



Full wwPDB EM Validation Report ⓘ

Jul 1, 2026 – 11:13 am BST

PDB ID : 9SBY / pdb_00009sby
EMDB ID : EMD-54743
Title : Structure of Yeast RNA polymerase II elongation complex with ATP frame-14
Authors : Yi, G.; Li, Q.; Zhang, P.; Wang, D.
Deposited on : 2025-08-08
Resolution : 3.41 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

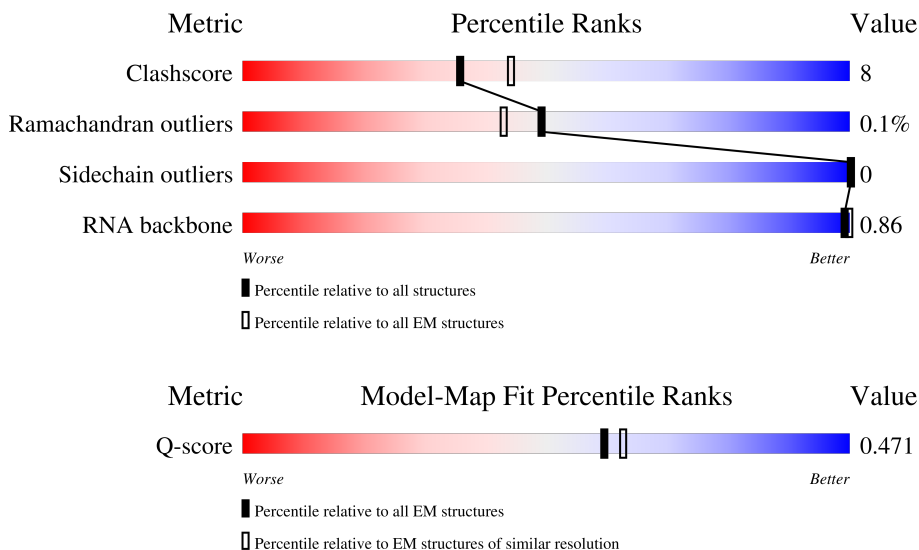
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.41 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	13997 (2.91 - 3.91)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	
2	B	1224	
3	C	318	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	74	
14	R	9	
15	T	74	

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 33083 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1390	10942	6911	1913	2056	62	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1150	9155	5787	1602	1711	55	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	266	2095	1317	348	417	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	167	1327	821	230	273	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	213	1744	1107	308	318	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	83	670	428	114	125	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	171	1340	861	222	249	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	134	1077	679	182	212	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	112	909	561	164	173	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	65	532	339	93	94	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	112	904	580	154	168	2	0	0

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

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

- Molecule 13 is a DNA chain called DNA (74-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
13	N	44	905	428	172	261	44	0	0

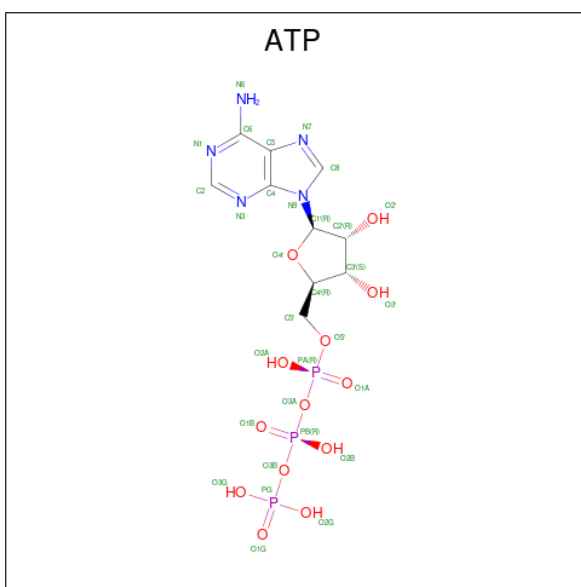
- Molecule 14 is a RNA chain called RNA (5'-R(P*AP*UP*CP*GP*AP*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			P
14	R	9	197	88	40	60	9	0	0

- Molecule 15 is a DNA chain called DNA (74-MER).

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			P
15	T	44	886	423	147	272	44	0	0

- Molecule 16 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



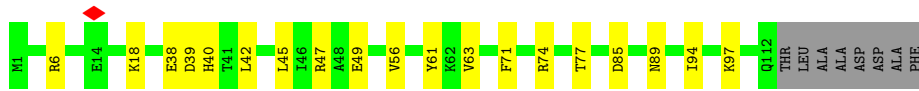
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
16	A	1	31	10	5	13	3	0

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

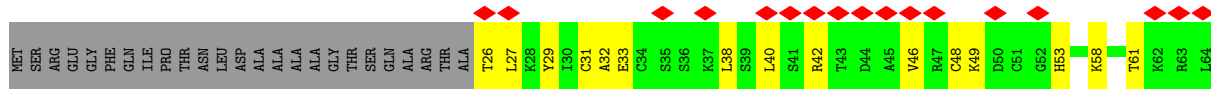
Mol	Chain	Residues	Atoms	AltConf
			Total	
17	A	2	Mg 2	0

- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

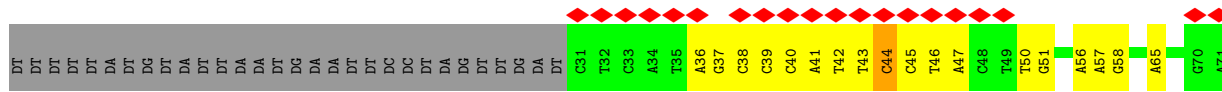
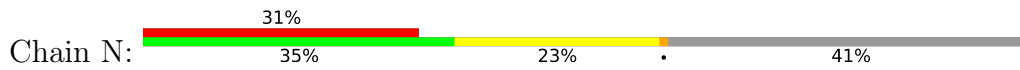
Mol	Chain	Residues	Atoms		AltConf
18	A	2	Total 2	Zn 2	0
18	B	1	Total 1	Zn 1	0
18	C	1	Total 1	Zn 1	0
18	I	2	Total 2	Zn 2	0
18	J	1	Total 1	Zn 1	0
18	L	1	Total 1	Zn 1	0



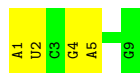
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 13: DNA (74-MER)



- Molecule 14: RNA (5'-R(P*AP*UP*CP*GP*AP*GP*AP*GP*G)-3')



- Molecule 15: DNA (74-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	89544	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.919	Depositor
Minimum map value	-0.433	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.16	Depositor
Map size (\AA)	348.18, 348.18, 348.18	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0880625, 1.0880625, 1.0880625	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.22	0/11139	0.33	0/15057
2	B	0.22	0/9332	0.30	0/12579
3	C	0.24	0/2133	0.30	0/2891
4	D	0.09	0/1336	0.21	0/1794
5	E	0.21	0/1780	0.30	0/2395
6	F	0.21	0/682	0.27	0/922
7	G	0.13	0/1368	0.26	0/1844
8	H	0.21	0/1095	0.26	0/1482
9	I	0.13	0/927	0.36	0/1249
10	J	0.25	0/541	0.32	0/727
11	K	0.22	0/922	0.26	0/1244
12	L	0.12	0/361	0.30	0/478
13	N	1.20	1/1016 (0.1%)	0.92	3/1566 (0.2%)
14	R	0.25	0/221	0.32	0/343
15	T	0.37	0/987	0.74	0/1518
All	All	0.30	1/33840 (0.0%)	0.37	3/46089 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	44	DC	O3'-P	36.85	2.16	1.61

