



Full wwPDB EM Validation Report ⓘ

Jul 1, 2026 – 11:20 am BST

PDB ID : 9SAY / pdb_00009say
EMDB ID : EMD-54704
Title : Structure of Yeast RNA polymerase II elongation complex apo-state-I
Authors : Yi, G.; Li, Q.; Zhang, P.; Wang, D.
Deposited on : 2025-08-08
Resolution : 3.44 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

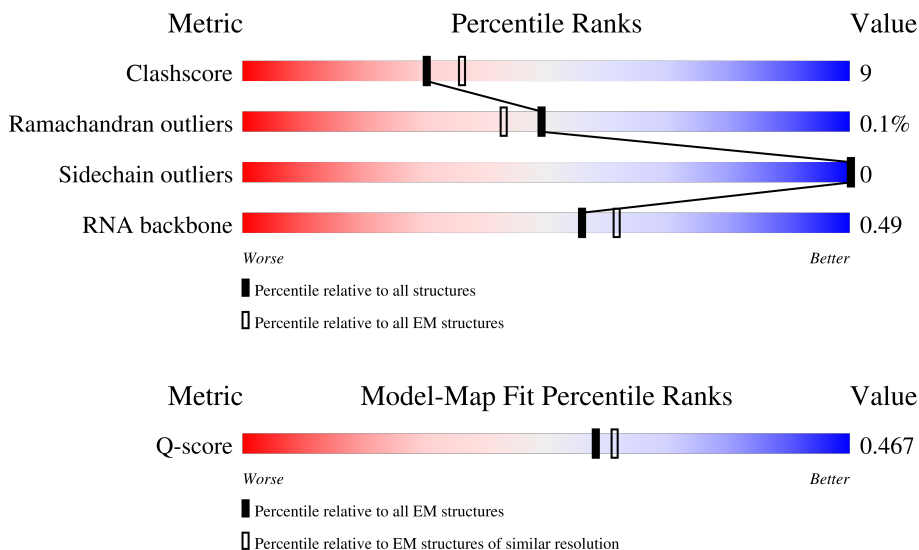
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.44 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	13877 (2.94 - 3.94)

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	

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

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 29640 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	1379	10859	6856	1899	2042	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	1148	9142	5779	1599	1709	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 polymerases I, II, and III subunit RPABC1.

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

- Molecule 5 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		
5	F	83	670	428	114	125	3	0	0

- Molecule 6 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		
6	H	134	1077	679	182	212	4	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 8 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		
8	J	65	532	339	93	94	6	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 10 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		
10	L	45	359	221	71	63	4	0	0

- Molecule 11 is a DNA chain called DNA (74-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	N	23	489	228	105	133	23	0	0

- Molecule 12 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		
12	R	9	198	88	40	61	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
13	T	33	653	314	100	206	33	0	0

- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of

Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
14	A	1	Total 1	Mg 1	0

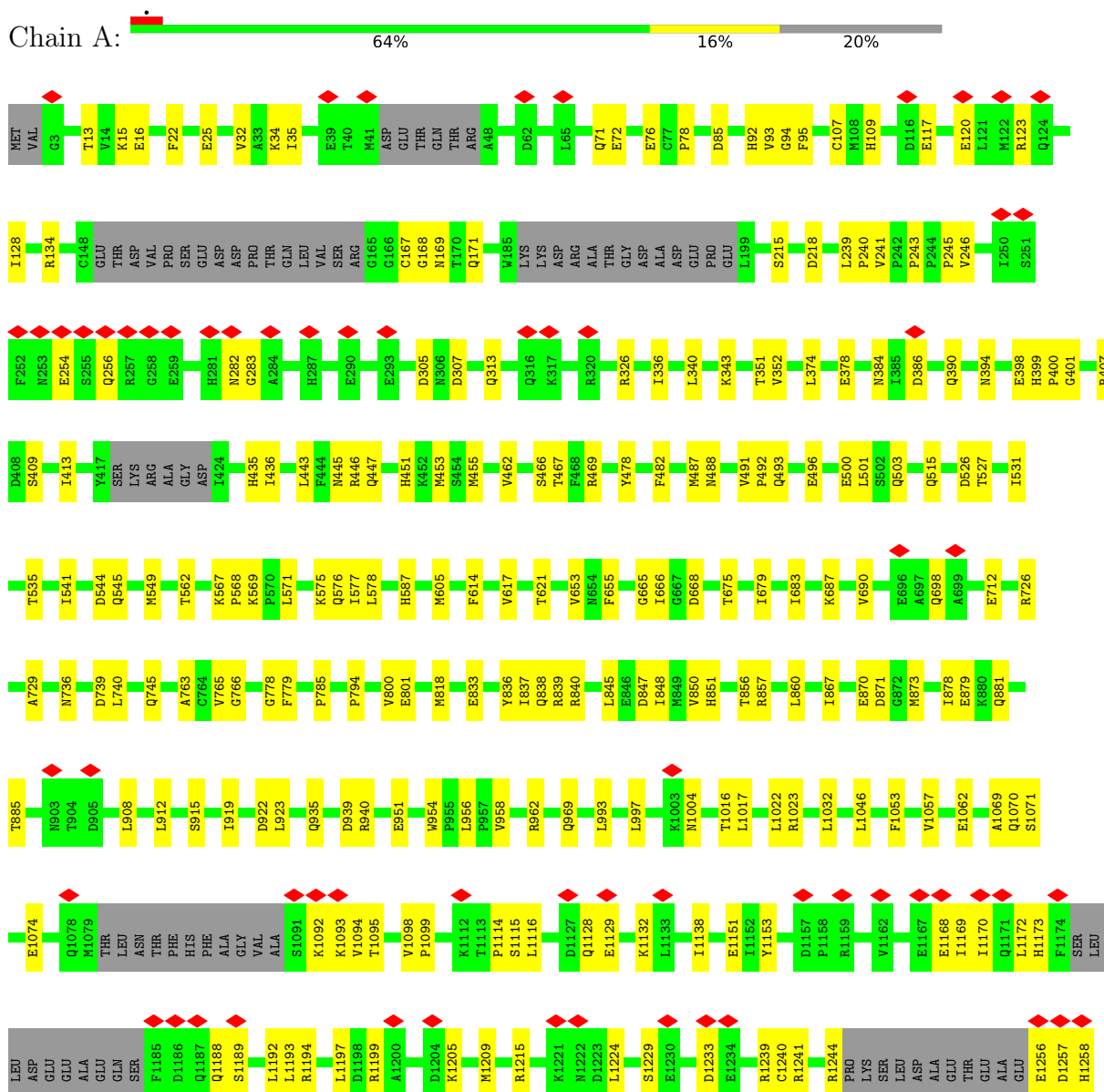
- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

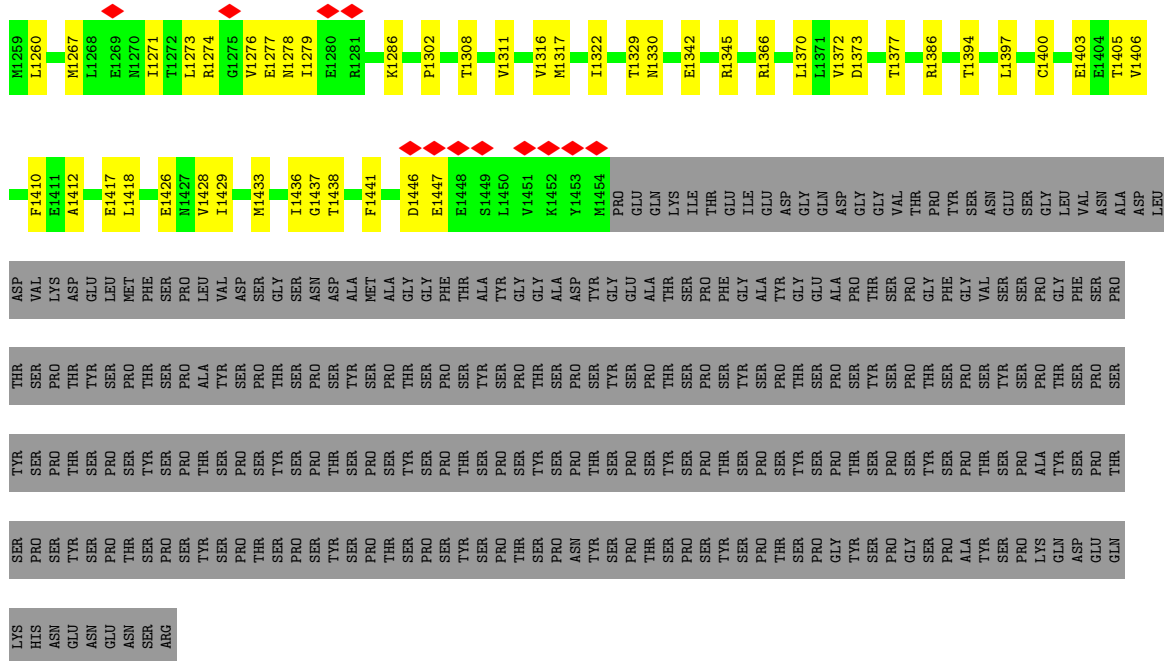
Mol	Chain	Residues	Atoms		AltConf
15	A	2	Total 2	Zn 2	0
15	B	1	Total 1	Zn 1	0
15	C	1	Total 1	Zn 1	0
15	I	2	Total 2	Zn 2	0
15	J	1	Total 1	Zn 1	0
15	L	1	Total 1	Zn 1	0

3 Residue-property plots

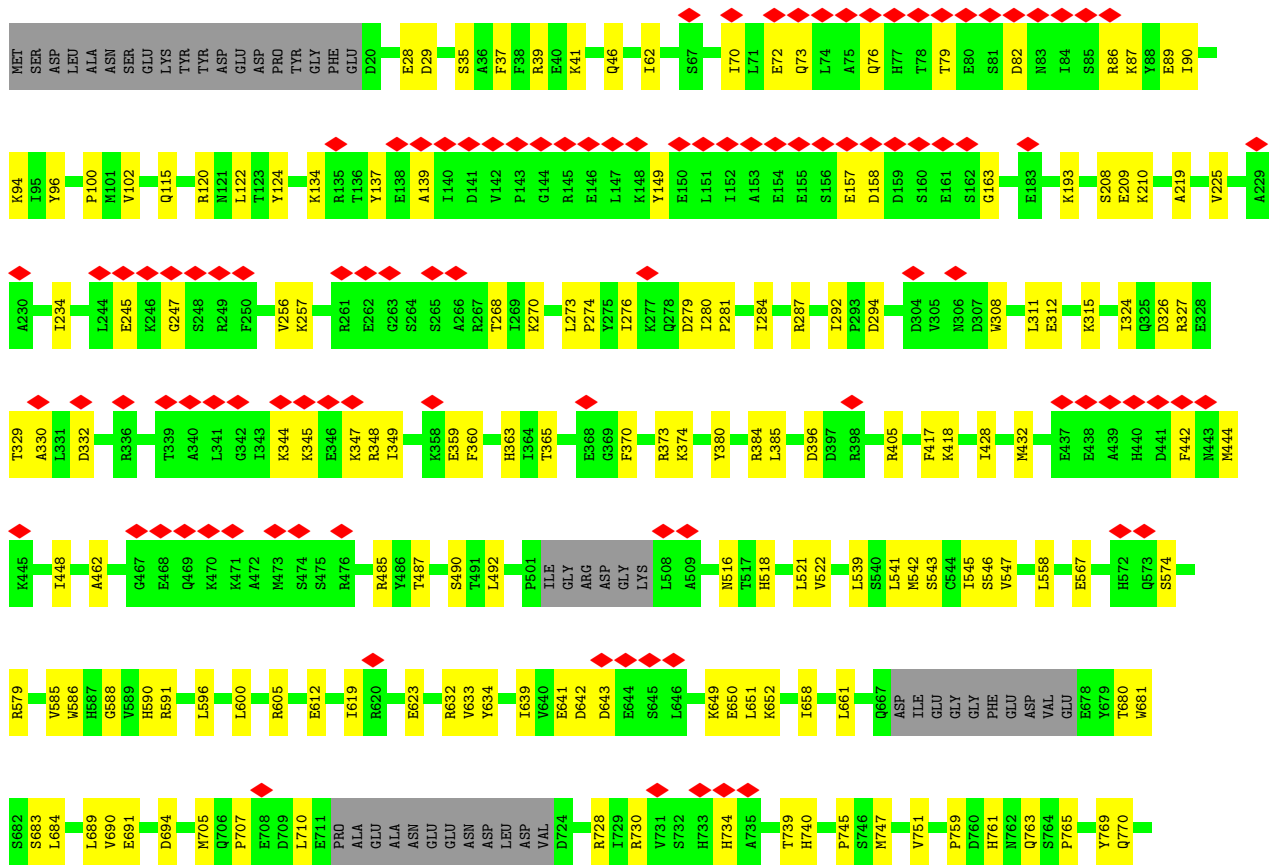
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 2: DNA-directed RNA polymerase II subunit RPB2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64243	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	1.217	Depositor
Minimum map value	-0.777	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.2	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

