Full wwPDB EM Validation Report

Mar 20, 2026 – 11:49 AM UTC

PDB ID	:	9K38 / pdb_00009k38
EMDB ID	:	EMD-62008
Title	:	Human RNA Polymerase III de novo transcribing complex 6 (TC6)
Authors	:	Wang, Q.; Ren, Y.; Jin, Q.; Chen, X.; Xu, Y.
Deposited on	:	2024-10-18
Resolution	:	3.10 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:

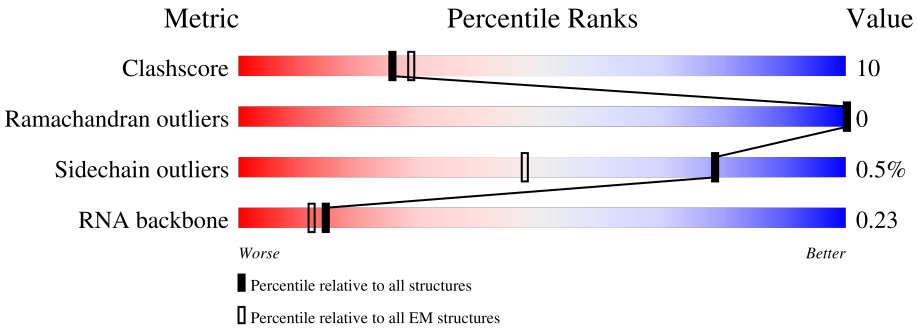
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

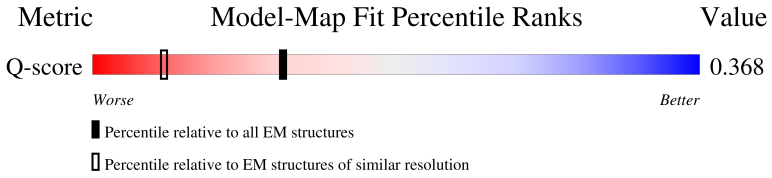
1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	1390	84% 15%
2	B	1133	5% 83% 15%
3	C	346	82% 17%

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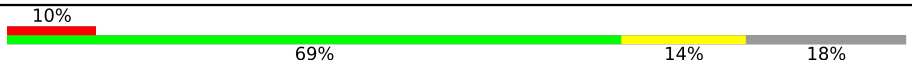
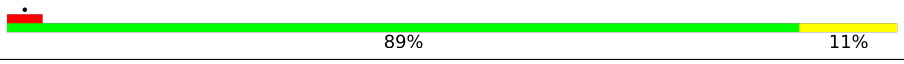
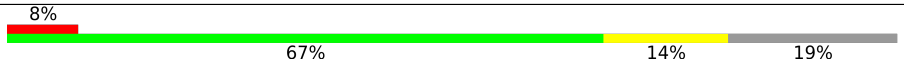
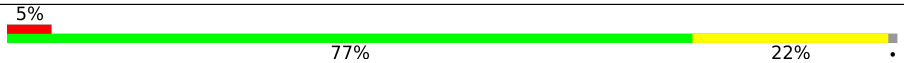
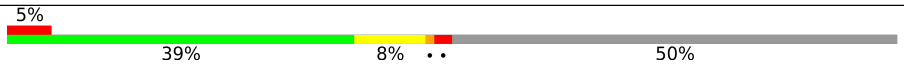
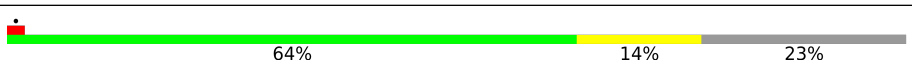
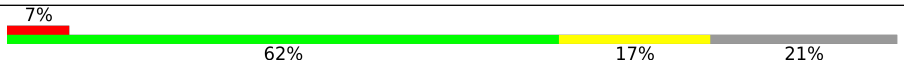
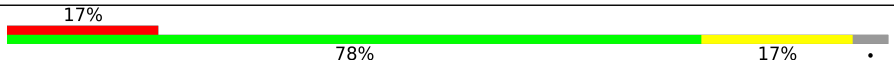
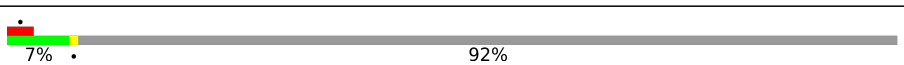
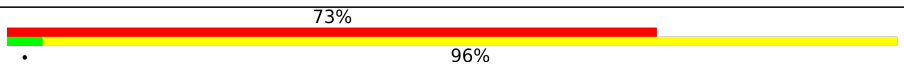
Mol	Chain	Length	Quality of chain
4	D	148	
5	E	210	
6	F	127	
7	G	204	
8	H	150	
9	I	108	
10	J	67	
11	K	133	
12	L	58	
13	M	708	
14	N	398	
15	O	534	
16	P	316	
17	Q	223	
18	V	419	
19	X	51	
20	Y	51	
21	Z	5	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	GTP	Z	101	-	-	X	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 44526 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 III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1378	10814	6850	1886	2005	73	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1105	8736	5535	1529	1603	69	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	343	2736	1723	488	514	11	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	122	985	614	172	196	3	0	0

- Molecule 5 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		
5	E	209	1715	1083	300	324	8	0	0

- Molecule 6 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		
6	F	76	610	392	103	110	5	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	166	Total	C	N	O	S	0	0
			1337	876	211	245	5		

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

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

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	54	Total	C	N	O	S	0	0
			426	267	79	74	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			512	331	87	88	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	103	Total	C	N	O	S	0	0
			822	513	145	157	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	422	Total	C	N	O	S	0	0
			3382	2138	588	636	20		

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	146	Total	C	N	O	S	0	0
			1128	710	191	221	6		

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	512	Total	C	N	O	S	0	0
			4075	2565	712	774	24		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	303	Total	C	N	O	S	0	0
			2403	1516	411	460	16		

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	87	Total	C	N	O	S	0	0
			754	488	126	134	6		

- Molecule 18 is a protein called Transcription factor IIIB 50 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	34	Total	C	N	O	S	0	0
			246	144	41	56	5		

- Molecule 19 is a DNA chain called DNA (51-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	51	Total	C	N	O	P	0	0
			1048	498	201	298	51		

- Molecule 20 is a DNA chain called DNA (51-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	51	Total	C	N	O	P	0	0
			1043	499	179	314	51		

- Molecule 21 is a RNA chain called RNA (5'-R(P*UP*GP*CP*UP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	5	Total	C	N	O	P	0	0
			103	46	15	37	5		

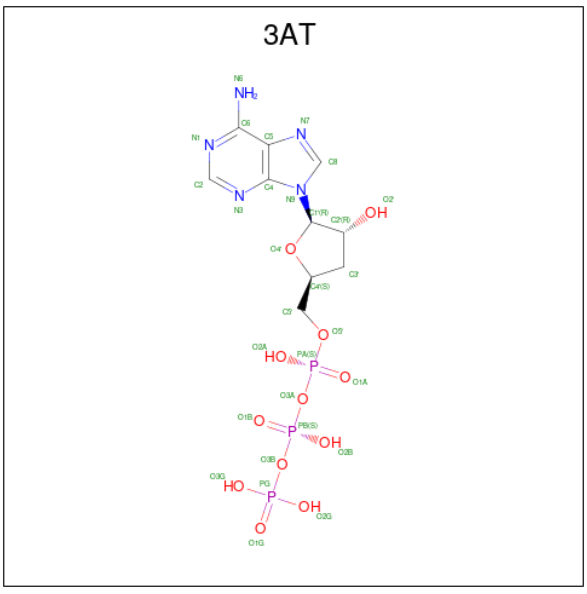
- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

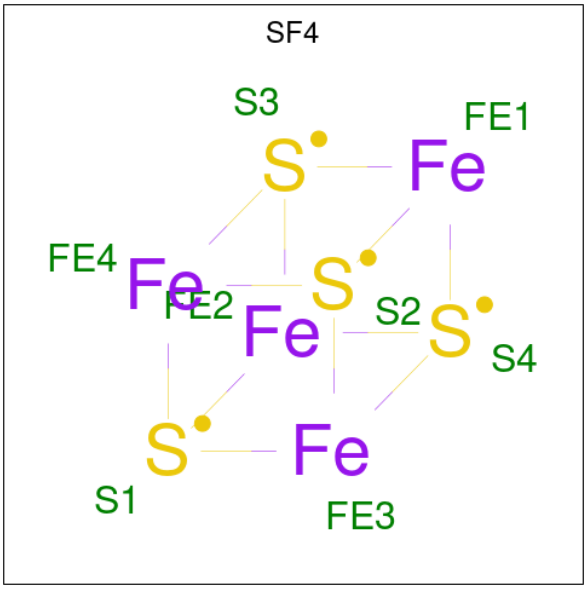
Mol	Chain	Residues	Atoms		AltConf
23	A	1	Total	Mg	0
			1	1	

- Molecule 24 is 3'-DEOXYADENOSINE-5'-TRIPHOSPHATE (CCD ID: 3AT) (formula: $C_{10}H_{16}N_5O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



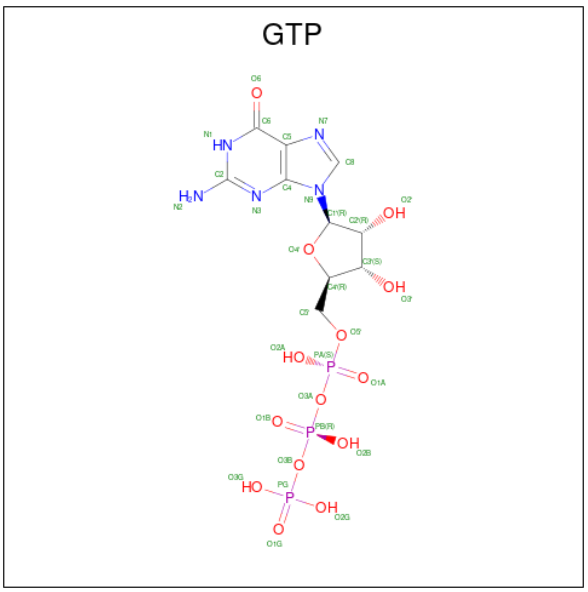
Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total	C	N	O	P	0
			30	10	5	12	3	

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
25	P	1	Total	Fe	S	0
			8	4	4	

- Molecule 26 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



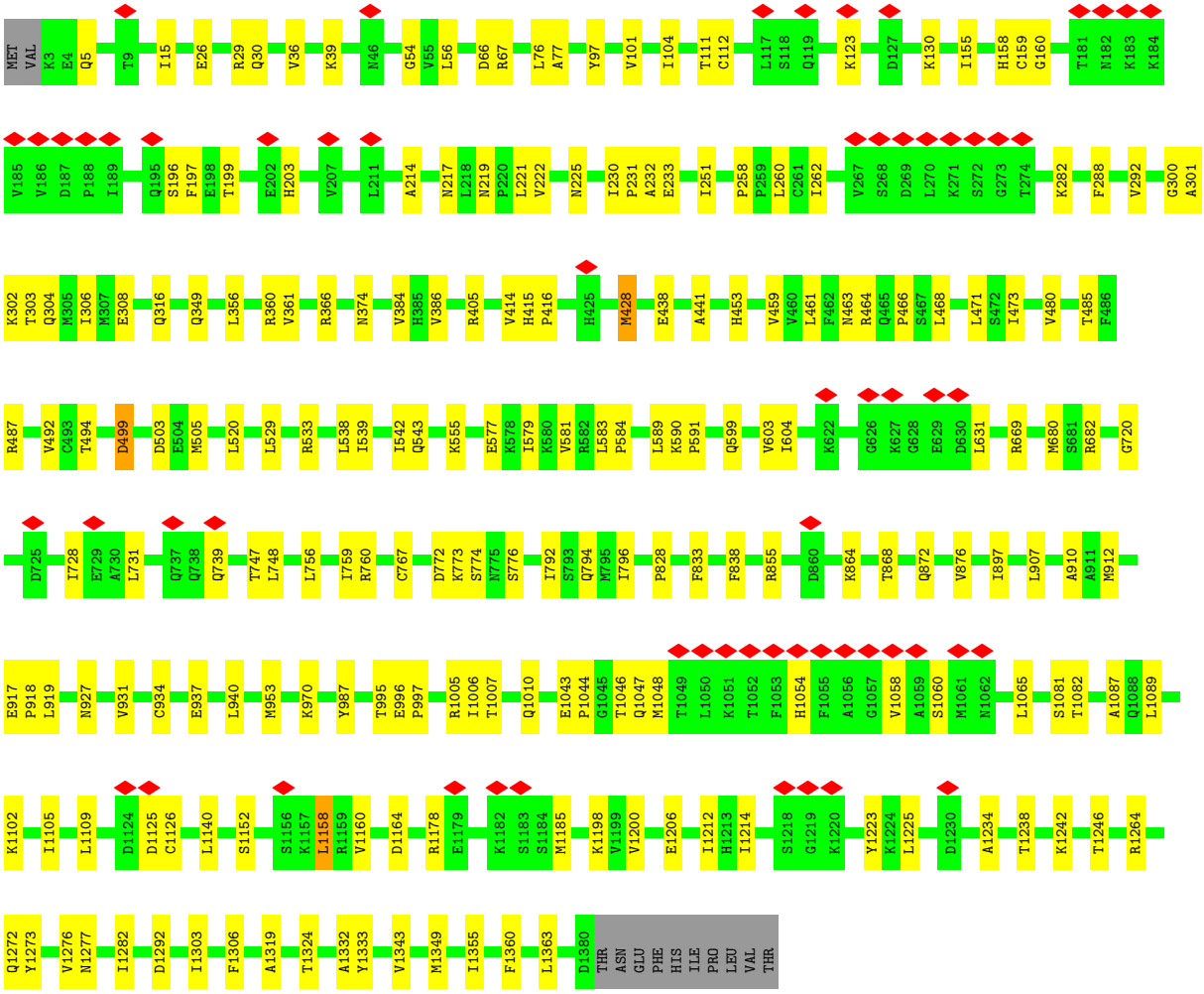
Mol	Chain	Residues	Atoms					AltConf
26	Z	1	Total	C	N	O	P	0
			32	10	5	14	3	

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.

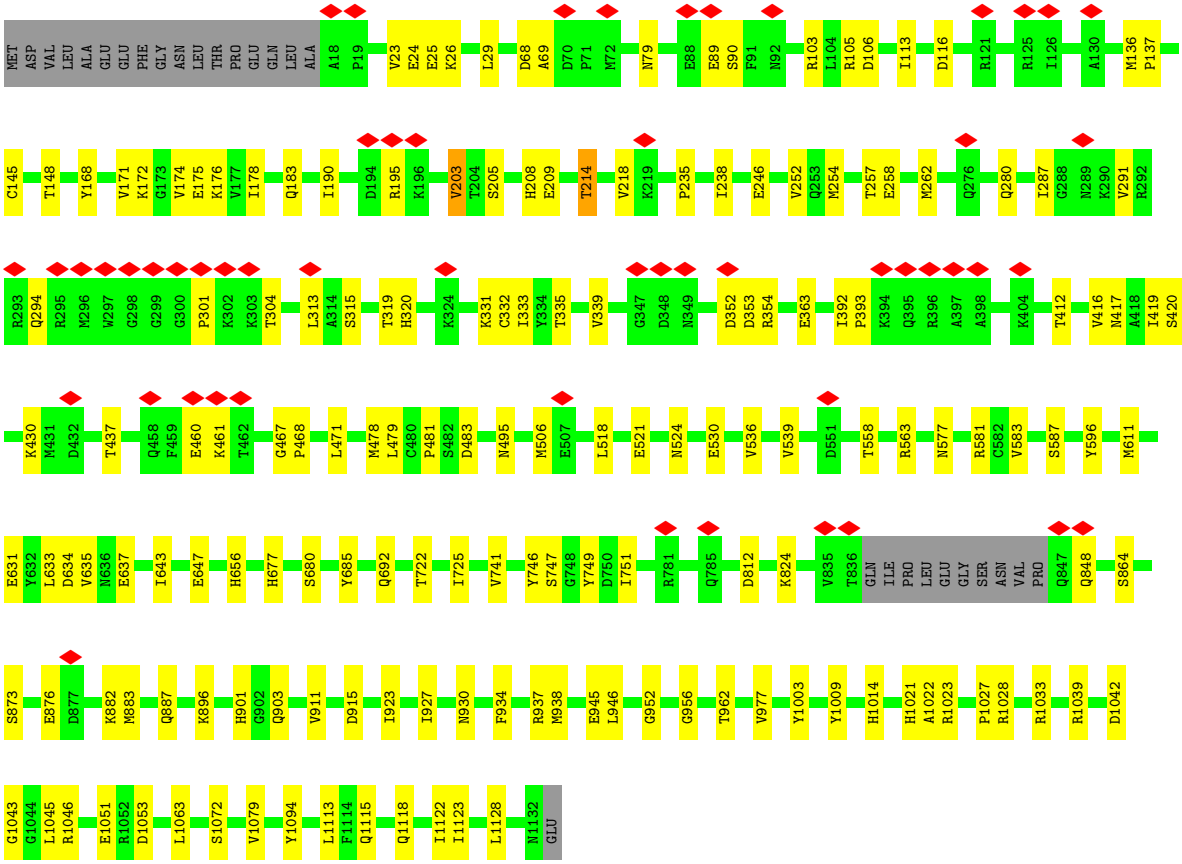
• Molecule 1: DNA-directed RNA polymerase III subunit RPC1

Chain A:

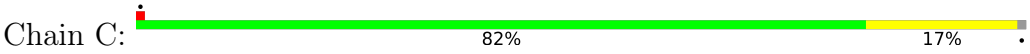


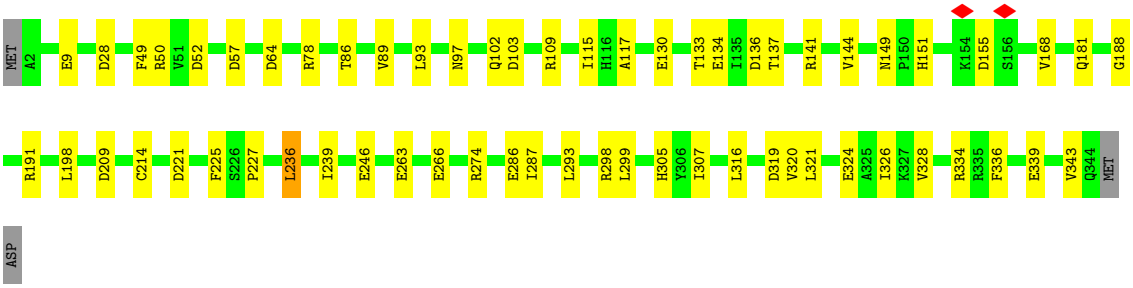
• Molecule 2: DNA-directed RNA polymerase III subunit RPC2

Chain B:

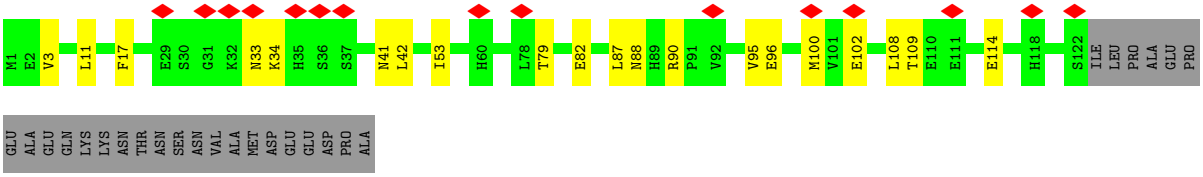


• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



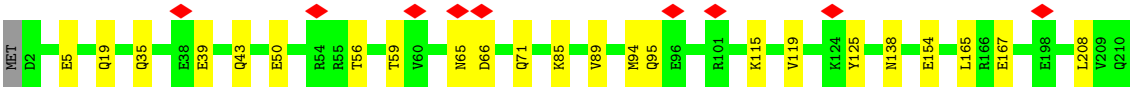


• Molecule 4: DNA-directed RNA polymerase III subunit RPC9



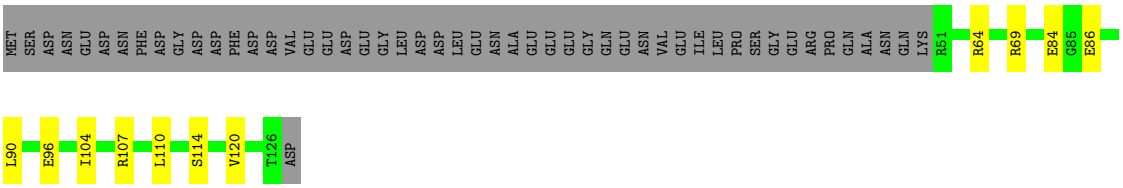
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



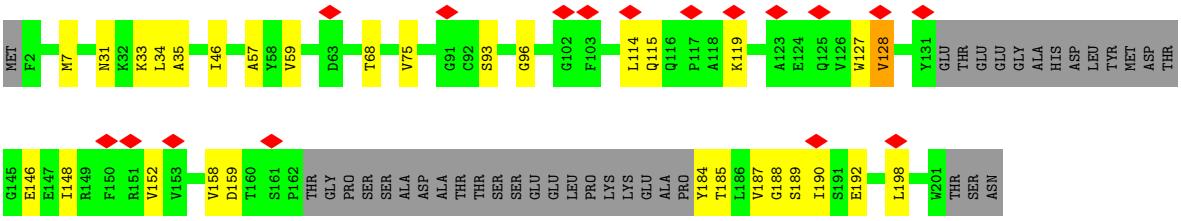
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



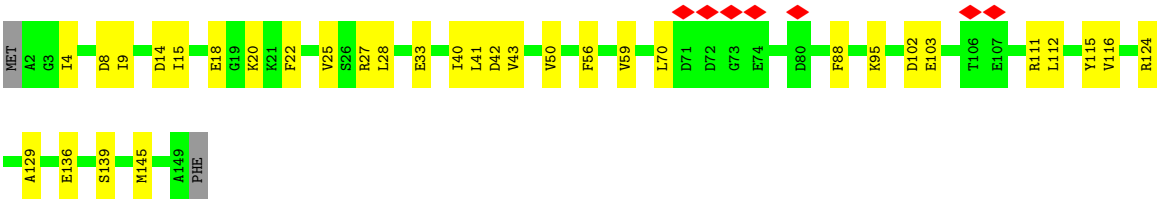
• Molecule 7: DNA-directed RNA polymerase III subunit RPC8

