Full wwPDB EM Validation Report

Feb 24, 2025 – 12:20 PM EST

PDB ID	:	9EHZ
EMDB ID	:	EMD-48071
Title	:	Cryo-EM structure of Human RNA polymerase II Elongation Complex in an Intermediate Translocation State
Authors	:	Florez Ariza, A.; Lue, N.; Nogales, E.
Deposited on	:	2024-11-25
Resolution	:	2.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

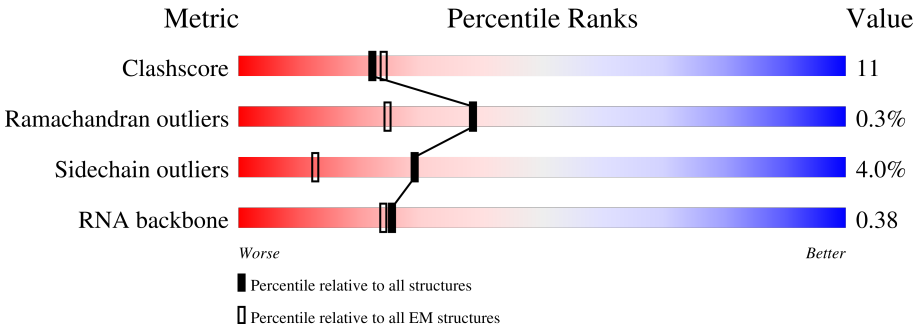
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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 >=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 <=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	D	142	47% 69% 21% 10%
2	E	210	77% 21%
3	F	127	50% 13% 35%
4	G	172	31% 66% 31%
5	H	150	66% 31%
6	I	125	6% 75% 15% 9%
7	J	67	66% 34%

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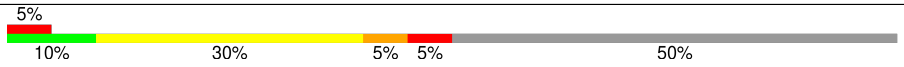
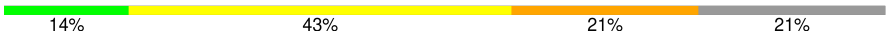
Mol	Chain	Length	Quality of chain
8	K	117	
9	L	58	
10	N	43	
11	P	20	
12	T	28	
13	A	1970	
14	B	1174	
15	C	275	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32125 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB4.

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

- Molecule 2 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	209	Total	C	N	O	S	0	0
			1711	1084	300	319	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	44	PHE	SER	conflict	UNP P19388

- Molecule 3 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	82	Total	C	N	O	S	0	0
			658	419	113	121	5		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	114	Total	C	N	O	S	0	0
			927	571	166	179	11		

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

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

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 10 is a DNA chain called Non-template DNA, nucleic acid scaffold.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	14	Total	C	N	O	P	0	0
			292	139	56	83	14		

- Molecule 11 is a RNA chain called RNA, nucleic acid scaffold.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	10	Total	C	N	O	P	0	0
			217	97	44	66	10		

- Molecule 12 is a DNA chain called Template DNA, nucleic acid scaffold.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	22	Total	C	N	O	P	0	0
			447	214	77	134	22		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	1437	Total	C	N	O	S	0	0
			11392	7162	2037	2120	73		

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	1134	Total	C	N	O	S	0	0
			9062	5732	1595	1671	64		

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	257	Total	C	N	O	S	0	0
			2060	1296	351	407	6		

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

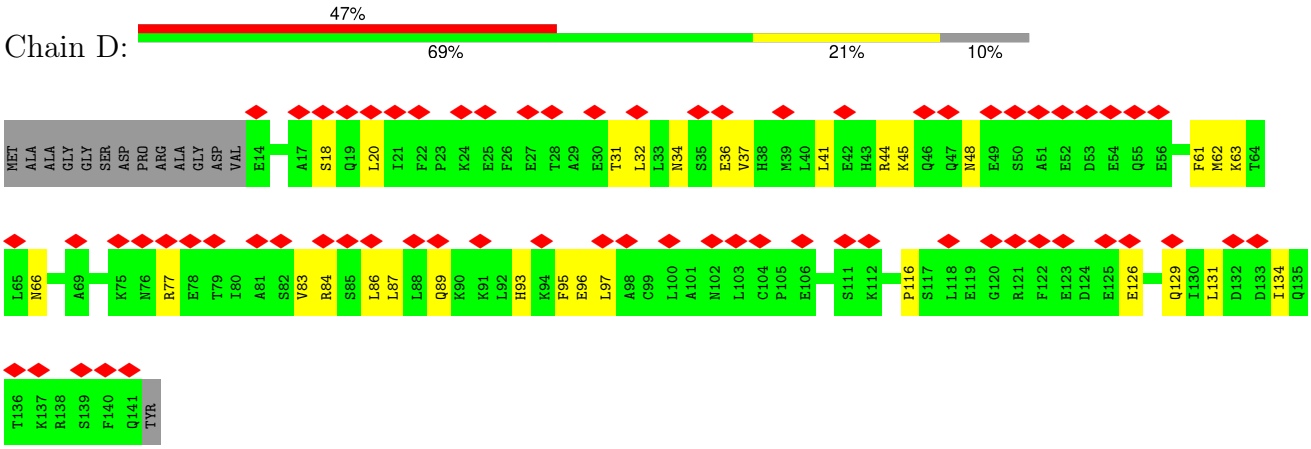
Mol	Chain	Residues	Atoms		AltConf
17	P	1	Total	Mg	0
			1	1	

3 Residue-property plots (i)

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

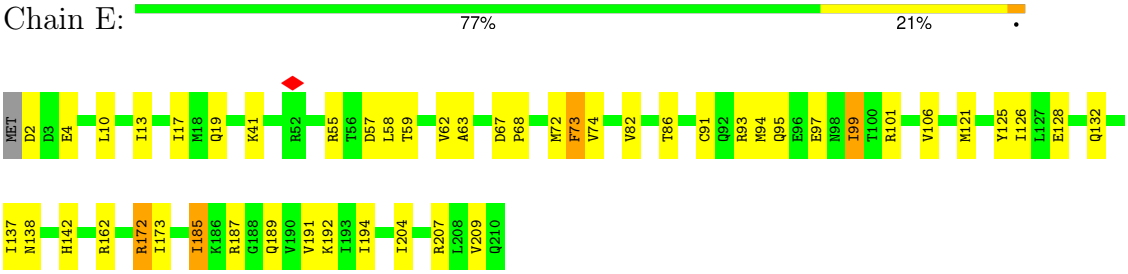
• Molecule 1: DNA-directed RNA polymerase II subunit RPB4

Chain D:



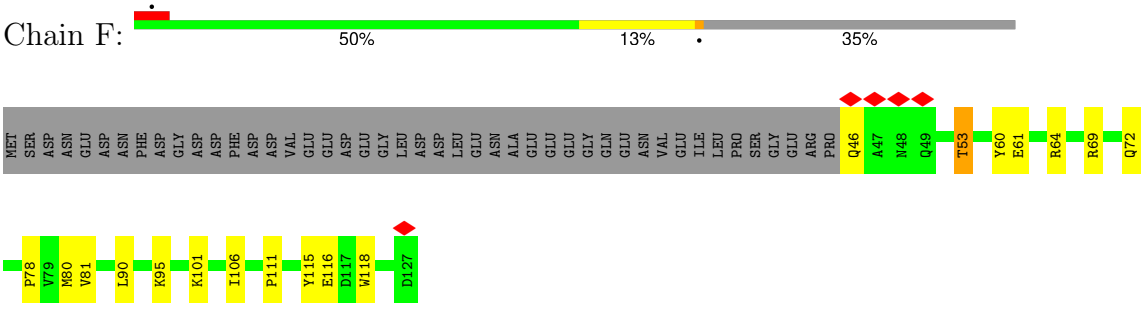
• Molecule 2: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



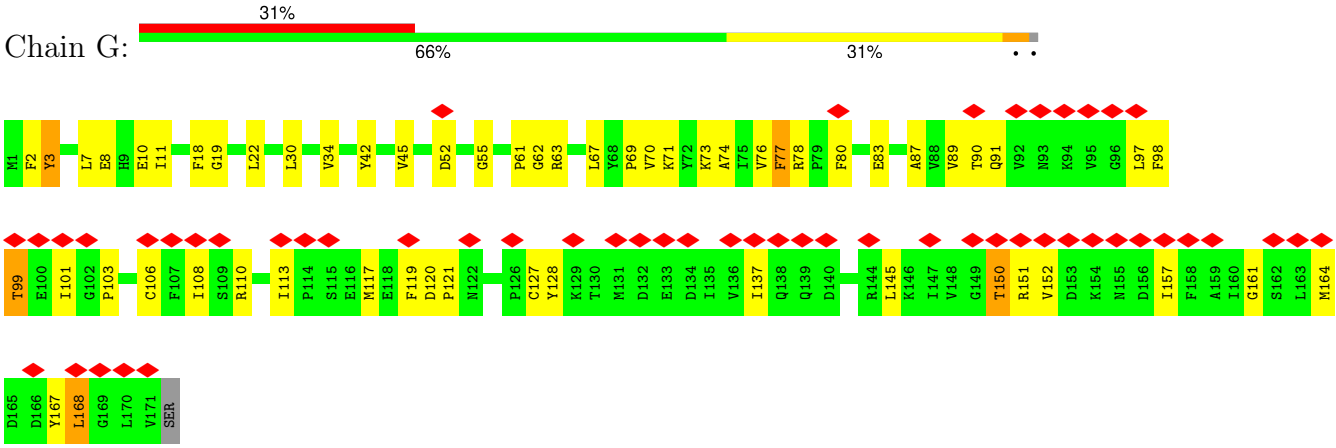
• Molecule 3: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



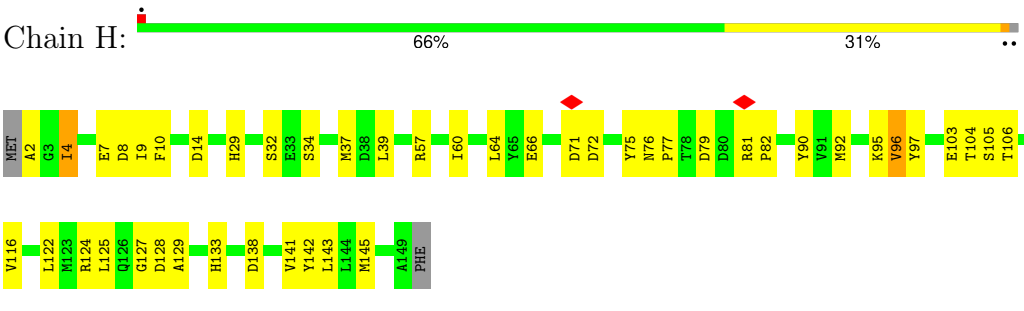
• Molecule 4: DNA-directed RNA polymerase II subunit RPB7

Chain G:



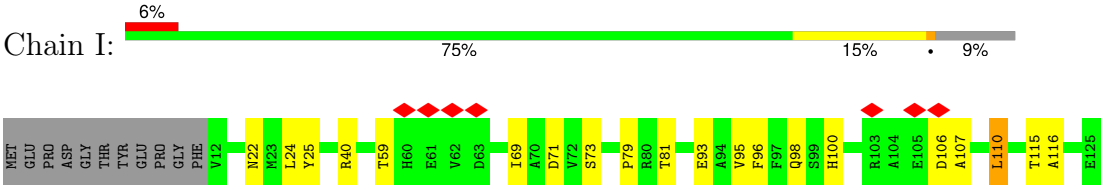
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



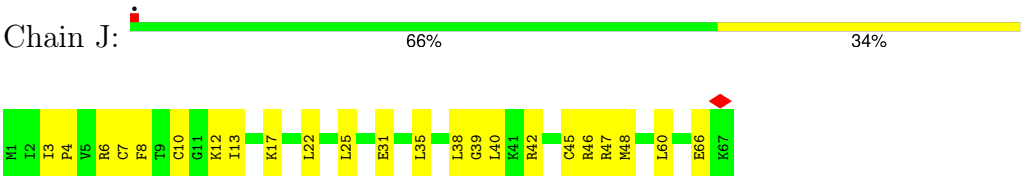
• Molecule 6: DNA-directed RNA polymerase II subunit RPB9

Chain I:



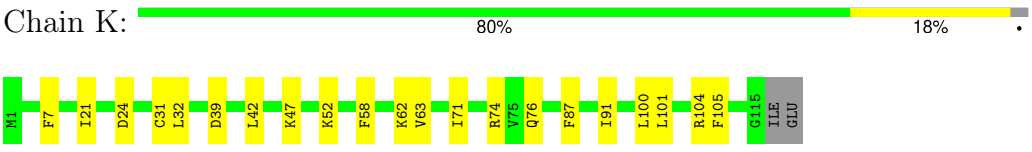
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



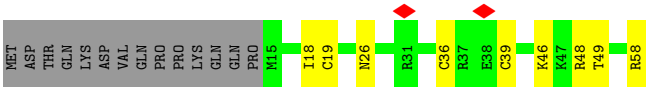
• Molecule 8: DNA-directed RNA polymerase II subunit RPB11-a

Chain K:



• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:

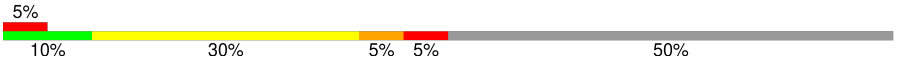


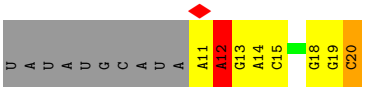
• Molecule 10: Non-template DNA, nucleic acid scaffold

Chain N:

• Molecule 11: RNA, nucleic acid scaffold

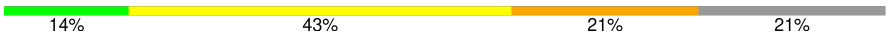
Chain P:





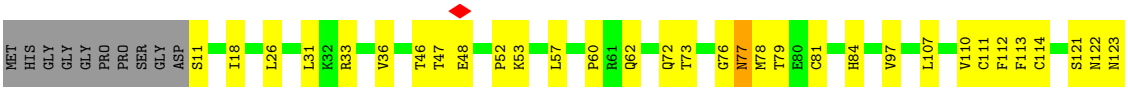
• Molecule 12: Template DNA, nucleic acid scaffold

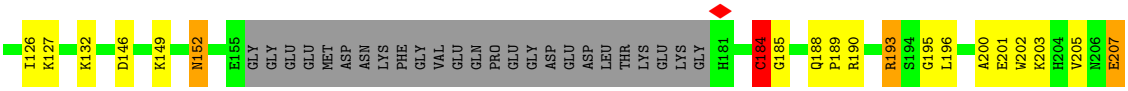
Chain T:

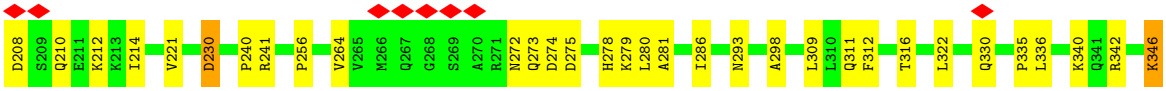


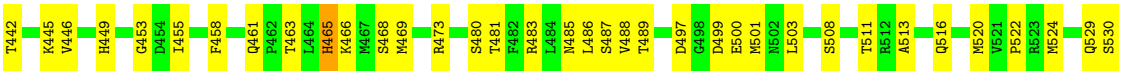
• Molecule 13: DNA-directed RNA polymerase II subunit RPB1