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	0/11049	0.31	0/14927
2	B	0.12	0/9319	0.27	0/12563
3	C	0.12	0/2133	0.26	0/2891
4	E	0.10	0/1780	0.30	0/2395
5	F	0.10	0/682	0.25	0/922
6	H	0.10	0/1095	0.24	0/1482
7	I	0.11	0/926	0.34	0/1246
8	J	0.13	0/541	0.32	0/727
9	K	0.11	0/922	0.22	0/1244
10	L	0.11	0/361	0.32	0/478
11	N	0.21	0/553	0.36	0/855
12	R	0.19	0/222	0.24	0/345
13	T	0.28	0/724	0.50	0/1110
All	All	0.12	0/30307	0.30	0/41185

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 [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	10859	0	10943	190	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	9142	0	9145	184	0
3	C	2095	0	2051	48	0
4	E	1744	0	1772	23	0
5	F	670	0	690	10	0
6	H	1077	0	1050	9	0
7	I	909	0	866	21	0
8	J	532	0	542	19	0
9	K	904	0	911	20	0
10	L	359	0	381	9	0
11	N	489	0	256	24	0
12	R	198	0	99	9	0
13	T	653	0	375	38	0
14	A	1	0	0	0	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
All	All	29640	0	29081	523	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 (523) 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:T:40:DA:H4'	13:T:41:DT:H5'	1.45	0.95
2:B:996:ARG:HH21	3:C:38:ILE:HG23	1.45	0.79
1:A:836:TYR:HB2	13:T:41:DT:H5''	1.65	0.77
1:A:1128:GLN:HE22	1:A:1132:LYS:HG3	1.50	0.76
3:C:10:ILE:HD13	3:C:20:PHE:HB3	1.66	0.76
11:N:71:DA:C2'	11:N:72:DT:H72	2.17	0.75
1:A:1197:LEU:HD12	1:A:1209:MET:HE1	1.71	0.72
2:B:996:ARG:NH1	8:J:10:CYS:O	2.21	0.72
1:A:1239:ARG:HH22	1:A:1241:ARG:HH21	1.36	0.72
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.22	0.72
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.71	0.71
2:B:276:ILE:HG21	2:B:280:ILE:HD11	1.72	0.71
13:T:39:DC:H2'	13:T:40:DA:C5	2.25	0.71
3:C:248:ILE:HG21	9:K:102:LYS:HB2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:GLN:HB3	2:B:86:ARG:HB2	1.72	0.70
11:N:68:DG:C2	13:T:23:DG:N1	2.60	0.70
2:B:46:GLN:OE1	2:B:545:ILE:N	2.23	0.69
1:A:1256:GLU:OE1	1:A:1258:HIS:ND1	2.25	0.69
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.26	0.69
3:C:101:LEU:HD23	3:C:155:LEU:HD12	1.75	0.68
3:C:258:ILE:HG13	9:K:42:LEU:HD21	1.74	0.68
2:B:209:GLU:OE1	2:B:485:ARG:NH1	2.27	0.68
13:T:39:DC:H2'	13:T:40:DA:C4	2.29	0.68
11:N:68:DG:C2	13:T:23:DG:C2	2.82	0.68
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.59	0.67
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.77	0.66
1:A:398:GLU:HG2	1:A:400:PRO:HD2	1.78	0.66
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.77	0.66
1:A:378:GLU:OE2	1:A:384:ASN:ND2	2.29	0.66
1:A:1138:ILE:HG22	1:A:1279:ILE:HG21	1.78	0.66
1:A:503:GLN:OE1	5:F:90:ARG:NH2	2.28	0.65
2:B:287:ARG:NH2	2:B:294:ASP:OD1	2.29	0.65
1:A:1093:LYS:HG3	1:A:1095:THR:HG23	1.77	0.65
4:E:88:VAL:HB	4:E:116:ILE:HG12	1.78	0.65
13:T:38:DC:H2''	13:T:39:DC:H5''	1.78	0.65
1:A:1004:ASN:HD22	4:E:167:ARG:HD2	1.62	0.65
4:E:155:ARG:NH1	4:E:194:GLU:OE2	2.30	0.64
8:J:36:LEU:HD11	8:J:51:LEU:HB2	1.78	0.64
1:A:879:GLU:OE2	1:A:962:ARG:NH2	2.28	0.64
1:A:1342:GLU:OE1	4:E:200:ARG:NH2	2.30	0.64
1:A:1151:GLU:OE2	1:A:1194:ARG:NH1	2.31	0.63
2:B:76:GLN:HB3	2:B:82:ASP:HB3	1.81	0.63
1:A:1062:GLU:OE1	5:F:88:TYR:OH	2.17	0.63
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.79	0.63
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.80	0.63
2:B:849:GLY:HA2	2:B:852:ARG:HD2	1.79	0.63
12:R:2:U:H2'	12:R:3:C:C6	2.33	0.63
1:A:93:VAL:HG11	1:A:305:ASP:HB3	1.81	0.62
1:A:390:GLN:O	1:A:394:ASN:ND2	2.32	0.62
1:A:549:MET:HE3	1:A:577:ILE:HG21	1.80	0.62
10:L:31:CYS:HB2	10:L:48:CYS:SG	2.38	0.62
1:A:562:THR:O	1:A:576:GLN:NE2	2.33	0.62
3:C:5:GLY:O	3:C:24:ASN:ND2	2.32	0.62
2:B:210:LYS:HE2	2:B:462:ALA:HA	1.81	0.62
1:A:1189:SER:HB3	1:A:1244:ARG:HH22	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:71:DA:N9	11:N:72:DT:H72	2.15	0.62
3:C:179:GLU:OE1	3:C:206:ASN:ND2	2.32	0.62
2:B:70:ILE:HG22	2:B:89:GLU:HG2	1.83	0.61
3:C:37:MET:HE3	3:C:176:ILE:HD13	1.83	0.61
3:C:75:MET:O	3:C:246:ARG:NH2	2.33	0.61
4:E:48:ASP:OD1	4:E:49:SER:N	2.34	0.61
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.82	0.61
2:B:287:ARG:NH1	2:B:292:ILE:O	2.34	0.61
8:J:10:CYS:SG	8:J:11:GLY:N	2.74	0.61
3:C:165:LYS:O	9:K:6:ARG:NH2	2.34	0.60
11:N:71:DA:C2'	11:N:72:DT:C7	2.79	0.60
1:A:469:ARG:NH2	2:B:991:GLY:O	2.23	0.60
2:B:1166:CYS:HB3	2:B:1185:CYS:SG	2.41	0.60
3:C:22:LEU:HD11	9:K:101:LEU:HD11	1.83	0.60
11:N:71:DA:H2''	11:N:72:DT:C7	2.32	0.60
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	1.84	0.60
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.84	0.59
1:A:1199:ARG:NH2	1:A:1233:ASP:O	2.35	0.59
13:T:32:DC:H2'	13:T:33:DT:H71	1.84	0.59
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.84	0.59
2:B:1006:ILE:HD11	8:J:43:ARG:HB3	1.85	0.59
7:I:28:GLU:HB3	7:I:35:VAL:HG22	1.85	0.59
4:E:127:ILE:HD11	4:E:132:ILE:HD11	1.84	0.59
8:J:8:PHE:H	8:J:49:MET:HE3	1.68	0.59
11:N:66:DG:H2''	11:N:67:DC:C6	2.38	0.58
1:A:447:GLN:OE1	1:A:488:ASN:ND2	2.37	0.58
2:B:898:LEU:HD11	2:B:964:VAL:HG21	1.84	0.58
2:B:87:LYS:HB3	2:B:137:TYR:HB2	1.85	0.58
11:N:51:DG:C8	11:N:51:DG:H5'	2.39	0.58
1:A:107:CYS:SG	1:A:171:GLN:NE2	2.76	0.57
1:A:1016:THR:HB	4:E:206:GLY:HA3	1.85	0.57
11:N:51:DG:H1	13:T:40:DA:H61	1.51	0.57
2:B:332:ASP:OD1	2:B:348:ARG:NH1	2.28	0.57
3:C:101:LEU:HB3	3:C:155:LEU:HB2	1.86	0.57
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.38	0.57
1:A:1169:ILE:HD11	1:A:1229:SER:HB3	1.86	0.57
1:A:614:PHE:HB3	6:H:122:LEU:HD21	1.86	0.57
9:K:100:ALA:O	9:K:104:ASN:ND2	2.34	0.57
1:A:120:GLU:OE1	1:A:123:ARG:NH1	2.37	0.56
4:E:80:VAL:HG22	4:E:109:ILE:HB	1.87	0.56
8:J:10:CYS:SG	8:J:43:ARG:NH2	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:68:DG:N1	13:T:23:DG:C6	2.73	0.56
1:A:32:VAL:HG12	2:B:1183:LYS:HZ1	1.69	0.56
1:A:282:ASN:OD1	1:A:283:GLY:N	2.38	0.56
11:N:62:DC:H2''	11:N:63:DA:C8	2.40	0.56
13:T:18:DA:H2'	13:T:19:DT:H71	1.88	0.56
2:B:739:THR:O	2:B:740:HIS:ND1	2.38	0.56
2:B:651:LEU:HD11	2:B:707:PRO:HB3	1.87	0.56
5:F:81:THR:HG21	5:F:136:ARG:HD3	1.88	0.56
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.88	0.56
2:B:326:ASP:OD2	2:B:327:ARG:N	2.38	0.56
13:T:37:DC:C4'	13:T:38:DC:H5'	2.36	0.56
1:A:492:PRO:HG3	1:A:501:LEU:HD12	1.87	0.56
1:A:839:ARG:NH1	2:B:1132:GLU:OE1	2.39	0.56
2:B:896:ASP:OD2	10:L:29:TYR:OH	2.24	0.56
1:A:1397:LEU:HB2	1:A:1426:GLU:HG3	1.87	0.55
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.71	0.55
2:B:1187:ASN:ND2	2:B:1190:ASP:O	2.39	0.55
6:H:59:ILE:HD11	6:H:123:MET:HE1	1.88	0.55
11:N:65:DA:H2''	11:N:66:DG:H5''	1.87	0.55
1:A:407:ARG:NH1	1:A:409:SER:OG	2.39	0.55
9:K:49:GLU:HG3	9:K:94:ILE:HG13	1.87	0.55
1:A:1116:LEU:HD23	1:A:1329:THR:HB	1.89	0.55
2:B:257:LYS:NZ	2:B:279:ASP:OD2	2.39	0.55
2:B:650:GLU:HA	2:B:710:LEU:HD13	1.89	0.55
2:B:1106:ARG:NH2	2:B:1111:MET:SD	2.80	0.55
2:B:37:PHE:HE1	2:B:41:LYS:HD2	1.71	0.55
10:L:32:ALA:HB3	10:L:53:HIS:HE1	1.71	0.55
3:C:56:THR:HG21	3:C:145:CYS:SG	2.47	0.55
9:K:85:ASP:O	9:K:89:ASN:ND2	2.32	0.55
1:A:13:THR:HB	1:A:15:LYS:HE3	1.88	0.55
1:A:605:MET:HE3	1:A:621:THR:HG21	1.88	0.55
1:A:698:GLN:HE21	7:I:99:LEU:HD22	1.72	0.55
1:A:445:ASN:HB2	1:A:455:MET:HG3	1.87	0.55
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.42	0.55
3:C:146:LYS:NZ	8:J:58:GLU:OE2	2.36	0.55
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.89	0.54
2:B:954:VAL:HG12	10:L:46:VAL:HG11	1.89	0.54
2:B:102:VAL:HG21	2:B:122:LEU:HD13	1.88	0.54
4:E:176:PRO:HB2	4:E:212:ARG:HD3	1.89	0.54
1:A:469:ARG:HH21	2:B:976:ILE:HD13	1.72	0.54
1:A:1205:LYS:O	1:A:1274:ARG:NH2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:GLY:O	2:B:418:LYS:NZ	2.35	0.54
2:B:579:ARG:NH2	2:B:623:GLU:OE2	2.30	0.54
2:B:872:GLU:HG2	2:B:916:THR:HG22	1.89	0.54
8:J:37:SER:OG	8:J:47:ARG:NH2	2.41	0.54
1:A:78:PRO:O	2:B:1205:GLN:NE2	2.40	0.54
1:A:535:THR:O	1:A:575:LYS:NZ	2.27	0.54
7:I:45:ARG:NE	7:I:47:GLU:OE2	2.31	0.54
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.90	0.54
1:A:246:VAL:HA	2:B:1202:LEU:HD11	1.89	0.54
2:B:137:TYR:HB3	2:B:149:TYR:HB3	1.90	0.54
1:A:939:ASP:OD2	1:A:1023:ARG:NH1	2.41	0.53
2:B:380:TYR:OH	2:B:384:ARG:NH2	2.41	0.53
2:B:852:ARG:NH2	10:L:70:ARG:OXT	2.41	0.53
2:B:157:GLU:HG3	2:B:163:GLY:HA2	1.89	0.53
2:B:586:TRP:CD1	2:B:588:GLY:H	2.25	0.53
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.89	0.53
13:T:40:DA:C4'	13:T:41:DT:H5'	2.28	0.53
1:A:443:LEU:HD11	1:A:455:MET:HG2	1.90	0.53
2:B:79:THR:H	2:B:82:ASP:HB2	1.73	0.53
11:N:71:DA:C8	11:N:72:DT:H72	2.44	0.53
2:B:796:LEU:HD12	2:B:853:SER:HB3	1.90	0.53
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.90	0.53
1:A:399:HIS:O	1:A:435:HIS:ND1	2.41	0.53
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.90	0.53
2:B:710:LEU:HA	2:B:734:HIS:HE2	1.72	0.53
11:N:62:DC:H2''	11:N:63:DA:N7	2.24	0.53
1:A:1115:SER:N	1:A:1330:ASN:OD1	2.40	0.53
2:B:1187:ASN:HD21	2:B:1190:ASP:HB2	1.72	0.53
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.91	0.53
1:A:665:GLY:N	1:A:668:ASP:OD2	2.40	0.53
1:A:1436:ILE:HG22	1:A:1437:GLY:H	1.74	0.53
2:B:373:ARG:NE	2:B:567:GLU:OE2	2.42	0.53
1:A:729:ALA:HB1	1:A:763:ALA:HB1	1.91	0.52
4:E:143:ASN:HD22	4:E:146:HIS:CD2	2.26	0.52
1:A:451:HIS:HD2	1:A:1074:GLU:HG3	1.74	0.52
1:A:569:LYS:HE2	1:A:571:LEU:HD21	1.90	0.52
2:B:365:THR:HG21	2:B:370:PHE:HB2	1.92	0.52
2:B:987:LYS:NZ	12:R:9:G:OP1	2.39	0.52
13:T:26:DC:H2''	13:T:27:DT:H72	1.92	0.52
13:T:43:DC:H2''	13:T:44:DT:H5'	1.91	0.52
1:A:343:LYS:HZ1	2:B:1156:ASP:HB3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:878:ILE:HD12	1:A:1366:ARG:HH12	1.74	0.52
2:B:158:ASP:HA	2:B:163:GLY:HA3	1.90	0.52
1:A:1286:LYS:HD2	1:A:1302:PRO:HB2	1.90	0.52
2:B:208:SER:OG	2:B:210:LYS:NZ	2.43	0.52
4:E:55:ARG:HB2	4:E:84:ASP:HB2	1.92	0.52
3:C:66:ARG:NH2	8:J:3:VAL:O	2.38	0.52
12:R:4:G:H2'	12:R:5:A:C8	2.45	0.52
2:B:605:ARG:NE	2:B:691:GLU:OE2	2.30	0.51
11:N:71:DA:H2'	11:N:72:DT:H72	1.93	0.51
1:A:307:ASP:OD1	1:A:313:GLN:NE2	2.44	0.51
1:A:836:TYR:HE2	1:A:840:ARG:HH11	1.56	0.51
2:B:134:LYS:HE3	2:B:442:PHE:HZ	1.75	0.51
1:A:851:HIS:CE1	1:A:857:ARG:HB2	2.46	0.51
6:H:8:ASP:OD1	6:H:9:ILE:N	2.42	0.51
7:I:2:THR:HG22	7:I:42:LEU:HG	1.91	0.51
12:R:1:A:H2'	12:R:2:U:C6	2.45	0.51
1:A:446:ARG:HB2	1:A:487:MET:HG2	1.92	0.51
1:A:666:ILE:HG21	2:B:1030:LEU:HD22	1.93	0.51
2:B:797:TYR:HE1	2:B:854:LEU:HG	1.76	0.51
13:T:40:DA:H1'	13:T:41:DT:C6	2.45	0.51
3:C:8:VAL:HG11	9:K:105:PHE:HD2	1.75	0.51
4:E:179:GLN:HG2	4:E:215:MET:HE2	1.94	0.50
1:A:466:SER:OG	9:K:2:ASN:ND2	2.38	0.50
1:A:1279:ILE:HD12	1:A:1308:THR:HG21	1.93	0.50
1:A:850:VAL:HG22	1:A:856:THR:HG22	1.93	0.50
13:T:39:DC:H5''	13:T:39:DC:H6	1.75	0.50
1:A:401:GLY:O	1:A:435:HIS:ND1	2.45	0.50
2:B:769:TYR:HB3	2:B:773:MET:HE3	1.94	0.50
1:A:935:GLN:NE2	1:A:939:ASP:OD1	2.43	0.50
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.12	0.50
2:B:825:VAL:HG22	2:B:1010:LEU:HB3	1.94	0.50
7:I:58:VAL:HG11	7:I:109:ILE:HD11	1.93	0.50
1:A:1215:ARG:HG3	1:A:1273:LEU:HA	1.94	0.49
2:B:308:TRP:HH2	7:I:47:GLU:HG2	1.76	0.49
1:A:492:PRO:O	1:A:493:GLN:NE2	2.45	0.49
4:E:124:VAL:HG13	4:E:132:ILE:HB	1.94	0.49
1:A:72:GLU:HB3	1:A:76:GLU:HB3	1.94	0.49
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.94	0.49
2:B:952:VAL:HG22	2:B:966:VAL:HG22	1.95	0.49
2:B:957:ASN:OD1	2:B:958:GLN:N	2.40	0.49
1:A:491:VAL:O	2:B:1150:ARG:NH2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LYS:NZ	1:A:85:ASP:OD2	2.40	0.49
1:A:675:THR:O	1:A:679:ILE:HG12	2.12	0.49
2:B:311:LEU:HB3	7:I:4:PHE:CE2	2.48	0.49
2:B:1163:CYS:HB3	2:B:1166:CYS:SG	2.53	0.49
2:B:944:THR:OG1	2:B:1122:ARG:NH2	2.46	0.49
5:F:97:ARG:NE	5:F:124:GLU:OE1	2.46	0.49
13:T:38:DC:P	13:T:38:DC:H3'	2.53	0.49
2:B:634:TYR:HA	2:B:694:ASP:HA	1.95	0.49
2:B:681:TRP:CH2	2:B:690:VAL:HG11	2.48	0.49
2:B:798:TYR:HE1	3:C:66:ARG:HH21	1.61	0.49
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.94	0.49
7:I:14:LEU:HB3	7:I:27:PHE:HB3	1.94	0.49
2:B:856:PHE:CE1	2:B:969:ARG:HG3	2.47	0.48
2:B:652:LYS:HB3	2:B:689:LEU:HD22	1.95	0.48
2:B:761:HIS:HB2	2:B:1024:ALA:HB2	1.95	0.48
1:A:675:THR:OG1	1:A:736:ASN:OD1	2.30	0.48
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.96	0.48
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.49	0.48
2:B:546:SER:OG	2:B:632:ARG:N	2.43	0.48
1:A:1224:LEU:HD21	1:A:1240:CYS:HB3	1.96	0.48
3:C:99:LEU:O	3:C:157:CYS:N	2.47	0.48
1:A:526:ASP:HB2	2:B:835:GLN:NE2	2.29	0.48
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.96	0.48
2:B:62:ILE:HG21	2:B:417:PHE:HD2	1.79	0.48
13:T:39:DC:H6	13:T:39:DC:C5'	2.27	0.48
1:A:871:ASP:CG	1:A:1366:ARG:HH21	2.22	0.48
2:B:37:PHE:CE1	2:B:41:LYS:HD2	2.48	0.48
3:C:26:ASP:OD1	3:C:26:ASP:N	2.45	0.48
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.95	0.47
1:A:1267:MET:HA	1:A:1271:ILE:HG12	1.96	0.47
2:B:485:ARG:NH2	2:B:782:LEU:HD11	2.29	0.47
4:E:190:LEU:HD13	4:E:214:CYS:HB2	1.96	0.47
13:T:36:DT:H2''	13:T:37:DC:C6	2.49	0.47
1:A:455:MET:O	2:B:1141:HIS:NE2	2.39	0.47
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.95	0.47
