



Full wwPDB EM Validation Report ⓘ

Jun 22, 2026 – 04:41 pm BST

PDB ID : 9SC4 / pdb_00009sc4
EMDB ID : EMD-54749
Title : Structure of Yeast RNA polymerase II elongation complex with ATP frame-20
Authors : Yi, G.; Li, Q.; Zhang, P.; Wang, D.
Deposited on : 2025-08-08
Resolution : 3.76 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
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) : 2.49

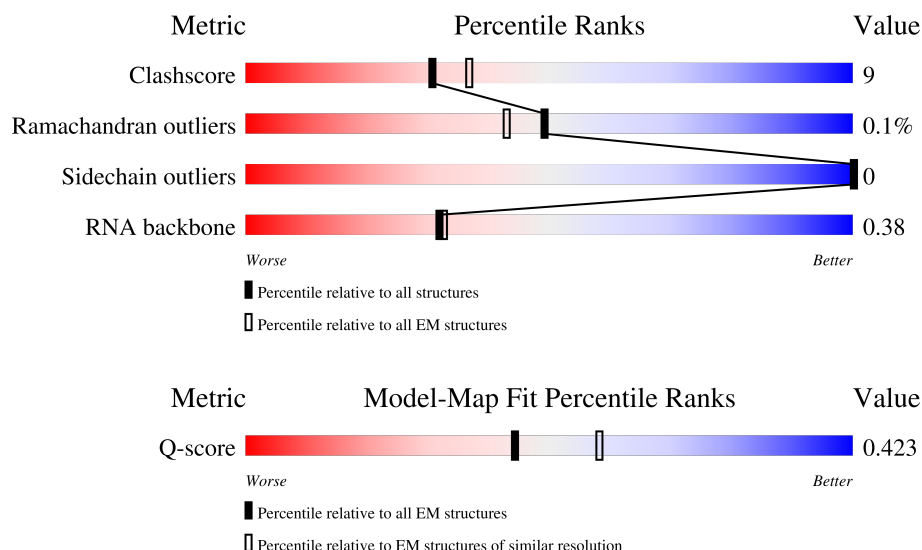
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.76 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	10214 (3.26 - 4.26)

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

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
1	A	1390	Total	C	N	O	S	0	0
			10942	6911	1913	2056	62		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
14	R	9	Total	C	N	O	P	
			197	88	40	60	9	
							0	0

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

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

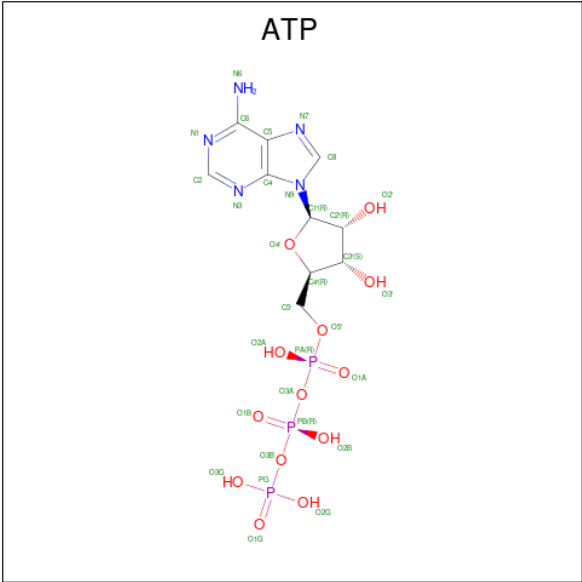
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 18 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

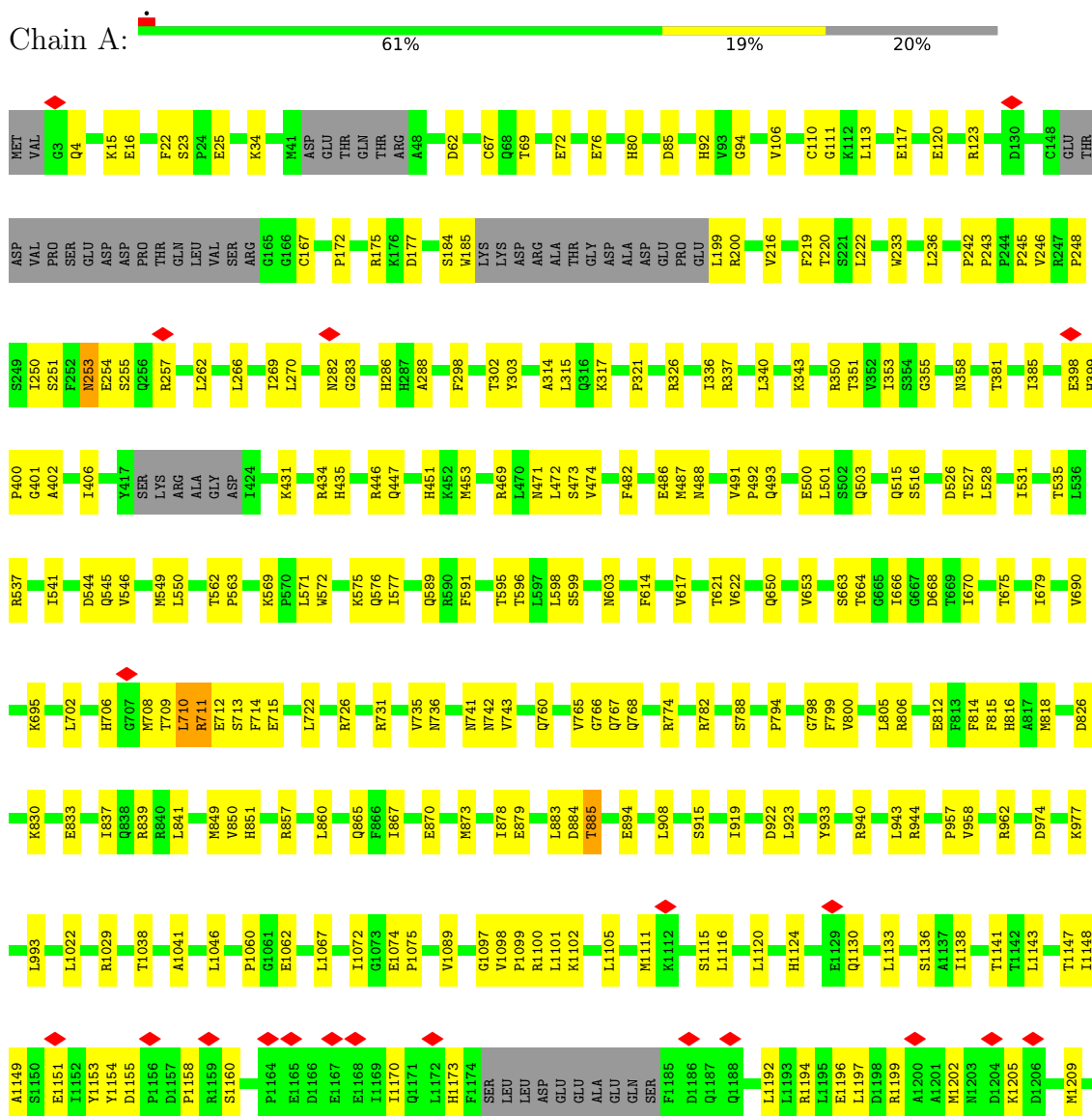


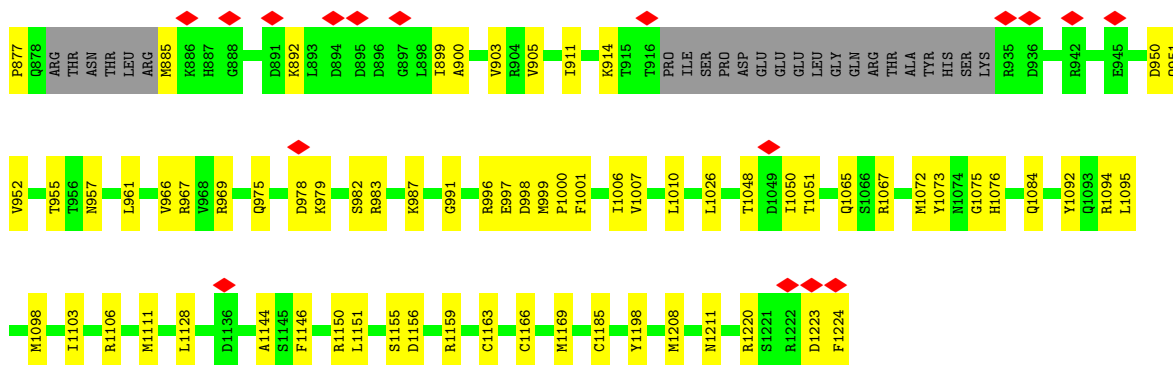
Mol	Chain	Residues	Atoms					AltConf
18	T	1	Total	C	N	O	P	0
			31	10	5	13	3	

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.

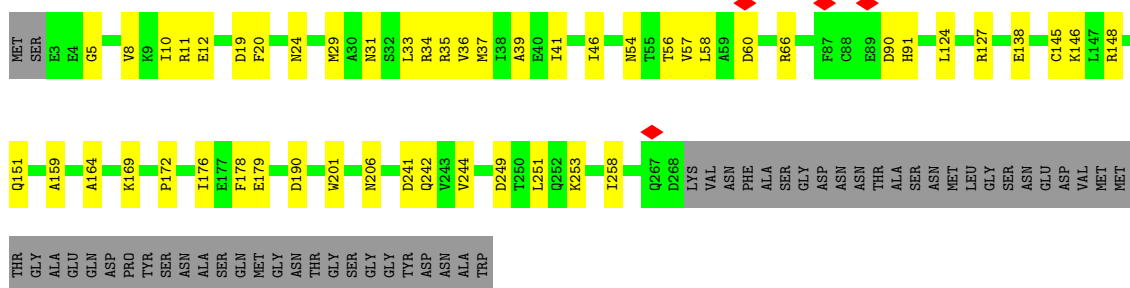
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1





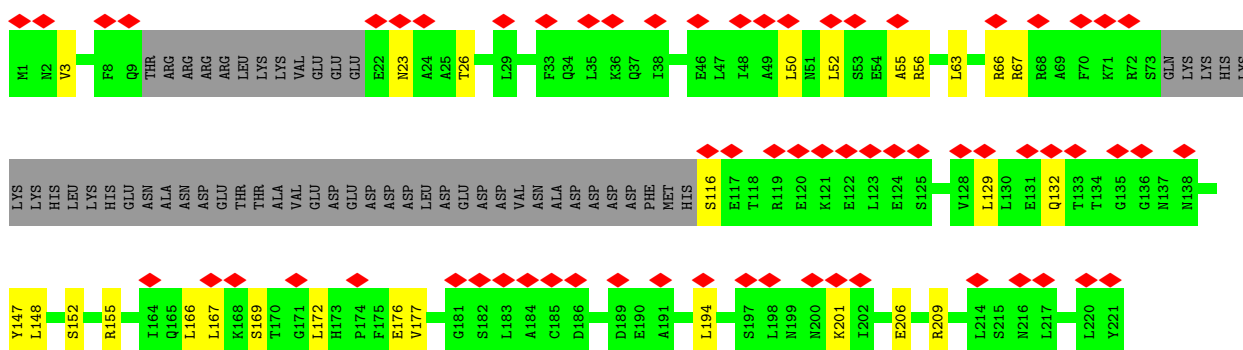
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 68% 16% 16%



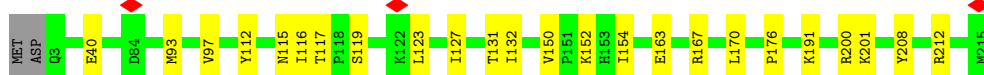
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D: 29% 63% 12% 24%



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

Chain E: 88% 11%




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

Chain F: 

MET SER ASP TTR GLU GLU ALA PHE ASN ASP GLY GLN ASN PHE GLU ASP PHE ASP VAL HIS PHE SER ASP GLU THR TYR GLU GLU PRO GLN PHE LYS ASP GLY THR THR ASP ALA ASN GLY LYS THR ILE VAL THR GLY ASN GLY PRO ASP PHE GLN


HIS GLU GLN ILE ARG ARG LYS THR LEU GLY K72 D77 Q78 T86 K87 Y88 E89 R90 A91 R92 R97 V107 L111 D116 T120 V133 R136 D140 G141 S142 D154 LEU

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

Chain G: 

M1 F2 D6 L9 L13 L26 K29 L30 E33 V34 T39 G43 Y44 I45 L46 V48 D52 D55 R58 K73 P81 F82 K83 G84 E85 V86 V87 V91 V92 S93 C94 I157 S95 Q96 H97 G98 F99 E100 V101 Q102 V103 G104 P105 M106 K107 K112 H113 L114 M115 P116 Q117 D118 L119 T120 F121 N122 A123 G124 S125 N126 P127 Y130 Q131 I132 S133 E134 D135 V136 I137 T138 I139 K140 S141 R142 I143 R144 V145 K146 I147 E148 G149 V154 S155 S156 I157 H158 A159 I160 G161 S162 I163 K164 E165 G169 A170 I171

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

Chain H: 

MET S2 D8 I9 F10 V15 R25 I26 D41 P48 I59 L65 GLU ASP THR PRO ALA ASN ASP SER THR R77 V96 Y98 K103 S108 K109 Y115 L121 L122 M123 N139 L143 R146

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

Chain I: 


M1 T2 T3 F4 R5 R8 D9 C10 L14 Y15 P16 A17 E18 D19 E20 E21 N22 N23 R24 L25 L26 F27 E28 C29 R30 T31 C32 S33 Y34 V35 E36 E37 A38 G39 S40 P41 L42 V43 Y44 R45 H46 E47 L48 L49 T50 N51 I52 E53 E54 T55 A56 Q57 V58 V59 Q60 D61 I62 Q63 S64 D65 F66 T67 L68 P69 R70 S71 D72 R73 E74 C75 P76 K77 C78 H79 S80 R81 E82 F85 F86 Q87 S88 Q89 Q90 R91 A92 K93 D94 T95 S96 L99 F100 F101 L104 S105 C106 S107 H108 I109 F110 T111 S112 ASP GLN LYS ASN LYS ARG THR GLN PHE SER

