



## Full wwPDB EM Validation Report ⓘ

Apr 7, 2025 – 01:34 pm BST

PDB ID : 8QQ2 / pdb\_00008qq2  
EMDB ID : EMD-18573  
Title : RNAPII elongation complex bound to RECQ5  
Authors : Skubnik, K.; Sebesta, M.; Stefl, R.  
Deposited on : 2023-10-03  
Resolution : 4.20 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.dev117  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

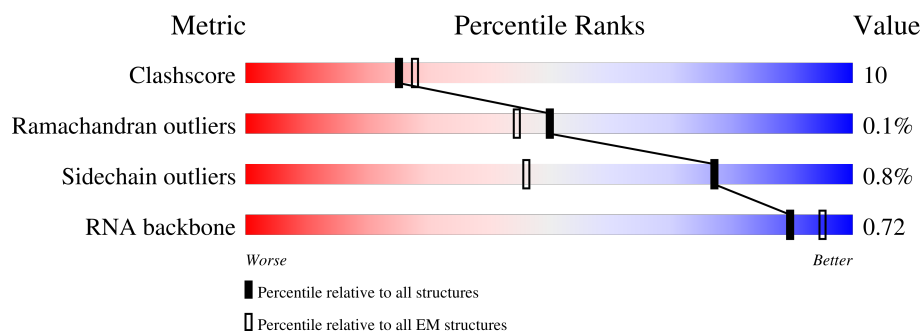
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.20 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.





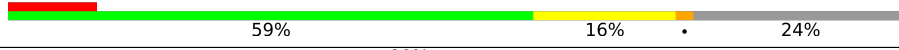




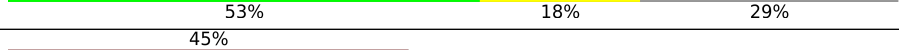
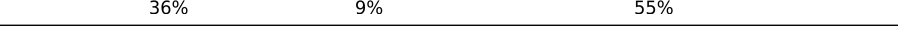
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1970	<div> <div>14%</div> <div>55%</div> <div>15%</div> <div>30%</div> </div>
2	B	1174	<div> <div>13%</div> <div>77%</div> <div>17%</div> <div>5%</div> </div>
3	C	275	<div> <div>73%</div> <div>20%</div> <div>7%</div> </div>
4	E	210	<div> <div>19%</div> <div>74%</div> <div>25%</div> </div>
5	F	127	<div> <div>5%</div> <div>54%</div> <div>7%</div> <div>39%</div> </div>
6	H	150	<div> <div>6%</div> <div>79%</div> <div>20%</div> </div>
7	I	125	<div> <div>23%</div> <div>70%</div> <div>22%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
8	J	67	 88% 9% ..
9	K	117	 81% 17% .
10	L	58	 10% 59% 16% . 24%
11	D	142	 90% 46% 44% 10%
12	G	172	 80% 52% 47% .
13	R	650	 11% 15% 84%
14	P	17	 35% 41% 29% 12% 18%
15	T	51	 51% 53% 18% 29%
16	N	55	 45% 36% 9% 55%

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 32595 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 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1383	Total	C	N	O	S	0	0
			10926	6881	1960	2019	66		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1114	Total	C	N	O	S	0	0
			8848	5602	1552	1630	64		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	255	Total	C	N	O	S	0	0
			2039	1283	348	402	6		

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	209	Total	C	N	O	S	0	0
			1687	1068	296	315	8		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	78	Total	C	N	O	S	0	0
			623	400	106	112	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	34	GLU	VAL	variant	UNP Q32PE0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	148	Total	C	N	O	S	0	0
			1172	743	191	233	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	114	Total	C	N	O	S	0	0
			921	569	165	176	11		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	66	Total	C	N	O	S	0	0
			520	337	88	89	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	44	Total	C	N	O	S	0	0
			368	228	71	63	6		

- Molecule 11 is a protein called Polymerase (RNA) II (DNA directed) polypeptide D.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	128	Total	C	N	O	S	0	0
			1005	632	172	197	4		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	171	Total	C	N	O	S	0	0
			1334	867	216	243	8		

- Molecule 13 is a protein called ATP-dependent DNA helicase Q5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	101	Total	C	N	O	S	0	0
			679	425	119	132	3		

- Molecule 14 is a RNA chain called RNA, DNA-RNA ELONGATION SCAFFOLD.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	14	Total	C	N	O	P	0	0
			293	131	46	102	14		

- Molecule 15 is a DNA chain called DNA, DNA-RNA ELONGATION SCAFFOLD.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	36	Total	C	N	O	P	0	0
			748	352	155	205	36		

- Molecule 16 is a DNA chain called DNA (55-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	25	Total	C	N	O	P	0	0
			503	242	76	160	25		

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

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

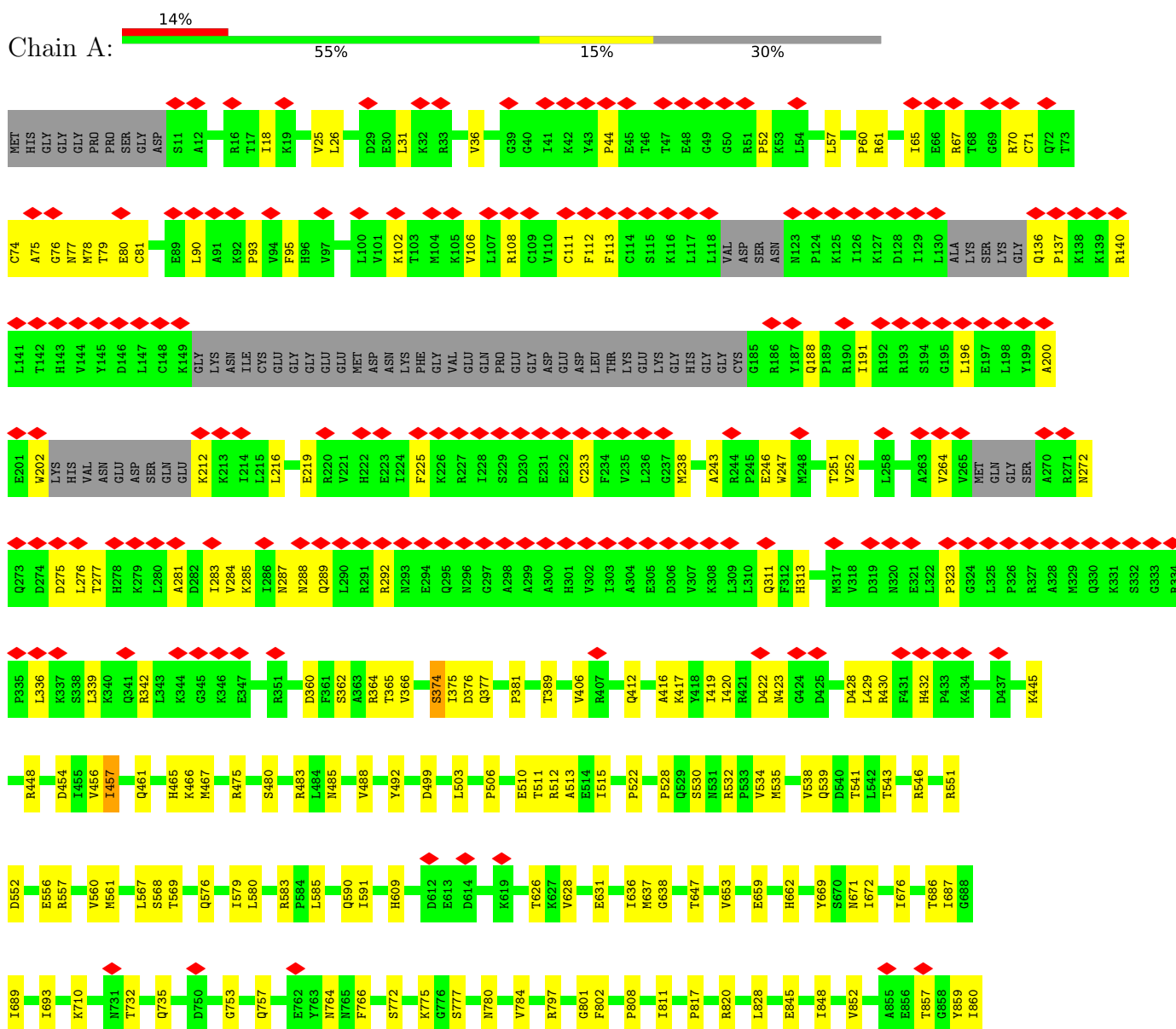
- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	P	1	Total	Mg	0
			1	1	

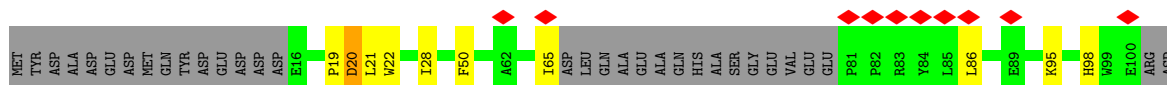
### 3 Residue-property plots

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

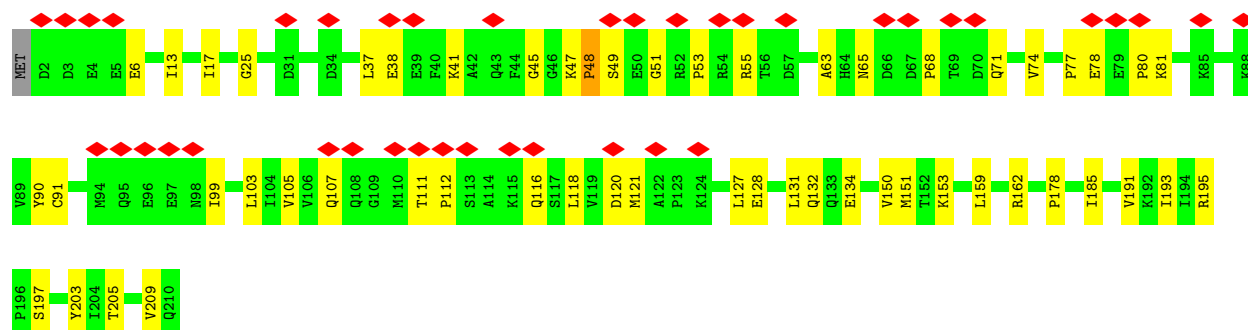
#### • Molecule 1: DNA-directed RNA polymerase subunit



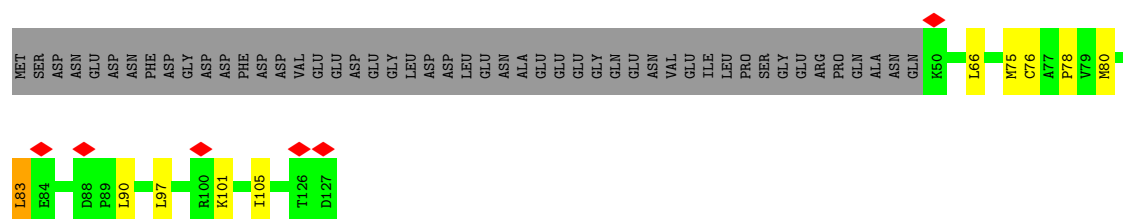




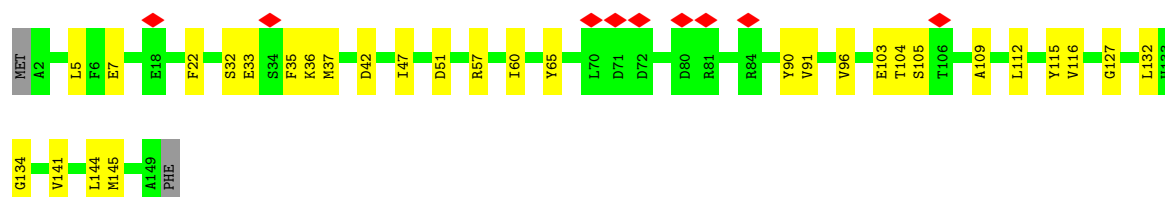




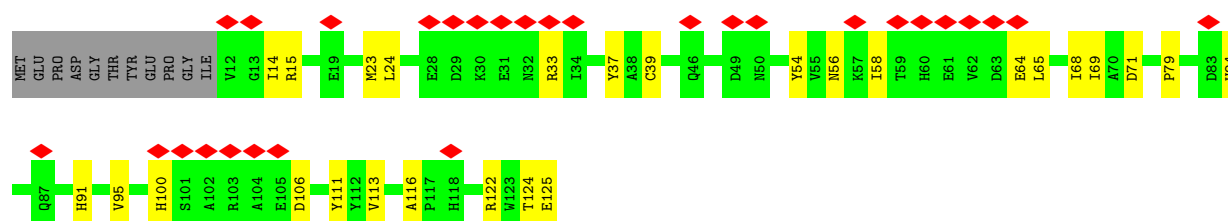
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



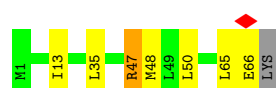
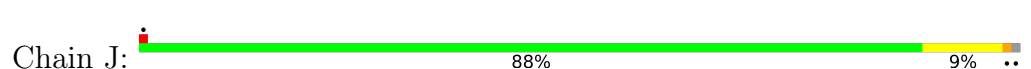
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



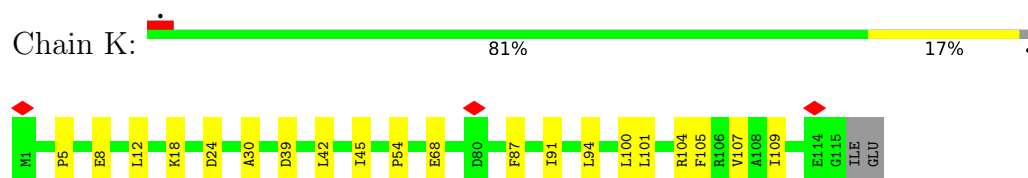
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



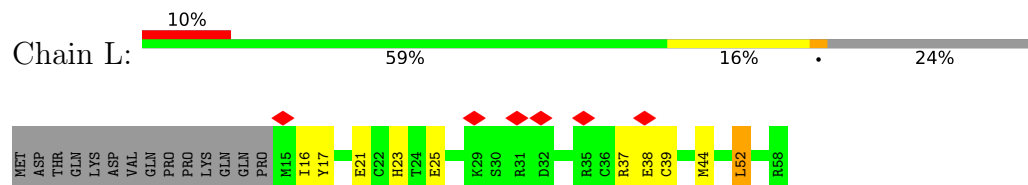
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



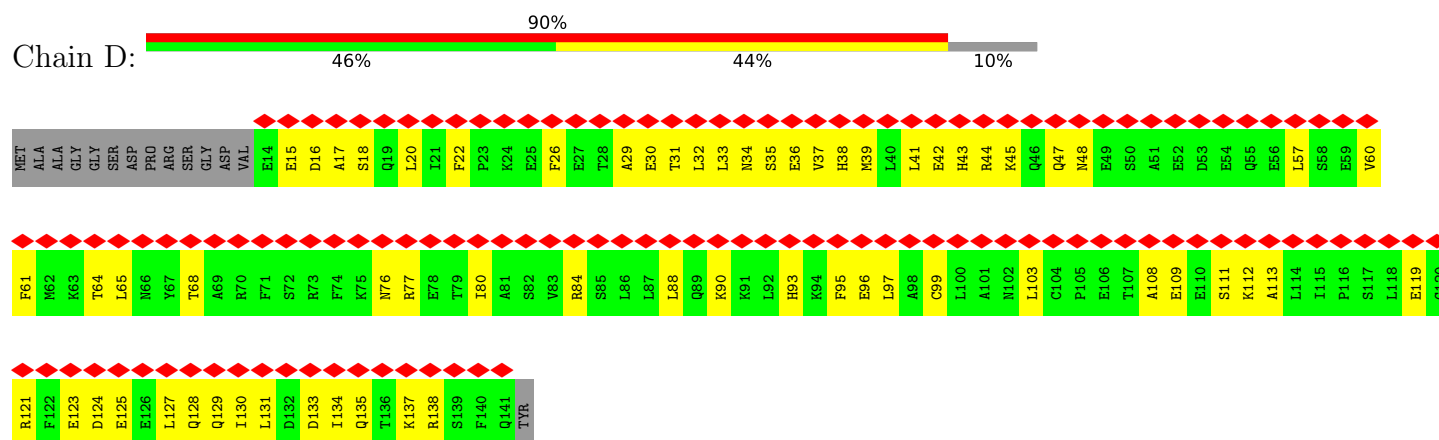
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