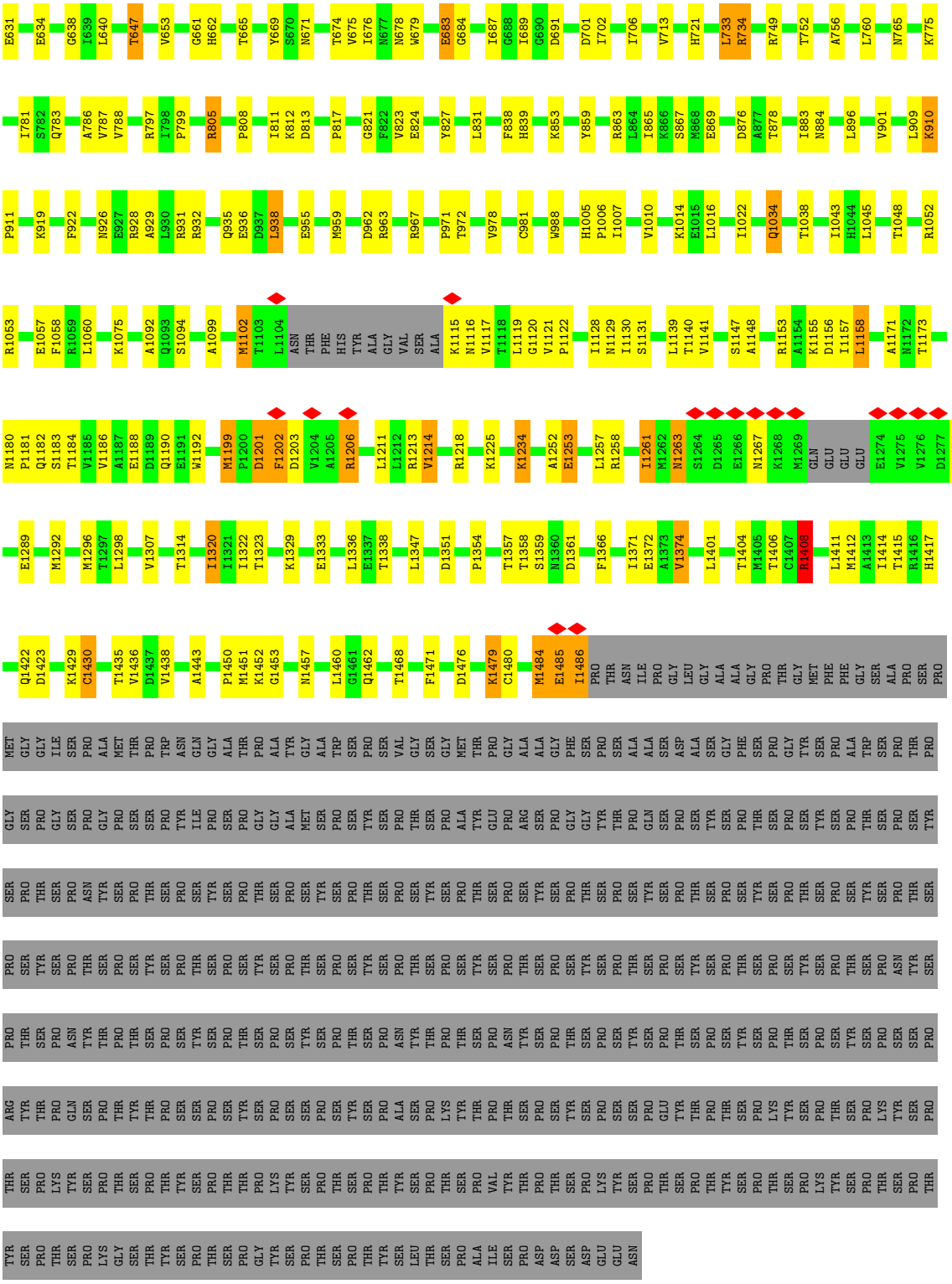
Chain A:





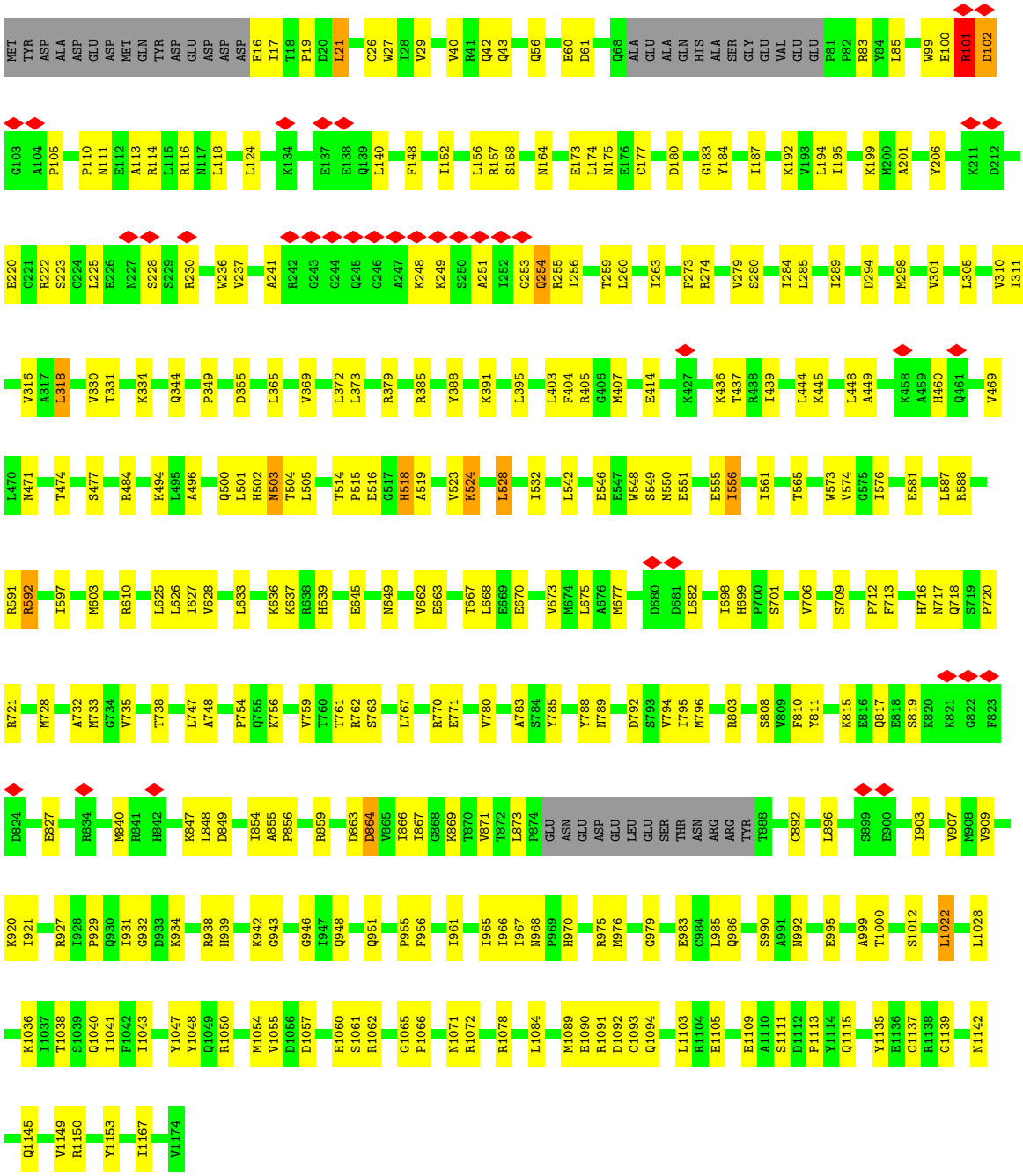






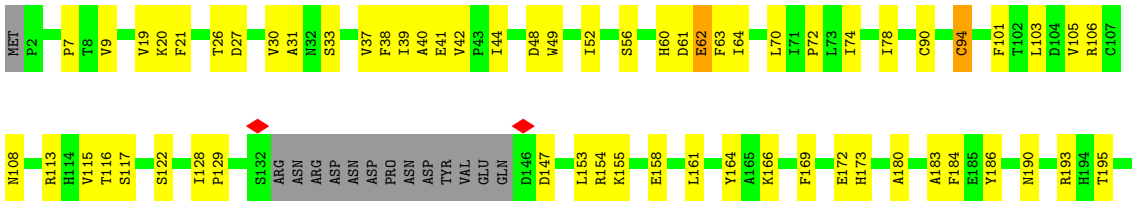
• Molecule 14: DNA-directed RNA polymerase II subunit RPB2

Chain B:



• Molecule 15: DNA-directed RNA polymerase II subunit RPB3

Chain C:




K205
E213
D214
E215
A218
F229
Y230
Y231
N232
V233
E234
P241
V245
Q260
L263
D270
V271
LEU
THR
ILE
ASN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	174428	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.003	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	D	0.24	0/1019	0.47	0/1374
2	E	0.28	0/1742	0.50	0/2353
3	F	0.29	0/668	0.51	0/903
4	G	0.26	0/1365	0.48	0/1853
5	H	0.28	0/1207	0.49	0/1628
6	I	0.28	0/948	0.49	0/1284
7	J	0.28	0/542	0.46	0/730
8	K	0.27	0/939	0.45	0/1271
9	L	0.29	0/377	0.59	0/500
10	N	0.71	0/328	1.32	3/505 (0.6%)
11	P	0.67	0/243	1.28	1/377 (0.3%)
12	T	0.73	0/499	1.41	9/767 (1.2%)
13	A	0.28	0/11599	0.50	0/15657
14	B	0.29	0/9243	0.51	0/12475
15	C	0.28	0/2103	0.48	0/2858
All	All	0.31	0/32822	0.55	13/44535 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1
13	A	0	3
14	B	0	1
All	All	0	5

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	T	13	DC	OP2-P-O3'	6.82	120.20	105.20
12	T	13	DC	P-O3'-C3'	6.71	127.76	119.70
12	T	16	DC	O4'-C4'-C3'	-6.45	101.92	104.50
10	N	25	DT	P-O3'-C3'	5.83	126.70	119.70
12	T	5	DA	OP1-P-O3'	5.80	117.97	105.20
12	T	9	DC	OP2-P-O3'	5.64	117.61	105.20
12	T	20	DT	OP2-P-O3'	5.51	117.32	105.20
11	P	12	A	O4'-C1'-N9	5.46	112.57	108.20
12	T	12	DA	OP1-P-O3'	5.42	117.11	105.20
10	N	15	DT	OP1-P-O3'	5.40	117.09	105.20
10	N	22	DA	OP2-P-O3'	5.39	117.06	105.20
12	T	2	DT	OP1-P-O3'	5.23	116.71	105.20
12	T	14	DG	OP1-P-O3'	5.01	116.21	105.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	A	1408	ARG	Sidechain
13	A	430	ARG	Sidechain
13	A	910	LYS	Peptide
14	B	101	ARG	Sidechain
2	E	172	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1005	0	964	25	0
2	E	1711	0	1729	33	0
3	F	658	0	686	15	0
4	G	1334	0	1333	35	0
5	H	1186	0	1147	31	0
6	I	927	0	859	13	0
7	J	533	0	553	17	0
8	K	920	0	942	17	0
9	L	372	0	378	9	0
10	N	292	0	159	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	P	217	0	111	19	0
12	T	447	0	250	50	0
13	A	11392	0	11515	300	0
14	B	9062	0	9106	240	0
15	C	2060	0	2011	50	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	P	1	0	0	0	0
All	All	32125	0	31743	720	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 11.

