



## Full wwPDB EM Validation Report ⓘ

Apr 22, 2025 – 03:38 pm BST

PDB ID : 8QW9 / pdb\_00008qw9  
EMDB ID : EMD-18683  
Title : RNAPII elongation complex bound to RECQ5\_R502E  
Authors : Skubnik, K.; Sebesta, M.; Stefl, R.  
Deposited on : 2023-10-19  
Resolution : 4.30 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

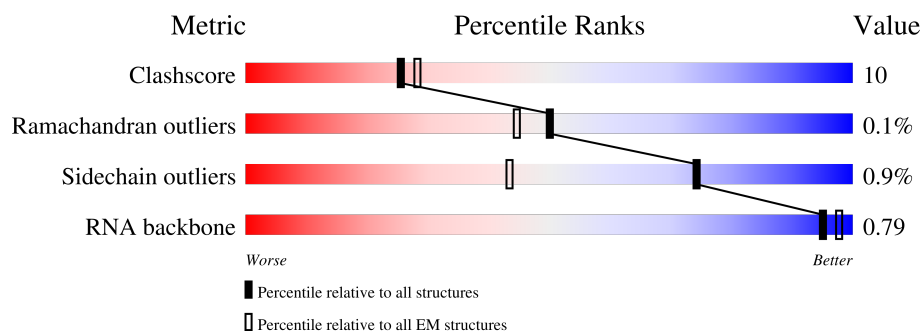
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.30 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	
2	B	1174	
3	C	275	
4	E	210	
5	F	127	
6	H	150	
7	I	125	

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Mol	Chain	Length	Quality of chain
8	J	67	 88% 9% ..
9	K	117	 82% 16% .
10	L	58	 59% 17% 24%
11	D	142	 82% 46% 44% 10%
12	G	172	 69% 52% 47% .
13	P	17	 12% 41% 6% 12% 41%
14	T	51	 18% 24% 14% 63%
15	N	55	 15% 11% . 85%
16	R	650	 15% . 84%

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 32356 atoms, of which 645 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	1371	Total	C	N	O	S	0	0
			10833	6821	1945	2002	65		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1106	Total	C	N	O	S	0	0
			8802	5576	1540	1622	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
			903	560	160	172	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 RNA chain called RNA, DNA-RNA ELONGATION SCAFFOLD.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	10	Total	C	N	O	P	0	0
			213	95	37	71	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	19	Total	C	N	O	P	0	0
			391	184	77	111	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	8	Total	C	N	O	P	0	0
			162	78	24	52	8		

- Molecule 16 is a protein called ATP-dependent DNA helicase Q5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	104	Total	C	H	N	O	S	
			1376	458	645	130	140	3	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	502	GLU	ARG	engineered mutation	UNP O94762

- 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	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	

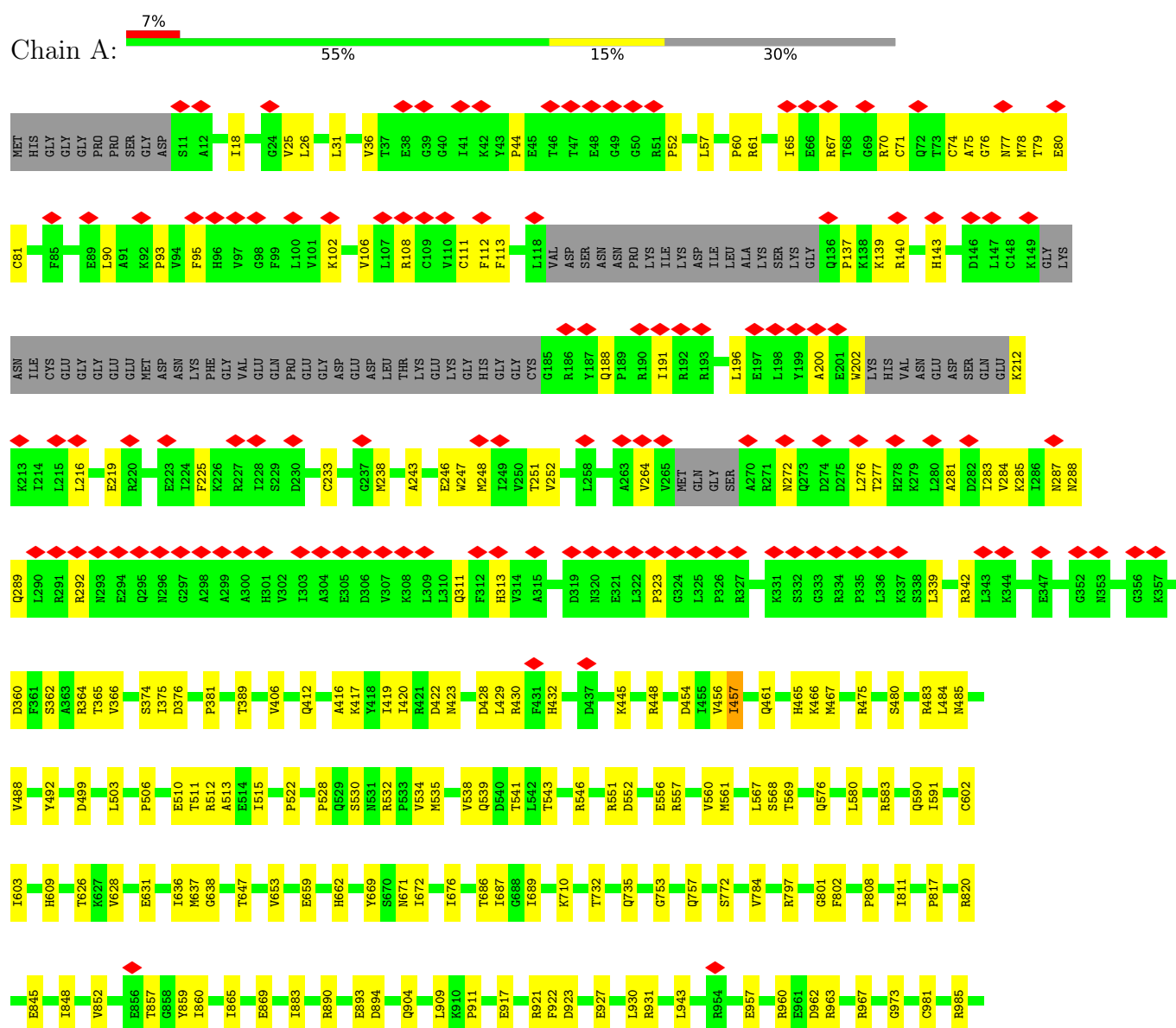
- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

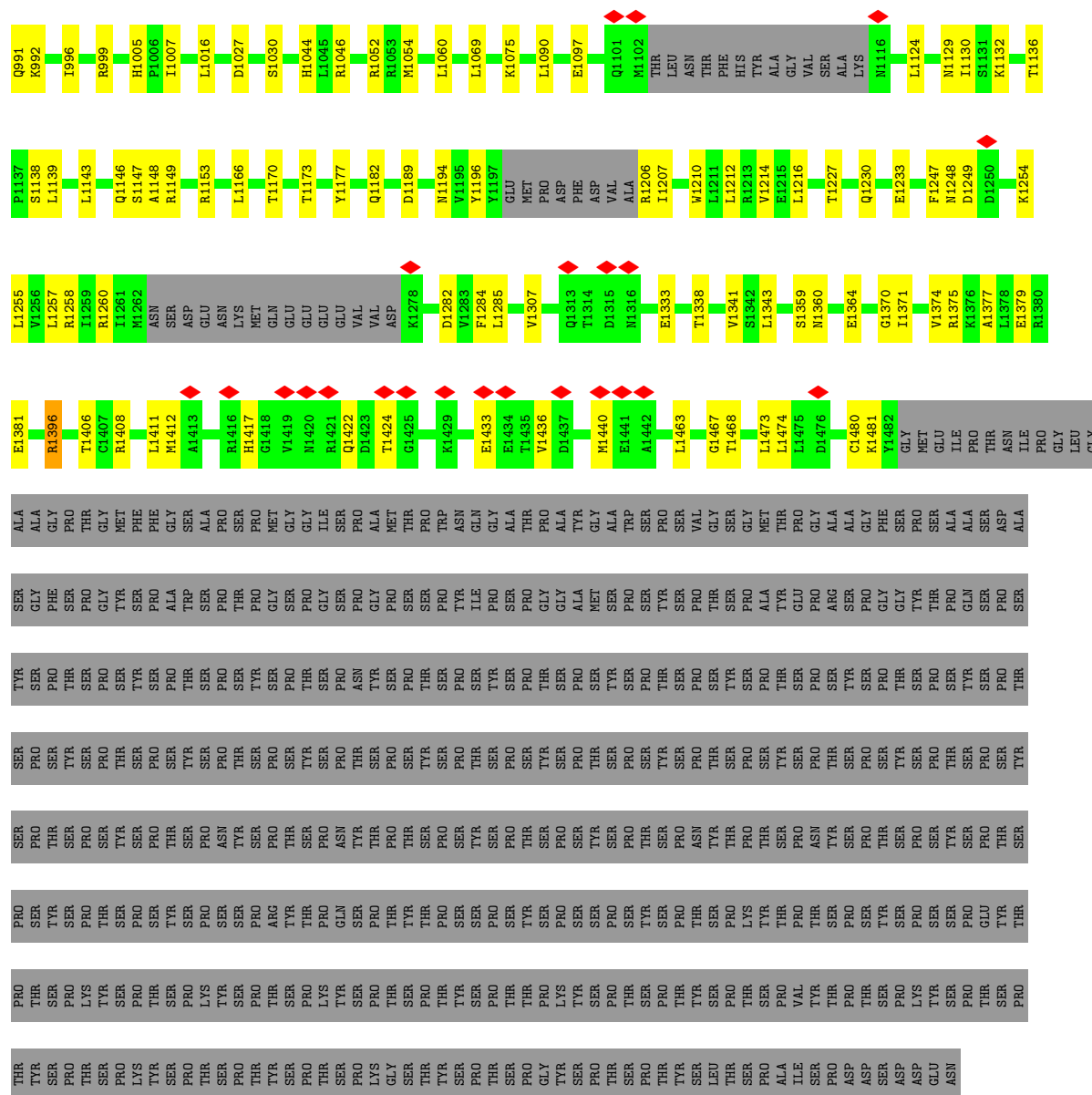
### 3 Residue-property plots

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.

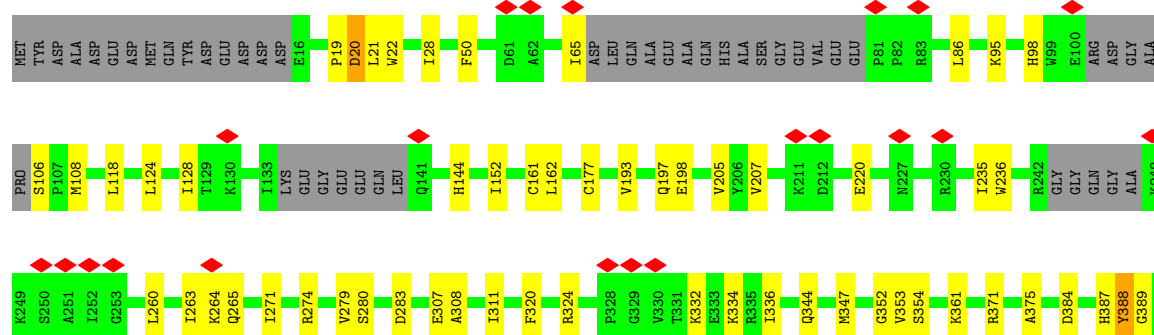
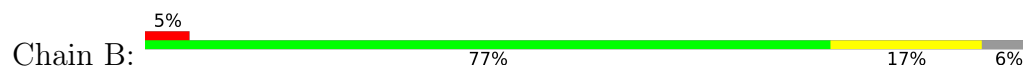
#### • Molecule 1: DNA-directed RNA polymerase subunit

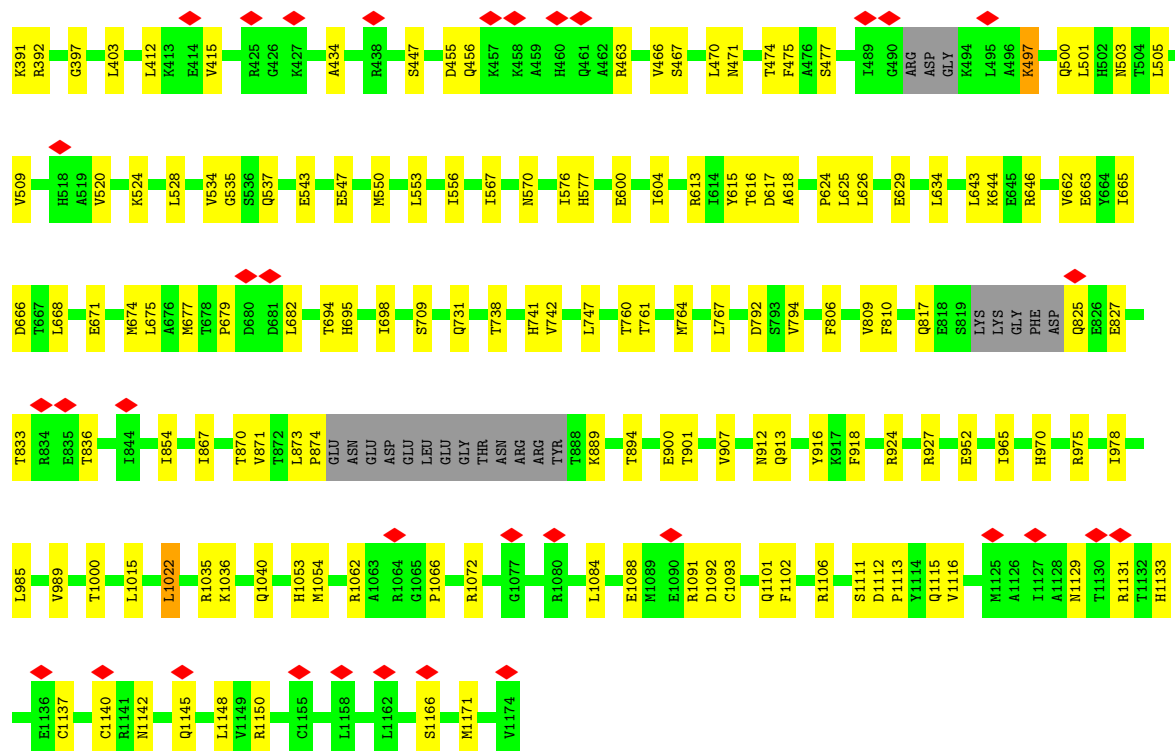






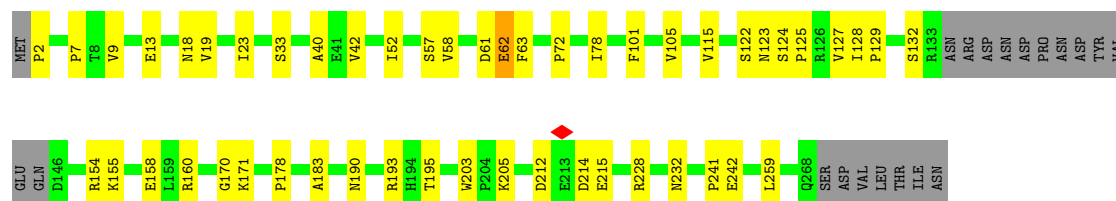
● Molecule 2: DNA-directed RNA polymerase subunit beta





