Full wwPDB EM Validation Report ⓘ

Sep 10, 2022 – 07:21 am BST

PDB ID	:	7Z1N
EMDB ID	:	EMD-14449
Title	:	Structure of yeast RNA Polymerase III Delta C53-C37-C11
Authors	:	Girbig, M.; Mueller, C.W.
Deposited on	:	2022-02-24
Resolution	:	3.90 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:

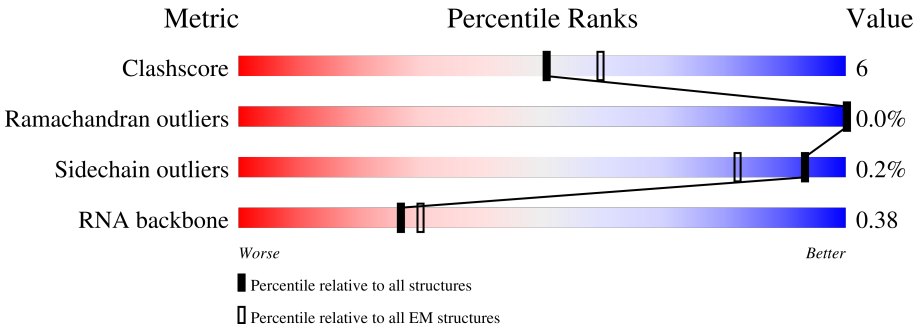
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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 3.90 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	1460	29% 84% 14% ·
2	B	1149	37% 81% 16% ·
3	C	335	35% 83% 16%
4	D	161	78% 68% 22% 10%
5	E	215	51% 81% 19%
6	F	155	10% 48% 5% 46%
7	G	212	54% 74% 20% 6%

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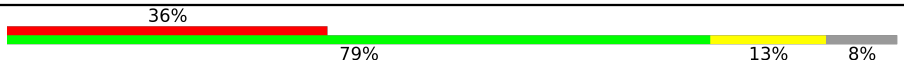
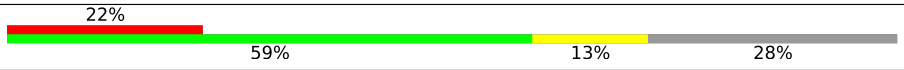
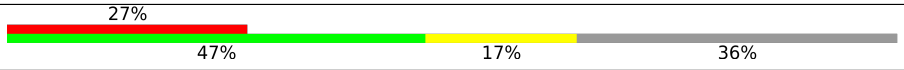
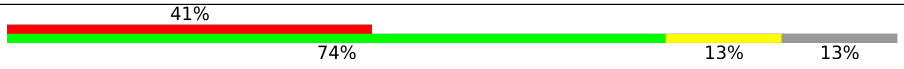
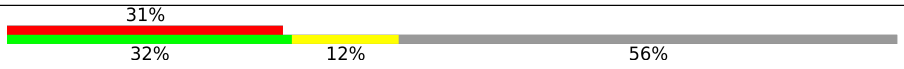
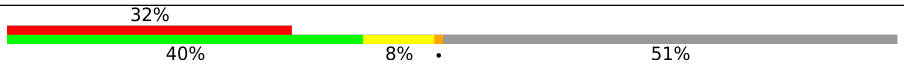
Mol	Chain	Length	Quality of chain
8	H	146	
9	J	70	
10	K	142	
11	L	70	
12	O	654	
13	P	317	
14	Q	251	
15	R	24	
16	S	44	
17	T	44	

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 38601 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	1433	11209	7067	1977	2104	61	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	1112	8771	5549	1514	1648	60	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	334	2647	1676	453	510	8	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	145	1185	755	200	224	6	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	215	1759	1116	310	321	12	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	83	671	429	114	125	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	199	Total	C	N	O	S	0	0
			1610	1046	258	298	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	135	Total	C	N	O	S	0	0
			1083	683	183	213	4		

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 10 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	102	Total	C	N	O	S	0	0
			801	501	131	164	5		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

- Molecule 12 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	570	Total	C	N	O	S	0	0
			4577	2908	787	863	19		

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	140	Total	C	N	O	S	0	0
			1162	757	180	221	4		

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	123	Total	C	N	O	S	0	0
			981	633	163	182	3		

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	9	Total	C	N	O	P	0	0
			195	87	39	60	9		

- Molecule 16 is a DNA chain called NT-DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	18	Total	C	N	O	P	0	0
			366	176	61	111	18		

- Molecule 17 is a DNA chain called T-DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	29	Total	C	N	O	P	0	0
			597	284	109	175	29		

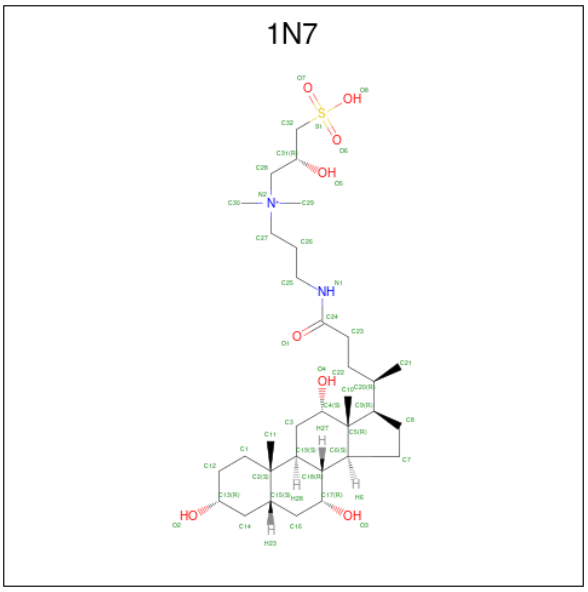
- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 20 is CHAPSO (three-letter code: 1N7) (formula: $C_{32}H_{59}N_2O_8S$).



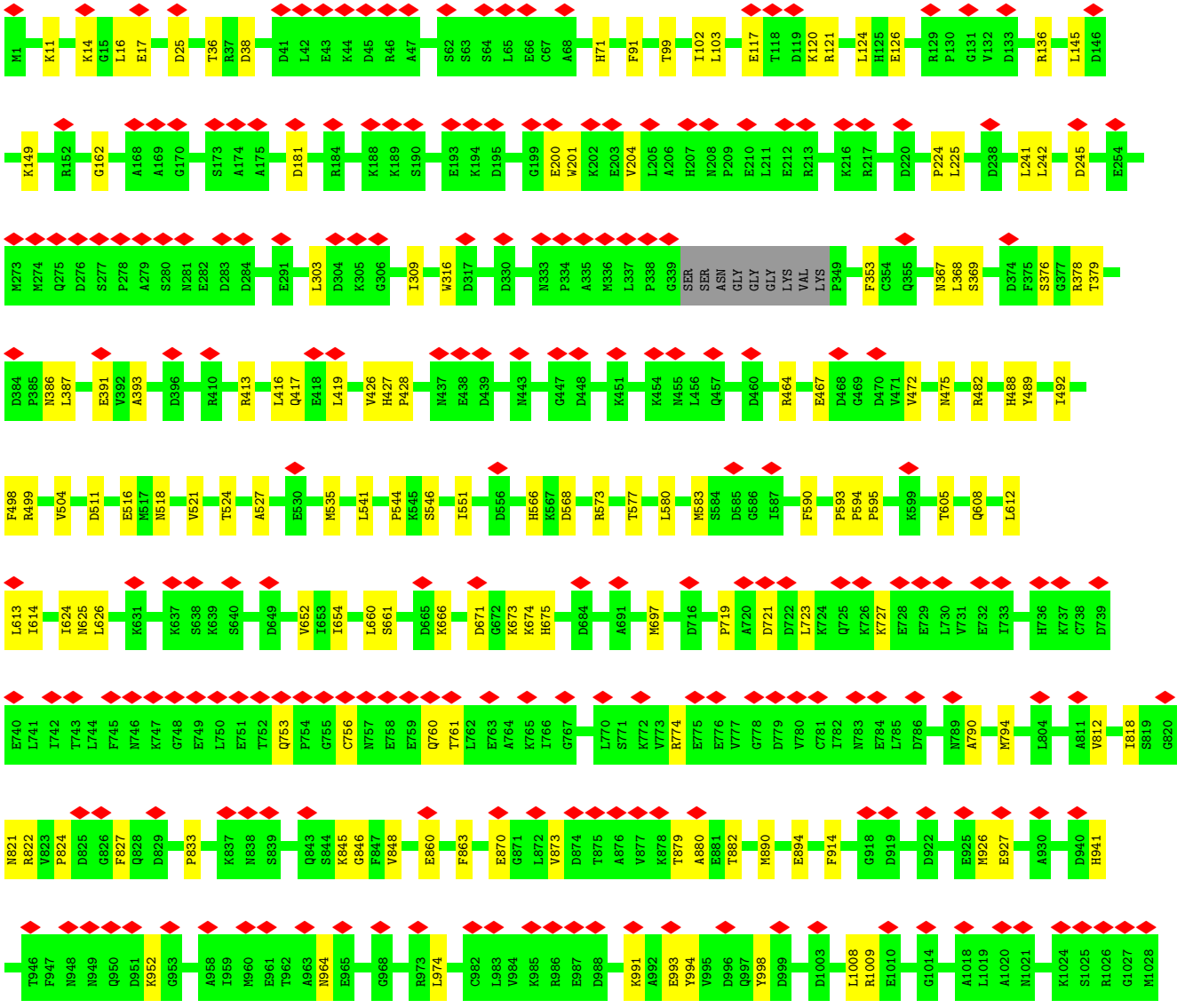
Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	C	O	0
			27	24	3	
20	K	1	Total	C	O	0
			27	24	3	

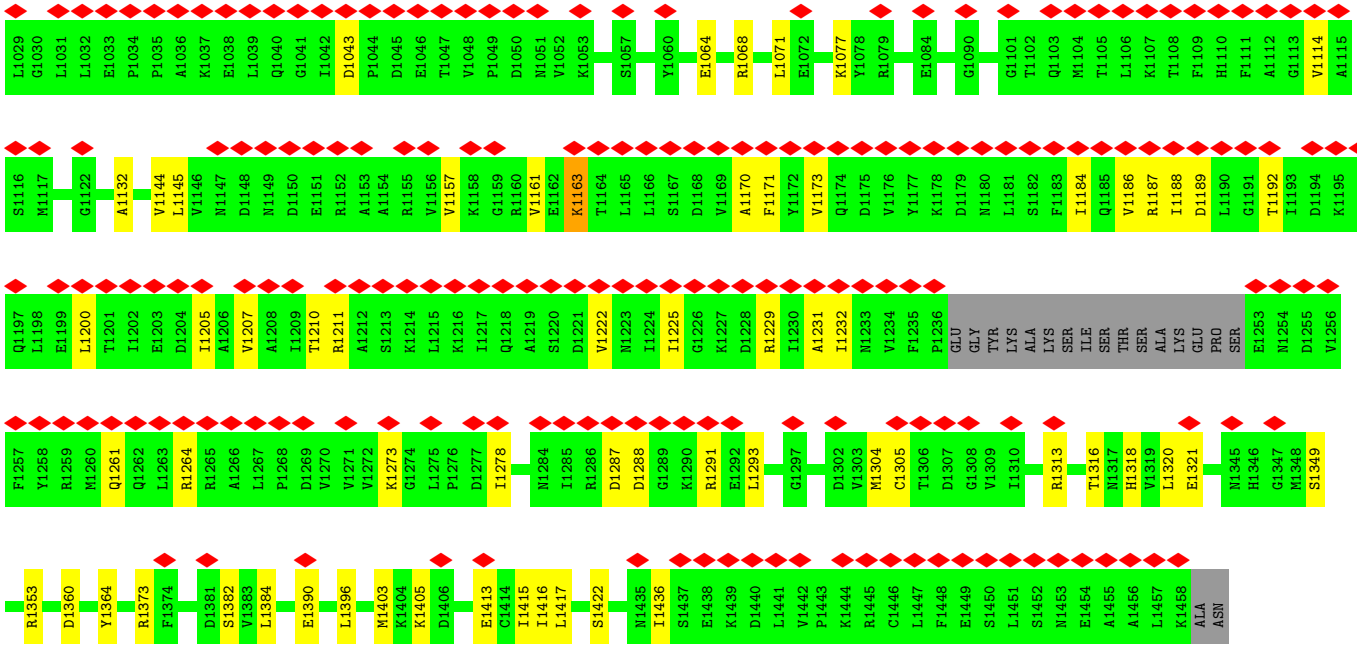
3 Residue-property plots (i)

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.

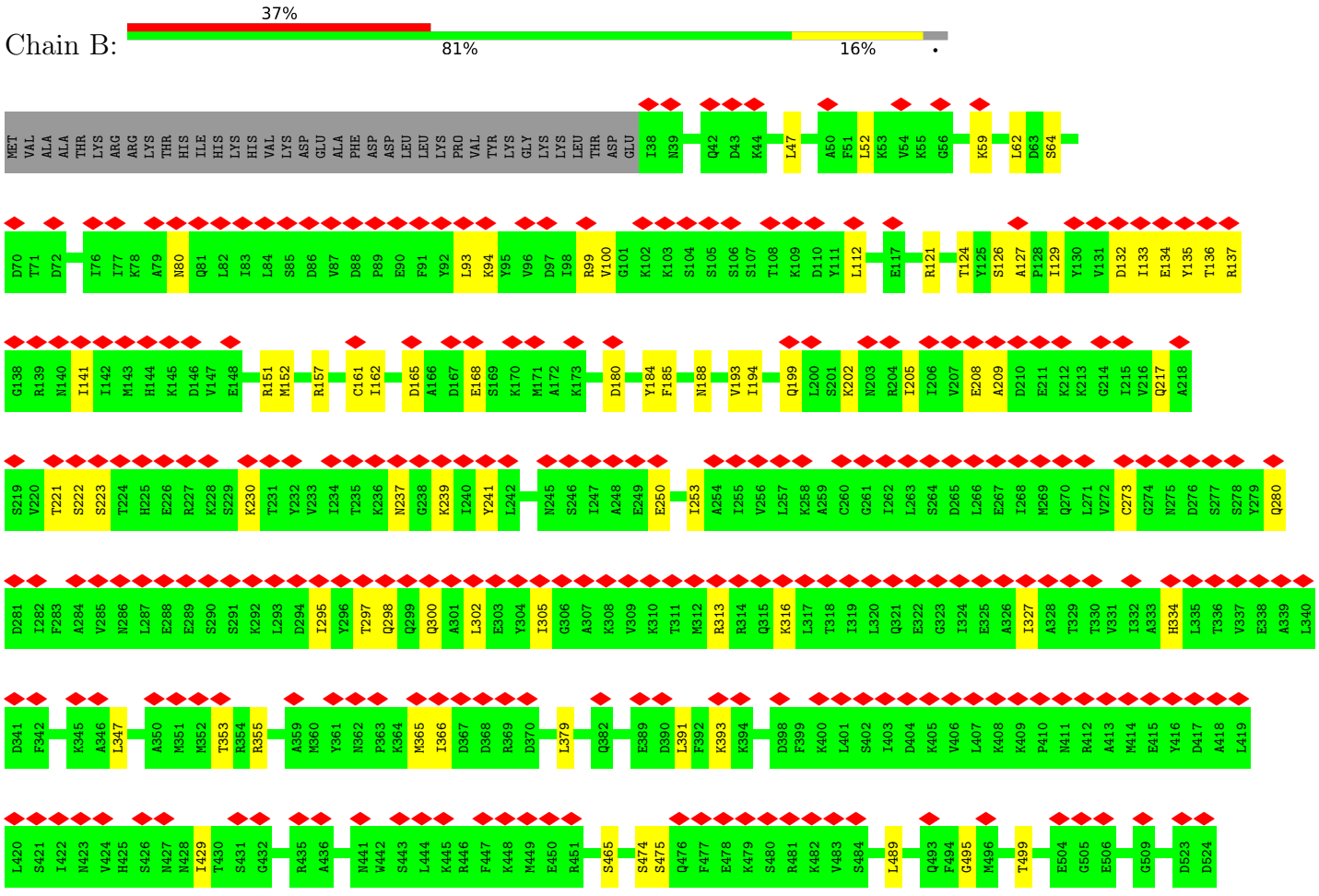
• Molecule 1: DNA-directed RNA polymerase III subunit RPC1