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	N	44	DC	P-O3'-C3'	-18.83	91.96	120.20
13	N	44	DC	O3'-P-O5'	-7.56	92.65	104.00
13	N	44	DC	OP2-P-O3'	6.28	126.83	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	10942	0	11025	181	0
2	B	9155	0	9161	166	0
3	C	2095	0	2051	35	0
4	D	1327	0	1331	19	0
5	E	1744	0	1772	18	0
6	F	670	0	690	7	0
7	G	1340	0	1357	29	0
8	H	1077	0	1050	9	0
9	I	909	0	867	23	0
10	J	532	0	542	13	0
11	K	904	0	911	15	0
12	L	359	0	381	18	0
13	N	905	0	494	26	0
14	R	197	0	97	2	0
15	T	886	0	498	10	0
16	A	31	0	12	0	0
17	A	2	0	0	0	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	C	1	0	0	0	0
18	I	2	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
All	All	33083	0	32239	505	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (505) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:44:DC:O3'	13:N:45:DC:P	2.16	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:44:DC:C3'	13:N:45:DC:P	2.62	0.86
2:B:996:ARG:HH21	3:C:38:ILE:HG23	1.39	0.85
3:C:35:ARG:HH12	11:K:40:HIS:HB2	1.42	0.83
12:L:31:CYS:HB2	12:L:48:CYS:SG	2.20	0.80
2:B:996:ARG:NH1	10:J:10:CYS:O	2.15	0.79
1:A:1308:THR:HG22	1:A:1310:GLY:H	1.48	0.76
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.67	0.75
3:C:66:ARG:NH2	10:J:3:VAL:O	2.17	0.74
2:B:380:TYR:OH	2:B:384:ARG:NH2	2.21	0.74
13:N:44:DC:H3'	13:N:45:DC:P	2.27	0.73
2:B:158:ASP:HA	2:B:163:GLY:HA3	1.70	0.72
1:A:399:HIS:O	1:A:435:HIS:ND1	2.23	0.72
1:A:1205:LYS:O	1:A:1274:ARG:NH2	2.21	0.72
5:E:97:VAL:HG13	5:E:127:ILE:HD13	1.71	0.72
1:A:939:ASP:OD2	1:A:1023:ARG:NH1	2.24	0.71
1:A:1277:GLU:OE1	1:A:1278:ASN:ND2	2.24	0.70
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.72	0.70
10:J:10:CYS:SG	10:J:11:GLY:N	2.64	0.70
2:B:276:ILE:HG21	2:B:280:ILE:HD11	1.74	0.69
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.74	0.69
2:B:739:THR:O	2:B:740:HIS:ND1	2.25	0.69
2:B:895:ASP:O	12:L:42:ARG:NH2	2.26	0.69
1:A:1256:GLU:OE1	1:A:1258:HIS:ND1	2.26	0.68
2:B:208:SER:OG	2:B:210:LYS:NZ	2.27	0.68
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.75	0.68
1:A:1199:ARG:NH2	1:A:1233:ASP:O	2.28	0.67
2:B:287:ARG:NH2	2:B:294:ASP:OD1	2.27	0.67
1:A:107:CYS:SG	1:A:171:GLN:NE2	2.66	0.67
2:B:90:ILE:HG12	2:B:134:LYS:HD3	1.77	0.67
3:C:10:ILE:HD13	3:C:20:PHE:HB3	1.75	0.67
4:D:148:LEU:O	4:D:152:SER:OG	2.13	0.66
2:B:903:VAL:HG13	12:L:61:THR:HG21	1.77	0.66
1:A:1423:GLY:O	1:A:1427:ASN:ND2	2.29	0.66
1:A:1124:HIS:O	1:A:1130:GLN:NE2	2.29	0.66
2:B:1006:ILE:HD11	10:J:43:ARG:HB3	1.78	0.65
13:N:37:DG:H4'	13:N:38:DC:H5'	1.78	0.65
2:B:345:LYS:HD3	2:B:348:ARG:HH22	1.60	0.65
1:A:541:ILE:HD13	1:A:549:MET:HE1	1.76	0.65
1:A:1194:ARG:HG2	1:A:1239:ARG:HG2	1.77	0.65
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.78	0.65
2:B:1156:ASP:HB3	2:B:1198:TYR:H	1.60	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:852:ARG:NH2	12:L:70:ARG:OXT	2.29	0.64
2:B:157:GLU:HG3	2:B:163:GLY:HA2	1.79	0.64
1:A:1286:LYS:HD2	1:A:1302:PRO:HB2	1.80	0.64
3:C:90:ASP:OD2	3:C:91:HIS:ND1	2.29	0.64
9:I:88:SER:O	9:I:91:ARG:NH2	2.30	0.64
4:D:66:ARG:NH2	7:G:47:CYS:SG	2.71	0.64
2:B:87:LYS:HB3	2:B:137:TYR:HB2	1.79	0.64
1:A:1197:LEU:HD12	1:A:1209:MET:HE1	1.78	0.63
7:G:101:VAL:N	7:G:108:VAL:O	2.30	0.63
2:B:400:HIS:NE2	2:B:699:GLU:OE2	2.28	0.63
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.81	0.62
1:A:115:LEU:HB2	1:A:122:MET:HE3	1.81	0.62
1:A:343:LYS:HD2	2:B:1151:LEU:HD22	1.82	0.62
1:A:1155:ASP:OD2	1:A:1241:ARG:NH2	2.32	0.62
13:N:38:DC:H4'	13:N:39:DC:OP1	2.00	0.62
7:G:116:PRO:HD3	7:G:163:ILE:HG13	1.81	0.61
1:A:711:ARG:HA	1:A:714:PHE:HB3	1.81	0.61
2:B:849:GLY:HA2	2:B:852:ARG:HD2	1.81	0.61
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.80	0.61
1:A:1278:ASN:HD22	1:A:1312:ASN:HD22	1.48	0.61
9:I:10:CYS:SG	9:I:31:THR:OG1	2.59	0.61
10:J:37:SER:OG	10:J:47:ARG:NH2	2.34	0.61
3:C:179:GLU:OE1	3:C:206:ASN:ND2	2.31	0.60
3:C:31:ASN:OD1	3:C:34:ARG:NH2	2.34	0.60
4:D:67:ARG:HH21	4:D:132:GLN:HB2	1.66	0.60
13:N:40:DC:H1'	13:N:41:DA:C6	2.37	0.60
2:B:780:VAL:HG22	2:B:795:ILE:HG23	1.83	0.60
1:A:605:MET:HE2	1:A:621:THR:HG21	1.82	0.60
1:A:840:ARG:NH2	1:A:1106:ASN:OD1	2.35	0.60
1:A:940:ARG:HH21	1:A:944:ARG:NH2	2.00	0.60
13:N:46:DT:H4'	13:N:47:DA:H5'	1.83	0.60
1:A:715:GLU:OE1	1:A:774:ARG:NE	2.31	0.59
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.84	0.59
2:B:102:VAL:HG21	2:B:122:LEU:HD13	1.83	0.59
2:B:259:TYR:OH	2:B:279:ASP:OD2	2.18	0.59
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.84	0.59
1:A:847:ASP:HB3	1:A:1398:MET:HE1	1.85	0.59
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.83	0.59
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.85	0.59
11:K:85:ASP:O	11:K:89:ASN:ND2	2.36	0.59
1:A:120:GLU:OE1	1:A:123:ARG:NH1	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:LYS:NZ	1:A:716:ASP:OD2	2.36	0.59
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.84	0.59
13:N:44:DC:O3'	13:N:45:DC:H5'	2.02	0.59
1:A:1144:LYS:HG3	9:I:48:LEU:HD12	1.86	0.58
11:K:49:GLU:OE2	11:K:97:LYS:NZ	2.25	0.58
1:A:1410:PHE:HD1	2:B:1212:ILE:HD11	1.69	0.58
4:D:66:ARG:NH1	7:G:35:GLU:OE2	2.31	0.58
8:H:48:PRO:O	8:H:146:ARG:NH2	2.37	0.58
14:R:1:A:H2'	14:R:2:U:C6	2.39	0.57
2:B:680:THR:O	2:B:683:SER:OG	2.21	0.57
7:G:114:LEU:HD13	7:G:162:SER:HB2	1.86	0.57
1:A:1192:LEU:HD13	1:A:1241:ARG:HE	1.68	0.57
2:B:951:GLN:OE1	2:B:967:ARG:NH2	2.37	0.57
9:I:74:GLU:OE2	9:I:79:HIS:ND1	2.36	0.57
1:A:922:ASP:OD1	1:A:923:LEU:N	2.37	0.57
1:A:72:GLU:HB3	1:A:76:GLU:HB3	1.87	0.57
2:B:65:GLU:OE1	2:B:418:LYS:NZ	2.36	0.57
9:I:65:ASP:OD2	9:I:67:THR:OG1	2.22	0.57
1:A:710:LEU:O	1:A:713:SER:N	2.38	0.57
7:G:86:VAL:HG22	7:G:146:LYS:HB2	1.87	0.57
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.87	0.56
1:A:445:ASN:HB2	1:A:455:MET:HG3	1.86	0.56
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.70	0.56
2:B:896:ASP:OD2	12:L:29:TYR:OH	2.22	0.56
1:A:842:VAL:O	1:A:846:GLU:HB3	2.05	0.56
1:A:1420:ASP:OD1	2:B:1220:ARG:NH1	2.38	0.56
2:B:86:ARG:HG3	2:B:138:GLU:HG2	1.87	0.56
5:E:152:LYS:HE3	5:E:154:ILE:HD11	1.86	0.56
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.70	0.56
13:N:46:DT:H1'	13:N:47:DA:C2	2.40	0.56
1:A:1279:ILE:HD12	1:A:1308:THR:HG21	1.87	0.56
1:A:706:HIS:HB2	1:A:1283:VAL:HG21	1.87	0.56
1:A:282:ASN:OD1	1:A:283:GLY:N	2.39	0.56
1:A:401:GLY:H	1:A:435:HIS:HD1	1.53	0.56
1:A:1066:VAL:O	1:A:1070:GLN:HG3	2.06	0.56
2:B:287:ARG:NH1	2:B:292:ILE:O	2.39	0.56
13:N:56:DA:H1'	13:N:57:DA:H5'	1.87	0.55
1:A:342:GLY:O	2:B:1129:ARG:NH1	2.38	0.55
12:L:26:THR:OG1	12:L:40:LEU:O	2.24	0.55
1:A:406:ILE:HB	1:A:431:LYS:HB2	1.89	0.55
1:A:833:GLU:O	1:A:837:ILE:HD12	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:101:VAL:HG21	7:G:145:VAL:HG21	1.87	0.55
2:B:864:LYS:O	2:B:871:THR:N	2.39	0.55
1:A:502:SER:OG	1:A:503:GLN:NE2	2.33	0.55
4:D:56:ARG:HB2	4:D:148:LEU:HB3	1.89	0.55
12:L:38:LEU:HD21	12:L:49:LYS:H	1.70	0.55
1:A:503:GLN:OE1	6:F:90:ARG:NH2	2.39	0.55
2:B:394:ASP:OD1	2:B:395:GLN:N	2.40	0.54
15:T:33:DT:H2"	15:T:34:DT:OP2	2.07	0.54
1:A:549:MET:HE3	1:A:577:ILE:HG21	1.88	0.54
1:A:668:ASP:OD2	1:A:742:ASN:ND2	2.39	0.54
2:B:332:ASP:OD1	2:B:348:ARG:NH1	2.39	0.54
1:A:771:GLU:N	1:A:822:GLU:OE2	2.40	0.54
1:A:1154:TYR:H	9:I:41:PRO:HB2	1.70	0.54
1:A:550:LEU:HD11	1:A:561:PRO:HD2	1.90	0.54
2:B:102:VAL:HB	2:B:112:LEU:HD22	1.90	0.54
2:B:842:ASN:OD1	2:B:845:SER:N	2.32	0.54
3:C:169:LYS:NZ	12:L:69:ALA:O	2.38	0.54
1:A:915:SER:O	1:A:919:ILE:HG12	2.08	0.54
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.90	0.53
1:A:443:LEU:HD21	1:A:455:MET:HE2	1.89	0.53
1:A:492:PRO:HG3	1:A:501:LEU:HD12	1.90	0.53
4:D:176:GLU:N	4:D:176:GLU:OE1	2.41	0.53
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.73	0.53
3:C:35:ARG:HH12	11:K:40:HIS:CB	2.19	0.53
2:B:165:VAL:HG11	2:B:448:ILE:HD13	1.90	0.53
2:B:1010:LEU:HD23	2:B:1092:TYR:CD2	2.44	0.53
12:L:32:ALA:HB3	12:L:53:HIS:HE1	1.72	0.53
2:B:637:LEU:HD13	2:B:740:HIS:HB3	1.91	0.53
4:D:153:ARG:NH1	4:D:183:LEU:O	2.41	0.53
1:A:694:THR:O	1:A:698:GLN:N	2.35	0.53
1:A:1116:LEU:HB2	1:A:1308:THR:HB	1.90	0.53
8:H:8:ASP:OD1	8:H:9:ILE:N	2.41	0.53
2:B:345:LYS:HG3	2:B:348:ARG:HH12	1.73	0.53
1:A:666:ILE:HG21	2:B:1030:LEU:HD22	1.90	0.53
2:B:682:SER:O	2:B:686:ASN:ND2	2.42	0.53
12:L:31:CYS:SG	12:L:32:ALA:N	2.82	0.52
13:N:39:DC:O2	15:T:52:DG:N1	2.43	0.52
