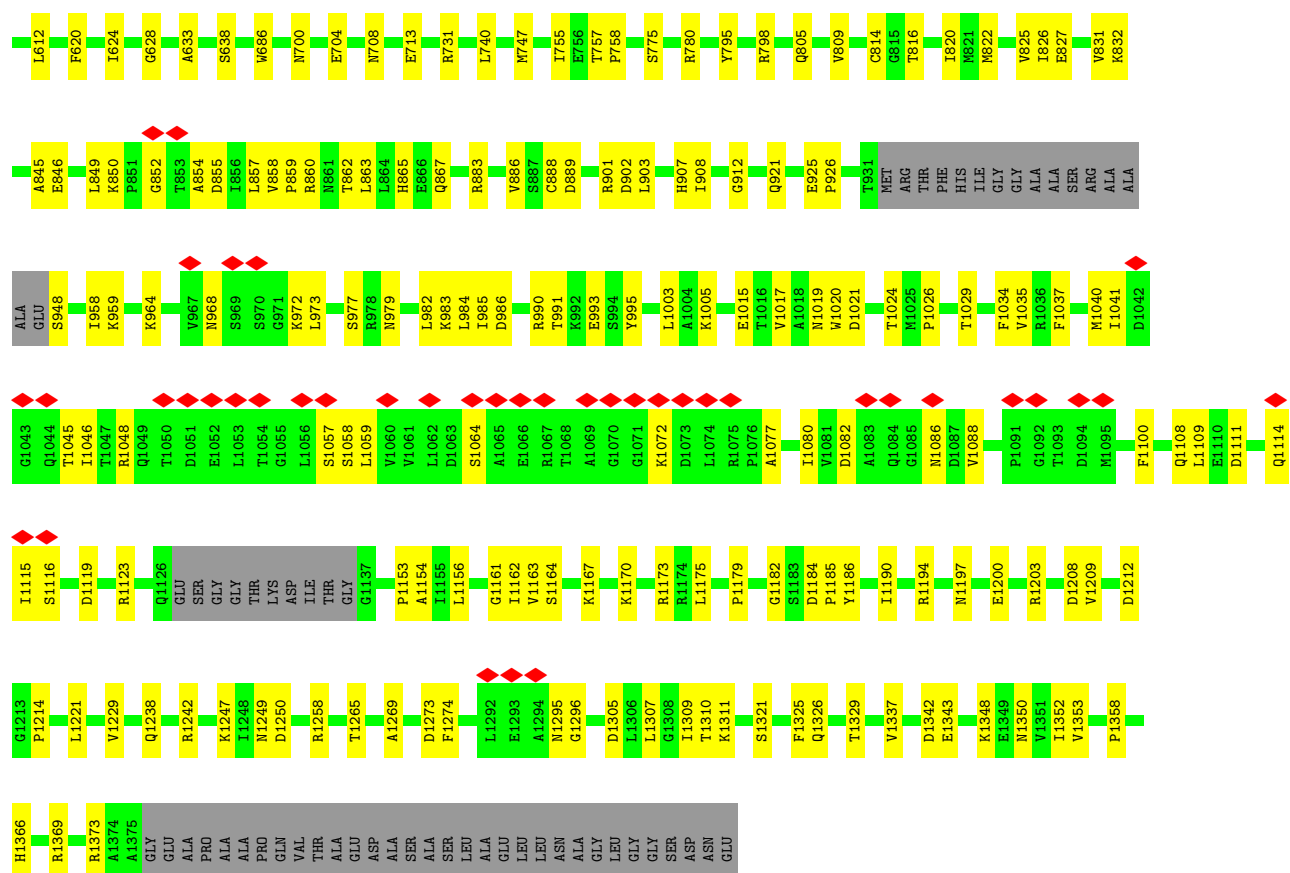
Mol	Chain	Residues	Atoms		AltConf
8	D	1	Total	Mg	0
			1	1	

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

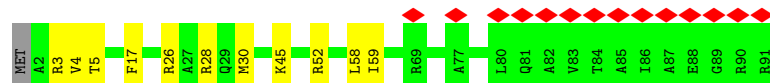
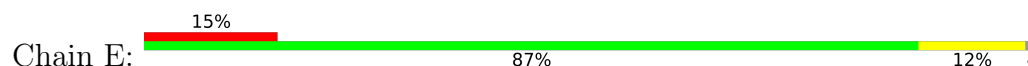
Mol	Chain	Residues	Atoms		AltConf
9	D	2	Total	Zn	0
			2	2	



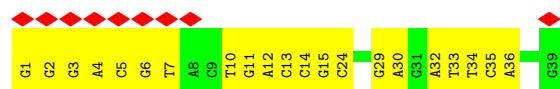
F461	M298	R123	MET
Q465	L306	D129	LYS
T473	L307	M130	ASP
L474	D308	S143	LEU
E475	N309	G149	LEU
A476	G310	M151	LYS
A482	R314	G150	PHE
M488	A315	M151	LEU
M495	L316	E155	ALA
P502	T317	R156	GLN
V506	K321	Q157	THR
M513	R322	Q158	LYS
T514	P323	I159	THR
A520	S326	L160	GLU
V526	S329	Q164	E16
L527	K332	D177	F17
T528	L342	D193	D18
K531	K345	L194	M29
E532	R362	E197	I30
A546	K370	L205	G36
K549	K378	L217	T43
V550	Y382	R220	Y46
D558	E405	S230	R47
A559	V408	G231	T48
N560	L412	N232	F49
T573	V415	P243	K50
R576	E418	V244	L56
L579	L423	P246	F57
P584	M424	L249	C58
K585	R425	R250	A59
G586	A426	V253	R60
L587	P427	P254	I61
I591	H430	D256	R77
V592	R431	G257	L78
L596	L432	C258	K79
I601	F437	R259	C85
M604	E443	F260	E86
		L268	V90
		R275	E91
			V92
			T93
			Q94
			R99
			E100
			R101
			W115
			L120
			G



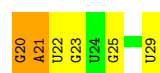
- Molecule 4: DNA-directed RNA polymerase subunit omega



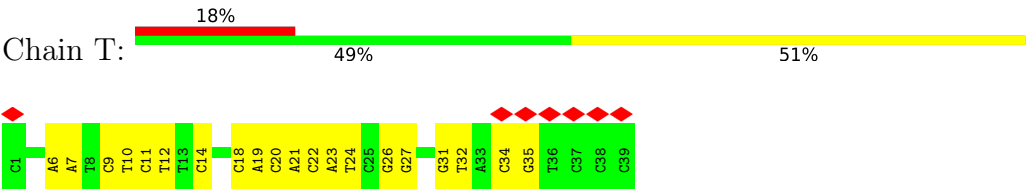
- Molecule 5: DNA (30-MER)



- Molecule 6: RNA (5'-R(P*GP*AP*UP*GP*UP*GP*UP*GP*CP*U)-3')



- Molecule 7: DNA (39-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	65966	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 ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.215	Depositor
Minimum map value	-0.502	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.27	Depositor
Map size (Å)	308.0, 308.0, 308.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.12	0/1789	0.37	0/2425
1	B	0.13	0/1686	0.40	0/2285
2	C	0.12	0/10528	0.34	1/14205 (0.0%)
3	D	0.12	0/10514	0.34	0/14199
4	E	0.11	0/711	0.33	0/956
5	N	0.19	0/728	0.40	0/1121
6	R	0.12	0/238	0.28	0/369
7	T	0.18	0/876	0.38	0/1346
All	All	0.12	0/27070	0.35	1/36906 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	630	VAL	N-CA-C	-5.72	106.82	111.91

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	57	PHE	Peptide

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	1767	0	1782	36	0
1	B	1667	0	1689	36	0
2	C	10363	0	10368	177	0
3	D	10357	0	10573	192	0
4	E	709	0	719	7	0
5	N	647	0	347	23	0
6	R	214	0	107	6	0
7	T	785	0	440	25	0
8	D	1	0	0	0	0
9	D	2	0	0	0	0
All	All	26512	0	26025	467	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 9.