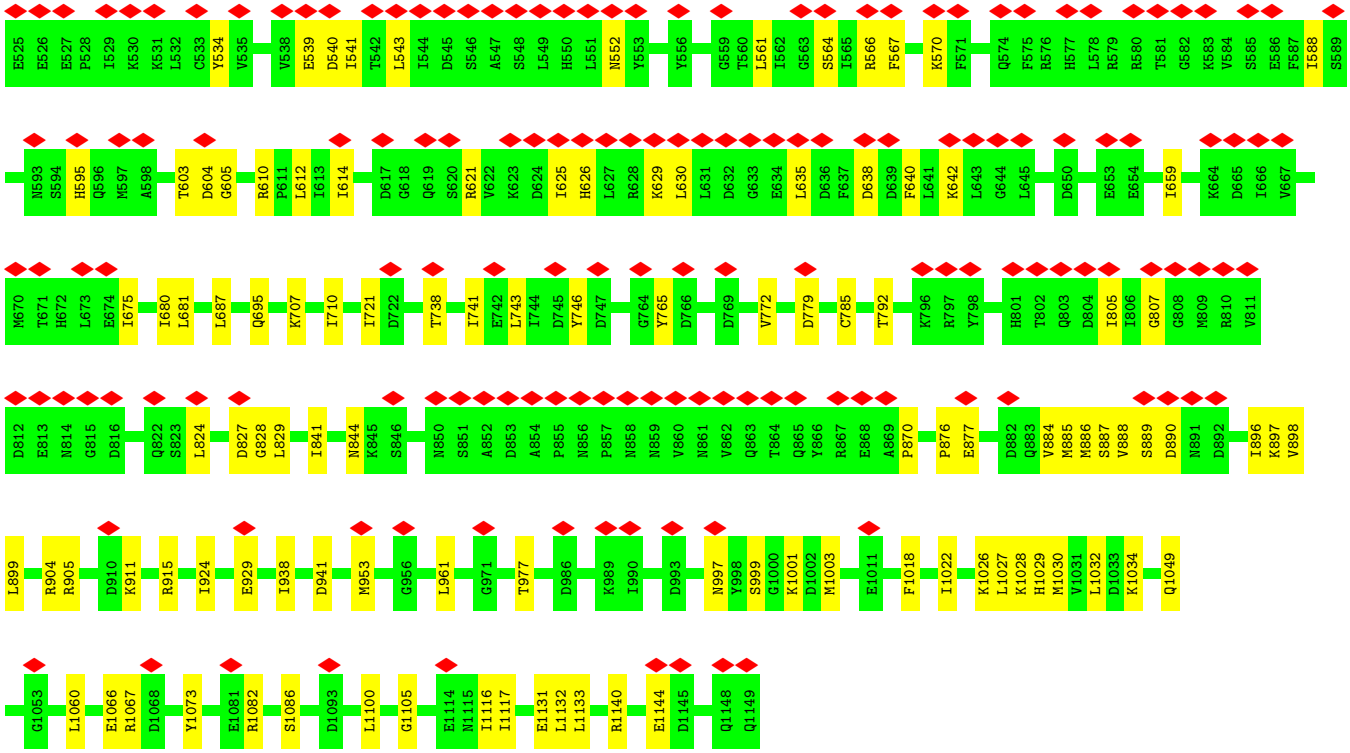
Chain A:





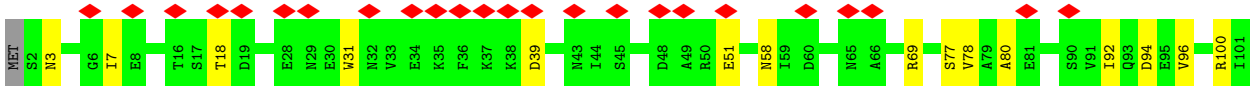
• Molecule 2: DNA-directed RNA polymerase III subunit RPC2





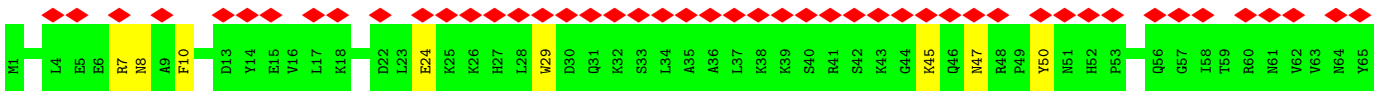
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

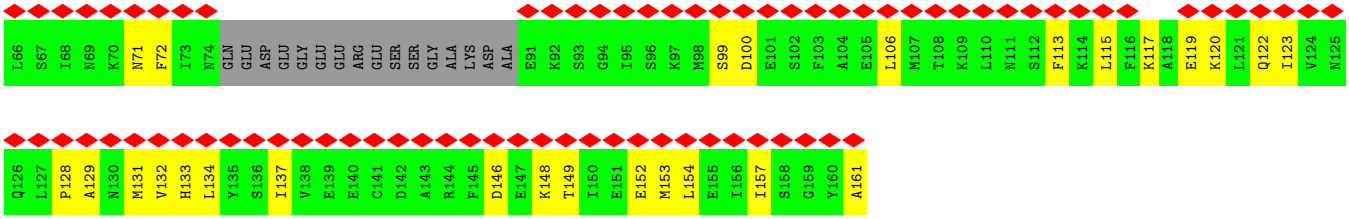
Chain C:



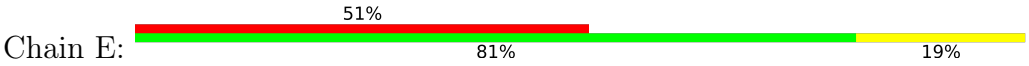
• Molecule 4: DNA-directed RNA polymerase III subunit RPC9

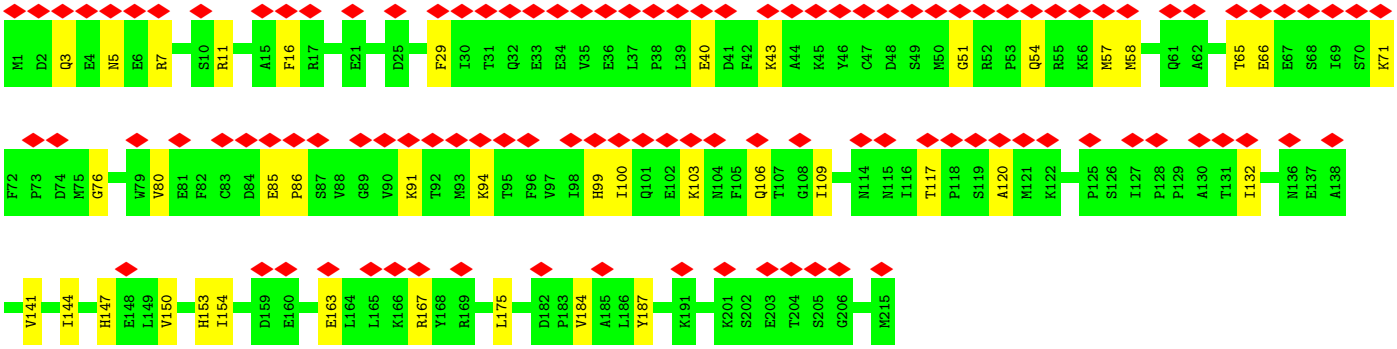
Chain D:



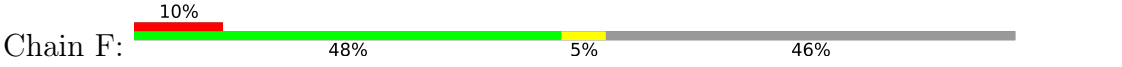


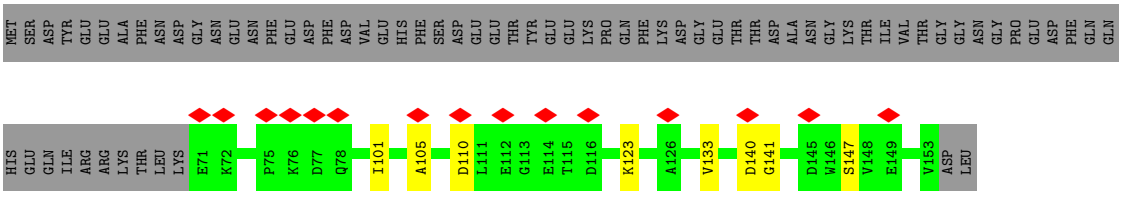
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



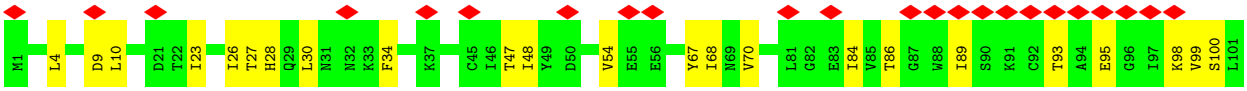


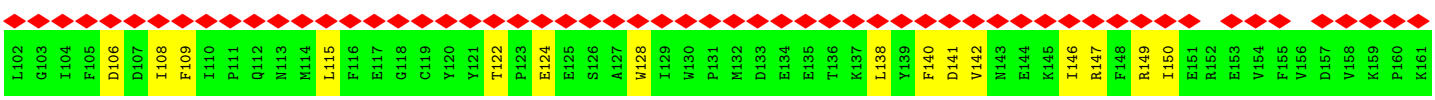
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

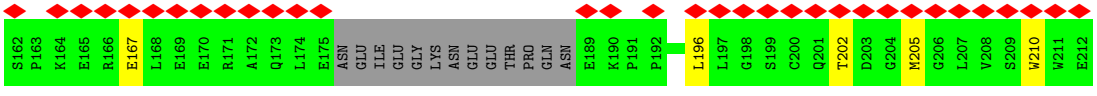




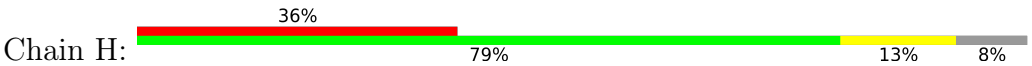
• Molecule 7: DNA-directed RNA polymerase III subunit RPC8

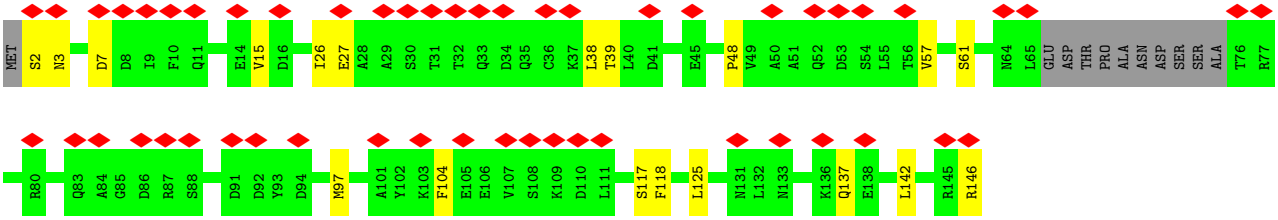




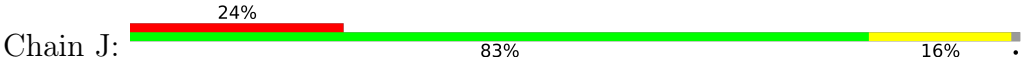


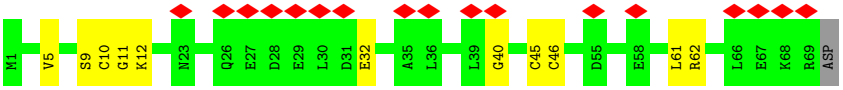
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



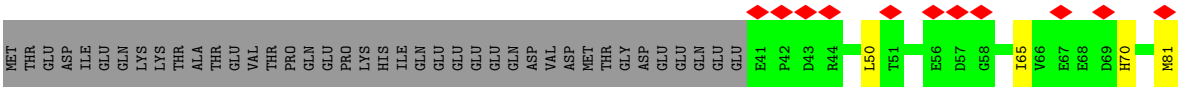


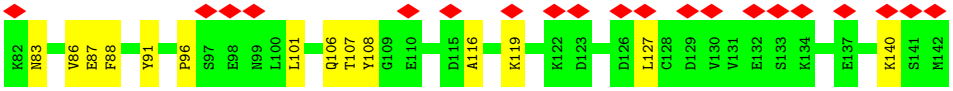
• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC5



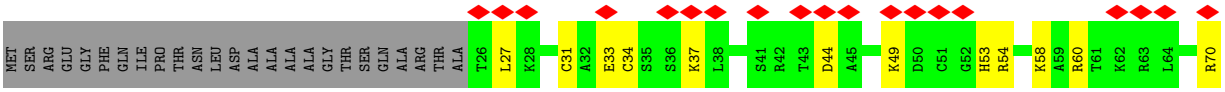


• Molecule 10: DNA-directed RNA polymerases I and III subunit RPAC2

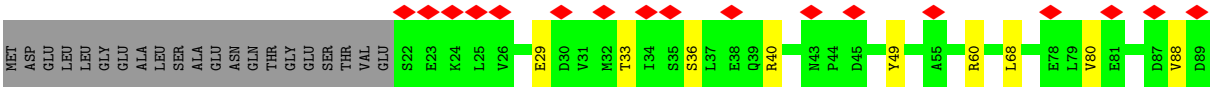


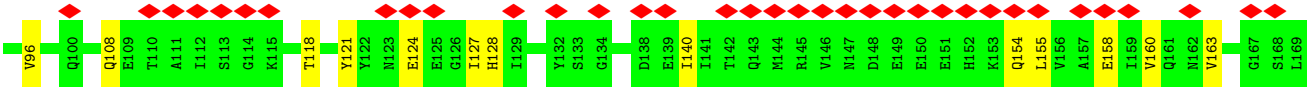


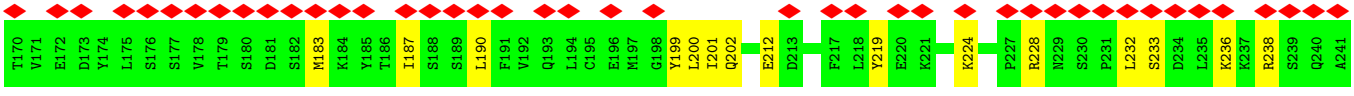
• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC4