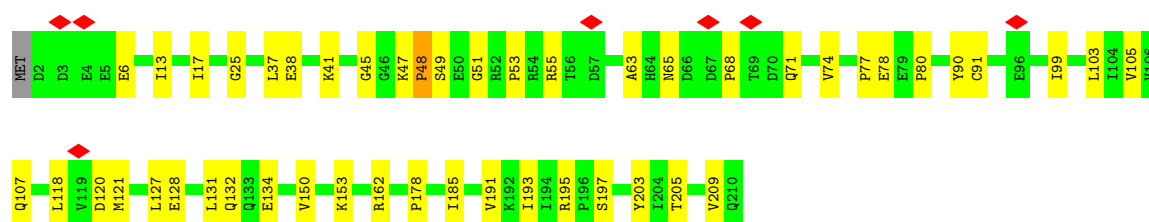
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 75% 18% 7%



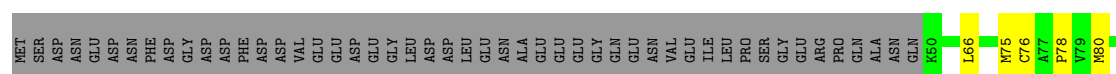
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 77% 22%



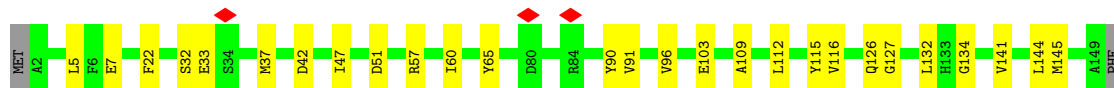
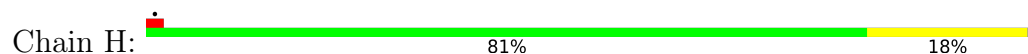
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 53% 8% 39%

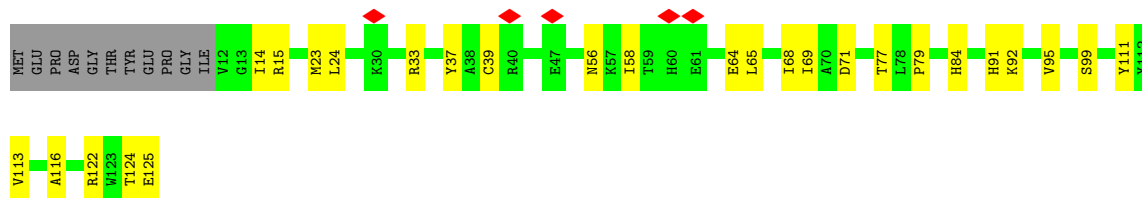




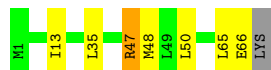
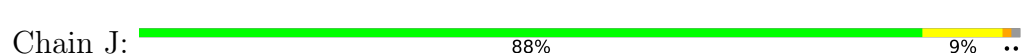
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



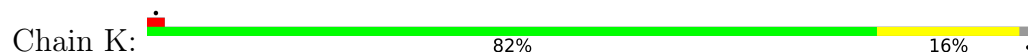
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



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



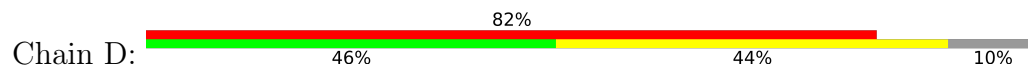
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



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



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

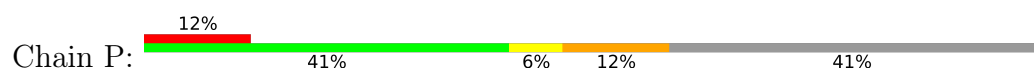




• Molecule 12: DNA-directed RNA polymerase II subunit RPB7



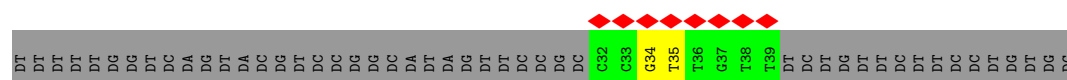
• Molecule 13: RNA, DNA-RNA ELONGATION SCAFFOLD



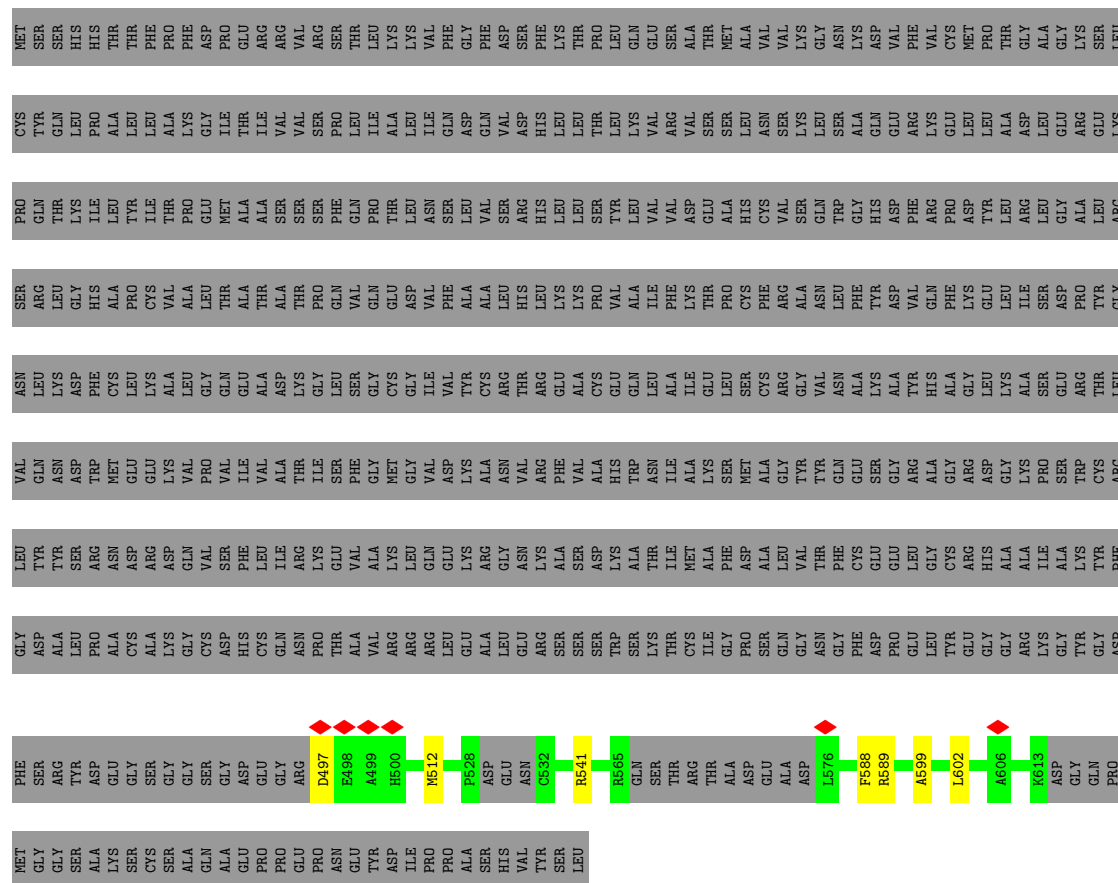
• Molecule 14: DNA, DNA-RNA ELONGATION SCAFFOLD



• Molecule 15: DNA, DNA-RNA ELONGATION SCAFFOLD



• Molecule 16: ATP-dependent DNA helicase Q5



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	19142	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	0.756	Depositor
Minimum map value	-0.422	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	333.44, 333.44, 333.44	wwPDB
Map dimensions	400, 400, 400	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	0.32	0/11028	0.47	0/14895
2	B	0.33	0/8975	0.44	0/12121
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	0.48	0/1611
7	I	0.36	0/923	0.46	0/1252
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	P	0.20	0/237	0.76	0/367
14	T	0.61	0/439	0.93	1/675 (0.1%)
15	N	0.52	0/179	1.08	0/274
16	R	0.54	0/741	0.88	2/1008 (0.2%)
All	All	0.34	0/32373	0.49	3/43921 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	28	DG	O4'-C4'-C3'	-6.25	102.00	104.50
16	R	589	ARG	NE-CZ-NH2	5.26	122.93	120.30
16	R	541	ARG	NE-CZ-NH2	5.14	122.87	120.30

