



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 06:36 AM UTC

PDB ID : 6F42 / pdb_00006f42
EMDB ID : EMD-4182
Title : RNA Polymerase III closed complex CC1.
Authors : Vorlaender, M.K.; Khatter, H.; Wetzel, R.; Hagen, W.J.H.; Mueller, C.W.
Deposited on : 2017-11-29
Resolution : 5.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

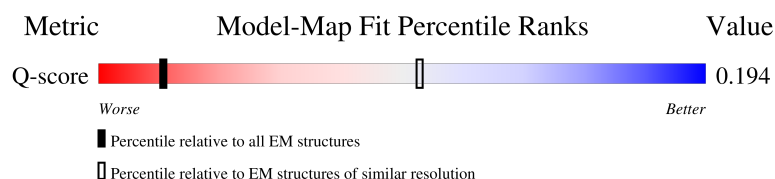
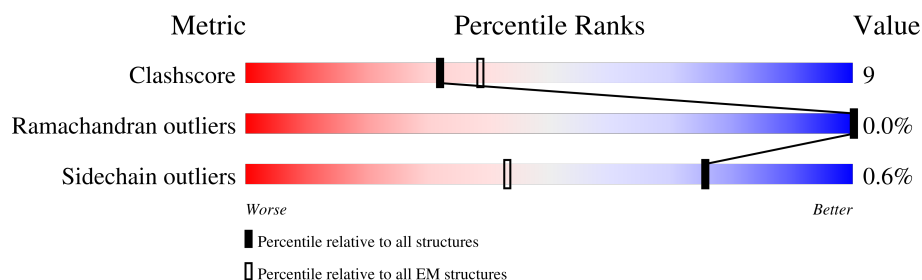
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 5.50 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	-
Q-score	-	25397	520 (5.00 - 6.00)

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	1460	11% 74% 21% .
2	B	1149	5% 71% 25% .
3	C	335	78% 21% .
4	D	161	13% 60% 14% 26%

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	212	
8	H	146	
9	I	110	
10	J	70	
11	K	142	
12	L	70	
13	M	282	
14	N	422	
15	O	654	
16	P	317	
17	Q	251	
18	U	240	
19	V	596	
20	W	594	
21	X	81	
22	Y	81	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 45046 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 III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1398	Total	C	N	O	S	0	0
			10972	6919	1936	2059	58		

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1114	Total	C	N	O	S	0	0
			8788	5558	1516	1654	60		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	335	Total	C	N	O	S	0	0
			2655	1681	454	511	9		

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	119	Total	C	N	O	S	0	0
			977	628	156	187	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1751	1111	309	320	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
			671	429	114	125	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	180	Total	C	N	O	S	0	0
			1448	950	231	261	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	140	Total	C	N	O	S	0	0
			1120	703	188	224	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total	C	N	O	S	0	0
			255	161	39	49	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			549	350	95	98	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			792	496	130	161	5		

- 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
			358	221	71	62	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	159	Total	C	N	O	S	0	0
			1300	835	218	246	1		

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	104	Total	C	N	O	S	0	0
			797	505	143	146	3		

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	534	Total	C	N	O	S	0	0
			4293	2733	736	806	18		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	99	Total	C	N	O	S	0	0
			827	538	127	158	4		

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	35	Total	C	N	O	0	0
			273	181	45	47		

- Molecule 18 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	180	Total	C	N	O	S	0	0
			1416	921	242	247	6		

- Molecule 19 is a protein called Transcription factor IIIB 70 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	332	Total	C	N	O	S	0	0
			2651	1661	481	495	14		

- Molecule 20 is a protein called Transcription factor TFIIB component B”.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	165	Total	C	N	O	S	0	0
			1383	882	245	249	7		

- Molecule 21 is a DNA chain called Non-template DNA.

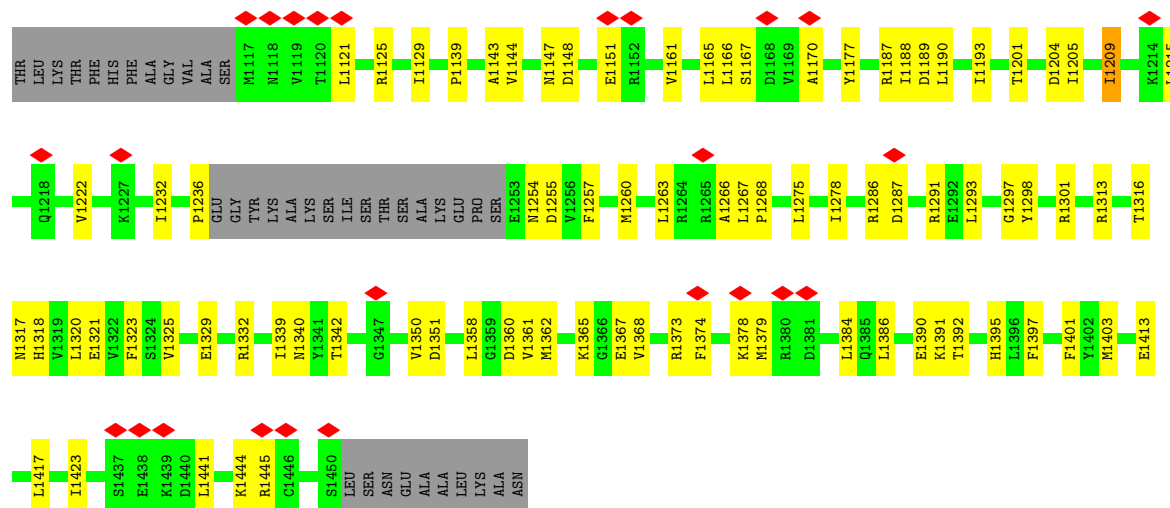
Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	43	Total	C	N	O	P	0	0
			877	424	146	264	43		

- Molecule 22 is a DNA chain called Template DNA.

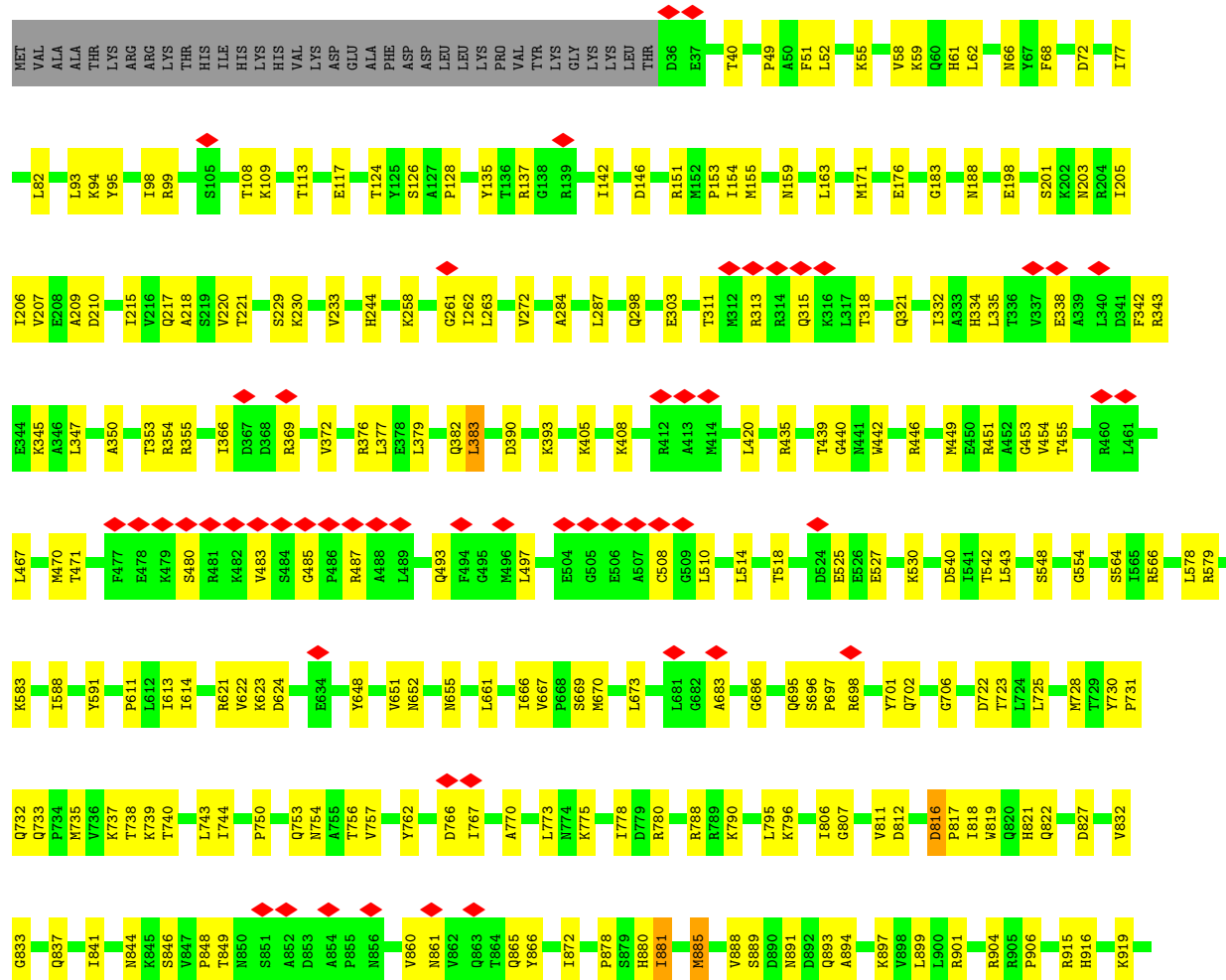
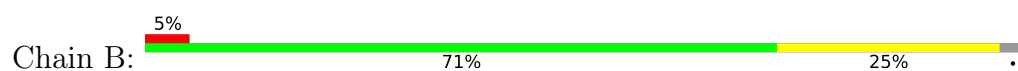
Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	43	Total	C	N	O	P	0	0
			886	425	166	252	43		

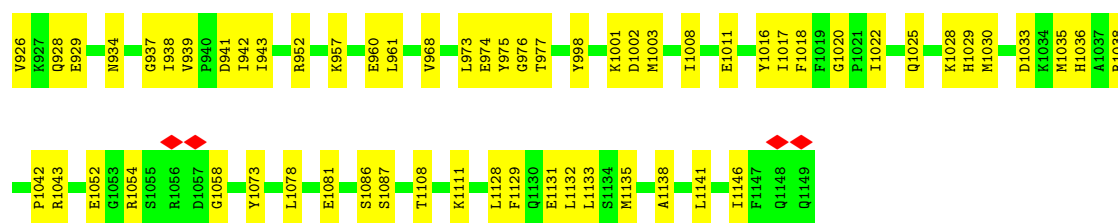
- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
23	A	2	Total	Zn	0
			2	2	
23	B	1	Total	Zn	0
			1	1	
23	I	1	Total	Zn	0
			1	1	
23	J	1	Total	Zn	0
			1	1	
23	L	1	Total	Zn	0
			1	1	
23	V	1	Total	Zn	0
			1	1	



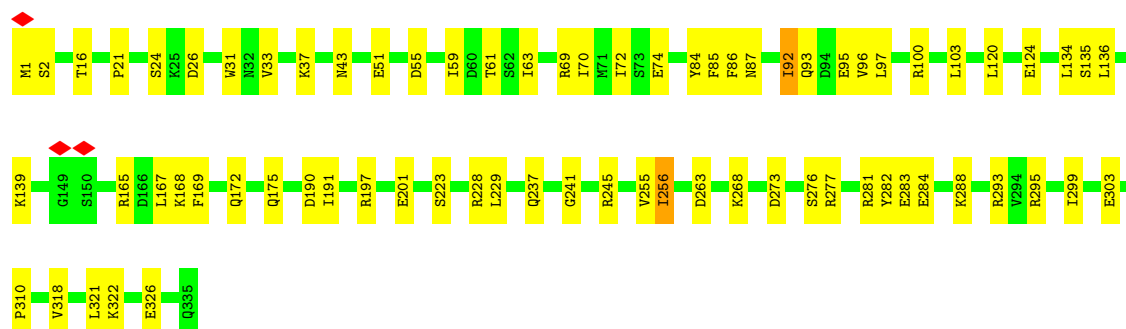
• Molecule 2: DNA-directed RNA polymerase III subunit RPC2





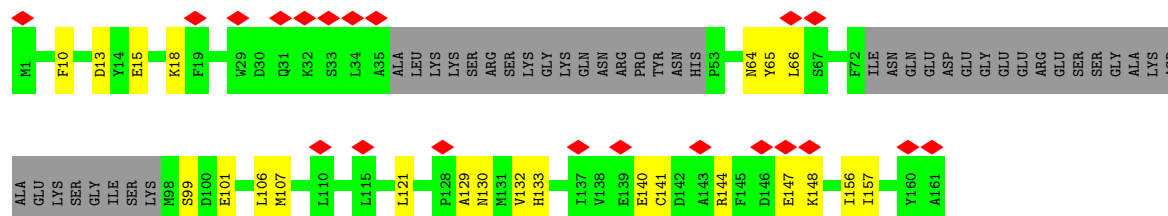
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C: 78% 21% .



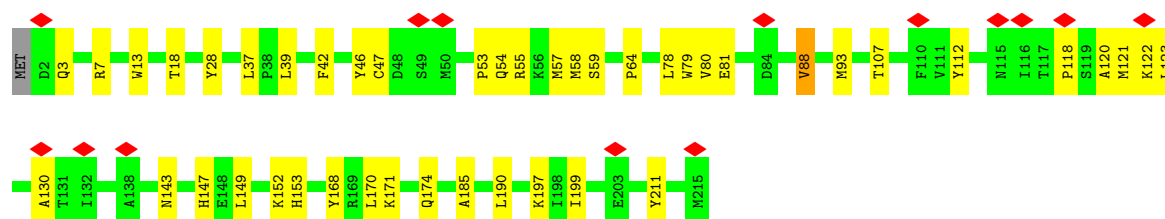
• Molecule 4: DNA-directed RNA polymerase III subunit RPC9

Chain D: 13% 60% 14% 26%



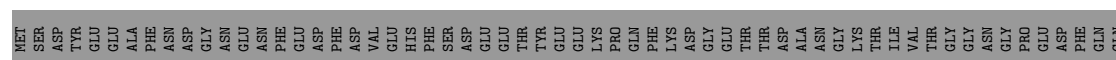
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 7% 79% 20%



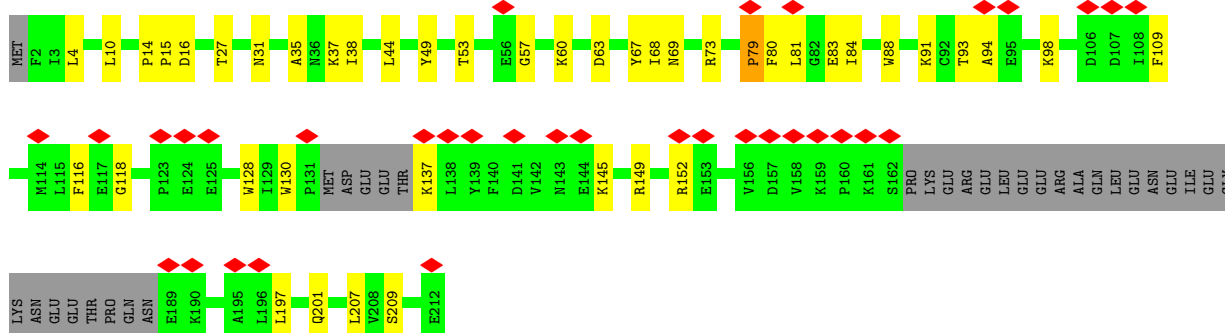
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 45% 8% 46%

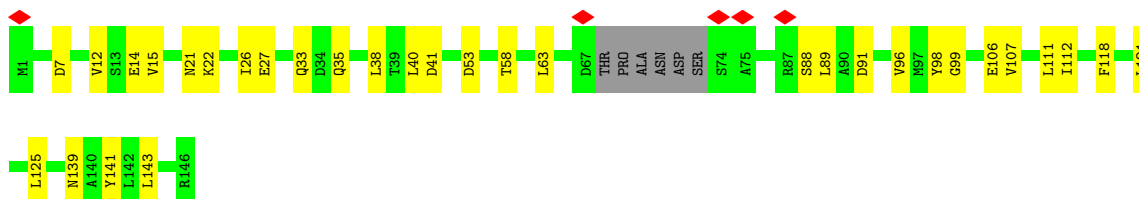
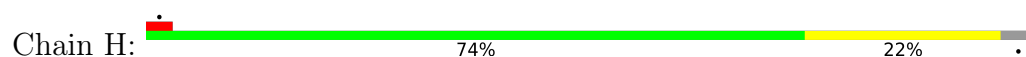




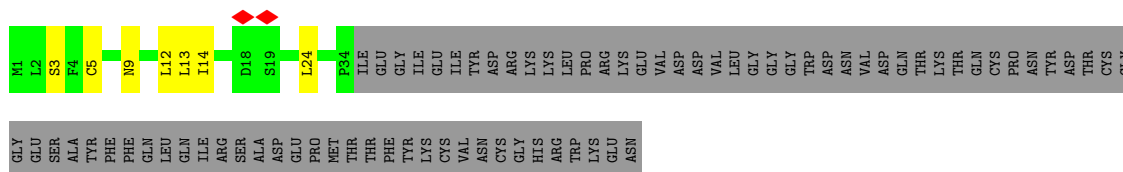
- Molecule 7: DNA-directed RNA polymerase III subunit RPC8