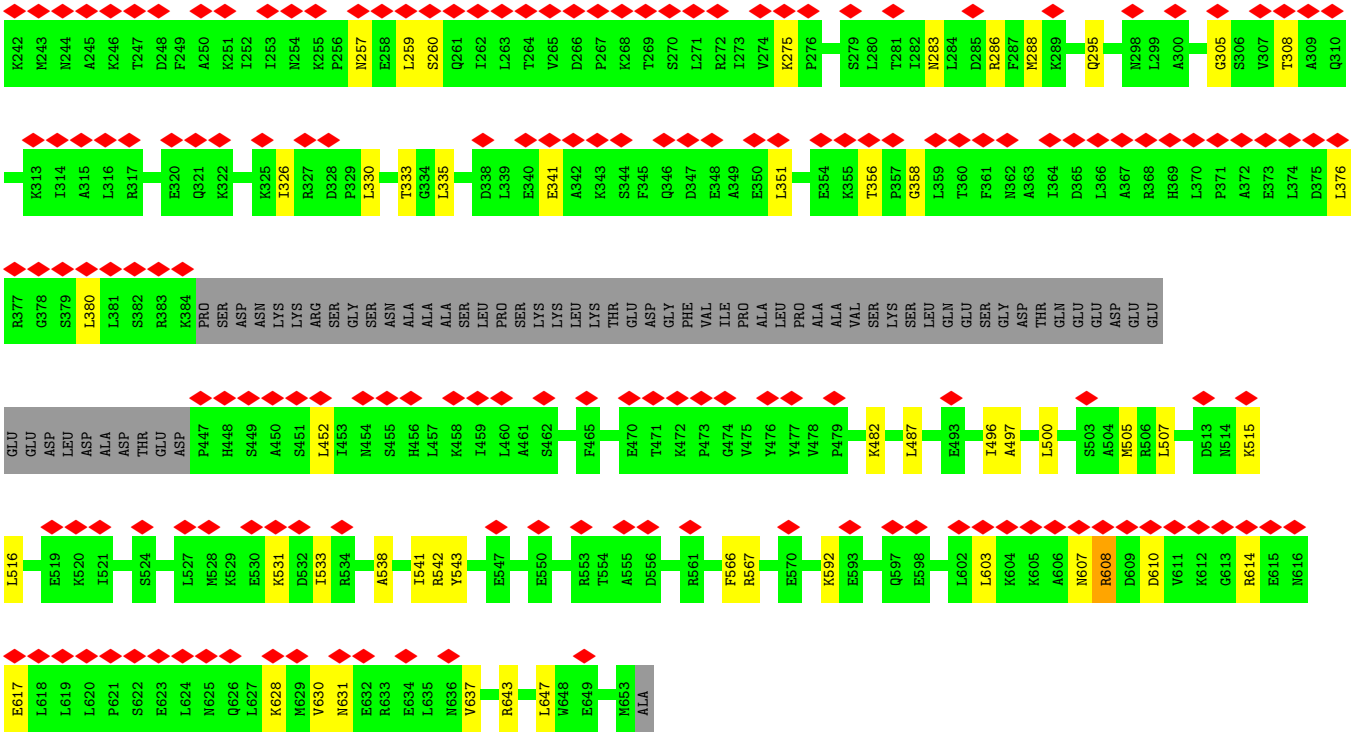


• Molecule 12: DNA-directed RNA polymerase III subunit RPC3



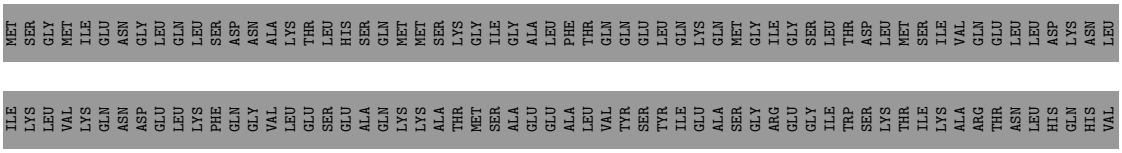


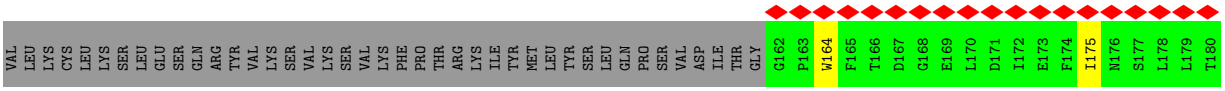


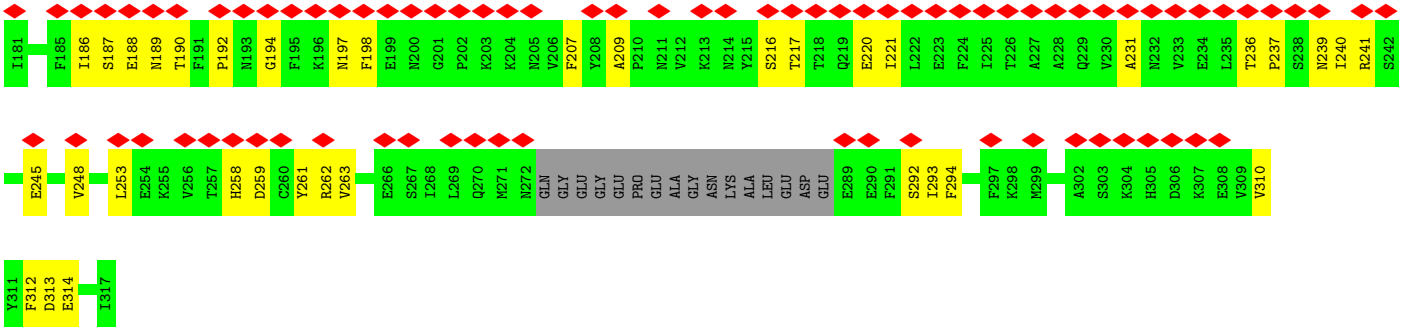


• Molecule 13: DNA-directed RNA polymerase III subunit RPC6

Chain P:

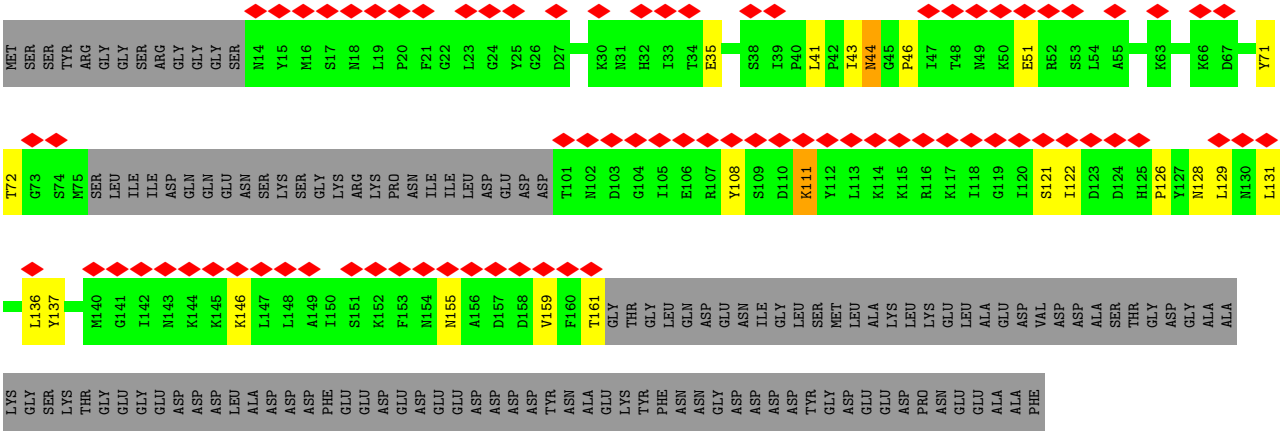






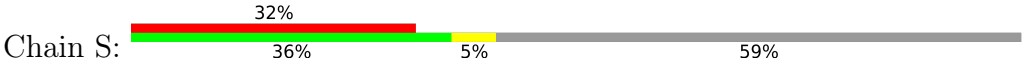
• Molecule 14: DNA-directed RNA polymerase III subunit RPC7

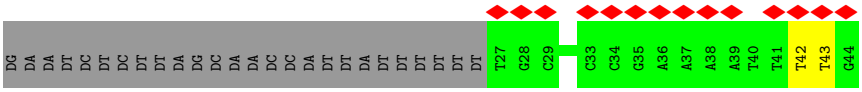
Chain Q:



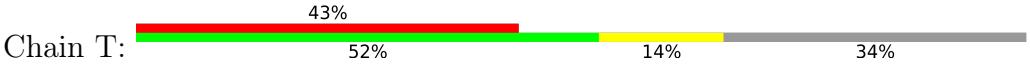
- Molecule 15: RNA

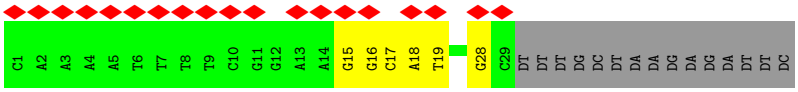
- Molecule 16: NT-DNA





- Molecule 17: T-DNA





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	18530	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 ($e^-/Å^2$)	39.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.362	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	364.33798, 364.33798, 364.33798	wwPDB
Map dimensions	346, 346, 346	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.053, 1.053, 1.053	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1N7, 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	0.32	0/11411	0.55	0/15417
2	B	0.30	0/8926	0.55	2/12045 (0.0%)
3	C	0.30	0/2703	0.55	0/3666
4	D	0.28	0/1203	0.56	0/1610
5	E	0.31	0/1795	0.60	0/2416
6	F	0.30	0/683	0.53	0/923
7	G	0.29	0/1650	0.53	1/2237 (0.0%)
8	H	0.31	0/1101	0.59	0/1492
9	J	0.34	0/578	0.59	0/775
10	K	0.28	0/812	0.51	0/1096
11	L	0.30	0/360	0.62	0/478
12	O	0.29	0/4646	0.53	1/6267 (0.0%)
13	P	0.29	0/1193	0.52	1/1620 (0.1%)
14	Q	0.29	0/1004	0.53	0/1354
15	R	0.31	0/218	0.76	0/338
16	S	0.57	0/408	0.99	0/627
17	T	0.60	0/669	0.92	0/1031
All	All	0.32	0/39360	0.57	5/53392 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	165	ASP	CB-CG-OD2	6.27	123.94	118.30
2	B	941	ASP	CB-CG-OD1	5.37	123.14	118.30
13	P	231	ALA	C-N-CA	5.29	134.91	121.70
7	G	115	LEU	CA-CB-CG	5.26	127.40	115.30
12	O	351	LEU	CA-CB-CG	5.26	127.39	115.30

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	11209	0	11339	138	0
2	B	8771	0	8891	114	0
3	C	2647	0	2616	35	0
4	D	1185	0	1206	23	0
5	E	1759	0	1788	25	0
6	F	671	0	692	4	0
7	G	1610	0	1602	28	0
8	H	1083	0	1057	12	0
9	J	569	0	585	9	0
10	K	801	0	795	16	0
11	L	358	0	381	8	0
12	O	4577	0	4754	62	0
13	P	1162	0	1113	23	0
14	Q	981	0	979	17	0
15	R	195	0	99	1	0
16	S	366	0	206	1	0
17	T	597	0	328	4	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
19	A	1	0	0	0	0
20	A	27	0	39	3	0
20	K	27	0	39	3	0
All	All	38601	0	38509	457	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 6.