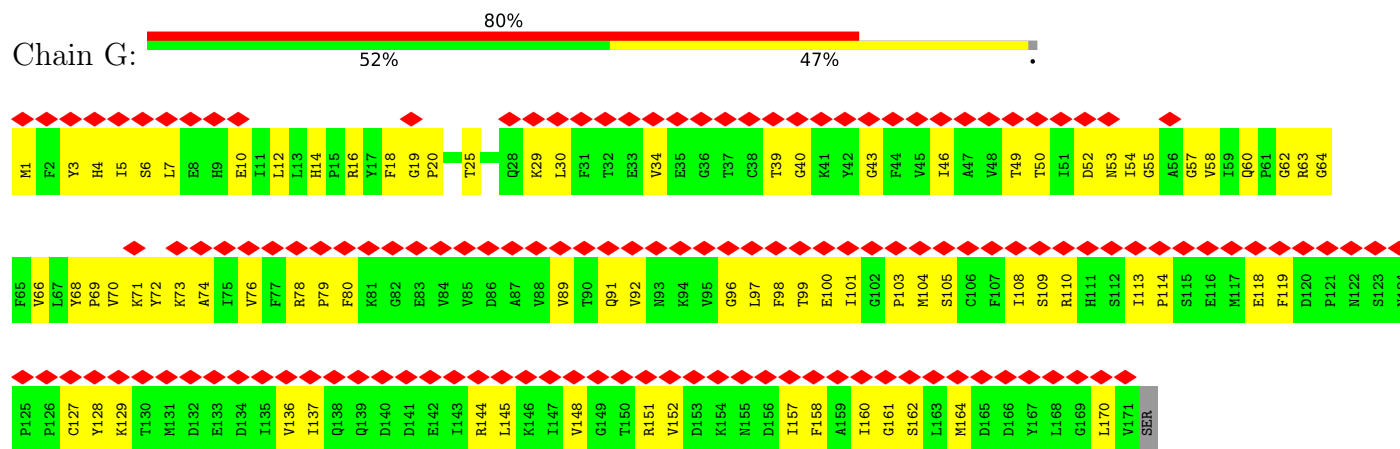
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



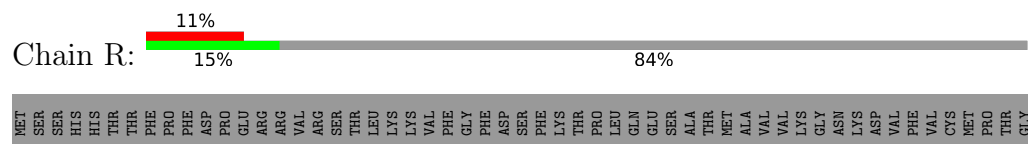
- Molecule 11: Polymerase (RNA) II (DNA directed) polypeptide D

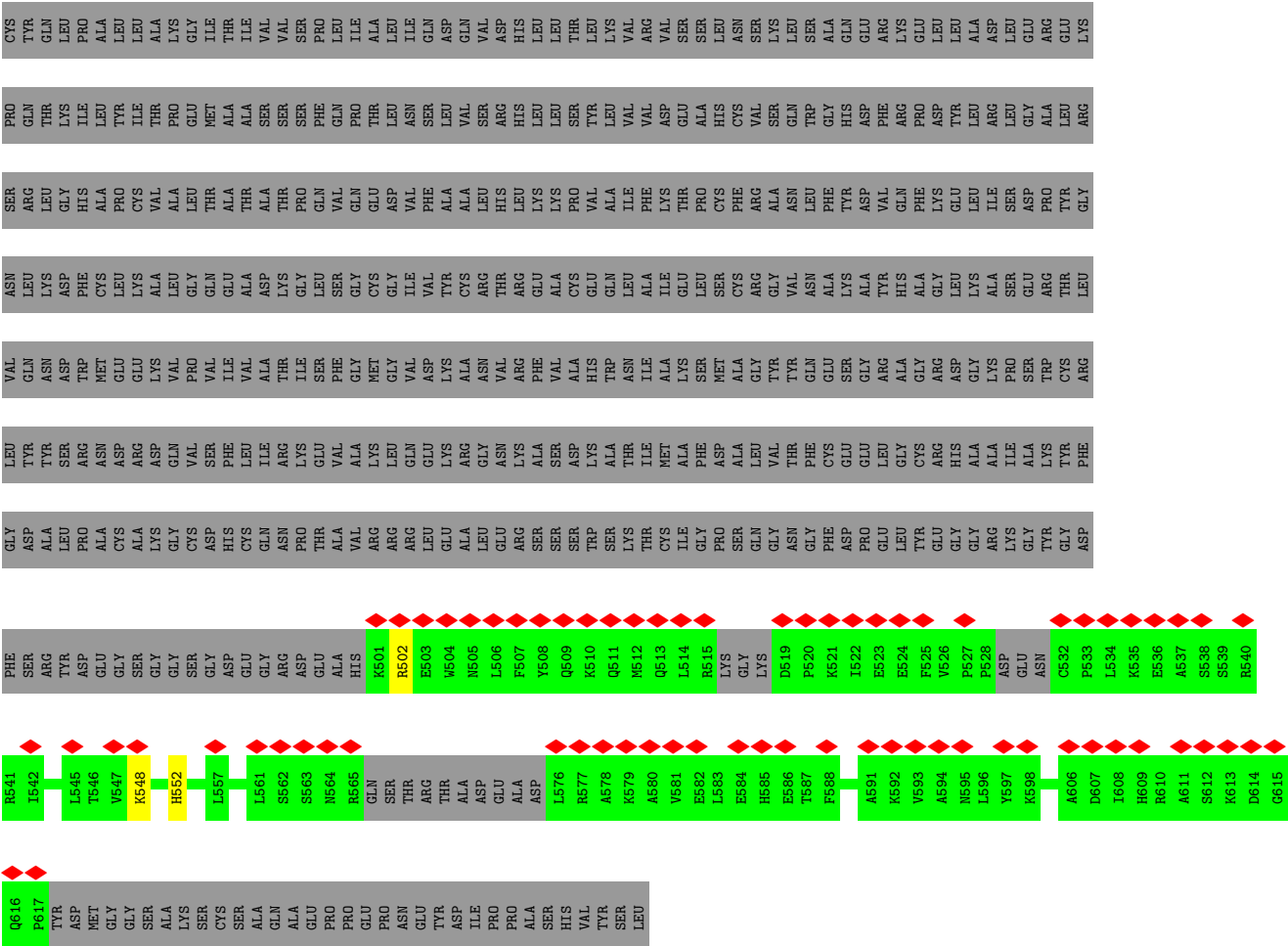


- Molecule 12: DNA-directed RNA polymerase II subunit RPB7

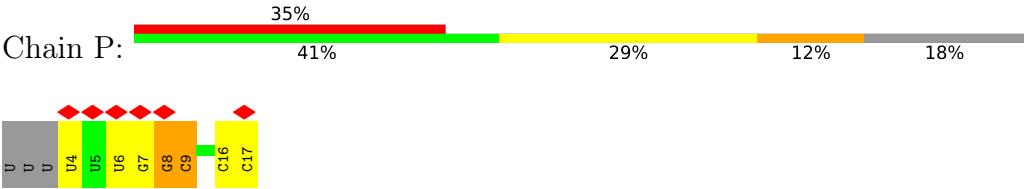


- Molecule 13: ATP-dependent DNA helicase Q5

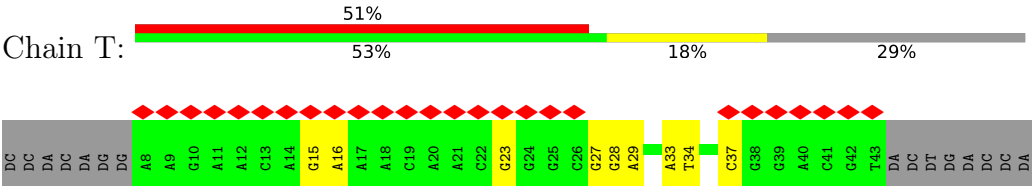




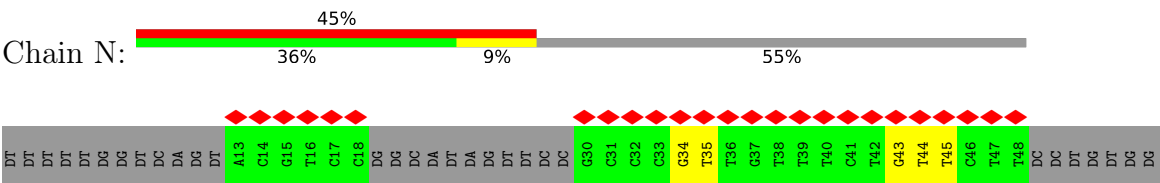
• Molecule 14: RNA, DNA-RNA ELONGATION SCAFFOLD



• Molecule 15: DNA, DNA-RNA ELONGATION SCAFFOLD



• Molecule 16: DNA (55-MER)



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24526	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.998	Depositor
Minimum map value	-0.523	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	400.128, 400.128, 400.128	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8336, 0.8336, 0.8336	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.31	0/11122	0.47	0/15020
2	B	0.33	0/9023	0.44	0/12186
3	C	0.36	0/2082	0.46	0/2830
4	E	0.32	0/1718	0.48	0/2324
5	F	0.32	0/633	0.43	0/856
6	H	0.35	0/1193	0.47	0/1611
7	I	0.31	0/942	0.43	0/1276
8	J	0.37	0/529	0.44	0/714
9	K	0.32	0/939	0.44	0/1271
10	L	0.34	0/373	0.51	0/496
11	D	0.28	0/1019	0.42	0/1374
12	G	0.35	0/1365	0.50	0/1853
13	R	0.56	0/687	0.85	1/939 (0.1%)
14	P	0.27	0/325	0.77	0/503
15	T	0.56	0/844	0.87	1/1301 (0.1%)
16	N	0.53	0/557	1.04	0/854
All	All	0.34	0/33351	0.51	2/45408 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	R	502	ARG	NE-CZ-NH2	7.38	123.99	120.30
15	T	28	DG	O4'-C4'-C3'	-6.21	102.02	104.50

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10926	0	11040	251	0
2	B	8848	0	8845	143	0
3	C	2039	0	1985	54	0
4	E	1687	0	1685	44	0
5	F	623	0	655	12	0
6	H	1172	0	1128	26	0
7	I	921	0	853	24	0
8	J	520	0	536	6	0
9	K	920	0	942	26	0
10	L	368	0	368	9	0
11	D	1005	0	964	54	0
12	G	1334	0	1333	75	0
13	R	679	0	576	2	0
14	P	293	0	149	4	0
15	T	748	0	400	12	0
16	N	503	0	288	11	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	P	1	0	0	0	0
All	All	32595	0	31747	654	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 10.

