



## Full wwPDB EM Validation Report ⓘ

Apr 28, 2024 – 12:53 AM JST

PDB ID : 8JCH  
EMDB ID : EMD-36162  
Title : Cryo-EM structure of yeast Rat1-bound Pol II pre-termination transcription complex 1 (Pol II Rat1-PTTC1)  
Authors : Zeng, Y.; Zhang, Y.  
Deposited on : 2023-05-11  
Resolution : 2.70 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

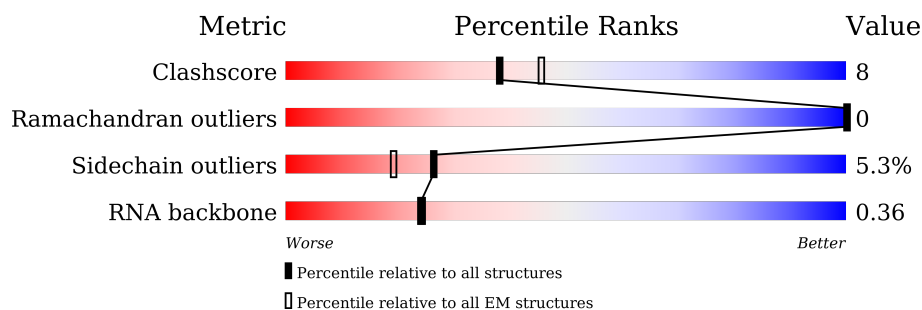
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.70 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.









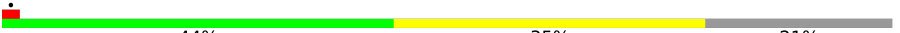




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 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	1259	
3	C	318	
4	D	221	
5	E	215	
6	F	155	
7	G	171	

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Mol	Chain	Length	Quality of chain
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	1019	
14	N	48	
15	O	387	
16	P	23	
17	T	48	
18	W	1063	

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 42732 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1419	Total	C	N	O	S	0	0
			11132	7019	1949	2106	58		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1157	Total	C	N	O	S	0	0
			9193	5819	1604	1714	56		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1225	GLU	-	expression tag	UNP P08518
B	1226	ASN	-	expression tag	UNP P08518
B	1227	LEU	-	expression tag	UNP P08518
B	1228	TYR	-	expression tag	UNP P08518
B	1229	PHE	-	expression tag	UNP P08518
B	1230	GLN	-	expression tag	UNP P08518
B	1231	GLY	-	expression tag	UNP P08518
B	1232	HIS	-	expression tag	UNP P08518
B	1233	HIS	-	expression tag	UNP P08518
B	1234	HIS	-	expression tag	UNP P08518
B	1235	HIS	-	expression tag	UNP P08518
B	1236	HIS	-	expression tag	UNP P08518
B	1237	HIS	-	expression tag	UNP P08518
B	1238	ASP	-	expression tag	UNP P08518
B	1239	TYR	-	expression tag	UNP P08518
B	1240	LYS	-	expression tag	UNP P08518
B	1241	ASP	-	expression tag	UNP P08518
B	1242	HIS	-	expression tag	UNP P08518
B	1243	ASP	-	expression tag	UNP P08518
B	1244	GLY	-	expression tag	UNP P08518
B	1245	ASP	-	expression tag	UNP P08518

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1246	TYR	-	expression tag	UNP P08518
B	1247	LYS	-	expression tag	UNP P08518
B	1248	ASP	-	expression tag	UNP P08518
B	1249	HIS	-	expression tag	UNP P08518
B	1250	ASP	-	expression tag	UNP P08518
B	1251	ILE	-	expression tag	UNP P08518
B	1252	ASP	-	expression tag	UNP P08518
B	1253	TYR	-	expression tag	UNP P08518
B	1254	LYS	-	expression tag	UNP P08518
B	1255	ASP	-	expression tag	UNP P08518
B	1256	ASP	-	expression tag	UNP P08518
B	1257	ASP	-	expression tag	UNP P08518
B	1258	ASP	-	expression tag	UNP P08518
B	1259	LYS	-	expression tag	UNP P08518

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	270	Total	C	N	O	S	0	0
			2125	1336	353	422	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	180	Total	C	N	O	S	0	0
			1455	899	262	292	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1704	1080	305	310	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			670	428	113	126	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	144	Total	C	N	O	S	0	0
			1104	695	184	221	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	115	Total	C	N	O	S	0	0
			871	542	147	171	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	66	Total	C	N	O	S	0	0
			540	345	94	95	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	111	Total	C	N	O	S	0	0
			895	575	152	166	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			364	224	72	64	4		

- Molecule 13 is a protein called 5'-3' exoribonuclease 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	721	Total	C	N	O	S	0	0
			5834	3756	994	1059	25		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-12	MET	-	initiating methionine	UNP Q02792
M	-11	GLY	-	expression tag	UNP Q02792
M	-10	SER	-	expression tag	UNP Q02792
M	-9	SER	-	expression tag	UNP Q02792
M	-8	HIS	-	expression tag	UNP Q02792
M	-7	HIS	-	expression tag	UNP Q02792
M	-6	HIS	-	expression tag	UNP Q02792
M	-5	HIS	-	expression tag	UNP Q02792
M	-4	HIS	-	expression tag	UNP Q02792
M	-3	HIS	-	expression tag	UNP Q02792
M	-2	SER	-	expression tag	UNP Q02792
M	-1	GLN	-	expression tag	UNP Q02792
M	0	ASP	-	expression tag	UNP Q02792

- Molecule 14 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	38	Total	C	N	O	P	0	0
			787	375	141	233	38		

- Molecule 15 is a protein called Decapping nuclease RAI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	350	Total	C	N	O	S	0	0
			2880	1841	487	544	8		

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	23	Total	C	N	O	P	0	0
			493	220	90	160	23		

- Molecule 17 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	38	Total	C	N	O	P	0	0
			769	367	137	227	38		

- Molecule 18 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	W	71	Total	C	N	O	0	0
			565	349	111	105		

- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 20 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

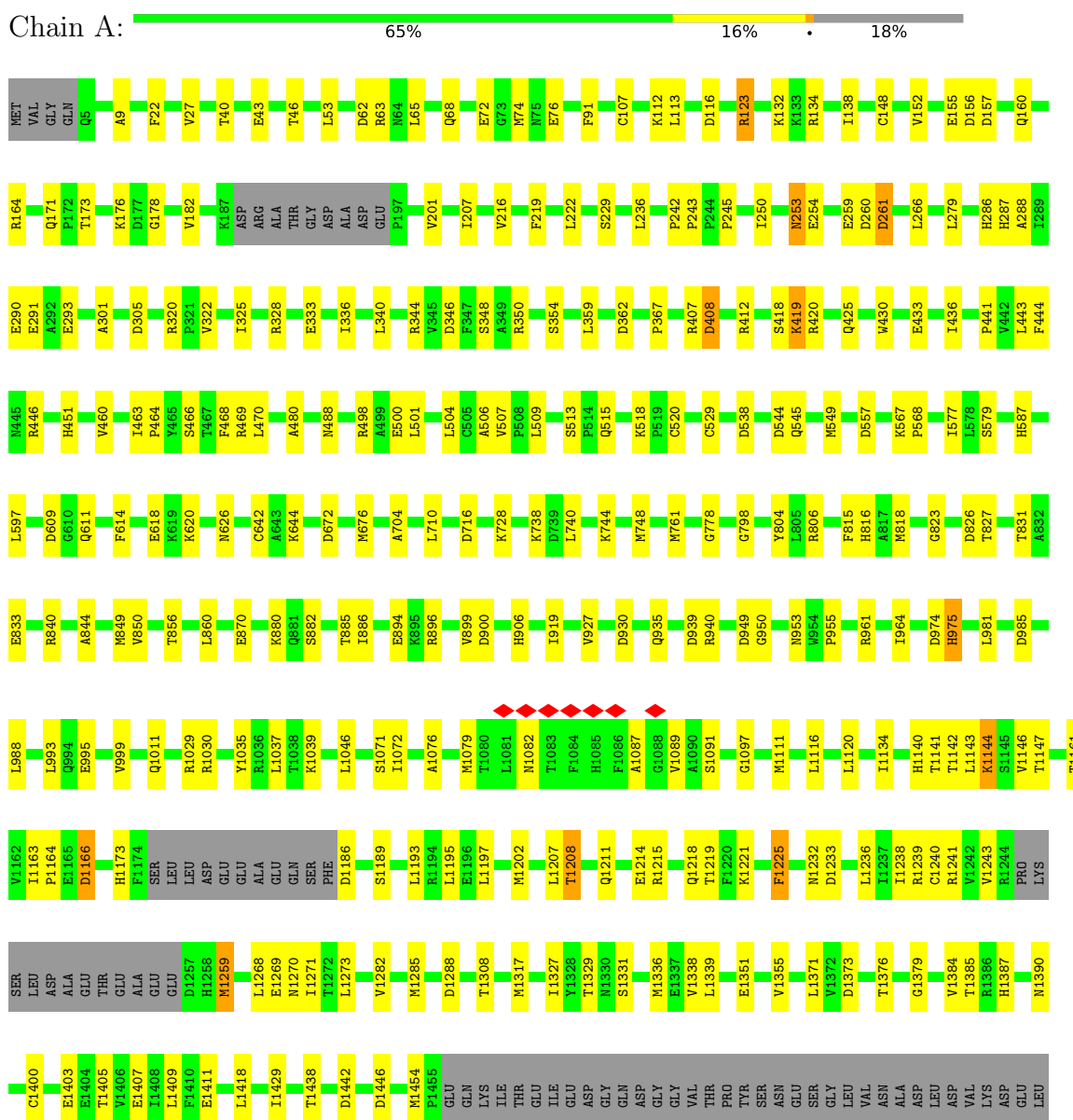
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total 1	Mg 1	0
20	M	1	Total 1	Mg 1	0
20	O	1	Total 1	Mg 1	0



### 3 Residue-property plots [i](#)

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

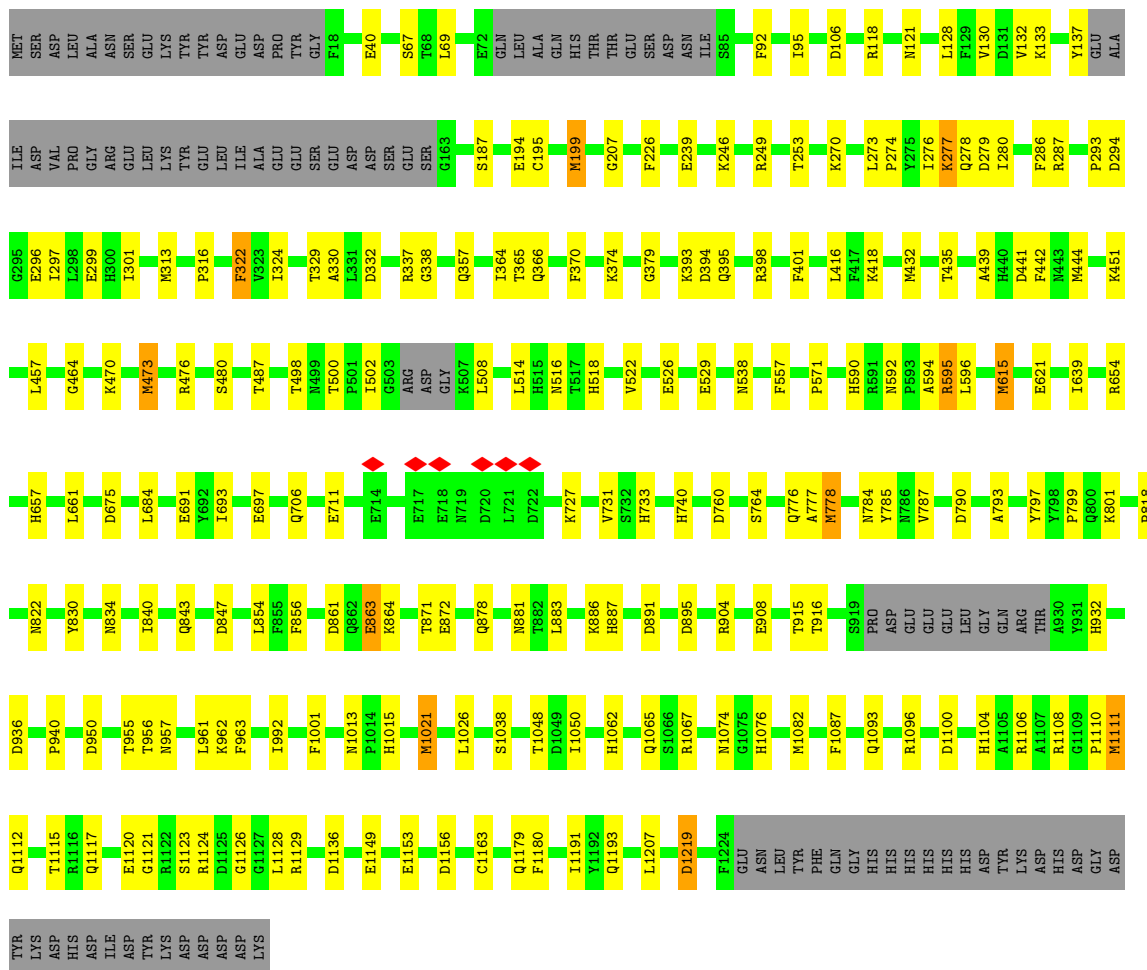
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



[illegible]

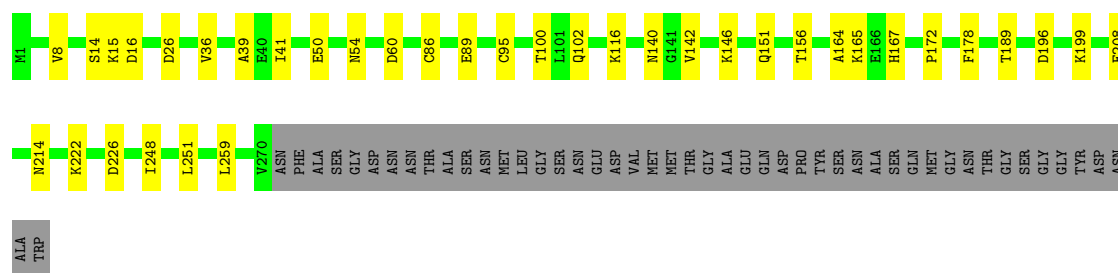
- Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:  76% 15% 8%

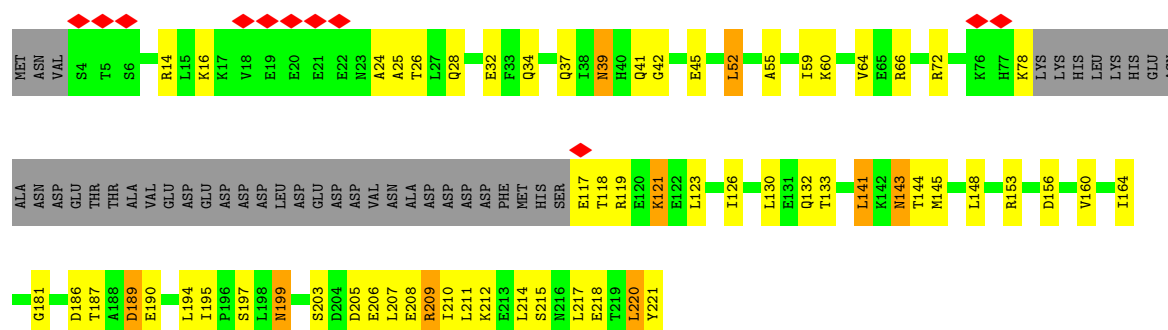


- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

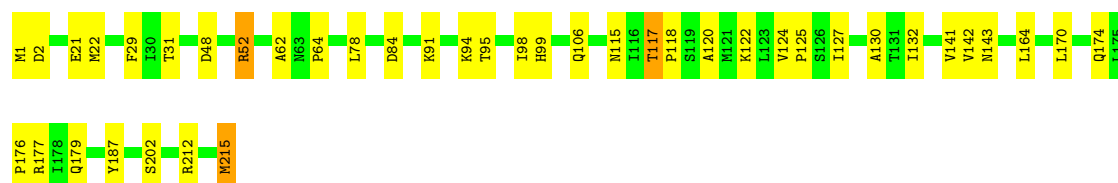
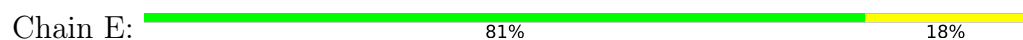
Chain C:  73% 12% 15%



