Full wwPDB EM Validation Report ⓘ

Aug 27, 2024 – 05:07 PM JST

PDB ID	:	9JA1
EMDB ID	:	EMD-61287
Title	:	The RNA polymerase II elongation complex from Saccharomyces cerevisiae
Authors	:	Yi, G.; Ma, J.; Zhang, P.
Deposited on	:	2024-08-23
Resolution	:	2.98 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:

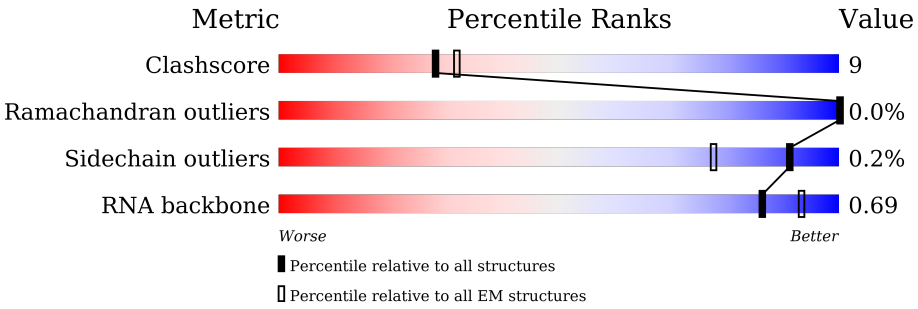
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance

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

The reported resolution of this entry is 2.98 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	A	1733	8% 58% 16% 26%
2	B	1224	17% 72% 18% 10%
3	C	318	5% 69% 15% 16%
4	E	215	13% 84% 14%
5	F	155	44% 10% 46%
6	H	146	10% 75% 17% 8%
7	J	70	71% 21% 7%

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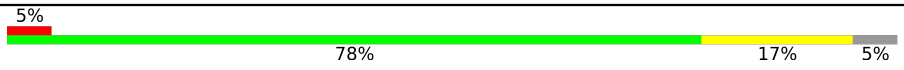
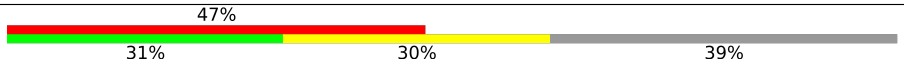
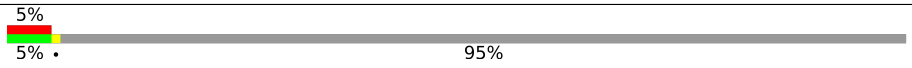
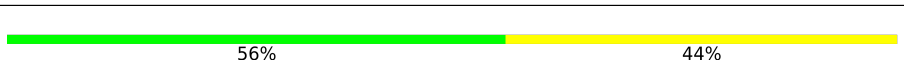
Mol	Chain	Length	Quality of chain
8	K	120	
9	L	70	
10	D	221	
11	G	171	
12	R	9	
13	T	74	
14	N	74	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 27832 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1286	10060	6346	1767	1892	55	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1100	8724	5525	1523	1621	55	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	266	2091	1315	347	416	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	210	1726	1097	305	314	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	83	670	428	114	125	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	134	1076	677	182	213	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	114	Total	C	N	O	S	0	0
			915	588	156	169	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	43	Total	C	N	O	S	0	0
			343	211	69	59	4		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	D	12	Total	C	N	O	0	0
			95	61	16	18		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	79	Total	C	N	O	S	0	0
			638	416	105	114	3		

- Molecule 12 is a RNA chain called RNA (5'-R(P*AP*UP*CP*GP*AP*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	9	Total	C	N	O	P	0	0
			194	88	40	58	8		

- Molecule 13 is a DNA chain called DNA (5'-D(P*GP*CP*TP*CP*CP*TP*TP*CP*TP*CP*CP*CP*AP*TP*CP*CP*TP*CP*TP*CP*GP*AP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	23	Total	C	N	O	P	0	0
			455	219	69	144	23		

- Molecule 14 is a DNA chain called DNA (5'-D(P*TP*GP*GP*GP*AP*GP*AP*AP*GP*GP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	13	Total	C	N	O	P	0	0
			274	129	60	73	12		

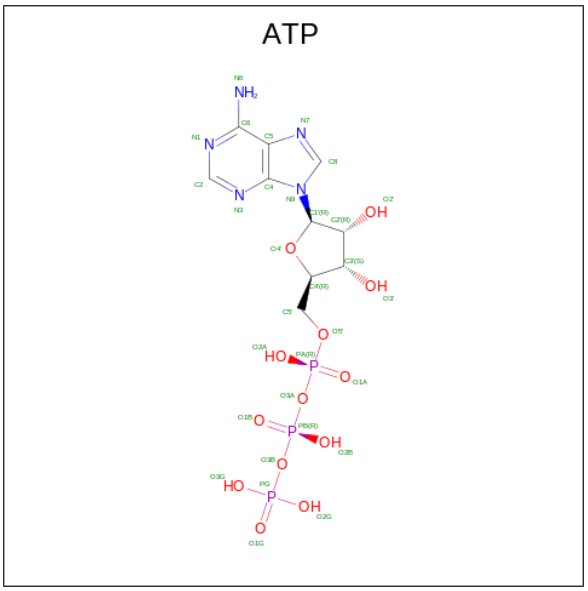
- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
16	A	1	Total	Mg	0
			1	1	
16	R	1	Total	Mg	0
			1	1	

- Molecule 17 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

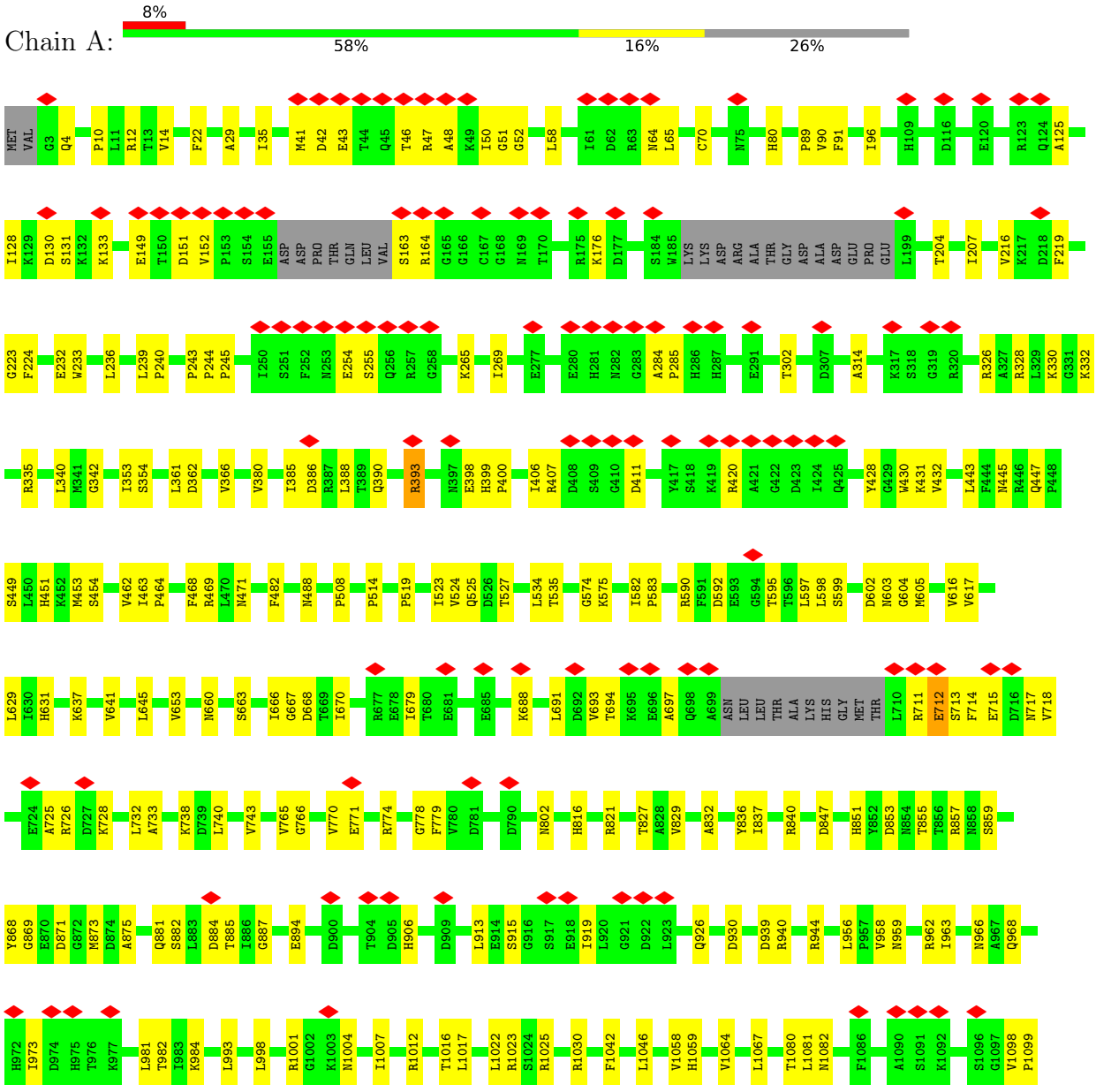


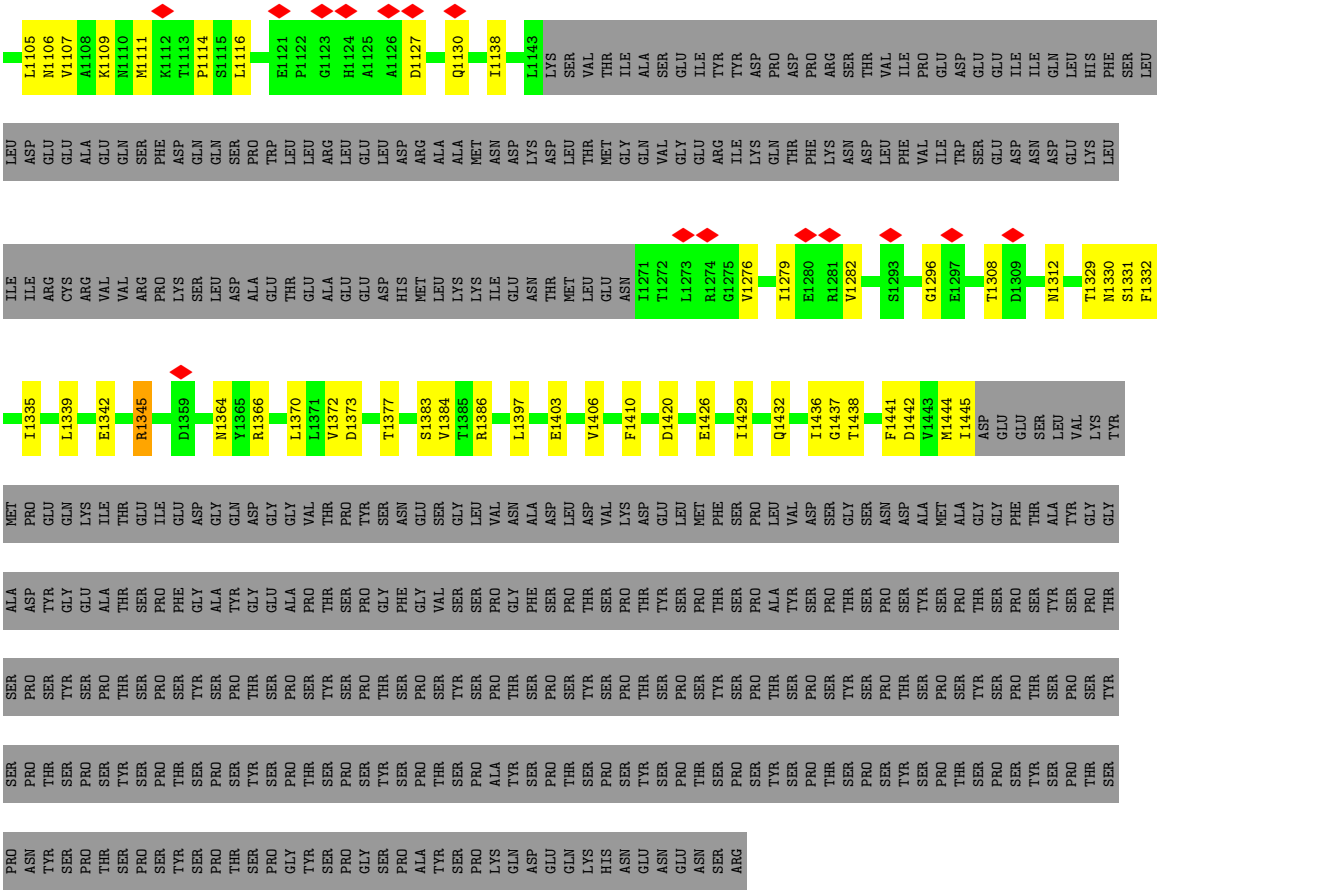
Mol	Chain	Residues	Atoms					AltConf
17	T	1	Total	C	N	O	P	0
			31	10	5	13	3	

3 Residue-property plots (i)

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

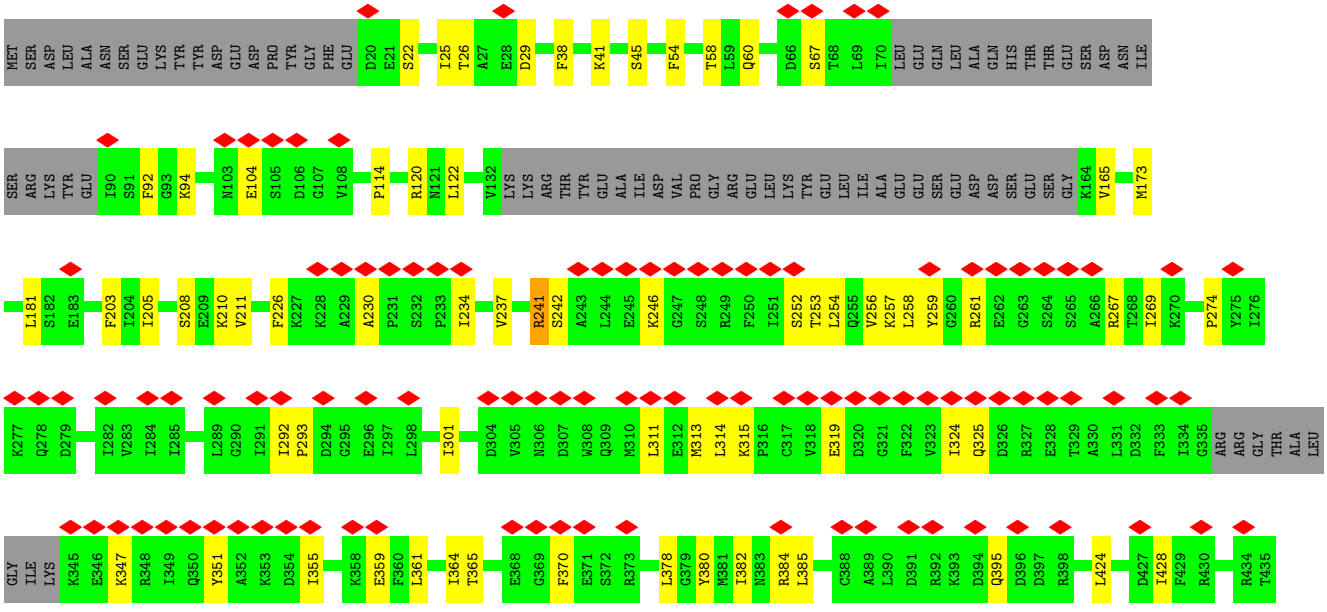
• Molecule 1: DNA-directed RNA polymerase II subunit RPB1