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



- Molecule 9: DNA-directed RNA polymerase III subunit RPC10



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



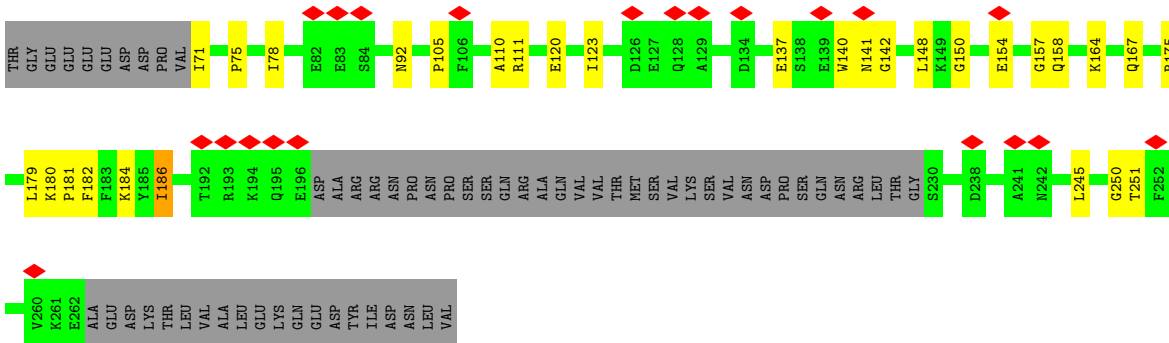
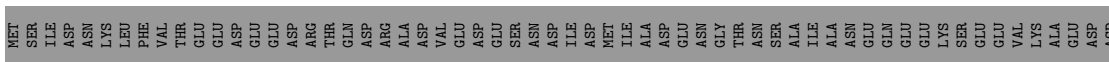
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2



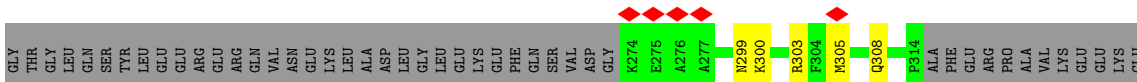
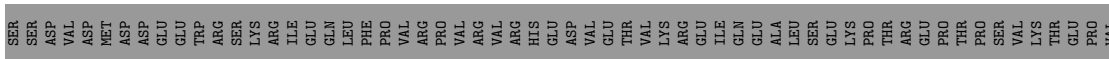
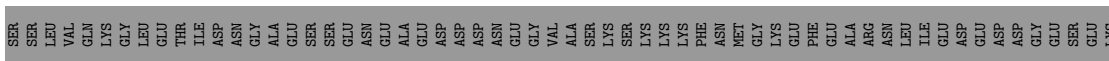
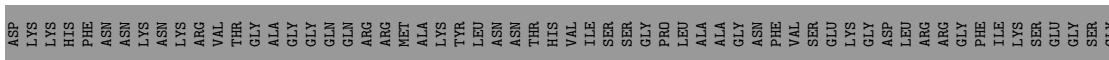
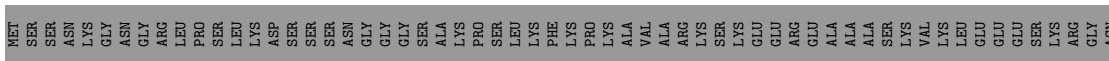
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

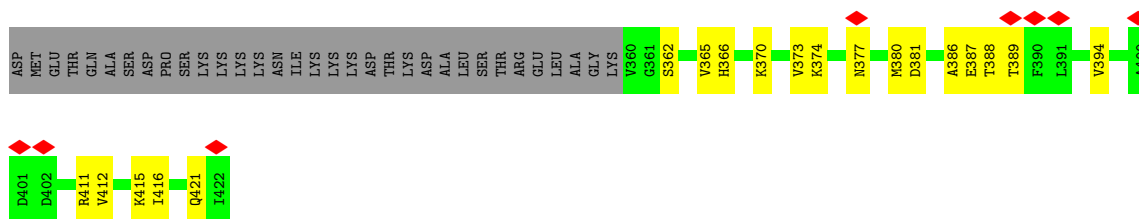


- Molecule 13: DNA-directed RNA polymerase III subunit RPC5

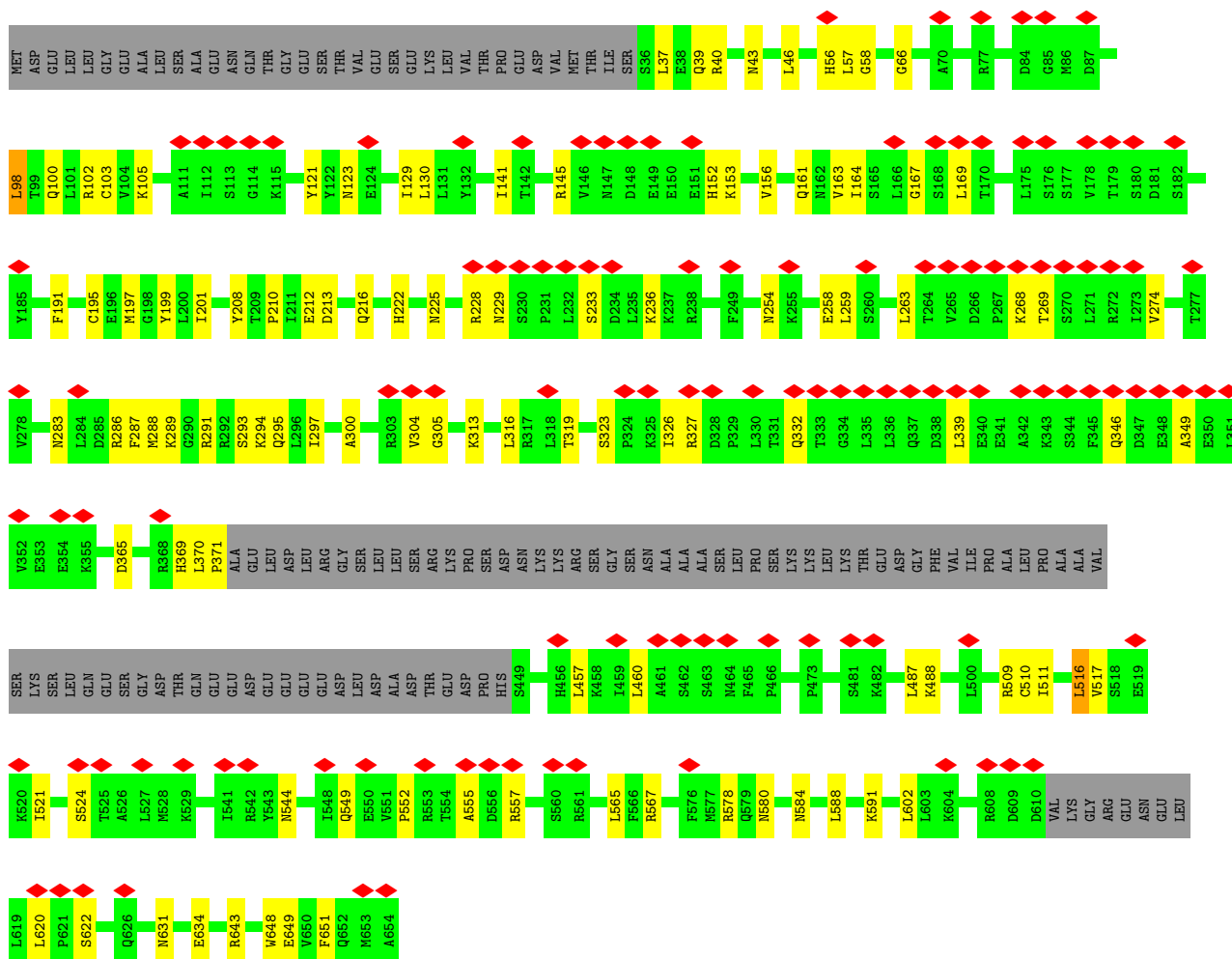


- Molecule 14: DNA-directed RNA polymerase III subunit RPC4

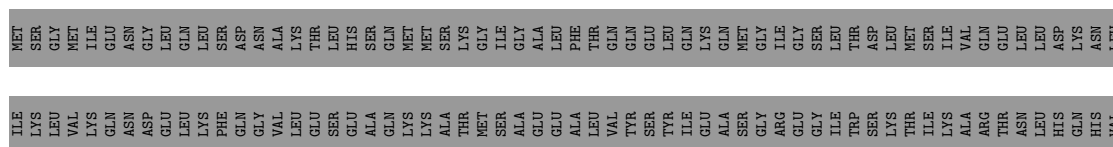


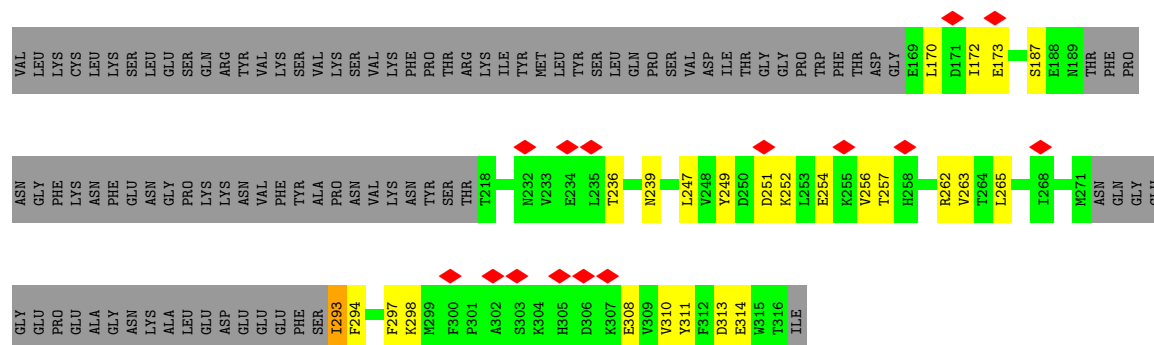


• Molecule 15: DNA-directed RNA polymerase III subunit RPC3

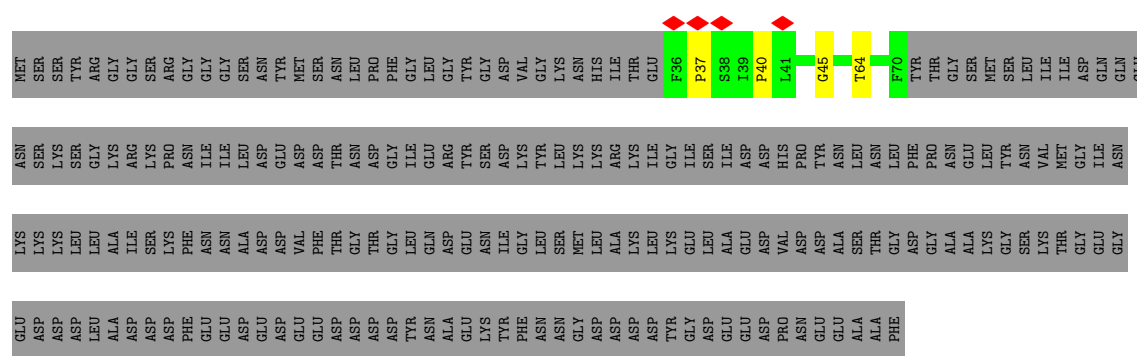


• Molecule 16: DNA-directed RNA polymerase III subunit RPC6





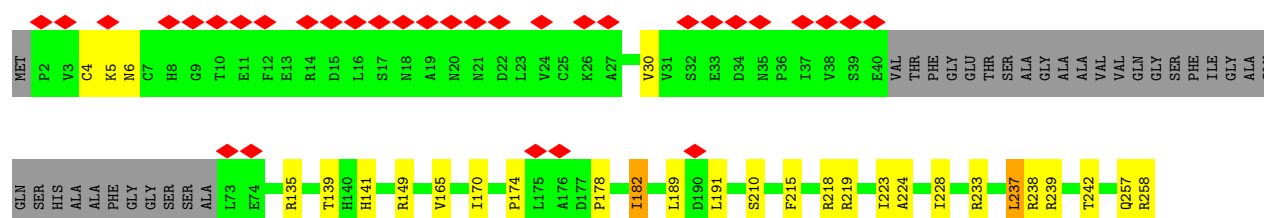
- Molecule 17: DNA-directed RNA polymerase III subunit RPC7



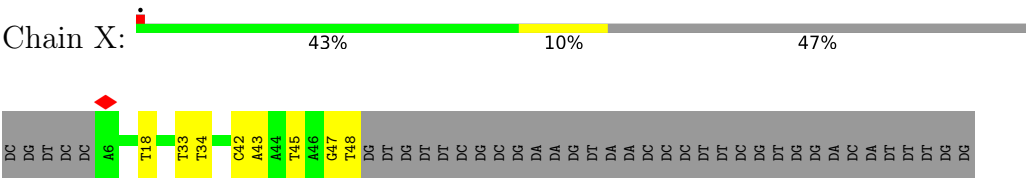
- Molecule 18: TATA-box-binding protein



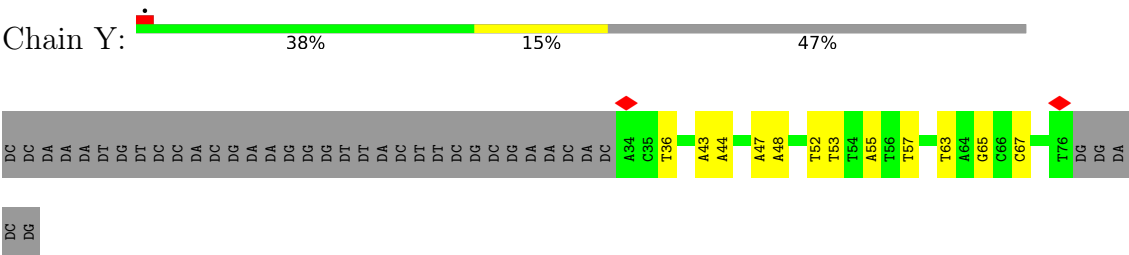
- Molecule 19: Transcription factor IIIB 70 kDa subunit



● Molecule 21: Non-template DNA



● Molecule 22: Template DNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	18760	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.097	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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: 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	0.09	0/11168	0.36	0/15086
2	B	0.09	0/8943	0.36	0/12068
3	C	0.10	0/2711	0.38	0/3676
4	D	0.09	0/991	0.31	0/1328
5	E	0.09	0/1787	0.33	0/2406
6	F	0.08	0/683	0.33	0/923
7	G	0.08	0/1486	0.29	0/2017
8	H	0.09	0/1138	0.37	0/1540
9	I	0.09	0/261	0.45	0/354
10	J	0.09	0/558	0.30	0/750
11	K	0.07	0/803	0.27	0/1083
12	L	0.09	0/360	0.38	0/478
13	M	0.08	0/1331	0.37	0/1800
14	N	0.09	0/805	0.34	0/1081
15	O	0.08	0/4358	0.31	0/5879
16	P	0.11	0/843	0.39	0/1142
17	Q	0.13	0/281	0.38	0/381
18	U	0.10	0/1443	0.34	0/1942
19	V	0.08	0/2693	0.33	0/3628
20	W	0.09	0/1413	0.39	0/1890
21	X	0.21	0/980	0.47	0/1510
22	Y	0.22	0/996	0.47	0/1535
All	All	0.10	0/46032	0.36	0/62497

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	70	CYS	Peptide
2	B	318	THR	Peptide