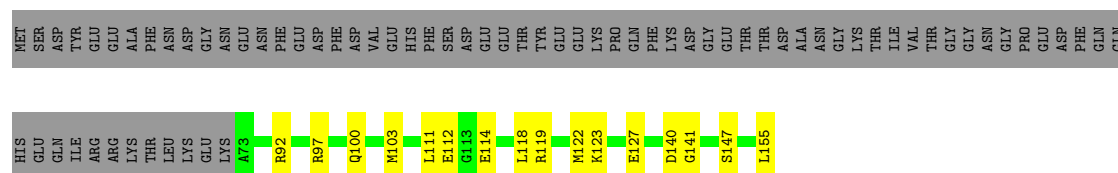
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4



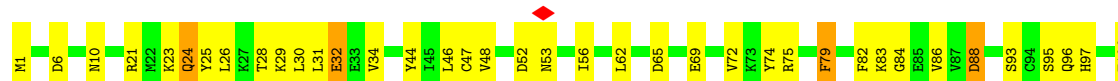
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



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



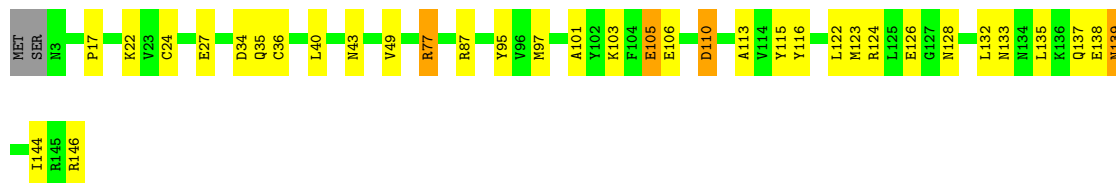
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7





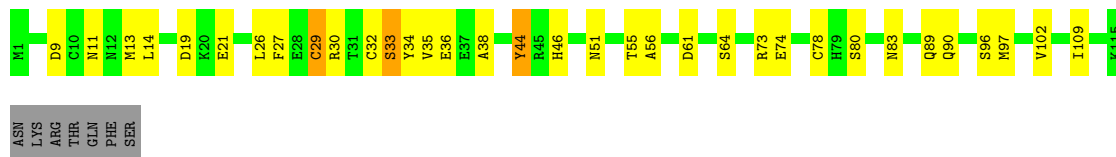
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 75% 21%



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

Chain I: 66% 25% 6%



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

Chain J: 71% 23% 6%



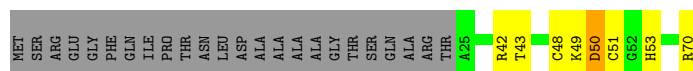
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K: 71% 21% 8%



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

Chain L: 54% 10% 34%

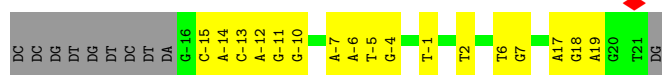


- Molecule 13: 5'-3' exoribonuclease 2

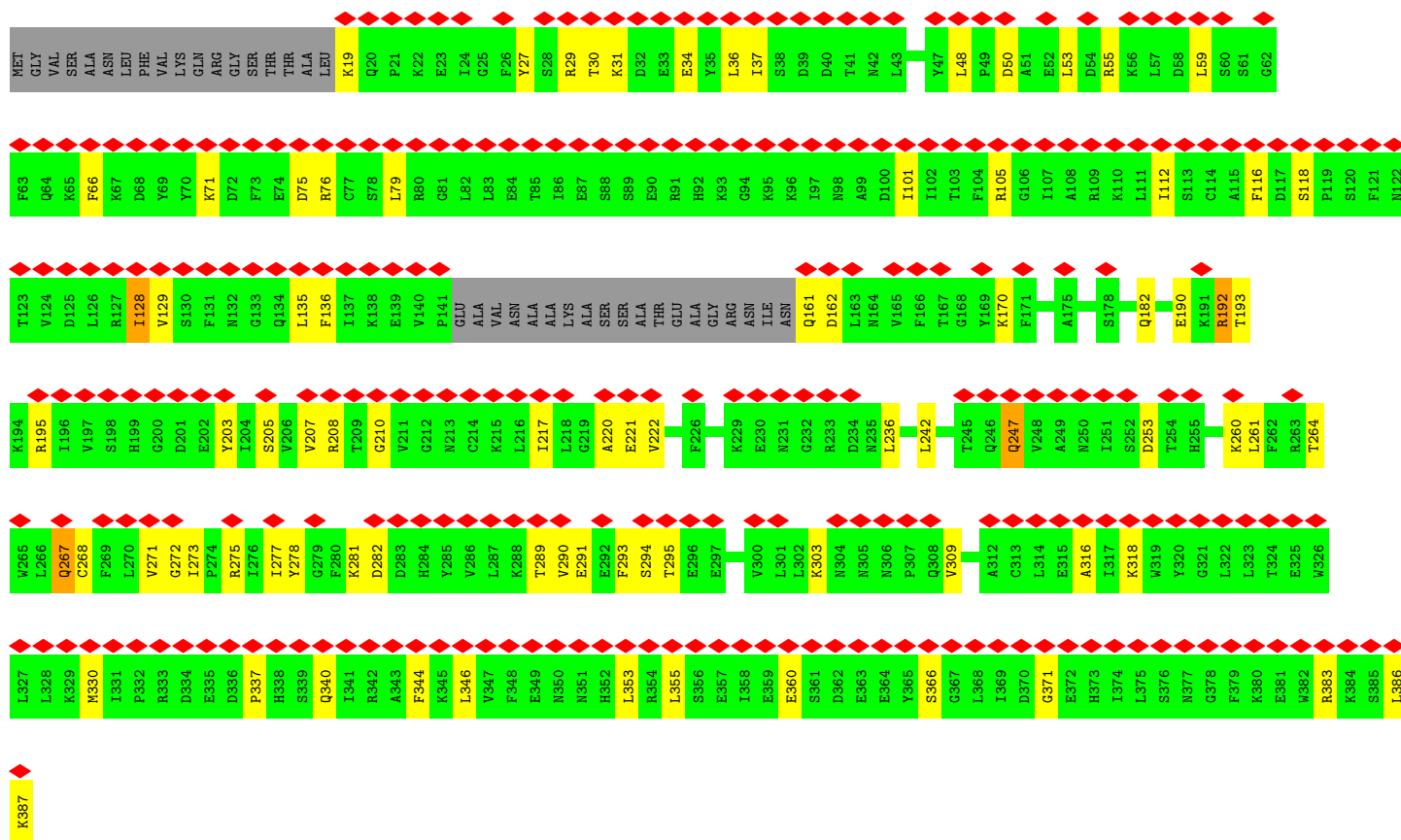
Chain M: 34% 51% 18% 29%



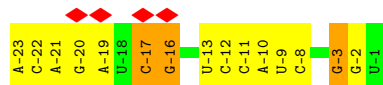
- Molecule 14: DNA (38-MER)



- Molecule 15: Decapping nuclease RAI1



- Molecule 16: RNA



- Molecule 17: DNA (38-MER)





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	416223	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.352	Depositor
Minimum map value	-0.895	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.15	Depositor
Map size ( $\text{\AA}$ )	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.1, 1.1, 1.1	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	0.25	0/11334	0.48	0/15335
2	B	0.25	0/9376	0.50	0/12647
3	C	0.24	0/2163	0.44	0/2930
4	D	0.24	0/1466	0.53	0/1963
5	E	0.25	0/1739	0.51	0/2347
6	F	0.24	0/682	0.54	0/922
7	G	0.27	0/1368	0.54	0/1844
8	H	0.26	0/1123	0.54	0/1529
9	I	0.26	0/889	0.53	0/1207
10	J	0.27	0/549	0.57	0/738
11	K	0.25	0/913	0.44	0/1232
12	L	0.27	0/366	0.64	0/485
13	M	0.27	0/5991	0.49	0/8129
14	N	0.50	0/882	0.92	0/1362
15	O	0.24	0/2941	0.47	0/3963
16	P	0.29	0/551	0.93	0/857
17	T	0.54	0/860	0.90	0/1322
18	W	0.22	0/571	0.52	0/762
All	All	0.27	0/43764	0.53	0/59574

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	11132	0	11172	181	0
2	B	9193	0	9182	117	0
3	C	2125	0	2090	25	0
4	D	1455	0	1477	41	0
5	E	1704	0	1687	20	0
6	F	670	0	688	10	0
7	G	1340	0	1357	32	0
8	H	1104	0	1047	19	0
9	I	871	0	777	18	0
10	J	540	0	553	11	0
11	K	895	0	903	18	0
12	L	364	0	386	5	0
13	M	5834	0	5727	135	0
14	N	787	0	432	15	0
15	O	2880	0	2849	47	0
16	P	493	0	248	16	0
17	T	769	0	428	18	0
18	W	565	0	580	3	0
19	A	2	0	0	0	0
19	B	1	0	0	0	0
19	C	1	0	0	0	0
19	I	2	0	0	0	0
19	J	1	0	0	0	0
19	L	1	0	0	0	0
20	A	1	0	0	0	0
20	M	1	0	0	0	0
20	O	1	0	0	0	0
All	All	42732	0	41583	678	0

