Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 09:58 pm GMT

PDB ID	:	6F40
EMDB ID	:	EMD-4180
Title	:	RNA Polymerase III open complex
Authors	:	Vorlaender, M.K.; Khatter, H.; Wetzel, R.; Hagen, W.J.H.; Mueller, C.W.
Deposited on	:	2017-11-29
Resolution	:	3.70 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 (i) 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 (i)) were used in the production of this report:

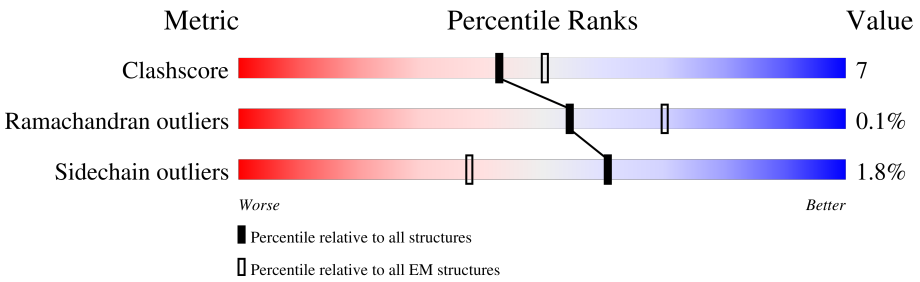
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 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

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	11% 77% 18% • •
2	B	1149	6% 76% 20% • •
3	C	335	• 86% 14%
4	D	161	48% 61% 12% 26%
5	E	215	14% 83% 16%
6	F	155	48% 6% 46%
7	G	212	38% 66% 19% 15%
8	H	146	6% 77% 19% •

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Mol	Chain	Length	Quality of chain
9	I	110	5% 23% 8% 69%
10	J	70	81% 14%
11	K	142	58% 13% 29%
12	L	70	54% 10% 36%
13	M	282	17% 51% 14% 35%
14	N	422	5% 19% 5% 75%
15	O	654	22% 64% 17% 18%
16	P	317	18% 61% 16% 22%
17	Q	251	12% 86%
18	U	240	21% 52% 23% 25%
19	V	596	12% 48% 8% 43%
20	W	594	16% 28% 8% 63%
21	X	81	23% 57% 12% 31%
22	Y	81	16% 57% 14% 30%

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 47396 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	1398	10972	6919	1936	2059	58	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	1114	8788	5558	1516	1654	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	335	2655	1681	454	511	9	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	119	977	628	156	187	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	214	1751	1111	309	320	11	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
			Total	C	N	O	S		
7	G	180	1448	950	231	261	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	140	1120	703	188	224	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	34	255	161	39	49	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	67	549	350	95	98	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	101	792	496	130	161	5	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	183	1484	942	257	283	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	104	797	505	143	146	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	534	4293	2733	736	806	18	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	246	1990	1276	326	377	11	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	Q	35	273	181	45	47	0	0

- Molecule 18 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	U	180	1416	921	242	247	6	0	0

- Molecule 19 is a protein called Transcription factor IIIB 70 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	V	337	2686	1682	486	504	14	0	0

- Molecule 20 is a protein called Transcription factor TFIIIB component B".

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	W	218	1798	1131	319	339	9	0	0

- Molecule 21 is a DNA chain called Non-Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
21	X	56	1137	549	186	346	56	0	0

- Molecule 22 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	Y	57	1179	563	226	333	57	0	0

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

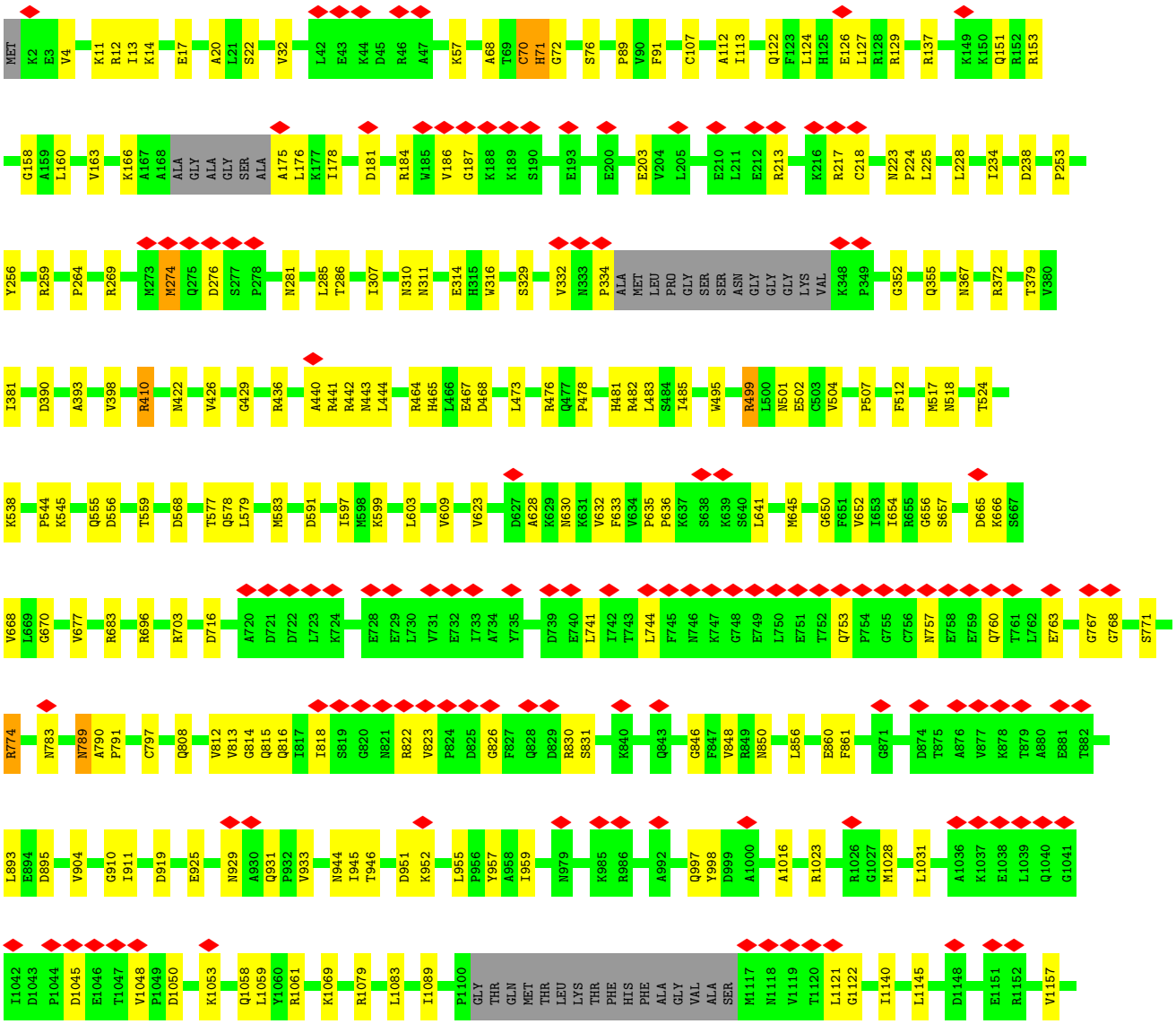
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
23	A	2	2	2	0
23	B	1	1	1	0
23	I	1	1	1	0
23	J	1	1	1	0
23	L	1	1	1	0
23	V	1	1	1	0

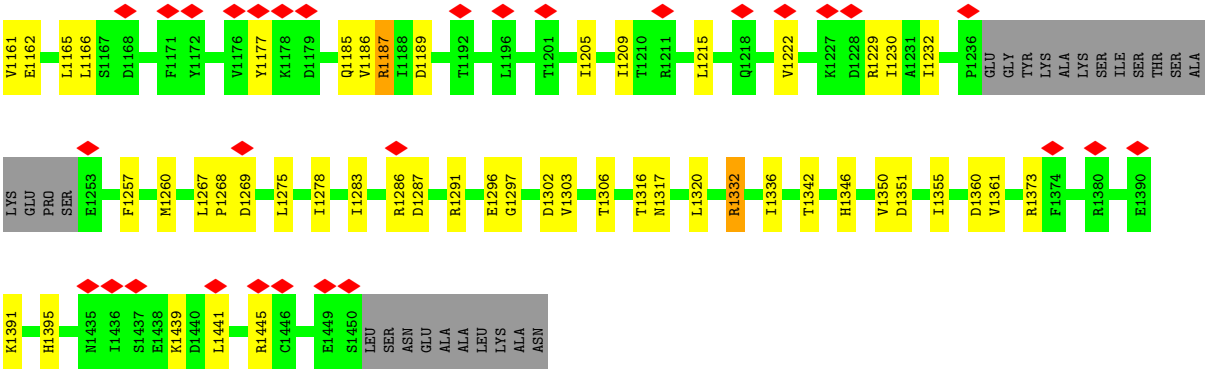
3 Residue-property plots (i)