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

Chain J: 

M1 V3 F8 S9 C10 G11 W18 Y21 L25 Q26 E27 L36 K42 R43 Y44 C46 C47 R48 N49 I50 L51 L56 I57 L61 F65 LEU GLU LYS ARG ASP

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

Chain K: 

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19500	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	0.831	Depositor
Minimum map value	-0.326	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.028	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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.12	0/11139	0.31	0/15057
2	B	0.12	0/9332	0.28	0/12579
3	C	0.11	0/2133	0.27	0/2891
4	D	0.08	0/1336	0.24	0/1794
5	E	0.10	0/1780	0.28	0/2395
6	F	0.10	0/682	0.26	0/922
7	G	0.10	0/1368	0.24	0/1844
8	H	0.10	0/1095	0.23	0/1482
9	I	0.11	0/927	0.32	0/1249
10	J	0.12	0/541	0.28	0/727
11	K	0.11	0/922	0.26	0/1244
12	L	0.09	0/361	0.33	0/478
13	N	0.29	0/1016	0.69	0/1566
14	R	0.13	0/221	0.26	0/343
15	T	0.37	0/987	0.76	0/1518
All	All	0.14	0/33840	0.33	0/46089

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	A	10942	0	11025	231	0
2	B	9155	0	9161	178	0
3	C	2095	0	2051	38	0
4	D	1327	0	1331	19	0
5	E	1744	0	1772	24	0
6	F	670	0	690	13	0
7	G	1340	0	1357	24	0
8	H	1077	0	1050	15	0
9	I	909	0	867	23	0
10	J	532	0	542	15	0
11	K	904	0	911	12	0
12	L	359	0	381	12	0
13	N	905	0	493	35	0
14	R	197	0	97	3	0
15	T	886	0	498	22	0
16	A	2	0	0	0	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	T	31	0	12	0	0
All	All	33083	0	32238	580	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (580) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:117:THR:HB	13:N:65:DA:OP1	1.35	1.25
5:E:117:THR:CB	13:N:65:DA:OP1	1.85	1.23
1:A:675:THR:OG1	1:A:736:ASN:ND2	2.01	0.93
2:B:1156:ASP:HB3	2:B:1198:TYR:H	1.48	0.78
5:E:117:THR:OG1	13:N:65:DA:OP1	2.02	0.76
13:N:45:DC:H2''	13:N:46:DT:H2'	1.66	0.75
2:B:1006:ILE:HD11	10:J:43:ARG:HB3	1.68	0.75
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.69	0.75
1:A:15:LYS:HB3	2:B:1220:ARG:HE	1.52	0.74
8:H:15:VAL:HG12	8:H:26:ILE:HG22	1.67	0.74
2:B:1166:CYS:HB3	2:B:1185:CYS:SG	2.27	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:ASN:ND2	1:A:650:GLN:OE1	2.18	0.74
1:A:537:ARG:HH12	8:H:25:ARG:HH21	1.36	0.73
5:E:119:SER:OG	13:N:65:DA:H5''	1.89	0.73
1:A:1199:ARG:NH2	1:A:1233:ASP:O	2.21	0.73
15:T:34:DT:H1'	15:T:35:DC:H5'	1.71	0.72
1:A:711:ARG:HA	1:A:714:PHE:HB3	1.72	0.72
2:B:849:GLY:HA2	2:B:852:ARG:HD2	1.71	0.71
12:L:32:ALA:HB3	12:L:53:HIS:HE1	1.54	0.71
15:T:52:DG:H1'	15:T:53:DC:H5''	1.72	0.71
1:A:1205:LYS:O	1:A:1274:ARG:NH2	2.23	0.71
1:A:1062:GLU:OE1	6:F:88:TYR:OH	2.09	0.71
1:A:67:CYS:SG	1:A:80:HIS:CD2	2.83	0.70
3:C:54:ASN:ND2	3:C:60:ASP:OD1	2.23	0.70
2:B:345:LYS:HG3	2:B:348:ARG:HH12	1.56	0.70
1:A:446:ARG:HB2	1:A:487:MET:HG2	1.72	0.70
1:A:1197:LEU:HD12	1:A:1209:MET:HE1	1.74	0.69
2:B:998:ASP:OD1	3:C:35:ARG:NH1	2.26	0.69
1:A:1256:GLU:OE1	1:A:1258:HIS:ND1	2.23	0.69
3:C:10:ILE:HD13	3:C:20:PHE:HB3	1.74	0.69
1:A:1154:TYR:H	9:I:41:PRO:HB2	1.58	0.69
1:A:1072:ILE:HD11	1:A:1356:ILE:HG13	1.74	0.68
10:J:10:CYS:SG	10:J:43:ARG:NH2	2.66	0.68
1:A:526:ASP:HB2	2:B:835:GLN:NE2	2.09	0.67
1:A:883:LEU:HD13	1:A:943:LEU:HD13	1.76	0.67
1:A:544:ASP:HB2	11:K:47:ARG:HH22	1.59	0.67
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.75	0.67
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.77	0.67
1:A:768:GLN:OE1	1:A:816:HIS:ND1	2.25	0.67
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.75	0.67
1:A:708:MET:HG2	1:A:709:THR:H	1.60	0.66
2:B:852:ARG:NH2	12:L:70:ARG:OXT	2.28	0.66
2:B:276:ILE:HG21	2:B:280:ILE:HD11	1.77	0.66
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.77	0.66
9:I:51:ASN:HB2	9:I:90:GLN:HG3	1.78	0.66
4:D:194:LEU:HD22	7:G:86:VAL:HG11	1.77	0.66
1:A:473:SER:OG	1:A:650:GLN:NE2	2.29	0.66
2:B:247:GLY:O	2:B:418:LYS:NZ	2.29	0.66
13:N:39:DC:O2	15:T:52:DG:N2	2.28	0.66
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.61	0.66
3:C:66:ARG:NH2	10:J:3:VAL:O	2.23	0.65
2:B:28:GLU:OE2	2:B:807:ARG:NH1	2.28	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.77	0.65
10:J:36:LEU:HD11	10:J:51:LEU:HB2	1.76	0.65
9:I:75:CYS:HB3	9:I:80:SER:H	1.62	0.65
8:H:25:ARG:NE	8:H:41:ASP:OD1	2.30	0.65
2:B:332:ASP:OD1	2:B:348:ARG:NH1	2.30	0.64
1:A:406:ILE:HB	1:A:431:LYS:HB2	1.78	0.64
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.79	0.64
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.78	0.64
3:C:179:GLU:OE1	3:C:206:ASN:ND2	2.30	0.64
5:E:152:LYS:HE3	5:E:154:ILE:HD11	1.78	0.64
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.79	0.64
2:B:237:VAL:HG23	2:B:257:LYS:HG2	1.78	0.64
15:T:42:DC:H2'	15:T:43:DC:C6	2.33	0.64
10:J:10:CYS:SG	10:J:11:GLY:N	2.70	0.64
3:C:33:LEU:HG	3:C:37:MET:HE2	1.78	0.63
1:A:710:LEU:O	1:A:713:SER:N	2.32	0.63
2:B:158:ASP:HA	2:B:163:GLY:HA3	1.79	0.63
2:B:380:TYR:OH	2:B:384:ARG:NH2	2.32	0.63
1:A:317:LYS:HE2	13:N:40:DC:H41	1.63	0.63
8:H:48:PRO:O	8:H:146:ARG:NH2	2.30	0.63
2:B:208:SER:OG	2:B:210:LYS:NZ	2.32	0.63
2:B:780:VAL:HG22	2:B:795:ILE:HG23	1.80	0.62
4:D:67:ARG:NH2	4:D:132:GLN:OE1	2.32	0.62
1:A:1286:LYS:HD2	1:A:1302:PRO:HB2	1.82	0.62
1:A:664:THR:HA	1:A:742:ASN:HD22	1.64	0.62
3:C:258:ILE:HG13	11:K:42:LEU:HD21	1.81	0.62
2:B:313:MET:HE3	2:B:390:LEU:HD21	1.82	0.61
7:G:102:GLN:OE1	7:G:107:LYS:NZ	2.32	0.61
8:H:8:ASP:OD1	8:H:9:ILE:N	2.34	0.61
1:A:110:CYS:HB3	1:A:167:CYS:SG	2.39	0.61
14:R:1:A:H2'	14:R:2:U:C6	2.35	0.61
1:A:336:ILE:HG13	1:A:340:LEU:HD12	1.83	0.61
1:A:1141:THR:HG23	1:A:1273:LEU:HB2	1.83	0.61
3:C:90:ASP:OD2	3:C:91:HIS:ND1	2.34	0.61
2:B:1075:GLY:O	3:C:35:ARG:NH2	2.34	0.61
2:B:259:TYR:OH	2:B:279:ASP:OD2	2.19	0.60
15:T:42:DC:H2'	15:T:43:DC:H6	1.65	0.60
1:A:1192:LEU:HD13	1:A:1241:ARG:HE	1.66	0.60
1:A:535:THR:O	1:A:575:LYS:NZ	2.27	0.60
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.82	0.60
6:F:107:VAL:HG11	6:F:111:LEU:HD21	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:900:ALA:HB2	12:L:58:LYS:HZ2	1.65	0.60
5:E:115:ASN:OD1	5:E:116:ILE:N	2.35	0.60
9:I:48:LEU:HD12	9:I:49:ILE:HG23	1.82	0.60
1:A:800:VAL:HA	1:A:812:GLU:HG2	1.83	0.60
1:A:857:ARG:HH22	5:E:170:LEU:HD21	1.67	0.60
2:B:703:ILE:HG12	2:B:740:HIS:HB2	1.84	0.59
1:A:1124:HIS:O	1:A:1130:GLN:NE2	2.35	0.59
2:B:169:ARG:H	2:B:454:THR:HG22	1.67	0.59
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.83	0.59
2:B:87:LYS:HB3	2:B:137:TYR:HB2	1.83	0.59
3:C:148:ARG:NE	10:J:61:LEU:O	2.29	0.59
2:B:371:GLU:OE1	2:B:371:GLU:N	2.33	0.59
2:B:1155:SER:OG	2:B:1156:ASP:N	2.35	0.59
1:A:549:MET:HE3	1:A:577:ILE:HG21	1.85	0.58
1:A:350:ARG:NE	1:A:486:GLU:OE1	2.36	0.58
1:A:1354:ASN:O	1:A:1358:SER:OG	2.20	0.58
1:A:503:GLN:OE1	6:F:90:ARG:NH2	2.36	0.58
1:A:715:GLU:OE1	1:A:774:ARG:NE	2.34	0.58
1:A:1116:LEU:HB2	1:A:1308:THR:HB	1.85	0.58
11:K:85:ASP:O	11:K:89:ASN:ND2	2.36	0.58
1:A:1151:GLU:OE2	1:A:1194:ARG:NH1	2.37	0.57
4:D:176:GLU:N	4:D:176:GLU:OE1	2.36	0.57
8:H:98:TYR:OH	8:H:139:ASN:ND2	2.31	0.57
1:A:851:HIS:CD2	1:A:857:ARG:HD2	2.39	0.57
9:I:15:TYR:N	9:I:28:GLU:O	2.38	0.57
1:A:767:GLN:NE2	1:A:768:GLN:O	2.37	0.57
5:E:93:MET:HG3	5:E:123:LEU:HD22	1.86	0.57
1:A:878:ILE:HD12	1:A:1366:ARG:HH12	1.69	0.57
2:B:750:GLY:O	2:B:754:SER:OG	2.21	0.57
2:B:825:VAL:HG22	2:B:1010:LEU:HB3	1.87	0.57
2:B:1048:THR:HG23	2:B:1050:ILE:H	1.70	0.57
1:A:472:LEU:HD22	2:B:835:GLN:OE1	2.04	0.56
4:D:148:LEU:O	4:D:152:SER:OG	2.17	0.56
7:G:119:LEU:HG	7:G:132:SER:HB3	1.86	0.56
1:A:282:ASN:OD1	1:A:283:GLY:N	2.37	0.56
2:B:682:SER:O	2:B:686:ASN:ND2	2.32	0.56
5:E:117:THR:CG2	13:N:65:DA:OP1	2.53	0.56
1:A:668:ASP:OD2	1:A:742:ASN:ND2	2.39	0.56
2:B:76:GLN:HB3	2:B:82:ASP:HB3	1.87	0.56
13:N:48:DC:H2"	13:N:49:DT:C2	2.40	0.56
4:D:66:ARG:NH2	7:G:48:VAL:O	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:940:ARG:HH21	1:A:944:ARG:NH2	2.03	0.56
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.87	0.56
1:A:4:GLN:NE2	1:A:76:GLU:OE1	2.35	0.56
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.86	0.56
1:A:23:SER:OG	1:A:25:GLU:OE1	2.25	0.55
1:A:399:HIS:O	1:A:435:HIS:ND1	2.39	0.55
1:A:471:ASN:O	1:A:474:VAL:HG12	2.06	0.55
2:B:137:TYR:HB3	2:B:149:TYR:HB3	1.88	0.55
1:A:894:GLU:OE1	1:A:933:TYR:OH	2.24	0.55
9:I:101:PHE:N	9:I:110:PHE:O	2.35	0.55
2:B:840:ILE:HG22	2:B:999:MET:HE1	1.88	0.55
5:E:127:ILE:HD11	5:E:132:ILE:HD11	1.87	0.55
2:B:290:GLY:HA3	2:B:327:ARG:HH21	1.70	0.55
2:B:842:ASN:OD1	2:B:845:SER:N	2.31	0.55
1:A:621:THR:HG22	1:A:622:VAL:HG13	1.89	0.55
1:A:706:HIS:CD2	1:A:1307:GLU:HB3	2.42	0.55
1:A:922:ASP:OD1	1:A:923:LEU:N	2.40	0.55
2:B:951:GLN:OE1	2:B:967:ARG:NH2	2.40	0.55
15:T:33:DT:H2'	15:T:34:DT:H71	1.89	0.55
15:T:44:DT:H2'	15:T:45:DC:H6	1.72	0.55
1:A:1446:ASP:OD1	1:A:1447:GLU:N	2.40	0.55
4:D:172:LEU:HD11	4:D:201:LYS:HB3	1.89	0.54
2:B:308:TRP:CG	9:I:1:MET:H2	2.26	0.54
1:A:690:VAL:HG11	1:A:794:PRO:HG3	1.88	0.54
1:A:120:GLU:OE1	1:A:123:ARG:NH1	2.41	0.54
1:A:251:SER:HB3	1:A:257:ARG:HD2	1.89	0.54
1:A:1060:PRO:HD2	6:F:86:THR:HG21	1.89	0.54
2:B:139:ALA:HB2	2:B:149:TYR:HA	1.90	0.54
1:A:492:PRO:O	1:A:493:GLN:NE2	2.40	0.54
2:B:637:LEU:HD13	2:B:740:HIS:HB3	1.90	0.54
1:A:1278:ASN:OD1	1:A:1312:ASN:ND2	2.40	0.54
2:B:287:ARG:NH1	2:B:292:ILE:O	2.41	0.54
10:J:8:PHE:H	10:J:49:MET:HE3	1.72	0.54
10:J:43:ARG:NH2	10:J:46:CYS:SG	2.81	0.54
15:T:43:DC:H2'	15:T:44:DT:C6	2.43	0.54
1:A:1136:SER:OG	1:A:1274:ARG:NH1	2.40	0.53
12:L:31:CYS:HB2	12:L:48:CYS:SG	2.48	0.53
1:A:1308:THR:HG22	1:A:1310:GLY:H	1.72	0.53
11:K:29:ASN:ND2	11:K:77:THR:O	2.41	0.53
13:N:36:DA:C8	13:N:36:DA:H5'	2.44	0.53
2:B:900:ALA:HB3	12:L:61:THR:HG22	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:637:LEU:HA	2:B:743:ILE:HG12	1.91	0.53
2:B:903:VAL:HG13	12:L:61:THR:HG21	1.90	0.53
15:T:38:DC:H2''	15:T:39:DC:C5	2.44	0.53
2:B:394:ASP:OD1	2:B:395:GLN:N	2.41	0.53
8:H:41:ASP:OD2	8:H:122:LEU:N	2.39	0.53
15:T:53:DC:H2''	15:T:54:DT:C6	2.44	0.53
1:A:451:HIS:CE1	1:A:453:MET:HB2	2.44	0.52
2:B:557:PHE:HB3	2:B:561:TRP:CZ3	2.45	0.52
1:A:589:GLN:HE21	1:A:591:PHE:HE1	1.57	0.52
1:A:668:ASP:O	1:A:741:ASN:ND2	2.40	0.52
1:A:915:SER:O	1:A:919:ILE:HG12	2.10	0.52
13:N:46:DT:H1'	13:N:47:DA:C4	2.44	0.52
2:B:481:GLN:NE2	2:B:494:HIS:NE2	2.57	0.52