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

All (678) 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:M:107:ARG:HG2	13:M:652:PHE:HB3	1.58	0.86
13:M:110:MET:HE2	13:M:685:GLN:HG3	1.63	0.81
13:M:615:VAL:HG23	13:M:620:ILE:HG22	1.66	0.77
8:H:35:GLN:N	8:H:35:GLN:OE1	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:113:GLN:HG3	13:M:116:ARG:HH22	1.53	0.73
2:B:1120:GLU:N	2:B:1120:GLU:OE2	2.22	0.73
13:M:732:TRP:CH2	16:P:-21:A:H2'	2.23	0.72
2:B:239:GLU:OE2	2:B:239:GLU:N	2.22	0.72
2:B:799:PRO:HB2	2:B:818:PRO:HG2	1.71	0.72
2:B:95:ILE:HD11	2:B:128:LEU:HD12	1.71	0.72
15:O:182:GLN:OE1	15:O:182:GLN:N	2.21	0.71
5:E:29:PHE:HB2	5:E:64:PRO:HG3	1.73	0.71
1:A:1215:ARG:HG2	1:A:1273:LEU:HA	1.73	0.71
14:N:19:DA:N1	17:T:-18:DC:N4	2.40	0.69
1:A:333:GLU:OE2	1:A:333:GLU:N	2.26	0.69
2:B:195:CYS:HB2	2:B:784:ASN:HB2	1.74	0.69
2:B:270:LYS:HB3	2:B:279:ASP:HB3	1.76	0.68
1:A:1195:LEU:HB2	1:A:1238:ILE:HB	1.76	0.68
13:M:874:ALA:HA	13:M:877:LEU:HD12	1.74	0.67
14:N:-5:DT:H4'	14:N:-4:DG:H5'	1.77	0.67
13:M:51:TYR:HB3	13:M:208:ILE:HD12	1.77	0.67
2:B:199:MET:SD	2:B:199:MET:N	2.68	0.67
15:O:105:ARG:HG2	15:O:267:GLN:HE22	1.60	0.66
7:G:44:TYR:HB2	7:G:79:PHE:HB3	1.77	0.66
13:M:869:GLU:HG3	13:M:909:LYS:HE2	1.77	0.66
1:A:1329:THR:HG22	1:A:1331:SER:H	1.60	0.66
1:A:961:ARG:HH11	1:A:961:ARG:HG3	1.61	0.66
12:L:49:LYS:HE3	12:L:49:LYS:HA	1.78	0.65
13:M:12:ARG:NH1	16:P:-17:C:O2	2.30	0.65
13:M:725:MET:SD	13:M:737:LEU:HB2	2.37	0.65
13:M:210:ASN:OD1	13:M:213:ARG:NH2	2.30	0.64
1:A:618:GLU:N	1:A:618:GLU:OE1	2.30	0.64
1:A:975:HIS:O	1:A:975:HIS:ND1	2.30	0.64
2:B:654:ARG:H	2:B:657:HIS:HD2	1.44	0.64
2:B:776:GLN:HE22	16:P:-2:G:H5'	1.62	0.64
1:A:1141:THR:HG22	1:A:1142:THR:H	1.63	0.64
1:A:804:TYR:HH	1:A:816:HIS:HE2	1.43	0.64
1:A:1407:GLU:N	1:A:1407:GLU:OE1	2.29	0.64
13:M:49:ASN:ND2	13:M:51:TYR:OH	2.31	0.64
1:A:544:ASP:N	1:A:544:ASP:OD1	2.31	0.64
7:G:88:ASP:OD1	7:G:88:ASP:N	2.31	0.64
2:B:277:LYS:H	2:B:277:LYS:HD2	1.64	0.63
1:A:157:ASP:HB2	1:A:160:GLN:HE21	1.64	0.63
14:N:-11:DG:H2'	14:N:-10:DG:C8	2.34	0.62
15:O:192:ARG:HG2	15:O:195:ARG:HD2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:729:LYS:HG2	13:M:733:GLN:HB3	1.81	0.62
2:B:908:GLU:N	2:B:908:GLU:OE2	2.31	0.62
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.81	0.62
2:B:278:GLN:HE21	2:B:337:ARG:HD2	1.65	0.62
1:A:62:ASP:OD1	1:A:63:ARG:N	2.32	0.62
2:B:287:ARG:NH1	2:B:324:ILE:O	2.32	0.62
13:M:632:ILE:HD11	13:M:670:LEU:HD23	1.80	0.62
17:T:-1:DT:H2'	17:T:0:DA:H8	1.65	0.62
4:D:164:ILE:HD12	4:D:164:ILE:H	1.65	0.62
14:N:18:DG:O6	14:N:19:DA:N6	2.33	0.62
1:A:123:ARG:HH22	1:A:155:GLU:HG2	1.65	0.61
17:T:7:DG:H2'	17:T:8:DA:C8	2.36	0.61
2:B:621:GLU:N	2:B:621:GLU:OE1	2.34	0.61
13:M:886:ASN:HD21	16:P:-16:G:H4'	1.65	0.61
1:A:1076:ALA:HA	1:A:1079:MET:HE2	1.81	0.61
1:A:464:PRO:HB2	11:K:4:PRO:HG3	1.83	0.60
7:G:24:GLN:O	7:G:28:THR:HG23	2.02	0.60
8:H:27:GLU:N	8:H:27:GLU:OE2	2.34	0.60
13:M:105:ALA:HB3	13:M:110:MET:SD	2.41	0.60
13:M:732:TRP:HH2	16:P:-21:A:H2'	1.66	0.60
2:B:1048:THR:HG23	2:B:1050:ILE:H	1.65	0.60
8:H:22:LYS:O	8:H:43:ASN:ND2	2.34	0.60
15:O:27:TYR:HH	15:O:29:ARG:HH11	1.50	0.60
17:T:-1:DT:H2'	17:T:0:DA:C8	2.36	0.59
17:T:-18:DC:H6	17:T:-18:DC:H5'	1.66	0.59
3:C:151:GLN:HE21	10:J:65:PRO:HB3	1.67	0.59
13:M:617:PRO:O	13:M:620:ILE:HG13	2.02	0.59
1:A:182:VAL:HG12	1:A:201:VAL:HG22	1.85	0.59
1:A:113:LEU:O	1:A:164:ARG:NH2	2.36	0.59
2:B:883:LEU:HD22	2:B:932:HIS:HB3	1.85	0.59
1:A:823:GLY:O	1:A:827:THR:HG23	2.02	0.59
1:A:433:GLU:OE2	2:B:1108:ARG:NH2	2.36	0.59
3:C:26:ASP:OD2	3:C:26:ASP:N	2.34	0.58
4:D:186:ASP:O	4:D:212:LYS:NZ	2.36	0.58
13:M:330:CYS:HA	13:M:341:LEU:HD23	1.85	0.58
2:B:957:ASN:HD21	2:B:961:LEU:HB2	1.68	0.58
13:M:19:SER:HB3	13:M:291:TRP:HB2	1.84	0.58
13:M:705:LEU:HD13	13:M:753:GLN:HE21	1.68	0.58
15:O:291:GLU:OE1	15:O:293:PHE:N	2.32	0.58
13:M:232:LEU:HA	13:M:252:ARG:HD3	1.85	0.58
8:H:105:GLU:HG2	8:H:113:ALA:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:ASP:N	1:A:672:ASP:OD1	2.37	0.58
2:B:296:GLU:OE1	9:I:11:ASN:ND2	2.37	0.58
13:M:680:PHE:HZ	13:M:743:GLN:HE22	1.52	0.58
15:O:268:CYS:O	15:O:272:GLY:N	2.35	0.58
1:A:831:THR:HG23	17:T:-1:DT:H72	1.86	0.58
13:M:381:LEU:HD22	13:M:664:PHE:HB3	1.85	0.58
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.86	0.58
13:M:107:ARG:O	13:M:110:MET:HB2	2.04	0.58
13:M:117:ARG:HH11	13:M:158:ASN:HA	1.69	0.57
13:M:122:ARG:NH1	13:M:721:PHE:O	2.37	0.57
3:C:100:THR:HG22	3:C:156:THR:HG23	1.86	0.57
1:A:1214:GLU:O	1:A:1218:GLN:NE2	2.38	0.57
2:B:286:PHE:HB3	2:B:297:ILE:HD12	1.87	0.57
1:A:219:PHE:HA	1:A:222:LEU:HB2	1.86	0.57
7:G:29:LYS:HA	7:G:29:LYS:HE2	1.87	0.57
1:A:587:HIS:HD2	1:A:609:ASP:H	1.52	0.57
9:I:44:TYR:HE2	9:I:46:HIS:HB2	1.69	0.57
1:A:1161:THR:HG21	1:A:1239:ARG:HH21	1.70	0.57
13:M:147:ASP:OD1	13:M:147:ASP:N	2.36	0.57
1:A:1146:VAL:HG23	1:A:1197:LEU:HD22	1.86	0.57
1:A:1269:GLU:OE1	1:A:1270:ASN:ND2	2.38	0.57
10:J:14:VAL:HG12	10:J:17:LYS:HG3	1.87	0.57
6:F:97:ARG:NH1	6:F:100:GLN:OE1	2.38	0.57
13:M:339:PRO:HG2	13:M:660:LEU:HD22	1.87	0.57
15:O:205:SER:O	15:O:220:ALA:N	2.38	0.57
1:A:1376:THR:O	5:E:212:ARG:NH2	2.38	0.56
2:B:881:ASN:OD1	2:B:881:ASN:N	2.38	0.56
15:O:340:GLN:NE2	15:O:360:GLU:OE2	2.38	0.56
1:A:91:PHE:HZ	1:A:207:ILE:HD12	1.70	0.56
13:M:122:ARG:NH1	13:M:720:GLU:OE2	2.38	0.56
1:A:107:CYS:SG	1:A:171:GLN:NE2	2.78	0.56
1:A:350:ARG:NH1	1:A:488:ASN:OD1	2.37	0.56
1:A:1390:ASN:HD21	1:A:1403:GLU:CD	2.09	0.56
7:G:100:GLU:OE2	7:G:100:GLU:N	2.38	0.56
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.87	0.56
3:C:165:LYS:HG2	11:K:9:LEU:HD11	1.88	0.56
8:H:110:ASP:OD1	8:H:110:ASP:N	2.36	0.56
13:M:615:VAL:HB	13:M:619:ASP:HB3	1.88	0.56
7:G:111:THR:HB	7:G:114:LEU:HD23	1.86	0.56
4:D:55:ALA:O	4:D:59:ILE:HG22	2.05	0.56
3:C:214:ASN:OD1	3:C:214:ASN:N	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:518:HIS:HB3	2:B:522:VAL:HG22	1.88	0.55
2:B:529:GLU:CD	2:B:529:GLU:H	2.08	0.55
1:A:579:SER:HB3	1:A:611:GLN:HA	1.88	0.55
1:A:1225:PHE:O	1:A:1241:ARG:N	2.39	0.55
2:B:639:ILE:HD11	2:B:691:GLU:HB3	1.88	0.55
15:O:53:LEU:HD11	15:O:290:VAL:HB	1.88	0.55
11:K:10:PHE:HA	11:K:37:LYS:HB3	1.88	0.55
1:A:336:ILE:HD12	1:A:1405:THR:HG21	1.89	0.55
2:B:955:THR:HG23	2:B:963:PHE:HB3	1.89	0.55
12:L:42:ARG:HG3	12:L:42:ARG:HH11	1.71	0.55
1:A:896:ARG:HD3	1:A:1030:ARG:HD3	1.87	0.55
3:C:196:ASP:HB3	3:C:199:LYS:HG3	1.88	0.55
1:A:76:GLU:N	1:A:76:GLU:OE1	2.38	0.55
15:O:337:PRO:HG2	15:O:387:LYS:HB2	1.88	0.55
2:B:1082:MET:HG2	3:C:189:THR:HA	1.89	0.55
13:M:71:GLU:HB2	13:M:75:GLU:HB2	1.87	0.55
14:N:6:DT:H2'	14:N:7:DG:C8	2.42	0.55
1:A:545:GLN:O	1:A:549:MET:HG3	2.07	0.54
5:E:177:ARG:HB3	5:E:215:MET:HG2	1.88	0.54
13:M:332:ASN:HD21	13:M:335:LEU:HB2	1.71	0.54
2:B:370:PHE:HB2	2:B:374:LYS:HE3	1.88	0.54
4:D:132:GLN:NE2	4:D:133:THR:OG1	2.40	0.54
13:M:816:ASP:HB2	13:M:846:MET:HA	1.88	0.54
13:M:730:MET:SD	13:M:730:MET:N	2.81	0.54
9:I:26:LEU:HD12	9:I:35:VAL:HG13	1.90	0.54
9:I:29:CYS:SG	9:I:30:ARG:N	2.80	0.54
13:M:108:ALA:O	13:M:112:GLN:HG2	2.06	0.54
4:D:60:LYS:O	4:D:64:VAL:HG22	2.08	0.54
7:G:29:LYS:HE2	7:G:32:GLU:OE1	2.07	0.54
1:A:43:GLU:O	1:A:46:THR:OG1	2.24	0.54
7:G:56:ILE:HG12	7:G:72:VAL:HG12	1.89	0.54
10:J:32:GLU:N	10:J:32:GLU:OE2	2.41	0.54
13:M:162:PRO:HB3	13:M:198:ALA:HB1	1.90	0.54
1:A:346:ASP:OD1	2:B:1106:ARG:NH1	2.40	0.54
1:A:325:ILE:HA	1:A:328:ARG:HB2	1.88	0.54
1:A:367:PRO:HB3	1:A:466:SER:HA	1.90	0.54
1:A:412:ARG:HG3	1:A:412:ARG:HH11	1.72	0.54
13:M:15:PRO:O	13:M:16:LYS:HG3	2.07	0.54
3:C:8:VAL:HG21	11:K:105:PHE:HA	1.90	0.53
7:G:83:LYS:HB2	7:G:149:GLY:HA2	1.90	0.53
9:I:102:VAL:HG22	9:I:109:ILE:HG12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:47:LEU:HD13	13:M:249:LYS:HE3	1.89	0.53
1:A:418:SER:O	1:A:420:ARG:NE	2.42	0.53
1:A:463:ILE:HD13	1:A:469:ARG:HG3	1.91	0.53
16:P:-10:A:H2'	16:P:-9:U:C6	2.42	0.53
1:A:626:ASN:N	1:A:626:ASN:OD1	2.42	0.53
2:B:594:ALA:HB3	2:B:595:ARG:HE	1.73	0.53
13:M:50:LEU:HD22	13:M:93:PRO:HG3	1.90	0.53
13:M:800:VAL:HG22	13:M:813:VAL:HG22	1.90	0.53
1:A:840:ARG:NH1	1:A:1384:VAL:O	2.41	0.53
2:B:693:ILE:HG23	2:B:697:GLU:HB3	1.91	0.53
2:B:895:ASP:N	2:B:895:ASP:OD1	2.41	0.53
3:C:248:ILE:HG21	11:K:102:LYS:HB2	1.90	0.53
2:B:301:ILE:HD13	2:B:379:GLY:HA2	1.91	0.53
13:M:88:LEU:HD21	13:M:97:LEU:HD22	1.91	0.53
13:M:773:LEU:HB3	13:M:843:ILE:HD11	1.90	0.53
14:N:-7:DA:H2''	14:N:-5:DT:H3	1.74	0.53
13:M:828:CYS:O	13:M:831:GLN:NE2	2.42	0.53
1:A:597:LEU:HD13	8:H:103:LYS:HG2	1.91	0.53
15:O:105:ARG:HB2	15:O:220:ALA:HA	1.91	0.53
2:B:95:ILE:HG13	2:B:130:VAL:HG12	1.89	0.52
13:M:233:ASP:HB3	13:M:236:LEU:HD23	1.92	0.52
13:M:917:ARG:HD2	15:O:53:LEU:HD13	1.90	0.52
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.92	0.52
8:H:95:TYR:HD2	8:H:144:ILE:HD12	1.74	0.52
5:E:21:GLU:OE1	5:E:143:ASN:ND2	2.42	0.52
3:C:54:ASN:ND2	3:C:60:ASP:OD1	2.43	0.52
6:F:112:GLU:N	6:F:112:GLU:OE2	2.42	0.52
13:M:107:ARG:HA	13:M:110:MET:HG2	1.92	0.52
15:O:208:ARG:HA	15:O:217:ILE:HA	1.91	0.52
13:M:621:GLU:O	13:M:624:ARG:HG2	2.10	0.52
1:A:1400:CYS:HB2	1:A:1405:THR:HG23	1.92	0.52
7:G:120:THR:OG1	7:G:122:ASN:OD1	2.28	0.52
8:H:124:ARG:NH1	8:H:126:GLU:OE2	2.37	0.52
15:O:30:THR:OG1	15:O:31:LYS:N	2.42	0.52
7:G:131:GLN:HE21	7:G:136:VAL:HG23	1.73	0.52
8:H:128:ASN:HB2	8:H:132:LEU:HD23	1.91	0.52
7:G:65:ASP:OD2	7:G:65:ASP:N	2.43	0.51
7:G:139:ILE:HG22	7:G:140:LYS:HG3	1.92	0.51
13:M:876:ASP:O	13:M:880:ILE:HG12	2.10	0.51
1:A:9:ALA:O	2:B:1193:GLN:NE2	2.42	0.51
9:I:14:LEU:HB3	9:I:27:PHE:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:917:ARG:HG3	15:O:289:THR:HG23	1.93	0.51
15:O:273:ILE:O	15:O:295:THR:OG1	2.28	0.51
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.92	0.51
4:D:118:THR:OG1	4:D:119:ARG:N	2.40	0.51
17:T:-12:DA:H2''	17:T:-11:DT:H5''	1.92	0.51
1:A:1143:LEU:HD22	1:A:1143:LEU:H	1.75	0.51
2:B:830:TYR:OH	2:B:1074:ASN:O	2.24	0.51
15:O:190:GLU:O	15:O:193:THR:OG1	2.28	0.51
2:B:435:THR:OG1	2:B:439:ALA:O	2.22	0.51
14:N:-12:DA:H2''	14:N:-11:DG:N7	2.26	0.51
1:A:618:GLU:HG2	1:A:620:LYS:H	1.75	0.51
1:A:1072:ILE:HD13	1:A:1371:LEU:HD22	1.91	0.51
1:A:744:LYS:O	1:A:748:MET:HG3	2.11	0.51
9:I:73:ARG:HB3	9:I:83:ASN:HD21	1.76	0.51
1:A:549:MET:HE2	1:A:577:ILE:HG21	1.93	0.51
4:D:37:GLN:N	4:D:45:GLU:O	2.44	0.51
17:T:7:DG:H2'	17:T:8:DA:H8	1.73	0.51
1:A:336:ILE:HA	1:A:340:LEU:HB2	1.91	0.50
1:A:900:ASP:OD1	1:A:900:ASP:N	2.44	0.50
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.92	0.50
15:O:383:ARG:HA	15:O:386:LEU:HD12	1.92	0.50
1:A:354:SER:N	1:A:468:PHE:O	2.43	0.50
1:A:567:LYS:HB3	1:A:568:PRO:HD3	1.92	0.50
1:A:806:ARG:NH1	2:B:727:LYS:O	2.43	0.50
4:D:220:LEU:HD13	4:D:221:TYR:HD1	1.76	0.50
7:G:95:SER:OG	7:G:96:GLN:N	2.44	0.50
11:K:1:MET:HG3	11:K:3:ALA:H	1.76	0.50