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	10972	0	11097	212	0
2	B	8788	0	8904	188	0
3	C	2655	0	2628	52	0
4	D	977	0	983	15	0
5	E	1751	0	1776	28	0
6	F	671	0	692	8	0
7	G	1448	0	1446	30	0
8	H	1120	0	1089	24	0
9	I	255	0	243	5	0
10	J	549	0	559	16	0
11	K	792	0	790	9	0
12	L	358	0	384	15	0
13	M	1300	0	1267	18	0
14	N	797	0	846	16	0
15	O	4293	0	4456	75	0
16	P	827	0	809	19	0
17	Q	273	0	285	4	0
18	U	1416	0	1493	41	0
19	V	2651	0	2673	50	0
20	W	1383	0	1388	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	X	877	0	493	7	0
22	Y	886	0	487	12	0
23	A	2	0	0	0	0
23	B	1	0	0	0	0
23	I	1	0	0	0	0
23	J	1	0	0	0	0
23	L	1	0	0	0	0
23	V	1	0	0	0	0
All	All	45046	0	44788	758	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 (758) 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)
15:O:201:ILE:HD13	15:O:283:ASN:HD22	1.46	0.80
2:B:667:VAL:HG12	2:B:669:SER:H	1.47	0.79
15:O:549:GLN:HE21	15:O:567:ARG:HH22	1.31	0.76
3:C:93:GLN:HE21	3:C:96:VAL:HG23	1.52	0.75
2:B:695:GLN:HG2	2:B:697:PRO:HD2	1.67	0.75
3:C:255:VAL:HG21	3:C:273:ASP:HB2	1.70	0.73
3:C:172:GLN:H	3:C:175:GLN:HE21	1.36	0.73
1:A:181:ASP:OD2	1:A:184:ARG:NH2	2.21	0.73
19:V:215:PHE:HB3	19:V:223:ILE:HG21	1.70	0.71
19:V:237:LEU:HB3	20:W:290:SER:HB3	1.71	0.71
1:A:630:ASN:ND2	1:A:650:GLY:O	2.24	0.71
5:E:3:GLN:HE21	5:E:7:ARG:HH22	1.38	0.71
1:A:482:ARG:HD3	1:A:544:PRO:HG3	1.72	0.70
1:A:1441:LEU:HD21	7:G:53:THR:HA	1.73	0.70
1:A:504:VAL:HA	1:A:551:ILE:HD11	1.74	0.69
14:N:366:HIS:HB2	14:N:370:LYS:HB3	1.74	0.69
1:A:151:GLN:NE2	1:A:153:ARG:O	2.24	0.68
16:P:256:VAL:HG22	16:P:257:THR:HG23	1.76	0.68
2:B:818:ILE:H	2:B:821:HIS:HB2	1.59	0.68
2:B:217:GLN:HB2	2:B:233:VAL:HB	1.75	0.68
4:D:129:ALA:H	4:D:157:ILE:HG22	1.59	0.68
2:B:888:VAL:HG11	12:L:54:ARG:HH21	1.58	0.67
3:C:70:ILE:HG23	3:C:74:GLU:HB2	1.75	0.67
15:O:591:LYS:HD2	16:P:308:GLU:HG3	1.77	0.67
1:A:757:ASN:HD22	1:A:760:GLN:HE21	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:732:GLN:NE2	2:B:733:GLN:O	2.28	0.66
19:V:257:GLN:OE1	19:V:258:ARG:NH1	2.28	0.66
1:A:599:LYS:HB2	8:H:96:VAL:HG22	1.76	0.66
15:O:293:SER:HB2	15:O:316:LEU:HD11	1.77	0.66
19:V:238:ARG:NH2	20:W:291:GLU:OE2	2.29	0.66
1:A:1362:MET:HE1	1:A:1368:VAL:HG23	1.76	0.66
2:B:483:VAL:HG12	2:B:485:GLY:H	1.60	0.66
15:O:39:GLN:O	15:O:43:ASN:ND2	2.28	0.66
13:M:148:LEU:HA	13:M:182:PHE:H	1.61	0.66
18:U:104:MET:HB2	18:U:113:ALA:HB3	1.77	0.66
11:K:88:PHE:HB3	11:K:106:GLN:HB3	1.77	0.65
15:O:511:ILE:HG12	15:O:517:VAL:HG11	1.78	0.65
15:O:40:ARG:NH2	16:P:314:GLU:OE1	2.28	0.65
9:I:3:SER:HB2	9:I:12:LEU:HB2	1.79	0.65
1:A:636:PRO:HB3	1:A:645:MET:HE3	1.77	0.65
2:B:833:GLY:H	2:B:881:ILE:HD11	1.62	0.65
3:C:191:ILE:HG23	10:J:15:GLY:HA3	1.77	0.65
1:A:753:GLN:HB2	1:A:757:ASN:HD21	1.62	0.64
18:U:84:THR:O	18:U:88:HIS:NE2	2.30	0.64
3:C:165:ARG:NH2	3:C:190:ASP:OD1	2.30	0.64
2:B:885:MET:HE2	2:B:897:LYS:HD3	1.79	0.64
2:B:915:ARG:H	2:B:1025:GLN:HE22	1.46	0.64
1:A:19:SER:HA	1:A:1403:MET:HG2	1.80	0.63
1:A:25:ASP:O	1:A:29:GLN:NE2	2.31	0.63
2:B:731:PRO:HB2	2:B:750:PRO:HG2	1.80	0.63
1:A:352:GLY:H	1:A:355:GLN:HB2	1.64	0.63
2:B:258:LYS:NZ	2:B:263:LEU:O	2.32	0.63
1:A:153:ARG:HH12	15:O:339:LEU:HB3	1.63	0.62
6:F:115:THR:HG22	6:F:116:ASP:H	1.64	0.62
16:P:187:SER:HA	16:P:263:VAL:HG21	1.81	0.62
13:M:92:ASN:HD21	13:M:181:PRO:HG3	1.64	0.62
19:V:6:ASN:HD22	19:V:30:VAL:HG21	1.64	0.62
2:B:207:VAL:HG12	2:B:217:GLN:HE22	1.64	0.62
13:M:164:LYS:HB3	13:M:167:GLN:HB2	1.81	0.62
15:O:588:LEU:HD21	16:P:310:VAL:HG22	1.81	0.62
1:A:1332:ARG:NH1	1:A:1360:ASP:OD1	2.33	0.62
1:A:929:ASN:O	1:A:931:GLN:NE2	2.33	0.61
2:B:728:MET:HE3	2:B:730:TYR:H	1.64	0.61
2:B:816:ASP:OD1	2:B:816:ASP:N	2.32	0.61
5:E:170:LEU:HB2	5:E:174:GLN:HE21	1.64	0.61
18:U:196:ARG:HG3	18:U:203:VAL:HG12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:VAL:HG13	1:A:334:PRO:HD3	1.81	0.61
4:D:140:GLU:HG3	4:D:144:ARG:HH12	1.66	0.61
8:H:99:GLY:HA3	8:H:118:PHE:HA	1.82	0.61
18:U:194:ILE:O	18:U:196:ARG:NH1	2.34	0.61
2:B:730:TYR:OH	3:C:100:ARG:NH1	2.33	0.61
18:U:195:TYR:HD2	18:U:204:LEU:HD21	1.66	0.61
3:C:43:ASN:HB2	3:C:55:ASP:HB2	1.83	0.61
2:B:155:MET:HE3	2:B:183:GLY:HA2	1.82	0.60
2:B:221:THR:HG21	2:B:334:HIS:H	1.66	0.60
2:B:827:ASP:OD2	12:L:29:TYR:OH	2.20	0.60
14:N:374:LYS:NZ	14:N:377:ASN:O	2.35	0.60
18:U:107:ARG:HB2	20:W:473:LEU:HD22	1.83	0.60
1:A:72:GLY:HA3	1:A:76:SER:HB2	1.84	0.60
1:A:379:THR:HG22	2:B:1035:MET:HA	1.82	0.60
7:G:80:PHE:HB3	7:G:83:GLU:HB2	1.84	0.60
1:A:601:TYR:HD1	3:C:24:SER:HB2	1.67	0.59
15:O:56:HIS:HE1	15:O:130:LEU:HD22	1.67	0.59
1:A:372:ARG:NH1	2:B:1052:GLU:OE1	2.35	0.59
5:E:55:ARG:HA	5:E:58:MET:HE1	1.84	0.59
18:U:188:GLU:OE2	19:V:219:ARG:NH2	2.35	0.59
7:G:149:ARG:HH21	7:G:201:GLN:HG2	1.67	0.59
1:A:1263:LEU:HA	1:A:1266:ALA:HB3	1.84	0.59
8:H:106:GLU:HA	8:H:112:ILE:HA	1.85	0.59
1:A:200:GLU:HG2	15:O:516:LEU:HB2	1.84	0.59
3:C:136:LEU:HB3	3:C:167:LEU:HA	1.85	0.58
1:A:493:ARG:HB3	1:A:499:ARG:HH21	1.68	0.58
18:U:93:GLU:OE2	20:W:439:PHE:N	2.33	0.58
20:W:407:ASN:ND2	22:Y:65:DG:OP1	2.33	0.58
1:A:637:LYS:HD3	1:A:645:MET:HE1	1.84	0.58
1:A:1023:ARG:NH2	1:A:1028:MET:SD	2.76	0.58
18:U:197:MET:HB2	18:U:202:ILE:HG22	1.85	0.58
1:A:409:THR:HG22	1:A:410:ARG:HD2	1.85	0.58
2:B:113:THR:OG1	2:B:117:GLU:OE1	2.21	0.58
3:C:87:ASN:ND2	12:L:61:THR:O	2.36	0.58
1:A:1048:VAL:O	1:A:1053:LYS:NZ	2.37	0.58
2:B:390:ASP:HA	2:B:393:LYS:HE3	1.85	0.58
8:H:33:GLN:HG3	8:H:35:GLN:H	1.69	0.58
2:B:210:ASP:H	2:B:215:ILE:HG22	1.68	0.58
2:B:683:ALA:HB1	2:B:744:ILE:HD13	1.86	0.58
1:A:815:GLN:NE2	1:A:816:GLN:O	2.37	0.58
2:B:807:GLY:O	2:B:844:ASN:ND2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:31:ASP:HB3	10:J:34:THR:HG22	1.84	0.57
16:P:263:VAL:HG12	16:P:265:LEU:H	1.69	0.57
18:U:68:GLN:HE22	18:U:163:SER:H	1.52	0.57
2:B:332:ILE:O	2:B:345:LYS:NZ	2.32	0.57
1:A:787:ASN:ND2	8:H:21:ASN:OD1	2.38	0.57
1:A:1254:ASN:HD21	9:I:13:LEU:HD21	1.69	0.57
2:B:1043:ARG:NH1	2:B:1087:SER:O	2.36	0.57
15:O:199:TYR:HD1	15:O:286:ARG:HD2	1.68	0.57
19:V:165:VAL:HG23	19:V:170:ILE:HB	1.87	0.57
1:A:473:LEU:HA	1:A:487:SER:HA	1.85	0.57
11:K:72:LEU:HG	11:K:76:LEU:HD23	1.87	0.57
1:A:945:ILE:HG23	1:A:946:THR:HG23	1.85	0.57
2:B:732:GLN:HB3	2:B:753:GLN:HA	1.84	0.56
2:B:1033:ASP:O	2:B:1054:ARG:NH2	2.36	0.56
19:V:476:ASN:HB3	19:V:479:ALA:HB3	1.87	0.56
1:A:872:LEU:HD21	2:B:701:TYR:HE1	1.70	0.56
1:A:1301:ARG:HH21	1:A:1325:VAL:HA	1.69	0.56
3:C:1:MET:HG3	3:C:2:SER:H	1.70	0.56
15:O:233:SER:HB3	15:O:236:LYS:HD3	1.88	0.56
15:O:288:MET:HG3	15:O:326:ILE:HD13	1.86	0.56
18:U:67:LEU:HB3	18:U:160:ILE:HD11	1.88	0.56
1:A:1386:LEU:HB3	1:A:1395:HIS:HD1	1.70	0.56
15:O:100:GLN:HG3	15:O:167:GLY:HA3	1.87	0.56
1:A:12:ARG:HB2	2:B:1146:ILE:HG13	1.87	0.56
1:A:555:GLN:NE2	2:B:767:ILE:O	2.39	0.56
1:A:859:PRO:HD3	2:B:661:LEU:HD11	1.86	0.56
2:B:40:THR:HB	2:B:624:ASP:HB3	1.86	0.56
5:E:118:PRO:O	5:E:122:LYS:NZ	2.36	0.56
10:J:22:LEU:O	10:J:26:GLN:NE2	2.39	0.56
19:V:275:PHE:HE2	19:V:279:ASP:HB2	1.71	0.56
15:O:620:LEU:HD23	15:O:622:SER:H	1.70	0.56
18:U:186:GLU:OE1	18:U:189:LEU:N	2.33	0.56
1:A:217:ARG:HH22	15:O:555:ALA:HA	1.70	0.56
1:A:993:GLU:O	5:E:197:LYS:NZ	2.37	0.56
16:P:170:LEU:HD13	16:P:172:ILE:H	1.71	0.56
1:A:179:ILE:HG12	15:O:557:ARG:HH22	1.71	0.56
1:A:951:ASP:O	1:A:1061:ARG:NH2	2.39	0.56
2:B:525:GLU:HG2	2:B:527:GLU:H	1.69	0.56
16:P:236:THR:HG23	16:P:239:ASN:H	1.71	0.56
18:U:94:TYR:HB2	18:U:102:VAL:HG22	1.86	0.56
6:F:138:LEU:HB2	6:F:142:SER:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:254:GLU:N	16:P:262:ARG:O	2.29	0.55
3:C:84:TYR:HB3	12:L:64:LEU:HD11	1.87	0.55
1:A:632:VAL:HG23	1:A:633:PHE:H	1.70	0.55
1:A:1147:ASN:ND2	1:A:1151:GLU:OE2	2.32	0.55
14:N:299:ASN:C	14:N:300:LYS:HD2	2.32	0.55
19:V:165:VAL:HA	19:V:170:ILE:HD13	1.88	0.55
13:M:75:PRO:HA	14:N:362:SER:HA	1.87	0.55
1:A:1445:ARG:NH2	4:D:10:PHE:O	2.40	0.55
2:B:66:ASN:HD21	2:B:159:ASN:HD21	1.53	0.55
2:B:372:VAL:HG23	2:B:651:VAL:HG11	1.88	0.55
18:U:138:LYS:NZ	19:V:465:VAL:O	2.32	0.55
8:H:98:TYR:OH	8:H:139:ASN:ND2	2.40	0.55
16:P:311:TYR:CD2	17:Q:37:PRO:HG2	2.42	0.55
1:A:483:LEU:HD11	1:A:540:ASN:HB3	1.88	0.55
15:O:161:GLN:NE2	17:Q:64:THR:OG1	2.40	0.55
1:A:624:ILE:HG22	1:A:625:ASN:H	1.72	0.55
1:A:683:ARG:NH1	1:A:925:GLU:OE2	2.40	0.55
2:B:795:LEU:HD21	2:B:806:ILE:HD11	1.89	0.55
15:O:129:ILE:HG21	15:O:164:ILE:HD13	1.88	0.55
20:W:467:ILE:HG13	20:W:468:LEU:HD12	1.88	0.55
2:B:723:THR:HA	2:B:790:LYS:HB3	1.88	0.54
19:V:485:ARG:HG3	20:W:498:PHE:HB2	1.88	0.54
21:X:42:DC:H2''	21:X:43:DA:C8	2.42	0.54
2:B:1008:ILE:HD11	11:K:70:HIS:CD2	2.43	0.54
2:B:1108:THR:HA	2:B:1111:LYS:HG2	1.90	0.54
19:V:258:ARG:NH2	22:Y:63:DT:OP2	2.40	0.54
1:A:364:PHE:HA	1:A:368:LEU:HB2	1.88	0.54
2:B:548:SER:OG	14:N:389:THR:O	2.26	0.54
4:D:141:CYS:SG	4:D:144:ARG:NH2	2.80	0.54
15:O:327:ARG:O	15:O:332:GLN:NE2	2.41	0.54
5:E:47:CYS:HB2	5:E:53:PRO:HA	1.90	0.54
15:O:98:LEU:HB2	15:O:103:CYS:HB2	1.89	0.54
7:G:130:TRP:HE3	7:G:137:LYS:HB3	1.73	0.54
20:W:450:SER:H	20:W:453:GLN:NE2	2.06	0.54
1:A:683:ARG:HH12	1:A:925:GLU:HG2	1.73	0.54
1:A:927:GLU:H	1:A:932:PRO:HA	1.73	0.54
3:C:197:ARG:HE	10:J:61:LEU:HD13	1.71	0.54
4:D:15:GLU:HG3	4:D:18:LYS:HE3	1.89	0.54
2:B:206:ILE:HD11	2:B:218:ALA:HB3	1.90	0.54
18:U:224:TYR:HB3	19:V:445:LEU:HD22	1.90	0.54
2:B:788:ARG:HB3	2:B:899:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:93:THR:HG22	7:G:94:ALA:H	1.72	0.53
15:O:457:LEU:HA	15:O:460:LEU:HD13	1.90	0.53
1:A:605:THR:HG23	1:A:607:LYS:H	1.73	0.53
2:B:258:LYS:HG2	2:B:263:LEU:HA	1.90	0.53
1:A:1318:HIS:HD2	1:A:1321:GLU:HB3	1.73	0.53
1:A:553:ALA:HB1	1:A:557:PHE:HB2	1.91	0.53
1:A:597:ILE:HB	1:A:603:LEU:HB2	1.89	0.53
19:V:233:ARG:HE	20:W:285:PRO:HG3	1.72	0.53
1:A:210:GLU:HG3	21:X:48:DT:H5''	1.91	0.53
2:B:667:VAL:HB	2:B:670:MET:HB2	1.90	0.53
2:B:1036:HIS:CE1	2:B:1058:GLY:HA3	2.43	0.53
3:C:31:TRP:HH2	11:K:127:LEU:HD13	1.74	0.53
7:G:57:GLY:HA2	7:G:68:ILE:HG13	1.89	0.53
18:U:88:HIS:HB2	19:V:475:LEU:HD22	1.91	0.53
1:A:186:VAL:HG13	1:A:187:GLY:H	1.74	0.53
1:A:664:MET:HE3	1:A:666:LYS:H	1.74	0.53
2:B:846:SER:HB3	2:B:866:TYR:HB3	1.91	0.53
3:C:21:PRO:HD2	11:K:82:LYS:HA	1.91	0.53
12:L:29:TYR:HB3	12:L:56:LEU:HD21	1.90	0.53
14:N:305:MET:HA	14:N:412:VAL:HG13	1.91	0.53
1:A:122:GLN:NE2	1:A:126:GLU:OE2	2.42	0.53
1:A:223:ASN:HB2	1:A:316:TRP:HH2	1.74	0.53
1:A:901:ASP:OD2	1:A:905:ARG:NH2	2.42	0.53
3:C:16:THR:O	3:C:295:ARG:NH1	2.42	0.53
18:U:109:PRO:O	18:U:110:LYS:HG3	2.09	0.53
1:A:1257:PHE:HB2	9:I:14:ILE:HB	1.92	0.52
3:C:237:GLN:HB2	3:C:288:LYS:HG3	1.91	0.52
5:E:168:TYR:HB2	5:E:170:LEU:HD22	1.91	0.52
2:B:686:GLY:HA3	2:B:740:THR:HG21	1.90	0.52
2:B:369:ARG:NH2	2:B:480:SER:OG	2.42	0.52
2:B:420:LEU:HD12	19:V:149:ARG:HG2	1.92	0.52
1:A:757:ASN:HD22	1:A:760:GLN:NE2	2.08	0.52
2:B:540:ASP:HB3	2:B:543:LEU:HD13	1.92	0.52
1:A:812:VAL:HG22	1:A:814:GLY:H	1.74	0.52
1:A:1190:LEU:HD22	1:A:1193:ILE:HD13	1.92	0.52
2:B:163:LEU:HD22	2:B:171:MET:HE2	1.90	0.52
8:H:41:ASP:HB2	8:H:121:LEU:HD12	1.91	0.52
2:B:811:VAL:HG12	2:B:816:ASP:HA	1.91	0.52
1:A:789:ASN:ND2	1:A:791:PRO:HD2	2.25	0.52
1:A:1286:ARG:HG2	1:A:1287:ASP:H	1.74	0.52
2:B:889:SER:OG	2:B:891:ASN:O	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:ALA:HA	8:H:98:TYR:HB3	1.93	0.51
1:A:1320:LEU:HD23	1:A:1320:LEU:H	1.75	0.51
12:L:38:LEU:HD11	12:L:49:LYS:H	1.75	0.51
1:A:84:LEU:HD12	1:A:261:LEU:HD23	1.92	0.51
2:B:49:PRO:HG3	2:B:743:LEU:HD21	1.92	0.51
1:A:815:GLN:HE21	1:A:846:GLY:HA3	1.75	0.51
15:O:488:LYS:HE2	15:O:651:PHE:HA	1.91	0.51
1:A:1350:VAL:HG23	1:A:1351:ASP:H	1.76	0.51
3:C:59:ILE:HB	3:C:63:ILE:HD11	1.91	0.51
18:U:164:CYS:SG	18:U:165:ASP:N	2.84	0.51
18:U:197:MET:HB3	18:U:200:PRO:HD2	1.92	0.51
19:V:485:ARG:HB2	20:W:499:ASN:HD21	1.76	0.51
13:M:154:GLU:HB3	13:M:175:ARG:HG2	1.93	0.51
1:A:83:HIS:HA	1:A:262:PRO:HA	1.93	0.51
1:A:892:SER:OG	1:A:1379:MET:SD	2.68	0.51
2:B:311:THR:HG23	2:B:313:ARG:HH22	1.76	0.51
2:B:754:ASN:HD21	10:J:48:ARG:HB2	1.74	0.51
11:K:62:SER:HB3	11:K:104:ARG:HH11	1.75	0.51
18:U:98:ARG:NH1	22:Y:55:DA:OP1	2.44	0.51
18:U:185:TYR:HB3	18:U:193:LEU:HG	1.93	0.51
1:A:1079:ARG:HD3	6:F:84:TYR:HE2	1.76	0.51
1:A:1267:LEU:HG	1:A:1268:PRO:HD3	1.93	0.51
2:B:611:PRO:HA	2:B:648:TYR:HA	1.93	0.51
4:D:147:GLU:CD	4:D:148:LYS:H	2.19	0.51
8:H:7:ASP:OD1	8:H:58:THR:OG1	2.27	0.51
20:W:311:ARG:NH2	22:Y:67:DC:OP1	2.44	0.51
20:W:420:TRP:CG	20:W:457:LYS:HZ2	2.28	0.51
20:W:450:SER:H	20:W:453:GLN:HE22	1.58	0.51
1:A:104:GLN:HB2	1:A:145:LEU:HD11	1.92	0.51
1:A:1050:ASP:HA	1:A:1053:LYS:HE2	1.92	0.51
1:A:1121:LEU:O	1:A:1342:THR:OG1	2.28	0.51
2:B:837:GLN:HG2	2:B:878:PRO:HB3	1.92	0.51
12:L:31:CYS:SG	12:L:32:ALA:N	2.84	0.51
1:A:1187:ARG:NH1	1:A:1189:ASP:OD1	2.43	0.50
1:A:1329:GLU:HG3	5:E:153:HIS:HE1	1.77	0.50
2:B:527:GLU:HA	2:B:530:LYS:HE3	1.93	0.50
2:B:614:ILE:HG23	2:B:621:ARG:HD2	1.91	0.50
2:B:796:LYS:HA	2:B:893:GLN:HE21	1.76	0.50
2:B:1081:GLU:OE2	2:B:1086:SER:OG	2.30	0.50
8:H:58:THR:HB	8:H:143:LEU:HB2	1.92	0.50
2:B:493:GLN:HE21	2:B:497:LEU:HG	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:722:ASP:HB2	2:B:725:LEU:HD21	1.94	0.50
2:B:766:ASP:HA	2:B:770:ALA:HB3	1.93	0.50
3:C:245:ARG:NH1	3:C:263:ASP:OD2	2.43	0.50
4:D:107:MET:HE1	4:D:121:LEU:HD23	1.93	0.50
2:B:272:VAL:O	2:B:354:ARG:NH1	2.44	0.50
2:B:315:GLN:NE2	21:X:45:DT:OP1	2.45	0.50
2:B:579:ARG:NH1	2:B:588:ILE:O	2.45	0.50
6:F:136:ARG:N	6:F:144:GLU:O	2.45	0.50
19:V:441:ASN:HB2	19:V:444:LEU:HB2	1.93	0.50
1:A:261:LEU:HD12	1:A:262:PRO:HD2	1.94	0.50
19:V:233:ARG:HG3	19:V:239:ARG:HH11	1.77	0.50
5:E:171:LYS:H	5:E:174:GLN:NE2	2.09	0.50
1:A:840:LYS:HA	1:A:845:LYS:HE3	1.94	0.50
7:G:207:LEU:HG	7:G:209:SER:H	1.77	0.50
18:U:93:GLU:HG3	18:U:105:ARG:HH12	1.75	0.50
20:W:311:ARG:HH22	20:W:314:ARG:NH2	2.10	0.50
1:A:225:LEU:HD13	1:A:228:LEU:HD21	1.94	0.50
2:B:405:LYS:HA	2:B:408:LYS:HE3	1.94	0.50
8:H:58:THR:O	8:H:143:LEU:N	2.41	0.50
12:L:26:THR:HB	12:L:28:LYS:HG2	1.94	0.49
2:B:819:TRP:HA	2:B:822:GLN:HE22	1.76	0.49
3:C:100:ARG:NH2	10:J:3:VAL:O	2.41	0.49
12:L:53:HIS:HE1	12:L:55:ILE:HB	1.76	0.49
1:A:145:LEU:HG	1:A:149:LYS:HE2	1.94	0.49
2:B:591:TYR:HB2	2:B:652:ASN:HB3	1.93	0.49
2:B:780:ARG:NH2	10:J:10:CYS:O	2.42	0.49
2:B:261:GLY:HA2	2:B:298:GLN:HG3	1.95	0.49
5:E:107:THR:HB	5:E:130:ALA:HB3	1.93	0.49
15:O:199:TYR:HA	15:O:283:ASN:HB3	1.93	0.49
21:X:18:DT:O2	22:Y:65:DG:N2	2.46	0.49
1:A:274:MET:HG2	1:A:276:ASP:H	1.76	0.49
1:A:914:PHE:HE2	5:E:211:TYR:H	1.60	0.49
1:A:1161:VAL:HA	1:A:1275:LEU:HD13	1.94	0.49
8:H:14:GLU:H	8:H:27:GLU:HB2	1.75	0.49
1:A:1205:ILE:O	1:A:1209:ILE:HD12	2.13	0.49
2:B:666:ILE:HD11	2:B:673:LEU:HD12	1.93	0.49
14:N:373:VAL:HG23	14:N:381:ASP:HB2	1.93	0.49
15:O:289:LYS:HD2	15:O:323:SER:HB2	1.94	0.49
1:A:666:LYS:HD2	1:A:670:GLY:HA3	1.94	0.49
2:B:1028:LYS:HG2	2:B:1029:HIS:H	1.78	0.49
2:B:1036:HIS:HE1	2:B:1058:GLY:HA3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:VAL:HA	7:G:38:ILE:HG22	1.93	0.49
1:A:166:LYS:HA	1:A:178:ILE:HG22	1.95	0.49
1:A:763:GLU:HG2	1:A:822:ARG:HE	1.77	0.49
1:A:830:ARG:NH2	2:B:655:ASN:O	2.46	0.49
1:A:1236:PRO:HB3	1:A:1255:ASP:HB3	1.93	0.49
2:B:303:GLU:HB2	2:B:321:GLN:HE21	1.77	0.49
8:H:63:LEU:HG	8:H:89:LEU:HD23	1.95	0.49
18:U:73:THR:HA	18:U:122:VAL:HA	1.95	0.49
19:V:265:THR:HG23	19:V:266:LYS:H	1.77	0.49
1:A:625:ASN:HD22	1:A:655:ARG:HA	1.78	0.49
18:U:142:ILE:HG12	19:V:473:HIS:HD2	1.76	0.49
1:A:19:SER:HB3	2:B:1138:ALA:HB3	1.95	0.49
1:A:703:ARG:NH2	11:K:93:ILE:O	2.42	0.49
18:U:129:GLU:HG2	18:U:133:LYS:HE2	1.93	0.49
1:A:921:LEU:HD11	1:A:926:MET:HE3	1.95	0.48
2:B:904:ARG:NH1	2:B:1030:MET:SD	2.86	0.48
7:G:10:LEU:HA	7:G:69:ASN:HA	1.95	0.48
1:A:431:ASN:OD1	1:A:465:HIS:NE2	2.46	0.48
2:B:566:ARG:HD3	14:N:387:GLU:HB3	1.93	0.48
15:O:549:GLN:N	15:O:565:LEU:O	2.42	0.48
1:A:1064:GLU:OE2	1:A:1068:ARG:NE	2.41	0.48
2:B:735:MET:HE3	2:B:968:VAL:HG22	1.96	0.48
2:B:739:LYS:H	2:B:977:THR:HG22	1.79	0.48
2:B:775:LYS:N	2:B:926:VAL:O	2.44	0.48
5:E:185:ALA:HA	5:E:190:LEU:HD23	1.94	0.48
12:L:29:TYR:CG	12:L:56:LEU:HD11	2.48	0.48
13:M:111:ARG:HD3	13:M:120:GLU:HB2	1.94	0.48
15:O:552:PRO:HB3	15:O:557:ARG:HG3	1.95	0.48
1:A:850:ASN:ND2	1:A:860:GLU:OE2	2.43	0.48
3:C:322:LYS:NZ	3:C:326:GLU:OE1	2.47	0.48
15:O:197:MET:HE2	15:O:199:TYR:HE1	1.79	0.48
2:B:137:ARG:HH11	2:B:142:ILE:HD13	1.78	0.48
13:M:110:ALA:HB3	13:M:245:LEU:HB2	1.94	0.48
1:A:37:ARG:HG3	1:A:294:TRP:HB2	1.94	0.48
2:B:77:ILE:HB	2:B:95:TYR:CE2	2.48	0.48
2:B:514:LEU:HD11	2:B:518:THR:HG21	1.96	0.48
1:A:427:HIS:CE1	1:A:492:ILE:HG13	2.49	0.48
2:B:849:THR:HG22	2:B:865:GLN:HB2	1.95	0.48
15:O:228:ARG:HG3	15:O:229:ASN:H	1.77	0.48
15:O:327:ARG:HE	15:O:332:GLN:HE22	1.60	0.48
19:V:178:PRO:HB2	19:V:224:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:W:488:ILE:HA	20:W:491:ASN:HB2	1.95	0.48
18:U:133:LYS:HE3	19:V:452:LEU:HA	1.95	0.48
2:B:128:PRO:HA	2:B:151:ARG:HA	1.96	0.48
8:H:12:VAL:HG22	8:H:53:ASP:H	1.79	0.48
19:V:219:ARG:HH11	22:Y:63:DT:H4'	1.79	0.48
1:A:107:CYS:HB3	1:A:112:ALA:H	1.79	0.47
1:A:544:PRO:HA	1:A:924:LEU:HD13	1.96	0.47
5:E:37:LEU:HD11	5:E:42:PHE:HB2	1.95	0.47
13:M:250:GLY:O	13:M:251:THR:HG22	2.13	0.47
19:V:242:THR:OG1	20:W:296:SER:OG	2.31	0.47
1:A:808:GLN:HG2	1:A:813:VAL:HA	1.96	0.47
15:O:259:LEU:HD23	15:O:259:LEU:H	1.78	0.47
18:U:149:ALA:HB1	18:U:151:LYS:HG2	1.96	0.47
1:A:482:ARG:HH21	2:B:1073:TYR:HA	1.79	0.47
1:A:818:ILE:HD12	1:A:823:VAL:HA	1.96	0.47
2:B:62:LEU:HD23	2:B:155:MET:HE2	1.95	0.47
2:B:229:SER:OG	2:B:244:HIS:NE2	2.32	0.47
3:C:135:SER:O	3:C:168:LYS:N	2.47	0.47
5:E:47:CYS:HA	5:E:54:GLN:HG3	1.96	0.47
15:O:580:ASN:O	15:O:584:ASN:ND2	2.47	0.47
19:V:189:LEU:HD21	19:V:238:ARG:HG2	1.96	0.47
2:B:126:SER:HA	2:B:153:PRO:HA	1.96	0.47
15:O:57:LEU:HD23	15:O:58:GLY:N	2.30	0.47
15:O:287:PHE:O	15:O:291:ARG:N	2.44	0.47
15:O:365:ASP:O	15:O:369:HIS:ND1	2.39	0.47
15:O:105:LYS:HE2	15:O:123:ASN:HA	1.96	0.47
15:O:199:TYR:CD1	15:O:286:ARG:HD2	2.48	0.47
14:N:386:ALA:HB2	14:N:416:ILE:HG22	1.96	0.47