All (654) 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)
3:C:78:ILE:HD11	3:C:127:VAL:CG2	1.59	1.29
3:C:78:ILE:HD11	3:C:127:VAL:HG22	1.34	1.05
1:A:465:HIS:HB3	1:A:1097:GLU:OE1	1.57	1.05
6:H:96:VAL:HG22	6:H:116:VAL:CG2	1.86	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:111:TYR:CD1	7:I:124:THR:HG21	1.93	1.03
6:H:96:VAL:CG2	6:H:116:VAL:HG22	1.89	1.01
6:H:91:VAL:HG22	6:H:144:LEU:CD2	1.94	0.98
4:E:116:GLN:HE22	15:T:15:DG:H4'	1.28	0.98
6:H:96:VAL:HG22	6:H:116:VAL:HG22	0.98	0.97
3:C:259:LEU:HD22	9:K:91:ILE:CD1	1.95	0.97
3:C:259:LEU:HD22	9:K:91:ILE:HD11	1.46	0.97
2:B:900:GLU:O	2:B:901:THR:HG22	1.68	0.94
3:C:78:ILE:CD1	3:C:127:VAL:CG2	2.46	0.93
9:K:45:ILE:HG22	9:K:94:LEU:CD1	1.98	0.93
4:E:111:THR:HG21	16:N:43:DG:H4'	1.52	0.91
7:I:111:TYR:CD1	7:I:124:THR:CG2	2.53	0.91
1:A:797:ARG:HH11	1:A:820:ARG:HB2	1.34	0.90
9:K:45:ILE:HG22	9:K:94:LEU:HD11	1.51	0.90
1:A:860:ILE:HD13	1:A:1124:LEU:HD23	1.54	0.90
1:A:461:GLN:OE1	15:T:29:DA:H2''	1.73	0.87
3:C:259:LEU:CD2	9:K:91:ILE:HD11	2.05	0.87
1:A:1027:ASP:OD1	1:A:1030:SER:HB2	1.74	0.86
4:E:116:GLN:HE22	15:T:15:DG:C4'	1.86	0.86
1:A:1480:CYS:O	12:G:19:GLY:C	2.14	0.86
4:E:195:ARG:HH22	4:E:205:THR:HG21	1.43	0.84
2:B:332:LYS:NZ	2:B:336:ILE:HD12	1.92	0.84
2:B:21:LEU:O	2:B:21:LEU:HD23	1.78	0.83
1:A:1027:ASP:OD1	1:A:1030:SER:CB	2.26	0.82
6:H:91:VAL:HG22	6:H:144:LEU:HD23	1.60	0.82
10:L:21:GLU:OE2	10:L:39:CYS:SG	2.38	0.82
3:C:128:ILE:HG23	3:C:129:PRO:HD2	1.62	0.82
7:I:111:TYR:CE1	7:I:124:THR:HG21	2.15	0.82
1:A:1374:VAL:HG21	1:A:1411:LEU:HD21	1.62	0.81
1:A:860:ILE:HD11	1:A:1124:LEU:HG	1.63	0.80
2:B:553:LEU:O	2:B:556:ILE:HG22	1.80	0.80
4:E:112:PRO:HB3	15:T:16:DA:H5'	1.63	0.80
3:C:259:LEU:CD2	9:K:91:ILE:CD1	2.60	0.79
1:A:1371:ILE:O	1:A:1374:VAL:HG12	1.83	0.79
1:A:797:ARG:NH1	1:A:820:ARG:HB2	1.99	0.78
4:E:111:THR:CG2	16:N:43:DG:H4'	2.13	0.77
1:A:1054:MET:SD	1:A:1060:LEU:HD12	2.26	0.76
1:A:465:HIS:CB	1:A:1097:GLU:OE1	2.34	0.76
1:A:488:VAL:O	1:A:488:VAL:HG12	1.86	0.76
3:C:78:ILE:HD11	3:C:127:VAL:HG21	1.66	0.75
1:A:375:ILE:HD13	1:A:485:ASN:HD22	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:89:VAL:HA	12:G:99:THR:HG22	1.68	0.74
1:A:200:ALA:HB2	1:A:216:LEU:HG	1.68	0.74
1:A:857:THR:O	1:A:860:ILE:HG22	1.87	0.74
2:B:332:LYS:HZ2	2:B:336:ILE:HD12	1.51	0.74
6:H:103:GLU:HG3	6:H:109:ALA:HB2	1.70	0.73
4:E:195:ARG:HH22	4:E:205:THR:CG2	2.01	0.73
4:E:13:ILE:HD11	4:E:132:GLN:HG3	1.70	0.73
12:G:40:GLY:HA2	12:G:157:ILE:HD11	1.71	0.73
2:B:264:LYS:HB3	2:B:324:ARG:HB3	1.71	0.73
2:B:344:GLN:NE2	2:B:354:SER:O	2.22	0.73
11:D:90:LYS:HE2	11:D:130:ILE:HD11	1.70	0.73
1:A:860:ILE:CD1	1:A:1124:LEU:HD23	2.18	0.72
1:A:323:PRO:HG3	15:T:23:DG:OP1	1.88	0.72
3:C:78:ILE:HD11	3:C:127:VAL:HG23	1.70	0.72
7:I:69:ILE:HG22	7:I:71:ASP:H	1.55	0.72
1:A:860:ILE:CD1	1:A:1124:LEU:CD2	2.67	0.72
4:E:185:ILE:HG21	4:E:209:VAL:HG21	1.72	0.72
2:B:747:LEU:HD22	2:B:810:PHE:CZ	2.25	0.71
4:E:116:GLN:NE2	15:T:15:DG:H4'	2.04	0.71
1:A:57:LEU:HD21	1:A:281:ALA:HB2	1.73	0.71
7:I:84:HIS:ND1	7:I:125:GLU:OE2	2.21	0.71
1:A:811:ILE:HD12	7:I:79:PRO:HB3	1.73	0.71
4:E:55:ARG:HB2	4:E:78:GLU:HG2	1.72	0.71
3:C:190:ASN:ND2	3:C:195:THR:O	2.24	0.71
9:K:45:ILE:CG2	9:K:94:LEU:HD13	2.21	0.70
9:K:45:ILE:CG2	9:K:94:LEU:CD1	2.69	0.70
1:A:1206:ARG:NH1	7:I:33:ARG:HH12	1.88	0.70
1:A:1474:LEU:HB2	5:F:105:ILE:HG13	1.73	0.70
1:A:67:ARG:HA	1:A:78:MET:HG3	1.73	0.70
1:A:860:ILE:HD13	1:A:1124:LEU:CD2	2.21	0.70
1:A:71:CYS:SG	1:A:74:CYS:O	2.50	0.70
5:F:76:CYS:O	12:G:16:ARG:HA	1.92	0.70
1:A:922:PHE:H	1:A:1052:ARG:HD2	1.57	0.69
2:B:86:LEU:HB3	2:B:128:ILE:HD11	1.73	0.69
12:G:100:GLU:HA	12:G:105:SER:HA	1.73	0.69
1:A:1148:ALA:HB1	1:A:1333:GLU:HB3	1.73	0.69
1:A:1371:ILE:HA	1:A:1374:VAL:HG12	1.75	0.69
1:A:845:GLU:OE2	2:B:500:GLN:NE2	2.25	0.69
6:H:32:SER:HB3	6:H:37:MET:H	1.58	0.69
1:A:511:THR:HG23	2:B:1102:PHE:HB2	1.75	0.68
1:A:360:ASP:OD1	2:B:1062:ARG:NH2	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:387:HIS:NE2	2:B:671:GLU:OE2	2.22	0.68
8:J:65:LEU:O	10:L:23:HIS:ND1	2.25	0.68
2:B:353:VAL:O	2:B:353:VAL:HG12	1.93	0.68
1:A:1417:HIS:HD2	16:N:34:DG:O3'	1.76	0.68
2:B:900:GLU:O	2:B:901:THR:CG2	2.40	0.68
3:C:259:LEU:HD22	9:K:91:ILE:HD13	1.73	0.68
12:G:148:VAL:N	12:G:160:ILE:O	2.27	0.68
6:H:91:VAL:HG22	6:H:144:LEU:HD22	1.76	0.68
11:D:34:ASN:O	11:D:68:THR:OG1	2.11	0.67
2:B:274:ARG:NH2	2:B:279:VAL:O	2.25	0.67
1:A:52:PRO:HG2	1:A:65:ILE:HD13	1.76	0.67
1:A:1227:THR:HB	1:A:1230:GLN:HG2	1.77	0.67
3:C:128:ILE:CG2	3:C:129:PRO:HD2	2.23	0.67
12:G:110:ARG:HA	12:G:113:ILE:HD12	1.77	0.67
12:G:152:VAL:HA	12:G:157:ILE:HA	1.76	0.67
1:A:1371:ILE:HD12	1:A:1374:VAL:CG1	2.25	0.67
5:F:75:MET:HE2	12:G:14:HIS:CE1	2.30	0.67
5:F:78:PRO:HD2	12:G:18:PHE:O	1.94	0.67
11:D:108:ALA:N	11:D:128:GLN:OE1	2.27	0.67
1:A:1417:HIS:CD2	16:N:34:DG:O3'	2.48	0.67
11:D:48:ASN:HD22	11:D:57:LEU:HG	1.60	0.67
1:A:79:THR:HA	2:B:1072:ARG:HH22	1.61	0.66
1:A:1343:LEU:N	1:A:1364:GLU:OE2	2.29	0.66
2:B:177:CYS:SG	2:B:738:THR:OG1	2.51	0.66
2:B:197:GLN:OE1	2:B:463:ARG:NH1	2.29	0.66
4:E:80:PRO:HA	4:E:107:GLN:HB2	1.77	0.66
1:A:848:ILE:O	1:A:852:VAL:HG23	1.96	0.66
1:A:883:ILE:HD11	1:A:1424:THR:HG22	1.76	0.66
3:C:205:LYS:NZ	3:C:212:ASP:O	2.22	0.66
1:A:381:PRO:HB3	1:A:480:SER:HA	1.77	0.65
2:B:205:VAL:O	2:B:371:ARG:NH2	2.30	0.65
10:L:37:ARG:O	10:L:38:GLU:HG2	1.97	0.65
11:D:34:ASN:O	11:D:38:HIS:HB2	1.96	0.65
1:A:1182:GLN:HA	1:A:1194:ASN:HD21	1.61	0.65
1:A:1132:LYS:NZ	16:N:34:DG:OP2	2.27	0.64
3:C:190:ASN:O	3:C:193:ARG:NH2	2.29	0.64
4:E:193:ILE:HB	4:E:205:THR:OG1	1.98	0.64
1:A:196:LEU:HD23	1:A:311:GLN:HG3	1.78	0.64
1:A:917:GLU:O	1:A:921:ARG:HB2	1.98	0.64
8:J:47:ARG:NH2	8:J:48:MET:SD	2.71	0.64
1:A:999:ARG:NH1	6:H:103:GLU:OE2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:352:GLY:O	2:B:361:LYS:NZ	2.31	0.63
1:A:904:GLN:NE2	1:A:981:CYS:O	2.31	0.63
1:A:1371:ILE:HD12	1:A:1374:VAL:HG11	1.79	0.63
7:I:111:TYR:HA	7:I:124:THR:HG22	1.80	0.63
3:C:259:LEU:HD21	9:K:87:PHE:HE2	1.62	0.63
4:E:131:LEU:HB2	4:E:134:GLU:HG3	1.81	0.63
2:B:912:ASN:HD21	2:B:916:TYR:HB2	1.64	0.63
2:B:1062:ARG:NH1	2:B:1066:PRO:O	2.32	0.63
1:A:75:ALA:HB2	2:B:1131:ARG:HD3	1.82	0.62
1:A:1341:VAL:HB	1:A:1364:GLU:OE1	1.99	0.62
12:G:91:GLN:HB3	12:G:98:PHE:HB2	1.80	0.62
3:C:78:ILE:CD1	3:C:127:VAL:HG23	2.28	0.62
1:A:26:LEU:HD12	2:B:1166:SER:HA	1.81	0.62
1:A:576:GLN:O	1:A:590:GLN:NE2	2.32	0.62
1:A:1248:ASN:OD1	1:A:1249:ASP:N	2.29	0.62
2:B:501:LEU:HD12	2:B:505:LEU:HD12	1.81	0.62
4:E:81:LYS:NZ	16:N:43:DG:OP1	2.32	0.62
2:B:794:VAL:HG13	2:B:965:ILE:HG23	1.82	0.62
12:G:39:THR:O	12:G:43:GLY:N	2.32	0.61
1:A:1027:ASP:OD1	1:A:1030:SER:N	2.28	0.61
2:B:792:ASP:OD2	2:B:975:ARG:NH1	2.34	0.61
1:A:1343:LEU:HB2	1:A:1364:GLU:OE2	2.01	0.60
5:F:75:MET:HE2	12:G:14:HIS:HE1	1.64	0.60
1:A:551:ARG:NH2	6:H:42:ASP:OD2	2.34	0.60
1:A:1170:THR:HB	7:I:58:ILE:HD11	1.82	0.60
2:B:1142:ASN:HD21	2:B:1145:GLN:HG3	1.67	0.60
4:E:185:ILE:CG2	4:E:209:VAL:HG21	2.31	0.60
11:D:32:LEU:HD11	12:G:4:HIS:HB2	1.83	0.60
9:K:5:PRO:HG2	9:K:8:GLU:HG3	1.84	0.60
11:D:26:PHE:CE2	12:G:78:ARG:HD3	2.35	0.60
3:C:228:ARG:HG2	3:C:228:ARG:O	2.02	0.60
11:D:95:PHE:O	11:D:99:CYS:HB2	2.02	0.60
1:A:1467:GLY:O	1:A:1468:THR:OG1	2.19	0.60
2:B:235:ILE:HD12	2:B:347:MET:HG3	1.83	0.60
4:E:111:THR:HG21	16:N:43:DG:C4'	2.29	0.60
7:I:113:VAL:HG22	7:I:122:ARG:HG2	1.83	0.60
12:G:129:LYS:HB2	12:G:136:VAL:HG22	1.84	0.59
1:A:375:ILE:HD13	1:A:485:ASN:ND2	2.17	0.59
1:A:1138:SER:OG	1:A:1360:ASN:ND2	2.35	0.59
1:A:1371:ILE:O	1:A:1374:VAL:CG1	2.50	0.59
2:B:193:VAL:HG21	2:B:470:LEU:HD13	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:41:LEU:HD12	11:D:68:THR:HG21	1.84	0.59
1:A:284:VAL:O	1:A:288:ASN:ND2	2.35	0.59
1:A:1212:LEU:HB2	1:A:1285:LEU:HD12	1.83	0.59
1:A:1170:THR:HA	1:A:1216:LEU:HD13	1.84	0.59
1:A:1343:LEU:CB	1:A:1364:GLU:OE2	2.51	0.59
2:B:626:LEU:HD23	2:B:662:VAL:HG12	1.83	0.59
11:D:38:HIS:O	11:D:42:GLU:HG2	2.02	0.59
3:C:2:PRO:HB3	9:K:54:PRO:HD2	1.84	0.59
7:I:100:HIS:ND1	7:I:100:HIS:O	2.35	0.59
1:A:1206:ARG:HG2	1:A:1207:ILE:N	2.18	0.59
1:A:506:PRO:HG3	1:A:515:ILE:HD12	1.84	0.59
2:B:198:GLU:OE2	2:B:388:TYR:OH	2.20	0.59
2:B:747:LEU:HD22	2:B:810:PHE:HZ	1.68	0.59
1:A:465:HIS:CG	1:A:1097:GLU:OE1	2.56	0.58
1:A:1480:CYS:O	12:G:19:GLY:CA	2.51	0.58
11:D:111:SER:HB2	11:D:131:LEU:HD21	1.85	0.58
12:G:55:GLY:HA3	12:G:69:PRO:HG2	1.84	0.58
1:A:488:VAL:CG1	1:A:492:TYR:CE2	2.86	0.58
1:A:732:THR:OG1	1:A:735:GLN:HG3	2.03	0.58
5:F:75:MET:CE	12:G:14:HIS:CE1	2.87	0.58
1:A:860:ILE:HD11	1:A:1124:LEU:CG	2.32	0.58
3:C:19:VAL:HG23	3:C:241:PRO:HB2	1.84	0.58
1:A:264:VAL:HB	1:A:272:ASN:HB2	1.86	0.58
7:I:65:LEU:HD21	7:I:124:THR:HG23	1.84	0.58
1:A:18:ILE:HD12	2:B:1171:MET:HB3	1.86	0.58
1:A:1417:HIS:CD2	16:N:34:DG:H4'	2.38	0.58
1:A:560:VAL:HG22	1:A:591:ILE:HD11	1.84	0.58
11:D:84:ARG:O	11:D:88:LEU:HB2	2.04	0.58
2:B:901:THR:HG23	2:B:901:THR:O	2.04	0.58
11:D:95:PHE:O	11:D:99:CYS:CB	2.52	0.58
12:G:4:HIS:CE1	12:G:73:LYS:HB3	2.39	0.58
1:A:376:ASP:HB3	1:A:522:PRO:HD3	1.85	0.57
4:E:45:GLY:HA3	4:E:53:PRO:HD3	1.87	0.57
11:D:31:THR:HG22	12:G:3:TYR:HE1	1.69	0.57
11:D:44:ARG:HH22	11:D:48:ASN:HB2	1.70	0.57
12:G:30:LEU:HD22	12:G:70:VAL:HG11	1.85	0.57
1:A:454:ASP:OD1	1:A:512:ARG:NH1	2.36	0.57
12:G:3:TYR:N	12:G:76:VAL:O	2.29	0.57
4:E:120:ASP:OD1	4:E:121:MET:N	2.38	0.57
1:A:488:VAL:O	1:A:488:VAL:CG1	2.52	0.57
2:B:207:VAL:HG11	2:B:375:ALA:CB	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:7:GLU:OE2	6:H:57:ARG:NH2	2.38	0.57
1:A:461:GLN:OE1	15:T:29:DA:C2'	2.48	0.57
2:B:827:GLU:HG2	2:B:871:VAL:HG22	1.85	0.57
6:H:5:LEU:HD22	6:H:134:GLY:HA3	1.87	0.57
11:D:135:GLN:HA	11:D:138:ARG:HD3	1.88	0.56
1:A:1480:CYS:O	12:G:19:GLY:HA2	2.04	0.56
2:B:617:ASP:OD1	2:B:618:ALA:N	2.37	0.56
1:A:528:PRO:HG2	1:A:1090:LEU:HD11	1.87	0.56
1:A:557:ARG:O	1:A:561:MET:HG2	2.05	0.56
2:B:761:THR:HG23	2:B:1000:THR:HA	1.87	0.56
12:G:101:ILE:N	12:G:104:MET:O	2.37	0.56
1:A:90:LEU:HA	1:A:287:ASN:HD21	1.70	0.56
2:B:98:HIS:O	2:B:106:SER:OG	2.24	0.56
2:B:332:LYS:HZ3	2:B:336:ILE:HD12	1.67	0.56
1:A:1130:ILE:HD11	1:A:1411:LEU:HB3	1.88	0.56
3:C:72:PRO:HG3	8:J:13:ILE:HD11	1.87	0.56
1:A:860:ILE:HD11	1:A:1124:LEU:CD2	2.36	0.55