All (467) 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)
5:N:29:DG:N2	7:T:11:DC:O2	2.06	0.87
2:C:200:ARG:NH2	5:N:24:DC:OP2	2.11	0.84
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.63	0.79
1:B:64:VAL:HG13	1:B:69:SER:HB2	1.68	0.75
2:C:1274:GLU:HG2	3:D:424:ASN:HD21	1.54	0.72
3:D:845:ALA:HA	3:D:883:ARG:HG3	1.73	0.71
6:R:20:G:H2'	6:R:21:A:C8	2.25	0.71
3:D:129:ASP:OD2	3:D:220:ARG:NH1	2.23	0.70
3:D:527:LEU:HB2	3:D:550:VAL:HG12	1.73	0.70
3:D:316:ILE:HG21	3:D:323:PRO:HA	1.73	0.70
3:D:959:LYS:HD2	3:D:985:ILE:HG13	1.73	0.70
3:D:93:THR:HG22	3:D:94:GLN:H	1.58	0.69
3:D:708:ASN:HA	3:D:713:GLU:HA	1.75	0.69
2:C:685:MET:HE3	2:C:1073:LYS:HD3	1.75	0.68
2:C:232:ILE:HB	2:C:331:LYS:HG3	1.75	0.68
2:C:808:ASN:H	3:D:633:ALA:HB2	1.59	0.68
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:130:MET:SD	3:D:157:GLN:NE2	2.66	0.68
7:T:9:DC:H2'	7:T:10:DT:H71	1.77	0.67
4:E:26:ARG:HG3	4:E:30:MET:HE2	1.75	0.67
7:T:31:DG:H2''	7:T:32:DT:H5'	1.77	0.67
2:C:93:SER:HA	2:C:128:PRO:HA	1.76	0.67
2:C:1288:GLN:O	2:C:1292:THR:HB	1.95	0.66
3:D:1154:ALA:HA	3:D:1194:ARG:HH12	1.60	0.66
1:A:45:ARG:HH22	1:B:37:HIS:HB2	1.61	0.65
7:T:20:DC:H2'	7:T:21:DA:H8	1.60	0.65
3:D:149:GLY:HA2	3:D:177:ASP:H	1.60	0.65
1:B:12:ARG:HG2	1:B:13:LEU:H	1.60	0.65
1:B:155:ALA:HB1	1:B:158:ARG:HH12	1.61	0.65
1:B:91:ARG:NH2	1:B:210:THR:O	2.30	0.65
3:D:1005:LYS:NZ	3:D:1015:GLU:OE2	2.29	0.65
3:D:245:LEU:O	3:D:250:ARG:NH1	2.28	0.64
2:C:1282:GLY:HA3	4:E:17:PHE:HE1	1.62	0.64
3:D:60:ARG:HB3	3:D:90:VAL:HG22	1.77	0.64
2:C:1122:LYS:NZ	2:C:1126:ASP:OD1	2.30	0.64
2:C:260:LYS:HG3	2:C:261:VAL:HG23	1.80	0.64
1:A:33:ARG:HE	1:A:197:ASP:HB2	1.63	0.64
1:A:125:LYS:HE2	1:A:127:GLN:HB2	1.79	0.64
2:C:801:ARG:NH1	2:C:1093:PRO:O	2.30	0.64
3:D:755:ILE:HG22	3:D:757:THR:H	1.62	0.63
3:D:46:TYR:O	3:D:47:ARG:HG2	1.97	0.63
2:C:198:ILE:HG22	2:C:199:ASP:H	1.65	0.62
3:D:120:LEU:HB3	5:N:30:DA:H4'	1.80	0.62
2:C:1069:ARG:NH2	2:C:1114:GLU:OE2	2.31	0.62
7:T:20:DC:H2'	7:T:21:DA:C8	2.34	0.62
2:C:296:VAL:HA	2:C:316:GLU:HA	1.82	0.61
3:D:230:SER:OG	3:D:232:ASN:ND2	2.33	0.61
3:D:473:THR:HG23	3:D:476:ALA:H	1.65	0.61
2:C:1230:MET:HG3	2:C:1231:TYR:H	1.66	0.61
3:D:903:LEU:HD21	3:D:1249:ASN:HD22	1.66	0.61
4:E:3:ARG:HE	4:E:52:ARG:HG2	1.64	0.61
2:C:97:ARG:HB3	2:C:121:GLU:HB2	1.82	0.60
4:E:58:LEU:HD12	4:E:59:ILE:HG12	1.83	0.60
3:D:1173:ARG:HB2	3:D:1190:ILE:HB	1.83	0.60
2:C:748:ILE:HG12	2:C:966:ILE:HD13	1.83	0.60
3:D:1080:ILE:HG23	3:D:1088:VAL:HB	1.83	0.60
2:C:237:LEU:HD21	2:C:289:VAL:HG23	1.83	0.59
3:D:814:CYS:SG	3:D:883:ARG:NH2	2.76	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1046:ILE:HD12	3:D:1059:LEU:HD21	1.84	0.59
3:D:197:GLU:OE2	3:D:220:ARG:NH2	2.35	0.59
1:B:107:ILE:HB	1:B:135:ASP:HA	1.85	0.59
2:C:17:LYS:HE3	2:C:1153:ALA:HB3	1.83	0.59
2:C:804:PHE:HB3	2:C:1100:PRO:HB3	1.85	0.59
2:C:10:ARG:HH21	2:C:791:LEU:HB2	1.66	0.59
2:C:212:ALA:HA	2:C:359:ARG:HG3	1.85	0.59
3:D:968:ASN:HD21	3:D:972:LYS:HB2	1.67	0.59
3:D:984:LEU:HB3	3:D:993:GLU:H	1.68	0.59
3:D:1048:ARG:NH2	3:D:1057:SER:O	2.36	0.59
2:C:600:THR:HG22	2:C:602:GLU:H	1.68	0.59
2:C:1142:ARG:NH2	2:C:1166:ASP:OD1	2.36	0.58
3:D:826:ILE:HG22	3:D:831:VAL:HA	1.84	0.58
5:N:33:DT:H2''	5:N:34:DT:H71	1.85	0.58
2:C:562:GLU:OE1	2:C:662:SER:OG	2.20	0.58
3:D:805:GLN:NE2	3:D:1321:SER:OG	2.36	0.58
2:C:149:LEU:HD11	2:C:451:ARG:HB3	1.84	0.58
5:N:6:DG:H2'	5:N:7:DT:H71	1.86	0.58
1:B:86:LYS:HD2	3:D:528:THR:HG23	1.86	0.58
3:D:1162:ILE:HA	3:D:1203:ARG:HA	1.86	0.58
1:B:188:GLU:OE2	1:B:200:LYS:NZ	2.34	0.58
2:C:589:THR:OG1	2:C:659:GLN:NE2	2.35	0.57
2:C:841:ARG:NH1	3:D:256:ASP:O	2.37	0.57
3:D:1161:GLY:HA3	3:D:1179:PRO:HA	1.87	0.57
5:N:10:DT:H2''	5:N:11:DG:C8	2.39	0.57
2:C:599:VAL:H	2:C:627:GLY:HA3	1.69	0.57
3:D:983:LYS:HB2	3:D:991:THR:HG23	1.87	0.57
2:C:10:ARG:HH11	2:C:697:LYS:HD3	1.69	0.57
3:D:255:LEU:H	3:D:260:PHE:HA	1.69	0.57
3:D:1035:VAL:HG21	3:D:1109:LEU:HD21	1.86	0.57
2:C:1134:GLN:HG3	2:C:1136:GLN:HG2	1.85	0.57
2:C:811:ASN:HB3	2:C:1099:ASN:HB2	1.87	0.57
2:C:935:THR:HG22	2:C:1048:LYS:HG2	1.86	0.57
2:C:864:LYS:HB3	2:C:871:VAL:HG23	1.86	0.56
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.87	0.56
3:D:1153:PRO:O	3:D:1194:ARG:NH2	2.34	0.56
5:N:29:DG:H2''	5:N:30:DA:C8	2.41	0.56
7:T:18:DC:H2'	7:T:19:DA:H8	1.71	0.56
3:D:1005:LYS:HD2	3:D:1017:VAL:HG12	1.85	0.56
1:B:47:LEU:HD21	1:B:180:VAL:HG11	1.88	0.56
2:C:14:ASP:HB3	2:C:1183:ALA:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:36:GLY:HA3	3:D:61:ILE:HD12	1.87	0.56
1:A:102:LEU:HD23	1:A:115:ILE:HD13	1.87	0.56
3:D:482:ALA:O	3:D:488:ASN:ND2	2.39	0.56
1:A:157:THR:O	1:A:160:HIS:ND1	2.26	0.56
3:D:275:ARG:NH1	3:D:298:MET:O	2.37	0.56
1:A:33:ARG:NH1	1:A:199:ASP:OD2	2.38	0.56
3:D:425:ARG:HG2	3:D:427:PRO:HD2	1.87	0.56
2:C:238:GLN:HG3	2:C:284:LEU:HD11	1.88	0.56
7:T:6:DA:H2''	7:T:7:DA:C8	2.41	0.56
5:N:4:DA:H2''	5:N:5:DC:C5	2.41	0.55
2:C:223:LEU:HD21	2:C:426:ILE:HD13	1.88	0.55
3:D:18:ASP:OD1	3:D:1369:ARG:NH2	2.39	0.55
6:R:21:A:H2'	6:R:22:U:C6	2.42	0.55
1:A:19:VAL:HG22	1:A:20:SER:H	1.72	0.55
1:A:182:ARG:NH1	2:C:1090:ASN:O	2.39	0.55
2:C:813:GLU:HB2	3:D:461:PHE:HD2	1.71	0.55
2:C:221:LEU:HD21	2:C:336:LEU:HD11	1.89	0.55
3:D:316:ILE:HG13	3:D:317:THR:H	1.72	0.55
1:B:18:GLN:NE2	1:B:19:VAL:O	2.40	0.54
2:C:1336:ASN:ND2	3:D:29:MET:SD	2.79	0.54
3:D:1197:ASN:ND2	3:D:1212:ASP:OD2	2.35	0.54
1:B:92:VAL:O	1:B:148:ARG:NH2	2.40	0.54
3:D:352:ARG:NH2	3:D:465:GLN:OE1	2.38	0.54
2:C:411:ARG:NH2	2:C:427:ASP:OD2	2.41	0.54
3:D:310:GLY:HA2	3:D:314:ARG:HG2	1.90	0.54
3:D:982:LEU:HB3	3:D:995:TYR:HB2	1.90	0.54
3:D:43:THR:HG22	3:D:56:LEU:HB2	1.88	0.54
3:D:205:LEU:HD13	3:D:217:LEU:HB2	1.89	0.54
3:D:1179:PRO:HB2	3:D:1182:GLY:H	1.73	0.54
2:C:133:ASN:O	2:C:527:LYS:NZ	2.41	0.54
3:D:48:THR:HB	3:D:50:LYS:HE2	1.90	0.54
5:N:13:DC:H2''	5:N:14:DC:C5	2.43	0.54
1:A:50:SER:OG	1:A:150:ARG:NH2	2.40	0.54
1:A:48:LEU:HG	1:A:183:ILE:HD12	1.90	0.53
2:C:201:ARG:NH1	2:C:370:MET:SD	2.81	0.53
2:C:297:VAL:HA	2:C:335:THR:HG22	1.90	0.53
3:D:514:THR:HG21	3:D:596:LEU:HD12	1.89	0.53
1:B:47:LEU:HA	1:B:51:MET:HE3	1.90	0.53
3:D:1369:ARG:HE	3:D:1373:ARG:HD3	1.73	0.53
1:A:29:GLU:HG3	1:A:30:PRO:HD2	1.91	0.53
1:B:192:VAL:HB	1:B:195:ARG:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:107:ARG:HH21	2:C:484:LEU:HD23	1.73	0.53
1:A:12:ARG:HB3	1:A:29:GLU:OE1	2.09	0.53
2:C:257:ALA:HA	2:C:282:VAL:HG11	1.91	0.53
2:C:1269:ARG:NH1	7:T:18:DC:OP1	2.42	0.53
3:D:827:GLU:HB3	3:D:832:LYS:HD2	1.90	0.53
3:D:1034:PHE:HA	3:D:1114:GLN:HA	1.91	0.53
2:C:1268:GLN:HE22	3:D:352:ARG:HD2	1.73	0.53
3:D:1154:ALA:N	3:D:1214:PRO:O	2.41	0.53
3:D:85:CYS:SG	3:D:86:GLU:N	2.81	0.53
1:B:57:THR:OG1	1:B:147:GLN:NE2	2.36	0.53
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.91	0.53
3:D:850:LYS:HB3	3:D:855:ASP:HB2	1.91	0.53
2:C:183:TRP:N	2:C:199:ASP:OD1	2.41	0.53
5:N:11:DG:C8	5:N:11:DG:H5'	2.43	0.53
2:C:149:LEU:HD21	2:C:451:ARG:HD3	1.91	0.52
3:D:495:ASN:HD22	3:D:1247:LYS:HB2	1.74	0.52
2:C:246:LEU:HD12	2:C:277:LEU:HD11	1.90	0.52
2:C:801:ARG:HB2	2:C:1095:ASP:HB2	1.92	0.52
3:D:123:ARG:HG3	3:D:1337:VAL:HG11	1.90	0.52
2:C:251:ALA:HB3	2:C:266:GLY:H	1.74	0.52
2:C:27:LEU:O	2:C:528:ARG:NH1	2.41	0.52
2:C:189:ASP:OD1	2:C:193:ASN:N	2.40	0.52
3:D:1058:SER:OG	3:D:1108:GLN:NE2	2.39	0.52
1:A:14:VAL:HG22	1:A:15:ASP:H	1.75	0.52
2:C:321:LEU:HD23	2:C:325:LEU:HD23	1.91	0.52
3:D:317:THR:HG21	5:N:15:DG:H2''	1.92	0.52
3:D:77:ARG:HG2	3:D:79:LYS:H	1.75	0.52
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.92	0.52
1:B:60:GLU:OE2	1:B:171:LEU:N	2.43	0.52
3:D:814:CYS:HB2	3:D:889:ASP:HB3	1.92	0.52
3:D:865:HIS:CE1	3:D:867:GLN:HB2	2.45	0.52
2:C:256:GLU:OE1	2:C:286:GLU:N	2.31	0.52
2:C:1143:GLU:OE2	2:C:1147:ARG:NE	2.43	0.52
4:E:4:VAL:HG13	4:E:5:THR:HG23	1.92	0.52
5:N:1:DG:H2''	5:N:2:DG:H5'	1.92	0.52
1:A:135:ASP:HB3	1:A:138:ALA:HB2	1.91	0.51
2:C:700:VAL:HG11	2:C:1114:GLU:HG3	1.92	0.51
3:D:160:LEU:HD22	3:D:164:GLN:HB3	1.91	0.51
3:D:948:SER:OG	3:D:1020:TRP:NE1	2.44	0.51
2:C:700:VAL:HG22	2:C:1117:LEU:HD22	1.91	0.51
2:C:49:LEU:HB3	2:C:53:PHE:HE2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:591:ILE:HG23	3:D:592:VAL:HG13	1.93	0.51
3:D:1029:THR:HG21	3:D:1115:ILE:HD13	1.92	0.51
7:T:31:DG:H2'	7:T:32:DT:H71	1.92	0.51
2:C:314:ASN:O	2:C:352:ARG:NH2	2.43	0.51
1:B:66:HIS:CD2	1:B:68:TYR:HB2	2.46	0.51
1:B:155:ALA:O	1:B:158:ARG:NH1	2.44	0.51
2:C:57:PHE:CD2	2:C:70:TYR:HB2	2.45	0.51
1:A:86:LYS:NZ	2:C:826:ASP:OD2	2.44	0.51
2:C:582:ASN:OD1	2:C:583:GLU:N	2.43	0.51
2:C:801:ARG:HG2	2:C:1229:TYR:HE1	1.76	0.51
2:C:1056:VAL:HG11	2:C:1058:ARG:HH21	1.76	0.51
2:C:799:ASN:O	2:C:827:ARG:NH2	2.34	0.51
3:D:964:LYS:HB3	3:D:977:SER:HB2	1.93	0.51
3:D:1269:ALA:HB2	3:D:1274:PHE:HA	1.92	0.50
2:C:246:LEU:HD21	2:C:255:ILE:HD12	1.93	0.50
2:C:538:LEU:H	2:C:538:LEU:HD23	1.77	0.50
3:D:857:LEU:HD12	3:D:858:VAL:HG13	1.93	0.50
2:C:514:PHE:HZ	7:T:22:DC:H4'	1.75	0.50
2:C:1185:PRO:HB2	2:C:1188:ASP:OD1	2.11	0.50
3:D:30:ILE:HG23	3:D:243:PRO:HG3	1.92	0.50
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.92	0.50
3:D:1164:SER:HA	3:D:1200:GLU:HG2	1.93	0.50
3:D:986:ASP:OD1	3:D:990:ARG:N	2.45	0.50
3:D:1021:ASP:OD2	3:D:1024:THR:OG1	2.26	0.50
2:C:59:ILE:HG22	2:C:60:GLN:H	1.77	0.50
2:C:102:LEU:N	2:C:117:ILE:O	2.36	0.50
2:C:177:ILE:HG12	2:C:183:TRP:CD1	2.46	0.50
2:C:49:LEU:HB3	2:C:53:PHE:CE2	2.47	0.50
1:A:195:ARG:HB3	1:A:198:LEU:HD13	1.94	0.50
2:C:69:GLN:HE21	2:C:101:ARG:CZ	2.24	0.50
1:A:23:HIS:ND1	1:A:205:MET:O	2.45	0.49
2:C:812:PHE:CD2	2:C:813:GLU:HG2	2.47	0.49
2:C:1246:ARG:HD2	2:C:1249:GLY:HA3	1.94	0.49
3:D:888:CYS:SG	3:D:889:ASP:N	2.86	0.49
2:C:230:PHE:HB2	2:C:333:ILE:HB	1.94	0.49
7:T:11:DC:H2''	7:T:12:DT:H71	1.95	0.49
1:B:101:THR:HG22	1:B:143:ARG:HG2	1.94	0.49
1:B:155:ALA:HB2	1:B:174:ASP:HA	1.93	0.49
2:C:733:VAL:HG13	2:C:748:ILE:HD13	1.95	0.49
3:D:584:PRO:HG2	3:D:587:LEU:HD13	1.94	0.49
3:D:850:LYS:HG2	3:D:852:GLY:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:102:LEU:HD22	2:C:489:PRO:HG3	1.94	0.49
3:D:437:PHE:HZ	3:D:453:VAL:HG11	1.77	0.49
3:D:809:VAL:HG23	3:D:912:GLY:H	1.78	0.49
2:C:1196:LYS:HD3	2:C:1199:LEU:HD12	1.93	0.49
7:T:23:DA:H2''	7:T:24:DT:O5'	2.13	0.49
3:D:423:LEU:HD13	3:D:437:PHE:HD2	1.78	0.49
6:R:22:U:H2'	6:R:23:G:C8	2.48	0.49
3:D:1307:LEU:HD23	3:D:1311:LYS:HG3	1.94	0.49
3:D:1350:ASN:HA	3:D:1353:VAL:HG12	1.94	0.49
5:N:29:DG:H2''	5:N:30:DA:OP2	2.13	0.49
3:D:316:ILE:HG13	3:D:317:THR:N	2.28	0.48
2:C:68:LEU:HD23	2:C:479:LEU:HD11	1.95	0.48
2:C:964:LEU:HD13	2:C:1025:PHE:HD2	1.78	0.48
2:C:1058:ARG:NH1	2:C:1240:ASP:OD2	2.47	0.48
