



Full wwPDB EM Validation Report ⓘ

Jul 14, 2026 – 04:05 AM JST

PDB ID : 9W8R / pdb_00009w8r
EMDB ID : EMD-65749
Title : Structure of yeast Pol II in complex with a short control scaffold lacking cisplatin-ICL lesion.
Authors : Xu, J.; Zhu, L.
Deposited on : 2025-08-08
Resolution : 2.68 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
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) : 2.50

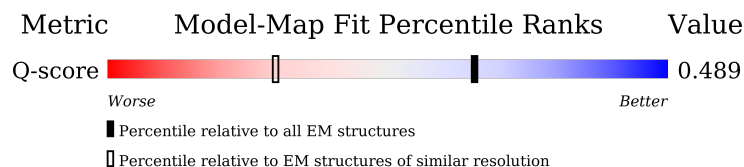
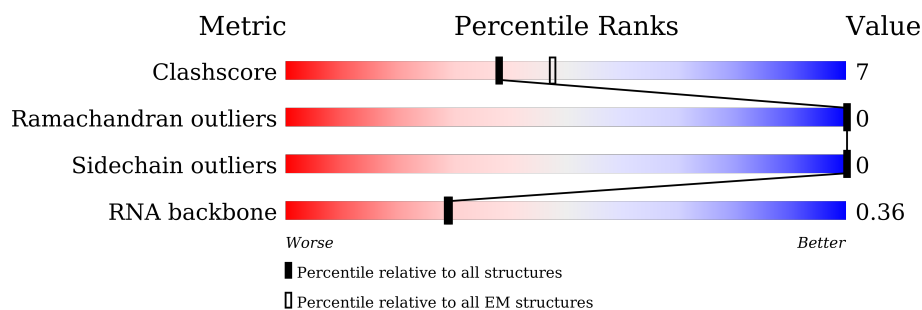
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.68 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	9255 (2.18 - 3.18)

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	C	318	
2	E	215	
3	F	155	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	G	171	
5	I	122	
6	J	70	
7	K	120	
8	L	70	
9	N	10	
10	P	15	
11	T	20	
12	A	1733	
13	B	1224	
14	D	221	
15	H	146	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32477 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 2 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 3 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 9 is a DNA chain called DNA (NTS, non-template strand).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	10	Total	C	N	O	P	0	0
			214	99	48	57	10		

- Molecule 10 is a RNA chain called RNA (5'-R(*UP*AP*UP*UP*AP*UP*GP*AP*GP*GP*GP*GP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	9	Total	C	N	O	P	0	0
			203	90	45	59	9		

- Molecule 11 is a DNA chain called DNA (TS, template strand).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	T	20	Total	C	N	O	P	0	0
			390	188	55	127	20		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	1418	Total	C	N	O	S	0	0
			11153	7029	1947	2115	62		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	1176	Total	C	N	O	S	0	0
			9378	5929	1638	1756	55		

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	166	Total	C	N	O	S	0	0
			1332	823	238	269	2		

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	140	Total	C	N	O	S	0	0
			1120	704	188	224	4		

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

Mol	Chain	Residues	Atoms		AltConf
16	C	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	
16	A	2	Total	Zn	0
			2	2	
16	B	1	Total	Zn	0
			1	1	

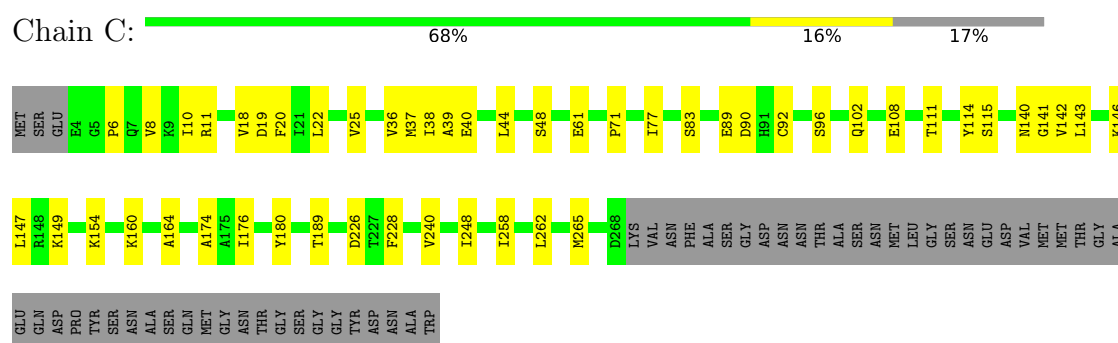
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

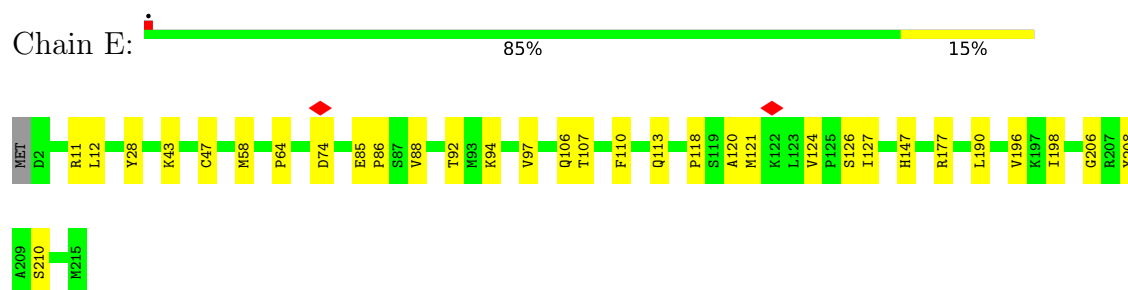
3 Residue-property plots [i](#)

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

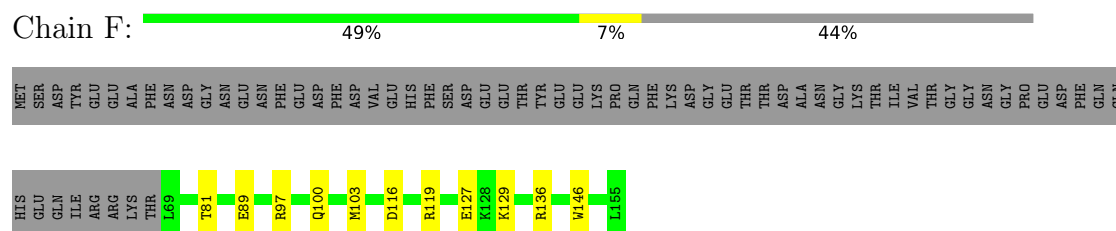
- Molecule 1: DNA-directed RNA polymerase II subunit RPB3



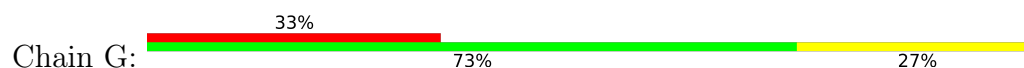
- Molecule 2: DNA-directed RNA polymerases I, II, and III subunit RPABC1

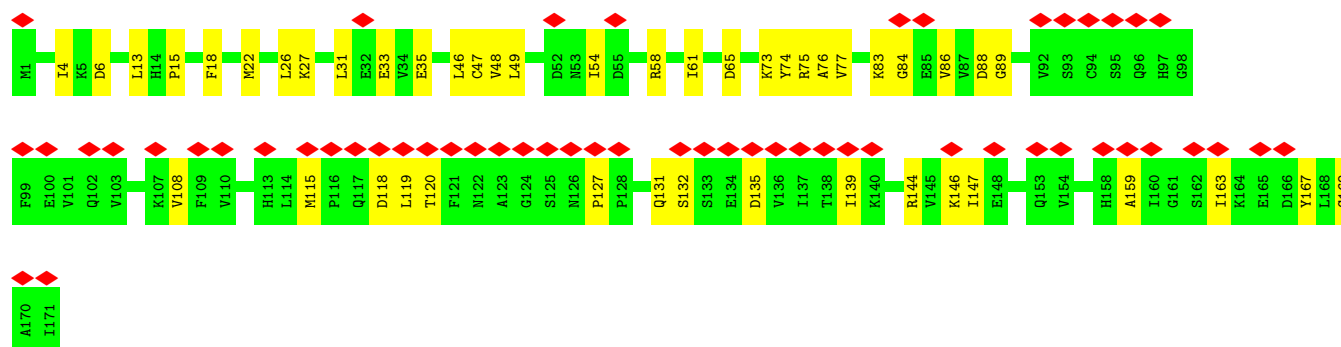


- Molecule 3: DNA-directed RNA polymerases I, II, and III subunit RPABC2



- Molecule 4: DNA-directed RNA polymerase II subunit RPB7

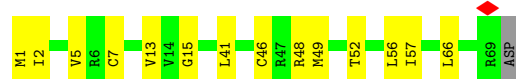
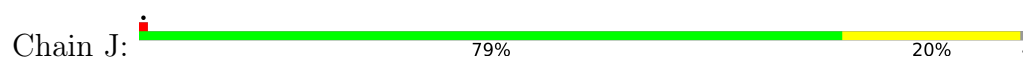




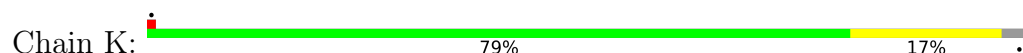
- Molecule 5: DNA-directed RNA polymerase II subunit RPB9



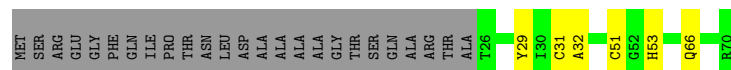
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC5



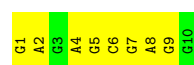
- Molecule 7: DNA-directed RNA polymerase II subunit RPB11



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 9: DNA (NTS, non-template strand)



- Molecule 10: RNA (5'-R(*UP*AP*UP*UP*AP*UP*GP*AP*GP*GP*GP*GP*AP*AP*A)-3')

Chain P: 13% 47% 40%

U A U U A U G7 A8 G9 G10 G11 G12 A13 A14 A15

- Molecule 11: DNA (TS, template strand)

Chain T: 5% 95%

C9 C10 T11 C12 G13 C14 T15 T16 T17 C18 C19 G11 T20 T21 T22 C23 C24 C25 C26 T27 C28

- Molecule 12: DNA-directed RNA polymerase II subunit RPB1

Chain A: 66% 16% 18%

MET V2 K15 E16 E43 R63 R64 E72 G73 M74 E76 C105 V106 C107 M108 H109 C110 L114 L115 D116 E120 R123 D130 W139 K145 M146 V147 C148 E149 E155 D156 D157 P158 T159 Q160 R164 C167 Q171 P172 V185 D188 ARG

ALA THR GLY ASP ALA ASP GLU P197 I207 I210 I214 S215 M75 E76 F219 P243 P244 P245 S249 ILE SER PHE ASN GLU SER ARG G268 K265 T302 R326 L329 R335 I336 R337 G338 N339 K343 D346 A349 G355 L359 D362

L374 R387 L388 T389 V392 R393 P396 A402 T406 R412 R415 R420 A421 G422 K431 R434 M437 D438 N439 L443 R446 Q447 H451 K452 M453 S454 R459 R469 L470 N471 L472 S473 V474 F482 D483 M487 H490 E500 A506

V507 P508 L509 K510 I511 V512 S513 P514 Q515 P519 L528 I531 R532 K533 L534 L547 N548 M549 D555 V556 D557 T562 P563 P568 W572 S573 G574 K575 Q576 S579 I582 H587 L588 Q589 R590 T595 T596 L597 N603 L606 I607 I608 Q611 I612 I613

F614 E618 K619 L620 K621 T622 V633 T634 K644 L645 Q650 W656 K657 I670 K687 V693 N700 G707 R711 E715 F721 R726 K744 M748 A749 G750 S751 K752 G766 Q767 Q768 R774 E795 Y804 H816 A832 G835

R840 I848 I867 H873 D874 A875 I878 Q881 D884 T885 R896 W899 D900 N903 T904 D905 L908 D909 L912 E918 D922 L923 L929 P939 L956 P957 V958 Q969 H975 L981 T982 I983 L993 L997 G1002 I1007

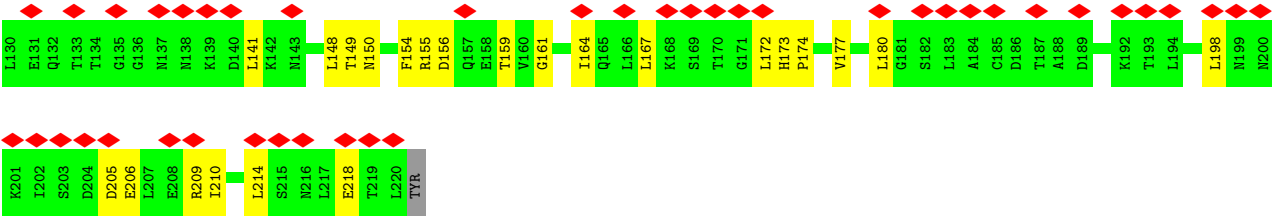
Q1008 N1009 A1010 Q1011 R1012 L1017 F1018 L1021 L1022 R1023 S1024 R1029 R1030 Y1035 R1036 F1042 L1046 G1065 I1072 G1073 E1074 M1079 THR LEU ASN THR PHE HIS PHE ALA GLY VAL ALA SER LYS K1093 V1094 T1095 M1106 M1111 K1112 P1113 P1114 S1115 L1116 L1120 A1131