All (457) 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)
1:A:827:PHE:HE2	1:A:833:PRO:HG3	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:10:CYS:SG	9:J:11:GLY:N	2.58	0.77
5:E:54:GLN:NE2	5:E:57:MET:SD	2.59	0.76
1:A:378:ARG:NE	1:A:516:GLU:OE1	2.22	0.72
2:B:904:ARG:HD3	2:B:1032:LEU:HD23	1.72	0.72
2:B:1026:LYS:NZ	2:B:1030:MET:SD	2.64	0.69
2:B:614:ILE:HG23	2:B:621:ARG:HG3	1.73	0.69
2:B:687:LEU:O	2:B:915:ARG:NH1	2.26	0.68
13:P:192:PRO:O	13:P:197:ASN:ND2	2.26	0.68
1:A:652:VAL:HA	1:A:661:SER:O	1.94	0.68
2:B:721:ILE:HG23	2:B:899:LEU:HD13	1.76	0.68
1:A:224:PRO:HD2	1:A:316:TRP:HZ2	1.58	0.67
17:T:17:DC:H2'	17:T:18:DA:H8	1.59	0.67
2:B:885:MET:SD	2:B:887:SER:OG	2.52	0.67
2:B:997:ASN:HD22	3:C:277:ARG:HH11	1.41	0.67
1:A:833:PRO:HB2	2:B:659:ILE:HD12	1.76	0.66
9:J:10:CYS:HB3	9:J:45:CYS:SG	2.34	0.66
1:A:573:ARG:HH21	10:K:87:GLU:HB2	1.60	0.66
11:L:31:CYS:HB3	11:L:34:CYS:SG	2.35	0.66
5:E:80:VAL:HG12	5:E:109:ILE:HB	1.79	0.64
11:L:33:GLU:OE1	11:L:53:HIS:ND1	2.30	0.64
2:B:80:ASN:HD22	2:B:393:LYS:HG2	1.60	0.64
1:A:14:LYS:HD2	2:B:1144:GLU:HB3	1.80	0.64
1:A:821:ASN:OD1	1:A:822:ARG:N	2.31	0.64
2:B:302:LEU:HD22	2:B:327:ILE:HG13	1.78	0.64
4:D:71:ASN:OD1	7:G:147:ARG:NH2	2.29	0.64
3:C:150:SER:HB2	3:C:156:LEU:HD11	1.80	0.63
3:C:103:LEU:HD23	3:C:218:LYS:HB3	1.81	0.63
1:A:464:ARG:NH1	1:A:467:GLU:OE2	2.32	0.63
3:C:39:ASP:HB3	3:C:58:ASN:HD22	1.63	0.63
1:A:200:GLU:HG2	12:O:515:LYS:HB3	1.80	0.62
12:O:376:LEU:HD23	12:O:452:LEU:HB3	1.81	0.62
1:A:580:LEU:HA	1:A:583:MET:HE3	1.81	0.62
1:A:993:GLU:HG3	5:E:154:ILE:HD13	1.82	0.62
1:A:1225:ILE:O	1:A:1229:ARG:HB2	1.99	0.62
13:P:188:GLU:HA	13:P:194:GLY:HA2	1.81	0.62
8:H:2:SER:OG	8:H:3:ASN:N	2.31	0.62
3:C:18:THR:HG22	3:C:295:ARG:HH22	1.64	0.61
1:A:546:SER:OG	1:A:1349:SER:O	2.17	0.61
2:B:738:THR:HG23	2:B:977:THR:HA	1.81	0.61
1:A:393:ALA:HB3	1:A:499:ARG:HB2	1.83	0.61
1:A:774:ARG:HG2	1:A:812:VAL:HG23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:ILE:HG12	2:B:353:THR:HG21	1.82	0.61
1:A:1171:PHE:N	1:A:1187:ARG:O	2.32	0.61
8:H:97:MET:HE2	8:H:118:PHE:HD1	1.65	0.60
2:B:474:SER:OG	2:B:475:SER:N	2.34	0.60
4:D:146:ASP:OD2	4:D:148:LYS:NZ	2.34	0.60
1:A:880:ALA:HB1	17:T:19:DT:H5"	1.84	0.60
12:O:201:ILE:HG12	12:O:283:ASN:HB2	1.83	0.60
12:O:608:ARG:NH1	12:O:610:ASP:OD1	2.36	0.59
3:C:51:GLU:OE2	3:C:301:ASN:ND2	2.35	0.59
1:A:1188:ILE:HD13	1:A:1205:ILE:HD13	1.84	0.59
2:B:1105:GLY:HA2	2:B:1116:ILE:HG21	1.84	0.59
1:A:535:MET:HG2	2:B:1073:TYR:CD1	2.37	0.59
2:B:136:THR:HG22	2:B:141:ILE:HG22	1.84	0.59
12:O:140:ILE:HG21	12:O:160:VAL:HG21	1.85	0.59
1:A:36:THR:HG22	1:A:38:ASP:H	1.68	0.58
2:B:59:LYS:HG2	2:B:62:LEU:HD12	1.85	0.58
12:O:356:THR:HG22	12:O:358:GLY:H	1.68	0.58
2:B:779:ASP:OD1	2:B:905:ARG:NH2	2.36	0.58
12:O:603:LEU:HD21	12:O:630:VAL:HG11	1.86	0.58
13:P:190:THR:HB	13:P:263:VAL:HG12	1.85	0.58
12:O:163:VAL:HG11	12:O:200:LEU:HD11	1.85	0.58
1:A:1163:LYS:NZ	1:A:1278:ILE:O	2.37	0.57
2:B:157:ARG:NH1	2:B:180:ASP:O	2.37	0.57
2:B:100:VAL:HG22	2:B:129:ILE:HG22	1.85	0.57
10:K:140:LYS:HZ1	20:K:401:1N7:H24	1.69	0.57
1:A:426:VAL:HG12	1:A:428:PRO:HD2	1.85	0.57
8:H:15:VAL:HG12	8:H:26:ILE:HG22	1.85	0.57
1:A:201:TRP:HA	1:A:204:VAL:HG12	1.85	0.57
1:A:225:LEU:HD23	12:O:541:ILE:HG22	1.85	0.57
12:O:108:GLN:HG2	12:O:118:THR:HG22	1.85	0.57
15:R:12:C:H42	17:T:28:DG:H1	1.52	0.57
2:B:911:LYS:HD3	2:B:1029:HIS:HB2	1.87	0.57
3:C:132:ILE:HB	3:C:208:CYS:HB2	1.87	0.57
13:P:236:THR:OG1	13:P:239:ASN:OD1	2.23	0.57
2:B:539:GLU:HB3	2:B:543:LEU:HD11	1.86	0.56
13:P:253:LEU:HD13	13:P:261:TYR:HB3	1.87	0.56
1:A:162:GLY:HA3	1:A:181:ASP:O	2.05	0.56
4:D:71:ASN:O	7:G:147:ARG:NH2	2.39	0.56
3:C:132:ILE:HG23	3:C:169:PHE:HE1	1.70	0.56
3:C:191:ILE:HG21	9:J:5:VAL:HG23	1.88	0.56
1:A:120:LYS:HG3	1:A:241:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:LEU:HD21	2:B:127:ALA:HB2	1.87	0.56
13:P:237:PRO:HA	13:P:240:ILE:HD12	1.88	0.56
12:O:592:LYS:HB2	12:O:637:VAL:HG11	1.88	0.55
2:B:552:ASN:HB3	2:B:564:SER:HB3	1.89	0.55
1:A:1132:ALA:HB1	1:A:1320:LEU:HD21	1.88	0.55
1:A:1170:ALA:HA	1:A:1188:ILE:HA	1.87	0.55
2:B:135:TYR:OH	2:B:137:ARG:NH2	2.40	0.55
2:B:889:SER:OG	2:B:890:ASP:N	2.39	0.55
3:C:215:ASP:OD1	11:L:70:ARG:NH1	2.40	0.55
13:P:187:SER:HA	13:P:263:VAL:HG11	1.88	0.55
1:A:367:ASN:ND2	2:B:1049:GLN:OE1	2.39	0.55
1:A:625:ASN:HA	1:A:654:ILE:O	2.07	0.55
11:L:53:HIS:CD2	11:L:54:ARG:H	2.25	0.55
1:A:368:LEU:HD23	1:A:1416:ILE:HG23	1.89	0.55
12:O:305:GLY:H	13:P:207:PHE:HE1	1.55	0.55
1:A:870:GLU:HA	1:A:873:VAL:HG12	1.88	0.54
12:O:631:ASN:HB3	14:Q:159:VAL:HG23	1.88	0.54
11:L:44:ASP:OD2	11:L:49:LYS:NZ	2.35	0.54
16:S:42:DT:H2"	16:S:43:DT:H5"	1.89	0.54
1:A:1373:ARG:NH1	1:A:1390:GLU:OE1	2.38	0.54
8:H:48:PRO:HD2	8:H:146:ARG:HH22	1.72	0.54
1:A:625:ASN:HD22	1:A:941:HIS:HA	1.72	0.54
1:A:1184:ILE:O	1:A:1231:ALA:HA	2.08	0.54
1:A:1316:THR:HG22	1:A:1318:HIS:H	1.73	0.54
3:C:157:TYR:HB2	3:C:160:ALA:HB2	1.89	0.54
8:H:3:ASN:OD1	8:H:61:SER:OG	2.25	0.54
3:C:3:ASN:ND2	3:C:296:ASN:OD1	2.40	0.54
1:A:225:LEU:HD21	12:O:542:ARG:HA	1.89	0.54
1:A:719:PRO:HB3	1:A:723:LEU:HD23	1.90	0.54
1:A:614:ILE:HD13	1:A:624:ILE:HD11	1.88	0.54
2:B:1003:MET:SD	3:C:293:ARG:NH1	2.81	0.53
5:E:117:THR:HG23	5:E:120:ALA:H	1.73	0.53
1:A:11:LYS:HG3	2:B:1117:ILE:HD13	1.89	0.53
1:A:1200:LEU:HD21	1:A:1273:LYS:HB2	1.90	0.53
2:B:126:SER:OG	2:B:151:ARG:NE	2.38	0.53
2:B:237:ASN:OD1	2:B:239:LYS:NZ	2.40	0.53
4:D:134:LEU:HA	4:D:137:ILE:HG22	1.89	0.53
4:D:72:PHE:HB2	4:D:129:ALA:HB2	1.90	0.53
12:O:380:LEU:HD23	13:P:209:ALA:HA	1.91	0.53
13:P:217:THR:HG22	13:P:220:GLU:HG3	1.90	0.53
14:Q:121:SER:OG	14:Q:122:ILE:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:829:LEU:HD21	2:B:896:ILE:HD13	1.90	0.53
7:G:26:ILE:HD11	7:G:68:ILE:HD12	1.91	0.53
2:B:124:THR:HG22	2:B:188:ASN:H	1.74	0.52
6:F:110:ASP:O	6:F:123:LYS:NZ	2.42	0.52
7:G:10:LEU:HD11	7:G:67:TYR:HB3	1.90	0.52
7:G:54:VAL:HG12	7:G:70:VAL:HG12	1.91	0.52
12:O:603:LEU:O	12:O:607:ASN:HB2	2.08	0.52
1:A:1415:ILE:HD13	2:B:1067:ARG:HD3	1.90	0.52
12:O:124:GLU:HB3	12:O:128:HIS:CD2	2.44	0.52
12:O:154:GLN:OE1	14:Q:155:ASN:ND2	2.41	0.52
9:J:12:LYS:NZ	9:J:40:GLY:O	2.42	0.52
2:B:202:LYS:HD2	2:B:223:SER:HB2	1.91	0.52
10:K:116:ALA:HA	10:K:119:LYS:HE3	1.91	0.52
2:B:695:GLN:HB2	2:B:953:MET:HB2	1.92	0.52
2:B:305:ILE:HG13	2:B:327:ILE:HD11	1.92	0.52
2:B:629:LYS:HB3	2:B:635:LEU:HD13	1.91	0.52
7:G:128:TRP:HB2	7:G:140:PHE:HB2	1.91	0.52
2:B:495:GLY:HA3	2:B:610:ARG:HH11	1.75	0.52
7:G:9:ASP:OD1	7:G:10:LEU:N	2.42	0.52
1:A:488:HIS:HE1	1:A:504:VAL:HG11	1.75	0.51
3:C:78:VAL:HG21	3:C:108:VAL:HB	1.91	0.51
12:O:507:LEU:HD21	12:O:533:ILE:HD12	1.90	0.51
1:A:1207:VAL:HA	1:A:1210:THR:HG22	1.93	0.51
2:B:52:LEU:HD12	2:B:743:LEU:HD23	1.91	0.51
2:B:626:HIS:HA	2:B:629:LYS:HD2	1.92	0.51
6:F:133:VAL:HG12	6:F:147:SER:HA	1.92	0.51
1:A:482:ARG:HD2	2:B:1073:TYR:CE2	2.45	0.51
1:A:1384:LEU:HB2	1:A:1413:GLU:HG2	1.93	0.51
3:C:7:ILE:HD13	3:C:275:VAL:HG11	1.92	0.51
7:G:27:THR:HG23	7:G:48:ILE:HD11	1.92	0.51
1:A:224:PRO:HD2	1:A:316:TRP:CZ2	2.44	0.51
1:A:753:GLN:HG2	1:A:761:THR:HG22	1.93	0.51
2:B:221:THR:OG1	2:B:230:LYS:NZ	2.36	0.51
2:B:588:ILE:HD12	2:B:603:THR:HG22	1.92	0.51
12:O:543:TYR:OH	13:P:313:ASP:OD1	2.26	0.51
4:D:24:GLU:HG3	4:D:29:TRP:HB2	1.93	0.51
7:G:93:THR:HG23	7:G:95:GLU:H	1.75	0.51
1:A:387:LEU:HG	1:A:391:GLU:HB3	1.92	0.51
1:A:427:HIS:CE1	1:A:492:ILE:HG13	2.46	0.51
2:B:241:TYR:HB3	2:B:250:GLU:HB3	1.93	0.51
4:D:154:LEU:HD23	4:D:157:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:330:LEU:O	12:O:333:THR:OG1	2.26	0.51
2:B:792:THR:HG22	2:B:897:LYS:HG2	1.91	0.51
2:B:961:LEU:HD12	2:B:1022:ILE:HD11	1.92	0.51
1:A:593:PRO:HD3	1:A:612:LEU:HD21	1.93	0.51
13:P:312:PHE:HB2	14:Q:41:LEU:HG	1.93	0.50
1:A:117:GLU:HG3	12:O:212:GLU:HG2	1.92	0.50
1:A:121:ARG:NH1	12:O:121:TYR:OH	2.33	0.50
1:A:303:LEU:HD13	12:O:542:ARG:HH21	1.77	0.50
1:A:674:LYS:NZ	1:A:926:MET:O	2.45	0.50
2:B:630:LEU:HD12	2:B:640:PHE:HE2	1.76	0.50
12:O:49:TYR:CD1	12:O:127:ILE:HG21	2.47	0.50
2:B:126:SER:HB2	2:B:151:ARG:HB3	1.94	0.50
5:E:163:GLU:OE2	5:E:167:ARG:NH1	2.44	0.50
6:F:101:ILE:HD13	6:F:105:ALA:HB3	1.94	0.50
12:O:29:GLU:OE2	12:O:33:THR:OG1	2.29	0.50
12:O:643:ARG:NH2	14:Q:46:PRO:O	2.33	0.50
2:B:94:LYS:HB3	2:B:134:GLU:HB3	1.93	0.50
12:O:643:ARG:NH2	14:Q:51:GLU:OE1	2.45	0.50
2:B:805:ILE:HG22	2:B:807:GLY:H	1.77	0.49
1:A:1261:GLN:OE1	1:A:1264:ARG:NH1	2.45	0.49
1:A:1173:VAL:HG13	1:A:1186:VAL:HG12	1.95	0.49
2:B:827:ASP:OD2	11:L:58:LYS:NZ	2.44	0.49
12:O:295:GLN:HB3	12:O:487:LEU:HD21	1.94	0.49
1:A:927:GLU:OE2	1:A:1077:LYS:NZ	2.31	0.49
4:D:128:PRO:HD2	4:D:157:ILE:HD12	1.95	0.49
7:G:150:ILE:HG21	7:G:196:LEU:HD22	1.94	0.49
2:B:205:ILE:HD13	2:B:355:ARG:CZ	2.43	0.49
12:O:260:SER:O	12:O:275:LYS:NZ	2.45	0.49
14:Q:44:ASN:ND2	14:Q:44:ASN:O	2.46	0.49
2:B:222:SER:HA	2:B:334:HIS:CE1	2.48	0.49
12:O:305:GLY:HA3	12:O:308:THR:HB	1.94	0.49
2:B:929:GLU:HB2	3:C:69:ARG:HD2	1.93	0.49
5:E:40:GLU:HA	5:E:43:LYS:HE2	1.95	0.49
2:B:489:LEU:HD21	2:B:499:THR:HG22	1.94	0.49
12:O:614:ARG:NH1	12:O:617:GLU:OE2	2.45	0.49
1:A:416:LEU:HD23	1:A:419:LEU:HD12	1.95	0.48
1:A:926:MET:SD	1:A:1353:ARG:NH1	2.86	0.48
1:A:964:ASN:OD1	1:A:1009:ARG:NH1	2.46	0.48
1:A:1396:LEU:HD13	2:B:1132:LEU:HD21	1.94	0.48
17:T:15:DG:H2'	17:T:16:DG:C8	2.48	0.48
1:A:91:PHE:CD2	1:A:224:PRO:HG3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1043:ASP:N	1:A:1043:ASP:OD1	2.45	0.48
1:A:511:ASP:OD1	1:A:511:ASP:N	2.46	0.48
7:G:86:THR:HA	7:G:146:ILE:O	2.12	0.48
20:K:401:1N7:H27	20:K:401:1N7:H13	1.57	0.48
12:O:233:SER:HB3	12:O:236:LYS:HG2	1.95	0.48
1:A:974:LEU:HD23	1:A:998:TYR:HB3	1.94	0.48
2:B:741:ILE:HG23	2:B:746:TYR:HB3	1.94	0.48
12:O:202:GLN:OE1	12:O:260:SER:OG	2.28	0.48
13:P:186:ILE:HD11	13:P:221:ILE:HD11	1.95	0.48
13:P:292:SER:HB3	13:P:294:PHE:HD2	1.76	0.48
5:E:16:PHE:CZ	5:E:58:MET:HB2	2.48	0.48
12:O:224:LYS:O	12:O:228:ARG:NH1	2.46	0.48
1:A:914:PHE:HZ	5:E:175:LEU:HD22	1.78	0.48
2:B:209:ALA:HB3	2:B:366:ILE:HD12	1.96	0.48
1:A:1161:VAL:HG21	1:A:1293:LEU:HD21	1.96	0.48
2:B:273:CYS:SG	2:B:280:GLN:HG2	2.54	0.48
1:A:309:ILE:HG13	12:O:566:PHE:HZ	1.79	0.48
12:O:288:MET:HB3	12:O:326:ILE:HG21	1.96	0.48
12:O:647:LEU:HD21	13:P:293:ILE:HB	1.96	0.48
13:P:189:ASN:HD22	13:P:216:SER:HG	1.55	0.48
14:Q:129:LEU:O	14:Q:137:TYR:OH	2.30	0.47
1:A:790:ALA:O	1:A:794:MET:HG3	2.14	0.47
12:O:80:VAL:HG21	12:O:88:VAL:HG12	1.96	0.47
1:A:391:GLU:HA	1:A:489:TYR:O	2.14	0.47
10:K:88:PHE:HB3	10:K:106:GLN:HB2	1.95	0.47
1:A:102:ILE:HG23	1:A:103:LEU:HD12	1.96	0.47
5:E:85:GLU:HG2	5:E:86:PRO:HD2	1.95	0.47
4:D:119:GLU:O	4:D:123:ILE:HG12	2.15	0.47
8:H:38:LEU:HD12	8:H:125:LEU:HD13	1.97	0.47
1:A:475:ASN:ND2	2:B:1066:GLU:OE2	2.48	0.47