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	10833	0	10940	257	0
2	B	8802	0	8802	142	0
3	C	2039	0	1985	50	0
4	E	1687	0	1685	33	0
5	F	623	0	655	14	0
6	H	1172	0	1128	24	0
7	I	903	0	831	23	0
8	J	520	0	536	6	0
9	K	920	0	942	25	0
10	L	368	0	368	8	0
11	D	1005	0	964	56	0
12	G	1334	0	1333	76	0
13	P	213	0	108	3	0
14	T	391	0	212	6	0
15	N	162	0	93	5	0
16	R	731	645	646	9	0
17	A	2	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	A	1	0	0	0	0
All	All	31711	645	31228	638	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 (638) 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	1.31
3:C:78:ILE:HD11	3:C:127:VAL:HG22	1.34	1.09
1:A:465:HIS:HB3	1:A:1097:GLU:OE1	1.57	1.04
6:H:96:VAL:HG22	6:H:116:VAL:CG2	1.86	1.04
7:I:111:TYR:CD1	7:I:124:THR:HG21	1.93	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:96:VAL:CG2	6:H:116:VAL:HG22	1.89	1.01
6:H:96:VAL:HG22	6:H:116:VAL:HG22	0.98	0.98
3:C:259:LEU:HD22	9:K:91:ILE:CD1	1.95	0.97
6:H:91:VAL:HG22	6:H:144:LEU:CD2	1.94	0.97
3:C:259:LEU:HD22	9:K:91:ILE:HD11	1.47	0.96
2:B:900:GLU:O	2:B:901:THR:HG22	1.68	0.94
9:K:45:ILE:HG22	9:K:94:LEU:CD1	1.98	0.93
9:K:45:ILE:HG22	9:K:94:LEU:HD11	1.51	0.93
3:C:78:ILE:CD1	3:C:127:VAL:CG2	2.46	0.92
1:A:797:ARG:HH11	1:A:820:ARG:HB2	1.35	0.91
7:I:111:TYR:CD1	7:I:124:THR:CG2	2.53	0.91
1:A:1196:TYR:CE1	16:R:602:LEU:HD13	2.08	0.89
1:A:860:ILE:HD13	1:A:1124:LEU:HD23	1.54	0.88
1:A:461:GLN:OE1	14:T:29:DA:H2"	1.73	0.87
1:A:1480:CYS:O	12:G:19:GLY:C	2.14	0.86
3:C:259:LEU:CD2	9:K:91:ILE:HD11	2.05	0.86
1:A:1027:ASP:OD1	1:A:1030:SER:HB2	1.74	0.86
1:A:1196:TYR:CE1	16:R:602:LEU:CD1	2.60	0.84
4:E:195:ARG:HH22	4:E:205:THR:HG21	1.43	0.84
6:H:91:VAL:HG22	6:H:144:LEU:HD23	1.60	0.84
2:B:332:LYS:NZ	2:B:336:ILE:HD12	1.92	0.84
1:A:1027:ASP:OD1	1:A:1030:SER:CB	2.26	0.83
1:A:1374:VAL:HG21	1:A:1411:LEU:HD21	1.62	0.82
7:I:111:TYR:CE1	7:I:124:THR:HG21	2.15	0.82
2:B:21:LEU:O	2:B:21:LEU:HD23	1.78	0.82
2:B:553:LEU:O	2:B:556:ILE:HG22	1.80	0.81
10:L:21:GLU:OE2	10:L:39:CYS:SG	2.38	0.81
1:A:860:ILE:HD11	1:A:1124:LEU:HG	1.63	0.81
3:C:128:ILE:HG23	3:C:129:PRO:HD2	1.62	0.81
1:A:1196:TYR:CZ	16:R:602:LEU:CD1	2.64	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	0.78
1:A:797:ARG:NH1	1:A:820:ARG:HB2	1.99	0.78
1:A:375:ILE:HD13	1:A:485:ASN:HD22	1.50	0.77
1:A:1054:MET:SD	1:A:1060:LEU:HD12	2.25	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
12:G:89:VAL:HA	12:G:99:THR:HG22	1.68	0.75
3:C:78:ILE:HD11	3:C:127:VAL:HG21	1.66	0.75
1:A:857:THR:O	1:A:860:ILE:HG22	1.87	0.74
1:A:200:ALA:HB2	1:A:216:LEU:HG	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:ILE:CD1	1:A:1124:LEU:HD23	2.18	0.74
2:B:344:GLN:NE2	2:B:354:SER:O	2.22	0.73
1:A:323:PRO:HG3	14:T:23:DG:OP1	1.88	0.73
6:H:103:GLU:HG3	6:H:109:ALA:HB2	1.71	0.73
2:B:264:LYS:HB3	2:B:324:ARG:HB3	1.71	0.73
4:E:195:ARG:HH22	4:E:205:THR:CG2	2.01	0.73
12:G:40:GLY:HA2	12:G:157:ILE:HD11	1.71	0.73
7:I:69:ILE:HG22	7:I:71:ASP:H	1.54	0.72
1:A:860:ILE:CD1	1:A:1124:LEU:CD2	2.67	0.72
11:D:90:LYS:HE2	11:D:130:ILE:HD11	1.70	0.72
1:A:57:LEU:HD21	1:A:281:ALA:HB2	1.72	0.71
1:A:811:ILE:HD12	7:I:79:PRO:HB3	1.73	0.71
1:A:1474:LEU:HB2	5:F:105:ILE:HG13	1.73	0.71
4:E:13:ILE:HD11	4:E:132:GLN:HG3	1.70	0.71
9:K:45:ILE:CG2	9:K:94:LEU:CD1	2.69	0.71
1:A:1148:ALA:HB1	1:A:1333:GLU:HB3	1.73	0.70
1:A:1206:ARG:NH1	7:I:33:ARG:HH12	1.88	0.70
4:E:185:ILE:HG21	4:E:209:VAL:HG21	1.71	0.70
3:C:205:LYS:NZ	3:C:212:ASP:O	2.22	0.70
1:A:67:ARG:HA	1:A:78:MET:HG3	1.73	0.70
9:K:45:ILE:CG2	9:K:94:LEU:HD13	2.21	0.70
2:B:747:LEU:HD22	2:B:810:PHE:CZ	2.25	0.70
4:E:55:ARG:HB2	4:E:78:GLU:HG2	1.72	0.70
12:G:100:GLU:HA	12:G:105:SER:HA	1.73	0.70
1:A:860:ILE:HD13	1:A:1124:LEU:CD2	2.21	0.70
1:A:922:PHE:H	1:A:1052:ARG:HD2	1.57	0.70
2:B:900:GLU:O	2:B:901:THR:CG2	2.40	0.70
7:I:84:HIS:ND1	7:I:125:GLU:OE2	2.21	0.70
3:C:78:ILE:HD11	3:C:127:VAL:HG23	1.70	0.69
5:F:76:CYS:O	12:G:16:ARG:HA	1.91	0.69
1:A:71:CYS:SG	1:A:74:CYS:O	2.50	0.69
1:A:511:THR:HG23	2:B:1102:PHE:HB2	1.75	0.69
1:A:845:GLU:OE2	2:B:500:GLN:NE2	2.26	0.69
1:A:1371:ILE:HA	1:A:1374:VAL:HG12	1.75	0.69
2:B:332:LYS:HZ3	2:B:336:ILE:HD12	1.55	0.69
2:B:387:HIS:NE2	2:B:671:GLU:OE2	2.22	0.69
11:D:34:ASN:O	11:D:68:THR:OG1	2.11	0.69
2:B:86:LEU:HB3	2:B:128:ILE:HD11	1.73	0.68
2:B:274:ARG:NH2	2:B:279:VAL:O	2.25	0.68
2:B:353:VAL:O	2:B:353:VAL:HG12	1.93	0.68
3:C:259:LEU:HD22	9:K:91:ILE:HD13	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:91:VAL:HG22	6:H:144:LEU:HD22	1.76	0.68
3:C:128:ILE:CG2	3:C:129:PRO:HD2	2.23	0.68
5:F:78:PRO:HD2	12:G:18:PHE:O	1.94	0.68
1:A:52:PRO:HG2	1:A:65:ILE:HD13	1.76	0.68
1:A:360:ASP:OD1	2:B:1062:ARG:NH2	2.26	0.68
6:H:32:SER:HB3	6:H:37:MET:H	1.58	0.68
1:A:1417:HIS:HD2	15:N:34:DG:O3'	1.76	0.68
12:G:152:VAL:HA	12:G:157:ILE:HA	1.76	0.68
8:J:65:LEU:O	10:L:23:HIS:ND1	2.25	0.67
11:D:108:ALA:N	11:D:128:GLN:OE1	2.27	0.67
1:A:883:ILE:HD11	1:A:1424:THR:HG22	1.76	0.67
12:G:110:ARG:HA	12:G:113:ILE:HD12	1.77	0.67
1:A:1227:THR:HB	1:A:1230:GLN:HG2	1.77	0.67
9:K:45:ILE:HG22	9:K:94:LEU:HD13	1.77	0.67
1:A:1371:ILE:HD12	1:A:1374:VAL:CG1	2.25	0.67
2:B:197:GLN:OE1	2:B:463:ARG:NH1	2.28	0.67
12:G:148:VAL:N	12:G:160:ILE:O	2.27	0.66
1:A:1417:HIS:CD2	15:N:34:DG:O3'	2.48	0.66
3:C:190:ASN:ND2	3:C:195:THR:O	2.24	0.66
4:E:80:PRO:HA	4:E:107:GLN:HB2	1.77	0.66
11:D:34:ASN:O	11:D:38:HIS:HB2	1.96	0.66
1:A:79:THR:HA	2:B:1072:ARG:HH22	1.61	0.66
1:A:381:PRO:HB3	1:A:480:SER:HA	1.77	0.66
1:A:1343:LEU:N	1:A:1364:GLU:OE2	2.29	0.66
11:D:48:ASN:HD22	11:D:57:LEU:HG	1.60	0.65
1:A:848:ILE:O	1:A:852:VAL:HG23	1.96	0.65
1:A:1182:GLN:HA	1:A:1194:ASN:HD21	1.61	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
1:A:1132:LYS:NZ	15:N:34:DG:OP2	2.27	0.65
3:C:190:ASN:O	3:C:193:ARG:NH2	2.29	0.65
3:C:259:LEU:HD21	9:K:87:PHE:HE2	1.62	0.65
2:B:332:LYS:HZ2	2:B:336:ILE:HD12	1.62	0.64
1:A:196:LEU:HD23	1:A:311:GLN:HG3	1.78	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	0.64
4:E:193:ILE:HB	4:E:205:THR:OG1	1.98	0.64
7:I:111:TYR:HA	7:I:124:THR:HG22	1.80	0.64
1:A:1027:ASP:OD1	1:A:1030:SER:N	2.28	0.63
1:A:576:GLN:O	1:A:590:GLN:NE2	2.31	0.63
2:B:912:ASN:HD21	2:B:916:TYR:HB2	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:91:GLN:HB3	12:G:98:PHE:HB2	1.80	0.63
12:G:39:THR:O	12:G:43:GLY:N	2.32	0.63
5:F:75:MET:HE2	12:G:14:HIS:CE1	2.34	0.63
1:A:1341:VAL:HB	1:A:1364:GLU:OE1	1.99	0.63
2:B:352:GLY:O	2:B:361:LYS:NZ	2.31	0.62
2:B:501:LEU:HD12	2:B:505:LEU:HD12	1.81	0.62
2:B:794:VAL:HG13	2:B:965:ILE:HG23	1.81	0.62
1:A:26:LEU:HD12	2:B:1166:SER:HA	1.81	0.62
1:A:75:ALA:HB2	2:B:1131:ARG:HD3	1.82	0.62
1:A:917:GLU:O	1:A:921:ARG:HB2	1.98	0.62
1:A:904:GLN:NE2	1:A:981:CYS:O	2.31	0.62
1:A:1248:ASN:OD1	1:A:1249:ASP:N	2.29	0.62
1:A:1371:ILE:HD12	1:A:1374:VAL:HG11	1.79	0.62
4:E:131:LEU:HB2	4:E:134:GLU:HG3	1.81	0.62
2:B:1062:ARG:NH1	2:B:1066:PRO:O	2.32	0.61
11:D:26:PHE:CE2	12:G:78:ARG:HD3	2.35	0.61
2:B:792:ASP:OD2	2:B:975:ARG:NH1	2.34	0.61
7:I:113:VAL:HG22	7:I:122:ARG:HG2	1.83	0.61
2:B:193:VAL:HG21	2:B:470:LEU:HD13	1.83	0.61
1:A:1343:LEU:HB2	1:A:1364:GLU:OE2	2.01	0.60
12:G:129:LYS:HB2	12:G:136:VAL:HG22	1.83	0.60
1:A:551:ARG:NH2	6:H:42:ASP:OD2	2.34	0.60
2:B:235:ILE:HD12	2:B:347:MET:HG3	1.84	0.60
1:A:284:VAL:O	1:A:288:ASN:ND2	2.35	0.60
2:B:177:CYS:SG	2:B:738:THR:OG1	2.51	0.60
11:D:32:LEU:HD11	12:G:4:HIS:HB2	1.83	0.60
1:A:1170:THR:HA	1:A:1216:LEU:HD13	1.84	0.60
1:A:1138:SER:OG	1:A:1360:ASN:ND2	2.35	0.60
11:D:95:PHE:O	11:D:99:CYS:HB2	2.02	0.60
1:A:461:GLN:OE1	14:T:29:DA:C2'	2.48	0.60
2:B:1142:ASN:HD21	2:B:1145:GLN:HG3	1.67	0.60
11:D:41:LEU:HD12	11:D:68:THR:HG21	1.84	0.60
1:A:1170:THR:HB	7:I:58:ILE:HD11	1.82	0.59
1:A:506:PRO:HG3	1:A:515:ILE:HD12	1.84	0.59
2:B:626:LEU:HD23	2:B:662:VAL:HG12	1.83	0.59
4:E:185:ILE:CG2	4:E:209:VAL:HG21	2.31	0.59
1:A:375:ILE:HD13	1:A:485:ASN:ND2	2.17	0.59
1:A:1284:PHE:HZ	16:R:512:MET:HE2	1.67	0.59
3:C:228:ARG:HG2	3:C:228:ARG:O	2.02	0.59
1:A:1371:ILE:O	1:A:1374:VAL:CG1	2.50	0.59
9:K:5:PRO:HG2	9:K:8:GLU:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1206:ARG:HG2	1:A:1207:ILE:N	2.18	0.59
3:C:19:VAL:HG23	3:C:241:PRO:HB2	1.84	0.59
5:F:75:MET:HE2	12:G:14:HIS:HE1	1.67	0.59
1:A:465:HIS:CG	1:A:1097:GLU:OE1	2.56	0.59
1:A:488:VAL:CG1	1:A:492:TYR:CE2	2.86	0.59
3:C:78:ILE:CD1	3:C:127:VAL:HG23	2.28	0.59
1:A:376:ASP:HB3	1:A:522:PRO:HD3	1.85	0.59
11:D:31:THR:HG22	12:G:3:TYR:HE1	1.68	0.59
12:G:55:GLY:HA3	12:G:69:PRO:HG2	1.84	0.59
1:A:1212:LEU:HB2	1:A:1285:LEU:HD12	1.83	0.58
1:A:560:VAL:HG22	1:A:591:ILE:HD11	1.84	0.58
1:A:1417:HIS:CD2	15:N:34:DG:H4'	2.38	0.58
3:C:2:PRO:HB3	9:K:54:PRO:HD2	1.84	0.58
11:D:38:HIS:O	11:D:42:GLU:HG2	2.02	0.58
1:A:454:ASP:OD1	1:A:512:ARG:NH1	2.36	0.58
7:I:65:LEU:HD21	7:I:124:THR:HG23	1.84	0.58
1:A:264:VAL:HB	1:A:272:ASN:HB2	1.86	0.58
1:A:1343:LEU:CB	1:A:1364:GLU:OE2	2.51	0.58
1:A:1480:CYS:O	12:G:19:GLY:CA	2.51	0.58
2:B:747:LEU:HD22	2:B:810:PHE:HZ	1.68	0.58
5:F:75:MET:CE	12:G:14:HIS:CE1	2.87	0.58
1:A:18:ILE:HD12	2:B:1171:MET:HB3	1.86	0.58
1:A:860:ILE:HD11	1:A:1124:LEU:CG	2.32	0.58
2:B:827:GLU:HG2	2:B:871:VAL:HG22	1.85	0.58
11:D:111:SER:HB2	11:D:131:LEU:HD21	1.85	0.58
12:G:4:HIS:CE1	12:G:73:LYS:HB3	2.39	0.58
12:G:30:LEU:HD22	12:G:70:VAL:HG11	1.85	0.58
1:A:732:THR:OG1	1:A:735:GLN:HG3	2.03	0.58
7:I:111:TYR:HD1	7:I:124:THR:CG2	2.14	0.57
11:D:84:ARG:O	11:D:88:LEU:HB2	2.04	0.57
11:D:95:PHE:O	11:D:99:CYS:CB	2.52	0.57
4:E:45:GLY:HA3	4:E:53:PRO:HD3	1.87	0.57
2:B:198:GLU:OE2	2:B:388:TYR:OH	2.20	0.57
1:A:1480:CYS:O	12:G:19:GLY:HA2	2.04	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	0.56
2:B:761:THR:HG23	2:B:1000:THR:HA	1.87	0.56
2:B:901:THR:HG23	2:B:901:THR:O	2.04	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
1:A:44:PRO:HG3	1:A:284:VAL:HG13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:44:ARG:HH22	11:D:48:ASN:HB2	1.69	0.56
2:B:207:VAL:HG11	2:B:375:ALA:CB	2.34	0.56
6:H:7:GLU:OE2	6:H:57:ARG:NH2	2.38	0.56
11:D:135:GLN:HA	11:D:138:ARG:HD3	1.88	0.56
1:A:1130:ILE:HD11	1:A:1411:LEU:HB3	1.88	0.56
2:B:98:HIS:O	2:B:106:SER:OG	2.24	0.56
1:A:860:ILE:HD11	1:A:1124:LEU:CD2	2.36	0.56
1:A:1481:LYS:HG2	12:G:20:PRO:HA	1.86	0.56
3:C:72:PRO:HG3	8:J:13:ILE:HD11	1.88	0.56
1:A:1216:LEU:HB2	1:A:1255:LEU:HD22	1.87	0.56
3:C:158:GLU:OE2	3:C:160:ARG:NH2	2.38	0.56
6:H:5:LEU:HD22	6:H:134:GLY:HA3	1.87	0.56
1:A:90:LEU:HA	1:A:287:ASN:HD21	1.70	0.55
11:D:96:GLU:OE2	11:D:121:ARG:NH2	2.40	0.55
11:D:124:ASP:O	11:D:128:GLN:HB3	2.06	0.55
1:A:1016:LEU:HD22	1:A:1069:LEU:HD22	1.89	0.55
1:A:1371:ILE:C	1:A:1374:VAL:HG12	2.26	0.55
1:A:1371:ILE:HD11	1:A:1406:THR:HB	1.88	0.55
11:D:123:GLU:O	11:D:127:LEU:N	2.27	0.55
3:C:154:ARG:HG2	3:C:155:LYS:H	1.72	0.55
2:B:617:ASP:OD1	2:B:618:ALA:N	2.37	0.55
11:D:33:LEU:O	11:D:37:VAL:N	2.37	0.55
1:A:422:ASP:OD1	1:A:423:ASN:N	2.40	0.55
1:A:539:GLN:O	2:B:970:HIS:NE2	2.40	0.55
1:A:289:GLN:HG2	1:A:292:ARG:HH11	1.72	0.54
1:A:475:ARG:NH1	9:K:68:GLU:OE1	2.39	0.54
1:A:1371:ILE:CA	1:A:1374:VAL:HG12	2.37	0.54
1:A:1480:CYS:O	12:G:20:PRO:N	2.40	0.54
3:C:9:VAL:HG12	3:C:23:ILE:HD13	1.89	0.54
1:A:77:ASN:HB3	1:A:80:GLU:HG2	1.88	0.54
1:A:609:HIS:ND1	1:A:626:THR:OG1	2.37	0.54
1:A:659:GLU:OE2	1:A:985:ARG:NH2	2.40	0.54
1:A:784:VAL:HG22	2:B:978:ILE:HD11	1.88	0.54
7:I:68:ILE:O	7:I:122:ARG:NH2	2.39	0.54
1:A:532:ARG:NH2	1:A:647:THR:O	2.40	0.54
1:A:1467:GLY:O	1:A:1468:THR:OG1	2.19	0.54
12:G:60:GLN:OE1	12:G:63:ARG:HD2	2.07	0.54
1:A:457:ILE:HG13	1:A:515:ILE:HD13	1.88	0.54
1:A:1196:TYR:CE1	16:R:602:LEU:HD11	2.41	0.54
3:C:123:ASN:OD1	3:C:124:SER:N	2.41	0.54
6:H:32:SER:OG	6:H:33:GLU:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:48:ASN:ND2	11:D:57:LEU:HG	2.22	0.54
3:C:128:ILE:CG2	3:C:129:PRO:CD	2.85	0.54
7:I:64:GLU:OE1	7:I:64:GLU:N	2.41	0.54
2:B:474:THR:HG22	2:B:475:PHE:N	2.23	0.54
9:K:45:ILE:HG21	9:K:94:LEU:HD13	1.90	0.54
2:B:265:GLN:HG2	2:B:324:ARG:HD3	1.90	0.53
3:C:125:PRO:O	3:C:128:ILE:CD1	2.56	0.53
10:L:16:ILE:CG2	10:L:25:GLU:HB2	2.38	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
6:H:96:VAL:HG13	6:H:115:TYR:O	2.08	0.53
1:A:957:GLU:OE2	1:A:960:ARG:NH1	2.40	0.53
1:A:1474:LEU:CD2	12:G:58:VAL:HG22	2.39	0.53
11:D:17:ALA:HB2	12:G:80:PHE:HB2	1.89	0.53
3:C:101:PHE:CE2	3:C:122:SER:HB3	2.43	0.53
2:B:353:VAL:O	2:B:353:VAL:CG1	2.56	0.53
1:A:1408:ARG:NH1	1:A:1412:MET:SD	2.81	0.53
12:G:3:TYR:N	12:G:76:VAL:O	2.29	0.53
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
11:D:16:ASP:OD2	11:D:18:SER:OG	2.17	0.53
1:A:488:VAL:CG1	1:A:492:TYR:HE2	2.22	0.53
11:D:15:GLU:OE1	12:G:78:ARG:NH2	2.41	0.52
1:A:860:ILE:CD1	1:A:1124:LEU:HG	2.38	0.52
12:G:108:ILE:HD11	12:G:145:LEU:HD22	1.92	0.52
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.90	0.52
12:G:101:ILE:N	12:G:104:MET:O	2.37	0.52
1:A:78:MET:O	2:B:1072:ARG:NH1	2.42	0.52
2:B:471:ASN:ND2	2:B:477:SER:OG	2.43	0.52
11:D:112:LYS:HB3	11:D:119:GLU:OE2	2.09	0.52
12:G:97:LEU:HB2	12:G:108:ILE:HB	1.92	0.52
1:A:552:ASP:OD1	6:H:22:PHE:HB3	2.09	0.52
1:A:923:ASP:H	1:A:1052:ARG:NH2	2.07	0.52
1:A:1146:GLN:HB3	1:A:1153:ARG:HH11	1.75	0.52
4:E:25:GLY:O	4:E:65:ASN:ND2	2.28	0.52
6:H:90:TYR:HB3	6:H:145:MET:HB2	1.92	0.52
1:A:859:TYR:OH	1:A:1433:GLU:OE2	2.27	0.52
4:E:17:ILE:HG21	4:E:74:VAL:HG11	1.91	0.52
12:G:79:PRO:HG3	12:G:104:MET:SD	2.50	0.52
2:B:391:LYS:O	2:B:392:ARG:NH2	2.42	0.51
11:D:124:ASP:O	11:D:128:GLN:CB	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:GLU:OE1	1:A:219:GLU:N	2.40	0.51
1:A:467:MET:HG2	1:A:534:VAL:HG11	1.92	0.51
4:E:37:LEU:O	4:E:41:LYS:HG3	2.10	0.51
5:F:80:MET:HB3	5:F:101:LYS:HB3	1.92	0.51
5:F:83:LEU:H	5:F:83:LEU:HD23	1.74	0.51
1:A:1130:ILE:CD1	1:A:1411:LEU:HB3	2.40	0.51
1:A:1139:LEU:HD13	1:A:1359:SER:HB3	1.93	0.51
2:B:629:GLU:HB2	2:B:634:LEU:HD21	1.93	0.51
1:A:285:LYS:HA	1:A:288:ASN:HD21	1.75	0.51
1:A:339:LEU:HD23	1:A:342:ARG:HD2	1.91	0.51
1:A:1005:HIS:CG	1:A:1007:ILE:HG22	2.46	0.51
1:A:1196:TYR:CZ	16:R:602:LEU:HD11	2.46	0.51
2:B:709:SER:HB2	2:B:767:LEU:HD11	1.91	0.51
12:G:6:SER:HG	12:G:73:LYS:HZ3	1.55	0.51
12:G:119:PHE:HB2	12:G:128:TYR:HE1	1.76	0.51
12:G:50:THR:O	12:G:73:LYS:N	2.39	0.51
1:A:428:ASP:OD1	1:A:430:ARG:N	2.39	0.50
1:A:753:GLY:O	1:A:757:GLN:HG2	2.11	0.50
2:B:760:THR:OG1	2:B:764:MET:SD	2.62	0.50
5:F:78:PRO:CD	12:G:18:PHE:O	2.59	0.50
1:A:57:LEU:HD23	1:A:277:THR:HG23	1.94	0.50
2:B:989:VAL:HG22	2:B:1015:LEU:HB2	1.93	0.50
12:G:151:ARG:O	12:G:158:PHE:N	2.28	0.50
2:B:415:VAL:HG23	2:B:434:ALA:HB1	1.93	0.50
2:B:456:GLN:NE2	14:T:37:DC:OP2	2.45	0.50
2:B:833:THR:HB	2:B:836:THR:HG22	1.92	0.50