T1147 T1161 E1165 D1166 E1167 I1170 L1176 L1177 ASP GLU GLU ALA ALA GLN S1184 F1185 D1186 Q1187 R1194 E1196 L1197 D1198 A1201 M1209 R1215 F1220 L1224 L1236 C1240 R1244 P1245 K1246 S1247 L1248 D1249 A1250 E1251 T1252 E1253 A1254 E1255 K1262 M1265

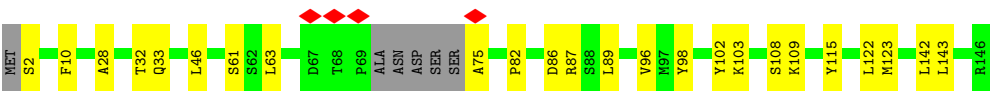
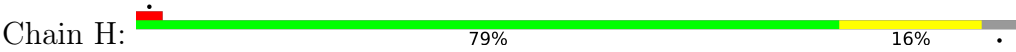
T1266 E1269 N1270 I1271 T1272 T1279 E1280 R1281 K1286 D1288 S1293 E1297 K1300 E1301 P1302 T1308 V1311 T1318 L1327 Y1328 T1329 N1330 S1331 V1363 R1366 L1370 L1371 Q1378 R1386 S1392 L1397 M1398 R1399 T1405 V1406 E1417 E1420 C1421 R1422

E1426 M1427 V1428 F1441 D1442 V1443 M1444 T1445 D1446 M1454 PRO GLU GLN LYS ILE THR GLU ILE ASP GLY GLN ASP GLY VAL THR PRO TYR SER ASN GLY GLY LEU VAL ASN ALA ASP LEU ASP VAL LYS ASP GLU LEU MET PHE SER PRO LEU VAL ASP SER GLY ASN





- Molecule 15: DNA-directed RNA polymerases I, II, and III subunit RPABC3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	116276	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.716	Depositor
Minimum map value	-0.288	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	297.6, 297.6, 297.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	C	0.13	0/2124	0.28	0/2879
2	E	0.10	0/1788	0.28	0/2406
3	F	0.13	0/717	0.29	0/967
4	G	0.11	0/1367	0.31	0/1844
5	I	0.09	0/962	0.29	0/1295
6	J	0.11	0/578	0.27	0/775
7	K	0.10	0/942	0.22	0/1272
8	L	0.12	0/361	0.32	0/478
9	N	0.56	0/242	0.81	0/373
10	P	0.59	0/229	0.67	0/357
11	T	0.33	0/430	0.67	0/657
12	A	0.12	0/11352	0.28	0/15350
13	B	0.12	0/9563	0.28	0/12900
14	D	0.12	0/1340	0.33	0/1797
15	H	0.10	0/1139	0.24	0/1544
All	All	0.14	0/33134	0.30	0/44894

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2086	0	2045	36	0
2	E	1752	0	1776	20	0
3	F	705	0	731	7	0
4	G	1339	0	1357	35	0
5	I	944	0	899	15	0
6	J	569	0	585	11	0
7	K	924	0	934	18	0
8	L	359	0	381	5	0
9	N	214	0	111	9	0
10	P	203	0	99	4	0
11	T	390	0	228	40	0
12	A	11153	0	11228	183	0
13	B	9378	0	9366	104	0
14	D	1332	0	1353	35	0
15	H	1120	0	1086	15	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	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	P	1	0	0	0	0
All	All	32477	0	32179	470	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 7.