Chain G:



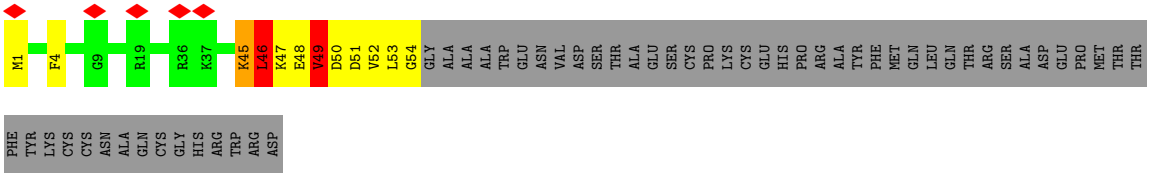
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



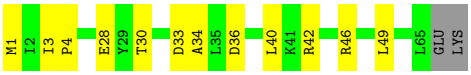
• Molecule 9: DNA-directed RNA polymerase III subunit RPC10

Chain I:



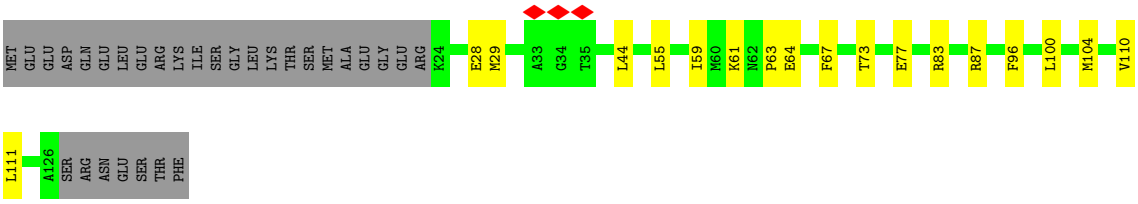
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



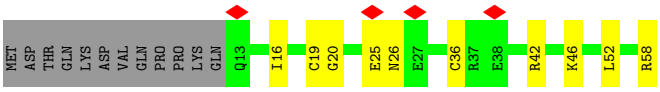
• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K:



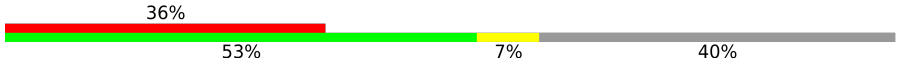
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

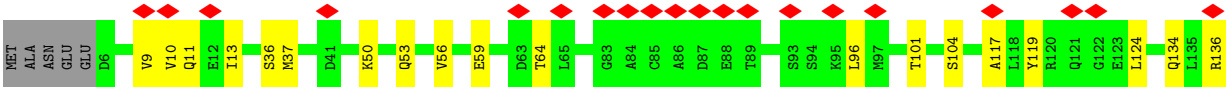
Chain L:

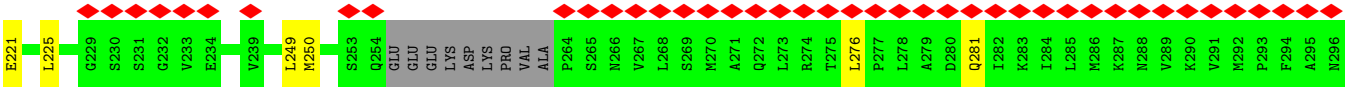


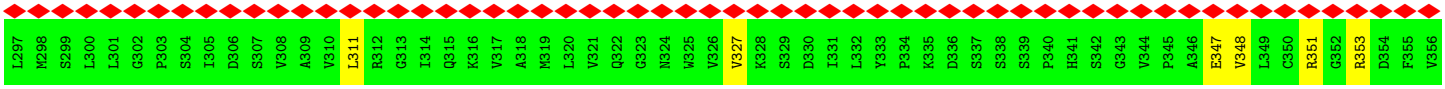
• Molecule 13: DNA-directed RNA polymerase III subunit RPC5

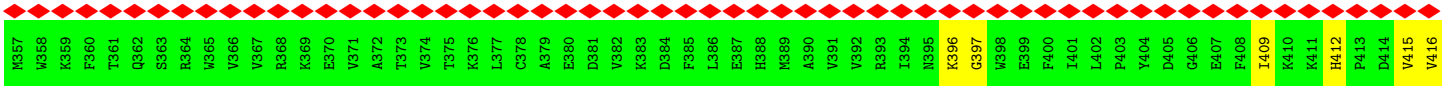
Chain M:

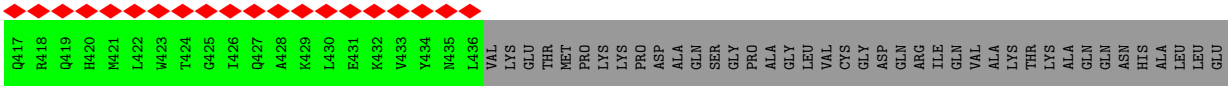


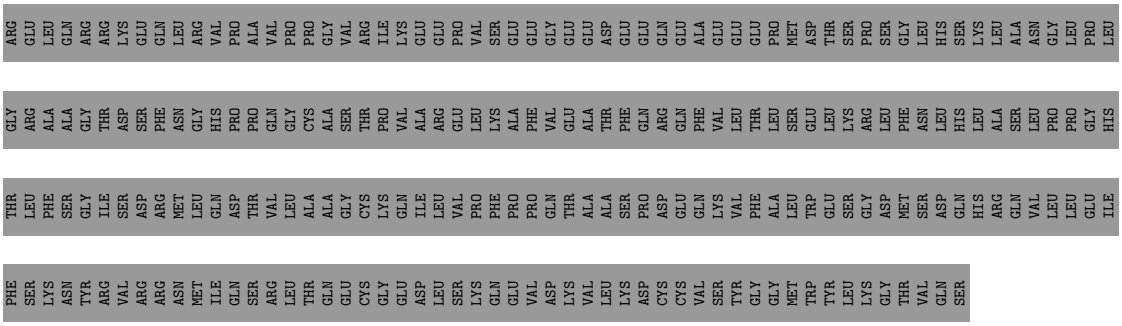






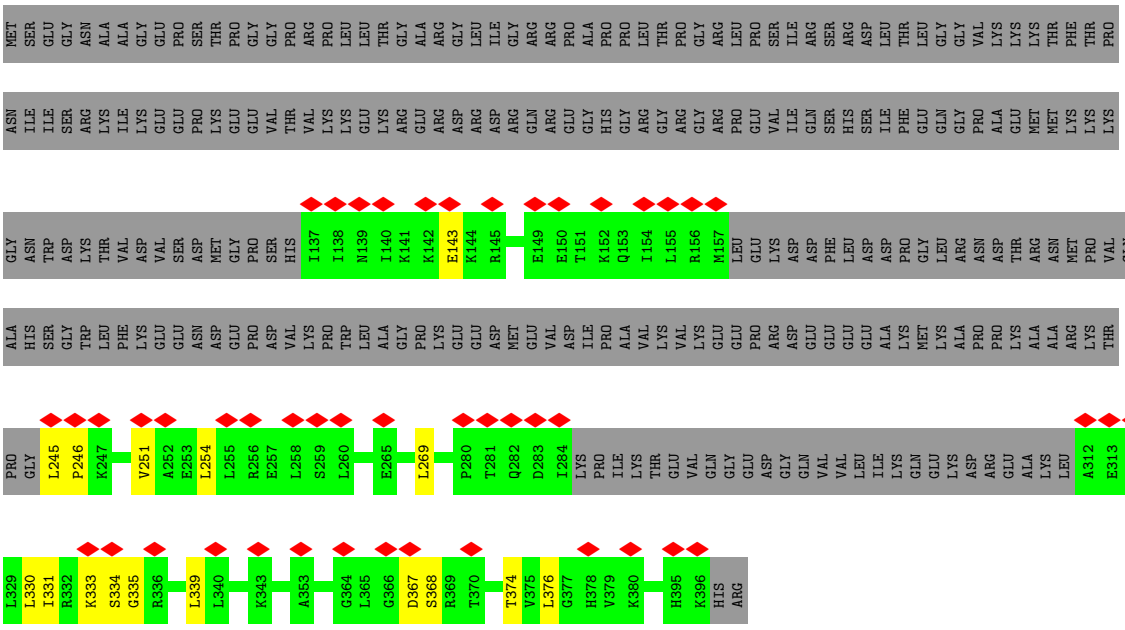






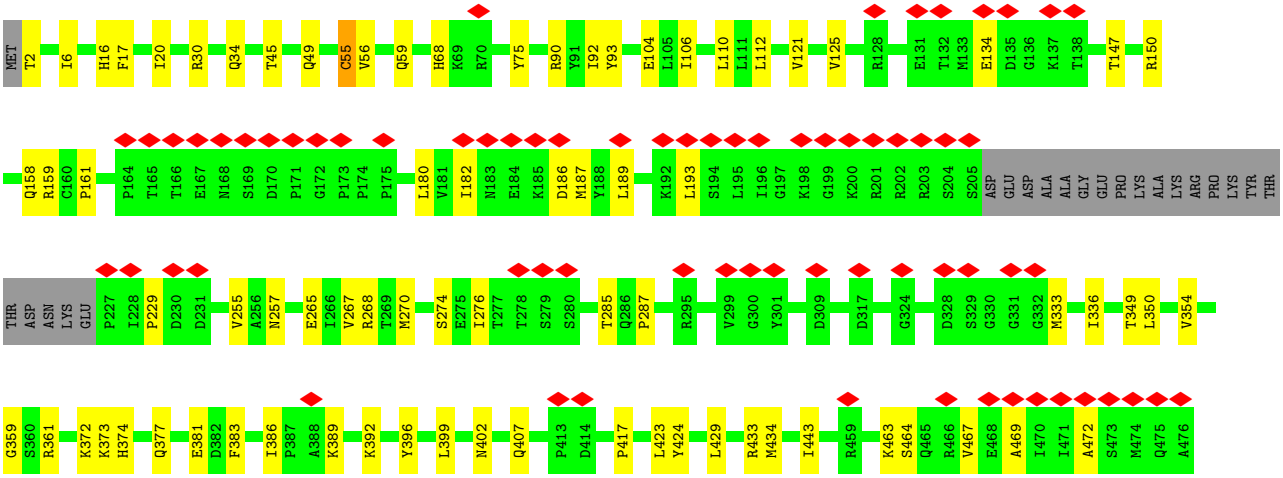
• Molecule 14: DNA-directed RNA polymerase III subunit RPC4

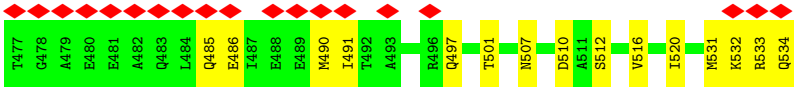
Chain N:



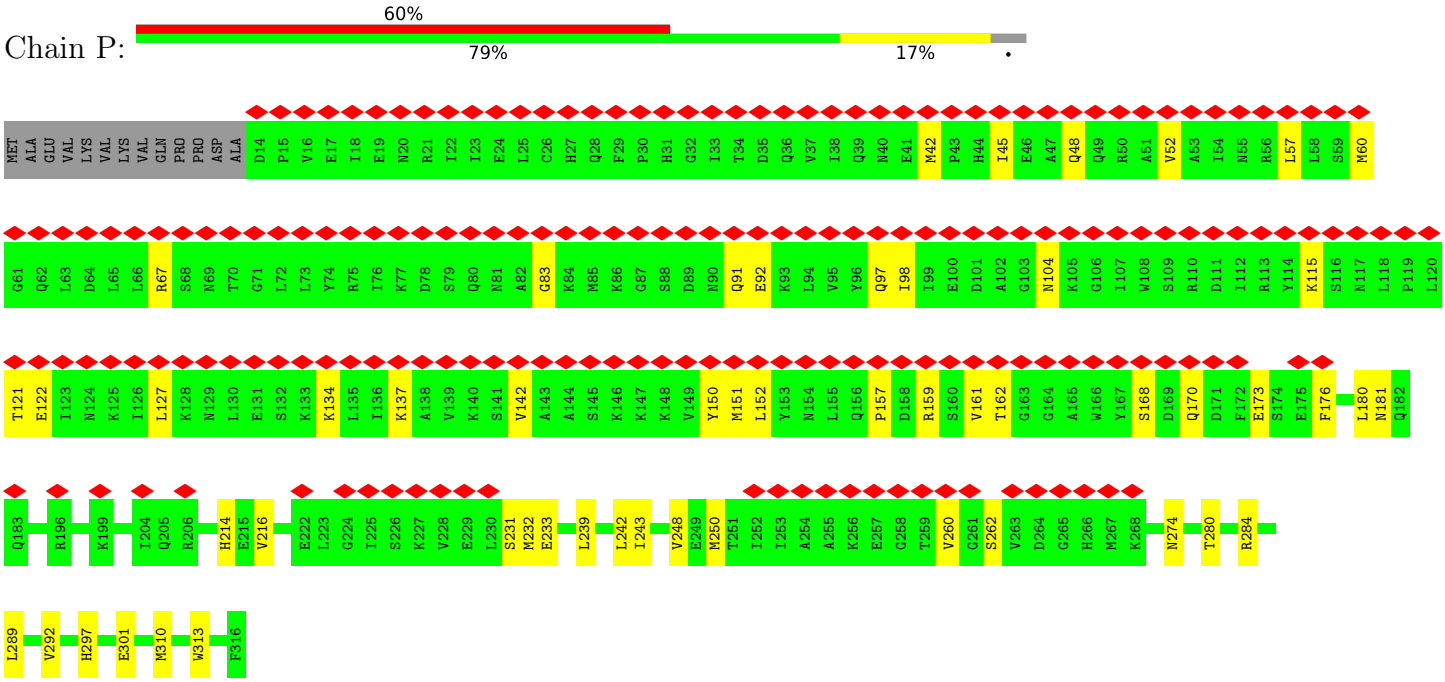
• Molecule 15: DNA-directed RNA polymerase III subunit RPC3

Chain O:

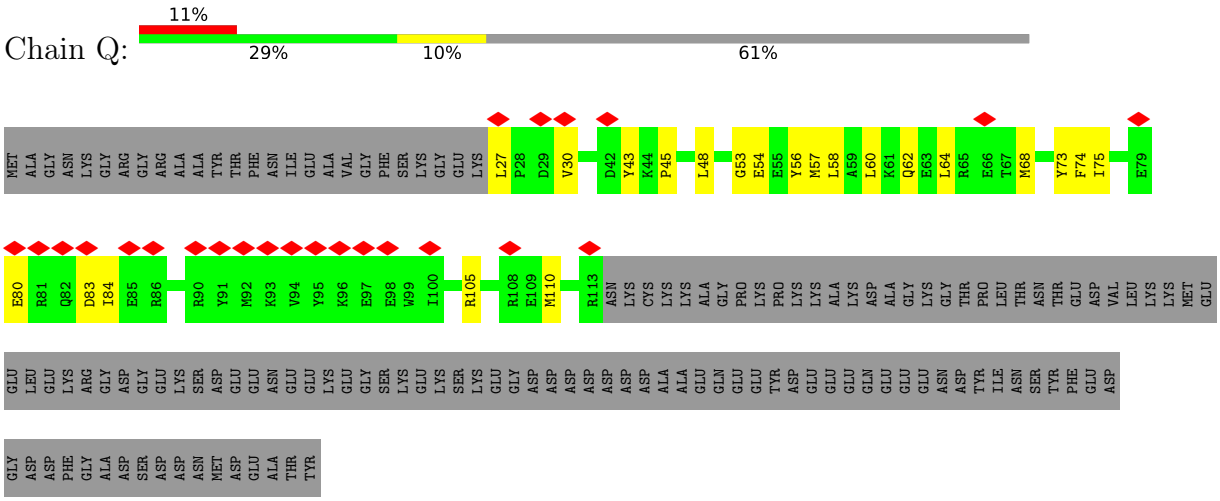




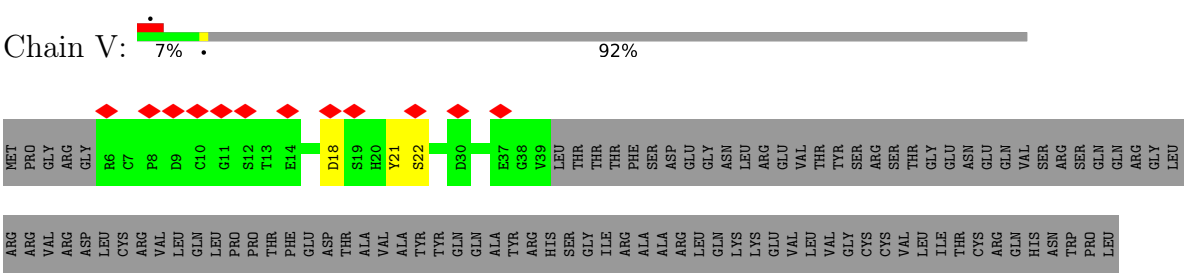
• Molecule 16: DNA-directed RNA polymerase III subunit RPC6

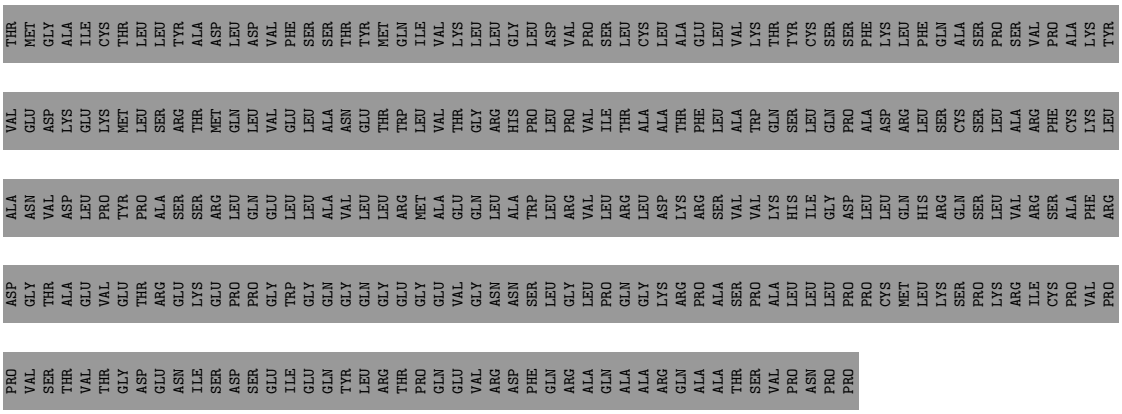


• Molecule 17: DNA-directed RNA polymerase III subunit RPC7



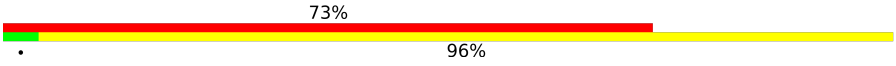
• Molecule 18: Transcription factor IIIB 50 kDa subunit

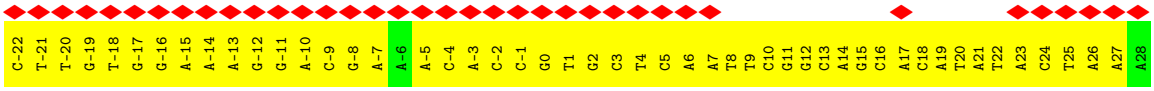




• Molecule 19: DNA (51-MER)

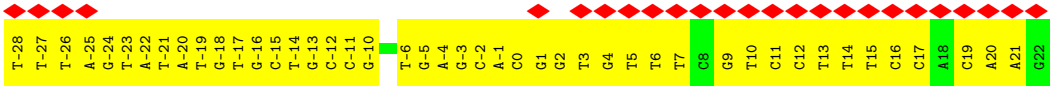
Chain X:





• Molecule 20: DNA (51-MER)

Chain Y:



• Molecule 21: RNA (5'-R(P*UP*GP*CP*UP*C)-3')