2:B:876:PRO:HG2	2:B:877:GLU:OE1	2.15	0.47
12:O:628:LYS:HB2	14:Q:161:THR:HG22	1.95	0.47
4:D:71:ASN:HB2	7:G:86:THR:HG21	1.96	0.47
8:H:7:ASP:OD1	8:H:7:ASP:N	2.48	0.47
1:A:1321:GLU:OE2	20:A:2003:1N7:H25	2.15	0.46
2:B:208:GLU:OE1	2:B:217:GLN:NE2	2.48	0.46
2:B:710:ILE:HD11	2:B:1028:LYS:HA	1.96	0.46
1:A:17:GLU:HG2	1:A:1405:LYS:HG3	1.98	0.46
2:B:161:CYS:SG	2:B:162:ILE:N	2.88	0.46
3:C:226:SER:OG	3:C:227:TYR:N	2.48	0.46
1:A:1145:LEU:HD22	1:A:1157:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:91:LYS:HA	5:E:94:LYS:HE3	1.97	0.46
12:O:232:LEU:HD23	12:O:236:LYS:HZ1	1.80	0.46
1:A:482:ARG:HE	1:A:544:PRO:HD3	1.80	0.46
2:B:99:ARG:NH1	2:B:132:ASP:OD1	2.41	0.46
2:B:313:ARG:O	2:B:316:LYS:NZ	2.45	0.46
3:C:290:LYS:HE3	3:C:290:LYS:HA	1.97	0.46
5:E:29:PHE:HB2	5:E:65:THR:HB	1.98	0.46
13:P:190:THR:HG21	13:P:262:ARG:HB2	1.96	0.46
1:A:879:THR:HA	1:A:882:THR:HG22	1.97	0.46
2:B:886:MET:HG2	2:B:896:ILE:HG12	1.97	0.46
14:Q:71:TYR:O	14:Q:72:THR:OG1	2.32	0.46
1:A:488:HIS:CE1	1:A:504:VAL:HG11	2.51	0.46
7:G:30:LEU:O	7:G:34:PHE:HB2	2.16	0.46
12:O:183:MET:O	12:O:187:ILE:HG12	2.15	0.46
14:Q:126:PRO:HA	14:Q:146:LYS:HD2	1.98	0.46
2:B:297:THR:OG1	2:B:300:GLN:O	2.34	0.46
2:B:604:ASP:OD1	2:B:605:GLY:N	2.49	0.46
4:D:7:ARG:HD2	4:D:10:PHE:CZ	2.51	0.46
2:B:567:PHE:HD2	2:B:570:LYS:HZ1	1.63	0.46
8:H:27:GLU:HG2	8:H:39:THR:HG22	1.98	0.46
1:A:666:LYS:NZ	1:A:671:ASP:O	2.49	0.45
1:A:1144:VAL:HG21	1:A:1313:ARG:HB2	1.99	0.45
2:B:911:LYS:HE3	2:B:1027:LEU:HD12	1.97	0.45
4:D:117:LYS:HA	4:D:120:LYS:HE2	1.99	0.45
1:A:245:ASP:HB3	1:A:1403:MET:HE2	1.98	0.45
2:B:391:LEU:HG	2:B:429:ILE:HD13	1.98	0.45
1:A:378:ARG:NH1	1:A:518:ASN:OD1	2.48	0.45
2:B:824:LEU:HD11	2:B:844:ASN:HB2	1.97	0.45
1:A:991:LYS:HZ3	1:A:994:TYR:HE2	1.65	0.45
2:B:884:VAL:HG22	2:B:898:VAL:HG22	1.98	0.45
4:D:50:TYR:OH	7:G:28:HIS:ND1	2.46	0.45
5:E:153:HIS:CD2	5:E:184:VAL:HG11	2.51	0.45
2:B:827:ASP:OD1	2:B:828:GLY:N	2.50	0.45
2:B:47:LEU:HB2	2:B:675:ILE:HD11	1.98	0.45
9:J:32:GLU:OE2	9:J:32:GLU:N	2.43	0.45
12:O:335:LEU:HD11	12:O:341:GLU:HG3	1.99	0.45
1:A:71:HIS:CE1	7:G:167:GLU:HG2	2.51	0.45
1:A:521:VAL:O	2:B:1082:ARG:NH2	2.50	0.45
7:G:141:ASP:N	7:G:141:ASP:OD1	2.50	0.45
10:K:87:GLU:HB3	10:K:108:TYR:CD1	2.51	0.45
1:A:1008:LEU:HD21	1:A:1071:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:99:SER:OG	4:D:100:ASP:N	2.49	0.45
1:A:541:LEU:HA	1:A:551:ILE:HD12	1.97	0.45
2:B:841:ILE:HD12	2:B:870:PRO:HB2	1.99	0.45
3:C:128:ASP:OD1	3:C:128:ASP:N	2.50	0.45
1:A:413:ARG:NH1	1:A:417:GLN:OE1	2.50	0.45
12:O:538:ALA:HA	12:O:541:ILE:HD12	1.99	0.44
1:A:848:VAL:HG13	1:A:860:GLU:HB3	1.99	0.44
12:O:40:ARG:NH1	14:Q:35:GLU:OE2	2.50	0.44
12:O:482:LYS:HE3	12:O:482:LYS:HA	1.99	0.44
1:A:472:VAL:HG12	1:A:521:VAL:HG22	1.99	0.44
1:A:1436:ILE:HG12	7:G:23:ILE:HD11	2.00	0.44
2:B:93:LEU:HD21	2:B:133:ILE:HD11	1.99	0.44
2:B:121:ARG:NH2	2:B:888:VAL:O	2.50	0.44
3:C:136:LEU:O	3:C:203:SER:HA	2.17	0.44
4:D:115:LEU:HD12	4:D:119:GLU:HG3	1.99	0.44
6:F:140:ASP:OD1	6:F:141:GLY:N	2.49	0.44
20:K:401:1N7:H34	20:K:401:1N7:H10	1.56	0.44
11:L:27:LEU:HD13	11:L:37:LYS:HB3	2.00	0.44
1:A:524:THR:HG23	1:A:527:ALA:H	1.82	0.44
2:B:1001:LYS:O	3:C:277:ARG:NH1	2.51	0.44
3:C:294:VAL:HG23	3:C:297:HIS:HB3	1.99	0.44
5:E:5:ASN:ND2	5:E:51:GLY:O	2.40	0.44
1:A:369:SER:OG	2:B:1067:ARG:NH2	2.33	0.44
5:E:16:PHE:CE1	5:E:58:MET:HB2	2.53	0.44
2:B:347:LEU:HD21	2:B:561:LEU:HD22	2.00	0.44
7:G:100:SER:HB2	7:G:106:ASP:HA	2.00	0.44
7:G:122:THR:OG1	7:G:124:GLU:OE1	2.33	0.44
2:B:680:ILE:HG23	2:B:681:LEU:HD22	2.00	0.43
5:E:147:HIS:HB3	5:E:150:VAL:HG12	2.00	0.43
10:K:83:ASN:HD22	10:K:86:VAL:HG23	1.82	0.43
1:A:580:LEU:HB3	1:A:590:PHE:HD1	1.83	0.43
2:B:126:SER:HA	2:B:152:MET:O	2.19	0.43
10:K:86:VAL:HG22	10:K:107:THR:HG22	2.00	0.43
1:A:613:LEU:HD11	1:A:697:MET:HA	2.01	0.43
2:B:1086:SER:O	2:B:1086:SER:OG	2.35	0.43
3:C:222:VAL:HG12	3:C:313:ILE:HD13	2.01	0.43
5:E:71:LYS:HB2	5:E:71:LYS:HE2	1.89	0.43
13:P:241:ARG:NE	13:P:259:ASP:OD1	2.45	0.43
13:P:310:VAL:HG11	14:Q:43:ILE:HD11	1.99	0.43
1:A:16:LEU:HD11	1:A:1417:LEU:HD11	2.01	0.43
3:C:100:ARG:NH2	3:C:192:LEU:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:ARG:HD2	1:A:845:LYS:HB3	2.01	0.43
1:A:952:LYS:HD3	1:A:952:LYS:HA	1.81	0.43
2:B:465:SER:HA	2:B:707:LYS:HG2	2.00	0.43
3:C:94:ASP:OD2	11:L:60:ARG:NH2	2.43	0.43
5:E:65:THR:OG1	5:E:66:GLU:N	2.52	0.43
12:O:96:VAL:HG23	14:Q:136:LEU:HD22	2.00	0.43
1:A:890:MET:SD	1:A:894:GLU:HB3	2.58	0.43
2:B:765:TYR:HE1	10:K:96:PRO:HG2	1.84	0.43
3:C:188:ASP:HB3	3:C:191:ILE:HD11	1.99	0.43
4:D:106:LEU:HB2	4:D:161:ALA:HB2	2.00	0.43
5:E:76:GLY:HA3	5:E:106:GLN:HB2	1.99	0.43
13:P:245:GLU:HA	13:P:248:VAL:HG12	2.01	0.43
1:A:580:LEU:HB3	1:A:590:PHE:CD1	2.53	0.43
1:A:1189:ASP:OD2	1:A:1192:THR:OG1	2.35	0.43
2:B:295:ILE:HD12	2:B:298:GLN:HA	2.01	0.43
7:G:4:LEU:HD23	7:G:4:LEU:HA	1.82	0.43
7:G:99:VAL:HG13	7:G:108:ILE:HB	2.00	0.43
2:B:540:ASP:OD1	2:B:541:ILE:N	2.52	0.42
2:B:610:ARG:HE	2:B:612:LEU:HD11	1.83	0.42
4:D:149:THR:HA	4:D:152:GLU:HG2	2.01	0.42
5:E:100:ILE:HG21	5:E:132:ILE:HD11	2.01	0.42
7:G:89:ILE:HG22	7:G:142:VAL:HG12	2.00	0.42
10:K:50:LEU:HD23	10:K:50:LEU:HA	1.92	0.42
1:A:376:SER:HB2	2:B:1060:LEU:HD12	2.00	0.42
1:A:386:ASN:HD22	10:K:96:PRO:HD3	1.84	0.42
1:A:605:THR:HG23	1:A:608:GLN:H	1.84	0.42
4:D:119:GLU:HA	4:D:122:GLN:OE1	2.20	0.42
12:O:507:LEU:HD23	12:O:507:LEU:HA	1.82	0.42
4:D:131:MET:O	4:D:133:HIS:N	2.52	0.42
5:E:3:GLN:HE22	5:E:7:ARG:HD2	1.84	0.42
5:E:99:HIS:CE1	5:E:103:LYS:HG3	2.53	0.42
10:K:87:GLU:HB3	10:K:108:TYR:HD1	1.83	0.42
1:A:126:GLU:OE2	1:A:136:ARG:NH2	2.52	0.42
2:B:552:ASN:OD1	2:B:566:ARG:HA	2.19	0.42
3:C:326:GLU:OE2	3:C:330:ASN:ND2	2.52	0.42
2:B:625:ILE:HG22	2:B:629:LYS:HE3	2.02	0.42
1:A:673:LYS:HD2	1:A:675:HIS:CE1	2.54	0.42
2:B:938:ILE:HD11	9:J:9:SER:OG	2.20	0.42
10:K:91:TYR:HB2	10:K:101:LEU:HD11	2.02	0.42
12:O:155:LEU:HA	12:O:158:GLU:HG2	2.02	0.42
1:A:660:LEU:HB3	8:H:117:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:LYS:HD2	1:A:812:VAL:HG13	2.01	0.42
20:A:2003:1N7:H27	20:A:2003:1N7:H13	1.59	0.42
12:O:68:LEU:HD23	12:O:68:LEU:HA	1.90	0.42
1:A:124:LEU:HA	1:A:124:LEU:HD23	1.87	0.42
1:A:594:PRO:HA	1:A:595:PRO:HD3	1.88	0.42
12:O:36:SER:OG	13:P:314:GLU:OE2	2.37	0.42
12:O:516:LEU:HD13	12:O:567:ARG:HB3	2.01	0.42
1:A:102:ILE:HG13	1:A:242:LEU:HD13	2.00	0.42
1:A:1305:CYS:SG	5:E:11:ARG:NH2	2.92	0.42
20:A:2003:1N7:H34	20:A:2003:1N7:H10	1.72	0.42
8:H:104:PHE:CE1	8:H:137:GLN:HB3	2.55	0.42
12:O:60:ARG:HE	14:Q:72:THR:HB	1.85	0.42
12:O:155:LEU:HD23	12:O:190:LEU:HD12	2.02	0.42
12:O:232:LEU:HD23	12:O:236:LYS:NZ	2.34	0.42
12:O:199:TYR:OH	12:O:286:ARG:NH1	2.52	0.41
12:O:610:ASP:OD1	12:O:610:ASP:N	2.52	0.41
1:A:848:VAL:HA	1:A:860:GLU:HG2	2.02	0.41
2:B:185:PHE:HE2	2:B:194:ILE:HD12	1.85	0.41
2:B:625:ILE:HG22	2:B:629:LYS:HZ1	1.86	0.41
2:B:785:CYS:SG	2:B:1026:LYS:NZ	2.77	0.41
5:E:144:ILE:HD11	5:E:187:TYR:HB2	2.01	0.41
7:G:202:THR:H	7:G:205:MET:HG3	1.84	0.41
1:A:25:ASP:OD2	2:B:1140:ARG:NH2	2.52	0.41
1:A:516:GLU:OE2	2:B:1034:LYS:HD3	2.20	0.41
1:A:566:HIS:ND1	1:A:568:ASP:OD1	2.53	0.41
1:A:756:CYS:HB3	1:A:760:GLN:HB2	2.03	0.41
1:A:818:ILE:HG21	1:A:824:PRO:HD3	2.01	0.41
1:A:846:GLY:HA2	1:A:863:PHE:CD2	2.55	0.41
3:C:77:SER:HB2	3:C:221:PRO:HB3	2.01	0.41
3:C:115:TRP:HH2	3:C:212:ILE:HG23	1.85	0.41
4:D:115:LEU:HB2	4:D:119:GLU:HG2	2.01	0.41
13:P:197:ASN:OD1	13:P:198:PHE:N	2.53	0.41
1:A:1207:VAL:O	1:A:1211:ARG:HB2	2.21	0.41
2:B:184:TYR:HB3	2:B:193:VAL:HG22	2.00	0.41
4:D:45:LYS:HZ3	4:D:47:ASN:HB3	1.85	0.41
4:D:146:ASP:OD1	4:D:146:ASP:N	2.53	0.41
7:G:98:LYS:HE2	7:G:109:PHE:HB2	2.02	0.41
3:C:69:ARG:HH22	10:K:70:HIS:HB2	1.85	0.41
4:D:113:PHE:HE1	4:D:153:MET:HB3	1.84	0.41
7:G:138:LEU:HD13	7:G:210:TRP:CD1	2.55	0.41
12:O:219:TYR:OH	12:O:238:ARG:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:497:ALA:HB2	12:O:505:MET:HB2	2.03	0.41
1:A:379:THR:HB	1:A:498:PHE:CD2	2.55	0.41
1:A:721:ASP:OD1	1:A:721:ASP:N	2.46	0.41
2:B:168:GLU:OE1	9:J:62:ARG:NH1	2.53	0.41
1:A:1287:ASP:OD1	1:A:1288:ASP:N	2.53	0.41
1:A:1305:CYS:SG	5:E:141:VAL:HG21	2.60	0.41
2:B:534:TYR:HE2	2:B:540:ASP:HA	1.86	0.41
1:A:1064:GLU:O	1:A:1068:ARG:HG2	2.20	0.41
2:B:199:GLN:OE1	2:B:202:LYS:NZ	2.53	0.41
12:O:496:ILE:HD12	12:O:496:ILE:HA	1.89	0.41
14:Q:128:ASN:ND2	14:Q:131:LEU:HD23	2.35	0.41
1:A:145:LEU:HD23	1:A:149:LYS:HE2	2.03	0.41
1:A:1382:SER:OG	1:A:1413:GLU:OE2	2.25	0.41
1:A:1422:SER:O	1:A:1422:SER:OG	2.29	0.41
2:B:638:ASP:O	2:B:642:LYS:HG2	2.20	0.41
3:C:80:ALA:HB3	3:C:102:GLY:HA2	2.02	0.41
3:C:92:ILE:HD11	3:C:96:VAL:HG11	2.02	0.41
7:G:84:ILE:HG22	7:G:149:ARG:HG3	2.03	0.41
8:H:57:VAL:HG13	8:H:142:LEU:HD11	2.03	0.41
8:H:118:PHE:HE1	8:H:142:LEU:HB3	1.86	0.41
9:J:45:CYS:SG	9:J:46:CYS:N	2.93	0.41
1:A:626:LEU:HD23	1:A:654:ILE:HB	2.03	0.41
1:A:1436:ILE:HD12	1:A:1436:ILE:HA	1.90	0.41
2:B:64:SER:HB2	2:B:379:LEU:HD13	2.03	0.41
3:C:162:VAL:HB	3:C:194:ALA:HB3	2.03	0.41
7:G:30:LEU:HA	7:G:30:LEU:HD23	1.86	0.41
12:O:259:LEU:HD12	12:O:259:LEU:HA	1.97	0.41
14:Q:108:TYR:CZ	14:Q:111:LYS:HG2	2.56	0.41
1:A:353:PHE:HE2	2:B:1131:GLU:HA	1.86	0.40
2:B:365:MET:SD	2:B:595:HIS:HB3	2.61	0.40
3:C:31:TRP:HH2	10:K:127:LEU:HD13	1.85	0.40
7:G:47:THR:OG1	7:G:48:ILE:N	2.53	0.40
1:A:1222:VAL:HG12	1:A:1232:ILE:HD12	2.02	0.40
2:B:961:LEU:HD22	2:B:1018:PHE:CZ	2.56	0.40
5:E:153:HIS:CG	5:E:184:VAL:HG11	2.56	0.40
10:K:65:ILE:HD12	10:K:101:LEU:HD23	2.03	0.40
12:O:500:LEU:HD11	12:O:543:TYR:HE2	1.86	0.40
1:A:1304:MET:HE2	1:A:1304:MET:HB2	1.89	0.40
1:A:1360:ASP:O	1:A:1364:TYR:HB3	2.21	0.40
2:B:772:VAL:HG22	2:B:924:ILE:HG22	2.04	0.40
3:C:195:LYS:HB3	9:J:61:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:P:164:TRP:HB3	13:P:175:ILE:HD11	2.03	0.40
1:A:99:THR:HA	1:A:102:ILE:HG22	2.03	0.40
1:A:577:THR:HG21	10:K:81:MET:HE3	2.03	0.40
2:B:999:SER:O	2:B:999:SER:OG	2.35	0.40
2:B:1100:LEU:HD11	2:B:1133:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1427/1460 (98%)	1351 (95%)	75 (5%)	1 (0%)	51 84
2	B	1110/1149 (97%)	1058 (95%)	52 (5%)	0	100 100
3	C	332/335 (99%)	320 (96%)	12 (4%)	0	100 100
4	D	141/161 (88%)	132 (94%)	8 (6%)	1 (1%)	22 60
5	E	213/215 (99%)	202 (95%)	11 (5%)	0	100 100
6	F	81/155 (52%)	78 (96%)	3 (4%)	0	100 100
7	G	195/212 (92%)	184 (94%)	11 (6%)	0	100 100
8	H	131/146 (90%)	123 (94%)	8 (6%)	0	100 100
9	J	67/70 (96%)	65 (97%)	2 (3%)	0	100 100
10	K	100/142 (70%)	99 (99%)	1 (1%)	0	100 100
11	L	43/70 (61%)	39 (91%)	4 (9%)	0	100 100
12	O	566/654 (86%)	544 (96%)	22 (4%)	0	100 100
13	P	136/317 (43%)	127 (93%)	9 (7%)	0	100 100
14	Q	119/251 (47%)	112 (94%)	7 (6%)	0	100 100
All	All	4661/5337 (87%)	4434 (95%)	225 (5%)	2 (0%)	100 100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1114	VAL
4	D	132	VAL