All (470) 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)
13:B:763:GLN:HG2	13:B:765:PRO:HD2	1.54	0.87
12:A:469:ARG:NH2	13:B:991:GLY:O	2.12	0.83
9:N:7:DG:H2'	9:N:8:DA:C8	2.13	0.82
14:D:119:ARG:HE	14:D:155:ARG:HH22	1.29	0.80
11:T:16:DC:H2'	11:T:17:DT:C6	2.19	0.78
5:I:78:CYS:SG	5:I:106:CYS:HB3	2.26	0.75
2:E:106:GLN:HG2	2:E:107:THR:HG23	1.68	0.74
10:P:7:G:H2'	10:P:8:A:C8	2.23	0.74
11:T:19:DC:H2'	11:T:20:DT:C6	2.22	0.73
13:B:837:ASP:OD1	13:B:1020:ARG:NH2	2.21	0.73
11:T:23:DC:H2'	11:T:24:DC:C6	2.24	0.73
10:P:7:G:H2'	10:P:8:A:H8	1.53	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:728:ARG:NH1	13:B:760:ASP:OD2	2.23	0.71
11:T:14:DC:H2'	11:T:15:DT:C6	2.25	0.71
9:N:8:DA:H2''	9:N:9:DG:H5'	1.74	0.69
12:A:107:CYS:SG	12:A:171:GLN:NE2	2.66	0.68
11:T:20:DT:H2'	11:T:21:DT:C6	2.28	0.68
1:C:39:ALA:HA	1:C:164:ALA:HB3	1.76	0.68
5:I:87:GLN:OE1	12:A:711:ARG:NH2	2.27	0.68
13:B:928:ARG:NH1	13:B:929:THR:O	2.26	0.68
11:T:17:DT:H2'	11:T:18:DC:C6	2.29	0.67
12:A:840:ARG:NH1	12:A:1106:ASN:OD1	2.27	0.67
13:B:287:ARG:NH2	13:B:294:ASP:OD1	2.28	0.67
2:E:177:ARG:NH1	12:A:1378:GLN:OE1	2.28	0.66
11:T:24:DC:H2'	11:T:25:DC:C6	2.31	0.66
12:A:909:ASP:HB3	12:A:912:LEU:HG	1.78	0.66
12:A:355:GLY:O	12:A:469:ARG:NH1	2.29	0.65
9:N:9:DG:OP2	9:N:9:DG:H3'	1.96	0.65
13:B:487:THR:OG1	13:B:777:ALA:O	2.15	0.65
3:F:97:ARG:NH1	3:F:100:GLN:OE1	2.30	0.65
12:A:875:ALA:HB2	12:A:1366:ARG:HD2	1.78	0.64
9:N:6:DC:H2'	9:N:7:DG:C8	2.32	0.64
5:I:74:GLU:OE1	5:I:81:ARG:NH2	2.31	0.64
6:J:48:ARG:NH1	6:J:49:MET:SD	2.70	0.64
11:T:25:DC:H2'	11:T:26:DC:C6	2.33	0.63
12:A:929:LEU:HD21	12:A:983:ILE:HG21	1.79	0.63
1:C:61:GLU:OE1	13:B:969:ARG:NH1	2.32	0.63
6:J:48:ARG:O	6:J:52:THR:OG1	2.17	0.63
12:A:120:GLU:OE1	12:A:123:ARG:NH2	2.32	0.63
5:I:52:ILE:HD11	13:B:309:GLN:HE22	1.64	0.63
11:T:19:DC:O4'	12:A:835:GLY:HA3	1.99	0.63
15:H:2:SER:N	15:H:61:SER:HG	1.97	0.62
4:G:108:VAL:HG22	4:G:159:ALA:HB3	1.82	0.62
12:A:597:LEU:HD21	15:H:103:LYS:HG2	1.81	0.62
13:B:287:ARG:NH1	13:B:324:ILE:O	2.33	0.62
1:C:10:ILE:HA	1:C:20:PHE:HA	1.82	0.62
12:A:707:GLY:HA2	12:A:1281:ARG:HD3	1.82	0.61
7:K:54:ARG:NH2	15:H:82:PRO:O	2.33	0.61
1:C:83:SER:HB3	1:C:160:LYS:HG2	1.83	0.61
4:G:4:ILE:HD11	14:D:48:ILE:HD11	1.82	0.61
1:C:174:ALA:O	13:B:996:ARG:NH1	2.27	0.61
15:H:75:ALA:N	15:H:98:TYR:HH	1.99	0.61
4:G:132:SER:OG	4:G:135:ASP:OD1	2.18	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:15:DT:H2''	11:T:16:DC:C6	2.36	0.60
4:G:84:GLY:N	4:G:147:ILE:O	2.32	0.60
12:A:147:VAL:HG13	12:A:149:GLU:HG2	1.83	0.60
5:I:115:LYS:NZ	12:A:700:ASN:O	2.35	0.60
12:A:1329:THR:HG22	12:A:1331:SER:H	1.67	0.60
12:A:1115:SER:OG	12:A:1330:ASN:OD1	2.16	0.60
12:A:402:ALA:HA	12:A:434:ARG:HA	1.83	0.59
12:A:326:ARG:HG3	12:A:1406:VAL:HG21	1.84	0.59
9:N:1:DG:H2'	9:N:2:DA:C8	2.38	0.59
11:T:13:DG:H2'	11:T:14:DC:H6	1.68	0.59
1:C:44:LEU:HB2	1:C:77:ILE:HD13	1.84	0.59
15:H:86:ASP:O	15:H:87:ARG:NH1	2.35	0.59
12:A:1286:LYS:HD2	12:A:1302:PRO:HB2	1.83	0.59
13:B:604:ARG:NH2	13:B:691:GLU:OE2	2.31	0.59
12:A:473:SER:OG	12:A:650:GLN:NE2	2.36	0.59
12:A:157:ASP:OD1	12:A:160:GLN:NE2	2.36	0.58
12:A:392:VAL:HG13	12:A:415:LEU:HD11	1.84	0.58
4:G:49:LEU:HD13	14:D:62:ALA:HB2	1.85	0.58
12:A:562:THR:O	12:A:576:GLN:NE2	2.37	0.58
13:B:133:LYS:HG3	13:B:157:GLU:HB3	1.86	0.58
1:C:36:VAL:HG13	1:C:40:GLU:HB2	1.86	0.58
13:B:229:ALA:O	13:B:261:ARG:NH1	2.37	0.58
11:T:22:DT:H2'	11:T:23:DC:C6	2.38	0.57
13:B:269:ILE:HD11	13:B:386:LEU:HD21	1.85	0.57
8:L:29:TYR:OH	13:B:896:ASP:OD2	2.21	0.57
13:B:307:ASP:OD2	13:B:392:ARG:NH1	2.36	0.57
1:C:258:ILE:HG13	7:K:42:LEU:HD21	1.85	0.57
11:T:16:DC:H3'	11:T:17:DT:H71	1.86	0.57
4:G:58:ARG:NH1	12:A:1446:ASP:OD1	2.38	0.57
2:E:121:MET:HE2	2:E:124:VAL:HG21	1.86	0.57
12:A:595:THR:HG22	12:A:603:ASN:OD1	2.05	0.57
12:A:1244:ARG:NH2	12:A:1249:ASP:OD2	2.37	0.57
14:D:56:ARG:HB2	14:D:148:LEU:HD22	1.85	0.57
12:A:568:PRO:HD2	15:H:46:LEU:HG	1.86	0.57
12:A:767:GLN:NE2	12:A:768:GLN:O	2.37	0.57
11:T:10:DC:H2'	11:T:11:DT:H72	1.87	0.56
12:A:116:ASP:H	12:A:164:ARG:HH12	1.52	0.56
11:T:16:DC:H2'	11:T:17:DT:H6	1.70	0.56
1:C:142:VAL:HG11	6:J:5:VAL:HG13	1.87	0.56
8:L:66:GLN:O	13:B:904:ARG:NH1	2.39	0.56
14:D:30:GLY:O	14:D:34:GLN:NE2	2.29	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:61:ASP:OD2	13:B:617:ARG:NH2	2.37	0.56
12:A:114:LEU:O	12:A:164:ARG:NH2	2.38	0.56
12:A:590:ARG:NH2	12:A:621:THR:OG1	2.38	0.56
5:I:10:CYS:SG	5:I:12:ASN:ND2	2.79	0.56
11:T:13:DG:H2'	11:T:14:DC:C6	2.40	0.56
12:A:1111:MET:HE3	12:A:1114:PRO:HA	1.86	0.56
13:B:165:VAL:HB	13:B:448:ILE:HD13	1.87	0.56
4:G:46:LEU:HD12	14:D:141:LEU:HA	1.86	0.56
11:T:12:DC:C2'	11:T:13:DG:C8	2.90	0.55
13:B:759:PRO:HG2	13:B:1046:PRO:HB3	1.88	0.55
13:B:102:VAL:HG21	13:B:122:LEU:HD13	1.88	0.55
11:T:27:DT:H2''	11:T:28:DC:H5'	1.87	0.55
12:A:396:PRO:HD3	12:A:415:LEU:HB3	1.89	0.55
11:T:14:DC:H2''	11:T:15:DT:H5'	1.89	0.55
12:A:896:ARG:HD2	12:A:1030:ARG:HH11	1.71	0.55
14:D:63:LEU:HB3	14:D:129:LEU:HD21	1.88	0.55
12:A:1030:ARG:NH2	12:A:1035:TYR:OH	2.36	0.55
12:A:922:ASP:OD1	12:A:923:LEU:N	2.40	0.54
1:C:71:PRO:HG3	6:J:13:VAL:HG21	1.88	0.54
1:C:143:LEU:HD21	1:C:146:LYS:HE3	1.90	0.54
4:G:35:GLU:OE2	14:D:66:ARG:NH1	2.40	0.54
11:T:12:DC:H2'	11:T:13:DG:C8	2.42	0.54
4:G:144:ARG:HH21	4:G:167:TYR:C	2.15	0.54
12:A:106:VAL:HG11	12:A:214:ILE:HG12	1.90	0.54
12:A:110:CYS:HB3	12:A:167:CYS:SG	2.47	0.54
12:A:116:ASP:H	12:A:164:ARG:NH1	2.05	0.54
4:G:15:PRO:HA	4:G:18:PHE:CE2	2.43	0.54
15:H:123:MET:HE2	15:H:142:LEU:HD13	1.88	0.54
12:A:881:GLN:NE2	12:A:958:VAL:O	2.41	0.54
12:A:884:ASP:HB3	12:A:896:ARG:HH12	1.71	0.54
12:A:446:ARG:HB2	12:A:487:MET:HG2	1.89	0.53
10:P:10:G:O2'	10:P:11:G:H5'	2.09	0.53
11:T:20:DT:H4'	13:B:1133:MET:SD	2.48	0.53
12:A:715:GLU:OE2	12:A:774:ARG:NH1	2.41	0.53
14:D:56:ARG:HG3	14:D:148:LEU:HB3	1.90	0.53
4:G:47:CYS:SG	4:G:48:VAL:N	2.81	0.53
4:G:73:LYS:HB3	14:D:40:HIS:CE1	2.44	0.53
12:A:362:ASP:HB3	12:A:508:PRO:HD3	1.89	0.53
1:C:102:GLN:HG2	1:C:154:LYS:HG2	1.91	0.52
7:K:29:ASN:ND2	7:K:77:THR:OG1	2.42	0.52
13:B:911:ILE:HG13	13:B:912:ILE:HG13	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:63:ARG:NE	12:A:63:ARG:O	2.43	0.52
12:A:346:ASP:OD1	13:B:1106:ARG:NE	2.38	0.52
13:B:979:LYS:HG2	13:B:1095:LEU:HD12	1.91	0.52
12:A:149:GLU:HB2	12:A:164:ARG:HH21	1.74	0.51
12:A:975:HIS:CD2	12:A:1036:ARG:HD2	2.45	0.51
13:B:205:ILE:HG13	13:B:461:LEU:HB3	1.92	0.51
1:C:89:GLU:HG2	1:C:90:ASP:H	1.76	0.51
4:G:61:ILE:HD11	12:A:1445:ILE:HG13	1.91	0.51
13:B:121:ASN:HA	13:B:207:GLY:HA3	1.91	0.51
11:T:15:DT:H2''	11:T:16:DC:C5	2.46	0.51
12:A:1279:ILE:HD12	12:A:1308:THR:HG21	1.92	0.51
12:A:693:VAL:HG21	12:A:721:PHE:HE2	1.75	0.51
14:D:174:PRO:HA	14:D:177:VAL:HG22	1.93	0.51
1:C:248:ILE:HG21	7:K:102:LYS:HB2	1.92	0.51
9:N:1:DG:H2'	9:N:2:DA:H8	1.76	0.51
4:G:6:ASP:OD2	14:D:39:ASN:HA	2.10	0.51
12:A:451:HIS:CD2	12:A:1074:GLU:HG3	2.46	0.51
12:A:993:LEU:HD23	12:A:1022:LEU:HD21	1.92	0.51
13:B:901:PRO:HA	13:B:949:VAL:HG13	1.92	0.51
2:E:88:VAL:HG21	2:E:110:PHE:HE2	1.76	0.51
12:A:329:LEU:HD23	12:A:335:ARG:HG3	1.92	0.51
12:A:1116:LEU:HD21	12:A:1327:ILE:HD11	1.93	0.50
14:D:56:ARG:HA	14:D:148:LEU:HD13	1.93	0.50
12:A:207:ILE:HA	12:A:210:ILE:HG22	1.93	0.50
12:A:687:LYS:NZ	12:A:795:GLU:OE1	2.42	0.50
13:B:287:ARG:NH1	13:B:321:GLY:O	2.45	0.50
1:C:22:LEU:HG	1:C:25:VAL:HG11	1.93	0.50
1:C:48:SER:OG	8:L:66:GLN:OE1	2.29	0.50
11:T:24:DC:H2'	11:T:25:DC:H6	1.74	0.50
13:B:600:LEU:HB3	13:B:615:MET:SD	2.50	0.50
14:D:53:SER:OG	14:D:154:PHE:N	2.41	0.50
1:C:8:VAL:HG11	7:K:105:PHE:HA	1.94	0.50
12:A:848:ILE:HG21	12:A:1370:LEU:HD11	1.94	0.50
13:B:643:ASP:OD2	13:B:654:ARG:NH2	2.45	0.50
2:E:86:PRO:HA	2:E:113:GLN:HB2	1.94	0.50
12:A:336:ILE:HG13	12:A:1405:THR:HG21	1.93	0.50
1:C:262:LEU:HD12	1:C:265:MET:HE2	1.94	0.50
9:N:4:DA:H2''	9:N:5:DG:C8	2.47	0.50
12:A:1187:GLN:O	12:A:1244:ARG:N	2.32	0.49
13:B:1171:VAL:HG22	13:B:1182:CYS:HB2	1.94	0.49
11:T:19:DC:H5''	12:A:832:ALA:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:ILE:HD11	7:K:112:GLN:HG3	1.94	0.49
12:A:981:LEU:HD11	12:A:1042:PHE:HB2	1.93	0.49
13:B:259:TYR:OH	13:B:279:ASP:OD2	2.30	0.49
13:B:311:LEU:O	13:B:315:LYS:HG2	2.12	0.49
14:D:119:ARG:NH1	14:D:150:ASN:O	2.45	0.49
5:I:101:PHE:HE1	5:I:112:SER:HB3	1.77	0.49
13:B:886:LYS:HD2	13:B:940:PRO:HG3	1.95	0.49
13:B:952:VAL:HG12	13:B:966:VAL:HG13	1.94	0.49
1:C:37:MET:HE3	1:C:176:ILE:HD13	1.94	0.49
7:K:59:ALA:H	12:A:547:LEU:HD13	1.78	0.49
12:A:406:ILE:HG12	12:A:412:ARG:HG2	1.94	0.49
12:A:514:PRO:HB3	12:A:875:ALA:HB3	1.93	0.49
13:B:80:GLU:OE1	13:B:83:ASN:ND2	2.46	0.49
13:B:135:ARG:HD3	13:B:155:GLU:HG3	1.94	0.49
1:C:18:VAL:HG12	1:C:240:VAL:HG22	1.95	0.48
4:G:127:PRO:HG2	4:G:139:ILE:HG12	1.95	0.48
12:A:804:TYR:OH	12:A:816:HIS:NE2	2.40	0.48
12:A:908:LEU:HA	12:A:1029:ARG:HH12	1.78	0.48
12:A:1279:ILE:HG23	12:A:1308:THR:HG23	1.95	0.48
14:D:214:LEU:O	14:D:218:GLU:HB2	2.13	0.48
12:A:446:ARG:HB2	12:A:487:MET:HE3	1.95	0.48
12:A:563:PRO:HG3	12:A:572:TRP:CZ2	2.48	0.48
4:G:83:LYS:O	14:D:24:ALA:N	2.35	0.48
8:L:51:CYS:SG	8:L:53:HIS:HB2	2.53	0.48
13:B:459:TYR:OH	13:B:465:ASN:ND2	2.34	0.48
12:A:359:LEU:O	12:A:471:ASN:ND2	2.44	0.48
4:G:49:LEU:N	4:G:75:ARG:O	2.41	0.48
9:N:7:DG:H2'	9:N:8:DA:H8	1.70	0.48
12:A:956:LEU:HD21	12:A:1017:LEU:HG	1.94	0.48
12:A:1252:THR:HA	12:A:1255:GLU:HG2	1.95	0.48
13:B:299:GLU:OE2	13:B:572:HIS:ND1	2.45	0.48
11:T:10:DC:H2'	11:T:11:DT:C7	2.44	0.48
11:T:21:DT:H2'	11:T:22:DT:C6	2.48	0.48
11:T:23:DC:H2'	11:T:24:DC:H6	1.74	0.48
2:E:126:SER:OG	2:E:127:ILE:N	2.46	0.48
12:A:534:LEU:O	12:A:574:GLY:HA3	2.12	0.48
12:A:848:ILE:HB	12:A:1065:GLY:HA3	1.94	0.48
12:A:1397:LEU:HB2	12:A:1426:GLU:HG3	1.94	0.48
13:B:51:PHE:HB2	13:B:173:MET:HE3	1.95	0.48
12:A:528:LEU:HD23	12:A:751:SER:HA	1.96	0.48
13:B:176:SER:O	13:B:182:SER:HB3	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:88:ASP:OD1	4:G:89:GLY:N	2.47	0.48
5:I:77:LYS:HD3	5:I:108:HIS:CG	2.49	0.48
12:A:1454:MET:SD	12:A:1454:MET:N	2.87	0.48
12:A:16:GLU:OE1	14:D:13:ARG:NH1	2.39	0.48
15:H:32:THR:OG1	15:H:33:GLN:OE1	2.32	0.48
12:A:114:LEU:HD23	12:A:145:LYS:HG3	1.94	0.47
12:A:956:LEU:HD13	12:A:1021:LEU:HD22	1.94	0.47
12:A:1420:ASP:OD1	12:A:1420:ASP:N	2.47	0.47
2:E:11:ARG:NH1	12:A:1318:THR:OG1	2.47	0.47
5:I:58:VAL:HA	5:I:62:ILE:HD12	1.95	0.47
7:K:77:THR:OG1	7:K:81:TYR:O	2.29	0.47
12:A:105:CYS:SG	12:A:139:TRP:HA	2.53	0.47
13:B:639:ILE:HD11	13:B:691:GLU:HB2	1.95	0.47
7:K:47:ARG:HH12	12:A:548:ASN:ND2	2.13	0.47
1:C:10:ILE:HD11	7:K:112:GLN:CG	2.45	0.47
12:A:1265:ASN:ND2	12:A:1269:GLU:OE2	2.47	0.47
13:B:63:ILE:O	13:B:67:SER:OG	2.17	0.47
15:H:63:LEU:O	15:H:89:LEU:N	2.38	0.47
4:G:86:VAL:HA	4:G:146:LYS:HA	1.97	0.47
12:A:608:ILE:HD12	12:A:613:ILE:HG13	1.95	0.47
12:A:993:LEU:HD22	12:A:1046:LEU:HD22	1.97	0.47
12:A:1095:THR:HG21	12:A:1112:LYS:HB2	1.97	0.47
12:A:1114:PRO:HB2	12:A:1311:VAL:HG23	1.96	0.47
15:H:10:PHE:HB3	15:H:28:ALA:HB1	1.96	0.47
1:C:111:THR:HB	1:C:147:LEU:HB2	1.96	0.47
1:C:114:TYR:CG	1:C:140:ASN:HB3	2.49	0.47
13:B:1041:GLU:OE1	13:B:1041:GLU:N	2.41	0.47
12:A:338:GLY:O	13:B:1129:ARG:NH1	2.45	0.47
1:C:6:PRO:O	7:K:104:ASN:ND2	2.46	0.47
7:K:114:LEU:H	7:K:114:LEU:HD23	1.80	0.47
12:A:900:ASP:OD2	12:A:903:ASN:ND2	2.48	0.47
13:B:924:GLU:O	13:B:928:ARG:HB3	2.15	0.47
15:H:2:SER:N	15:H:61:SER:OG	2.48	0.47
13:B:644:GLU:OE1	13:B:644:GLU:N	2.44	0.47
13:B:899:ILE:HD12	13:B:911:ILE:HG22	1.96	0.47
14:D:31:GLN:N	14:D:31:GLN:OE1	2.48	0.46
4:G:88:ASP:HA	4:G:144:ARG:HA	1.97	0.46
12:A:15:LYS:HB3	13:B:1220:ARG:HE	1.80	0.46
12:A:451:HIS:O	12:A:454:SER:OG	2.25	0.46
12:A:512:VAL:HA	12:A:519:PRO:HA	1.98	0.46
1:C:38:ILE:HG12	1:C:176:ILE:HD12	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:18:LYS:NZ	7:K:38:GLU:OE2	2.39	0.46