3:D:1064:SER:O	3:D:1072:LYS:NZ	2.45	0.48
5:N:30:DA:OP2	5:N:30:DA:H8	1.96	0.48
2:C:880:GLY:O	2:C:919:ARG:NH1	2.42	0.48
3:D:143:SER:OG	3:D:160:LEU:O	2.29	0.48
3:D:863:LEU:HD21	3:D:901:ARG:HE	1.78	0.48
1:A:30:PRO:HB2	1:A:198:LEU:HB3	1.96	0.48
3:D:620:PHE:CE2	3:D:624:ILE:HD11	2.48	0.48
1:A:192:VAL:HB	1:A:195:ARG:HB2	1.95	0.48
1:B:25:LYS:HA	1:B:204:GLU:HA	1.95	0.48
2:C:102:LEU:HB3	2:C:117:ILE:HB	1.96	0.48
1:A:61:ILE:HD13	1:A:142:MET:HB3	1.96	0.48
3:D:430:HIS:NE2	3:D:432:LEU:HB2	2.29	0.48
3:D:528:THR:N	3:D:532:GLU:OE2	2.29	0.48
3:D:1184:ASP:N	3:D:1185:PRO:HD3	2.29	0.48
2:C:957:LYS:HG2	2:C:1029:LEU:HD11	1.96	0.47
3:D:1156:LEU:HA	3:D:1209:VAL:HA	1.96	0.47
7:T:26:DG:H1'	7:T:27:DG:N7	2.29	0.47
2:C:803:ALA:HB3	2:C:1097:VAL:HG22	1.96	0.47
1:A:46:ILE:HD11	1:A:224:LEU:HD13	1.96	0.47
2:C:158:ASP:OD1	2:C:159:SER:N	2.47	0.47
2:C:1070:HIS:HD2	2:C:1230:MET:HE1	1.80	0.47
3:D:1342:ASP:OD1	3:D:1343:GLU:N	2.43	0.47
3:D:795:TYR:OH	3:D:1326:GLN:NE2	2.46	0.47
3:D:1040:MET:HB3	3:D:1046:ILE:HD13	1.96	0.47
1:A:60:GLU:HG2	1:A:170:ARG:HG3	1.96	0.47
1:A:66:HIS:CE1	1:A:69:SER:HB3	2.50	0.47
1:A:153:VAL:HB	1:A:175:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LEU:HB2	1:B:144:ILE:HD11	1.97	0.47
2:C:242:VAL:HB	2:C:245:ARG:HB2	1.97	0.47
2:C:720:ARG:NH2	2:C:749:ASP:OD1	2.47	0.47
2:C:798:GLN:HB2	2:C:828:PHE:HE1	1.79	0.47
3:D:1238:GLN:O	3:D:1242:ARG:HG2	2.15	0.47
2:C:160:ASP:HB3	2:C:163:LYS:HG3	1.96	0.47
2:C:264:GLU:HG2	2:C:265:LYS:H	1.79	0.47
2:C:388:LEU:HD22	2:C:389:PHE:HD1	1.79	0.47
3:D:246:PRO:HB2	3:D:249:LEU:HD23	1.97	0.47
3:D:47:ARG:HH11	5:N:11:DG:P	2.37	0.47
2:C:453:ILE:HD12	2:C:587:LEU:HD21	1.97	0.46
2:C:706:ARG:HE	2:C:793:GLU:HG2	1.80	0.46
2:C:706:ARG:NH2	2:C:793:GLU:OE2	2.45	0.46
2:C:1107:MET:HG2	3:D:740:LEU:HD11	1.96	0.46
2:C:189:ASP:OD2	2:C:193:ASN:HB2	2.16	0.46
2:C:976:ARG:O	2:C:980:VAL:HG23	2.16	0.46
2:C:1105:SER:HB3	3:D:731:ARG:HB3	1.97	0.46
2:C:582:ASN:HB3	2:C:586:PHE:H	1.80	0.46
2:C:487:LEU:HD12	2:C:491:ASP:HB2	1.97	0.46
2:C:1072:ASN:ND2	2:C:1111:GLN:OE1	2.49	0.46
2:C:560:PRO:O	3:D:780:ARG:NH2	2.47	0.46
3:D:308:ASP:OD1	3:D:309:ASN:N	2.43	0.46
2:C:255:ILE:HB	2:C:262:TYR:CD2	2.51	0.46
2:C:117:ILE:HD12	2:C:117:ILE:H	1.81	0.46
2:C:817:LEU:HD11	2:C:1080:ASN:ND2	2.31	0.46
3:D:973:LEU:O	3:D:1003:LEU:N	2.47	0.46
3:D:1037:PHE:CE2	3:D:1111:ASP:HB2	2.51	0.46
7:T:22:DC:H2"	7:T:23:DA:H8	1.80	0.46
2:C:1256:GLN:HG2	3:D:99:ARG:HH12	1.81	0.46
3:D:514:THR:HG21	3:D:596:LEU:HB2	1.98	0.46
3:D:850:LYS:N	3:D:855:ASP:O	2.49	0.46
3:D:886:VAL:HA	3:D:1258:ARG:HD2	1.97	0.46
3:D:1041:ILE:N	3:D:1045:THR:OG1	2.46	0.46
2:C:516:ASP:OD1	2:C:761:GLN:NE2	2.49	0.45
3:D:193:ASP:OD1	3:D:194:LEU:N	2.46	0.45
3:D:1163:VAL:HG23	3:D:1175:LEU:HD21	1.97	0.45
3:D:1273:ASP:OD1	3:D:1274:PHE:N	2.41	0.45
2:C:1165:SER:HB2	2:C:1168:GLU:HB2	1.98	0.45
3:D:1116:SER:N	3:D:1119:ASP:OD2	2.39	0.45
2:C:56:VAL:HG11	2:C:468:LEU:HB3	1.96	0.45
2:C:413:GLU:HG2	2:C:415:GLU:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1246:ARG:HH22	2:C:1258:PRO:HB3	1.80	0.45
3:D:253:VAL:HG21	6:R:20:G:C2	2.52	0.45
3:D:430:HIS:HA	3:D:921:GLN:HB3	1.99	0.45
3:D:700:ASN:O	3:D:704:GLU:HB2	2.15	0.45
3:D:1048:ARG:NE	3:D:1057:SER:OG	2.50	0.45
2:C:544:GLY:H	2:C:548:ARG:HE	1.63	0.45
3:D:979:ASN:ND2	3:D:1208:ASP:OD2	2.40	0.45
5:N:3:DG:H2''	5:N:4:DA:C8	2.52	0.45
2:C:577:VAL:HG23	2:C:662:SER:HA	1.99	0.45
3:D:686:TRP:CE3	3:D:758:PRO:HG3	2.51	0.45
3:D:1077:ALA:HB2	3:D:1100:PHE:HA	1.99	0.45
7:T:34:DC:H2''	7:T:35:DG:H5'	1.98	0.45
2:C:10:ARG:NH2	2:C:791:LEU:HB2	2.29	0.45
3:D:586:GLY:HA3	3:D:612:LEU:HD11	1.98	0.45
3:D:58:CYS:SG	3:D:59:ALA:N	2.90	0.45
3:D:1249:ASN:OD1	3:D:1250:ASP:N	2.49	0.45
5:N:29:DG:H2''	5:N:30:DA:H8	1.80	0.45
2:C:522:SER:HA	2:C:525:THR:HG22	1.98	0.45
3:D:825:VAL:HG23	3:D:832:LYS:HB2	1.99	0.44
1:B:91:ARG:NE	1:B:122:GLU:OE1	2.50	0.44
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.82	0.44
3:D:798:ARG:HH22	3:D:1325:PHE:HA	1.82	0.44
3:D:849:LEU:HD13	3:D:854:ALA:HA	1.99	0.44
6:R:20:G:O2'	6:R:21:A:OP1	2.35	0.44
7:T:19:DA:H2'	7:T:20:DC:H6	1.81	0.44
1:A:135:ASP:OD1	1:A:136:GLU:N	2.51	0.44
1:A:167:PRO:HG2	1:A:170:ARG:HD3	2.00	0.44
1:B:102:LEU:HB3	1:B:142:MET:SD	2.58	0.44
2:C:1333:LEU:HD21	3:D:115:TRP:CH2	2.53	0.44
3:D:18:ASP:OD2	3:D:1373:ARG:NH2	2.50	0.44
3:D:747:MET:HE2	3:D:775:SER:HA	1.99	0.44
5:N:35:DC:H2''	5:N:36:DA:C8	2.53	0.44
3:D:245:LEU:HD23	3:D:250:ARG:HB3	2.00	0.44
3:D:902:ASP:OD1	3:D:903:LEU:N	2.50	0.44
2:C:91:THR:HG22	2:C:138:ILE:HA	1.99	0.44
2:C:841:ARG:HA	2:C:1046:VAL:HA	1.99	0.44
5:N:30:DA:OP2	5:N:30:DA:H2'	2.17	0.44
2:C:959:ASP:OD1	2:C:960:LEU:N	2.50	0.44
3:D:342:LEU:HD23	3:D:1352:ILE:HD12	1.98	0.44
3:D:46:TYR:C	3:D:48:THR:H	2.25	0.44
1:A:30:PRO:HA	1:A:200:LYS:HA	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:60:GLN:HA	2:C:67:GLU:HG3	1.99	0.43
3:D:1295:ASN:OD1	3:D:1296:GLY:N	2.49	0.43
1:A:23:HIS:CE1	1:A:204:GLU:HB2	2.52	0.43
1:A:66:HIS:HD2	1:A:68:TYR:HB2	1.82	0.43
1:B:182:ARG:HH11	3:D:531:LYS:HE3	1.83	0.43
7:T:18:DC:H2'	7:T:19:DA:C8	2.51	0.43
2:C:447:HIS:CD2	2:C:553:THR:HG21	2.54	0.43
2:C:559:CYS:HB2	2:C:662:SER:HB3	2.00	0.43
1:B:27:THR:HG22	1:B:202:VAL:HG12	1.99	0.43
2:C:95:PRO:HB3	2:C:123:TYR:HE1	1.83	0.43
2:C:293:ALA:HA	2:C:317:LEU:HB2	2.00	0.43
3:D:520:ALA:HB3	3:D:546:ALA:HB2	2.01	0.43
1:B:133:LEU:HD12	1:B:134:THR:O	2.19	0.43
2:C:797:GLY:N	2:C:1231:TYR:OH	2.50	0.43
5:N:32:DA:H2'	5:N:33:DT:H71	2.00	0.43
2:C:1312:ASN:OD1	2:C:1313:HIS:N	2.52	0.43
1:A:45:ARG:NH2	1:B:37:HIS:HB2	2.31	0.43
2:C:1291:LEU:HB2	3:D:345:LYS:HD2	2.01	0.43
3:D:513:MET:HE1	3:D:579:LEU:HD13	2.00	0.43
1:B:30:PRO:HG3	1:B:190:ALA:HB1	2.01	0.43
1:B:195:ARG:HD2	1:B:198:LEU:HD11	2.01	0.43
2:C:99:LYS:HG2	2:C:121:GLU:H	1.84	0.43
2:C:264:GLU:OE1	2:C:267:ARG:NH2	2.51	0.43
3:D:91:GLU:OE2	3:D:101:ARG:NH2	2.49	0.43
3:D:907:HIS:ND1	3:D:908:ILE:O	2.51	0.43
5:N:33:DT:H2'	5:N:33:DT:OP2	2.19	0.43
7:T:34:DC:H2''	7:T:35:DG:C8	2.53	0.43
2:C:358:ASP:OD1	2:C:359:ARG:N	2.52	0.43
3:D:865:HIS:HE1	3:D:867:GLN:HB2	1.83	0.43
3:D:1221:LEU:HD12	3:D:1229:VAL:HG11	2.01	0.43
3:D:47:ARG:NH1	5:N:11:DG:O5'	2.52	0.42
3:D:255:LEU:HB2	3:D:259:ARG:HG3	2.00	0.42
3:D:958:ILE:HG23	3:D:982:LEU:HD21	2.01	0.42
3:D:1167:LYS:HZ2	3:D:1170:LYS:HB2	1.84	0.42
1:B:113:ALA:HA	1:B:117:HIS:NE2	2.34	0.42
3:D:326:SER:H	3:D:329:ASP:HB2	1.85	0.42
3:D:502:PRO:HG3	3:D:601:ILE:HD13	2.01	0.42
2:C:996:ARG:HD3	2:C:999:GLU:HB2	2.01	0.42
2:C:1268:GLN:NE2	3:D:352:ARG:HD2	2.34	0.42
2:C:10:ARG:NH2	2:C:790:ASP:O	2.53	0.42
2:C:1030:GLU:OE2	2:C:1033:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1225:VAL:HG13	3:D:638:SER:HB2	2.01	0.42
3:D:1194:ARG:NH1	3:D:1212:ASP:O	2.47	0.42
7:T:6:DA:H2"	7:T:7:DA:H8	1.83	0.42
2:C:69:GLN:HE22	2:C:103:VAL:HG13	1.84	0.42
2:C:269:ILE:HG23	2:C:273:HIS:HB2	2.02	0.42
2:C:805:MET:HE1	2:C:1221:PHE:CZ	2.54	0.42
2:C:934:PHE:HB2	2:C:1049:ILE:HB	2.00	0.42
2:C:57:PHE:HB3	2:C:58:PRO:HD3	2.01	0.42
3:D:418:GLU:H	4:E:45:LYS:NZ	2.17	0.42
3:D:526:VAL:HG12	3:D:549:LYS:HB2	2.01	0.42
1:B:12:ARG:HB3	1:B:29:GLU:CB	2.50	0.42
2:C:230:PHE:CE1	2:C:239:MET:HB3	2.55	0.42
2:C:1304:MET:HE3	2:C:1308:ILE:HD11	2.01	0.42
3:D:591:ILE:HD11	3:D:604:MET:HA	2.01	0.42
1:A:225:ALA:O	1:A:229:GLU:HG2	2.20	0.42
1:B:12:ARG:HG2	1:B:13:LEU:HD23	2.01	0.42
2:C:387:ASN:HD21	2:C:394:ARG:NH1	2.18	0.42
3:D:370:LYS:HE2	3:D:443:GLU:HA	2.02	0.42
1:A:165:GLU:C	1:A:166:ARG:HD3	2.45	0.42
1:A:167:PRO:CG	1:A:170:ARG:HD3	2.50	0.42
1:B:73:GLY:O	1:B:134:THR:N	2.53	0.42
3:D:573:THR:HB	3:D:576:ARG:HG3	2.02	0.42
3:D:859:PRO:HG2	3:D:862:THR:HG23	2.02	0.42
1:B:33:ARG:NH2	2:C:1081:PRO:HG3	2.35	0.41
2:C:1288:GLN:O	2:C:1292:THR:CB	2.65	0.41
2:C:59:ILE:HG22	2:C:60:GLN:N	2.34	0.41
2:C:106:GLU:HB3	2:C:109:ALA:HB3	2.02	0.41
3:D:332:LYS:HD2	3:D:1329:THR:OG1	2.20	0.41
3:D:378:LYS:NZ	3:D:382:TYR:OH	2.41	0.41
3:D:1019:ASN:OD1	3:D:1020:TRP:N	2.52	0.41
3:D:1309:ILE:HG13	3:D:1310:THR:N	2.35	0.41
2:C:128:PRO:HG2	2:C:506:PHE:HD2	1.85	0.41
3:D:123:ARG:HH11	3:D:223:LEU:HD13	1.84	0.41
7:T:19:DA:H2'	7:T:20:DC:C6	2.55	0.41
3:D:584:PRO:HD3	3:D:620:PHE:CD1	2.55	0.41
3:D:1184:ASP:O	3:D:1186:TYR:N	2.53	0.41
7:T:11:DC:H2"	7:T:12:DT:OP2	2.21	0.41
2:C:764:CYS:SG	2:C:765:ILE:N	2.93	0.41
3:D:1026:PRO:HA	3:D:1123:ARG:HA	2.03	0.41
2:C:171:LEU:HB2	2:C:188:PHE:HB2	2.03	0.41
2:C:840:SER:HB3	2:C:1048:LYS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:971:LEU:HD23	2:C:974:ARG:HD2	2.03	0.41
3:D:1265:THR:HG23	3:D:1305:ASP:OD2	2.20	0.41
3:D:1348:LYS:O	3:D:1352:ILE:HG12	2.19	0.41
7:T:26:DG:H1'	7:T:27:DG:C5	2.56	0.41
2:C:74:ARG:NH2	2:C:97:ARG:HD2	2.36	0.41
2:C:956:ALA:O	2:C:960:LEU:HD13	2.21	0.41
3:D:979:ASN:HD21	3:D:1208:ASP:CG	2.28	0.41
2:C:84:GLU:O	2:C:88:ARG:HG2	2.21	0.41
2:C:222:ASP:OD2	2:C:227:LYS:NZ	2.54	0.41
2:C:256:GLU:CD	2:C:285:ILE:H	2.29	0.41
2:C:300:ASP:OD1	2:C:313:ALA:N	2.54	0.41
2:C:932:GLN:HB2	2:C:1051:LYS:HB2	2.02	0.41
2:C:1103:VAL:HB	2:C:1104:PRO:HD3	2.03	0.41
3:D:405:GLU:O	3:D:408:VAL:HG22	2.21	0.41
3:D:430:HIS:CD2	3:D:432:LEU:H	2.38	0.41
3:D:820:ILE:HB	3:D:822:MET:HE2	2.01	0.41
3:D:832:LYS:HB3	3:D:1242:ARG:HH12	1.86	0.41
3:D:846:GLU:HA	3:D:860:ARG:HG2	2.02	0.41
7:T:11:DC:C2'	7:T:12:DT:H71	2.51	0.41
7:T:14:DC:H6	7:T:14:DC:H2'	1.68	0.41
1:A:35:PHE:HE1	1:B:46:ILE:HD13	1.86	0.41
3:D:93:THR:HG22	3:D:94:GLN:N	2.32	0.41
3:D:814:CYS:SG	3:D:816:THR:HG22	2.61	0.41
3:D:1082:ASP:OD1	3:D:1086:ASN:N	2.48	0.41
6:R:22:U:H2'	6:R:23:G:H8	1.86	0.41
7:T:23:DA:H2'	7:T:24:DT:H71	2.03	0.41
2:C:165:HIS:NE2	2:C:190:PRO:HG3	2.36	0.40
2:C:993:PRO:HB2	2:C:995:ASP:OD1	2.21	0.40
1:A:6:THR:OG1	1:A:7:GLU:N	2.53	0.40
1:A:45:ARG:HH12	1:B:37:HIS:HB2	1.87	0.40
2:C:101:ARG:HD3	2:C:118:LYS:HE2	2.03	0.40
2:C:177:ILE:HG12	2:C:183:TRP:HD1	1.83	0.40
2:C:518:ASN:O	2:C:691:PRO:HD3	2.22	0.40
3:D:378:LYS:HB3	3:D:378:LYS:HZ2	1.86	0.40
3:D:412:LEU:HA	3:D:415:VAL:HG22	2.02	0.40
2:C:551:HIS:H	2:C:554:HIS:CE1	2.39	0.40
3:D:475:GLU:OE2	4:E:28:ARG:NH2	2.39	0.40
3:D:1358:PRO:HB3	3:D:1366:HIS:CG	2.56	0.40
2:C:838:CYS:N	2:C:1050:VAL:O	2.54	0.40
5:N:12:DA:H2''	5:N:13:DC:C5	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	227/329 (69%)	204 (90%)	23 (10%)	0	100	100
1	B	213/329 (65%)	192 (90%)	21 (10%)	0	100	100
2	C	1310/1342 (98%)	1221 (93%)	87 (7%)	2 (0%)	43	76
3	D	1328/1407 (94%)	1264 (95%)	64 (5%)	0	100	100
4	E	88/91 (97%)	84 (96%)	4 (4%)	0	100	100
All	All	3166/3498 (90%)	2965 (94%)	199 (6%)	2 (0%)	49	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	58	PRO
2	C	57	PHE