All (720) 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)
12:T:15:DC:C1'	13:A:461:GLN:OE1	1.69	1.39
10:N:15:DT:O4	14:B:391:LYS:NZ	1.58	1.35
12:T:13:DC:N4	14:B:518:HIS:CE1	1.96	1.34
10:N:15:DT:O2	14:B:385:ARG:HD3	1.25	1.31
12:T:13:DC:C4	14:B:518:HIS:NE2	1.98	1.30
11:P:11:A:H5"	13:A:264:VAL:CG1	1.71	1.20
11:P:11:A:C5'	13:A:264:VAL:HG13	1.72	1.18
12:T:13:DC:N4	14:B:518:HIS:NE2	1.92	1.13
12:T:15:DC:O4'	13:A:461:GLN:OE1	1.65	1.12
12:T:15:DC:C4'	13:A:461:GLN:OE1	1.97	1.11
12:T:14:DG:OP1	13:A:346:LYS:CD	2.02	1.06
12:T:15:DC:C2'	13:A:461:GLN:OE1	2.04	1.05
12:T:13:DC:C4	14:B:518:HIS:CE1	2.42	1.02
12:T:16:DC:OP1	13:A:358:ARG:NH1	1.96	0.98
14:B:515:PRO:HG3	14:B:523:VAL:HB	1.43	0.98
11:P:11:A:H5"	13:A:264:VAL:HG13	0.97	0.97
11:P:12:A:H61	12:T:22:DA:H61	1.15	0.94
12:T:15:DC:H1'	13:A:461:GLN:OE1	1.65	0.93
12:T:14:DG:OP1	13:A:346:LYS:HD2	1.68	0.92
13:A:184:CYS:SG	13:A:185:GLY:N	2.40	0.91
10:N:15:DT:O2	14:B:385:ARG:CD	2.17	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:20:C:H4'	13:A:499:ASP:OD1	1.72	0.89
12:T:13:DC:H42	14:B:518:HIS:CE1	1.89	0.88
9:L:36:CYS:HB3	9:L:39:CYS:SG	2.16	0.84
3:F:78:PRO:HG3	13:A:1486:ILE:HA	1.58	0.83
14:B:285:LEU:HD11	14:B:301:VAL:HG11	1.62	0.82
14:B:866:ILE:HG22	14:B:867:ILE:HG13	1.63	0.81
11:P:11:A:C5'	13:A:264:VAL:CG1	2.44	0.81
6:I:79:PRO:HB3	13:A:811:ILE:HD12	1.64	0.80
12:T:15:DC:H4'	13:A:461:GLN:OE1	1.82	0.79
15:C:37:VAL:HG13	15:C:41:GLU:HB2	1.65	0.78
6:I:106:ASP:HB2	13:A:733:LEU:HB2	1.65	0.78
11:P:11:A:C4'	13:A:264:VAL:HG13	2.13	0.78
14:B:733:MET:HE1	14:B:1050:ARG:HH11	1.49	0.78
13:A:783:GLN:HB2	14:B:976:MET:HE1	1.66	0.77
15:C:183:ALA:HB3	15:C:232:ASN:HB3	1.68	0.76
12:T:14:DG:OP1	13:A:346:LYS:HD3	1.86	0.76
12:T:15:DC:H4'	13:A:461:GLN:NE2	2.01	0.76
11:P:12:A:H61	12:T:22:DA:N6	1.85	0.74
13:A:111:CYS:SG	13:A:114:CYS:HB3	2.27	0.74
14:B:636:LYS:H	14:B:639:HIS:HD2	1.35	0.74
11:P:12:A:N6	12:T:22:DA:H61	1.85	0.73
13:A:78:MET:O	14:B:1072:ARG:NH2	2.22	0.72
13:A:1022:ILE:H	13:A:1034:GLN:HE22	1.37	0.72
13:A:1211:LEU:HD11	13:A:1258:ARG:HB3	1.72	0.72
12:T:13:DC:C5	14:B:518:HIS:NE2	2.41	0.72
6:I:69:ILE:HG22	6:I:71:ASP:H	1.55	0.71
12:T:6:DG:H2"	12:T:7:DT:H5'	1.72	0.71
14:B:273:PHE:HB3	14:B:284:ILE:HD12	1.71	0.71
12:T:15:DC:H4'	13:A:461:GLN:CD	2.11	0.71
7:J:47:ARG:NH1	7:J:48:MET:SD	2.64	0.71
12:T:14:DG:H2"	14:B:1089:MET:HE2	1.73	0.71
11:P:20:C:H5"	13:A:497:ASP:O	1.90	0.70
12:T:15:DC:H2"	13:A:461:GLN:OE1	1.88	0.69
7:J:10:CYS:SG	7:J:42:ARG:NH1	2.66	0.69
14:B:718:GLN:HG2	14:B:720:PRO:HD2	1.75	0.69
12:T:13:DC:H2"	12:T:14:DG:H5'	1.75	0.68
14:B:709:SER:HB2	14:B:767:LEU:HD11	1.75	0.68
12:T:14:DG:H2"	14:B:1089:MET:CE	2.23	0.68
13:A:1128:ILE:HD12	13:A:1414:ILE:HD12	1.76	0.68
4:G:89:VAL:HA	4:G:99:THR:HA	1.76	0.68
13:A:589:LYS:HZ3	13:A:638:GLY:H	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:11:A:C4'	13:A:264:VAL:CG1	2.71	0.67
12:T:15:DC:H4'	13:A:461:GLN:HE22	1.59	0.67
14:B:1036:LYS:NZ	15:C:186:TYR:O	2.25	0.67
6:I:73:SER:HA	6:I:95:VAL:HG11	1.75	0.67
13:A:1128:ILE:HG23	13:A:1414:ILE:HB	1.75	0.66
13:A:1218:ARG:NH2	13:A:1252:ALA:O	2.29	0.66
13:A:1206:ARG:O	13:A:1263:ASN:ND2	2.29	0.66
14:B:260:LEU:HB2	14:B:263:ILE:HD12	1.77	0.66
14:B:274:ARG:NH1	14:B:279:VAL:O	2.27	0.66
14:B:848:LEU:HD23	14:B:854:ILE:HG23	1.76	0.66
4:G:145:LEU:HA	4:G:168:LEU:HD21	1.78	0.65
7:J:17:LYS:HB3	7:J:38:LEU:HD13	1.77	0.65
13:A:1102:MET:HG2	13:A:1120:GLY:HA2	1.77	0.65
2:E:55:ARG:HA	2:E:58:LEU:HD12	1.77	0.65
14:B:677:MET:H	14:B:682:LEU:HD12	1.61	0.65
14:B:854:ILE:HD11	14:B:866:ILE:HD13	1.77	0.65
13:A:674:THR:O	13:A:678:ASN:ND2	2.29	0.65
14:B:404:PHE:HA	14:B:407:MET:HE2	1.77	0.64
14:B:1012:SER:HB3	14:B:1022:LEU:HB2	1.78	0.64
13:A:869:GLU:OE1	14:B:1091:ARG:NH2	2.30	0.64
14:B:395:LEU:HD21	14:B:532:ILE:HD13	1.79	0.64
14:B:1040:GLN:NE2	15:C:195:THR:OG1	2.30	0.64
13:A:36:VAL:HG21	13:A:73:THR:HG21	1.80	0.64
1:D:44:ARG:HH12	1:D:45:LYS:HE2	1.63	0.64
1:D:44:ARG:O	1:D:48:ASN:ND2	2.31	0.64
15:C:90:CYS:SG	15:C:94:CYS:HB3	2.38	0.64
8:K:24:ASP:OD2	8:K:74:ARG:NH1	2.31	0.63
13:A:364:ARG:HB2	14:B:1084:LEU:HD21	1.79	0.63
13:A:749:ARG:HH22	13:A:783:GLN:HE21	1.45	0.63
13:A:605:THR:HA	13:A:627:LYS:HA	1.80	0.63
13:A:1182:GLN:O	13:A:1190:GLN:NE2	2.28	0.63
13:A:146:ASP:HA	13:A:149:LYS:HE3	1.81	0.63
9:L:26:ASN:ND2	9:L:36:CYS:SG	2.72	0.63
13:A:805:ARG:HD2	13:A:812:LYS:HG2	1.80	0.63
13:A:938:LEU:HD21	13:A:1005:HIS:HA	1.81	0.62
13:A:522:PRO:HB2	13:A:662:HIS:HB2	1.82	0.62
7:J:46:ARG:NH1	14:B:992:ASN:O	2.33	0.62
13:A:1261:ILE:HD11	13:A:1285:LEU:HG	1.81	0.62
10:N:15:DT:H3	14:B:385:ARG:HB3	1.64	0.62
14:B:528:LEU:HD11	14:B:767:LEU:HD21	1.81	0.62
12:T:14:DG:OP1	13:A:346:LYS:CE	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:T:19:DG:OP1	14:B:747:LEU:HD21	1.99	0.62
2:E:207:ARG:NH1	13:A:1372:GLU:OE2	2.33	0.61
7:J:3:ILE:HD12	7:J:4:PRO:HD2	1.81	0.61
13:A:1048:THR:HA	13:A:1053:ARG:HH21	1.65	0.61
13:A:1429:LYS:HB2	13:A:1438:VAL:HG11	1.81	0.61
14:B:1028:LEU:HD11	14:B:1043:ILE:HD11	1.80	0.61
13:A:911:PRO:O	13:A:963:ARG:NH2	2.30	0.61
14:B:955:PRO:HB2	14:B:1028:LEU:HD13	1.82	0.61
13:A:545:VAL:O	13:A:549:THR:OG1	2.16	0.61
8:K:100:LEU:HD21	8:K:104:ARG:HH21	1.65	0.61
13:A:576:GLN:O	13:A:590:GLN:NE2	2.34	0.61
14:B:330:VAL:H	14:B:334:LYS:HD2	1.66	0.61
14:B:748:ALA:HB3	14:B:811:TYR:HB2	1.82	0.61
10:N:21:DT:H5"	13:A:1417:HIS:ND1	2.16	0.60
5:H:106:THR:HG22	13:A:926:ASN:HD21	1.66	0.60
14:B:1062:ARG:HE	14:B:1065:GLY:H	1.50	0.60
5:H:95:LYS:HE3	5:H:138:ASP:HA	1.83	0.60
13:A:79:THR:HA	14:B:1072:ARG:HH21	1.67	0.60
2:E:207:ARG:NH2	13:A:1406:THR:O	2.34	0.60
14:B:636:LYS:H	14:B:639:HIS:CD2	2.19	0.60
13:A:76:GLY:HA2	13:A:81:CYS:HB2	1.83	0.60
13:A:11:SER:N	14:B:1135:TYR:HH	2.00	0.59
14:B:407:MET:HE1	14:B:444:LEU:HG	1.84	0.59
7:J:42:ARG:NH1	7:J:45:CYS:SG	2.74	0.59
12:T:14:DG:OP1	13:A:346:LYS:NZ	2.35	0.59
13:A:1148:ALA:HB1	13:A:1333:GLU:HB3	1.83	0.59
13:A:264:VAL:HB	13:A:272:ASN:HB3	1.83	0.59
13:A:349:ARG:NH1	14:B:1071:ASN:OD1	2.35	0.59
14:B:311:ILE:HG23	14:B:316:VAL:HG13	1.85	0.59
5:H:96:VAL:HB	5:H:116:VAL:HG22	1.85	0.59
14:B:1091:ARG:NH1	14:B:1092:ASP:OD1	2.36	0.59
15:C:19:VAL:HG23	15:C:241:PRO:HB2	1.84	0.59
13:A:863:ARG:NH2	13:A:1129:ASN:OD1	2.35	0.59
2:E:13:ILE:HD11	2:E:132:GLN:HG3	1.84	0.59
4:G:97:LEU:HB3	4:G:108:ILE:HB	1.84	0.59
8:K:105:PHE:HD1	15:C:9:VAL:HG11	1.68	0.59
13:A:193:ARG:NH1	13:A:195:GLY:O	2.35	0.59
13:A:455:ILE:HD13	13:A:516:GLN:HB2	1.85	0.59
11:P:12:A:N1	12:T:22:DA:N1	2.51	0.59
14:B:706:VAL:HG13	14:B:767:LEU:HD22	1.85	0.59
14:B:471:ASN:ND2	14:B:477:SER:OG	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:17:ILE:HG13	14:B:19:PRO:HD3	1.85	0.58
14:B:927:ARG:HB3	14:B:1054:MET:HE1	1.84	0.58
14:B:113:ALA:HA	14:B:118:LEU:HB2	1.83	0.58
14:B:310:VAL:HG13	14:B:311:ILE:HD12	1.84	0.58
13:A:827:TYR:HH	13:A:839:HIS:HE2	1.52	0.58
14:B:248:LYS:HB3	14:B:255:ARG:HH21	1.69	0.58
13:A:1141:VAL:HB	13:A:1336:LEU:HB2	1.84	0.58
14:B:111:ASN:ND2	14:B:175:ASN:O	2.37	0.58
3:F:81:VAL:HG11	3:F:95:LYS:HG3	1.85	0.58
14:B:21:LEU:HD22	14:B:637:LYS:HE3	1.86	0.58
14:B:938:ARG:HD2	14:B:1047:TYR:HD2	1.69	0.58
14:B:192:LYS:HE2	14:B:469:VAL:HG22	1.86	0.57
4:G:62:GLY:O	4:G:63:ARG:HG2	2.04	0.57
13:A:972:THR:HG22	13:A:1320:ILE:HG12	1.86	0.57
13:A:1435:THR:OG1	13:A:1436:VAL:N	2.37	0.57
14:B:668:LEU:HD23	14:B:668:LEU:H	1.70	0.57
4:G:3:TYR:N	4:G:76:VAL:O	2.38	0.57
13:A:1173:THR:HG21	13:A:1289:GLU:HG3	1.86	0.57
14:B:795:ILE:HB	14:B:966:ILE:HB	1.87	0.57
4:G:52:ASP:OD2	4:G:73:LYS:NZ	2.38	0.56
13:A:420:ILE:HG13	13:A:426:ARG:HG2	1.87	0.56
14:B:194:LEU:HD11	14:B:448:LEU:HD22	1.86	0.56
4:G:18:PHE:HA	4:G:22:LEU:HD13	1.87	0.56
11:P:11:A:O4'	13:A:264:VAL:HG11	2.04	0.56
13:A:340:LYS:HG3	13:A:1436:VAL:HG11	1.86	0.56
14:B:808:SER:OG	14:B:1050:ARG:NH1	2.38	0.56
7:J:12:LYS:NZ	7:J:39:GLY:O	2.36	0.56
13:A:1155:LYS:HD2	13:A:1158:LEU:HD23	1.87	0.56
13:A:1188:GLU:OE2	13:A:1213:ARG:NH2	2.38	0.56
14:B:591:ARG:NH2	14:B:663:GLU:OE2	2.36	0.56
14:B:747:LEU:HD13	14:B:810:PHE:HE1	1.70	0.56
14:B:934:LYS:HZ1	14:B:942:LYS:HD2	1.69	0.56
15:C:190:ASN:ND2	15:C:195:THR:O	2.38	0.56
12:T:18:DG:H2'	12:T:19:DG:C8	2.40	0.56
13:A:330:GLN:HB3	13:A:336:LEU:HD21	1.88	0.56
13:A:1214:VAL:HG13	13:A:1257:LEU:HB3	1.87	0.56
14:B:789:ASN:HB3	14:B:795:ILE:HG13	1.87	0.56
12:T:13:DC:N3	14:B:494:LYS:NZ	2.53	0.56
13:A:205:VAL:HG11	13:A:210:GLN:HG3	1.88	0.56
15:C:52:ILE:HD13	15:C:64:ILE:HD11	1.87	0.56
13:A:107:LEU:HD21	13:A:221:VAL:HG13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:783:ALA:O	14:B:789:ASN:ND2	2.38	0.56
12:T:6:DG:H2'	12:T:7:DT:C6	2.40	0.55
13:A:429:LEU:HA	13:A:433:PRO:HG3	1.88	0.55
13:A:760:LEU:HD11	13:A:781:ILE:HG21	1.88	0.55
13:A:972:THR:HA	13:A:1320:ILE:HG21	1.88	0.55
13:A:631:GLU:HG2	13:A:988:TRP:HZ2	1.71	0.55
14:B:1115:GLN:HE21	14:B:1150:ARG:HH11	1.53	0.55
14:B:761:THR:HG23	14:B:1000:THR:HA	1.87	0.55
1:D:63:LYS:HA	1:D:66:ASN:HD21	1.72	0.55
5:H:75:TYR:HB2	13:A:576:GLN:HA	1.87	0.55
13:A:508:SER:HB2	13:A:511:THR:HG22	1.87	0.55
13:A:653:VAL:HG11	13:A:669:TYR:CZ	2.42	0.55
13:A:1453:GLY:O	13:A:1457:ASN:ND2	2.38	0.55
14:B:588:ARG:O	14:B:592:ARG:HD3	2.06	0.55
1:D:41:LEU:O	1:D:44:ARG:NH2	2.40	0.55
13:A:706:ILE:HD11	13:A:787:VAL:HG21	1.88	0.55
13:A:1366:PHE:HB2	13:A:1374:VAL:HG21	1.88	0.55
14:B:40:VAL:HG21	14:B:183:GLY:HA3	1.89	0.55
14:B:939:HIS:NE2	14:B:983:GLU:OE1	2.31	0.55
14:B:249:LYS:HZ2	14:B:254:GLN:H	1.53	0.55
13:A:274:ASP:OD1	13:A:275:ASP:N	2.38	0.54
13:A:466:LYS:HA	14:B:1093:CYS:SG	2.47	0.54
13:A:592:PHE:HA	13:A:595:ILE:HD12	1.89	0.54
5:H:103:GLU:HB3	5:H:109:ALA:HB2	1.89	0.54
13:A:827:TYR:OH	13:A:839:HIS:NE2	2.40	0.54
1:D:44:ARG:NH1	1:D:48:ASN:HD21	2.05	0.54
13:A:551:ARG:NH2	13:A:622:SER:O	2.41	0.54
13:A:1147:SER:HA	13:A:1153:ARG:HB2	1.90	0.54
2:E:192:LYS:HE3	2:E:204:ILE:HD13	1.89	0.54
9:L:19:CYS:HB2	9:L:36:CYS:SG	2.46	0.54
12:T:2:DT:H1'	12:T:3:DC:H5'	1.89	0.54
13:A:1412:MET:SD	13:A:1422:GLN:NE2	2.80	0.54
13:A:427:ILE:HG21	13:A:437:ASP:HB3	1.88	0.54
14:B:403:LEU:HD23	14:B:444:LEU:HD23	1.88	0.54
4:G:8:GLU:OE2	4:G:71:LYS:NZ	2.39	0.54
13:A:922:PHE:H	13:A:1052:ARG:HD2	1.72	0.54
14:B:116:ARG:HB2	14:B:118:LEU:HG	1.88	0.54
14:B:1115:GLN:HG2	14:B:1150:ARG:HG2	1.88	0.54
1:D:93:HIS:HB3	1:D:96:GLU:HB3	1.89	0.54
13:A:1451:MET:HE3	13:A:1460:LEU:HD22	1.89	0.54
14:B:735:VAL:HG23	14:B:754:PRO:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:228:SER:O	14:B:405:ARG:NH1	2.40	0.54
14:B:780:VAL:HG22	14:B:965:ILE:HB	1.89	0.54
1:D:87:LEU:HB3	1:D:97:LEU:HD11	1.89	0.54
13:A:1130:ILE:HD13	13:A:1411:LEU:HB3	1.89	0.54
14:B:157:ARG:NH1	14:B:180:ASP:O	2.41	0.54
13:A:394:VAL:HG23	13:A:442:THR:HA	1.90	0.53
13:A:481:THR:O	13:A:483:ARG:NH2	2.40	0.53
13:A:867:SER:HB2	13:A:1414:ILE:HG23	1.90	0.53
13:A:1016:LEU:HD23	13:A:1045:LEU:HD21	1.90	0.53
4:G:10:GLU:HB3	4:G:67:LEU:HD11	1.90	0.53
13:A:691:ASP:OD2	13:A:765:ASN:ND2	2.41	0.53
13:A:876:ASP:OD1	13:A:878:THR:OG1	2.23	0.53
13:A:679:TRP:CZ2	13:A:683:GLU:HG3	2.43	0.53
2:E:73:PHE:HZ	2:E:93:ARG:HH21	1.55	0.53
5:H:10:PHE:CE2	5:H:32:SER:HB3	2.44	0.53
13:A:256:PRO:HD2	13:A:280:LEU:HD11	1.90	0.53
14:B:99:TRP:HD1	14:B:105:PRO:HA	1.74	0.53