11:D:124:ASP:O	11:D:128:GLN:HB3	2.06	0.55
1:A:44:PRO:HG3	1:A:284:VAL:HG13	1.87	0.55
1:A:784:VAL:HG22	2:B:978:ILE:HD11	1.88	0.55
1:A:1371:ILE:CA	1:A:1374:VAL:HG12	2.37	0.55
7:I:111:TYR:HD1	7:I:124:THR:CG2	2.14	0.55
11:D:16:ASP:OD2	11:D:18:SER:OG	2.17	0.55
3:C:128:ILE:HG23	3:C:129:PRO:CD	2.36	0.55
1:A:539:GLN:O	2:B:970:HIS:NE2	2.40	0.55
3:C:154:ARG:HG2	3:C:155:LYS:H	1.72	0.55
3:C:158:GLU:OE2	3:C:160:ARG:NH2	2.38	0.55
1:A:77:ASN:HB3	1:A:80:GLU:HG2	1.88	0.55
1:A:289:GLN:HG2	1:A:292:ARG:HH11	1.72	0.55
1:A:422:ASP:OD1	1:A:423:ASN:N	2.40	0.55
1:A:457:ILE:HG13	1:A:515:ILE:HD13	1.88	0.55
11:D:96:GLU:OE2	11:D:121:ARG:NH2	2.40	0.55
6:H:32:SER:OG	6:H:33:GLU:N	2.40	0.55
12:G:60:GLN:OE1	12:G:63:ARG:HD2	2.07	0.55
1:A:659:GLU:OE2	1:A:985:ARG:NH2	2.40	0.54
3:C:9:VAL:HG12	3:C:23:ILE:HD13	1.89	0.54
1:A:1016:LEU:HD22	1:A:1069:LEU:HD22	1.89	0.54
2:B:265:GLN:HG2	2:B:324:ARG:HD3	1.90	0.54
1:A:532:ARG:NH2	1:A:647:THR:O	2.40	0.54
3:C:128:ILE:CG2	3:C:129:PRO:CD	2.85	0.54
1:A:1216:LEU:HB2	1:A:1255:LEU:HD22	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1371:ILE:HD11	1:A:1406:THR:HB	1.88	0.54
1:A:1371:ILE:C	1:A:1374:VAL:HG12	2.26	0.54
6:H:96:VAL:HG13	6:H:115:TYR:O	2.08	0.54
11:D:33:LEU:O	11:D:37:VAL:N	2.37	0.54
2:B:474:THR:HG22	2:B:475:PHE:N	2.23	0.54
1:A:1408:ARG:NH1	1:A:1412:MET:SD	2.81	0.54
9:K:45:ILE:HG21	9:K:94:LEU:HD13	1.90	0.54
2:B:900:GLU:C	2:B:901:THR:HG22	2.28	0.53
4:E:63:ALA:HB1	4:E:68:PRO:HA	1.90	0.53
1:A:1480:CYS:O	12:G:20:PRO:N	2.40	0.53
3:C:9:VAL:HG21	9:K:105:PHE:HA	1.89	0.53
1:A:364:ARG:HB2	2:B:1084:LEU:HD11	1.91	0.53
7:I:64:GLU:OE1	7:I:64:GLU:N	2.41	0.53
10:L:16:ILE:CG2	10:L:25:GLU:HB2	2.38	0.53
2:B:353:VAL:O	2:B:353:VAL:CG1	2.56	0.53
3:C:123:ASN:OD1	3:C:124:SER:N	2.41	0.53
3:C:125:PRO:O	3:C:128:ILE:CD1	2.56	0.53
4:E:25:GLY:O	4:E:65:ASN:ND2	2.28	0.53
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.90	0.53
11:D:48:ASN:ND2	11:D:57:LEU:HG	2.22	0.53
1:A:923:ASP:H	1:A:1052:ARG:NH2	2.07	0.53
1:A:957:GLU:OE2	1:A:960:ARG:NH1	2.40	0.53
3:C:101:PHE:CE2	3:C:122:SER:HB3	2.43	0.53
2:B:491:ARG:O	2:B:499:ARG:NH1	2.42	0.53
7:I:68:ILE:O	7:I:122:ARG:NH2	2.39	0.52
4:E:17:ILE:HG21	4:E:74:VAL:HG11	1.91	0.52
5:F:83:LEU:H	5:F:83:LEU:HD23	1.74	0.52
6:H:37:MET:HE2	6:H:127:GLY:HA3	1.91	0.52
1:A:488:VAL:CG1	1:A:492:TYR:HE2	2.22	0.52
1:A:552:ASP:OD1	6:H:22:PHE:HB3	2.10	0.52
1:A:1474:LEU:CD2	12:G:58:VAL:HG22	2.39	0.52
11:D:17:ALA:HB2	12:G:80:PHE:HB2	1.89	0.52
1:A:609:HIS:ND1	1:A:626:THR:OG1	2.37	0.52
11:D:112:LYS:HB3	11:D:119:GLU:OE2	2.09	0.52
1:A:475:ARG:NH1	9:K:68:GLU:OE1	2.39	0.52
1:A:1146:GLN:HB3	1:A:1153:ARG:HH11	1.75	0.52
12:G:108:ILE:HD11	12:G:145:LEU:HD22	1.92	0.52
1:A:467:MET:HG2	1:A:534:VAL:HG11	1.92	0.52
1:A:1371:ILE:HA	1:A:1374:VAL:CG1	2.40	0.52
1:A:78:MET:O	2:B:1072:ARG:NH1	2.43	0.52
1:A:285:LYS:HA	1:A:288:ASN:HD21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:ILE:CD1	1:A:1411:LEU:HB3	2.40	0.51
2:B:471:ASN:ND2	2:B:477:SER:OG	2.43	0.51
2:B:709:SER:HB2	2:B:767:LEU:HD11	1.91	0.51
3:C:7:PRO:HB2	9:K:101:LEU:HD13	1.92	0.51
2:B:840:MET:O	14:P:4:U:H4'	2.11	0.51
11:D:15:GLU:OE1	12:G:78:ARG:NH2	2.41	0.51
12:G:79:PRO:HG3	12:G:104:MET:SD	2.50	0.51
2:B:760:THR:OG1	2:B:764:MET:SD	2.62	0.51
1:A:1005:HIS:CG	1:A:1007:ILE:HG22	2.46	0.51
1:A:1182:GLN:HA	1:A:1194:ASN:ND2	2.26	0.51
6:H:90:TYR:HB3	6:H:145:MET:HB2	1.92	0.51
11:D:124:ASP:O	11:D:128:GLN:CB	2.59	0.51
5:F:78:PRO:CD	12:G:18:PHE:O	2.59	0.51
1:A:339:LEU:HD23	1:A:342:ARG:HD2	1.91	0.51
1:A:1199:MET:HG2	13:R:552:HIS:CB	2.40	0.51
4:E:37:LEU:O	4:E:41:LYS:HG3	2.10	0.51
2:B:833:THR:HB	2:B:836:THR:HG22	1.93	0.51
1:A:1139:LEU:HD13	1:A:1359:SER:HB3	1.92	0.51
1:A:428:ASP:OD1	1:A:430:ARG:N	2.39	0.50
2:B:50:PHE:HB2	2:B:397:GLY:HA2	1.93	0.50
2:B:415:VAL:HG23	2:B:434:ALA:HB1	1.93	0.50
9:K:104:ARG:HA	9:K:107:VAL:HG12	1.93	0.50
1:A:628:VAL:HA	1:A:638:GLY:HA3	1.93	0.50
1:A:1030:SER:OG	4:E:162:ARG:NE	2.43	0.50
12:G:97:LEU:HB2	12:G:108:ILE:HB	1.92	0.50
12:G:129:LYS:HB3	12:G:136:VAL:HG13	1.93	0.50
2:B:629:GLU:HB2	2:B:634:LEU:HD21	1.93	0.50
1:A:753:GLY:O	1:A:757:GLN:HG2	2.10	0.50
1:A:1173:THR:HG23	7:I:56:ASN:HB3	1.94	0.50
2:B:694:THR:O	2:B:695:HIS:ND1	2.43	0.50
5:F:80:MET:HB3	5:F:101:LYS:HB3	1.92	0.50
7:I:106:ASP:N	7:I:106:ASP:OD1	2.44	0.50
9:K:45:ILE:HG22	9:K:94:LEU:HD13	1.77	0.50
11:D:109:GLU:O	11:D:113:ALA:CB	2.60	0.50
1:A:57:LEU:HD23	1:A:277:THR:HG23	1.94	0.50
2:B:391:LYS:O	2:B:392:ARG:NH2	2.42	0.50
1:A:1206:ARG:HG2	1:A:1207:ILE:H	1.76	0.50
1:A:26:LEU:HD13	1:A:31:LEU:HD21	1.94	0.49
2:B:456:GLN:NE2	15:T:37:DC:OP2	2.45	0.49
3:C:128:ILE:HG22	3:C:132:SER:HB2	1.94	0.49
12:G:52:ASP:H	12:G:72:TYR:HA	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1377:ALA:O	1:A:1381:GLU:HG2	2.12	0.49
4:E:118:LEU:HD22	4:E:127:LEU:HB2	1.93	0.49
12:G:119:PHE:HB2	12:G:128:TYR:HE1	1.76	0.49
2:B:989:VAL:HG22	2:B:1015:LEU:HB2	1.93	0.49
6:H:60:ILE:HG23	6:H:141:VAL:CG1	2.42	0.49
2:B:455:ASP:OD1	2:B:456:GLN:N	2.45	0.49
14:P:8:G:O2'	14:P:9:C:P	2.70	0.49
2:B:677:MET:H	2:B:682:LEU:HD22	1.77	0.49
11:D:134:ILE:O	11:D:138:ARG:HG3	2.12	0.49
12:G:7:LEU:HB2	12:G:72:TYR:CZ	2.47	0.49
1:A:522:PRO:HB2	1:A:662:HIS:HB2	1.93	0.49
6:H:91:VAL:CG2	6:H:144:LEU:CD2	2.82	0.49
12:G:30:LEU:O	12:G:34:VAL:HG22	2.13	0.49
2:B:625:LEU:HD12	2:B:665:ILE:HG13	1.94	0.49
3:C:62:GLU:H	3:C:62:GLU:HG2	1.34	0.49
4:E:71:GLN:HB2	4:E:99:ILE:HD12	1.95	0.49
12:G:1:MET:HB3	12:G:3:TYR:CZ	2.47	0.49
1:A:689:ILE:HD12	2:B:985:LEU:HD22	1.95	0.48
1:A:225:PHE:HB3	1:A:246:GLU:HB3	1.95	0.48
1:A:513:ALA:HB2	5:F:90:LEU:HD21	1.94	0.48
2:B:260:LEU:HB2	2:B:263:ILE:HD12	1.94	0.48
4:E:203:TYR:CE2	4:E:205:THR:CG2	2.97	0.48
1:A:102:LYS:O	1:A:106:VAL:HG12	2.12	0.48
1:A:1258:ARG:NH1	1:A:1260:ARG:HH11	2.10	0.48
11:D:84:ARG:NH2	11:D:97:LEU:HD22	2.27	0.48
11:D:125:GLU:O	11:D:129:GLN:HB2	2.12	0.48
12:G:52:ASP:N	12:G:71:LYS:O	2.46	0.48
2:B:570:ASN:ND2	2:B:616:THR:OG1	2.45	0.48
11:D:42:GLU:OE2	11:D:65:LEU:HD11	2.14	0.48
1:A:1370:GLY:HA2	4:E:178:PRO:HD2	1.96	0.48
10:L:17:TYR:HB3	10:L:44:MET:HB3	1.96	0.48
1:A:859:TYR:HB2	15:T:27:DG:H5''	1.95	0.48
1:A:1481:LYS:HD3	12:G:20:PRO:HA	1.95	0.48
2:B:613:ARG:NH1	2:B:615:TYR:OH	2.42	0.48
11:D:76:ASN:OD1	11:D:77:ARG:N	2.47	0.48
12:G:25:THR:O	12:G:29:LYS:HG2	2.13	0.48
1:A:219:GLU:OE1	1:A:219:GLU:N	2.40	0.48
1:A:488:VAL:HG12	1:A:492:TYR:CE2	2.48	0.48
2:B:731:GLN:OE1	2:B:1053:HIS:NE2	2.44	0.48
2:B:741:HIS:ND1	2:B:742:VAL:HG13	2.29	0.48
2:B:543:GLU:O	2:B:547:GLU:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:870:THR:CG2	2:B:889:LYS:HB3	2.43	0.48
12:G:49:THR:H	12:G:74:ALA:HA	1.78	0.48
1:A:93:PRO:HG2	1:A:219:GLU:HG3	1.96	0.47
1:A:859:TYR:OH	1:A:1433:GLU:OE2	2.27	0.47
1:A:801:GLY:HA3	2:B:503:ASN:HB2	1.96	0.47
1:A:857:THR:O	1:A:860:ILE:CG2	2.59	0.47
4:E:77:PRO:HD2	4:E:105:VAL:O	2.14	0.47
12:G:97:LEU:HD22	12:G:108:ILE:HD12	1.95	0.47
12:G:50:THR:O	12:G:73:LYS:N	2.39	0.47
12:G:114:PRO:HG3	12:G:164:MET:HA	1.96	0.47
1:A:202:TRP:HB2	1:A:212:LYS:N	2.29	0.47
1:A:1230:GLN:O	1:A:1233:GLU:HG3	2.14	0.47
3:C:105:VAL:HG11	3:C:115:VAL:HG22	1.96	0.47
4:E:185:ILE:HD13	4:E:191:VAL:CG1	2.43	0.47
12:G:6:SER:HG	12:G:73:LYS:HZ3	1.55	0.47
1:A:420:ILE:HB	1:A:445:LYS:HB2	1.95	0.47
12:G:92:VAL:HG11	12:G:127:CYS:HA	1.95	0.47
16:N:34:DG:H2'	16:N:35:DT:H72	1.97	0.47
1:A:251:THR:HG23	1:A:252:VAL:HG23	1.95	0.47
1:A:860:ILE:CD1	1:A:1124:LEU:HG	2.38	0.47
2:B:1112:ASP:OD1	2:B:1112:ASP:N	2.47	0.47
11:D:123:GLU:O	11:D:127:LEU:N	2.27	0.47
12:G:162:SER:OG	12:G:164:MET:HG2	2.14	0.47
1:A:808:PRO:HB2	2:B:675:LEU:HD12	1.97	0.47
1:A:927:GLU:OE2	1:A:931:ARG:NH2	2.48	0.47
2:B:924:ARG:NH2	3:C:62:GLU:OE2	2.48	0.47
1:A:488:VAL:HG12	1:A:492:TYR:CD2	2.50	0.47
4:E:112:PRO:CB	15:T:16:DA:H5'	2.39	0.47
1:A:963:ARG:NH1	1:A:967:ARG:HH11	2.12	0.47
2:B:643:LEU:O	2:B:646:ARG:HB2	2.14	0.47
12:G:10:GLU:HG2	12:G:69:PRO:HA	1.96	0.47
1:A:60:PRO:HA	1:A:65:ILE:HD11	1.97	0.46
2:B:1137:CYS:SG	2:B:1140:CYS:HB2	2.55	0.46
1:A:36:VAL:O	1:A:61:ARG:NH1	2.48	0.46
2:B:128:ILE:HG23	2:B:144:HIS:HB2	1.97	0.46
2:B:357:CYS:SG	2:B:361:LYS:NZ	2.74	0.46
2:B:550:MET:HG3	2:B:567:ILE:HD12	1.96	0.46
2:B:867:ILE:HB	2:B:894:THR:HG22	1.97	0.46
4:E:6:GLU:HB3	4:E:48:PRO:HG2	1.97	0.46
1:A:466:LYS:HA	2:B:1093:CYS:SG	2.56	0.46
2:B:95:LYS:HD3	2:B:162:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:VAL:HG12	1:A:243:ALA:HA	1.97	0.46
2:B:528:LEU:HA	2:B:528:LEU:HD23	1.80	0.46
3:C:52:ILE:HD12	3:C:61:ASP:HB3	1.97	0.46
10:L:37:ARG:C	10:L:38:GLU:HG2	2.36	0.46
11:D:45:LYS:HB2	11:D:61:PHE:HZ	1.80	0.46
1:A:927:GLU:HA	1:A:930:LEU:HB2	1.97	0.46
1:A:962:ASP:OD2	1:A:1046:ARG:NH1	2.44	0.46
12:G:137:ILE:HG12	12:G:170:LEU:HB2	1.97	0.46
2:B:1022:LEU:HD23	2:B:1022:LEU:H	1.80	0.46
8:J:35:LEU:HD11	8:J:50:LEU:HG	1.97	0.46
1:A:111:CYS:SG	1:A:188:GLN:NE2	2.79	0.46
2:B:384:ASP:OD1	2:B:384:ASP:N	2.48	0.46
12:G:108:ILE:HG12	12:G:161:GLY:C	2.36	0.46
1:A:631:GLU:OE1	1:A:992:LYS:NZ	2.35	0.46
7:I:14:ILE:HG23	7:I:23:MET:HG3	1.97	0.46
5:F:66:LEU:HD21	5:F:97:LEU:HD22	1.98	0.45
11:D:125:GLU:O	11:D:129:GLN:CB	2.64	0.45
11:D:131:LEU:O	11:D:135:GLN:HG2	2.16	0.45
1:A:25:VAL:HG13	1:A:247:TRP:HE3	1.81	0.45
1:A:70:ARG:HB3	1:A:76:GLY:H	1.82	0.45
1:A:406:VAL:HG11	1:A:419:ILE:HD11	1.98	0.45
3:C:40:ALA:O	3:C:170:GLY:N	2.48	0.45
4:E:151:MET:HE1	4:E:159:LEU:HD13	1.98	0.45
6:H:112:LEU:HB2	6:H:132:LEU:HD23	1.97	0.45
8:J:66:GLU:HA	10:L:23:HIS:HB3	1.97	0.45
9:K:12:LEU:HD11	9:K:18:LYS:HD3	1.98	0.45
1:A:996:ILE:HD13	1:A:1060:LEU:HA	1.98	0.45
1:A:1147:SER:HB3	1:A:1153:ARG:HB3	1.98	0.45
2:B:161:CYS:SG	2:B:162:LEU:N	2.89	0.45
12:G:10:GLU:HA	12:G:68:TYR:O	2.16	0.45
15:T:33:DA:H2'	15:T:34:DT:H71	1.99	0.45
4:E:116:GLN:HE22	15:T:15:DG:C3'	2.27	0.45
4:E:203:TYR:CE2	4:E:205:THR:HG22	2.52	0.45
11:D:109:GLU:O	11:D:113:ALA:HB2	2.17	0.45
14:P:8:G:O2'	14:P:9:C:OP1	2.33	0.45
2:B:747:LEU:HD22	2:B:810:PHE:CE1	2.52	0.45
7:I:91:HIS:ND1	7:I:116:ALA:HB2	2.31	0.45
1:A:860:ILE:CD1	1:A:1124:LEU:CG	2.94	0.45
7:I:111:TYR:CD1	7:I:124:THR:HG22	2.49	0.45
1:A:1474:LEU:HA	12:G:57:GLY:O	2.17	0.45
11:D:84:ARG:O	11:D:88:LEU:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:93:HIS:HB3	11:D:96:GLU:HG3	1.98	0.45