1:A:25:GLU:OE1	1:A:25:GLU:N	2.41	0.47
1:A:778:GLY:HA3	2:B:516:ASN:HB2	1.95	0.47
2:B:28:GLU:OE2	2:B:807:ARG:NH1	2.47	0.47
2:B:1000:PRO:HB2	2:B:1072:MET:HE2	1.95	0.47
1:A:22:PHE:HE2	2:B:1208:MET:HA	1.80	0.47
1:A:541:ILE:HD13	1:A:549:MET:HE1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:133:VAL:HG23	5:F:147:SER:HA	1.96	0.47
13:T:44:DT:H2''	13:T:45:DC:H5'	1.95	0.47
2:B:590:HIS:CD2	2:B:596:LEU:HD22	2.49	0.47
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.15	0.47
2:B:983:ARG:NH2	2:B:1028:GLU:OE2	2.43	0.47
5:F:79:ARG:NH2	5:F:150:GLU:OE2	2.48	0.47
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.97	0.47
2:B:642:ASP:HB3	2:B:649:LYS:HZ3	1.79	0.47
2:B:797:TYR:O	8:J:1:MET:N	2.47	0.47
2:B:120:ARG:HA	2:B:963:PHE:HZ	1.79	0.47
2:B:219:ALA:HB2	2:B:405:ARG:HG2	1.97	0.47
1:A:1170:ILE:HA	1:A:1173:HIS:CD2	2.49	0.46
3:C:262:LEU:HD22	9:K:87:LEU:HD23	1.98	0.46
6:H:103:LYS:HB3	6:H:115:TYR:HB2	1.97	0.46
13:T:37:DC:H4'	13:T:38:DC:H5'	1.96	0.46
2:B:950:ASP:HB2	2:B:969:ARG:HB2	1.98	0.46
9:K:47:ARG:HD3	9:K:61:TYR:HD1	1.80	0.46
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.15	0.46
2:B:680:THR:O	2:B:683:SER:OG	2.27	0.46
1:A:779:PHE:CE2	1:A:785:PRO:HD3	2.51	0.46
1:A:836:TYR:CB	13:T:41:DT:H5''	2.43	0.46
8:J:47:ARG:O	8:J:51:LEU:HB3	2.15	0.46
2:B:822:ASN:O	8:J:48:ARG:NH1	2.48	0.46
3:C:255:VAL:HG21	9:K:94:ILE:HG21	1.97	0.46
9:K:47:ARG:HH11	9:K:47:ARG:HG2	1.80	0.46
1:A:336:ILE:HD12	1:A:1405:THR:HG21	1.97	0.46
1:A:818:MET:SD	2:B:516:ASN:ND2	2.88	0.46
1:A:1170:ILE:HA	1:A:1173:HIS:HD2	1.81	0.46
2:B:778:MET:HG3	2:B:794:ASN:HB3	1.98	0.46
2:B:895:ASP:O	10:L:42:ARG:NH2	2.48	0.46
1:A:500:GLU:OE1	1:A:1438:THR:HG21	2.16	0.46
1:A:848:ILE:HG21	1:A:1370:LEU:HD11	1.98	0.46
1:A:1153:TYR:HE1	7:I:42:LEU:HD13	1.80	0.46
2:B:780:VAL:HG22	2:B:795:ILE:HG23	1.98	0.46
7:I:50:THR:OG1	7:I:51:ASN:N	2.49	0.46
1:A:386:ASP:OD1	1:A:386:ASP:N	2.48	0.46
1:A:1412:ALA:HA	1:A:1417:GLU:HG3	1.98	0.46
2:B:139:ALA:HB2	2:B:149:TYR:HA	1.97	0.46
4:E:196:VAL:HG23	4:E:198:ILE:HD11	1.98	0.46
11:N:59:DG:H2''	11:N:60:DA:C8	2.51	0.46
11:N:68:DG:N2	13:T:23:DG:C2	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:PHE:CD2	2:B:836:GLU:HB2	2.51	0.46
1:A:873:MET:HB2	1:A:1366:ARG:NH2	2.31	0.46
1:A:997:LEU:HB3	1:A:1053:PHE:CE2	2.51	0.46
3:C:34:ARG:HA	3:C:37:MET:HE2	1.98	0.46
13:T:39:DC:H5''	13:T:39:DC:C6	2.51	0.46
1:A:765:VAL:HB	1:A:800:VAL:HB	1.99	0.45
1:A:847:ASP:OD1	1:A:847:ASP:N	2.46	0.45
2:B:234:ILE:HD13	2:B:257:LYS:HD2	1.96	0.45
2:B:1001:PHE:CE2	3:C:178:PHE:HB3	2.49	0.45
3:C:145:CYS:SG	3:C:146:LYS:N	2.89	0.45
1:A:94:GLY:HA3	1:A:1410:PHE:CD2	2.50	0.45
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.51	0.45
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.51	0.45
1:A:117:GLU:O	1:A:123:ARG:NE	2.50	0.45
1:A:1094:VAL:HG23	1:A:1095:THR:H	1.81	0.45
2:B:225:VAL:N	2:B:396:ASP:OD2	2.45	0.45
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.97	0.45
2:B:877:PRO:HB2	2:B:885:MET:HE1	1.97	0.45
7:I:17:ARG:N	7:I:26:LEU:O	2.37	0.45
7:I:71:SER:OG	7:I:83:ASN:OD1	2.24	0.45
1:A:215:SER:OG	1:A:218:ASP:OD2	2.33	0.45
1:A:436:ILE:O	1:A:436:ILE:HG13	2.15	0.45
1:A:451:HIS:ND1	1:A:453:MET:HE2	2.31	0.45
1:A:867:ILE:HG23	1:A:870:GLU:HA	1.98	0.45
2:B:324:ILE:HD13	2:B:330:ALA:HA	1.98	0.45
2:B:542:MET:HE2	2:B:747:MET:HG3	1.98	0.45
1:A:478:TYR:CD2	1:A:487:MET:HE1	2.51	0.45
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.98	0.45
2:B:72:GLU:OE2	2:B:149:TYR:OH	2.34	0.45
2:B:94:LYS:HD3	2:B:96:TYR:HE1	1.82	0.45
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.99	0.45
10:L:31:CYS:SG	10:L:32:ALA:N	2.89	0.45
1:A:739:ASP:OD2	6:H:19:ARG:HD2	2.16	0.45
1:A:740:LEU:HA	1:A:745:GLN:HE21	1.81	0.45
2:B:487:THR:HG23	2:B:490:SER:H	1.82	0.45
3:C:52:GLU:OE1	3:C:52:GLU:N	2.49	0.45
1:A:1004:ASN:ND2	4:E:167:ARG:HD2	2.30	0.45
1:A:1094:VAL:HG23	1:A:1095:THR:N	2.32	0.45
1:A:1428:VAL:HG21	2:B:1135:ARG:HD2	1.99	0.45
2:B:100:PRO:HG2	2:B:124:TYR:CZ	2.52	0.45
2:B:444:MET:HE2	2:B:444:MET:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:58:VAL:HG12	7:I:58:VAL:O	2.16	0.45
1:A:128:ILE:O	1:A:134:ARG:NH1	2.51	0.45
1:A:956:LEU:HD21	1:A:1017:LEU:HD23	1.99	0.45
2:B:428:ILE:HD11	2:B:448:ILE:HG13	1.99	0.45
2:B:1150:ARG:HA	2:B:1154:ALA:HB3	1.99	0.45
8:J:21:TYR:CZ	8:J:25:LEU:HD11	2.52	0.45
12:R:7:A:H2'	12:R:8:G:H8	1.82	0.45
2:B:315:LYS:HE2	7:I:4:PHE:CE1	2.52	0.44
2:B:485:ARG:HH21	2:B:782:LEU:HD21	1.82	0.44
2:B:539:LEU:HB3	2:B:543:SER:OG	2.17	0.44
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.99	0.44
13:T:26:DC:H2''	13:T:27:DT:C7	2.47	0.44
2:B:1149:GLU:HA	2:B:1153:GLU:OE1	2.17	0.44
7:I:49:ILE:HG13	7:I:50:THR:HA	1.99	0.44
1:A:109:HIS:HB2	1:A:169:ASN:HD21	1.81	0.44
2:B:541:LEU:HD23	2:B:541:LEU:HA	1.84	0.44
7:I:29:CYS:SG	7:I:31:THR:OG1	2.76	0.44
1:A:92:HIS:HB3	1:A:95:PHE:HB2	2.00	0.44
1:A:683:ILE:HG21	1:A:801:GLU:HG2	1.98	0.44
1:A:712:GLU:OE2	1:A:1092:LYS:NZ	2.32	0.44
3:C:67:LEU:HD11	3:C:155:LEU:HD13	2.00	0.44
2:B:29:ASP:HB3	2:B:658:ILE:HD13	2.00	0.44
2:B:344:LYS:NZ	2:B:347:LYS:HG2	2.33	0.44
2:B:345:LYS:O	2:B:349:ILE:HG12	2.18	0.44
2:B:856:PHE:HB3	2:B:967:ARG:HD2	2.00	0.44
2:B:1084:GLN:OE1	3:C:192:TRP:N	2.44	0.44
5:F:110:ASP:N	5:F:110:ASP:OD1	2.50	0.44
1:A:690:VAL:HG11	1:A:794:PRO:HG3	1.99	0.44
1:A:912:LEU:HD13	1:A:1032:LEU:HB3	1.99	0.44
2:B:619:ILE:HG21	7:I:62:ILE:HA	2.00	0.44
10:L:33:GLU:HG3	10:L:53:HIS:CE1	2.52	0.44
2:B:832:GLY:CA	2:B:835:GLN:HE21	2.31	0.43
1:A:1317:MET:HA	1:A:1322:ILE:HD11	2.00	0.43
2:B:832:GLY:HA2	2:B:835:GLN:HE21	1.83	0.43
3:C:44:LEU:HD22	3:C:129:ILE:HG12	1.99	0.43
8:J:28:ASP:OD1	8:J:28:ASP:N	2.51	0.43
13:T:38:DC:C6	13:T:39:DC:C4	3.05	0.43
1:A:445:ASN:O	1:A:488:ASN:N	2.49	0.43
1:A:549:MET:HG2	1:A:655:PHE:CD2	2.54	0.43
2:B:842:ASN:OD1	2:B:845:SER:N	2.45	0.43
4:E:96:PHE:CZ	4:E:100:ILE:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:915:SER:O	1:A:919:ILE:HG12	2.19	0.43
1:A:1114:PRO:HB2	1:A:1311:VAL:HG23	2.00	0.43
11:N:53:DG:H2''	11:N:54:DA:C8	2.53	0.43
11:N:66:DG:H2''	11:N:67:DC:H6	1.81	0.43
1:A:1274:ARG:O	1:A:1276:VAL:N	2.52	0.43
4:E:143:ASN:HB3	4:E:146:HIS:HD2	1.83	0.43
13:T:38:DC:H2''	13:T:39:DC:C6	2.54	0.43
1:A:860:LEU:HG	1:A:1394:THR:HG22	2.01	0.43
1:A:873:MET:HE1	1:A:1057:VAL:HG22	1.99	0.43
2:B:518:HIS:HB3	2:B:522:VAL:HG22	2.01	0.43
8:J:57:ILE:O	8:J:61:LEU:HG	2.19	0.43
1:A:527:THR:HG23	1:A:653:VAL:HB	2.01	0.43
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.99	0.43
11:N:68:DG:H2''	11:N:69:DG:H8	1.84	0.43
1:A:76:GLU:OE2	2:B:1159:ARG:NH2	2.48	0.43
1:A:833:GLU:O	1:A:837:ILE:HG12	2.19	0.43
2:B:792:MET:SD	2:B:857:ARG:NH2	2.92	0.43
9:K:39:ASP:OD1	9:K:39:ASP:N	2.52	0.43
2:B:840:ILE:HB	2:B:1011:ILE:HB	2.00	0.43
2:B:558:LEU:HD21	2:B:600:LEU:HD11	2.00	0.43
2:B:801:LYS:O	8:J:52:THR:HG23	2.19	0.43
2:B:1152:MET:O	2:B:1157:ALA:HB2	2.19	0.43
1:A:544:ASP:OD1	1:A:545:GLN:N	2.51	0.42
2:B:158:ASP:OD1	2:B:158:ASP:N	2.49	0.42
3:C:169:LYS:NZ	10:L:69:ALA:O	2.39	0.42
7:I:65:ASP:OD1	7:I:67:THR:OG1	2.33	0.42
7:I:72:ASP:O	7:I:81:ARG:HD2	2.19	0.42
1:A:1410:PHE:CD1	2:B:1212:ILE:HD11	2.54	0.42
3:C:116:LYS:HE2	3:C:116:LYS:HB3	1.83	0.42
11:N:53:DG:N2	13:T:38:DC:O2	2.52	0.42
1:A:401:GLY:H	1:A:435:HIS:HD1	1.66	0.42
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.99	0.42
6:H:96:VAL:HG22	6:H:143:LEU:HG	2.01	0.42
12:R:2:U:H2'	12:R:3:C:H6	1.79	0.42
12:R:3:C:H2'	12:R:4:G:O4'	2.19	0.42
1:A:399:HIS:NE2	1:A:462:VAL:HG21	2.35	0.42
1:A:531:ILE:HD11	1:A:578:LEU:HD21	2.02	0.42
2:B:799:PRO:HB2	2:B:818:PRO:HG2	2.01	0.42
2:B:862:GLN:OE1	2:B:957:ASN:ND2	2.53	0.42
12:R:9:G:C2	13:T:43:DC:C2	3.07	0.42
13:T:31:DC:H2''	13:T:32:DC:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:37:DC:P	13:T:37:DC:H3'	2.59	0.42
1:A:446:ARG:HB2	1:A:487:MET:HE3	2.01	0.42
2:B:360:PHE:O	2:B:374:LYS:NZ	2.45	0.42
2:B:547:VAL:HG12	2:B:612:GLU:OE1	2.19	0.42
13:T:33:DT:C2'	13:T:34:DT:H71	2.50	0.42
1:A:352:VAL:HG23	1:A:467:THR:HG22	2.00	0.42
1:A:488:ASN:OD1	2:B:1128:LEU:HD13	2.20	0.42
1:A:951:GLU:O	1:A:954:TRP:NE1	2.52	0.42
1:A:1446:ASP:OD1	1:A:1447:GLU:N	2.50	0.42
7:I:76:PRO:HG2	7:I:110:PHE:CE1	2.55	0.42
1:A:71:GLN:OE1	1:A:71:GLN:HA	2.19	0.42
1:A:254:GLU:O	1:A:256:GLN:HG2	2.19	0.42
1:A:1168:GLU:O	1:A:1172:LEU:HD23	2.20	0.42
2:B:1013:ASN:OD1	2:B:1015:HIS:ND1	2.51	0.42
6:H:25:ARG:HD2	6:H:39:THR:HG23	2.01	0.42
1:A:587:HIS:CE1	1:A:969:GLN:HG3	2.55	0.42
1:A:838:GLN:HE22	1:A:1070:GLN:HG2	1.83	0.42
2:B:90:ILE:HD12	2:B:432:MET:SD	2.60	0.42
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.85	0.42
2:B:600:LEU:HD23	2:B:600:LEU:HA	1.88	0.42
2:B:957:ASN:N	2:B:961:LEU:O	2.41	0.42
12:R:7:A:H2'	12:R:8:G:C8	2.55	0.42
1:A:351:THR:OG1	2:B:1103:ILE:HG13	2.19	0.42
1:A:567:LYS:HB3	1:A:568:PRO:HD3	2.02	0.42
4:E:61:GLN:HE21	4:E:105:PHE:HE1	1.68	0.42
7:I:71:SER:HB3	7:I:85:PHE:CD2	2.55	0.42
9:K:47:ARG:HG2	9:K:47:ARG:NH1	2.35	0.42
11:N:54:DA:H2''	11:N:55:DG:C8	2.55	0.42
1:A:167:CYS:SG	1:A:168:GLY:N	2.93	0.41
1:A:515:GLN:HG3	1:A:1071:SER:HB3	2.01	0.41
1:A:1277:GLU:HG2	1:A:1278:ASN:OD1	2.19	0.41
2:B:728:ARG:HG3	2:B:730:ARG:HG3	2.02	0.41
3:C:37:MET:SD	3:C:244:VAL:HG12	2.60	0.41
9:K:56:VAL:HG22	9:K:77:THR:HG22	2.02	0.41
1:A:881:GLN:NE2	1:A:956:LEU:O	2.47	0.41
3:C:46:ILE:HG23	3:C:157:CYS:HB3	2.02	0.41
3:C:54:ASN:ND2	3:C:60:ASP:OD1	2.52	0.41
3:C:107:SER:OG	3:C:111:THR:OG1	2.38	0.41
1:A:605:MET:HE1	1:A:617:VAL:HG22	2.02	0.41
1:A:1386:ARG:HD3	1:A:1403:GLU:OE1	2.20	0.41
1:A:1098:VAL:HB	1:A:1099:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:186:LEU:HD21	3:C:224:GLN:C	2.44	0.41
1:A:922:ASP:OD1	1:A:923:LEU:N	2.52	0.41
2:B:35:SER:O	2:B:39:ARG:NH1	2.53	0.41
2:B:312:GLU:HA	2:B:315:LYS:HG3	2.01	0.41
2:B:639:ILE:HD11	2:B:691:GLU:HG3	2.03	0.41
2:B:889:THR:HG22	2:B:891:ASP:H	1.85	0.41
6:H:63:LEU:HB3	6:H:88:SER:OG	2.21	0.41
1:A:15:LYS:HB3	2:B:1220:ARG:HE	1.84	0.41
1:A:908:LEU:H	1:A:908:LEU:HD23	1.85	0.41
2:B:641:GLU:HG2	2:B:643:ASP:H	1.85	0.41
2:B:1138:MET:HE2	2:B:1146:PHE:CD2	2.55	0.41
1:A:496:GLU:O	1:A:500:GLU:HG3	2.21	0.41
1:A:1256:GLU:CD	1:A:1257:ASP:H	2.29	0.41
1:A:1276:VAL:HG11	1:A:1316:VAL:HG22	2.03	0.41
2:B:120:ARG:HB2	2:B:122:LEU:HG	2.03	0.41
2:B:1168:LEU:HB3	2:B:1170:THR:HG23	2.03	0.41
3:C:163:ILE:HG13	3:C:165:LYS:H	1.86	0.41
4:E:201:LYS:HB2	4:E:201:LYS:HE3	1.80	0.41
4:E:157:SER:OG	4:E:160:GLU:OE1	2.27	0.41
1:A:1188:GLN:OE1	1:A:1241:ARG:HD2	2.21	0.41
1:A:1193:LEU:HB2	1:A:1260:LEU:HD12	2.03	0.41
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	2.03	0.41
1:A:1436:ILE:HG22	1:A:1437:GLY:N	2.36	0.41
2:B:324:ILE:HG23	2:B:329:THR:OG1	2.20	0.41
2:B:574:SER:OG	2:B:591:ARG:NH2	2.46	0.41
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.54	0.41
3:C:11:ARG:NE	3:C:19:ASP:OD1	2.44	0.41
5:F:107:VAL:HG12	5:F:109:VAL:H	1.86	0.41
13:T:30:DT:H2''	13:T:31:DC:C6	2.56	0.41
13:T:36:DT:C4	13:T:37:DC:N4	2.89	0.41
1:A:683:ILE:O	1:A:687:LYS:HG2	2.21	0.41
2:B:268:THR:OG1	2:B:270:LYS:NZ	2.53	0.41
3:C:204:SER:HG	3:C:207:CYS:HG	1.56	0.41
3:C:241:ASP:OD2	9:K:109:TRP:NE1	2.54	0.41
4:E:118:PRO:HA	4:E:121:MET:HE2	2.02	0.41
13:T:39:DC:H3'	13:T:40:DA:C8	2.56	0.41
11:N:54:DA:H2''	11:N:55:DG:H8	1.86	0.40
1:A:500:GLU:CD	2:B:1145:SER:HB2	2.47	0.40
1:A:845:LEU:HB2	1:A:1069:ALA:HB2	2.03	0.40
2:B:256:VAL:HG12	2:B:385:LEU:HD22	2.03	0.40
3:C:244:VAL:HG21	9:K:105:PHE:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:36:DT:H4'	13:T:37:DC:OP1	2.21	0.40
1:A:451:HIS:CE1	1:A:453:MET:HB2	2.57	0.40
2:B:73:GLN:N	2:B:86:ARG:O	2.54	0.40
2:B:273:LEU:HB2	2:B:276:ILE:HG13	2.02	0.40
2:B:492:LEU:HB3	2:B:751:VAL:HG11	2.04	0.40
2:B:822:ASN:ND2	8:J:52:THR:HG21	2.35	0.40
1:A:885:THR:HG22	1:A:940:ARG:HB2	2.03	0.40
1:A:1189:SER:HB3	1:A:1244:ARG:HH12	1.85	0.40
2:B:759:PRO:HD2	2:B:1046:PRO:HA	2.04	0.40
2:B:770:GLN:HE22	2:B:1093:GLN:HE22	1.70	0.40
3:C:127:ARG:HG3	3:C:129:ILE:HG22	2.04	0.40
11:N:68:DG:H2''	11:N:69:DG:C8	2.56	0.40
13:T:39:DC:H2'	13:T:40:DA:C6	2.56	0.40
1:A:374:LEU:HD13	1:A:491:VAL:HG21	2.03	0.40
1:A:833:GLU:HG3	1:A:1098:VAL:HG11	2.04	0.40
1:A:1400:CYS:HB2	1:A:1405:THR:HG23	2.03	0.40
1:A:1433:MET:HE1	5:F:92:ARG:NH2	2.36	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	1358/1733 (78%)	1299 (96%)	57 (4%)	2 (0%)	48 78
2	B	1134/1224 (93%)	1093 (96%)	40 (4%)	1 (0%)	48 78
3	C	264/318 (83%)	259 (98%)	5 (2%)	0	100 100
4	E	211/215 (98%)	204 (97%)	6 (3%)	1 (0%)	24 56
5	F	81/155 (52%)	80 (99%)	1 (1%)	0	100 100
6	H	130/146 (89%)	128 (98%)	2 (2%)	0	100 100
7	I	108/122 (88%)	99 (92%)	9 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	J	63/70 (90%)	61 (97%)	2 (3%)	0	100	100
9	K	110/120 (92%)	108 (98%)	2 (2%)	0	100	100
10	L	43/70 (61%)	38 (88%)	5 (12%)	0	100	100
All	All	3502/4173 (84%)	3369 (96%)	129 (4%)	4 (0%)	49	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1129	GLU
1	A	958	VAL
2	B	245	GLU
4	E	52	ARG