12:A:557:ASP:OD1	12:A:557:ASP:N	2.48	0.46
13:B:839:MET:O	13:B:991:GLY:N	2.43	0.46
12:A:483:ASP:HA	13:B:988:GLY:HA2	1.96	0.46
14:D:15:LEU:O	14:D:16:LYS:HG2	2.16	0.46
11:T:12:DC:H2''	11:T:13:DG:O4'	2.15	0.46
12:A:997:LEU:O	12:A:1011:GLN:NE2	2.39	0.46
11:T:28:DC:H5''	13:B:463:THR:HG21	1.97	0.46
12:A:500:GLU:OE2	13:B:1146:PHE:N	2.42	0.46
12:A:939:ASP:OD2	12:A:1023:ARG:NE	2.35	0.46
5:I:8:ARG:NH1	5:I:9:ASP:HB2	2.31	0.46
7:K:49:GLU:HB2	7:K:94:ILE:HD11	1.96	0.46
11:T:14:DC:H2''	11:T:15:DT:C5'	2.45	0.46
12:A:265:LYS:NZ	12:A:302:THR:OG1	2.42	0.46
12:A:515:GLN:NE2	12:A:1363:VAL:HG22	2.31	0.46
12:A:1215:ARG:NH2	12:A:1272:THR:O	2.43	0.46
1:C:10:ILE:HG22	1:C:20:PHE:HB3	1.98	0.46
4:G:115:MET:HG3	4:G:163:ILE:HD11	1.98	0.45
6:J:66:LEU:HD21	13:B:787:VAL:HG12	1.98	0.45
11:T:19:DC:H2'	11:T:20:DT:H6	1.77	0.45
12:A:918:GLU:N	12:A:918:GLU:OE1	2.49	0.45
13:B:258:LEU:HB2	13:B:385:LEU:HD21	1.98	0.45
14:D:123:LEU:HA	14:D:126:ILE:HG12	1.97	0.45
12:A:587:HIS:HE1	12:A:969:GLN:HG3	1.81	0.45
12:A:618:GLU:OE1	12:A:619:LYS:N	2.49	0.45
4:G:120:THR:O	4:G:131:GLN:N	2.43	0.45
12:A:528:LEU:O	12:A:531:ILE:HG22	2.17	0.45
12:A:873:MET:HB3	12:A:878:ILE:HD11	1.98	0.45
12:A:1009:ASN:OD1	12:A:1012:ARG:NH2	2.49	0.45
13:B:848:ARG:HH22	13:B:996:ARG:HE	1.64	0.45
14:D:167:LEU:HD12	14:D:177:VAL:HG12	1.99	0.45
15:H:108:SER:OG	15:H:109:LYS:N	2.48	0.45
2:E:190:LEU:HD11	2:E:196:VAL:HG13	1.99	0.45
12:A:443:LEU:HB3	12:A:490:HIS:HB2	1.99	0.45
13:B:25:ILE:HA	13:B:655:LYS:HD3	1.99	0.45
14:D:161:GLY:HA2	14:D:164:ILE:HG22	1.99	0.45
7:K:49:GLU:HG2	7:K:94:ILE:HG12	1.99	0.45
1:C:92:CYS:O	1:C:96:SER:OG	2.29	0.45
12:A:387:ARG:HH21	12:A:437:MET:HE1	1.81	0.45
3:F:136:ARG:HD2	3:F:146:TRP:CD1	2.52	0.45
12:A:1197:LEU:HB2	12:A:1236:LEU:HB2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:96:VAL:HG13	15:H:143:LEU:HG	1.98	0.45
2:E:28:TYR:HA	2:E:64:PRO:HA	1.99	0.45
2:E:198:ILE:HB	2:E:210:SER:HB3	1.98	0.45
12:A:439:ASN:OD1	12:A:459:ARG:NH1	2.45	0.45
14:D:154:PHE:HB3	14:D:159:THR:HG23	1.99	0.45
13:B:101:MET:HE2	13:B:109:THR:HG22	1.98	0.44
13:B:841:MET:HE3	13:B:1010:LEU:HD21	1.97	0.44
12:A:74:MET:O	13:B:1116:ARG:NH2	2.47	0.44
12:A:406:ILE:HB	12:A:431:LYS:HB2	1.99	0.44
12:A:470:LEU:HD12	12:A:474:VAL:HG13	1.98	0.44
12:A:1399:ARG:NH2	12:A:1417:GLU:OE1	2.50	0.44
11:T:13:DG:H2''	11:T:14:DC:C5'	2.47	0.44
12:A:338:GLY:C	13:B:1129:ARG:HH12	2.25	0.44
13:B:281:PRO:HD2	13:B:284:ILE:HD12	1.99	0.44
10:P:8:A:H2'	10:P:9:G:C8	2.52	0.44
14:D:210:ILE:O	14:D:214:LEU:HD23	2.18	0.44
6:J:56:LEU:HD13	13:B:780:VAL:HG21	1.99	0.44
12:A:905:ASP:OD1	12:A:905:ASP:N	2.50	0.44
12:A:1161:THR:HG22	12:A:1170:ILE:HD13	1.98	0.44
13:B:936:ASP:OD1	13:B:938:SER:OG	2.27	0.44
14:D:20:GLU:OE1	14:D:20:GLU:N	2.46	0.44
12:A:579:SER:HB3	12:A:611:GLN:HA	1.99	0.44
12:A:1224:LEU:HD21	12:A:1240:CYS:HB3	2.00	0.44
12:A:1288:ASP:OD2	12:A:1300:LYS:HB3	2.17	0.44
1:C:11:ARG:N	1:C:19:ASP:O	2.51	0.44
4:G:15:PRO:HA	4:G:18:PHE:CD2	2.52	0.44
5:I:17:ARG:N	5:I:26:LEU:O	2.39	0.44
1:C:189:THR:HG22	13:B:1081:LEU:O	2.17	0.44
2:E:43:LYS:O	2:E:47:CYS:HB3	2.18	0.44
3:F:89:GLU:HA	12:A:1441:PHE:CZ	2.53	0.44
9:N:8:DA:C2'	9:N:9:DG:H5'	2.45	0.44
12:A:1002:GLY:HA3	12:A:1007:ILE:HG21	1.99	0.44
13:B:757:PRO:HG2	13:B:984:HIS:CE1	2.53	0.44
13:B:883:LEU:HG	13:B:932:HIS:HB3	2.00	0.44
13:B:903:VAL:O	13:B:949:VAL:HG12	2.18	0.44
12:A:579:SER:HA	12:A:582:ILE:HD12	1.99	0.44
13:B:120:ARG:HA	13:B:963:PHE:HZ	1.82	0.44
3:F:127:GLU:HG3	3:F:129:LYS:HG2	2.00	0.43
12:A:216:VAL:HA	12:A:219:PHE:CE2	2.53	0.43
13:B:661:LEU:HD11	13:B:684:LEU:HD11	1.98	0.43
1:C:115:SER:OG	1:C:141:GLY:HA3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:7:CYS:HA	6:J:49:MET:HG3	2.01	0.43
11:T:17:DT:O4'	12:A:1386:ARG:NH2	2.51	0.43
12:A:752:LYS:HG2	13:B:1015:HIS:O	2.17	0.43
8:L:31:CYS:SG	8:L:32:ALA:N	2.91	0.43
11:T:25:DC:H5'	13:B:792:MET:HE2	2.00	0.43
12:A:1220:PHE:HD2	12:A:1224:LEU:HD22	1.83	0.43
13:B:105:SER:HB2	13:B:960:GLY:HA3	2.01	0.43
13:B:244:LEU:HD23	13:B:244:LEU:H	1.84	0.43
1:C:226:ASP:HA	1:C:228:PHE:CE1	2.54	0.43
6:J:41:LEU:HD22	6:J:46:CYS:HB3	2.01	0.43
11:T:22:DT:H2'	11:T:23:DC:H6	1.81	0.43
12:A:512:VAL:HG23	12:A:634:THR:HG21	2.00	0.43
4:G:31:LEU:C	4:G:33:GLU:H	2.25	0.43
12:A:451:HIS:ND1	12:A:453:MET:HB2	2.34	0.43
12:A:589:GLN:HG3	12:A:606:LEU:HD13	2.01	0.43
12:A:1147:THR:HG21	12:A:1195:LEU:HD23	1.99	0.43
13:B:1138:MET:HE2	13:B:1146:PHE:CD2	2.54	0.43
2:E:94:LYS:HA	2:E:97:VAL:HG12	2.00	0.43
3:F:116:ASP:HB3	3:F:119:ARG:HG2	2.00	0.43
4:G:61:ILE:HD13	12:A:1443:VAL:HG12	2.01	0.43
12:A:451:HIS:ND1	12:A:453:MET:HE2	2.34	0.43
12:A:1120:LEU:HD11	12:A:1131:ALA:HB2	2.01	0.43
12:A:1266:THR:O	12:A:1270:ASN:HB3	2.19	0.43
13:B:237:VAL:HG13	13:B:257:LYS:HG2	2.01	0.43
13:B:1056:SER:HB2	13:B:1066:SER:HB2	2.00	0.43
1:C:180:TYR:HB3	1:C:228:PHE:CD2	2.53	0.42
13:B:54:PHE:HA	13:B:58:THR:HB	2.01	0.42
13:B:541:LEU:HD23	13:B:541:LEU:HA	1.89	0.42
12:A:555:ASP:OD2	12:A:644:LYS:NZ	2.32	0.42
13:B:216:GLU:OE1	13:B:500:THR:OG1	2.37	0.42
14:D:205:ASP:OD1	14:D:206:GLU:N	2.52	0.42
11:T:16:DC:H2''	11:T:17:DT:O5'	2.19	0.42
12:A:532:ARG:HD3	12:A:749:ALA:HB2	2.01	0.42
12:A:726:ARG:HD3	12:A:766:GLY:HA3	2.01	0.42
2:E:74:ASP:N	2:E:74:ASP:OD1	2.50	0.42
12:A:149:GLU:HB2	12:A:164:ARG:NH2	2.35	0.42
12:A:958:VAL:HB	12:A:1018:PHE:CE1	2.54	0.42
13:B:408:LEU:HD23	13:B:545:ILE:HG21	2.01	0.42
14:D:206:GLU:HA	14:D:209:ARG:HG2	2.01	0.42
2:E:206:GLY:N	12:A:1017:LEU:HB2	2.34	0.42
4:G:27:LYS:HG2	4:G:54:ILE:HD12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:19:ASP:OD2	5:I:24:ARG:NH1	2.51	0.42
6:J:1:MET:HA	6:J:56:LEU:HB2	2.01	0.42
11:T:21:DT:H4'	12:A:447:GLN:OE1	2.20	0.42
12:A:72:GLU:HB3	12:A:76:GLU:HB2	2.02	0.42
12:A:339:ASN:O	12:A:343:LYS:HE2	2.19	0.42
12:A:1293:SER:N	12:A:1297:GLU:O	2.41	0.42
14:D:126:ILE:HD13	14:D:149:THR:HG21	2.01	0.42
2:E:12:LEU:HG	2:E:58:MET:HE1	2.02	0.42
3:F:103:MET:HE1	4:G:65:ASP:O	2.20	0.42
12:A:108:MET:H	12:A:171:GLN:HE21	1.68	0.42
12:A:243:PRO:HB2	12:A:245:PRO:HD2	2.02	0.42
12:A:667:GLY:HA2	12:A:670:ILE:HD12	2.01	0.42
12:A:1196:GLU:N	12:A:1196:GLU:OE1	2.52	0.42
13:B:641:GLU:OE2	13:B:654:ARG:NH2	2.53	0.42
13:B:999:MET:HE3	13:B:1008:PRO:HG2	2.01	0.42
1:C:111:THR:O	1:C:147:LEU:N	2.47	0.42
2:E:85:GLU:OE2	2:E:92:THR:HG21	2.20	0.42
2:E:120:ALA:O	2:E:124:VAL:HG23	2.20	0.42
12:A:172:PRO:HB3	12:A:185:TRP:CD2	2.54	0.42
12:A:549:MET:HE3	12:A:656:TRP:HB2	2.01	0.42
11:T:14:DC:H2'	11:T:15:DT:C5	2.55	0.42
12:A:614:PHE:HB3	15:H:122:LEU:HD21	2.02	0.42
12:A:744:LYS:HG3	12:A:748:MET:HE2	2.01	0.42
7:K:58:PHE:CD2	12:A:547:LEU:HD22	2.55	0.42
12:A:451:HIS:CE1	12:A:453:MET:HB2	2.55	0.42
12:A:470:LEU:HD21	12:A:482:PHE:HE1	1.83	0.42
12:A:1198:ASP:HB3	12:A:1201:ALA:HB3	2.01	0.42
13:B:138:GLU:N	13:B:138:GLU:OE1	2.52	0.42
13:B:363:HIS:HD2	13:B:585:VAL:HG22	1.85	0.42
13:B:1169:MET:SD	13:B:1201:LYS:HG2	2.60	0.42
2:E:147:HIS:NE2	12:A:1327:ILE:O	2.49	0.41
4:G:13:LEU:HD11	4:G:26:LEU:HG	2.01	0.41
7:K:24:ASP:OD2	7:K:74:ARG:NE	2.38	0.41
13:B:1163:CYS:HB2	13:B:1187:ASN:HD21	1.84	0.41
12:A:884:ASP:HB2	12:A:1024:SER:OG	2.20	0.41
12:A:1422:ARG:HD3	13:B:1224:PHE:CD2	2.54	0.41
13:B:102:VAL:HB	13:B:112:LEU:HD22	2.02	0.41
13:B:465:ASN:HA	13:B:477:ALA:HA	2.01	0.41
12:A:130:ASP:OD1	12:A:130:ASP:N	2.52	0.41
12:A:389:THR:O	12:A:393:ARG:HG2	2.20	0.41
12:A:1072:ILE:HD13	12:A:1371:LEU:HD22	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1209:MET:SD	12:A:1236:LEU:HB3	2.60	0.41
13:B:764:SER:OG	13:B:765:PRO:HD3	2.20	0.41
14:D:156:ASP:OD1	14:D:159:THR:HG22	2.20	0.41
2:E:118:PRO:HA	2:E:121:MET:HB2	2.01	0.41
2:E:208:TYR:HE1	12:A:867:ILE:HG22	1.85	0.41
4:G:118:ASP:OD1	4:G:119:LEU:N	2.54	0.41
12:A:471:ASN:O	12:A:474:VAL:HG12	2.21	0.41
13:B:1008:PRO:HB3	13:B:1087:PHE:HE1	1.86	0.41
14:D:69:ALA:HA	14:D:72:ARG:HG2	2.03	0.41
11:T:25:DC:H2'	11:T:26:DC:H6	1.80	0.41
12:A:1392:SER:O	12:A:1399:ARG:HD3	2.20	0.41
13:B:839:MET:HE1	13:B:980:PHE:HB2	2.02	0.41
4:G:74:TYR:CE2	4:G:76:ALA:HB2	2.56	0.41
4:G:86:VAL:HG22	4:G:146:LYS:HB2	2.01	0.41
12:A:159:THR:OG1	12:A:160:GLN:OE1	2.35	0.41
12:A:506:ALA:O	12:A:510:GLN:HG2	2.20	0.41
12:A:1165:GLU:OE1	12:A:1194:ARG:NH2	2.54	0.41
12:A:1428:VAL:HG13	13:B:1151:LEU:HD13	2.03	0.41
12:A:633:VAL:HG21	12:A:645:LEU:HD22	2.02	0.41
13:B:910:VAL:HA	13:B:940:PRO:HA	2.01	0.41
1:C:142:VAL:HG13	6:J:15:GLY:HA3	2.02	0.41
11:T:19:DC:C4'	12:A:835:GLY:HA3	2.50	0.41
12:A:885:THR:HG23	12:A:1024:SER:HB2	2.01	0.41
12:A:899:VAL:HB	12:A:929:LEU:HD12	2.02	0.41
13:B:840:ILE:HB	13:B:1011:ILE:HB	2.03	0.41
14:D:180:LEU:HD21	14:D:198:LEU:HD11	2.02	0.41
4:G:4:ILE:HG22	4:G:77:VAL:HA	2.02	0.41
4:G:18:PHE:HD1	4:G:22:MET:SD	2.44	0.41
4:G:77:VAL:HG11	14:D:59:ILE:HD11	2.02	0.41
5:I:6:PHE:CE1	13:B:298:LEU:HD12	2.56	0.41
12:A:157:ASP:OD2	12:A:159:THR:OG1	2.39	0.41
12:A:349:ALA:HB2	12:A:374:LEU:HD11	2.03	0.41
12:A:528:LEU:HB3	12:A:751:SER:HB3	2.03	0.41
12:A:1262:LYS:O	12:A:1266:THR:HG22	2.21	0.41
15:H:102:TYR:CZ	15:H:115:TYR:HB3	2.56	0.41
4:G:144:ARG:NH1	4:G:169:GLY:O	2.54	0.41
6:J:2:ILE:HD12	6:J:57:ILE:HD13	2.03	0.41
13:B:883:LEU:HD21	13:B:928:ARG:HD3	2.03	0.40
3:F:81:THR:OG1	3:F:146:TRP:NE1	2.55	0.40
14:D:33:PHE:HD1	14:D:47:LEU:HD21	1.86	0.40
13:B:424:LEU:O	13:B:428:ILE:HG12	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:1106:ARG:NH1	13:B:1125:ASP:O	2.55	0.40
5:I:84:VAL:HG13	5:I:104:LEU:HD11	2.03	0.40
13:B:136:THR:HG23	13:B:152:ILE:HG22	2.03	0.40
1:C:108:GLU:HA	1:C:149:LYS:HD2	2.03	0.40
7:K:102:LYS:NZ	7:K:106:GLU:OE2	2.41	0.40
13:B:314:LEU:HD12	13:B:317:CYS:SG	2.61	0.40
14:D:172:LEU:HG	14:D:173:HIS:H	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	263/318 (83%)	254 (97%)	9 (3%)	0	100	100
2	E	212/215 (99%)	204 (96%)	8 (4%)	0	100	100
3	F	85/155 (55%)	84 (99%)	1 (1%)	0	100	100
4	G	169/171 (99%)	162 (96%)	7 (4%)	0	100	100
5	I	114/122 (93%)	110 (96%)	4 (4%)	0	100	100
6	J	67/70 (96%)	67 (100%)	0	0	100	100
7	K	113/120 (94%)	112 (99%)	1 (1%)	0	100	100
8	L	43/70 (61%)	42 (98%)	1 (2%)	0	100	100
12	A	1408/1733 (81%)	1387 (98%)	21 (2%)	0	100	100
13	B	1164/1224 (95%)	1135 (98%)	29 (2%)	0	100	100
14	D	162/221 (73%)	157 (97%)	5 (3%)	0	100	100
15	H	136/146 (93%)	132 (97%)	4 (3%)	0	100	100
All	All	3936/4565 (86%)	3846 (98%)	90 (2%)	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	C	233/274 (85%)	233 (100%)	0	100	100
2	E	196/197 (100%)	196 (100%)	0	100	100
3	F	77/137 (56%)	77 (100%)	0	100	100
4	G	152/152 (100%)	152 (100%)	0	100	100
5	I	110/116 (95%)	110 (100%)	0	100	100
6	J	64/65 (98%)	64 (100%)	0	100	100
7	K	99/102 (97%)	99 (100%)	0	100	100
8	L	40/57 (70%)	40 (100%)	0	100	100
12	A	1240/1520 (82%)	1240 (100%)	0	100	100
13	B	1022/1061 (96%)	1022 (100%)	0	100	100
14	D	148/200 (74%)	148 (100%)	0	100	100
15	H	123/128 (96%)	123 (100%)	0	100	100
All	All	3504/4009 (87%)	3504 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	73	GLN
1	C	195	GLN
2	E	115	ASN
4	G	24	GLN
4	G	96	GLN
4	G	153	GLN
5	I	90	GLN
6	J	53	HIS
7	K	29	ASN
8	L	53	HIS
12	A	4	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	A	92	HIS
12	A	118	HIS
12	A	169	ASN
12	A	171	GLN
12	A	339	ASN
12	A	435	HIS
12	A	479	ASN
12	A	515	GLN
12	A	587	HIS
12	A	877	HIS
12	A	975	HIS
12	A	1078	GLN
12	A	1265	ASN
12	A	1387	HIS
13	B	110	HIS
13	B	115	GLN
13	B	300	HIS
13	B	357	GLN
13	B	449	ASN
13	B	538	ASN
13	B	1104	HIS
15	H	83	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	P	8/15 (53%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	P	13	A
10	P	15	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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](#)