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	194/286 (68%)	193 (100%)	1 (0%)	81	82
1	B	183/286 (64%)	183 (100%)	0	100	100
2	C	1132/1157 (98%)	1132 (100%)	0	100	100
3	D	1114/1168 (95%)	1114 (100%)	0	100	100
4	E	74/75 (99%)	74 (100%)	0	100	100
All	All	2697/2972 (91%)	2696 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	103	ASN
1	B	66	HIS
2	C	65	ASN
2	C	69	GLN
2	C	387	ASN
2	C	513	GLN
2	C	551	HIS
2	C	604	HIS
2	C	628	HIS
2	C	658	GLN
2	C	659	GLN
2	C	688	GLN
2	C	725	GLN
2	C	808	ASN
2	C	832	HIS
2	C	1136	GLN
2	C	1146	GLN
2	C	1257	GLN
2	C	1268	GLN
2	C	1288	GLN
3	D	113	HIS
3	D	186	GLN
3	D	232	ASN
3	D	274	ASN
3	D	341	ASN
3	D	365	GLN
3	D	424	ASN
3	D	469	HIS
3	D	477	GLN
3	D	488	ASN
3	D	805	GLN
3	D	1326	GLN
4	E	31	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	R	10/10 (100%)	3 (30%)	1 (10%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	R	21	A
6	R	25	G
6	R	29	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	R	20	G