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

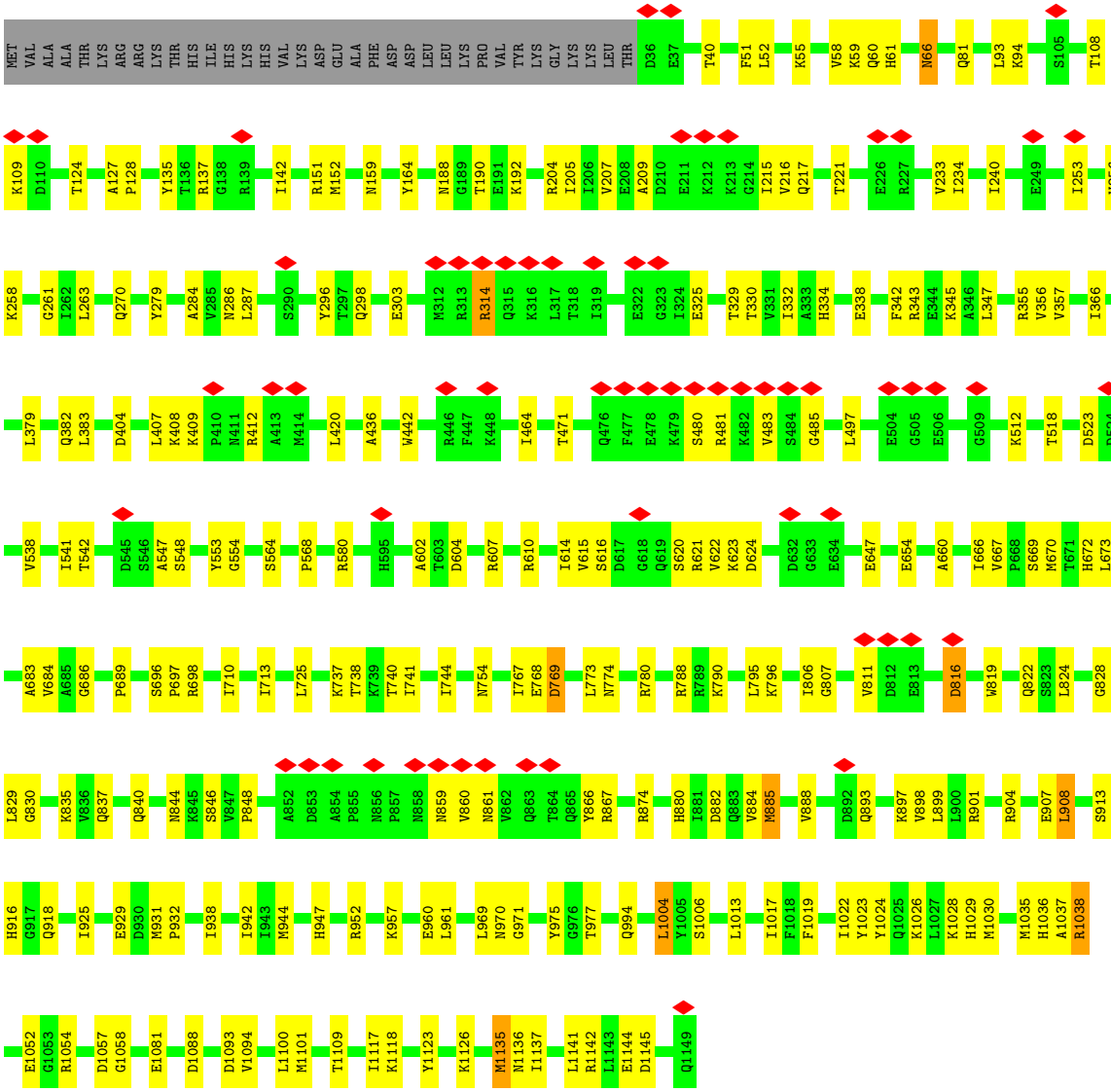
Chain A:





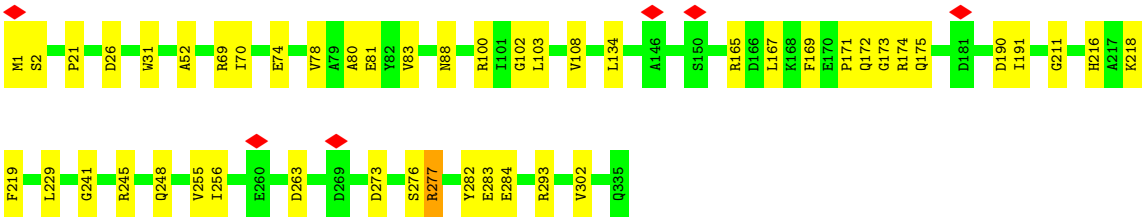
• Molecule 2: DNA-directed RNA polymerase III subunit RPC2

Chain B:



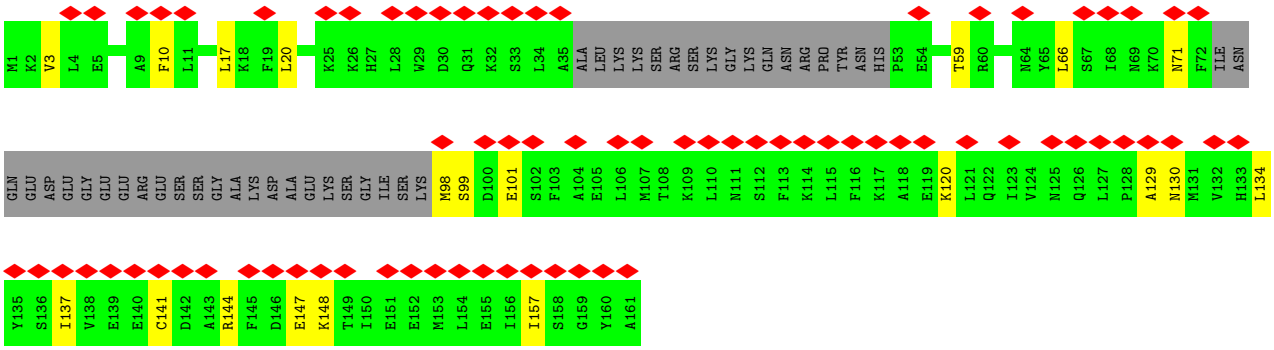
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C:



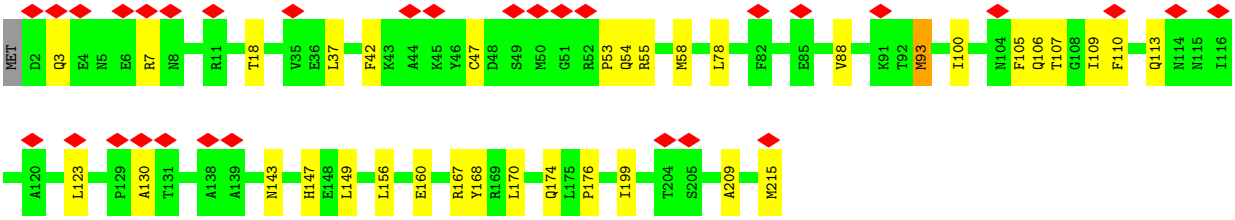
- Molecule 4: DNA-directed RNA polymerase III subunit RPC9

Chain D:



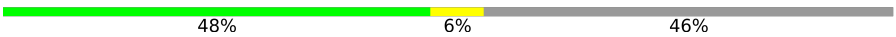
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

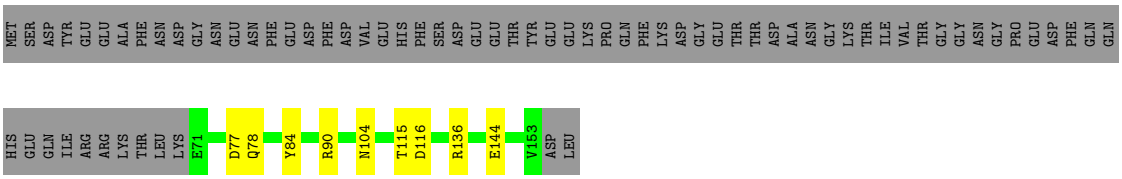
Chain E:



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

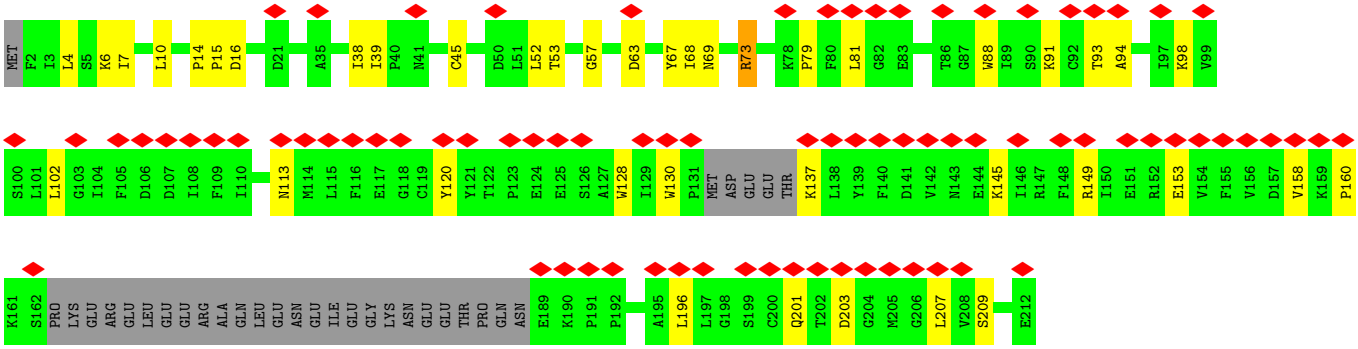
Chain F:





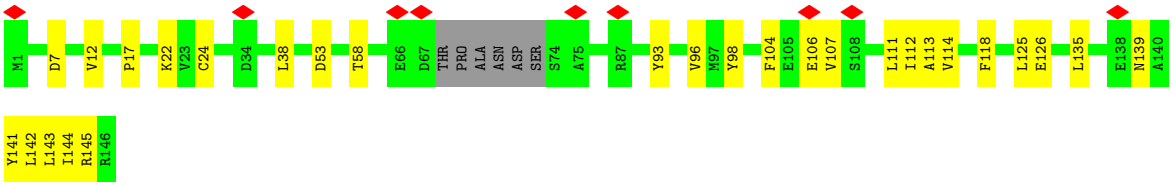
- Molecule 7: DNA-directed RNA polymerase III subunit RPC8

Chain G:



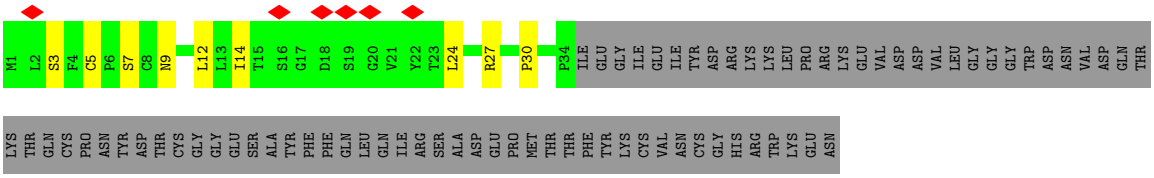
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



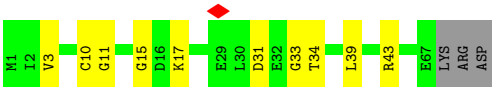
- Molecule 9: DNA-directed RNA polymerase III subunit RPC10

Chain I:



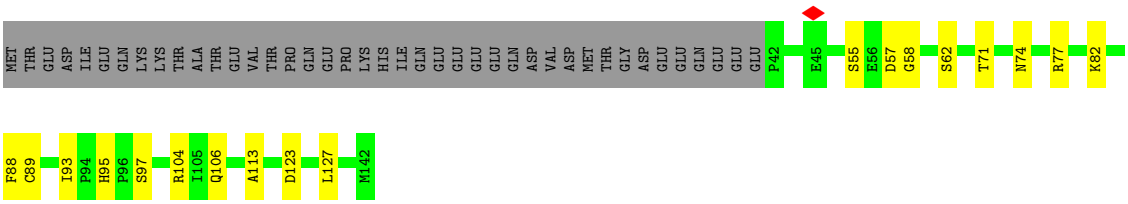
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

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: 54% 10% 36%

MET SER ARG GLU GLY PHE GLN ILE PRO THR ASN LEU ASP ALA ALA ALA ALA GLY THR SER GLN ALA ARG THR ALA T26 L27 C31 A32 R54 L57 R60 A69 R70

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

Chain M: 17% 51% 14% 35%

MET SER ILE ASP ASN LYS LEU PHE VAL THR GLU GLU GLU ASP GLU GLU ASP ARG THR GLN ASP ARG ALA ASP VAL GLU ASP GLU SER ASN ASP ILE ASP MET ILE ALA ASP GLU ASN GLY THR ASN SER ALA ILE ALA ASN GLU GLN GLU GLU LYS SER GLU GLU VAL LYS ALA GLU ASP

THR GLY GLU GLU GLU ASP ASP PRO VAL I71 L76 K77 I78 E81 E82 E83 N92 R93 V97 G98 R99 E103 H104 P105 F106 A110 R111 Y112 K113 L118 I123 P124 L125 D126 E127 Q128 A129 K133 D134 K135 A136 E137 S138 E139 W140 N141 G142 V143 N144 V145

L148 V153 Q158 Y159 K164 D165 M166 Q167 Q178 P181 F182 I186 A189 T192 R193 K194 Q195 E196 D197 A198 R199 R200 N201 P202 N203 P204 SER SER GLN ARG ALA GLN VAL VAL THR M214 S215 V216 K217 S218 V219 N220 D221 Q224 N225 R226 L227 T228 L231

N242 L245 Q250 T251 F252 E253 Q254 V260 K261 E262 ALA GLU ASP LYS THR LEU VAL ALA LEU GLU LYS GLN GLU ASP TYR ILE ASP ASN LEU VAL

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

Chain N: 5% 19% 5% 75%

MET SER SER ASN LYS GLY ASN GLY ARG LEU PRO SER LEU LYS ASP SER SER SER ASN GLY GLY GLY SER ALA LYS PRO SER LEU LYS PHE LYS PRO LYS ALA VAL ALA ARG LYS SER LYS GLU GLU ARG GLU ALA ALA ALA SER LYS VAL LYS LEU GLU GLU GLU SER LYS ARG GLY ASN

ASP LYS LYS HIS PHE ASN ASN LYS ASN LYS ARG VAL THR GLY ALA GLY GLY GLN GLN ARG ARG MET ALA LYS TYR LEU ASN ASN THR HIS VAL ILE SER SER GLY PRO LEU ALA ALA GLY ASN PHE VAL SER GLU LYS GLY ASP LEU ARG ARG GLY PHE ILE LYS SER GLU GLY SER GLY

SER SER LEU VAL GLN LYS GLY LEU GLU THR ILE ASP ASN GLY ALA GLU SER SER GLU ASN GLU ALA GLU ASP ASP ASP ASN GLU GLY VAL ALA SER LYS SER LYS LYS LYS PHE ASN MET GLY LYS GLU PHE GLU ALA ARG ASN LEU ILE GLU ASP GLU ASP ASP GLY GLU SER GLU LYS

SER SER ASP VAL ASP MET ASP ASP GLU GLU TRP ARG SER LYS ARG ILE GLU GLN LEU PHE PRO VAL ARG PRO VAL ARG VAL ARG HIS GLU ASP VAL GLU THR VAL LYS ARG GLU ILE GLN GLU ALA LEU SER GLU LYS PRO THR ARG GLU PRO THR PRO SER VAL LYS THR GLU PRO VAL