1:A:289:LEU:HA	1:A:292:ILE:HD12	1.96	0.47
2:B:284:ALA:HA	2:B:287:LEU:HD13	1.96	0.47
2:B:510:LEU:HD23	2:B:510:LEU:H	1.80	0.47
2:B:773:LEU:HB3	2:B:942:ILE:HG22	1.97	0.47
5:E:78:LEU:HD13	5:E:107:THR:HG23	1.97	0.47
7:G:79:PRO:HB2	7:G:83:GLU:HG2	1.96	0.47
13:M:158:GLN:H	14:N:308:GLN:HA	1.80	0.47
19:V:218:ARG:HH22	19:V:288:PRO:HG2	1.79	0.47
5:E:147:HIS:HE1	5:E:149:LEU:HD23	1.78	0.47
1:A:393:ALA:HB3	1:A:499:ARG:HB2	1.97	0.47
1:A:1373:ARG:HB3	1:A:1391:LYS:HE2	1.97	0.47
2:B:756:THR:H	2:B:941:ASP:HB2	1.80	0.47
3:C:100:ARG:HH12	10:J:4:PRO:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:37:LEU:HA	15:O:40:ARG:HE	1.79	0.47
2:B:841:ILE:HG12	2:B:872:ILE:HG12	1.97	0.47
15:O:254:ASN:O	15:O:258:GLU:N	2.48	0.47
16:P:172:ILE:HG22	16:P:173:GLU:H	1.80	0.47
2:B:929:GLU:HB3	3:C:72:ILE:HD11	1.97	0.46
15:O:121:TYR:HD2	15:O:210:PRO:HG2	1.80	0.46
20:W:318:ARG:NH1	20:W:448:TYR:HB2	2.31	0.46
21:X:34:DT:O4	22:Y:47:DA:N6	2.48	0.46
2:B:420:LEU:O	19:V:149:ARG:NH2	2.44	0.46
8:H:63:LEU:HD21	8:H:143:LEU:HD11	1.98	0.46
15:O:102:ARG:HG3	15:O:208:TYR:HD1	1.79	0.46
18:U:67:LEU:HD12	18:U:160:ILE:HG13	1.97	0.46
20:W:488:ILE:HG22	20:W:492:ILE:HG23	1.97	0.46
2:B:99:ARG:NH2	2:B:146:ASP:OD1	2.48	0.46
13:M:105:PRO:HB2	13:M:123:ILE:HD11	1.97	0.46
1:A:403:THR:OG1	1:A:464:ARG:O	2.19	0.46
1:A:1278:ILE:HG22	1:A:1297:GLY:HA3	1.97	0.46
2:B:201:SER:HA	2:B:376:ARG:HG2	1.97	0.46
8:H:107:VAL:N	8:H:111:LEU:O	2.47	0.46
15:O:191:PHE:O	15:O:195:CYS:N	2.47	0.46
1:A:774:ARG:HH21	1:A:804:LEU:HD11	1.80	0.46
1:A:1125:ARG:HH12	1:A:1129:ILE:HD11	1.80	0.46
1:A:1177:TYR:OH	1:A:1260:MET:SD	2.73	0.46
21:X:47:DG:N2	22:Y:36:DT:O2	2.47	0.46
1:A:882:THR:O	1:A:886:SER:N	2.44	0.46
1:A:1170:ALA:HA	1:A:1188:ILE:HA	1.98	0.46
2:B:968:VAL:O	10:J:47:ARG:NE	2.45	0.46
13:M:150:GLY:HA3	13:M:179:LEU:HD23	1.98	0.46
18:U:90:ARG:HB3	19:V:473:HIS:CE1	2.51	0.46
2:B:220:VAL:HA	2:B:230:LYS:HA	1.98	0.46
1:A:107:CYS:SG	1:A:108:LYS:N	2.89	0.46
1:A:440:ALA:O	1:A:441:ARG:HG3	2.16	0.46
1:A:513:ASP:HB2	2:B:919:LYS:HE2	1.98	0.46
1:A:1139:PRO:HG3	1:A:1298:TYR:CZ	2.51	0.46
2:B:51:PHE:HD2	2:B:52:LEU:HD12	1.79	0.46
2:B:393:LYS:HE2	2:B:446:ARG:HG2	1.98	0.46
2:B:737:LYS:HE2	2:B:973:LEU:HB3	1.97	0.46
2:B:915:ARG:N	2:B:1025:GLN:HE22	2.10	0.46
4:D:15:GLU:HA	4:D:18:LYS:HB3	1.97	0.46
16:P:247:LEU:HD12	16:P:252:LYS:HB2	1.98	0.46
2:B:698:ARG:NH2	2:B:952:ARG:HG2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:737:LYS:N	2:B:974:GLU:O	2.46	0.46
8:H:15:VAL:HG22	8:H:26:ILE:HG22	1.97	0.46
1:A:5:VAL:HB	7:G:37:LYS:HB3	1.98	0.46
1:A:89:PRO:HG3	1:A:259:ARG:HG3	1.98	0.46
2:B:696:SER:OG	2:B:697:PRO:HD3	2.16	0.46
15:O:521:ILE:HA	15:O:524:SER:HB3	1.98	0.46
1:A:120:LYS:HB2	1:A:241:LEU:HD21	1.98	0.45
1:A:884:TYR:OH	1:A:888:ARG:NH2	2.49	0.45
2:B:55:LYS:HG2	2:B:59:LYS:HD3	1.99	0.45
3:C:241:GLY:O	3:C:245:ARG:NH1	2.49	0.45
18:U:140:ALA:HA	18:U:143:ILE:HD12	1.98	0.45
21:X:33:DT:O4	22:Y:48:DA:N6	2.49	0.45
1:A:329:SER:HB3	1:A:355:GLN:HG3	1.98	0.45
2:B:467:LEU:HA	2:B:470:MET:HE2	1.98	0.45
13:M:182:PHE:HE2	13:M:184:LYS:HD3	1.82	0.45
19:V:458:ASP:OD1	19:V:458:ASP:N	2.47	0.45
1:A:163:VAL:O	1:A:181:ASP:N	2.50	0.45
2:B:198:GLU:HB3	2:B:377:LEU:HD12	1.98	0.45
2:B:778:ILE:HD11	2:B:906:PRO:HD2	1.98	0.45
3:C:228:ARG:HB2	3:C:299:ILE:HB	1.98	0.45
7:G:88:TRP:HE1	7:G:145:LYS:HG2	1.82	0.45
8:H:38:LEU:HB3	8:H:125:LEU:HB3	1.97	0.45
15:O:631:ASN:ND2	15:O:634:GLU:OE2	2.50	0.45
20:W:287:GLY:O	20:W:288:GLN:HG3	2.16	0.45
1:A:442:ARG:HG2	19:V:30:VAL:HG22	1.98	0.45
1:A:633:PHE:HE1	1:A:651:PHE:HB2	1.81	0.45
1:A:1045:ASP:O	1:A:1053:LYS:NZ	2.44	0.45
2:B:622:VAL:HG23	2:B:623:LYS:H	1.81	0.45
1:A:84:LEU:N	1:A:261:LEU:O	2.43	0.45
1:A:88:LEU:HB2	1:A:225:LEU:HD21	1.98	0.45
2:B:82:LEU:HD23	2:B:94:LYS:HB3	1.98	0.45
1:A:229:ASN:OD1	15:O:544:ASN:ND2	2.49	0.45
1:A:1444:LYS:O	7:G:49:TYR:OH	2.32	0.45
2:B:860:VAL:HG23	2:B:861:ASN:H	1.82	0.45
10:J:10:CYS:SG	10:J:11:GLY:N	2.89	0.45
15:O:291:ARG:NE	15:O:649:GLU:OE2	2.40	0.45
18:U:68:GLN:NE2	18:U:163:SER:OG	2.49	0.45
20:W:473:LEU:O	20:W:476:LYS:NZ	2.46	0.45
1:A:552:ALA:HB1	1:A:670:GLY:HA2	1.98	0.45
1:A:1031:LEU:HD23	1:A:1031:LEU:H	1.81	0.45
1:A:1166:LEU:HD21	1:A:1268:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:ARG:HD3	2:B:542:THR:HG22	1.99	0.45
2:B:812:ASP:OD1	2:B:812:ASP:N	2.48	0.45
4:D:106:LEU:HB2	4:D:156:ILE:HG23	1.98	0.45
15:O:295:GLN:HG3	15:O:487:LEU:HD21	1.98	0.45
19:V:239:ARG:NH2	20:W:284:PHE:H	2.14	0.45
1:A:531:ALA:HA	1:A:535:MET:SD	2.57	0.45
2:B:205:ILE:HD11	2:B:355:ARG:NH2	2.32	0.45
2:B:816:ASP:OD1	2:B:817:PRO:HD3	2.17	0.45
13:M:140:TRP:CD1	13:M:142:GLY:H	2.35	0.45
15:O:263:LEU:HA	15:O:274:VAL:HA	1.98	0.45
19:V:274:LYS:HG2	19:V:275:PHE:H	1.81	0.45
2:B:338:GLU:HB2	2:B:342:PHE:HD1	1.81	0.45
2:B:737:LYS:O	2:B:976:GLY:N	2.45	0.45
12:L:53:HIS:CE1	12:L:55:ILE:HB	2.51	0.45
1:A:1148:ASP:O	1:A:1291:ARG:NH1	2.50	0.45
3:C:134:LEU:HB2	3:C:169:PHE:HA	1.99	0.45
15:O:268:LYS:O	15:O:269:THR:HG22	2.17	0.45
18:U:154:ASP:OD1	18:U:154:ASP:N	2.50	0.45
2:B:915:ARG:NH2	2:B:960:GLU:OE2	2.50	0.44
3:C:223:SER:HB3	3:C:303:GLU:HG2	1.99	0.44
9:I:5:CYS:O	9:I:9:ASN:N	2.39	0.44
14:N:380:MET:HB3	14:N:421:GLN:HE22	1.82	0.44
15:O:141:ILE:O	15:O:145:ARG:NE	2.48	0.44
18:U:238:ARG:C	18:U:239:LYS:HD3	2.41	0.44
1:A:1358:LEU:HA	1:A:1361:VAL:HG22	2.00	0.44
1:A:1386:LEU:HB3	1:A:1395:HIS:ND1	2.32	0.44
4:D:133:HIS:NE2	7:G:84:ILE:HG21	2.33	0.44
7:G:116:PHE:HZ	7:G:128:TRP:HE1	1.65	0.44
15:O:105:LYS:HB3	15:O:210:PRO:HD3	1.99	0.44
2:B:487:ARG:HD2	2:B:508:CYS:HB3	2.00	0.44
3:C:256:ILE:HA	3:C:268:LYS:H	1.82	0.44
7:G:31:ASN:O	7:G:35:ALA:N	2.50	0.44
2:B:961:LEU:HB2	2:B:1022:ILE:HD11	1.99	0.44
3:C:139:LYS:HG3	3:C:201:GLU:HB3	2.00	0.44
5:E:46:TYR:HA	5:E:57:MET:HE1	2.00	0.44
13:M:157:GLY:HA3	14:N:308:GLN:HG3	2.00	0.44
2:B:435:ARG:O	2:B:439:THR:OG1	2.32	0.44
2:B:795:LEU:HB2	2:B:894:ALA:HB3	1.99	0.44
15:O:163:VAL:HA	15:O:169:LEU:HG	2.00	0.44
15:O:294:LYS:HD2	15:O:297:ILE:HD11	1.99	0.44
19:V:135:ARG:HG2	19:V:174:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:LEU:HA	1:A:566:HIS:HB2	2.00	0.44
2:B:934:ASN:OD1	2:B:938:ILE:N	2.42	0.44
3:C:93:GLN:NE2	3:C:96:VAL:HG23	2.26	0.44
5:E:147:HIS:CE1	5:E:149:LEU:HD23	2.52	0.44
13:M:71:ILE:N	14:N:365:VAL:O	2.50	0.44
16:P:311:TYR:HA	17:Q:40:PRO:HA	2.00	0.44
1:A:57:LYS:HB3	1:A:68:ALA:HB3	1.98	0.44
1:A:386:ASN:O	1:A:699:LYS:NZ	2.50	0.44
1:A:1373:ARG:HH21	1:A:1390:GLU:HB3	1.82	0.44
2:B:928:GLN:HE21	2:B:939:VAL:HG21	1.81	0.44
15:O:319:THR:O	15:O:323:SER:OG	2.36	0.44
1:A:103:LEU:HD12	1:A:164:VAL:HG11	2.00	0.44
1:A:1365:LYS:NZ	1:A:1378:LYS:O	2.27	0.44
2:B:142:ILE:HD11	20:W:399:GLU:HB2	1.99	0.44
3:C:276:SER:C	3:C:277:ARG:HD2	2.42	0.44
4:D:130:ASN:ND2	4:D:132:VAL:HG12	2.33	0.44
5:E:59:SER:OG	5:E:80:VAL:O	2.29	0.44
18:U:219:GLN:HG3	18:U:221:GLU:H	1.83	0.44
1:A:16:LEU:HD13	1:A:17:GLU:N	2.33	0.44
1:A:164:VAL:HA	1:A:180:HIS:HA	2.00	0.44
1:A:258:TRP:HH2	2:B:1135:MET:HA	1.82	0.44
1:A:400:LYS:HA	1:A:465:HIS:CD2	2.53	0.44
2:B:1001:LYS:HA	2:B:1018:PHE:HA	2.00	0.44
15:O:152:HIS:HD2	15:O:156:VAL:HB	1.82	0.44
2:B:176:GLU:O	10:J:63:TYR:OH	2.35	0.43
19:V:182:ILE:HG23	19:V:228:ILE:HD11	2.00	0.43
1:A:364:PHE:HE2	1:A:1392:THR:HG21	1.83	0.43
2:B:203:ASN:HB3	2:B:335:LEU:HD11	1.99	0.43
2:B:379:LEU:H	2:B:382:GLN:NE2	2.16	0.43
3:C:86:PHE:HE1	12:L:64:LEU:HD12	1.83	0.43
10:J:17:LYS:HB3	10:J:39:LEU:HD21	1.99	0.43
18:U:87:LEU:HD11	19:V:487:TRP:CE3	2.53	0.43
1:A:73:ASN:OD1	1:A:74:LEU:N	2.47	0.43
8:H:121:LEU:H	8:H:121:LEU:HD23	1.84	0.43
1:A:808:GLN:HB3	1:A:813:VAL:HG12	2.00	0.43
3:C:282:TYR:O	3:C:283:GLU:HG3	2.19	0.43
5:E:79:TRP:NE1	5:E:81:GLU:OE2	2.52	0.43
1:A:503:CYS:HB3	1:A:551:ILE:HG13	2.00	0.43
3:C:86:PHE:CE1	12:L:64:LEU:HD12	2.54	0.43
5:E:93:MET:HG2	5:E:123:LEU:HD11	2.01	0.43
5:E:121:MET:HE3	5:E:122:LYS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:117:PRO:HA	6:F:120:ILE:HG22	2.00	0.43
13:M:137:GLU:O	13:M:141:ASN:ND2	2.52	0.43
15:O:210:PRO:HD2	15:O:213:ASP:OD2	2.18	0.43
19:V:4:CYS:SG	19:V:5:LYS:N	2.91	0.43
19:V:237:LEU:HD21	20:W:285:PRO:O	2.18	0.43
1:A:407:LYS:HA	1:A:461:VAL:HA	2.00	0.43
2:B:848:PRO:HG3	2:B:866:TYR:HE1	1.84	0.43
3:C:93:GLN:HE22	3:C:95:GLU:HG2	1.83	0.43
15:O:643:ARG:HH22	17:Q:45:GLY:HA3	1.84	0.43
18:U:75:THR:HA	18:U:120:LYS:HG3	2.01	0.43
19:V:139:THR:HG23	19:V:141:HIS:H	1.83	0.43
1:A:81:PHE:CZ	2:B:1133:LEU:HD23	2.53	0.43
1:A:1397:PHE:O	1:A:1401:PHE:N	2.46	0.43
14:N:394:VAL:HG23	14:N:412:VAL:HB	2.00	0.43
15:O:212:GLU:OE2	15:O:216:GLN:NE2	2.44	0.43
1:A:1028:MET:HE2	1:A:1048:VAL:HG21	2.00	0.43
2:B:880:HIS:O	2:B:901:ARG:N	2.49	0.43
3:C:33:VAL:O	3:C:37:LYS:N	2.51	0.43
7:G:81:LEU:HD23	7:G:81:LEU:H	1.84	0.43
7:G:152:ARG:H	7:G:197:LEU:HB2	1.83	0.43
15:O:578:ARG:HG3	15:O:648:TRP:HE1	1.83	0.43
16:P:313:ASP:C	16:P:314:GLU:HG3	2.44	0.43
18:U:68:GLN:HA	18:U:127:LYS:HD2	2.00	0.43
1:A:468:ASP:OD1	1:A:468:ASP:N	2.52	0.43
1:A:1318:HIS:CD2	1:A:1321:GLU:HB3	2.52	0.43
2:B:738:THR:HG23	2:B:977:THR:HA	2.01	0.43
5:E:93:MET:HE3	5:E:120:ALA:HA	2.00	0.43
7:G:10:LEU:HD23	7:G:10:LEU:H	1.84	0.43
15:O:304:VAL:HG22	15:O:305:GLY:H	1.84	0.43
15:O:510:CYS:HA	16:P:249:TYR:CZ	2.54	0.43
22:Y:52:DT:H2"	22:Y:53:DT:H5"	2.00	0.43
1:A:327:ILE:HD12	2:B:1135:MET:HE3	2.01	0.42
2:B:702:GLN:O	2:B:706:GLY:N	2.37	0.42
2:B:998:TYR:CD1	3:C:281:ARG:HD2	2.54	0.42
2:B:1011:GLU:HB3	3:C:61:THR:HG21	2.00	0.42
2:B:1078:LEU:H	2:B:1078:LEU:HD23	1.84	0.42
3:C:318:VAL:HA	3:C:321:LEU:HD13	2.00	0.42
15:O:370:LEU:HD12	15:O:371:PRO:HD2	2.00	0.42
20:W:503:ILE:O	20:W:506:GLN:HG2	2.19	0.42
3:C:26:ASP:OD1	3:C:26:ASP:N	2.50	0.42
7:G:84:ILE:HD13	7:G:149:ARG:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:116:PHE:HD2	7:G:118:GLY:H	1.65	0.42
8:H:26:ILE:HG13	8:H:40:LEU:O	2.19	0.42
15:O:102:ARG:HG3	15:O:208:TYR:CD1	2.54	0.42
16:P:297:PHE:O	16:P:298:LYS:HD3	2.19	0.42
19:V:210:SER:HA	19:V:215:PHE:HZ	1.84	0.42
1:A:1374:PHE:O	1:A:1378:LYS:NZ	2.47	0.42
2:B:1003:MET:HB3	2:B:1016:TYR:CD1	2.55	0.42
11:K:58:GLY:O	11:K:113:ALA:N	2.40	0.42
1:A:1143:ALA:HB3	1:A:1293:LEU:HD11	2.00	0.42
1:A:1144:VAL:HG21	1:A:1313:ARG:HH12	1.84	0.42
2:B:61:HIS:HB3	2:B:155:MET:HE1	2.01	0.42
2:B:262:ILE:HA	13:M:180:LYS:NZ	2.34	0.42
3:C:92:ILE:H	3:C:92:ILE:HG13	1.72	0.42
5:E:88:VAL:HG13	5:E:112:TYR:HE1	1.84	0.42
14:N:388:THR:HG21	14:N:415:LYS:HB3	2.02	0.42
20:W:483:GLU:O	20:W:487:GLU:N	2.51	0.42
1:A:70:CYS:SG	1:A:71:HIS:N	2.91	0.42
1:A:613:LEU:O	1:A:696:ARG:NH1	2.50	0.42
1:A:895:ASP:OD1	1:A:895:ASP:N	2.53	0.42
2:B:124:THR:HG22	2:B:188:ASN:H	1.83	0.42
15:O:222:HIS:HA	15:O:225:ASN:HD22	1.84	0.42
15:O:300:ALA:O	15:O:304:VAL:N	2.49	0.42
19:V:485:ARG:NH2	20:W:487:GLU:OE2	2.52	0.42
1:A:264:PRO:O	1:A:269:ARG:NH1	2.34	0.42
1:A:1384:LEU:HD11	1:A:1413:GLU:HG2	2.01	0.42
2:B:108:THR:HG22	2:B:109:LYS:H	1.83	0.42
2:B:383:LEU:HD21	2:B:442:TRP:CH2	2.55	0.42
2:B:613:ILE:HD11	2:B:673:LEU:HD22	2.02	0.42
2:B:737:LYS:HE3	2:B:975:TYR:HE1	1.84	0.42
2:B:1038:ARG:NH2	2:B:1042:PRO:O	2.40	0.42
3:C:276:SER:O	3:C:277:ARG:HD2	2.20	0.42
1:A:636:PRO:HG2	1:A:643:ASN:HA	2.02	0.42
1:A:753:GLN:N	1:A:757:ASN:OD1	2.52	0.42
1:A:933:VAL:HG23	1:A:934:ASN:H	1.85	0.42
1:A:1222:VAL:HG22	1:A:1232:ILE:HD13	2.02	0.42
2:B:578:LEU:HD22	2:B:583:LYS:HD3	2.00	0.42
2:B:1129:PHE:HA	2:B:1132:LEU:HG	2.01	0.42
8:H:63:LEU:HD13	8:H:141:TYR:CD2	2.54	0.42
1:A:16:LEU:HD23	2:B:1141:LEU:HD23	2.01	0.42
1:A:1097:ILE:H	1:A:1097:ILE:HG13	1.76	0.42
1:A:1201:THR:HG23	1:A:1204:ASP:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:303:ARG:HH12	14:N:411:ARG:CZ	2.32	0.42
15:O:46:LEU:HD21	15:O:66:GLY:HA2	2.00	0.42
1:A:90:VAL:HG21	1:A:323:VAL:HG11	2.02	0.42
1:A:107:CYS:N	1:A:112:ALA:O	2.44	0.42
1:A:563:LEU:HD11	1:A:708:ARG:HD2	2.01	0.42
2:B:68:PHE:HA	2:B:72:ASP:HB2	2.01	0.42
2:B:832:VAL:HG13	12:L:60:ARG:HA	2.02	0.42
2:B:916:HIS:HD1	2:B:957:LYS:HD3	1.85	0.42
19:V:219:ARG:HD3	20:W:408:TYR:CE2	2.54	0.42
2:B:881:ILE:H	2:B:881:ILE:HG13	1.51	0.41
3:C:85:PHE:HE1	3:C:97:LEU:HD11	1.85	0.41
4:D:64:ASN:OD1	4:D:65:TYR:N	2.53	0.41
16:P:293:ILE:HD12	16:P:294:PHE:N	2.35	0.41
19:V:210:SER:HA	19:V:215:PHE:CZ	2.55	0.41
1:A:31:GLU:HG3	1:A:32:VAL:HG13	2.01	0.41
1:A:524:THR:HG23	2:B:1081:GLU:HG3	2.01	0.41
1:A:897:SER:HB3	1:A:1423:ILE:HG13	2.02	0.41
2:B:554:GLY:HA2	2:B:564:SER:HA	2.02	0.41
2:B:1036:HIS:CD2	2:B:1054:ARG:HG2	2.55	0.41
7:G:60:LYS:HD3	7:G:63:ASP:HB2	2.02	0.41
19:V:268:ALA:O	19:V:272:VAL:HG23	2.20	0.41
7:G:38:ILE:HD12	7:G:44:LEU:HB2	2.03	0.41
11:K:107:THR:OG1	11:K:108:TYR:N	2.54	0.41
13:M:186:ILE:H	13:M:186:ILE:HG13	1.64	0.41
15:O:313:LYS:HE2	15:O:313:LYS:HB3	1.91	0.41
1:A:635:PRO:HA	1:A:636:PRO:HD3	1.96	0.41
1:A:1263:LEU:O	1:A:1267:LEU:N	2.53	0.41
2:B:93:LEU:HD13	2:B:135:TYR:HB3	2.03	0.41
2:B:757:VAL:N	2:B:1020:GLY:O	2.51	0.41
7:G:14:PRO:HA	7:G:15:PRO:HD3	1.90	0.41
18:U:105:ARG:HB2	20:W:437:THR:HG21	2.01	0.41
15:O:346:GLN:HA	15:O:349:ALA:HB3	2.02	0.41
1:A:438:GLU:OE2	1:A:441:ARG:N	2.53	0.41
1:A:906:THR:HG23	1:A:908:ALA:H	1.86	0.41
1:A:1373:ARG:NE	1:A:1390:GLU:OE1	2.53	0.41
3:C:120:LEU:HD23	3:C:124:GLU:HG2	2.02	0.41
7:G:63:ASP:OD2	7:G:67:TYR:OH	2.24	0.41
15:O:98:LEU:H	15:O:98:LEU:HG	1.70	0.41
20:W:420:TRP:NE1	20:W:457:LYS:HD3	2.35	0.41
1:A:384:ASP:HB3	1:A:387:LEU:HD22	2.02	0.41
1:A:716:ASP:HB2	1:A:789:ASN:ND2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1059:LEU:HD11	8:H:112:ILE:HG21	2.02	0.41
1:A:1391:LYS:HE3	1:A:1395:HIS:NE2	2.36	0.41
2:B:449:MET:HE1	2:B:451:ARG:NE	2.35	0.41
2:B:1003:MET:HB3	2:B:1016:TYR:HD1	1.86	0.41
2:B:1128:LEU:O	2:B:1131:GLU:HG3	2.20	0.41
4:D:99:SER:OG	4:D:101:GLU:OE1	2.38	0.41
5:E:18:THR:HG23	5:E:143:ASN:HB3	2.02	0.41
6:F:104:ASN:HB3	7:G:16:ASP:HB3	2.02	0.41
1:A:665:ASP:HB2	1:A:797:CYS:HA	2.02	0.41
2:B:929:GLU:HB2	3:C:69:ARG:HG2	2.03	0.41
2:B:934:ASN:OD1	2:B:937:GLY:N	2.54	0.41
5:E:152:LYS:H	5:E:199:ILE:HD11	1.86	0.41
19:V:287:PRO:HD2	19:V:290:PHE:HE1	1.86	0.41
20:W:480:ASN:O	20:W:482:ASP:N	2.52	0.41
1:A:196:ILE:O	1:A:200:GLU:N	2.47	0.41
1:A:1042:ILE:H	1:A:1042:ILE:HG13	1.67	0.41
2:B:209:ALA:HB2	2:B:366:ILE:HG21	2.01	0.41
2:B:347:LEU:HD22	2:B:350:ALA:HB3	2.03	0.41
2:B:471:THR:HB	2:B:514:LEU:HB3	2.02	0.41
2:B:762:TYR:HB3	2:B:943:ILE:HD13	2.02	0.41
3:C:229:LEU:HB2	3:C:293:ARG:HD3	2.02	0.41
10:J:48:ARG:O	10:J:52:THR:OG1	2.39	0.41
16:P:263:VAL:HG12	16:P:265:LEU:N	2.35	0.41
19:V:474:LEU:HD22	19:V:475:LEU:H	1.85	0.41
20:W:289:ILE:HD12	20:W:289:ILE:H	1.86	0.41
1:A:476:ARG:NH1	1:A:508:TYR:O	2.54	0.41
3:C:103:LEU:HB3	10:J:6:ARG:HE	1.85	0.41
3:C:282:TYR:C	3:C:284:GLU:H	2.29	0.41
18:U:69:ASN:ND2	22:Y:57:DT:H1'	2.36	0.41
2:B:454:VAL:HG13	2:B:455:THR:HG23	2.03	0.40
2:B:1078:LEU:HA	2:B:1081:GLU:HB3	2.03	0.40
5:E:28:TYR:HA	5:E:64:PRO:HA	2.03	0.40
15:O:509:ARG:NH1	16:P:251:ASP:OD1	2.54	0.40
15:O:602:LEU:H	15:O:602:LEU:HD23	1.87	0.40
22:Y:43:DA:H2''	22:Y:44:DA:C8	2.55	0.40
1:A:382:SER:N	1:A:498:PHE:O	2.54	0.40
1:A:535:MET:SD	1:A:535:MET:N	2.95	0.40
1:A:1165:LEU:HG	1:A:1167:SER:H	1.86	0.40
1:A:1339:ILE:HD12	1:A:1340:ASN:N	2.36	0.40
2:B:58:VAL:HG12	2:B:61:HIS:HB2	2.03	0.40
6:F:81:THR:OG1	6:F:144:GLU:OE2	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:57:LEU:HD23	15:O:58:GLY:H	1.86	0.40
18:U:63:ILE:H	18:U:63:ILE:HG13	1.69	0.40
1:A:223:ASN:HB2	1:A:316:TRP:CH2	2.56	0.40
1:A:300:LYS:HE2	1:A:300:LYS:HB3	1.87	0.40
1:A:787:ASN:HD21	8:H:21:ASN:CG	2.28	0.40
2:B:77:ILE:HG21	2:B:98:ILE:HD13	2.03	0.40
2:B:733:GLN:HE21	10:J:52:THR:HA	1.87	0.40
4:D:13:ASP:HB3	4:D:66:LEU:HD21	2.02	0.40
4:D:130:ASN:HD21	4:D:132:VAL:HG12	1.87	0.40
5:E:13:TRP:CD2	5:E:39:LEU:HD23	2.56	0.40
7:G:27:THR:HG22	7:G:31:ASN:HD21	1.86	0.40
7:G:91:LYS:NZ	7:G:93:THR:OG1	2.55	0.40
8:H:88:SER:N	8:H:91:ASP:OD2	2.54	0.40
10:J:7:CYS:HB3	10:J:11:GLY:H	1.87	0.40
1:A:599:LYS:HB3	1:A:600:PRO:HD3	2.02	0.40
1:A:1316:THR:OG1	1:A:1317:ASN:N	2.55	0.40
1:A:1323:PHE:CZ	1:A:1367:GLU:HA	2.57	0.40
2:B:350:ALA:HA	2:B:353:THR:HG22	2.03	0.40
2:B:440:GLY:O	2:B:453:GLY:N	2.54	0.40
2:B:1002:ASP:O	2:B:1017:ILE:N	2.42	0.40
7:G:4:LEU:HD13	7:G:73:ARG:HG3	2.04	0.40
12:L:40:LEU:HD13	12:L:41:SER:O	2.22	0.40
15:O:102:ARG:HA	15:O:208:TYR:HE1	1.86	0.40
19:V:233:ARG:NH2	20:W:280:CYS:O	2.54	0.40
1:A:789:ASN:HD22	1:A:790:ALA:N	2.19	0.40
1:A:832:LEU:HD23	1:A:834:HIS:H	1.86	0.40
3:C:51:GLU:N	3:C:310:PRO:HG3	2.37	0.40
3:C:282:TYR:C	3:C:283:GLU:HG3	2.46	0.40
6:F:99:LEU:HG	6:F:103:MET:HE2	2.03	0.40
7:G:98:LYS:HD3	7:G:109:PHE:HD1	1.87	0.40
9:I:14:ILE:HD13	9:I:24:LEU:HB3	2.03	0.40
15:O:141:ILE:HD12	15:O:153:LYS:NZ	2.36	0.40
18:U:66:THR:HG23	18:U:68:GLN:NE2	2.36	0.40
19:V:191:LEU:HA	19:V:238:ARG:HH22	1.85	0.40
19:V:273:GLN:HG2	19:V:274:LYS:HB2	2.03	0.40
20:W:489:LYS:HB3	20:W:489:LYS:HE2	1.91	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	1388/1460 (95%)	1263 (91%)	125 (9%)	0	100	100
2	B	1112/1149 (97%)	1011 (91%)	101 (9%)	0	100	100
3	C	333/335 (99%)	303 (91%)	30 (9%)	0	100	100
4	D	113/161 (70%)	101 (89%)	12 (11%)	0	100	100
5	E	212/215 (99%)	198 (93%)	14 (7%)	0	100	100
6	F	81/155 (52%)	72 (89%)	9 (11%)	0	100	100
7	G	174/212 (82%)	157 (90%)	16 (9%)	1 (1%)	21	59
8	H	136/146 (93%)	121 (89%)	15 (11%)	0	100	100
9	I	32/110 (29%)	25 (78%)	7 (22%)	0	100	100
10	J	65/70 (93%)	57 (88%)	8 (12%)	0	100	100
11	K	99/142 (70%)	93 (94%)	6 (6%)	0	100	100
12	L	43/70 (61%)	40 (93%)	3 (7%)	0	100	100
13	M	155/282 (55%)	143 (92%)	12 (8%)	0	100	100
14	N	100/422 (24%)	89 (89%)	11 (11%)	0	100	100
15	O	528/654 (81%)	497 (94%)	31 (6%)	0	100	100
16	P	93/317 (29%)	84 (90%)	9 (10%)	0	100	100
17	Q	33/251 (13%)	29 (88%)	4 (12%)	0	100	100
18	U	178/240 (74%)	169 (95%)	9 (5%)	0	100	100
19	V	326/596 (55%)	303 (93%)	23 (7%)	0	100	100
20	W	161/594 (27%)	142 (88%)	19 (12%)	0	100	100
All	All	5362/7581 (71%)	4897 (91%)	464 (9%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	79	PRO