2:B:274:ARG:HH11	2:B:308:ALA:HB1	1.81	0.45
2:B:809:VAL:HG12	2:B:810:PHE:N	2.32	0.45
3:C:57:SER:OG	3:C:58:VAL:N	2.50	0.45
1:A:535:MET:O	1:A:669:TYR:OH	2.26	0.45
1:A:1054:MET:SD	1:A:1060:LEU:CD1	2.99	0.45
1:A:893:GLU:OE1	4:E:197:SER:OG	2.21	0.44
1:A:911:PRO:O	1:A:963:ARG:NH1	2.40	0.44
2:B:466:VAL:HG12	2:B:467:SER:N	2.32	0.44
3:C:40:ALA:HB1	3:C:171:LYS:HG3	1.99	0.44
6:H:51:ASP:OD1	6:H:51:ASP:N	2.50	0.44
2:B:389:GLY:O	2:B:668:LEU:HD23	2.17	0.44
3:C:42:VAL:HB	3:C:178:PRO:HG3	2.00	0.44
1:A:44:PRO:HA	1:A:57:LEU:HD11	2.00	0.44
2:B:534:VAL:N	2:B:600:GLU:OE2	2.31	0.44
1:A:488:VAL:HG11	1:A:492:TYR:HE2	1.82	0.44
1:A:1282:ASP:OD1	1:A:1282:ASP:N	2.50	0.44
4:E:38:GLU:OE1	4:E:41:LYS:HD2	2.18	0.44
11:D:22:PHE:CE2	11:D:93:HIS:HE1	2.35	0.44
2:B:280:SER:OG	2:B:283:ASP:OD2	2.35	0.44
2:B:332:LYS:HE3	2:B:332:LYS:HB3	1.86	0.44
12:G:53:ASN:OD1	12:G:54:ILE:N	2.51	0.44
1:A:511:THR:HG21	2:B:1102:PHE:HD1	1.83	0.44
2:B:220:GLU:HB3	2:B:236:TRP:CD1	2.53	0.44
2:B:1040:GLN:HG2	3:C:203:TRP:CH2	2.53	0.44
4:E:103:LEU:HD23	4:E:128:GLU:HB2	1.99	0.44
10:L:52:LEU:H	10:L:52:LEU:HG	1.72	0.44
11:D:43:HIS:O	11:D:47:GLN:HG3	2.18	0.44
12:G:12:LEU:HA	12:G:66:VAL:O	2.18	0.44
1:A:456:VAL:HG21	1:A:503:LEU:HD11	2.00	0.44
1:A:1436:VAL:O	1:A:1440:MET:HG3	2.17	0.44
2:B:28:ILE:HD13	2:B:644:LYS:HB3	2.00	0.44
7:I:95:VAL:HG12	7:I:113:VAL:O	2.18	0.44
11:D:65:LEU:HA	11:D:68:THR:HG22	1.99	0.44
1:A:583:ARG:HH22	6:H:47:ILE:HD12	1.83	0.43
2:B:19:PRO:C	2:B:21:LEU:H	2.20	0.43
2:B:22:TRP:CE2	2:B:679:PRO:HG2	2.52	0.43
2:B:98:HIS:HB2	2:B:108:MET:HB2	2.00	0.43
4:E:77:PRO:HG3	4:E:90:TYR:HE2	1.83	0.43
11:D:20:LEU:HD22	11:D:93:HIS:ND1	2.33	0.43
1:A:636:ILE:HG22	1:A:637:MET:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:VAL:HG11	1:A:669:TYR:CZ	2.52	0.43
2:B:412:LEU:HD23	2:B:412:LEU:HA	1.82	0.43
2:B:509:VAL:HG11	2:B:524:LYS:HD2	2.00	0.43
4:E:55:ARG:CZ	4:E:107:GLN:HE22	2.31	0.43
11:D:35:SER:O	11:D:39:MET:HG3	2.18	0.43
1:A:569:THR:HG23	1:A:671:ASN:HD21	1.83	0.43
2:B:271:ILE:HG21	2:B:320:PHE:CD2	2.54	0.43
7:I:24:LEU:HD23	7:I:39:CYS:HB3	2.00	0.43
2:B:1088:GLU:O	2:B:1091:ARG:HG3	2.19	0.43
3:C:128:ILE:CG2	3:C:132:SER:HB2	2.48	0.43
5:F:75:MET:HE1	12:G:14:HIS:ND1	2.33	0.43
16:N:44:DT:H2'	16:N:45:DT:H72	2.00	0.43
1:A:76:GLY:HA2	1:A:81:CYS:HB2	1.99	0.43
1:A:1307:VAL:HG13	1:A:1338:THR:HG22	2.01	0.43
11:D:29:ALA:HA	12:G:5:ILE:HG22	1.99	0.43
12:G:12:LEU:HD21	12:G:60:GLN:HE22	1.83	0.43
1:A:583:ARG:HH12	6:H:47:ILE:HD11	1.84	0.43
1:A:1214:VAL:HG22	1:A:1257:LEU:HB3	2.01	0.43
1:A:44:PRO:HA	1:A:57:LEU:CD1	2.49	0.43
1:A:108:ARG:HG3	1:A:191:ILE:HD12	2.00	0.43
1:A:1136:THR:HG22	1:A:1136:THR:O	2.19	0.43
3:C:61:ASP:N	3:C:61:ASP:OD1	2.51	0.43
12:G:152:VAL:HB	12:G:157:ILE:HG12	1.99	0.43
1:A:137:PRO:O	1:A:140:ARG:HG2	2.19	0.42
1:A:276:LEU:HD11	1:A:339:LEU:HD21	2.00	0.42
1:A:686:THR:OG1	1:A:687:ILE:N	2.52	0.42
1:A:1146:GLN:OE1	1:A:1149:ARG:NH1	2.42	0.42
2:B:567:ILE:HD11	2:B:577:HIS:HB2	2.01	0.42
2:B:666:ASP:OD1	2:B:666:ASP:N	2.43	0.42
9:K:24:ASP:HB3	9:K:30:ALA:HB3	2.01	0.42
11:D:64:THR:HG21	12:G:46:ILE:HG23	2.01	0.42
11:D:108:ALA:HB2	11:D:128:GLN:HB2	2.01	0.42
1:A:136:GLN:HA	1:A:137:PRO:HD2	1.93	0.42
1:A:362:SER:HA	1:A:503:LEU:O	2.19	0.42
1:A:389:THR:HG21	1:A:417:LYS:HE2	2.00	0.42
1:A:541:THR:HG23	1:A:676:ILE:HB	2.01	0.42
1:A:890:ARG:HD3	1:A:890:ARG:HA	1.93	0.42
1:A:1130:ILE:O	1:A:1130:ILE:HG13	2.19	0.42
9:K:100:LEU:HD11	9:K:104:ARG:HE	1.84	0.42
1:A:510:GLU:OE2	2:B:1101:GLN:NE2	2.52	0.42
2:B:537:GLN:OE1	2:B:537:GLN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1035:ARG:NH2	2:B:1036:LYS:O	2.52	0.42
4:E:47:LYS:O	4:E:51:GLY:HA3	2.18	0.42
2:B:403:LEU:HD21	2:B:447:SER:HB2	2.01	0.42
3:C:33:SER:CB	9:K:45:ILE:HD11	2.48	0.42
12:G:62:GLY:O	12:G:64:GLY:N	2.50	0.42
1:A:416:ALA:HA	1:A:448:ARG:HA	2.01	0.42
1:A:465:HIS:ND1	1:A:1097:GLU:OE2	2.52	0.42
1:A:797:ARG:NH1	1:A:820:ARG:CB	2.78	0.42
1:A:1375:ARG:NH1	1:A:1379:GLU:OE1	2.49	0.42
11:D:103:LEU:HB3	12:G:144:ARG:HH22	1.85	0.42
1:A:365:THR:OG1	1:A:366:VAL:N	2.53	0.42
1:A:922:PHE:HB2	1:A:1052:ARG:HB2	2.02	0.42
1:A:927:GLU:HG3	1:A:943:LEU:HD11	2.01	0.42
1:A:1075:LYS:HD3	1:A:1075:LYS:HA	1.79	0.42
12:G:62:GLY:O	12:G:63:ARG:HG2	2.20	0.42
12:G:62:GLY:C	12:G:64:GLY:H	2.22	0.42
1:A:568:SER:OG	1:A:671:ASN:OD1	2.33	0.42
1:A:894:ASP:OD1	1:A:1396:ARG:NH1	2.53	0.42
2:B:118:LEU:HD23	2:B:913:GLN:HG2	2.01	0.42
2:B:556:ILE:CD1	2:B:576:ILE:HD11	2.50	0.42
2:B:1115:GLN:HG2	2:B:1150:ARG:HD2	2.00	0.42
1:A:465:HIS:CG	1:A:1097:GLU:OE2	2.73	0.42
1:A:991:GLN:HA	1:A:996:ILE:HD12	2.01	0.42
1:A:1195:VAL:O	1:A:1198:GLU:HG3	2.19	0.42
2:B:825:GLN:HB2	2:B:826:GLU:H	1.72	0.42
12:G:151:ARG:O	12:G:158:PHE:N	2.28	0.42
3:C:13:GLU:OE2	3:C:18:ASN:ND2	2.53	0.42
3:C:72:PRO:HG3	8:J:13:ILE:CD1	2.50	0.42
7:I:15:ARG:HD2	7:I:37:TYR:CE2	2.55	0.42
11:D:20:LEU:HD12	11:D:121:ARG:HH12	1.85	0.42
1:A:710:LYS:HG2	1:A:817:PRO:HG3	2.01	0.41
2:B:1129:ASN:O	2:B:1133:HIS:N	2.52	0.41
3:C:242:GLU:HG2	9:K:109:ILE:HD12	2.01	0.41
9:K:42:LEU:HD23	9:K:42:LEU:HA	1.90	0.41
1:A:465:HIS:CG	1:A:1097:GLU:CD	2.94	0.41
1:A:465:HIS:CE1	1:A:1097:GLU:OE2	2.73	0.41
1:A:546:ARG:HD3	1:A:772:SER:HB3	2.02	0.41
2:B:520:VAL:HG13	2:B:520:VAL:O	2.20	0.41
2:B:626:LEU:HG	2:B:698:ILE:HD13	2.02	0.41
12:G:96:GLY:HA3	12:G:109:SER:HA	2.01	0.41
1:A:283:ILE:HG12	1:A:313:HIS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:VAL:O	1:A:539:GLN:HG2	2.20	0.41
1:A:556:GLU:HG3	1:A:557:ARG:H	1.83	0.41
1:A:580:LEU:HD23	1:A:580:LEU:O	2.21	0.41
1:A:865:ILE:HG21	2:B:1092:ASP:CG	2.41	0.41
12:G:52:ASP:OD1	12:G:73:LYS:HG2	2.19	0.41
1:A:233:CYS:SG	1:A:238:MET:HG3	2.60	0.41
11:D:60:VAL:HG13	12:G:103:PRO:HB3	2.01	0.41
1:A:499:ASP:OD1	14:P:16:C:H4'	2.21	0.41
1:A:1408:ARG:HH22	1:A:1422:GLN:HA	1.86	0.41
1:A:543:THR:HB	2:B:970:HIS:HE2	1.84	0.41
1:A:1226:LEU:HD23	1:A:1226:LEU:HA	1.91	0.41
2:B:870:THR:HG21	2:B:889:LYS:HB3	2.03	0.41
2:B:1116:VAL:O	2:B:1148:LEU:HD12	2.21	0.41
11:D:30:GLU:O	12:G:3:TYR:HA	2.20	0.41
12:G:118:GLU:HG2	12:G:129:LYS:O	2.20	0.41
12:G:119:PHE:HA	12:G:128:TYR:HD1	1.85	0.41
1:A:57:LEU:HD23	1:A:277:THR:CG2	2.50	0.41
1:A:541:THR:HG21	1:A:672:ILE:HG22	2.03	0.41
1:A:802:PHE:HD2	2:B:671:GLU:HG2	1.86	0.41
1:A:1143:LEU:HD13	1:A:1147:SER:HB2	2.03	0.41
2:B:124:LEU:HD22	2:B:152:ILE:HD11	2.02	0.41
2:B:535:GLY:HA3	2:B:618:ALA:HB2	2.03	0.41
2:B:699:HIS:CE1	2:B:701:SER:HG	2.33	0.41
6:H:36:LYS:HA	6:H:36:LYS:HD3	1.90	0.41
10:L:37:ARG:O	10:L:38:GLU:CG	2.66	0.41
1:A:777:SER:OG	1:A:780:ASN:OD1	2.32	0.41
2:B:20:ASP:OD1	2:B:20:ASP:N	2.53	0.41
2:B:274:ARG:HD2	2:B:311:ILE:HG22	2.03	0.41
2:B:624:PRO:HA	2:B:663:GLU:O	2.21	0.41
2:B:1111:SER:O	2:B:1113:PRO:HD3	2.21	0.41
3:C:205:LYS:NZ	3:C:213:GLU:HA	2.36	0.41
3:C:214:ASP:OD1	3:C:215:GLU:N	2.54	0.41
4:E:195:ARG:NH2	4:E:205:THR:CG2	2.77	0.41
11:D:33:LEU:HB2	11:D:36:GLU:HG3	2.02	0.41
11:D:34:ASN:O	11:D:38:HIS:CB	2.66	0.41
1:A:412:GLN:OE1	1:A:412:GLN:N	2.53	0.41
1:A:428:ASP:OD1	1:A:429:LEU:N	2.54	0.41
1:A:530:SER:O	1:A:532:ARG:HG3	2.20	0.41
1:A:917:GLU:OE2	1:A:921:ARG:NH2	2.54	0.41
2:B:604:ILE:CD1	2:B:668:LEU:CD1	2.99	0.41
12:G:97:LEU:HB3	12:G:99:THR:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:334:LYS:HD3	2:B:334:LYS:HA	1.73	0.40
2:B:553:LEU:HD23	2:B:553:LEU:HA	1.88	0.40
2:B:817:GLN:HB3	2:B:918:PHE:HD1	1.86	0.40
4:E:150:VAL:HG22	4:E:185:ILE:HD11	2.03	0.40
11:D:35:SER:HB3	11:D:80:ILE:HD11	2.02	0.40
1:A:374:SER:OG	1:A:377:GLN:OE1	2.37	0.40
1:A:775:LYS:HE2	1:A:775:LYS:HB2	1.95	0.40
2:B:604:ILE:HG12	2:B:668:LEU:HD12	2.03	0.40
2:B:854:ILE:O	2:B:907:VAL:HG21	2.21	0.40
2:B:912:ASN:ND2	2:B:916:TYR:HB2	2.33	0.40
3:C:128:ILE:HG22	3:C:129:PRO:N	2.36	0.40
3:C:188:PRO:HD3	3:C:230:TYR:HE1	1.87	0.40
3:C:203:TRP:HA	3:C:204:PRO:HD3	1.98	0.40
6:H:104:THR:OG1	6:H:105:SER:N	2.55	0.40
9:K:45:ILE:CG2	9:K:94:LEU:CD2	2.99	0.40
1:A:275:ASP:HB3	1:A:336:LEU:HD22	2.03	0.40
1:A:865:ILE:O	1:A:869:GLU:HB3	2.21	0.40
1:A:909:LEU:HD21	1:A:973:GLY:HA2	2.02	0.40
1:A:1199:MET:CE	13:R:548:LYS:O	2.69	0.40
1:A:1353:ASP:HA	1:A:1354:PRO:HD3	1.95	0.40
9:K:39:ASP:N	9:K:39:ASP:OD1	2.53	0.40
12:G:43:GLY:HA2	12:G:157:ILE:HD12	2.03	0.40
1:A:579:ILE:HB	1:A:585:LEU:HB2	2.03	0.40
1:A:693:ILE:HG12	1:A:828:LEU:HD21	2.04	0.40
1:A:764:ASN:OD1	1:A:766:PHE:HB2	2.22	0.40
1:A:1228:MET:SD	1:A:1255:LEU:HD21	2.62	0.40
2:B:65:ILE:HD11	2:B:412:LEU:HD22	2.02	0.40
3:C:240:ARG:HE	3:C:240:ARG:HB2	1.70	0.40
4:E:17:ILE:HD13	4:E:17:ILE:HA	1.93	0.40
6:H:35:PHE:HB3	6:H:37:MET:HG3	2.04	0.40
16:N:43:DG:H2'	16:N:44:DT:H72	2.03	0.40
1:A:1422:GLN:H	1:A:1422:GLN:HG3	1.71	0.40
2:B:1062:ARG:CZ	2:B:1074:PRO:HB3	2.52	0.40
7:I:54:TYR:CE2	7:I:56:ASN:HB2	2.57	0.40
11:D:133:ASP:O	11:D:137:LYS:HG2	2.21	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	1365/1970 (69%)	1282 (94%)	82 (6%)	1 (0%)	48	82
2	B	1102/1174 (94%)	1033 (94%)	69 (6%)	0	100	100
3	C	251/275 (91%)	238 (95%)	13 (5%)	0	100	100
4	E	207/210 (99%)	205 (99%)	1 (0%)	1 (0%)	25	62
5	F	76/127 (60%)	72 (95%)	4 (5%)	0	100	100
6	H	146/150 (97%)	137 (94%)	9 (6%)	0	100	100
7	I	112/125 (90%)	107 (96%)	5 (4%)	0	100	100
8	J	64/67 (96%)	62 (97%)	2 (3%)	0	100	100
9	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
10	L	42/58 (72%)	39 (93%)	3 (7%)	0	100	100
11	D	126/142 (89%)	121 (96%)	5 (4%)	0	100	100
12	G	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
13	R	93/650 (14%)	93 (100%)	0	0	100	100
All	All	3866/5237 (74%)	3663 (95%)	201 (5%)	2 (0%)	50	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	PHE
4	E	48	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	1208/1749 (69%)	1198 (99%)	10 (1%)	79	84
2	B	963/1027 (94%)	955 (99%)	8 (1%)	79	84
3	C	230/252 (91%)	228 (99%)	2 (1%)	75	83
4	E	183/190 (96%)	180 (98%)	3 (2%)	58	73
5	F	67/111 (60%)	66 (98%)	1 (2%)	60	74
6	H	126/131 (96%)	125 (99%)	1 (1%)	79	84
7	I	101/112 (90%)	101 (100%)	0	100	100
8	J	54/56 (96%)	53 (98%)	1 (2%)	52	69
9	K	104/106 (98%)	104 (100%)	0	100	100
10	L	40/55 (73%)	39 (98%)	1 (2%)	42	62
11	D	106/127 (84%)	106 (100%)	0	100	100
12	G	147/153 (96%)	147 (100%)	0	100	100
13	R	57/545 (10%)	57 (100%)	0	100	100
All	All	3386/4614 (73%)	3359 (99%)	27 (1%)	77	84