There are no chain breaks in this entry.

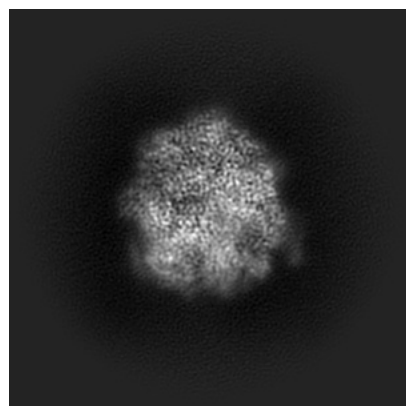
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65749. These allow visual inspection of the internal detail of the map and identification of artifacts.

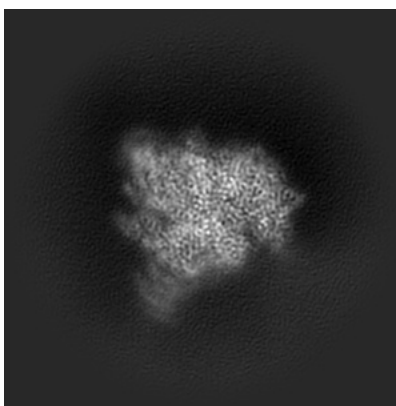
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

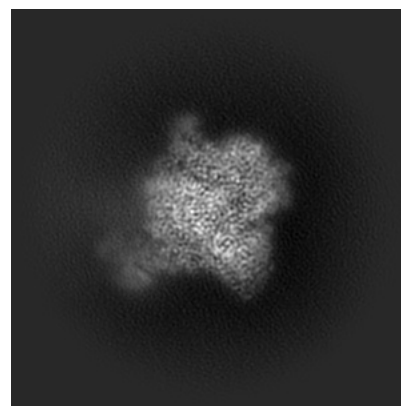
6.1.1 Primary map



X

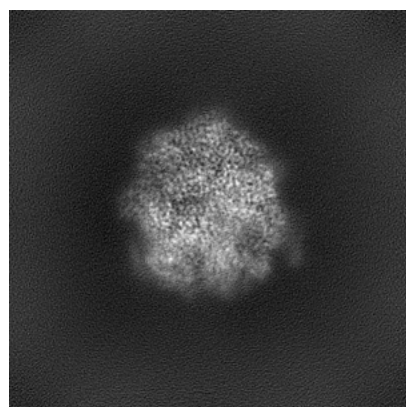


Y

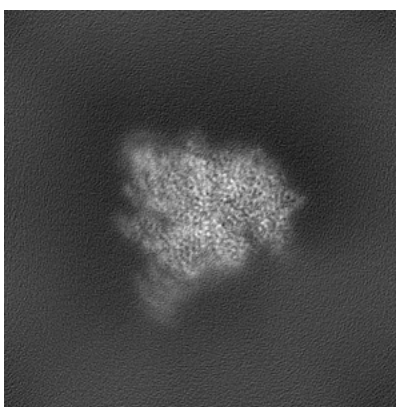


Z

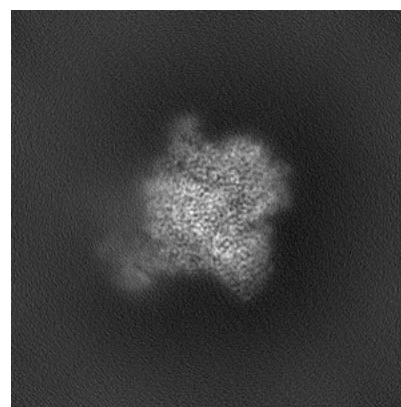
6.1.2 Raw map



X



Y

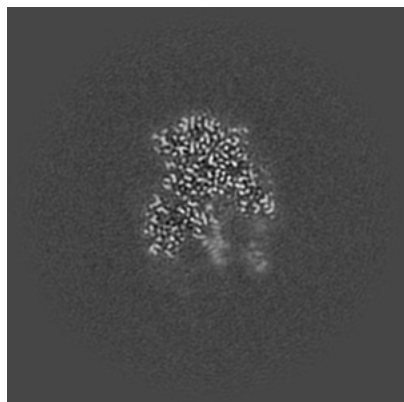


Z

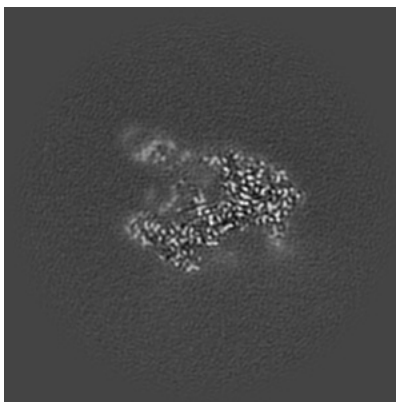
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