13:M:18:ILE:HG23	13:M:290:LEU:HB2	1.92	0.50
13:M:98:VAL:HG22	13:M:194:ILE:HB	1.92	0.50
16:P:-23:A:H3'	16:P:-22:C:H6	1.76	0.50
1:A:176:LYS:NZ	1:A:178:GLY:O	2.44	0.50
2:B:590:HIS:CD2	2:B:596:LEU:HD22	2.47	0.50
1:A:513:SER:HB3	1:A:520:CYS:HB3	1.93	0.50
1:A:1259:MET:SD	1:A:1259:MET:N	2.79	0.50
11:K:30:ALA:HB2	11:K:76:GLN:HG3	1.92	0.50
13:M:735:ILE:HG22	13:M:736:ALA:N	2.26	0.50
16:P:-9:U:H2'	16:P:-8:C:C6	2.47	0.50
1:A:443:LEU:HD13	1:A:501:LEU:HD11	1.93	0.50
9:I:78:CYS:SG	9:I:80:SER:OG	2.67	0.50
15:O:75:ASP:OD1	15:O:75:ASP:N	2.44	0.50
1:A:259:GLU:HA	1:A:259:GLU:OE2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:LYS:HA	1:A:955:PRO:HA	1.94	0.50
13:M:110:MET:HE1	13:M:685:GLN:HE21	1.77	0.50
2:B:595:ARG:H	2:B:595:ARG:NE	2.09	0.50
5:E:118:PRO:HB3	17:T:-13:DG:H4'	1.94	0.50
14:N:17:DA:H2''	14:N:18:DG:C8	2.47	0.50
1:A:557:ASP:N	1:A:557:ASP:OD1	2.38	0.50
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.93	0.50
2:B:464:GLY:HA2	2:B:480:SER:HB3	1.94	0.50
2:B:1156:ASP:OD1	2:B:1156:ASP:N	2.45	0.50
1:A:65:LEU:HD23	1:A:65:LEU:H	1.77	0.49
1:A:818:MET:HG2	2:B:514:LEU:HB3	1.94	0.49
1:A:1116:LEU:HD21	1:A:1327:ILE:HD11	1.94	0.49
1:A:1438:THR:O	6:F:92:ARG:NH1	2.44	0.49
1:A:348:SER:HB2	2:B:1128:LEU:HD23	1.92	0.49
2:B:654:ARG:H	2:B:657:HIS:CD2	2.28	0.49
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.93	0.49
5:E:94:LYS:O	5:E:98:ILE:HG13	2.13	0.49
9:I:56:ALA:HB2	9:I:89:GLN:HE21	1.78	0.49
13:M:110:MET:CE	13:M:685:GLN:HE21	2.25	0.49
1:A:961:ARG:O	1:A:964:ILE:HG13	2.12	0.49
4:D:181:GLY:HA2	4:D:214:LEU:HD21	1.94	0.49
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.95	0.49
2:B:487:THR:OG1	2:B:777:ALA:O	2.31	0.49
13:M:604:TYR:HA	13:M:607:ARG:HH21	1.78	0.49
13:M:629:LYS:HG3	13:M:670:LEU:HD21	1.95	0.49
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.95	0.49
4:D:208:GLU:O	4:D:212:LYS:HG2	2.13	0.49
13:M:104:VAL:HB	13:M:201:PRO:HB3	1.95	0.49
1:A:419:LYS:HD2	1:A:419:LYS:O	2.13	0.49
1:A:1166:ASP:HB3	1:A:1239:ARG:HH12	1.77	0.49
7:G:131:GLN:NE2	7:G:137:ILE:O	2.35	0.49
13:M:118:PHE:HA	13:M:691:PRO:HB3	1.93	0.49
2:B:277:LYS:NZ	2:B:338:GLY:O	2.45	0.49
8:H:138:GLU:HG2	8:H:139:ASN:HB2	1.94	0.49
10:J:36:LEU:HD22	10:J:47:ARG:HG2	1.95	0.49
13:M:79:ALA:O	13:M:82:GLU:HG3	2.13	0.49
13:M:310:LEU:HD11	13:M:314:PHE:HB2	1.93	0.49
13:M:772:LEU:HD12	13:M:773:LEU:H	1.77	0.49
2:B:324:ILE:HG23	2:B:329:THR:HG23	1.95	0.48
2:B:872:GLU:HG2	2:B:916:THR:HB	1.94	0.48
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.95	0.48
12:L:51:CYS:SG	12:L:53:HIS:HB2	2.53	0.48
13:M:197:ASP:N	13:M:197:ASP:OD1	2.45	0.48
1:A:518:LYS:HG2	1:A:626:ASN:HB3	1.94	0.48
4:D:66:ARG:NH2	7:G:48:VAL:O	2.45	0.48
13:M:233:ASP:HA	16:P:-22:C:H4'	1.94	0.48
15:O:105:ARG:HD3	15:O:221:GLU:H	1.77	0.48
1:A:72:GLU:N	1:A:72:GLU:OE1	2.46	0.48
1:A:882:SER:OG	1:A:953:ASN:OD1	2.31	0.48
2:B:276:ILE:HG21	2:B:280:ILE:HD11	1.95	0.48
13:M:182:LEU:HD23	13:M:188:TRP:HB3	1.95	0.48
15:O:128:ILE:HG12	15:O:344:PHE:HB2	1.95	0.48
1:A:961:ARG:HG3	1:A:961:ARG:NH1	2.27	0.48
1:A:1142:THR:OG1	1:A:1268:LEU:O	2.26	0.48
13:M:192:GLN:NE2	13:M:807:SER:OG	2.46	0.48
7:G:165:GLU:HB3	7:G:168:LEU:HD22	1.95	0.48
1:A:885:THR:HG22	1:A:940:ARG:HB2	1.95	0.48
13:M:9:TRP:HA	13:M:12:ARG:HE	1.78	0.48
13:M:112:GLN:HG3	13:M:333:ASP:O	2.14	0.48
15:O:19:LYS:N	15:O:210:GLY:O	2.46	0.48
13:M:117:ARG:O	13:M:118:PHE:C	2.52	0.48
13:M:233:ASP:O	13:M:252:ARG:NH1	2.47	0.48
1:A:418:SER:O	1:A:419:LYS:HG3	2.14	0.48
15:O:366:SER:O	15:O:371:GLY:N	2.46	0.48
2:B:508:LEU:HD11	14:N:2:DT:H5'	1.95	0.48
8:H:40:LEU:HD11	8:H:97:MET:HE1	1.96	0.48
13:M:125:GLN:HA	13:M:128:ASN:ND2	2.28	0.48
1:A:260:ASP:OD1	1:A:261:ASP:N	2.47	0.47
1:A:407:ARG:HG2	1:A:430:TRP:CE2	2.49	0.47
16:P:-10:A:H2'	16:P:-9:U:H6	1.79	0.47
1:A:242:PRO:HD2	1:A:266:LEU:HD11	1.96	0.47
1:A:1446:ASP:OD1	1:A:1446:ASP:N	2.39	0.47
2:B:1104:HIS:NE2	2:B:1126:GLY:O	2.36	0.47
4:D:144:THR:HG21	7:G:46:LEU:HD22	1.95	0.47
16:P:-20:G:P	16:P:-20:G:H21	2.37	0.47
1:A:738:LYS:HD3	1:A:740:LEU:HD11	1.97	0.47
1:A:1189:SER:HB3	1:A:1241:ARG:HD3	1.96	0.47
13:M:119:ARG:O	13:M:122:ARG:N	2.47	0.47
15:O:346:LEU:HD21	15:O:353:LEU:HD13	1.95	0.47
1:A:587:HIS:CD2	1:A:609:ASP:H	2.33	0.47
1:A:886:ILE:HD11	1:A:950:GLY:HA2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:VAL:HG22	1:A:1029:ARG:HE	1.80	0.47
2:B:299:GLU:HG2	2:B:571:PRO:HG2	1.96	0.47
4:D:25:ALA:HB2	7:G:84:GLY:HA3	1.96	0.47
13:M:37:ASP:O	13:M:92:ARG:NH1	2.47	0.47
2:B:797:TYR:HE1	2:B:854:LEU:HG	1.79	0.47
18:W:819:VAL:HG12	18:W:829:VAL:HG22	1.96	0.47
1:A:538:ASP:OD1	1:A:538:ASP:N	2.43	0.47
1:A:1379:GLY:HA3	5:E:179:GLN:HG2	1.95	0.47
2:B:249:ARG:NH1	14:N:-1:DT:O4	2.47	0.47
13:M:114:ARG:HH22	13:M:717:TYR:HD1	1.62	0.47
13:M:118:PHE:CD1	13:M:721:PHE:HD2	2.31	0.47
2:B:287:ARG:NH2	2:B:294:ASP:OD2	2.35	0.47
2:B:441:ASP:OD1	2:B:441:ASP:N	2.47	0.47
4:D:209:ARG:HD3	4:D:210:ILE:HG23	1.96	0.47
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.97	0.47
13:M:315:ASP:OD1	13:M:315:ASP:N	2.46	0.47
2:B:760:ASP:OD1	2:B:760:ASP:N	2.35	0.47
2:B:801:LYS:O	2:B:822:ASN:ND2	2.48	0.47
7:G:101:VAL:HB	7:G:108:VAL:HG13	1.97	0.47
2:B:364:ILE:HG22	2:B:365:THR:HG22	1.97	0.47
2:B:1112:GLN:HB2	2:B:1117:GLN:O	2.15	0.47
5:E:48:ASP:OD1	5:E:52:ARG:N	2.48	0.47
5:E:176:PRO:HB2	5:E:212:ARG:HG2	1.96	0.47
17:T:14:DT:H2''	17:T:15:DG:H5''	1.97	0.47
1:A:116:ASP:OD1	1:A:116:ASP:N	2.48	0.47
1:A:999:VAL:HG12	1:A:1011:GLN:HG2	1.95	0.47
1:A:1385:THR:HG23	1:A:1387:HIS:H	1.80	0.47
4:D:194:LEU:HD22	7:G:86:VAL:HG11	1.96	0.47
7:G:30:LEU:O	7:G:34:VAL:HG22	2.15	0.47
8:H:137:GLN:HG2	8:H:138:GLU:H	1.79	0.47
16:P:-3:G:H2'	16:P:-2:G:C8	2.50	0.47
18:W:857:THR:OG1	18:W:858:TYR:N	2.48	0.47
1:A:500:GLU:O	1:A:504:LEU:HB2	2.14	0.46
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.96	0.46
3:C:14:SER:OG	3:C:15:LYS:N	2.48	0.46
9:I:61:ASP:O	9:I:64:SER:OG	2.33	0.46
13:M:125:GLN:HA	13:M:128:ASN:HD21	1.80	0.46
14:N:-6:DA:H1'	14:N:-5:DT:H2'	1.97	0.46
15:O:207:VAL:HG21	15:O:236:LEU:HD21	1.97	0.46
1:A:250:ILE:HG23	16:P:-10:A:H1'	1.97	0.46
3:C:142:VAL:HG13	10:J:15:GLY:HA3	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:91:LYS:O	5:E:95:THR:HG23	2.15	0.46
1:A:1087:ALA:HB1	1:A:1091:SER:HA	1.97	0.46
2:B:322:PHE:CZ	9:I:30:ARG:HG3	2.50	0.46
3:C:86:CYS:SG	3:C:95:CYS:HB3	2.55	0.46
1:A:336:ILE:HG23	1:A:340:LEU:HD12	1.97	0.46
1:A:935:GLN:NE2	1:A:939:ASP:OD2	2.46	0.46
1:A:1166:ASP:OD1	1:A:1166:ASP:N	2.49	0.46
3:C:36:VAL:HG21	3:C:251:LEU:HD13	1.98	0.46
6:F:155:LEU:HD23	6:F:155:LEU:H	1.80	0.46
13:M:107:ARG:O	13:M:107:ARG:HG3	2.16	0.46
15:O:203:TYR:HB3	15:O:222:VAL:HB	1.98	0.46
1:A:340:LEU:HD13	1:A:1429:ILE:HG12	1.96	0.46
1:A:1143:LEU:O	1:A:1147:THR:N	2.42	0.46
8:H:49:VAL:HA	8:H:146:ARG:HH22	1.80	0.46
9:I:96:SER:OG	9:I:97:MET:N	2.49	0.46
13:M:110:MET:HE3	13:M:110:MET:HA	1.98	0.46
13:M:313:THR:OG1	15:O:55:ARG:NH1	2.49	0.46
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.80	0.46
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.96	0.46
5:E:29:PHE:HB3	5:E:62:ALA:HB3	1.97	0.46
6:F:103:MET:O	6:F:103:MET:HG3	2.15	0.46
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.97	0.46
4:D:207:LEU:O	4:D:210:ILE:HD12	2.16	0.46
1:A:156:ASP:OD1	1:A:156:ASP:N	2.38	0.46
2:B:1128:LEU:HD22	2:B:1128:LEU:H	1.81	0.46
1:A:1120:LEU:HD11	1:A:1134:ILE:HG21	1.98	0.46
4:D:32:GLU:O	4:D:37:GLN:NE2	2.34	0.46
4:D:39:ASN:OD1	4:D:42:GLY:N	2.29	0.46
4:D:195:ILE:HD12	4:D:195:ILE:O	2.16	0.46
5:E:170:LEU:HD22	5:E:174:GLN:HB3	1.98	0.46
13:M:912:THR:HG22	13:M:914:TYR:H	1.81	0.46
15:O:116:PHE:HE2	15:O:316:ALA:HB2	1.81	0.46
15:O:247:GLN:N	15:O:281:LYS:O	2.49	0.46
2:B:915:THR:HG22	2:B:936:ASP:HA	1.97	0.46
1:A:134:ARG:O	1:A:138:ILE:HG12	2.15	0.45
2:B:818:PRO:HG3	10:J:54:VAL:HG21	1.98	0.45
8:H:35:GLN:HE21	8:H:128:ASN:ND2	2.14	0.45
13:M:126:ILE:O	13:M:129:GLU:HG3	2.15	0.45
15:O:267:GLN:O	15:O:271:VAL:HG12	2.16	0.45
1:A:1082:ASN:HB3	1:A:1097:GLY:HA3	1.98	0.45
1:A:1193:LEU:O	1:A:1240:CYS:N	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:141:VAL:HG12	5:E:142:VAL:HG23	1.99	0.45
6:F:97:ARG:HD2	6:F:97:ARG:HA	1.75	0.45
8:H:77:ARG:HB3	8:H:77:ARG:CZ	2.46	0.45
9:I:33:SER:OG	9:I:34:TYR:N	2.48	0.45
1:A:290:GLU:O	1:A:293:GLU:HG3	2.16	0.45
4:D:199:ASN:OD1	4:D:199:ASN:N	2.49	0.45
10:J:42:LYS:HB3	10:J:42:LYS:HE3	1.84	0.45
1:A:362:ASP:OD1	1:A:362:ASP:N	2.39	0.45
1:A:927:VAL:HA	1:A:930:ASP:OD2	2.15	0.45
8:H:17:PRO:HB3	8:H:24:CYS:HA	1.99	0.45
2:B:776:GLN:HB3	2:B:1096:ARG:HG2	1.97	0.45
7:G:62:LEU:HD21	7:G:69:GLU:HG3	1.98	0.45
13:M:18:ILE:HG13	13:M:290:LEU:HD13	1.98	0.45
14:N:-15:DC:H2'	14:N:-14:DA:C8	2.51	0.45
1:A:614:PHE:HB3	8:H:122:LEU:HD21	1.99	0.45
1:A:1189:SER:HB2	1:A:1243:VAL:HG22	1.98	0.45
3:C:86:CYS:O	18:W:813:LYS:NZ	2.50	0.45
4:D:52:LEU:HD13	4:D:148:LEU:HD23	1.99	0.45
13:M:249:LYS:HB3	13:M:293:HIS:ND1	2.32	0.45
15:O:101:ILE:HG12	15:O:135:LEU:HB2	1.98	0.45
15:O:162:ASP:OD1	15:O:162:ASP:N	2.48	0.45
15:O:346:LEU:HD11	15:O:353:LEU:HB3	1.99	0.45
1:A:261:ASP:N	1:A:261:ASP:OD1	2.50	0.45
1:A:408:ASP:N	1:A:408:ASP:OD1	2.48	0.45
4:D:205:ASP:O	4:D:208:GLU:HG3	2.17	0.45
7:G:53:ASN:ND2	7:G:53:ASN:O	2.50	0.45
13:M:687:MET:HB2	13:M:702:PHE:HE2	1.81	0.45
16:P:-23:A:H3'	16:P:-22:C:C6	2.52	0.45
1:A:229:SER:O	1:A:229:SER:OG	2.35	0.45
2:B:293:PRO:HB2	9:I:11:ASN:HB3	1.99	0.45
13:M:179:ALA:HA	13:M:843:ILE:HD12	1.98	0.45
2:B:1180:PHE:HB2	2:B:1191:ILE:HG13	1.99	0.45
4:D:153:ARG:HH21	4:D:218:GLU:HG2	1.82	0.45
5:E:117:THR:HG23	5:E:120:ALA:HB2	1.99	0.45
13:M:295:ASN:HD21	13:M:906:VAL:HG12	1.81	0.45
1:A:894:GLU:OE2	1:A:906:HIS:NE2	2.51	0.45
2:B:1111:MET:HE3	2:B:1112:GLN:H	1.82	0.45
12:L:50:ASP:OD1	12:L:50:ASP:N	2.50	0.45
1:A:288:ALA:O	1:A:291:GLU:HG3	2.16	0.44
1:A:320:ARG:HB2	1:A:320:ARG:NH1	2.32	0.44
1:A:850:VAL:HG22	1:A:856:THR:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:843:GLN:NE2	2:B:847:ASP:OD1	2.49	0.44
13:M:725:MET:CE	13:M:737:LEU:HD13	2.47	0.44
1:A:761:MET:HG3	2:B:1021:MET:HG3	1.99	0.44
1:A:1116:LEU:HB3	1:A:1308:THR:HB	2.00	0.44
17:T:1:DC:H2'	17:T:2:DC:C6	2.52	0.44
1:A:1163:ILE:HD12	1:A:1164:PRO:HD2	1.99	0.44
1:A:1208:THR:HB	1:A:1211:GLN:HB2	1.99	0.44
2:B:778:MET:HE2	2:B:778:MET:HB2	1.87	0.44
4:D:117:GLU:HA	4:D:121:LYS:HB2	1.99	0.44
4:D:206:GLU:O	4:D:210:ILE:HG13	2.18	0.44
5:E:122:LYS:O	5:E:125:PRO:HD2	2.17	0.44
11:K:51:LEU:HA	11:K:51:LEU:HD23	1.80	0.44
15:O:59:LEU:HA	15:O:170:LYS:HG2	1.99	0.44
2:B:273:LEU:HD13	2:B:274:PRO:HD2	2.00	0.44
2:B:1013:ASN:HD22	2:B:1015:HIS:HB2	1.83	0.44
2:B:1219:ASP:OD1	4:D:14:ARG:NH2	2.50	0.44
11:K:39:ASP:OD1	11:K:39:ASP:N	2.51	0.44
13:M:729:LYS:HG2	13:M:733:GLN:CG	2.47	0.44
1:A:63:ARG:HA	1:A:74:MET:HG3	1.98	0.44