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	PHE
1	A	112	PHE
1	A	374	SER
1	A	432	HIS
1	A	457	ILE
1	A	483	ARG
1	A	567	LEU
1	A	1129	ASN
1	A	1189	ASP
1	A	1396	ARG
2	B	20	ASP
2	B	307	GLU
2	B	388	TYR
2	B	806	PHE
2	B	825	GLN
2	B	952	GLU
2	B	1022	LEU
2	B	1106	ARG
3	C	62	GLU
3	C	63	PHE

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Mol	Chain	Res	Type
4	E	49	SER
4	E	91	CYS
4	E	153	LYS
5	F	83	LEU
6	H	65	TYR
8	J	47	ARG
10	L	52	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	288	ASN
1	A	1129	ASN
1	A	1190	GLN
1	A	1194	ASN
1	A	1360	ASN
1	A	1417	HIS
2	B	790	GLN
3	C	217	GLN
4	E	116	GLN
11	D	48	ASN
11	D	93	HIS
12	G	4	HIS
12	G	14	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	13/17 (76%)	3 (23%)	2 (15%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	7	G
14	P	9	C
14	P	17	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	P	6	U
14	P	8	G

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

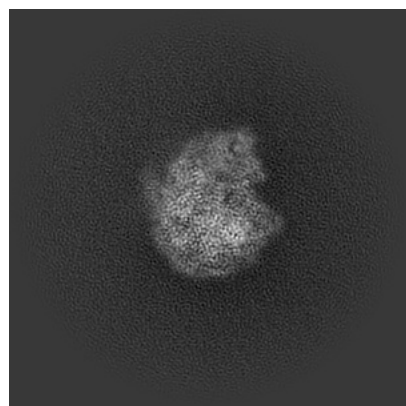
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18573. These allow visual inspection of the internal detail of the map and identification of artifacts.

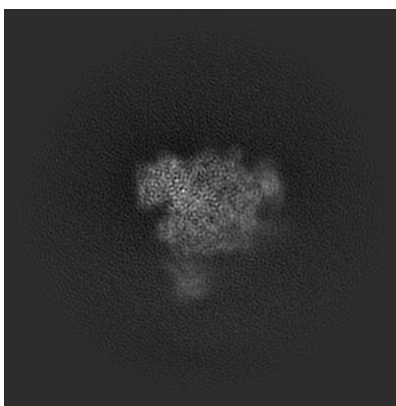
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

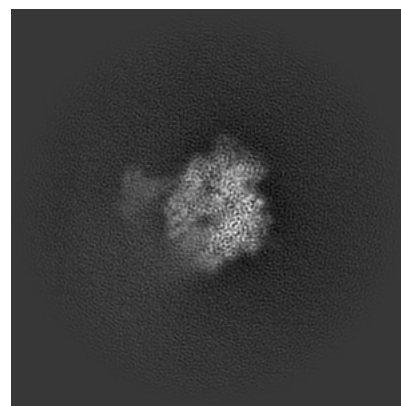
#### 6.1.1 Primary map



X

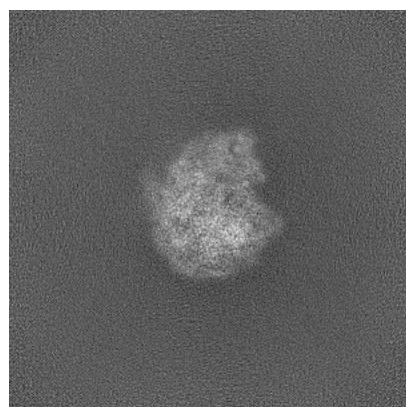


Y

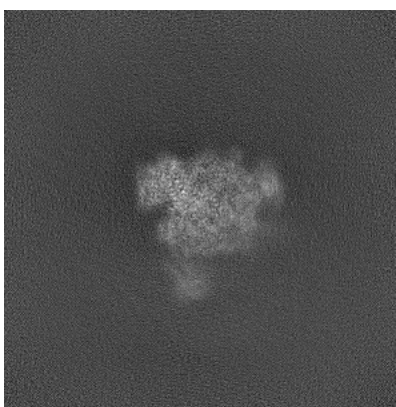


Z

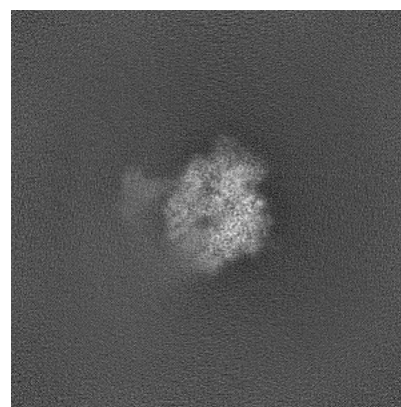
#### 6.1.2 Raw map



X



Y

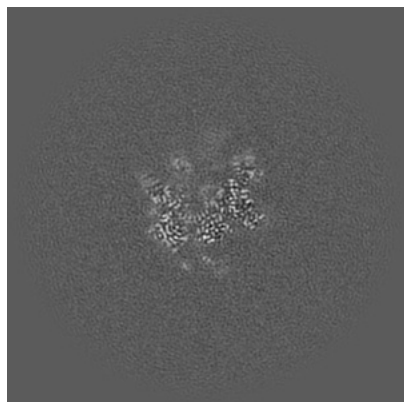


Z

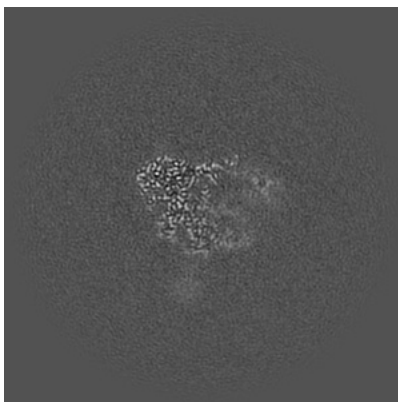
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

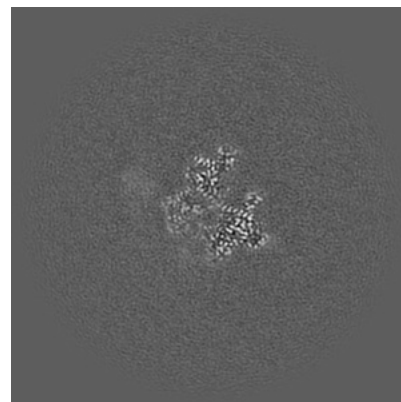
### 6.2.1 Primary map



X Index: 240



Y Index: 240

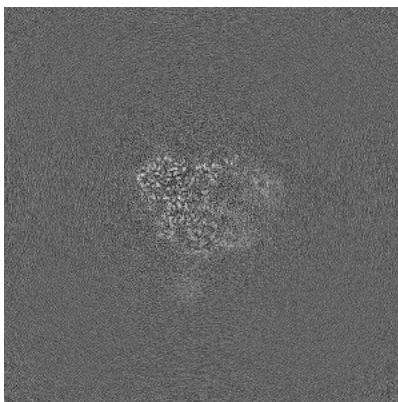


Z Index: 240

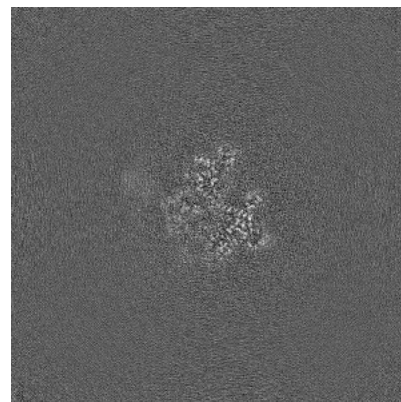
### 6.2.2 Raw map



X Index: 240



Y Index: 240



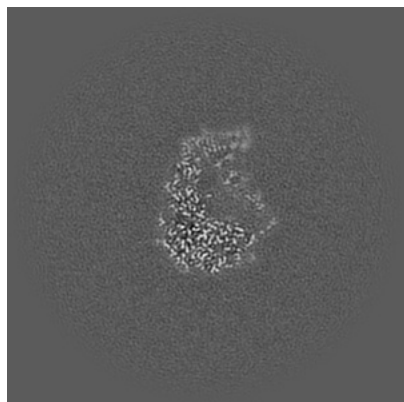
Z Index: 240

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

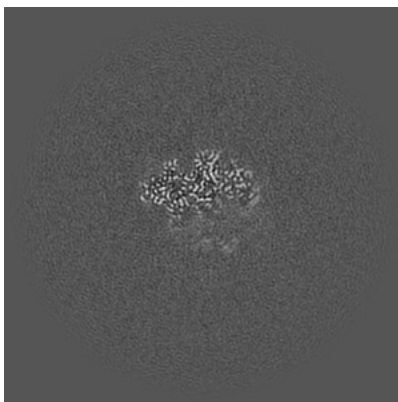


## 6.3 Largest variance slices [i](#)

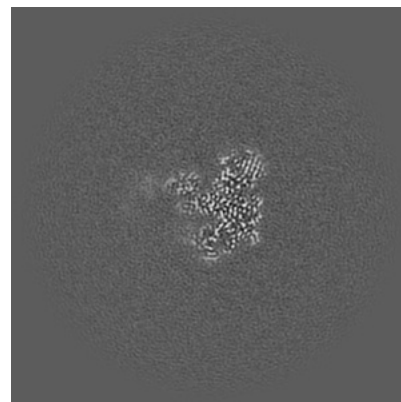
### 6.3.1 Primary map



X Index: 269

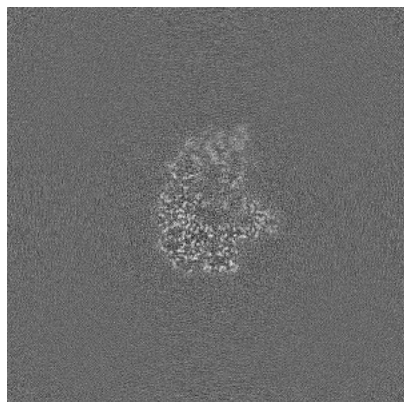


Y Index: 208

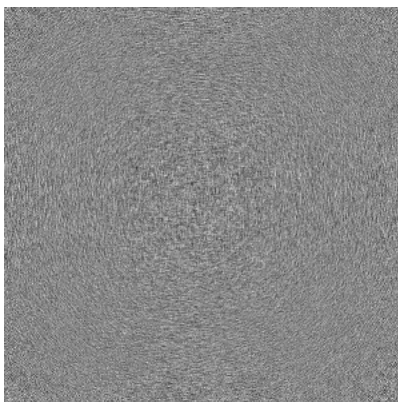


Z Index: 204

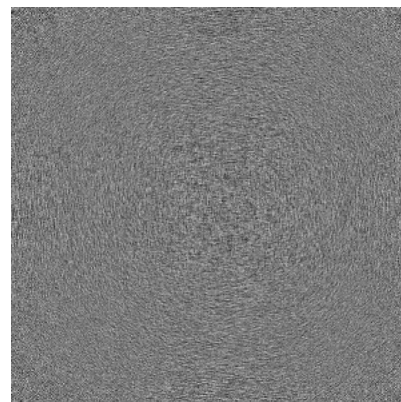
### 6.3.2 Raw map



X Index: 260



Y Index: 0

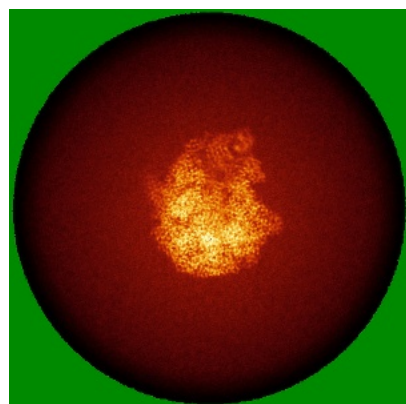


Z Index: 0

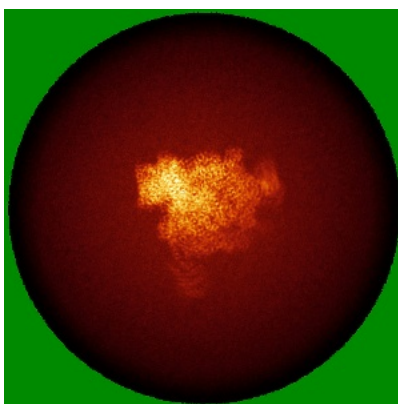
The images above show the largest variance slices of the map in three orthogonal directions.