5:H:2:ALA:N	5:H:66:GLU:O	2.42	0.53
13:A:431:PHE:O	13:A:432:HIS:C	2.46	0.53
14:B:929:PRO:HA	14:B:1050:ARG:HH21	1.73	0.53
15:C:205:LYS:NZ	15:C:215:GLU:O	2.35	0.53
2:E:82:VAL:HG13	2:E:86:THR:HB	1.91	0.53
13:A:1443:ALA:HB2	14:B:1167:ILE:HG23	1.91	0.53
14:B:721:ARG:CZ	14:B:975:ARG:HD2	2.38	0.53
1:D:131:LEU:O	1:D:134:ILE:HG13	2.08	0.52
12:T:4:DA:H1'	12:T:5:DA:C8	2.43	0.52
13:A:1199:MET:SD	13:A:1199:MET:N	2.82	0.52
14:B:236:TRP:HB2	14:B:259:THR:HB	1.90	0.52
13:A:275:ASP:HB3	13:A:336:LEU:HD22	1.92	0.52
14:B:294:ASP:OD2	14:B:379:ARG:NH1	2.41	0.52
12:T:17:DT:OP1	14:B:1078:ARG:N	2.43	0.52
13:A:560:VAL:HG22	13:A:591:ILE:HD11	1.90	0.52
13:A:713:VAL:HG11	13:A:817:PRO:HD3	1.90	0.52
13:A:286:ILE:HD13	13:A:309:LEU:HD23	1.91	0.52
8:K:91:ILE:HG21	15:C:260:GLN:HB2	1.91	0.52
15:C:31:ALA:O	15:C:231:TYR:OH	2.28	0.52
4:G:91:GLN:HB2	4:G:98:PHE:HD2	1.75	0.52
13:A:274:ASP:OD2	13:A:342:ARG:NH2	2.43	0.52
13:A:279:LYS:HE2	13:A:316:THR:HB	1.92	0.52
14:B:285:LEU:HD21	14:B:305:LEU:HD11	1.92	0.52
14:B:759:VAL:HG12	14:B:999:ALA:HB2	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:47:LYS:HE2	13:A:562:ASN:HD21	1.75	0.52
13:A:549:THR:HG21	13:A:640:LEU:HG	1.92	0.52
13:A:1058:PHE:HB3	13:A:1060:LEU:HD13	1.92	0.52
12:T:18:DG:H2'	12:T:19:DG:H8	1.73	0.52
14:B:503:ASN:OD1	14:B:503:ASN:N	2.42	0.52
14:B:938:ARG:HD2	14:B:1047:TYR:CD2	2.44	0.52
2:E:82:VAL:HG23	2:E:106:VAL:HG13	1.91	0.51
10:N:21:DT:H5"	13:A:1417:HIS:CE1	2.44	0.51
11:P:20:C:O3'	13:A:499:ASP:OD1	2.25	0.51
11:P:20:C:OP1	14:B:942:LYS:NZ	2.29	0.51
15:C:48:ASP:HB3	15:C:166:LYS:HD3	1.93	0.51
5:H:97:TYR:CZ	5:H:115:TYR:HB3	2.45	0.51
2:E:91:CYS:HA	2:E:94:MET:HE2	1.93	0.51
12:T:22:DA:H2"	12:T:23:DT:H5"	1.91	0.51
7:J:35:LEU:HD13	7:J:46:ARG:HB3	1.92	0.51
8:K:39:ASP:O	8:K:71:ILE:HD11	2.11	0.51
12:T:18:DG:H2"	12:T:19:DG:C5'	2.41	0.51
13:A:626:THR:OG1	13:A:627:LYS:N	2.40	0.51
13:A:1307:VAL:HG13	13:A:1338:THR:HG22	1.93	0.51
13:A:97:VAL:HG21	13:A:322:LEU:HD11	1.93	0.51
3:F:61:GLU:HA	13:A:1471:PHE:CZ	2.46	0.51
14:B:550:MET:HG2	14:B:551:GLU:H	1.77	0.51
15:C:60:HIS:ND1	15:C:62:GLU:HG2	2.26	0.51
9:L:46:LYS:NZ	14:B:849:ASP:OD2	2.44	0.50
14:B:713:PHE:O	14:B:717:ASN:ND2	2.44	0.50
14:B:938:ARG:NH1	14:B:983:GLU:OE2	2.43	0.50
14:B:1094:GLN:HB2	14:B:1103:LEU:HD13	1.93	0.50
2:E:59:THR:HB	2:E:73:PHE:HE1	1.77	0.50
7:J:35:LEU:HB2	7:J:46:ARG:HH21	1.77	0.50
13:A:60:PRO:HB2	13:A:72:GLN:HG3	1.93	0.50
8:K:105:PHE:CD1	15:C:9:VAL:HG11	2.46	0.50
10:N:15:DT:H71	14:B:199:LYS:HA	1.94	0.50
14:B:907:VAL:HG13	14:B:921:ILE:HG12	1.93	0.50
2:E:97:GLU:HB3	2:E:99:ILE:HD13	1.93	0.50
5:H:90:TYR:HB3	5:H:145:MET:HG3	1.93	0.50
5:H:124:ARG:HB2	13:A:621:ILE:HD11	1.93	0.50
12:T:15:DC:H2"	13:A:461:GLN:CD	2.31	0.50
13:A:112:PHE:HD1	13:A:113:PHE:HD2	1.58	0.50
13:A:293:ASN:HB3	13:A:298:ALA:HB2	1.94	0.50
13:A:465:HIS:O	13:A:468:SER:OG	2.24	0.50
15:C:52:ILE:HD12	15:C:61:ASP:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:931:ARG:NH1	13:A:936:GLU:OE2	2.45	0.50
13:A:1156:ASP:OD1	13:A:1225:LYS:NZ	2.32	0.50
14:B:220:GLU:OE2	14:B:222:ARG:NH2	2.45	0.50
12:T:18:DG:H2"	12:T:19:DG:H5'	1.93	0.50
13:A:610:PRO:HG2	13:A:613:GLU:HG3	1.93	0.50
2:E:63:ALA:HB1	2:E:68:PRO:HA	1.94	0.49
11:P:20:C:C4'	13:A:499:ASP:OD1	2.52	0.49
2:E:2:ASP:N	2:E:2:ASP:OD1	2.44	0.49
4:G:99:THR:HG23	4:G:106:CYS:HB3	1.94	0.49
12:T:12:DA:H4'	13:A:859:TYR:CD1	2.47	0.49
12:T:17:DT:H2'	12:T:18:DG:C8	2.47	0.49
2:E:101:ARG:NH1	2:E:128:GLU:OE2	2.45	0.49
2:E:173:ILE:O	2:E:209:VAL:HA	2.12	0.49
5:H:112:LEU:HD13	5:H:129:ALA:HB2	1.94	0.49
15:C:116:THR:HB	15:C:147:ASP:HB3	1.94	0.49
9:L:46:LYS:HB2	14:B:907:VAL:HB	1.94	0.49
13:A:547:LYS:NZ	13:A:684:GLY:O	2.45	0.49
10:N:21:DT:H5"	13:A:1417:HIS:CG	2.48	0.49
15:C:20:LYS:HB2	15:C:232:ASN:HD22	1.78	0.49
11:P:11:A:H4'	13:A:264:VAL:HG13	1.92	0.49
14:B:587:LEU:HB3	14:B:603:MET:SD	2.53	0.49
15:C:105:VAL:HG11	15:C:115:VAL:HG22	1.94	0.49
3:F:111:PRO:O	13:A:884:ASN:ND2	2.46	0.49
13:A:335:PRO:HD3	14:B:460:HIS:NE2	2.28	0.49
13:A:532:ARG:NH1	13:A:647:THR:O	2.45	0.49
9:L:48:ARG:HA	14:B:856:PRO:HG2	1.93	0.49
13:A:62:GLN:HG3	13:A:84:HIS:O	2.12	0.49
13:A:808:PRO:HB2	14:B:675:LEU:HD12	1.94	0.49
14:B:114:ARG:NH2	14:B:184:TYR:OH	2.46	0.49
14:B:1062:ARG:NH2	14:B:1066:PRO:O	2.46	0.49
4:G:42:TYR:HA	4:G:78:ARG:HH21	1.78	0.48
5:H:71:ASP:OD2	5:H:142:TYR:OH	2.31	0.48
13:A:111:CYS:HB3	13:A:114:CYS:O	2.13	0.48
13:A:543:THR:HG1	14:B:970:HIS:CE1	2.31	0.48
14:B:515:PRO:CG	14:B:523:VAL:HB	2.29	0.48
15:C:56:SER:HB2	15:C:158:GLU:H	1.77	0.48
13:A:865:ILE:HD12	13:A:1092:ALA:HB3	1.94	0.48
14:B:187:ILE:HG21	14:B:449:ALA:HB2	1.95	0.48
14:B:474:THR:OG1	14:B:732:ALA:O	2.23	0.48
15:C:37:VAL:O	15:C:42:VAL:HG23	2.13	0.48
3:F:80:MET:HB2	3:F:101:LYS:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:1430:CYS:O	13:A:1435:THR:HG22	2.13	0.48
15:C:113:ARG:HB3	15:C:153:LEU:HB2	1.95	0.48
2:E:172:ARG:HH21	13:A:1408:ARG:NH2	2.12	0.48
6:I:106:ASP:OD1	6:I:106:ASP:N	2.46	0.48
6:I:110:LEU:HD22	13:A:721:HIS:HB3	1.94	0.48
13:A:207:GLU:OE1	13:A:208:ASP:N	2.47	0.48
14:B:187:ILE:HG23	14:B:445:LYS:HG3	1.95	0.48
14:B:331:THR:HG22	14:B:334:LYS:HE3	1.95	0.48
1:D:87:LEU:HB3	1:D:97:LEU:HD21	1.95	0.48
13:A:111:CYS:SG	13:A:188:GLN:NE2	2.81	0.48
13:A:121:SER:HA	13:A:126:ILE:HG21	1.95	0.48
13:A:420:ILE:HB	13:A:445:LYS:HB2	1.95	0.48
14:B:549:SER:OG	14:B:550:MET:N	2.45	0.48
14:B:819:SER:H	14:B:827:GLU:HB2	1.79	0.48
15:C:106:ARG:NH1	15:C:108:ASN:OD1	2.44	0.48
5:H:122:LEU:HD13	13:A:551:ARG:HH21	1.79	0.48
13:A:823:VAL:HG11	13:A:831:LEU:HD22	1.95	0.48
5:H:64:LEU:HD11	13:A:580:LEU:HD13	1.95	0.48
9:L:58:ARG:HD2	15:C:173:HIS:CD2	2.49	0.48
12:T:13:DC:H42	14:B:494:LYS:HZ3	1.62	0.48
13:A:1450:PRO:HB2	13:A:1452:LYS:HG2	1.96	0.48
14:B:148:PHE:CD2	14:B:437:THR:HG21	2.48	0.48
14:B:1060:HIS:HB2	14:B:1078:ARG:HG3	1.96	0.48
13:A:375:ILE:HD11	13:A:487:SER:HB2	1.94	0.48
13:A:1292:MET:O	13:A:1296:MET:HB2	2.14	0.48
14:B:436:LYS:O	14:B:439:ILE:HG22	2.13	0.48
4:G:120:ASP:N	4:G:120:ASP:OD1	2.45	0.47
13:A:575:PRO:HG3	13:A:594:LEU:HD11	1.96	0.47
14:B:747:LEU:HD13	14:B:810:PHE:CE1	2.49	0.47
1:D:126:GLU:O	1:D:129:GLN:HG3	2.14	0.47
14:B:556:ILE:HD13	14:B:556:ILE:HA	1.78	0.47
2:E:73:PHE:HD2	2:E:99:ILE:HD12	1.80	0.47
13:A:46:THR:HG22	13:A:47:THR:HG23	1.97	0.47
13:A:121:SER:O	13:A:127:LYS:NZ	2.43	0.47
13:A:392:GLU:OE2	13:A:401:ARG:NH2	2.42	0.47
14:B:1105:GLU:HA	14:B:1109:GLU:HB2	1.94	0.47
10:N:21:DT:H2"	10:N:22:DA:C8	2.49	0.47
13:A:805:ARG:NH2	13:A:808:PRO:O	2.46	0.47
14:B:556:ILE:HD11	14:B:576:ILE:HD11	1.95	0.47
5:H:105:SER:O	13:A:932:ARG:HD3	2.14	0.47
6:I:25:TYR:CD1	6:I:40:ARG:HD3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:971:PRO:O	13:A:972:THR:OG1	2.23	0.47
14:B:16:GLU:HG3	14:B:636:LYS:HB3	1.97	0.47
14:B:1062:ARG:NE	14:B:1065:GLY:H	2.11	0.47
4:G:150:THR:HG22	4:G:157:ILE:HD11	1.97	0.47
5:H:92:MET:HB2	5:H:143:LEU:HB3	1.97	0.47
14:B:628:VAL:HG22	14:B:633:LEU:HD23	1.97	0.47
14:B:866:ILE:HG12	14:B:896:LEU:HD22	1.97	0.47
5:H:60:ILE:HG23	5:H:141:VAL:HG13	1.97	0.47
12:T:14:DG:H1'	14:B:1089:MET:HE1	1.97	0.47
13:A:18:ILE:H	13:A:1462:GLN:HE22	1.62	0.47
13:A:312:PHE:O	13:A:316:THR:OG1	2.17	0.47
13:A:381:PRO:HB3	13:A:480:SER:HA	1.97	0.47
13:A:955:GLU:O	13:A:959:MET:HG3	2.14	0.47
14:B:110:PRO:HB3	14:B:156:LEU:HD21	1.96	0.47
8:K:31:CYS:SG	8:K:32:LEU:N	2.87	0.47
2:E:137:ILE:HG21	13:A:1347:LEU:HB3	1.97	0.47
13:A:376:ASP:O	13:A:473:ARG:N	2.48	0.47
1:D:32:LEU:HB3	1:D:36:GLU:HB2	1.97	0.47
13:A:48:GLU:OE1	13:A:48:GLU:N	2.48	0.47
13:A:901:VAL:HB	13:A:978:VAL:HG12	1.97	0.47
14:B:100:GLU:O	14:B:101:ARG:C	2.53	0.47
4:G:108:ILE:HD11	4:G:145:LEU:HD22	1.97	0.46
5:H:128:ASP:N	5:H:128:ASP:OD1	2.46	0.46
6:I:100:HIS:NE2	13:A:813:ASP:OD2	2.49	0.46
14:B:756:LYS:HD3	14:B:770:ARG:HG3	1.96	0.46
15:C:26:THR:HG23	15:C:229:PHE:HE2	1.80	0.46
1:D:93:HIS:O	1:D:97:LEU:N	2.39	0.46
4:G:152:VAL:HA	4:G:157:ILE:HA	1.96	0.46
13:A:367:ILE:HG21	13:A:501:MET:HG3	1.97	0.46
5:H:105:SER:OG	5:H:106:THR:N	2.46	0.46
14:B:548:TRP:O	14:B:549:SER:OG	2.28	0.46
4:G:34:VAL:HG12	4:G:45:VAL:HG11	1.97	0.46
8:K:21:ILE:HD11	15:C:263:LEU:HD12	1.97	0.46
14:B:26:CYS:O	14:B:29:VAL:HG22	2.16	0.46
14:B:177:CYS:SG	14:B:738:THR:OG1	2.62	0.46
7:J:60:LEU:HD22	15:C:154:ARG:HB2	1.98	0.46
13:A:364:ARG:NH1	13:A:500:GLU:OE1	2.48	0.46
13:A:1022:ILE:H	13:A:1034:GLN:NE2	2.10	0.46
14:B:927:ARG:NH2	14:B:1057:ASP:OD1	2.49	0.46
2:E:192:LYS:HE2	2:E:194:ILE:HD11	1.98	0.46
14:B:524:LYS:HB2	14:B:524:LYS:HE2	1.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:VAL:HA	1:D:86:LEU:HG	1.98	0.46
5:H:14:ASP:HB2	5:H:29:HIS:HB2	1.96	0.46
13:A:919:LYS:NZ	13:A:1057:GLU:OE2	2.29	0.46
14:B:192:LYS:NZ	14:B:449:ALA:O	2.49	0.46
14:B:555:GLU:OE1	14:B:555:GLU:N	2.48	0.46
15:C:38:PHE:HE1	15:C:245:VAL:HA	1.81	0.46
2:E:142:HIS:HE1	13:A:1358:THR:HG22	1.81	0.46
13:A:18:ILE:H	13:A:1462:GLN:NE2	2.14	0.46
13:A:52:PRO:HB2	13:A:60:PRO:HD3	1.98	0.46
13:A:926:ASN:HD22	13:A:928:ARG:H	1.63	0.46
14:B:699:HIS:HD2	14:B:701:SER:H	1.64	0.46
15:C:180:ALA:N	15:C:234:GLU:O	2.44	0.46
4:G:30:LEU:HD22	4:G:70:VAL:HG11	1.98	0.45
13:A:402:LEU:HD23	13:A:405:LEU:HD12	1.98	0.45
14:B:788:TYR:O	14:B:946:GLY:HA3	2.16	0.45
13:A:1099:ALA:HA	13:A:1102:MET:SD	2.55	0.45
14:B:789:ASN:O	14:B:968:ASN:HB2	2.16	0.45
14:B:817:GLN:O	14:B:869:LYS:NZ	2.38	0.45
11:P:11:A:C4'	13:A:264:VAL:HG11	2.46	0.45
13:A:77:ASN:O	13:A:77:ASN:ND2	2.47	0.45
13:A:1371:ILE:O	13:A:1374:VAL:HG12	2.17	0.45
14:B:285:LEU:O	14:B:289:ILE:N	2.43	0.45
14:B:496:ALA:O	14:B:500:GLN:HG3	2.16	0.45
2:E:19:GLN:NE2	2:E:138:ASN:HD22	2.14	0.45
4:G:110:ARG:NH2	4:G:113:ILE:HG21	2.30	0.45
13:A:152:ASN:O	13:A:152:ASN:ND2	2.42	0.45
15:C:19:VAL:HG12	15:C:21:PHE:HD1	1.80	0.45
13:A:372:ASN:ND2	14:B:788:TYR:OH	2.42	0.45
14:B:330:VAL:N	14:B:334:LYS:HD2	2.29	0.45
14:B:967:ILE:HG21	14:B:1048:TYR:OH	2.17	0.45
2:E:10:LEU:HD13	2:E:58:LEU:HD11	1.98	0.45
14:B:313:GLU:HB3	14:B:316:VAL:HG12	1.99	0.45
14:B:515:PRO:HD2	14:B:523:VAL:O	2.17	0.45
14:B:770:ARG:NH2	14:B:771:GLU:OE2	2.49	0.45
4:G:110:ARG:NH2	4:G:117:MET:SD	2.89	0.45
4:G:119:PHE:HB2	4:G:128:TYR:CZ	2.52	0.45
5:H:81:ARG:HB2	5:H:82:PRO:HD3	1.99	0.45
11:P:14:A:H2'	11:P:15:C:O4'	2.16	0.45
15:C:205:LYS:HE3	15:C:213:GLU:HA	1.99	0.45
3:F:60:TYR:HB3	13:A:1468:THR:H	1.82	0.45
13:A:545:VAL:HG23	13:A:676:ILE:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:1180:ASN:O	13:A:1183:SER:OG	2.24	0.45
14:B:713:PHE:HB3	14:B:716:HIS:CD2	2.52	0.45
14:B:794:VAL:HG12	14:B:967:ILE:HG22	1.98	0.45
14:B:859:ARG:HA	14:B:903:ILE:HG12	1.98	0.45
14:B:1072:ARG:HD2	14:B:1153:TYR:CE1	2.52	0.45
4:G:119:PHE:CE2	4:G:121:PRO:HG3	2.51	0.44
8:K:87:PHE:HD2	15:C:263:LEU:HD22	1.82	0.44
13:A:556:GLU:OE2	13:A:583:ARG:NH1	2.37	0.44
13:A:1408:ARG:HD3	13:A:1408:ARG:HA	1.71	0.44
14:B:810:PHE:HB2	14:B:927:ARG:HD2	1.99	0.44
15:C:40:ALA:O	15:C:169:PHE:HB2	2.17	0.44
1:D:62:MET:O	1:D:66:ASN:ND2	2.50	0.44
5:H:57:ARG:O	5:H:145:MET:HA	2.17	0.44
6:I:59:THR:HG23	13:A:1171:ALA:HA	1.97	0.44
14:B:101:ARG:O	14:B:102:ASP:C	2.56	0.44
14:B:733:MET:HE1	14:B:1050:ARG:NH1	2.26	0.44
14:B:794:VAL:O	14:B:946:GLY:N	2.46	0.44
14:B:796:MET:HB2	14:B:948:GLN:HG2	1.99	0.44