Chain Z:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	300000	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)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.214	Depositor
Minimum map value	-0.115	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	429.07724, 429.07724, 429.07724	wwPDB
Map dimensions	322, 322, 322	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.332538, 1.332538, 1.332538	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, ZN, 3AT, GTP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.11	0/11008	0.24	0/14842
2	B	0.11	0/8905	0.24	0/12011
3	C	0.12	0/2790	0.25	0/3782
4	D	0.13	0/997	0.27	0/1343
5	E	0.12	0/1745	0.22	0/2358
6	F	0.13	0/620	0.24	0/839
7	G	0.12	0/1374	0.27	0/1868
8	H	0.11	0/1207	0.24	0/1628
9	I	0.83	2/434 (0.5%)	0.83	3/584 (0.5%)
10	J	0.13	0/521	0.23	0/703
11	K	0.13	0/837	0.28	0/1129
12	L	0.16	0/394	0.29	0/524
13	M	0.11	0/3455	0.23	0/4673
14	N	0.12	0/1137	0.23	0/1530
15	O	0.11	0/4141	0.23	0/5592
16	P	0.11	0/2446	0.22	0/3301
17	Q	0.14	0/777	0.24	0/1050
18	V	0.14	0/248	0.21	0/336
19	X	0.43	0/1178	0.41	0/1815
20	Y	0.43	0/1166	0.44	0/1798
21	Z	1.90	3/113 (2.7%)	2.77	10/173 (5.8%)
All	All	0.19	5/45493 (0.0%)	0.30	13/61879 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Z	4	C	O3'-P	-9.43	1.47	1.61
9	I	46	LEU	C-O	-7.99	1.15	1.23
21	Z	2	U	O3'-P	-6.63	1.51	1.61
21	Z	5	U	O3'-P	-5.93	1.52	1.61
9	I	47	LYS	CA-C	-5.29	1.45	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	Z	2	U	P-O3'-C3'	-14.61	98.29	120.20
21	Z	2	U	O3'-P-O5'	14.47	125.70	104.00
21	Z	5	U	C3'-C2'-O2'	13.27	130.60	110.70
9	I	51	ASP	N-CA-C	7.80	121.95	110.17
21	Z	6	C	O4'-C4'-C3'	-7.06	96.94	104.00
21	Z	2	U	C2'-C3'-O3'	6.99	124.19	113.70
21	Z	6	C	C4'-C3'-O3'	-6.82	102.78	113.00
9	I	47	LYS	N-CA-C	-5.89	100.95	110.32
21	Z	2	U	C4'-C3'-O3'	-5.80	104.30	113.00
21	Z	6	C	C1'-C2'-O2'	-5.76	99.75	108.40
21	Z	6	C	C2'-C3'-O3'	5.60	122.10	113.70
9	I	49	VAL	N-CA-C	-5.50	101.64	108.89
21	Z	5	U	C4'-C3'-O3'	5.17	120.75	113.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10814	0	11058	244	0
2	B	8736	0	8861	129	0
3	C	2736	0	2712	45	0
4	D	985	0	1006	14	0
5	E	1715	0	1733	14	0
6	F	610	0	642	8	0
7	G	1337	0	1306	21	0
8	H	1186	0	1147	23	0
9	I	426	0	428	9	0
10	J	512	0	525	9	0
11	K	822	0	810	15	0
12	L	388	0	393	7	0
13	M	3382	0	3376	59	0
14	N	1128	0	1181	15	0
15	O	4075	0	4149	172	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	P	2403	0	2408	66	0
17	Q	754	0	759	35	0
18	V	246	0	221	2	0
19	X	1048	0	572	173	0
20	Y	1043	0	580	109	0
21	Z	103	0	53	27	0
22	A	2	0	0	0	0
22	B	1	0	0	0	0
22	I	1	0	0	0	0
22	J	1	0	0	0	0
22	L	1	0	0	0	0
23	A	1	0	0	0	0
24	B	30	0	12	6	0
25	P	8	0	0	1	0
26	Z	32	0	11	12	0
All	All	44526	0	43943	918	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (918) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:177:PHE:CE2	16:P:98:ILE:HD12	1.37	1.55
2:B:427:LYS:HD2	19:X:-3:DA:C2	1.41	1.54
21:Z:2:U:P	26:Z:101:GTP:C3'	2.10	1.39
19:X:24:DC:C2'	19:X:25:DT:H72	1.54	1.38
2:B:427:LYS:HD2	19:X:-3:DA:N1	1.40	1.35
13:M:177:PHE:CE1	16:P:98:ILE:HG13	1.64	1.33
2:B:427:LYS:CD	19:X:-3:DA:C2	2.15	1.26
1:A:303:THR:OG1	15:O:377:GLN:NE2	1.68	1.24
1:A:203:HIS:CE1	15:O:383:PHE:CZ	2.26	1.23
13:M:171:LYS:NZ	16:P:67:ARG:HD2	1.54	1.22
1:A:203:HIS:NE2	15:O:383:PHE:CZ	2.10	1.20
19:X:24:DC:H2"	19:X:25:DT:C7	1.72	1.19
19:X:24:DC:C2'	19:X:25:DT:C7	2.19	1.19
19:X:21:DA:H2"	19:X:22:DT:C7	1.72	1.18
13:M:177:PHE:CD2	16:P:98:ILE:HD12	1.77	1.18
19:X:-22:DC:H2'	19:X:-21:DT:C7	1.77	1.13
19:X:11:DG:O6	20:Y:-11:DC:N4	1.83	1.11
13:M:177:PHE:CE2	16:P:98:ILE:CD1	2.33	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:PHE:CE2	15:O:374:HIS:CD2	2.39	1.10
19:X:-2:DC:C5	19:X:-1:DC:N4	2.18	1.10
19:X:-22:DC:H2'	19:X:-21:DT:H72	1.14	1.10
1:A:196:SER:O	15:O:373:LYS:HB2	1.51	1.09
19:X:24:DC:H2'	19:X:25:DT:H72	1.13	1.09
13:M:177:PHE:CZ	16:P:98:ILE:HD12	1.85	1.08
1:A:197:PHE:CZ	15:O:374:HIS:NE2	2.21	1.08
19:X:21:DA:H2"	19:X:22:DT:H71	1.14	1.08
19:X:3:DC:H2"	19:X:4:DT:H5"	1.35	1.07
1:A:231:PRO:HA	15:O:2:THR:OG1	1.53	1.07
13:M:177:PHE:CZ	16:P:98:ILE:CG1	2.38	1.06
1:A:230:ILE:O	15:O:2:THR:N	1.88	1.06
19:X:6:DA:H5'	19:X:7:DA:H5"	1.39	1.05
13:M:177:PHE:CE1	16:P:98:ILE:CG1	2.40	1.04
19:X:-22:DC:C2'	19:X:-21:DT:H72	1.87	1.04
19:X:-2:DC:C5	19:X:-1:DC:C4	2.46	1.04
1:A:203:HIS:NE2	15:O:383:PHE:HZ	1.47	1.03
19:X:21:DA:C2'	19:X:22:DT:H71	1.87	1.03
13:M:177:PHE:CZ	16:P:98:ILE:HB	1.95	1.00
1:A:232:ALA:HB3	15:O:6:ILE:HD11	1.43	1.00
13:M:171:LYS:HZ2	16:P:67:ARG:HD2	1.14	1.00
13:M:171:LYS:HZ3	16:P:67:ARG:CB	1.75	0.99
20:Y:-24:DG:C2'	20:Y:-23:DT:H71	1.90	0.99
13:M:171:LYS:HZ3	16:P:67:ARG:CD	1.74	0.99
19:X:-19:DG:H2"	19:X:-18:DT:C5	1.97	0.99
13:M:171:LYS:HG3	16:P:67:ARG:HD3	1.45	0.97
13:M:177:PHE:CZ	16:P:98:ILE:CD1	2.46	0.97
13:M:171:LYS:NZ	16:P:67:ARG:CD	2.26	0.96
1:A:203:HIS:CE1	15:O:383:PHE:HZ	1.76	0.96
1:A:199:THR:OG1	15:O:372:LYS:HD2	1.66	0.96
1:A:130:LYS:CE	15:O:34:GLN:NE2	2.29	0.95
1:A:159:CYS:HB2	15:O:531:MET:HG2	1.49	0.95
20:Y:5:DT:H1'	20:Y:6:DT:H5'	1.49	0.95
19:X:9:DT:H2"	19:X:10:DC:H5'	1.51	0.92
19:X:21:DA:H2"	19:X:22:DT:C5	2.04	0.92
13:M:177:PHE:CZ	16:P:98:ILE:CB	2.52	0.92
1:A:196:SER:HB2	15:O:373:LYS:HG3	1.51	0.92
20:Y:-24:DG:H2'	20:Y:-23:DT:H71	1.52	0.90
1:A:196:SER:HB2	15:O:373:LYS:CB	2.02	0.90
19:X:7:DA:C2'	19:X:8:DT:H72	2.02	0.89
21:Z:2:U:P	26:Z:101:GTP:C2'	2.61	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:X:11:DG:H1	20:Y:-11:DC:H5	1.14	0.89
1:A:196:SER:HB2	15:O:373:LYS:CG	2.03	0.89
2:B:685:TYR:CE2	24:B:1202:3AT:O1G	2.26	0.88
1:A:159:CYS:CB	15:O:531:MET:SD	2.61	0.88
15:O:92:ILE:HG21	17:Q:60:LEU:HD11	1.53	0.88
13:M:177:PHE:HZ	16:P:98:ILE:HB	1.37	0.86
13:M:171:LYS:HZ3	16:P:67:ARG:HB2	1.40	0.86
13:M:171:LYS:NZ	16:P:67:ARG:HB2	1.91	0.85
20:Y:5:DT:H2"	20:Y:6:DT:OP2	1.76	0.85
20:Y:-19:DT:H1'	20:Y:-18:DG:H5'	1.57	0.85
1:A:26:GLU:HG2	16:P:297:HIS:HB2	1.59	0.85
9:I:45:LYS:NZ	9:I:45:LYS:HB2	1.88	0.85
19:X:7:DA:C2'	19:X:8:DT:C7	2.55	0.84
1:A:155:ILE:HB	15:O:534:GLN:HE21	1.41	0.84
1:A:159:CYS:HB3	15:O:531:MET:SD	2.17	0.84
13:M:177:PHE:CD2	16:P:98:ILE:CD1	2.54	0.84
2:B:685:TYR:HE2	24:B:1202:3AT:O1G	1.61	0.83
15:O:274:SER:HG	15:O:285:THR:HG1	1.19	0.83
19:X:11:DG:N1	20:Y:-11:DC:H5	1.76	0.83
20:Y:5:DT:H1'	20:Y:6:DT:C5'	2.08	0.83
20:Y:-24:DG:H2"	20:Y:-23:DT:H71	1.56	0.83
1:A:123:LYS:HD2	15:O:68:HIS:CD2	2.13	0.83
19:X:21:DA:C2'	19:X:22:DT:C7	2.49	0.83
1:A:196:SER:CB	15:O:373:LYS:HG3	2.08	0.82
19:X:24:DC:H2"	19:X:25:DT:C5	2.13	0.82
1:A:203:HIS:NE2	15:O:383:PHE:CE2	2.46	0.82
19:X:24:DC:H2'	19:X:25:DT:C7	1.94	0.82
19:X:-22:DC:C2'	19:X:-21:DT:C7	2.52	0.82
19:X:24:DC:H2"	19:X:25:DT:H73	1.62	0.82
19:X:-2:DC:H5	19:X:-1:DC:N4	1.76	0.81
19:X:-17:DG:N1	19:X:-16:DG:C6	2.48	0.81
19:X:1:DT:H2"	19:X:2:DG:H3'	1.61	0.81
20:Y:-24:DG:C2'	20:Y:-23:DT:C7	2.59	0.81
1:A:159:CYS:HA	15:O:531:MET:HB3	1.63	0.81
1:A:232:ALA:HB3	15:O:6:ILE:CD1	2.10	0.80
19:X:15:DG:H2"	19:X:16:DC:C6	2.15	0.80
19:X:11:DG:N1	20:Y:-11:DC:C5	2.50	0.80
1:A:232:ALA:CB	15:O:6:ILE:HD11	2.12	0.80
19:X:-19:DG:H2"	19:X:-18:DT:C7	2.12	0.80
1:A:197:PHE:CZ	15:O:374:HIS:CE1	2.69	0.79
19:X:-17:DG:C2	19:X:-16:DG:C5	2.71	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:95:GLN:OE1	5:E:125:TYR:OH	2.01	0.79
20:Y:-16:DG:H2"	20:Y:-15:DC:C6	2.18	0.79
1:A:130:LYS:HE2	15:O:34:GLN:NE2	1.97	0.79
2:B:172:LYS:NZ	20:Y:3:DT:OP2	2.16	0.79
1:A:233:GLU:HA	15:O:30:ARG:O	1.81	0.78
13:M:36:SER:OG	13:M:37:MET:SD	2.41	0.78
1:A:196:SER:HB2	15:O:373:LYS:HB3	1.66	0.78
1:A:232:ALA:CB	15:O:6:ILE:CD1	2.61	0.78
17:Q:27:LEU:HD23	19:X:-7:DA:H2'	1.65	0.78
1:A:111:THR:HG23	15:O:429:LEU:CD2	2.14	0.78
16:P:137:LYS:NZ	16:P:152:LEU:O	2.17	0.78
1:A:303:THR:OG1	15:O:424:TYR:OH	1.83	0.78
20:Y:11:DC:H2"	20:Y:12:DC:C5	2.19	0.78
19:X:-14:DA:H2"	19:X:-13:DA:C8	2.20	0.77
20:Y:-24:DG:H2'	20:Y:-23:DT:C7	2.13	0.77
20:Y:16:DC:H2"	20:Y:17:DC:C6	2.19	0.77
21:Z:2:U:O5'	26:Z:101:GTP:C2'	2.33	0.77
19:X:-2:DC:C4	19:X:-1:DC:N4	2.53	0.77
2:B:427:LYS:CD	19:X:-3:DA:N1	2.33	0.77
1:A:123:LYS:CD	15:O:68:HIS:CD2	2.69	0.76
2:B:195:ARG:NH1	19:X:9:DT:H73	2.00	0.76
19:X:13:DC:H2"	19:X:14:DA:O5'	1.85	0.76
1:A:464:ARG:NH1	24:B:1202:3AT:O2'	2.17	0.76
1:A:282:LYS:NZ	1:A:316:GLN:OE1	2.16	0.75
1:A:374:ASN:ND2	2:B:749:TYR:OH	2.19	0.75
1:A:197:PHE:CZ	15:O:374:HIS:CD2	2.70	0.75
19:X:-9:DC:H2"	19:X:-8:DG:N7	2.01	0.75
19:X:16:DC:H4'	19:X:17:DA:OP1	1.86	0.75
15:O:112:LEU:HD11	17:Q:64:LEU:HD22	1.69	0.75
2:B:427:LYS:HD3	19:X:-3:DA:C2	2.21	0.74
19:X:3:DC:H2'	19:X:4:DT:H72	1.69	0.74
2:B:313:LEU:O	2:B:331:LYS:NZ	2.20	0.74
19:X:19:DA:C2'	19:X:20:DT:H71	2.17	0.74
2:B:427:LYS:HD2	19:X:-3:DA:H2	1.46	0.74
1:A:159:CYS:HB2	15:O:531:MET:CG	2.17	0.74
1:A:855:ARG:NH2	2:B:481:PRO:O	2.21	0.73
2:B:89:GLU:OE2	12:L:42:ARG:NE	2.21	0.73
20:Y:15:DT:H2"	20:Y:16:DC:C6	2.24	0.73
1:A:197:PHE:CE1	15:O:374:HIS:CE1	2.76	0.73
19:X:7:DA:H2'	19:X:8:DT:C7	2.18	0.73
19:X:24:DC:H2"	19:X:25:DT:C6	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:X:7:DA:N9	19:X:8:DT:H72	2.03	0.72
20:Y:-24:DG:H2"	20:Y:-23:DT:C6	2.24	0.72
19:X:2:DG:C1'	19:X:3:DC:H5"	2.19	0.72
4:D:108:LEU:O	4:D:109:THR:OG1	2.07	0.72
9:I:46:LEU:HD13	9:I:46:LEU:N	2.03	0.72
20:Y:-14:DT:H2"	20:Y:-13:DG:C8	2.25	0.72
1:A:155:ILE:HB	15:O:534:GLN:NE2	2.04	0.71
1:A:720:GLY:HA3	1:A:759:ILE:HD11	1.72	0.71
15:O:20:ILE:HD11	17:Q:75:ILE:HG13	1.73	0.71
19:X:-17:DG:C2	19:X:-16:DG:C6	2.78	0.71
20:Y:16:DC:H2"	20:Y:17:DC:C5	2.26	0.71
19:X:-4:DC:H5"	19:X:-4:DC:H6	1.54	0.71
4:D:87:LEU:O	4:D:90:ARG:NH1	2.23	0.71
19:X:2:DG:H4'	19:X:3:DC:OP1	1.91	0.71
20:Y:3:DT:H2"	20:Y:4:DG:O4'	1.91	0.71
2:B:1023:ARG:NH1	2:B:1042:ASP:O	2.24	0.70
19:X:19:DA:H2"	19:X:20:DT:H71	1.70	0.70
1:A:1273:TYR:O	1:A:1277:ASN:ND2	2.23	0.70
19:X:18:DC:H1'	19:X:19:DA:C8	2.26	0.70
21:Z:2:U:P	26:Z:101:GTP:O3'	2.48	0.70
2:B:483:ASP:OD2	2:B:495:ASN:ND2	2.25	0.70
10:J:28:GLU:OE2	13:M:396:LYS:N	2.23	0.70
1:A:203:HIS:HE1	15:O:383:PHE:CZ	2.04	0.70
13:M:171:LYS:HZ3	16:P:67:ARG:CG	2.04	0.70
15:O:20:ILE:HD11	17:Q:75:ILE:CG1	2.22	0.70
1:A:995:THR:HG22	1:A:997:PRO:HD2	1.73	0.70
1:A:221:LEU:HD13	15:O:399:LEU:O	1.92	0.69
19:X:-5:DA:H4'	19:X:-4:DC:OP2	1.92	0.69
19:X:5:DC:H2"	19:X:6:DA:H4'	1.74	0.69
1:A:111:THR:HG23	15:O:429:LEU:HD21	1.73	0.69
20:Y:-2:DC:H2'	20:Y:-1:DA:H8	1.57	0.69
3:C:141:ARG:NH1	3:C:209:ASP:OD1	2.26	0.69
7:G:115:GLN:NE2	7:G:192:GLU:O	2.25	0.69
20:Y:-1:DA:H2'	20:Y:0:DC:C6	2.28	0.69
19:X:-21:DT:H2"	19:X:-20:DT:H5'	1.75	0.69
19:X:26:DA:C2	20:Y:-25:DA:C2	2.80	0.69
1:A:197:PHE:CE2	15:O:374:HIS:CG	2.81	0.68
19:X:7:DA:H2'	19:X:8:DT:H72	1.75	0.68
19:X:17:DA:H1'	19:X:18:DC:H5'	1.76	0.68
20:Y:11:DC:H2"	20:Y:12:DC:C6	2.28	0.68
2:B:903:GLN:OE1	2:B:937:ARG:NH1	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1023:ARG:NH2	2:B:1027:PRO:O	2.27	0.68
19:X:9:DT:C2'	19:X:10:DC:H5'	2.24	0.68
4:D:96:GLU:HA	4:D:100:MET:HE2	1.74	0.68
19:X:-2:DC:H5	19:X:-1:DC:C4	2.02	0.68
1:A:199:THR:CG2	15:O:372:LYS:HD2	2.23	0.68
1:A:130:LYS:CE	15:O:34:GLN:HE21	2.05	0.68
1:A:503:ASP:OD1	21:Z:6:C:O3'	2.12	0.68
19:X:7:DA:H2"	19:X:8:DT:C7	2.22	0.68
16:P:83:GLY:N	16:P:92:GLU:OE2	2.27	0.67
2:B:190:ILE:HG21	2:B:354:ARG:HE	1.59	0.67
19:X:-12:DG:H2"	19:X:-11:DG:C8	2.29	0.67
20:Y:-20:DA:H2"	20:Y:-19:DT:O5'	1.94	0.67
19:X:17:DA:C1'	19:X:18:DC:H5'	2.25	0.67
10:J:3:ILE:HD12	10:J:4:PRO:HD2	1.77	0.67
19:X:26:DA:H2"	19:X:27:DA:C8	2.29	0.67
1:A:29:ARG:NH1	16:P:301:GLU:OE1	2.28	0.66
1:A:464:ARG:HB2	1:A:505:MET:HE3	1.77	0.66
2:B:203:VAL:HG13	2:B:214:THR:HG23	1.77	0.66
1:A:756:LEU:HD22	1:A:833:PHE:CD1	2.31	0.66
19:X:17:DA:C2	20:Y:-16:DG:N2	2.64	0.66
16:P:216:VAL:HG21	16:P:239:LEU:HD11	1.77	0.66
3:C:149:ASN:ND2	3:C:151:HIS:O	2.29	0.65
19:X:-22:DC:H2'	19:X:-21:DT:H73	1.75	0.65
20:Y:-16:DG:C5	20:Y:-15:DC:N4	2.64	0.65
16:P:122:GLU:OE1	16:P:122:GLU:N	2.27	0.65
6:F:69:ARG:NE	6:F:96:GLU:OE1	2.30	0.65
20:Y:-24:DG:H2"	20:Y:-23:DT:C7	2.23	0.65
1:A:159:CYS:O	15:O:531:MET:HA	1.97	0.65
13:M:50:LYS:NZ	13:M:200:HIS:O	2.30	0.65
15:O:92:ILE:HG21	17:Q:60:LEU:CD1	2.26	0.65
20:Y:1:DG:H1'	20:Y:2:DG:H5'	1.79	0.65
21:Z:2:U:P	26:Z:101:GTP:H2'	2.36	0.65
1:A:303:THR:HG1	15:O:377:GLN:HE21	1.45	0.64
1:A:199:THR:CB	15:O:372:LYS:HD2	2.27	0.64
3:C:9:GLU:OE2	3:C:298:ARG:NH1	2.30	0.64
8:H:8:ASP:OD1	8:H:9:ILE:N	2.29	0.64
19:X:-2:DC:N4	19:X:-1:DC:N4	2.46	0.64
19:X:5:DC:O2	19:X:6:DA:H2"	1.98	0.64
1:A:199:THR:HG21	15:O:372:LYS:HD2	1.78	0.64
21:Z:2:U:O5'	26:Z:101:GTP:H2'	1.97	0.64
2:B:254:MET:HE1	2:B:332:CYS:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:177:PHE:CE1	16:P:98:ILE:CD1	2.78	0.64
2:B:741:VAL:HG22	2:B:927:ILE:HB	1.78	0.64
10:J:36:ASP:OD1	10:J:46:ARG:NH1	2.31	0.64
19:X:2:DG:C4'	19:X:3:DC:H5"	2.28	0.64
1:A:485:THR:OG1	1:A:487:ARG:NH1	2.31	0.64
16:P:284:ARG:HD3	17:Q:48:LEU:HA	1.81	0.63
17:Q:80:GLU:N	17:Q:80:GLU:OE1	2.32	0.63
1:A:876:VAL:HG11	2:B:1053:ASP:CG	2.23	0.63
8:H:33:GLU:OE1	8:H:33:GLU:N	2.31	0.63
1:A:159:CYS:O	15:O:531:MET:CA	2.47	0.63
9:I:45:LYS:HB2	9:I:45:LYS:HZ3	1.63	0.63
13:M:221:GLU:HB3	14:N:374:THR:HG21	1.80	0.63
19:X:21:DA:H2"	19:X:22:DT:C6	2.32	0.63
1:A:130:LYS:NZ	15:O:34:GLN:HE21	1.96	0.63
1:A:230:ILE:C	15:O:2:THR:N	2.55	0.63
20:Y:-24:DG:H2"	20:Y:-23:DT:C5	2.34	0.63
1:A:159:CYS:HA	15:O:531:MET:SD	2.38	0.63
1:A:471:LEU:HD22	1:A:538:LEU:HD12	1.81	0.63
2:B:195:ARG:HH12	19:X:9:DT:H73	1.63	0.63
1:A:159:CYS:O	15:O:531:MET:HB3	1.99	0.63
1:A:590:LYS:NZ	8:H:88:PHE:O	2.32	0.63
1:A:203:HIS:HE2	15:O:383:PHE:HZ	1.08	0.62
1:A:499:ASP:OD1	1:A:499:ASP:N	2.32	0.62
1:A:1054:HIS:CD2	1:A:1065:LEU:HD12	2.33	0.62
16:P:151:MET:HE1	16:P:157:PRO:HA	1.81	0.62
19:X:-19:DG:H2"	19:X:-18:DT:C6	2.34	0.62
4:D:33:ASN:OD1	4:D:34:LYS:N	2.32	0.62
19:X:11:DG:C2	20:Y:-10:DG:N2	2.67	0.62
1:A:130:LYS:HE3	15:O:34:GLN:NE2	2.14	0.62
1:A:159:CYS:CA	15:O:531:MET:HB3	2.29	0.62
1:A:384:VAL:HG13	1:A:415:HIS:CD2	2.34	0.62
1:A:760:ARG:NH2	1:A:794:GLN:OE1	2.32	0.62
2:B:1014:HIS:CE1	21:Z:5:U:H4'	2.34	0.62
20:Y:-6:DT:H2'	20:Y:-5:DG:C8	2.35	0.62
1:A:199:THR:OG1	15:O:372:LYS:CD	2.46	0.62
13:M:59:GLU:OE1	13:M:101:THR:HG22	2.00	0.62
1:A:196:SER:O	15:O:373:LYS:CB	2.39	0.62
2:B:633:LEU:HD11	2:B:656:HIS:CD2	2.34	0.62
15:O:270:MET:HE2	15:O:336:ILE:HD11	1.81	0.62
19:X:1:DT:H4'	19:X:2:DG:OP1	1.98	0.62
19:X:23:DA:H2"	19:X:24:DC:C6	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:GLN:NE2	2:B:363:GLU:OE2	2.33	0.61
11:K:64:GLU:OE1	11:K:64:GLU:N	2.33	0.61
19:X:3:DC:H2'	19:X:4:DT:C7	2.30	0.61
1:A:306:ILE:HG13	15:O:396:TYR:CE2	2.34	0.61
1:A:415:HIS:CE1	1:A:480:VAL:HG11	2.35	0.61
7:G:93:SER:OG	7:G:96:GLY:O	2.16	0.61
1:A:1234:ALA:O	1:A:1238:THR:HG23	1.98	0.61
2:B:539:VAL:HG12	2:B:583:VAL:HB	1.82	0.61
2:B:741:VAL:HG21	2:B:1009:TYR:CE1	2.35	0.61
3:C:144:VAL:HG21	3:C:168:VAL:HG13	1.81	0.61
14:N:251:VAL:HG23	14:N:331:ILE:HG21	1.83	0.61
19:X:12:DG:H2'	19:X:13:DC:C6	2.35	0.61
1:A:937:GLU:OE1	1:A:1007:THR:OG1	2.17	0.61