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	1237/1257 (98%)	1235 (100%)	2 (0%)	93 96
2	B	973/1006 (97%)	973 (100%)	0	100 100
3	C	295/296 (100%)	294 (100%)	1 (0%)	92 95
4	D	133/145 (92%)	132 (99%)	1 (1%)	81 89
5	E	197/197 (100%)	197 (100%)	0	100 100
6	F	73/137 (53%)	73 (100%)	0	100 100
7	G	178/190 (94%)	178 (100%)	0	100 100
8	H	119/128 (93%)	119 (100%)	0	100 100
9	J	64/65 (98%)	64 (100%)	0	100 100
10	K	92/130 (71%)	92 (100%)	0	100 100
11	L	40/57 (70%)	40 (100%)	0	100 100
12	O	524/593 (88%)	521 (99%)	3 (1%)	86 91
13	P	131/285 (46%)	130 (99%)	1 (1%)	81 89
14	Q	109/212 (51%)	107 (98%)	2 (2%)	59 77
All	All	4165/4698 (89%)	4155 (100%)	10 (0%)	93 96

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1163	LYS
1	A	1291	ARG
3	C	148	LYS
4	D	8	ASN

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Mol	Chain	Res	Type
12	O	257	ASN
12	O	531	LYS
12	O	608	ARG
13	P	258	HIS
14	Q	44	ASN
14	Q	111	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	899	GLN
2	B	80	ASN
2	B	334	HIS
3	C	301	ASN
5	E	54	GLN
12	O	128	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	R	8/24 (33%)	3 (37%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	R	12	C
15	R	13	C
15	R	15	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
20	1N7	A	2003	-	30,30,46	1.92	10 (33%)	47,48,72	3.57	26 (55%)
20	1N7	K	401	-	30,30,46	1.81	11 (36%)	47,48,72	3.44	26 (55%)

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
20	1N7	A	2003	-	-	1/7/72/92	0/4/4/4
20	1N7	K	401	-	-	1/7/72/92	0/4/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	2003	1N7	C16-C15	4.19	1.60	1.53
20	K	401	1N7	C16-C15	3.68	1.59	1.53
20	A	2003	1N7	C16-C17	3.54	1.58	1.52
20	K	401	1N7	C16-C17	3.39	1.58	1.52
20	A	2003	1N7	C7-C6	-3.30	1.47	1.54
20	A	2003	1N7	C5-C6	-3.21	1.50	1.55
20	K	401	1N7	C7-C6	-3.19	1.47	1.54
20	A	2003	1N7	C1-C2	2.75	1.59	1.54
20	K	401	1N7	C5-C6	-2.72	1.50	1.55
20	K	401	1N7	C14-C13	2.69	1.56	1.51
20	A	2003	1N7	C3-C4	-2.61	1.48	1.53
20	A	2003	1N7	C18-C6	-2.55	1.48	1.53
20	A	2003	1N7	O4-C4	-2.51	1.39	1.43
20	K	401	1N7	C18-C6	-2.43	1.49	1.53
20	K	401	1N7	C1-C2	2.42	1.58	1.54
20	K	401	1N7	C2-C19	2.36	1.60	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	K	401	1N7	O4-C4	-2.33	1.39	1.43
20	K	401	1N7	O3-C17	-2.33	1.38	1.43
20	A	2003	1N7	O3-C17	-2.29	1.38	1.43
20	K	401	1N7	C3-C4	-2.17	1.49	1.53
20	A	2003	1N7	C2-C15	2.07	1.58	1.55

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	2003	1N7	C10-C5-C4	9.11	118.34	109.07
20	K	401	1N7	C10-C5-C4	8.30	117.51	109.07
20	A	2003	1N7	C1-C2-C15	6.63	117.57	107.77
20	K	401	1N7	C5-C9-C20	-6.49	111.75	119.50
20	K	401	1N7	C10-C5-C6	-6.43	101.15	111.21
20	A	2003	1N7	C11-C2-C1	-6.28	98.13	108.26
20	K	401	1N7	C5-C6-C18	-6.12	106.92	114.74
20	A	2003	1N7	C10-C5-C6	-6.10	101.67	111.21
20	A	2003	1N7	C6-C18-C17	-5.97	103.89	111.81
20	K	401	1N7	C1-C2-C15	5.95	116.57	107.77
20	A	2003	1N7	C5-C6-C18	-5.82	107.31	114.74
20	K	401	1N7	C11-C2-C1	-5.49	99.41	108.26
20	A	2003	1N7	C9-C5-C4	-5.11	113.00	117.67
20	A	2003	1N7	C3-C19-C2	-5.06	108.51	113.73
20	A	2003	1N7	C5-C9-C20	-5.04	113.47	119.50
20	K	401	1N7	C6-C18-C17	-5.04	105.12	111.81
20	K	401	1N7	C9-C5-C4	-4.90	113.19	117.67
20	K	401	1N7	C19-C2-C15	-4.85	101.77	108.58
20	K	401	1N7	C2-C19-C18	4.81	116.98	111.82
20	A	2003	1N7	C7-C6-C5	4.81	108.27	103.55
20	A	2003	1N7	C19-C18-C6	4.64	116.08	109.71
20	A	2003	1N7	C9-C5-C6	-4.54	95.52	100.09
20	K	401	1N7	C16-C15-C14	4.44	116.30	111.19
20	A	2003	1N7	C16-C15-C2	4.37	117.30	112.66
20	K	401	1N7	C7-C6-C5	4.09	107.56	103.55
20	K	401	1N7	C3-C19-C2	-4.00	109.61	113.73
20	K	401	1N7	C8-C7-C6	-3.97	97.26	105.13
20	A	2003	1N7	C16-C17-C18	-3.86	107.36	111.48
20	A	2003	1N7	C2-C19-C18	3.85	115.96	111.82
20	K	401	1N7	C16-C17-C18	-3.80	107.42	111.48
20	A	2003	1N7	C8-C7-C6	-3.77	97.65	105.13
20	K	401	1N7	C14-C15-C2	-3.76	108.66	112.66
20	K	401	1N7	C11-C2-C19	3.71	116.29	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	K	401	1N7	C9-C5-C6	-3.69	96.37	100.09
20	A	2003	1N7	C19-C2-C15	-3.65	103.45	108.58
20	A	2003	1N7	C10-C5-C9	3.60	116.84	111.21
20	K	401	1N7	C19-C18-C6	3.58	114.62	109.71
20	A	2003	1N7	C15-C16-C17	3.56	118.39	114.46
20	A	2003	1N7	O3-C17-C18	-3.19	102.29	109.43
20	A	2003	1N7	C21-C20-C9	3.05	117.59	112.92
20	A	2003	1N7	C16-C15-C14	3.03	114.67	111.19
20	K	401	1N7	O3-C17-C18	-3.02	102.69	109.43
20	K	401	1N7	C10-C5-C9	3.01	115.93	111.21
20	K	401	1N7	C21-C20-C9	2.95	117.43	112.92
20	A	2003	1N7	C11-C2-C19	2.80	115.04	111.18
20	A	2003	1N7	C14-C15-C2	-2.59	109.91	112.66
20	A	2003	1N7	C15-C14-C13	2.52	116.46	112.76
20	K	401	1N7	C15-C14-C13	2.38	116.25	112.76
20	A	2003	1N7	C8-C9-C20	-2.30	108.58	112.15
20	K	401	1N7	C16-C15-C2	2.20	115.00	112.66
20	K	401	1N7	C8-C9-C20	-2.15	108.82	112.15
20	K	401	1N7	C6-C5-C4	2.05	109.31	107.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	K	401	1N7	C22-C20-C9-C5
20	A	2003	1N7	C21-C20-C22-C23

There are no ring outliers.

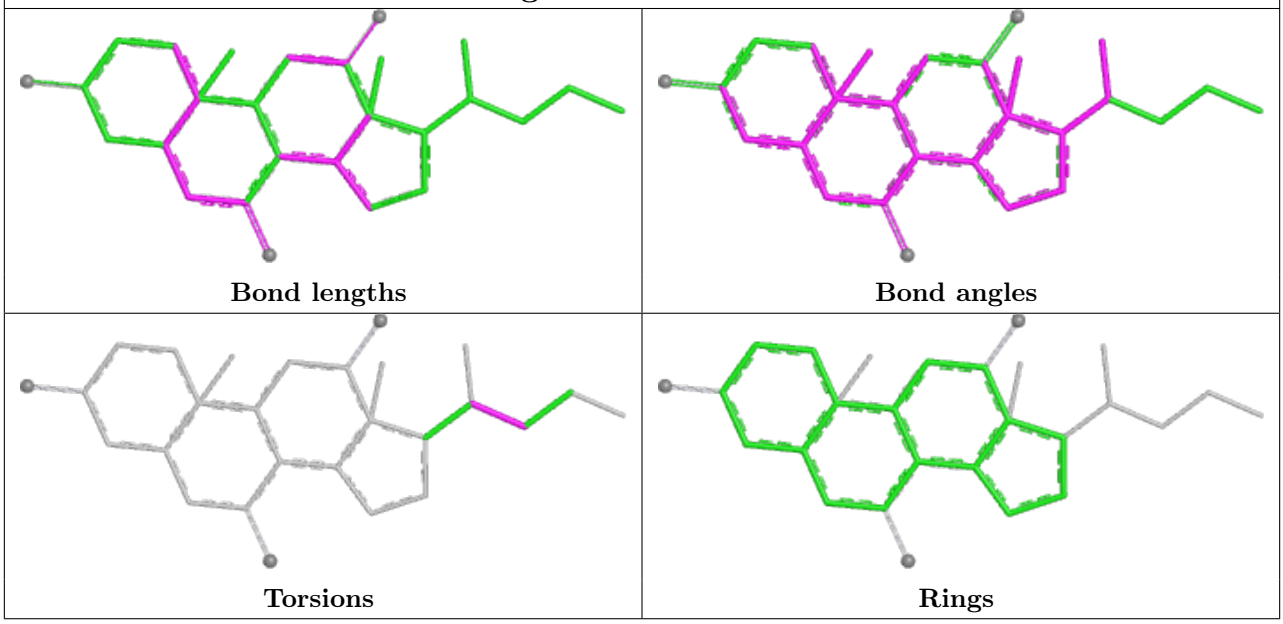
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	2003	1N7	3	0
20	K	401	1N7	3	0

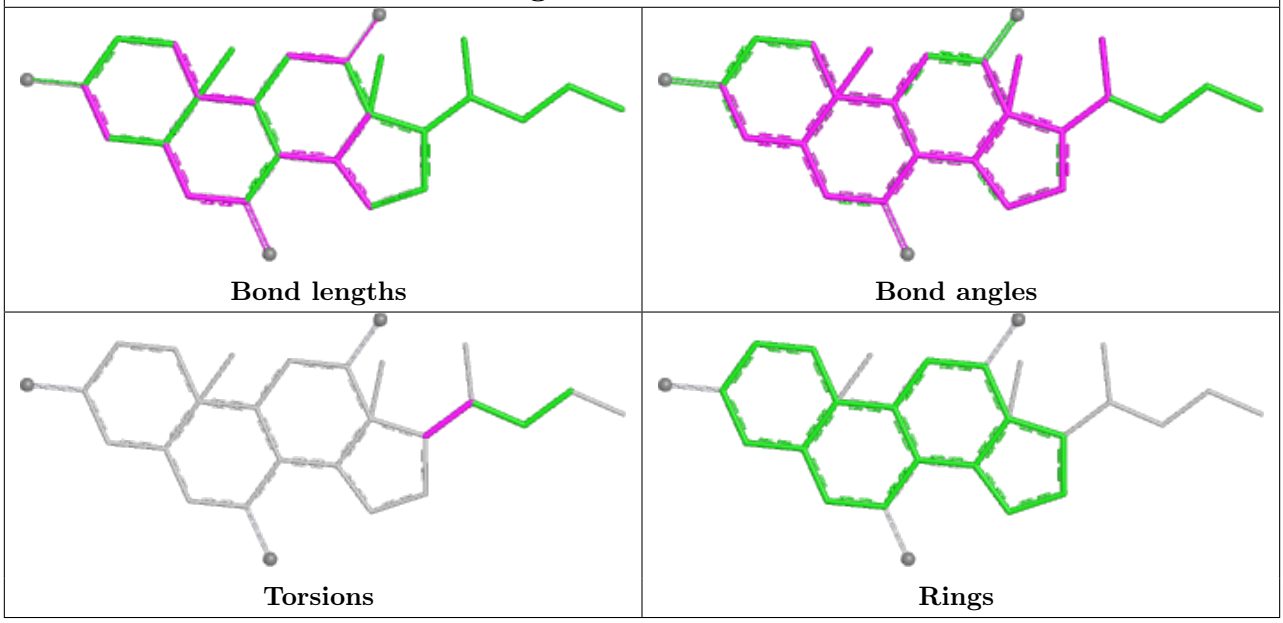
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 1N7 A 2003



Ligand 1N7 K 401



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

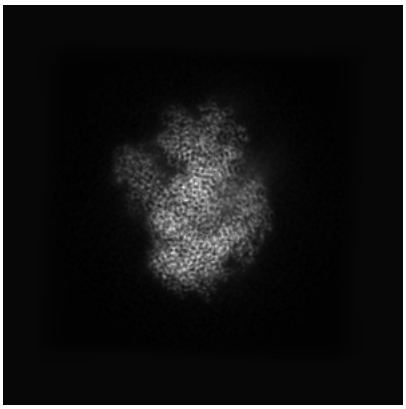
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14449. These allow visual inspection of the internal detail of the map and identification of artifacts.