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	15:DG	O3'	24:DC	P	28.77

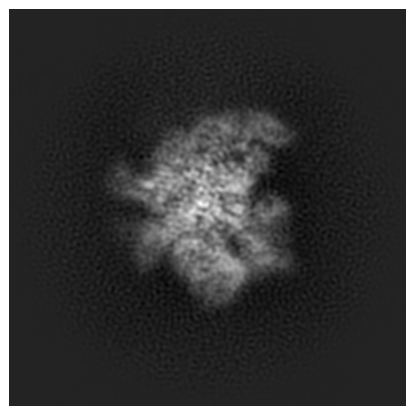
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4274. These allow visual inspection of the internal detail of the map and identification of artifacts.

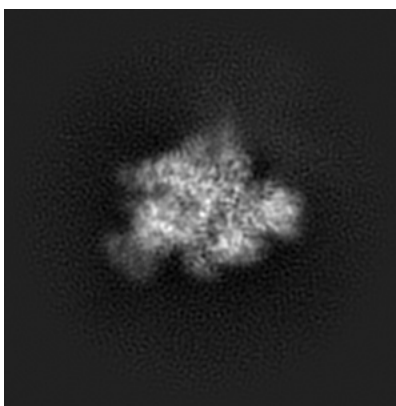
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

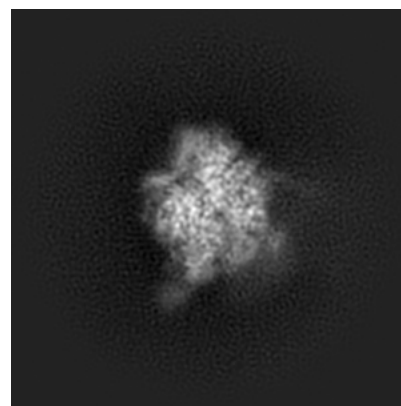
6.1.1 Primary map



X

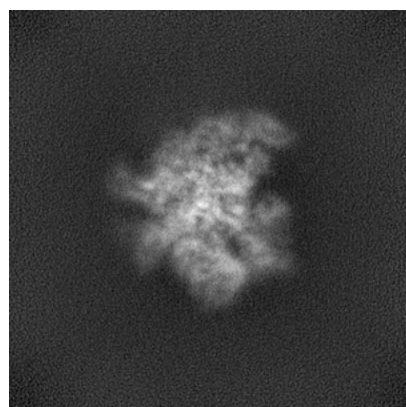


Y

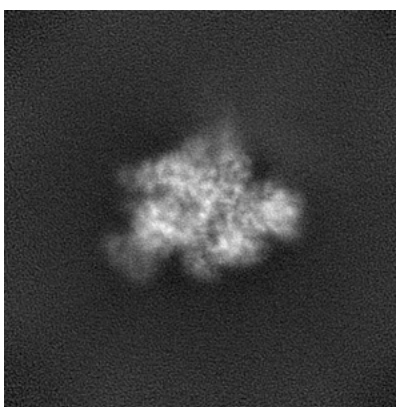


Z

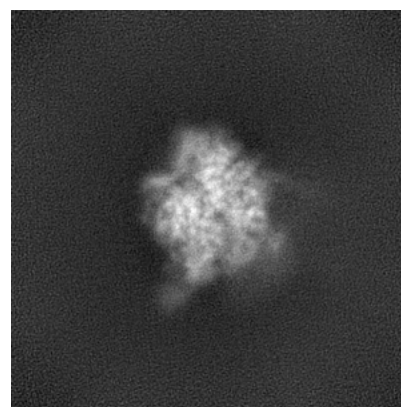
6.1.2 Raw map



X



Y

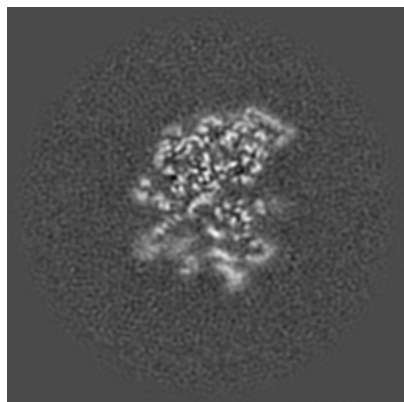


Z

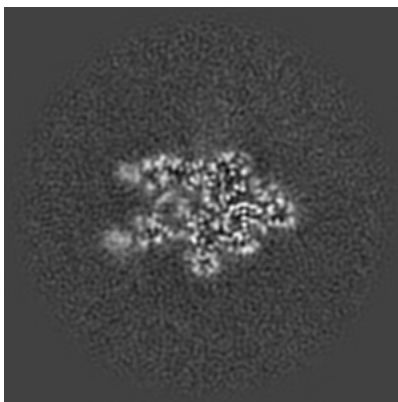
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

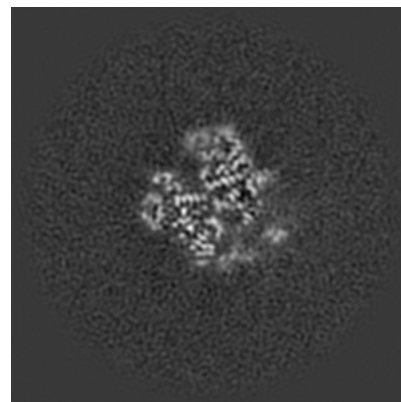
6.2.1 Primary map



X Index: 140

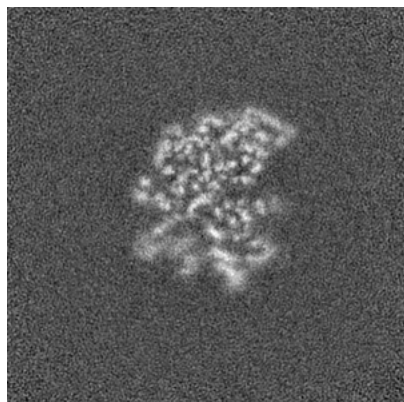


Y Index: 140

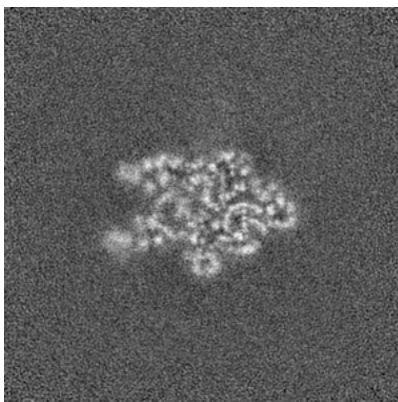


Z Index: 140

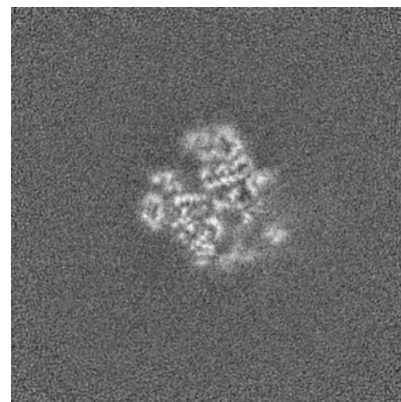
6.2.2 Raw map



X Index: 140



Y Index: 140

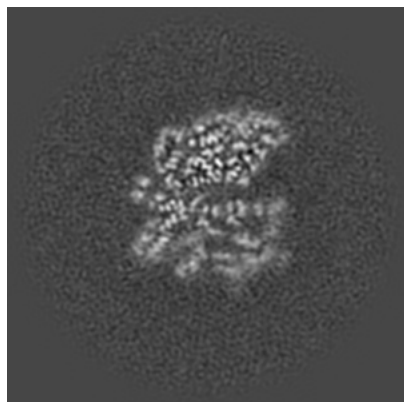


Z Index: 140

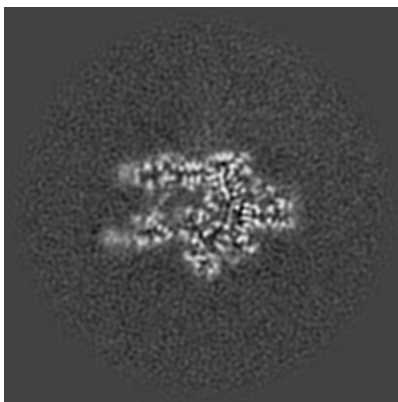
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