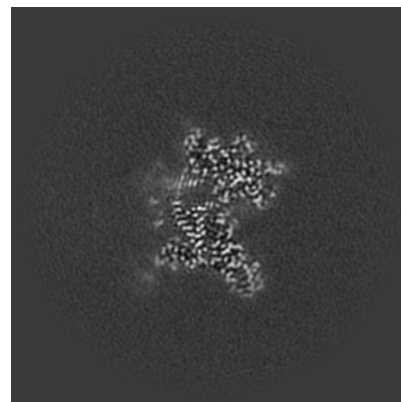
6.2.1 Primary map



X Index: 160

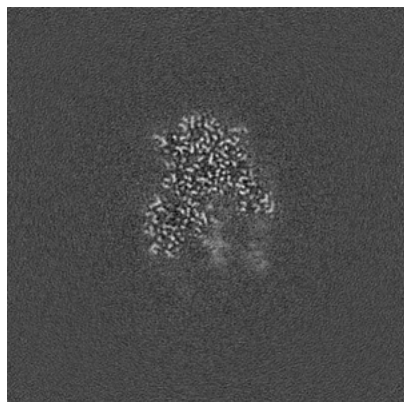


Y Index: 160

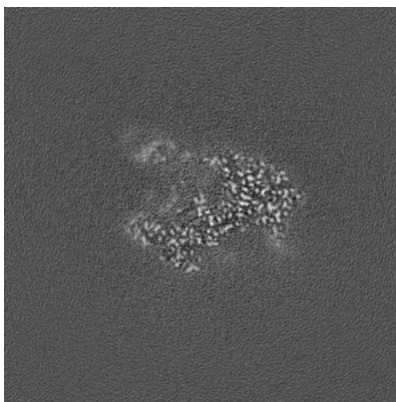


Z Index: 160

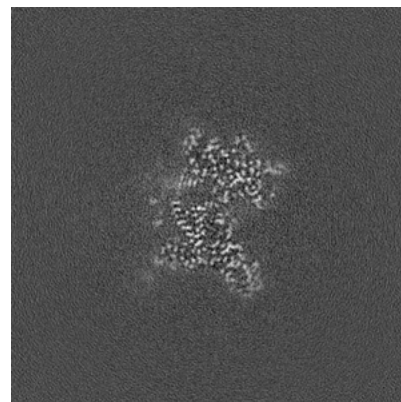
6.2.2 Raw map



X Index: 160



Y Index: 160

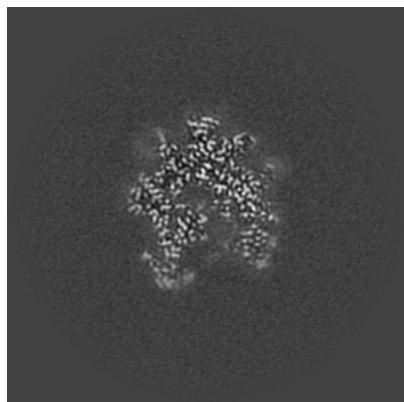


Z Index: 160

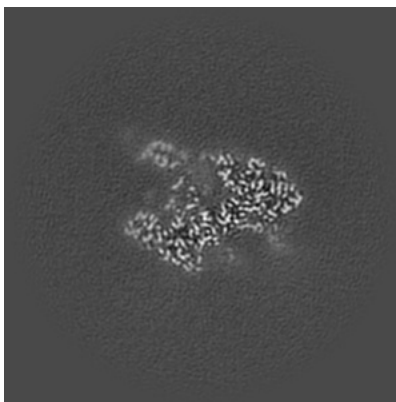
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

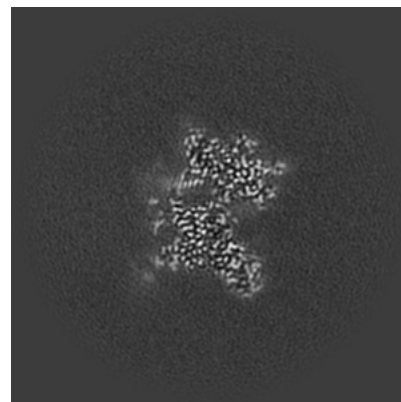
6.3.1 Primary map



X Index: 174

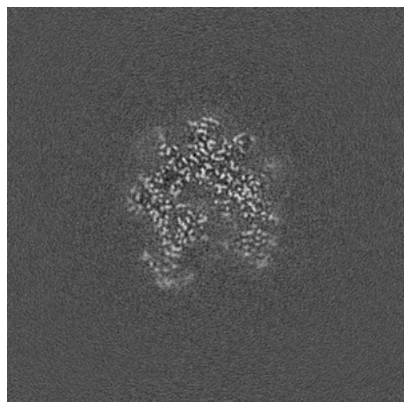


Y Index: 158

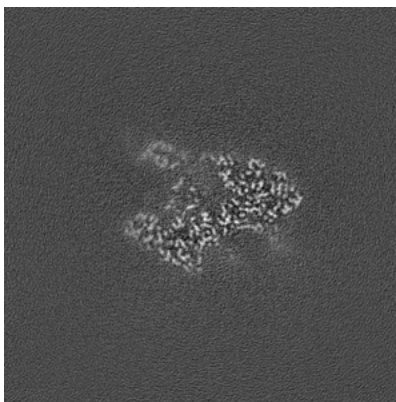


Z Index: 159

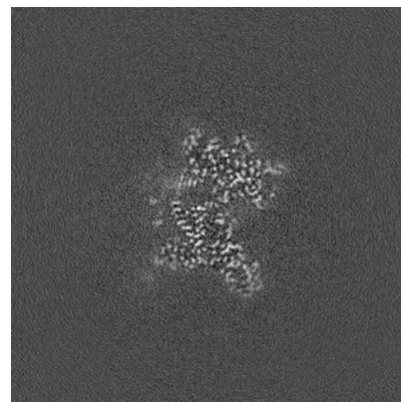
6.3.2 Raw map



X Index: 174



Y Index: 158

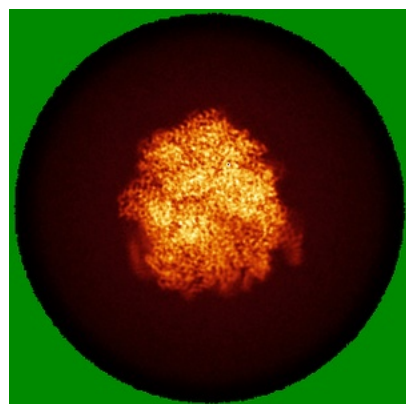


Z Index: 160

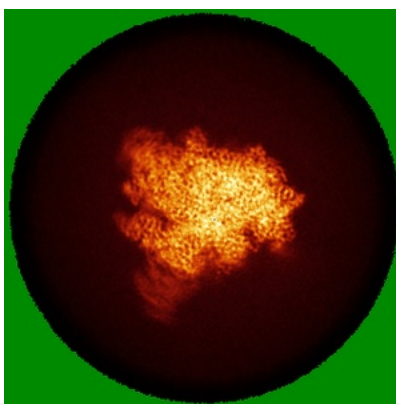
The images above show the largest variance slices of the map in three orthogonal directions.

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

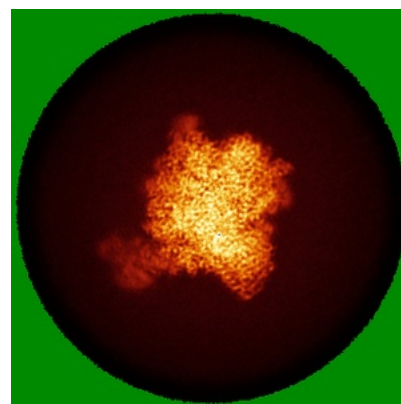
6.4.1 Primary map



X

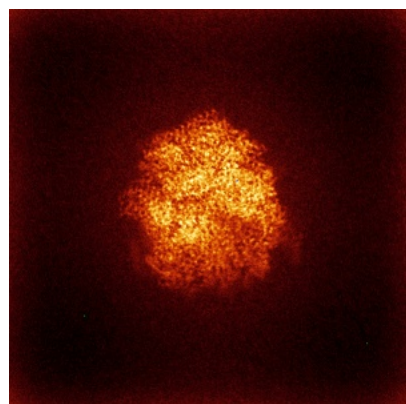


Y

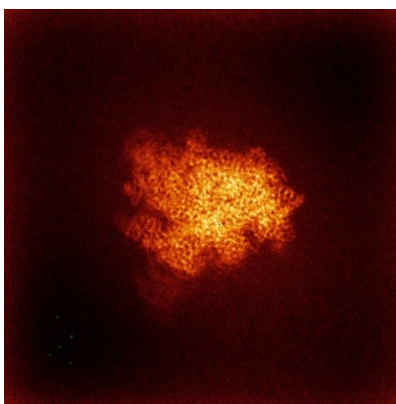


Z

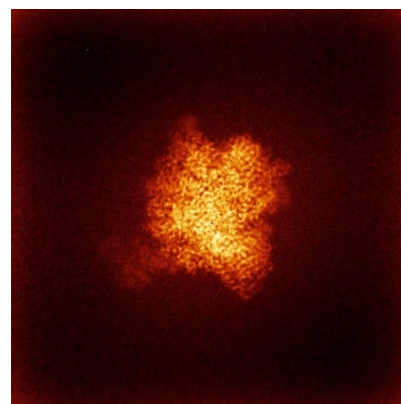
6.4.2 Raw map



X



Y

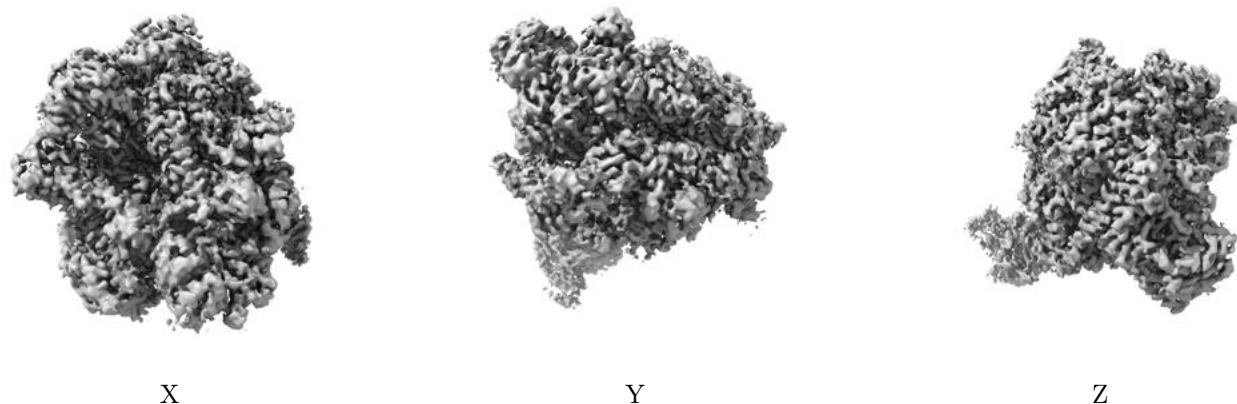


Z

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.

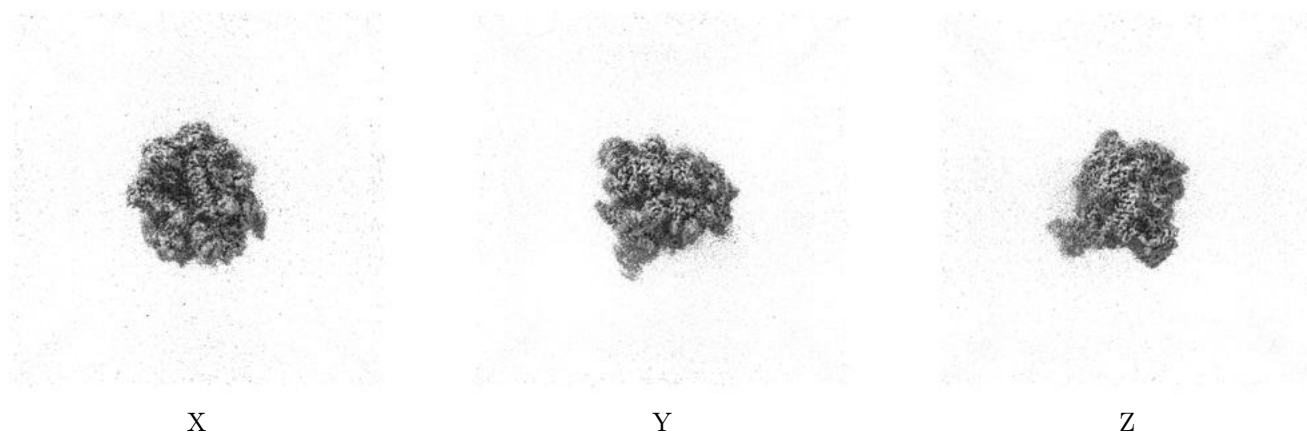
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. 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.