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	1214/1257 (97%)	1205 (99%)	9 (1%)	76	80
2	B	975/1006 (97%)	970 (100%)	5 (0%)	81	82
3	C	296/296 (100%)	294 (99%)	2 (1%)	76	80
4	D	110/145 (76%)	110 (100%)	0	100	100
5	E	196/197 (100%)	195 (100%)	1 (0%)	81	82
6	F	73/137 (53%)	73 (100%)	0	100	100
7	G	160/190 (84%)	160 (100%)	0	100	100
8	H	123/128 (96%)	122 (99%)	1 (1%)	73	79
9	I	31/98 (32%)	31 (100%)	0	100	100
10	J	62/65 (95%)	61 (98%)	1 (2%)	55	69
11	K	91/130 (70%)	91 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
13	M	138/249 (55%)	136 (99%)	2 (1%)	59	72
14	N	88/360 (24%)	88 (100%)	0	100	100
15	O	490/593 (83%)	488 (100%)	2 (0%)	84	83
16	P	95/285 (33%)	94 (99%)	1 (1%)	65	75
17	Q	31/212 (15%)	31 (100%)	0	100	100
18	U	152/205 (74%)	149 (98%)	3 (2%)	48	66
19	V	292/513 (57%)	290 (99%)	2 (1%)	76	80
20	W	149/534 (28%)	148 (99%)	1 (1%)	76	80
All	All	4806/6657 (72%)	4776 (99%)	30 (1%)	76	82