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.92	0.52
1:A:1120:LEU:HD23	1:A:1130:GLN:HE22	1.75	0.52
2:B:952:VAL:HG22	2:B:966:VAL:HG22	1.91	0.52
2:B:1106:ARG:NH2	2:B:1111:MET:SD	2.83	0.52
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	1.90	0.51
2:B:311:LEU:HB3	9:I:4:PHE:CE2	2.45	0.51
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.90	0.51
2:B:950:ASP:OD1	2:B:969:ARG:NH2	2.43	0.51
1:A:1143:LEU:HD13	1:A:1271:ILE:HG12	1.92	0.51
2:B:232:SER:N	2:B:261:ARG:HH21	2.08	0.51
5:E:176:PRO:HB2	5:E:212:ARG:HD3	1.93	0.51
2:B:142:VAL:HG11	2:B:145:ARG:HD3	1.92	0.51
3:C:169:LYS:NZ	12:L:69:ALA:O	2.42	0.51
13:N:47:DA:H2'	13:N:48:DC:C2	2.45	0.51
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.93	0.51
1:A:1158:PRO:HA	1:A:1241:ARG:NH1	2.25	0.51
7:G:91:VAL:HG12	7:G:101:VAL:HG22	1.92	0.51
13:N:38:DC:H4'	13:N:39:DC:OP1	2.11	0.51
2:B:424:LEU:HD11	2:B:448:ILE:HG23	1.92	0.51
2:B:773:MET:HE1	2:B:987:LYS:HD3	1.92	0.51
1:A:184:SER:HG	1:A:199:LEU:N	2.08	0.51
1:A:818:MET:SD	2:B:516:ASN:ND2	2.83	0.51
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.91	0.51
1:A:1328:TYR:OH	1:A:1351:GLU:OE2	2.22	0.51
1:A:491:VAL:O	2:B:1150:ARG:NH2	2.36	0.51
2:B:796:LEU:HD12	2:B:853:SER:HB3	1.93	0.51
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	1.93	0.51
2:B:957:ASN:N	2:B:961:LEU:O	2.39	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:11:ARG:HE	3:C:19:ASP:CG	2.20	0.51
9:I:49:ILE:HG13	9:I:50:THR:N	2.26	0.51
2:B:102:VAL:HG21	2:B:122:LEU:HD13	1.92	0.50
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.93	0.50
3:C:56:THR:HG22	3:C:58:LEU:H	1.76	0.50
13:N:60:DA:H61	15:T:30:DT:H3	1.59	0.50
1:A:663:SER:O	1:A:742:ASN:ND2	2.44	0.50
1:A:833:GLU:O	1:A:837:ILE:HD12	2.11	0.50
7:G:116:PRO:HB2	7:G:119:LEU:HD13	1.93	0.50
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.47	0.50
1:A:544:ASP:OD1	1:A:545:GLN:N	2.41	0.50
2:B:792:MET:SD	2:B:857:ARG:NH2	2.84	0.50
2:B:1163:CYS:HB3	2:B:1166:CYS:SG	2.51	0.50
1:A:34:LYS:NZ	1:A:85:ASP:OD2	2.39	0.50
2:B:253:THR:HG22	2:B:253:THR:O	2.12	0.50
2:B:951:GLN:HE21	12:L:57:LEU:HD21	1.77	0.50
1:A:72:GLU:HB3	1:A:76:GLU:HB3	1.94	0.50
1:A:94:GLY:HA3	1:A:1410:PHE:CD2	2.47	0.50
1:A:974:ASP:OD2	1:A:977:LYS:N	2.40	0.50
2:B:134:LYS:HE3	2:B:442:PHE:CZ	2.47	0.50
13:N:56:DA:H1'	13:N:57:DA:H5'	1.94	0.50
2:B:899:ILE:HD12	2:B:911:ILE:HG22	1.94	0.49
1:A:469:ARG:NH2	2:B:991:GLY:O	2.35	0.49
1:A:806:ARG:HG2	2:B:728:ARG:HA	1.94	0.49
8:H:108:SER:OG	8:H:109:LYS:N	2.45	0.49
1:A:1148:ILE:HD12	1:A:1196:GLU:HB3	1.94	0.49
3:C:124:LEU:O	3:C:127:ARG:HG2	2.13	0.49
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.95	0.49
1:A:879:GLU:OE2	1:A:962:ARG:NH2	2.33	0.49
1:A:666:ILE:HD13	2:B:1026:LEU:HB2	1.95	0.49
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.94	0.49
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.95	0.49
1:A:614:PHE:HB3	8:H:122:LEU:HD21	1.93	0.49
1:A:833:GLU:OE1	1:A:1102:LYS:NZ	2.32	0.49
2:B:629:ASP:OD1	2:B:630:ALA:N	2.46	0.49
13:N:55:DG:H1'	13:N:56:DA:H5'	1.93	0.49
1:A:355:GLY:O	1:A:469:ARG:NH1	2.46	0.49
3:C:145:CYS:SG	3:C:146:LYS:N	2.86	0.49
1:A:1062:GLU:OE2	1:A:1067:LEU:HD11	2.11	0.48
2:B:278:GLN:N	2:B:278:GLN:OE1	2.43	0.48
4:D:166:LEU:O	4:D:169:SER:OG	2.30	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:42:DT:H2''	13:N:43:DT:H5''	1.95	0.48
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.48	0.48
15:T:45:DC:H2''	15:T:46:DT:H5'	1.95	0.48
1:A:598:LEU:O	1:A:598:LEU:HD23	2.12	0.48
2:B:209:GLU:OE1	2:B:485:ARG:NH1	2.42	0.48
9:I:42:LEU:HD11	9:I:45:ARG:HB2	1.96	0.48
4:D:3:VAL:HG13	7:G:9:LEU:HD11	1.95	0.48
1:A:317:LYS:HE3	1:A:317:LYS:HA	1.94	0.48
1:A:1279:ILE:HD12	1:A:1308:THR:HG21	1.94	0.48
1:A:1397:LEU:HB2	1:A:1426:GLU:HG3	1.95	0.48
2:B:546:SER:OG	2:B:632:ARG:N	2.45	0.48
2:B:1084:GLN:NE2	3:C:190:ASP:O	2.37	0.48
1:A:1115:SER:O	1:A:1329:THR:OG1	2.22	0.48
2:B:855:PHE:HZ	2:B:857:ARG:HH21	1.62	0.48
2:B:975:GLN:N	2:B:978:ASP:OD2	2.36	0.48
15:T:52:DG:H4'	15:T:53:DC:OP1	2.13	0.48
1:A:884:ASP:O	1:A:885:THR:OG1	2.25	0.48
3:C:5:GLY:O	3:C:24:ASN:ND2	2.46	0.48
1:A:1138:ILE:HG22	1:A:1279:ILE:HG21	1.95	0.48
2:B:1076:HIS:O	3:C:31:ASN:ND2	2.46	0.48
2:B:211:VAL:HG21	2:B:495:LEU:HD23	1.96	0.48
3:C:57:VAL:HG13	3:C:151:GLN:HE22	1.79	0.48
8:H:59:ILE:HD11	8:H:123:MET:HE1	1.94	0.48
2:B:234:ILE:HD11	2:B:259:TYR:CZ	2.49	0.48
2:B:861:ASP:OD1	2:B:862:GLN:N	2.47	0.47
1:A:788:SER:HB3	9:I:69:PRO:HG3	1.96	0.47
1:A:1342:GLU:OE1	5:E:200:ARG:NH2	2.47	0.47
2:B:900:ALA:HA	12:L:58:LYS:HD3	1.96	0.47
5:E:117:THR:HB	13:N:65:DA:P	2.45	0.47
7:G:118:ASP:OD1	7:G:118:ASP:N	2.47	0.47
2:B:567:GLU:OE1	2:B:567:GLU:N	2.41	0.47
9:I:28:GLU:HB3	9:I:35:VAL:HG22	1.95	0.47
1:A:185:TRP:HH2	1:A:200:ARG:HH21	1.62	0.47
3:C:249:ASP:O	3:C:253:LYS:HG2	2.14	0.47
9:I:1:MET:SD	9:I:45:ARG:HD3	2.54	0.47
1:A:873:MET:HG3	1:A:957:PRO:HG3	1.97	0.47
9:I:14:LEU:HD23	9:I:29:CYS:HB3	1.97	0.47
1:A:255:SER:O	1:A:255:SER:OG	2.31	0.47
1:A:317:LYS:CE	13:N:40:DC:H41	2.27	0.47
1:A:562:THR:O	1:A:576:GLN:NE2	2.47	0.47
1:A:814:PHE:CD2	1:A:818:MET:HE2	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:46:DT:H4'	13:N:47:DA:O4'	2.14	0.47
1:A:248:PRO:HG2	1:A:250:ILE:HD11	1.97	0.47
1:A:286:HIS:C	1:A:288:ALA:H	2.22	0.47
2:B:892:LYS:HD3	2:B:905:VAL:HG12	1.96	0.47
5:E:163:GLU:OE2	5:E:167:ARG:NE	2.46	0.47
1:A:175:ARG:HH12	1:A:177:ASP:HB2	1.80	0.47
11:K:90:ALA:O	11:K:94:ILE:HG13	2.15	0.47
1:A:841:LEU:HD21	1:A:1105:LEU:HD13	1.97	0.47
2:B:485:ARG:NH2	2:B:782:LEU:HD11	2.30	0.47
1:A:1149:ALA:HB2	9:I:47:GLU:HG3	1.98	0.47
2:B:373:ARG:NE	2:B:567:GLU:OE2	2.30	0.47
7:G:121:PHE:HA	7:G:130:TYR:HA	1.96	0.47
1:A:883:LEU:HD12	1:A:883:LEU:O	2.15	0.46
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.97	0.46
1:A:849:MET:HG2	1:A:850:VAL:H	1.80	0.46
11:K:47:ARG:HD2	11:K:61:TYR:CD1	2.50	0.46
15:T:32:DC:H2''	15:T:33:DT:C6	2.51	0.46
1:A:402:ALA:HA	1:A:434:ARG:HA	1.97	0.46
1:A:546:VAL:HG21	1:A:572:TRP:CE3	2.50	0.46
1:A:1336:MET:SD	1:A:1381:LEU:HG	2.56	0.46
1:A:1452:LYS:HE3	1:A:1454:MET:HB2	1.96	0.46
2:B:499:ASN:OD1	2:B:500:THR:N	2.48	0.46
1:A:782:ARG:NH2	2:B:699:GLU:O	2.48	0.46
1:A:873:MET:HB2	1:A:1366:ARG:NH2	2.31	0.46
2:B:238:ALA:O	2:B:256:VAL:N	2.45	0.46
1:A:92:HIS:HD2	1:A:236:LEU:HD21	1.79	0.46
1:A:253:ASN:CG	1:A:254:GLU:H	2.23	0.46
1:A:254:GLU:OE1	2:B:864:LYS:NZ	2.45	0.46
1:A:908:LEU:HA	1:A:1029:ARG:HH12	1.81	0.46
2:B:90:ILE:HG12	2:B:134:LYS:HD3	1.97	0.46
3:C:138:GLU:OE1	3:C:138:GLU:N	2.44	0.46
1:A:1297:GLU:OE1	1:A:1297:GLU:N	2.46	0.46
15:T:45:DC:H2'	15:T:46:DT:H71	1.98	0.46
1:A:343:LYS:HD2	2:B:1151:LEU:HD22	1.97	0.46
2:B:997:GLU:HB2	3:C:35:ARG:HG3	1.98	0.46
4:D:116:SER:O	4:D:155:ARG:NH2	2.48	0.46
1:A:599:SER:OG	1:A:603:ASN:ND2	2.49	0.46
1:A:857:ARG:NH2	5:E:170:LEU:HD21	2.31	0.46
1:A:1155:ASP:OD2	1:A:1241:ARG:NH2	2.43	0.46
1:A:1196:GLU:HG2	1:A:1237:ILE:HG22	1.98	0.46
2:B:365:THR:HG21	2:B:370:PHE:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:600:LEU:HB3	2:B:615:MET:SD	2.55	0.46
2:B:798:TYR:HE2	3:C:66:ARG:HH21	1.64	0.46
3:C:12:GLU:HB2	3:C:19:ASP:HB3	1.98	0.46
3:C:37:MET:SD	3:C:244:VAL:HG12	2.56	0.46
7:G:46:LEU:HD21	7:G:105:PRO:HG3	1.98	0.46
9:I:54:GLU:HA	9:I:90:GLN:HG2	1.97	0.46
1:A:569:LYS:HE2	1:A:571:LEU:HD21	1.97	0.46
2:B:34:ILE:HD12	2:B:747:MET:HE2	1.97	0.46
2:B:309:GLN:OE1	2:B:309:GLN:N	2.46	0.46
1:A:337:ARG:HD2	1:A:839:ARG:HH22	1.81	0.45
2:B:234:ILE:HD13	2:B:257:LYS:HB3	1.98	0.45
4:D:63:LEU:HB3	4:D:129:LEU:HD21	1.97	0.45
7:G:96:GLN:O	7:G:130:TYR:OH	2.28	0.45
9:I:65:ASP:OD2	9:I:67:THR:OG1	2.29	0.45
1:A:358:ASN:OD1	2:B:833:TYR:OH	2.23	0.45
1:A:1158:PRO:HA	1:A:1241:ARG:HH12	1.80	0.45
1:A:353:ILE:HG13	1:A:482:PHE:HD1	1.80	0.45
2:B:778:MET:SD	2:B:853:SER:OG	2.71	0.45
2:B:877:PRO:HB2	2:B:885:MET:HE1	1.97	0.45
2:B:101:MET:O	2:B:169:ARG:NH2	2.49	0.45
10:J:9:SER:OG	10:J:48:ARG:NH2	2.30	0.45
10:J:21:TYR:CE2	10:J:25:LEU:HD11	2.52	0.45
12:L:53:HIS:CE1	12:L:55:ILE:HB	2.52	0.45
2:B:345:LYS:HD2	2:B:348:ARG:HH22	1.82	0.45
3:C:46:ILE:HD13	3:C:159:ALA:HB2	1.99	0.45
1:A:106:VAL:HG12	1:A:113:LEU:HD23	1.98	0.45
1:A:528:LEU:O	1:A:531:ILE:HG22	2.16	0.45
2:B:345:LYS:O	2:B:349:ILE:HG12	2.16	0.45
13:N:59:DG:H2''	13:N:60:DA:OP2	2.17	0.45
1:A:482:PHE:HD2	2:B:836:GLU:HB2	1.82	0.45
1:A:527:THR:HG23	1:A:653:VAL:HB	1.98	0.45
1:A:726:ARG:NH1	1:A:1089:VAL:HG22	2.31	0.45
1:A:867:ILE:HG23	1:A:870:GLU:HA	1.99	0.45
2:B:443:ASN:O	2:B:447:ALA:N	2.48	0.45
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.51	0.45
15:T:44:DT:H2'	15:T:45:DC:C6	2.51	0.45
2:B:336:ARG:HH22	2:B:345:LYS:HE3	1.82	0.45
3:C:8:VAL:HG11	11:K:105:PHE:HD1	1.81	0.45
7:G:30:LEU:O	7:G:34:VAL:HG22	2.17	0.45
11:K:47:ARG:HD2	11:K:61:TYR:HD1	1.81	0.45
13:N:58:DG:H2''	13:N:59:DG:OP2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:43:DC:H2'	15:T:44:DT:H6	1.80	0.45
1:A:315:LEU:HA	1:A:321:PRO:HA	1.99	0.44
1:A:336:ILE:HG23	1:A:337:ARG:H	1.82	0.44
1:A:535:THR:HG21	1:A:617:VAL:HG23	1.98	0.44
2:B:634:TYR:HA	2:B:694:ASP:HA	1.99	0.44
2:B:1169:MET:HE3	2:B:1169:MET:HB2	1.93	0.44
1:A:336:ILE:HG23	1:A:337:ARG:N	2.32	0.44
2:B:80:GLU:HA	2:B:83:ASN:ND2	2.32	0.44
2:B:501:PRO:HB2	13:N:49:DT:C2	2.52	0.44
4:D:56:ARG:HB2	4:D:148:LEU:HB3	1.98	0.44
5:E:40:GLU:OE1	5:E:40:GLU:N	2.48	0.44
9:I:10:CYS:SG	9:I:31:THR:OG1	2.62	0.44
1:A:62:ASP:OD1	1:A:62:ASP:N	2.50	0.44
2:B:141:ASP:HA	2:B:147:LEU:HD22	1.99	0.44
5:E:117:THR:HG21	13:N:65:DA:P	2.58	0.44
11:K:7:PHE:HB2	11:K:11:LEU:HD12	1.98	0.44
7:G:131:GLN:HG2	7:G:136:VAL:HG13	1.99	0.44
1:A:401:GLY:H	1:A:435:HIS:HD1	1.63	0.44
1:A:537:ARG:HH12	8:H:25:ARG:NH2	2.10	0.44
2:B:326:ASP:OD1	2:B:327:ARG:N	2.50	0.44
2:B:384:ARG:HD2	2:B:393:LYS:NZ	2.33	0.44
2:B:1223:ASP:OD1	2:B:1224:PHE:N	2.45	0.44
1:A:865:GLN:NE2	1:A:1373:ASP:OD2	2.46	0.44
2:B:37:PHE:CZ	2:B:41:LYS:HD2	2.53	0.44
2:B:176:SER:O	2:B:182:SER:HB3	2.17	0.44
13:N:33:DC:H2''	13:N:34:DA:C8	2.52	0.44
1:A:563:PRO:HB3	1:A:572:TRP:CE2	2.52	0.44
1:A:596:THR:C	1:A:598:LEU:H	2.24	0.44
1:A:1038:THR:H	1:A:1041:ALA:HB3	1.82	0.44
1:A:1426:GLU:OE1	1:A:1426:GLU:N	2.51	0.44
4:D:67:ARG:NH2	4:D:129:LEU:HA	2.33	0.44
7:G:102:GLN:NE2	7:G:104:GLY:O	2.45	0.44