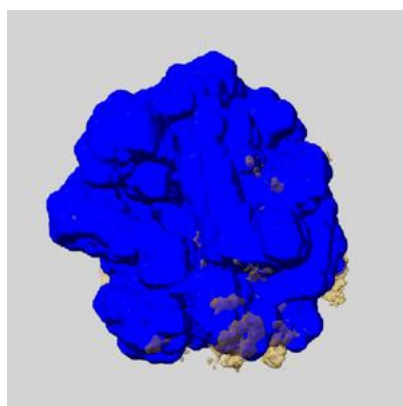
6.6 Mask visualisation [i](#)

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

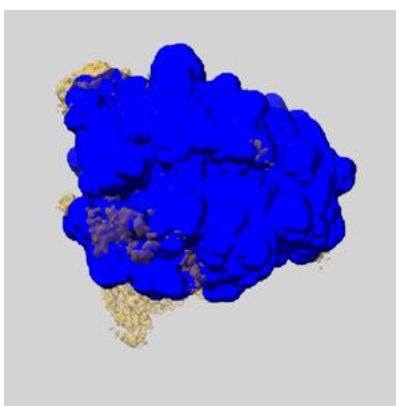
A mask typically either:

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

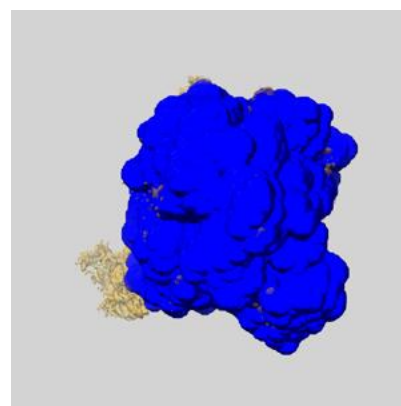
6.6.1 emd_65749_msk_1.map [i](#)



X



Y

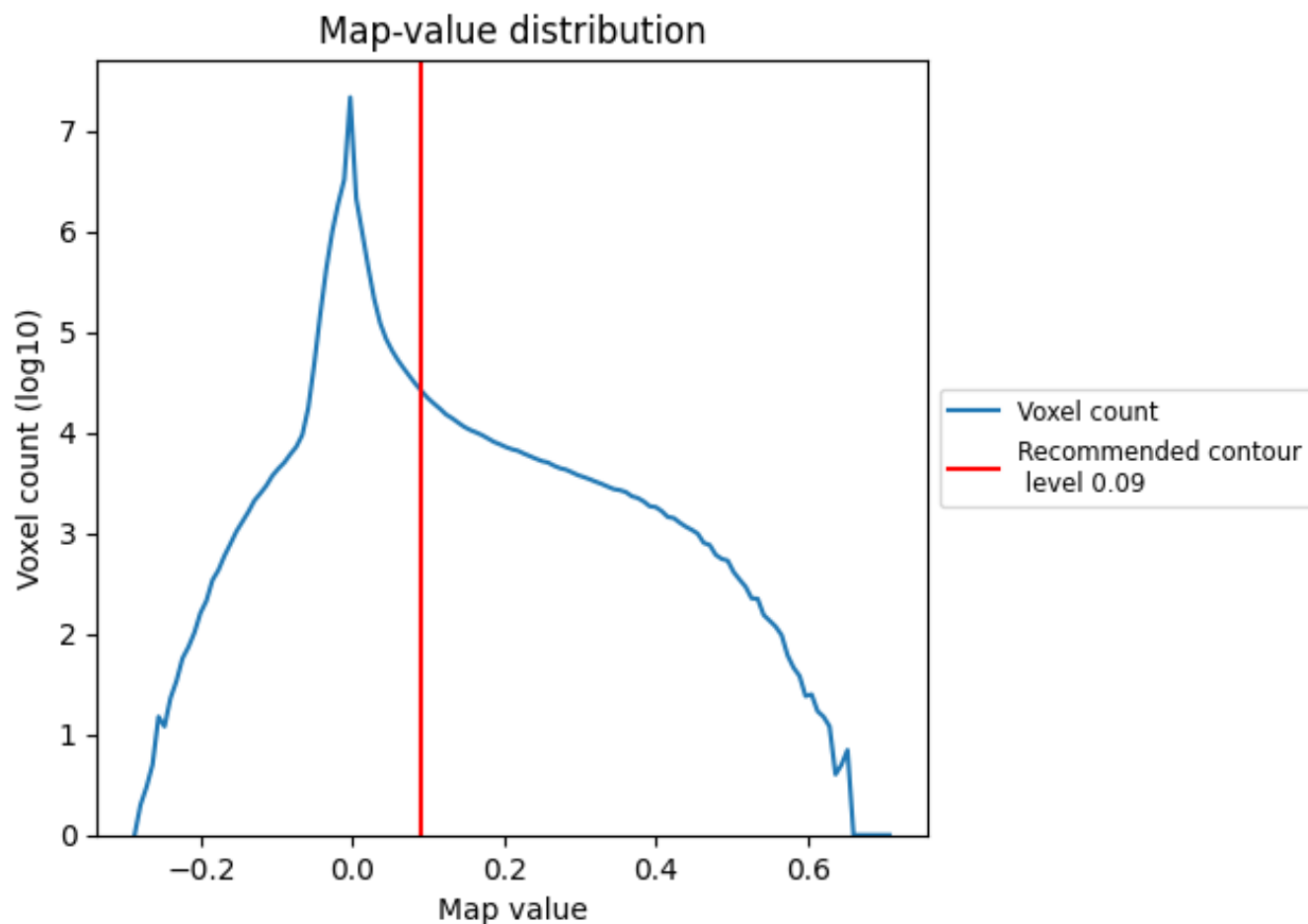


Z

7 Map analysis [i](#)

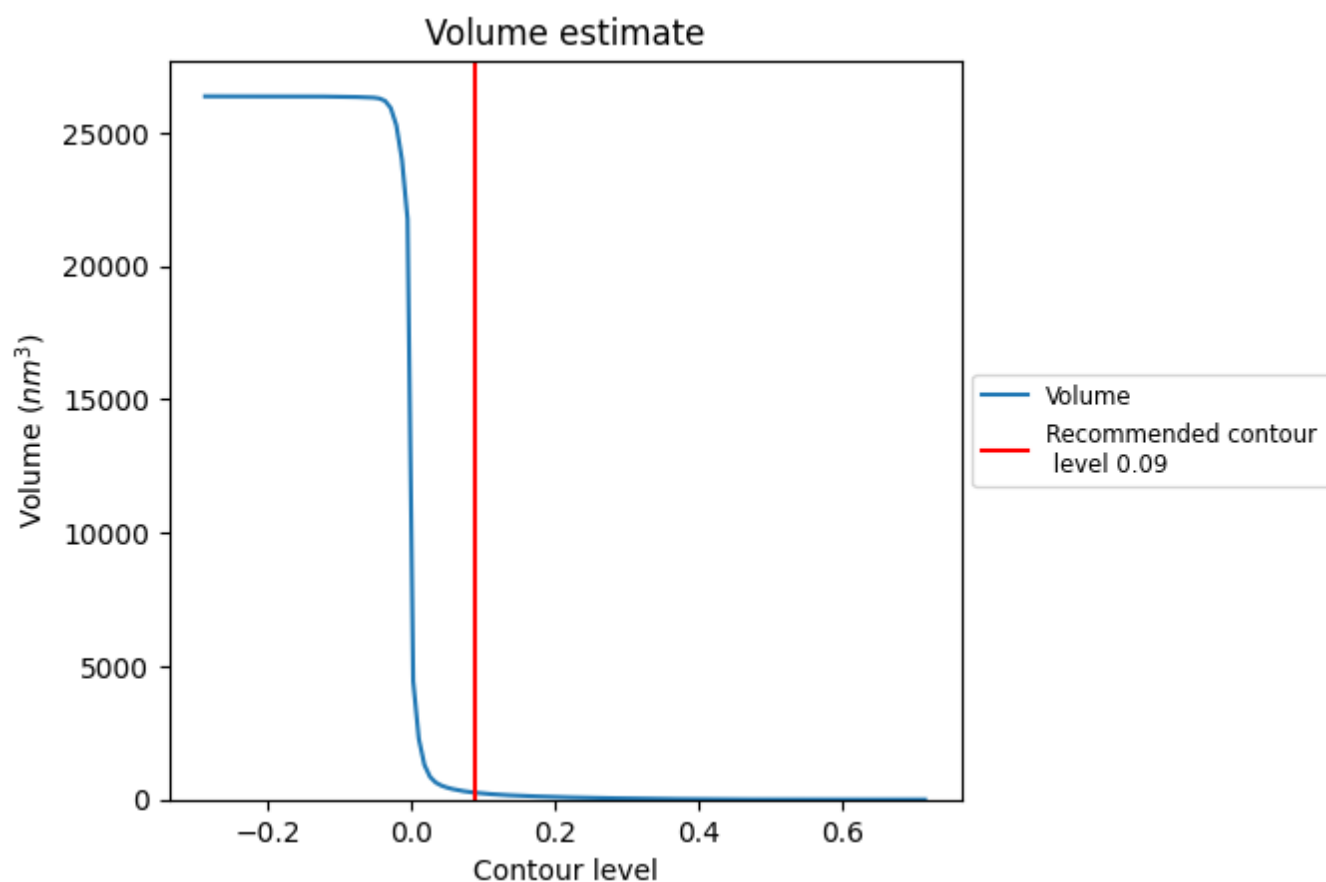
This section contains the results of statistical analysis of the map.

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.

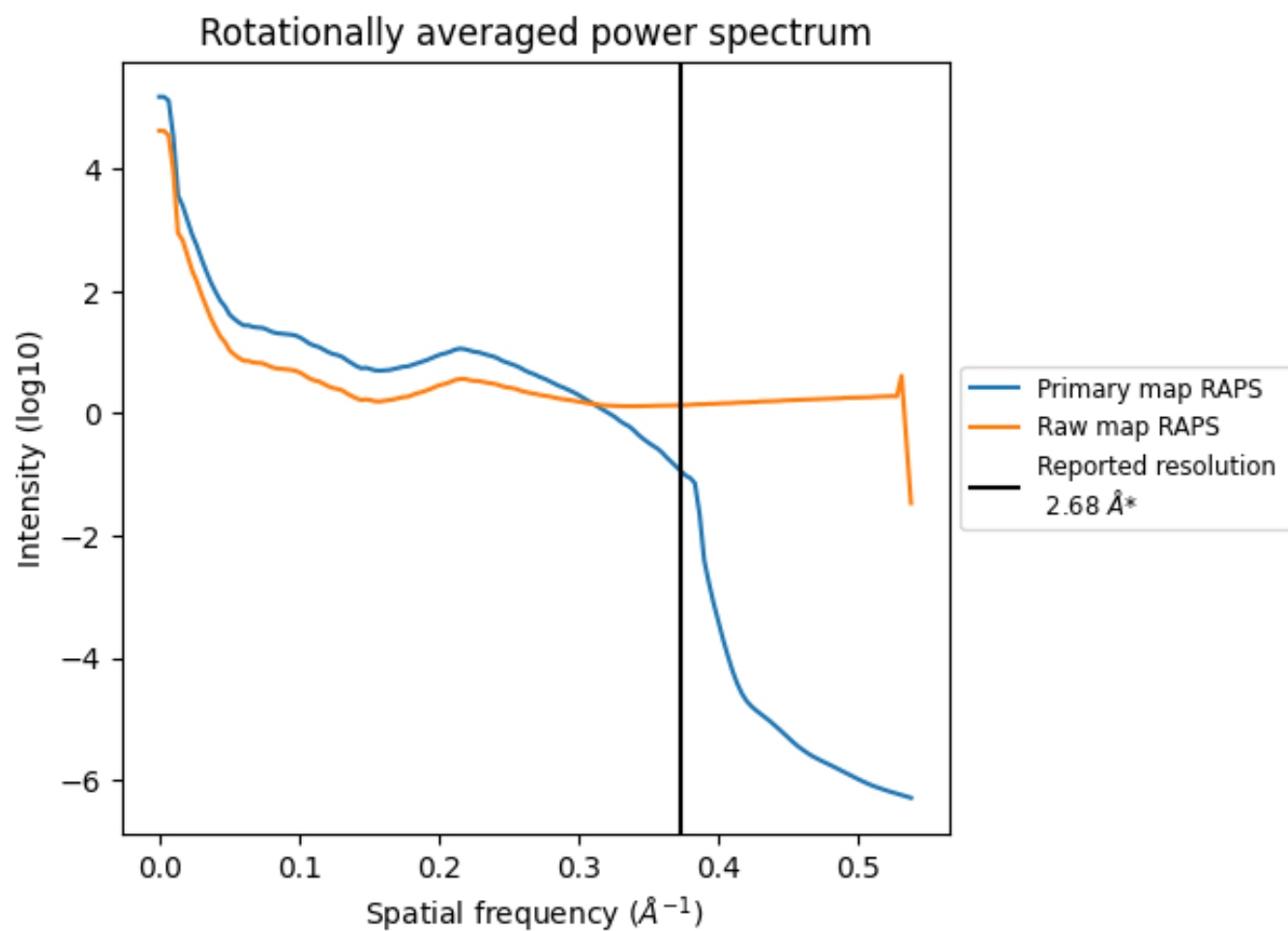
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 254 nm^3 ; this corresponds to an approximate mass of 230 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 ⓘ