19:X:13:DC:H4'	19:X:14:DA:OP1	2.00	0.61
1:A:231:PRO:HA	15:O:2:THR:CB	2.30	0.61
19:X:-15:DA:H2"	19:X:-14:DA:C8	2.35	0.61
19:X:7:DA:C2'	19:X:8:DT:H73	2.29	0.61
21:Z:2:U:OP2	26:Z:101:GTP:O3'	2.18	0.61
7:G:184:TYR:O	7:G:185:THR:OG1	2.17	0.61
19:X:2:DG:H1'	19:X:3:DC:H5"	1.83	0.61
19:X:19:DA:C2'	19:X:20:DT:C7	2.78	0.61
1:A:225:ASN:HD21	15:O:434:MET:HB2	1.64	0.61
20:Y:11:DC:C2	20:Y:12:DC:C4	2.89	0.61
1:A:773:LYS:O	1:A:774:SER:OG	2.16	0.60
13:M:177:PHE:HE1	16:P:97:GLN:HB3	1.65	0.60
15:O:159:ARG:NH2	15:O:189:LEU:O	2.33	0.60
2:B:915:ASP:OD1	3:C:78:ARG:NH2	2.34	0.60
19:X:7:DA:C4	19:X:8:DT:H72	2.36	0.60
20:Y:-16:DG:H2"	20:Y:-15:DC:H6	1.65	0.60
19:X:8:DT:H6	19:X:8:DT:H5'	1.66	0.60
1:A:158:HIS:O	15:O:533:ARG:HG3	2.01	0.60
20:Y:-28:DT:H2'	20:Y:-27:DT:H72	1.82	0.60
2:B:685:TYR:HE2	24:B:1202:3AT:PG	2.23	0.60
16:P:159:ARG:NH1	16:P:233:GLU:OE2	2.33	0.60
13:M:249:LEU:HD12	13:M:250:MET:HG2	1.82	0.60
16:P:127:LEU:HD13	16:P:150:TYR:CZ	2.37	0.60
16:P:310:MET:HG3	25:P:401:SF4:S2	2.42	0.60
1:A:1319:ALA:O	1:A:1324:THR:HG22	2.02	0.60
4:D:41:ASN:ND2	7:G:35:ALA:O	2.35	0.60
1:A:5:GLN:HB2	7:G:185:THR:HG21	1.84	0.60
1:A:159:CYS:O	15:O:531:MET:CB	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:5:GLU:N	5:E:5:GLU:OE1	2.35	0.59
1:A:232:ALA:HB2	15:O:6:ILE:CD1	2.32	0.59
6:F:110:LEU:HD12	6:F:114:SER:HB3	1.83	0.59
1:A:97:TYR:O	1:A:101:VAL:HG23	2.03	0.59
2:B:1046:ARG:HD3	20:Y:-4:DA:H5'	1.84	0.59
7:G:115:GLN:O	7:G:119:LYS:NZ	2.31	0.59
19:X:2:DG:H4'	19:X:3:DC:H5"	1.85	0.59
20:Y:14:DT:H2"	20:Y:15:DT:H71	1.84	0.59
3:C:93:LEU:HD23	12:L:52:LEU:HD11	1.85	0.59
19:X:3:DC:OP1	19:X:3:DC:H4'	2.01	0.59
20:Y:-22:DA:H2"	20:Y:-21:DT:C6	2.37	0.59
15:O:361:ARG:HH21	15:O:386:ILE:HG23	1.68	0.59
1:A:1125:ASP:OD1	1:A:1126:CYS:N	2.36	0.59
1:A:461:LEU:HD21	2:B:1063:LEU:HD21	1.85	0.58
13:M:412:HIS:O	13:M:416:VAL:HG23	2.03	0.58
1:A:1105:ILE:HG22	1:A:1238:THR:HG21	1.83	0.58
15:O:104:GLU:OE2	17:Q:56:TYR:OH	2.16	0.58
19:X:7:DA:C1'	19:X:8:DT:H72	2.33	0.58
1:A:306:ILE:HG13	15:O:396:TYR:CZ	2.37	0.58
20:Y:6:DT:H4'	20:Y:7:DT:OP1	2.03	0.58
2:B:79:ASN:N	2:B:116:ASP:OD1	2.36	0.58
1:A:772:ASP:OD1	1:A:773:LYS:N	2.36	0.58
14:N:333:LYS:O	14:N:334:SER:OG	2.18	0.58
19:X:17:DA:C2	20:Y:-16:DG:C2	2.92	0.58
1:A:1152:SER:OG	1:A:1200:VAL:O	2.19	0.58
3:C:266:GLU:N	3:C:266:GLU:OE1	2.37	0.58
13:M:53:GLN:OE1	13:M:200:HIS:ND1	2.36	0.58
1:A:111:THR:CG2	15:O:429:LEU:HD21	2.34	0.58
13:M:177:PHE:CG	16:P:98:ILE:CD1	2.87	0.58
16:P:232:MET:SD	16:P:262:SER:OG	2.57	0.58
20:Y:15:DT:H2"	20:Y:16:DC:C5	2.38	0.58
1:A:1214:ILE:HG12	9:I:54:GLY:HA3	1.86	0.58
6:F:84:GLU:N	6:F:86:GLU:OE1	2.36	0.58
15:O:147:THR:HG22	15:O:150:ARG:HH22	1.67	0.58
1:A:159:CYS:CA	15:O:531:MET:SD	2.91	0.58
1:A:196:SER:CA	15:O:373:LYS:HG3	2.33	0.58
1:A:111:THR:HG23	15:O:429:LEU:HD22	1.85	0.57
1:A:303:THR:HG1	15:O:424:TYR:HH	1.12	0.57
2:B:634:ASP:OD1	2:B:635:VAL:N	2.36	0.57
19:X:1:DT:C2'	19:X:2:DG:H3'	2.33	0.57
19:X:19:DA:H2'	19:X:20:DT:C7	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:171:LYS:HB2	16:P:67:ARG:HB3	1.86	0.57
20:Y:-22:DA:H2"	20:Y:-21:DT:H71	1.86	0.57
20:Y:-2:DC:H2'	20:Y:-1:DA:C8	2.37	0.57
8:H:27:ARG:NE	8:H:42:ASP:OD1	2.38	0.57
20:Y:11:DC:C2'	20:Y:12:DC:C5	2.86	0.57
20:Y:13:DT:H2"	20:Y:14:DT:C6	2.39	0.57
1:A:159:CYS:CB	15:O:531:MET:CG	2.83	0.57
1:A:1206:GLU:OE1	1:A:1206:GLU:N	2.38	0.57
16:P:121:THR:OG1	16:P:122:GLU:OE1	2.22	0.57
19:X:1:DT:H2"	19:X:2:DG:C3'	2.32	0.57
21:Z:2:U:O5'	26:Z:101:GTP:O2'	2.21	0.57
1:A:123:LYS:HE2	15:O:68:HIS:HD2	1.68	0.57
5:E:115:LYS:O	5:E:119:VAL:HG23	2.05	0.57
2:B:647:GLU:N	2:B:647:GLU:OE1	2.37	0.56
19:X:-4:DC:H5"	19:X:-4:DC:C6	2.39	0.56
19:X:19:DA:H2'	19:X:20:DT:H71	1.85	0.56
16:P:57:LEU:HD23	16:P:60:MET:HE2	1.87	0.56
16:P:284:ARG:HB3	17:Q:48:LEU:HD13	1.86	0.56
19:X:2:DG:C2'	19:X:3:DC:H5"	2.35	0.56
19:X:5:DC:C2'	19:X:6:DA:H4'	2.35	0.56
16:P:214:HIS:HB3	16:P:260:VAL:HG22	1.87	0.56
19:X:-17:DG:C6	19:X:-16:DG:O6	2.58	0.56
1:A:360:ARG:NH1	20:Y:-3:DG:OP1	2.36	0.56
1:A:361:VAL:HG12	2:B:1072:SER:HB3	1.86	0.56
19:X:24:DC:C2'	19:X:25:DT:C5	2.83	0.56
20:Y:-6:DT:H2'	20:Y:-5:DG:H8	1.69	0.56
19:X:24:DC:C2'	19:X:25:DT:H73	2.24	0.56
1:A:288:PHE:O	1:A:292:VAL:HG23	2.05	0.56
2:B:24:GLU:OE1	2:B:24:GLU:N	2.38	0.56
1:A:868:THR:HG21	1:A:1046:THR:HG23	1.86	0.56
1:A:912:MET:HE3	1:A:917:GLU:C	2.31	0.56
2:B:178:ILE:HG12	2:B:437:THR:HG22	1.88	0.56
8:H:20:LYS:NZ	8:H:22:PHE:O	2.39	0.56
8:H:70:LEU:HD23	8:H:70:LEU:H	1.71	0.56
16:P:42:MET:HG2	16:P:45:ILE:HD12	1.88	0.56
3:C:109:ARG:NH2	3:C:198:LEU:O	2.39	0.55
4:D:88:ASN:O	4:D:90:ARG:NH2	2.40	0.55
13:M:225:LEU:HD11	14:N:376:LEU:HD13	1.89	0.55
15:O:17:PHE:C	17:Q:74:PHE:CD1	2.84	0.55
3:C:49:PHE:CZ	11:K:110:VAL:HG23	2.40	0.55
19:X:7:DA:H2'	19:X:8:DT:H73	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:-12:DC:H2"	20:Y:-11:DC:OP2	2.06	0.55
2:B:205:SER:OG	2:B:320:HIS:N	2.36	0.55
4:D:3:VAL:HG12	7:G:7:MET:HG2	1.88	0.55
21:Z:2:U:P	26:Z:101:GTP:HO3'	2.25	0.55
6:F:104:ILE:O	6:F:120:VAL:HG23	2.07	0.55
2:B:530:GLU:OE1	2:B:530:GLU:N	2.36	0.55
2:B:1039:ARG:N	20:Y:-2:DC:OP1	2.40	0.55
19:X:15:DG:H2"	19:X:16:DC:H6	1.66	0.55
2:B:258:GLU:OE1	2:B:258:GLU:N	2.40	0.55
4:D:114:GLU:OE1	4:D:114:GLU:N	2.38	0.55
19:X:-13:DA:H2"	19:X:-12:DG:C8	2.42	0.55
1:A:104:ILE:HD11	1:A:1333:TYR:HE1	1.70	0.55
1:A:1360:PHE:O	6:F:64:ARG:NH1	2.40	0.55
3:C:130:GLU:OE1	3:C:130:GLU:N	2.40	0.55
7:G:148:ILE:HG23	7:G:190:ILE:HG23	1.88	0.55
19:X:8:DT:H2"	19:X:9:DT:O5'	2.06	0.55
1:A:77:ALA:O	2:B:1033:ARG:NH1	2.40	0.55
2:B:23:VAL:HG23	2:B:26:LYS:HB2	1.89	0.55
2:B:722:THR:HG23	2:B:962:THR:HA	1.87	0.55
13:M:311:LEU:HD21	13:M:415:VAL:HG21	1.88	0.55
13:M:347:GLU:OE2	13:M:351:ARG:NH2	2.40	0.55
20:Y:-15:DC:H2'	20:Y:-14:DT:H72	1.89	0.55
15:O:45:THR:OG1	15:O:49:GLN:OE1	2.25	0.55
19:X:12:DG:N1	20:Y:-11:DC:C5	2.75	0.55
1:A:123:LYS:CD	15:O:68:HIS:HD2	2.19	0.55
15:O:158:GLN:HB2	15:O:187:MET:HE3	1.89	0.55
1:A:302:LYS:C	15:O:396:TYR:OH	2.50	0.54
8:H:28:LEU:HD21	8:H:50:VAL:HG21	1.88	0.54
19:X:-4:DC:H4'	19:X:-3:DA:OP2	2.06	0.54
19:X:-2:DC:N4	19:X:-1:DC:H41	2.05	0.54
2:B:294:GLN:N	2:B:294:GLN:OE1	2.40	0.54
12:L:26:ASN:ND2	12:L:36:CYS:SG	2.78	0.54
20:Y:-1:DA:C6	21:Z:3:G:N1	2.74	0.54
20:Y:14:DT:C2'	20:Y:15:DT:H71	2.37	0.54
1:A:26:GLU:CG	16:P:297:HIS:HB2	2.35	0.54
1:A:438:GLU:N	1:A:438:GLU:OE1	2.38	0.54
19:X:7:DA:H2"	19:X:8:DT:H73	1.88	0.54
20:Y:-12:DC:H1'	20:Y:-11:DC:H5"	1.89	0.54
1:A:529:LEU:HA	1:A:539:ILE:HD13	1.89	0.54
2:B:427:LYS:CD	19:X:-3:DA:H2	2.02	0.54
2:B:1051:GLU:OE1	2:B:1051:GLU:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:17:PHE:HB2	4:D:53:ILE:HG21	1.90	0.54
1:A:130:LYS:NZ	15:O:34:GLN:NE2	2.55	0.54
2:B:209:GLU:N	2:B:209:GLU:OE1	2.41	0.54
3:C:339:GLU:O	3:C:343:VAL:HG23	2.08	0.54
19:X:3:DC:C2'	19:X:4:DT:H5"	2.23	0.54
19:X:13:DC:H2'	19:X:14:DA:C8	2.42	0.54
15:O:374:HIS:HB3	15:O:423:LEU:HD23	1.90	0.54
7:G:33:LYS:C	7:G:34:LEU:HD22	2.33	0.54
19:X:24:DC:C1'	19:X:25:DT:H72	2.34	0.54
15:O:121:VAL:O	15:O:125:VAL:HG23	2.07	0.54
1:A:304:GLN:N	1:A:304:GLN:OE1	2.40	0.53
1:A:1343:VAL:HG21	1:A:1355:ILE:HD13	1.89	0.53
3:C:50:ARG:NH1	3:C:52:ASP:OD2	2.41	0.53
14:N:328:LYS:O	14:N:339:LEU:HD12	2.07	0.53
15:O:349:THR:HG23	16:P:280:THR:HG21	1.89	0.53
15:O:485:GLN:N	15:O:485:GLN:OE1	2.42	0.53
1:A:1185:MET:SD	1:A:1185:MET:N	2.81	0.53
19:X:-17:DG:N2	19:X:-16:DG:C2	2.76	0.53
20:Y:-2:DC:H2'	20:Y:-1:DA:H5"	1.91	0.53
2:B:252:VAL:HG21	9:I:4:PHE:HZ	1.72	0.53
2:B:254:MET:HE3	2:B:333:ILE:HD13	1.90	0.53
19:X:25:DT:H2"	19:X:26:DA:H8	1.73	0.53
2:B:287:ILE:O	2:B:291:VAL:HG23	2.08	0.53
5:E:65:ASN:OD1	5:E:66:ASP:N	2.42	0.53
1:A:155:ILE:HD12	15:O:534:GLN:NE2	2.24	0.53
1:A:1054:HIS:HD2	1:A:1065:LEU:HD12	1.73	0.53
10:J:28:GLU:OE2	13:M:397:GLY:N	2.40	0.53
13:M:13:ILE:HD13	13:M:119:TYR:HE1	1.74	0.53
19:X:19:DA:C2	20:Y:-18:DG:N2	2.77	0.53
1:A:1087:ALA:HA	1:A:1246:THR:HG22	1.91	0.53
13:M:9:VAL:HG23	13:M:10:VAL:HG22	1.91	0.53
20:Y:-1:DA:H2'	20:Y:0:DC:H6	1.70	0.53
1:A:1158:LEU:HD12	1:A:1160:VAL:HG23	1.90	0.53
1:A:1306:PHE:CE2	19:X:11:DG:H4'	2.44	0.53
5:E:39:GLU:OE2	5:E:43:GLN:NE2	2.41	0.53
15:O:350:LEU:O	15:O:354:VAL:HG23	2.09	0.53
20:Y:-3:DG:N2	21:Z:5:U:C2	2.77	0.53
1:A:1158:LEU:HD12	1:A:1160:VAL:CG2	2.39	0.53
2:B:427:LYS:CE	19:X:-3:DA:C2	2.91	0.53
3:C:86:THR:HG21	3:C:227:PRO:HB3	1.90	0.53
15:O:255:VAL:HG21	15:O:267:VAL:HG11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:X:24:DC:C6	19:X:25:DT:H72	2.44	0.53
1:A:1044:PRO:HG2	1:A:1282:ILE:HD11	1.90	0.52
2:B:864:SER:OG	2:B:887:GLN:NE2	2.40	0.52
3:C:89:VAL:HG22	3:C:214:CYS:SG	2.50	0.52
1:A:159:CYS:HB2	15:O:531:MET:SD	2.48	0.52
3:C:188:GLY:O	3:C:191:ARG:NH1	2.42	0.52
10:J:40:LEU:HD11	10:J:49:LEU:HD12	1.91	0.52
14:N:245:LEU:HD12	14:N:246:PRO:HD2	1.90	0.52
2:B:876:GLU:N	2:B:876:GLU:OE1	2.41	0.52
2:B:946:LEU:HD22	2:B:1003:TYR:CZ	2.44	0.52
3:C:133:THR:O	3:C:137:THR:HG22	2.08	0.52
11:K:28:GLU:N	11:K:28:GLU:OE1	2.43	0.52
15:O:20:ILE:HD11	17:Q:75:ILE:HG12	1.92	0.52
19:X:-9:DC:H2"	19:X:-8:DG:C8	2.44	0.52
19:X:-1:DC:OP2	19:X:-1:DC:H2'	2.10	0.52
19:X:18:DC:OP2	19:X:18:DC:H3'	2.09	0.52
19:X:-2:DC:H41	19:X:-1:DC:N4	2.07	0.52
20:Y:14:DT:H2"	20:Y:15:DT:C6	2.45	0.52
1:A:414:VAL:HG12	1:A:416:PRO:HD2	1.90	0.52
1:A:604:ILE:HG23	1:A:682:ARG:HB2	1.91	0.52
2:B:824:LYS:NZ	18:V:18:ASP:OD1	2.42	0.52
19:X:25:DT:H2"	19:X:26:DA:C8	2.44	0.52
2:B:412:THR:O	2:B:416:VAL:HG23	2.10	0.52
3:C:263:GLU:OE2	3:C:274:ARG:NH1	2.41	0.52
15:O:180:LEU:HD23	17:Q:105:ARG:NH2	2.24	0.52
1:A:1363:LEU:HD11	6:F:107:ARG:HH11	1.74	0.52
1:A:589:LEU:HD12	1:A:590:LYS:N	2.26	0.51
20:Y:-22:DA:H2"	20:Y:-21:DT:C5	2.44	0.51
20:Y:9:DG:C8	20:Y:10:DT:H72	2.45	0.51
1:A:123:LYS:CE	15:O:68:HIS:HD2	2.24	0.51
2:B:901:HIS:NE2	2:B:945:GLU:OE1	2.40	0.51
3:C:97:ASN:ND2	3:C:103:ASP:OD1	2.42	0.51
14:N:367:ASP:OD1	14:N:368:SER:N	2.43	0.51
1:A:1264:ARG:NE	1:A:1292:ASP:OD1	2.43	0.51
3:C:326:ILE:HG21	11:K:111:LEU:HB2	1.92	0.51
14:N:254:LEU:HD12	14:N:331:ILE:HD11	1.93	0.51
19:X:-16:DG:H2"	19:X:-15:DA:C8	2.45	0.51
19:X:18:DC:H3'	19:X:18:DC:P	2.51	0.51
1:A:26:GLU:OE1	1:A:26:GLU:N	2.41	0.51
19:X:-19:DG:H2"	19:X:-18:DT:H71	1.91	0.51
1:A:160:GLY:HA3	15:O:532:LYS:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:PRO:HG2	2:B:419:ILE:HD12	1.90	0.51
19:X:-19:DG:C2'	19:X:-18:DT:C7	2.85	0.51
1:A:918:PRO:C	1:A:919:LEU:HD12	2.35	0.51
3:C:155:ASP:HB3	13:M:348:VAL:HG21	1.92	0.51
15:O:486:GLU:N	15:O:486:GLU:OE1	2.43	0.51
20:Y:6:DT:P	20:Y:6:DT:H3'	2.50	0.51
1:A:428:MET:HA	1:A:428:MET:HE2	1.93	0.51
13:M:177:PHE:CD1	16:P:98:ILE:HG13	2.36	0.51
16:P:91:GLN:OE1	16:P:91:GLN:N	2.43	0.51
20:Y:5:DT:P	20:Y:5:DT:H3'	2.51	0.51
2:B:257:THR:O	2:B:262:MET:HE1	2.11	0.51
3:C:115:ILE:HG22	3:C:117:ALA:H	1.76	0.51
13:M:215:ASP:OD1	13:M:216:SER:N	2.42	0.51
19:X:11:DG:C6	20:Y:-11:DC:N4	2.58	0.51
20:Y:-18:DG:H2"	20:Y:-17:DT:O5'	2.09	0.51
2:B:68:ASP:OD1	2:B:69:ALA:N	2.44	0.51
3:C:144:VAL:HG11	3:C:168:VAL:HG22	1.93	0.51
19:X:22:DT:H2"	19:X:23:DA:C8	2.46	0.51
1:A:159:CYS:HA	15:O:531:MET:CB	2.37	0.50
1:A:300:GLY:HA3	15:O:389:LYS:HA	1.93	0.50
7:G:189:SER:C	7:G:190:ILE:HD12	2.36	0.50
19:X:-3:DA:OP2	19:X:-3:DA:H3'	2.12	0.50
1:A:197:PHE:CD2	15:O:374:HIS:CG	3.00	0.50
3:C:236:LEU:HD12	3:C:307:ILE:HD11	1.94	0.50
13:M:134:GLN:OE1	13:M:136:ARG:NH2	2.43	0.50
13:M:327:VAL:O	13:M:353:ARG:NH1	2.42	0.50
20:Y:-16:DG:C4	20:Y:-15:DC:C4	2.99	0.50
1:A:214:ALA:HB1	15:O:407:GLN:HE21	1.75	0.50
2:B:105:ARG:NH2	2:B:873:SER:O	2.44	0.50
7:G:152:VAL:HG22	7:G:189:SER:OG	2.11	0.50
26:Z:101:GTP:O1A	26:Z:101:GTP:H8	1.93	0.50
1:A:232:ALA:HB1	15:O:30:ARG:HG3	1.93	0.50
2:B:106:ASP:OD1	2:B:882:LYS:NZ	2.33	0.50
4:D:102:GLU:OE1	4:D:102:GLU:N	2.43	0.50
20:Y:-23:DT:H2"	20:Y:-22:DA:C8	2.47	0.50
3:C:236:LEU:HD13	3:C:305:HIS:CE1	2.46	0.50
3:C:319:ASP:OD1	3:C:320:VAL:N	2.45	0.50
5:E:59:THR:OG1	5:E:71:GLN:OE1	2.29	0.50
13:M:56:VAL:N	13:M:104:SER:OG	2.44	0.50
18:V:21:TYR:O	18:V:22:SER:OG	2.27	0.50
20:Y:-21:DT:H2"	20:Y:-20:DA:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:-20:DA:H2"	20:Y:-19:DT:C5'	2.42	0.50
2:B:315:SER:O	2:B:319:THR:HG22	2.11	0.50
19:X:19:DA:H2"	19:X:20:DT:C6	2.46	0.50
1:A:231:PRO:HA	15:O:2:THR:CG2	2.42	0.50
15:O:59:GLN:HG2	17:Q:73:TYR:CE1	2.47	0.50
19:X:-21:DT:H2"	19:X:-20:DT:C5'	2.42	0.50
20:Y:-24:DG:C2'	20:Y:-23:DT:C5	2.94	0.50
1:A:232:ALA:HB2	15:O:6:ILE:HD12	1.94	0.50
8:H:111:ARG:C	8:H:112:LEU:HD12	2.37	0.50
15:O:510:ASP:HB2	17:Q:58:LEU:CD1	2.42	0.50
19:X:21:DA:C2	20:Y:-20:DA:C2	2.99	0.50
20:Y:-1:DA:H2"	20:Y:0:DC:H5'	1.93	0.50
1:A:56:LEU:HA	1:A:260:LEU:HD21	1.93	0.49
1:A:756:LEU:HD21	1:A:828:PRO:HB3	1.94	0.49
1:A:1272:GLN:O	1:A:1276:VAL:HG23	2.12	0.49
1:A:539:ILE:HG22	1:A:680:MET:HE1	1.94	0.49
2:B:524:ASN:O	13:M:134:GLN:NE2	2.44	0.49
1:A:155:ILE:HD12	15:O:534:GLN:CD	2.37	0.49
3:C:102:GLN:HE22	10:J:1:MET:HE1	1.76	0.49
3:C:324:GLU:O	3:C:328:VAL:HG23	2.12	0.49
1:A:159:CYS:C	15:O:531:MET:HB3	2.36	0.49
1:A:1043:GLU:OE2	1:A:1047:GLN:NE2	2.45	0.49
2:B:746:TYR:O	2:B:747:SER:OG	2.23	0.49
2:B:1079:VAL:HB	2:B:1128:LEU:HD11	1.94	0.49
13:M:11:GLN:CB	14:N:331:ILE:HD12	2.43	0.49
19:X:17:DA:C4'	19:X:18:DC:H5'	2.42	0.49
7:G:46:ILE:HB	7:G:75:VAL:HG23	1.95	0.49
3:C:49:PHE:HZ	11:K:110:VAL:HG23	1.78	0.49
1:A:1303:ILE:O	1:A:1303:ILE:HG22	2.12	0.49
2:B:29:LEU:HG	2:B:611:MET:HE1	1.95	0.49
8:H:95:LYS:C	8:H:116:VAL:HG13	2.36	0.49
20:Y:-20:DA:OP2	20:Y:-20:DA:H3'	2.13	0.49
20:Y:6:DT:H1'	20:Y:7:DT:C6	2.48	0.49
2:B:946:LEU:HD23	2:B:946:LEU:C	2.38	0.49
17:Q:54:GLU:OE1	17:Q:54:GLU:N	2.42	0.49
17:Q:83:ASP:OD1	17:Q:84:ILE:N	2.45	0.49
1:A:838:PHE:O	2:B:677:HIS:ND1	2.42	0.49
2:B:692:GLN:NE2	21:Z:4:C:O3'	2.45	0.49
16:P:104:ASN:HA	16:P:151:MET:HE3	1.95	0.49
20:Y:-1:DA:C4	21:Z:3:G:N2	2.80	0.49
1:A:631:LEU:HD11	8:H:115:TYR:HE2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:LYS:NZ	2:B:420:SER:O	2.46	0.48
20:Y:-3:DG:H2"	20:Y:-2:DC:H5'	1.94	0.48
20:Y:-28:DT:C2'	20:Y:-27:DT:H72	2.43	0.48
1:A:669:ARG:NH2	1:A:910:ALA:O	2.45	0.48
16:P:142:VAL:HG23	16:P:170:GLN:HA	1.95	0.48
19:X:2:DG:H4'	19:X:3:DC:C5'	2.42	0.48
20:Y:13:DT:H2"	20:Y:14:DT:H71	1.95	0.48
1:A:303:THR:N	15:O:377:GLN:HE22	2.11	0.48
8:H:14:ASP:OD1	8:H:15:ILE:N	2.46	0.48
1:A:405:ARG:NH1	1:A:441:ALA:O	2.47	0.48
12:L:19:CYS:SG	12:L:20:GLY:N	2.86	0.48
20:Y:12:DC:H2'	20:Y:13:DT:H72	1.94	0.48
3:C:133:THR:OG1	3:C:136:ASP:OD1	2.31	0.48
1:A:76:LEU:O	2:B:1033:ARG:NH2	2.47	0.48
8:H:112:LEU:HD13	8:H:129:ALA:HB2	1.96	0.48
20:Y:2:DG:H2"	20:Y:3:DT:C6	2.49	0.48
1:A:728:ILE:HD13	1:A:748:LEU:HD21	1.93	0.48
3:C:336:PHE:HE1	11:K:44:LEU:HD22	1.79	0.48
5:E:85:LYS:O	5:E:89:VAL:HG23	2.13	0.48
15:O:377:GLN:HE21	15:O:424:TYR:HH	1.59	0.48
16:P:98:ILE:HD13	16:P:115:LYS:HD3	1.95	0.48
19:X:1:DT:H2"	19:X:2:DG:O5'	2.14	0.48
1:A:579:ILE:O	11:K:83:ARG:NH2	2.46	0.48
1:A:1102:LYS:HB2	1:A:1212:ILE:HD11	1.96	0.48
2:B:946:LEU:HD22	2:B:1003:TYR:CE2	2.48	0.48
15:O:359:GLY:HA3	17:Q:43:TYR:OH	2.14	0.48