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	VAL
1	A	486	LEU
1	A	624	ILE

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Mol	Chain	Res	Type
1	A	645	MET
1	A	848	VAL
1	A	1042	ILE
1	A	1209	ILE
1	A	1215	LEU
1	A	1417	LEU
2	B	154	ILE
2	B	383	LEU
2	B	816	ASP
2	B	881	ILE
2	B	885	MET
3	C	92	ILE
3	C	256	ILE
5	E	88	VAL
8	H	22	LYS
10	J	56	LEU
13	M	78	ILE
13	M	186	ILE
15	O	98	LEU
15	O	516	LEU
16	P	293	ILE
18	U	106	ILE
18	U	157	ILE
18	U	170	ILE
19	V	182	ILE
19	V	237	LEU
20	W	502	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	71	HIS
1	A	147	GLN
1	A	367	ASN
1	A	477	GLN
1	A	533	ASN
1	A	578	GLN
1	A	625	ASN
1	A	630	ASN
1	A	692	ASN
1	A	725	GLN

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Mol	Chain	Res	Type
1	A	757	ASN
1	A	783	ASN
1	A	789	ASN
1	A	805	ASN
1	A	815	GLN
1	A	899	GLN
1	A	934	ASN
1	A	944	ASN
1	A	1058	GLN
1	A	1131	ASN
1	A	1254	ASN
1	A	1262	GLN
1	A	1354	HIS
2	B	66	ASN
2	B	144	HIS
2	B	159	ASN
2	B	217	GLN
2	B	225	HIS
2	B	298	GLN
2	B	299	GLN
2	B	300	GLN
2	B	315	GLN
2	B	321	GLN
2	B	427	ASN
2	B	519	HIS
2	B	574	GLN
2	B	596	GLN
2	B	600	HIS
2	B	655	ASN
2	B	693	HIS
2	B	733	GLN
2	B	753	GLN
2	B	801	HIS
2	B	893	GLN
2	B	928	GLN
2	B	936	GLN
2	B	970	ASN
2	B	1036	HIS
2	B	1136	ASN
2	B	1149	GLN
3	C	99	HIS
3	C	172	GLN

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Mol	Chain	Res	Type
3	C	207	HIS
3	C	234	ASN
3	C	296	ASN
4	D	71	ASN
4	D	130	ASN
5	E	3	GLN
5	E	99	HIS
5	E	153	HIS
5	E	174	GLN
7	G	31	ASN
7	G	113	ASN
8	H	134	ASN
8	H	139	ASN
10	J	53	HIS
11	K	74	ASN
13	M	92	ASN
13	M	128	GLN
13	M	141	ASN
15	O	152	HIS
15	O	154	GLN
15	O	161	GLN
15	O	225	ASN
15	O	332	GLN
15	O	549	GLN
15	O	580	ASN
15	O	584	ASN
15	O	631	ASN
15	O	636	ASN
16	P	189	ASN
16	P	219	GLN
16	P	239	ASN
18	U	68	GLN
18	U	91	ASN
18	U	159	ASN
19	V	6	ASN
19	V	82	ASN
19	V	95	HIS
19	V	114	ASN
19	V	115	ASN
19	V	183	GLN
19	V	473	HIS
20	W	292	ASN

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Mol	Chain	Res	Type
20	W	491	ASN
20	W	499	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

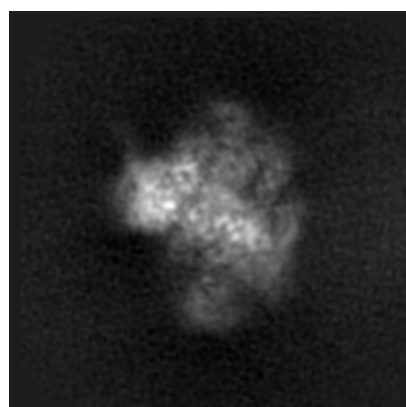
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4182. These allow visual inspection of the internal detail of the map and identification of artifacts.