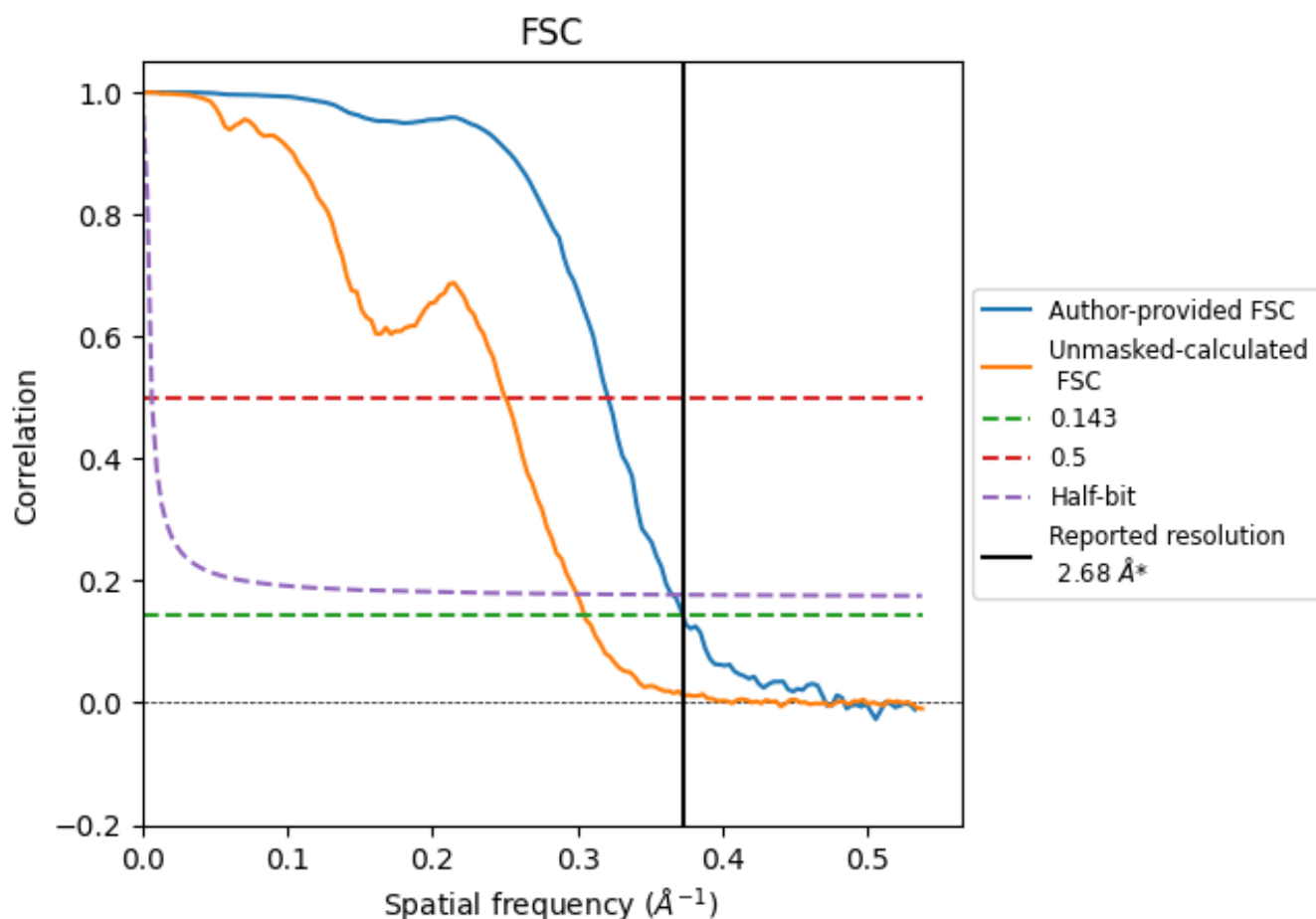


*Reported resolution corresponds to spatial frequency of 0.373 Å⁻¹

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 0.373 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

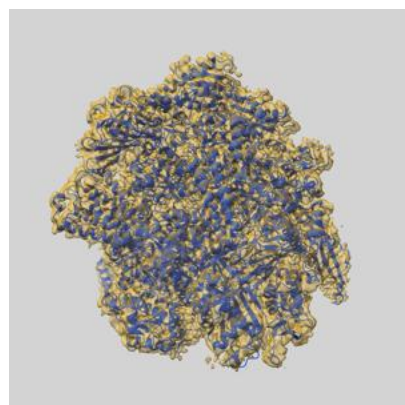
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	2.68	3.11	2.74
Unmasked-calculated*	3.28	4.00	3.34

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.28 differs from the reported value 2.68 by more than 10 %

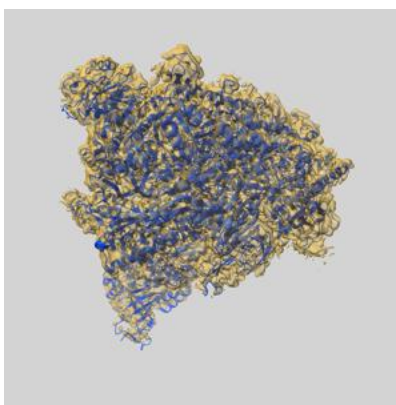
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-65749 and PDB model 9W8R. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

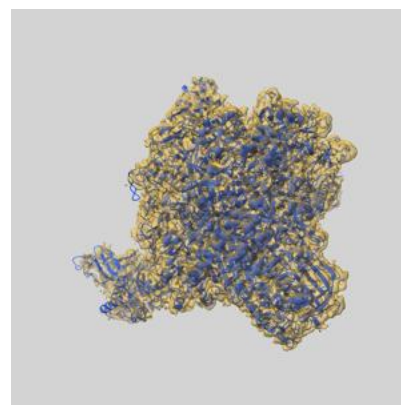
9.1 Map-model overlay [i](#)



X



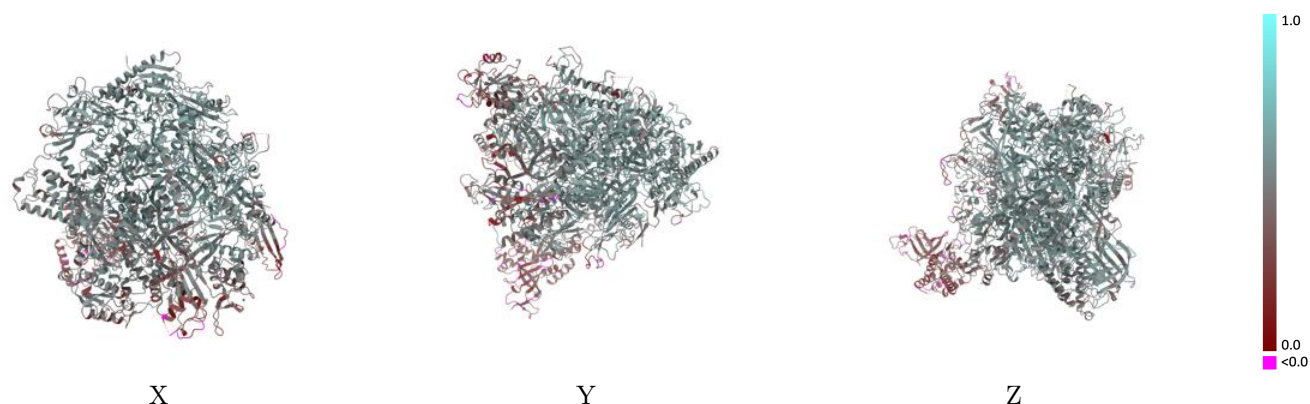
Y



Z

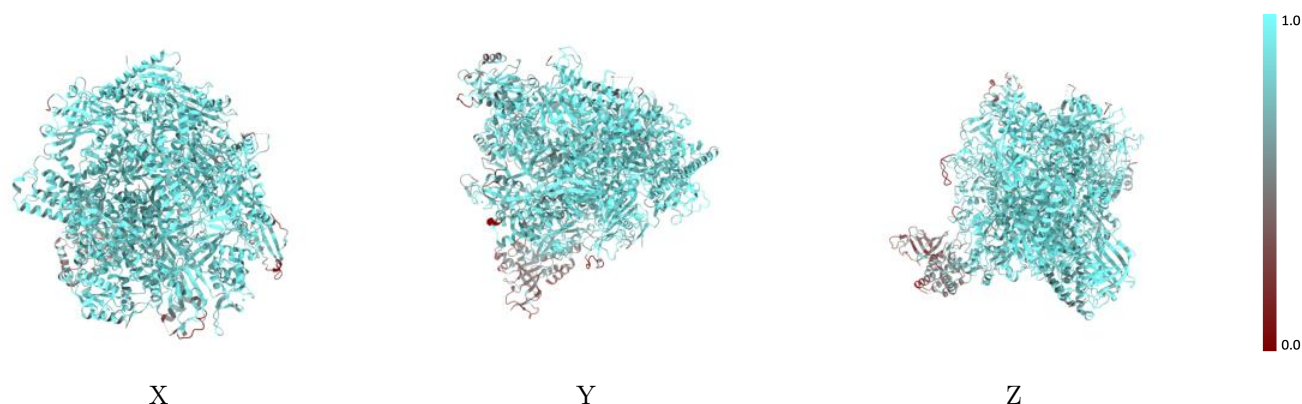
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



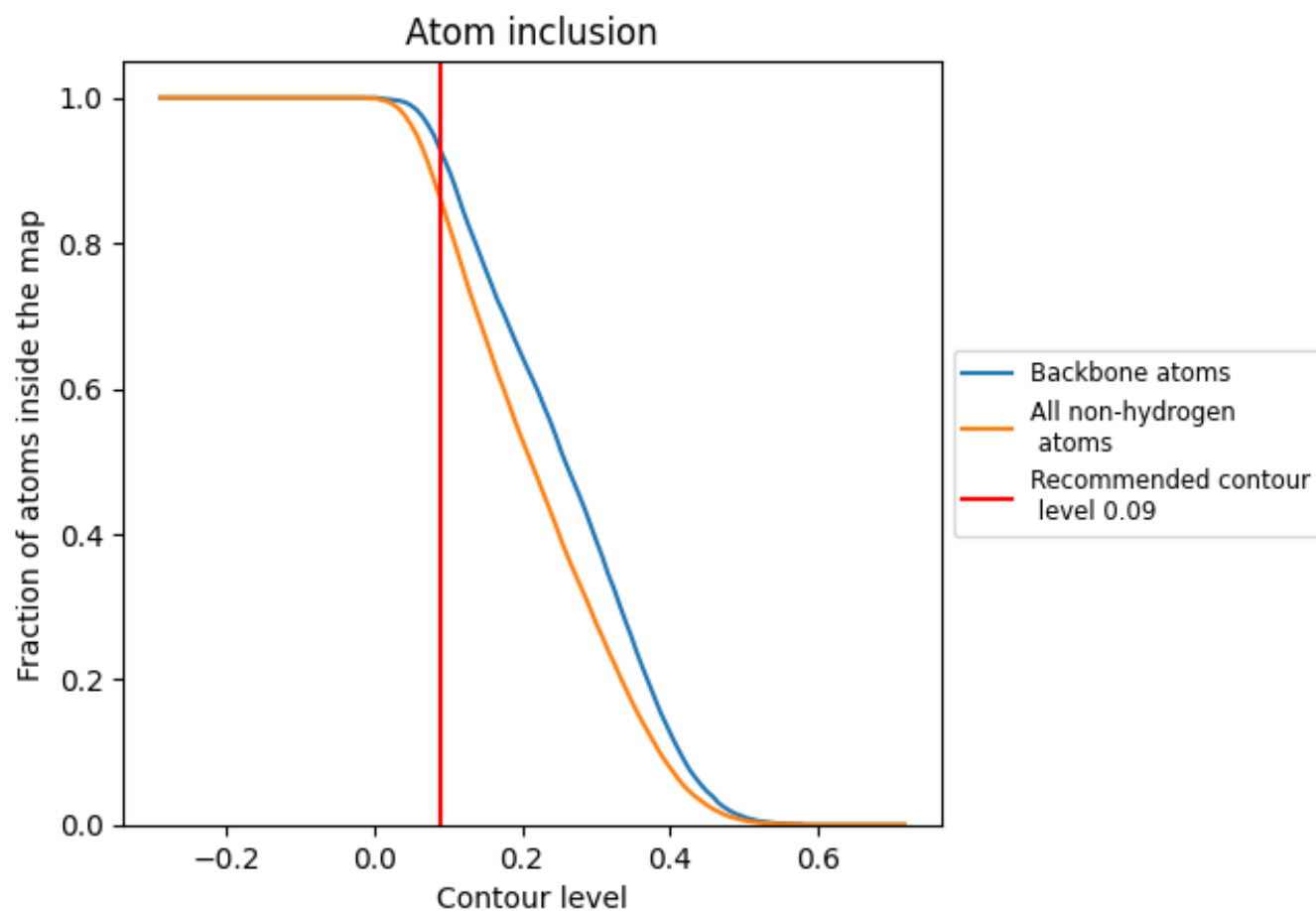
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 86% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8610	0.4890
A	0.8910	0.5090
B	0.8920	0.5180
C	0.9170	0.5360
D	0.4420	0.2030
E	0.9000	0.4810
F	0.8810	0.5110
G	0.5380	0.2820
H	0.8700	0.5080
I	0.8490	0.4370
J	0.9110	0.5490
K	0.9280	0.5390
L	0.8500	0.4700
N	0.9060	0.4020
P	1.0000	0.5900
T	0.9490	0.4910

1.0

0.0

<0.0