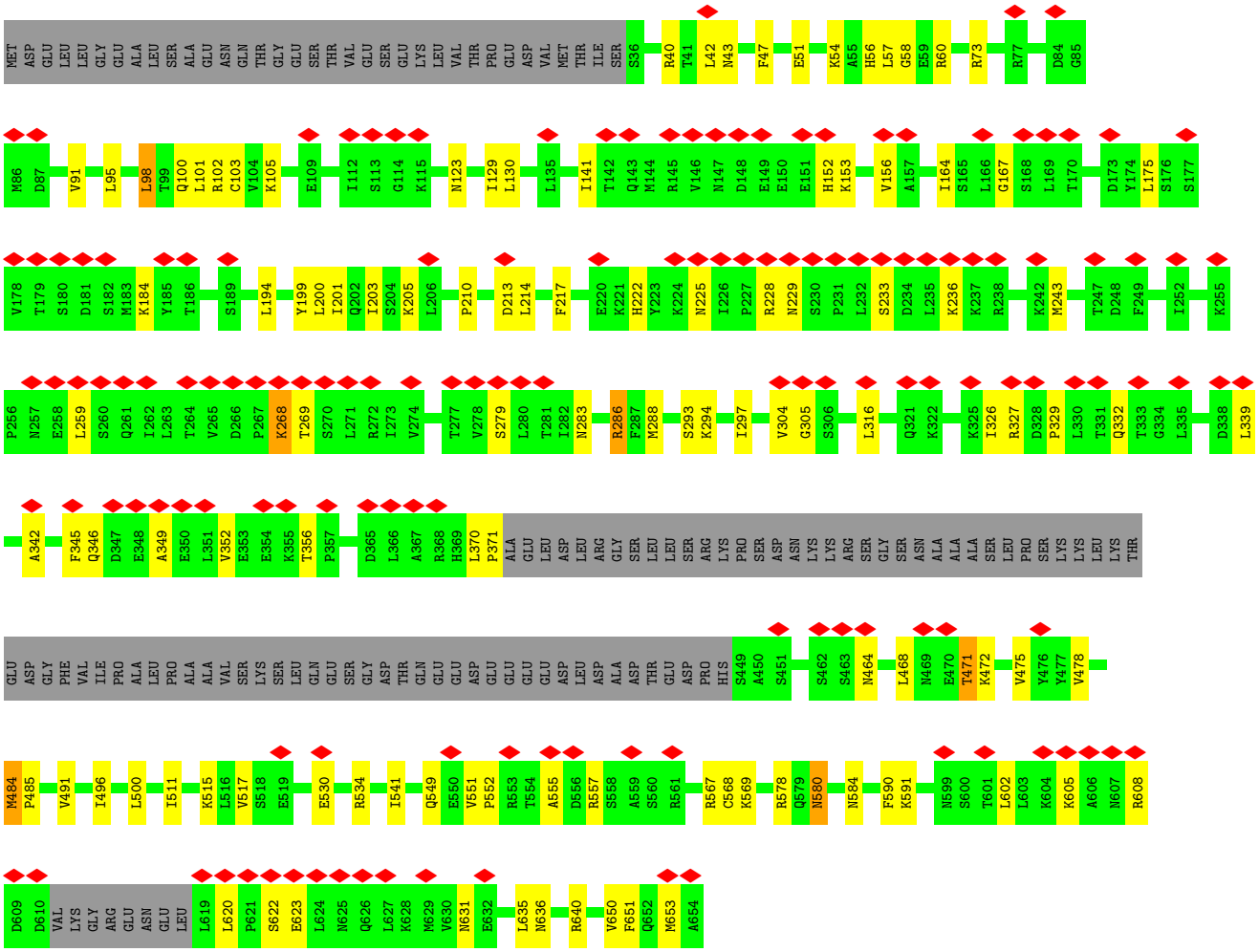
GLY THR GLY LEU GLN SER TYR LEU GLU GLU GLU ARG GLU ARG GLN VAL ASN GLU LYS LEU ALA ASP LEU GLY LEU GLU LYS GLU PHE GLN SER VAL ASP GLY K274 A277 A278 E279 L280 E281 H287 I290 M297 N298 N299 K300 M305 V306 F307 Q308 L309 R312 L313 P314 ALA

PHE GLU ARG PRO ALA VAL LYS GLU LYS GLU ASP MET GLU THR GLN ALA SER ASP PRO SER LYS LYS LYS LYS ASN ILE LYS LYS LYS ASP THR LYS ASP ALA LEU SER THR ARG GLU LEU ALA GLY LYS V360 I363 H366 K370 V373 K374 I375 G376 N377 M380 D381

I382 A386 T389 F390 L391 V394 I399 A400 D401 D402 A403 S404 V412 I416 Q421 I422

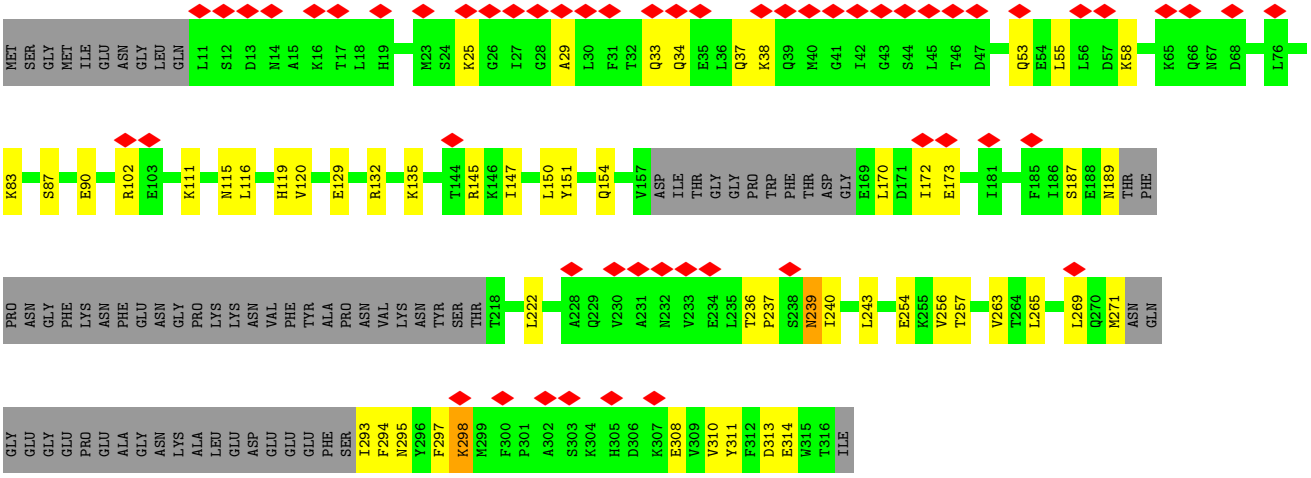
• Molecule 15: DNA-directed RNA polymerase III subunit RPC3

Chain O:



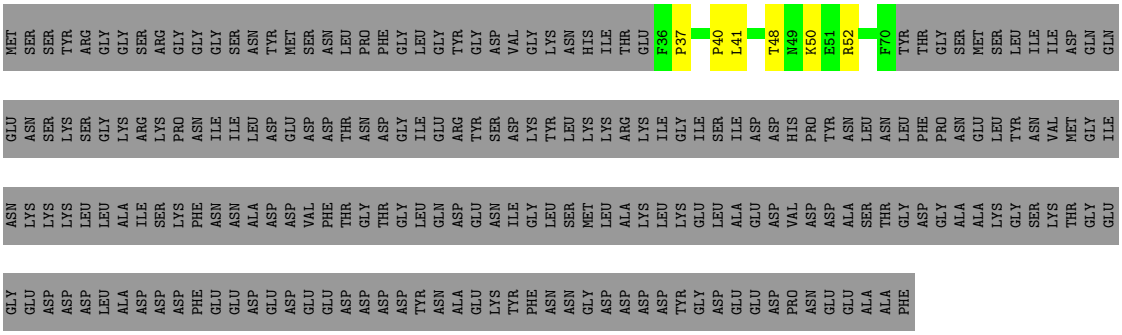
• Molecule 16: DNA-directed RNA polymerase III subunit RPC6

Chain P:



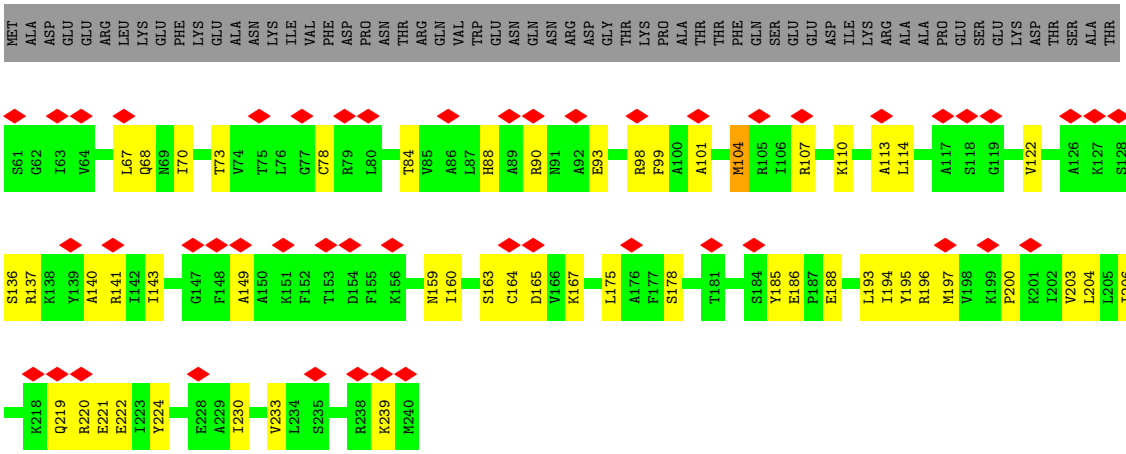
• Molecule 17: DNA-directed RNA polymerase III subunit RPC7

Chain Q:



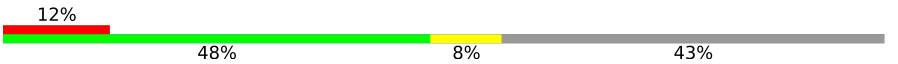
• Molecule 18: TATA-box-binding protein

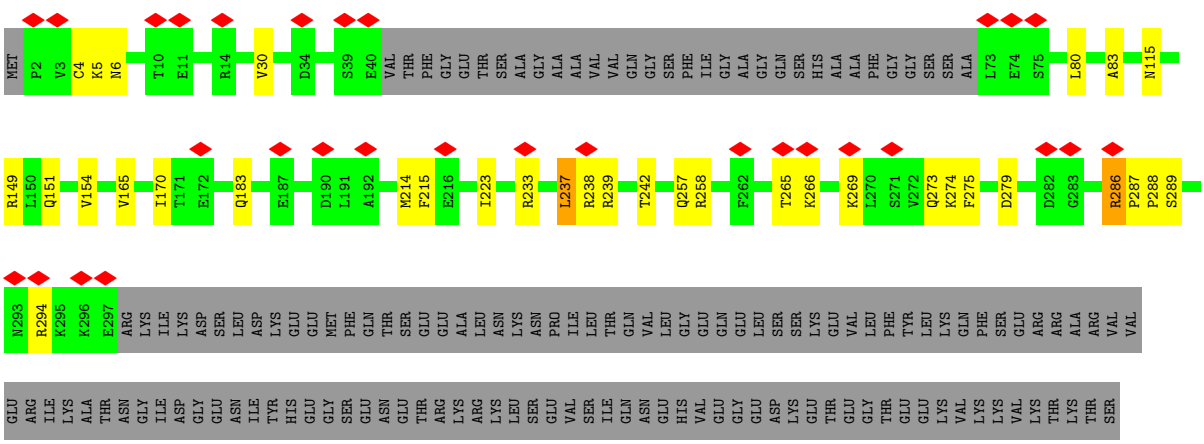
Chain U:

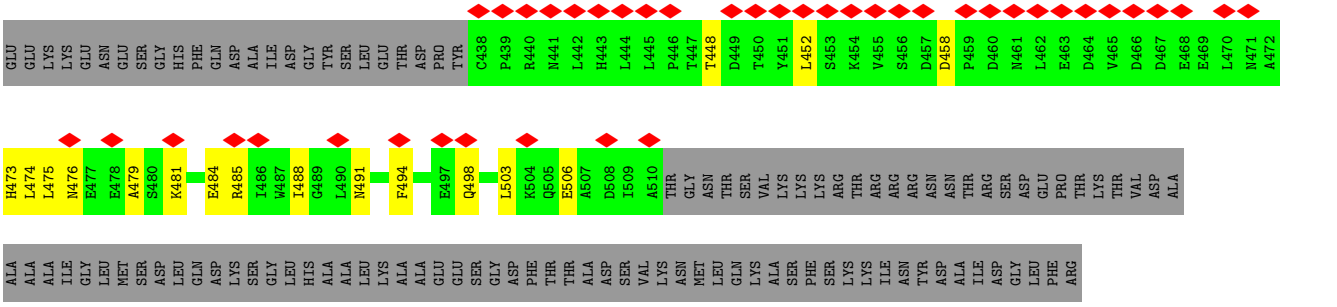


• Molecule 19: Transcription factor IIIB 70 kDa subunit

Chain V:

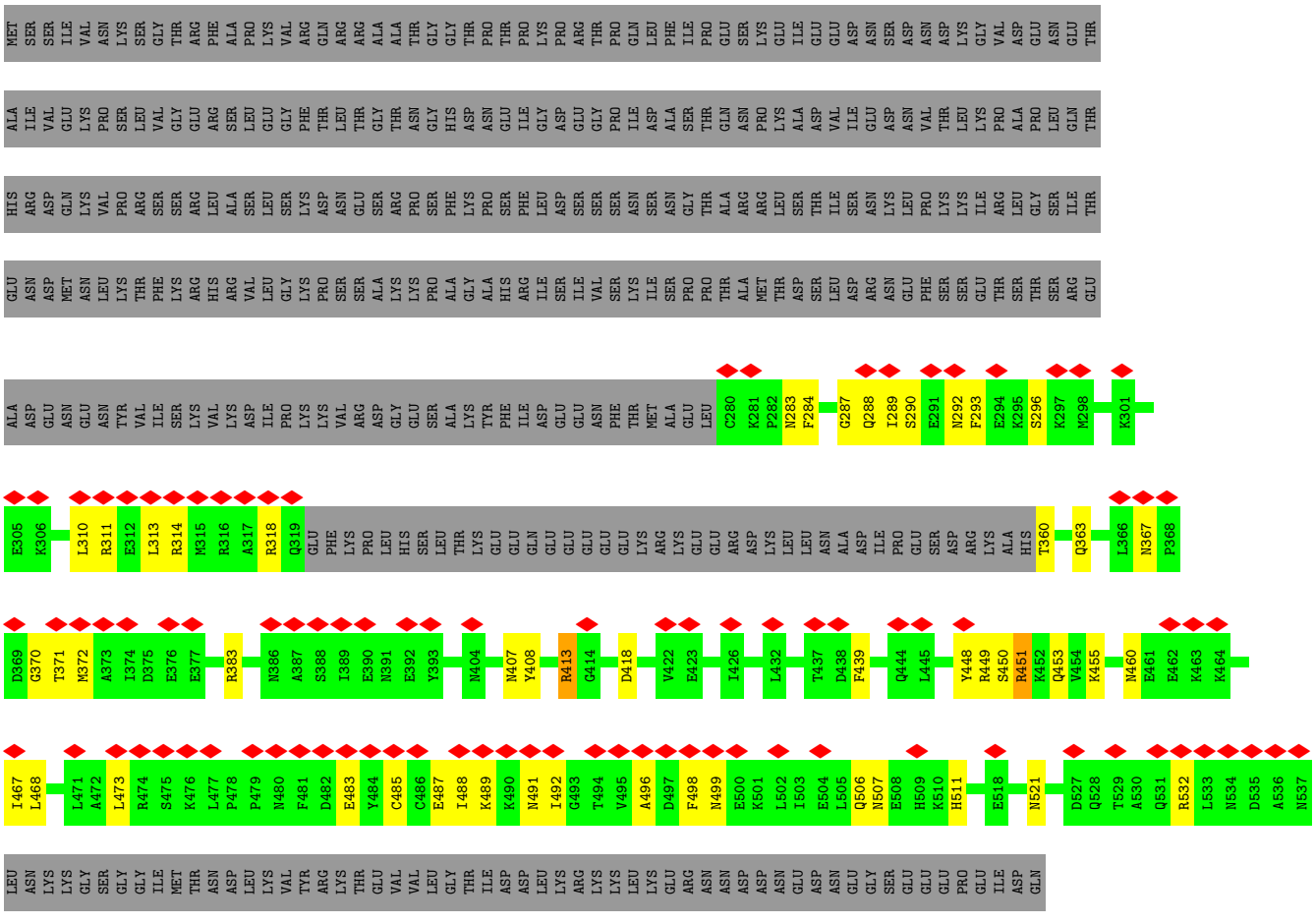






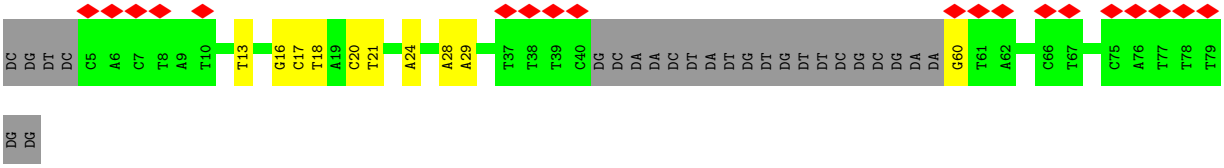
• Molecule 20: Transcription factor TFIIIB component B"

Chain W: 16% 28% 8% 63%



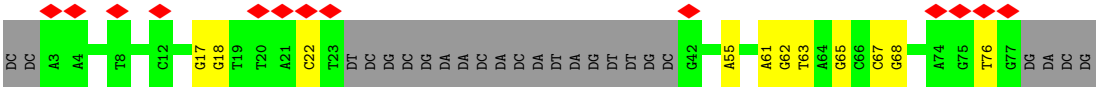
• Molecule 21: Non-Template DNA

Chain X: 23% 57% 12% 31%



• Molecule 22: Template DNA

Chain Y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	62751	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.311	Depositor
Minimum map value	-0.172	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.24	0/11168	0.47	0/15086
2	B	0.24	0/8943	0.47	0/12068
3	C	0.25	0/2711	0.47	0/3676
4	D	0.23	0/991	0.42	0/1328
5	E	0.24	0/1787	0.45	0/2406
6	F	0.23	0/683	0.44	0/923
7	G	0.24	0/1486	0.45	0/2017
8	H	0.24	0/1138	0.52	0/1540
9	I	0.25	0/261	0.57	0/354
10	J	0.23	0/558	0.43	0/750
11	K	0.23	0/803	0.44	0/1083
12	L	0.22	0/360	0.47	0/478
13	M	0.24	0/1518	0.47	0/2054
14	N	0.23	0/805	0.48	0/1081
15	O	0.23	0/4358	0.45	1/5879 (0.0%)
16	P	0.23	0/2020	0.47	0/2718
17	Q	0.26	0/281	0.45	0/381
18	U	0.25	0/1443	0.47	0/1942
19	V	0.23	0/2728	0.44	0/3676
20	W	0.23	0/1831	0.42	0/2454
21	X	0.55	0/1268	1.06	0/1951
22	Y	0.56	0/1326	0.96	0/2043
All	All	0.26	0/48467	0.51	1/65888 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	O	471	THR	C-N-CA	6.69	138.43	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	70	CYS	Peptide
2	B	1057	ASP	Peptide