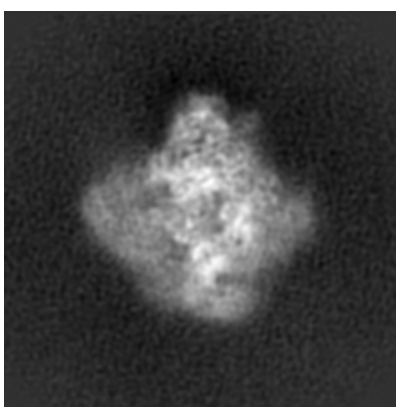
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

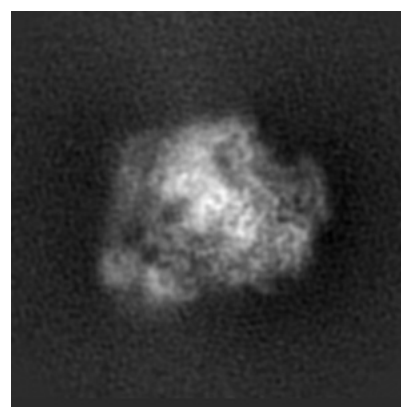
6.1.1 Primary map



X



Y

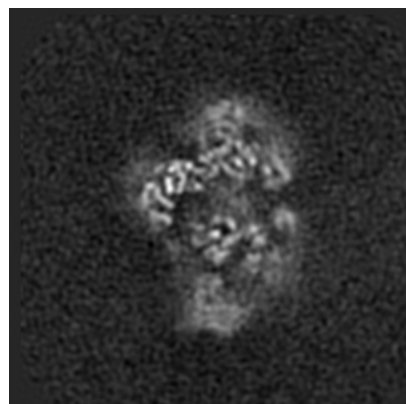


Z

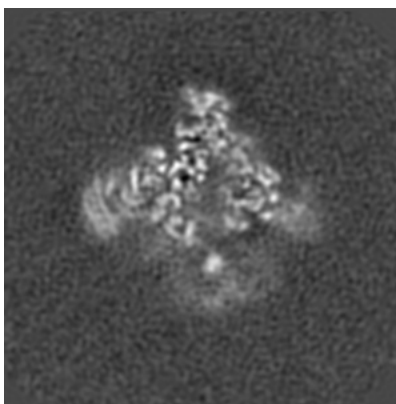
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

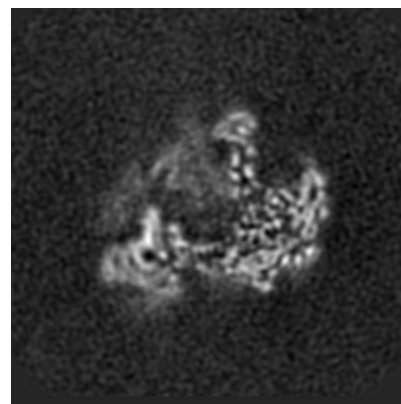
6.2.1 Primary map



X Index: 120



Y Index: 120

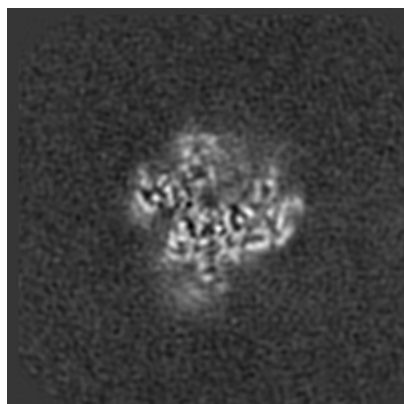


Z Index: 120

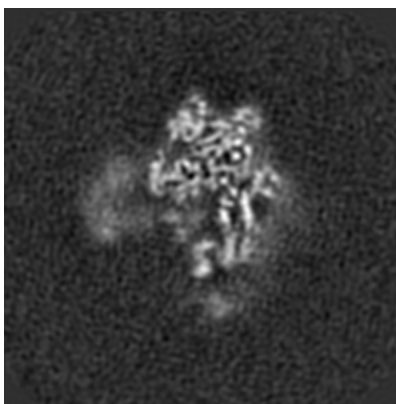
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

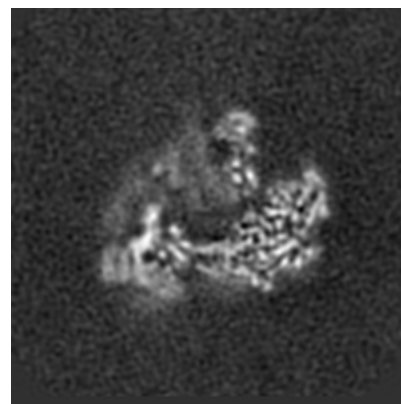
6.3.1 Primary map



X Index: 140



Y Index: 108

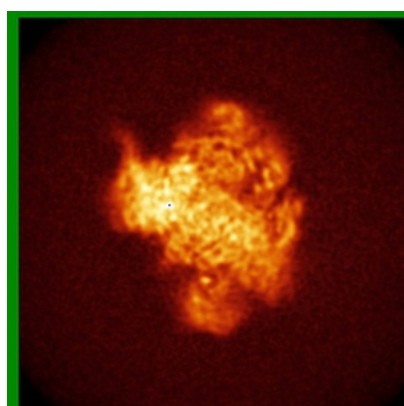


Z Index: 122

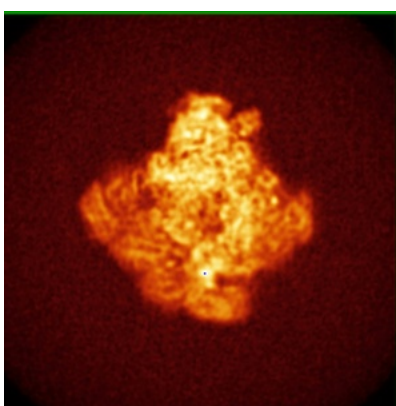
The images above show the largest variance slices of the map in three orthogonal directions.

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

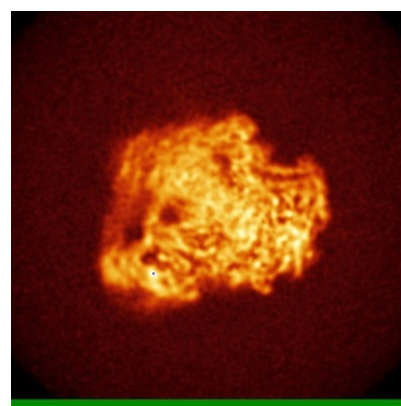
6.4.1 Primary map



X



Y

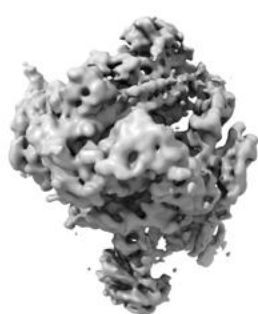


Z

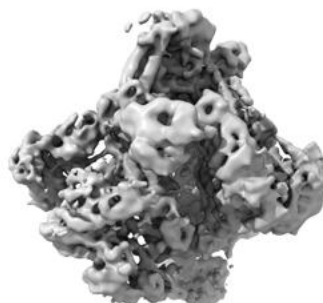
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

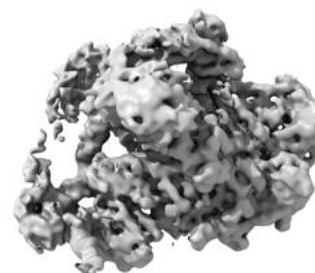
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

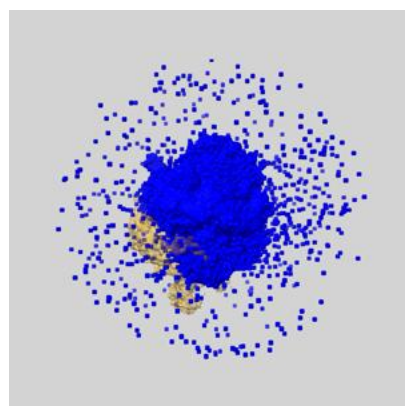
6.6 Mask visualisation [i](#)

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

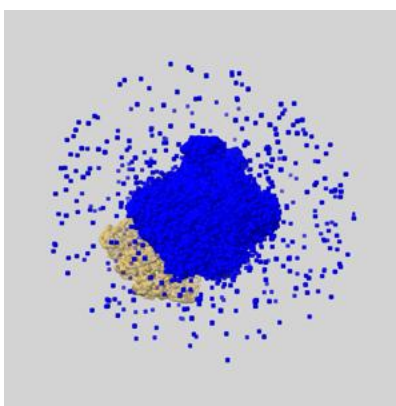
A mask typically either:

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

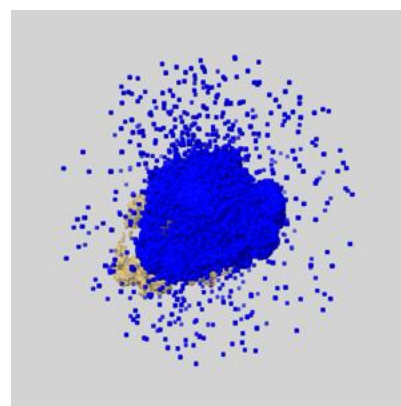
6.6.1 emd_4182_msk_1.map [i](#)



X



Y

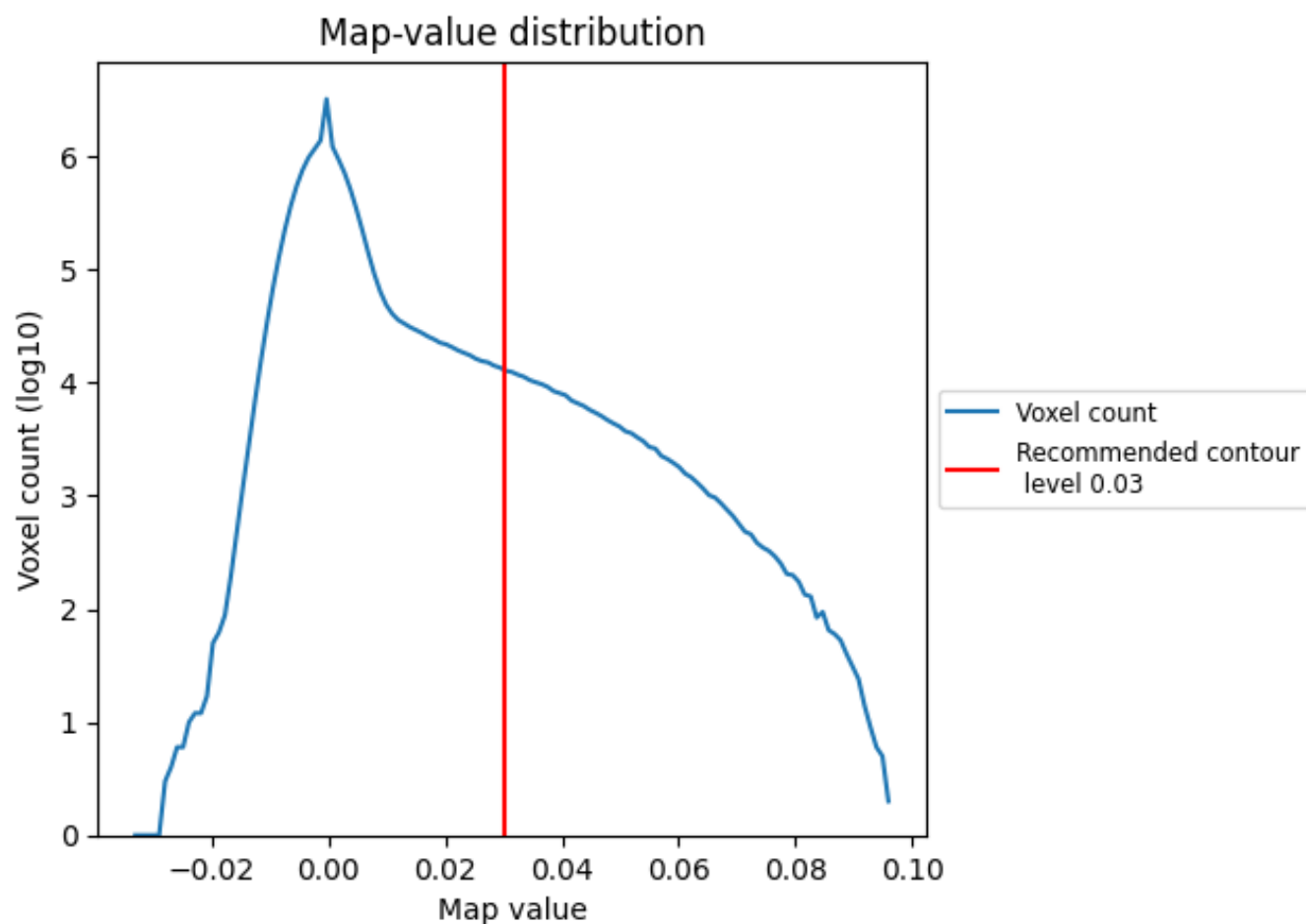


Z

7 Map analysis [i](#)

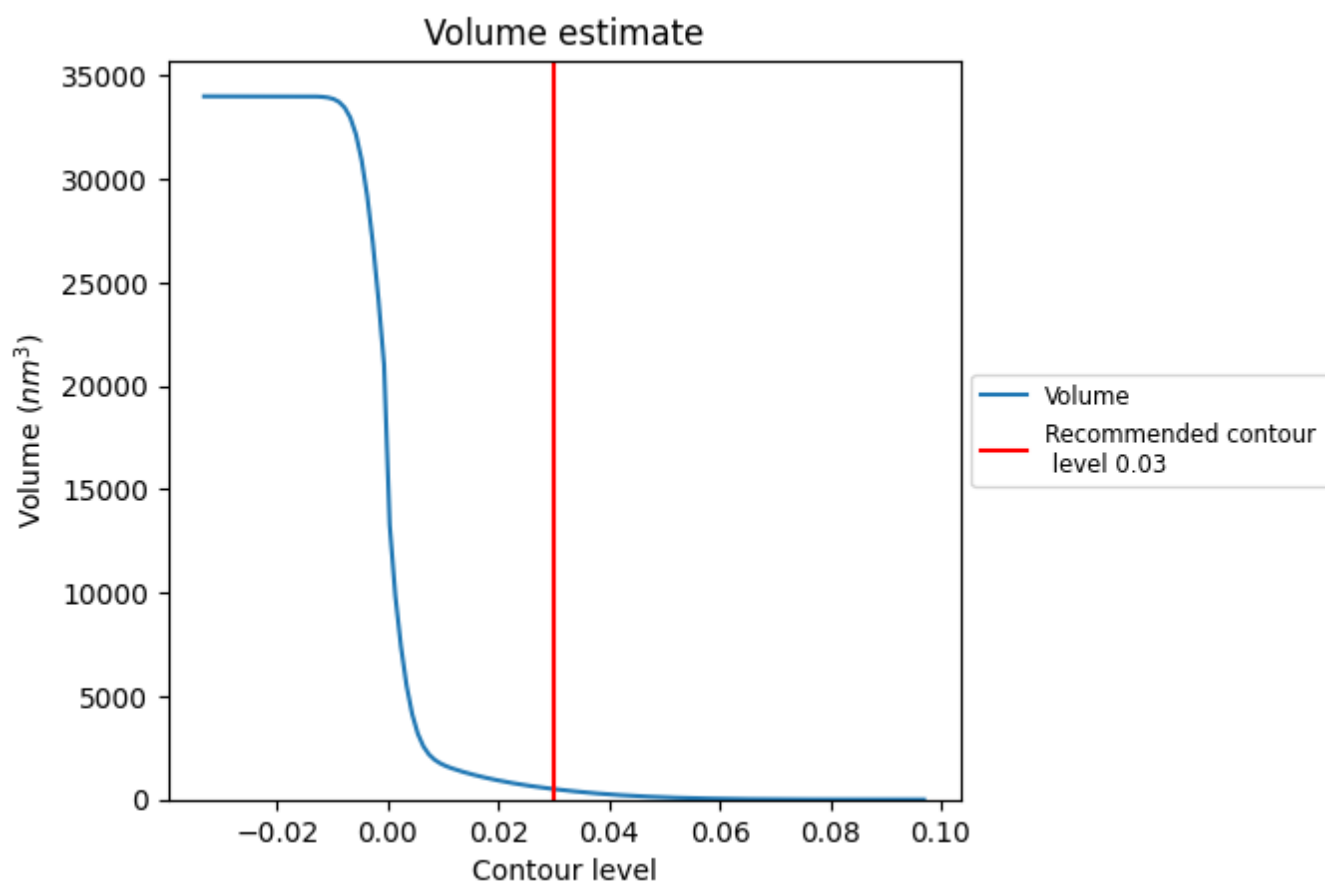
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