1:A:351:THR:HG22	2:B:1103:ILE:HA	1.99	0.44
1:A:546:VAL:O	1:A:550:LEU:HD23	2.18	0.43
6:F:133:VAL:HG21	7:G:58:ARG:NH1	2.32	0.43
1:A:1097:GLY:O	1:A:1101:LEU:N	2.37	0.43
6:F:89:GLU:OE2	6:F:136:ARG:NE	2.52	0.43
1:A:1147:THR:HB	9:I:48:LEU:HD11	2.00	0.43
1:A:1268:LEU:HD11	9:I:48:LEU:HD22	1.99	0.43
2:B:734:HIS:C	2:B:736:THR:H	2.27	0.43
1:A:4:GLN:NE2	2:B:1159:ARG:HB3	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LEU:HD23	1:A:270:LEU:HA	1.88	0.43
1:A:1436:ILE:O	1:A:1440:ALA:N	2.50	0.43
6:F:77:ASP:OD1	6:F:78:GLN:N	2.49	0.43
2:B:344:LYS:NZ	2:B:347:LYS:HG2	2.34	0.43
7:G:116:PRO:HD3	7:G:163:ILE:HG13	2.00	0.43
1:A:269:ILE:HD11	1:A:303:TYR:HB2	2.01	0.43
1:A:1160:SER:HA	1:A:1170:ILE:HG21	2.00	0.43
2:B:45:SER:OG	2:B:46:GLN:OE1	2.36	0.43
3:C:41:ILE:HB	3:C:172:PRO:HG3	2.00	0.43
1:A:117:GLU:OE1	1:A:117:GLU:N	2.51	0.43
1:A:451:HIS:ND1	1:A:453:MET:HE2	2.32	0.43
1:A:482:PHE:CD2	2:B:836:GLU:HB2	2.54	0.43
1:A:710:LEU:O	1:A:712:GLU:N	2.52	0.43
2:B:217:ARG:NH2	2:B:407:ASP:OD1	2.51	0.43
2:B:217:ARG:NE	2:B:407:ASP:OD2	2.46	0.43
2:B:825:VAL:HG21	2:B:1092:TYR:CE2	2.54	0.43
5:E:97:VAL:HG13	5:E:127:ILE:HD13	2.01	0.43
7:G:29:LYS:O	7:G:33:GLU:HG2	2.19	0.43
1:A:216:VAL:HA	1:A:219:PHE:CE2	2.54	0.43
1:A:381:THR:O	1:A:385:ILE:HG13	2.19	0.43
2:B:739:THR:O	2:B:740:HIS:ND1	2.50	0.43
8:H:41:ASP:HB2	8:H:121:LEU:HB3	2.00	0.43
1:A:860:LEU:HG	1:A:1394:THR:HG22	2.00	0.43
1:A:1398:MET:N	1:A:1426:GLU:OE2	2.50	0.43
2:B:539:LEU:HB3	2:B:543:SER:OG	2.18	0.43
1:A:731:ARG:O	1:A:735:VAL:HG13	2.19	0.42
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	2.01	0.42
1:A:1153:TYR:HE1	9:I:42:LEU:HB2	1.84	0.42
1:A:1447:GLU:N	1:A:1447:GLU:OE1	2.51	0.42
8:H:96:VAL:HG22	8:H:143:LEU:HG	2.01	0.42
10:J:1:MET:HA	10:J:56:LEU:HB2	2.00	0.42
1:A:447:GLN:HE22	1:A:488:ASN:ND2	2.17	0.42
1:A:488:ASN:OD1	2:B:1128:LEU:HD13	2.19	0.42
1:A:1224:LEU:HD12	1:A:1241:ARG:C	2.44	0.42
2:B:157:GLU:HG3	2:B:163:GLY:HA2	2.01	0.42
13:N:57:DA:H2"	13:N:58:DG:H8	1.84	0.42
1:A:298:PHE:O	1:A:302:THR:HG23	2.19	0.42
1:A:765:VAL:HB	1:A:800:VAL:HB	2.01	0.42
1:A:1111:MET:HE1	1:A:1331:SER:HA	2.01	0.42
1:A:1407:GLU:N	1:A:1407:GLU:OE1	2.51	0.42
2:B:29:ASP:HB3	2:B:658:ILE:HD13	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:ARG:HG3	3:C:176:ILE:HG21	2.01	0.42
15:T:35:DC:H2''	15:T:36:DT:H71	2.01	0.42
1:A:1098:VAL:HB	1:A:1099:PRO:HD3	2.01	0.42
1:A:67:CYS:SG	1:A:69:THR:HB	2.60	0.42
1:A:702:LEU:HD23	1:A:702:LEU:H	1.84	0.42
5:E:117:THR:HG22	13:N:64:DG:H3'	2.01	0.42
1:A:398:GLU:HG2	1:A:400:PRO:HD2	2.00	0.42
2:B:396:ASP:OD1	2:B:397:ASP:N	2.53	0.42
2:B:508:LEU:HD21	13:N:51:DG:H5''	2.02	0.42
2:B:558:LEU:HD13	2:B:580:VAL:HG11	2.01	0.42
2:B:1094:ARG:HH21	2:B:1098:MET:HG2	1.84	0.42
3:C:34:ARG:HA	3:C:37:MET:HE3	2.02	0.42
1:A:110:CYS:SG	1:A:111:GLY:N	2.93	0.42
1:A:219:PHE:HA	1:A:222:LEU:HD12	2.00	0.42
2:B:550:ASP:HA	2:B:551:PRO:HD3	1.90	0.42
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.55	0.42
8:H:103:LYS:HB3	8:H:115:TYR:HB2	2.01	0.42
1:A:1436:ILE:HB	2:B:1144:ALA:HB2	2.01	0.42
2:B:982:SER:OG	2:B:983:ARG:N	2.53	0.42
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.85	0.42
7:G:139:ILE:HD12	7:G:139:ILE:H	1.85	0.42
9:I:85:PHE:HB3	9:I:101:PHE:CD1	2.55	0.42
10:J:42:LYS:HG3	10:J:43:ARG:H	1.84	0.42
15:T:55:DA:H2''	15:T:56:DT:H71	2.02	0.42
1:A:595:THR:OG1	1:A:603:ASN:OD1	2.28	0.42
1:A:943:LEU:HD23	1:A:943:LEU:HA	1.89	0.42
4:D:56:ARG:HA	4:D:148:LEU:HD13	2.02	0.42
1:A:1148:ILE:N	1:A:1196:GLU:O	2.44	0.42
2:B:469:GLN:NE2	15:T:51:DG:H5''	2.35	0.42
4:D:50:LEU:HB2	7:G:2:PHE:HB2	2.00	0.42
13:N:55:DG:C2	13:N:56:DA:C4	3.07	0.42
14:R:2:U:H2'	14:R:3:C:C6	2.55	0.42
15:T:33:DT:H6	15:T:33:DT:OP2	2.03	0.42
15:T:57:DG:H2''	15:T:58:DA:C8	2.55	0.42
1:A:760:GLN:HG2	1:A:765:VAL:HA	2.01	0.41
1:A:826:ASP:HA	1:A:830:LYS:HB2	2.02	0.41
1:A:1100:ARG:HH12	1:A:1111:MET:HE2	1.84	0.41
1:A:1441:PHE:CE2	6:F:89:GLU:HG2	2.55	0.41
1:A:22:PHE:HE2	2:B:1208:MET:HA	1.85	0.41
1:A:262:LEU:O	1:A:266:LEU:HD23	2.20	0.41
1:A:1202:MET:HE2	1:A:1202:MET:HB3	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:GLU:OE1	2:B:80:GLU:N	2.48	0.41
2:B:863:GLU:O	2:B:961:LEU:HD13	2.19	0.41
2:B:874:PHE:HE1	2:B:914:LYS:HD3	1.86	0.41
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	2.02	0.41
6:F:116:ASP:O	6:F:120:ILE:HG12	2.20	0.41
7:G:114:LEU:HD13	7:G:162:SER:HB2	2.02	0.41
1:A:515:GLN:OE1	1:A:516:SER:OG	2.22	0.41
2:B:115:GLN:O	2:B:119:LEU:HG	2.21	0.41
2:B:705:MET:HE3	2:B:742:GLU:HG3	2.02	0.41
12:L:49:LYS:C	12:L:51:CYS:H	2.28	0.41
13:N:58:DG:C2	13:N:59:DG:C4	3.08	0.41
1:A:1433:MET:HE1	6:F:92:ARG:HH22	1.84	0.41
2:B:227:LYS:HE3	2:B:236:HIS:CE1	2.55	0.41
8:H:8:ASP:HB3	8:H:10:PHE:CE1	2.55	0.41
1:A:526:ASP:HB2	2:B:835:GLN:HE21	1.82	0.41
1:A:675:THR:O	1:A:679:ILE:HG12	2.20	0.41
1:A:1143:LEU:HD13	1:A:1271:ILE:HG21	2.03	0.41
3:C:58:LEU:HD21	10:J:57:ILE:HD13	2.02	0.41
5:E:200:ARG:HD2	5:E:208:TYR:HD2	1.85	0.41
1:A:302:THR:HG21	1:A:314:ALA:HB2	2.03	0.41
1:A:1170:ILE:HA	1:A:1173:HIS:CD2	2.55	0.41
4:D:206:GLU:HA	4:D:209:ARG:HG2	2.01	0.41
11:K:81:TYR:CE2	11:K:86:ALA:HB2	2.56	0.41
12:L:31:CYS:SG	12:L:32:ALA:N	2.93	0.41
13:N:48:DC:H6	13:N:48:DC:H2'	1.71	0.41
1:A:670:ILE:HG12	1:A:805:LEU:HD21	2.02	0.41
1:A:1343:ALA:HB2	5:E:150:VAL:HG22	2.02	0.41
2:B:87:LYS:HD2	2:B:137:TYR:HD2	1.85	0.41
2:B:521:LEU:HD22	2:B:633:VAL:HG12	2.03	0.41
2:B:773:MET:HE1	2:B:987:LYS:HB3	2.03	0.41
4:D:52:LEU:HD11	4:D:147:TYR:CE2	2.55	0.41
4:D:167:LEU:HB3	4:D:177:VAL:HG13	2.03	0.41
7:G:13:LEU:HD11	7:G:26:LEU:HD21	2.01	0.41
7:G:85:GLU:HG2	7:G:87:VAL:HG13	2.03	0.41
2:B:41:LYS:O	2:B:45:SER:HB3	2.20	0.41
2:B:1000:PRO:HB2	2:B:1072:MET:HE2	2.03	0.41
5:E:201:LYS:HE3	5:E:201:LYS:HB2	1.87	0.41
1:A:23:SER:HB2	1:A:233:TRP:CE2	2.56	0.41
1:A:216:VAL:O	1:A:220:THR:OG1	2.36	0.41
2:B:73:GLN:N	2:B:86:ARG:O	2.54	0.41
2:B:1065:GLN:OE1	2:B:1067:ARG:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1220:ARG:HA	2:B:1220:ARG:HD3	1.92	0.41
3:C:241:ASP:OD1	3:C:242:GLN:N	2.53	0.41
4:D:23:ASN:HB3	4:D:26:THR:HG22	2.03	0.41
4:D:50:LEU:HB3	4:D:55:ALA:HB2	2.03	0.41
6:F:111:LEU:HD22	6:F:120:ILE:HD12	2.03	0.41
13:N:42:DT:C6	13:N:43:DT:H72	2.56	0.41
1:A:695:LYS:HD3	1:A:695:LYS:HA	1.84	0.41
1:A:798:GLY:HA2	1:A:815:PHE:CD2	2.56	0.41
1:A:1130:GLN:HA	1:A:1133:LEU:HG	2.03	0.41
1:A:1427:ASN:HB2	1:A:1434:ALA:HB2	2.03	0.41
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.85	0.41
1:A:242:PRO:HB2	1:A:246:VAL:HB	2.03	0.40
1:A:722:LEU:HD13	1:A:799:PHE:CD1	2.56	0.40
1:A:1364:ASN:OD1	1:A:1365:TYR:N	2.54	0.40
7:G:39:THR:O	7:G:43:GLY:N	2.51	0.40
3:C:36:VAL:HG21	3:C:251:LEU:HD13	2.03	0.40
10:J:3:VAL:HG21	10:J:18:TRP:HB2	2.03	0.40
1:A:492:PRO:HG3	1:A:501:LEU:HD12	2.02	0.40
1:A:1386:ARG:HD2	1:A:1404:GLU:OE2	2.22	0.40
2:B:121:ASN:HA	2:B:207:GLY:HA3	2.04	0.40
2:B:739:THR:HG22	2:B:740:HIS:CE1	2.57	0.40
3:C:37:MET:HA	3:C:41:ILE:HD11	2.04	0.40
5:E:131:THR:HG21	5:E:191:LYS:HE3	2.03	0.40
7:G:81:PRO:HG3	7:G:106:MET:SD	2.62	0.40
9:I:49:ILE:HG13	9:I:50:THR:H	1.87	0.40
13:N:53:DG:H2''	13:N:54:DA:C8	2.56	0.40
1:A:500:GLU:OE1	2:B:1146:PHE:N	2.52	0.40
2:B:261:ARG:O	2:B:264:SER:OG	2.25	0.40
5:E:112:TYR:CD1	5:E:116:ILE:HD11	2.57	0.40
6:F:140:ASP:OD1	6:F:142:SER:OG	2.38	0.40
13:N:56:DA:C4	13:N:57:DA:C8	3.10	0.40
1:A:236:LEU:CD2	2:B:1211:ASN:HD22	2.34	0.40
1:A:541:ILE:HG22	1:A:546:VAL:HG23	2.03	0.40
3:C:29:MET:HE3	3:C:29:MET:HB2	1.92	0.40
13:N:49:DT:H6	13:N:49:DT:H2'	1.63	0.40
14:R:3:C:H2'	14:R:4:G:O4'	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1376/1733 (79%)	1311 (95%)	60 (4%)	5 (0%)	30	61
2	B	1136/1224 (93%)	1097 (97%)	39 (3%)	0	100	100
3	C	264/318 (83%)	256 (97%)	8 (3%)	0	100	100
4	D	161/221 (73%)	161 (100%)	0	0	100	100
5	E	211/215 (98%)	203 (96%)	8 (4%)	0	100	100
6	F	81/155 (52%)	78 (96%)	3 (4%)	0	100	100
7	G	169/171 (99%)	164 (97%)	5 (3%)	0	100	100
8	H	130/146 (89%)	128 (98%)	2 (2%)	0	100	100
9	I	110/122 (90%)	101 (92%)	9 (8%)	0	100	100
10	J	63/70 (90%)	62 (98%)	1 (2%)	0	100	100
11	K	110/120 (92%)	109 (99%)	1 (1%)	0	100	100
12	L	43/70 (61%)	35 (81%)	8 (19%)	0	100	100
All	All	3854/4565 (84%)	3705 (96%)	144 (4%)	5 (0%)	49	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	710	LEU
1	A	711	ARG
1	A	885	THR
1	A	253	ASN
1	A	958	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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 (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
1	A	287	HIS
1	A	313	GLN
1	A	488	ASN
1	A	589	GLN
1	A	611	GLN
1	A	660	ASN
1	A	698	GLN
1	A	736	ASN
1	A	742	ASN
1	A	1128	GLN
1	A	1218	GLN
2	B	60	GLN
2	B	300	HIS
2	B	357	GLN
2	B	481	GLN
2	B	762	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	763	GLN
2	B	770	GLN
2	B	776	GLN
2	B	862	GLN
3	C	252	GLN
5	E	63	ASN
7	G	10	ASN
7	G	122	ASN
9	I	23	ASN
9	I	89	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	R	7/9 (77%)	2 (28%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	R	4	G
14	R	6	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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
18	ATP	T	101	16	29,33,33	2.92	8 (27%)	44,52,52	2.74	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
18	ATP	T	101	16	-	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)
18	T	101	ATP	C8-N9	-9.02	1.21	1.37
18	T	101	ATP	C4-N9	-8.67	1.18	1.37
18	T	101	ATP	C6-N6	4.42	1.45	1.34
18	T	101	ATP	C5-N7	3.55	1.45	1.39
18	T	101	ATP	C8-N7	2.99	1.37	1.31
18	T	101	ATP	O4'-C1'	2.91	1.48	1.42
18	T	101	ATP	C2'-C3'	-2.63	1.46	1.53
18	T	101	ATP	C5-C6	-2.61	1.33	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	T	101	ATP	C4-N9-C8	12.80	119.60	105.73
18	T	101	ATP	N3-C2-N1	-5.29	120.32	128.60
18	T	101	ATP	PB-O3B-PG	-4.12	118.68	132.83
18	T	101	ATP	C5-C4-N3	-3.71	121.92	126.75
18	T	101	ATP	N3-C4-N9	3.62	133.05	127.08
18	T	101	ATP	N9-C8-N7	-3.42	109.23	113.91
18	T	101	ATP	PA-O3A-PB	-3.41	121.11	132.83
18	T	101	ATP	C5-N7-C8	-3.24	98.90	103.51
18	T	101	ATP	C1'-N9-C8	-3.11	120.10	127.14
18	T	101	ATP	C4-C5-N7	-2.78	107.23	110.62
18	T	101	ATP	C4-N9-C1'	-2.64	120.29	126.59
18	T	101	ATP	C2-N3-C4	2.48	117.61	111.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	T	101	ATP	C3'-C2'-C1'	2.10	105.41	101.43