2:B:50:PHE:HB2	2:B:397:GLY:HA2	1.93	0.50
3:C:7:PRO:HB2	9:K:101:LEU:HD13	1.92	0.50
12:G:129:LYS:HB3	12:G:136:VAL:HG13	1.93	0.50
11:D:109:GLU:O	11:D:113:ALA:CB	2.60	0.50
1:A:1182:GLN:HA	1:A:1194:ASN:ND2	2.26	0.50
1:A:1206:ARG:HG2	1:A:1207:ILE:H	1.76	0.50
1:A:1377:ALA:O	1:A:1381:GLU:HG2	2.12	0.50
4:E:118:LEU:HD22	4:E:127:LEU:HB2	1.93	0.50
9:K:104:ARG:HA	9:K:107:VAL:HG12	1.93	0.50
1:A:1054:MET:SD	1:A:1060:LEU:CD1	2.99	0.49
2:B:694:THR:O	2:B:695:HIS:ND1	2.44	0.49
1:A:535:MET:O	1:A:669:TYR:OH	2.26	0.49
1:A:628:VAL:HA	1:A:638:GLY:HA3	1.93	0.49
2:B:570:ASN:ND2	2:B:616:THR:OG1	2.45	0.49
2:B:625:LEU:HD12	2:B:665:ILE:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:PRO:HB2	1:A:662:HIS:HB2	1.93	0.49
6:H:60:ILE:HG23	6:H:141:VAL:CG1	2.42	0.49
11:D:125:GLU:O	11:D:129:GLN:HB2	2.12	0.49
1:A:26:LEU:HD13	1:A:31:LEU:HD21	1.94	0.49
1:A:857:THR:O	1:A:860:ILE:CG2	2.59	0.49
1:A:1030:SER:OG	4:E:162:ARG:NE	2.43	0.49
1:A:420:ILE:HB	1:A:445:LYS:HB2	1.95	0.49
3:C:128:ILE:HG22	3:C:132:SER:HB2	1.94	0.49
11:D:134:ILE:O	11:D:138:ARG:HG3	2.12	0.49
13:P:8:G:O2'	13:P:9:C:P	2.70	0.49
1:A:513:ALA:HB2	5:F:90:LEU:HD21	1.94	0.49
2:B:260:LEU:HB2	2:B:263:ILE:HD12	1.93	0.49
1:A:1258:ARG:NH1	1:A:1260:ARG:HH11	2.10	0.49
1:A:1371:ILE:HA	1:A:1374:VAL:CG1	2.40	0.49
1:A:1173:THR:HG23	7:I:56:ASN:HB3	1.94	0.49
2:B:455:ASP:OD1	2:B:456:GLN:N	2.45	0.49
2:B:870:THR:CG2	2:B:889:LYS:HB3	2.43	0.49
11:D:84:ARG:NH2	11:D:97:LEU:HD22	2.27	0.49
12:G:1:MET:HB3	12:G:3:TYR:CZ	2.47	0.49
12:G:30:LEU:O	12:G:34:VAL:HG22	2.13	0.49
12:G:52:ASP:H	12:G:72:TYR:HA	1.76	0.49
1:A:689:ILE:HD12	2:B:985:LEU:HD22	1.95	0.49
2:B:677:MET:H	2:B:682:LEU:HD22	1.77	0.49
1:A:1196:TYR:HE1	16:R:602:LEU:HD13	1.75	0.48
6:H:37:MET:HE2	6:H:127:GLY:HA3	1.95	0.48
1:A:488:VAL:HG12	1:A:492:TYR:CE2	2.48	0.48
1:A:801:GLY:HA3	2:B:503:ASN:HB2	1.96	0.48
3:C:128:ILE:HG23	3:C:129:PRO:CD	2.36	0.48
4:E:203:TYR:CE2	4:E:205:THR:CG2	2.97	0.48
12:G:25:THR:O	12:G:29:LYS:HG2	2.13	0.48
12:G:7:LEU:HB2	12:G:72:TYR:CZ	2.47	0.48
12:G:52:ASP:N	12:G:71:LYS:O	2.46	0.48
1:A:225:PHE:HB3	1:A:246:GLU:HB3	1.95	0.48
1:A:1230:GLN:O	1:A:1233:GLU:HG3	2.14	0.48
11:D:76:ASN:OD1	11:D:77:ARG:N	2.47	0.48
12:G:114:PRO:HG3	12:G:164:MET:HA	1.96	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	2.28	0.48
3:C:105:VAL:HG11	3:C:115:VAL:HG22	1.96	0.48
10:L:17:TYR:HB3	10:L:44:MET:HB3	1.96	0.48
11:D:42:GLU:OE2	11:D:65:LEU:HD11	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LYS:O	1:A:106:VAL:HG12	2.12	0.48
1:A:1370:GLY:HA2	4:E:178:PRO:HD2	1.96	0.48
4:E:71:GLN:HB2	4:E:99:ILE:HD12	1.95	0.48
4:E:185:ILE:HD13	4:E:191:VAL:CG1	2.43	0.48
1:A:962:ASP:OD2	1:A:1046:ARG:NH1	2.44	0.48
12:G:97:LEU:HD22	12:G:108:ILE:HD12	1.95	0.48
1:A:1146:GLN:OE1	1:A:1149:ARG:NH1	2.42	0.47
1:A:111:CYS:SG	1:A:188:GLN:NE2	2.79	0.47
2:B:550:MET:HG3	2:B:567:ILE:HD12	1.96	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
12:G:10:GLU:HG2	12:G:69:PRO:HA	1.95	0.47
13:P:8:G:O2'	13:P:9:C:OP1	2.33	0.47
1:A:25:VAL:HG12	1:A:243:ALA:HA	1.96	0.47
1:A:911:PRO:O	1:A:963:ARG:NH1	2.40	0.47
12:G:49:THR:H	12:G:74:ALA:HA	1.78	0.47
1:A:93:PRO:HG2	1:A:219:GLU:HG3	1.96	0.47
1:A:202:TRP:HB2	1:A:212:LYS:N	2.29	0.47
1:A:251:THR:HG23	1:A:252:VAL:HG23	1.95	0.47
1:A:808:PRO:HB2	2:B:675:LEU:HD12	1.97	0.47
1:A:859:TYR:HB2	14:T:27:DG:H5''	1.95	0.47
2:B:1022:LEU:HD23	2:B:1022:LEU:H	1.80	0.47
2:B:1112:ASP:OD1	2:B:1112:ASP:N	2.47	0.47
4:E:77:PRO:HD2	4:E:105:VAL:O	2.14	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
2:B:867:ILE:HB	2:B:894:THR:HG22	1.97	0.47
12:G:162:SER:OG	12:G:164:MET:HG2	2.14	0.47
2:B:543:GLU:O	2:B:547:GLU:HG2	2.14	0.47
2:B:1137:CYS:SG	2:B:1140:CYS:HB2	2.55	0.47
4:E:6:GLU:HB3	4:E:48:PRO:HG2	1.97	0.47
12:G:137:ILE:HG12	12:G:170:LEU:HB2	1.97	0.47
3:C:52:ILE:HD12	3:C:61:ASP:HB3	1.97	0.47
1:A:568:SER:OG	1:A:671:ASN:OD1	2.33	0.46
2:B:128:ILE:HG23	2:B:144:HIS:HB2	1.97	0.46
2:B:384:ASP:OD1	2:B:384:ASP:N	2.48	0.46
11:D:45:LYS:HB2	11:D:61:PHE:HZ	1.80	0.46
12:G:92:VAL:HG11	12:G:127:CYS:HA	1.95	0.46
15:N:34:DG:H2'	15:N:35:DT:H72	1.97	0.46
1:A:631:GLU:OE1	1:A:992:LYS:NZ	2.35	0.46
2:B:613:ARG:NH1	2:B:615:TYR:OH	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:75:MET:HE1	12:G:14:HIS:ND1	2.30	0.46
1:A:488:VAL:HG12	1:A:492:TYR:CD2	2.50	0.46
1:A:927:GLU:HA	1:A:930:LEU:HB2	1.97	0.46
8:J:35:LEU:HD11	8:J:50:LEU:HG	1.97	0.46
1:A:406:VAL:HG11	1:A:419:ILE:HD11	1.98	0.46
2:B:161:CYS:SG	2:B:162:LEU:N	2.89	0.46
10:L:37:ARG:C	10:L:38:GLU:HG2	2.36	0.46
8:J:66:GLU:HA	10:L:23:HIS:HB3	1.97	0.46
12:G:108:ILE:HG12	12:G:161:GLY:C	2.36	0.46
1:A:36:VAL:O	1:A:61:ARG:NH1	2.48	0.46
1:A:860:ILE:CD1	1:A:1124:LEU:CG	2.94	0.46
7:I:14:ILE:HG23	7:I:23:MET:HG3	1.96	0.46
12:G:10:GLU:HA	12:G:68:TYR:O	2.16	0.46
1:A:466:LYS:HA	2:B:1093:CYS:SG	2.56	0.46
1:A:1147:SER:HB3	1:A:1153:ARG:HB3	1.98	0.46
11:D:125:GLU:O	11:D:129:GLN:CB	2.64	0.46
11:D:131:LEU:O	11:D:135:GLN:HG2	2.16	0.46
1:A:60:PRO:HA	1:A:65:ILE:HD11	1.97	0.45
11:D:93:HIS:HB3	11:D:96:GLU:HG3	1.98	0.45
7:I:91:HIS:ND1	7:I:116:ALA:HB2	2.31	0.45
2:B:95:LYS:HD3	2:B:162:LEU:HD23	1.98	0.45
14:T:33:DA:H2'	14:T:34:DT:H71	1.99	0.45
1:A:25:VAL:HG13	1:A:247:TRP:HE3	1.81	0.45
1:A:1474:LEU:HA	12:G:57:GLY:O	2.17	0.45
5:F:66:LEU:HD21	5:F:97:LEU:HD22	1.98	0.45
2:B:334:LYS:HA	2:B:334:LYS:HD3	1.73	0.45
2:B:809:VAL:HG12	2:B:810:PHE:N	2.32	0.45
11:D:109:GLU:O	11:D:113:ALA:HB2	2.17	0.45
2:B:747:LEU:HD22	2:B:810:PHE:CE1	2.52	0.45
6:H:112:LEU:HB2	6:H:132:LEU:HD23	1.97	0.45
1:A:996:ILE:HD13	1:A:1060:LEU:HA	1.99	0.45
2:B:19:PRO:C	2:B:21:LEU:H	2.20	0.45
3:C:62:GLU:H	3:C:62:GLU:HG2	1.34	0.45
1:A:488:VAL:HG11	1:A:492:TYR:HE2	1.82	0.45
4:E:203:TYR:CE2	4:E:205:THR:HG22	2.52	0.44
9:K:12:LEU:HD11	9:K:18:LYS:HD3	1.98	0.44
3:C:57:SER:OG	3:C:58:VAL:N	2.50	0.44
2:B:389:GLY:O	2:B:668:LEU:HD23	2.17	0.44
3:C:40:ALA:HB1	3:C:171:LYS:HG3	1.99	0.44
7:I:111:TYR:CD1	7:I:124:THR:HG22	2.49	0.44
1:A:653:VAL:HG11	1:A:669:TYR:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:VAL:HB	3:C:178:PRO:HG3	2.00	0.44
4:E:38:GLU:OE1	4:E:41:LYS:HD2	2.18	0.44
1:A:44:PRO:HA	1:A:57:LEU:HD11	2.00	0.44
1:A:511:THR:HG21	2:B:1102:PHE:HD1	1.83	0.44
2:B:274:ARG:HH11	2:B:308:ALA:HB1	1.81	0.44
1:A:70:ARG:HB3	1:A:76:GLY:H	1.82	0.44
1:A:389:THR:HG21	1:A:417:LYS:HE2	2.00	0.44
11:D:43:HIS:O	11:D:47:GLN:HG3	2.18	0.44
11:D:35:SER:O	11:D:39:MET:HG3	2.18	0.44
11:D:65:LEU:HA	11:D:68:THR:HG22	1.99	0.44
2:B:22:TRP:CE2	2:B:679:PRO:HG2	2.52	0.44
4:E:77:PRO:HG3	4:E:90:TYR:HE2	1.83	0.44
2:B:28:ILE:HD13	2:B:644:LYS:HB3	2.00	0.44
2:B:466:VAL:HG12	2:B:467:SER:N	2.32	0.44
1:A:76:GLY:HA2	1:A:81:CYS:HB2	1.99	0.43
4:E:103:LEU:HD23	4:E:128:GLU:HB2	1.99	0.43
6:H:91:VAL:CG2	6:H:144:LEU:CD2	2.82	0.43
7:I:95:VAL:HG12	7:I:113:VAL:O	2.18	0.43
12:G:12:LEU:HA	12:G:66:VAL:O	2.18	0.43
1:A:276:LEU:HD11	1:A:339:LEU:HD21	2.01	0.43
2:B:220:GLU:HB3	2:B:236:TRP:CD1	2.53	0.43
3:C:33:SER:CB	9:K:45:ILE:HD11	2.48	0.43
11:D:22:PHE:CE2	11:D:93:HIS:HE1	2.35	0.43
1:A:1166:LEU:O	1:A:1170:THR:OG1	2.31	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
12:G:53:ASN:OD1	12:G:54:ILE:N	2.51	0.43
12:G:152:VAL:HB	12:G:157:ILE:HG12	2.00	0.43
1:A:569:THR:HG23	1:A:671:ASN:HD21	1.84	0.43
2:B:537:GLN:OE1	2:B:537:GLN:N	2.51	0.43
6:H:51:ASP:OD1	6:H:51:ASP:N	2.50	0.43
11:D:20:LEU:HD22	11:D:93:HIS:ND1	2.33	0.43
1:A:1075:LYS:HA	1:A:1075:LYS:HD3	1.79	0.43
1:A:1436:VAL:O	1:A:1440:MET:HG3	2.17	0.43
2:B:98:HIS:HB2	2:B:108:MET:HB2	2.00	0.43
3:C:128:ILE:CG2	3:C:132:SER:HB2	2.48	0.43
4:E:47:LYS:O	4:E:51:GLY:HA3	2.18	0.43
12:G:62:GLY:C	12:G:64:GLY:H	2.22	0.43
1:A:248:MET:HE2	1:A:248:MET:HB2	1.88	0.43
2:B:1088:GLU:O	2:B:1091:ARG:HG3	2.19	0.43
11:D:29:ALA:HA	12:G:5:ILE:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:ILE:HG22	1:A:637:MET:HG2	2.00	0.43
1:A:1136:THR:HG22	1:A:1136:THR:O	2.18	0.43
2:B:118:LEU:HD23	2:B:913:GLN:HG2	2.01	0.43
1:A:139:LYS:O	1:A:143:HIS:ND1	2.48	0.43
11:D:84:ARG:O	11:D:88:LEU:CB	2.65	0.43
1:A:583:ARG:HH22	6:H:47:ILE:HD12	1.83	0.43
1:A:583:ARG:HH12	6:H:47:ILE:HD11	1.84	0.43
2:B:1035:ARG:NH2	2:B:1036:LYS:O	2.52	0.43
7:I:24:LEU:HD23	7:I:39:CYS:HB3	2.00	0.43
12:G:12:LEU:HD21	12:G:60:GLN:HE22	1.84	0.43
1:A:456:VAL:HG21	1:A:503:LEU:HD11	2.00	0.43
1:A:510:GLU:OE2	2:B:1101:GLN:NE2	2.52	0.43
1:A:541:THR:HG23	1:A:676:ILE:HB	2.01	0.43
1:A:556:GLU:HG3	1:A:557:ARG:H	1.83	0.43
1:A:991:GLN:HA	1:A:996:ILE:HD12	2.01	0.43
1:A:1130:ILE:O	1:A:1130:ILE:HG13	2.19	0.43
1:A:1247:PHE:CZ	16:R:599:ALA:HB1	2.53	0.43
2:B:271:ILE:HG21	2:B:320:PHE:CD2	2.54	0.43
2:B:280:SER:OG	2:B:283:ASP:OD2	2.35	0.43
11:D:108:ALA:HB2	11:D:128:GLN:HB2	2.01	0.43
1:A:44:PRO:HA	1:A:57:LEU:CD1	2.49	0.42
1:A:137:PRO:O	1:A:140:ARG:HG2	2.19	0.42
2:B:1040:GLN:HG2	3:C:203:TRP:CH2	2.53	0.42
1:A:108:ARG:HG3	1:A:191:ILE:HD12	2.00	0.42
1:A:686:THR:OG1	1:A:687:ILE:N	2.53	0.42
1:A:797:ARG:NH1	1:A:820:ARG:CB	2.78	0.42
1:A:1307:VAL:HG13	1:A:1338:THR:HG22	2.01	0.42
2:B:412:LEU:HD23	2:B:412:LEU:HA	1.82	0.42
10:L:37:ARG:O	10:L:38:GLU:CG	2.66	0.42
2:B:1115:GLN:HG2	2:B:1150:ARG:HD2	2.00	0.42
11:D:34:ASN:O	11:D:38:HIS:CB	2.66	0.42
12:G:97:LEU:N	12:G:108:ILE:O	2.35	0.42
1:A:543:THR:HB	2:B:970:HIS:HE2	1.84	0.42
2:B:567:ILE:HD11	2:B:577:HIS:HB2	2.01	0.42
9:K:100:LEU:HD11	9:K:104:ARG:HE	1.84	0.42
11:D:39:MET:HE2	11:D:39:MET:HB3	1.93	0.42
2:B:403:LEU:HD21	2:B:447:SER:HB2	2.01	0.42
9:K:24:ASP:HB3	9:K:30:ALA:HB3	2.01	0.42
11:D:103:LEU:HB3	12:G:144:ARG:HH22	1.85	0.42
1:A:894:ASP:OD1	1:A:1396:ARG:NH1	2.53	0.42
3:C:40:ALA:O	3:C:170:GLY:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:195:ARG:NH2	4:E:205:THR:CG2	2.77	0.42
11:D:64:THR:HG21	12:G:46:ILE:HG23	2.01	0.42
12:G:52:ASP:OD1	12:G:73:LYS:HG2	2.19	0.42
1:A:465:HIS:ND1	1:A:1097:GLU:OE2	2.52	0.42
1:A:927:GLU:HG3	1:A:943:LEU:HD11	2.01	0.42
11:D:33:LEU:HB2	11:D:36:GLU:HG3	2.01	0.42
11:D:30:GLU:O	12:G:3:TYR:HA	2.20	0.42
2:B:626:LEU:HG	2:B:698:ILE:HD13	2.02	0.42
3:C:61:ASP:N	3:C:61:ASP:OD1	2.51	0.42
12:G:62:GLY:O	12:G:63:ARG:HG2	2.20	0.42
12:G:119:PHE:HA	12:G:128:TYR:HD1	1.85	0.42
1:A:283:ILE:HG12	1:A:313:HIS:HB3	2.02	0.42
1:A:465:HIS:CE1	1:A:1097:GLU:OE2	2.73	0.42
1:A:865:ILE:HG21	2:B:1092:ASP:CG	2.41	0.42
1:A:893:GLU:OE1	4:E:197:SER:OG	2.21	0.42
1:A:922:PHE:HB2	1:A:1052:ARG:HB2	2.02	0.42
2:B:520:VAL:HG13	2:B:520:VAL:O	2.20	0.42
2:B:870:THR:HG21	2:B:889:LYS:HB3	2.02	0.42
3:C:72:PRO:HG3	8:J:13:ILE:CD1	2.50	0.42
5:F:75:MET:HE1	12:G:14:HIS:CE1	2.54	0.42
7:I:15:ARG:HD2	7:I:37:TYR:CE2	2.55	0.42
11:D:60:VAL:HG13	12:G:103:PRO:HB3	2.01	0.42
12:G:62:GLY:O	12:G:64:GLY:N	2.50	0.42
1:A:365:THR:OG1	1:A:366:VAL:N	2.53	0.41
1:A:710:LYS:HG2	1:A:817:PRO:HG3	2.01	0.41
1:A:909:LEU:HD21	1:A:973:GLY:HA2	2.02	0.41
1:A:362:SER:HA	1:A:503:LEU:O	2.19	0.41
1:A:465:HIS:CG	1:A:1097:GLU:CD	2.94	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
1:A:233:CYS:SG	1:A:238:MET:HG3	2.60	0.41
1:A:416:ALA:HA	1:A:448:ARG:HA	2.01	0.41
2:B:332:LYS:HE3	2:B:332:LYS:HB3	1.86	0.41
2:B:817:GLN:HB3	2:B:918:PHE:HD1	1.86	0.41
12:G:96:GLY:HA3	12:G:109:SER:HA	2.01	0.41
1:A:538:VAL:O	1:A:539:GLN:HG2	2.20	0.41
1:A:546:ARG:HD3	1:A:772:SER:HB3	2.02	0.41
1:A:1143:LEU:HD13	1:A:1147:SER:HB2	2.03	0.41
1:A:1214:VAL:HG22	1:A:1257:LEU:HB3	2.01	0.41
1:A:1282:ASP:OD1	1:A:1282:ASP:N	2.50	0.41
2:B:124:LEU:HD22	2:B:152:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:274:ARG:HD2	2:B:311:ILE:HG22	2.03	0.41
2:B:528:LEU:HD23	2:B:528:LEU:HA	1.80	0.41
2:B:1111:SER:O	2:B:1113:PRO:HD3	2.21	0.41
2:B:1116:VAL:O	2:B:1148:LEU:HD12	2.21	0.41
1:A:1254:LYS:HD3	1:A:1254:LYS:HA	1.93	0.41
3:C:13:GLU:OE2	3:C:18:ASN:ND2	2.53	0.41
1:A:465:HIS:CG	1:A:1097:GLU:OE2	2.73	0.41
3:C:128:ILE:HG22	3:C:129:PRO:N	2.36	0.41
6:H:37:MET:HE2	6:H:126:GLN:O	2.20	0.41
1:A:499:ASP:OD1	13:P:16:C:H4'	2.21	0.41
2:B:20:ASP:N	2:B:20:ASP:OD1	2.52	0.41
2:B:535:GLY:HA3	2:B:618:ALA:HB2	2.03	0.41
4:E:118:LEU:HD23	4:E:118:LEU:HA	1.90	0.41
1:A:412:GLN:OE1	1:A:412:GLN:N	2.53	0.41
1:A:802:PHE:HD2	2:B:671:GLU:HG2	1.86	0.41
1:A:1463:LEU:HD23	1:A:1463:LEU:HA	1.85	0.41
2:B:624:PRO:HA	2:B:663:GLU:O	2.21	0.41
2:B:666:ASP:OD1	2:B:666:ASP:N	2.43	0.41
1:A:530:SER:O	1:A:532:ARG:HG3	2.21	0.41
1:A:541:THR:HG21	1:A:672:ILE:HG22	2.03	0.41
1:A:1177:TYR:HB2	1:A:1210:TRP:CZ3	2.56	0.41
1:A:1408:ARG:HH22	1:A:1422:GLN:HA	1.86	0.41
2:B:497:LYS:HE2	2:B:497:LYS:HB3	1.48	0.41
2:B:534:VAL:N	2:B:600:GLU:OE2	2.31	0.41
2:B:556:ILE:CD1	2:B:576:ILE:HD11	2.50	0.41
2:B:912:ASN:ND2	2:B:916:TYR:HB2	2.33	0.41
3:C:214:ASP:OD1	3:C:215:GLU:N	2.54	0.41
7:I:92:LYS:HE2	7:I:92:LYS:HB2	1.91	0.41
11:D:20:LEU:HD12	11:D:121:ARG:HH12	1.85	0.41
11:D:35:SER:HB3	11:D:80:ILE:HD11	2.02	0.41
1:A:890:ARG:HD3	1:A:890:ARG:HA	1.93	0.41
1:A:894:ASP:OD1	1:A:894:ASP:N	2.54	0.41
2:B:854:ILE:O	2:B:907:VAL:HG21	2.21	0.41
2:B:873:LEU:HD12	2:B:874:PRO:HD2	2.03	0.41
1:A:580:LEU:HD23	1:A:580:LEU:O	2.21	0.40
2:B:604:ILE:HG12	2:B:668:LEU:HD12	2.03	0.40
4:E:150:VAL:HG22	4:E:185:ILE:HD11	2.03	0.40
11:D:133:ASP:O	11:D:137:LYS:HG2	2.21	0.40
1:A:1422:GLN:H	1:A:1422:GLN:HG3	1.71	0.40
9:K:45:ILE:CG2	9:K:94:LEU:CD2	2.99	0.40
12:G:43:GLY:HA2	12:G:157:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:118:GLU:HG2	12:G:129:LYS:O	2.20	0.40
1:A:428:ASP:OD1	1:A:429:LEU:N	2.54	0.40
1:A:484:LEU:HD12	1:A:485:ASN:O	2.22	0.40
1:A:865:ILE:O	1:A:869:GLU:HB3	2.21	0.40
2:B:65:ILE:HD11	2:B:412:LEU:HD22	2.02	0.40
2:B:604:ILE:CD1	2:B:668:LEU:CD1	2.99	0.40
2:B:1129:ASN:OD1	2:B:1131:ARG:HG2	2.22	0.40
1:A:992:LYS:HD3	1:A:992:LYS:HA	1.85	0.40
1:A:1196:TYR:OH	16:R:602:LEU:HD12	2.22	0.40
1:A:1375:ARG:NH1	1:A:1379:GLU:OE1	2.49	0.40
1:A:1473:LEU:HD22	5:F:104:ILE:HG21	2.03	0.40
2:B:674:MET:HG2	7:I:77:THR:HG22	2.03	0.40
2:B:927:ARG:NH2	2:B:1054:MET:SD	2.92	0.40
9:K:39:ASP:OD1	9:K:39:ASP:N	2.53	0.40
1:A:539:GLN:O	2:B:970:HIS:CE1	2.75	0.40
1:A:602:CYS:SG	1:A:603:ILE:N	2.95	0.40
1:A:904:GLN:OE1	1:A:1044:HIS:NE2	2.54	0.40
11:D:33:LEU:HD12	11:D:80:ILE:HG23	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1355/1970 (69%)	1272 (94%)	82 (6%)	1 (0%)	48	83
2	B	1090/1174 (93%)	1022 (94%)	68 (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	63
5	F	76/127 (60%)	72 (95%)	4 (5%)	0	100	100
6	H	146/150 (97%)	137 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	I	112/125 (90%)	104 (93%)	8 (7%)	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
16	R	98/650 (15%)	95 (97%)	3 (3%)	0	100	100
All	All	3849/5237 (74%)	3641 (95%)	206 (5%)	2 (0%)	50	83