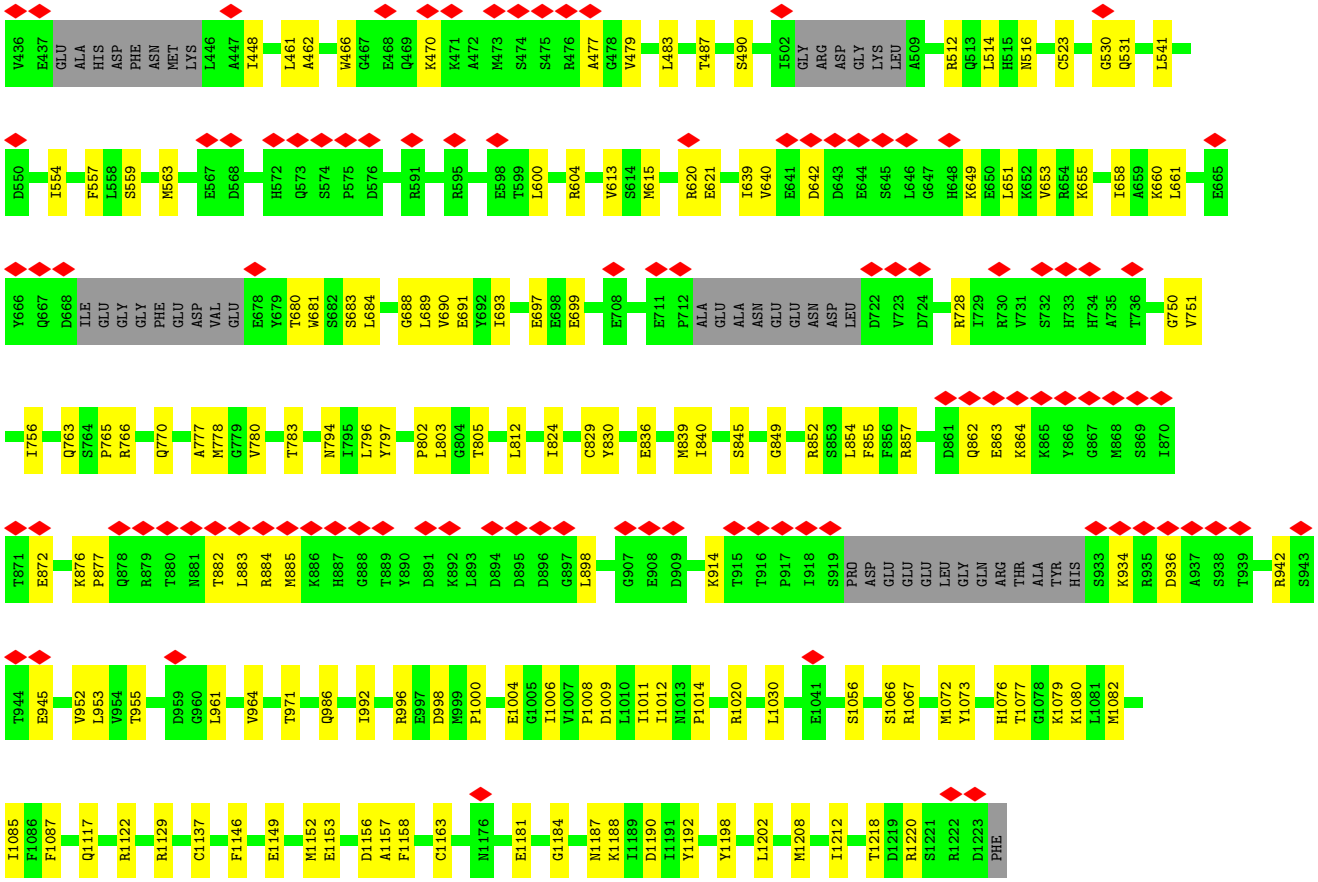




• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

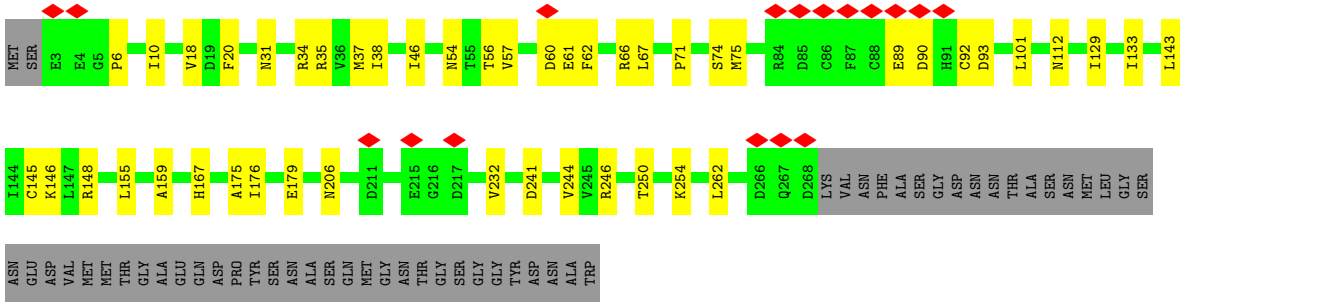
Chain B:





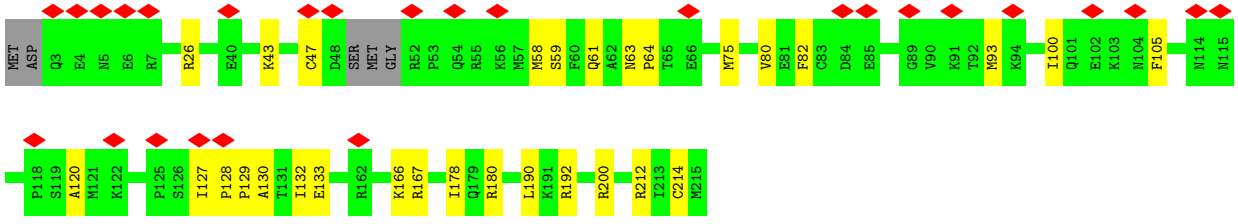
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



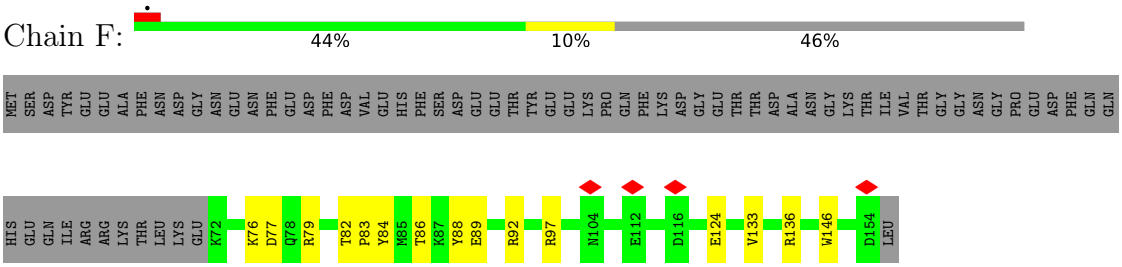
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



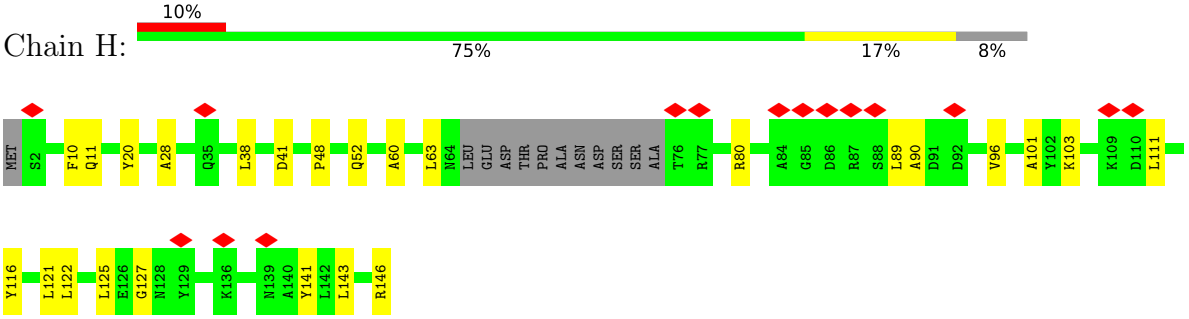
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



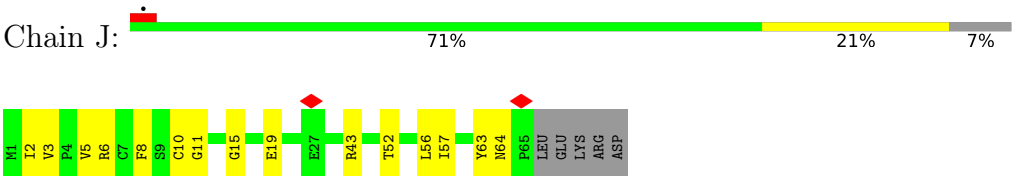
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



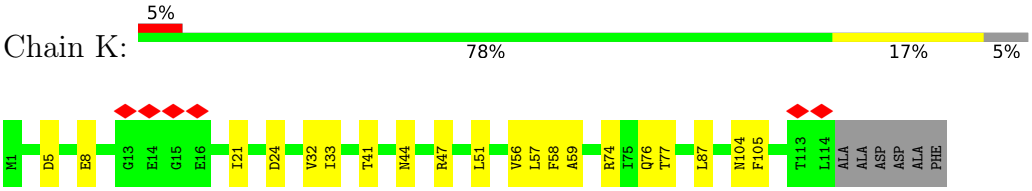
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



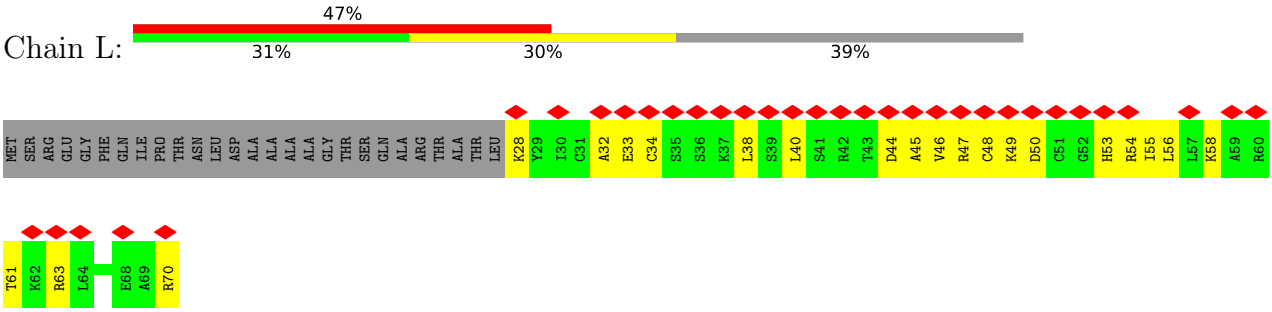
• Molecule 8: DNA-directed RNA polymerase II subunit RPB11

Chain K:



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

Chain L:

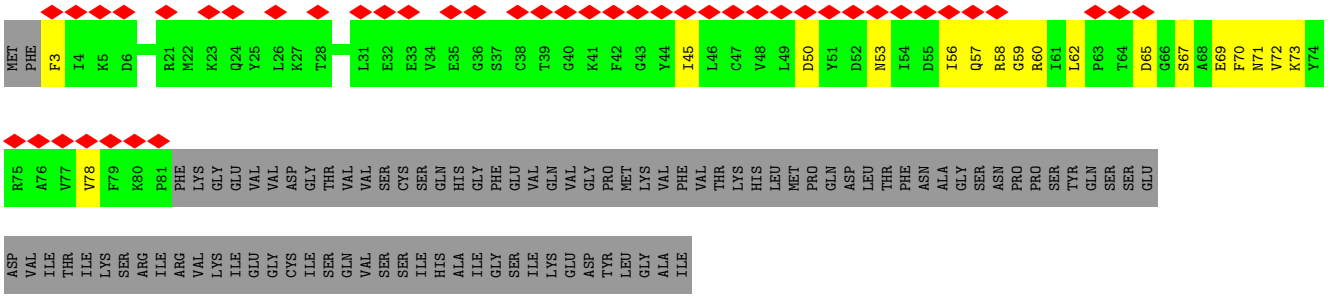


• Molecule 10: DNA-directed RNA polymerase II subunit RPB4

Chain D:

• Molecule 11: DNA-directed RNA polymerase II subunit RPB7

Chain G:

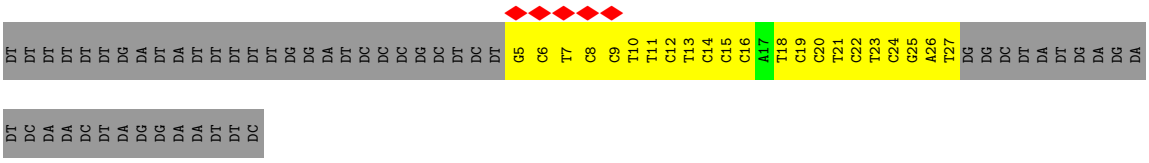


• Molecule 12: RNA (5'-R(P*AP*UP*CP*GP*AP*GP*AP*GP*G)-3')

Chain R:

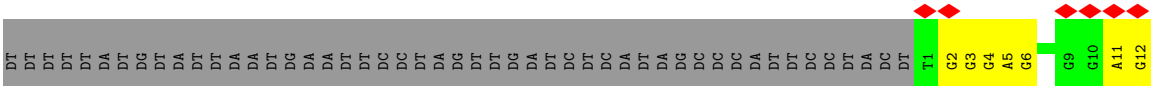
• Molecule 13: DNA (5'-D(P*GP*CP*TP*CP*CP*TP*TP*CP*TP*CP*CP*CP*AP*TP*CP*CP*TP*CP*TP*CP*GP*AP*T)-3')

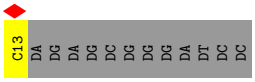
Chain T:



• Molecule 14: DNA (5'-D(P*TP*GP*GP*GP*AP*GP*AP*AP*GP*GP*AP*GP*C)-3')