2:B:886:LYS:HE3	2:B:940:PRO:HD3	1.99	0.44
13:M:44:ASN:HD22	13:M:291:TRP:HE1	1.66	0.44
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.81	0.44
1:A:744:LYS:HG2	1:A:748:MET:HE2	1.98	0.44
1:A:1186:ASP:N	1:A:1186:ASP:OD1	2.51	0.44
2:B:132:VAL:HG23	2:B:133:LYS:H	1.82	0.44
4:D:39:ASN:OD1	4:D:41:GLN:N	2.49	0.44
7:G:25:TYR:O	7:G:29:LYS:HG2	2.18	0.44
13:M:292:LEU:HD23	13:M:292:LEU:HA	1.89	0.44
13:M:648:SER:HB3	13:M:674:PHE:HB3	2.00	0.44
14:N:6:DT:H2'	14:N:7:DG:H8	1.81	0.44
1:A:1111:MET:H	1:A:1111:MET:HG2	1.66	0.44
13:M:259:ASP:OD1	13:M:259:ASP:N	2.49	0.44
15:O:261:LEU:HA	15:O:264:THR:HG22	1.98	0.44
17:T:12:DT:H2''	17:T:13:DG:C8	2.53	0.44
2:B:473:MET:SD	2:B:473:MET:N	2.91	0.44
2:B:691:GLU:OE2	2:B:740:HIS:NE2	2.35	0.44
4:D:186:ASP:OD2	4:D:187:THR:N	2.50	0.44
7:G:132:SER:OG	7:G:133:SER:N	2.50	0.44
17:T:3:DT:H2'	17:T:4:DC:H6	1.83	0.44
1:A:362:ASP:HB3	1:A:507:VAL:HB	2.00	0.43
1:A:870:GLU:OE1	5:E:202:SER:OG	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1141:THR:HG22	1:A:1142:THR:N	2.30	0.43
2:B:357:GLN:NE2	2:B:366:GLN:O	2.51	0.43
2:B:526:GLU:HG2	2:B:538:ASN:HB2	2.00	0.43
5:E:124:VAL:HG13	5:E:132:ILE:HB	2.00	0.43
9:I:19:ASP:O	9:I:21:GLU:N	2.51	0.43
2:B:67:SER:HB2	2:B:92:PHE:HB2	1.99	0.43
2:B:863:GLU:OE1	2:B:962:LYS:HB2	2.17	0.43
6:F:112:GLU:OE2	6:F:123:LYS:NZ	2.51	0.43
11:K:2:ASN:OD1	11:K:2:ASN:N	2.51	0.43
13:M:107:ARG:CG	13:M:652:PHE:HB3	2.39	0.43
7:G:96:GLN:HE22	7:G:97:HIS:CD2	2.36	0.43
9:I:36:GLU:HG2	9:I:38:ALA:H	1.83	0.43
13:M:213:ARG:NH2	13:M:645:GLY:H	2.15	0.43
13:M:229:ILE:HD13	13:M:248:PHE:CZ	2.54	0.43
13:M:325:PHE:HB2	13:M:639:LEU:HD11	2.00	0.43
14:N:-13:DC:H2"	14:N:-12:DA:C8	2.53	0.43
15:O:36:LEU:HD22	15:O:37:ILE:H	1.83	0.43
13:M:298:ARG:HG2	13:M:316:LEU:HD21	2.00	0.43
1:A:506:ALA:HB3	1:A:509:LEU:HG	2.01	0.43
1:A:644:LYS:HD2	1:A:644:LYS:HA	1.83	0.43
1:A:1351:GLU:O	1:A:1355:VAL:HG23	2.18	0.43
2:B:313:MET:O	2:B:316:PRO:HD2	2.18	0.43
2:B:1149:GLU:HA	2:B:1153:GLU:HG2	2.00	0.43
11:K:12:LEU:HD12	11:K:12:LEU:HA	1.92	0.43
1:A:515:GLN:HG3	1:A:1071:SER:HB3	2.00	0.43
1:A:1202:MET:HA	1:A:1207:LEU:HG	2.00	0.43
2:B:106:ASP:OD1	2:B:106:ASP:N	2.52	0.43
13:M:109:LYS:HA	13:M:109:LYS:HD3	1.73	0.43
13:M:701:ILE:HG12	13:M:757:LEU:HD13	2.01	0.43
1:A:152:VAL:HG23	1:A:164:ARG:HB2	2.01	0.43
4:D:164:ILE:HD12	4:D:164:ILE:N	2.33	0.43
6:F:140:ASP:OD1	6:F:141:GLY:N	2.51	0.43
13:M:722:PRO:HG2	13:M:737:LEU:HB3	2.01	0.43
1:A:1219:THR:HG21	1:A:1271:ILE:HG23	1.99	0.43
2:B:1106:ARG:NH2	2:B:1110:PRO:O	2.52	0.43
4:D:189:ASP:OD2	4:D:190:GLU:N	2.52	0.43
8:H:101:ALA:HB2	8:H:116:TYR:CZ	2.53	0.43
11:K:26:LYS:HD2	11:K:26:LYS:HA	1.78	0.43
13:M:616:THR:O	13:M:620:ILE:HG23	2.19	0.43
1:A:1144:LYS:HA	1:A:1147:THR:HG22	2.01	0.42
3:C:226:ASP:N	3:C:226:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:98:ILE:HD12	5:E:99:HIS:N	2.34	0.42
13:M:725:MET:SD	13:M:735:ILE:HB	2.59	0.42
1:A:1259:MET:H	1:A:1259:MET:CE	2.32	0.42
2:B:950:ASP:OD1	2:B:950:ASP:N	2.46	0.42
4:D:130:LEU:HD13	4:D:141:LEU:HD12	2.01	0.42
4:D:215:SER:O	4:D:218:GLU:HG3	2.19	0.42
6:F:119:ARG:HA	6:F:122:MET:HG3	2.01	0.42
11:K:91:CYS:O	11:K:95:ILE:HG12	2.20	0.42
1:A:53:LEU:HD23	1:A:53:LEU:HA	1.91	0.42
1:A:1282:VAL:HG22	1:A:1308:THR:HG23	2.00	0.42
2:B:329:THR:HA	2:B:332:ASP:OD2	2.20	0.42
2:B:711:GLU:HB2	2:B:733:HIS:HE1	1.85	0.42
4:D:212:LYS:N	4:D:212:LYS:HE2	2.35	0.42
10:J:62:ARG:HD2	10:J:62:ARG:HA	1.83	0.42
13:M:599:LEU:O	13:M:602:PRO:HD2	2.19	0.42
9:I:55:THR:OG1	9:I:56:ALA:N	2.52	0.42
13:M:686:LEU:HD11	13:M:690:LEU:HD22	2.01	0.42
1:A:340:LEU:HD23	1:A:340:LEU:HA	1.92	0.42
2:B:246:LYS:HD3	2:B:246:LYS:HA	1.90	0.42
2:B:293:PRO:O	2:B:297:ILE:HG12	2.18	0.42
2:B:955:THR:OG1	2:B:956:THR:N	2.50	0.42
7:G:31:LEU:HD23	7:G:31:LEU:HA	1.81	0.42
13:M:162:PRO:HA	13:M:167:MET:HG3	2.01	0.42
13:M:751:ARG:HA	13:M:751:ARG:HD2	1.86	0.42
1:A:844:ALA:HB2	1:A:1384:VAL:HG13	2.02	0.42
1:A:1035:TYR:O	1:A:1037:LEU:HG	2.20	0.42
4:D:24:ALA:HB3	4:D:28:GLN:HB3	2.01	0.42
7:G:26:LEU:HD12	7:G:56:ILE:HD13	2.02	0.42
8:H:103:LYS:HB3	8:H:115:TYR:HB2	2.02	0.42
14:N:-14:DA:H2''	14:N:-13:DC:H5'	2.00	0.42
2:B:118:ARG:NH2	2:B:194:GLU:OE2	2.53	0.42
2:B:595:ARG:HE	2:B:595:ARG:H	1.65	0.42
3:C:146:LYS:HE3	10:J:57:ILE:HG21	2.02	0.42
15:O:53:LEU:HD21	15:O:290:VAL:HG23	2.01	0.42
1:A:1268:LEU:HD12	1:A:1268:LEU:HA	1.87	0.42
2:B:1074:ASN:ND2	2:B:1076:HIS:HB2	2.35	0.42
9:I:51:ASN:OD1	9:I:51:ASN:N	2.53	0.42
17:T:-17:DT:H2''	17:T:-16:DA:C8	2.55	0.42
17:T:4:DC:H2'	17:T:5:DT:H6	1.84	0.42
1:A:112:LYS:HE3	1:A:112:LYS:HB3	1.88	0.42
1:A:173:THR:O	1:A:173:THR:OG1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:PRO:HG2	1:A:498:ARG:HG2	2.00	0.42
13:M:299:GLU:H	13:M:299:GLU:HG3	1.71	0.42
13:M:372:LEU:HD12	13:M:372:LEU:HA	1.94	0.42
17:T:-19:DT:H2'	17:T:-18:DC:C5	2.55	0.42
1:A:253:ASN:O	1:A:254:GLU:HB3	2.20	0.41
1:A:279:LEU:HD11	1:A:288:ALA:HB1	2.01	0.41
1:A:676:MET:HE2	1:A:806:ARG:HH21	1.86	0.41
1:A:728:LYS:HB2	1:A:728:LYS:HE3	1.75	0.41
13:M:44:ASN:N	13:M:44:ASN:OD1	2.52	0.41
13:M:330:CYS:SG	13:M:351:LEU:HD21	2.60	0.41
1:A:704:ALA:HB2	1:A:710:LEU:HG	2.01	0.41
1:A:778:GLY:HA3	2:B:516:ASN:HB2	2.01	0.41
1:A:860:LEU:HD23	1:A:860:LEU:HA	1.90	0.41
3:C:89:GLU:OE2	3:C:89:GLU:N	2.30	0.41
6:F:127:GLU:H	6:F:127:GLU:HG2	1.69	0.41
7:G:6:ASP:OD1	7:G:75:ARG:NH1	2.53	0.41
13:M:120:SER:HA	13:M:123:ASP:OD2	2.20	0.41
13:M:124:ALA:O	13:M:127:GLU:HG3	2.19	0.41
1:A:436:ILE:HG22	1:A:460:VAL:HG11	2.02	0.41
2:B:878:GLN:HG3	13:M:401:ARG:HH22	1.85	0.41
13:M:729:LYS:HG2	13:M:733:GLN:CB	2.48	0.41
15:O:192:ARG:HA	15:O:195:ARG:HB3	2.02	0.41
16:P:-23:A:C5	16:P:-22:C:C4	3.08	0.41
1:A:1207:LEU:HD23	1:A:1207:LEU:HA	1.95	0.41
15:O:346:LEU:HD13	15:O:355:LEU:HD13	2.02	0.41
1:A:849:MET:O	1:A:856:THR:HA	2.20	0.41
7:G:23:LYS:HE2	7:G:23:LYS:HB3	1.91	0.41
15:O:129:VAL:HB	15:O:136:PHE:HB2	2.02	0.41
15:O:242:LEU:HA	15:O:277:ILE:O	2.20	0.41
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.91	0.41
1:A:919:ILE:H	1:A:919:ILE:HG13	1.69	0.41
1:A:1269:GLU:OE2	1:A:1269:GLU:N	2.52	0.41
4:D:217:LEU:HD23	4:D:220:LEU:HD21	2.02	0.41
13:M:830:ILE:HG23	13:M:832:GLY:H	1.86	0.41
15:O:318:LYS:HA	15:O:318:LYS:HD2	1.76	0.41
1:A:1317:MET:HG2	1:A:1327:ILE:HG21	2.02	0.41
1:A:1338:VAL:HG23	1:A:1339:LEU:HG	2.01	0.41
2:B:592:ASN:HB3	2:B:595:ARG:CZ	2.50	0.41
13:M:23:GLU:O	13:M:25:GLN:NE2	2.53	0.41
13:M:632:ILE:HG13	13:M:633:GLU:N	2.35	0.41
15:O:34:GLU:OE1	15:O:36:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:-11:DT:H2''	17:T:-10:DA:C8	2.56	0.41
1:A:974:ASP:OD1	1:A:974:ASP:N	2.54	0.41
2:B:1038:SER:HB3	2:B:1062:HIS:CE1	2.55	0.41
3:C:222:LYS:HE2	3:C:222:LYS:HB2	1.90	0.41
13:M:364:THR:OG1	13:M:365:TYR:N	2.54	0.41
13:M:598:LYS:HA	13:M:598:LYS:HD3	1.79	0.41
1:A:216:VAL:HA	1:A:219:PHE:CE2	2.56	0.41
1:A:301:ALA:O	1:A:305:ASP:N	2.49	0.41
1:A:344:ARG:HA	2:B:1129:ARG:HA	2.03	0.41
1:A:798:GLY:HA2	1:A:815:PHE:CD2	2.56	0.41
1:A:1039:LYS:HE3	1:A:1039:LYS:HB2	1.87	0.41
2:B:416:LEU:HD23	2:B:457:LEU:HD23	2.03	0.41
2:B:418:LYS:HE3	2:B:418:LYS:HB2	1.85	0.41
2:B:886:LYS:HB2	2:B:886:LYS:HE2	1.75	0.41
2:B:1121:GLY:O	2:B:1126:GLY:N	2.54	0.41
3:C:89:GLU:H	3:C:89:GLU:CD	2.16	0.41
4:D:143:ASN:OD1	4:D:143:ASN:N	2.51	0.41
5:E:127:ILE:HG22	5:E:130:ALA:HB3	2.03	0.41
11:K:11:LEU:HD23	11:K:11:LEU:HA	1.91	0.41
11:K:37:LYS:HA	11:K:37:LYS:HD3	1.92	0.41
11:K:110:ASN:HD22	11:K:110:ASN:HA	1.68	0.41
13:M:34:LEU:HD13	13:M:35:PRO:HD2	2.03	0.41
13:M:156:ASP:OD2	13:M:158:ASN:ND2	2.54	0.41
13:M:222:ASN:HB3	13:M:225:THR:HG23	2.01	0.41
16:P:-22:C:H2'	16:P:-21:A:C8	2.56	0.41
1:A:236:LEU:HD13	1:A:236:LEU:HA	1.94	0.41
4:D:156:ASP:O	4:D:160:VAL:HG12	2.20	0.41
5:E:22:MET:HE2	5:E:187:TYR:CD2	2.56	0.41
7:G:96:GLN:O	7:G:112:LYS:NZ	2.39	0.41
10:J:10:CYS:SG	10:J:11:GLY:N	2.94	0.41
13:M:279:PHE:HA	13:M:282:LYS:HZ2	1.87	0.41
13:M:320:ILE:H	13:M:320:ILE:HG12	1.69	0.41
13:M:695:GLY:HA2	13:M:698:LEU:HD12	2.02	0.41
15:O:260:LYS:HA	15:O:260:LYS:HD2	1.87	0.41
1:A:1221:LYS:HE3	1:A:1221:LYS:HB3	1.92	0.40
2:B:133:LYS:HE2	2:B:133:LYS:HA	2.03	0.40
13:M:117:ARG:O	13:M:120:SER:N	2.55	0.40
13:M:232:LEU:H	13:M:232:LEU:HD23	1.86	0.40
13:M:350:ILE:HG21	13:M:391:ILE:HD11	2.03	0.40
13:M:883:LYS:NZ	13:M:885:ASN:HB2	2.36	0.40
15:O:161:GLN:HB2	15:O:162:ASP:H	1.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:4:DC:H2'	17:T:5:DT:C6	2.56	0.40
1:A:827:THR:O	1:A:831:THR:HG22	2.22	0.40
2:B:834:ASN:HB3	2:B:840:ILE:HG13	2.03	0.40
3:C:167:HIS:CD2	12:L:70:ARG:HG3	2.56	0.40
10:J:50:ILE:HD12	10:J:50:ILE:C	2.41	0.40
15:O:282:ASP:OD1	15:O:282:ASP:N	2.52	0.40
2:B:324:ILE:HG21	2:B:330:ALA:HB2	2.03	0.40
4:D:60:LYS:HB3	4:D:60:LYS:HE2	1.92	0.40
4:D:78:LYS:HG2	15:O:303:LYS:HD3	2.03	0.40
13:M:178:THR:HG21	13:M:773:LEU:HD13	2.03	0.40
13:M:333:ASP:OD1	13:M:333:ASP:N	2.53	0.40
2:B:615:MET:H	2:B:615:MET:HG2	1.79	0.40
4:D:211:LEU:HD23	4:D:211:LEU:HA	1.90	0.40
13:M:104:VAL:O	13:M:202:GLY:N	2.44	0.40
13:M:107:ARG:HA	13:M:110:MET:HB2	2.03	0.40
13:M:898:ASP:HA	13:M:901:GLN:NE2	2.36	0.40
1:A:1089:VAL:HG21	1:A:1285:MET:HE1	2.03	0.40
4:D:123:LEU:HA	4:D:126:ILE:HD11	2.03	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	1411/1733 (81%)	1356 (96%)	55 (4%)	0	100	100
2	B	1147/1259 (91%)	1106 (96%)	41 (4%)	0	100	100
3	C	268/318 (84%)	261 (97%)	7 (3%)	0	100	100
4	D	176/221 (80%)	168 (96%)	8 (4%)	0	100	100
5	E	213/215 (99%)	206 (97%)	7 (3%)	0	100	100
6	F	81/155 (52%)	78 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	169/171 (99%)	154 (91%)	15 (9%)	0	100	100
8	H	142/146 (97%)	132 (93%)	10 (7%)	0	100	100
9	I	113/122 (93%)	103 (91%)	10 (9%)	0	100	100
10	J	64/70 (91%)	60 (94%)	4 (6%)	0	100	100
11	K	109/120 (91%)	108 (99%)	1 (1%)	0	100	100
12	L	44/70 (63%)	41 (93%)	3 (7%)	0	100	100
13	M	713/1019 (70%)	677 (95%)	36 (5%)	0	100	100
15	O	346/387 (89%)	333 (96%)	13 (4%)	0	100	100
18	W	69/1063 (6%)	64 (93%)	5 (7%)	0	100	100
All	All	5065/7069 (72%)	4847 (96%)	218 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1231/1520 (81%)	1185 (96%)	46 (4%)	34	63
2	B	998/1094 (91%)	945 (95%)	53 (5%)	22	48
3	C	238/274 (87%)	233 (98%)	5 (2%)	53	80
4	D	162/200 (81%)	146 (90%)	16 (10%)	8	18
5	E	181/197 (92%)	170 (94%)	11 (6%)	18	41
6	F	73/137 (53%)	69 (94%)	4 (6%)	21	46
7	G	152/152 (100%)	131 (86%)	21 (14%)	3	8
8	H	116/128 (91%)	105 (90%)	11 (10%)	8	20
9	I	95/116 (82%)	87 (92%)	8 (8%)	11	25
10	J	61/65 (94%)	59 (97%)	2 (3%)	38	67
11	K	96/102 (94%)	92 (96%)	4 (4%)	30	58
12	L	40/57 (70%)	37 (92%)	3 (8%)	13	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	632/909 (70%)	600 (95%)	32 (5%)	24	50
15	O	320/346 (92%)	302 (94%)	18 (6%)	21	45
18	W	59/876 (7%)	58 (98%)	1 (2%)	60	84
All	All	4454/6173 (72%)	4219 (95%)	235 (5%)	26	48