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	1205/1520 (79%)	1205 (100%)	0	100	100
2	B	996/1061 (94%)	996 (100%)	0	100	100
3	C	234/274 (85%)	234 (100%)	0	100	100
4	E	195/197 (99%)	195 (100%)	0	100	100
5	F	73/137 (53%)	73 (100%)	0	100	100
6	H	118/128 (92%)	118 (100%)	0	100	100
7	I	106/116 (91%)	106 (100%)	0	100	100
8	J	60/65 (92%)	60 (100%)	0	100	100
9	K	97/102 (95%)	97 (100%)	0	100	100
10	L	40/57 (70%)	40 (100%)	0	100	100
All	All	3124/3657 (85%)	3124 (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 (23)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	ASN
1	A	287	HIS
1	A	490	HIS
1	A	698	GLN
1	A	996	ASN
1	A	1211	GLN
1	A	1387	HIS
1	A	1427	ASN
2	B	47	GLN
2	B	73	GLN
2	B	115	GLN
2	B	178	ASN
2	B	224	GLN
2	B	366	GLN
2	B	770	GLN
2	B	776	GLN
2	B	843	GLN
2	B	1211	ASN
3	C	73	GLN
3	C	264	GLN
4	E	101	GLN
4	E	143	ASN
5	F	104	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	R	8/9 (88%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	R	4	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
7	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1274:ARG	C	1275:GLY	N	5.96
1	A	1275:GLY	C	1276:VAL	N	5.30
1	I	49:ILE	C	50:THR	N	3.89
1	A	1141:THR	C	1142:THR	N	3.79