Chain N:




C13
DA
DG
DA
DG
DC
DG
DG
DG
DA
DT
DC
DC

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	146186	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.910	Depositor
Minimum map value	-0.520	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	348.18, 348.18, 348.18	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.829, 0.829, 0.829	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.25	0/10242	0.48	0/13850
2	B	0.26	0/8894	0.49	0/11999
3	C	0.26	0/2129	0.46	0/2886
4	E	0.25	0/1761	0.48	0/2369
5	F	0.26	0/682	0.49	0/922
6	H	0.25	0/1094	0.49	0/1481
7	J	0.25	0/541	0.48	0/727
8	K	0.25	0/933	0.47	0/1260
9	L	0.23	0/345	0.52	0/457
10	D	0.22	0/94	0.43	0/125
11	G	0.24	0/652	0.42	0/878
12	R	0.29	0/218	0.62	0/339
13	T	0.32	0/504	0.68	0/772
14	N	0.26	0/310	0.75	0/479
All	All	0.26	0/28399	0.49	0/38544

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	10060	0	10131	211	0
2	B	8724	0	8735	158	0
3	C	2091	0	2046	39	0
4	E	1726	0	1754	17	0
5	F	670	0	690	15	0
6	H	1076	0	1046	20	0
7	J	532	0	542	16	0
8	K	915	0	925	13	0
9	L	343	0	363	19	0
10	D	95	0	104	1	0
11	G	638	0	650	17	0
12	R	194	0	98	6	0
13	T	455	0	262	52	0
14	N	274	0	146	21	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	A	1	0	0	0	0
16	R	1	0	0	0	0
17	T	31	0	12	1	0
All	All	27832	0	27504	521	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (521) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:8:DC:H1’	13:T:9:DC:H5’	1.17	1.12
13:T:8:DC:C1’	13:T:9:DC:H5’	1.82	1.10
13:T:7:DT:H2”	13:T:8:DC:H5”	1.31	1.09
1:A:832:ALA:HB2	13:T:18:DT:H72	1.41	1.02
2:B:242:SER:O	2:B:252:SER:HB3	1.65	0.97
1:A:583:PRO:HB2	1:A:637:LYS:HE3	1.46	0.94
13:T:8:DC:H1’	13:T:9:DC:C5’	1.97	0.94
14:N:3:DG:H2”	14:N:4:DG:H5’	1.50	0.93
14:N:3:DG:H2”	14:N:4:DG:C5’	1.99	0.93
7:J:5:VAL:HG12	7:J:6:ARG:HG2	1.52	0.92
1:A:43:GLU:H	1:A:50:ILE:HD11	1.38	0.88
6:H:60:ALA:HB2	6:H:143:LEU:HD11	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:8:DC:H2”	13:T:9:DC:C6	2.12	0.85
13:T:8:DC:H4’	13:T:9:DC:OP1	1.74	0.84
9:L:40:LEU:HA	9:L:44:ASP:HB3	1.59	0.84
1:A:832:ALA:HB2	13:T:18:DT:C7	2.07	0.83
13:T:7:DT:C2’	13:T:8:DC:H5”	2.08	0.83
1:A:152:VAL:HB	1:A:164:ARG:HD2	1.60	0.81
6:H:63:LEU:HG	6:H:89:LEU:HB3	1.65	0.78
13:T:7:DT:H2”	13:T:8:DC:C5’	2.13	0.78
13:T:13:DT:H3	14:N:5:DA:H62	1.33	0.77
9:L:47:ARG:NH1	9:L:54:ARG:HG3	2.00	0.77
13:T:6:DC:H2”	13:T:7:DT:H5’	1.65	0.77
13:T:8:DC:O3’	13:T:9:DC:H3’	1.84	0.76
1:A:1329:THR:HG22	1:A:1331:SER:H	1.50	0.75
2:B:797:TYR:HE1	2:B:854:LEU:HG	1.51	0.75
1:A:1444:MET:HA	11:G:60:ARG:HA	1.69	0.75
1:A:1386:ARG:NH2	13:T:15:DC:H1’	2.01	0.75
13:T:9:DC:H2”	13:T:10:DT:O5’	1.85	0.74
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.70	0.73
9:L:49:LYS:HG3	9:L:50:ASP:H	1.54	0.72
5:F:82:THR:HG22	5:F:84:TYR:H	1.55	0.72
1:A:666:ILE:HD13	2:B:1030:LEU:HD22	1.71	0.72
14:N:3:DG:H2”	14:N:4:DG:O5’	1.87	0.71
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.71	0.71
3:C:35:ARG:NH1	8:K:41:THR:OG1	2.24	0.71
1:A:535:THR:HG21	1:A:617:VAL:HG23	1.72	0.70
2:B:1006:ILE:HD11	7:J:43:ARG:HB3	1.73	0.70
2:B:802:PRO:HG2	2:B:805:THR:HG22	1.73	0.70
2:B:642:ASP:HA	2:B:649:LYS:HG2	1.73	0.69
3:C:6:PRO:O	8:K:104:ASN:ND2	2.25	0.69
9:L:28:LYS:N	9:L:38:LEU:O	2.25	0.69
2:B:604:ARG:NH2	2:B:691:GLU:OE2	2.24	0.69
6:H:60:ALA:HB3	6:H:141:TYR:HB2	1.75	0.69
7:J:2:ILE:HG23	7:J:3:VAL:H	1.58	0.69
3:C:179:GLU:OE1	3:C:206:ASN:ND2	2.27	0.68
1:A:1081:LEU:HD21	17:T:101:ATP:H2’	1.75	0.68
2:B:365:THR:HG21	2:B:370:PHE:HB2	1.75	0.68
2:B:845:SER:HB2	7:J:8:PHE:HB3	1.75	0.67
2:B:530:GLY:O	2:B:531:GLN:HG2	1.94	0.67
4:E:190:LEU:HD23	4:E:214:CYS:HB2	1.76	0.67
6:H:48:PRO:O	6:H:146:ARG:NH2	2.28	0.67
2:B:986:GLN:OE1	2:B:1020:ARG:NH1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:GLN:HE22	2:B:1158:PHE:HD1	1.42	0.66
2:B:241:ARG:HG3	2:B:253:THR:HG22	1.78	0.66
6:H:90:ALA:HB1	6:H:96:VAL:HG21	1.77	0.66
1:A:1001:ARG:HH12	5:F:83:PRO:HD2	1.61	0.65
14:N:11:DA:H2'	14:N:12:DG:C8	2.32	0.65
2:B:1156:ASP:HB3	2:B:1198:TYR:H	1.61	0.65
13:T:6:DC:C2'	13:T:7:DT:H5'	2.26	0.65
12:R:6:G:O2'	12:R:7:A:H5'	1.96	0.65
5:F:76:LYS:HG3	5:F:79:ARG:HH21	1.61	0.64
2:B:259:TYR:O	2:B:267:ARG:HA	1.97	0.64
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.78	0.64
4:E:26:ARG:NH2	4:E:133:GLU:OE1	2.31	0.64
13:T:19:DC:H2'	13:T:20:DC:C6	2.32	0.64
1:A:326:ARG:HG2	1:A:1406:VAL:HG21	1.79	0.63
2:B:849:GLY:HA2	2:B:852:ARG:HD2	1.81	0.63
14:N:12:DG:H2'	14:N:13:DC:C6	2.34	0.63
1:A:868:TYR:HD2	1:A:1058:VAL:HG11	1.64	0.63
8:K:24:ASP:OD2	8:K:74:ARG:NH1	2.32	0.62
1:A:884:ASP:OD2	1:A:1030:ARG:NH2	2.28	0.62
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.32	0.62
13:T:6:DC:H1'	13:T:7:DT:H5'	1.82	0.61
1:A:149:GLU:O	1:A:164:ARG:NH1	2.33	0.61
1:A:1064:VAL:HG12	1:A:1370:LEU:HD22	1.81	0.61
9:L:46:VAL:HG13	9:L:56:LEU:HD12	1.81	0.61
8:K:21:ILE:HG12	8:K:33:ILE:HG23	1.82	0.61
1:A:43:GLU:N	1:A:50:ILE:HD11	2.12	0.61
1:A:43:GLU:H	1:A:50:ILE:CD1	2.13	0.60
1:A:873:MET:HB2	1:A:1366:ARG:HH21	1.66	0.60
1:A:1004:ASN:HD22	4:E:167:ARG:HD2	1.65	0.60
1:A:1127:ASP:OD2	1:A:1130:GLN:NE2	2.29	0.60
11:G:57:GLN:HE22	11:G:71:ASN:HD22	1.48	0.60
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.84	0.60
1:A:29:ALA:HB1	2:B:1184:GLY:HA2	1.84	0.59
2:B:477:ALA:CB	12:R:4:G:H4'	2.33	0.59
11:G:57:GLN:NE2	11:G:73:LYS:HE3	2.17	0.59
1:A:1403:GLU:OE1	13:T:16:DC:OP1	2.21	0.59
9:L:32:ALA:HB2	9:L:55:ILE:HD11	1.85	0.59
1:A:1342:GLU:OE2	4:E:200:ARG:NH2	2.36	0.59
2:B:211:VAL:HG21	2:B:483:LEU:HD13	1.83	0.59
3:C:54:ASN:ND2	3:C:60:ASP:OD1	2.30	0.59
3:C:143:LEU:HD21	3:C:146:LYS:HE3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:5:DG:H2'	13:T:6:DC:C6	2.38	0.58
1:A:691:LEU:O	1:A:694:THR:HG22	2.04	0.58
1:A:939:ASP:OD2	1:A:1023:ARG:NH1	2.37	0.58
1:A:998:LEU:HB3	1:A:1001:ARG:HE	1.68	0.58
2:B:67:SER:HB2	2:B:92:PHE:HD2	1.68	0.58
2:B:655:LYS:HA	2:B:658:ILE:HD12	1.84	0.58
8:K:44:ASN:OD1	8:K:47:ARG:NH1	2.35	0.58
9:L:46:VAL:HG13	9:L:56:LEU:CD1	2.34	0.58
1:A:882:SER:O	1:A:1025:ARG:NH2	2.36	0.58
1:A:398:GLU:HG2	1:A:400:PRO:HD2	1.86	0.58
1:A:131:SER:HB2	1:A:223:GLY:HA2	1.86	0.58
9:L:53:HIS:CE1	9:L:55:ILE:HG12	2.39	0.58
14:N:5:DA:H2'	14:N:6:DG:C8	2.39	0.58
2:B:1072:MET:HB2	2:B:1085:ILE:HD13	1.85	0.57
9:L:49:LYS:HG3	9:L:50:ASP:N	2.19	0.57
14:N:11:DA:H2"	14:N:12:DG:O4'	2.04	0.57
2:B:208:SER:OG	2:B:210:LYS:NZ	2.38	0.57
13:T:26:DA:H2"	13:T:27:DT:H5"	1.87	0.57
1:A:868:TYR:CD2	1:A:1058:VAL:HG11	2.40	0.57
3:C:92:CYS:SG	3:C:93:ASP:N	2.76	0.57
13:T:6:DC:H42	14:N:11:DA:H61	1.52	0.57
1:A:913:LEU:HD23	1:A:915:SER:H	1.69	0.57
2:B:38:PHE:HZ	2:B:541:LEU:HB3	1.70	0.57
1:A:885:THR:HG22	1:A:940:ARG:HB2	1.87	0.56
9:L:40:LEU:HA	9:L:44:ASP:CB	2.34	0.56
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.87	0.56
1:A:451:HIS:CD2	1:A:453:MET:HB2	2.39	0.56
4:E:61:GLN:NE2	4:E:63:ASN:OD1	2.39	0.56
1:A:361:LEU:HA	1:A:471:ASN:HD22	1.70	0.56
1:A:887:GLY:O	1:A:940:ARG:NH2	2.38	0.56
1:A:535:THR:HG23	1:A:575:LYS:HG2	1.87	0.56
2:B:778:MET:HE3	2:B:794:ASN:HB3	1.86	0.56
11:G:58:ARG:O	11:G:70:PHE:HA	2.06	0.56
1:A:1445:ILE:HG22	11:G:59:GLY:O	2.05	0.56
2:B:29:ASP:OD2	2:B:655:LYS:NZ	2.39	0.56
1:A:354:SER:O	1:A:469:ARG:HA	2.06	0.56
2:B:680:THR:O	2:B:683:SER:OG	2.21	0.56
2:B:378:LEU:O	2:B:382:ILE:HG12	2.06	0.55
13:T:8:DC:C2'	13:T:9:DC:C6	2.88	0.55
1:A:445:ASN:ND2	1:A:454:SER:O	2.37	0.55
8:K:32:VAL:HG22	8:K:74:ARG:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:7:DT:H2"	13:T:8:DC:O4'	2.06	0.55
1:A:660:ASN:OD1	2:B:1082:MET:HB2	2.07	0.55
1:A:968:GLN:HA	1:A:973:ILE:HD12	1.88	0.55
2:B:165:VAL:HG11	2:B:448:ILE:HG13	1.89	0.55
13:T:7:DT:OP2	13:T:7:DT:H2'	2.06	0.55
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.88	0.55
13:T:12:DC:H2"	13:T:13:DT:O5'	2.07	0.55
2:B:952:VAL:HB	9:L:58:LYS:HG2	1.89	0.54
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.89	0.54
2:B:301:ILE:HG21	2:B:314:LEU:HD21	1.88	0.54
2:B:1149:GLU:HG3	2:B:1153:GLU:HB2	1.89	0.54
2:B:996:ARG:HH22	3:C:175:ALA:HA	1.71	0.54
7:J:10:CYS:SG	7:J:11:GLY:N	2.81	0.54
3:C:56:THR:HG21	3:C:145:CYS:SG	2.48	0.54
2:B:60:GLN:HE22	2:B:94:LYS:HD2	1.72	0.54
9:L:61:THR:HG22	9:L:63:ARG:H	1.71	0.54
14:N:4:DG:H4'	14:N:5:DA:OP1	2.08	0.54
3:C:262:LEU:HD22	8:K:87:LEU:HD23	1.89	0.54
2:B:1004:GLU:O	7:J:43:ARG:NH1	2.40	0.54
2:B:487:THR:OG1	2:B:777:ALA:O	2.23	0.54
3:C:66:ARG:NH2	7:J:5:VAL:HG23	2.23	0.54
2:B:267:ARG:HH22	2:B:313:MET:HG2	1.72	0.54
2:B:173:MET:HB2	2:B:203:PHE:HE1	1.73	0.53