All (235) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	PHE
1	A	27	VAL
1	A	40	THR
1	A	68	GLN
1	A	123	ARG
1	A	132	LYS
1	A	148	CYS
1	A	253	ASN
1	A	261	ASP
1	A	286	HIS
1	A	287	HIS
1	A	322	VAL
1	A	408	ASP
1	A	419	LYS
1	A	425	GLN
1	A	444	PHE
1	A	451	HIS
1	A	470	LEU
1	A	529	CYS
1	A	642	CYS
1	A	716	ASP
1	A	826	ASP
1	A	833	GLU
1	A	949	ASP
1	A	975	HIS
1	A	981	LEU
1	A	985	ASP
1	A	988	LEU
1	A	995	GLU
1	A	1140	HIS
1	A	1144	LYS
1	A	1166	ASP
1	A	1173	HIS

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Mol	Chain	Res	Type
1	A	1208	THR
1	A	1225	PHE
1	A	1232	ASN
1	A	1233	ASP
1	A	1236	LEU
1	A	1259	MET
1	A	1288	ASP
1	A	1336	MET
1	A	1373	ASP
1	A	1411	GLU
1	A	1418	LEU
1	A	1442	ASP
1	A	1454	MET
2	B	40	GLU
2	B	69	LEU
2	B	137	TYR
2	B	187	SER
2	B	199	MET
2	B	253	THR
2	B	277	LYS
2	B	322	PHE
2	B	393	LYS
2	B	394	ASP
2	B	398	ARG
2	B	401	PHE
2	B	432	MET
2	B	442	PHE
2	B	444	MET
2	B	451	LYS
2	B	470	LYS
2	B	473	MET
2	B	476	ARG
2	B	498	THR
2	B	500	THR
2	B	502	ILE
2	B	557	PHE
2	B	595	ARG
2	B	615	MET
2	B	675	ASP
2	B	706	GLN
2	B	731	VAL
2	B	764	SER

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Mol	Chain	Res	Type
2	B	778	MET
2	B	785	TYR
2	B	787	VAL
2	B	790	ASP
2	B	861	ASP
2	B	863	GLU
2	B	864	LYS
2	B	871	THR
2	B	887	HIS
2	B	891	ASP
2	B	904	ARG
2	B	1021	MET
2	B	1026	LEU
2	B	1087	PHE
2	B	1093	GLN
2	B	1100	ASP
2	B	1111	MET
2	B	1115	THR
2	B	1123	SER
2	B	1124	ARG
2	B	1136	ASP
2	B	1163	CYS
2	B	1179	GLN
2	B	1219	ASP
3	C	16	ASP
3	C	50	GLU
3	C	102	GLN
3	C	208	GLU
3	C	259	LEU
4	D	16	LYS
4	D	26	THR
4	D	34	GLN
4	D	39	ASN
4	D	52	LEU
4	D	72	ARG
4	D	121	LYS
4	D	141	LEU
4	D	143	ASN
4	D	145	MET
4	D	189	ASP
4	D	197	SER
4	D	199	ASN

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Mol	Chain	Res	Type
4	D	203	SER
4	D	209	ARG
4	D	220	LEU
5	E	1	MET
5	E	2	ASP
5	E	31	THR
5	E	52	ARG
5	E	78	LEU
5	E	84	ASP
5	E	106	GLN
5	E	115	ASN
5	E	117	THR
5	E	164	LEU
5	E	215	MET
6	F	111	LEU
6	F	114	GLU
6	F	118	LEU
6	F	147	SER
7	G	1	MET
7	G	10	ASN
7	G	21	ARG
7	G	24	GLN
7	G	32	GLU
7	G	47	CYS
7	G	52	ASP
7	G	74	TYR
7	G	79	PHE
7	G	82	PHE
7	G	88	ASP
7	G	93	SER
7	G	102	GLN
7	G	108	VAL
7	G	109	PHE
7	G	115	MET
7	G	131	GLN
7	G	134	GLU
7	G	138	THR
7	G	158	HIS
7	G	167	TYR
8	H	34	ASP
8	H	36	CYS
8	H	77	ARG

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Mol	Chain	Res	Type
8	H	87	ARG
8	H	105	GLU
8	H	106	GLU
8	H	110	ASP
8	H	123	MET
8	H	133	ASN
8	H	135	LEU
8	H	139	ASN
9	I	9	ASP
9	I	13	MET
9	I	29	CYS
9	I	32	CYS
9	I	33	SER
9	I	44	TYR
9	I	74	GLU
9	I	90	GLN
10	J	16	ASP
10	J	28	ASP
11	K	2	ASN
11	K	54	ARG
11	K	68	PHE
11	K	70	ARG
12	L	43	THR
12	L	48	CYS
12	L	50	ASP
13	M	3	VAL
13	M	12	ARG
13	M	16	LYS
13	M	44	ASN
13	M	61	CYS
13	M	73	GLU
13	M	83	TYR
13	M	96	VAL
13	M	107	ARG
13	M	109	LYS
13	M	110	MET
13	M	111	ASN
13	M	150	ARG
13	M	209	MET
13	M	227	HIS
13	M	325	PHE
13	M	327	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
13	M	390	ASP
13	M	604	TYR
13	M	607	ARG
13	M	614	HIS
13	M	640	MET
13	M	649	TRP
13	M	660	LEU
13	M	706	MET
13	M	730	MET
13	M	745	ARG
13	M	754	TYR
13	M	773	LEU
13	M	788	LEU
13	M	917	ARG
13	M	924	PHE
15	O	48	LEU
15	O	50	ASP
15	O	66	PHE
15	O	71	LYS
15	O	76	ARG
15	O	79	LEU
15	O	112	ILE
15	O	118	SER
15	O	128	ILE
15	O	192	ARG
15	O	247	GLN
15	O	253	ASP
15	O	267	GLN
15	O	275	ARG
15	O	278	TYR
15	O	294	SER
15	O	309	VAL
15	O	330	MET
18	W	845	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	HIS
1	A	160	GLN
1	A	576	GLN
1	A	587	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	589	GLN
1	A	802	ASN
1	A	903	ASN
1	A	1278	ASN
1	A	1390	ASN
1	A	1432	GLN
2	B	236	HIS
2	B	531	GLN
2	B	657	HIS
2	B	716	ASN
2	B	733	HIS
2	B	762	ASN
2	B	776	GLN
2	B	1013	ASN
2	B	1062	HIS
2	B	1074	ASN
2	B	1076	HIS
2	B	1117	GLN
2	B	1141	HIS
3	C	135	GLN
3	C	151	GLN
3	C	195	GLN
4	D	34	GLN
4	D	132	GLN
4	D	137	ASN
4	D	200	ASN
7	G	10	ASN
7	G	71	ASN
7	G	96	GLN
8	H	71	ASN
8	H	128	ASN
9	I	87	GLN
9	I	89	GLN
9	I	90	GLN
10	J	23	ASN
10	J	53	HIS
11	K	40	HIS
11	K	96	ASN
11	K	104	ASN
11	K	110	ASN
13	M	49	ASN
13	M	192	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
13	M	287	GLN
13	M	373	ASN
13	M	383	HIS
13	M	685	GLN
13	M	743	GLN
13	M	776	ASN
13	M	886	ASN
13	M	901	GLN
15	O	42	ASN
15	O	267	GLN
15	O	308	GLN
18	W	863	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	22/23 (95%)	7 (31%)	0

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	-19	A
16	P	-17	C
16	P	-16	G
16	P	-13	U
16	P	-12	C
16	P	-11	C
16	P	-3	G

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 11 ligands modelled in this entry, 11 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

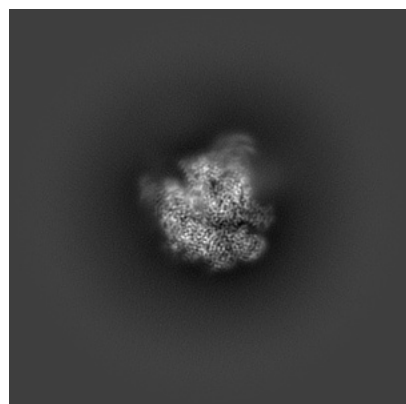
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36162. These allow visual inspection of the internal detail of the map and identification of artifacts.

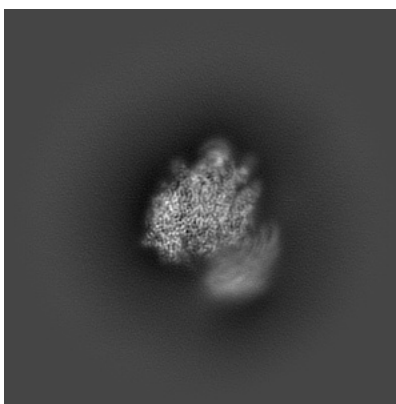
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

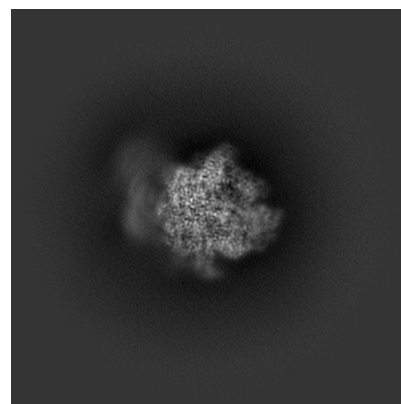
#### 6.1.1 Primary map



X

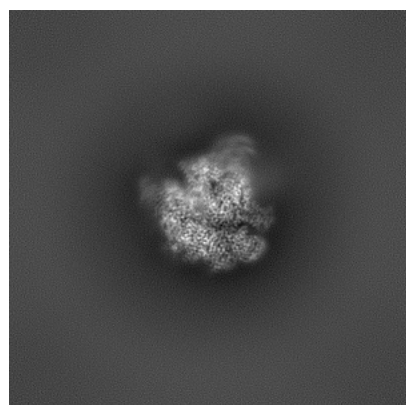


Y

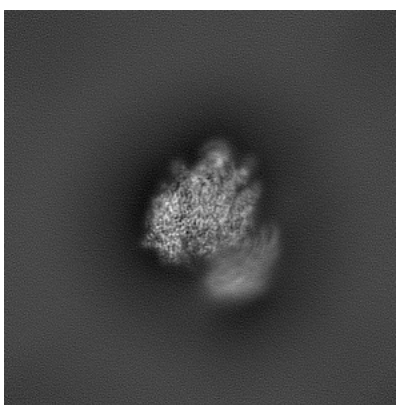


Z

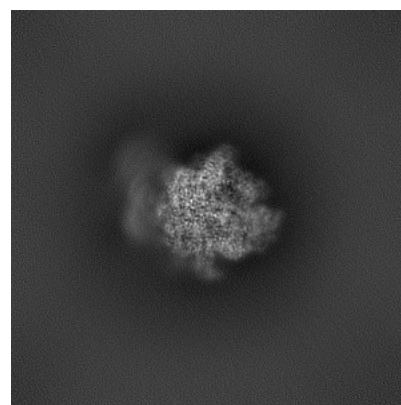
#### 6.1.2 Raw map



X



Y

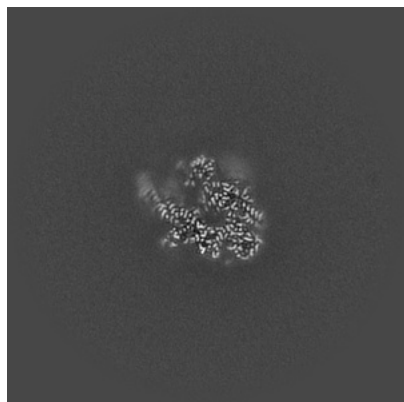


Z

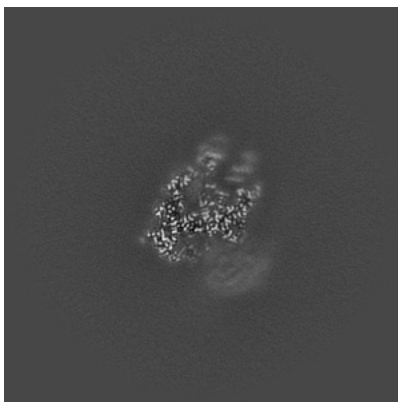
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