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	1197/1749 (68%)	1187 (99%)	10 (1%)	79	85
2	B	961/1027 (94%)	952 (99%)	9 (1%)	75	83
3	C	230/252 (91%)	228 (99%)	2 (1%)	75	83
4	E	183/190 (96%)	180 (98%)	3 (2%)	58	74
5	F	67/111 (60%)	66 (98%)	1 (2%)	60	75
6	H	126/131 (96%)	125 (99%)	1 (1%)	79	85
7	I	97/112 (87%)	96 (99%)	1 (1%)	73	82
8	J	54/56 (96%)	53 (98%)	1 (2%)	52	70
9	K	104/106 (98%)	104 (100%)	0	100	100
10	L	40/55 (73%)	39 (98%)	1 (2%)	42	63
11	D	106/127 (84%)	106 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	G	147/153 (96%)	147 (100%)	0	100	100
16	R	64/545 (12%)	62 (97%)	2 (3%)	35	56
All	All	3376/4614 (73%)	3345 (99%)	31 (1%)	74	83

All (31) 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	497	LYS
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
4	E	49	SER
4	E	91	CYS
4	E	153	LYS
5	F	83	LEU
6	H	65	TYR
7	I	99	SER
8	J	47	ARG
10	L	52	LEU
16	R	497	ASP
16	R	588	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) 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
1	A	1457	ASN
1	A	1462	GLN
2	B	471	ASN
2	B	500	GLN
2	B	790	GLN
2	B	1009	GLN
3	C	217	GLN
11	D	48	ASN
11	D	93	HIS
12	G	4	HIS
12	G	14	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	P	9/17 (52%)	1 (11%)	1 (11%)