2:B:883:LEU:HG	2:B:934:LYS:O	2.07	0.53
2:B:1004:GLU:HG3	2:B:1006:ILE:HG12	1.91	0.53
1:A:41:MET:O	1:A:46:THR:HA	2.09	0.53
1:A:679:ILE:HD11	1:A:733:ALA:HB2	1.91	0.53
3:C:71:PRO:HB2	3:C:133:ILE:HD12	1.90	0.53
12:R:4:G:O2'	12:R:5:A:H5'	2.08	0.53
14:N:11:DA:H2"	14:N:12:DG:C5'	2.38	0.53
13:T:8:DC:H2"	13:T:9:DC:H6	1.70	0.52
1:A:725:ALA:HA	1:A:728:LYS:HE2	1.91	0.52
13:T:7:DT:O2	14:N:11:DA:C2	2.63	0.52
1:A:693:VAL:HG12	1:A:714:PHE:CE1	2.44	0.52
1:A:829:VAL:HG22	2:B:512:ARG:HH11	1.74	0.52
1:A:1080:THR:C	1:A:1082:ASN:H	2.12	0.52
2:B:1073:TYR:CE1	2:B:1080:LYS:HG2	2.44	0.52
1:A:956:LEU:HD21	1:A:1017:LEU:HD22	1.92	0.52
11:G:59:GLY:HA2	11:G:69:GLU:O	2.10	0.52
2:B:953:LEU:HD11	9:L:55:ILE:HB	1.92	0.52
7:J:2:ILE:HD12	7:J:57:ILE:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ILE:HB	1:A:431:LYS:HB2	1.91	0.51
1:A:714:PHE:HA	1:A:717:ASN:ND2	2.25	0.51
2:B:864:LYS:HA	2:B:961:LEU:HD13	1.90	0.51
1:A:125:ALA:O	1:A:128:ILE:HG22	2.11	0.51
1:A:232:GLU:HG3	1:A:233:TRP:CD1	2.46	0.51
1:A:667:GLY:HA2	1:A:670:ILE:HD12	1.92	0.51
1:A:1276:VAL:HB	1:A:1279:ILE:HD12	1.92	0.51
13:T:10:DT:C6	13:T:11:DT:H72	2.45	0.51
1:A:130:ASP:OD2	1:A:133:LYS:HG2	2.10	0.51
1:A:715:GLU:HG3	1:A:774:ARG:HD2	1.92	0.51
2:B:1117:GLN:HG2	2:B:1156:ASP:OD1	2.11	0.51
3:C:89:GLU:HG2	3:C:90:ASP:H	1.76	0.51
1:A:22:PHE:HE2	2:B:1208:MET:HA	1.76	0.51
1:A:451:HIS:HD2	1:A:453:MET:HB2	1.76	0.51
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.93	0.51
3:C:75:MET:O	3:C:246:ARG:NH2	2.40	0.51
14:N:11:DA:C2'	14:N:12:DG:C8	2.93	0.51
1:A:597:LEU:HD13	6:H:103:LYS:HG2	1.92	0.51
2:B:1163:CYS:SG	2:B:1187:ASN:ND2	2.70	0.50
4:E:178:ILE:HB	4:E:212:ARG:HD3	1.93	0.50
1:A:50:ILE:HG22	1:A:51:GLY:N	2.26	0.50
2:B:653:VAL:HB	2:B:689:LEU:HB3	1.92	0.50
3:C:101:LEU:HD23	3:C:155:LEU:HD12	1.92	0.50
12:R:6:G:C2'	12:R:7:A:H5'	2.41	0.50
13:T:8:DC:C2	13:T:9:DC:C2	3.00	0.50
1:A:598:LEU:O	6:H:122:LEU:HD12	2.11	0.50
2:B:104:GLU:OE2	2:B:120:ARG:NH1	2.39	0.50
2:B:824:ILE:H	2:B:1009:ASP:HB2	1.76	0.50
2:B:226:PHE:HA	2:B:395:GLN:HE21	1.76	0.50
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.93	0.50
2:B:863:GLU:HB2	2:B:872:GLU:HB2	1.94	0.50
1:A:265:LYS:O	1:A:269:ILE:HG12	2.11	0.50
1:A:342:GLY:O	2:B:1129:ARG:NH1	2.44	0.50
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.11	0.50
2:B:876:LYS:HD2	2:B:877:PRO:HD2	1.93	0.50
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.12	0.49
2:B:477:ALA:HB1	12:R:4:G:O2'	2.12	0.49
2:B:898:LEU:HD22	2:B:964:VAL:HG11	1.94	0.49
6:H:41:ASP:HB2	6:H:121:LEU:HB3	1.93	0.49
2:B:971:THR:OG1	3:C:61:GLU:OE2	2.26	0.49
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ILE:HG22	1:A:176:LYS:HE3	1.95	0.49
5:F:92:ARG:HH22	11:G:60:ARG:HH22	1.58	0.49
6:H:89:LEU:HG	6:H:90:ALA:H	1.77	0.49
1:A:43:GLU:HB2	1:A:48:ALA:H	1.77	0.49
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.93	0.49
13:T:13:DT:H3	14:N:5:DA:N6	2.07	0.49
3:C:244:VAL:HG21	8:K:105:PHE:CZ	2.47	0.49
1:A:592:ASP:N	1:A:595:THR:OG1	2.43	0.49
1:A:1420:ASP:OD1	2:B:1220:ARG:NH1	2.45	0.49
13:T:6:DC:C1'	13:T:7:DT:H5'	2.41	0.49
1:A:697:ALA:HB2	1:A:714:PHE:CE1	2.48	0.49
2:B:120:ARG:HB2	2:B:122:LEU:HG	1.94	0.49
3:C:18:VAL:HG12	3:C:20:PHE:HD1	1.78	0.49
10:D:64:VAL:HG23	10:D:65:GLU:HG2	1.94	0.49
11:G:57:GLN:HE22	11:G:71:ASN:ND2	2.10	0.49
2:B:884:ARG:HB2	2:B:936:ASP:HB3	1.95	0.48
1:A:738:LYS:HB3	1:A:740:LEU:HD23	1.95	0.48
1:A:1397:LEU:HB2	1:A:1426:GLU:HG2	1.95	0.48
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.94	0.48
4:E:127:ILE:HD12	4:E:130:ALA:HB3	1.95	0.48
1:A:688:LYS:O	1:A:691:LEU:HB3	2.12	0.48
2:B:466:TRP:HB2	2:B:479:VAL:HG21	1.95	0.48
13:T:13:DT:H2"	13:T:14:DC:OP2	2.13	0.48
1:A:778:GLY:HA3	2:B:516:ASN:HB2	1.96	0.48
2:B:25:ILE:HD11	2:B:653:VAL:HG13	1.96	0.48
2:B:855:PHE:HZ	2:B:857:ARG:HH11	1.62	0.48
2:B:1187:ASN:HD21	2:B:1190:ASP:HB2	1.78	0.48
11:G:50:ASP:HB3	11:G:53:ASN:HB2	1.95	0.48
1:A:779:PHE:HD2	2:B:699:GLU:HG2	1.78	0.48
2:B:203:PHE:CD2	2:B:461:LEU:HD21	2.49	0.48
11:G:56:ILE:HA	11:G:72:VAL:HG13	1.95	0.48
1:A:399:HIS:NE2	1:A:462:VAL:HG21	2.28	0.48
1:A:1111:MET:HE1	1:A:1330:ASN:O	2.13	0.48
2:B:796:LEU:HD12	2:B:852:ARG:O	2.14	0.48
4:E:59:SER:HA	4:E:80:VAL:O	2.13	0.48
11:G:3:PHE:N	11:G:78:VAL:O	2.47	0.48
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.96	0.48
2:B:862:GLN:O	2:B:914:LYS:NZ	2.34	0.48
3:C:46:ILE:HD13	3:C:159:ALA:HB2	1.96	0.48
3:C:67:LEU:HD11	3:C:155:LEU:HD13	1.95	0.48
3:C:241:ASP:N	3:C:241:ASP:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:40:LEU:HD23	9:L:44:ASP:CG	2.34	0.48
14:N:4:DG:H2"	14:N:5:DA:O5'	2.13	0.48
1:A:871:ASP:OD2	1:A:1366:ARG:NH2	2.47	0.48
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.96	0.48
8:K:5:ASP:HB2	8:K:8:GLU:HG3	1.95	0.48
9:L:48:CYS:SG	9:L:49:LYS:N	2.86	0.48
13:T:8:DC:C4'	13:T:9:DC:OP1	2.56	0.48
13:T:25:DG:H2'	13:T:26:DA:C8	2.48	0.48
1:A:847:ASP:HB2	1:A:859:SER:HB3	1.96	0.47
2:B:942:ARG:HB2	2:B:945:GLU:HB2	1.96	0.47
13:T:18:DT:H2'	13:T:19:DC:C6	2.49	0.47
1:A:407:ARG:HH21	1:A:411:ASP:HB3	1.79	0.47
1:A:590:ARG:HG2	1:A:604:GLY:HA2	1.96	0.47
1:A:1438:THR:HG23	5:F:92:ARG:HB2	1.95	0.47
1:A:70:CYS:SG	1:A:80:HIS:CE1	3.06	0.47
1:A:254:GLU:OE1	1:A:255:SER:OG	2.28	0.47
1:A:827:THR:HG23	1:A:1081:LEU:HD12	1.95	0.47
1:A:944:ARG:NH2	1:A:1296:GLY:O	2.47	0.47
2:B:256:VAL:HG12	2:B:385:LEU:HD13	1.95	0.47
2:B:477:ALA:HB1	12:R:4:G:H4'	1.96	0.47
11:G:62:LEU:HG	11:G:67:SER:O	2.15	0.47
1:A:1001:ARG:NH1	5:F:82:THR:HA	2.28	0.47
1:A:1410:PHE:CD1	2:B:1212:ILE:HD11	2.49	0.47
1:A:1438:THR:H	5:F:88:TYR:HB3	1.79	0.47
8:K:56:VAL:HG22	8:K:77:THR:HG22	1.95	0.47
1:A:694:THR:HA	1:A:714:PHE:CE1	2.50	0.47
4:E:64:PRO:HB3	4:E:75:MET:HG2	1.96	0.47
11:G:45:ILE:HA	11:G:78:VAL:HG12	1.96	0.47
13:T:16:DC:N4	14:N:2:DG:H1	2.12	0.47
1:A:22:PHE:HZ	2:B:1208:MET:HG2	1.79	0.47
1:A:597:LEU:CD1	6:H:103:LYS:HG2	2.45	0.47
1:A:982:THR:HG22	1:A:984:LYS:H	1.80	0.47
2:B:25:ILE:HD13	2:B:658:ILE:HD11	1.97	0.47
2:B:54:PHE:HA	2:B:58:THR:HB	1.97	0.47
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.50	0.47
2:B:839:MET:HG2	2:B:1012:ILE:HG22	1.97	0.47
2:B:996:ARG:NH2	3:C:175:ALA:HA	2.30	0.47
1:A:962:ARG:O	1:A:966:ASN:ND2	2.48	0.47
1:A:1012:ARG:O	1:A:1016:THR:OG1	2.32	0.47
13:T:12:DC:H2'	13:T:13:DT:H71	1.96	0.47
1:A:869:GLY:HA3	1:A:1366:ARG:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:962:ARG:HG2	1:A:966:ASN:HD21	1.80	0.46
2:B:780:VAL:HG21	7:J:56:LEU:HD13	1.97	0.46
6:H:80:ARG:HG2	8:K:57:LEU:HD22	1.97	0.46
1:A:332:LYS:HD2	13:T:19:DC:OP1	2.15	0.46
13:T:12:DC:H2'	13:T:13:DT:C7	2.45	0.46
1:A:385:ILE:HD11	1:A:428:TYR:HE1	1.80	0.46
2:B:205:ILE:HG21	2:B:462:ALA:HB2	1.97	0.46
8:K:51:LEU:HD12	8:K:59:ALA:HB3	1.96	0.46
5:F:97:ARG:NE	5:F:124:GLU:OE1	2.47	0.46
13:T:26:DA:C2'	13:T:27:DT:H5"	2.46	0.46
1:A:679:ILE:HG13	1:A:732:LEU:HD22	1.97	0.46
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.96	0.46
2:B:600:LEU:HB3	2:B:615:MET:SD	2.56	0.46
1:A:152:VAL:HB	1:A:164:ARG:CD	2.39	0.46
1:A:1386:ARG:CZ	13:T:15:DC:H1'	2.46	0.46
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.97	0.46
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.98	0.46
1:A:393:ARG:O	1:A:420:ARG:NH1	2.44	0.46
2:B:855:PHE:HZ	2:B:857:ARG:NH1	2.13	0.46
1:A:523:ILE:HG23	1:A:527:THR:HB	1.99	0.45
1:A:981:LEU:HD11	1:A:1042:PHE:HB2	1.98	0.45
1:A:1279:ILE:HG23	1:A:1308:THR:HB	1.99	0.45
11:G:62:LEU:HB2	11:G:65:ASP:O	2.16	0.45
3:C:167:HIS:CD2	9:L:70:ARG:HB2	2.52	0.45
1:A:666:ILE:HD11	2:B:1067:ARG:HA	1.99	0.45
1:A:712:GLU:HB3	1:A:713:SER:H	1.60	0.45
2:B:364:ILE:HG22	2:B:365:THR:HG22	1.98	0.45
1:A:770:VAL:HG22	1:A:771:GLU:HG3	1.97	0.45
1:A:840:ARG:HB3	1:A:1384:VAL:HG12	1.99	0.45
1:A:1109:LYS:NZ	14:N:5:DA:H5'	2.31	0.45
1:A:1109:LYS:HZ2	14:N:5:DA:H5'	1.82	0.45
1:A:1282:VAL:HG13	1:A:1308:THR:HG22	1.97	0.45
2:B:681:TRP:CH2	2:B:690:VAL:HG11	2.51	0.45
1:A:802:ASN:ND2	2:B:728:ARG:HB2	2.32	0.45
1:A:1438:THR:N	5:F:88:TYR:HB3	2.32	0.45
2:B:311:LEU:O	2:B:315:LYS:HG3	2.16	0.45
2:B:347:LYS:O	2:B:351:TYR:N	2.40	0.45
2:B:620:ARG:HG3	2:B:621:GLU:OE1	2.16	0.45
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.81	0.45
1:A:388:LEU:HD12	1:A:432:VAL:HB	1.99	0.45
1:A:534:LEU:O	1:A:574:GLY:HA3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:THR:HG21	1:A:857:ARG:HE	1.82	0.45
2:B:559:SER:HA	2:B:563:MET:HG2	1.98	0.45
4:E:58:MET:HB3	4:E:82:PHE:CD1	2.52	0.45
3:C:250:THR:O	3:C:254:LYS:HG3	2.16	0.45
6:H:89:LEU:HG	6:H:90:ALA:N	2.31	0.45
1:A:12:ARG:HD2	2:B:1218:THR:HG21	1.99	0.45