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.91	0.52
7:G:122:ASN:ND2	7:G:125:SER:HB3	2.24	0.52
1:A:318:SER:OG	1:A:320:ARG:NH1	2.42	0.52
1:A:1446:ASP:OD1	1:A:1447:GLU:N	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:75:MET:O	3:C:246:ARG:NH2	2.29	0.52
4:D:194:LEU:HD22	7:G:86:VAL:HG11	1.91	0.52
11:K:56:VAL:HG22	11:K:77:THR:HG22	1.91	0.52
1:A:348:SER:HB2	2:B:1128:LEU:HD12	1.92	0.52
2:B:895:ASP:HB2	12:L:27:LEU:HD21	1.92	0.52
13:N:37:DG:H2 [?]	13:N:38:DC:C6	2.45	0.52
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.46	0.51
1:A:443:LEU:HD11	1:A:455:MET:HG2	1.91	0.51
4:D:175:PHE:CE2	7:G:1:MET:HG3	2.44	0.51
1:A:1111:MET:HE1	1:A:1331:SER:HA	1.91	0.51
2:B:87:LYS:HD2	2:B:137:TYR:HD2	1.76	0.51
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.92	0.51
1:A:402:ALA:HA	1:A:434:ARG:HA	1.92	0.51
1:A:380:VAL:HG23	1:A:428:TYR:HA	1.92	0.51
5:E:131:THR:HG21	5:E:191:LYS:HE3	1.92	0.51
1:A:614:PHE:HB3	8:H:122:LEU:HD21	1.93	0.51
2:B:801:LYS:O	10:J:52:THR:HG23	2.10	0.51
8:H:110:ASP:OD1	8:H:110:ASP:N	2.43	0.51
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.92	0.51
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.91	0.50
1:A:492:PRO:O	1:A:493:GLN:NE2	2.44	0.50
2:B:137:TYR:HE1	2:B:151:LEU:HD13	1.76	0.50
3:C:258:ILE:HG13	11:K:42:LEU:HD21	1.91	0.50
11:K:47:ARG:HD2	11:K:61:TYR:CD1	2.46	0.50
13:N:40:DC:H4 [']	13:N:41:DA:C8	2.46	0.50
4:D:5:THR:HG21	7:G:7:LEU:HD13	1.93	0.50
1:A:1206:ASP:O	1:A:1274:ARG:NH2	2.37	0.50
9:I:15:TYR:N	9:I:28:GLU:O	2.43	0.50
2:B:37:PHE:HE1	2:B:41:LYS:HD2	1.76	0.50
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.76	0.50
3:C:36:VAL:HG21	3:C:251:LEU:HD13	1.93	0.50
7:G:122:ASN:HD22	7:G:131:GLN:CD	2.19	0.50
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.94	0.50
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.93	0.50
4:D:190:GLU:HA	4:D:193:THR:HG22	1.94	0.50
1:A:1129:GLU:OE1	1:A:1132:LYS:NZ	2.32	0.49
10:J:1:MET:HA	10:J:56:LEU:HB2	1.94	0.49
1:A:873:MET:HG3	1:A:957:PRO:HG3	1.95	0.49
1:A:1120:LEU:HD23	1:A:1130:GLN:HE22	1.77	0.49
7:G:131:GLN:HG2	7:G:136:VAL:HG13	1.93	0.49
7:G:144:ARG:HB2	7:G:171:ILE:HD11	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:31:ASP:OD1	10:J:31:ASP:N	2.45	0.49
2:B:237:VAL:HG23	2:B:257:LYS:HG2	1.94	0.49
2:B:557:PHE:HB3	2:B:561:TRP:CZ3	2.48	0.49
13:N:37:DG:H2''	13:N:38:DC:C5	2.47	0.49
3:C:166:GLU:OE2	12:L:70:ARG:NH2	2.44	0.49
2:B:908:GLU:N	2:B:908:GLU:OE1	2.45	0.49
7:G:143:ILE:HG23	7:G:169:GLY:HA2	1.94	0.49
1:A:286:HIS:C	1:A:288:ALA:H	2.21	0.48
2:B:900:ALA:HB3	12:L:61:THR:HG22	1.95	0.48
2:B:45:SER:OG	2:B:46:GLN:OE1	2.31	0.48
2:B:877:PRO:HB2	2:B:885:MET:HE1	1.94	0.48
15:T:35:DC:H2'	15:T:36:DT:H71	1.94	0.48
2:B:629:ASP:OD1	2:B:630:ALA:N	2.46	0.48
11:K:18:LYS:NZ	11:K:38:GLU:OE2	2.40	0.48
9:I:94:ASP:OD1	9:I:94:ASP:N	2.45	0.48
1:A:789:LYS:HG3	9:I:67:THR:HB	1.95	0.48
1:A:894:GLU:OE1	1:A:933:TYR:OH	2.28	0.48
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.95	0.48
2:B:856:PHE:CE1	2:B:969:ARG:HG3	2.49	0.48
2:B:120:ARG:HB2	2:B:122:LEU:HG	1.96	0.48
2:B:604:ARG:HD2	2:B:615:MET:HE2	1.96	0.48
1:A:526:ASP:HB2	2:B:835:GLN:NE2	2.29	0.47
1:A:544:ASP:OD1	1:A:545:GLN:N	2.47	0.47
2:B:352:ALA:O	2:B:355:ILE:HG22	2.14	0.47
7:G:119:LEU:HA	7:G:132:SER:HB3	1.95	0.47
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.96	0.47
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	1.95	0.47
2:B:840:ILE:HG22	2:B:999:MET:HE1	1.96	0.47
1:A:771:GLU:H	1:A:822:GLU:CD	2.22	0.47
2:B:1117:GLN:HG2	2:B:1156:ASP:OD1	2.13	0.47
13:N:45:DC:H2''	13:N:46:DT:H2'	1.96	0.47
1:A:350:ARG:NE	1:A:486:GLU:OE1	2.47	0.47
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.97	0.47
2:B:600:LEU:HB3	2:B:615:MET:SD	2.54	0.47
2:B:889:THR:HG22	2:B:891:ASP:H	1.80	0.47
3:C:99:LEU:HG	3:C:120:ILE:HD13	1.97	0.47
5:E:26:ARG:NH2	5:E:133:GLU:OE1	2.35	0.47
9:I:70:ARG:HG2	9:I:84:VAL:HG12	1.97	0.47
1:A:890:ASP:HA	1:A:940:ARG:HH12	1.79	0.47
2:B:487:THR:O	2:B:490:SER:OG	2.27	0.47
11:K:39:ASP:OD1	11:K:39:ASP:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:MET:HE3	1:A:607:ILE:HD11	1.97	0.47
2:B:169:ARG:N	2:B:454:THR:OG1	2.45	0.47
4:D:184:ALA:H	7:G:144:ARG:HH22	1.63	0.47
9:I:75:CYS:HB3	9:I:80:SER:H	1.79	0.47
2:B:343:ILE:O	2:B:348:ARG:NH2	2.48	0.47
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.97	0.47
2:B:957:ASN:OD1	2:B:958:GLN:N	2.44	0.47
1:A:535:THR:HG21	1:A:617:VAL:HG23	1.96	0.46
2:B:35:SER:HG	2:B:811:TYR:HH	1.58	0.46
13:N:37:DG:C4'	13:N:38:DC:H5'	2.44	0.46
1:A:1116:LEU:HD23	1:A:1329:THR:HB	1.97	0.46
6:F:76:LYS:O	6:F:79:ARG:NE	2.46	0.46
9:I:76:PRO:HD2	9:I:110:PHE:CE2	2.50	0.46
1:A:446:ARG:HB2	1:A:487:MET:HE3	1.97	0.46
1:A:896:ARG:O	1:A:1029:ARG:HG2	2.15	0.46
1:A:1106:ASN:O	1:A:1107:VAL:C	2.59	0.46
2:B:499:ASN:OD1	2:B:500:THR:N	2.47	0.46
7:G:55:ASP:HB3	7:G:73:LYS:HB2	1.97	0.46
9:I:51:ASN:HB2	9:I:90:GLN:HG3	1.97	0.46
1:A:401:GLY:O	1:A:435:HIS:ND1	2.48	0.46
1:A:704:ALA:HB3	1:A:1281:ARG:HH22	1.79	0.46
2:B:496:ARG:HD3	2:B:751:VAL:HG21	1.97	0.46
1:A:683:ILE:O	1:A:687:LYS:HG2	2.15	0.46
1:A:929:LEU:HD11	1:A:983:ILE:HD13	1.97	0.46
9:I:48:LEU:HD23	9:I:48:LEU:H	1.80	0.46
1:A:379:VAL:HG12	1:A:431:LYS:HG2	1.98	0.46
1:A:845:LEU:HB2	1:A:848:ILE:HD12	1.98	0.46
2:B:734:HIS:C	2:B:736:THR:H	2.23	0.46
1:A:34:LYS:NZ	1:A:85:ASP:OD2	2.47	0.46
1:A:956:LEU:HD21	1:A:1017:LEU:HD23	1.98	0.46
1:A:1171:GLN:HG3	1:A:1172:LEU:HD22	1.97	0.46
2:B:798:TYR:O	2:B:821:GLN:NE2	2.37	0.46
4:D:8:PHE:CZ	4:D:40:HIS:HA	2.50	0.46
2:B:315:LYS:HE2	9:I:4:PHE:HE1	1.81	0.46
3:C:17:ASN:OD1	3:C:233:GLU:HG2	2.16	0.46
3:C:241:ASP:OD1	3:C:242:GLN:N	2.49	0.46
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.97	0.46
1:A:1170:ILE:HA	1:A:1173:HIS:HD2	1.80	0.45
4:D:39:ASN:ND2	4:D:43:GLU:OE2	2.48	0.45
1:A:22:PHE:HB3	1:A:27:VAL:HG23	1.98	0.45
6:F:116:ASP:O	6:F:120:ILE:HG12	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:LEU:HD21	10:J:57:ILE:HD13	1.97	0.45
1:A:336:ILE:HD12	1:A:1405:THR:HG21	1.99	0.45
1:A:675:THR:O	1:A:679:ILE:HG12	2.16	0.45
2:B:766:ARG:HG3	2:B:1022:THR:HG22	1.97	0.45
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.50	0.45
1:A:1016:THR:HB	5:E:206:GLY:HA3	1.98	0.45
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.51	0.45
2:B:326:ASP:OD1	2:B:327:ARG:N	2.49	0.45
2:B:518:HIS:HB3	2:B:522:VAL:HG22	1.99	0.45
13:N:42:DT:H2''	13:N:43:DT:H5''	1.99	0.45
1:A:268:ASP:OD1	1:A:299:HIS:NE2	2.50	0.45
1:A:879:GLU:OE2	1:A:962:ARG:NH2	2.37	0.45
1:A:1397:LEU:HB2	1:A:1426:GLU:HG3	1.98	0.45
1:A:260:ASP:OD2	1:A:328:ARG:NH2	2.49	0.45
1:A:535:THR:HG23	1:A:575:LYS:HG2	1.99	0.45
1:A:851:HIS:CE1	1:A:857:ARG:HB2	2.51	0.45
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.42	0.44
1:A:544:ASP:HB2	11:K:47:ARG:HH22	1.81	0.44
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.52	0.44
2:B:1223:ASP:OD1	2:B:1224:PHE:N	2.50	0.44
5:E:86:PRO:O	5:E:114:ASN:HB2	2.17	0.44
7:G:13:LEU:HD11	7:G:26:LEU:HG	1.98	0.44
13:N:44:DC:HO3'	13:N:45:DC:P	2.36	0.44
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.16	0.44
2:B:46:GLN:NE2	2:B:545:ILE:H	2.15	0.44
2:B:384:ARG:HD2	2:B:393:LYS:NZ	2.32	0.44
2:B:605:ARG:NE	2:B:691:GLU:OE2	2.49	0.44
3:C:178:PHE:CE1	3:C:230:MET:HE2	2.52	0.44
7:G:139:ILE:HG22	7:G:140:LYS:HG3	1.99	0.44
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.99	0.44
1:A:398:GLU:HG2	1:A:400:PRO:HD2	1.98	0.44
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.99	0.44
4:D:188:ALA:HB2	4:D:208:GLU:HG3	1.98	0.44
5:E:143:ASN:OD1	5:E:145:THR:OG1	2.30	0.44
15:T:53:DC:H2''	15:T:54:DT:H2'	1.99	0.44
1:A:1128:GLN:HB2	1:A:1304:TRP:NE1	2.33	0.44
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.18	0.44
1:A:698:GLN:HG2	9:I:99:LEU:HB2	1.99	0.44
3:C:37:MET:HE3	3:C:176:ILE:HD13	2.00	0.44
5:E:117:THR:OG1	13:N:65:DA:OP1	2.29	0.44
6:F:133:VAL:HG23	6:F:147:SER:HA	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:85:PHE:HB3	9:I:101:PHE:CD2	2.53	0.44
1:A:446:ARG:HB2	1:A:487:MET:HG2	2.00	0.44
1:A:677:ARG:O	1:A:681:GLU:HG2	2.17	0.44
1:A:1199:ARG:HH22	1:A:1234:GLU:C	2.26	0.44
2:B:617:ARG:NH2	9:I:61:ASP:OD2	2.50	0.44
2:B:900:ALA:HB2	12:L:58:LYS:HZ2	1.83	0.44
2:B:1152:MET:HE3	2:B:1152:MET:HB3	1.85	0.44
3:C:165:LYS:O	11:K:6:ARG:NH2	2.50	0.44
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.98	0.44