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	P	9	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
13	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

Of 8 ligands modelled in this entry, 8 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.

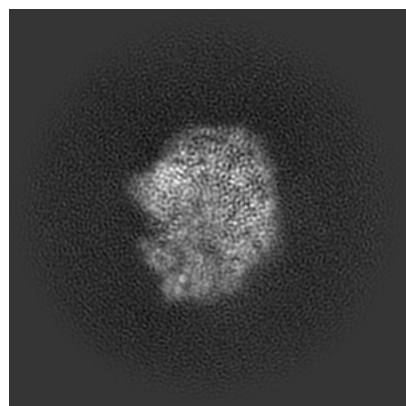
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18683. These allow visual inspection of the internal detail of the map and identification of artifacts.

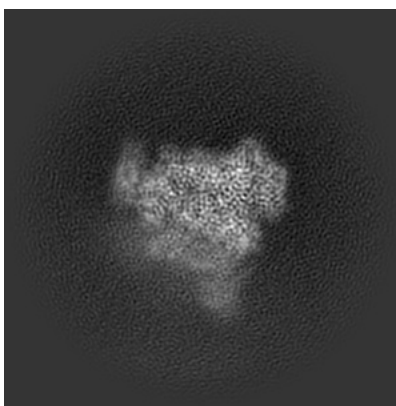
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

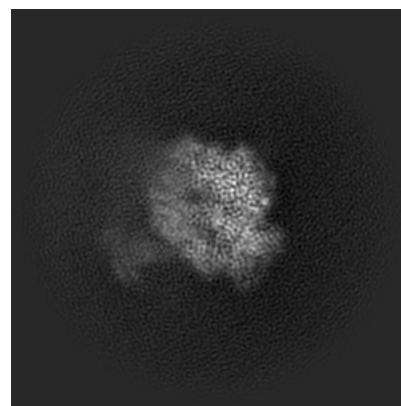
#### 6.1.1 Primary map



X

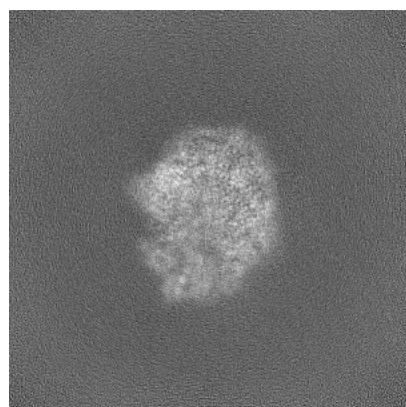


Y

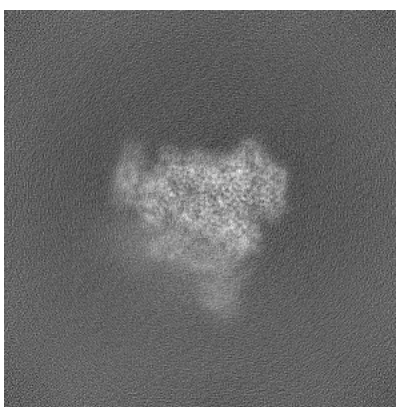


Z

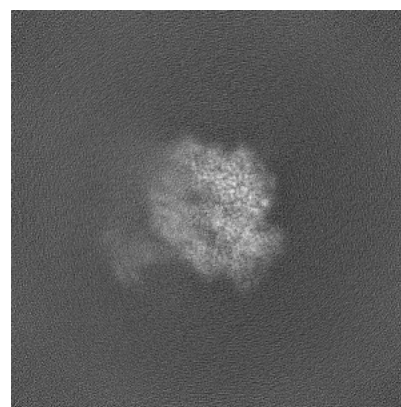
#### 6.1.2 Raw map



X



Y

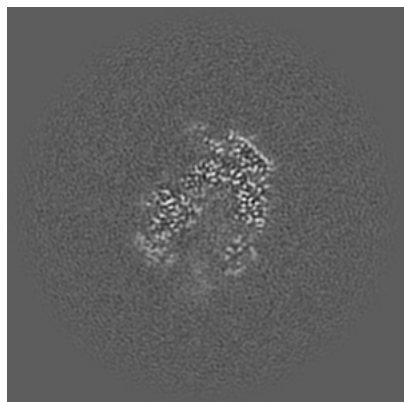


Z

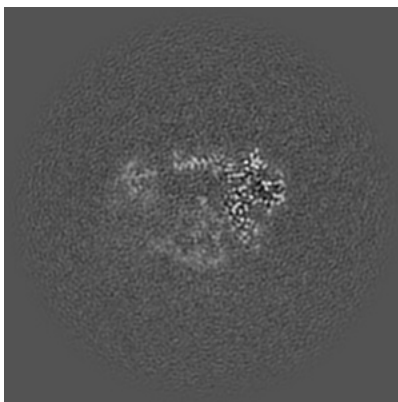
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

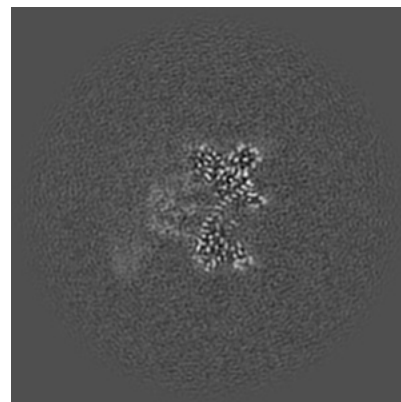
### 6.2.1 Primary map



X Index: 200

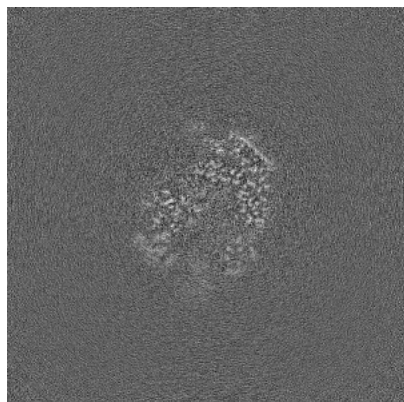


Y Index: 200

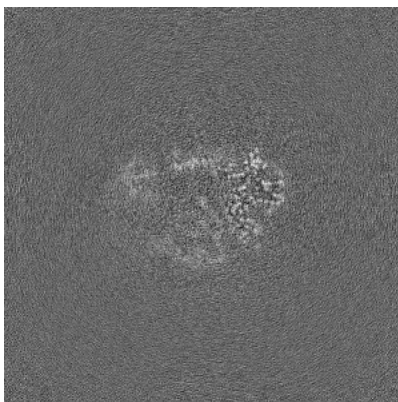


Z Index: 200

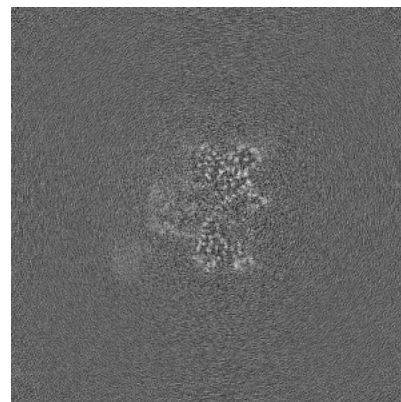
### 6.2.2 Raw map



X Index: 200



Y Index: 200



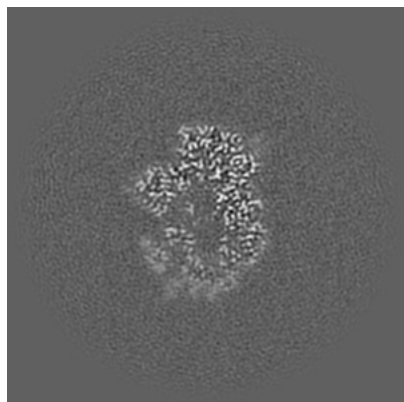
Z Index: 200

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

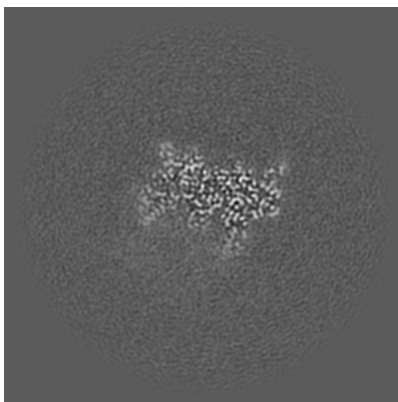


## 6.3 Largest variance slices [i](#)

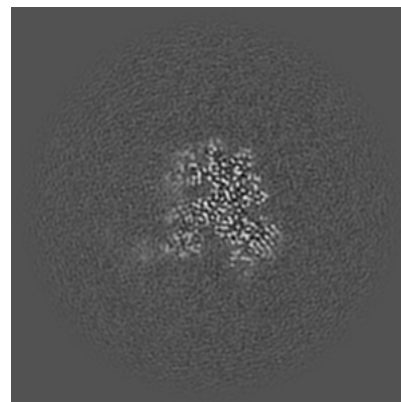
### 6.3.1 Primary map



X Index: 222

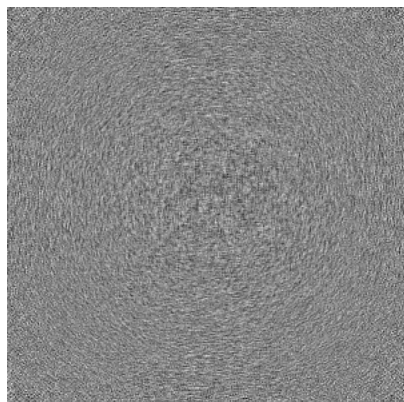


Y Index: 233

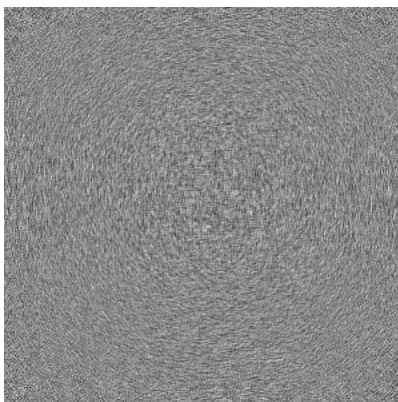


Z Index: 237

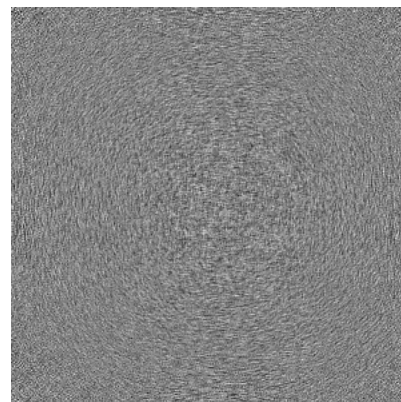
### 6.3.2 Raw map



X Index: 0



Y Index: 399

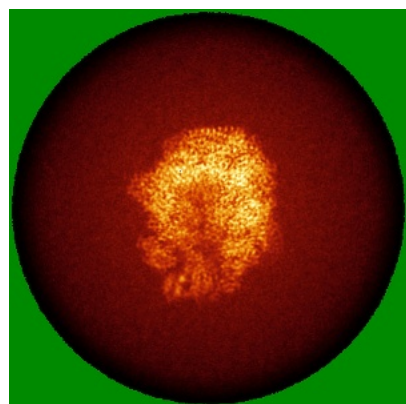


Z Index: 0

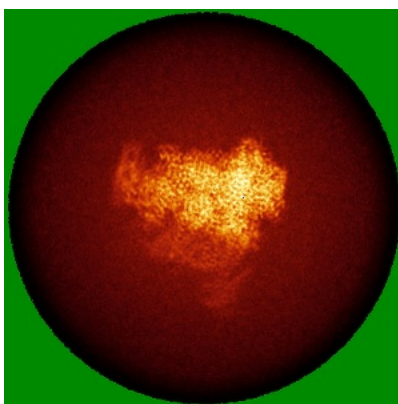
The images above show the largest variance slices of the map in three orthogonal directions.