2:B:766:ARG:HA	2:B:766:ARG:HD3	1.86	0.45
2:B:604:ARG:NH1	2:B:613:VAL:O	2.39	0.44
2:B:1122:ARG:HB2	13:T:22:DC:OP1	2.17	0.44
8:K:58:PHE:HB3	8:K:76:GLN:HB3	1.98	0.44
6:H:101:ALA:HB2	6:H:116:TYR:CE2	2.53	0.44
14:N:11:DA:H2'	14:N:12:DG:H8	1.80	0.44
1:A:42:ASP:O	1:A:43:GLU:C	2.55	0.44
1:A:89:PRO:O	1:A:204:THR:HG21	2.17	0.44
1:A:1410:PHE:HD1	2:B:1212:ILE:HD11	1.82	0.44
2:B:756:ILE:HG12	2:B:770:GLN:HG2	2.00	0.44
6:H:63:LEU:HA	6:H:89:LEU:HB3	1.99	0.44
7:J:2:ILE:O	7:J:3:VAL:HG23	2.17	0.44
1:A:151:ASP:HA	1:A:163:SER:N	2.32	0.44
1:A:152:VAL:H	1:A:164:ARG:HG2	1.83	0.44
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.99	0.44
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.18	0.44
2:B:301:ILE:HD13	2:B:382:ILE:HG21	2.00	0.44
2:B:523:CYS:SG	2:B:750:GLY:N	2.90	0.44
1:A:881:GLN:HE22	1:A:958:VAL:C	2.21	0.44
2:B:639:ILE:HD12	2:B:688:GLY:O	2.17	0.44
7:J:3:VAL:CG1	7:J:15:GLY:HA2	2.47	0.44
13:T:7:DT:C3'	13:T:8:DC:H5"	2.47	0.44
1:A:302:THR:HG21	1:A:314:ALA:HB3	2.00	0.44
1:A:527:THR:HG23	1:A:653:VAL:HB	2.00	0.44
1:A:666:ILE:HG13	1:A:667:GLY:N	2.33	0.44
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.98	0.44
2:B:246:LYS:HA	2:B:246:LYS:HD2	1.85	0.44
1:A:43:GLU:HG2	1:A:47:ARG:CB	2.48	0.44
2:B:829:CYS:SG	2:B:1014:PRO:HD2	2.58	0.44
3:C:37:MET:HE3	3:C:176:ILE:HD13	2.00	0.44
3:C:176:ILE:HG23	3:C:232:VAL:HG22	1.99	0.44
6:H:38:LEU:HD13	6:H:125:LEU:HD13	1.99	0.44
1:A:855:THR:HG23	1:A:857:ARG:HG3	2.00	0.43
2:B:554:ILE:O	2:B:557:PHE:HB2	2.18	0.43
3:C:37:MET:SD	3:C:244:VAL:HG12	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:60:ALA:HB2	6:H:143:LEU:CD1	2.39	0.43
13:T:7:DT:H1'	13:T:8:DC:O4'	2.18	0.43
1:A:443:LEU:HD22	2:B:1146:PHE:CE2	2.53	0.43
1:A:482:PHE:CD2	2:B:836:GLU:HB3	2.53	0.43
1:A:740:LEU:HD23	1:A:740:LEU:H	1.84	0.43
1:A:765:VAL:HG11	1:A:816:HIS:HD2	1.84	0.43
2:B:1076:HIS:O	3:C:31:ASN:ND2	2.51	0.43
1:A:524:VAL:HG12	1:A:525:GLN:N	2.33	0.43
1:A:602:ASP:HB3	1:A:616:VAL:HG23	2.01	0.43
1:A:406:ILE:N	1:A:431:LYS:O	2.49	0.43
1:A:598:LEU:O	1:A:599:SER:C	2.56	0.43
1:A:712:GLU:C	1:A:714:PHE:N	2.72	0.43
2:B:1181:GLU:HG2	2:B:1188:LYS:HG2	2.00	0.43
1:A:335:ARG:HE	2:B:1202:LEU:HD22	1.82	0.43
2:B:1073:TYR:HE2	3:C:179:GLU:HA	1.83	0.43
3:C:31:ASN:OD1	3:C:34:ARG:NH1	2.47	0.43
4:E:93:MET:HG3	4:E:120:ALA:HB1	2.00	0.43
6:H:11:GLN:NE2	6:H:52:GLN:OE1	2.52	0.43
1:A:216:VAL:HA	1:A:219:PHE:CE2	2.53	0.43
1:A:894:GLU:OE2	1:A:906:HIS:NE2	2.52	0.43
2:B:642:ASP:OD1	2:B:642:ASP:N	2.52	0.43
4:E:128:PRO:N	4:E:129:PRO:HD2	2.33	0.43
1:A:514:PRO:HG2	1:A:1067:LEU:HD11	2.01	0.43
1:A:926:GLN:HE21	1:A:930:ASP:HB3	1.84	0.43
2:B:315:LYS:O	2:B:319:GLU:HG2	2.18	0.43
9:L:40:LEU:HD22	9:L:45:ALA:O	2.19	0.43
1:A:366:VAL:O	1:A:463:ILE:HG12	2.19	0.43
1:A:1106:ASN:HA	1:A:1383:SER:HB2	2.01	0.43
2:B:29:ASP:HB3	2:B:658:ILE:HD13	2.01	0.43
2:B:883:LEU:N	2:B:934:LYS:O	2.48	0.43
5:F:92:ARG:NH2	11:G:60:ARG:HH22	2.17	0.43
1:A:90:VAL:O	1:A:236:LEU:N	2.49	0.42
1:A:663:SER:HB3	2:B:1085:ILE:HA	2.00	0.42
1:A:959:ASN:O	1:A:963:ILE:HG13	2.18	0.42
2:B:25:ILE:HG22	2:B:26:THR:O	2.19	0.42
2:B:351:TYR:O	2:B:355:ILE:HG12	2.19	0.42
14:N:3:DG:C6	14:N:4:DG:C6	3.06	0.42
1:A:64:ASN:OD1	1:A:65:LEU:N	2.53	0.42
1:A:330:LYS:HE2	1:A:330:LYS:HB3	1.81	0.42
1:A:386:ASP:OD1	1:A:386:ASP:N	2.50	0.42
1:A:602:ASP:OD2	6:H:20:TYR:OH	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1116:LEU:HB3	1:A:1308:THR:OG1	2.19	0.42
3:C:38:ILE:HG13	3:C:176:ILE:HD12	2.01	0.42
9:L:33:GLU:N	9:L:33:GLU:OE1	2.51	0.42
1:A:915:SER:O	1:A:919:ILE:HG12	2.18	0.42
3:C:74:SER:HA	3:C:129:ILE:HG13	1.99	0.42
4:E:127:ILE:HD11	4:E:132:ILE:HD11	2.01	0.42
1:A:35:ILE:HD12	1:A:52:GLY:O	2.19	0.42
5:F:133:VAL:HG11	11:G:58:ARG:HH12	1.85	0.42
1:A:64:ASN:OD1	1:A:65:LEU:HG	2.20	0.42
1:A:583:PRO:HD3	1:A:645:LEU:HD13	2.02	0.42
2:B:25:ILE:CD1	2:B:653:VAL:HG13	2.50	0.42
13:T:10:DT:H2'	13:T:11:DT:H72	2.02	0.42
1:A:362:ASP:HB3	1:A:508:PRO:HD3	2.02	0.42
1:A:1107:VAL:HG13	1:A:1332:PHE:CE2	2.54	0.42
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.55	0.42
2:B:424:LEU:O	2:B:428:ILE:HG12	2.19	0.42
3:C:148:ARG:NH1	7:J:64:ASN:HA	2.34	0.42
1:A:58:LEU:HB3	1:A:244:PRO:HD3	2.02	0.42
1:A:840:ARG:NH2	1:A:1106:ASN:OD1	2.53	0.42
2:B:640:VAL:HG22	2:B:651:LEU:HD23	2.02	0.42
2:B:660:LYS:HE2	2:B:660:LYS:HB3	1.92	0.42
1:A:219:PHE:HD1	1:A:224:PHE:HB2	1.85	0.42
1:A:590:ARG:HB3	1:A:605:MET:HB3	2.01	0.42
1:A:851:HIS:CD2	1:A:857:ARG:HB2	2.55	0.42
2:B:292:ILE:HB	2:B:293:PRO:HD3	2.02	0.42
6:H:10:PHE:HB3	6:H:28:ALA:HB1	2.01	0.42
1:A:284:ALA:O	1:A:285:PRO:C	2.58	0.42
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	2.01	0.42
3:C:66:ARG:NH2	7:J:3:VAL:O	2.44	0.42
3:C:112:ASN:ND2	7:J:19:GLU:OE2	2.53	0.42
4:E:43:LYS:O	4:E:47:CYS:HB3	2.20	0.42
13:T:15:DC:C2'	13:T:16:DC:O5'	2.67	0.42
2:B:22:SER:O	2:B:22:SER:OG	2.36	0.41
2:B:258:LEU:HD13	2:B:269:ILE:HG12	2.01	0.41
2:B:693:ILE:HG23	2:B:697:GLU:HB3	2.01	0.41
2:B:803:LEU:HG	7:J:52:THR:HG21	2.02	0.41
13:T:23:DT:H2"	13:T:24:DC:C5'	2.50	0.41
1:A:10:PRO:HG2	2:B:1192:TYR:HD1	1.85	0.41
1:A:836:TYR:OH	1:A:1403:GLU:OE2	2.34	0.41
1:A:837:ILE:HD12	1:A:1105:LEU:HD22	2.02	0.41
5:F:77:ASP:N	5:F:77:ASP:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:VAL:HB	1:A:1432:GLN:HE22	1.84	0.41
1:A:821:ARG:HE	2:B:514:LEU:HB2	1.85	0.41
1:A:875:ALA:HB1	1:A:1364:ASN:HD22	1.84	0.41
2:B:230:ALA:O	2:B:261:ARG:NH2	2.54	0.41
2:B:234:ILE:HD13	2:B:257:LYS:HD2	2.03	0.41
1:A:91:PHE:HZ	1:A:207:ILE:HD12	1.85	0.41
1:A:447:GLN:OE1	1:A:488:ASN:ND2	2.54	0.41
1:A:1004:ASN:OD1	1:A:1007:ILE:HB	2.20	0.41
2:B:1152:MET:O	2:B:1157:ALA:HB2	2.21	0.41
9:L:32:ALA:CB	9:L:55:ILE:HD11	2.50	0.41
1:A:717:ASN:OD1	1:A:718:VAL:N	2.53	0.41
1:A:1442:ASP:HA	11:G:60:ARG:HH21	1.86	0.41
2:B:94:LYS:HE2	2:B:94:LYS:HB3	1.93	0.41
2:B:237:VAL:HG22	2:B:257:LYS:HG2	2.01	0.41
2:B:487:THR:O	2:B:490:SER:OG	2.28	0.41
14:N:4:DG:H1’	14:N:5:DA:O4’	2.20	0.41
2:B:380:TYR:O	2:B:384:ARG:HG2	2.20	0.41
1:A:380:VAL:HG22	1:A:430:TRP:O	2.20	0.41
1:A:519:PRO:HD3	1:A:631:HIS:ND1	2.35	0.41
1:A:582:ILE:HD12	1:A:629:LEU:HD21	2.03	0.41
1:A:637:LYS:HD3	1:A:641:VAL:HG11	2.02	0.41
1:A:829:VAL:HG22	2:B:512:ARG:NH1	2.36	0.41
1:A:1059:HIS:HB3	5:F:86:THR:HB	2.02	0.41
1:A:1276:VAL:HG12	1:A:1312:ASN:HD22	1.85	0.41
4:E:180:ARG:HE	4:E:192:ARG:HH21	1.68	0.41
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.36	0.41
2:B:384:ARG:HA	2:B:384:ARG:HD2	1.92	0.41
3:C:37:MET:HE3	3:C:37:MET:HB2	1.95	0.41
6:H:111:LEU:HA	6:H:127:GLY:O	2.20	0.41
1:A:385:ILE:HD11	1:A:428:TYR:CE1	2.55	0.41
1:A:449:SER:HB3	2:B:1137:CYS:SG	2.60	0.41
1:A:592:ASP:H	1:A:595:THR:HG1	1.68	0.41
1:A:1111:MET:HB3	1:A:1114:PRO:HG3	2.02	0.41
1:A:1138:ILE:HA	1:A:1276:VAL:HG23	2.03	0.41
2:B:41:LYS:O	2:B:45:SER:HB3	2.21	0.41
2:B:840:ILE:HB	2:B:1011:ILE:HB	2.03	0.41
2:B:882:THR:HG21	2:B:885:MET:SD	2.61	0.41
5:F:136:ARG:HD2	5:F:146:TRP:CD1	2.56	0.41
13:T:20:DC:H2”	13:T:21:DT:H5’	2.02	0.41
13:T:23:DT:H2’	13:T:24:DC:C6	2.56	0.41
1:A:328:ARG:HH21	1:A:335:ARG:HH21	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1436:ILE:HG22	1:A:1437:GLY:N	2.36	0.41
2:B:783:THR:HG22	7:J:63:TYR:HE2	1.85	0.41
3:C:10:ILE:HD13	3:C:20:PHE:HB3	2.03	0.41
1:A:1127:ASP:OD1	1:A:1127:ASP:N	2.55	0.40
3:C:62:PHE:CE2	3:C:66:ARG:HD2	2.56	0.40
13:T:7:DT:H2"	13:T:8:DC:C4'	2.50	0.40
13:T:14:DC:H2'	13:T:15:DC:C2	2.57	0.40
1:A:50:ILE:HG22	1:A:51:GLY:H	1.85	0.40
1:A:711:ARG:O	1:A:712:GLU:C	2.59	0.40
2:B:751:VAL:HG22	2:B:812:LEU:HD11	2.03	0.40
2:B:254:LEU:HD22	2:B:361:LEU:HD11	2.04	0.40
2:B:313:MET:HB2	2:B:313:MET:HE3	1.89	0.40
2:B:470:LYS:HE2	2:B:470:LYS:HB2	1.84	0.40
3:C:56:THR:HG22	3:C:57:VAL:N	2.37	0.40
1:A:524:VAL:HG12	1:A:525:GLN:HG2	2.03	0.40
2:B:324:ILE:O	2:B:325:GLN:NE2	2.54	0.40
4:E:166:LYS:HE2	4:E:166:LYS:HB3	1.78	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	1276/1733 (74%)	1227 (96%)	48 (4%)	1 (0%)	48	79
2	B	1082/1224 (88%)	1033 (96%)	49 (4%)	0	100	100
3	C	264/318 (83%)	249 (94%)	15 (6%)	0	100	100
4	E	206/215 (96%)	199 (97%)	7 (3%)	0	100	100
5	F	81/155 (52%)	79 (98%)	2 (2%)	0	100	100
6	H	130/146 (89%)	117 (90%)	13 (10%)	0	100	100
7	J	63/70 (90%)	58 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	K	112/120 (93%)	112 (100%)	0	0	100	100
9	L	41/70 (59%)	32 (78%)	9 (22%)	0	100	100
10	D	10/221 (4%)	10 (100%)	0	0	100	100
11	G	77/171 (45%)	74 (96%)	3 (4%)	0	100	100
All	All	3342/4443 (75%)	3190 (96%)	151 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	464	PRO