15:T:42:DC:H2'	15:T:43:DC:C6	2.52	0.44
1:A:551:TYR:CE1	11:K:74:ARG:HD2	2.53	0.44
1:A:1128:GLN:CD	1:A:1129:GLU:H	2.25	0.44
1:A:1328:TYR:OH	1:A:1351:GLU:OE2	2.28	0.44
13:N:36:DA:H1'	13:N:37:DG:O4'	2.18	0.44
15:T:33:DT:H2''	15:T:34:DT:H71	2.00	0.44
1:A:434:ARG:HH22	1:A:498:ARG:NH2	2.15	0.43
2:B:134:LYS:HG2	2:B:442:PHE:HZ	1.82	0.43
10:J:8:PHE:HB2	10:J:48:ARG:HH22	1.83	0.43
1:A:1220:PHE:HB3	1:A:1223:ASP:OD1	2.18	0.43
2:B:158:ASP:N	2:B:158:ASP:OD1	2.51	0.43
2:B:604:ARG:CD	2:B:615:MET:HE2	2.48	0.43
2:B:798:TYR:HE1	3:C:66:ARG:HH21	1.66	0.43
12:L:33:GLU:HG3	12:L:53:HIS:CE1	2.53	0.43
2:B:641:GLU:OE1	2:B:652:LYS:HE2	2.18	0.43
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	2.00	0.43
7:G:81:PRO:HB3	7:G:106:MET:HE1	1.99	0.43
12:L:32:ALA:HB3	12:L:53:HIS:CE1	2.53	0.43
1:A:840:ARG:NE	1:A:1384:VAL:O	2.51	0.43
10:J:41:LEU:HD22	10:J:46:CYS:HB3	2.01	0.43
1:A:472:LEU:HD13	2:B:835:GLN:CD	2.44	0.43
3:C:178:PHE:HE1	3:C:230:MET:HE2	1.84	0.43
9:I:7:CYS:N	9:I:12:ASN:O	2.30	0.43
1:A:596:THR:C	1:A:598:LEU:H	2.25	0.43
1:A:704:ALA:HB3	1:A:1281:ARG:HH12	1.84	0.43
1:A:883:LEU:HD13	1:A:943:LEU:HD13	2.00	0.43
2:B:954:VAL:HG12	12:L:46:VAL:HG11	2.00	0.43
4:D:167:LEU:HB3	4:D:177:VAL:HG13	2.01	0.43
5:E:102:GLU:HG3	5:E:103:LYS:HG3	2.01	0.43
7:G:26:LEU:HD23	7:G:26:LEU:HA	1.80	0.43
2:B:175:ARG:NH2	2:B:198:ASP:O	2.52	0.43
2:B:335:GLY:HA3	2:B:348:ARG:HB3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:642:ASP:HB3	2:B:649:LYS:HG3	2.01	0.43
2:B:1072:MET:HG3	2:B:1085:ILE:HB	2.00	0.43
5:E:96:PHE:CE2	5:E:100:ILE:HD11	2.54	0.43
2:B:1010:LEU:HD23	2:B:1092:TYR:HD2	1.82	0.43
1:A:733:ALA:O	1:A:737:LEU:HG	2.19	0.43
1:A:778:GLY:HA3	2:B:516:ASN:HB2	2.00	0.43
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	2.00	0.43
5:E:43:LYS:O	5:E:47:CYS:HB2	2.18	0.43
8:H:15:VAL:HG23	8:H:26:ILE:HG22	2.01	0.43
14:R:4:G:H2'	14:R:5:A:C8	2.54	0.43
2:B:258:LEU:HD21	2:B:267:ARG:NH2	2.34	0.43
5:E:176:PRO:HB2	5:E:212:ARG:HD3	2.01	0.43
11:K:63:VAL:HG22	11:K:71:PHE:HB3	2.01	0.43
1:A:567:LYS:HB3	1:A:568:PRO:HD3	2.01	0.42
2:B:355:ILE:HD12	2:B:359:GLU:OE1	2.19	0.42
2:B:759:PRO:HD2	2:B:1046:PRO:HA	2.01	0.42
2:B:996:ARG:NH2	3:C:38:ILE:HG23	2.20	0.42
4:D:193:THR:HG21	7:G:167:TYR:CE2	2.54	0.42
7:G:113:HIS:O	7:G:164:LYS:HE3	2.19	0.42
13:N:40:DC:H4'	13:N:41:DA:C4	2.54	0.42
15:T:53:DC:C6	15:T:53:DC:H5''	2.55	0.42
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.86	0.42
1:A:845:LEU:HD12	1:A:845:LEU:O	2.19	0.42
2:B:37:PHE:CE1	2:B:41:LYS:HD2	2.54	0.42
2:B:597:MET:HE1	2:B:615:MET:HB2	2.00	0.42
1:A:1129:GLU:CD	1:A:1132:LYS:HZ1	2.20	0.42
2:B:293:PRO:HB2	9:I:11:ASN:HB3	2.02	0.42
4:D:214:LEU:HA	4:D:217:LEU:HG	2.00	0.42
11:K:47:ARG:HD2	11:K:61:TYR:HD1	1.83	0.42
15:T:39:DC:H6	15:T:39:DC:H2'	1.66	0.42
1:A:451:HIS:ND1	1:A:453:MET:HE2	2.33	0.42
1:A:1079:MET:O	1:A:1083:THR:HG23	2.18	0.42
2:B:134:LYS:HZ3	2:B:135:ARG:C	2.27	0.42
2:B:756:ILE:HG23	2:B:983:ARG:O	2.19	0.42
5:E:127:ILE:O	5:E:127:ILE:HG13	2.18	0.42
1:A:586:ILE:HD13	1:A:586:ILE:HA	1.88	0.42
1:A:1436:ILE:HG22	1:A:1437:GLY:N	2.34	0.42
7:G:139:ILE:HD12	7:G:139:ILE:H	1.85	0.42
13:N:41:DA:H8	13:N:42:DT:H72	1.83	0.42
1:A:251:SER:HB3	1:A:257:ARG:NH1	2.34	0.42
1:A:1153:TYR:HD2	1:A:1163:ILE:HD11	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:101:LEU:HD23	3:C:155:LEU:HD12	2.01	0.42
1:A:76:GLU:OE2	2:B:1159:ARG:NH2	2.52	0.42
2:B:345:LYS:HA	2:B:348:ARG:NH1	2.34	0.42
2:B:550:ASP:HA	2:B:551:PRO:HD3	1.95	0.42
1:A:1354:ASN:O	1:A:1358:SER:OG	2.31	0.42
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.54	0.42
2:B:79:THR:HB	2:B:82:ASP:CG	2.45	0.42
2:B:270:LYS:HG2	2:B:281:PRO:HA	2.01	0.42
2:B:541:LEU:HD23	2:B:541:LEU:HA	1.91	0.42
7:G:23:LYS:HE2	7:G:27:LYS:NZ	2.35	0.42
10:J:48:ARG:O	10:J:52:THR:HB	2.20	0.42
13:N:40:DC:H1'	13:N:41:DA:N6	2.34	0.42
13:N:57:DA:H2''	13:N:58:DG:C8	2.55	0.42
15:T:42:DC:H2'	15:T:43:DC:H6	1.82	0.42
1:A:1128:GLN:C	1:A:1130:GLN:H	2.28	0.42
1:A:1173:HIS:CE1	1:A:1174:PHE:HB2	2.55	0.42
2:B:211:VAL:HG11	2:B:494:HIS:CD2	2.55	0.42
2:B:1081:LEU:HD23	2:B:1081:LEU:HA	1.88	0.42
3:C:86:CYS:SG	3:C:87:PHE:N	2.93	0.42
5:E:43:LYS:HA	5:E:47:CYS:SG	2.60	0.42
6:F:94:LEU:HD23	6:F:94:LEU:HA	1.90	0.42
6:F:103:MET:HE1	7:G:65:ASP:HB2	2.02	0.41
1:A:368:LYS:HE3	1:A:368:LYS:HB2	1.87	0.41
1:A:486:GLU:OE2	2:B:1102:LYS:HD3	2.19	0.41
2:B:139:ALA:HB2	2:B:149:TYR:HA	2.02	0.41
2:B:1084:GLN:NE2	3:C:190:ASP:O	2.37	0.41
3:C:77:ILE:HD12	3:C:77:ILE:HA	1.88	0.41
1:A:355:GLY:O	1:A:469:ARG:NH1	2.53	0.41
1:A:1161:THR:HB	1:A:1170:ILE:HG13	2.02	0.41
2:B:597:MET:HE3	2:B:601:ARG:HE	1.85	0.41
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.55	0.41
2:B:214:ALA:HB2	2:B:408:LEU:HD23	2.03	0.41
2:B:807:ARG:HG3	2:B:1045:SER:OG	2.20	0.41
3:C:73:GLN:OE1	3:C:75:MET:N	2.53	0.41
8:H:38:LEU:HD13	8:H:123:MET:HE3	2.02	0.41
1:A:286:HIS:CG	1:A:287:HIS:H	2.39	0.41
1:A:304:MET:HE2	2:B:1210:MET:HA	2.02	0.41
2:B:59:LEU:O	2:B:63:ILE:HG12	2.20	0.41
2:B:330:ALA:O	2:B:334:ILE:HG12	2.20	0.41
2:B:485:ARG:NH2	2:B:782:LEU:HD11	2.35	0.41
1:A:1364:ASN:OD1	1:A:1365:TYR:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:LYS:HA	2:B:246:LYS:HD2	1.83	0.41
2:B:634:TYR:HA	2:B:694:ASP:HA	2.01	0.41
7:G:26:LEU:HD13	7:G:56:ILE:HD11	2.02	0.41
1:A:257:ARG:HA	1:A:257:ARG:HH11	1.86	0.41
1:A:326:ARG:NH2	1:A:1407:GLU:OE2	2.45	0.41
1:A:843:LYS:HA	1:A:843:LYS:HD2	1.77	0.41
1:A:949:ASP:OD1	1:A:949:ASP:N	2.49	0.41
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	2.02	0.41
12:L:26:THR:OG1	12:L:27:LEU:N	2.53	0.41
13:N:39:DC:H6	13:N:39:DC:H2'	1.65	0.41
1:A:362:ASP:HB3	1:A:508:PRO:HD3	2.02	0.41
2:B:37:PHE:C	2:B:39:ARG:H	2.29	0.41
2:B:840:ILE:O	2:B:1010:LEU:HD12	2.20	0.41
3:C:29:MET:HB2	3:C:29:MET:HE3	1.84	0.41
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.60	0.41
15:T:52:DG:H4'	15:T:53:DC:OP1	2.19	0.41
1:A:95:PHE:HE1	1:A:1414:ALA:HB2	1.86	0.41
1:A:443:LEU:HB3	1:A:490:HIS:HB2	2.03	0.41
1:A:814:PHE:HB2	2:B:519:TRP:HZ3	1.85	0.41
1:A:1259:MET:HE2	1:A:1259:MET:HA	2.01	0.41
2:B:283:VAL:O	2:B:287:ARG:HG3	2.20	0.41
2:B:705:MET:HE3	2:B:742:GLU:HG3	2.03	0.41
2:B:800:GLN:HB2	2:B:821:GLN:HA	2.03	0.41
2:B:839:MET:SD	2:B:1010:LEU:HD21	2.61	0.41
2:B:994:TYR:HB2	2:B:999:MET:HE2	2.03	0.41
3:C:196:ASP:HB3	3:C:199:LYS:HB3	2.02	0.41
3:C:262:LEU:HD12	3:C:262:LEU:HA	1.90	0.41
1:A:526:ASP:CG	2:B:1013:ASN:HD21	2.29	0.41
2:B:365:THR:HG21	2:B:370:PHE:HB2	2.03	0.41
2:B:652:LYS:HD2	2:B:688:GLY:O	2.21	0.41
2:B:1138:MET:HE2	2:B:1146:PHE:CD1	2.56	0.41
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.56	0.40
1:A:501:LEU:HD23	1:A:501:LEU:HA	1.82	0.40
1:A:512:VAL:HA	1:A:519:PRO:HA	2.03	0.40
2:B:171:PRO:HG2	2:B:461:LEU:HD12	2.03	0.40
9:I:108:HIS:CD2	9:I:109:ILE:H	2.38	0.40
13:N:50:DT:H1'	13:N:51:DG:C8	2.56	0.40
1:A:286:HIS:C	1:A:288:ALA:N	2.79	0.40
1:A:688:LYS:HD3	1:A:688:LYS:HA	1.72	0.40
1:A:1128:GLN:HB2	1:A:1304:TRP:HE1	1.87	0.40
2:B:1163:CYS:HB3	2:B:1166:CYS:SG	2.62	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:311:LEU:HB3	9:I:4:PHE:CZ	2.57	0.40
2:B:324:ILE:HD13	2:B:330:ALA:HA	2.04	0.40
2:B:679:TYR:OH	2:B:687:GLU:OE1	2.37	0.40
2:B:731:VAL:O	2:B:731:VAL:HG13	2.21	0.40
2:B:911:ILE:HG13	2:B:912:ILE:HG13	2.03	0.40
1:A:549:MET:HG2	1:A:655:PHE:CD2	2.57	0.40
2:B:238:ALA:HB2	2:B:385:LEU:HD13	2.03	0.40
2:B:1002:THR:HG22	2:B:1072:MET:SD	2.61	0.40
5:E:176:PRO:O	5:E:213:ILE:HG22	2.21	0.40
9:I:28:GLU:HB3	9:I:35:VAL:HG22	2.03	0.40
1:A:95:PHE:CE1	1:A:1414:ALA:HB2	2.56	0.40
1:A:353:ILE:HD13	1:A:487:MET:SD	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1376/1733 (79%)	1303 (95%)	69 (5%)	4 (0%)	36	65
2	B	1136/1224 (93%)	1099 (97%)	37 (3%)	0	100	100
3	C	264/318 (83%)	256 (97%)	8 (3%)	0	100	100
4	D	161/221 (73%)	158 (98%)	3 (2%)	0	100	100
5	E	211/215 (98%)	203 (96%)	8 (4%)	0	100	100
6	F	81/155 (52%)	80 (99%)	1 (1%)	0	100	100
7	G	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
8	H	130/146 (89%)	129 (99%)	1 (1%)	0	100	100
9	I	110/122 (90%)	99 (90%)	11 (10%)	0	100	100
10	J	63/70 (90%)	61 (97%)	2 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	110/120 (92%)	109 (99%)	1 (1%)	0	100	100
12	L	43/70 (61%)	36 (84%)	7 (16%)	0	100	100
All	All	3854/4565 (84%)	3696 (96%)	154 (4%)	4 (0%)	49	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	710	LEU
1	A	711	ARG
1	A	1107	VAL
1	A	958	VAL