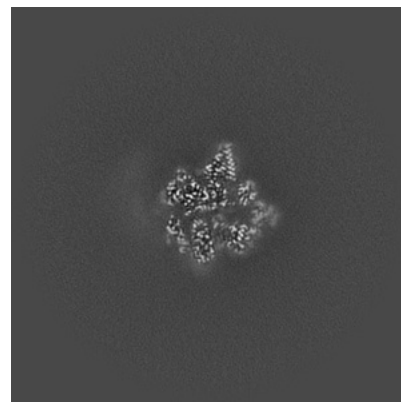
### 6.2.1 Primary map



X Index: 200

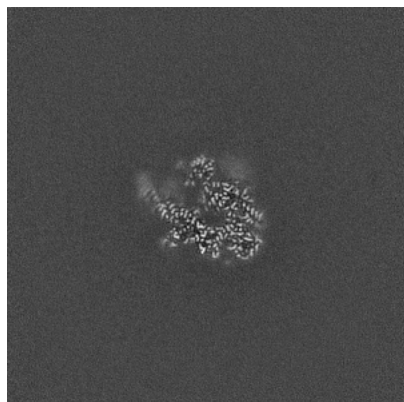


Y Index: 200

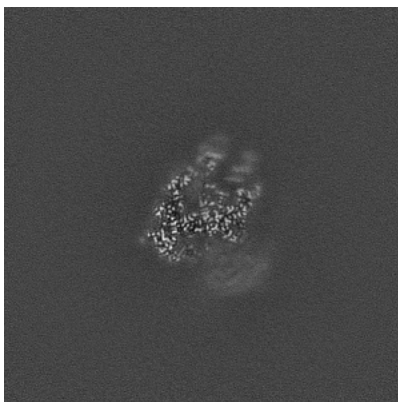


Z Index: 200

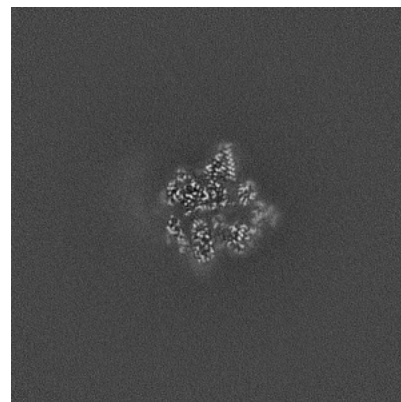
### 6.2.2 Raw map



X Index: 200



Y Index: 200

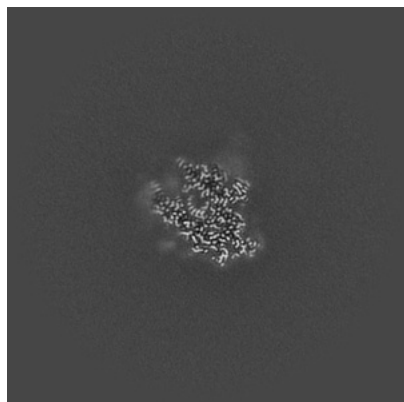


Z Index: 200

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

## 6.3 Largest variance slices [i](#)

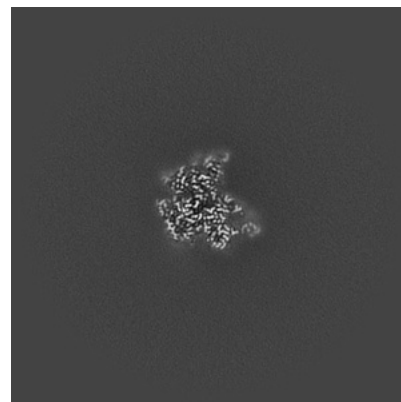
### 6.3.1 Primary map



X Index: 190

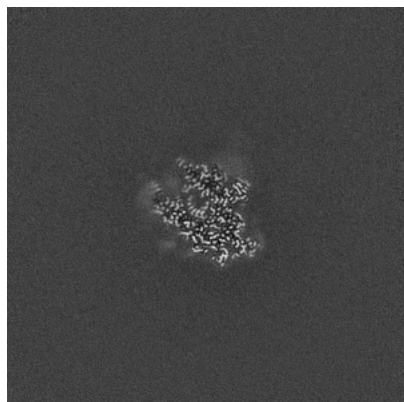


Y Index: 195



Z Index: 171

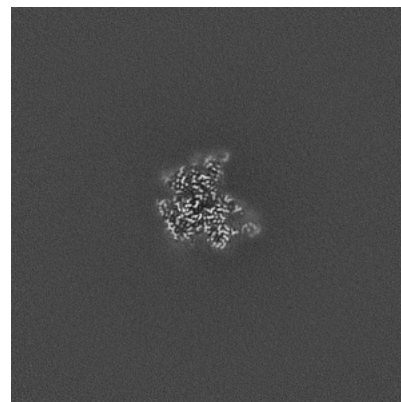
### 6.3.2 Raw map



X Index: 190



Y Index: 195



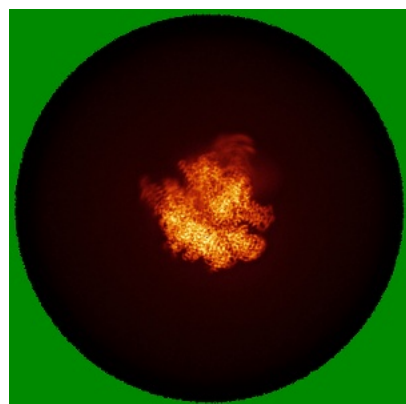
Z Index: 171

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

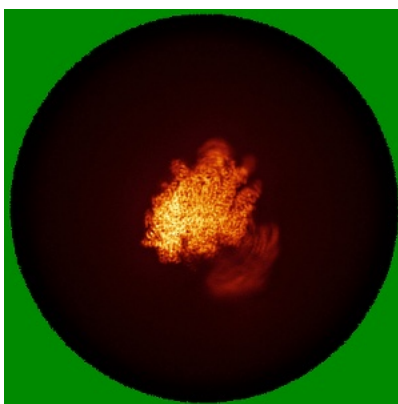


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

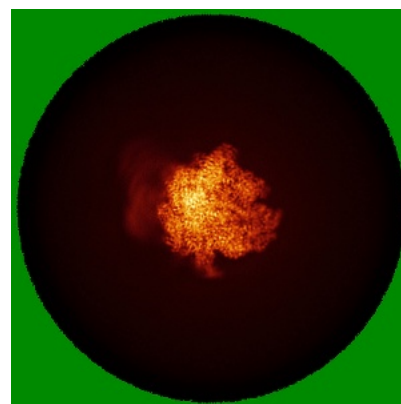
### 6.4.1 Primary map



X

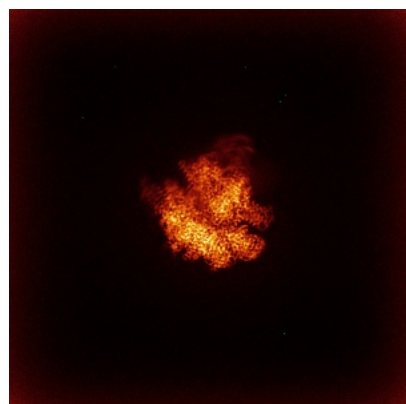


Y

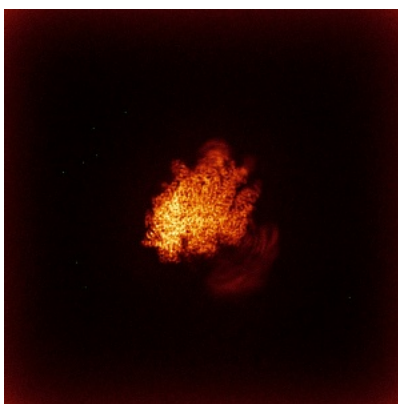


Z

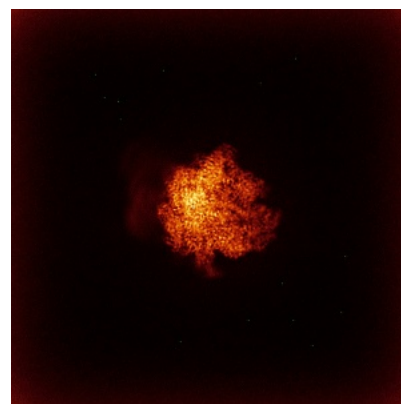
### 6.4.2 Raw map



X



Y

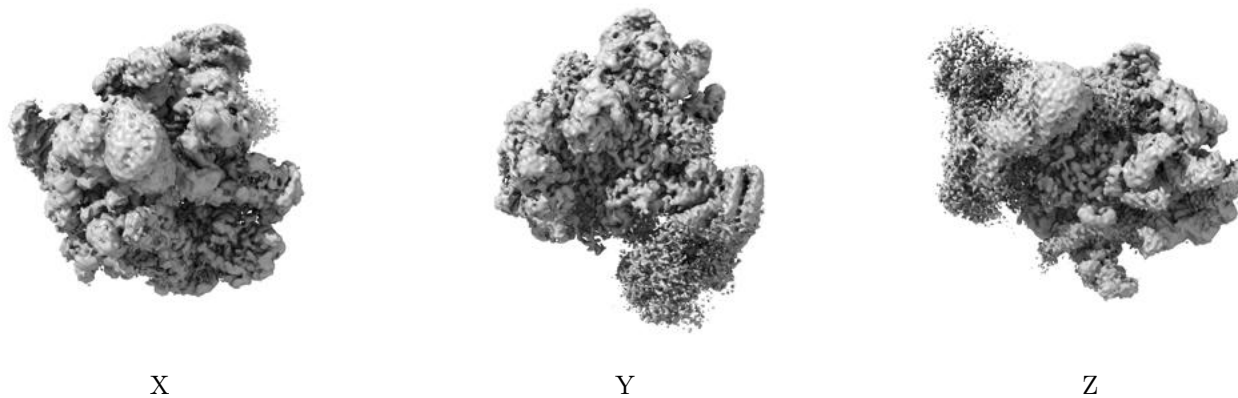


Z

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

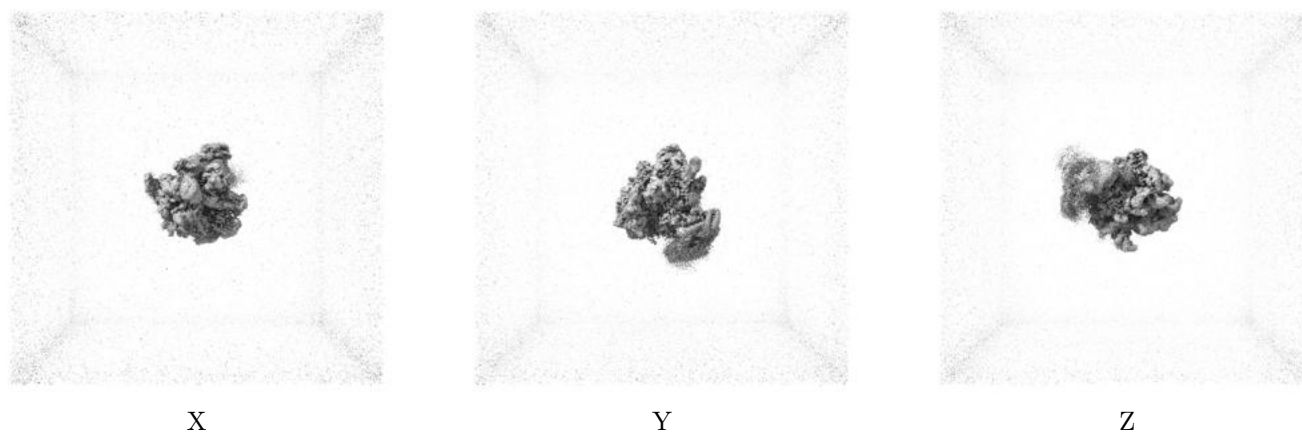
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

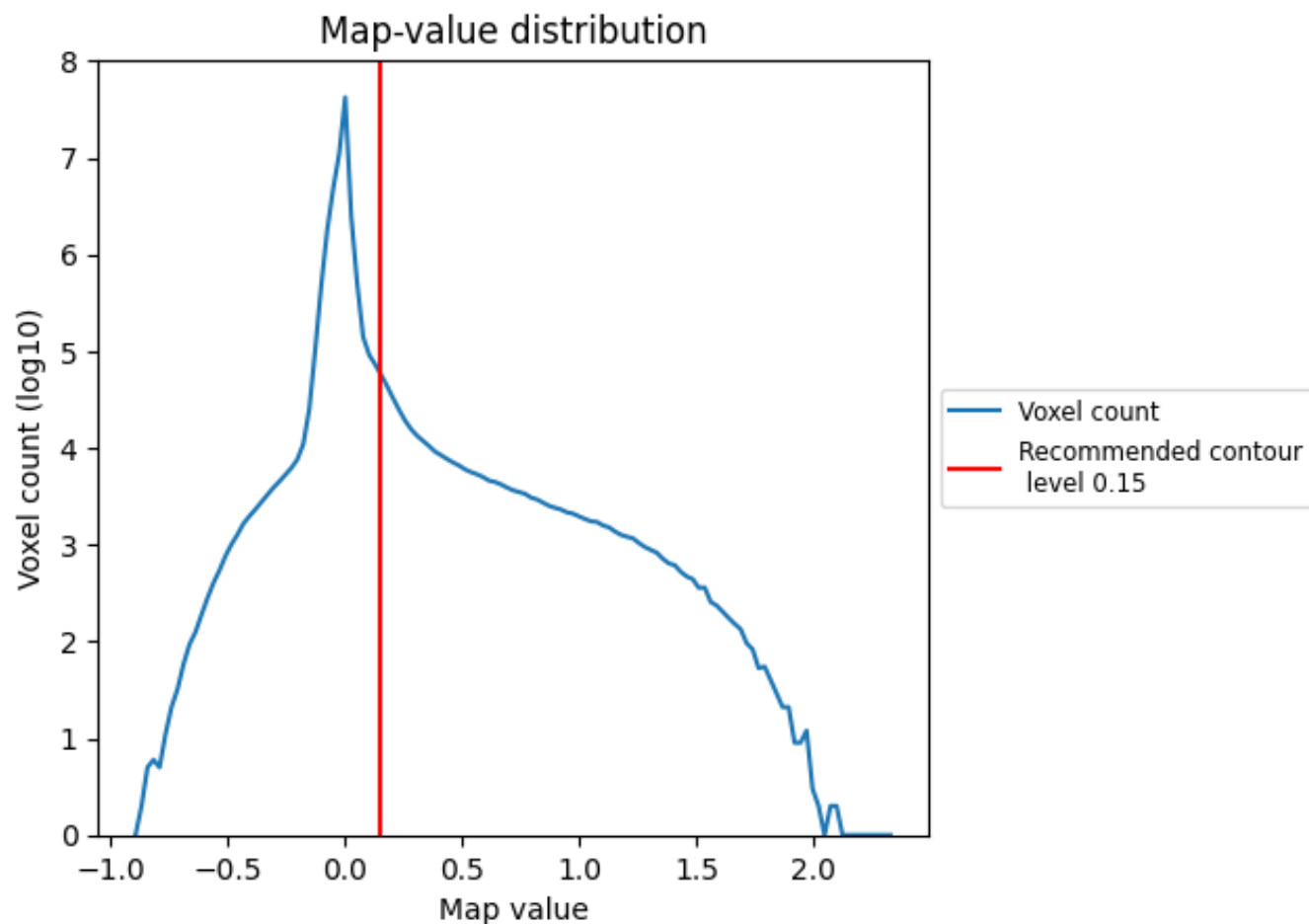
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

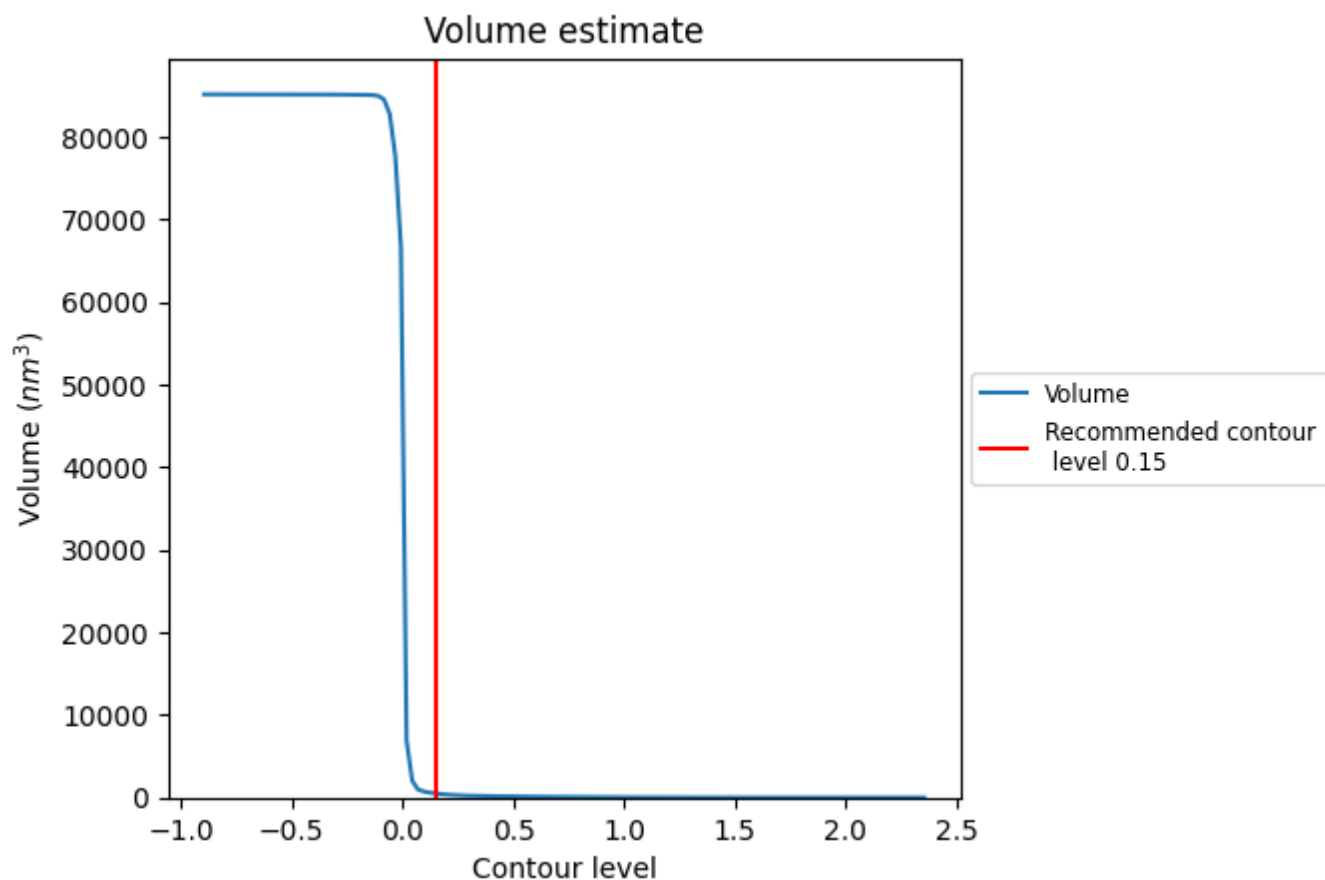
This section contains the results of statistical analysis of the map.