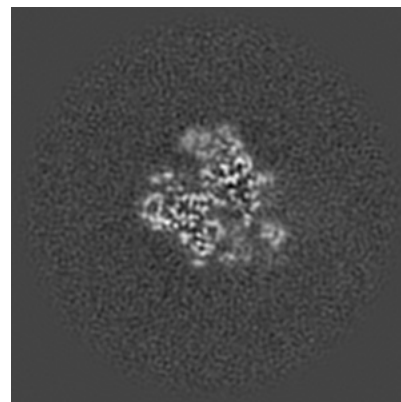
6.3.1 Primary map



X Index: 136

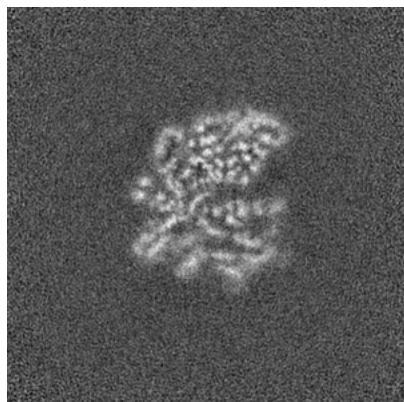


Y Index: 138

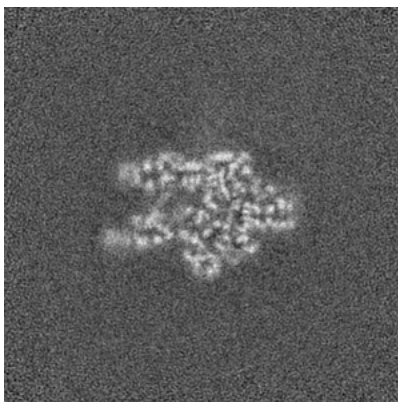


Z Index: 138

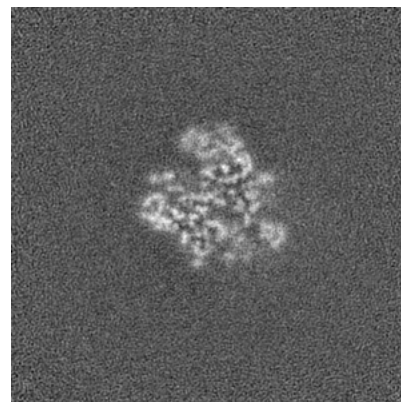
6.3.2 Raw map



X Index: 137



Y Index: 138

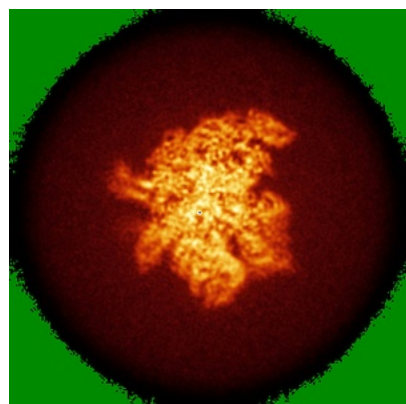


Z Index: 137

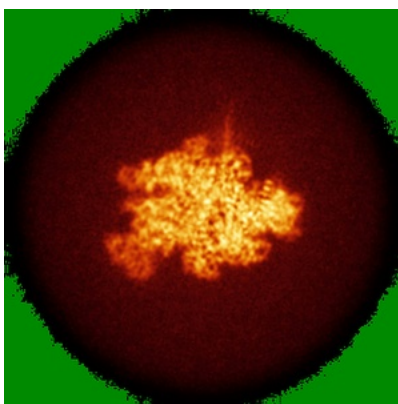
The images above show the largest variance slices of the map in three orthogonal directions.

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

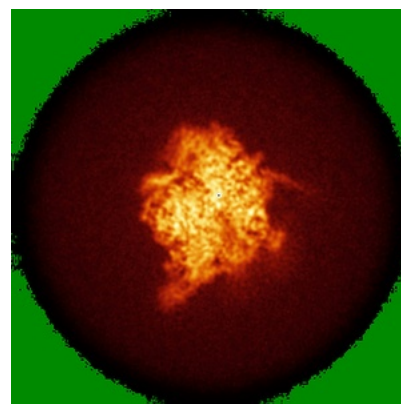
6.4.1 Primary map



X

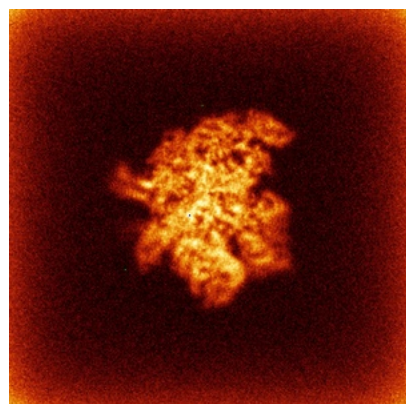


Y

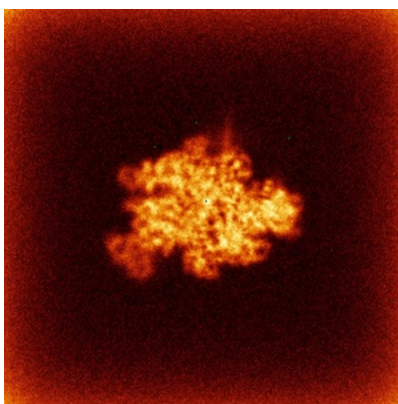


Z

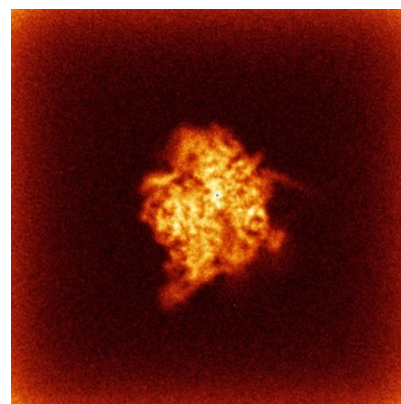
6.4.2 Raw map



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.

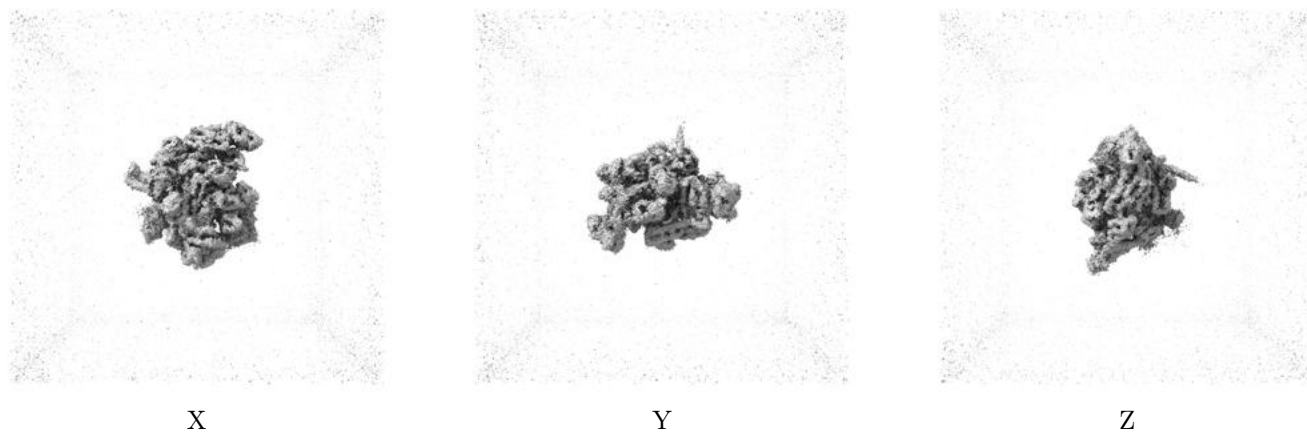
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.27. 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



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

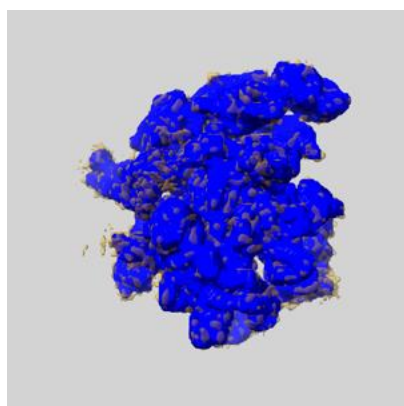
6.6 Mask visualisation [i](#)

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

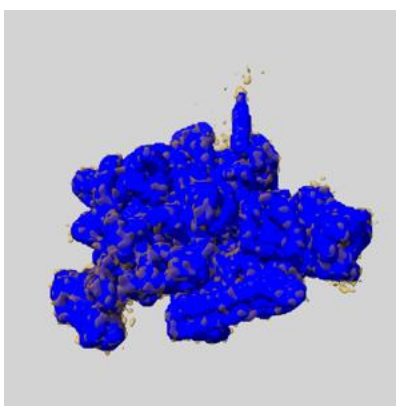
A mask typically either:

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

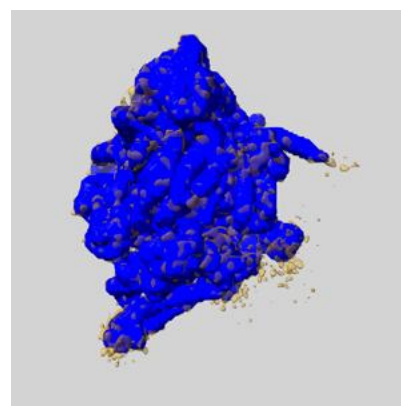
6.6.1 emd_4274_msk_1.map [i](#)