5.3.2 Protein sidechains [i](#)

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	1213/1520 (80%)	1213 (100%)	0	100	100
2	B	997/1061 (94%)	997 (100%)	0	100	100
3	C	234/274 (85%)	234 (100%)	0	100	100
4	D	149/200 (74%)	149 (100%)	0	100	100
5	E	195/197 (99%)	195 (100%)	0	100	100
6	F	73/137 (53%)	73 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	118/128 (92%)	118 (100%)	0	100	100
9	I	106/116 (91%)	106 (100%)	0	100	100
10	J	60/65 (92%)	60 (100%)	0	100	100
11	K	97/102 (95%)	97 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
All	All	3434/4009 (86%)	3434 (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 (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	287	HIS
1	A	445	ASN
1	A	458	HIS
1	A	471	ASN
1	A	479	ASN
1	A	493	GLN
1	A	650	GLN
1	A	660	ASN
1	A	851	HIS
1	A	1128	GLN
1	A	1130	GLN
1	A	1173	HIS
1	A	1278	ASN
2	B	83	ASN
2	B	236	HIS
2	B	366	GLN
2	B	572	HIS
2	B	686	ASN
2	B	822	ASN
3	C	65	HIS
3	C	264	GLN
4	D	2	ASN
5	E	63	ASN
6	F	100	GLN
6	F	104	ASN
7	G	122	ASN
11	K	104	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	R	7/9 (77%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	ATP	A	1801	17	29,33,33	2.91	8 (27%)	44,52,52	2.70	13 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	ATP	A	1801	17	-	4/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	1801	ATP	C8-N9	-9.00	1.21	1.37
16	A	1801	ATP	C4-N9	-8.50	1.18	1.37
16	A	1801	ATP	C6-N6	4.44	1.45	1.34
16	A	1801	ATP	C5-N7	3.57	1.45	1.39
16	A	1801	ATP	C8-N7	3.00	1.37	1.31
16	A	1801	ATP	O4'-C1'	2.80	1.48	1.42
16	A	1801	ATP	C2'-C3'	-2.80	1.45	1.53
16	A	1801	ATP	C5-C6	-2.71	1.33	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	1801	ATP	C4-N9-C8	12.59	119.38	105.73
16	A	1801	ATP	N3-C2-N1	-5.26	120.38	128.60
16	A	1801	ATP	C5-C4-N3	-3.71	121.91	126.75
16	A	1801	ATP	N3-C4-N9	3.66	133.11	127.08
16	A	1801	ATP	C1'-N9-C8	-3.59	119.03	127.14
16	A	1801	ATP	PB-O3B-PG	-3.32	121.42	132.83
16	A	1801	ATP	C5-N7-C8	-3.31	98.80	103.51
16	A	1801	ATP	N9-C8-N7	-3.23	109.50	113.91
16	A	1801	ATP	PA-O3A-PB	-3.03	122.43	132.83
16	A	1801	ATP	C3'-C2'-C1'	2.69	106.55	101.43
16	A	1801	ATP	C4-C5-N7	-2.68	107.35	110.62
16	A	1801	ATP	C2-N3-C4	2.43	117.50	111.75
16	A	1801	ATP	C4-N9-C1'	-2.10	121.58	126.59

There are no chirality outliers.

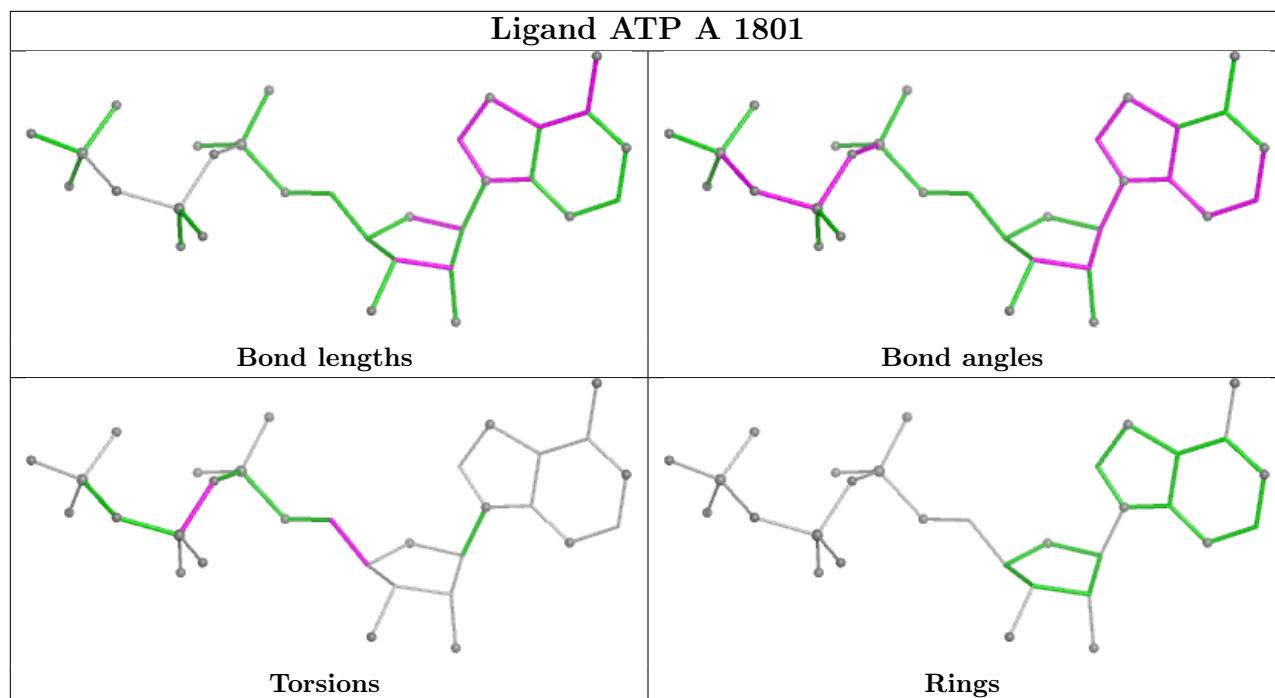
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	A	1801	ATP	C3'-C4'-C5'-O5'
16	A	1801	ATP	O4'-C4'-C5'-O5'
16	A	1801	ATP	PA-O3A-PB-O2B
16	A	1801	ATP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	44:DC	O3'	45:DC	P	2.16

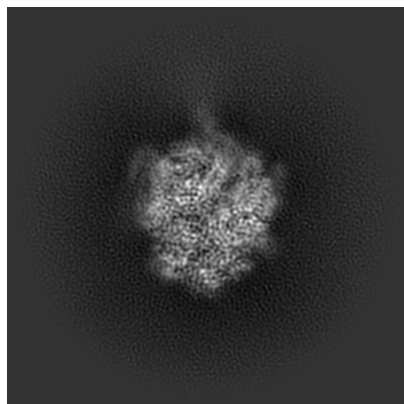
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54743. These allow visual inspection of the internal detail of the map and identification of artifacts.

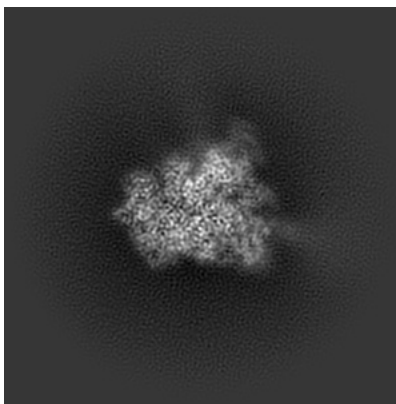
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

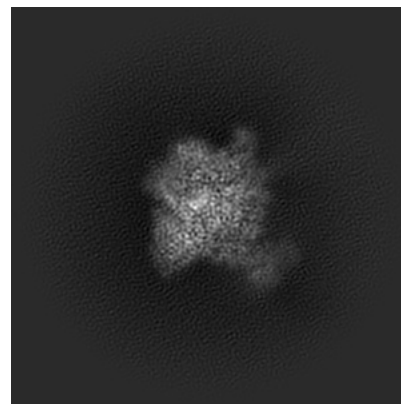
6.1.1 Primary map



X

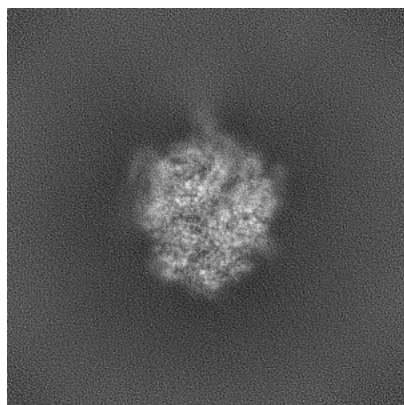


Y

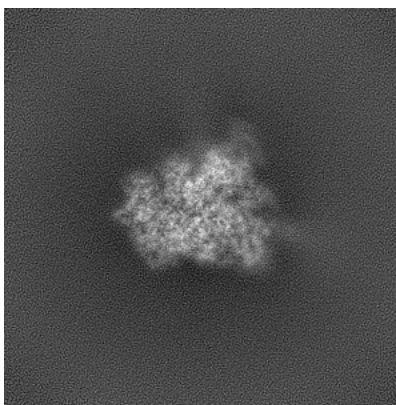


Z

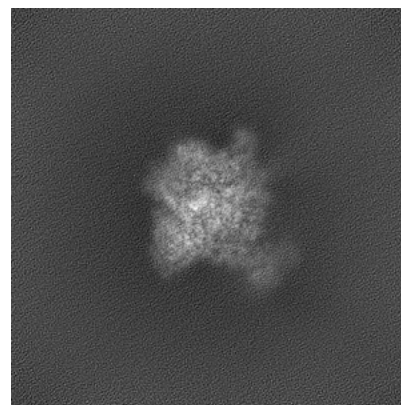
6.1.2 Raw map



X



Y

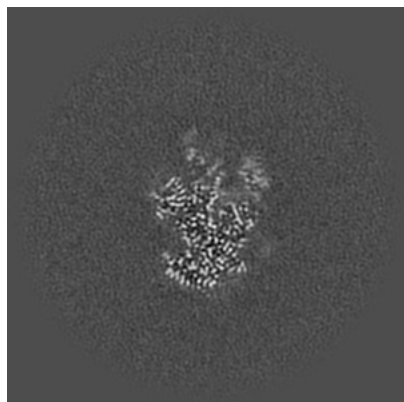


Z

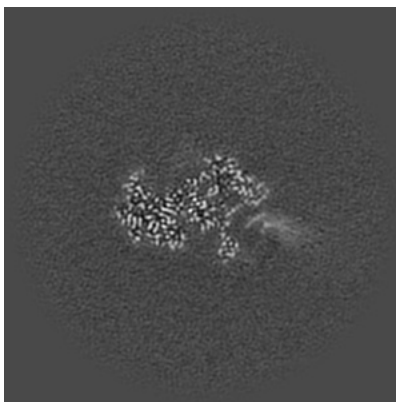
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