There are no chirality outliers.

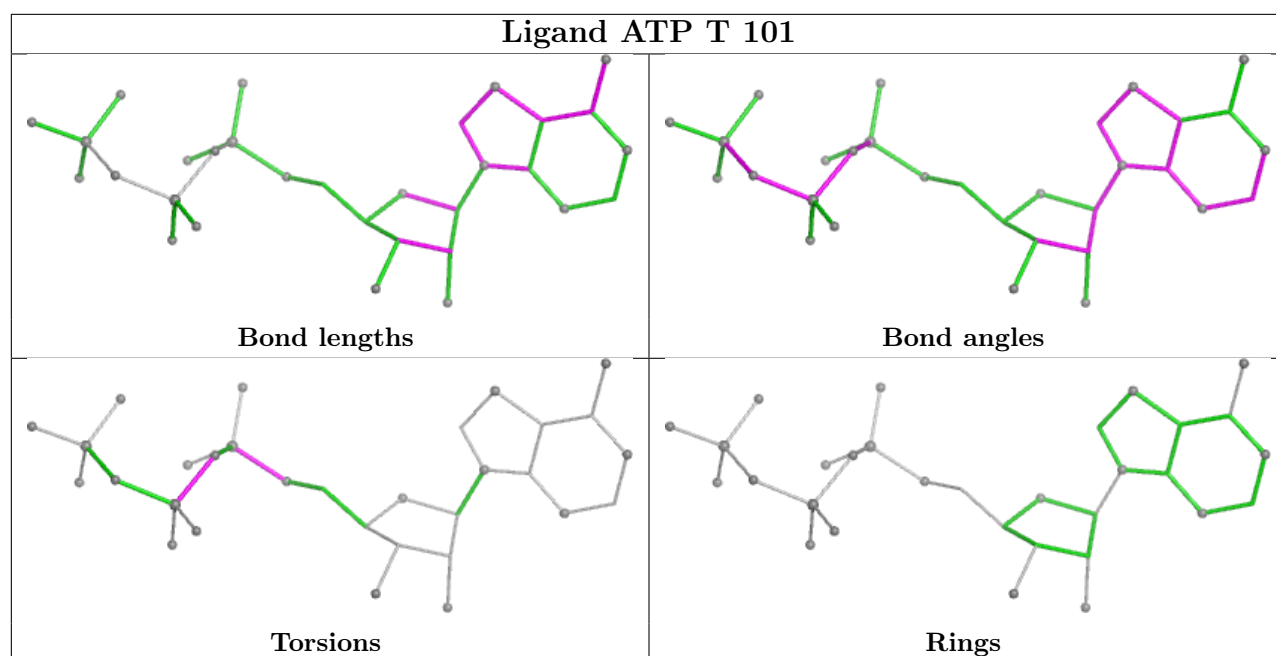
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	T	101	ATP	C5'-O5'-PA-O1A
18	T	101	ATP	C5'-O5'-PA-O3A
18	T	101	ATP	PA-O3A-PB-O1B
18	T	101	ATP	PA-O3A-PB-O2B

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](#)

There are no chain breaks in this entry.

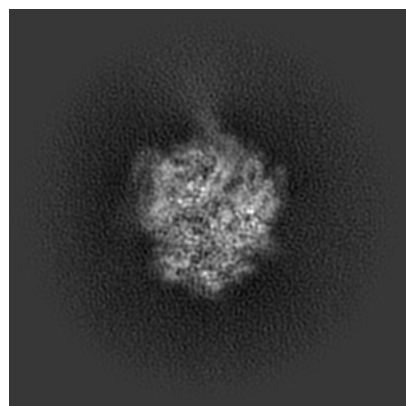
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54749. These allow visual inspection of the internal detail of the map and identification of artifacts.