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	10972	0	11096	177	0
2	B	8788	0	8901	160	0
3	C	2655	0	2628	32	0
4	D	977	0	983	9	0
5	E	1751	0	1776	23	0
6	F	671	0	692	6	0
7	G	1448	0	1446	23	0
8	H	1120	0	1089	19	0
9	I	255	0	243	8	0
10	J	549	0	559	7	0
11	K	792	0	790	12	0
12	L	358	0	384	6	0
13	M	1484	0	1448	25	0
14	N	797	0	846	13	0
15	O	4293	0	4456	70	0
16	P	1990	0	2030	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Q	273	0	285	6	0
18	U	1416	0	1493	37	0
19	V	2686	0	2704	42	0
20	W	1798	0	1789	39	0
21	X	1137	0	642	8	0
22	Y	1179	0	644	9	0
23	A	2	0	0	0	0
23	B	1	0	0	0	0
23	I	1	0	0	0	0
23	J	1	0	0	0	0
23	L	1	0	0	0	0
23	V	1	0	0	0	0
All	All	47396	0	46924	659	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 7.

All (659) 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)
20:W:371:THR:HG22	20:W:372:MET:HG3	1.68	0.76
2:B:667:VAL:HG12	2:B:669:SER:H	1.51	0.74
13:M:164:LYS:HB3	13:M:167:GLN:HB2	1.70	0.74
1:A:181:ASP:OD2	1:A:184:ARG:NH2	2.21	0.73
5:E:170:LEU:HB2	5:E:174:GLN:HE21	1.51	0.73
1:A:464:ARG:NH1	1:A:467:GLU:OE2	2.23	0.72
1:A:757:ASN:HD22	1:A:760:GLN:HE21	1.36	0.71
2:B:128:PRO:HA	2:B:151:ARG:HA	1.73	0.71
15:O:549:GLN:HE21	15:O:567:ARG:HH22	1.36	0.71
5:E:3:GLN:HE21	5:E:7:ARG:HH22	1.38	0.70
16:P:256:VAL:HG22	16:P:257:THR:HG23	1.72	0.70
1:A:274:MET:HG2	1:A:276:ASP:H	1.57	0.69
9:I:14:ILE:HD13	9:I:24:LEU:HB3	1.75	0.69
1:A:228:LEU:HD11	1:A:259:ARG:HH11	1.57	0.69
1:A:1441:LEU:HD21	7:G:53:THR:HA	1.73	0.69
14:N:366:HIS:HB2	14:N:370:LYS:HB3	1.75	0.69
20:W:450:SER:H	20:W:453:GLN:HE22	1.42	0.68
15:O:100:GLN:HG3	15:O:167:GLY:HA3	1.75	0.68
19:V:233:ARG:HG3	19:V:239:ARG:HH11	1.58	0.68
15:O:40:ARG:NH2	16:P:314:GLU:OE1	2.25	0.68
8:H:98:TYR:OH	8:H:139:ASN:ND2	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:ASN:ND2	1:A:650:GLY:O	2.28	0.67
3:C:165:ARG:NH2	3:C:190:ASP:OD1	2.27	0.66
1:A:269:ARG:HE	1:A:286:THR:HG22	1.61	0.66
19:V:491:ASN:HD21	19:V:494:PHE:HB2	1.60	0.66
2:B:888:VAL:HG11	12:L:54:ARG:HH21	1.61	0.66
4:D:141:CYS:SG	4:D:144:ARG:NH2	2.69	0.66
2:B:55:LYS:HG2	2:B:59:LYS:HD3	1.77	0.66
2:B:713:ILE:HG13	2:B:725:LEU:HD11	1.77	0.66
13:M:148:LEU:HA	13:M:182:PHE:H	1.61	0.66
1:A:668:VAL:HG12	1:A:677:VAL:HG23	1.78	0.65
1:A:1023:ARG:NH2	1:A:1028:MET:SD	2.68	0.65
13:M:217:LYS:NZ	20:W:360:THR:O	2.29	0.65
1:A:390:ASP:OD2	1:A:538:LYS:NZ	2.29	0.65
1:A:153:ARG:HH12	15:O:339:LEU:HB3	1.62	0.65
9:I:3:SER:HB2	9:I:12:LEU:HB2	1.78	0.65
1:A:815:GLN:HE21	1:A:846:GLY:HA3	1.61	0.65
13:M:92:ASN:HD21	13:M:181:PRO:HG3	1.62	0.65
10:J:31:ASP:HB3	10:J:34:THR:HG22	1.79	0.65
16:P:222:LEU:HD11	16:P:237:PRO:HG3	1.79	0.65
2:B:215:ILE:HD11	2:B:356:VAL:HG13	1.78	0.65
11:K:62:SER:HB3	11:K:104:ARG:HH11	1.62	0.65
1:A:512:PHE:HD2	2:B:768:GLU:HB2	1.61	0.64
1:A:597:ILE:HB	1:A:603:LEU:HB2	1.78	0.64
2:B:610:ARG:NH2	2:B:654:GLU:OE2	2.30	0.64
15:O:293:SER:HB3	15:O:316:LEU:HD11	1.80	0.64
3:C:31:TRP:HH2	11:K:127:LEU:HD13	1.60	0.64
1:A:703:ARG:NH2	11:K:93:ILE:O	2.26	0.64
20:W:460:ASN:ND2	21:X:18:DT:OP2	2.31	0.64
22:Y:67:DC:H2"	22:Y:68:DG:H2'	1.80	0.64
1:A:599:LYS:HB2	8:H:96:VAL:HG22	1.80	0.64
2:B:1004:LEU:HD21	2:B:1017:ILE:HB	1.80	0.64
16:P:170:LEU:HD13	16:P:172:ILE:H	1.63	0.64
1:A:151:GLN:NE2	1:A:153:ARG:O	2.30	0.64
1:A:568:ASP:O	8:H:22:LYS:NZ	2.31	0.64
1:A:1350:VAL:HG23	1:A:1351:ASP:H	1.63	0.63
15:O:620:LEU:HD23	15:O:622:SER:H	1.62	0.63
2:B:1028:LYS:HG2	2:B:1029:HIS:H	1.63	0.63
15:O:201:ILE:HD13	15:O:283:ASN:HD22	1.64	0.63
1:A:379:THR:HG22	2:B:1035:MET:HA	1.80	0.63
18:U:104:MET:HB2	18:U:113:ALA:HB3	1.80	0.63
16:P:135:LYS:NZ	16:P:150:LEU:O	2.26	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:185:TYR:HB3	18:U:193:LEU:HG	1.81	0.63
2:B:483:VAL:HG12	2:B:485:GLY:H	1.63	0.62
14:N:374:LYS:NZ	14:N:377:ASN:O	2.32	0.62
18:U:133:LYS:HE3	19:V:452:LEU:HA	1.81	0.62
19:V:215:PHE:HB3	19:V:223:ILE:HG21	1.81	0.62
3:C:191:ILE:HG23	10:J:15:GLY:HA3	1.80	0.62
1:A:683:ARG:NH1	1:A:925:GLU:OE2	2.33	0.62
3:C:1:MET:HG3	3:C:2:SER:H	1.64	0.62
7:G:93:THR:HG22	7:G:94:ALA:H	1.64	0.62
15:O:228:ARG:HG3	15:O:229:ASN:H	1.64	0.62
18:U:70:ILE:HG22	18:U:160:ILE:HD13	1.82	0.61
7:G:149:ARG:HH21	7:G:201:GLN:HG2	1.65	0.61
13:M:113:LYS:HD2	13:M:118:LEU:HD12	1.82	0.61
18:U:167:LYS:HD3	19:V:294:ARG:HH12	1.66	0.61
2:B:137:ARG:HH11	2:B:142:ILE:HD13	1.66	0.61
2:B:932:PRO:HB2	2:B:1004:LEU:HD12	1.81	0.61
18:U:107:ARG:HB2	20:W:473:LEU:HD22	1.82	0.61
18:U:93:GLU:OE2	20:W:439:PHE:N	2.31	0.61
18:U:195:TYR:HD2	18:U:204:LEU:HD21	1.66	0.61
2:B:60:GLN:HE22	2:B:471:THR:HG22	1.65	0.61