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

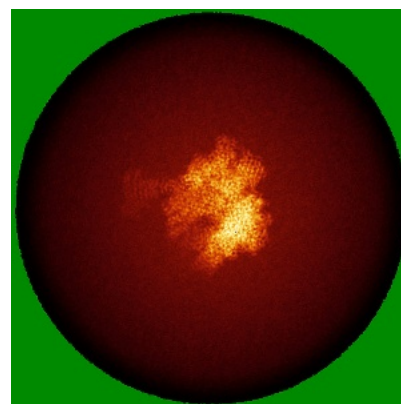
### 6.4.1 Primary map



X

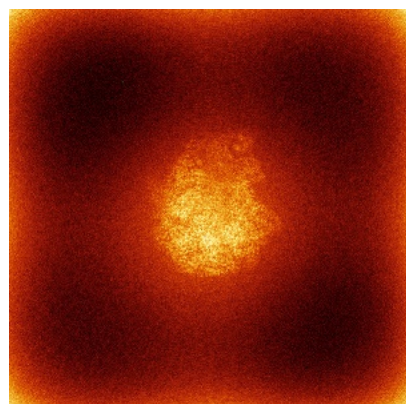


Y

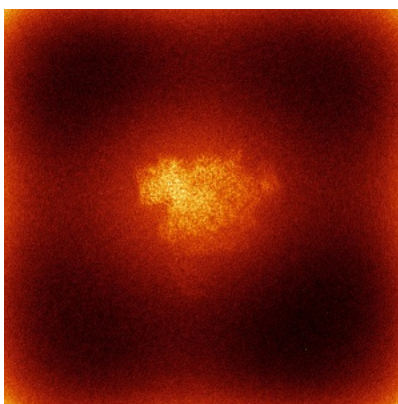


Z

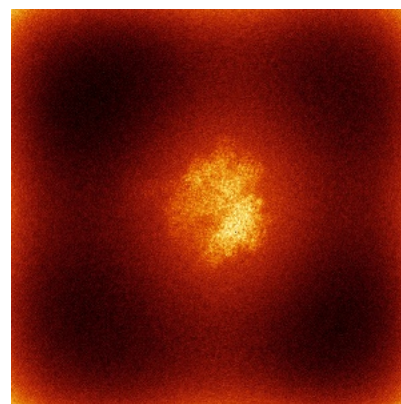
### 6.4.2 Raw map



X



Y



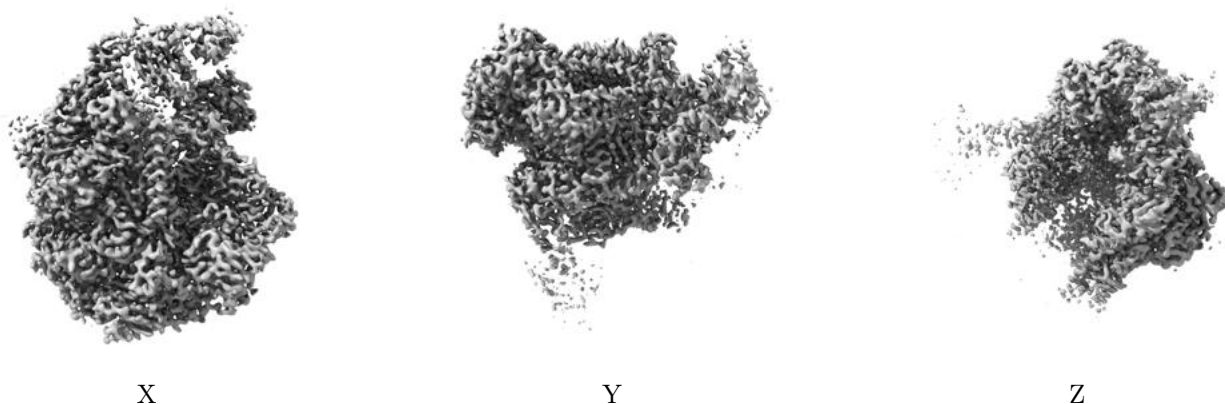
Z

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



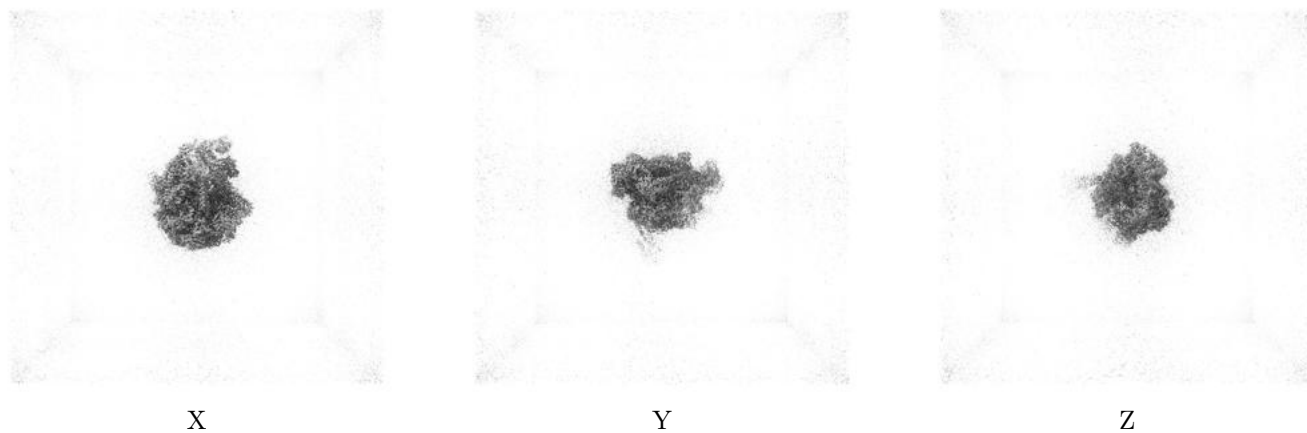
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. 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.

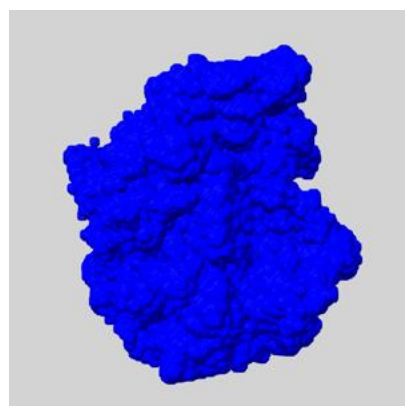
## 6.6 Mask visualisation [i](#)

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

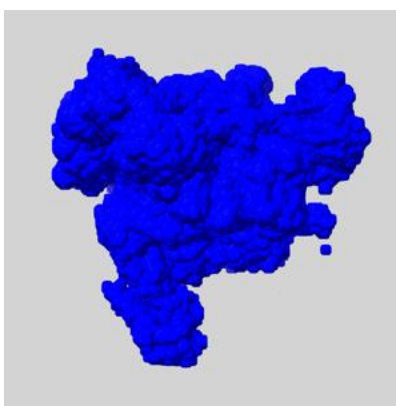
A mask typically either:

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

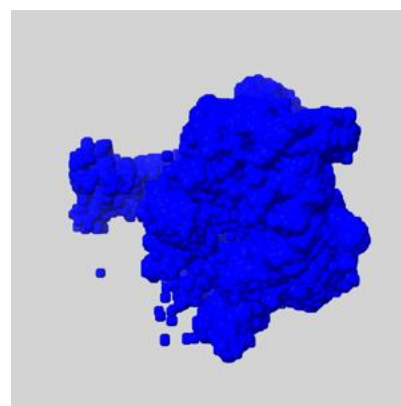
### 6.6.1 emd\_18573\_msk\_1.map [i](#)



X



Y

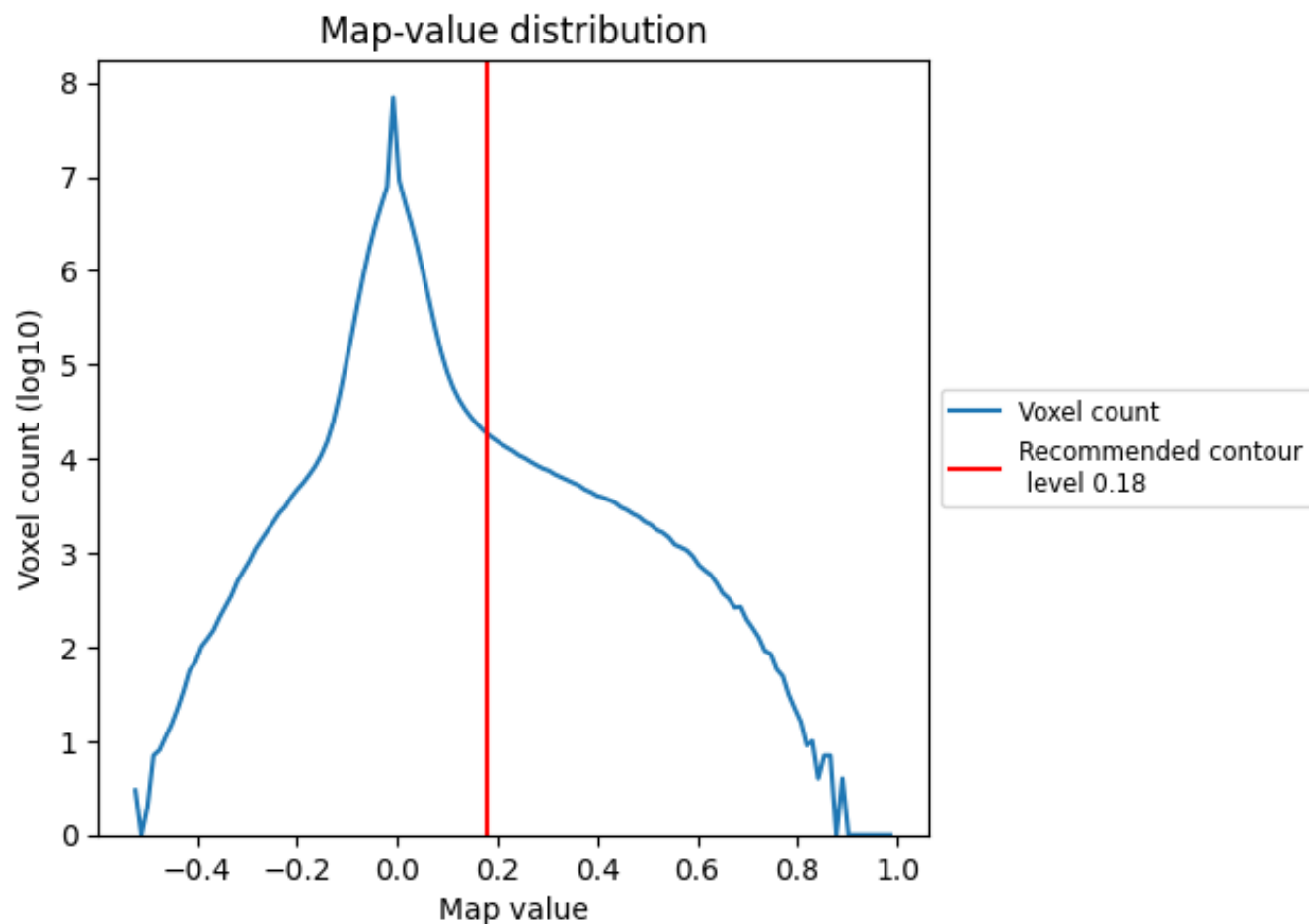


Z

## 7 Map analysis [i](#)

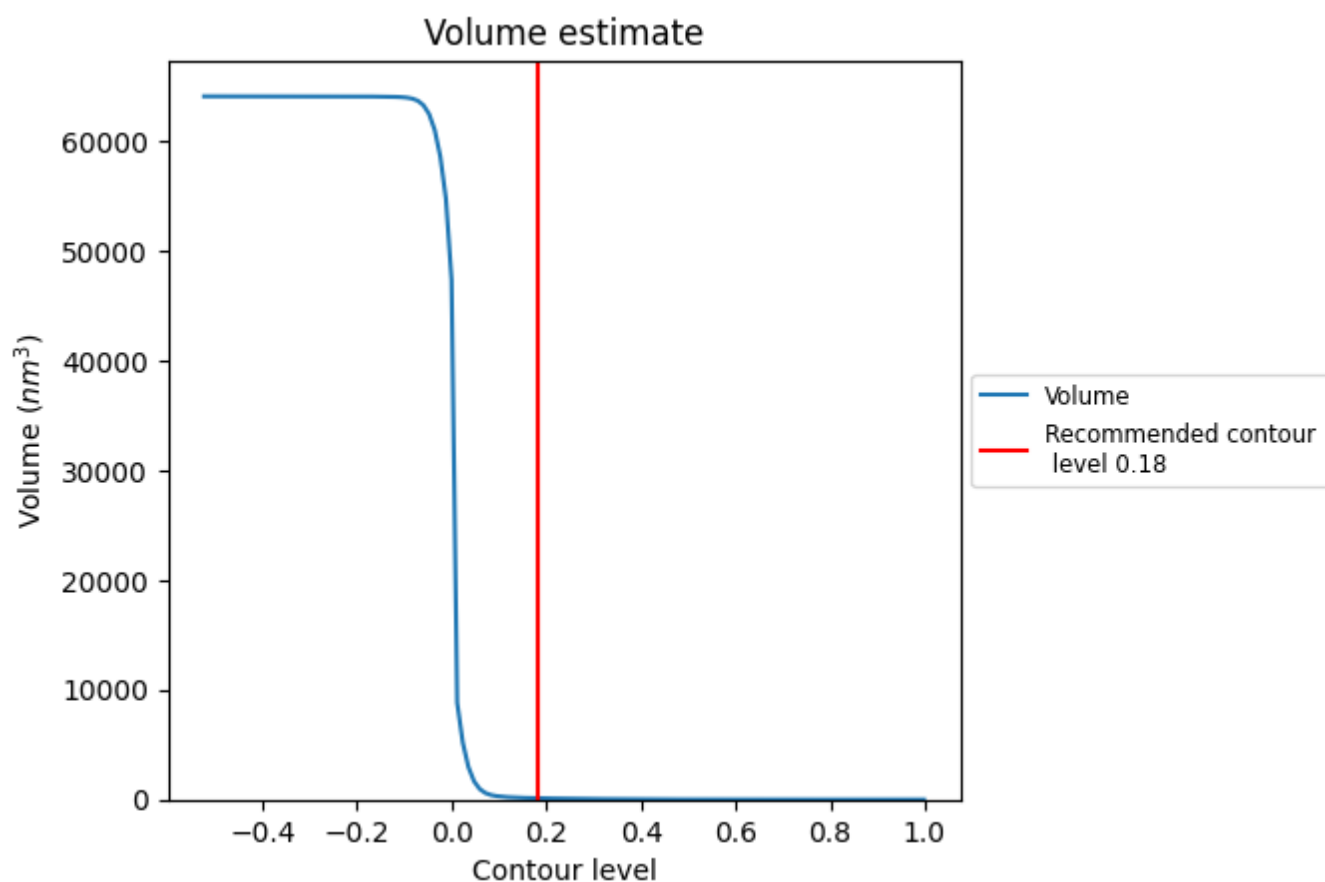
This section contains the results of statistical analysis of the map.