14:B:932:GLY:HA3	14:B:1055:VAL:HB	1.98	0.44
13:A:1476:ASP:HB3	13:A:1479:LYS:HB2	1.99	0.44
15:C:101:PHE:CE2	15:C:122:SER:HB3	2.53	0.44
5:H:39:LEU:HD13	5:H:125:LEU:HD13	1.99	0.44
13:A:273:GLN:HB2	13:A:278:HIS:CE1	2.52	0.44
13:A:346:LYS:C	13:A:348:GLY:H	2.20	0.44
13:A:485:ASN:OD1	13:A:486:LEU:N	2.50	0.44
13:A:1234:LYS:NZ	13:A:1298:LEU:O	2.51	0.44
2:E:187:ARG:HH22	13:A:132:LYS:HZ3	1.64	0.44
8:K:101:LEU:HD13	15:C:7:PRO:HB2	2.00	0.44
14:B:501:LEU:HD12	14:B:505:LEU:HD22	1.99	0.44
15:C:49:TRP:CE3	15:C:164:TYR:HD2	2.35	0.44
2:E:185:ILE:HG22	2:E:189:GLN:HB2	2.00	0.44
13:A:353:ASN:O	13:A:357:LYS:HE2	2.18	0.44
13:A:433:PRO:HB2	13:A:438:LEU:HD21	2.00	0.44
14:B:249:LYS:NZ	14:B:254:GLN:H	2.14	0.44
14:B:253:GLY:H	14:B:254:GLN:NE2	2.16	0.44
6:I:81:THR:HG23	6:I:96:PHE:HE1	1.82	0.44
13:A:363:ALA:HB3	13:A:503:LEU:HB3	1.99	0.44
13:A:368:THR:HG21	14:B:931:ILE:O	2.18	0.44
13:A:375:ILE:HD13	13:A:375:ILE:HA	1.86	0.44
13:A:631:GLU:HG2	13:A:988:TRP:CZ2	2.51	0.44
13:A:671:ASN:O	13:A:675:VAL:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:1121:VAL:N	13:A:1122:PRO:HD2	2.33	0.44
13:A:1484:MET:O	13:A:1485:GLU:C	2.55	0.44
14:B:56:GLN:HE21	14:B:60:GLU:HG3	1.82	0.44
5:H:75:TYR:CZ	5:H:77:PRO:HG3	2.53	0.44
13:A:469:MET:HB3	14:B:1093:CYS:SG	2.58	0.44
13:A:530:SER:O	13:A:532:ARG:HG3	2.18	0.44
14:B:101:ARG:HD2	14:B:101:ARG:HA	1.40	0.44
15:C:193:ARG:NH2	15:C:218:ALA:O	2.48	0.44
3:F:53:THR:OG1	3:F:116:GLU:OE1	2.20	0.44
13:A:1141:VAL:HA	13:A:1357:THR:HG23	1.99	0.44
1:D:63:LYS:NZ	4:G:103:PRO:HA	2.33	0.43
4:G:2:PHE:HA	4:G:77:PHE:HA	1.99	0.43
7:J:40:LEU:HD22	7:J:45:CYS:HB3	2.00	0.43
13:A:230:ASP:HB3	13:A:240:PRO:HG3	2.00	0.43
13:A:1347:LEU:HD22	13:A:1354:PRO:HA	2.00	0.43
14:B:61:ASP:OD2	14:B:228:SER:HB3	2.18	0.43
14:B:627:ILE:HD11	14:B:663:GLU:HB2	2.00	0.43
15:C:26:THR:HG23	15:C:229:PHE:CE2	2.53	0.43
13:A:335:PRO:HD3	14:B:460:HIS:CE1	2.53	0.43
13:A:581:LYS:HG2	13:A:582:PRO:HA	1.99	0.43
14:B:827:GLU:OE1	14:B:871:VAL:HG22	2.18	0.43
7:J:6:ARG:HB2	15:C:70:LEU:HD13	2.00	0.43
7:J:66:GLU:HG2	9:L:18:ILE:HG21	1.99	0.43
13:A:1180:ASN:OD1	13:A:1183:SER:N	2.51	0.43
13:A:1253:GLU:H	13:A:1253:GLU:HG3	1.64	0.43
13:A:1320:ILE:H	13:A:1320:ILE:HG13	1.73	0.43
13:A:1484:MET:HB3	13:A:1485:GLU:H	1.61	0.43
14:B:626:LEU:HD23	14:B:662:VAL:HG22	2.01	0.43
14:B:1137:CYS:HB3	14:B:1142:ASN:HB3	2.01	0.43
4:G:3:TYR:HD2	4:G:78:ARG:HD2	1.83	0.43
13:A:413:TYR:O	13:A:449:HIS:HD2	2.02	0.43
13:A:909:LEU:O	13:A:910:LYS:HG2	2.18	0.43
4:G:89:VAL:HG12	4:G:99:THR:HB	2.00	0.43
5:H:96:VAL:HA	5:H:116:VAL:HA	2.00	0.43
1:D:18:SER:HA	1:D:116:PRO:HG2	2.01	0.43
1:D:93:HIS:NE2	1:D:95:PHE:HB3	2.33	0.43
4:G:80:PHE:HB2	4:G:83:GLU:HG3	2.00	0.43
4:G:127:CYS:HB2	4:G:137:ILE:O	2.19	0.43
13:A:497:ASP:OD1	13:A:497:ASP:N	2.51	0.43
13:A:1423:ASP:OD1	13:A:1423:ASP:N	2.48	0.43
14:B:717:ASN:HD21	14:B:979:GLY:HA3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4:GLU:OE2	2:E:41:LYS:NZ	2.33	0.43
3:F:46:GLN:N	3:F:115:TYR:O	2.51	0.43
7:J:25:LEU:HD11	7:J:31:GLU:HA	2.01	0.43
13:A:593:SER:HB2	13:A:634:GLU:HA	2.01	0.43
1:D:44:ARG:NH2	1:D:45:LYS:HB2	2.33	0.43
12:T:14:DG:P	13:A:346:LYS:HZ2	2.41	0.43
13:A:201:GLU:HA	13:A:212:LYS:O	2.18	0.43
13:A:1155:LYS:HE3	13:A:1155:LYS:HB3	1.84	0.43
14:B:195:ILE:HD12	14:B:484:ARG:HB3	2.01	0.43
3:F:90:LEU:HD11	13:A:513:ALA:HB2	2.00	0.43
13:A:967:ARG:HD3	13:A:1322:ILE:HD13	2.01	0.43
14:B:223:SER:OG	14:B:349:PRO:HD2	2.18	0.43
14:B:587:LEU:HD22	14:B:597:ILE:HD11	2.00	0.43
3:F:69:ARG:HH11	3:F:72:GLN:NE2	2.17	0.43
13:A:453:GLY:HA2	13:A:473:ARG:HG2	2.01	0.43
13:A:689:ILE:HG13	14:B:985:LEU:HD22	2.01	0.43
13:A:1157:ILE:HD11	13:A:1351:ASP:HB2	2.01	0.43
14:B:785:TYR:CZ	14:B:955:PRO:HD3	2.54	0.43
2:E:67:ASP:OD1	2:E:67:ASP:N	2.51	0.42
7:J:13:ILE:HD11	15:C:72:PRO:HG3	2.00	0.42
13:A:821:GLY:HA2	13:A:838:PHE:CD2	2.54	0.42
14:B:27:TRP:CD2	14:B:762:ARG:HG2	2.54	0.42
14:B:929:PRO:O	14:B:948:GLN:NE2	2.43	0.42
15:C:33:SER:O	15:C:37:VAL:HG23	2.19	0.42
2:E:17:ILE:HG21	2:E:74:VAL:HG11	2.00	0.42
6:I:98:GLN:HE21	13:A:721:HIS:HE1	1.67	0.42
9:L:49:THR:HB	14:B:855:ALA:HB3	2.01	0.42
13:A:384:ILE:HG12	14:B:1061:SER:HB2	2.01	0.42
13:A:564:LEU:HD13	13:A:570:TRP:CZ2	2.54	0.42
13:A:962:ASP:HB3	13:A:1043:ILE:HG23	2.01	0.42
15:C:117:SER:HB2	15:C:129:PRO:HB2	2.00	0.42
13:A:601:ASN:HA	13:A:630:VAL:O	2.19	0.42
13:A:799:PRO:O	14:B:503:ASN:ND2	2.51	0.42
13:A:1192:TRP:HH2	13:A:1258:ARG:HG3	1.83	0.42
14:B:251:ALA:HB3	14:B:254:GLN:NE2	2.34	0.42
14:B:294:ASP:O	14:B:298:MET:HG3	2.19	0.42
14:B:344:GLN:NE2	14:B:355:ASP:H	2.18	0.42
1:D:77:ARG:H	1:D:77:ARG:HG2	1.63	0.42
3:F:106:ILE:N	3:F:118:TRP:O	2.44	0.42
6:I:93:GLU:HB3	6:I:115:THR:OG1	2.19	0.42
12:T:14:DG:C2'	14:B:1089:MET:HE2	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:561:ILE:HD11	14:B:573:TRP:CZ2	2.54	0.42
15:C:103:LEU:HB3	15:C:161:LEU:HG	2.00	0.42
13:A:18:ILE:HD11	14:B:1149:VAL:HG21	2.01	0.42
14:B:201:ALA:HB3	14:B:206:TYR:OH	2.20	0.42
14:B:542:LEU:HD21	14:B:574:VAL:HG11	2.01	0.42
14:B:792:ASP:O	14:B:943:GLY:HA3	2.19	0.42
8:K:7:PHE:HB3	15:C:172:GLU:OE2	2.20	0.42
13:A:425:ASP:OD1	13:A:425:ASP:N	2.53	0.42
13:A:1181:PRO:O	13:A:1184:THR:OG1	2.32	0.42
14:B:759:VAL:HG13	14:B:986:GLN:HG2	2.01	0.42
2:E:95:GLN:OE1	2:E:125:TYR:OH	2.25	0.42
5:H:37:MET:HE3	5:H:127:GLY:HA3	2.02	0.42
5:H:79:ASP:O	5:H:82:PRO:HD2	2.20	0.42
5:H:97:TYR:OH	5:H:122:LEU:HD23	2.19	0.42
13:A:463:THR:HG21	14:B:1090:GLU:HG3	2.01	0.42
13:A:972:THR:H	13:A:1320:ILE:HD13	1.84	0.42
14:B:256:ILE:HD11	14:B:373:LEU:HD21	2.02	0.42
14:B:847:LYS:NZ	14:B:864:ASP:OD2	2.43	0.42
14:B:956:PHE:HE2	15:C:184:PHE:HB3	1.84	0.42
4:G:55:GLY:HA3	4:G:69:PRO:HG2	2.01	0.42
13:A:604:ARG:O	13:A:628:VAL:N	2.52	0.42
13:A:926:ASN:ND2	13:A:929:ALA:H	2.18	0.42
14:B:515:PRO:HG2	14:B:519:ALA:O	2.19	0.42
14:B:565:THR:HG22	14:B:610:ARG:HB3	2.01	0.42
2:E:172:ARG:HH21	13:A:1408:ARG:HH21	1.68	0.42
4:G:7:LEU:HD23	4:G:74:ALA:HB3	2.02	0.42
13:A:26:LEU:HD13	13:A:31:LEU:HD21	2.01	0.42
13:A:399:ILE:HD11	13:A:440:LEU:O	2.19	0.42
13:A:752:THR:HB	13:A:786:ALA:HB1	2.01	0.42
14:B:83:ARG:HH21	14:B:85:LEU:HD21	1.85	0.42
12:T:13:DC:N3	14:B:518:HIS:CE1	2.83	0.41
13:A:601:ASN:HB3	13:A:988:TRP:CD2	2.55	0.41
13:A:1201:ASP:OD1	13:A:1202:PHE:N	2.45	0.41
14:B:502:HIS:HB3	14:B:505:LEU:HD13	2.02	0.41
14:B:504:THR:HB	14:B:667:THR:HG21	2.01	0.41
14:B:542:LEU:O	14:B:546:GLU:HG2	2.19	0.41
14:B:625:LEU:HD13	14:B:675:LEU:HD21	2.02	0.41
8:K:21:ILE:HG23	8:K:31:CYS:SG	2.60	0.41
13:A:756:ALA:HB2	13:A:786:ALA:HB2	2.01	0.41
13:A:1323:THR:HG21	13:A:1329:LYS:HE2	2.02	0.41
1:D:44:ARG:HH22	1:D:45:LYS:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:62:VAL:HG23	2:E:72:MET:HB3	2.02	0.41
3:F:64:ARG:NH2	4:G:61:PRO:HG3	2.34	0.41
7:J:42:ARG:HB3	14:B:961:ILE:HD11	2.02	0.41
8:K:100:LEU:HG	8:K:104:ARG:HE	1.85	0.41
13:A:702:ILE:HD13	13:A:786:ALA:HA	2.01	0.41
14:B:124:LEU:HD22	14:B:152:ILE:HD11	2.01	0.41
3:F:60:TYR:HB3	13:A:1468:THR:N	2.35	0.41
3:F:69:ARG:HH11	3:F:72:GLN:HE21	1.67	0.41
10:N:20:DG:OP1	13:A:1131:SER:CB	2.69	0.41
13:A:196:LEU:HD13	13:A:311:GLN:HG3	2.02	0.41
13:A:1484:MET:O	13:A:1486:ILE:N	2.53	0.41
13:A:520:MET:O	13:A:524:MET:HG2	2.20	0.41
13:A:865:ILE:HG12	14:B:1092:ASP:CG	2.41	0.41
15:C:154:ARG:HG2	15:C:155:LYS:N	2.35	0.41
13:A:200:ALA:HB3	13:A:214:ILE:HG12	2.01	0.41
13:A:469:MET:HE3	14:B:1094:GLN:HE21	1.86	0.41
14:B:19:PRO:C	14:B:21:LEU:H	2.23	0.41
14:B:990:SER:HB2	14:B:995:GLU:O	2.21	0.41
4:G:87:ALA:HB2	4:G:101:ILE:HG13	2.03	0.41
8:K:58:PHE:HB3	8:K:76:GLN:HB3	2.02	0.41
13:A:57:LEU:HD11	13:A:281:ALA:HB2	2.02	0.41
14:B:158:SER:O	14:B:164:ASN:HB2	2.21	0.41
14:B:803:ARG:NH2	14:B:951:GLN:OE1	2.45	0.41
1:D:63:LYS:HA	1:D:66:ASN:ND2	2.36	0.41
1:D:86:LEU:O	1:D:89:GLN:HG2	2.21	0.41
2:E:173:ILE:HB	2:E:207:ARG:HD3	2.02	0.41
5:H:8:ASP:OD1	5:H:9:ILE:N	2.54	0.41
5:H:76:ASN:OD1	5:H:76:ASN:N	2.54	0.41
13:A:189:PRO:HB3	13:A:202:TRP:CE2	2.56	0.41
13:A:421:ARG:HB2	13:A:425:ASP:OD1	2.21	0.41
13:A:1139:LEU:HD13	13:A:1359:SER:HB3	2.02	0.41
14:B:40:VAL:HG22	14:B:43:GLN:HB2	2.02	0.41
14:B:156:LEU:HD22	14:B:184:TYR:CE1	2.55	0.41
14:B:237:VAL:HG12	14:B:372:LEU:HD22	2.01	0.41
14:B:280:SER:O	14:B:284:ILE:HG12	2.21	0.41
14:B:645:GLU:O	14:B:649:ASN:HB2	2.20	0.41
14:B:1111:SER:O	14:B:1113:PRO:HD3	2.20	0.41
6:I:107:ALA:H	13:A:734:ARG:HH11	1.69	0.41
8:K:62:LYS:HB2	13:A:566:PHE:CZ	2.56	0.41
12:T:19:DG:OP1	14:B:747:LEU:CD2	2.66	0.41
13:A:48:GLU:OE1	13:A:53:LYS:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:413:TYR:O	13:A:415:GLY:N	2.53	0.41
13:A:535:MET:O	13:A:669:TYR:OH	2.36	0.41
13:A:661:GLY:O	13:A:665:THR:OG1	2.31	0.41
13:A:783:GLN:HA	13:A:787:VAL:O	2.20	0.41
14:B:254:GLN:HB3	14:B:255:ARG:H	1.70	0.41
14:B:670:GLU:O	14:B:673:VAL:HG12	2.21	0.41
14:B:712:PRO:HG2	14:B:939:HIS:CE1	2.56	0.41
14:B:815:LYS:HG3	14:B:920:LYS:HG2	2.02	0.41
14:B:854:ILE:O	14:B:907:VAL:HG21	2.21	0.41
15:C:27:ASP:HB2	15:C:30:VAL:HG23	2.03	0.41
4:G:11:ILE:HD11	4:G:30:LEU:HB2	2.02	0.40
13:A:33:ARG:HH11	14:B:1139:GLY:HA2	1.87	0.40
13:A:427:ILE:CG2	13:A:437:ASP:HB3	2.50	0.40
13:A:788:VAL:HG21	13:A:831:LEU:HD21	2.02	0.40
14:B:1028:LEU:HD12	14:B:1041:ILE:HG13	2.03	0.40
13:A:122:ASN:HA	13:A:127:LYS:HZ3	1.85	0.40
13:A:1128:ILE:HD13	13:A:1128:ILE:HA	1.89	0.40
14:B:561:ILE:HG13	14:B:576:ILE:HG21	2.01	0.40
1:D:34:ASN:HA	1:D:37:VAL:HG22	2.03	0.40
2:E:126:ILE:H	2:E:126:ILE:HG12	1.65	0.40
7:J:8:PHE:O	14:B:803:ARG:NH1	2.50	0.40
8:K:52:LYS:HE2	15:C:27:ASP:OD2	2.21	0.40
13:A:683:GLU:HA	14:B:1038:THR:HB	2.03	0.40
14:B:365:LEU:O	14:B:369:VAL:HG23	2.21	0.40
3:F:64:ARG:HD3	13:A:1471:PHE:CE2	2.57	0.40
4:G:19:GLY:HA2	13:A:1480:CYS:O	2.21	0.40
4:G:106:CYS:SG	4:G:161:GLY:N	2.95	0.40
5:H:4:ILE:HD11	5:H:7:GLU:HB2	2.03	0.40
13:A:543:THR:OG1	14:B:970:HIS:NE2	2.45	0.40
13:A:938:LEU:HD21	13:A:1006:PRO:HD2	2.03	0.40
13:A:1010:VAL:HG12	13:A:1014:LYS:HE2	2.04	0.40
14:B:318:LEU:HD13	14:B:318:LEU:HA	1.93	0.40
14:B:864:ASP:HB2	14:B:896:LEU:HD23	2.03	0.40
1:D:36:GLU:OE1	1:D:84:ARG:NH1	2.55	0.40
1:D:44:ARG:HH11	1:D:48:ASN:HD21	1.68	0.40
2:E:41:LYS:HB2	2:E:41:LYS:HE3	1.87	0.40
13:A:279:LYS:HA	13:A:279:LYS:HD2	1.83	0.40
13:A:408:ARG:HH21	13:A:414:PRO:HD2	1.86	0.40
13:A:529:GLN:HG3	13:A:1094:SER:HB3	2.02	0.40
13:A:787:VAL:HG22	13:A:824:GLU:O	2.22	0.40
13:A:1401:LEU:O	13:A:1404:THR:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:951:GLN:HB3	15:C:39:ILE:HG21	2.03	0.40
15:C:74:ILE:HD12	15:C:128:ILE:HB	2.04	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	D	126/142 (89%)	122 (97%)	4 (3%)	0	100	100
2	E	207/210 (99%)	198 (96%)	9 (4%)	0	100	100
3	F	80/127 (63%)	78 (98%)	2 (2%)	0	100	100
4	G	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
5	H	146/150 (97%)	138 (94%)	7 (5%)	1 (1%)	19	38
6	I	112/125 (90%)	102 (91%)	9 (8%)	1 (1%)	14	31
7	J	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
8	K	113/117 (97%)	113 (100%)	0	0	100	100
9	L	42/58 (72%)	38 (90%)	4 (10%)	0	100	100
13	A	1429/1970 (72%)	1352 (95%)	72 (5%)	5 (0%)	37	59
14	B	1128/1174 (96%)	1057 (94%)	68 (6%)	3 (0%)	37	59
15	C	253/275 (92%)	246 (97%)	7 (3%)	0	100	100
All	All	3870/4587 (84%)	3666 (95%)	194 (5%)	10 (0%)	38	59