X



Y

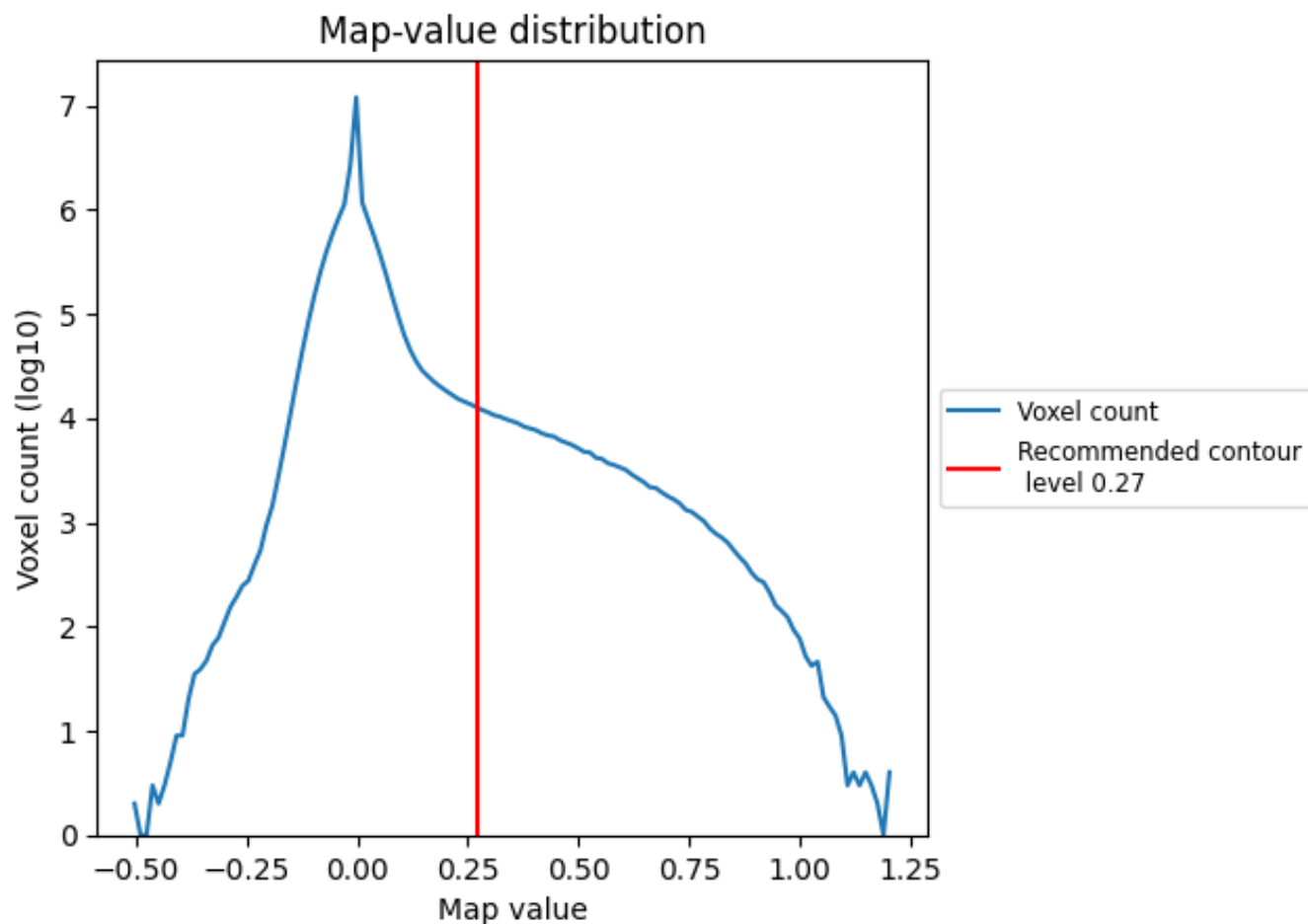


Z

7 Map analysis [i](#)

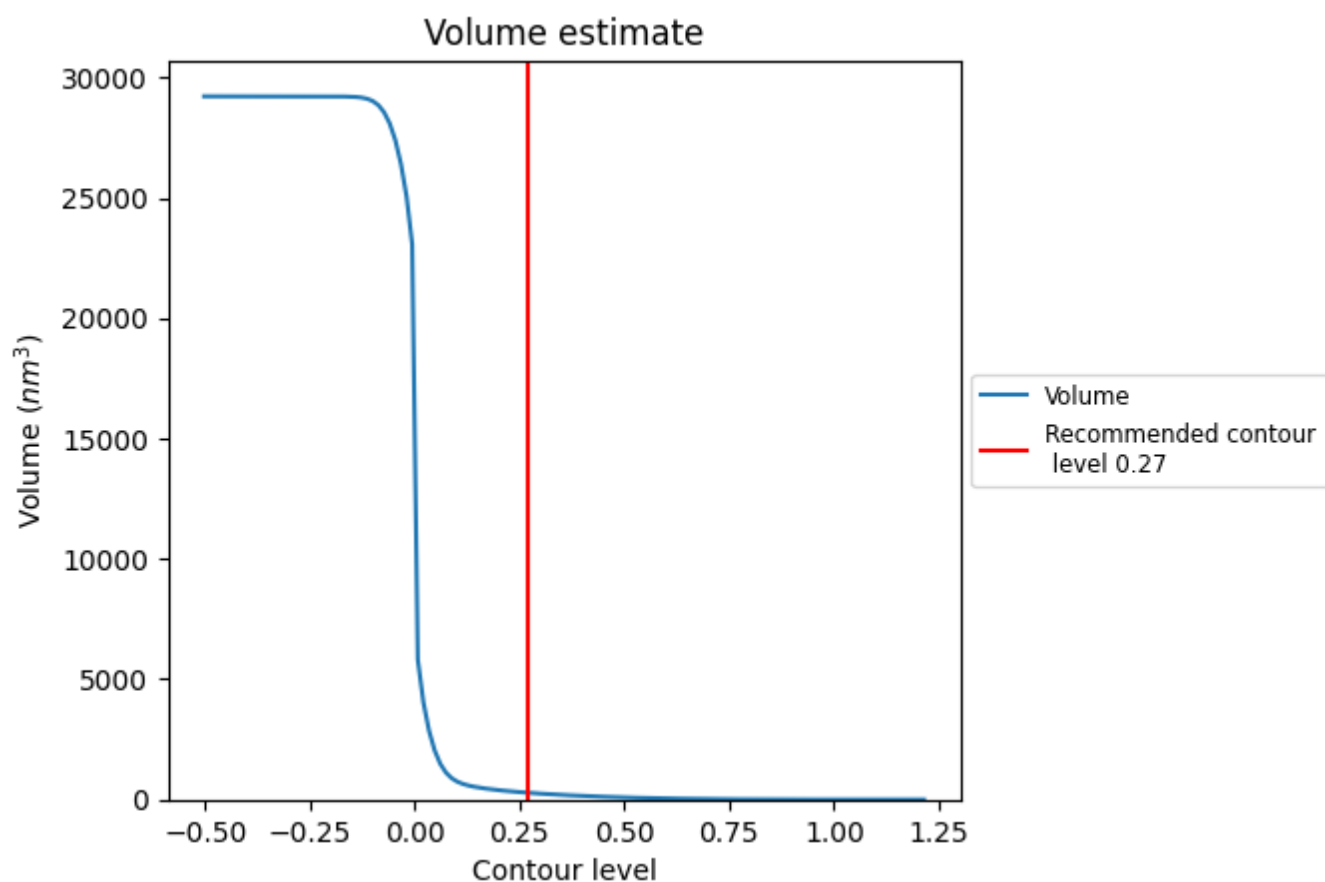
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

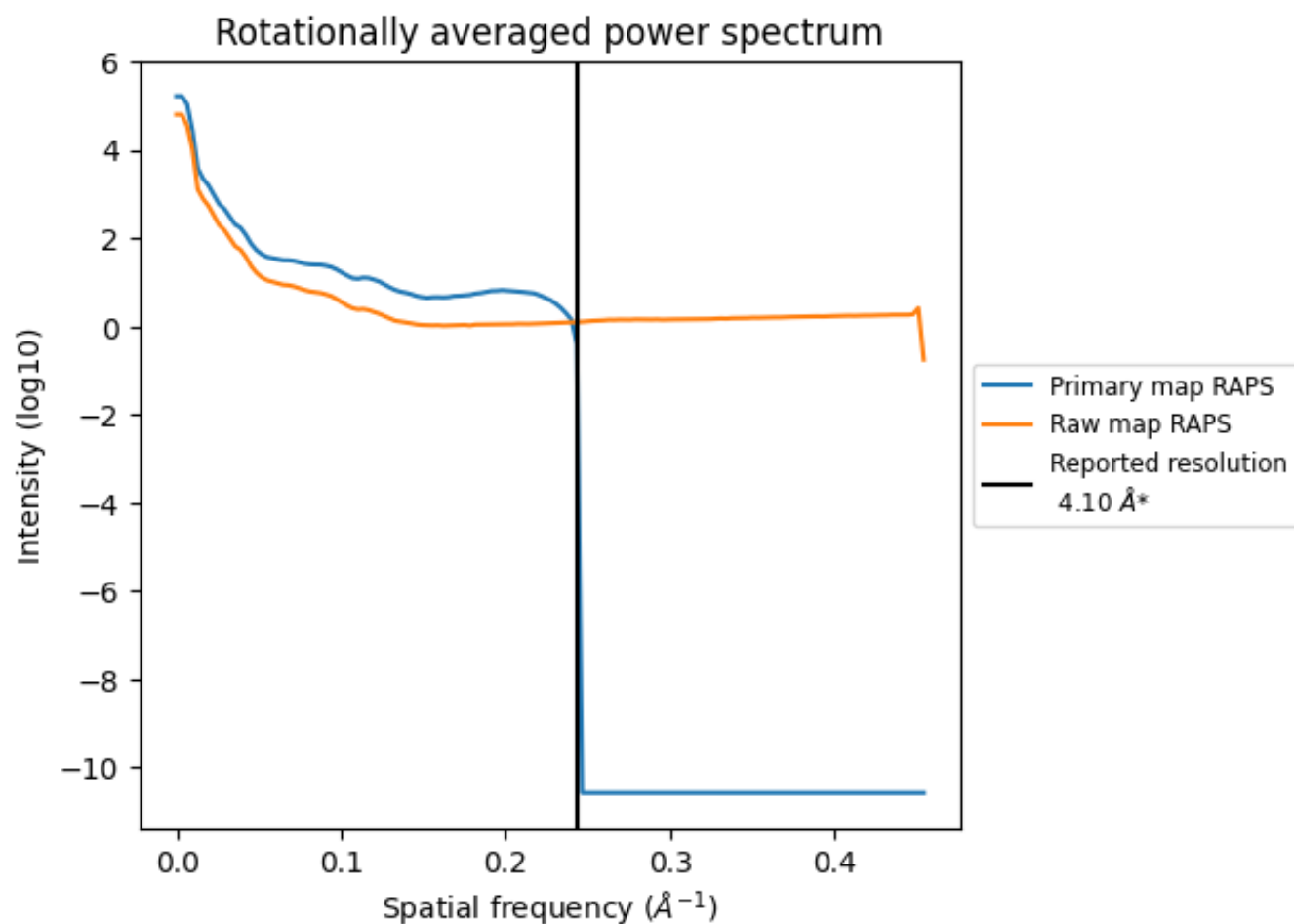
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 283 nm³; this corresponds to an approximate mass of 256 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 ⓘ