15:O:468:LEU:HD22	15:O:478:VAL:HB	1.83	0.61
2:B:221:THR:HG21	2:B:334:HIS:H	1.66	0.60
13:M:110:ALA:HB3	13:M:245:LEU:HB2	1.83	0.60
1:A:124:LEU:HA	1:A:127:LEU:HD23	1.84	0.60
2:B:40:THR:HB	2:B:624:ASP:HB3	1.83	0.60
16:P:187:SER:HA	16:P:263:VAL:HG21	1.83	0.60
21:X:60:DG:H1	22:Y:22:DC:H2'	1.65	0.60
7:G:4:LEU:HD13	7:G:73:ARG:HG3	1.82	0.60
2:B:258:LYS:HG2	2:B:263:LEU:HA	1.82	0.60
1:A:1257:PHE:HB2	9:I:14:ILE:HB	1.84	0.60
2:B:379:LEU:H	2:B:382:GLN:HE21	1.49	0.59
3:C:69:ARG:HE	11:K:71:THR:HG22	1.67	0.59
19:V:476:ASN:HB3	19:V:479:ALA:HB3	1.84	0.59
2:B:616:SER:OG	2:B:621:ARG:NE	2.35	0.59
3:C:255:VAL:HG21	3:C:273:ASP:HB2	1.84	0.59
2:B:796:LYS:HA	2:B:893:GLN:HE21	1.66	0.59
2:B:258:LYS:NZ	2:B:263:LEU:O	2.35	0.59
2:B:666:ILE:HD11	2:B:673:LEU:HD12	1.83	0.59
1:A:72:GLY:HA3	1:A:76:SER:HB2	1.84	0.59
1:A:166:LYS:HA	1:A:178:ILE:HG22	1.84	0.59
2:B:686:GLY:HA3	2:B:740:THR:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:194:ILE:O	18:U:196:ARG:NH1	2.36	0.59
19:V:265:THR:HG23	19:V:266:LYS:H	1.68	0.59
2:B:816:ASP:OD1	2:B:816:ASP:N	2.28	0.58
18:U:164:CYS:SG	18:U:165:ASP:N	2.76	0.58
21:X:21:DT:O2	22:Y:62:DG:N2	2.35	0.58
1:A:12:ARG:HG2	1:A:13:ILE:H	1.68	0.58
16:P:132:ARG:HD2	19:V:503:LEU:HD21	1.84	0.58
7:G:63:ASP:OD2	7:G:67:TYR:OH	2.17	0.58
1:A:70:CYS:SG	1:A:71:HIS:N	2.77	0.58
2:B:314:ARG:NH1	13:M:225:ASN:O	2.34	0.58
2:B:790:LYS:HD2	2:B:897:LYS:HE3	1.86	0.58
1:A:945:ILE:HG23	1:A:946:THR:HG23	1.83	0.58
13:M:158:GLN:H	14:N:308:GLN:HA	1.68	0.58
13:M:219:VAL:HG11	20:W:383:ARG:HE	1.69	0.58
7:G:158:VAL:HG22	7:G:160:PRO:HD3	1.86	0.58
13:M:128:GLN:HE22	13:M:133:LYS:HG2	1.69	0.57
16:P:313:ASP:O	16:P:314:GLU:HG3	2.04	0.57
1:A:929:ASN:O	1:A:931:GLN:NE2	2.37	0.57
5:E:78:LEU:HD13	5:E:107:THR:HG23	1.86	0.57
1:A:225:LEU:HD23	15:O:541:ILE:HG22	1.86	0.57
3:C:248:GLN:HA	3:C:256:ILE:HD11	1.86	0.57
12:L:31:CYS:SG	12:L:32:ALA:N	2.77	0.57
16:P:25:LYS:HD3	16:P:29:ALA:HB3	1.87	0.57
18:U:84:THR:O	18:U:88:HIS:NE2	2.37	0.57
1:A:393:ALA:HB3	1:A:499:ARG:HB2	1.85	0.57
2:B:1006:SER:HB2	2:B:1013:LEU:HD21	1.87	0.57
16:P:34:GLN:O	16:P:38:LYS:NZ	2.34	0.57
18:U:67:LEU:HB3	18:U:160:ILE:HD11	1.86	0.57
7:G:130:TRP:HE3	7:G:137:LYS:HB3	1.70	0.57
1:A:1185:GLN:HE22	1:A:1229:ARG:HD2	1.69	0.56
6:F:115:THR:HG22	6:F:116:ASP:H	1.70	0.56
1:A:11:LYS:HD2	2:B:1117:ILE:HG13	1.87	0.56
1:A:826:GLY:H	1:A:831:SER:HA	1.69	0.56
5:E:107:THR:HB	5:E:130:ALA:HB3	1.87	0.56
20:W:488:ILE:HG22	20:W:492:ILE:HG23	1.87	0.56
8:H:106:GLU:HA	8:H:112:ILE:HA	1.86	0.56
2:B:436:ALA:O	2:B:442:TRP:NE1	2.39	0.56
1:A:1336:ILE:HD13	1:A:1355:ILE:HG22	1.86	0.56
1:A:812:VAL:HG22	1:A:814:GLY:H	1.71	0.56
2:B:604:ASP:OD1	2:B:607:ARG:NH1	2.38	0.56
1:A:482:ARG:HH11	1:A:544:PRO:HG3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:THR:HG22	2:B:109:LYS:H	1.71	0.56
18:U:68:GLN:NE2	18:U:163:SER:OG	2.39	0.56
1:A:372:ARG:NH1	2:B:1052:GLU:OE1	2.39	0.56
2:B:207:VAL:HG12	2:B:217:GLN:HE22	1.71	0.56
1:A:122:GLN:NE2	1:A:126:GLU:OE2	2.38	0.55
1:A:1222:VAL:HG22	1:A:1232:ILE:HD13	1.87	0.55
1:A:1332:ARG:NH1	1:A:1360:ASP:OD1	2.39	0.55
3:C:245:ARG:NH1	3:C:263:ASP:OD2	2.40	0.55
15:O:484:MET:SD	15:O:485:PRO:HD3	2.46	0.55
18:U:175:LEU:HA	18:U:178:SER:HB2	1.89	0.55
1:A:524:THR:HG23	2:B:1081:GLU:HG3	1.88	0.55
1:A:789:ASN:HD22	1:A:790:ALA:N	2.03	0.55
9:I:30:PRO:HG2	13:M:125:LEU:HD11	1.89	0.55
1:A:186:VAL:HG13	1:A:187:GLY:H	1.70	0.55
15:O:233:SER:HB3	15:O:236:LYS:HD3	1.88	0.55
2:B:404:ASP:HA	2:B:407:LEU:HB2	1.88	0.55
16:P:311:TYR:HA	17:Q:40:PRO:HA	1.88	0.55
1:A:332:VAL:HG13	1:A:334:PRO:HD3	1.88	0.55
1:A:952:LYS:O	1:A:1061:ARG:NH2	2.40	0.55
2:B:769:ASP:OD2	2:B:952:ARG:NH2	2.39	0.55
20:W:450:SER:H	20:W:453:GLN:NE2	2.05	0.55
1:A:1187:ARG:NH1	1:A:1189:ASP:OD1	2.40	0.55
1:A:1048:VAL:O	1:A:1053:LYS:NZ	2.40	0.54
2:B:882:ASP:HB2	2:B:901:ARG:HB2	1.88	0.54
15:O:43:ASN:HB3	15:O:47:PHE:HB2	1.89	0.54
10:J:10:CYS:SG	10:J:11:GLY:N	2.80	0.54
1:A:632:VAL:HG23	1:A:633:PHE:H	1.71	0.54
2:B:553:TYR:CD2	2:B:568:PRO:HG3	2.43	0.54
16:P:87:SER:OG	16:P:90:GLU:OE1	2.23	0.54
3:C:80:ALA:HB3	3:C:102:GLY:HA2	1.89	0.54
1:A:22:SER:HB2	15:O:42:LEU:HD21	1.90	0.54
2:B:209:ALA:HB2	2:B:366:ILE:HG21	1.89	0.54
2:B:738:THR:HG23	2:B:977:THR:HA	1.88	0.54
2:B:795:LEU:HD21	2:B:806:ILE:HD11	1.90	0.54
3:C:241:GLY:O	3:C:245:ARG:NH1	2.41	0.54
1:A:1286:ARG:HG2	1:A:1287:ASP:H	1.73	0.54
13:M:250:GLY:O	13:M:251:THR:HG22	2.08	0.54
1:A:1445:ARG:NH2	4:D:10:PHE:O	2.41	0.54
2:B:904:ARG:NH1	2:B:1030:MET:SD	2.80	0.54