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	A	184	CYS
13	A	207	GLU

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Mol	Chain	Res	Type
13	A	1203	ASP
13	A	1485	GLU
14	B	101	ARG
14	B	241	ALA
5	H	34	SER
13	A	1267	ASN
14	B	230	ARG
6	I	116	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	106/126 (84%)	103 (97%)	3 (3%)	38	65
2	E	189/192 (98%)	182 (96%)	7 (4%)	29	55
3	F	71/111 (64%)	70 (99%)	1 (1%)	62	82
4	G	147/153 (96%)	138 (94%)	9 (6%)	15	34
5	H	129/131 (98%)	124 (96%)	5 (4%)	27	53
6	I	103/112 (92%)	100 (97%)	3 (3%)	37	64
7	J	56/56 (100%)	54 (96%)	2 (4%)	30	56
8	K	104/106 (98%)	102 (98%)	2 (2%)	52	75
9	L	41/55 (74%)	41 (100%)	0	100	100
13	A	1268/1748 (72%)	1200 (95%)	68 (5%)	18	39
14	B	993/1028 (97%)	961 (97%)	32 (3%)	34	60
15	C	234/252 (93%)	229 (98%)	5 (2%)	48	73
All	All	3441/4070 (84%)	3304 (96%)	137 (4%)	29	52

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	20	LEU
1	D	31	THR

Continued on next page...

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Mol	Chain	Res	Type
1	D	61	PHE
2	E	57	ASP
2	E	73	PHE
2	E	99	ILE
2	E	121	MET
2	E	162	ARG
2	E	185	ILE
2	E	191	VAL
3	F	53	THR
4	G	3	TYR
4	G	77	PHE
4	G	90	THR
4	G	99	THR
4	G	150	THR
4	G	151	ARG
4	G	164	MET
4	G	167	TYR
4	G	168	LEU
5	H	4	ILE
5	H	72	ASP
5	H	96	VAL
5	H	104	THR
5	H	133	HIS
6	I	22	ASN
6	I	24	LEU
6	I	110	LEU
7	J	7	CYS
7	J	22	LEU
8	K	42	LEU
8	K	63	VAL
13	A	77	ASN
13	A	110	VAL
13	A	123	ASN
13	A	152	ASN
13	A	184	CYS
13	A	190	ARG
13	A	193	ARG
13	A	203	LYS
13	A	230	ASP
13	A	241	ARG
13	A	346	LYS
13	A	434	LYS

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Mol	Chain	Res	Type
13	A	439	HIS
13	A	446	VAL
13	A	458	PHE
13	A	465	HIS
13	A	488	VAL
13	A	489	THR
13	A	549	THR
13	A	565	MET
13	A	626	THR
13	A	647	THR
13	A	683	GLU
13	A	687	ILE
13	A	701	ASP
13	A	733	LEU
13	A	734	ARG
13	A	775	LYS
13	A	797	ARG
13	A	805	ARG
13	A	853	LYS
13	A	883	ILE
13	A	896	LEU
13	A	935	GLN
13	A	938	LEU
13	A	981	CYS
13	A	1007	ILE
13	A	1034	GLN
13	A	1038	THR
13	A	1075	LYS
13	A	1102	MET
13	A	1115	LYS
13	A	1116	ASN
13	A	1117	VAL
13	A	1119	LEU
13	A	1140	THR
13	A	1158	LEU
13	A	1186	VAL
13	A	1199	MET
13	A	1201	ASP
13	A	1202	PHE
13	A	1206	ARG
13	A	1214	VAL
13	A	1234	LYS

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Mol	Chain	Res	Type
13	A	1253	GLU
13	A	1261	ILE
13	A	1263	ASN
13	A	1278	LYS
13	A	1314	THR
13	A	1320	ILE
13	A	1361	ASP
13	A	1374	VAL
13	A	1408	ARG
13	A	1415	THR
13	A	1430	CYS
13	A	1479	LYS
13	A	1484	MET
13	A	1486	ILE
14	B	21	LEU
14	B	42	GLN
14	B	101	ARG
14	B	102	ASP
14	B	140	LEU
14	B	173	GLU
14	B	174	LEU
14	B	225	LEU
14	B	254	GLN
14	B	318	LEU
14	B	388	TYR
14	B	414	GLU
14	B	503	ASN
14	B	514	THR
14	B	516	GLU
14	B	518	HIS
14	B	524	LYS
14	B	528	LEU
14	B	556	ILE
14	B	581	GLU
14	B	592	ARG
14	B	698	ILE
14	B	728	MET
14	B	763	SER
14	B	840	MET
14	B	863	ASP
14	B	864	ASP
14	B	873	LEU

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Mol	Chain	Res	Type
14	B	892	CYS
14	B	909	VAL
14	B	1022	LEU
14	B	1145	GLN
15	C	44	ILE
15	C	62	GLU
15	C	63	PHE
15	C	78	ILE
15	C	94	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	48	ASN
1	D	66	ASN
1	D	128	GLN
2	E	19	GLN
2	E	98	ASN
3	F	72	GLN
4	G	9	HIS
4	G	91	GLN
5	H	87	GLN
5	H	133	HIS
6	I	46	GLN
6	I	67	GLN
6	I	98	GLN
7	J	52	HIS
8	K	49	GLN
9	L	26	ASN
13	A	210	GLN
13	A	273	GLN
13	A	278	HIS
13	A	341	GLN
13	A	531	ASN
13	A	576	GLN
13	A	700	GLN
13	A	780	ASN
13	A	792	ASN
13	A	926	ASN
13	A	949	GLN
13	A	1034	GLN
13	A	1077	ASN

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Mol	Chain	Res	Type
13	A	1230	GLN
13	A	1244	ASN
13	A	1263	ASN
13	A	1299	GLN
13	A	1310	HIS
13	A	1422	GLN
13	A	1462	GLN
14	B	42	GLN
14	B	90	GLN
14	B	143	GLN
14	B	144	HIS
14	B	245	GLN
14	B	254	GLN
14	B	344	GLN
14	B	471	ASN
14	B	585	ASN
14	B	639	HIS
14	B	699	HIS
14	B	717	ASN
14	B	725	GLN
14	B	731	GLN
14	B	817	GLN
14	B	838	GLN
14	B	980	HIS
14	B	1021	HIS
14	B	1068	GLN
14	B	1094	GLN
14	B	1115	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	P	9/20 (45%)	5 (55%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	P	12	A
11	P	13	G
11	P	18	G
11	P	19	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	P	20	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

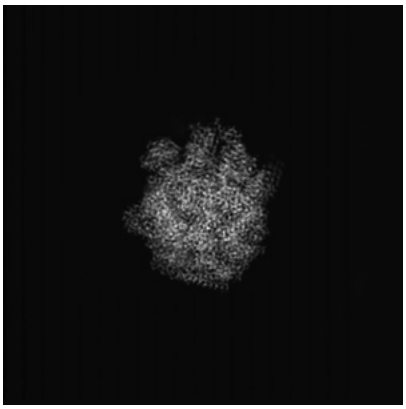
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-48071. 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.

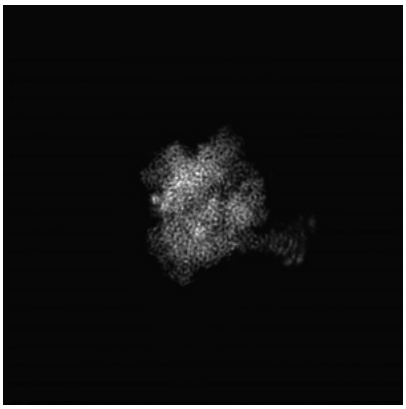
6.1 Orthogonal projections

6.1.1 Primary map



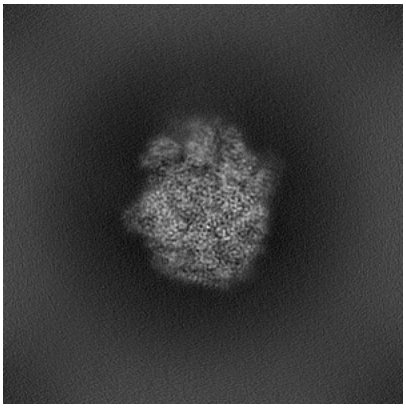
X

Y

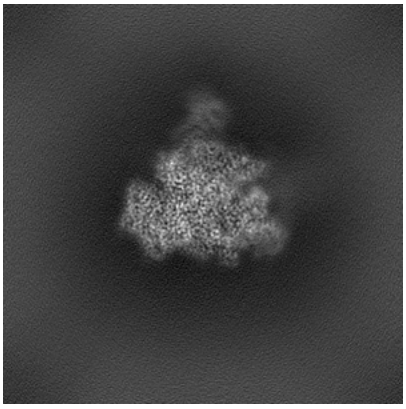


Z

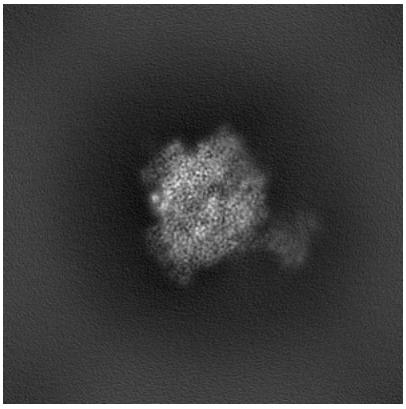
6.1.2 Raw map



X



Y



Z

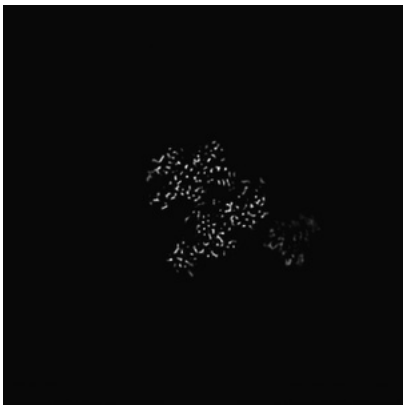
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