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	A	1111/1520 (73%)	1107 (100%)	4 (0%)	89	95
2	B	952/1061 (90%)	951 (100%)	1 (0%)	92	97
3	C	233/274 (85%)	233 (100%)	0	100	100
4	E	193/197 (98%)	193 (100%)	0	100	100
5	F	73/137 (53%)	73 (100%)	0	100	100
6	H	118/128 (92%)	118 (100%)	0	100	100
7	J	60/65 (92%)	60 (100%)	0	100	100
8	K	98/102 (96%)	98 (100%)	0	100	100
9	L	38/57 (67%)	37 (97%)	1 (3%)	41	70
10	D	10/200 (5%)	10 (100%)	0	100	100
11	G	71/152 (47%)	71 (100%)	0	100	100
All	All	2957/3893 (76%)	2951 (100%)	6 (0%)	91	97

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	390	GLN
1	A	393	ARG
1	A	712	GLU
1	A	1345	ARG
2	B	241	ARG
9	L	34	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	281	HIS
1	A	451	HIS
1	A	479	ASN
1	A	525	GLN
1	A	760	GLN
1	A	881	GLN
2	B	325	GLN
2	B	763	GLN
2	B	881	ASN
11	G	57	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	R	7/9 (77%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	ATP	T	101	-	26,33,33	0.92	1 (3%)	31,52,52	1.57	5 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	ATP	T	101	-	-	3/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	T	101	ATP	C5-C4	2.44	1.47	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	101	ATP	PA-O3A-PB	-3.68	120.20	132.83
17	T	101	ATP	C3'-C2'-C1'	3.42	106.12	100.98
17	T	101	ATP	PB-O3B-PG	-3.28	121.57	132.83
17	T	101	ATP	N3-C2-N1	-3.16	123.75	128.68
17	T	101	ATP	C4-C5-N7	-2.69	106.59	109.40

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	T	101	ATP	PB-O3A-PA-O5'
17	T	101	ATP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
17	T	101	ATP	O4'-C4'-C5'-O5'

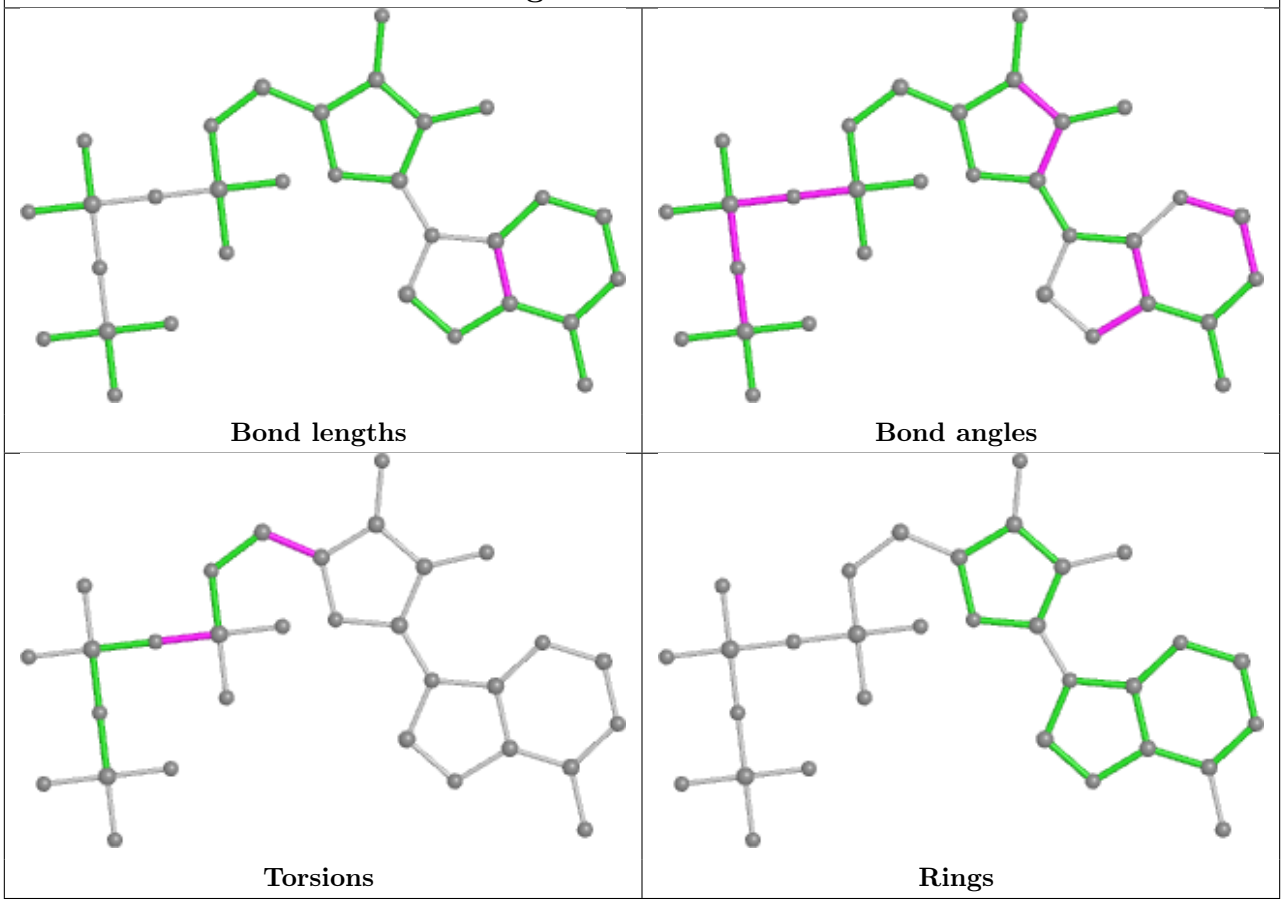
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	T	101	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP T 101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

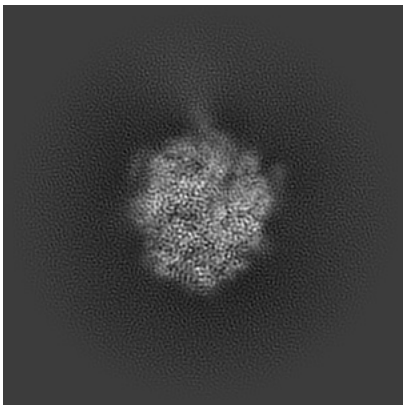
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-61287. These allow visual inspection of the internal detail of the map and identification of artifacts.

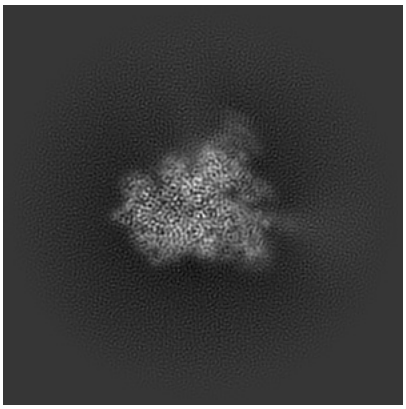
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

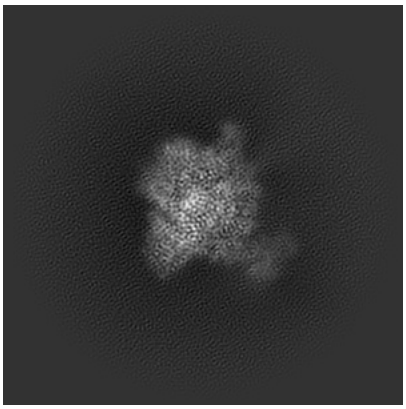
6.1.1 Primary map



X

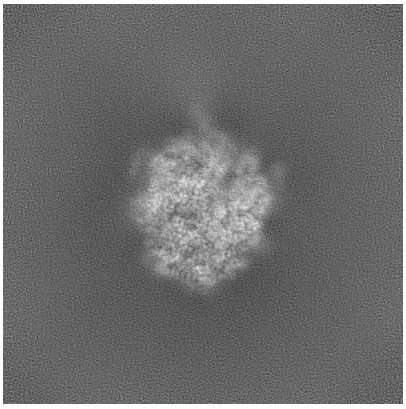


Y

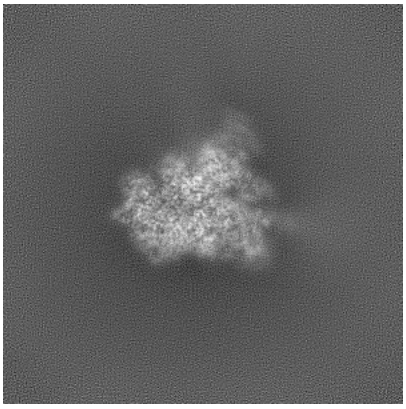


Z

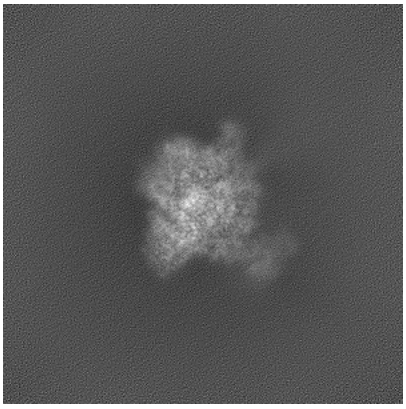
6.1.2 Raw map



X



Y

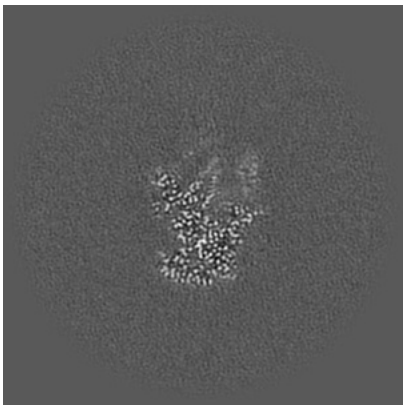


Z

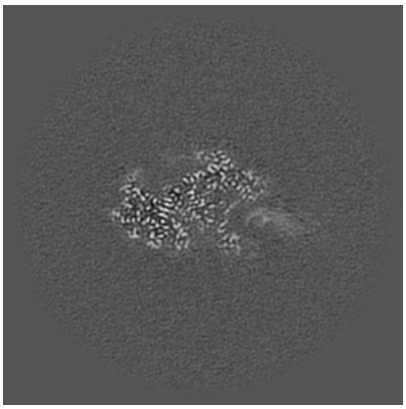
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

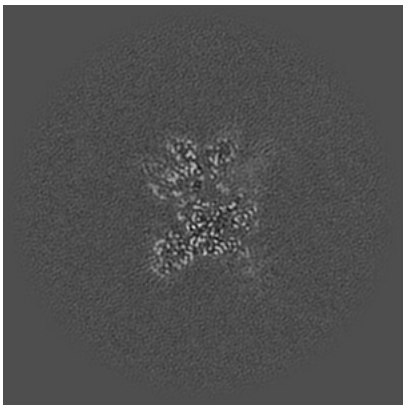
6.2.1 Primary map



X Index: 210

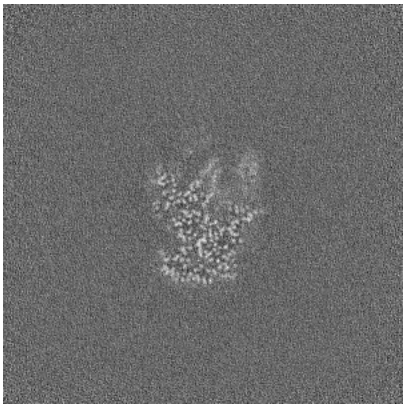


Y Index: 210

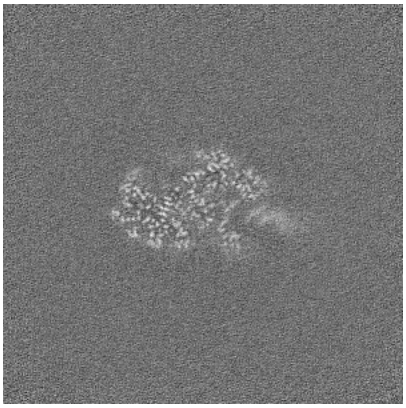


Z Index: 210

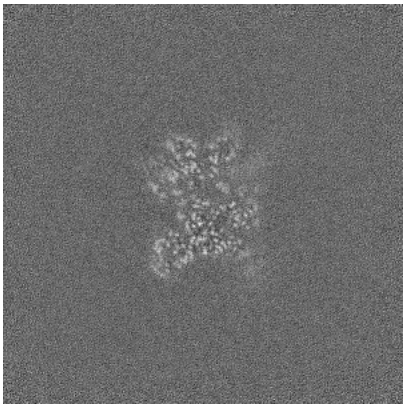
6.2.2 Raw map



X Index: 210



Y Index: 210

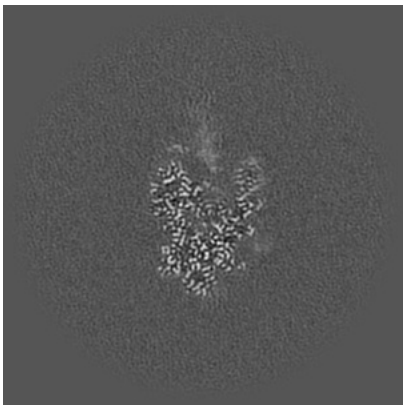


Z Index: 210

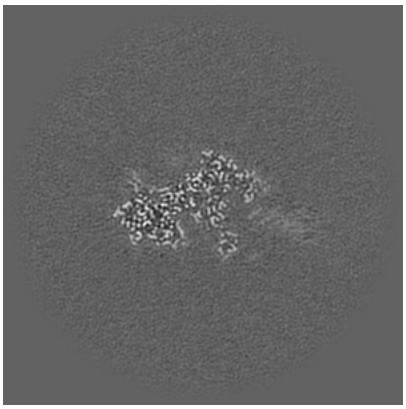
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