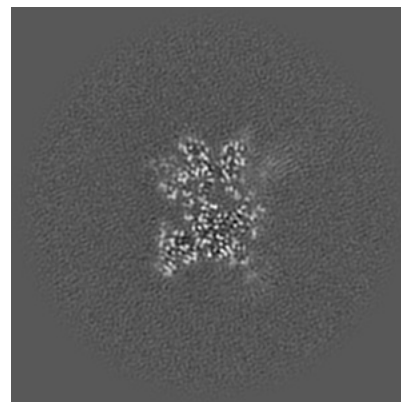
6.2.1 Primary map



X Index: 160

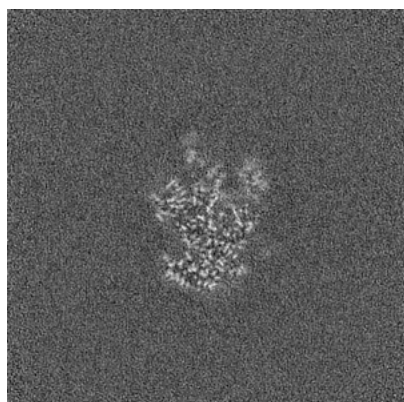


Y Index: 160

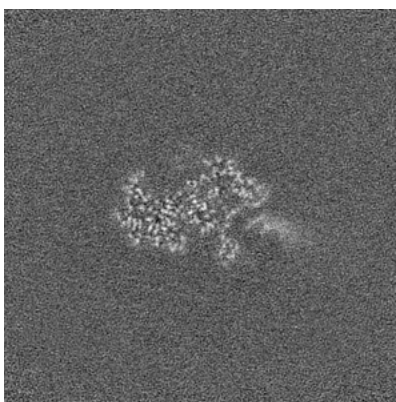


Z Index: 160

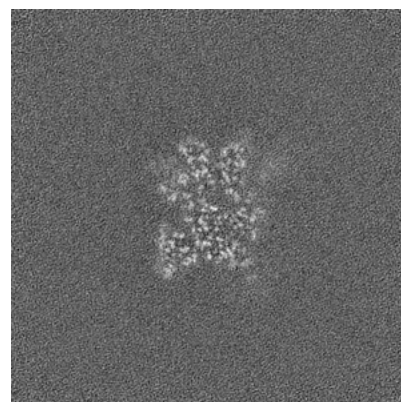
6.2.2 Raw map



X Index: 160



Y Index: 160

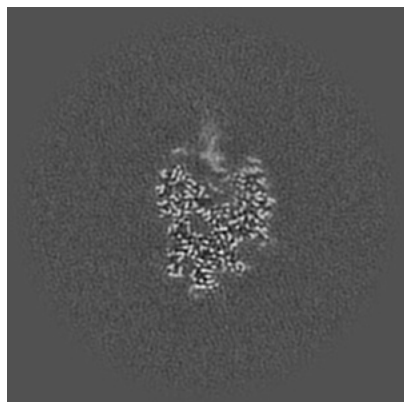


Z Index: 160

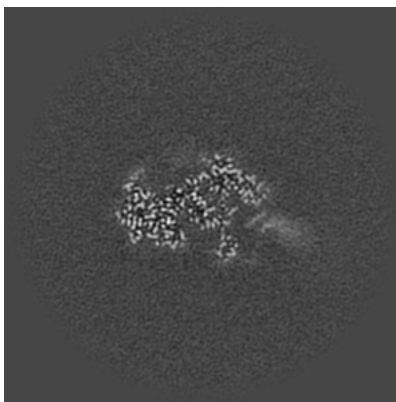
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

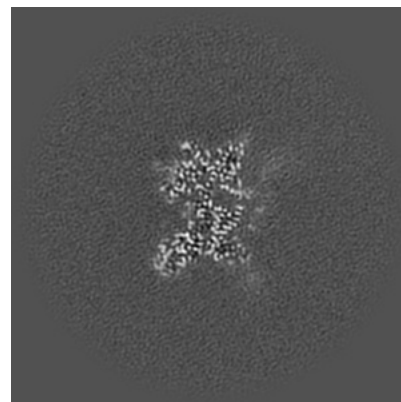
6.3.1 Primary map



X Index: 150

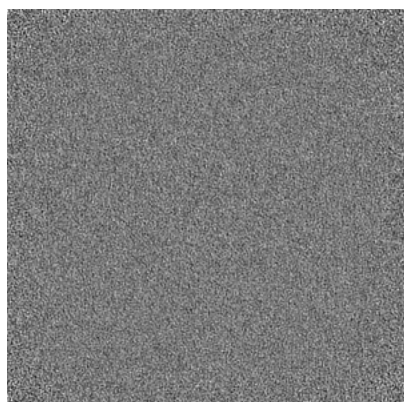


Y Index: 159

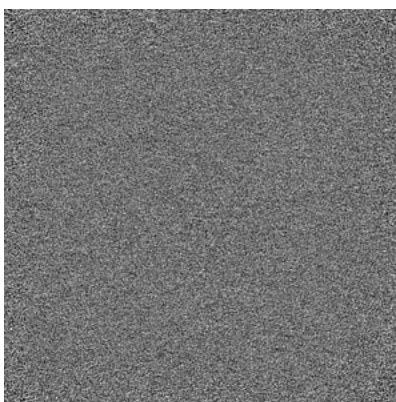


Z Index: 157

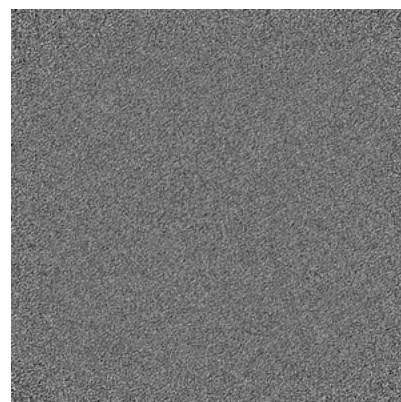
6.3.2 Raw map



X Index: 0



Y Index: 0

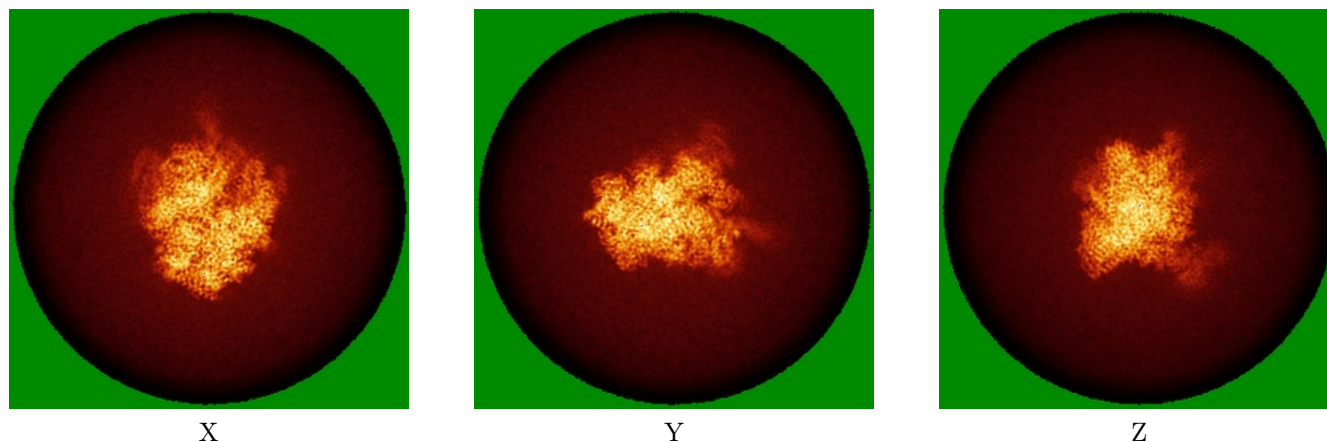


Z Index: 0

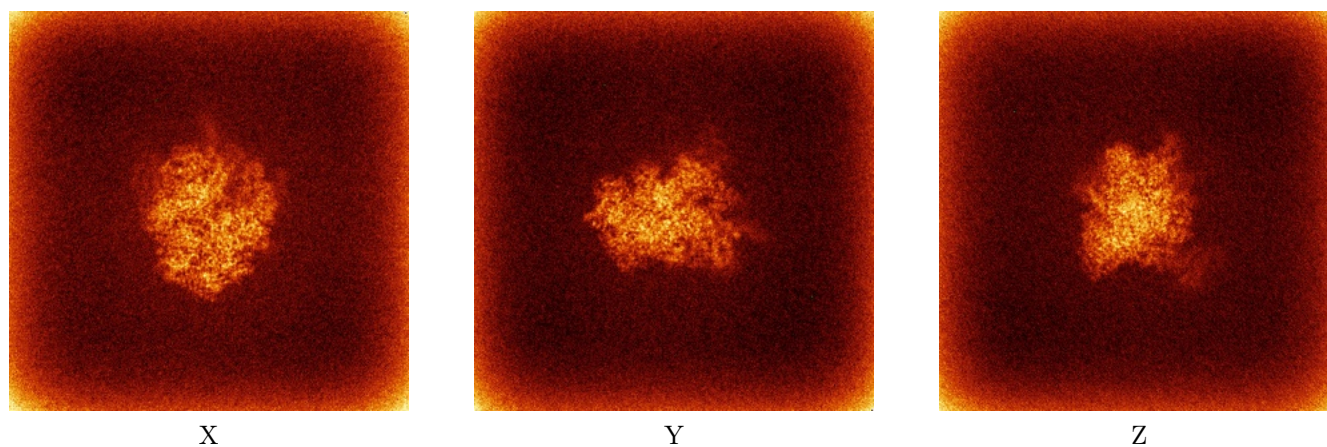
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



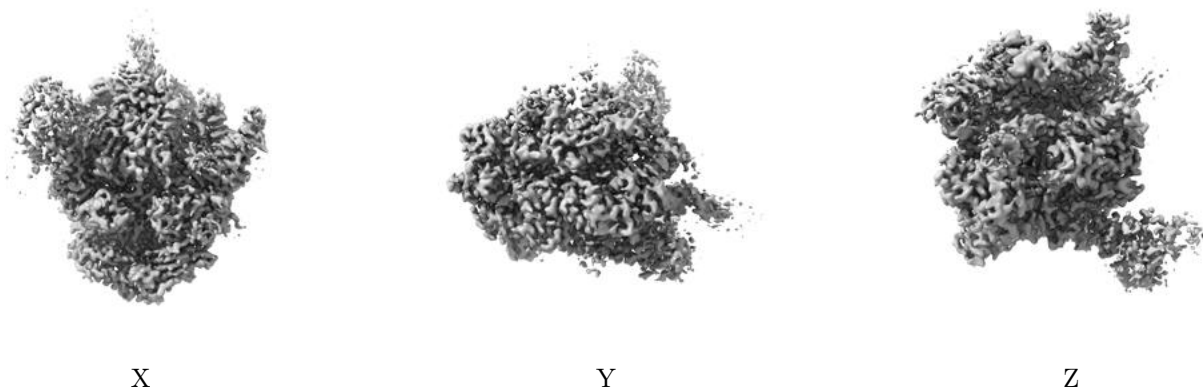
6.4.2 Raw map



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.

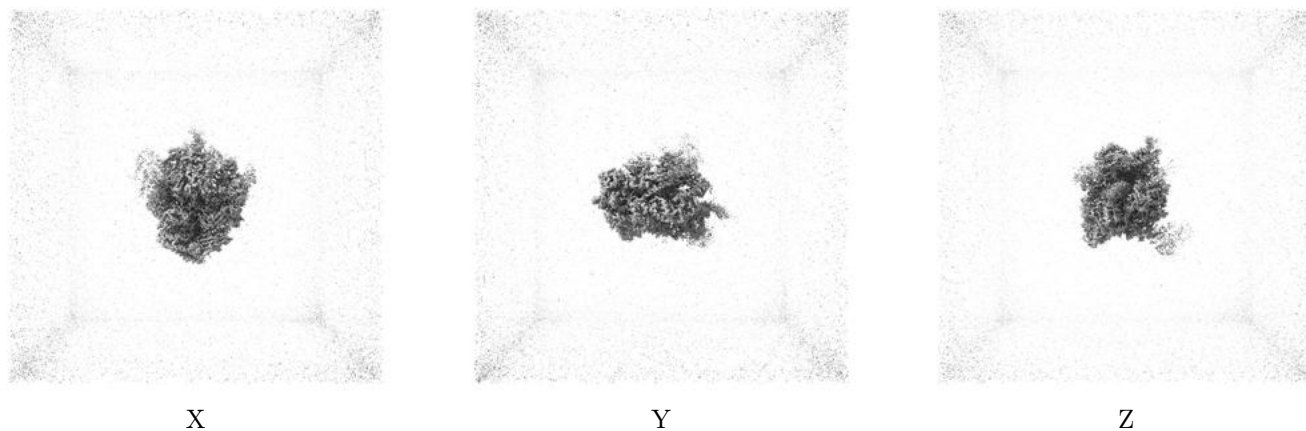
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. 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.