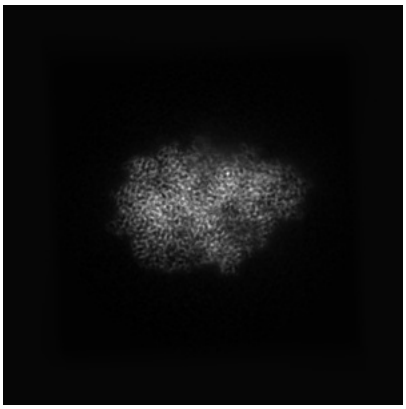
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

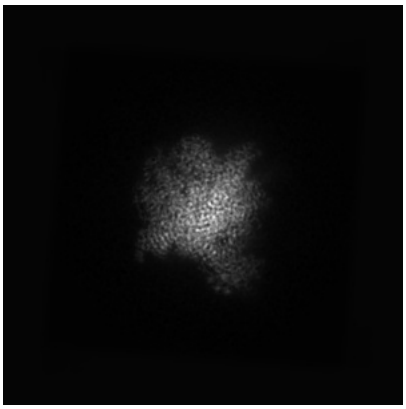
6.1.1 Primary map



X

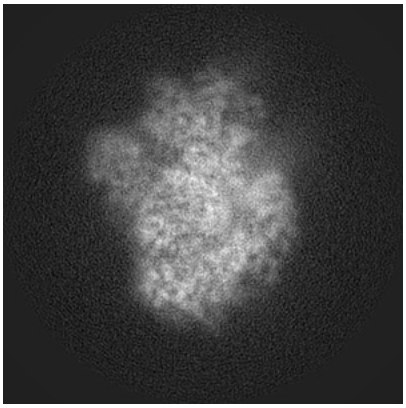


Y

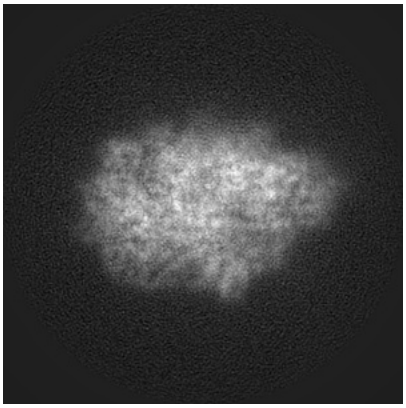


Z

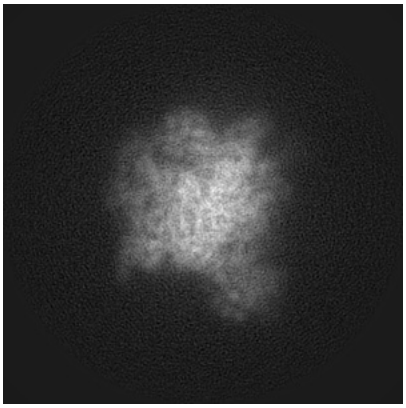
6.1.2 Raw map



X



Y

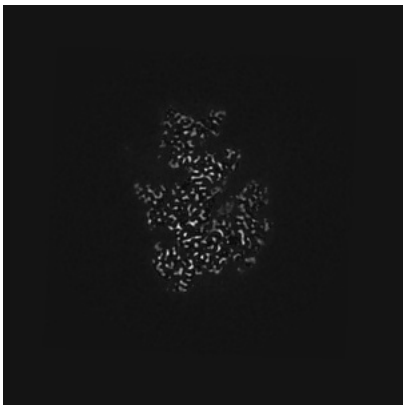


Z

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

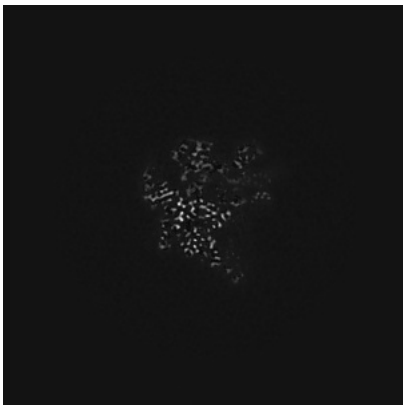
6.2 Central slices (i)

6.2.1 Primary map



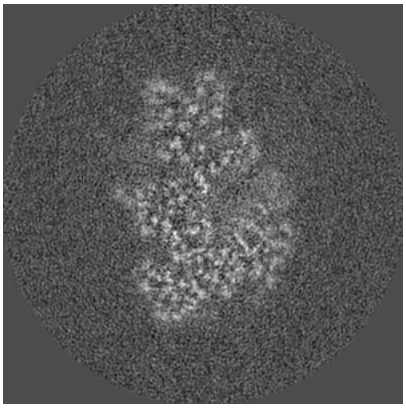
X Index: 173

Y Index: 173

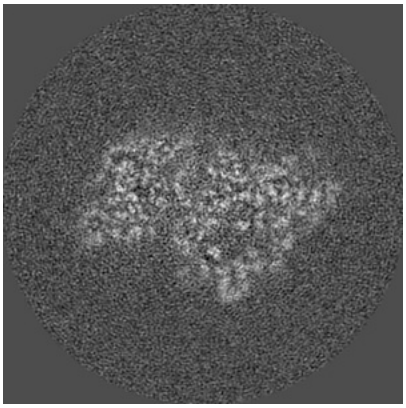


Z Index: 173

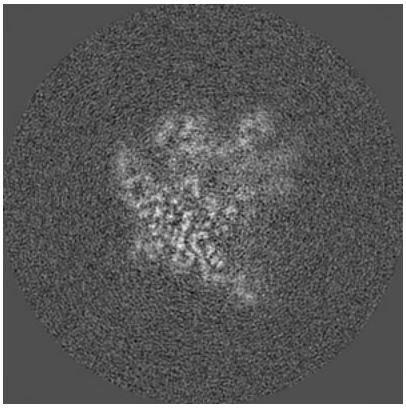
6.2.2 Raw map



X Index: 130



Y Index: 130

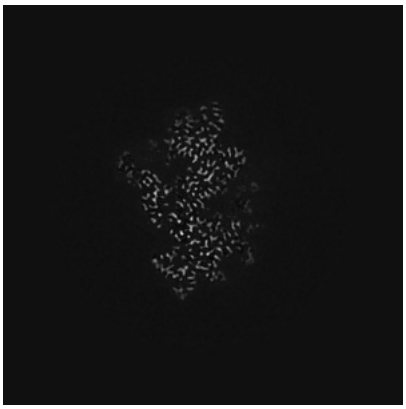


Z Index: 130

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

6.3 Largest variance slices (i)

6.3.1 Primary map

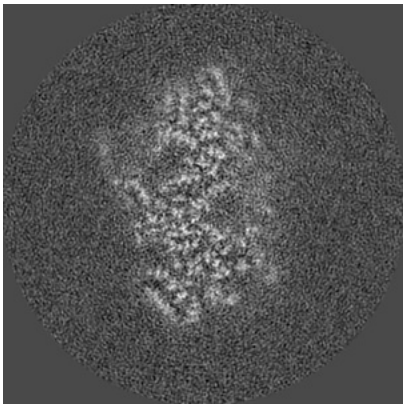


X Index: 182

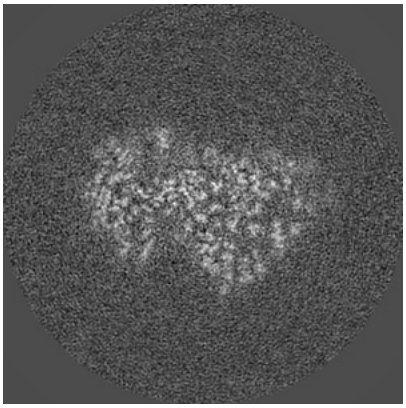
Y Index: 161

Z Index: 145

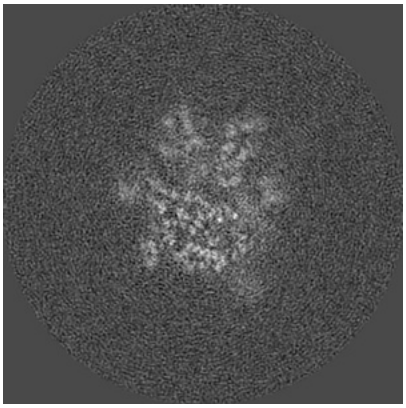
6.3.2 Raw map



X Index: 136



Y Index: 123



Z Index: 120

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

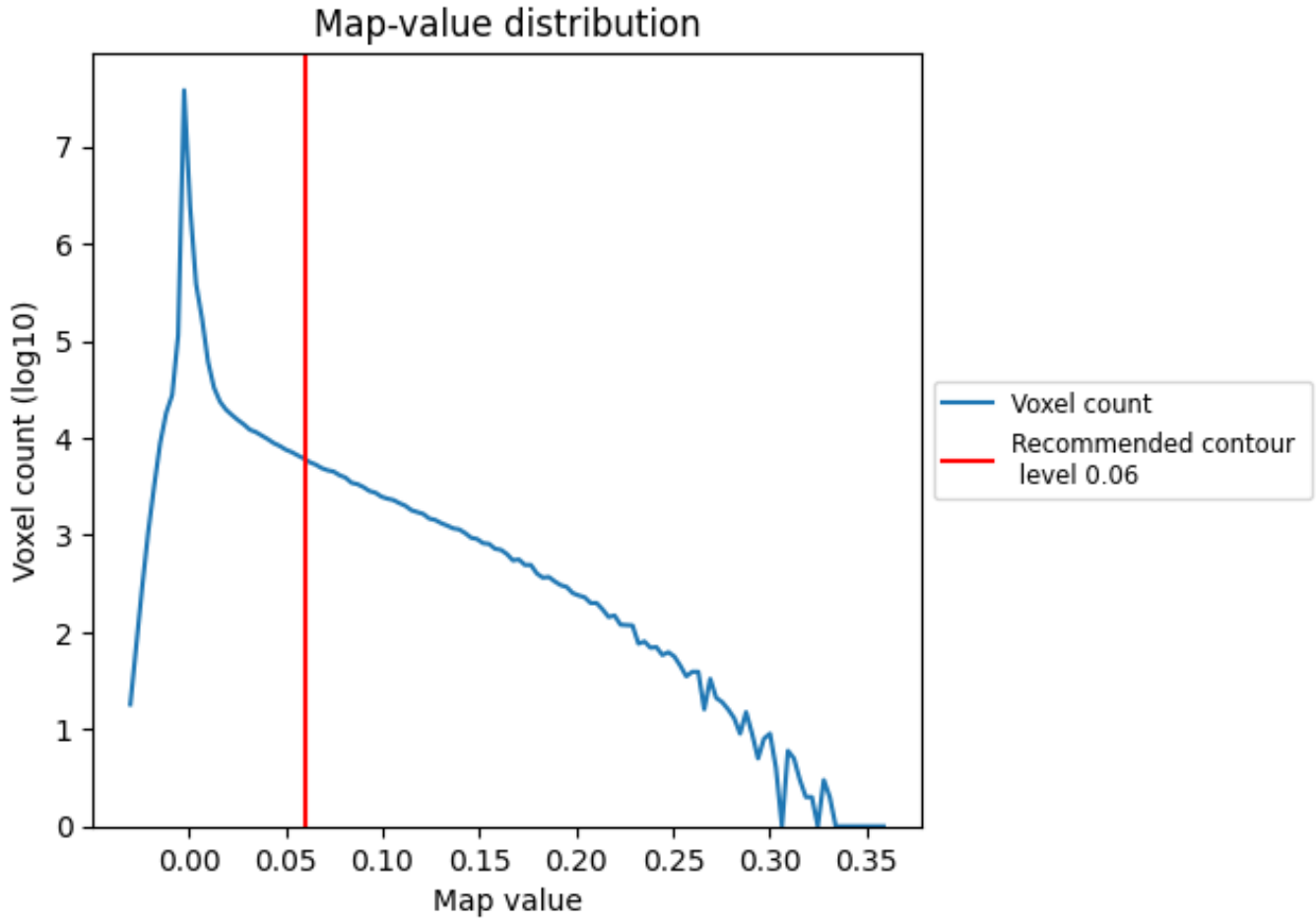
6.5 Mask visualisation (i)

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

7 Map analysis

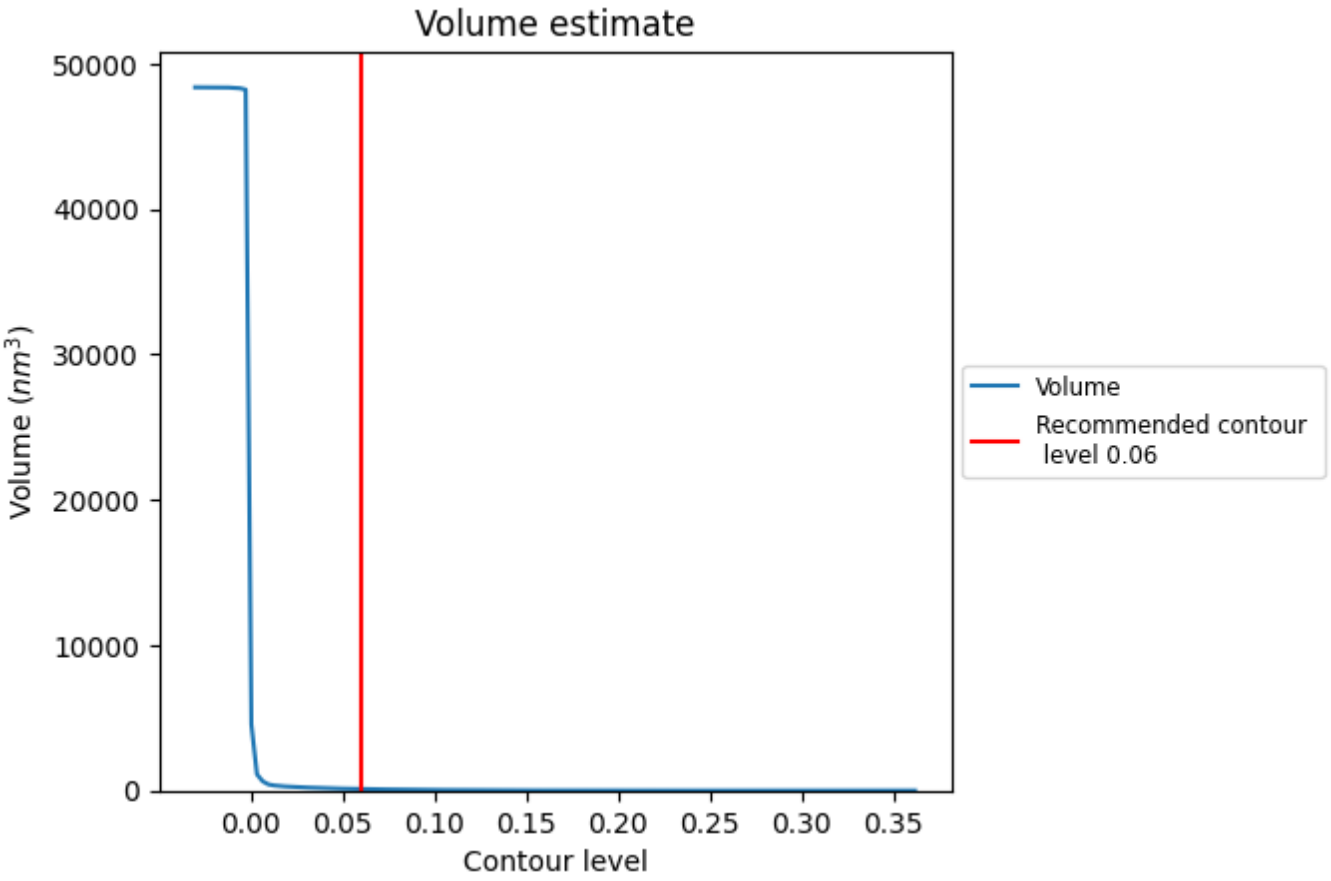
This section contains the results of statistical analysis of the map.