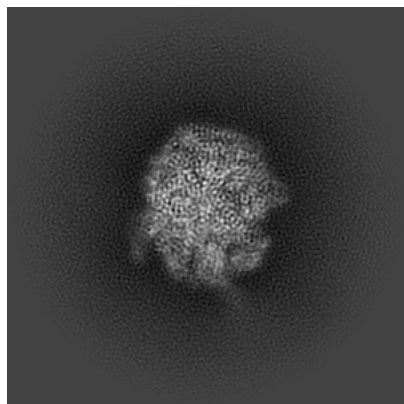
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54704. These allow visual inspection of the internal detail of the map and identification of artifacts.

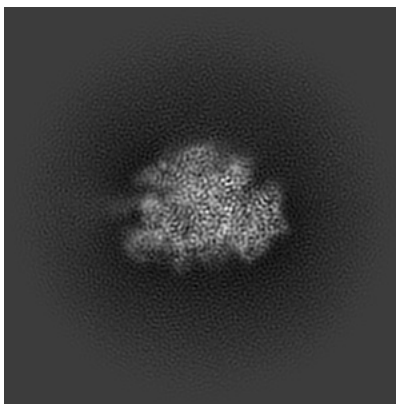
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

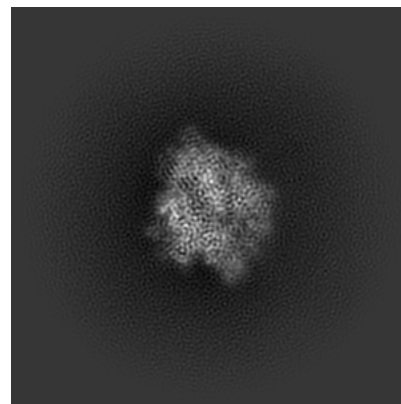
6.1.1 Primary map



X

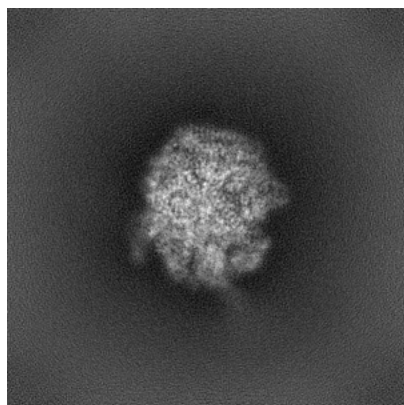


Y

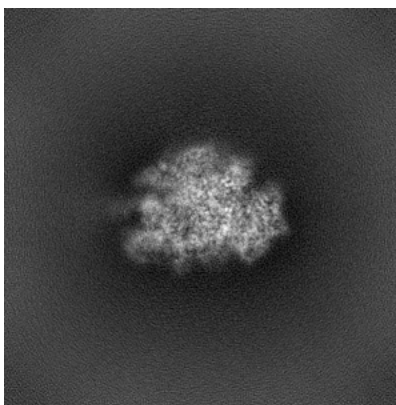


Z

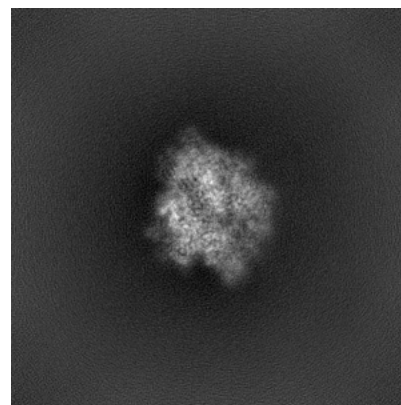
6.1.2 Raw map



X



Y

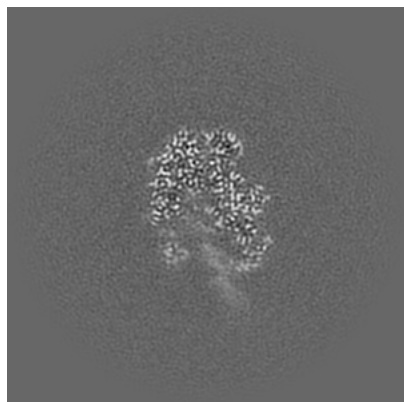


Z

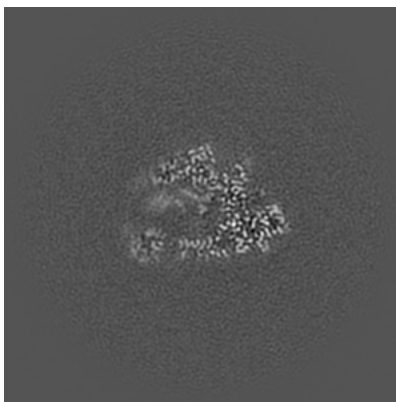
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