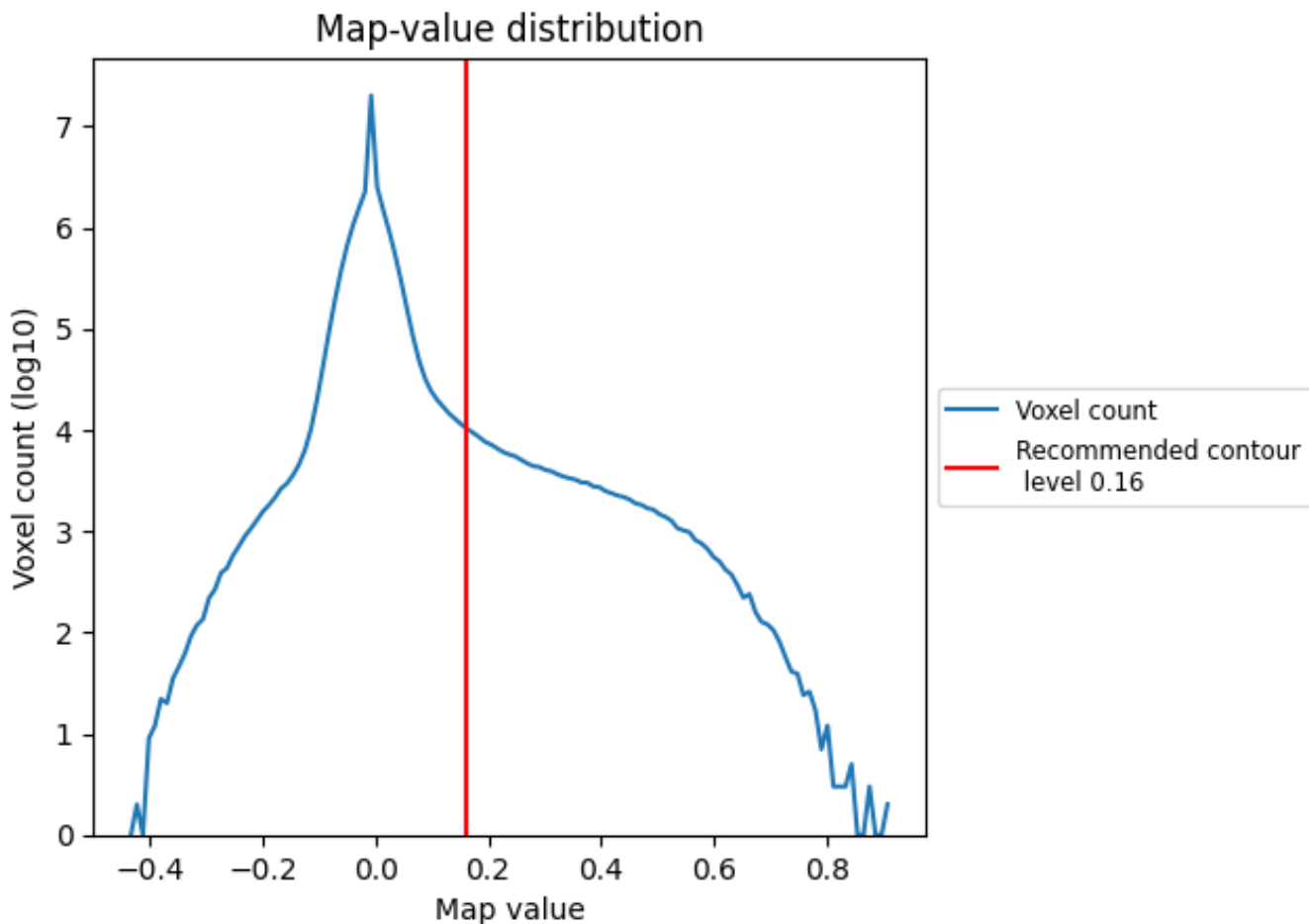
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

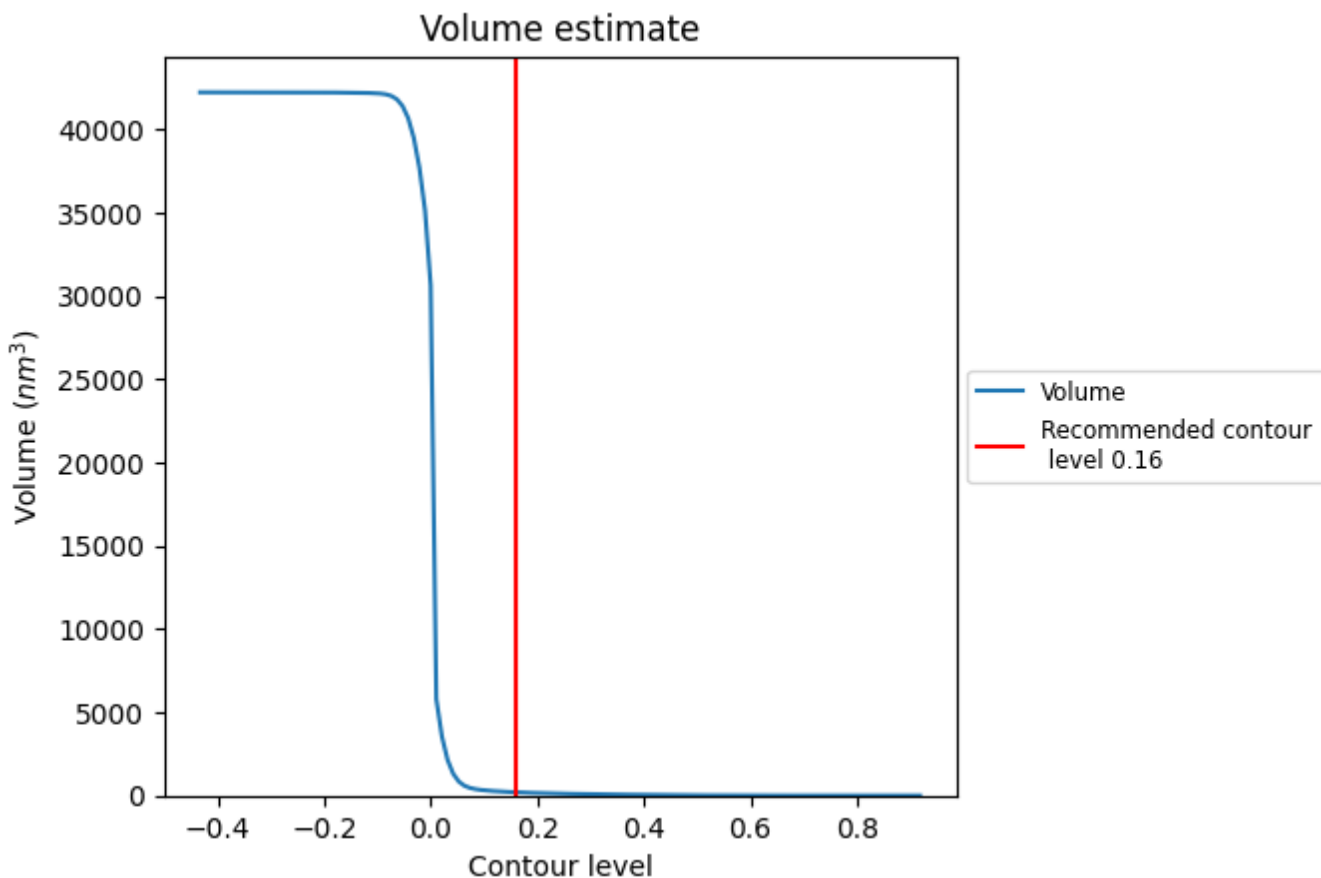
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

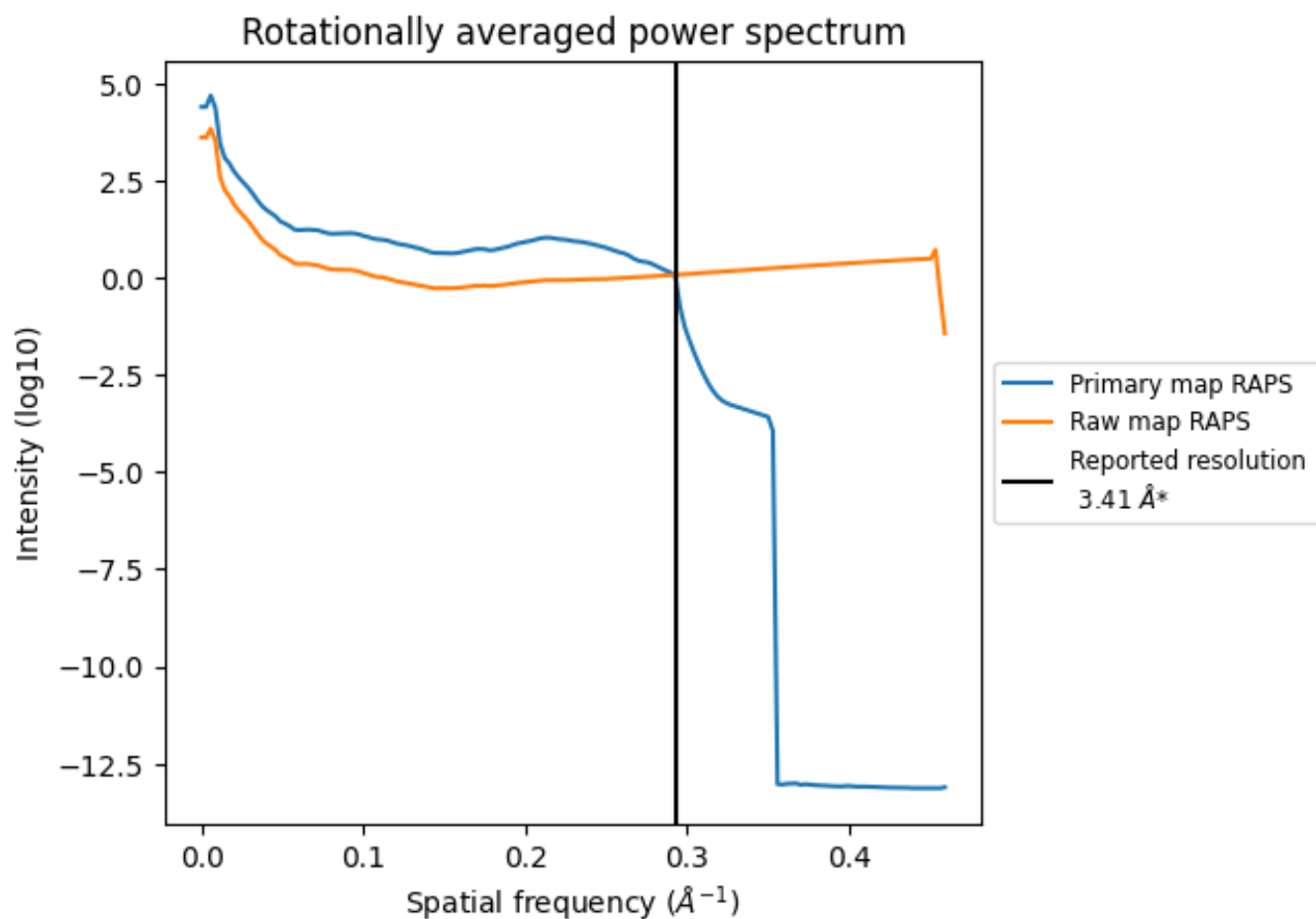
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 196 nm³; this corresponds to an approximate mass of 177 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 i