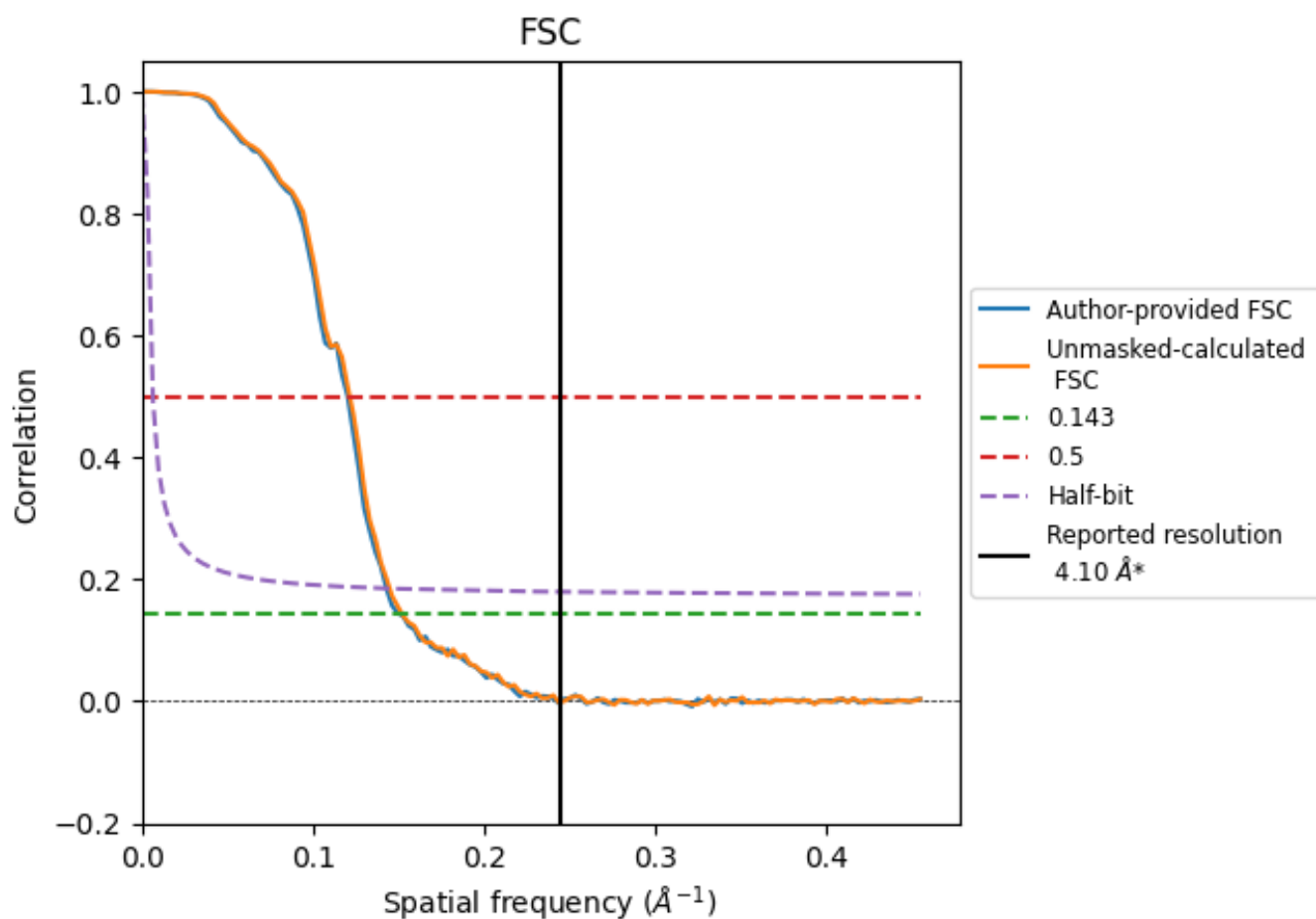


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	6.65	8.32	7.00
Unmasked-calculated*	6.58	8.24	6.91

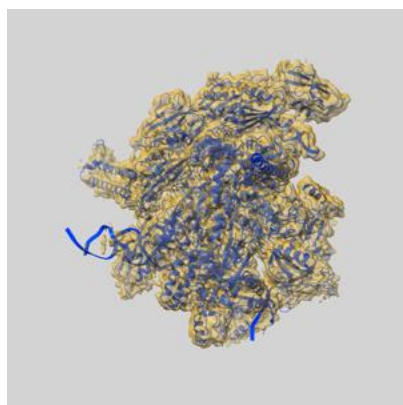
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 6.65 differs from the reported value 4.1 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.58 differs from the reported value 4.1 by more than 10 %

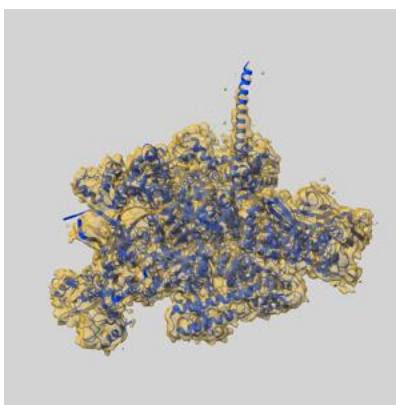
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4274 and PDB model 6FLP. Per-residue inclusion information can be found in section [3](#) on page [6](#).

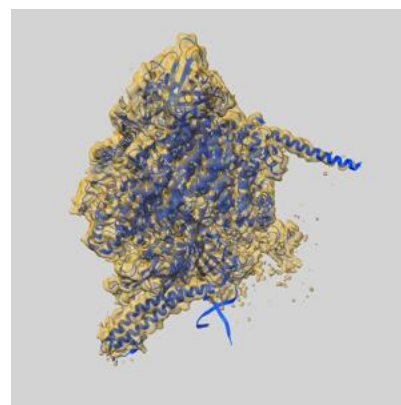
9.1 Map-model overlay [i](#)



X



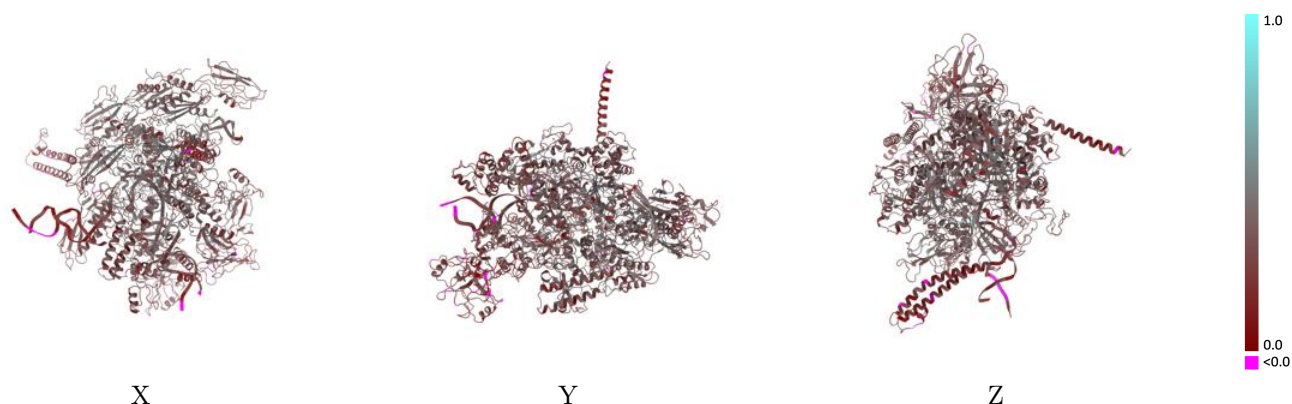
Y



Z

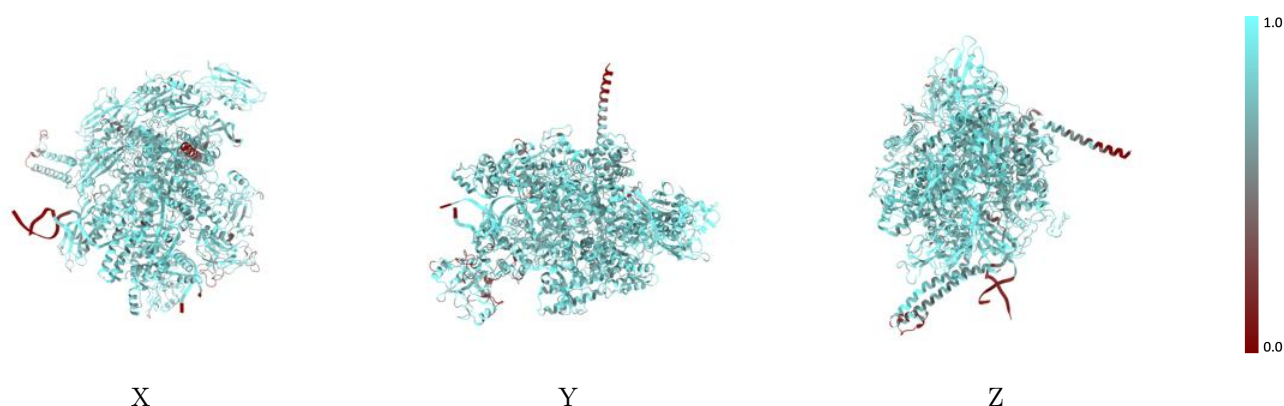
The images above show the 3D surface view of the map at the recommended contour level 0.27 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



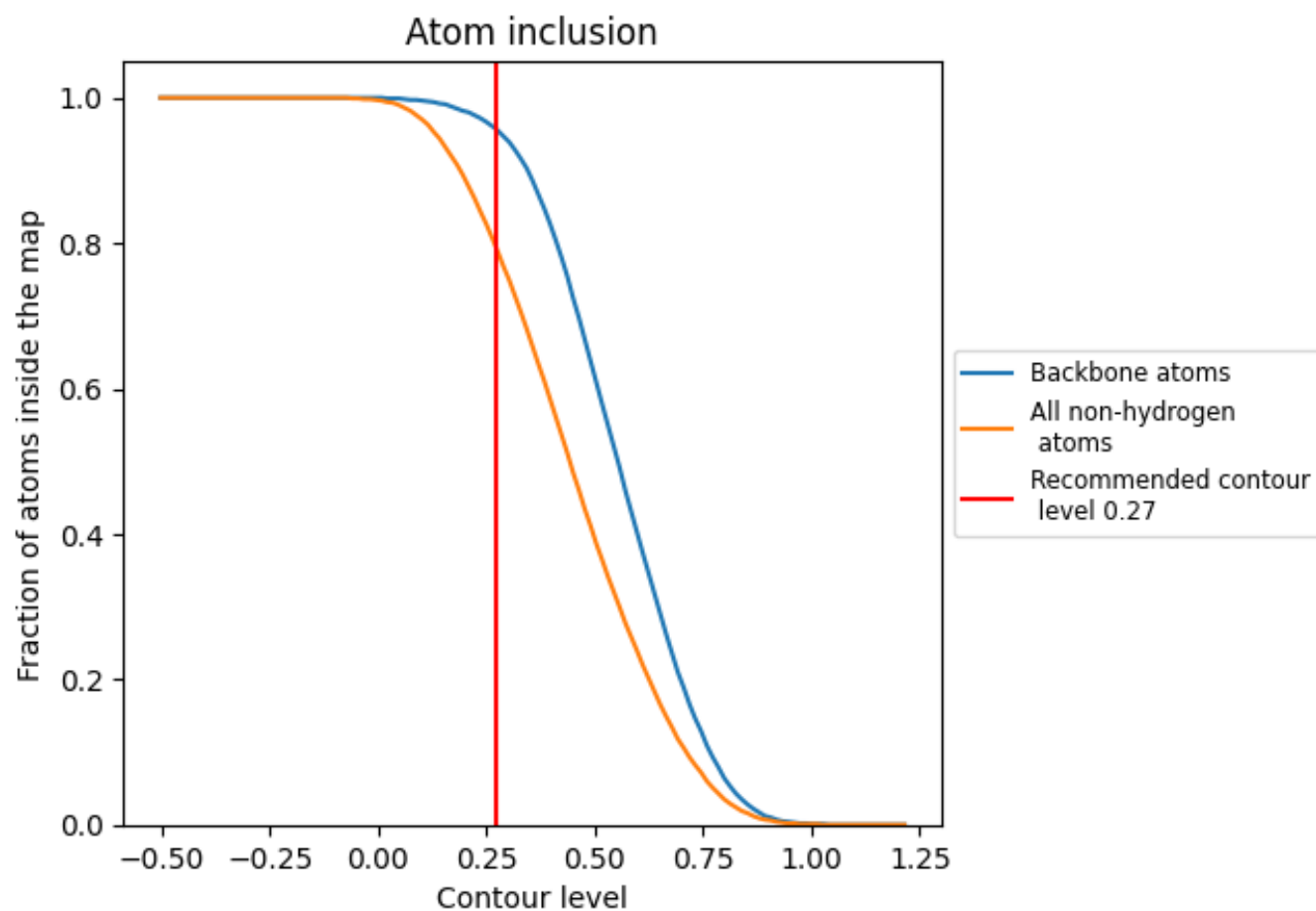
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.27).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 80% 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 (0.27) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7970	0.3340
A	0.8200	0.3650
B	0.8430	0.3380
C	0.8090	0.3460
D	0.7960	0.3330
E	0.6200	0.2870
N	0.6440	0.2000
R	0.9110	0.3350
T	0.7490	0.2650

1.0

0.0

<0.0