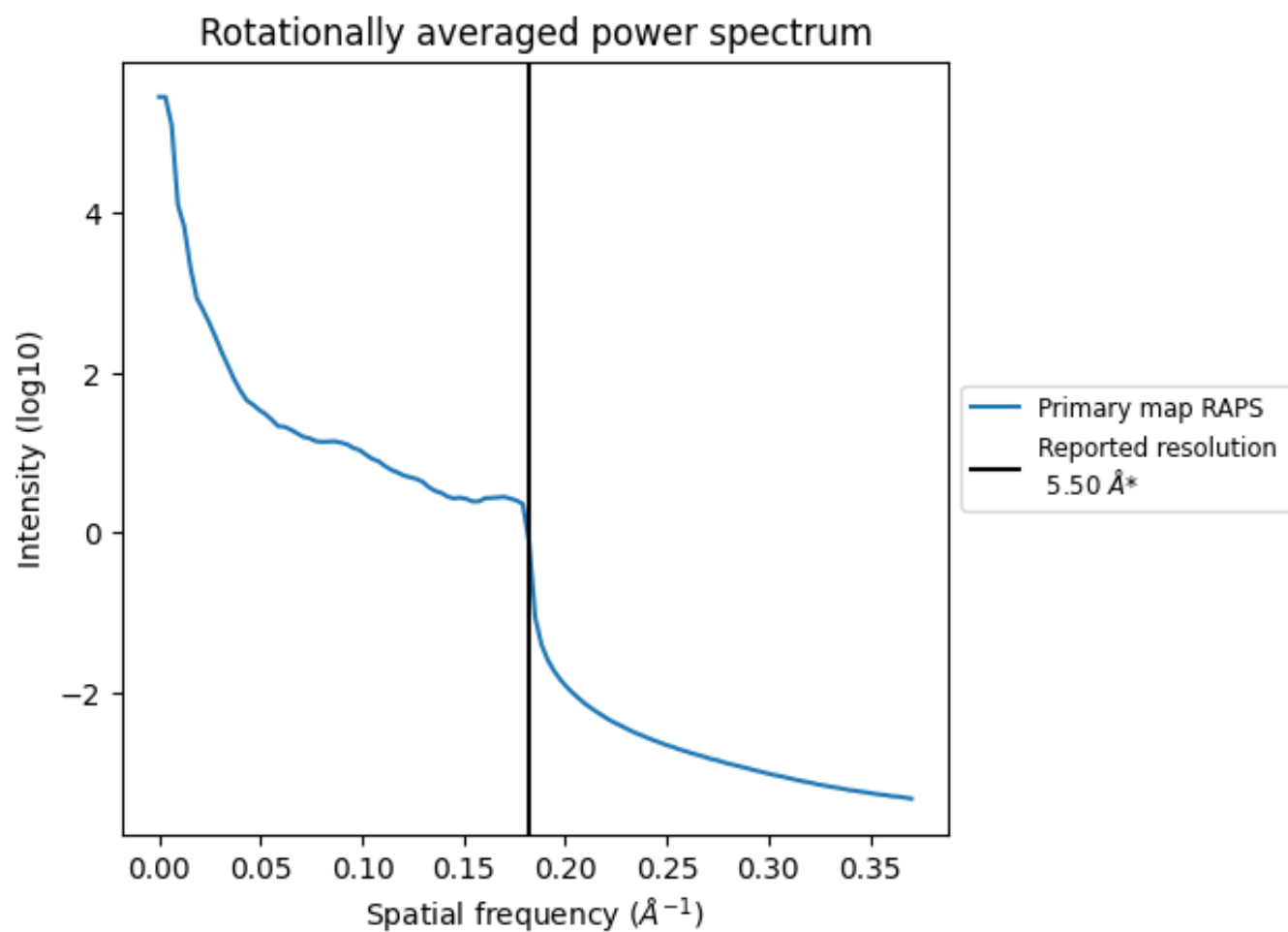
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 510 nm³; this corresponds to an approximate mass of 461 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 ⓘ

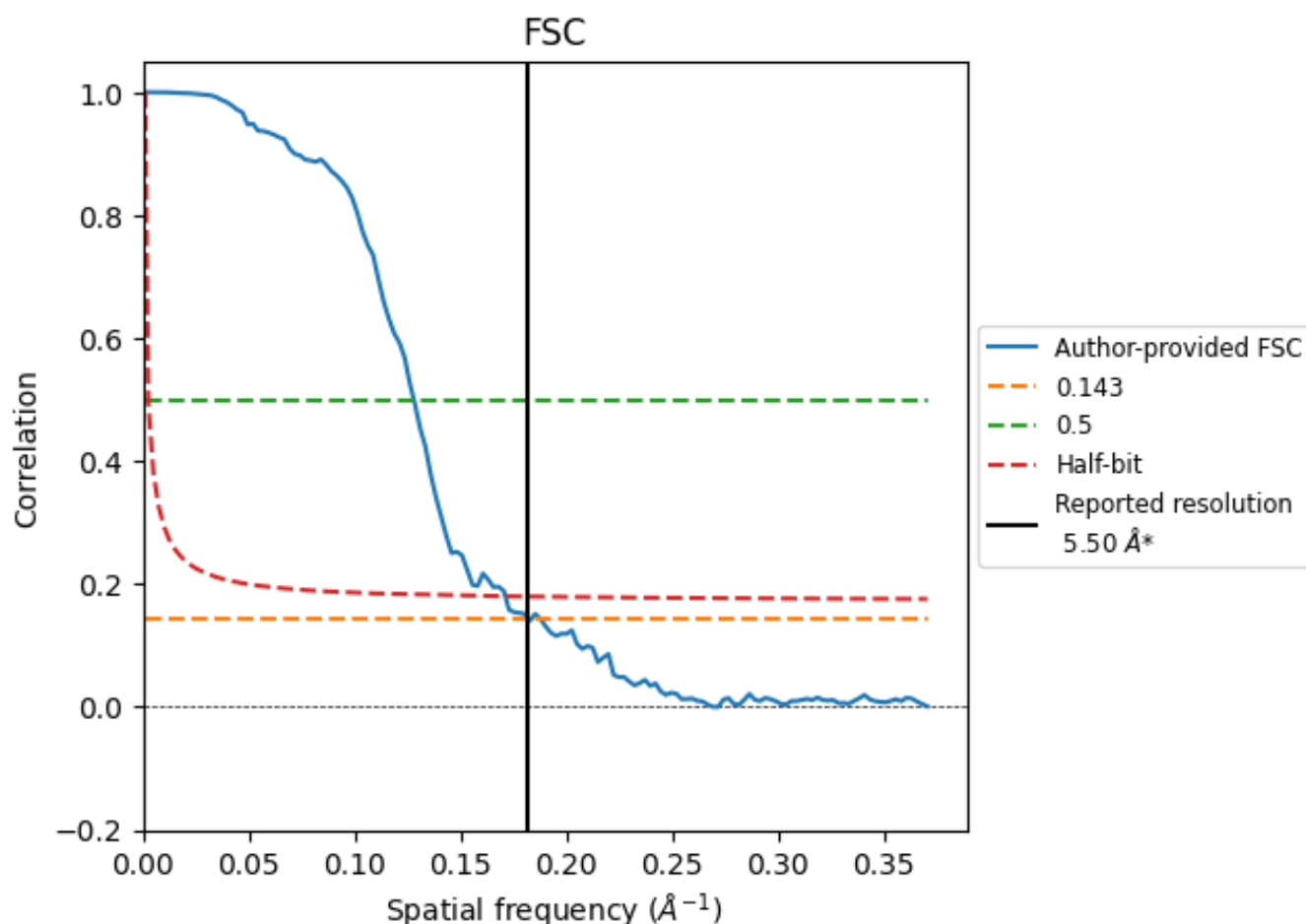


*Reported resolution corresponds to spatial frequency of 0.182 $\text{\AA}^{-1}$

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 0.182 Å⁻¹

8.2 Resolution estimates [i](#)

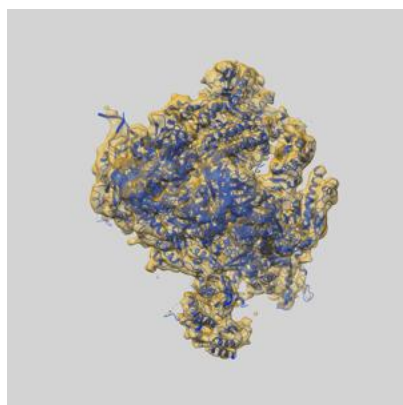
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.50	-	-
Author-provided FSC curve	5.49	7.82	5.85
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

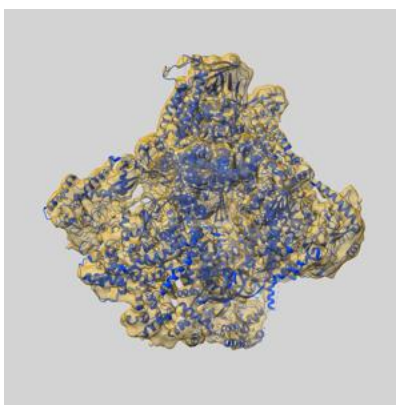
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4182 and PDB model 6F42. Per-residue inclusion information can be found in section 3 on page 8.

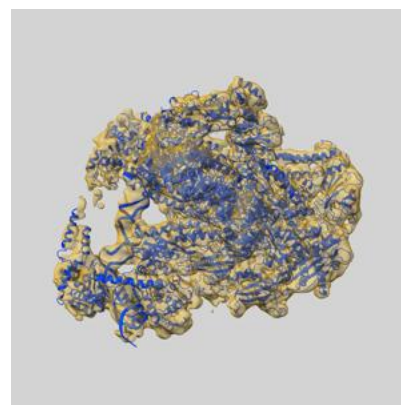
9.1 Map-model overlay [i](#)



X



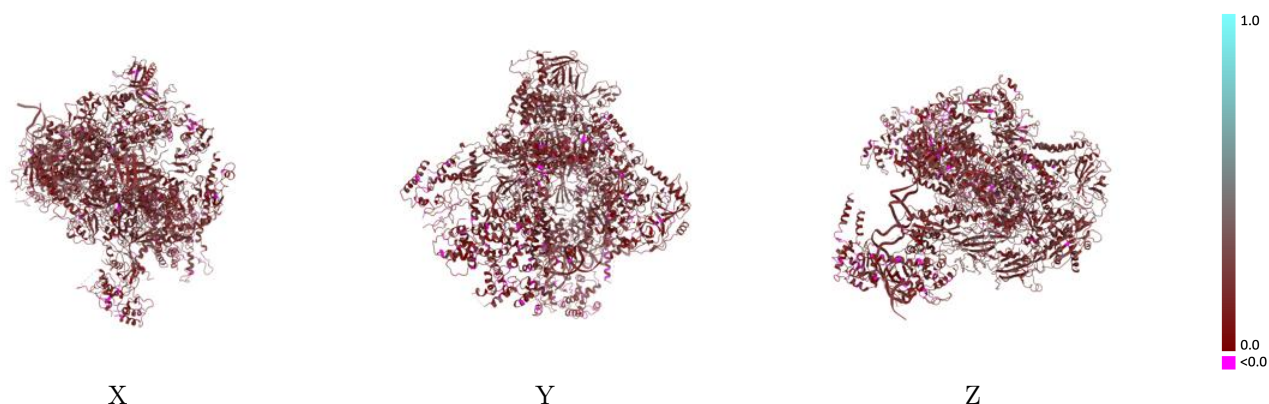
Y



Z

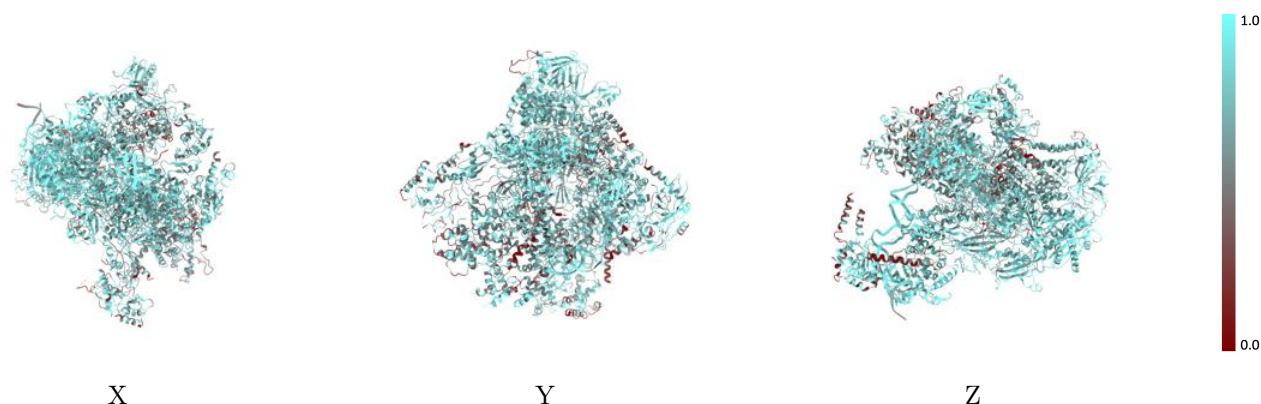
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



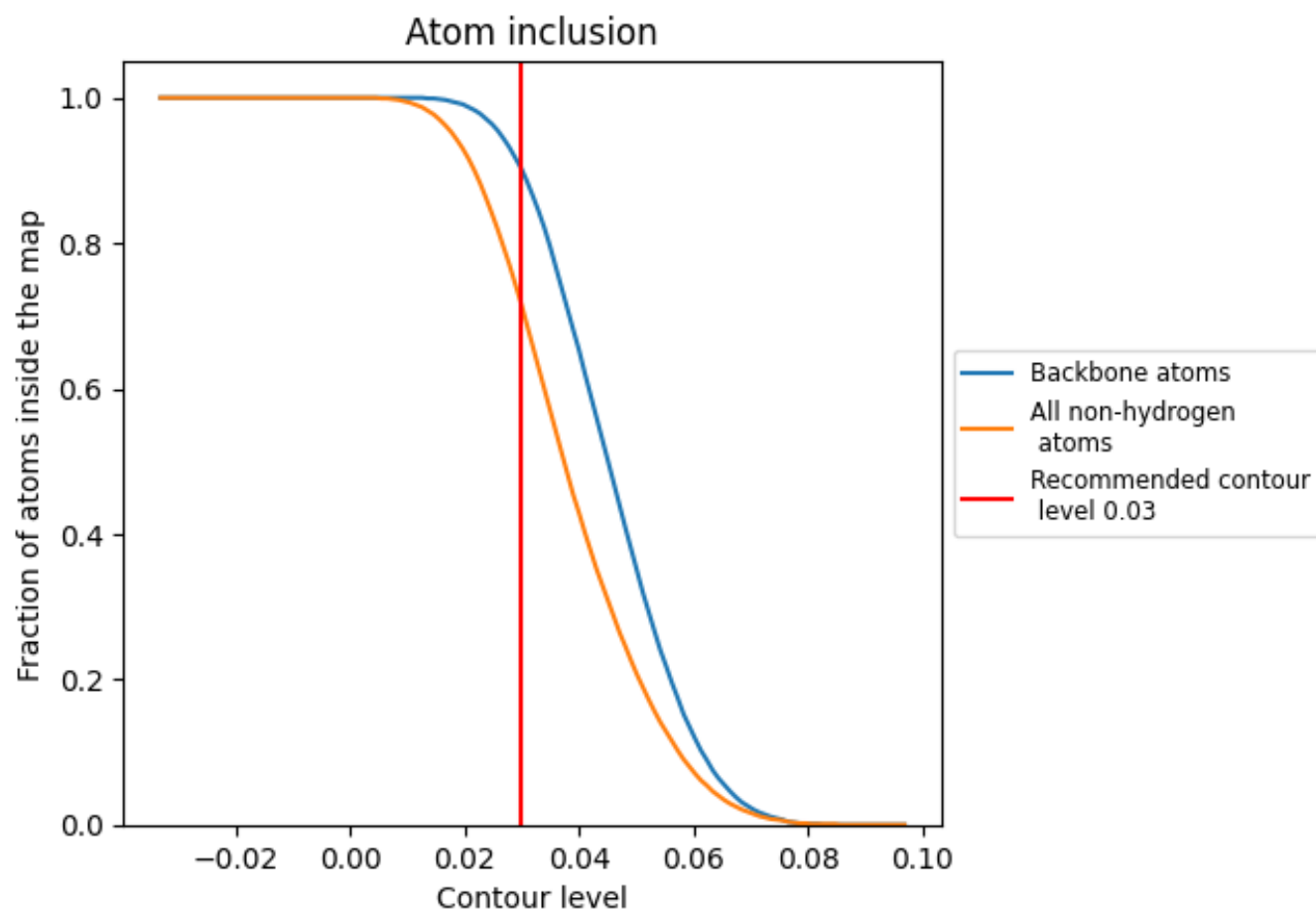
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7150	 0.1940
A	 0.6860	 0.2060
B	 0.7300	 0.2140
C	 0.8590	 0.2270
D	 0.6610	 0.1610
E	 0.7660	 0.1920
F	 0.8240	 0.2250
G	 0.6630	 0.1650
H	 0.8300	 0.2250
I	 0.8610	 0.1940
J	 0.7920	 0.1920
K	 0.8390	 0.2070
L	 0.8120	 0.2300
M	 0.6940	 0.1760
N	 0.7070	 0.1740
O	 0.5810	 0.1560
P	 0.6270	 0.1850
Q	 0.7000	 0.1960
U	 0.8500	 0.1490
V	 0.7010	 0.1690
W	 0.4820	 0.1310
X	 0.8710	 0.2120
Y	 0.8700	 0.2170