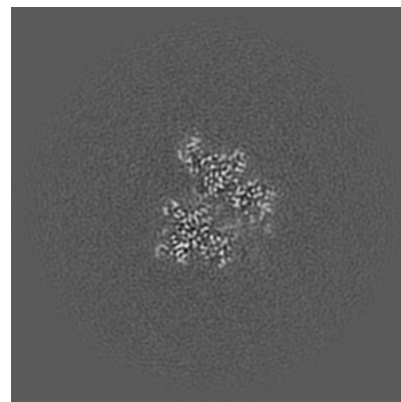
6.2.1 Primary map



X Index: 160

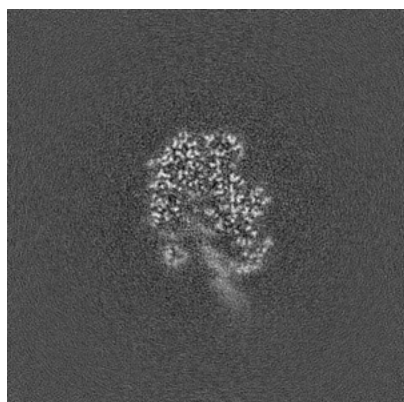


Y Index: 160

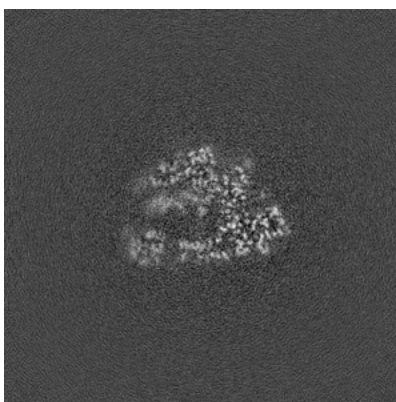


Z Index: 160

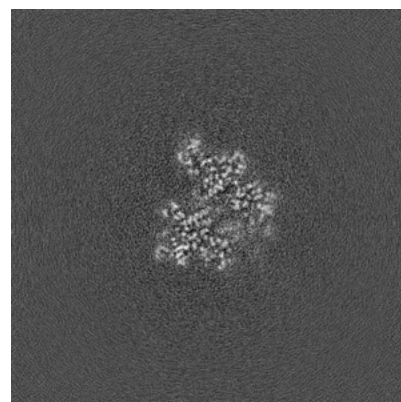
6.2.2 Raw map



X Index: 160



Y Index: 160

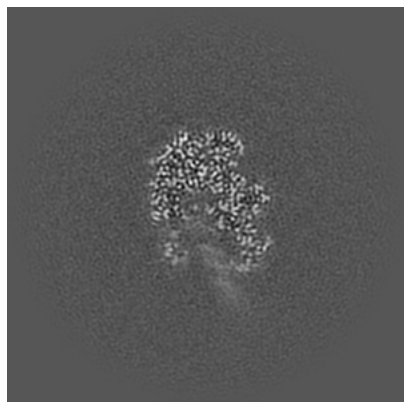


Z Index: 160

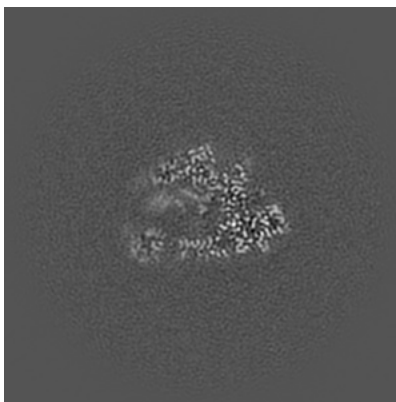
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

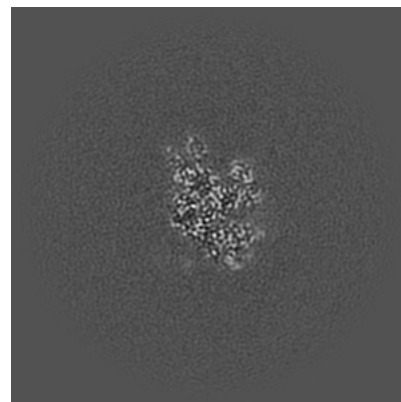
6.3.1 Primary map



X Index: 159

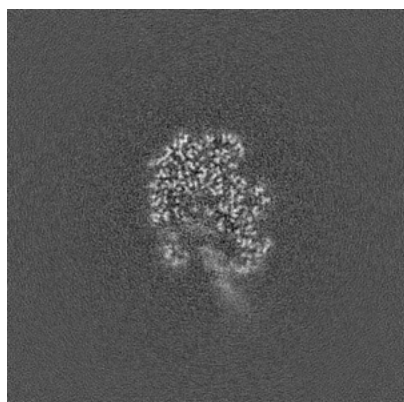


Y Index: 160

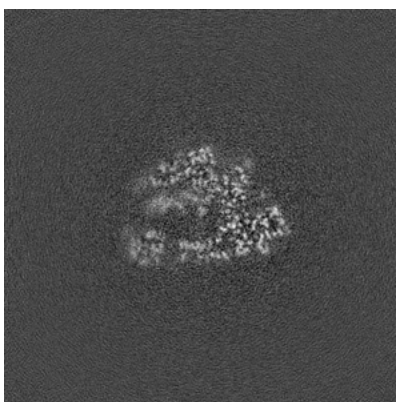


Z Index: 183

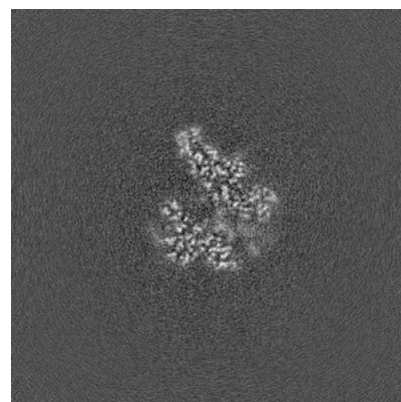
6.3.2 Raw map



X Index: 159



Y Index: 160

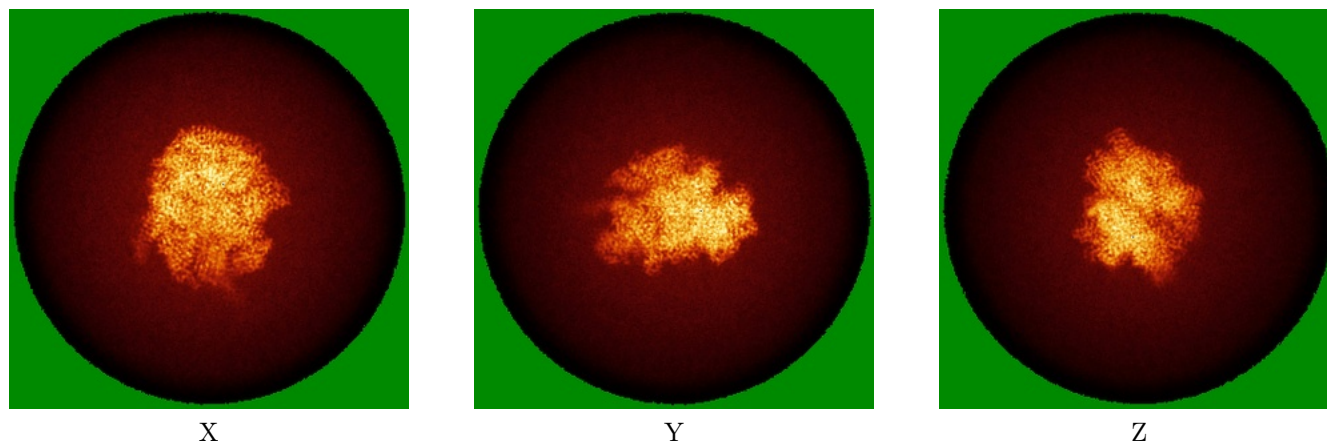


Z Index: 165

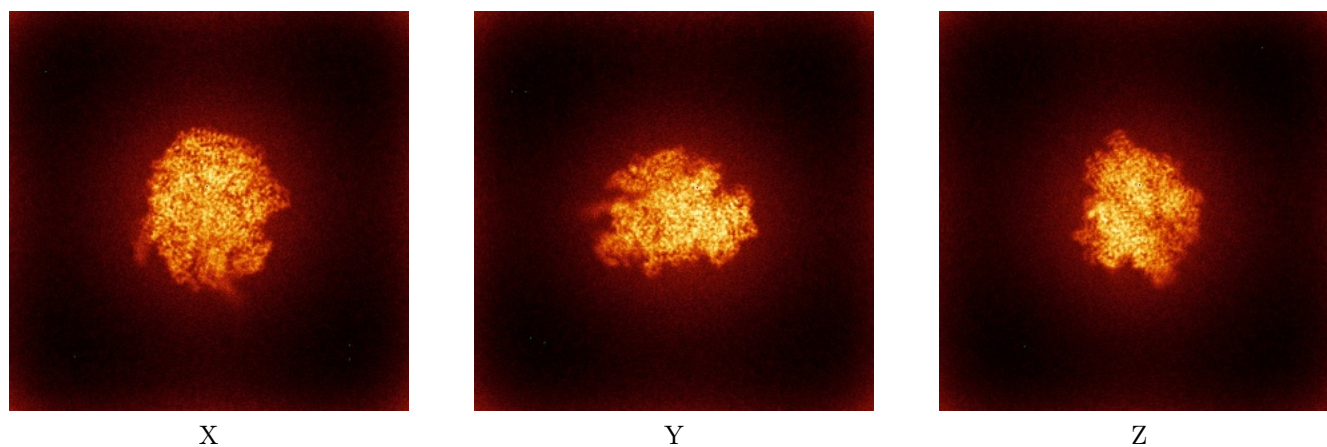
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



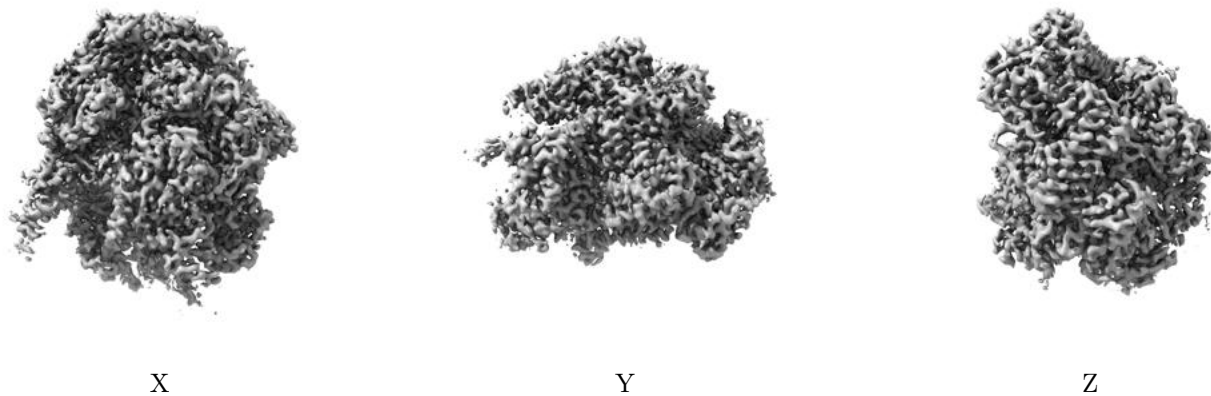
6.4.2 Raw map



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.