### 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.

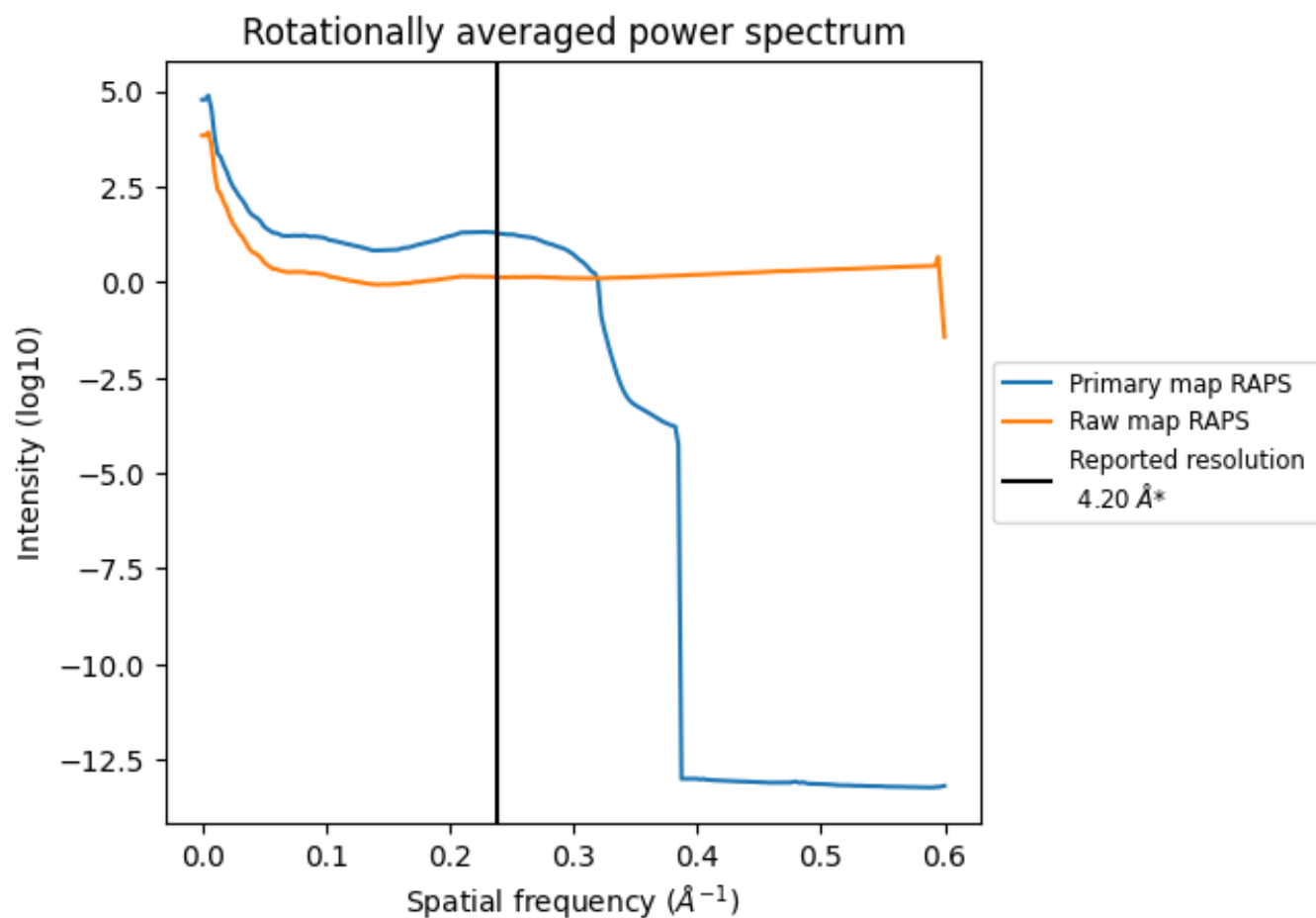
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 125 nm<sup>3</sup>; this corresponds to an approximate mass of 113 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 ⓘ

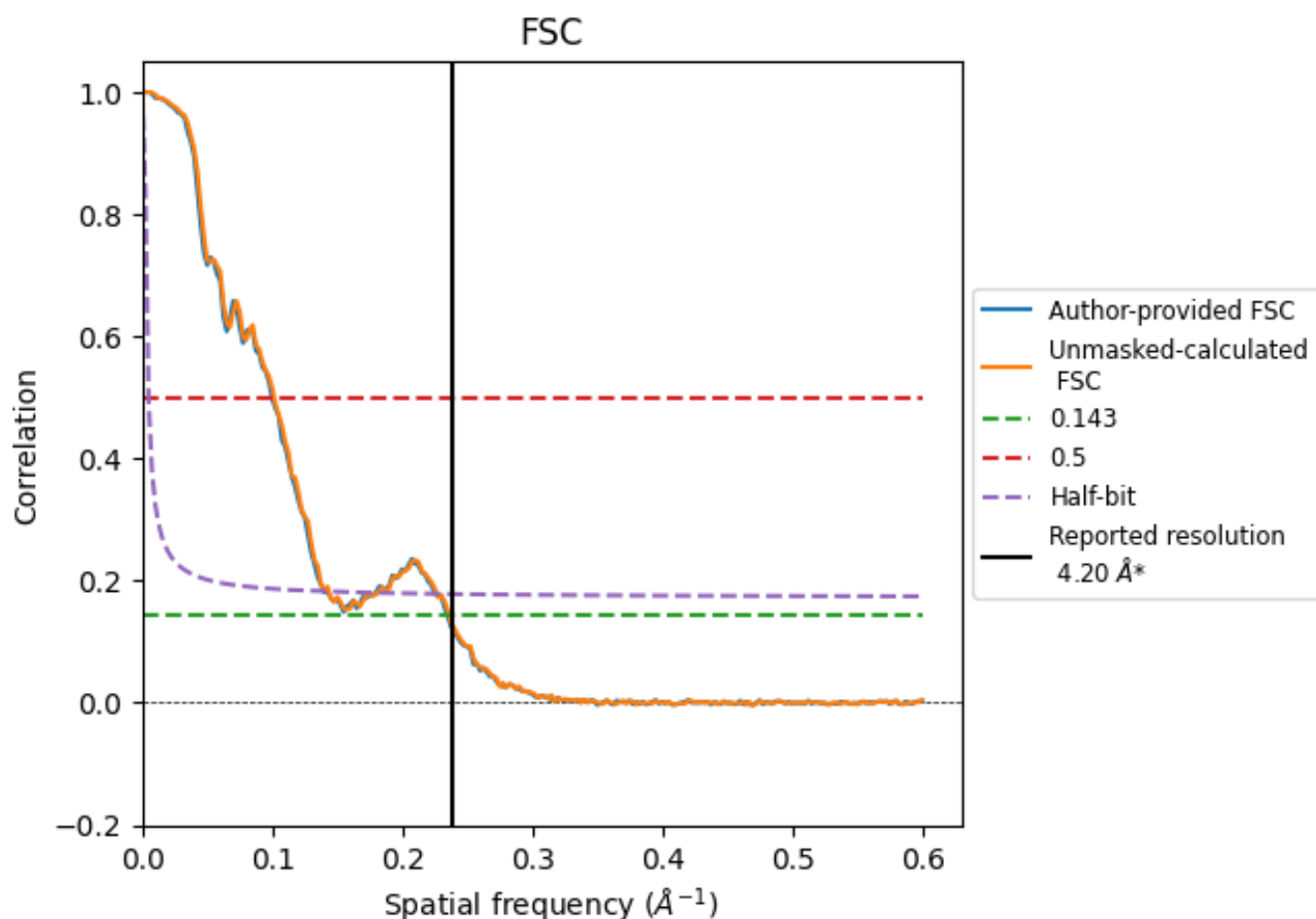


\*Reported resolution corresponds to spatial frequency of 0.238 Å<sup>-1</sup>

## 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  $0.238 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

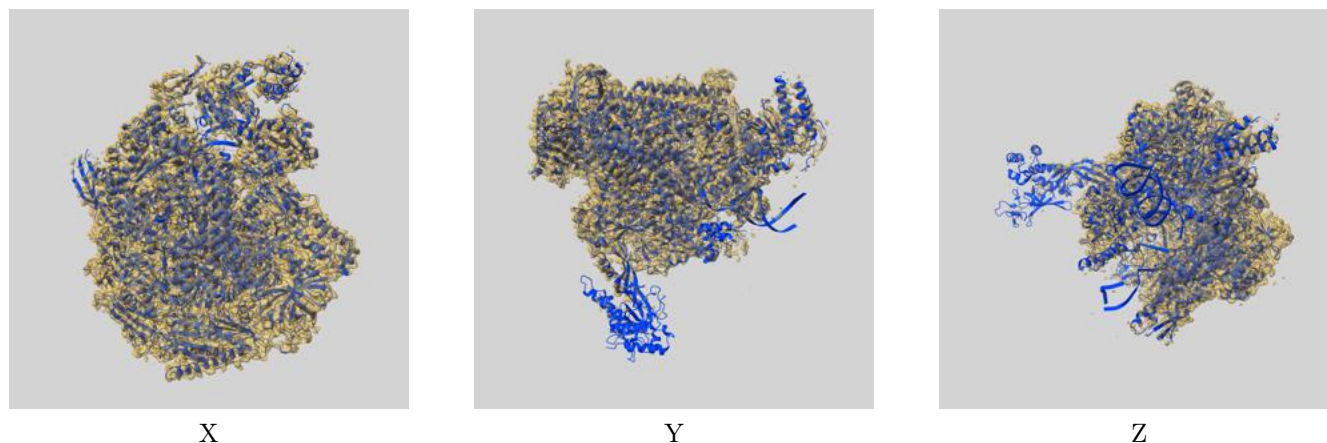
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.26	10.03	7.16
Unmasked-calculated*	4.24	9.86	6.97

\*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-18573 and PDB model 8QQ2. Per-residue inclusion information can be found in section 3 on page 8.

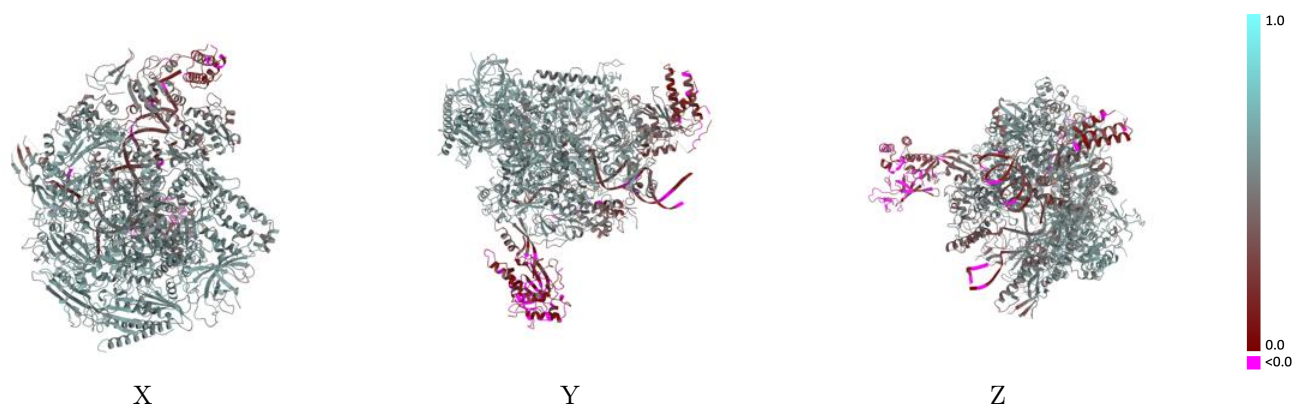
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.18 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.

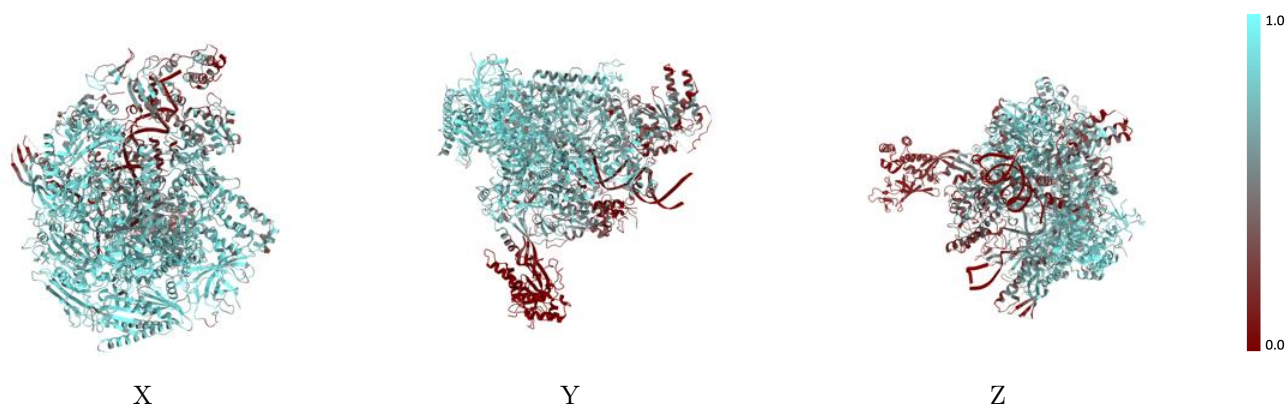


## 9.2 Q-score mapped to coordinate model [i](#)



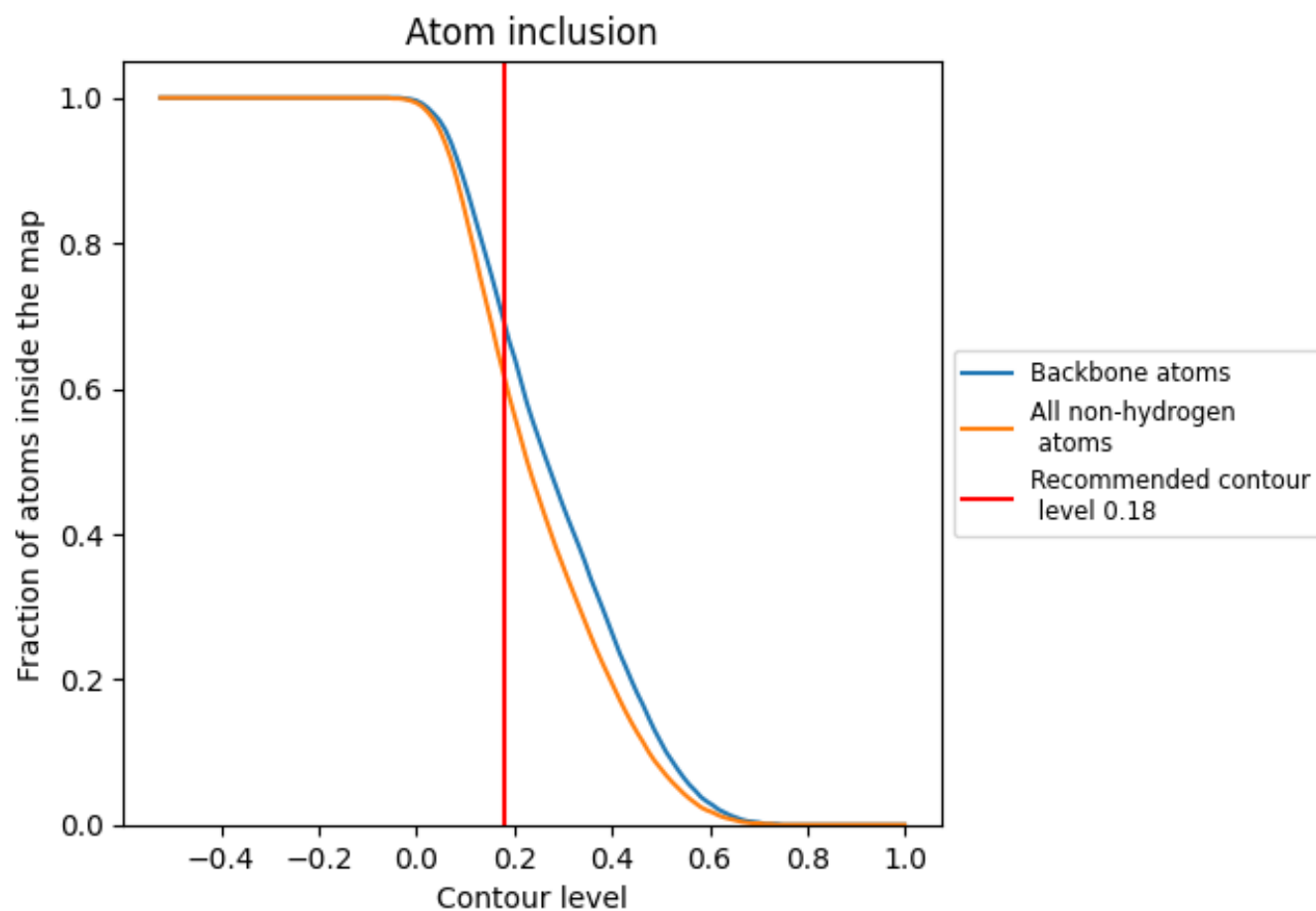
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).



































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 62% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6150	 0.4870
A	 0.6370	 0.5240
B	 0.7180	 0.5470
C	 0.8220	 0.5740
D	 0.0070	 0.0810
E	 0.6500	 0.5110
F	 0.7700	 0.5580
G	 0.1520	 0.1470
H	 0.7560	 0.5550
I	 0.6020	 0.5060
J	 0.8370	 0.5850
K	 0.7970	 0.5650
L	 0.6900	 0.5160
N	 0.0340	 0.1570
P	 0.3400	 0.3710
R	 0.2730	 0.1840
T	 0.1800	 0.2720