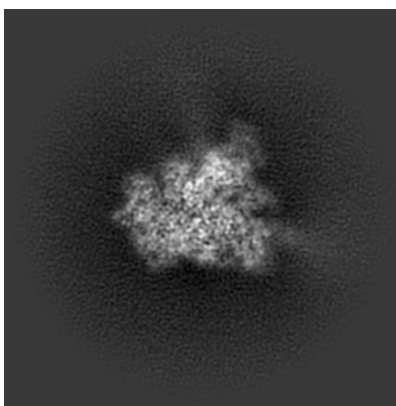
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

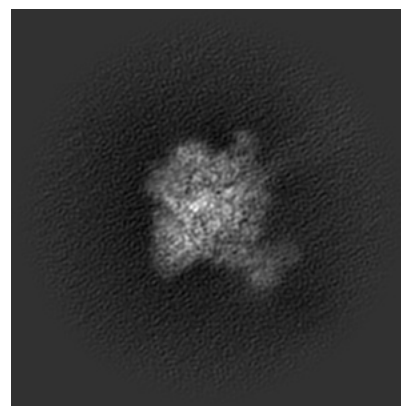
6.1.1 Primary map



X

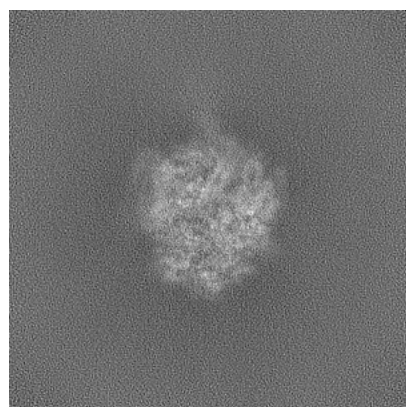


Y

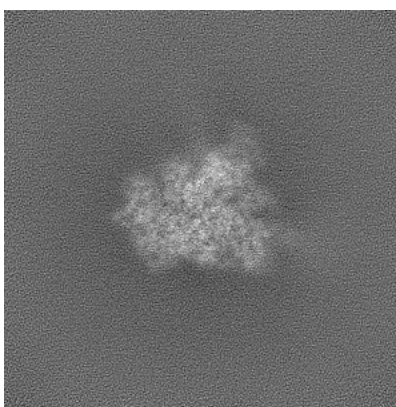


Z

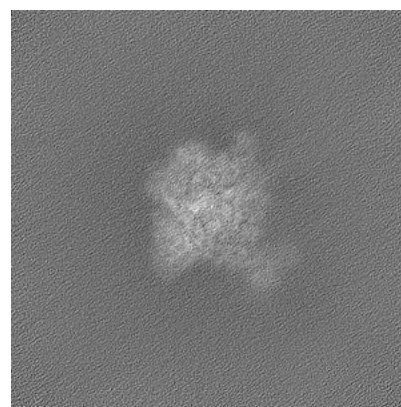
6.1.2 Raw map



X



Y

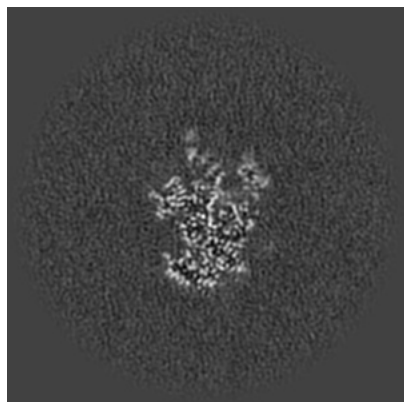


Z

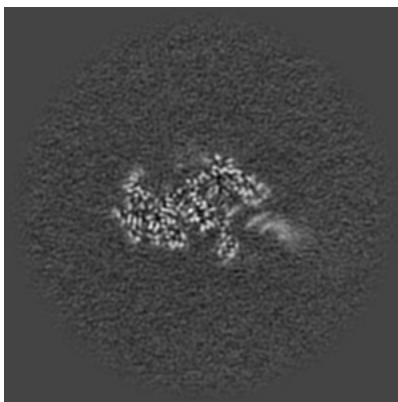
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

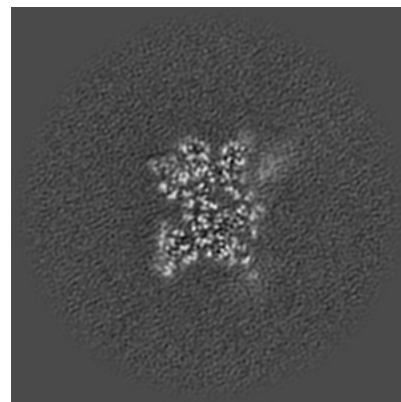
6.2.1 Primary map



X Index: 160

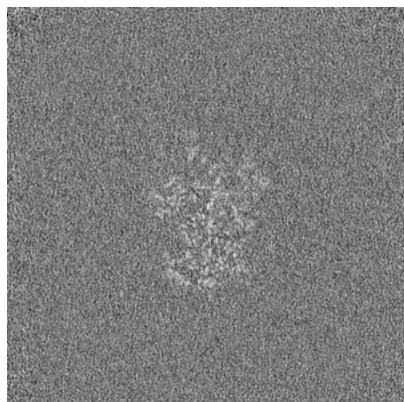


Y Index: 160

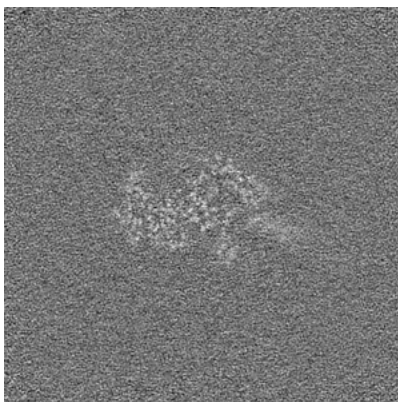


Z Index: 160

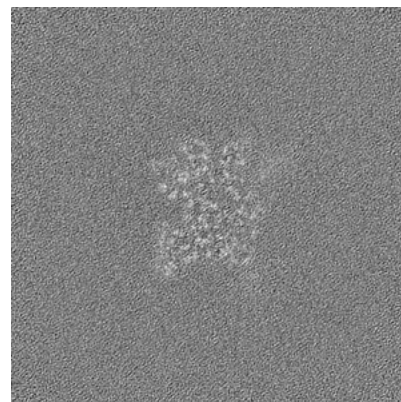
6.2.2 Raw map



X Index: 160



Y Index: 160

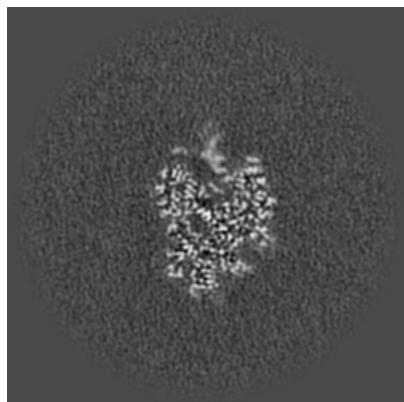


Z Index: 160

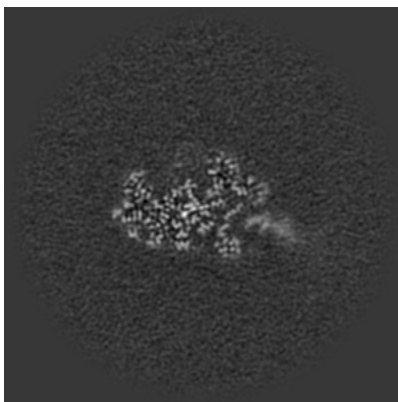
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

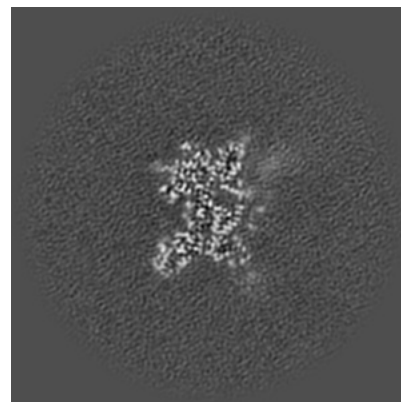
6.3.1 Primary map



X Index: 150

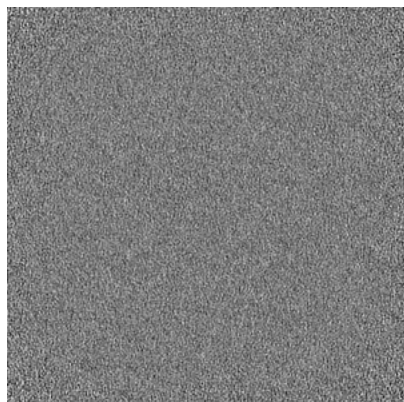


Y Index: 162

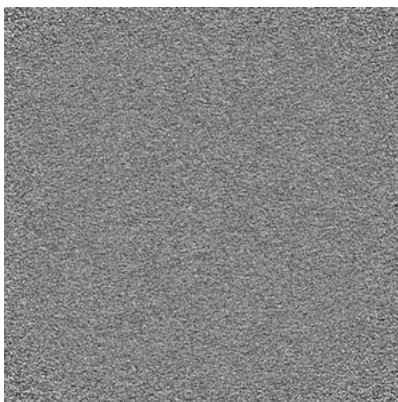


Z Index: 157

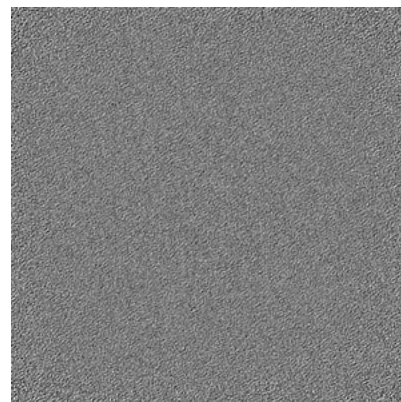
6.3.2 Raw map



X Index: 0



Y Index: 0

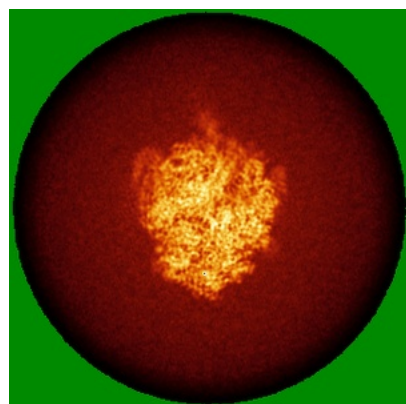


Z Index: 0

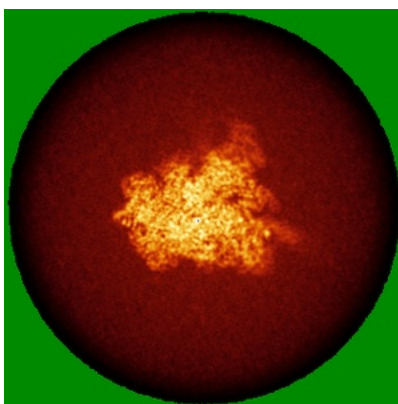
The images above show the largest variance slices of the map in three orthogonal directions.

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

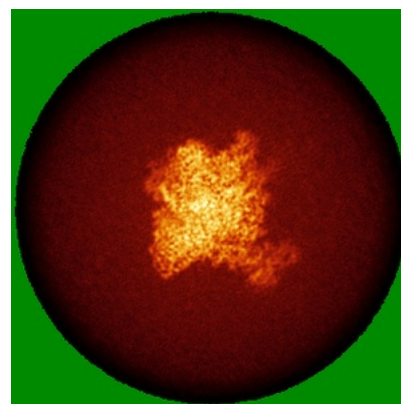
6.4.1 Primary map



X

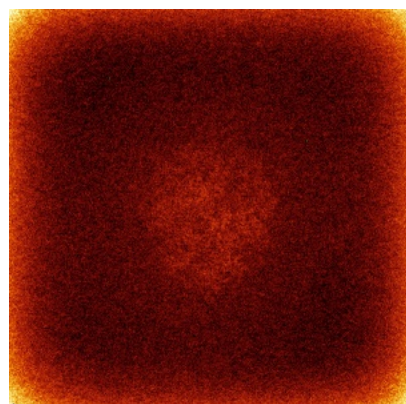


Y

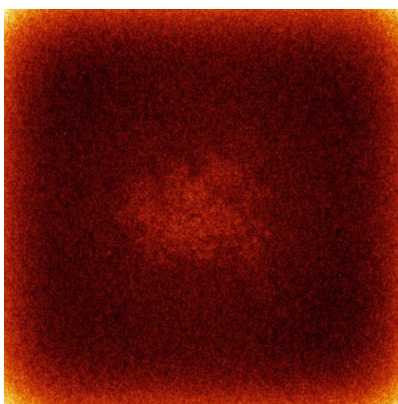


Z

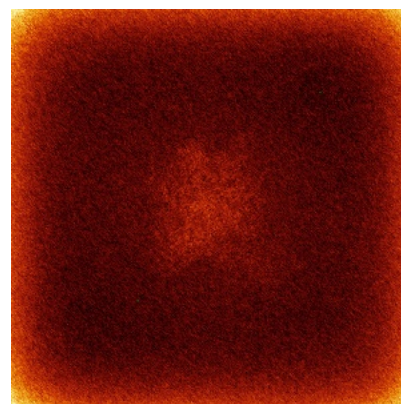
6.4.2 Raw map



X



Y

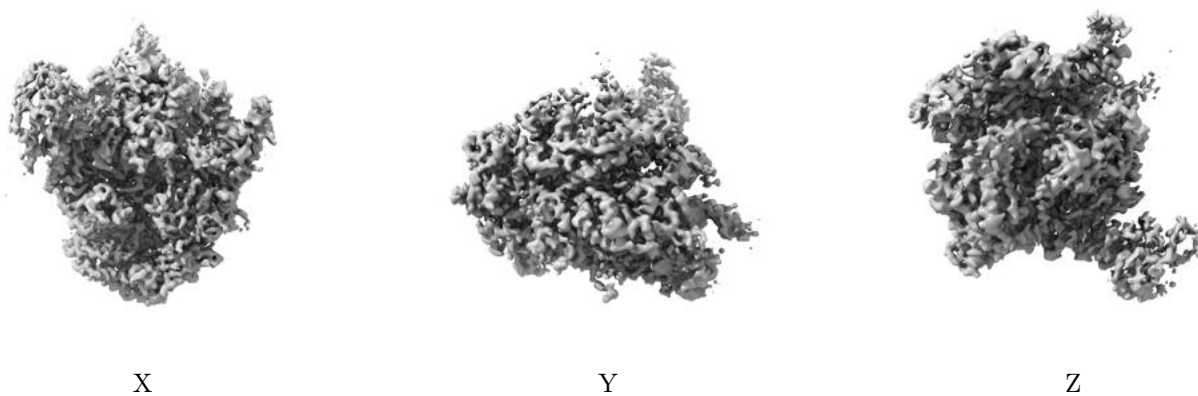


Z

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.