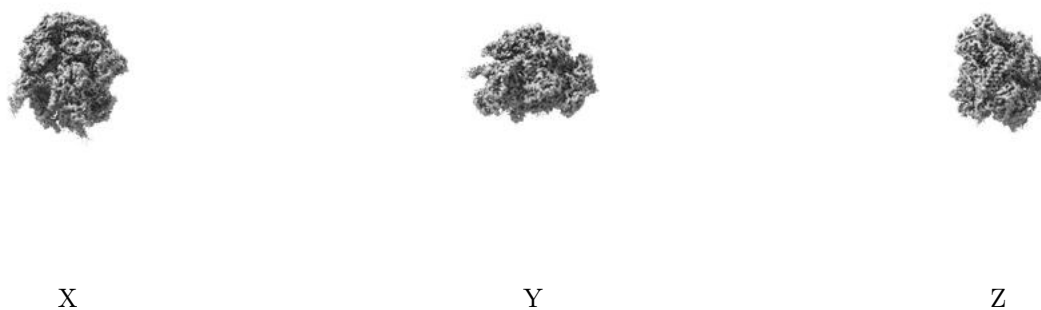
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

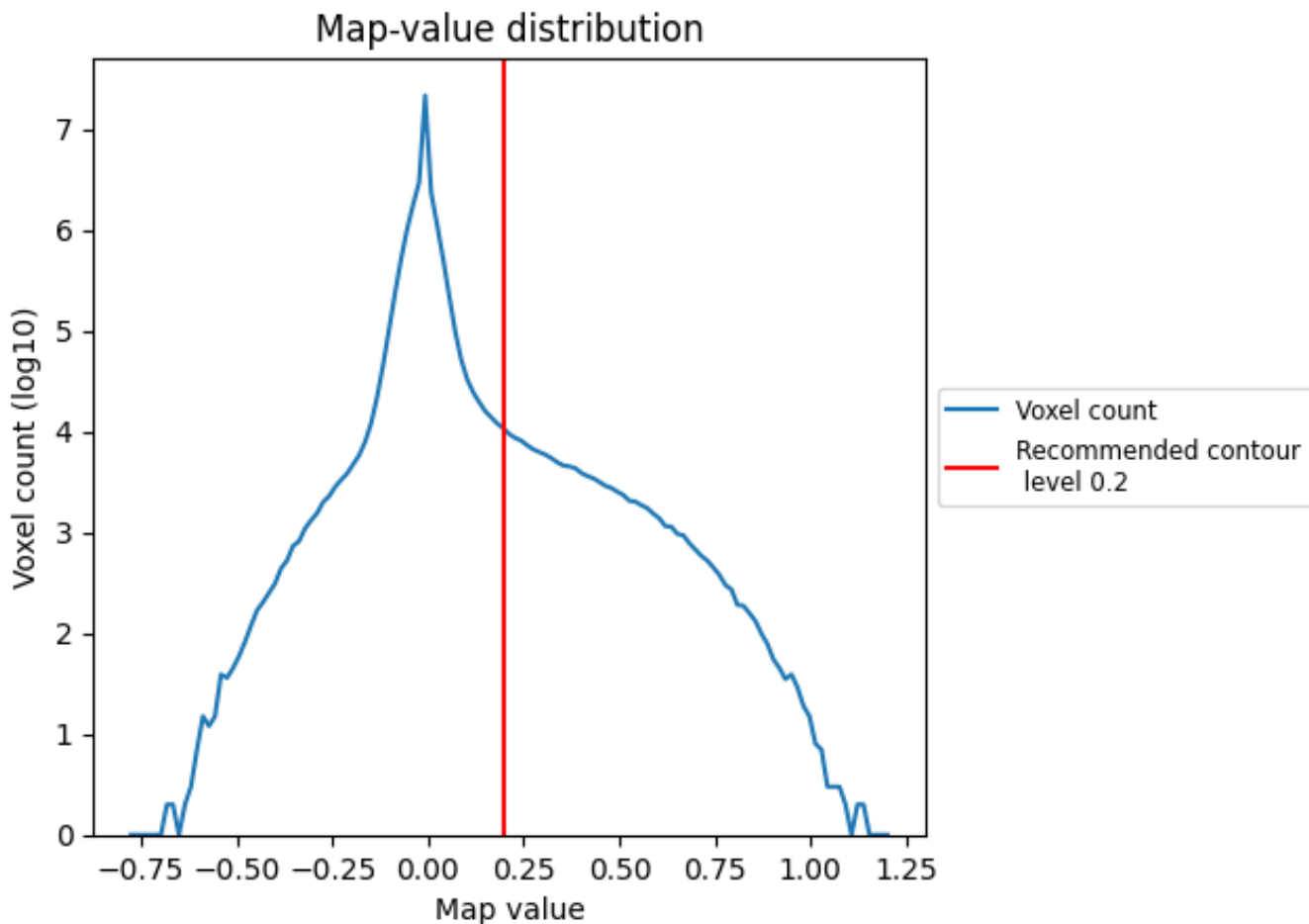
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

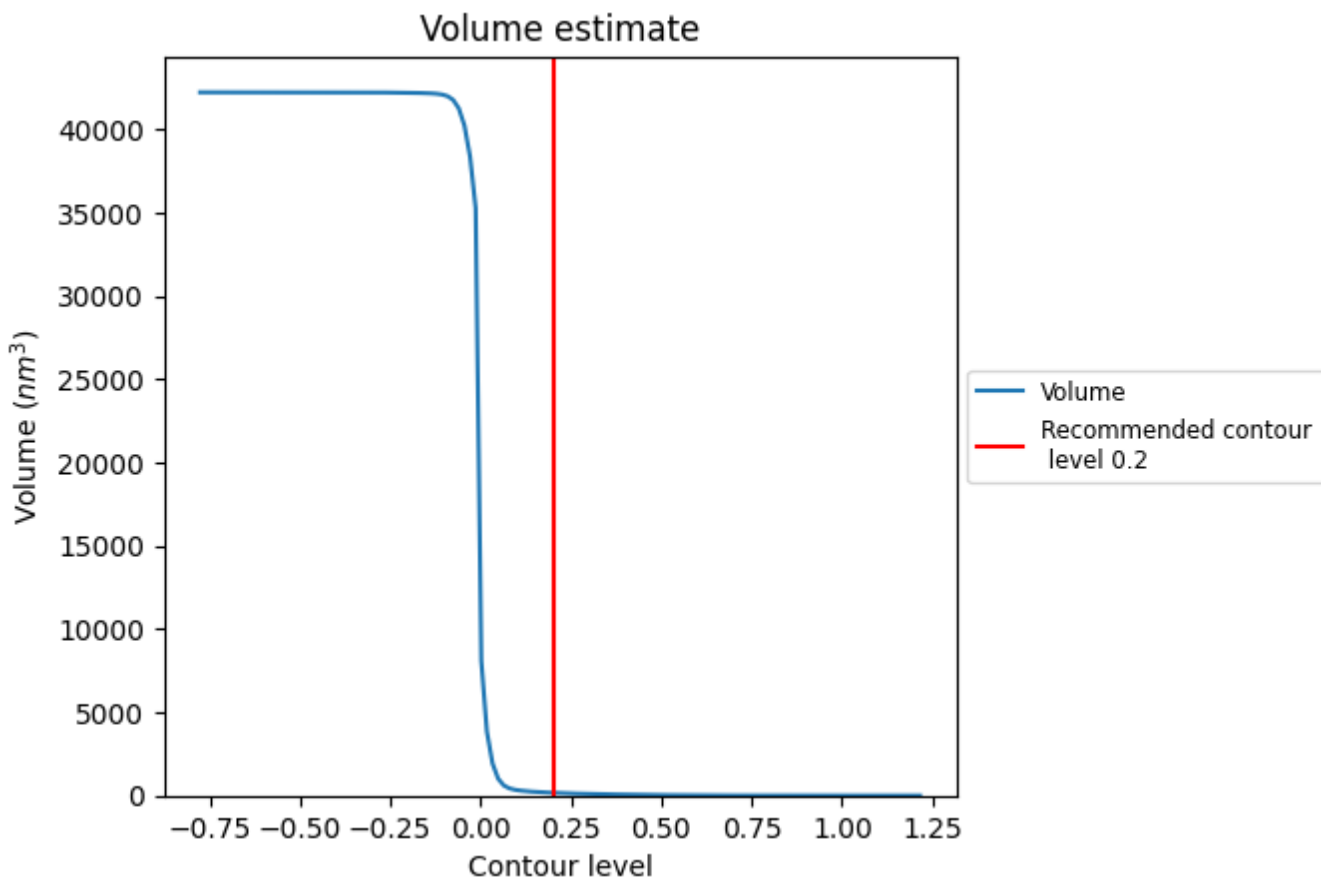
This section contains the results of statistical analysis of the map.

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.

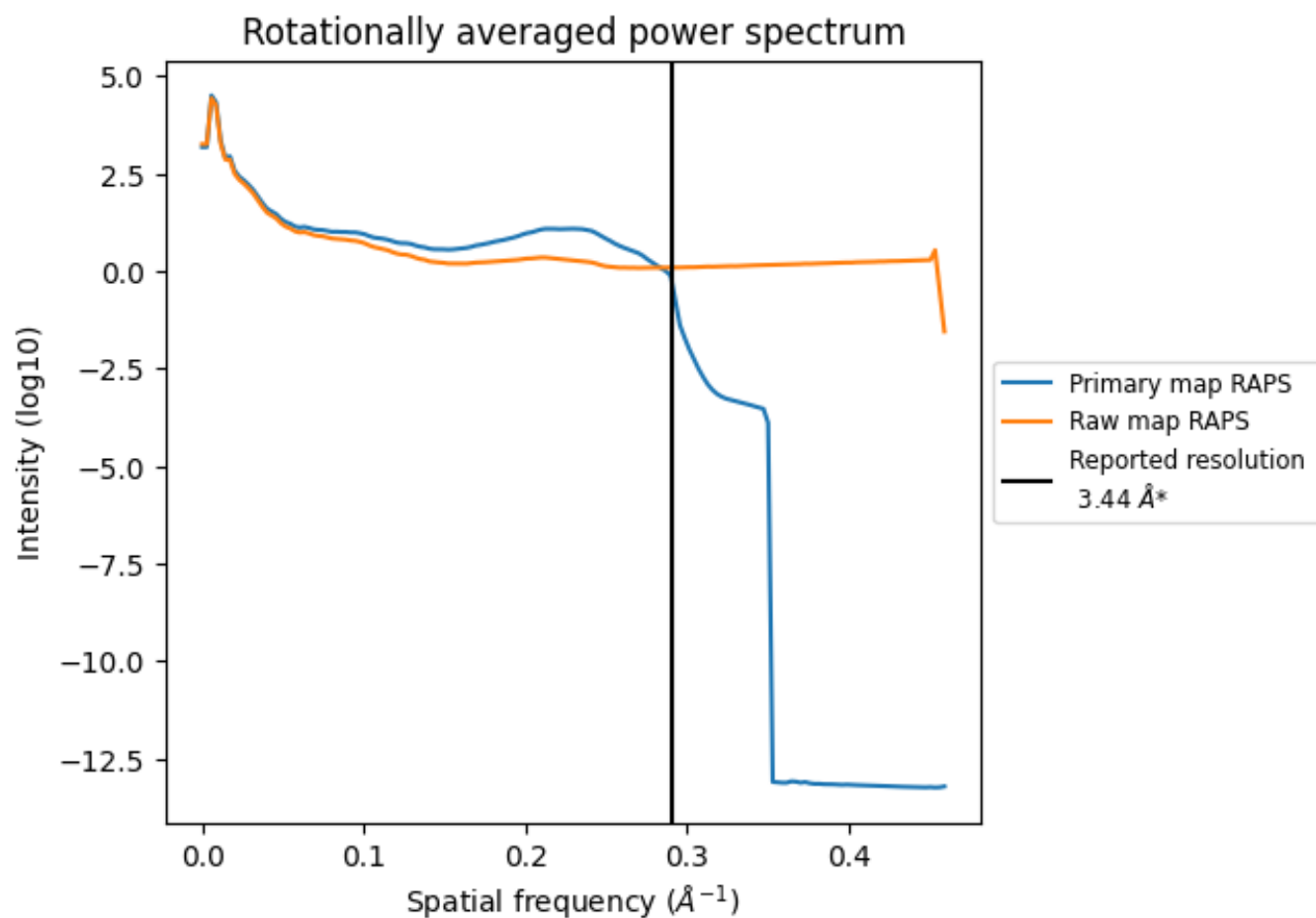
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 166 nm^3 ; this corresponds to an approximate mass of 150 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