1:A:111:THR:O	15:O:433:ARG:NE	2.47	0.48
2:B:536:VAL:O	2:B:581:ARG:NH1	2.47	0.48
8:H:103:GLU:N	8:H:103:GLU:OE1	2.47	0.47
11:K:73:THR:OG1	11:K:77:GLU:OE2	2.27	0.47
1:A:415:HIS:O	1:A:453:HIS:ND1	2.47	0.47
2:B:923:ILE:HD11	10:J:42:ARG:HB2	1.95	0.47
2:B:1118:GLN:HA	2:B:1123:ILE:HD13	1.96	0.47
13:M:177:PHE:CD1	16:P:98:ILE:CD1	2.97	0.47
13:M:409:ILE:HG23	13:M:416:VAL:HG21	1.96	0.47
15:O:512:SER:O	15:O:516:VAL:HG23	2.13	0.47
20:Y:-20:DA:H3'	20:Y:-20:DA:P	2.54	0.47
20:Y:-16:DG:C6	20:Y:-15:DC:N4	2.82	0.47
2:B:89:GLU:OE1	2:B:90:SER:N	2.47	0.47
2:B:235:PRO:HD2	2:B:238:ILE:HD12	1.95	0.47
15:O:443:ILE:HD12	15:O:520:ILE:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:-22:DA:H2"	20:Y:-21:DT:C7	2.44	0.47
1:A:231:PRO:CA	15:O:2:THR:HG23	2.42	0.47
2:B:103:ARG:NE	2:B:175:GLU:OE2	2.45	0.47
24:B:1202:3AT:H2'1	24:B:1202:3AT:N3	2.27	0.47
6:F:84:GLU:N	6:F:84:GLU:OE1	2.47	0.47
15:O:159:ARG:NH1	15:O:186:ASP:OD2	2.46	0.47
2:B:246:GLU:OE2	2:B:280:GLN:N	2.46	0.47
2:B:631:GLU:OE2	2:B:656:HIS:NE2	2.44	0.47
1:A:503:ASP:OD1	21:Z:6:C:H4'	2.15	0.47
2:B:252:VAL:HG21	9:I:4:PHE:CZ	2.49	0.47
5:E:50:GLU:OE2	5:E:56:THR:OG1	2.31	0.47
15:O:93:TYR:CE1	17:Q:53:GLY:HA2	2.50	0.47
16:P:243:ILE:CG1	16:P:248:VAL:HG23	2.44	0.47
19:X:-12:DG:H2"	19:X:-11:DG:H8	1.77	0.47
19:X:26:DA:H2"	19:X:27:DA:N7	2.29	0.47
20:Y:-2:DC:C2'	20:Y:-1:DA:H5"	2.45	0.47
20:Y:20:DA:H1'	20:Y:21:DA:H5'	1.97	0.47
21:Z:2:U:H2'	21:Z:3:G:C5'	2.45	0.47
1:A:308:GLU:OE1	15:O:417:PRO:HG2	2.15	0.47
14:N:251:VAL:HG11	14:N:335:GLY:HA2	1.97	0.47
15:O:381:GLU:OE2	15:O:392:LYS:NZ	2.28	0.47
1:A:459:VAL:HG21	1:A:520:LEU:HB2	1.96	0.47
15:O:161:PRO:O	17:Q:105:ARG:NH2	2.48	0.47
15:O:274:SER:OG	15:O:285:THR:OG1	2.14	0.47
1:A:366:ARG:CD	20:Y:-3:DG:H4'	2.45	0.47
2:B:195:ARG:HH12	19:X:9:DT:C7	2.29	0.47
15:O:16:HIS:CG	17:Q:68:MET:HE3	2.50	0.47
20:Y:-20:DA:H2"	20:Y:-19:DT:C6	2.50	0.47
8:H:27:ARG:HD2	8:H:40:ILE:HG22	1.97	0.46
15:O:16:HIS:CG	17:Q:68:MET:CE	2.98	0.46
15:O:17:PHE:O	17:Q:74:PHE:CD1	2.67	0.46
1:A:231:PRO:N	15:O:2:THR:HG23	2.31	0.46
1:A:555:LYS:HG2	8:H:25:VAL:HG21	1.97	0.46
19:X:-1:DC:H2"	19:X:0:DG:H4'	1.98	0.46
19:X:12:DG:N2	20:Y:-11:DC:C6	2.82	0.46
20:Y:1:DG:C2	20:Y:2:DG:C5	3.03	0.46
1:A:258:PRO:HB2	1:A:262:ILE:HD12	1.96	0.46
9:I:46:LEU:H	9:I:46:LEU:HD22	1.81	0.46
15:O:180:LEU:HD21	17:Q:105:ARG:CZ	2.44	0.46
15:O:265:GLU:OE1	15:O:268:ARG:NH1	2.48	0.46
16:P:292:VAL:O	16:P:292:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:LEU:HD12	1:A:584:PRO:HD2	1.98	0.46
1:A:927:ASN:O	1:A:931:VAL:HG23	2.16	0.46
3:C:28:ASP:O	11:K:61:LYS:NZ	2.48	0.46
4:D:79:THR:HG23	4:D:82:GLU:H	1.79	0.46
4:D:95:VAL:HG11	7:G:198:LEU:HD22	1.98	0.46
19:X:6:DA:N3	19:X:6:DA:H2'	2.30	0.46
1:A:112:CYS:HA	15:O:433:ARG:CZ	2.45	0.46
2:B:25:GLU:O	2:B:611:MET:HE2	2.15	0.46
3:C:86:THR:OG1	3:C:225:PHE:O	2.33	0.46
8:H:136:GLU:O	8:H:139:SER:OG	2.32	0.46
1:A:590:LYS:HB3	1:A:591:PRO:HD3	1.97	0.46
2:B:478:MET:C	2:B:479:LEU:HD12	2.41	0.46
13:M:117:ALA:HB1	13:M:124:LEU:HD11	1.97	0.46
15:O:287:PRO:HB2	15:O:333:MET:HE3	1.98	0.46
16:P:168:SER:OG	16:P:173:GLU:OE2	2.32	0.46
19:X:8:DT:H2'	19:X:9:DT:H72	1.98	0.46
1:A:1140:LEU:HD23	9:I:49:VAL:HG13	1.98	0.46
3:C:316:LEU:HD21	3:C:321:LEU:HD21	1.97	0.45
7:G:187:VAL:HG13	7:G:188:GLY:H	1.81	0.45
11:K:63:PRO:O	11:K:87:ARG:NE	2.42	0.45
1:A:533:ARG:NH1	1:A:1043:GLU:OE1	2.50	0.45
1:A:953:MET:HE3	1:A:970:LYS:HE3	1.98	0.45
7:G:146:GLU:N	7:G:146:GLU:OE1	2.49	0.45
19:X:17:DA:H4'	19:X:18:DC:OP1	2.15	0.45
1:A:940:LEU:HB2	1:A:1006:ILE:HG23	1.99	0.45
2:B:335:THR:O	2:B:339:VAL:HG23	2.17	0.45
5:E:94:MET:HE2	5:E:94:MET:HA	1.98	0.45
20:Y:1:DG:C2	20:Y:2:DG:C4	3.05	0.45
1:A:221:LEU:HB3	15:O:402:ASN:HD21	1.80	0.45
2:B:506:MET:HE2	2:B:587:SER:O	2.17	0.45
2:B:518:LEU:HD21	2:B:558:THR:HG21	1.97	0.45
20:Y:-27:DT:H2"	20:Y:-26:DT:C7	2.46	0.45
21:Z:2:U:C5'	26:Z:101:GTP:O2'	2.65	0.45
1:A:15:ILE:HD13	1:A:1349:MET:HE2	1.98	0.45
1:A:466:PRO:HD3	20:Y:-5:DG:H21	1.81	0.45
13:M:161:SER:OG	13:M:164:ASP:OD1	2.35	0.45
1:A:987:TYR:OH	8:H:102:ASP:N	2.49	0.45
5:E:35:GLN:NE2	5:E:39:GLU:OE1	2.49	0.45
13:M:177:PHE:CG	16:P:98:ILE:HD11	2.50	0.45
19:X:11:DG:H2"	19:X:12:DG:O5'	2.16	0.45
1:A:203:HIS:CE1	15:O:383:PHE:CE2	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:VAL:HG13	1:A:415:HIS:HD2	1.79	0.45
1:A:756:LEU:HD22	1:A:833:PHE:CE1	2.52	0.45
1:A:792:ILE:HG23	1:A:796:ILE:HD12	1.99	0.45
19:X:8:DT:H5'	19:X:8:DT:C6	2.47	0.45
1:A:160:GLY:HA3	15:O:532:LYS:HB2	1.98	0.45
2:B:171:VAL:O	2:B:174:VAL:HG22	2.16	0.45
2:B:1021:HIS:NE2	2:B:1043:GLY:O	2.46	0.45
19:X:19:DA:H2"	19:X:20:DT:C7	2.40	0.45
13:M:276:LEU:O	13:M:281:GLN:NE2	2.50	0.45
16:P:231:SER:OG	16:P:233:GLU:OE2	2.34	0.45
19:X:18:DC:H1'	19:X:19:DA:N7	2.31	0.45
20:Y:-3:DG:H2'	20:Y:-2:DC:O4'	2.16	0.45
2:B:1028:ARG:NH1	2:B:1072:SER:O	2.50	0.45
15:O:510:ASP:HB2	17:Q:58:LEU:HD13	1.99	0.44
1:A:301:ALA:O	15:O:392:LYS:HD3	2.17	0.44
1:A:1332:ALA:HB2	2:B:1122:ILE:HG23	1.99	0.44
2:B:934:PHE:O	2:B:938:MET:N	2.44	0.44
2:B:218:VAL:HG22	2:B:218:VAL:O	2.16	0.44
3:C:134:GLU:O	3:C:181:GLN:NE2	2.47	0.44
15:O:56:VAL:HG23	17:Q:73:TYR:HD1	1.81	0.44
15:O:257:ASN:O	16:P:274:ASN:HB2	2.17	0.44
20:Y:-5:DG:H2'	20:Y:-4:DA:O4'	2.18	0.44
1:A:872:GLN:O	1:A:876:VAL:HG23	2.18	0.44
12:L:16:ILE:HD11	12:L:25:GLU:HB3	1.98	0.44
20:Y:3:DT:H4'	20:Y:4:DG:OP1	2.16	0.44
1:A:386:VAL:HG13	2:B:1022:ALA:HB2	2.00	0.44
1:A:577:GLU:HB3	11:K:29:MET:HE1	1.99	0.44
1:A:731:LEU:HD23	1:A:748:LEU:HD22	1.98	0.44
3:C:287:ILE:HD11	3:C:293:LEU:HB3	1.99	0.44
19:X:-15:DA:H2"	19:X:-14:DA:H8	1.79	0.44
19:X:-13:DA:H2"	19:X:-12:DG:H8	1.82	0.44
11:K:55:LEU:O	11:K:59:ILE:HG22	2.17	0.44
13:M:177:PHE:CE1	16:P:97:GLN:HB3	2.49	0.44
19:X:-17:DG:C2	19:X:-16:DG:C4	3.06	0.44
19:X:19:DA:H2"	19:X:20:DT:OP2	2.18	0.44
1:A:356:LEU:HD11	2:B:1113:LEU:HD22	1.99	0.44
13:M:171:LYS:HZ1	16:P:67:ARG:HB2	1.78	0.44
15:O:507:ASN:OD1	17:Q:62:GLN:NE2	2.47	0.44
19:X:-17:DG:C6	19:X:-16:DG:C6	3.06	0.44
19:X:19:DA:C2'	19:X:20:DT:C5	3.01	0.44
1:A:464:ARG:HH22	24:B:1202:3AT:H1'	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:18:GLU:N	8:H:18:GLU:OE1	2.51	0.44
1:A:303:THR:N	15:O:377:GLN:NE2	2.66	0.44
2:B:471:LEU:HD21	2:B:481:PRO:HB3	1.99	0.44
8:H:41:LEU:HG	8:H:43:VAL:HG13	1.99	0.44
13:M:37:MET:SD	13:M:37:MET:N	2.91	0.44
19:X:20:DT:H2"	19:X:21:DA:C8	2.53	0.44
1:A:196:SER:HA	15:O:373:LYS:HG3	1.99	0.43
1:A:221:LEU:C	15:O:402:ASN:HD21	2.25	0.43
1:A:262:ILE:HD11	2:B:1115:GLN:HB3	1.99	0.43
1:A:39:LYS:HE3	17:Q:30:VAL:HG12	1.99	0.43
1:A:739:GLN:HG3	1:A:747:THR:HG23	2.00	0.43
1:A:1164:ASP:OD1	1:A:1178:ARG:NE	2.44	0.43
3:C:239:ILE:HD12	3:C:239:ILE:N	2.33	0.43
5:E:167:GLU:O	5:E:208:LEU:HD22	2.18	0.43
15:O:16:HIS:CB	17:Q:68:MET:HE3	2.48	0.43
19:X:-14:DA:H2"	19:X:-13:DA:H8	1.74	0.43
1:A:934:CYS:O	1:A:1005:ARG:NH2	2.45	0.43
1:A:996:GLU:HB3	1:A:997:PRO:HD3	2.01	0.43
1:A:1007:THR:HG23	1:A:1010:GLN:H	1.83	0.43
2:B:113:ILE:HD11	2:B:136:MET:HG2	2.01	0.43
2:B:145:CYS:O	2:B:148:THR:HG22	2.18	0.43
3:C:57:ASP:N	3:C:57:ASP:OD1	2.50	0.43
5:E:19:GLN:OE1	5:E:138:ASN:ND2	2.51	0.43
16:P:313:TRP:HZ2	17:Q:48:LEU:HD21	1.83	0.43
19:X:21:DA:C2'	19:X:22:DT:C5	2.88	0.43
1:A:631:LEU:HD11	8:H:124:ARG:HD3	2.01	0.43
1:A:864:LYS:NZ	1:A:1048:MET:O	2.47	0.43
2:B:751:ILE:O	2:B:930:ASN:ND2	2.52	0.43
4:D:11:LEU:HD23	4:D:11:LEU:H	1.84	0.43
15:O:75:TYR:OH	17:Q:110:MET:HE1	2.18	0.43
15:O:531:MET:O	15:O:533:ARG:NH1	2.51	0.43
19:X:-4:DC:H2"	19:X:-3:DA:OP1	2.19	0.43
19:X:19:DA:C8	19:X:19:DA:H5'	2.54	0.43
1:A:599:GLN:O	1:A:603:VAL:HG23	2.18	0.43
15:O:106:ILE:O	15:O:110:LEU:HD23	2.19	0.43
15:O:193:LEU:HD22	15:O:229:PRO:HG2	2.00	0.43
2:B:301:PRO:O	2:B:304:THR:HG23	2.19	0.43
3:C:109:ARG:NH1	10:J:3:ILE:O	2.49	0.43
8:H:9:ILE:N	8:H:9:ILE:HD12	2.33	0.43
2:B:352:ASP:OD1	2:B:353:ASP:N	2.52	0.43
10:J:33:ASP:OD1	10:J:34:ALA:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:X:5:DC:H2"	19:X:6:DA:C4'	2.46	0.43
19:X:12:DG:C2	20:Y:-11:DC:C5	3.07	0.43
20:Y:-20:DA:C2'	20:Y:-19:DT:C6	3.02	0.43
1:A:217:ASN:OD1	15:O:407:GLN:O	2.37	0.43
2:B:812:ASP:OD2	12:L:46:LYS:NZ	2.52	0.43
2:B:848:GLN:OE1	2:B:848:GLN:N	2.46	0.43
1:A:130:LYS:HE3	15:O:34:GLN:HE22	1.83	0.42
2:B:746:TYR:HE2	2:B:911:VAL:HG11	1.84	0.42
16:P:243:ILE:HD11	16:P:250:MET:HB2	2.01	0.42
20:Y:1:DG:C6	20:Y:2:DG:C6	3.07	0.42
3:C:246:GLU:N	3:C:246:GLU:OE1	2.52	0.42
9:I:45:LYS:HB2	9:I:45:LYS:HZ2	1.80	0.42
15:O:464:SER:HA	15:O:467:VAL:HG22	2.01	0.42
20:Y:19:DC:H2"	20:Y:20:DA:C8	2.54	0.42
2:B:467:GLY:H	2:B:468:PRO:HD2	1.84	0.42
15:O:182:ILE:HD11	15:O:187:MET:SD	2.59	0.42
19:X:-1:DC:OP2	19:X:-1:DC:H6	2.01	0.42
21:Z:2:U:C2'	21:Z:3:G:H5'	2.49	0.42
1:A:160:GLY:C	15:O:532:LYS:HE2	2.44	0.42
14:N:143:GLU:OE1	14:N:143:GLU:N	2.44	0.42
19:X:-11:DG:H2"	19:X:-10:DA:C8	2.54	0.42
20:Y:-17:DT:H2"	20:Y:-16:DG:C8	2.55	0.42
20:Y:-16:DG:H2"	20:Y:-15:DC:C5	2.53	0.42
20:Y:20:DA:H2"	20:Y:21:DA:O5'	2.19	0.42
2:B:521:GLU:OE1	2:B:521:GLU:N	2.48	0.42
15:O:463:LYS:HD3	15:O:490:MET:HE1	2.02	0.42
2:B:883:MET:SD	2:B:883:MET:N	2.92	0.42
3:C:334:ARG:NH2	11:K:104:MET:SD	2.93	0.42
16:P:181:ASN:HB3	16:P:242:LEU:HD21	2.00	0.42
1:A:366:ARG:HB2	2:B:1045:LEU:HD11	2.00	0.42
2:B:392:ILE:N	2:B:393:PRO:CD	2.83	0.42
2:B:430:LYS:HG3	19:X:3:DC:H1'	2.02	0.42
7:G:114:LEU:HD23	7:G:114:LEU:H	1.84	0.42
20:Y:-16:DG:C2'	20:Y:-15:DC:C5	3.03	0.42
20:Y:-1:DA:C6	21:Z:3:G:C6	3.08	0.42
1:A:66:ASP:OD1	1:A:67:ARG:N	2.53	0.42
15:O:134:GLU:N	15:O:134:GLU:OE1	2.53	0.42
1:A:1214:ILE:HG22	1:A:1223:TYR:CD1	2.55	0.42
2:B:692:GLN:OE1	2:B:1014:HIS:NE2	2.51	0.42
1:A:897:ILE:HD11	5:E:165:LEU:HD21	2.02	0.41
7:G:57:ALA:CB	7:G:68:THR:HG22	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:187:VAL:HG13	7:G:188:GLY:N	2.34	0.41
15:O:429:LEU:HD21	15:O:433:ARG:HE	1.84	0.41
21:Z:4:C:H2'	21:Z:5:U:C6	2.55	0.41
14:N:269:LEU:O	14:N:269:LEU:HD12	2.20	0.41
21:Z:2:U:C4'	26:Z:101:GTP:HO2'	2.32	0.41
1:A:159:CYS:O	15:O:532:LYS:N	2.49	0.41
2:B:417:ASN:O	2:B:421:THR:OG1	2.37	0.41
3:C:221:ASP:OD2	12:L:58:ARG:NH2	2.54	0.41
13:M:173:ILE:HG22	13:M:175:VAL:HG22	2.01	0.41
1:A:155:ILE:CB	15:O:534:GLN:NE2	2.80	0.41
1:A:520:LEU:HD23	6:F:90:LEU:HD21	2.02	0.41
1:A:604:ILE:HG23	1:A:682:ARG:CB	2.50	0.41
4:D:42:LEU:HD11	7:G:31:ASN:HB3	2.03	0.41
20:Y:-1:DA:H8	20:Y:-1:DA:H5"	1.86	0.41
1:A:349:GLN:OE1	1:A:349:GLN:N	2.54	0.41
8:H:4:ILE:HG23	8:H:59:VAL:HG13	2.03	0.41
15:O:276:ILE:HD12	15:O:276:ILE:N	2.35	0.41
19:X:-17:DG:N2	19:X:-16:DG:C4	2.88	0.41
2:B:208:HIS:O	2:B:208:HIS:ND1	2.54	0.41
14:N:251:VAL:HG23	14:N:331:ILE:CG2	2.49	0.41
1:A:463:ASN:OD1	1:A:464:ARG:N	2.53	0.41
1:A:464:ARG:NH2	21:Z:6:C:O2'	2.53	0.41
1:A:542:ILE:HG13	1:A:543:GLN:H	1.86	0.41
1:A:581:VAL:HG21	11:K:67:PHE:CE1	2.56	0.41
2:B:460:GLU:O	2:B:461:LYS:C	2.63	0.41
3:C:299:LEU:HD12	3:C:299:LEU:H	1.85	0.41
15:O:443:ILE:HD12	15:O:520:ILE:HD12	2.03	0.41
16:P:48:GLN:O	16:P:52:VAL:HG23	2.21	0.41
16:P:161:VAL:HG23	16:P:162:THR:HG22	2.03	0.41
19:X:-10:DA:H2"	19:X:-9:DC:C6	2.56	0.41
1:A:36:VAL:HG13	1:A:54:GLY:C	2.45	0.41
1:A:1081:SER:O	1:A:1082:THR:OG1	2.33	0.41
2:B:596:TYR:CE1	2:B:643:ILE:HD13	2.56	0.41
2:B:952:GLY:O	2:B:956:GLY:N	2.54	0.41
15:O:59:GLN:HG2	17:Q:73:TYR:HE1	1.85	0.41
15:O:497:GLN:O	15:O:501:THR:HG23	2.21	0.41
20:Y:12:DC:H2"	20:Y:13:DT:C6	2.56	0.41
21:Z:2:U:O5'	21:Z:2:U:H6	2.02	0.41
1:A:468:LEU:HD22	1:A:1046:THR:HG21	2.03	0.41
1:A:1109:LEU:HD12	1:A:1198:LYS:O	2.19	0.41
2:B:1014:HIS:CE1	21:Z:5:U:C4'	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:93:LEU:HD12	3:C:93:LEU:N	2.36	0.41
11:K:96:PHE:CE2	11:K:100:LEU:HD11	2.55	0.41
15:O:17:PHE:O	17:Q:74:PHE:HA	2.20	0.41
15:O:55:CYS:SG	15:O:56:VAL:N	2.94	0.41
16:P:176:PHE:CE2	16:P:180:LEU:HD11	2.56	0.41
16:P:243:ILE:HG13	16:P:248:VAL:HG23	2.02	0.41
16:P:289:LEU:CD1	17:Q:45:PRO:HA	2.50	0.41
20:Y:-1:DA:C2	21:Z:3:G:C2	3.09	0.41
2:B:577:ASN:O	2:B:581:ARG:N	2.53	0.41
2:B:977:VAL:HG23	3:C:286:GLU:HG3	2.03	0.41
14:N:330:LEU:N	14:N:330:LEU:HD12	2.36	0.41
19:X:12:DG:H2'	19:X:13:DC:H6	1.83	0.41
19:X:19:DA:H2"	19:X:20:DT:C5	2.55	0.41
1:A:1058:VAL:HG23	1:A:1060:SER:H	1.87	0.40
13:M:64:THR:HG21	13:M:96:LEU:HD13	2.03	0.40
1:A:30:GLN:NE2	2:B:1094:TYR:O	2.54	0.40
1:A:219:ASN:OD1	1:A:222:VAL:HG23	2.21	0.40
1:A:251:ILE:N	1:A:251:ILE:HD12	2.36	0.40
1:A:461:LEU:HD23	1:A:473:ILE:HD11	2.03	0.40
2:B:103:ARG:NH2	2:B:168:TYR:OH	2.54	0.40
7:G:127:TRP:O	7:G:128:VAL:HG23	2.20	0.40
7:G:158:VAL:HG23	7:G:159:ASP:N	2.37	0.40
1:A:1089:LEU:HD21	1:A:1225:LEU:HG	2.03	0.40
1:A:1242:LYS:O	1:A:1246:THR:HG23	2.21	0.40
8:H:56:PHE:CG	8:H:145:MET:HE3	2.56	0.40
1:A:130:LYS:HE2	15:O:34:GLN:HE21	1.74	0.40
1:A:221:LEU:HB3	15:O:402:ASN:ND2	2.35	0.40
2:B:896:LYS:NZ	21:Z:6:C:OP1	2.54	0.40
3:C:299:LEU:HD12	3:C:299:LEU:N	2.37	0.40
5:E:154:GLU:OE1	5:E:154:GLU:N	2.47	0.40
13:M:218:SER:HA	14:N:374:THR:HG23	2.02	0.40
15:O:90:ARG:HA	17:Q:57:MET:HE3	2.04	0.40
19:X:11:DG:H2"	19:X:12:DG:H8	1.87	0.40
1:A:199:THR:HG21	15:O:372:LYS:CD	2.47	0.40
1:A:907:LEU:HD12	1:A:912:MET:HE1	2.03	0.40
2:B:563:ARG:NH2	2:B:637:GLU:OE2	2.47	0.40
2:B:722:THR:H	2:B:725:ILE:HD12	1.86	0.40
15:O:469:ALA:HA	15:O:472:ALA:HB3	2.04	0.40
15:O:491:ILE:HG22	15:O:491:ILE:O	2.21	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	1376/1390 (99%)	1349 (98%)	27 (2%)	0	100	100
2	B	1101/1133 (97%)	1076 (98%)	25 (2%)	0	100	100
3	C	341/346 (99%)	336 (98%)	5 (2%)	0	100	100
4	D	120/148 (81%)	117 (98%)	3 (2%)	0	100	100
5	E	207/210 (99%)	202 (98%)	5 (2%)	0	100	100
6	F	74/127 (58%)	70 (95%)	4 (5%)	0	100	100
7	G	160/204 (78%)	146 (91%)	14 (9%)	0	100	100
8	H	146/150 (97%)	145 (99%)	1 (1%)	0	100	100
9	I	52/108 (48%)	49 (94%)	3 (6%)	0	100	100
10	J	63/67 (94%)	60 (95%)	3 (5%)	0	100	100
11	K	101/133 (76%)	100 (99%)	1 (1%)	0	100	100
12	L	44/58 (76%)	41 (93%)	3 (7%)	0	100	100
13	M	418/708 (59%)	401 (96%)	17 (4%)	0	100	100
14	N	140/398 (35%)	138 (99%)	2 (1%)	0	100	100
15	O	508/534 (95%)	498 (98%)	10 (2%)	0	100	100
16	P	301/316 (95%)	294 (98%)	7 (2%)	0	100	100
17	Q	85/223 (38%)	82 (96%)	3 (4%)	0	100	100
18	V	32/419 (8%)	29 (91%)	3 (9%)	0	100	100
All	All	5269/6672 (79%)	5133 (97%)	136 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	1200/1212 (99%)	1193 (99%)	7 (1%)	78 83
2	B	963/988 (98%)	960 (100%)	3 (0%)	86 87
3	C	299/302 (99%)	297 (99%)	2 (1%)	76 82
4	D	114/136 (84%)	114 (100%)	0	100 100
5	E	191/192 (100%)	191 (100%)	0	100 100
6	F	66/111 (60%)	66 (100%)	0	100 100
7	G	149/181 (82%)	147 (99%)	2 (1%)	61 77
8	H	129/131 (98%)	129 (100%)	0	100 100
9	I	48/93 (52%)	40 (83%)	8 (17%)	2 10
10	J	53/56 (95%)	52 (98%)	1 (2%)	50 73
11	K	92/119 (77%)	92 (100%)	0	100 100
12	L	43/55 (78%)	43 (100%)	0	100 100
13	M	377/622 (61%)	377 (100%)	0	100 100
14	N	131/347 (38%)	131 (100%)	0	100 100
15	O	458/476 (96%)	457 (100%)	1 (0%)	87 89
16	P	269/280 (96%)	268 (100%)	1 (0%)	84 86
17	Q	84/195 (43%)	84 (100%)	0	100 100
18	V	31/365 (8%)	31 (100%)	0	100 100
All	All	4697/5861 (80%)	4672 (100%)	25 (0%)	78 85