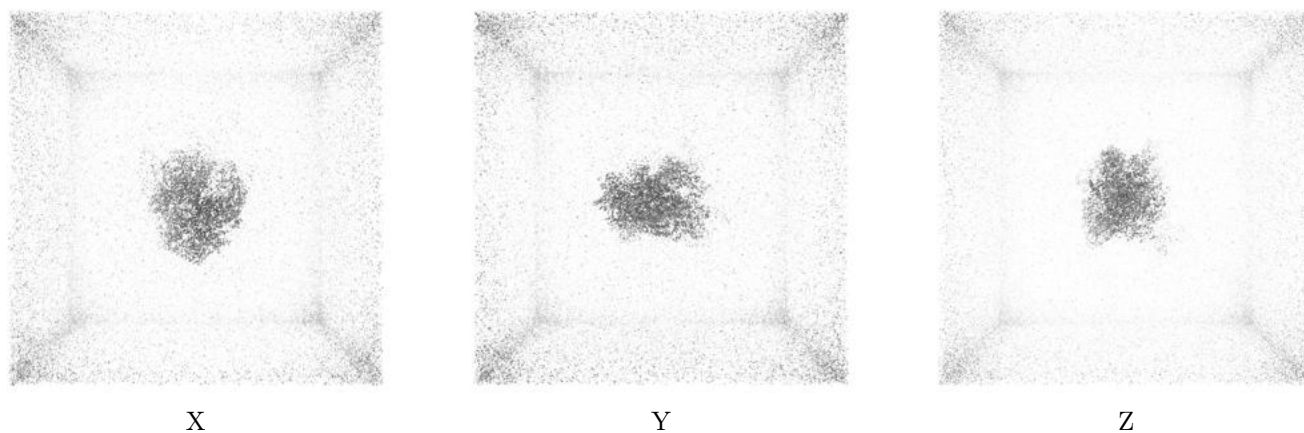
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

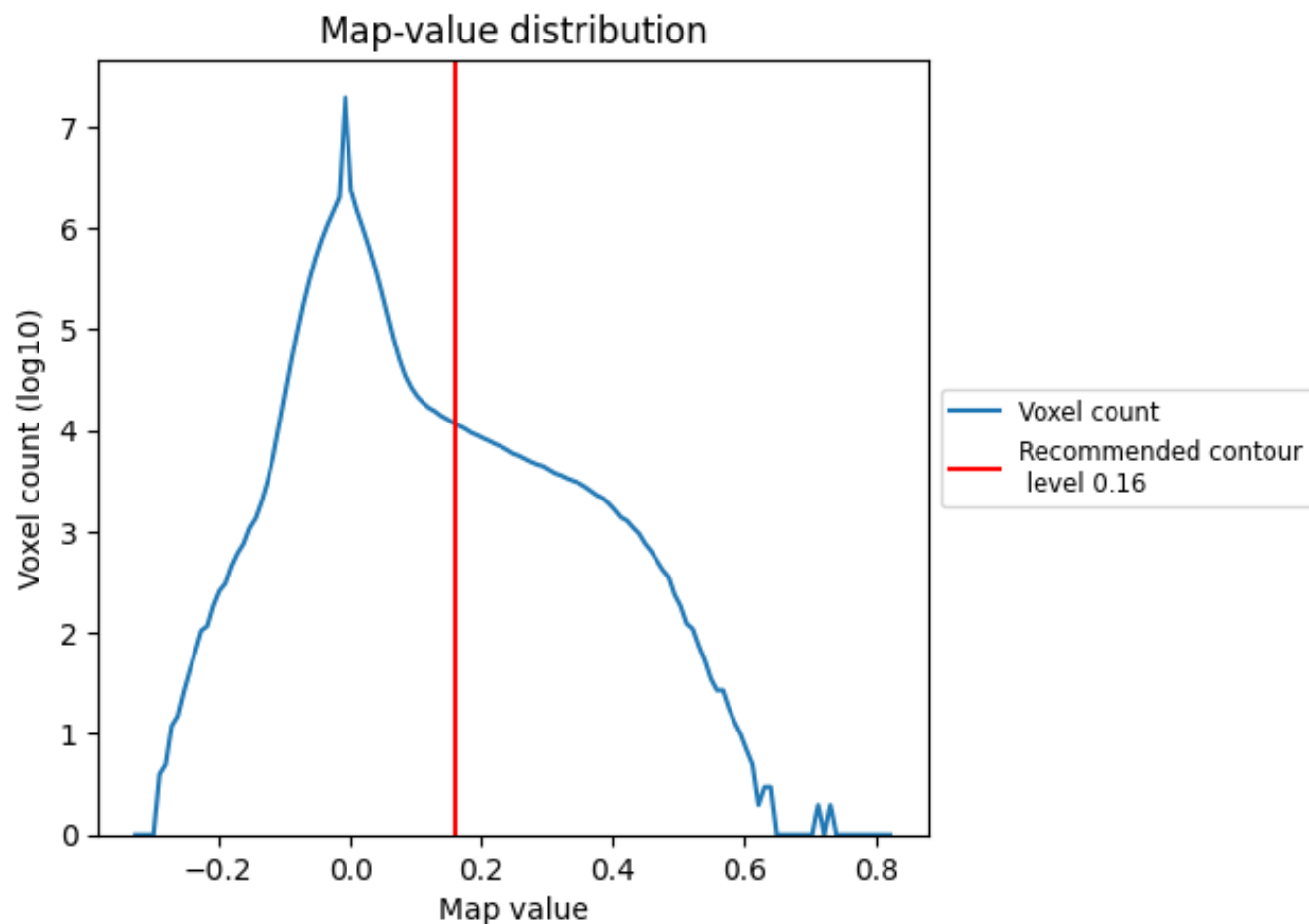
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

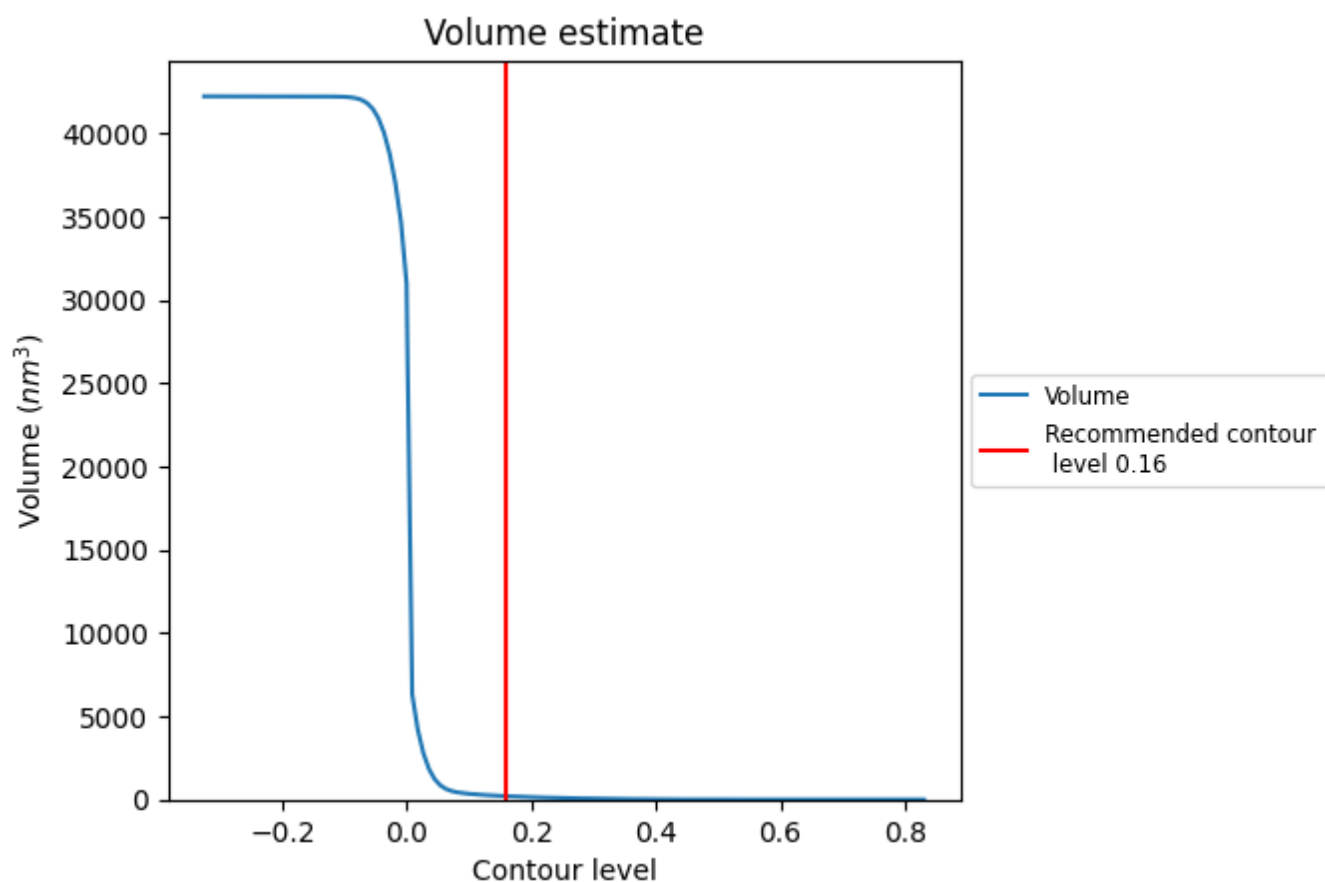
This section contains the results of statistical analysis of the map.

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.

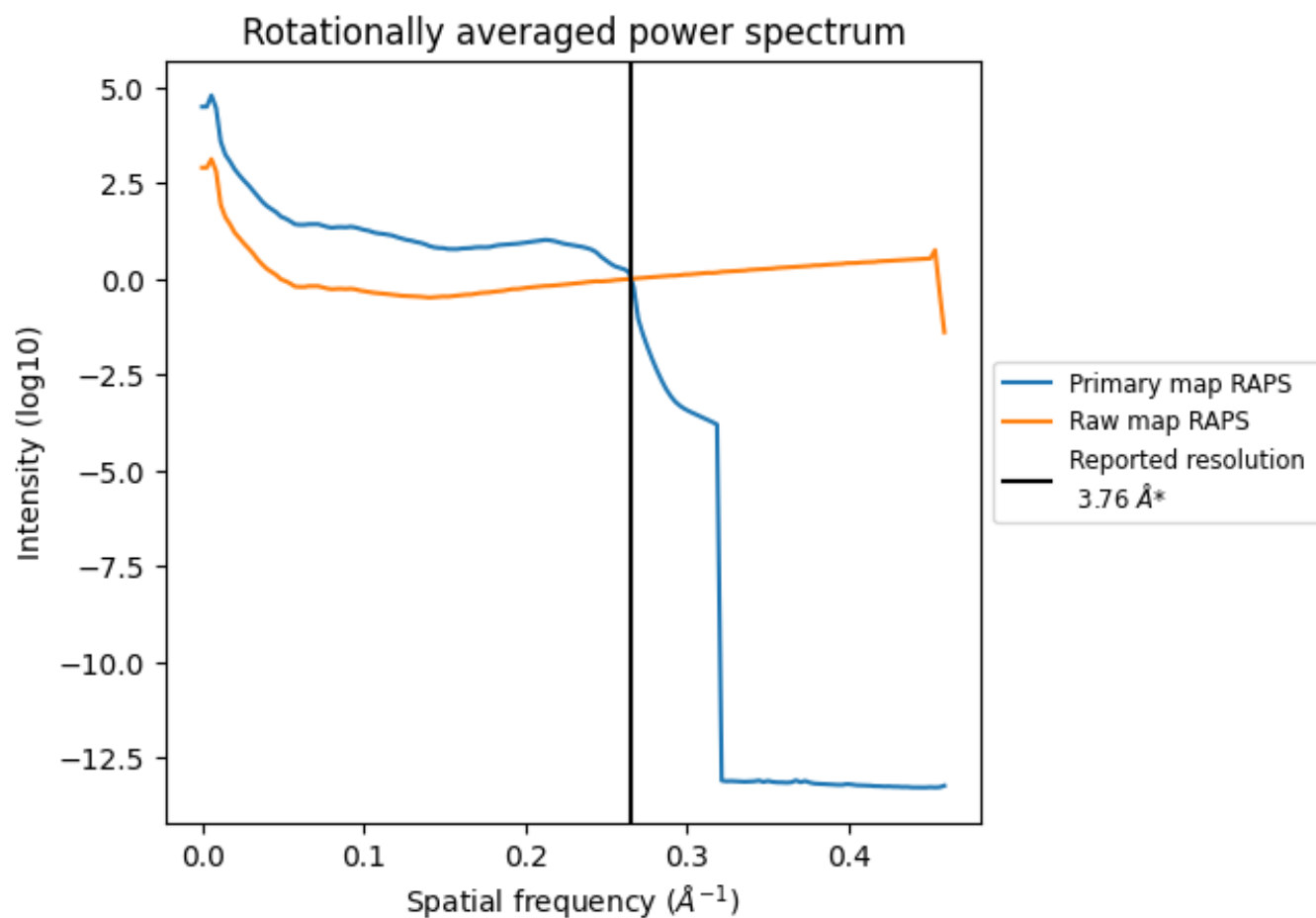
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 203 nm³; this corresponds to an approximate mass of 184 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 ⓘ