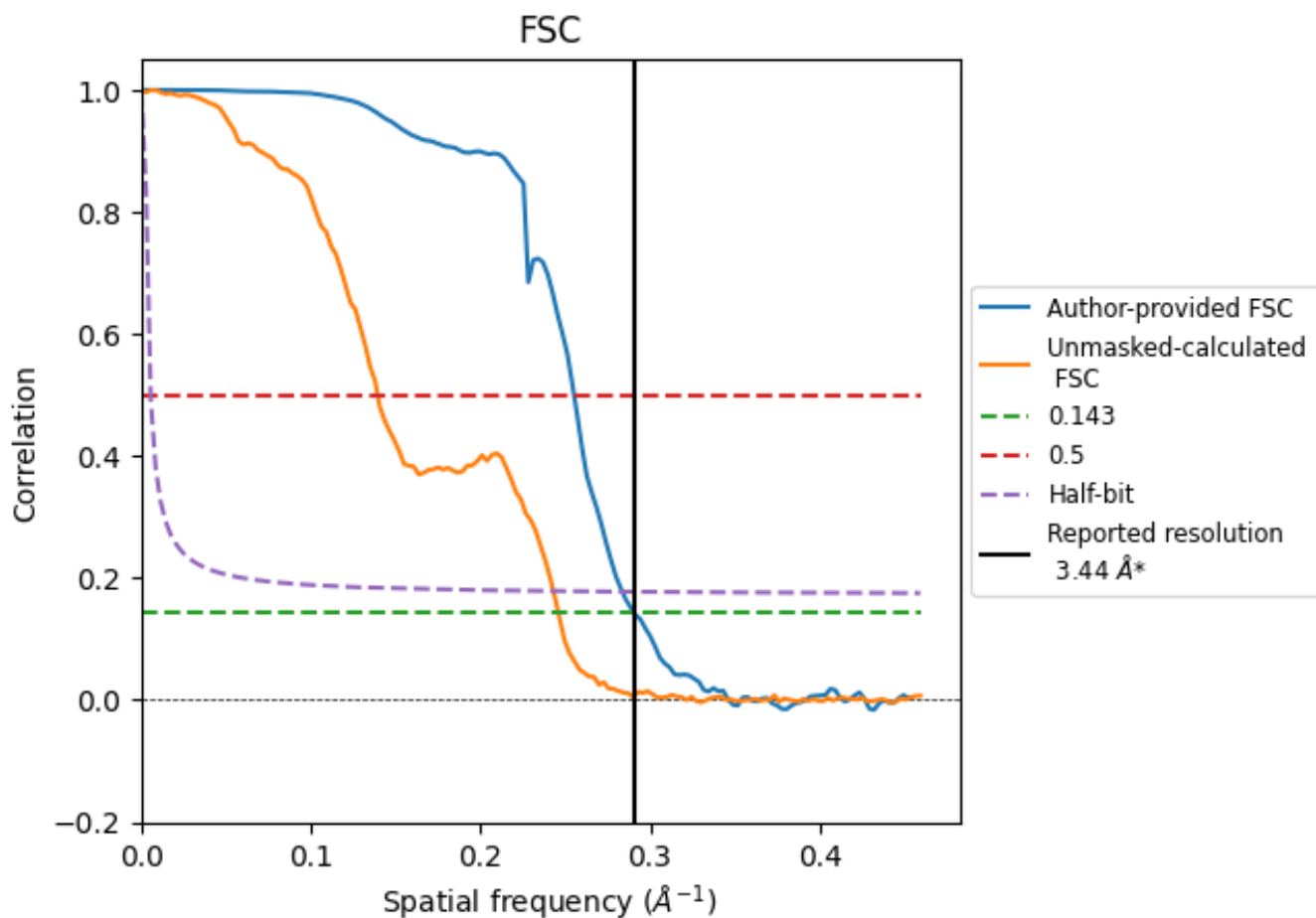


*Reported resolution corresponds to spatial frequency of 0.291 Å⁻¹

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 0.291 Å⁻¹

8.2 Resolution estimates [i](#)

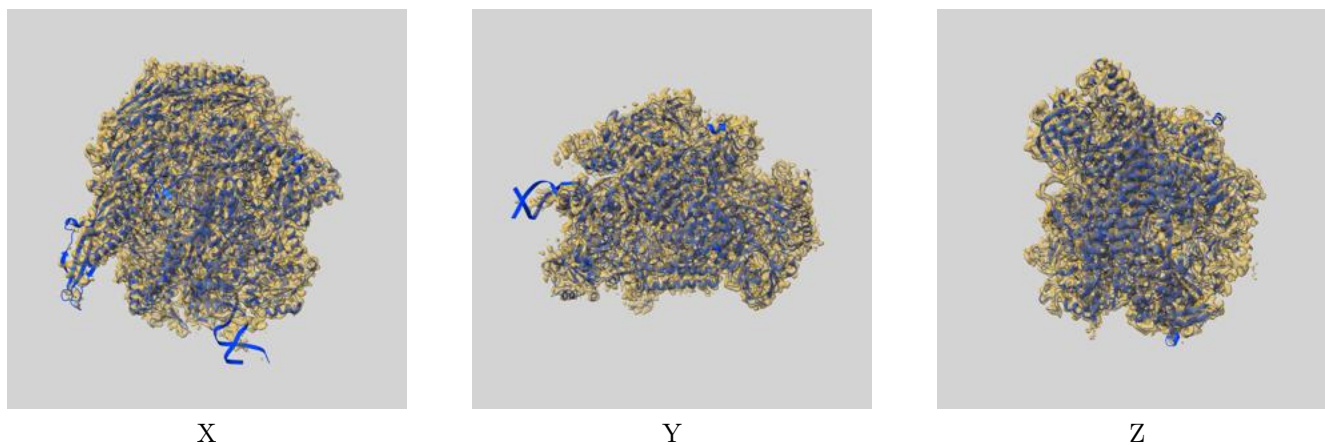
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.44	-	-
Author-provided FSC curve	3.44	3.92	3.52
Unmasked-calculated*	4.07	7.17	4.11

*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 4.07 differs from the reported value 3.44 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54704 and PDB model 9SAY. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



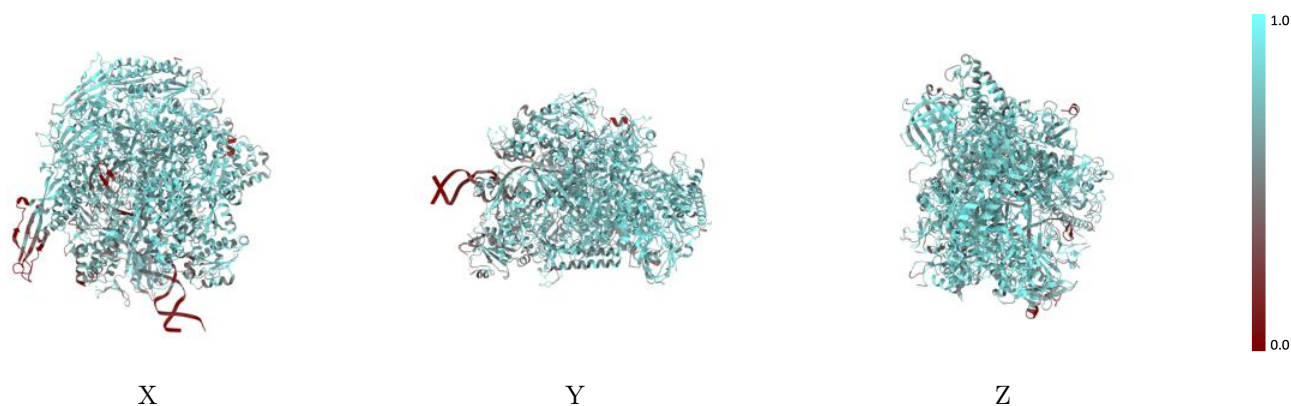
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



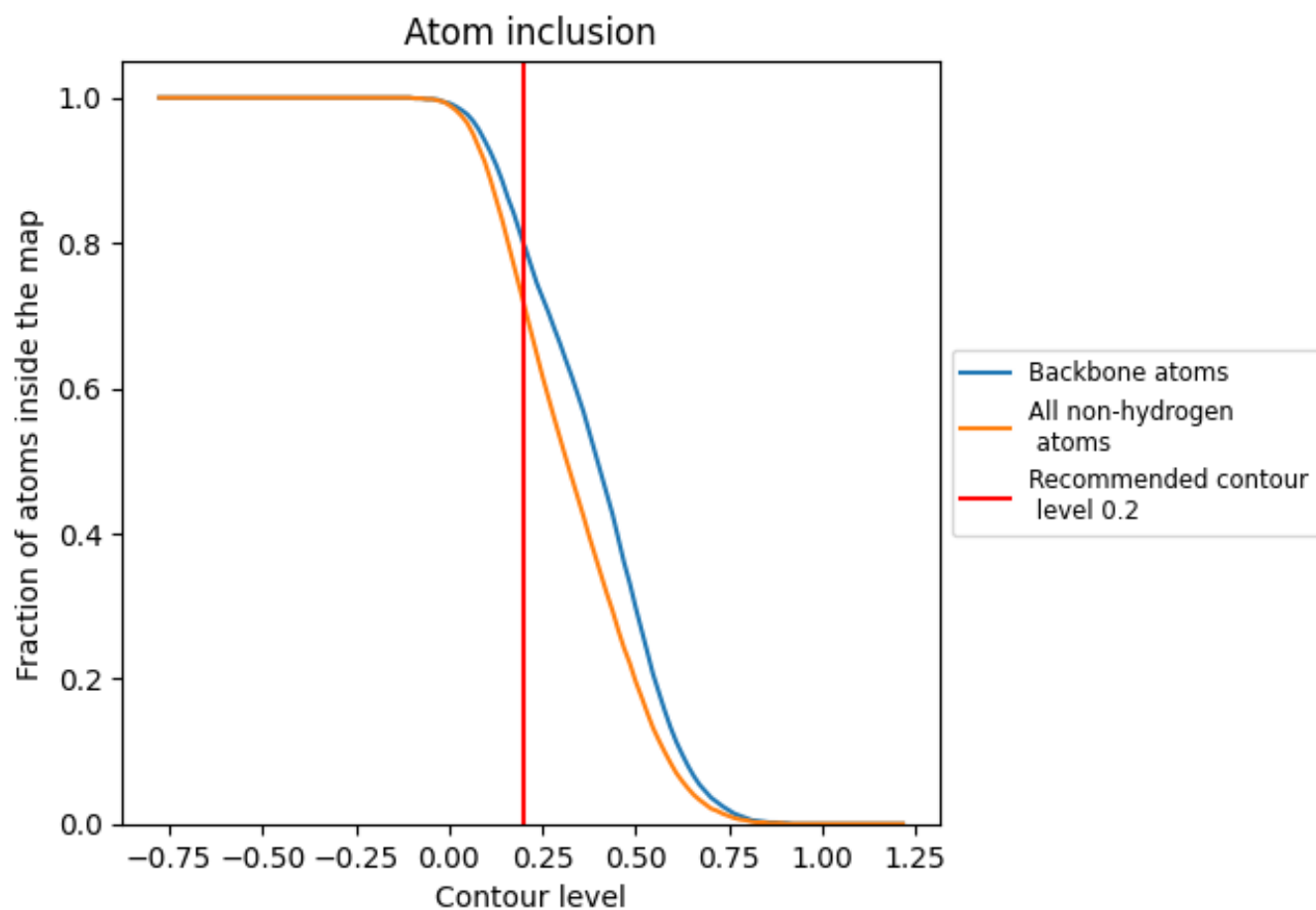
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7160	 0.4670
A	 0.7330	 0.4780
B	 0.7160	 0.4720
C	 0.7910	 0.5030
E	 0.7300	 0.4640
F	 0.7590	 0.4900
H	 0.7310	 0.4900
I	 0.6620	 0.4240
J	 0.8180	 0.5000
K	 0.7960	 0.5080
L	 0.7060	 0.4730
N	 0.2990	 0.1830
R	 0.5250	 0.3680
T	 0.3770	 0.2580