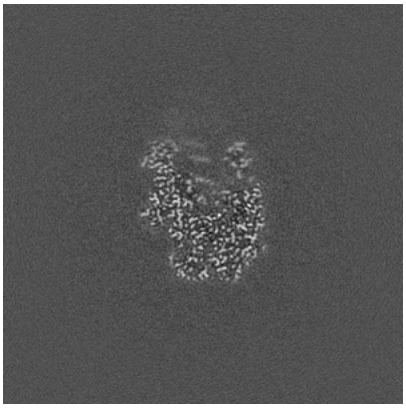
X Index: 160

Y Index: 160

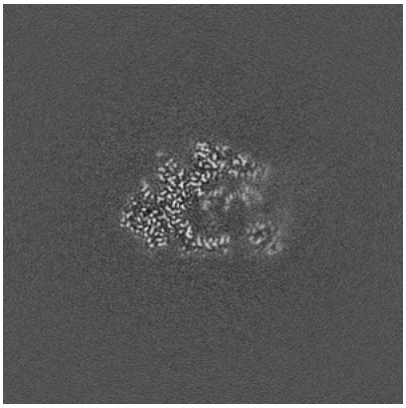


Z Index: 160

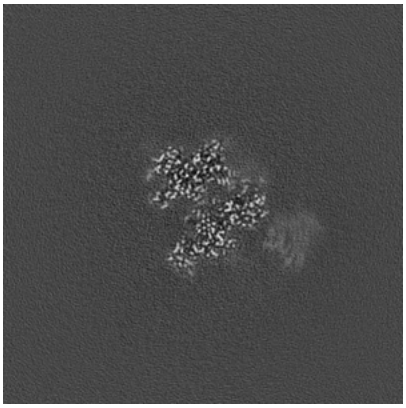
6.2.2 Raw map



X Index: 160



Y Index: 160



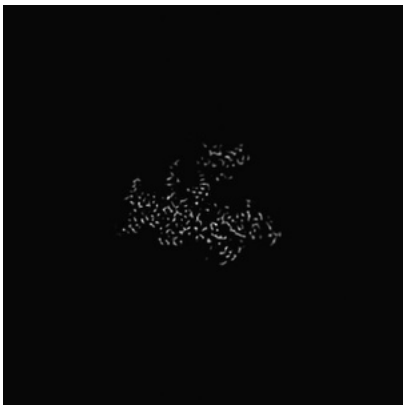
Z Index: 160

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

6.3 Largest variance slices (i)

6.3.1 Primary map

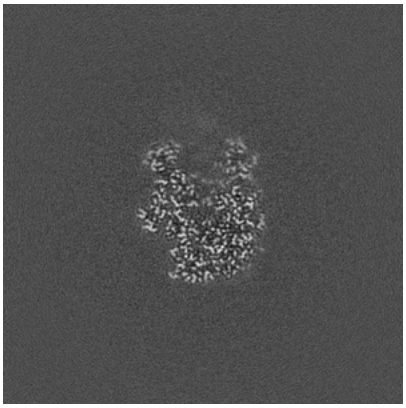
X Index: 138



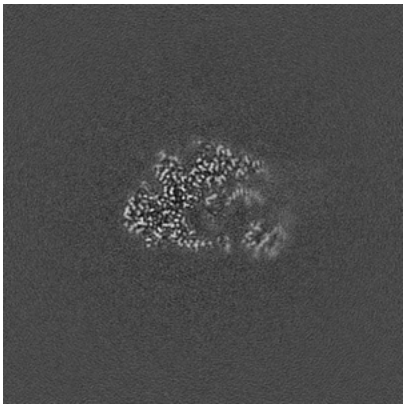
Y Index: 177

Z Index: 158

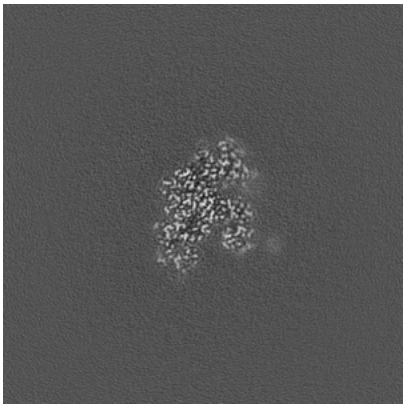
6.3.2 Raw map



X Index: 156



Y Index: 157

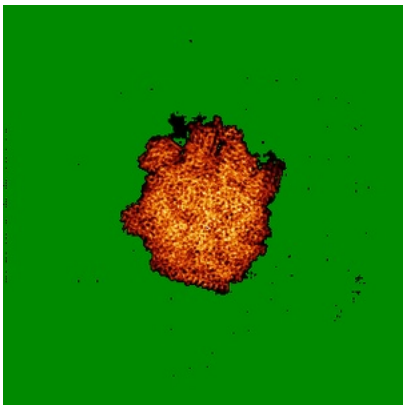


Z Index: 136

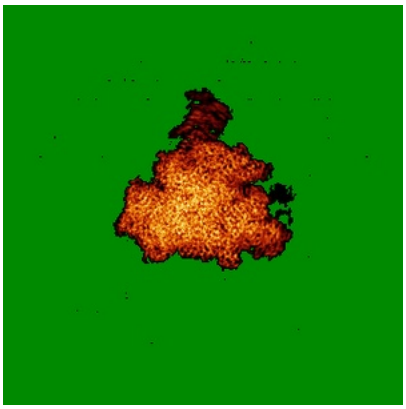
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

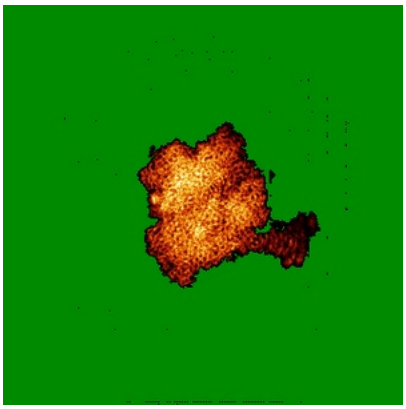
6.4.1 Primary map



X

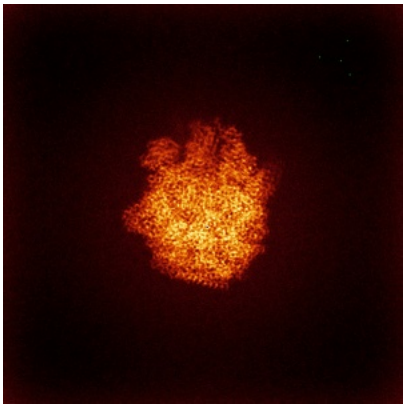


Y

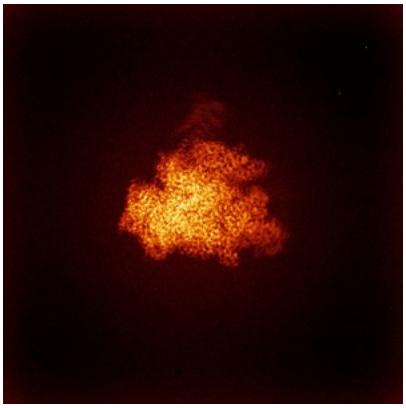


Z

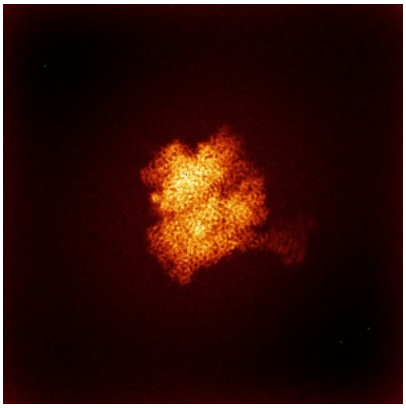
6.4.2 Raw map



X



Y

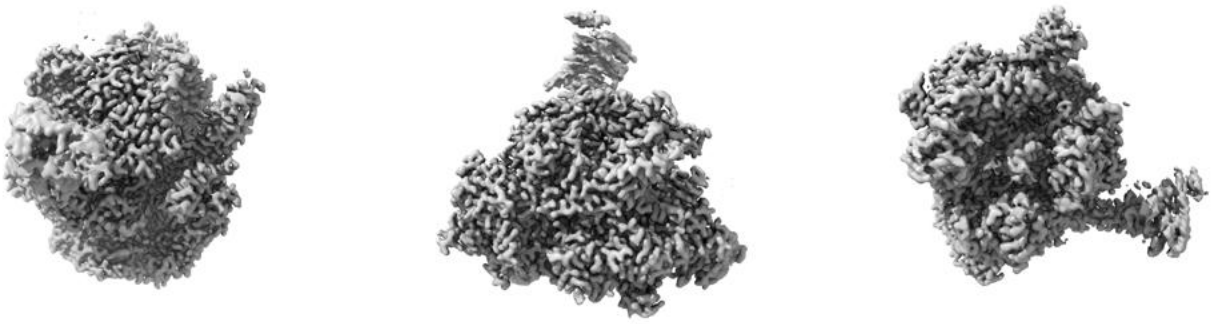


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. 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

X Y Z

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.

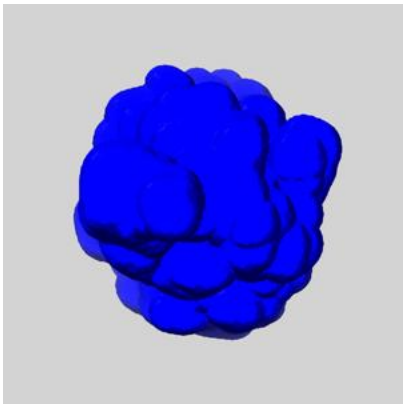
6.6 Mask visualisation

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

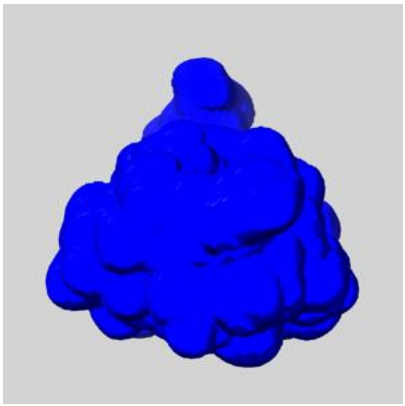
A mask typically either:

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

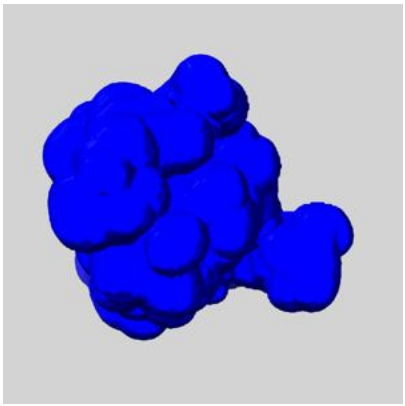
6.6.1 emd_48071_msk_1.map



X



Y

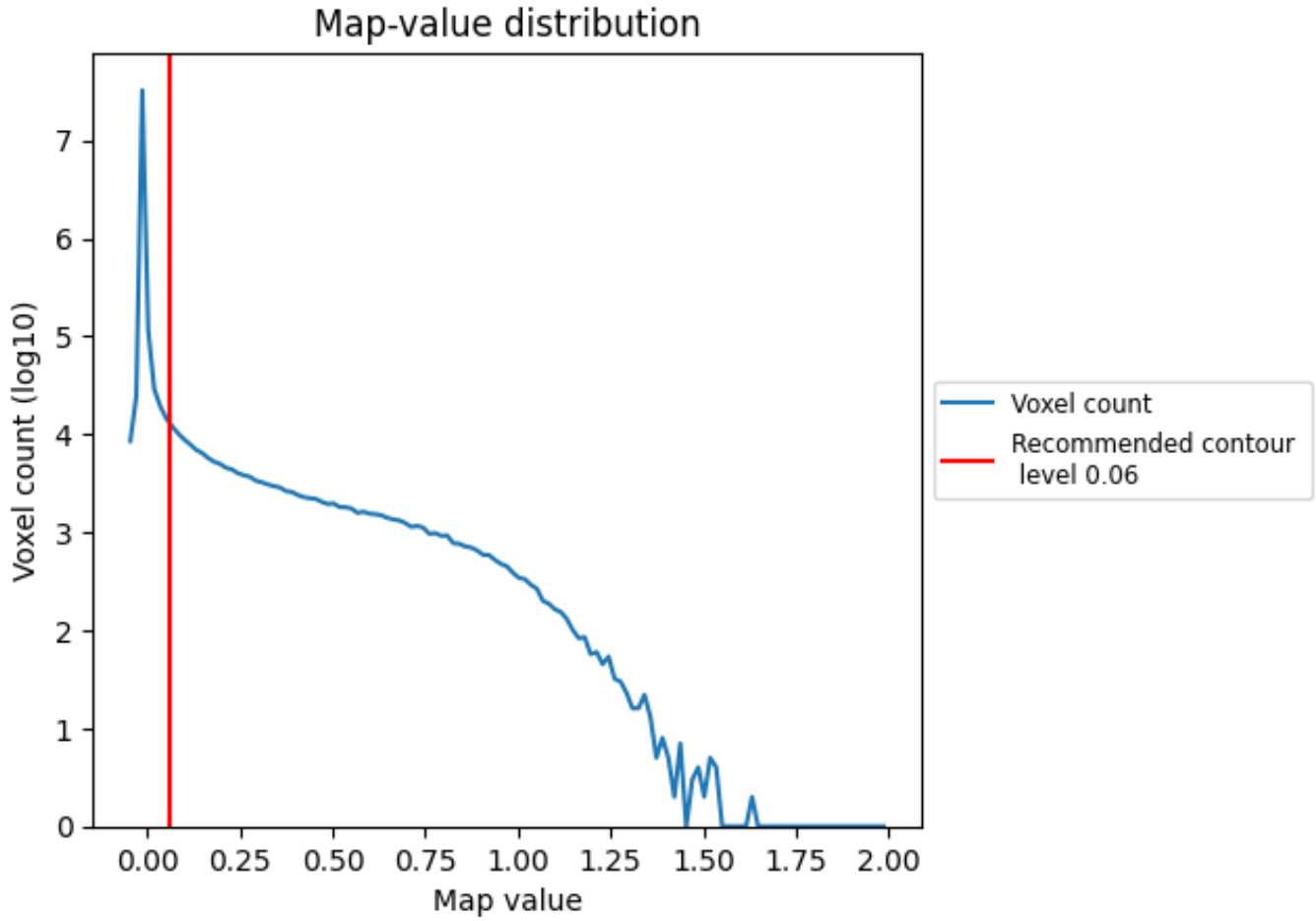


Z

7 Map analysis

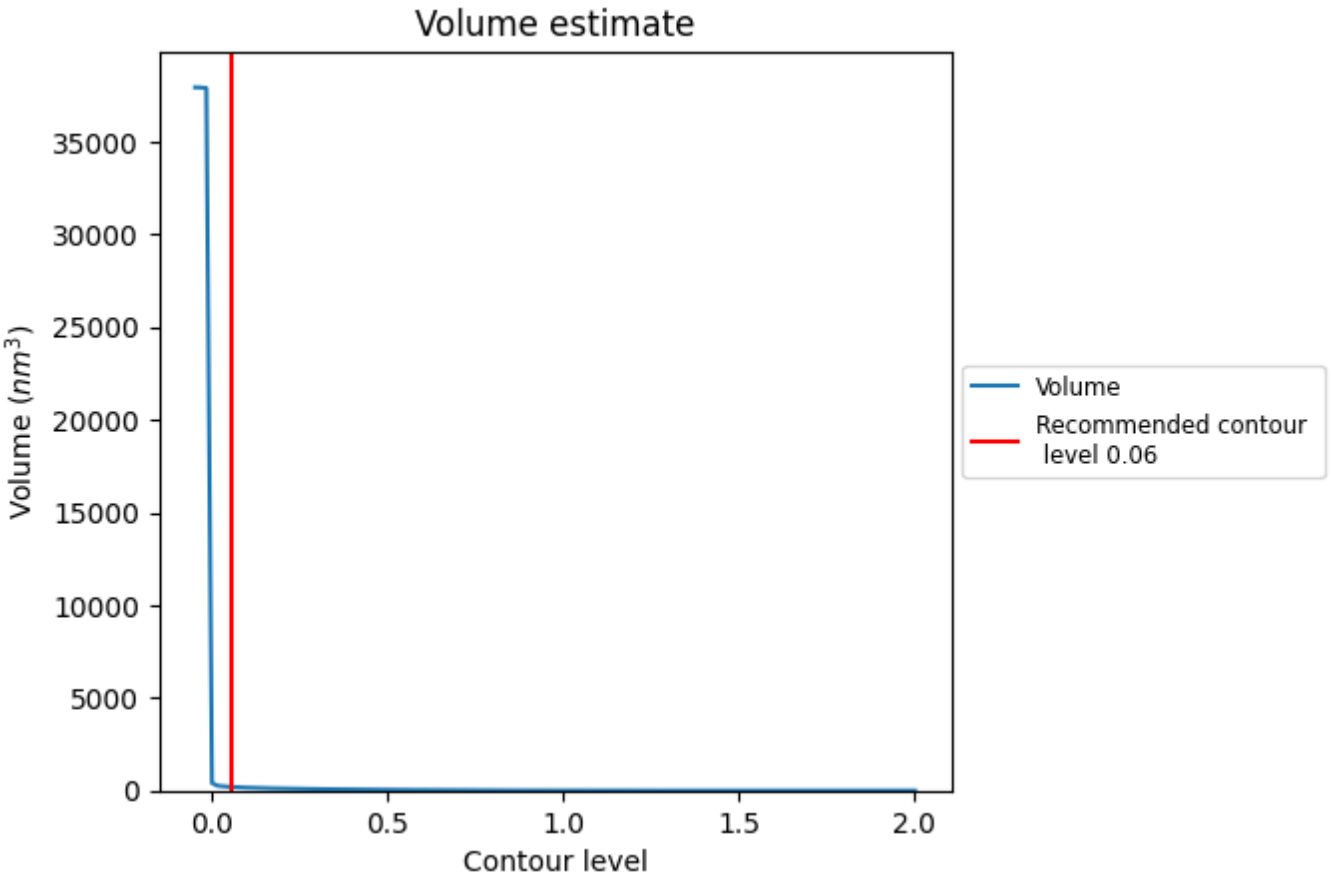
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