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

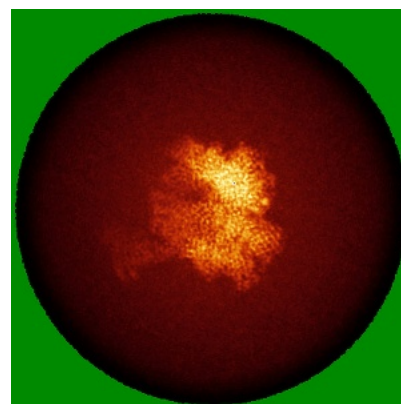
### 6.4.1 Primary map



X

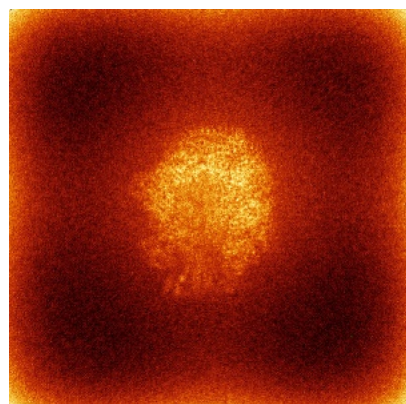


Y

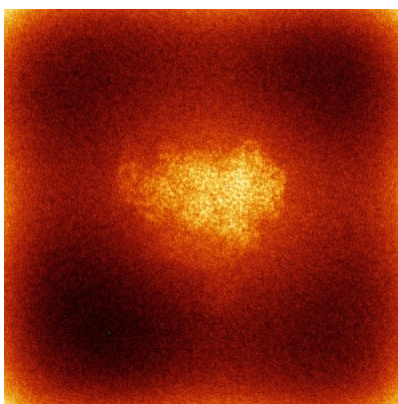


Z

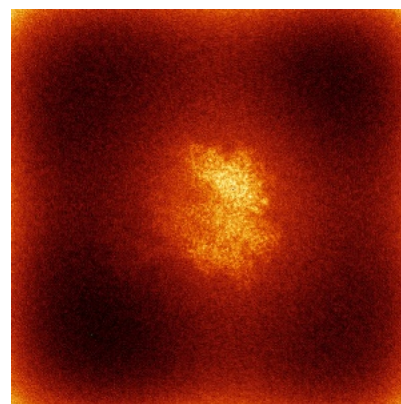
### 6.4.2 Raw map



X



Y



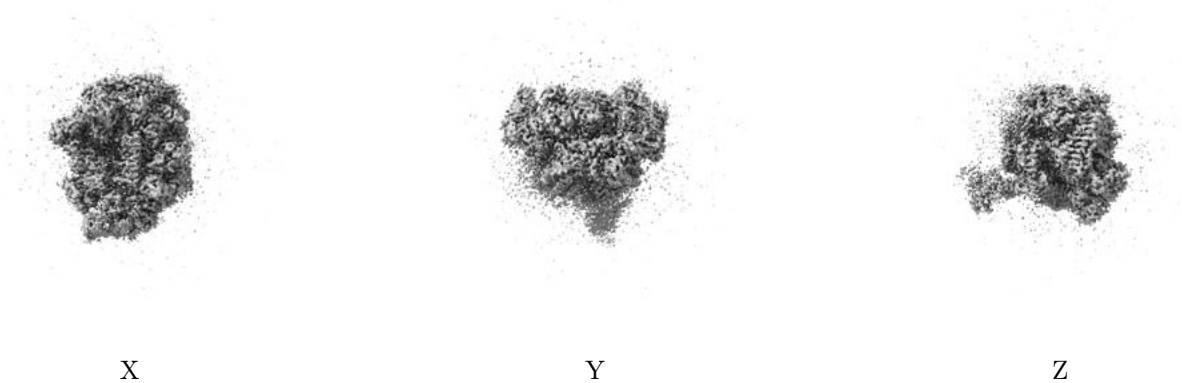
Z

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.



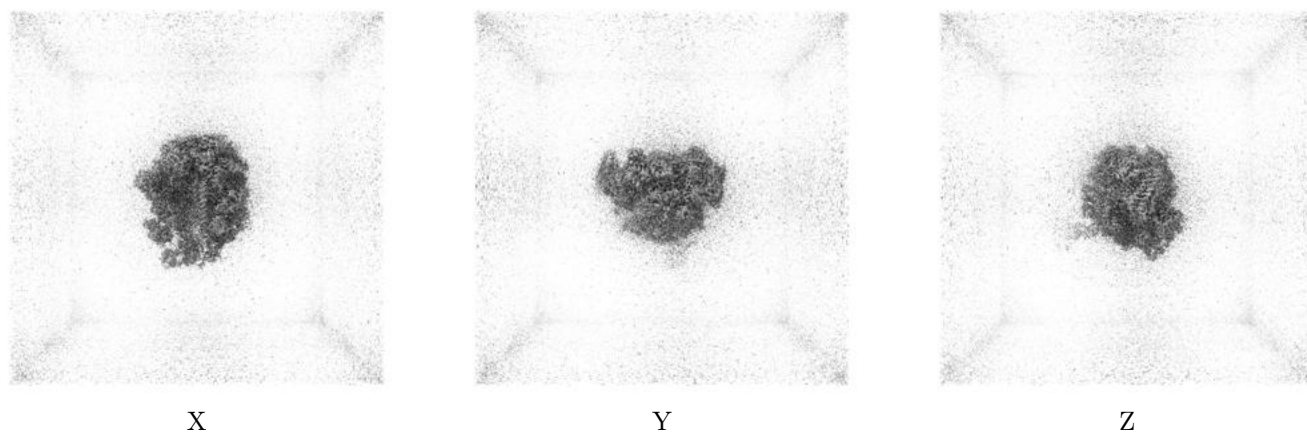
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

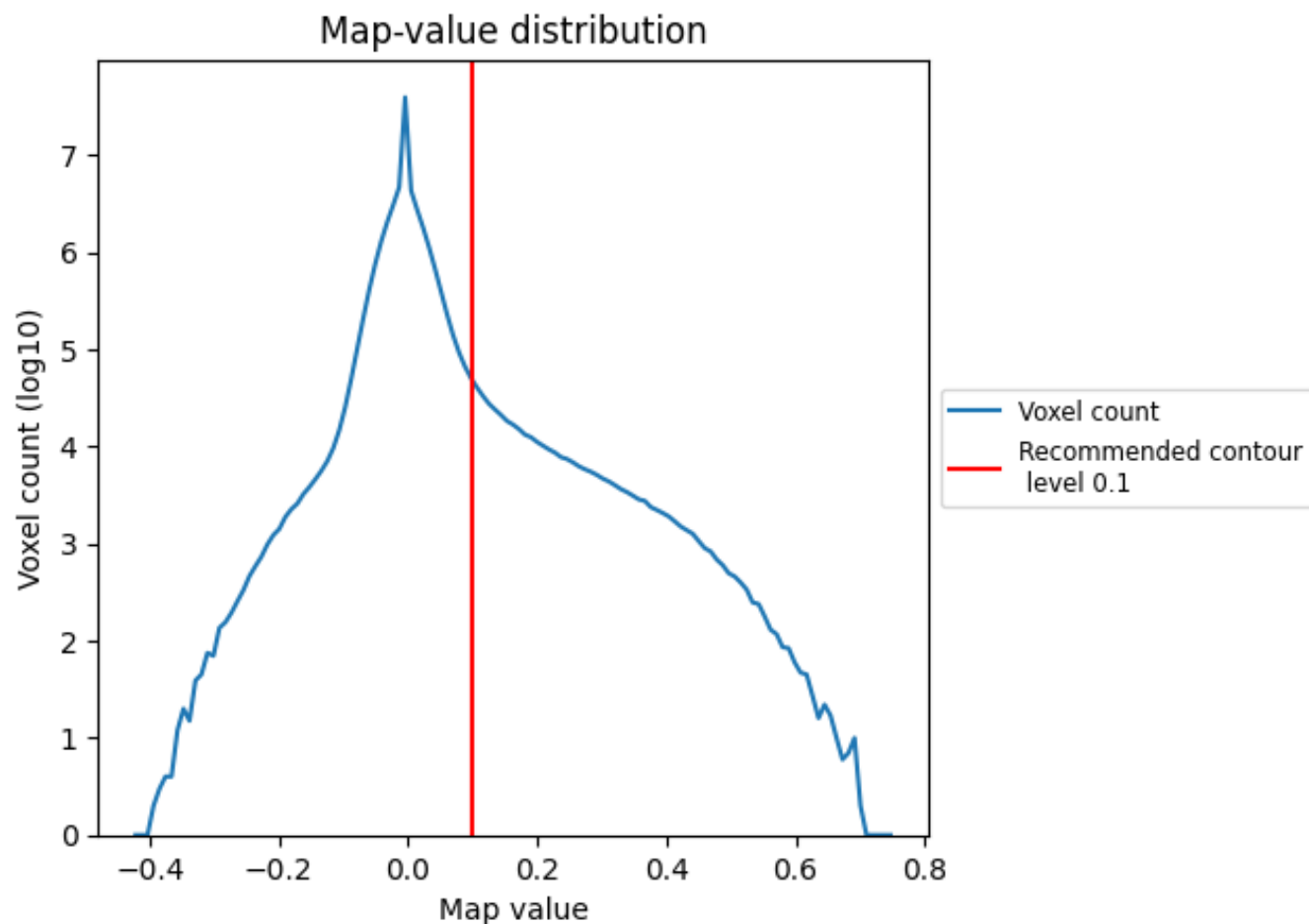
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

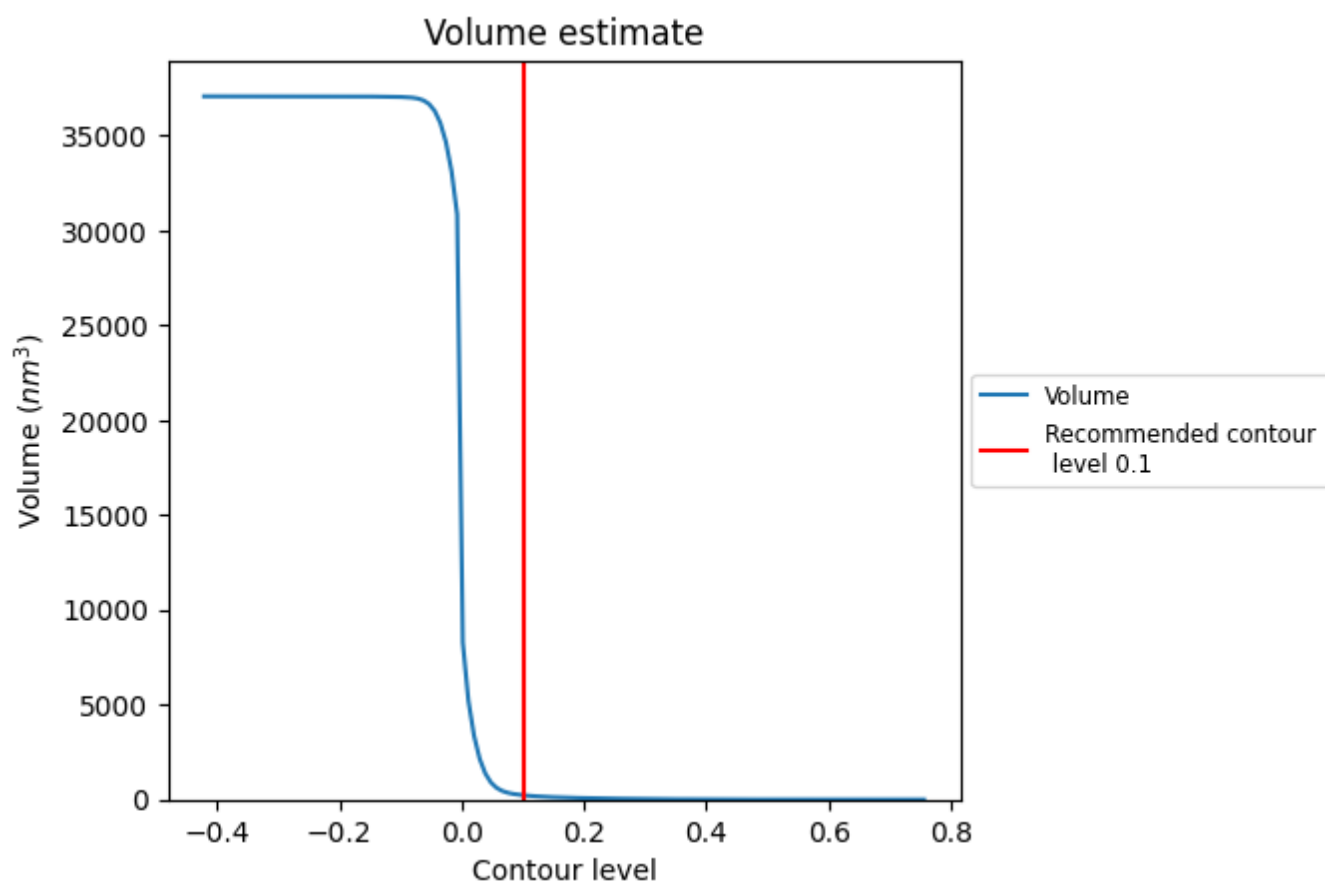
This section contains the results of statistical analysis of the map.

### 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.

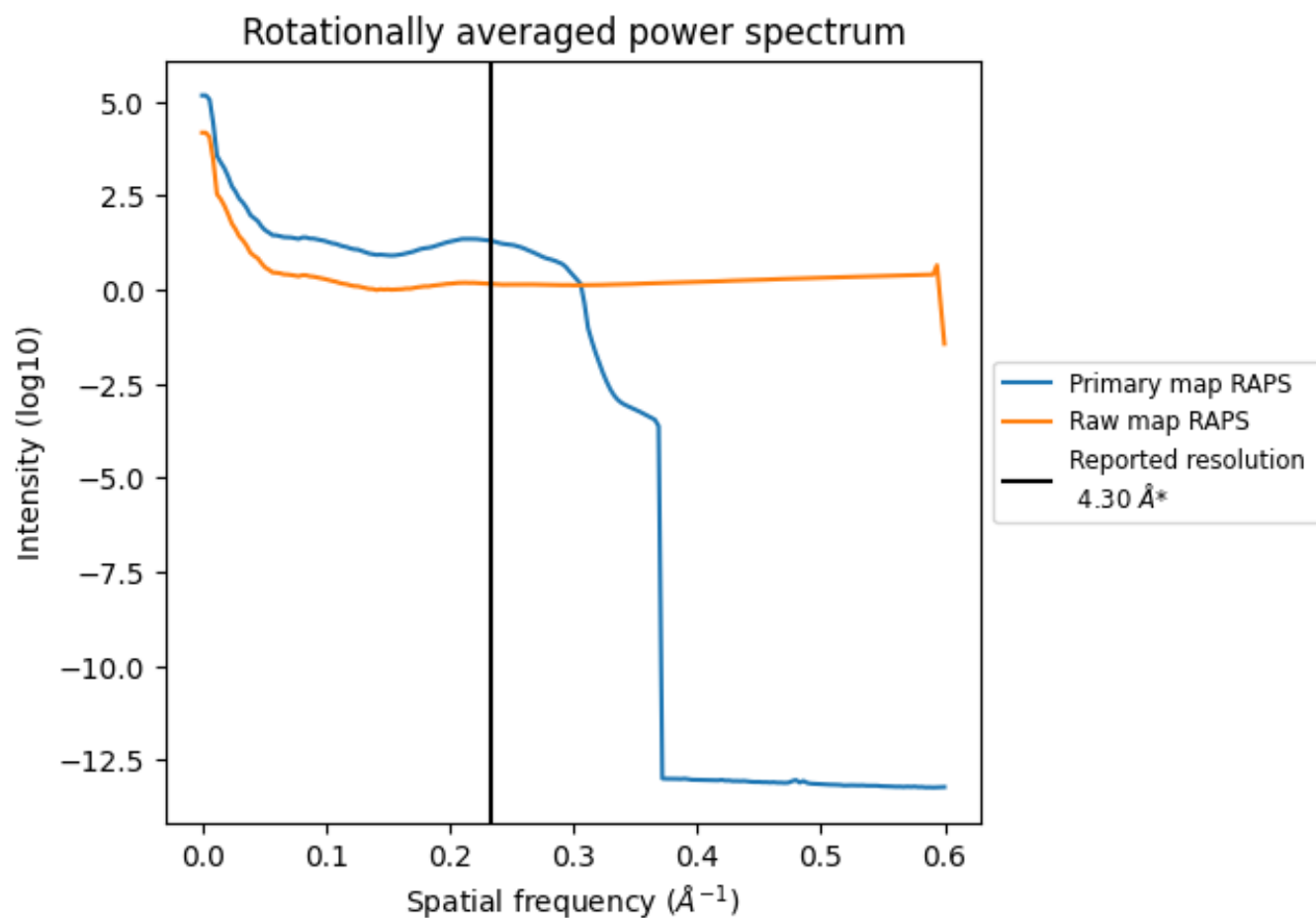
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 229 nm<sup>3</sup>; this corresponds to an approximate mass of 206 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 ⓘ