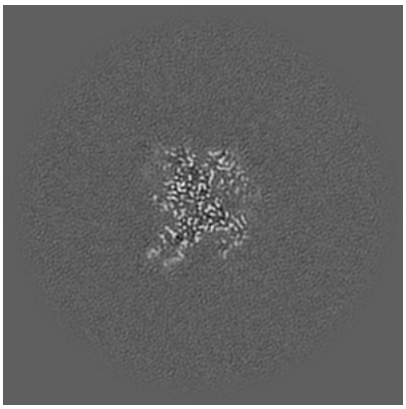
6.3.1 Primary map



X Index: 200

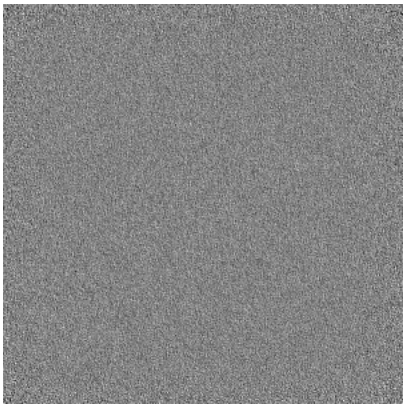


Y Index: 205

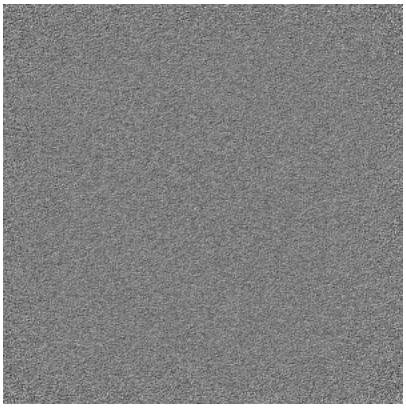


Z Index: 182

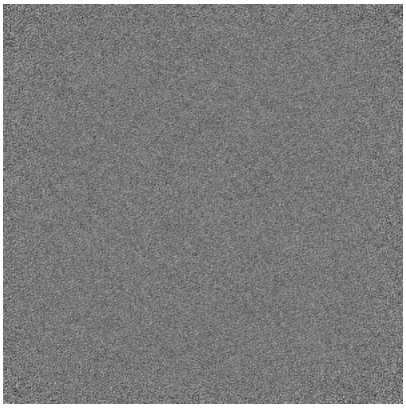
6.3.2 Raw map



X Index: 0



Y Index: 0

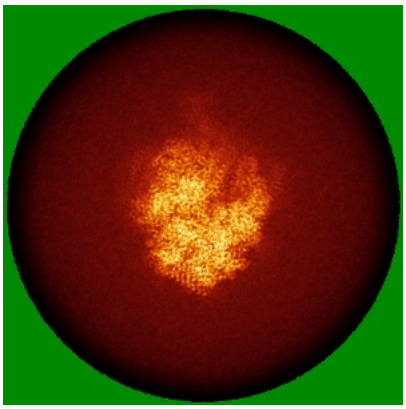


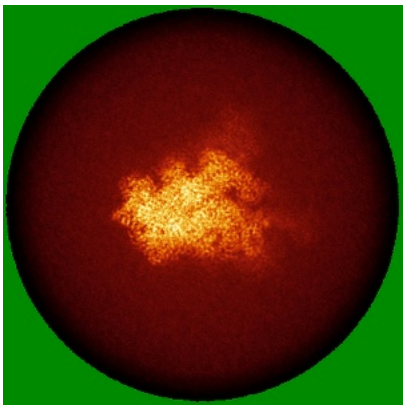
Z Index: 419

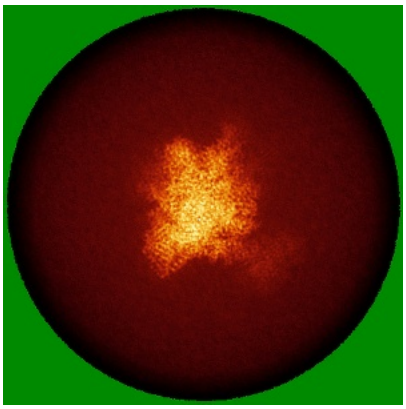
The images above show the largest variance slices of the map in three orthogonal directions.

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

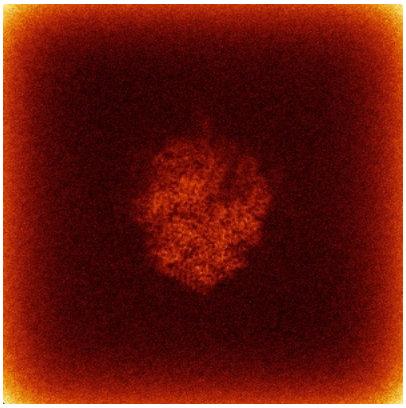
6.4.1 Primary map

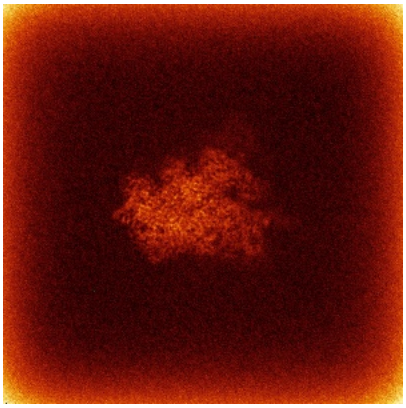

X

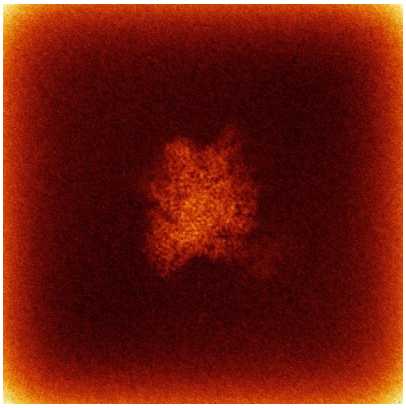

Y


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 0.2. 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.

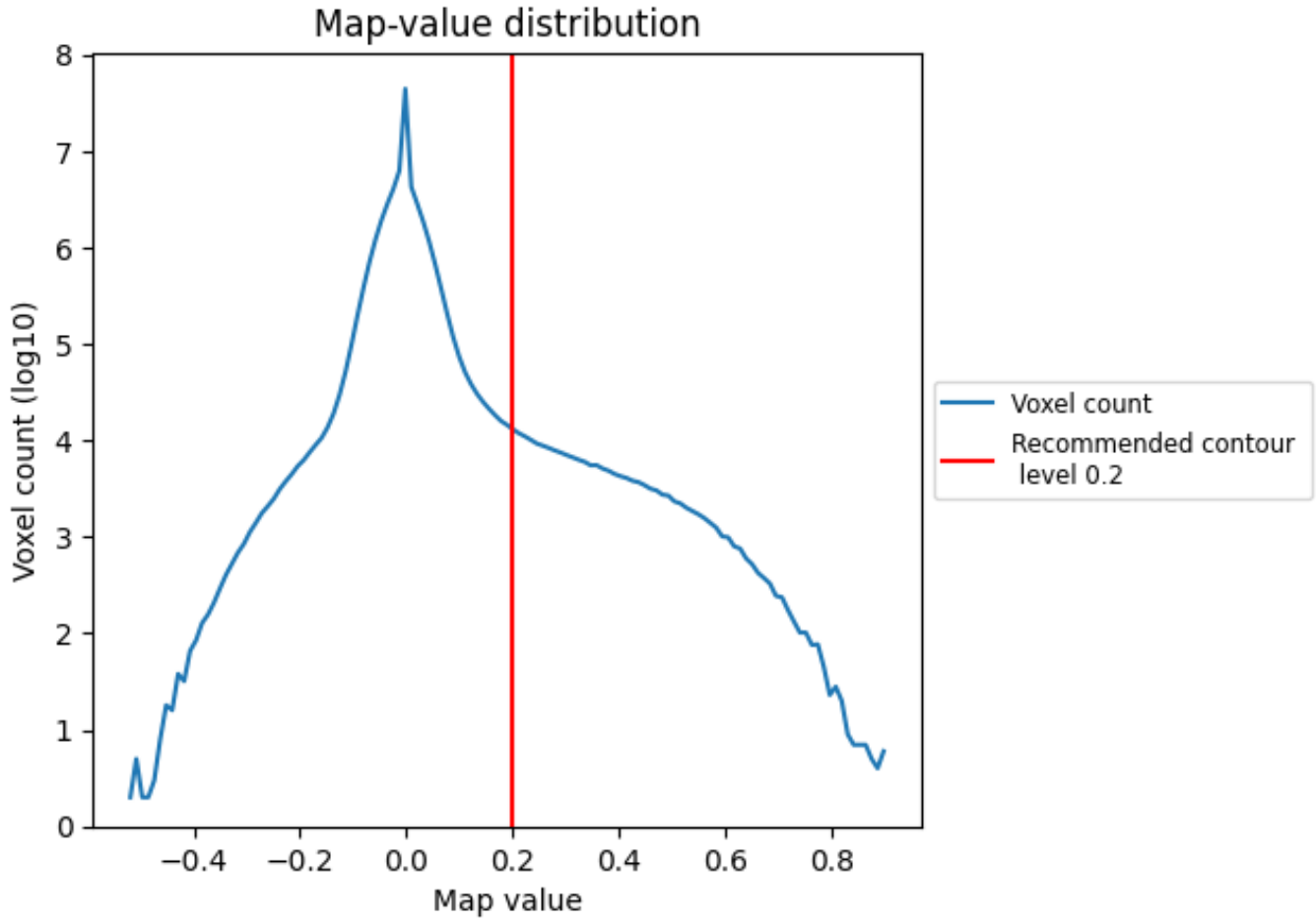
6.6 Mask visualisation (i)

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

7 Map analysis

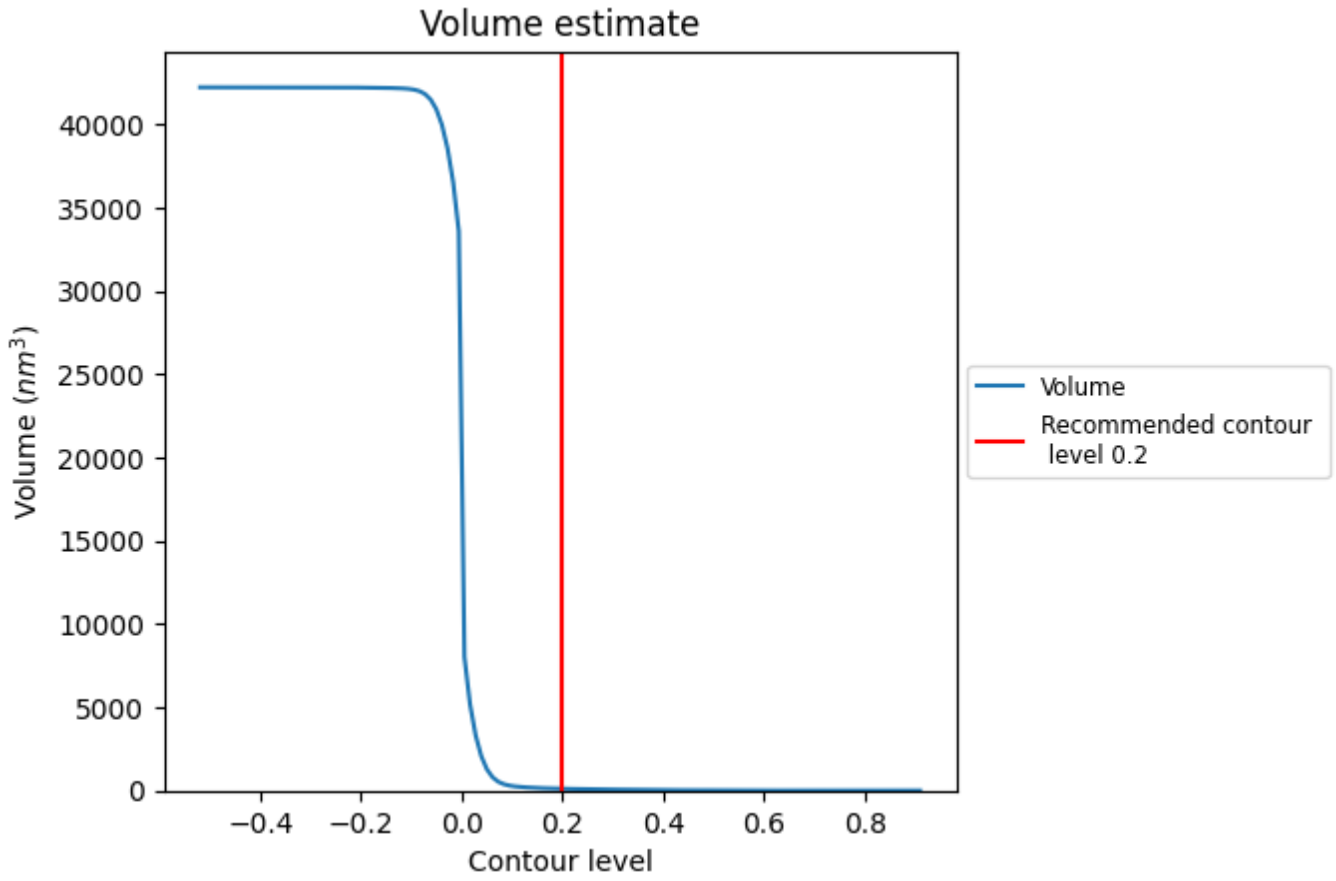
This section contains the results of statistical analysis of the map.

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.

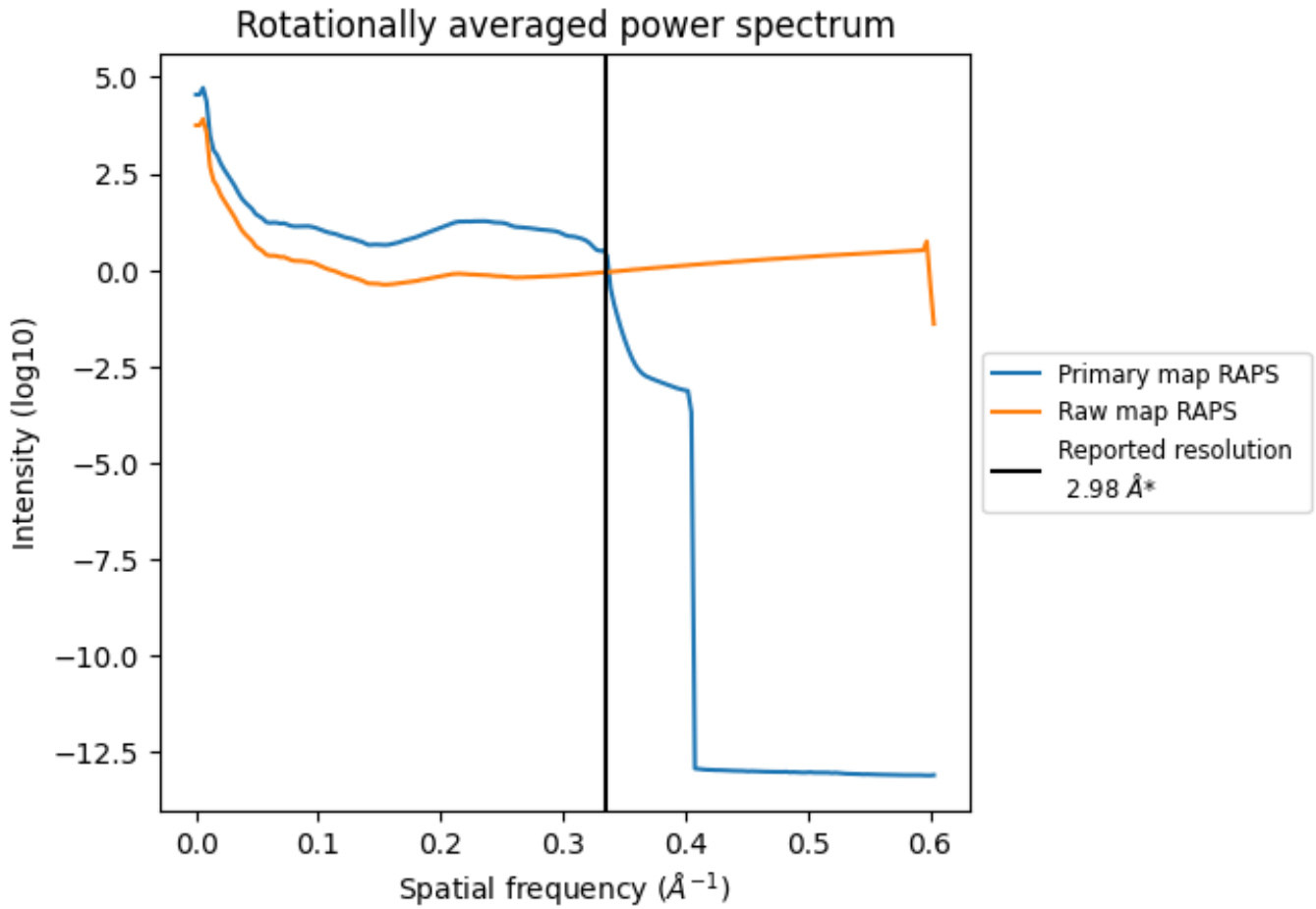
7.2 Volume estimate



The volume at the recommended contour level is 110 nm^3; this corresponds to an approximate mass of 100 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)