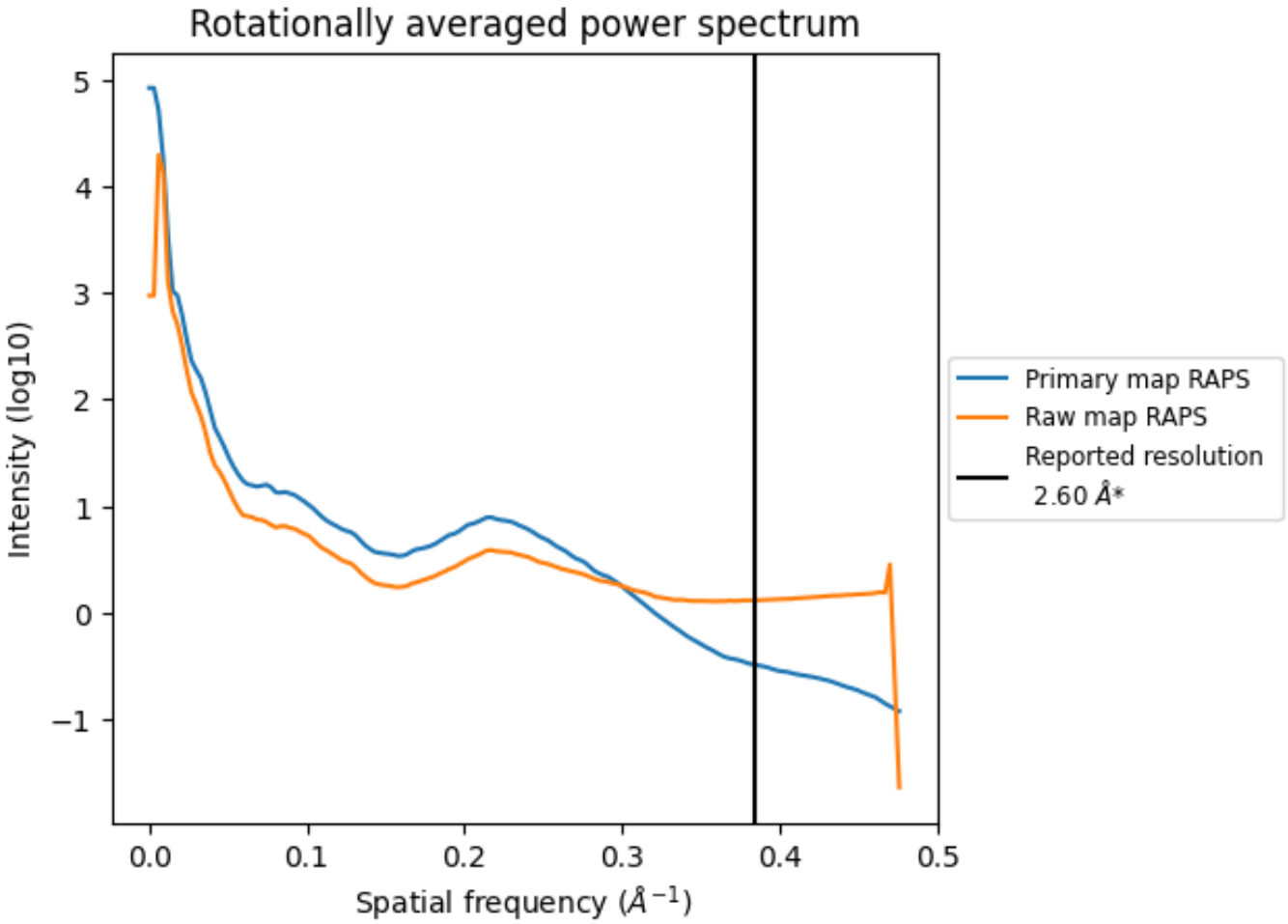
7.2 Volume estimate



The volume at the recommended contour level is 192 nm^3; this corresponds to an approximate mass of 173 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

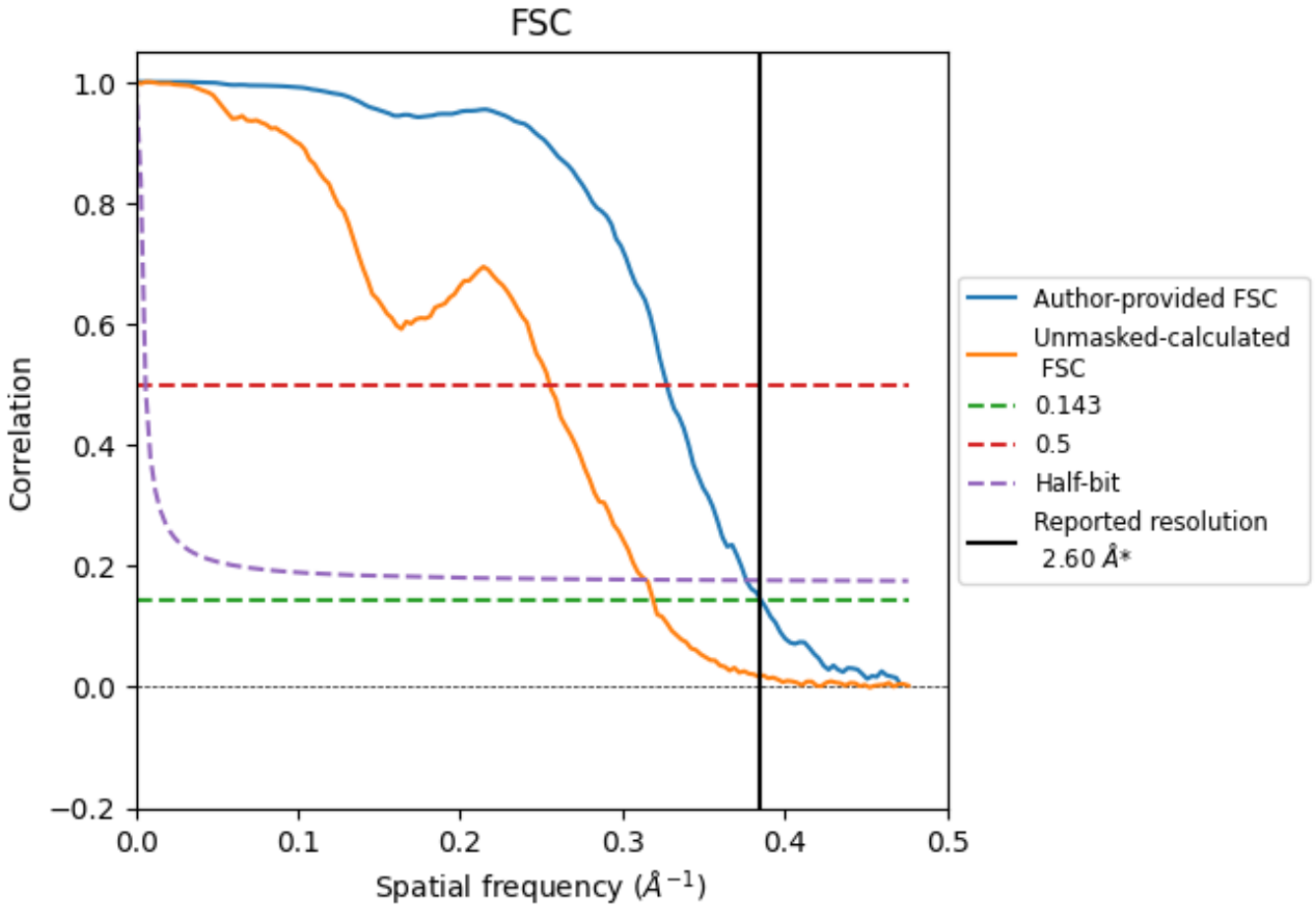


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8.2 Resolution estimates (i)

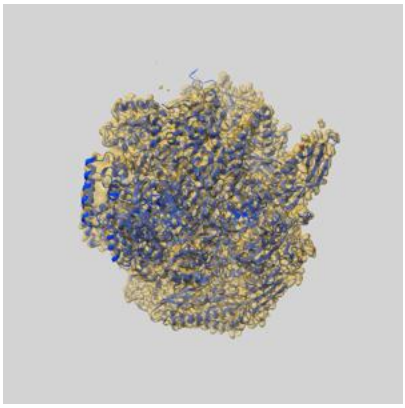
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.59	3.06	2.66
Unmasked-calculated*	3.14	3.92	3.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.14 differs from the reported value 2.6 by more than 10 %

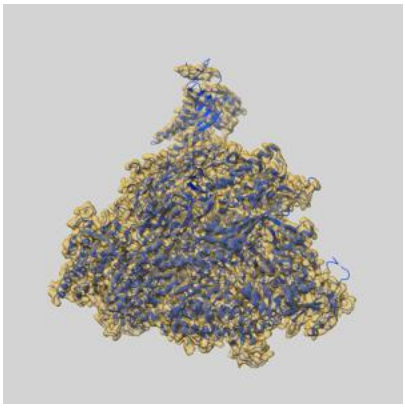
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-48071 and PDB model 9EHZ. Per-residue inclusion information can be found in section 3 on page 7.

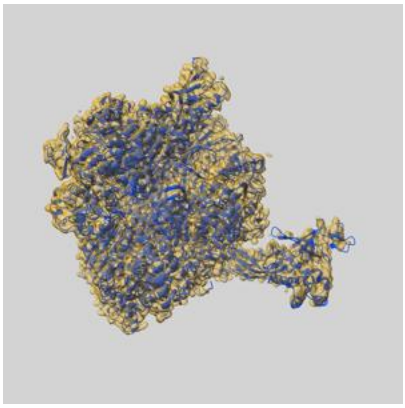
9.1 Map-model overlay



X



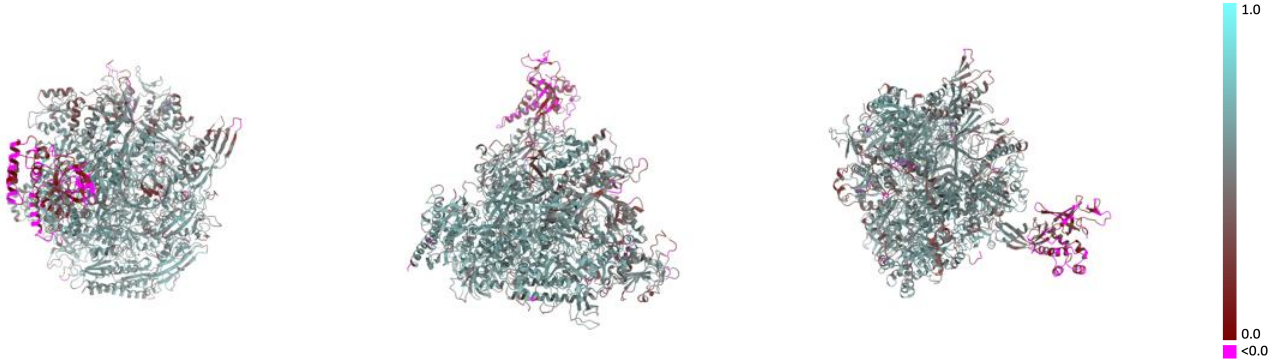
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

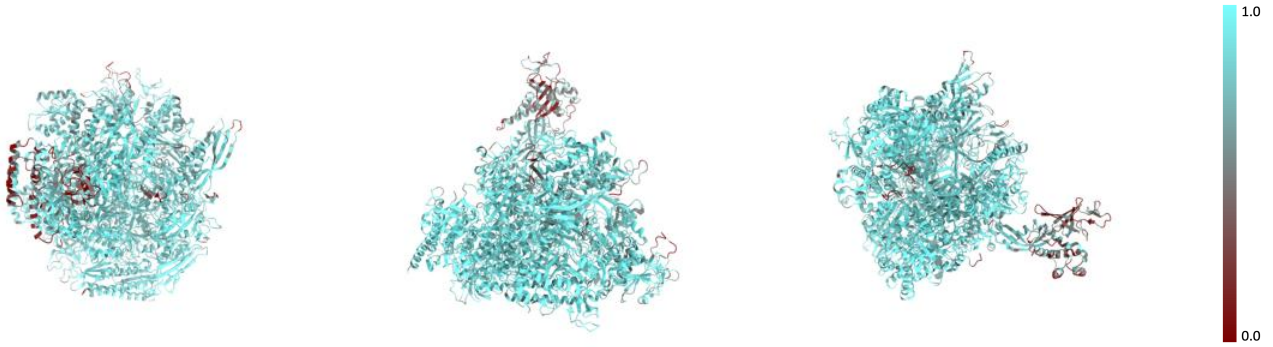
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

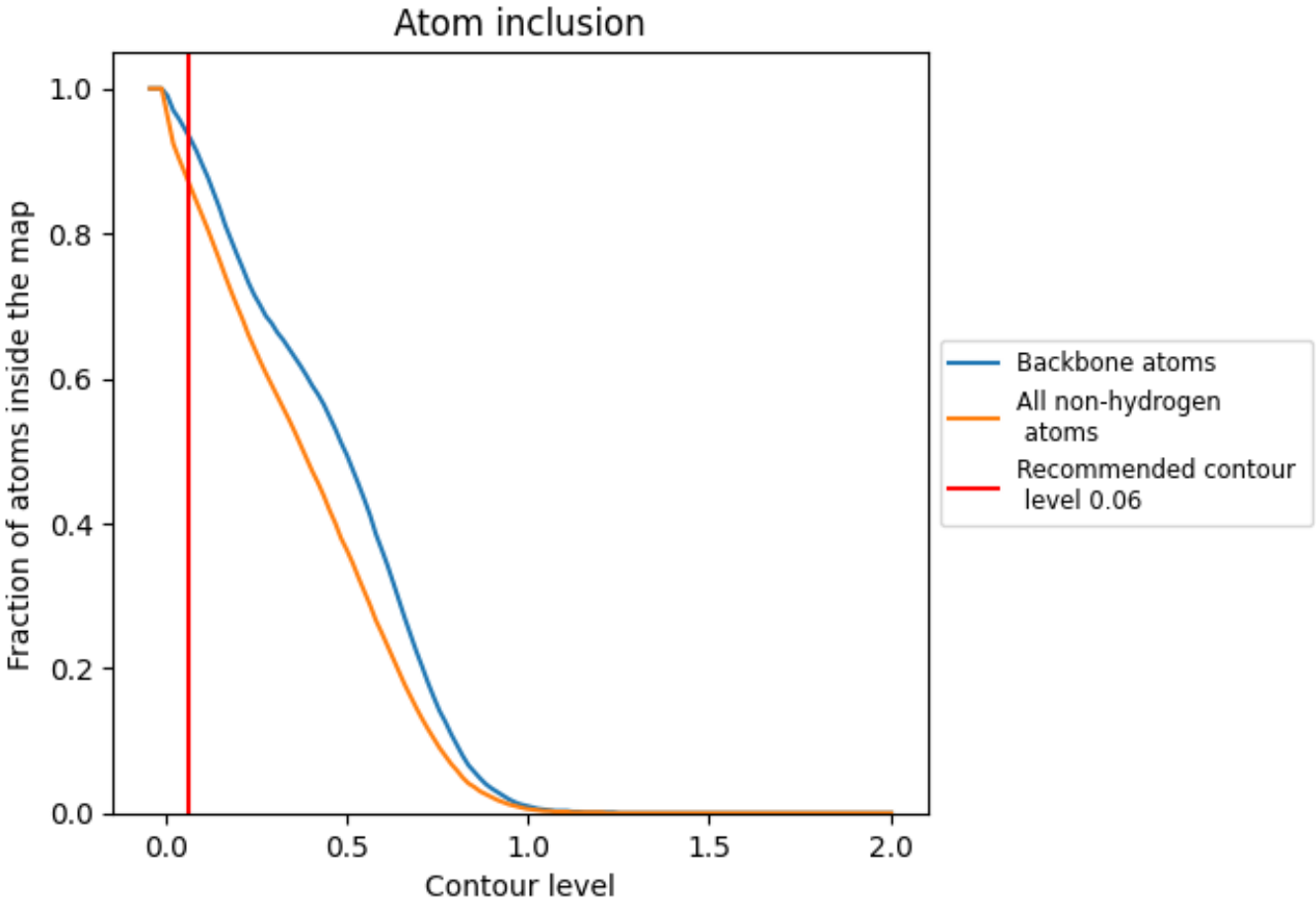
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 87% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8710	0.5260
A	0.9040	0.5580
B	0.8990	0.5550
C	0.9230	0.5850
D	0.4320	0.0630
E	0.8920	0.5260
F	0.8750	0.5510
G	0.5670	0.2570
H	0.8890	0.5410
I	0.8410	0.4920
J	0.9210	0.5820
K	0.9350	0.5840
L	0.8150	0.4790
N	0.9110	0.5340
P	0.8670	0.5380
T	0.8930	0.4930