### 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.

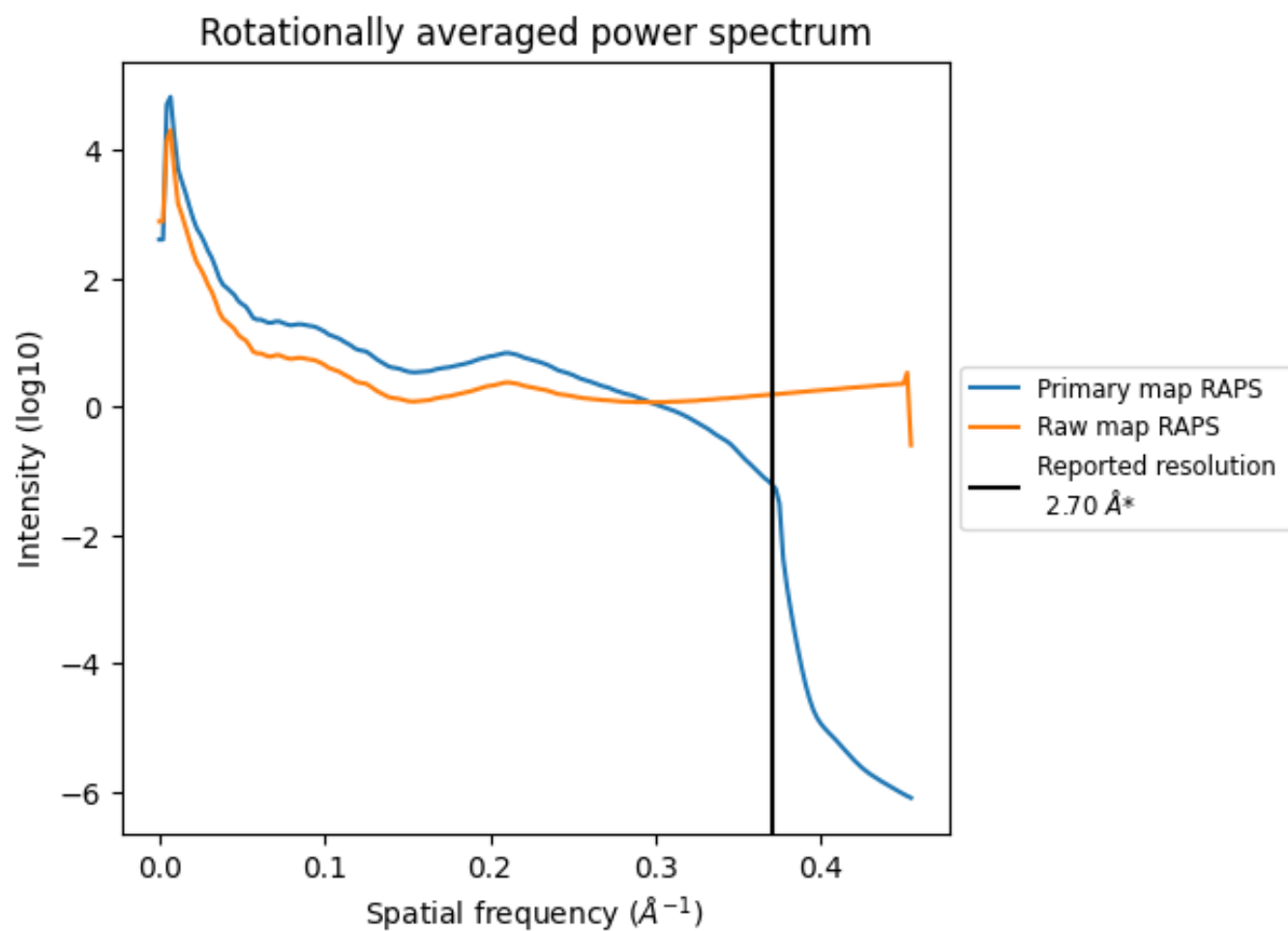
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 493  $\text{nm}^3$ ; this corresponds to an approximate mass of 445 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 ⓘ

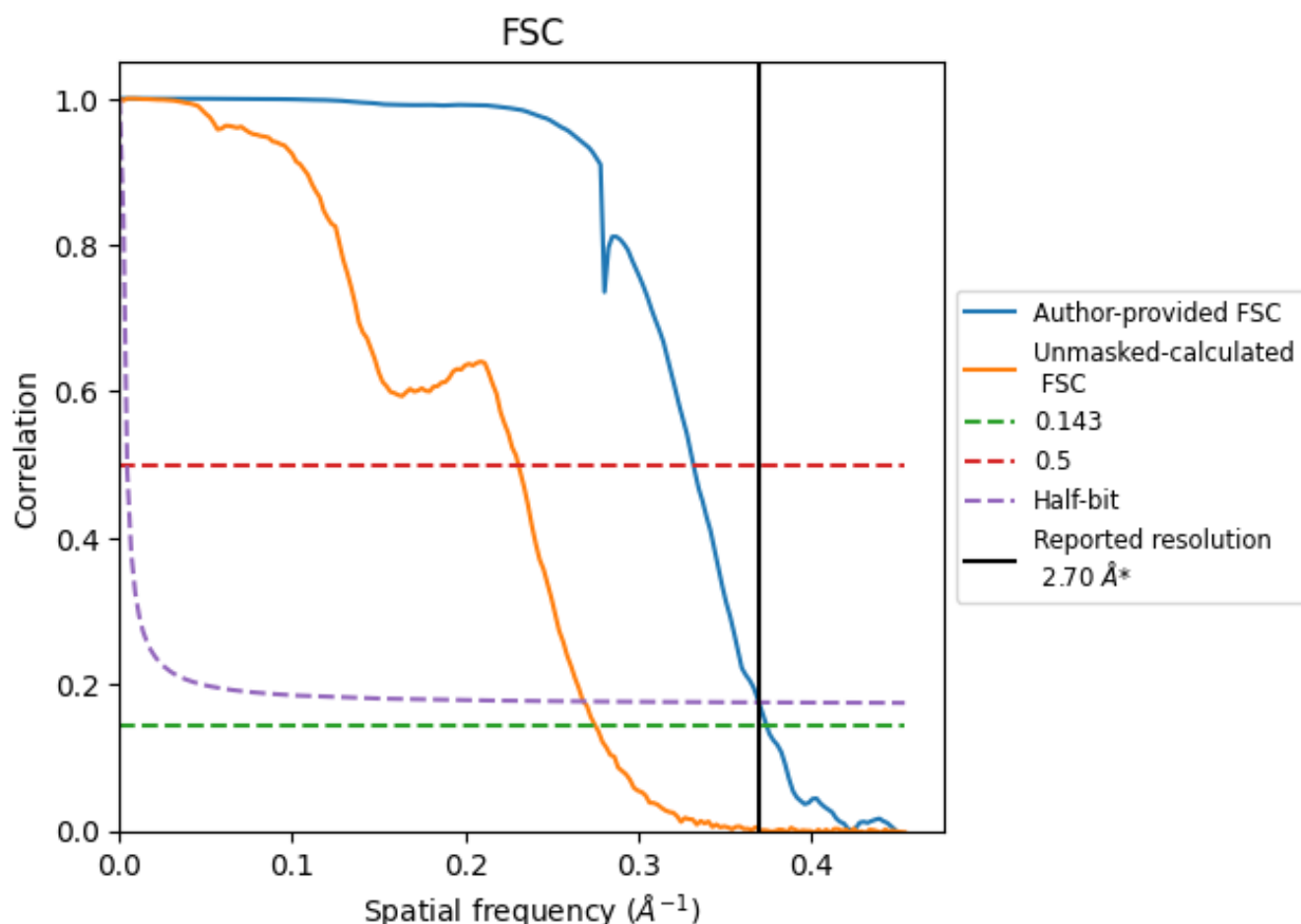


\*Reported resolution corresponds to spatial frequency of  $0.370 \text{ \AA}^{-1}$

## 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 0.370  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

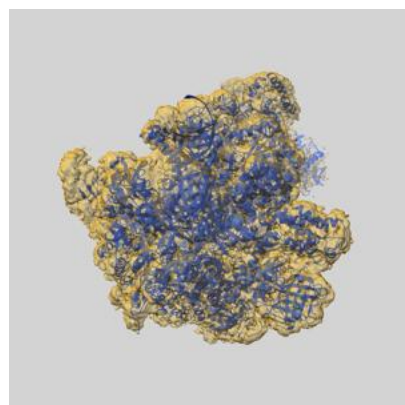
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.67	3.01	2.70
Unmasked-calculated*	3.63	4.33	3.73

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.63 differs from the reported value 2.7 by more than 10 %

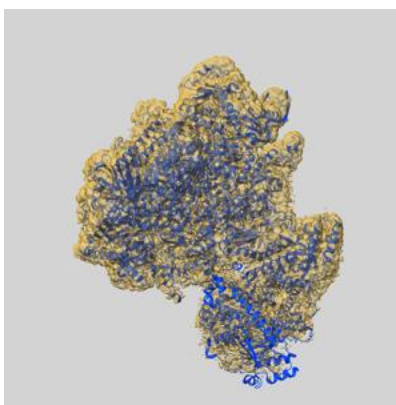
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36162 and PDB model 8JCH. Per-residue inclusion information can be found in section [3](#) on page [9](#).

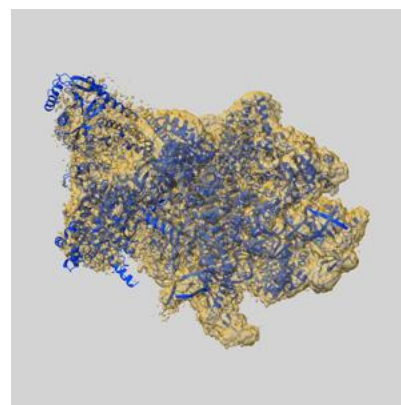
### 9.1 Map-model overlay [i](#)



X



Y

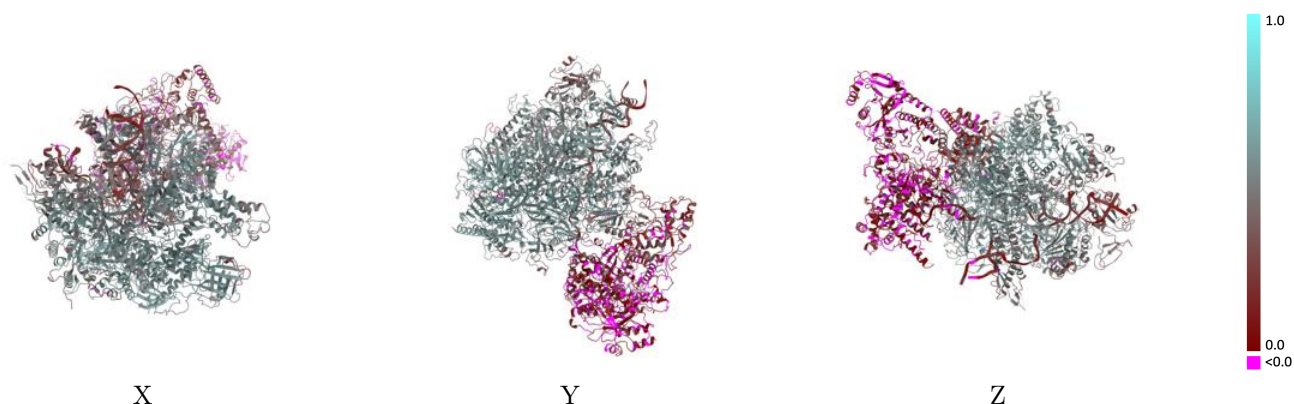


Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

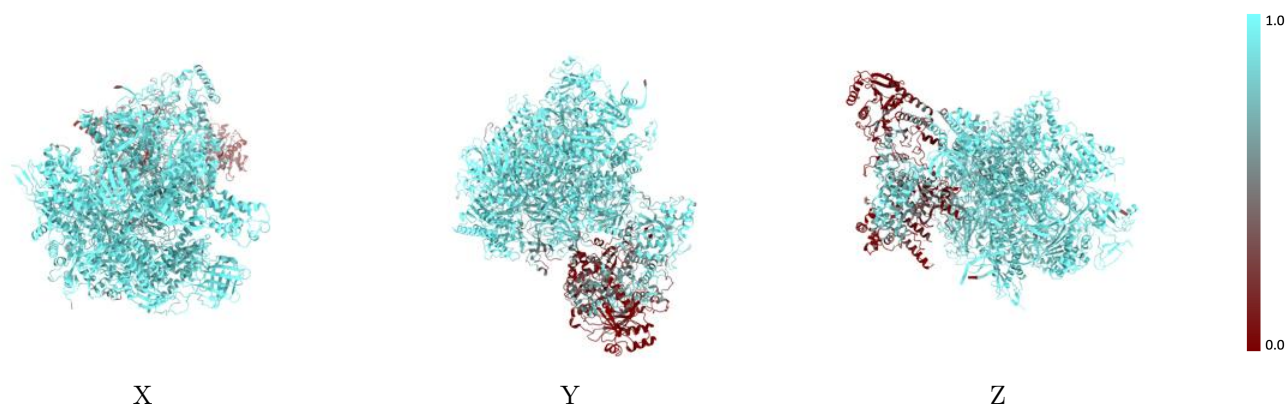


## 9.2 Q-score mapped to coordinate model [i](#)



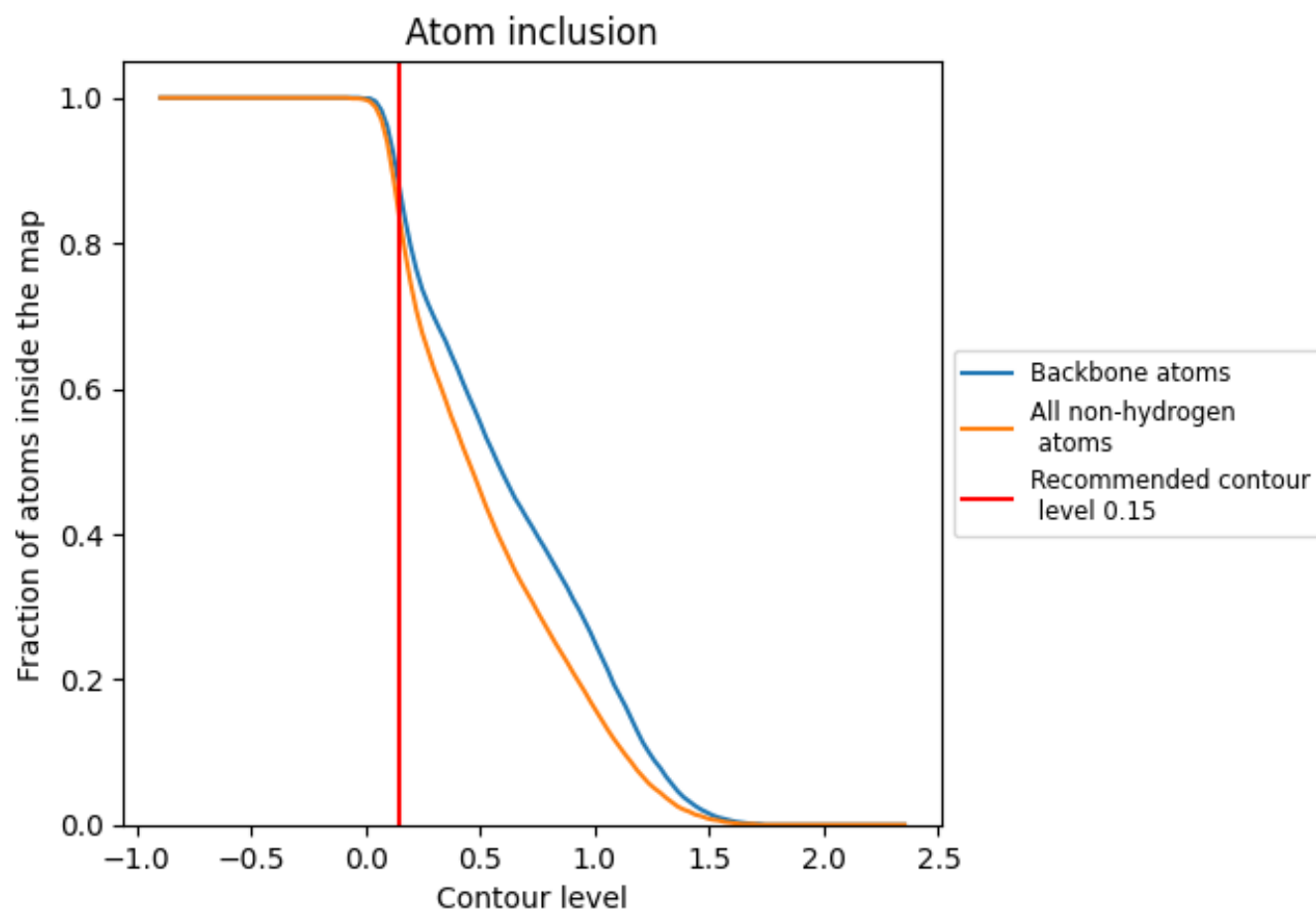
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).







































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 83% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8300	 0.4030
A	 0.9650	 0.5180
B	 0.9660	 0.5310
C	 0.9860	 0.5660
D	 0.7970	 0.2000
E	 0.9870	 0.5190
F	 0.9760	 0.5550
G	 0.8830	 0.2850
H	 0.9830	 0.5160
I	 0.9780	 0.4450
J	 0.9910	 0.5730
K	 0.9750	 0.5730
L	 0.9460	 0.5030
M	 0.4500	 0.0850
N	 0.9080	 0.2150
O	 0.2250	 0.0740
P	 0.6770	 0.2550
T	 0.8970	 0.3010
W	 0.6400	 0.4680