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	428	MET
1	A	492	VAL
1	A	494	THR
1	A	499	ASP
1	A	767	CYS
1	A	776	SER
1	A	1158	LEU
2	B	203	VAL
2	B	214	THR
2	B	680	SER
3	C	64	ASP

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Mol	Chain	Res	Type
3	C	236	LEU
7	G	59	VAL
7	G	128	VAL
9	I	1	MET
9	I	45	LYS
9	I	46	LEU
9	I	48	GLU
9	I	49	VAL
9	I	50	ASP
9	I	52	VAL
9	I	53	LEU
10	J	30	THR
15	O	55	CYS
16	P	134	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	119	GLN
1	A	158	HIS
1	A	225	ASN
1	A	296	HIS
1	A	374	ASN
1	A	415	HIS
1	A	423	GLN
1	A	739	GLN
1	A	1054	HIS
1	A	1371	ASN
2	B	100	HIS
2	B	253	GLN
2	B	395	GLN
2	B	408	GLN
2	B	501	HIS
2	B	517	ASN
2	B	552	HIS
2	B	737	GLN
2	B	1115	GLN
3	C	206	GLN
5	E	35	GLN
5	E	189	GLN
8	H	29	HIS

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Mol	Chain	Res	Type
8	H	131	ASN
13	M	11	GLN
15	O	34	GLN
15	O	68	HIS
15	O	249	GLN
15	O	402	ASN
15	O	407	GLN
15	O	497	GLN
15	O	534	GLN
18	V	20	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	Z	4/5 (80%)	2 (50%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	Z	4	C
21	Z	6	C

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 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
26	GTP	Z	101	-	33,34,34	1.19	4 (12%)	50,54,54	1.77	7 (14%)
24	3AT	B	1202	-	30,32,32	1.45	4 (13%)	42,50,50	1.87	9 (21%)
25	SF4	P	401	16	0,12,12	-	-	-		

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
25	SF4	P	401	16	-	-	0/6/5/5
24	3AT	B	1202	-	-	8/22/34/34	0/3/3/3
26	GTP	Z	101	-	-	2/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	1202	3AT	C5-C4	4.81	1.47	1.39
26	Z	101	GTP	C5-C4	3.14	1.47	1.38
24	B	1202	3AT	C5-C6	2.80	1.48	1.41
26	Z	101	GTP	C6-N1	-2.37	1.34	1.38
24	B	1202	3AT	C5-N7	-2.37	1.34	1.39
24	B	1202	3AT	C8-N7	2.33	1.36	1.31
26	Z	101	GTP	PB-O3A	2.08	1.61	1.59
26	Z	101	GTP	C5-N7	-2.02	1.35	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Z	101	GTP	C5-C4-N3	-6.23	118.47	128.39
24	B	1202	3AT	C5-C4-N3	-5.81	118.72	126.72
26	Z	101	GTP	C2-N3-C4	5.06	121.01	112.30
26	Z	101	GTP	N9-C4-N3	4.65	135.26	125.95
24	B	1202	3AT	N3-C4-N9	4.58	134.96	127.17
24	B	1202	3AT	C2-N3-C4	3.69	120.85	111.83
24	B	1202	3AT	C4-C5-N7	-3.44	106.64	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Z	101	GTP	C6-C5-N7	3.26	136.22	130.29
24	B	1202	3AT	N3-C2-N1	-3.17	123.78	128.58
26	Z	101	GTP	C4-C5-N7	-2.62	106.52	110.67
24	B	1202	3AT	C5-N7-C8	2.58	107.51	103.45
24	B	1202	3AT	C4-N9-C8	2.50	108.36	105.74
26	Z	101	GTP	C3'-C2'-C1'	2.42	106.05	101.46
24	B	1202	3AT	O4'-C4'-C3'	2.17	107.83	105.07
26	Z	101	GTP	O6-C6-C5	-2.12	120.95	126.53
24	B	1202	3AT	C6-C5-N7	2.11	136.15	132.09

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	1202	3AT	C5'-O5'-PA-O2A
24	B	1202	3AT	C5'-O5'-PA-O3A
24	B	1202	3AT	O4'-C4'-C5'-O5'
24	B	1202	3AT	C3'-C4'-C5'-O5'
26	Z	101	GTP	O4'-C4'-C5'-O5'
26	Z	101	GTP	C3'-C4'-C5'-O5'
24	B	1202	3AT	PG-O3B-PB-O2B
24	B	1202	3AT	C2'-C1'-N9-C8
24	B	1202	3AT	C2'-C1'-N9-C4
24	B	1202	3AT	PG-O3B-PB-O1B

There are no ring outliers.