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.

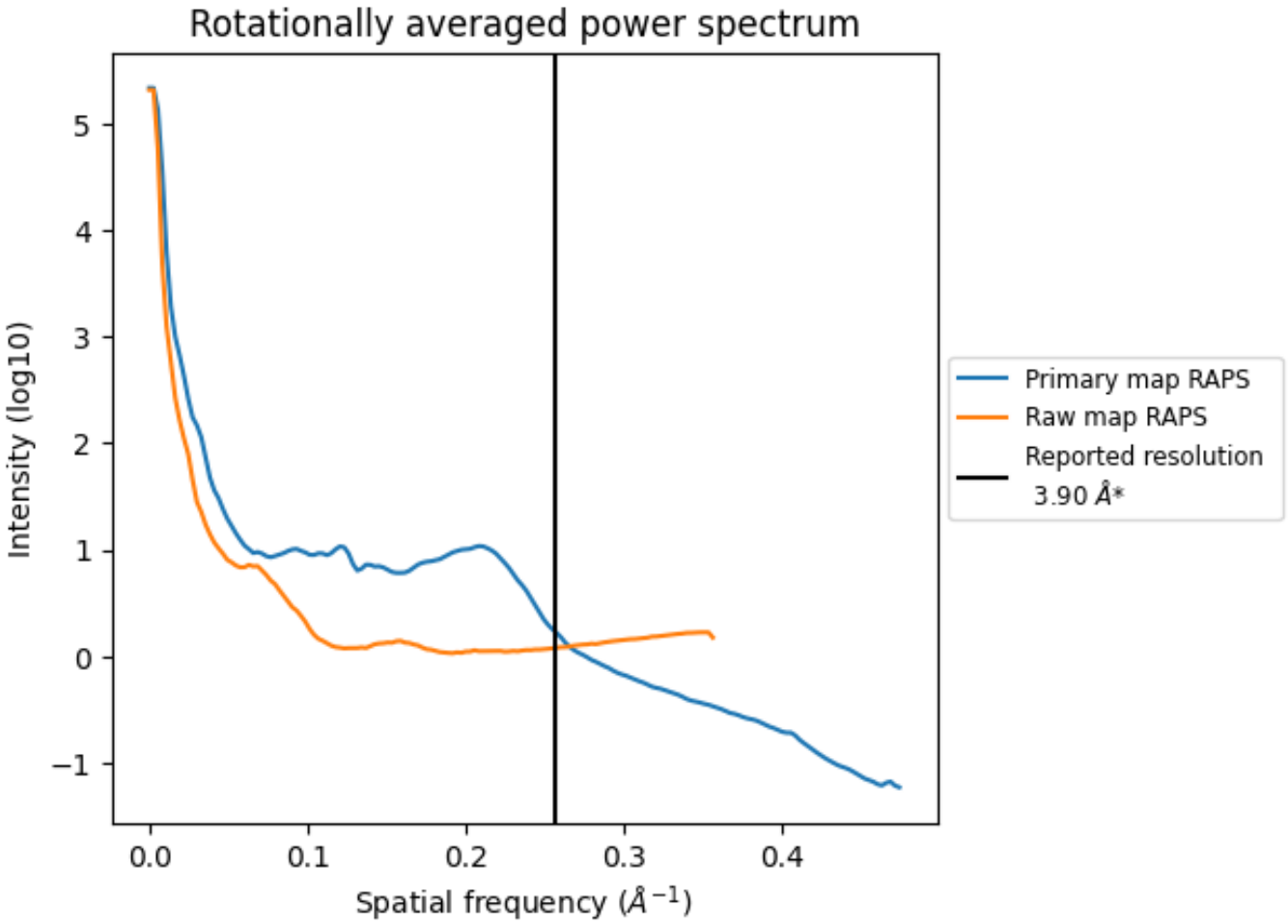
7.2 Volume estimate



The volume at the recommended contour level is 106 nm^3; this corresponds to an approximate mass of 96 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)

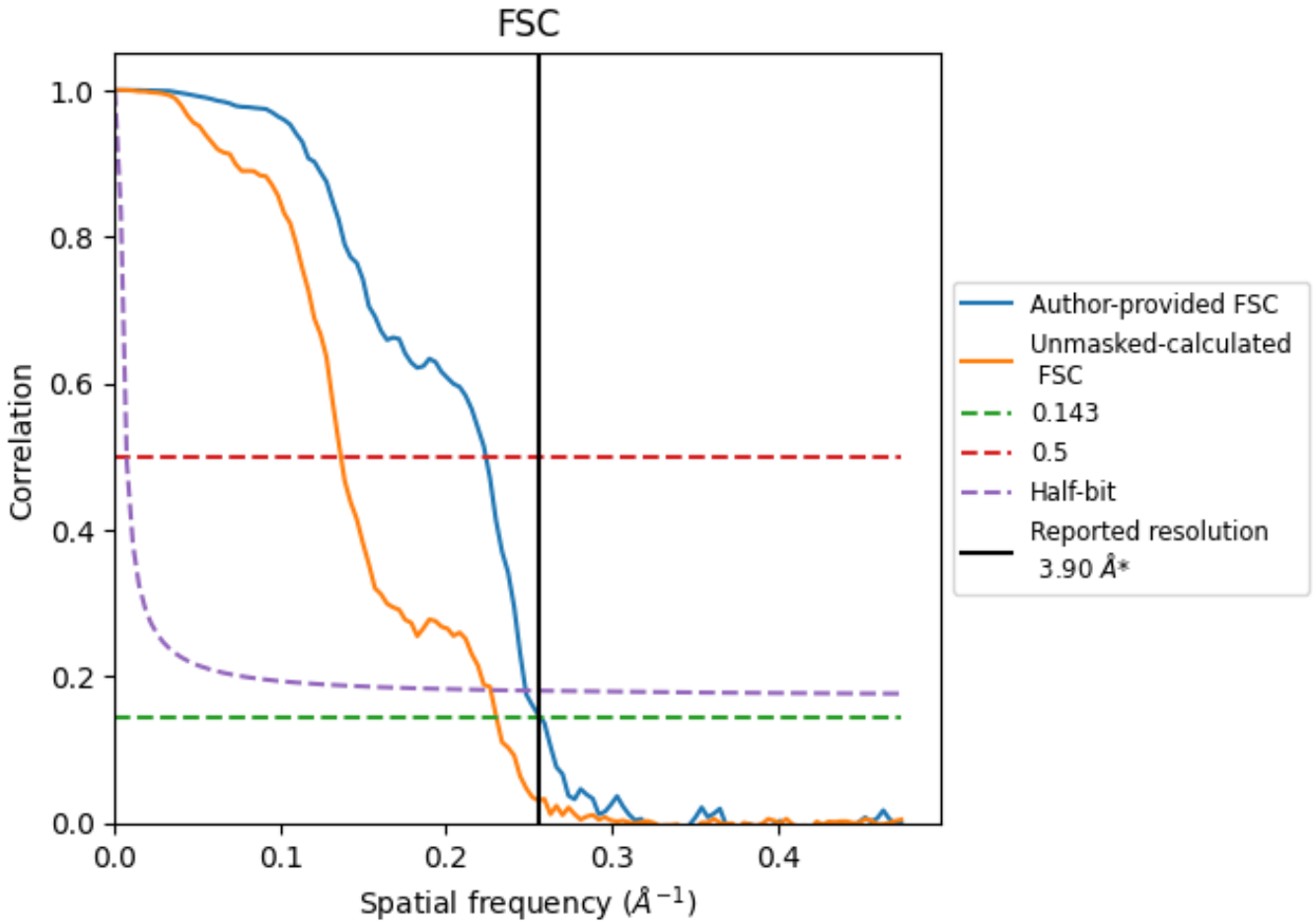


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

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 0.256 Å^{-1}

8.2 Resolution estimates (i)

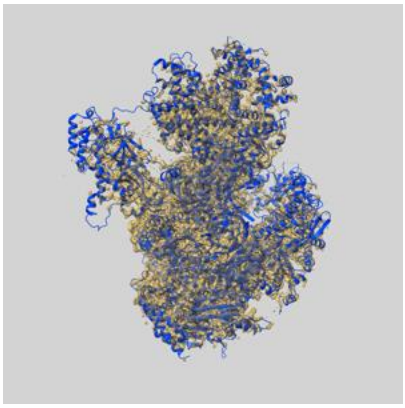
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.89	4.46	4.03
Unmasked-calculated*	4.34	7.33	4.41

*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 4.34 differs from the reported value 3.9 by more than 10 %

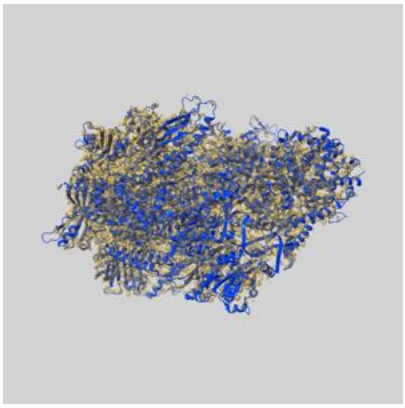
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14449 and PDB model 7Z1N. Per-residue inclusion information can be found in section 3 on page 8.

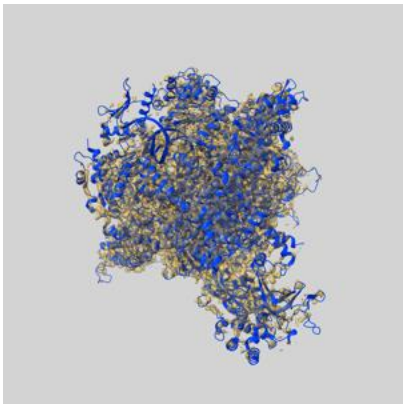
9.1 Map-model overlay



X



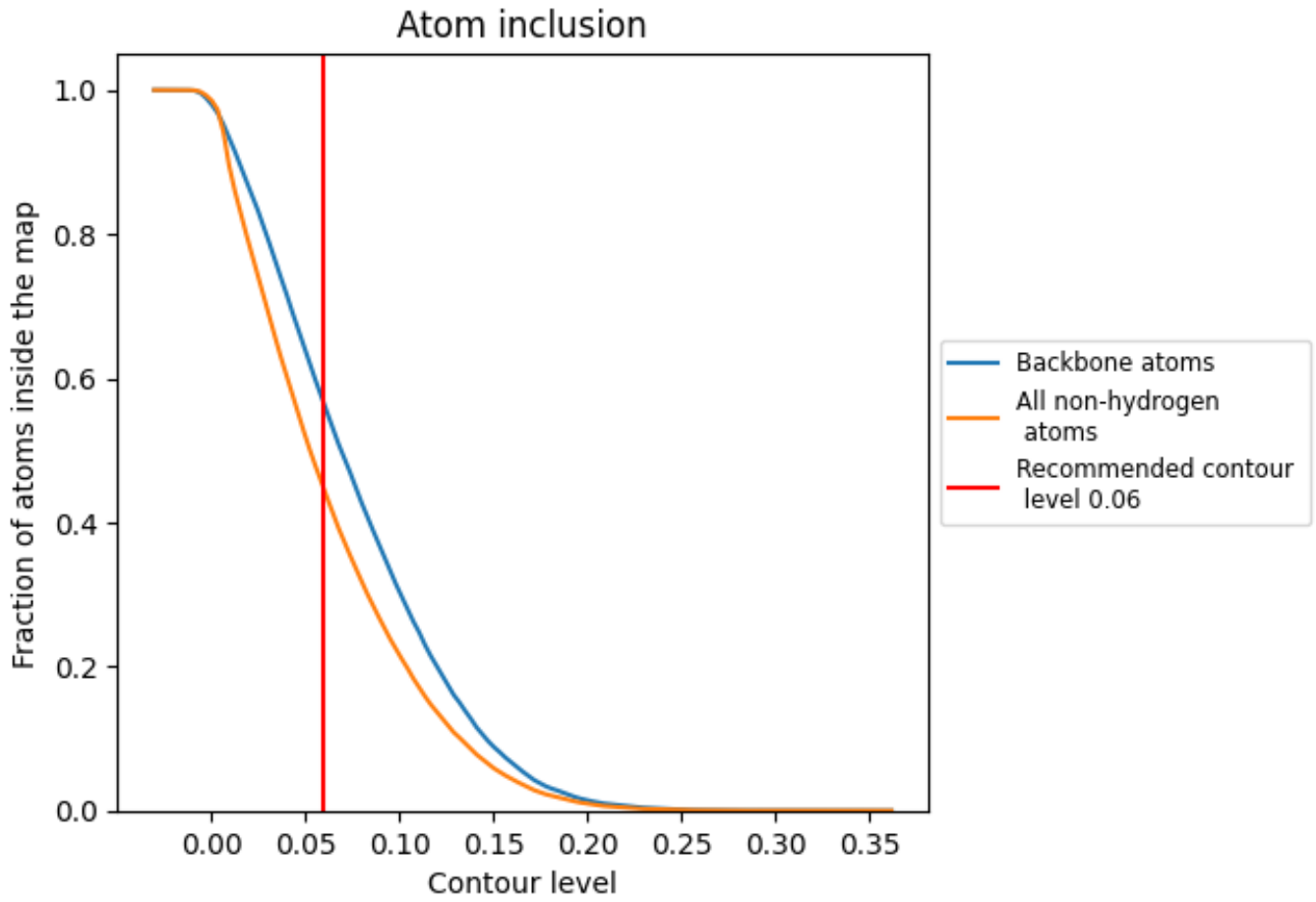
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion (i)



At the recommended contour level, 57% of all backbone atoms, 45% of all non-hydrogen atoms, are inside the map.