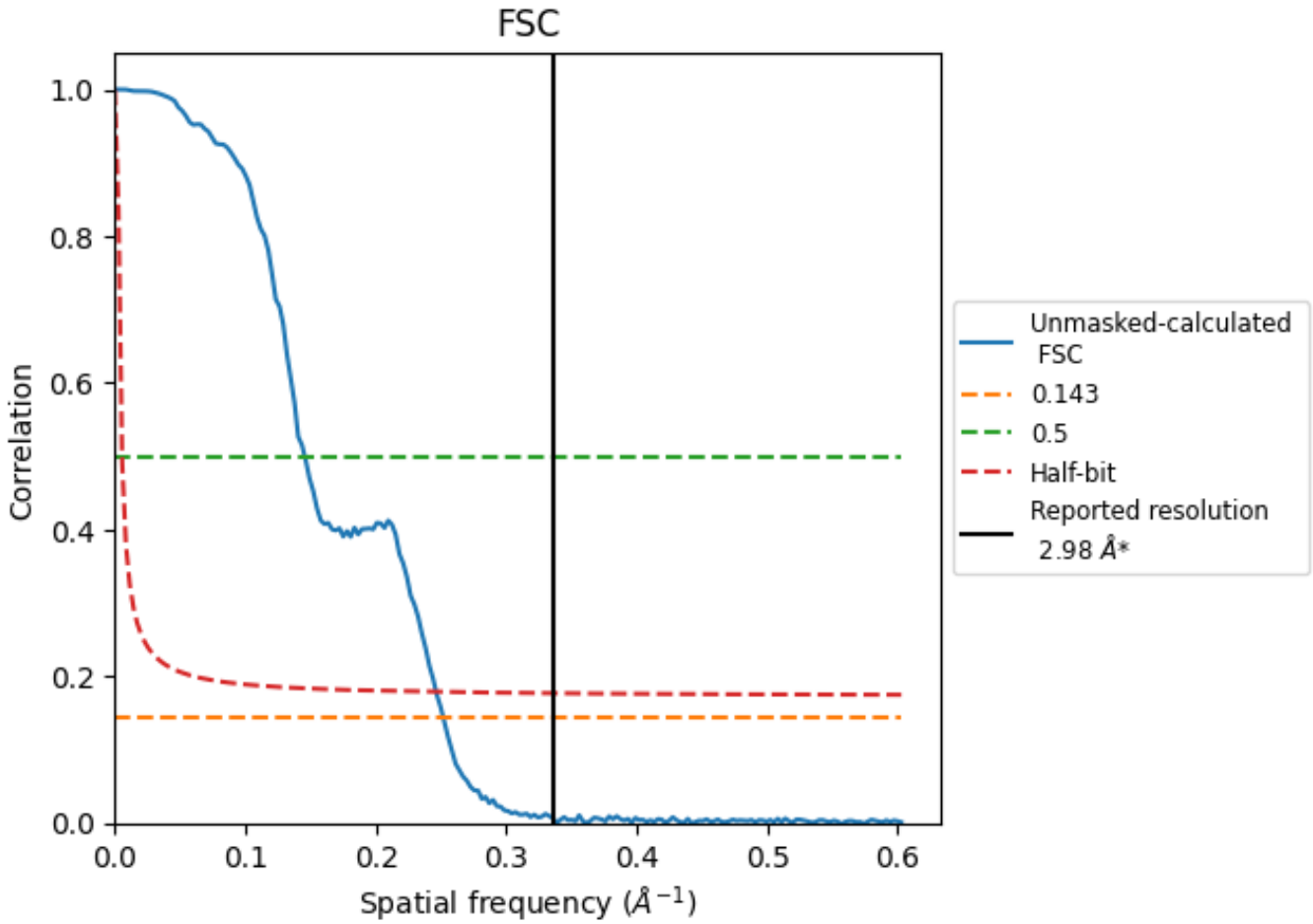


*Reported resolution corresponds to spatial frequency of 0.336 $Å^{-1}$

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 0.336 Å^{-1}

8.2 Resolution estimates (i)

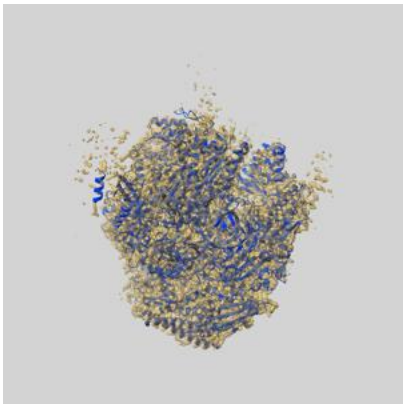
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.97	6.87	4.06

*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 3.97 differs from the reported value 2.98 by more than 10 %

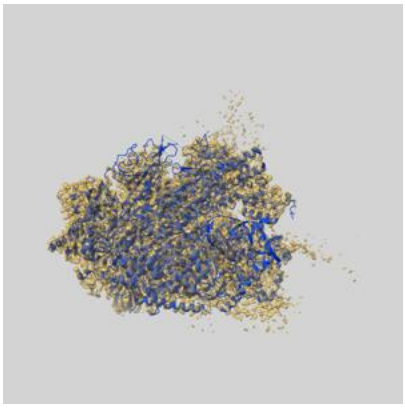
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-61287 and PDB model 9JA1. Per-residue inclusion information can be found in section 3 on page 8.

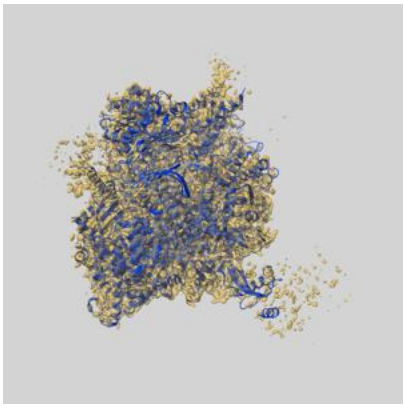
9.1 Map-model overlay



X



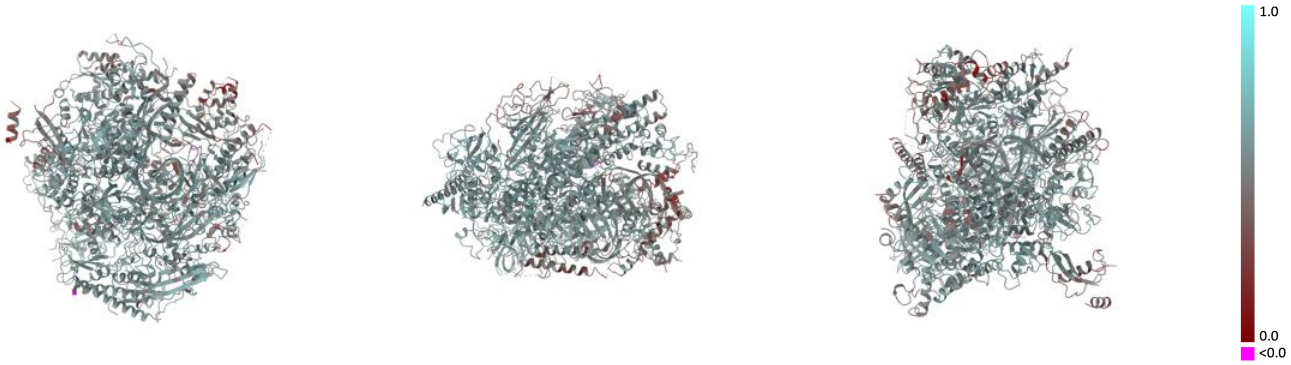
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

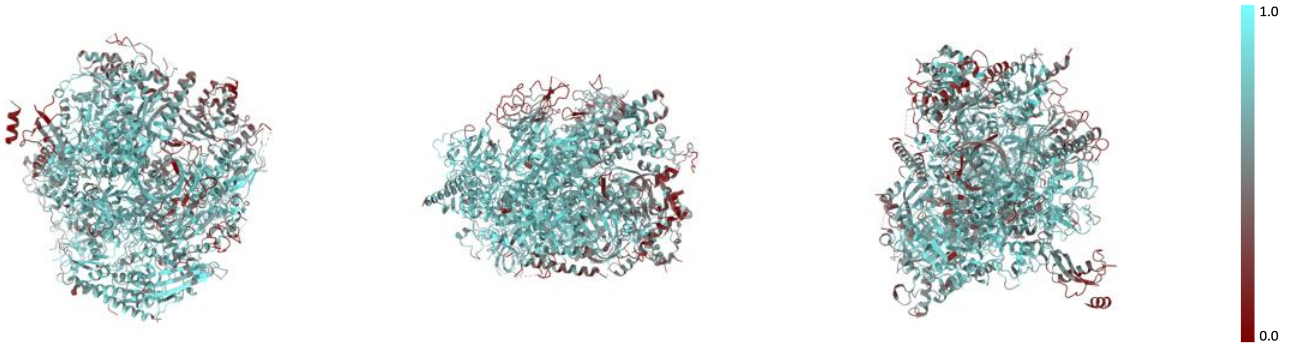
9.2 Q-score mapped to coordinate model (i)



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.

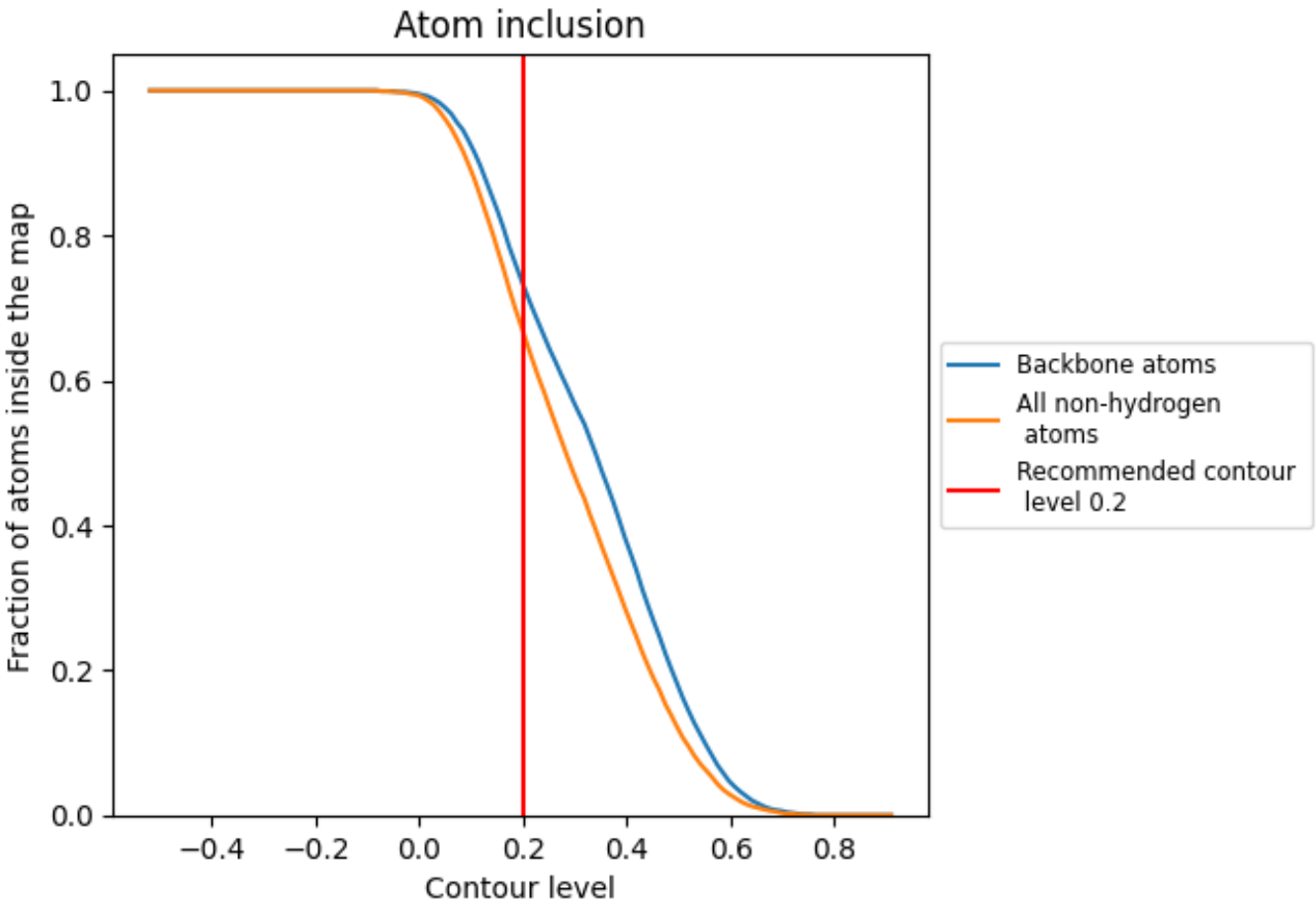
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 67% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6670	0.5370
A	0.6910	0.5440
B	0.6510	0.5340
C	0.7360	0.5580
D	0.1290	0.3500
E	0.6710	0.5320
F	0.7210	0.5640
G	0.3500	0.4380
H	0.6810	0.5360
J	0.7740	0.5560
K	0.7510	0.5720
L	0.2600	0.4320
N	0.4020	0.4690
R	0.8210	0.5830
T	0.6340	0.5120