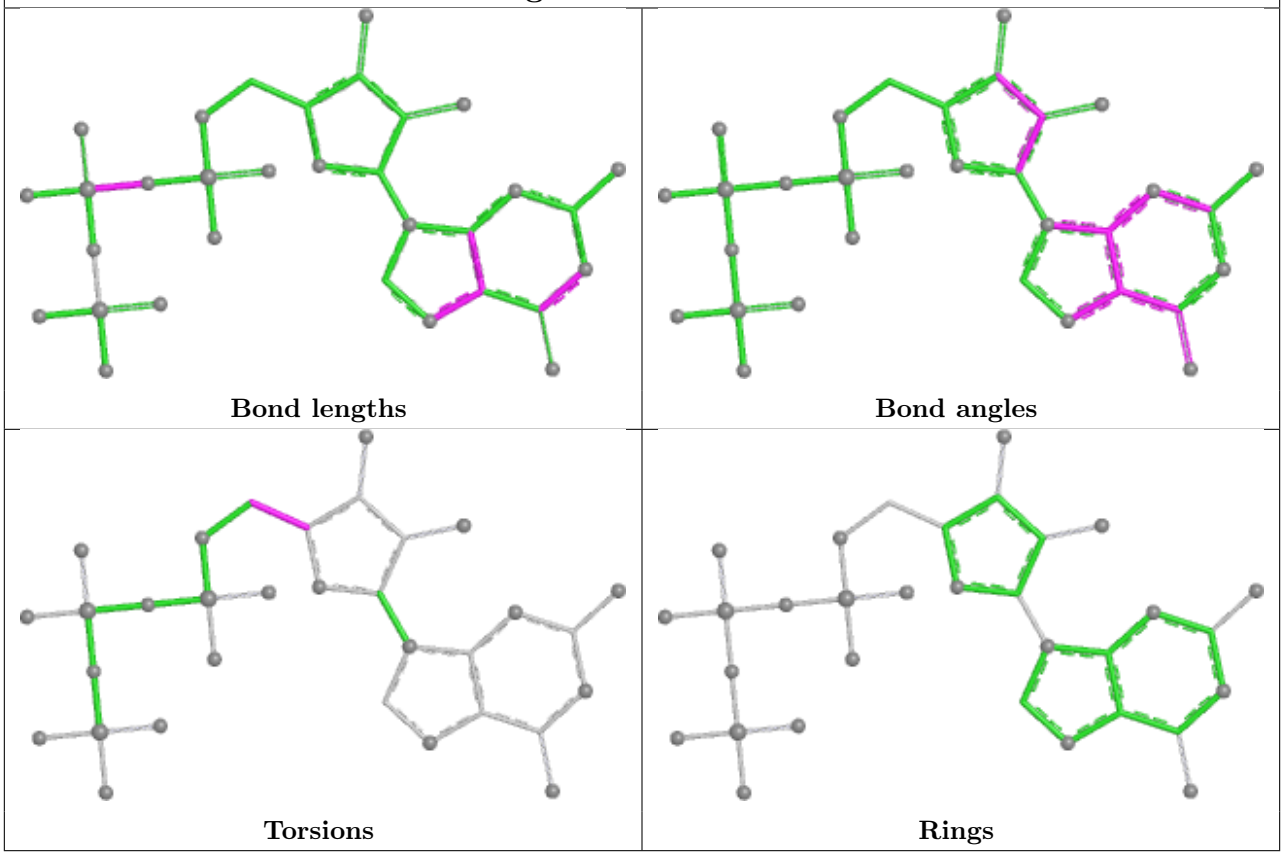
3 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	Z	101	GTP	12	0
24	B	1202	3AT	6	0
25	P	401	SF4	1	0

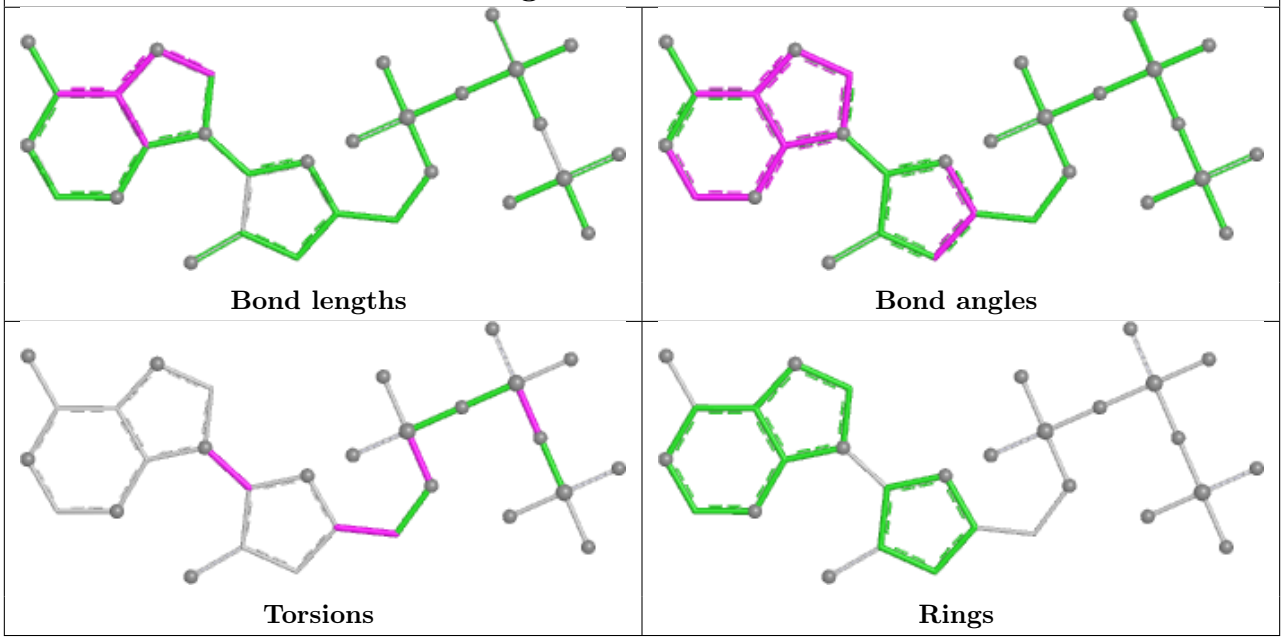
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 GTP Z 101



Ligand 3AT B 1202



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.

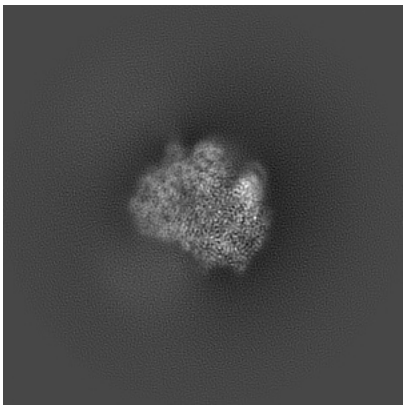
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-62008. These allow visual inspection of the internal detail of the map and identification of artifacts.

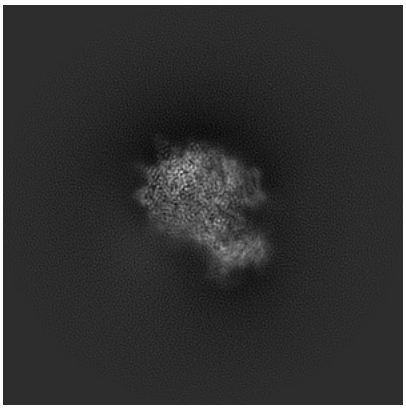
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

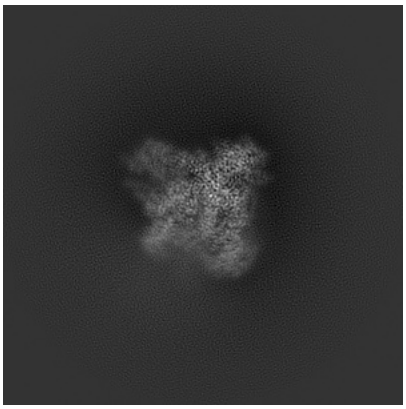
6.1.1 Primary map



X

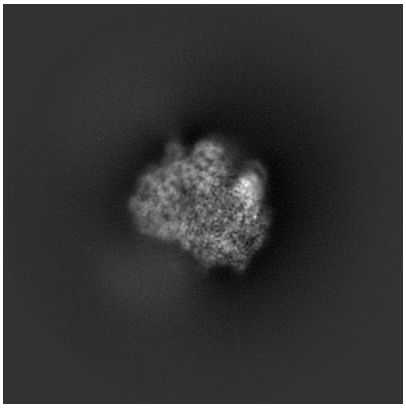


Y

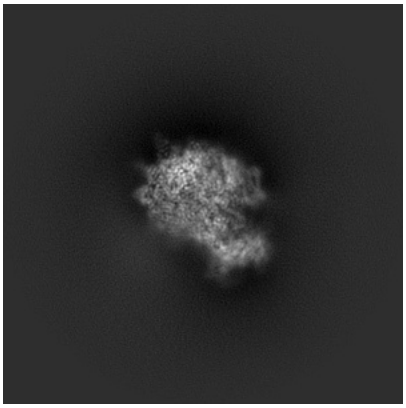


Z

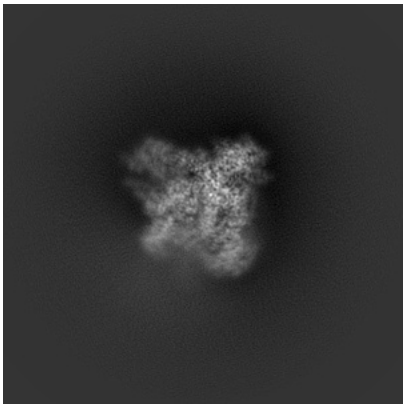
6.1.2 Raw map



X



Y

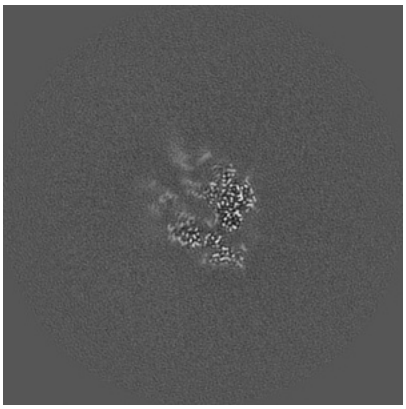


Z

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

6.2 Central slices (i)

6.2.1 Primary map



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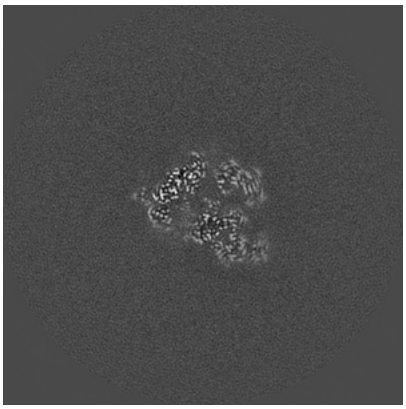
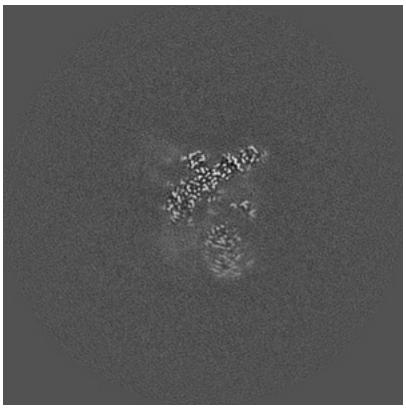
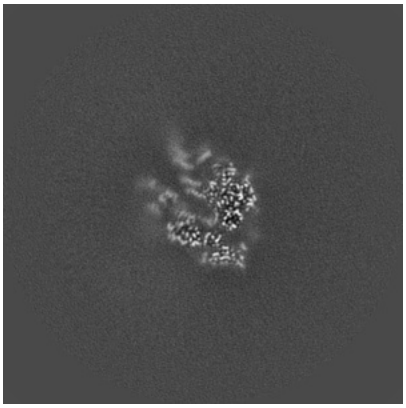


Y Index: 161

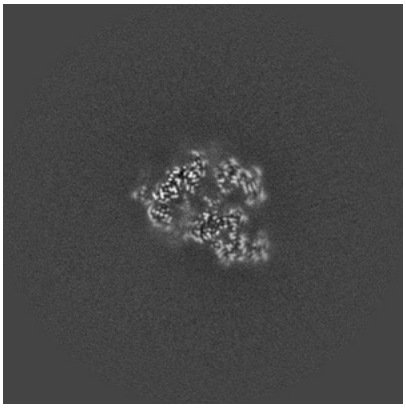


Z Index: 161

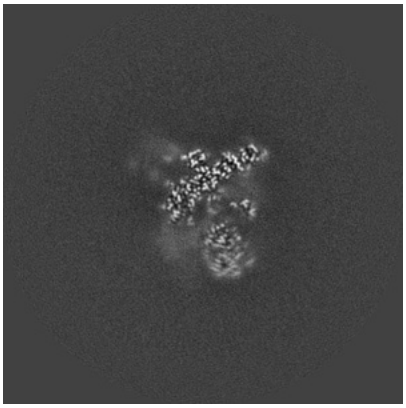
6.2.2 Raw map



X Index: 161



Y Index: 161

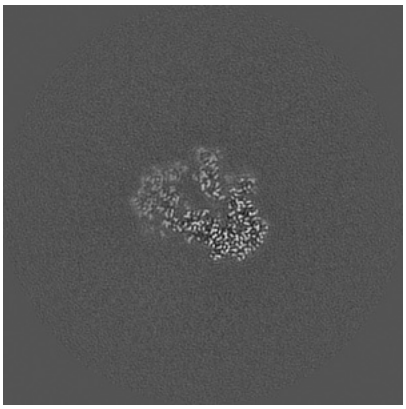


Z Index: 161

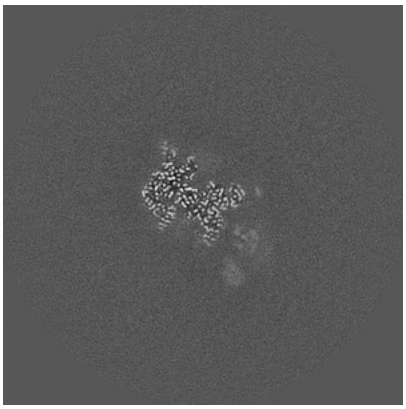
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

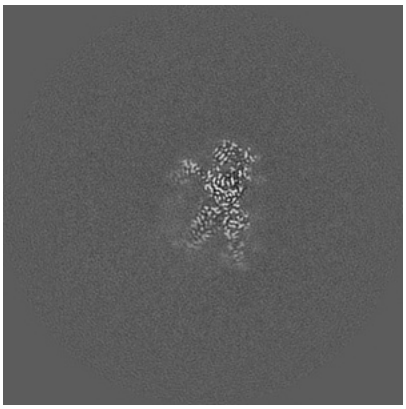
6.3.1 Primary map



X Index: 179

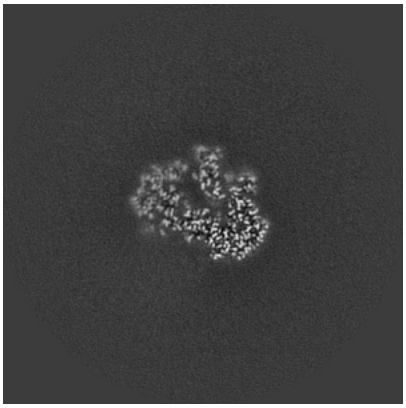


Y Index: 177

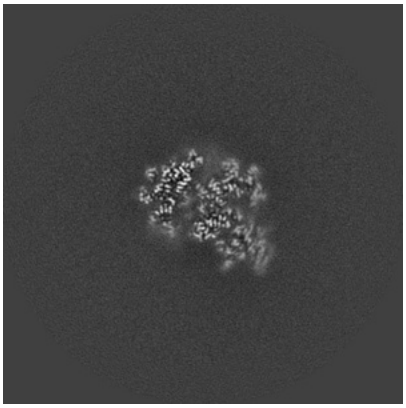


Z Index: 141

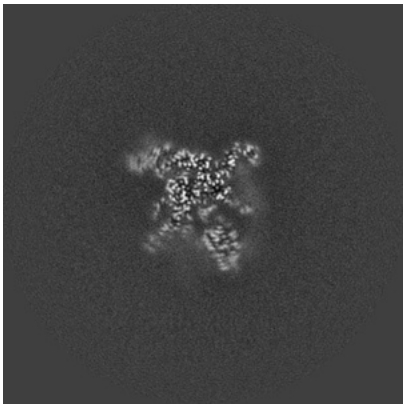
6.3.2 Raw map



X Index: 179



Y Index: 166

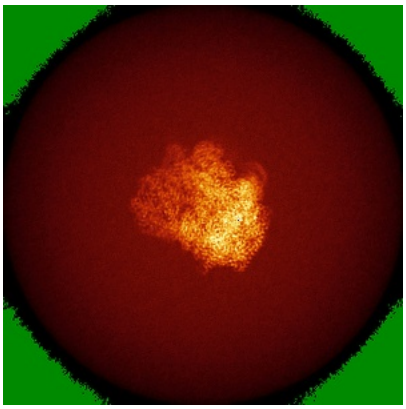


Z Index: 170

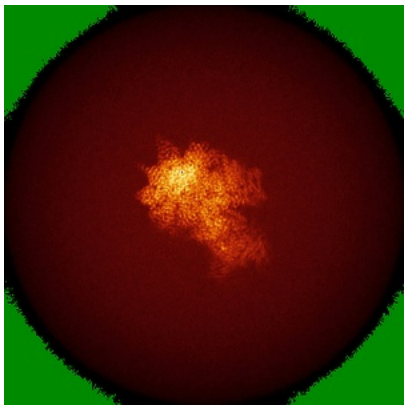
The images above show the largest variance slices of the map in three orthogonal directions.

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

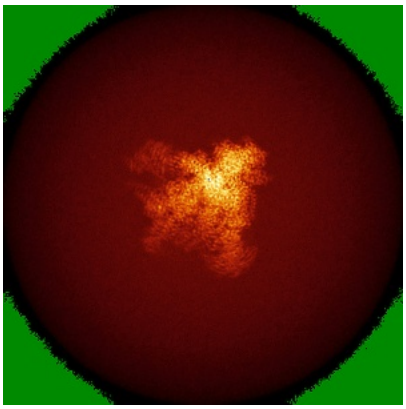
6.4.1 Primary map



X

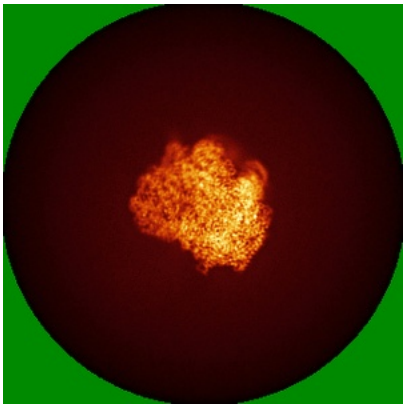


Y

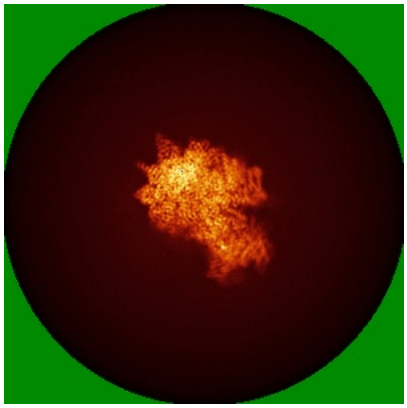


Z

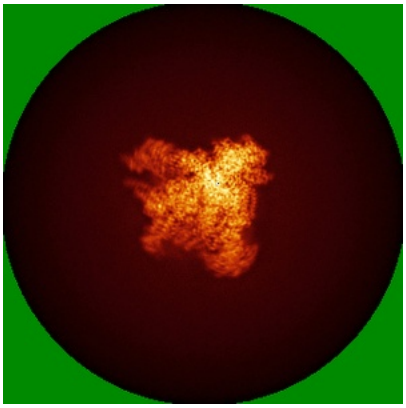
6.4.2 Raw map



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.

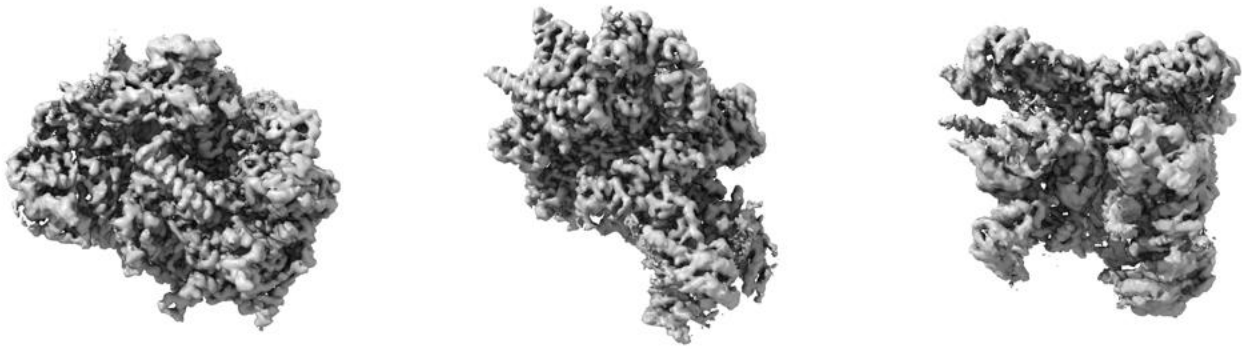
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

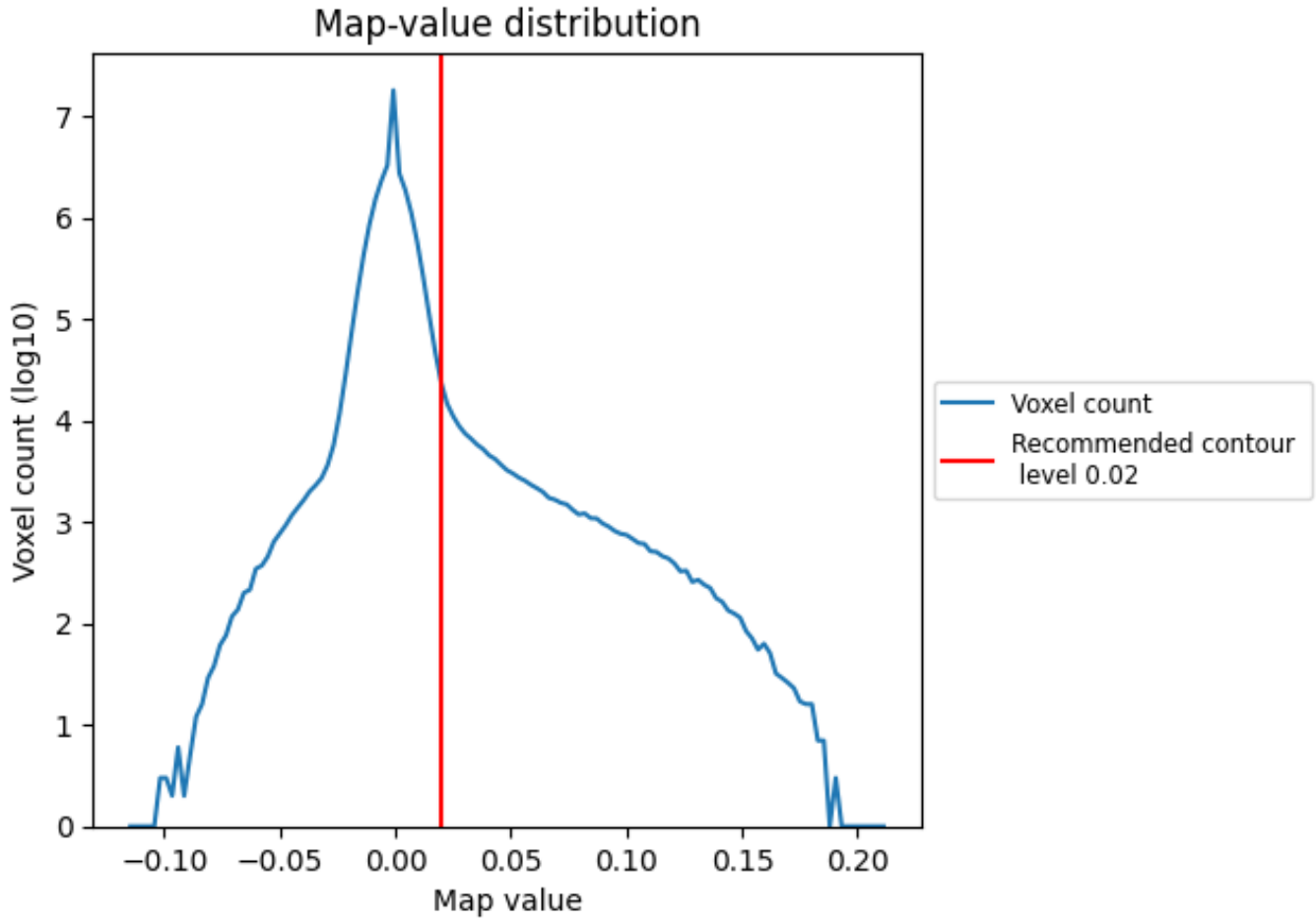
6.6 Mask visualisation (i)