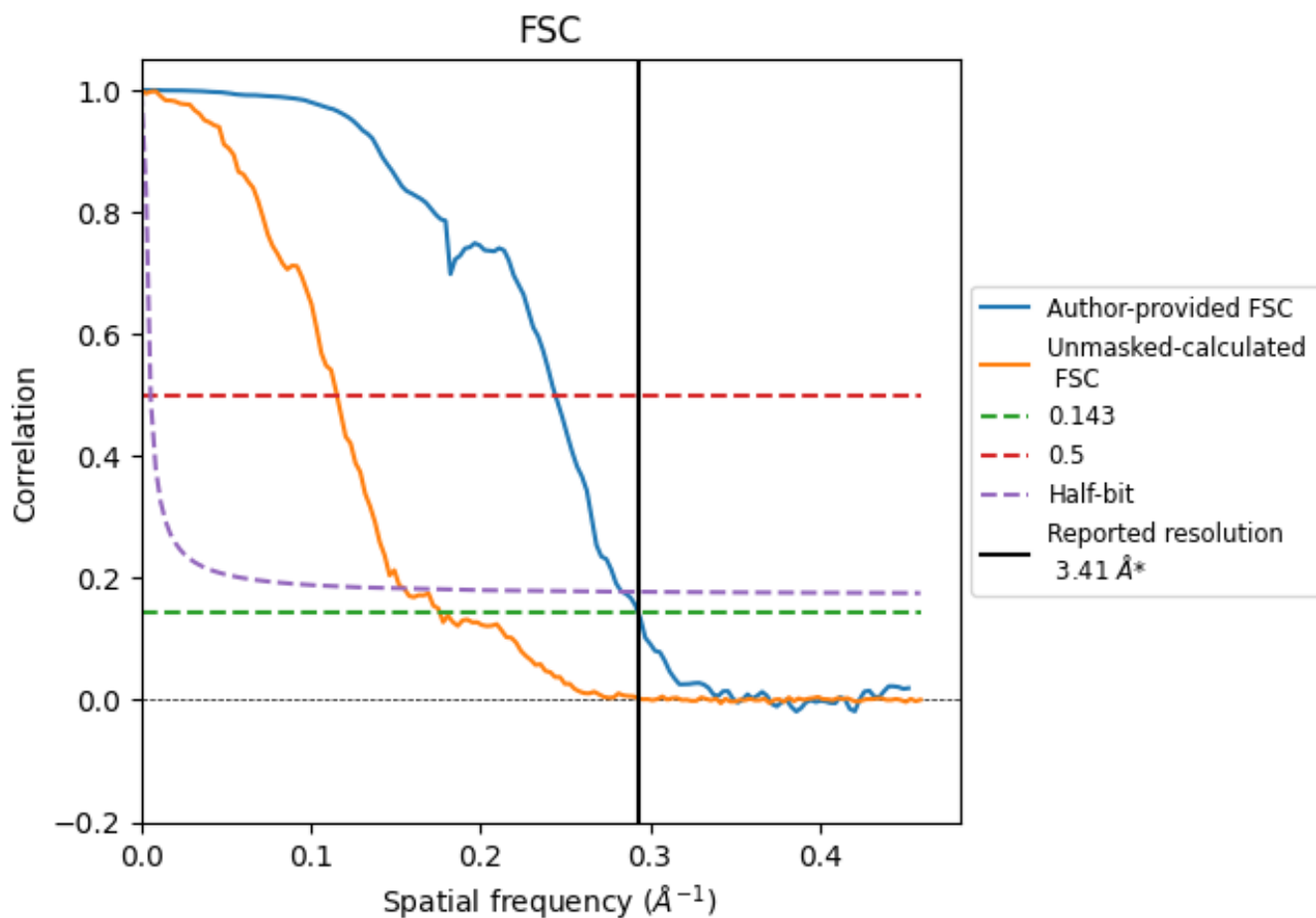


*Reported resolution corresponds to spatial frequency of 0.293 Å⁻¹

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 0.293 Å⁻¹

8.2 Resolution estimates [i](#)

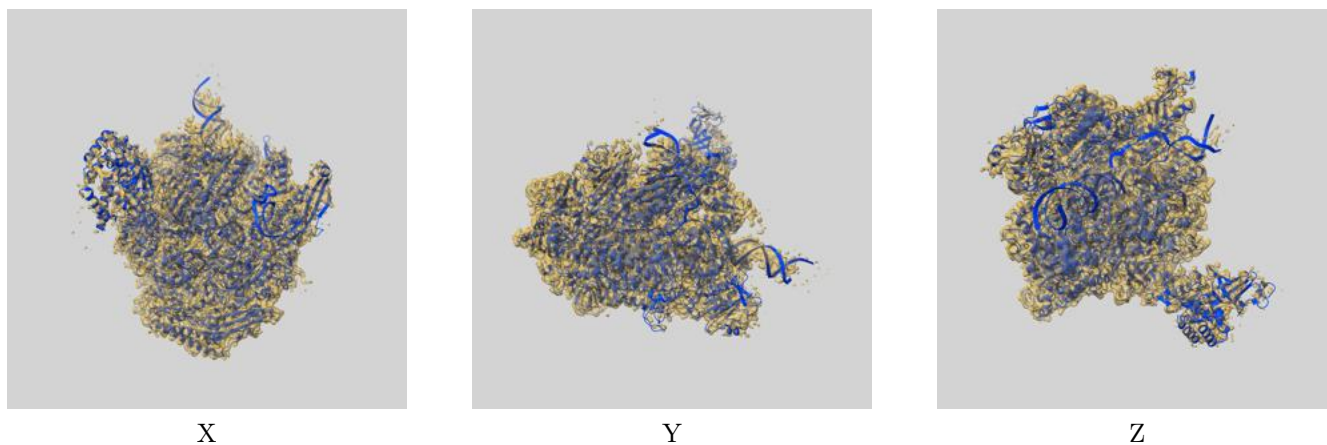
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.41	-	-
Author-provided FSC curve	3.41	4.10	3.53
Unmasked-calculated*	5.68	8.67	6.44

*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 5.68 differs from the reported value 3.41 by more than 10 %

9 Map-model fit [i](#)

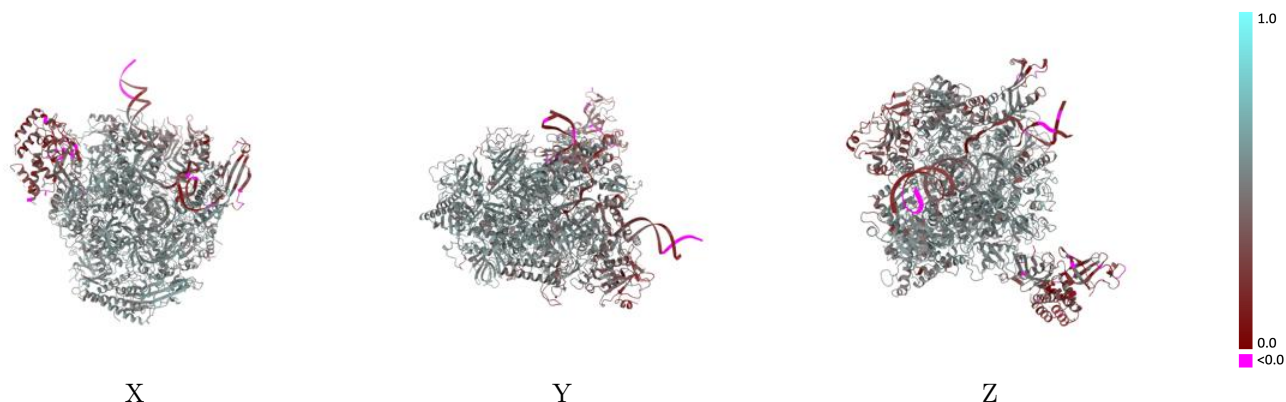
This section contains information regarding the fit between EMDB map EMD-54743 and PDB model 9SBY. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



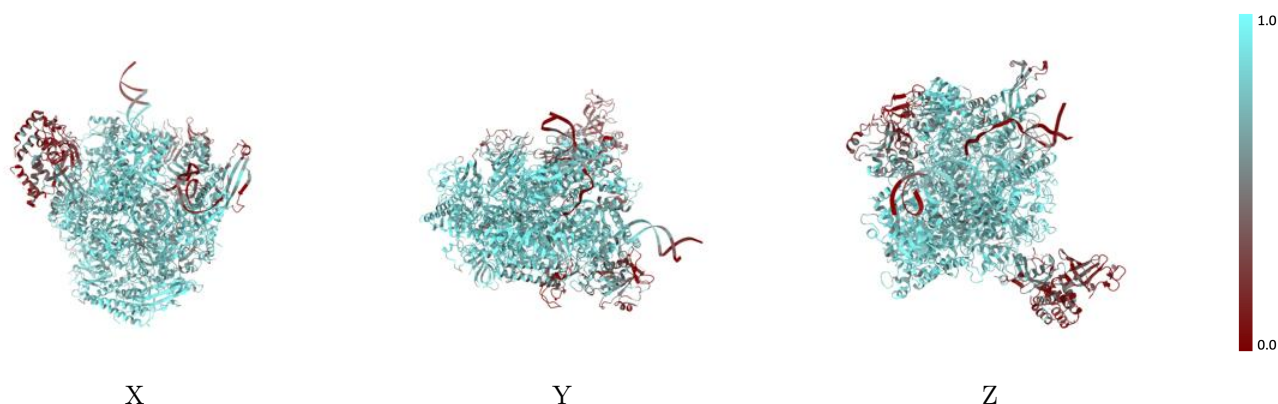
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



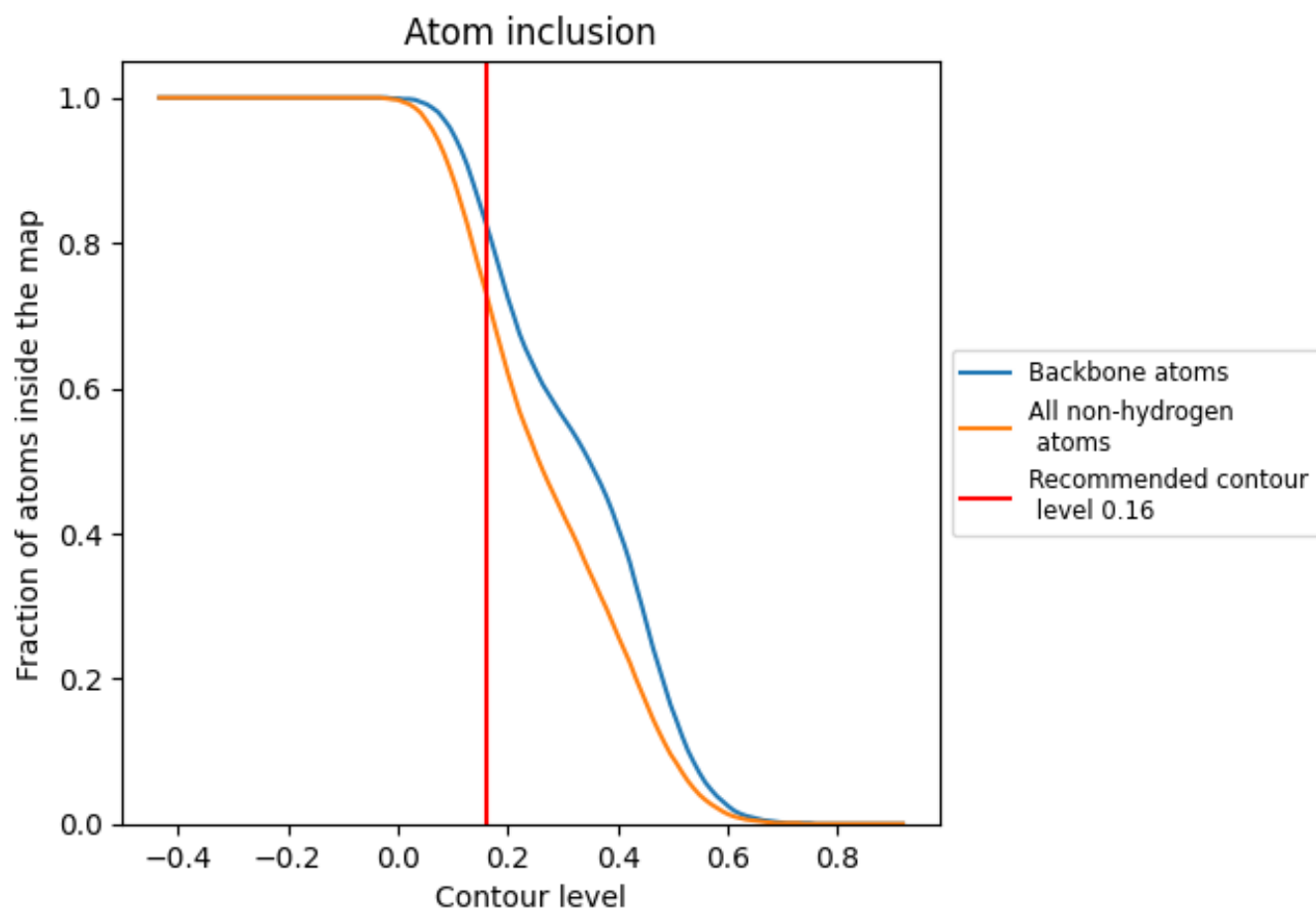
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 73% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7330	 0.4710
A	 0.8000	 0.5010
B	 0.7880	 0.4960
C	 0.8410	 0.5190
D	 0.2770	 0.2730
E	 0.8280	 0.5000
F	 0.8600	 0.5260
G	 0.4190	 0.3640
H	 0.8320	 0.5230
I	 0.1660	 0.3570
J	 0.8740	 0.5330
K	 0.8360	 0.5270
L	 0.4580	 0.4490
N	 0.4330	 0.2390
R	 0.9090	 0.4900
T	 0.5990	 0.2850