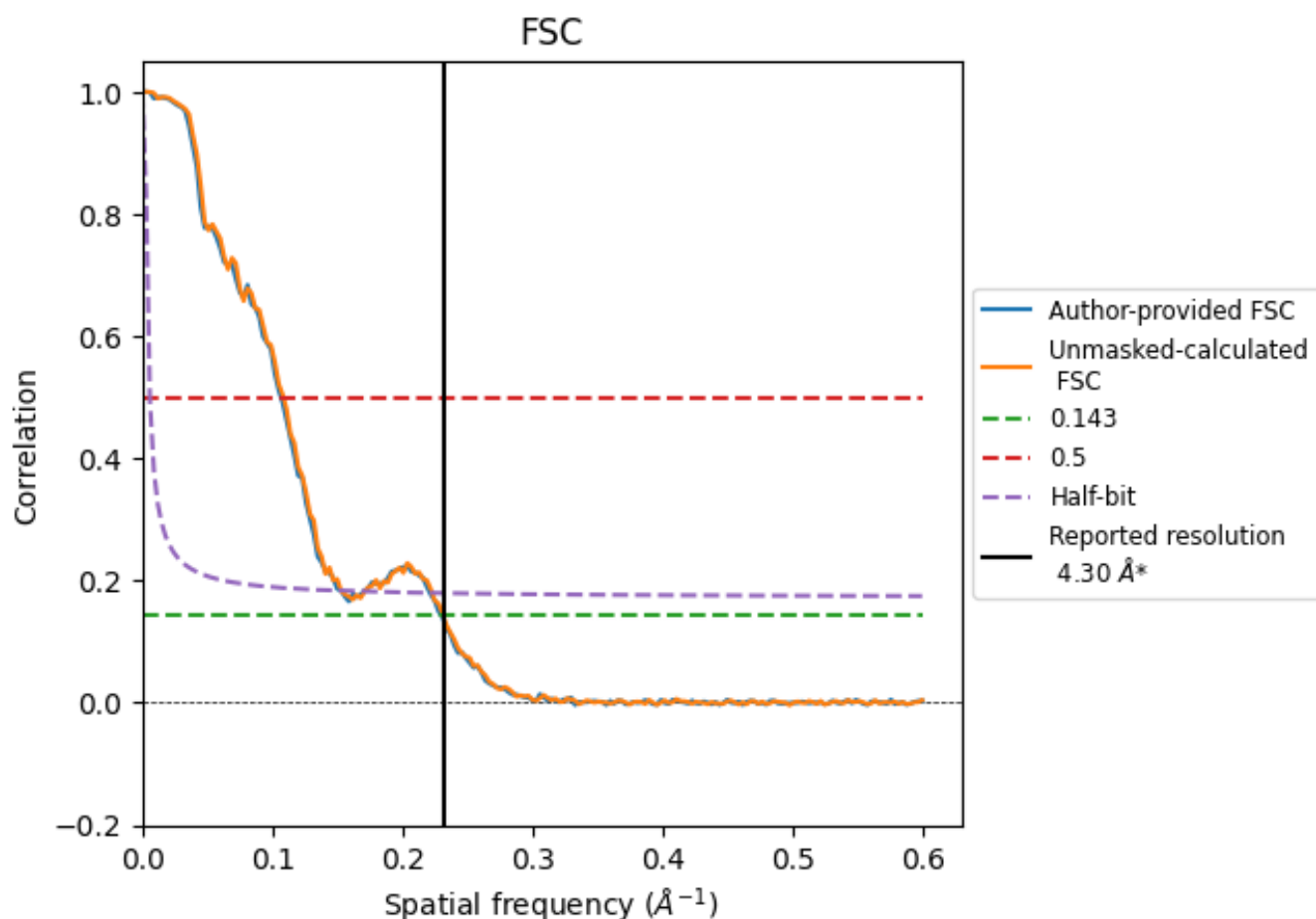


\*Reported resolution corresponds to spatial frequency of 0.233 Å<sup>-1</sup>

## 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 0.233 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

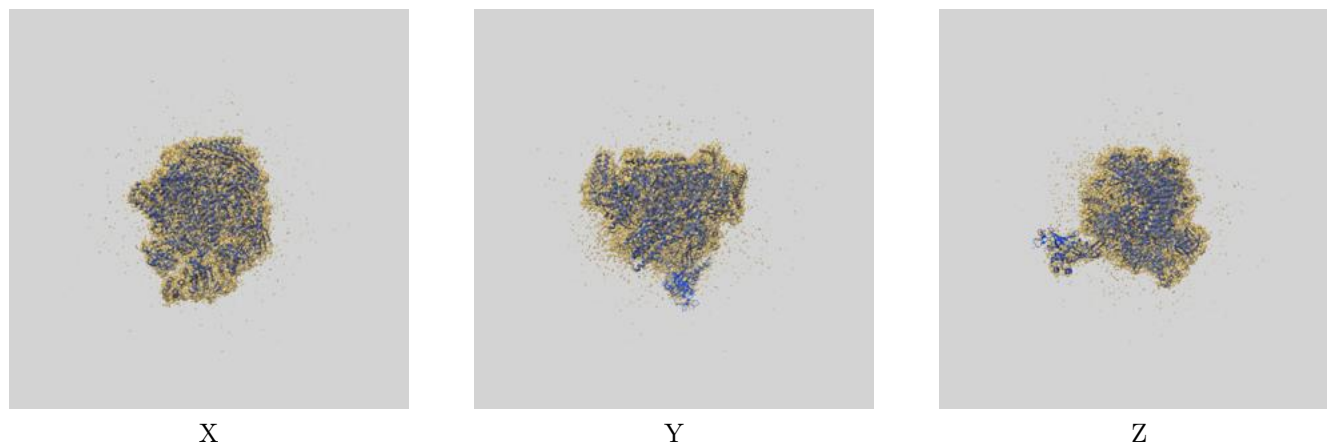
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.35	9.38	6.53
Unmasked-calculated*	4.32	9.22	6.54

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

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

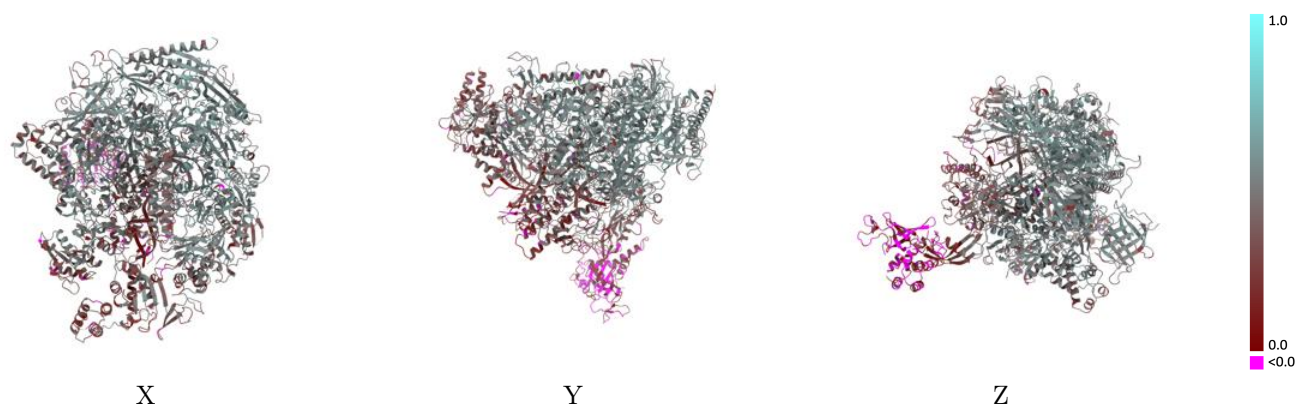
This section contains information regarding the fit between EMDB map EMD-18683 and PDB model 8QW9. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

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



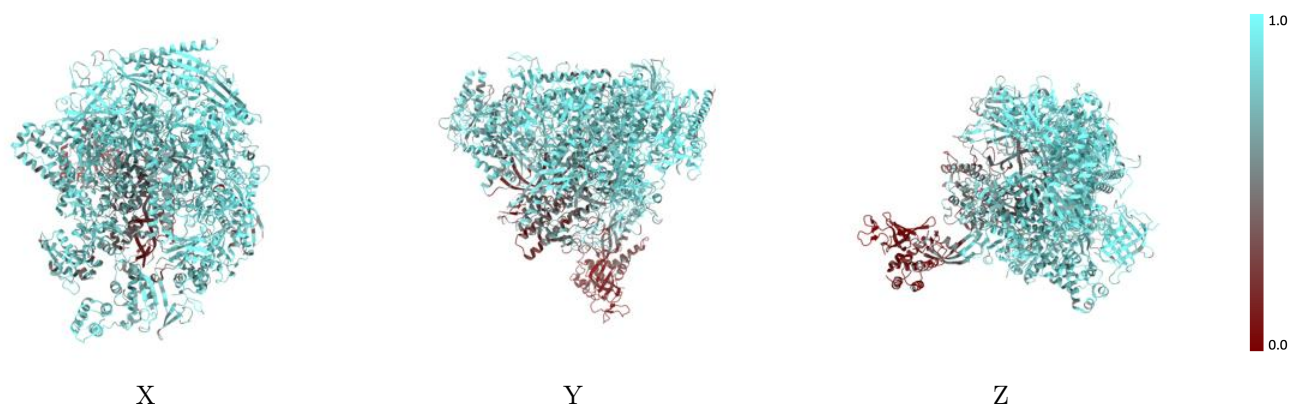
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

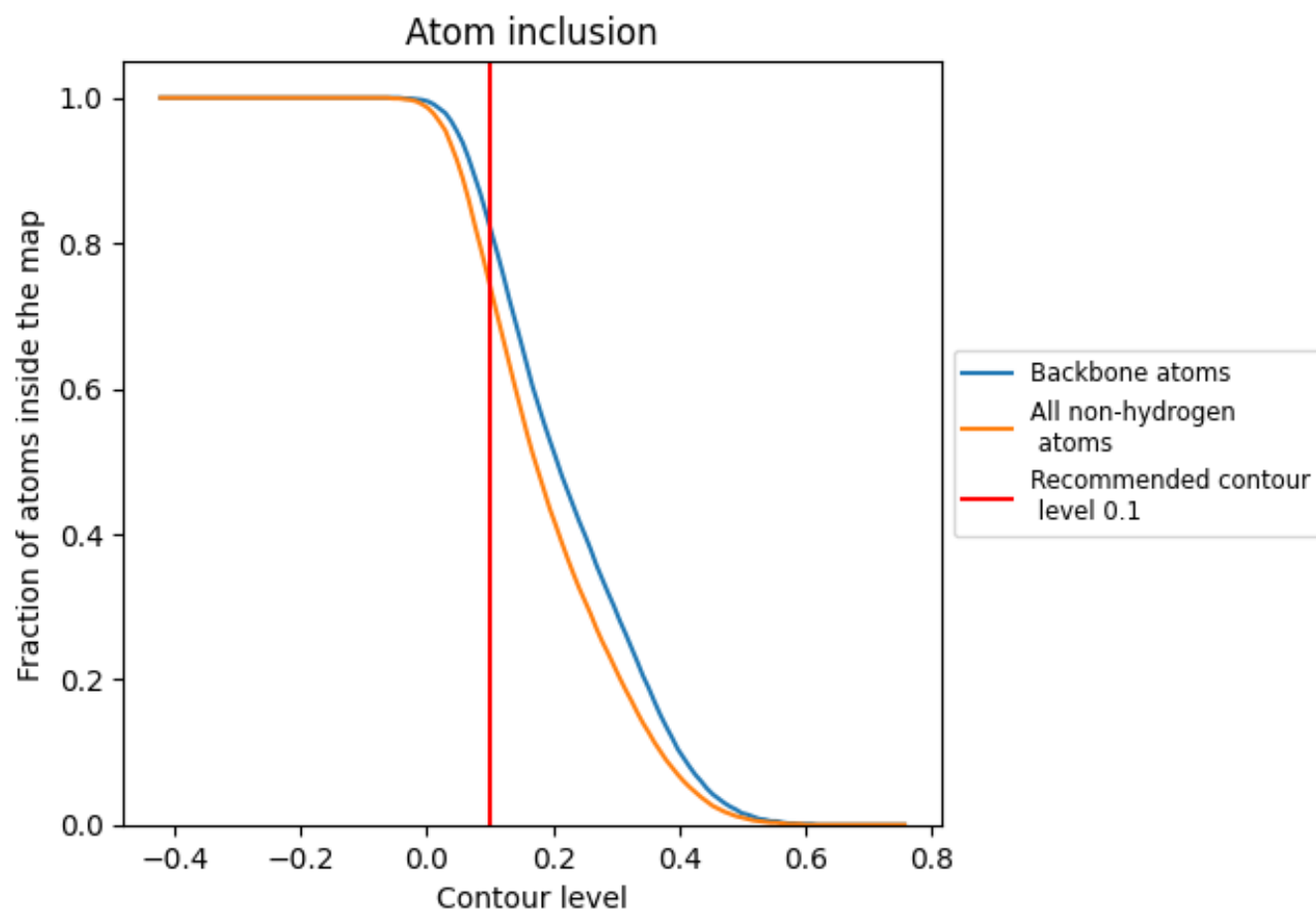
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.1).





































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 74% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7410	 0.4170
A	 0.7360	 0.4170
B	 0.8150	 0.4730
C	 0.8960	 0.5250
D	 0.1470	 0.0390
E	 0.8020	 0.4220
F	 0.8660	 0.4860
G	 0.2730	 0.1300
H	 0.8410	 0.4760
I	 0.7790	 0.4020
J	 0.9210	 0.5420
K	 0.8790	 0.5100
L	 0.8180	 0.4390
N	 0.1730	 0.1180
P	 0.4600	 0.2930
R	 0.7780	 0.2910
T	 0.4070	 0.2830