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

7 Map analysis

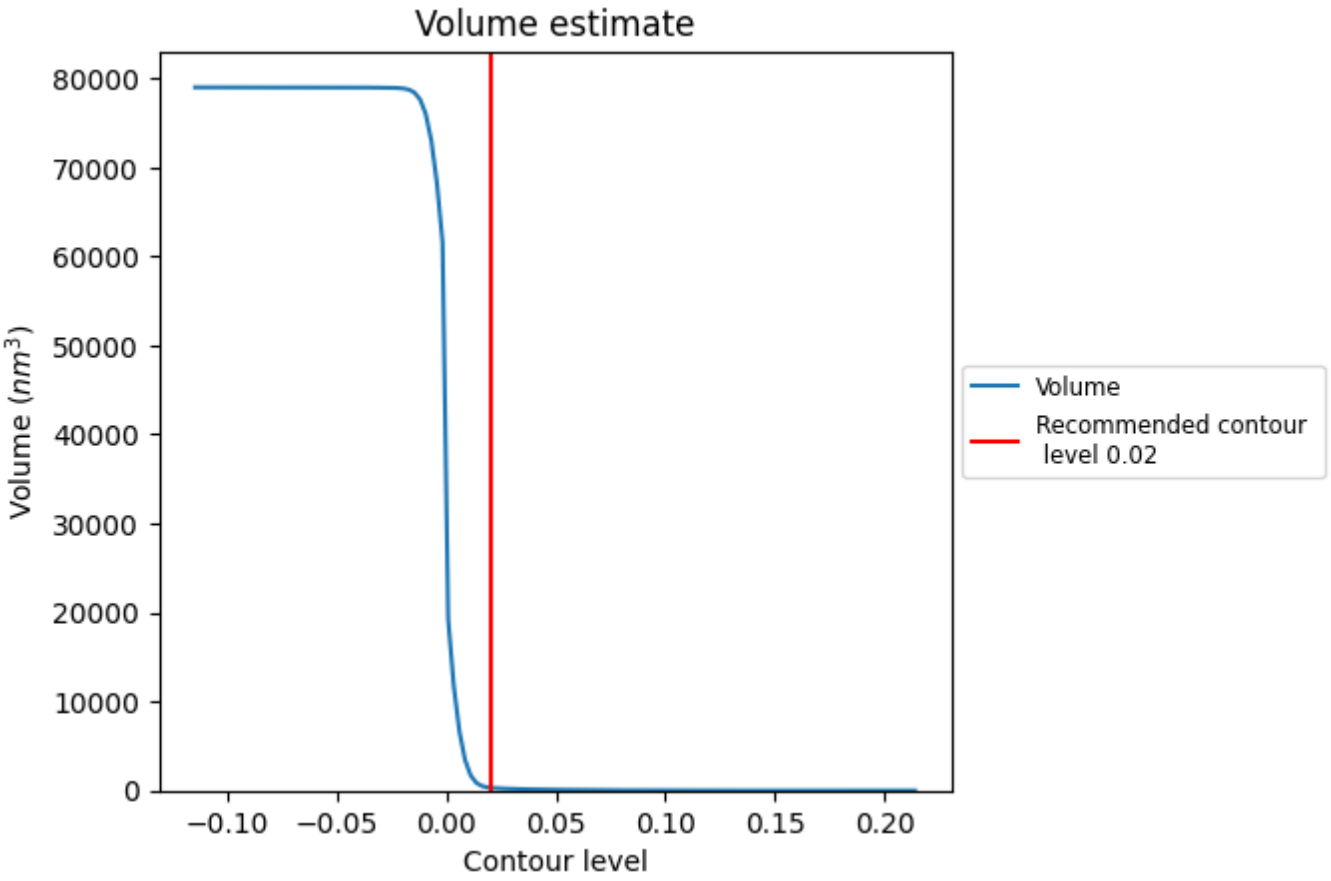
This section contains the results of statistical analysis of the map.

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.

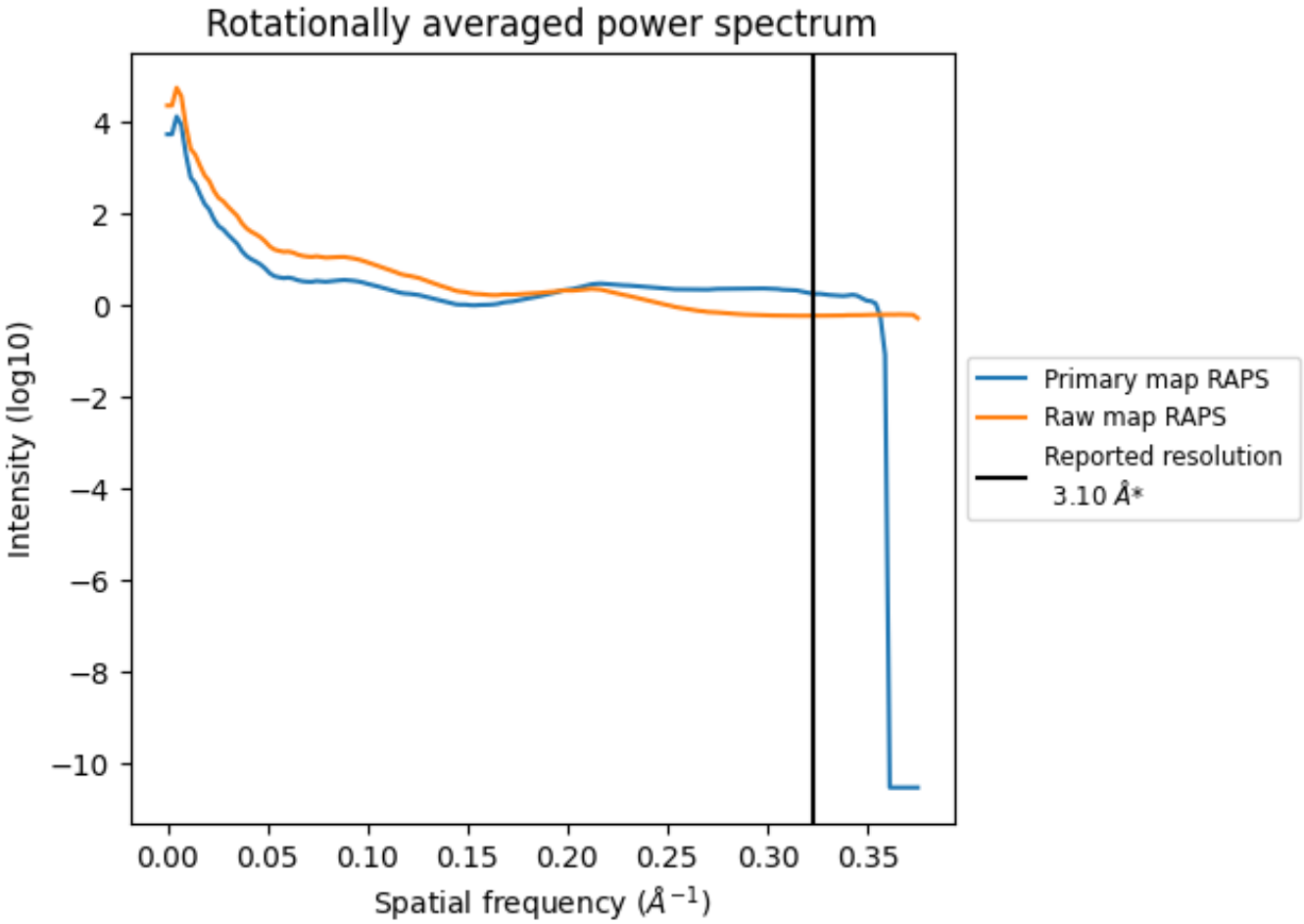
7.2 Volume estimate (i)



The volume at the recommended contour level is 326 nm^3; this corresponds to an approximate mass of 294 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)

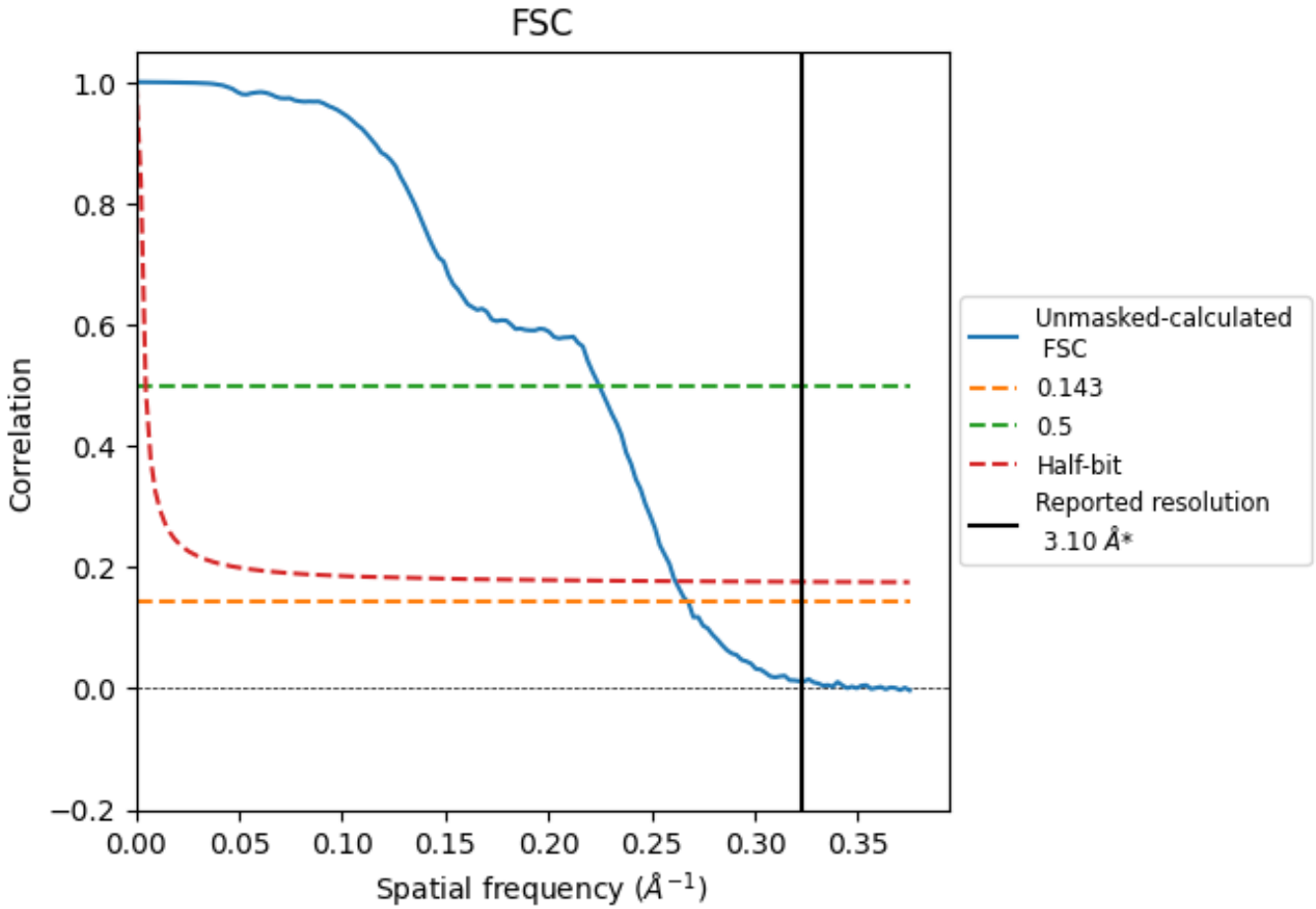


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

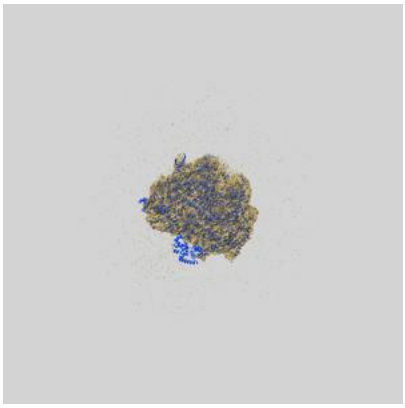
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.74	4.45	3.82

*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 3.74 differs from the reported value 3.1 by more than 10 %

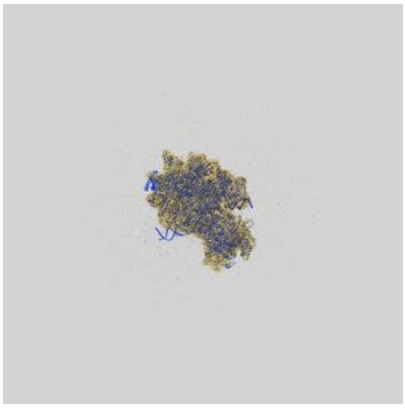
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-62008 and PDB model 9K38. Per-residue inclusion information can be found in section 3 on page 10.

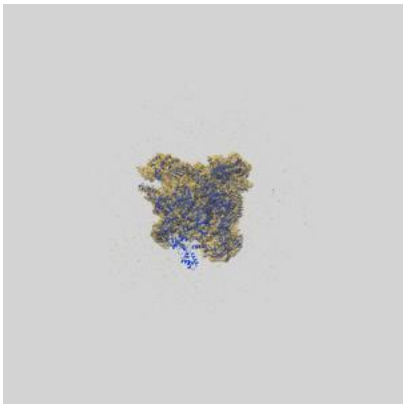
9.1 Map-model overlay



X



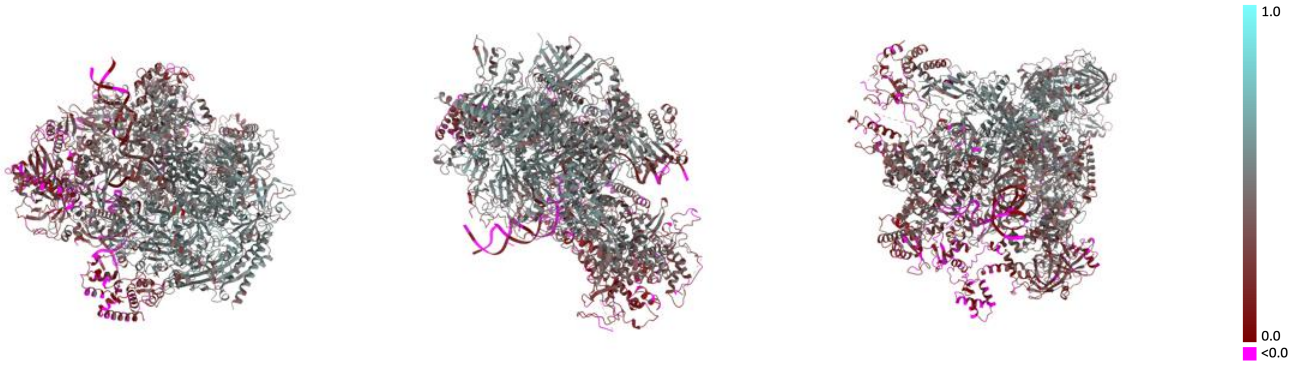
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

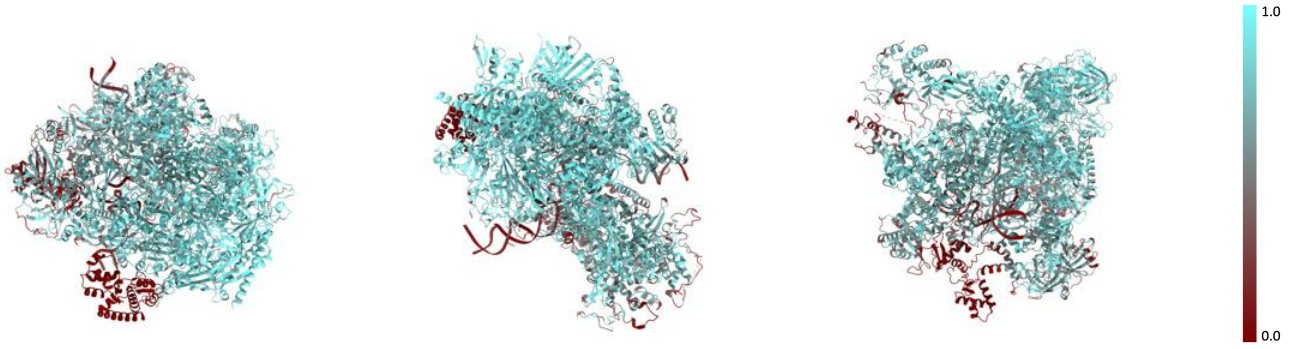
9.2 Q-score mapped to coordinate model (i)



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.

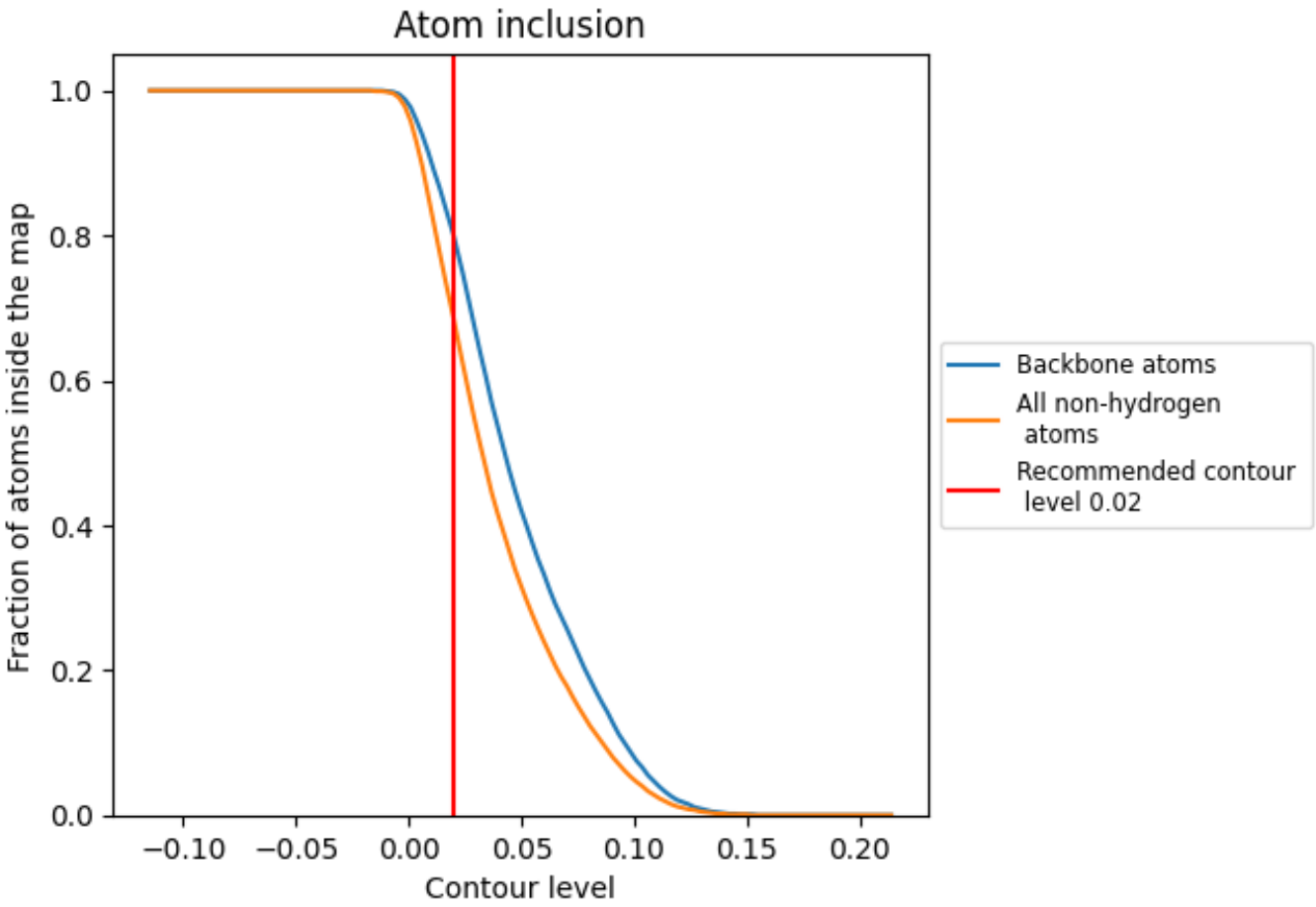
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 68% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6840	0.3680
A	0.7910	0.4450
B	0.8000	0.4450
C	0.8660	0.4870
D	0.6210	0.2410
E	0.7560	0.3680
F	0.8950	0.5080
G	0.7260	0.3250
H	0.8230	0.4690
I	0.7220	0.3640
J	0.8860	0.4840
K	0.8600	0.4770
L	0.7930	0.3960
M	0.3220	0.1890
N	0.5360	0.2000
O	0.6460	0.3420
P	0.2930	0.1570
Q	0.5840	0.2900
V	0.5640	0.3950
X	0.2350	0.0490
Y	0.3850	0.1480
Z	0.6590	0.4840