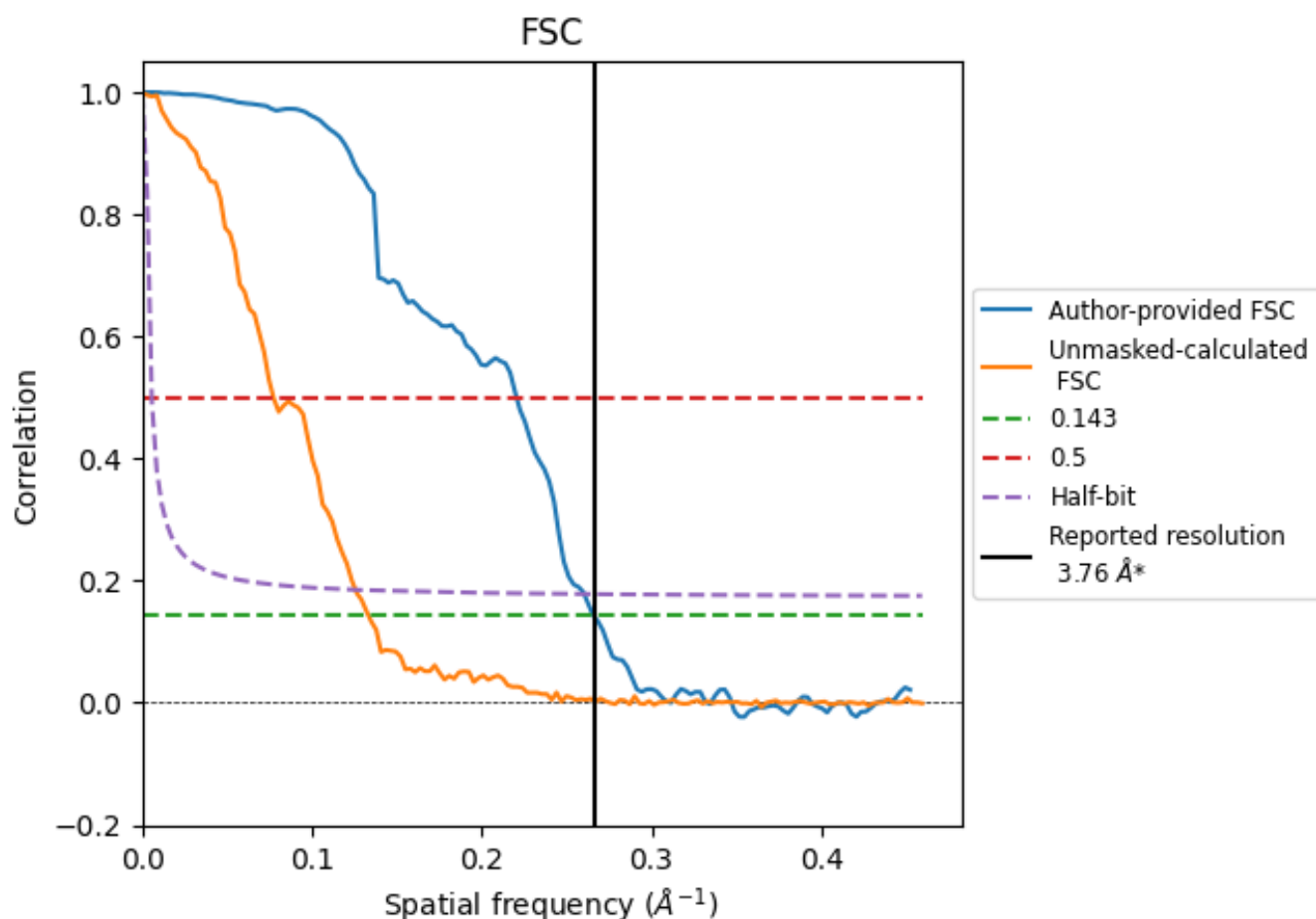


*Reported resolution corresponds to spatial frequency of 0.266 Å⁻¹

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 0.266 \AA^{-1}

8.2 Resolution estimates [i](#)

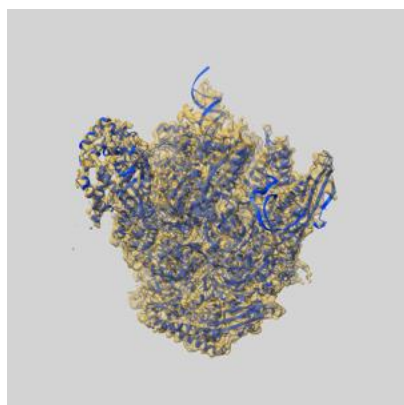
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.76	-	-
Author-provided FSC curve	3.77	4.53	3.84
Unmasked-calculated*	7.50	12.92	7.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.50 differs from the reported value 3.76 by more than 10 %

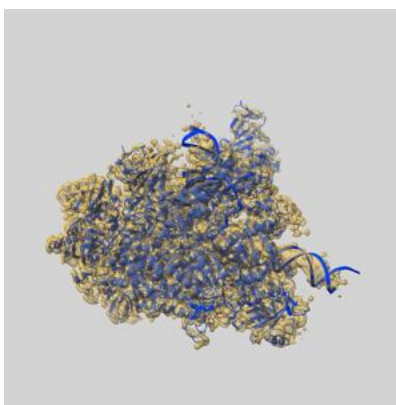
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54749 and PDB model 9SC4. Per-residue inclusion information can be found in section [3](#) on page [8](#).

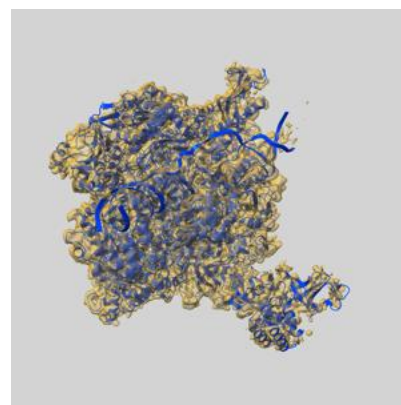
9.1 Map-model overlay [i](#)



X



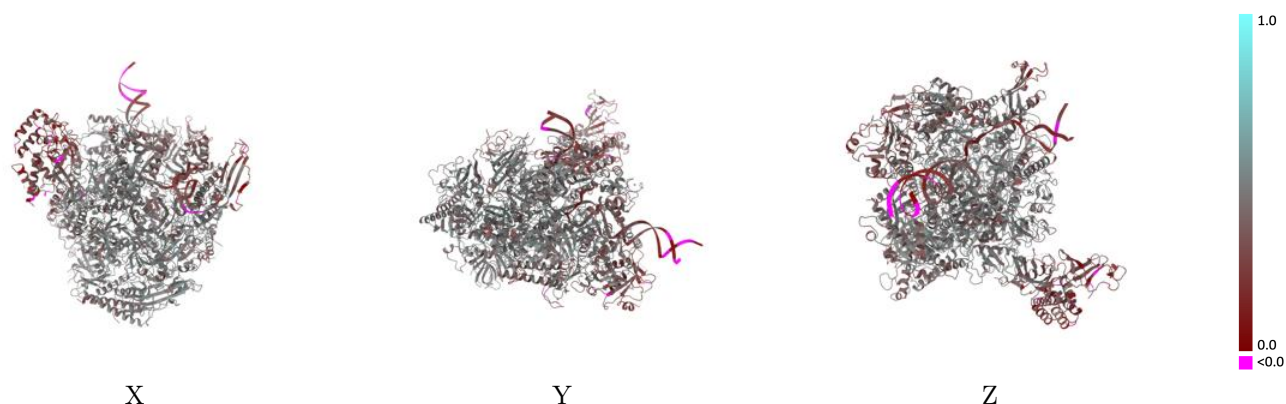
Y



Z

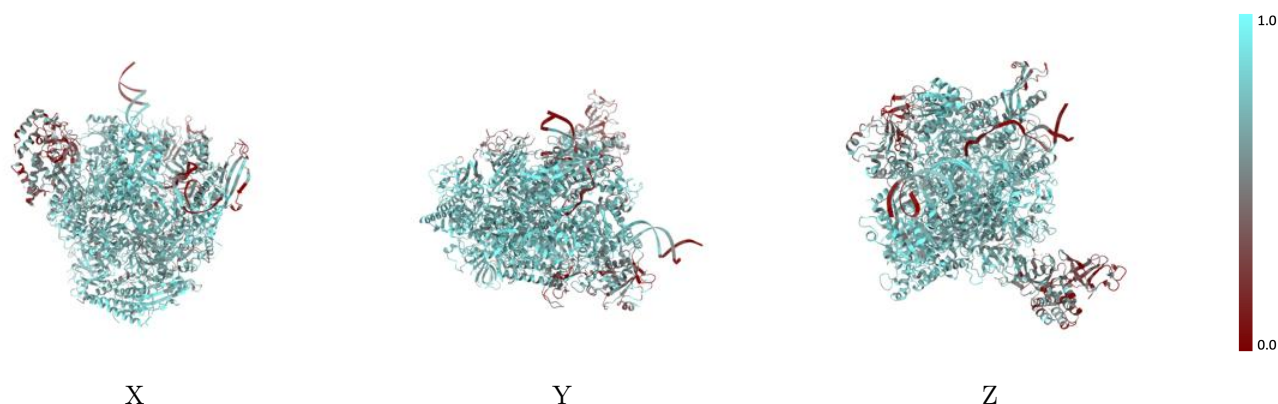
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



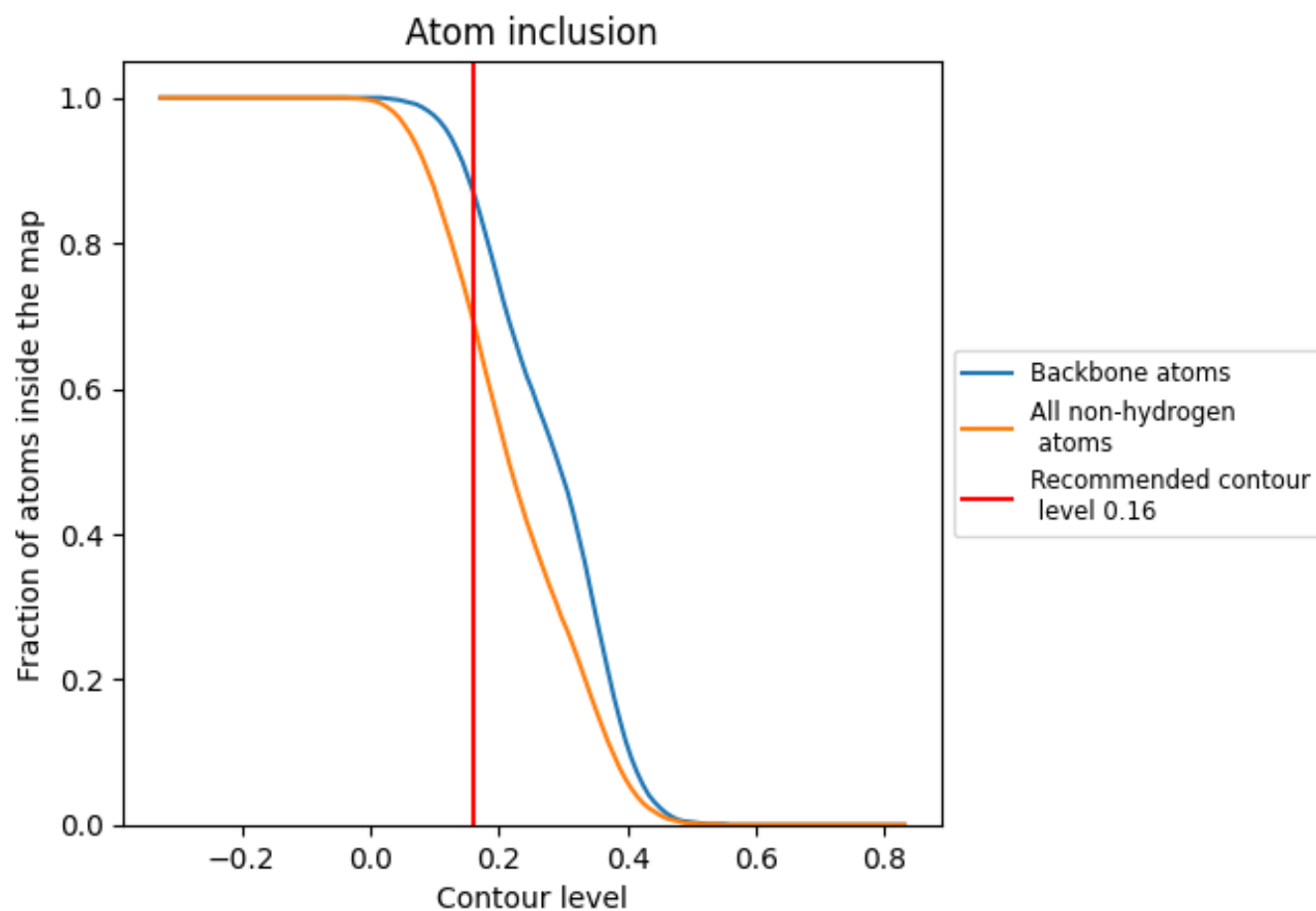
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 87% of all backbone atoms, 69% 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	 0.6940	 0.4230
A	 0.7420	 0.4430
B	 0.7230	 0.4450
C	 0.7690	 0.4650
D	 0.4160	 0.2790
E	 0.7540	 0.4440
F	 0.7710	 0.4660
G	 0.4690	 0.3380
H	 0.7630	 0.4560
I	 0.2950	 0.3510
J	 0.7970	 0.4690
K	 0.7610	 0.4600
L	 0.4580	 0.3990
N	 0.5020	 0.2240
R	 0.8980	 0.4470
T	 0.6530	 0.2860