15:O:288:MET:HG3	15:O:326:ILE:HD13	1.89	0.54
1:A:264:PRO:O	1:A:269:ARG:NH1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1094:VAL:HG21	2:B:1141:LEU:HD12	1.90	0.53
7:G:207:LEU:HG	7:G:209:SER:H	1.73	0.53
1:A:1059:LEU:HD11	8:H:112:ILE:HG21	1.90	0.53
15:O:640:ARG:NH2	16:P:308:GLU:O	2.41	0.53
19:V:214:MET:N	19:V:214:MET:SD	2.82	0.53
5:E:47:CYS:HB2	5:E:53:PRO:HA	1.90	0.53
2:B:1093:ASP:HB3	2:B:1118:LYS:HD2	1.89	0.53
15:O:57:LEU:HD23	15:O:58:GLY:H	1.73	0.53
16:P:269:LEU:HG	16:P:297:PHE:HE1	1.74	0.53
19:V:242:THR:OG1	20:W:296:SER:OG	2.27	0.53
1:A:579:LEU:HD23	1:A:609:VAL:HG21	1.91	0.53
20:W:467:ILE:HG13	20:W:468:LEU:HD12	1.89	0.53
1:A:997:GLN:HB3	5:E:167:ARG:HH12	1.74	0.53
15:O:199:TYR:HD1	15:O:286:ARG:HD2	1.74	0.53
3:C:100:ARG:NH1	10:J:3:VAL:O	2.39	0.52
5:E:106:GLN:HG2	5:E:107:THR:HG22	1.90	0.52
15:O:98:LEU:HB2	15:O:103:CYS:HB2	1.92	0.52
1:A:666:LYS:HD2	1:A:670:GLY:HA3	1.91	0.52
1:A:1278:ILE:HA	1:A:1297:GLY:HA3	1.91	0.52
19:V:484:GLU:OE1	20:W:499:ASN:ND2	2.42	0.52
16:P:145:ARG:HE	16:P:147:ILE:HD11	1.74	0.52
19:V:257:GLN:OE1	19:V:258:ARG:NH1	2.42	0.52
20:W:407:ASN:ND2	22:Y:65:DG:OP1	2.42	0.52
7:G:88:TRP:HB2	7:G:102:LEU:HD13	1.91	0.52
19:V:239:ARG:NH2	20:W:284:PHE:H	2.08	0.52
2:B:93:LEU:HD13	2:B:135:TYR:HB3	1.90	0.52
2:B:409:LYS:HB2	2:B:412:ARG:HB2	1.92	0.52
16:P:172:ILE:HG22	16:P:173:GLU:H	1.75	0.52
1:A:818:ILE:HD12	1:A:823:VAL:HA	1.91	0.52
2:B:1038:ARG:NH1	2:B:1058:GLY:O	2.43	0.52
15:O:591:LYS:HD2	16:P:308:GLU:HG3	1.91	0.52
18:U:129:GLU:OE1	19:V:448:THR:OG1	2.26	0.52
20:W:487:GLU:O	20:W:491:ASN:ND2	2.43	0.52
1:A:1166:LEU:HD21	1:A:1268:PRO:HA	1.92	0.52
19:V:6:ASN:HD22	19:V:30:VAL:HG21	1.75	0.52
1:A:654:ILE:HD11	1:A:657:SER:HA	1.91	0.51
1:A:757:ASN:HD22	1:A:760:GLN:NE2	2.07	0.51
3:C:70:ILE:HG23	3:C:74:GLU:HB2	1.92	0.51
2:B:938:ILE:HD11	10:J:43:ARG:HB2	1.91	0.51
5:E:78:LEU:HD21	5:E:109:ILE:HD11	1.91	0.51
15:O:605:LYS:HA	15:O:608:ARG:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:299:ASN:C	14:N:300:LYS:HD2	2.30	0.51
15:O:346:GLN:HA	15:O:349:ALA:HB3	1.92	0.51
16:P:311:TYR:CD2	17:Q:37:PRO:HG2	2.45	0.51
1:A:473:LEU:HD23	1:A:485:ILE:HD11	1.93	0.51
1:A:1283:ILE:HD11	1:A:1291:ARG:HD3	1.91	0.51
15:O:222:HIS:HA	15:O:225:ASN:HD22	1.74	0.51
18:U:88:HIS:HB2	19:V:475:LEU:HD13	1.92	0.51
20:W:483:GLU:O	20:W:487:GLU:N	2.41	0.51
2:B:261:GLY:HA2	2:B:298:GLN:HG3	1.91	0.51
2:B:944:MET:SD	2:B:1024:TYR:OH	2.69	0.51
3:C:172:GLN:H	3:C:175:GLN:HE21	1.59	0.51
1:A:808:GLN:HG2	1:A:813:VAL:HA	1.92	0.51
2:B:754:ASN:HA	2:B:1023:TYR:HA	1.91	0.51
2:B:835:LYS:HB3	2:B:880:HIS:CE1	2.46	0.51
2:B:915:ARG:NH2	2:B:960:GLU:OE2	2.44	0.51
11:K:88:PHE:HB3	11:K:106:GLN:HB3	1.92	0.51
1:A:440:ALA:O	1:A:441:ARG:HG3	2.11	0.51
1:A:468:ASP:OD1	1:A:468:ASP:N	2.43	0.51
1:A:946:THR:HG21	1:A:1069:LYS:HG3	1.93	0.51
1:A:1267:LEU:HG	1:A:1268:PRO:HD3	1.92	0.51
2:B:806:ILE:HG22	2:B:828:GLY:HA3	1.93	0.51
19:V:498:GLN:HG2	20:W:506:GLN:HE21	1.76	0.51
1:A:1121:LEU:O	1:A:1342:THR:OG1	2.29	0.51
18:U:193:LEU:HB3	18:U:206:ILE:HG13	1.92	0.50
2:B:343:ARG:NH1	2:B:541:ILE:O	2.39	0.50
2:B:1036:HIS:CE1	2:B:1058:GLY:HA3	2.47	0.50
1:A:153:ARG:HG2	1:A:160:LEU:HA	1.92	0.50
1:A:442:ARG:HG2	19:V:30:VAL:HG22	1.92	0.50
2:B:918:GLN:HG2	2:B:952:ARG:HD3	1.93	0.50
14:N:380:MET:HB3	14:N:421:GLN:HE22	1.76	0.50
15:O:329:PRO:HA	15:O:332:GLN:HG2	1.93	0.50
2:B:332:ILE:O	2:B:345:LYS:NZ	2.34	0.50
2:B:807:GLY:O	2:B:844:ASN:ND2	2.44	0.50
3:C:83:VAL:HG23	12:L:69:ALA:HB2	1.94	0.50
9:I:7:SER:HA	13:M:93:ARG:HH22	1.77	0.50
15:O:342:ALA:HA	15:O:345:PHE:HD2	1.75	0.50
2:B:738:THR:HG22	2:B:740:THR:H	1.76	0.50
2:B:217:GLN:HB2	2:B:233:VAL:HB	1.93	0.50
1:A:1205:ILE:O	1:A:1209:ILE:HD12	2.12	0.50
3:C:216:HIS:CE1	3:C:218:LYS:HG3	2.47	0.50
13:M:93:ARG:HE	13:M:105:PRO:HG3	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:408:LYS:HB2	16:P:119:HIS:CD2	2.47	0.50
2:B:824:LEU:HA	2:B:830:GLY:HA2	1.94	0.50
15:O:530:GLU:OE2	15:O:534:ARG:NH1	2.44	0.50
20:W:451:ARG:HH22	20:W:455:LYS:HD2	1.77	0.50
1:A:741:LEU:HD12	1:A:744:LEU:HD21	1.94	0.49
1:A:763:GLU:HG2	1:A:822:ARG:HE	1.75	0.49
15:O:496:ILE:HG23	15:O:500:LEU:HD21	1.94	0.49
1:A:476:ARG:HG3	1:A:478:PRO:HD2	1.94	0.49
1:A:577:THR:HG21	11:K:89:CYS:H	1.77	0.49
2:B:819:TRP:HA	2:B:822:GLN:HE22	1.76	0.49
1:A:11:LYS:HA	2:B:1145:ASP:HA	1.92	0.49
1:A:665:ASP:HB2	1:A:797:CYS:HA	1.93	0.49
1:A:113:ILE:HD12	1:A:238:ASP:HB2	1.94	0.49
15:O:304:VAL:HG22	15:O:305:GLY:H	1.78	0.49
16:P:295:ASN:HB2	16:P:298:LYS:HE2	1.94	0.49
20:W:318:ARG:NH1	20:W:448:TYR:HB2	2.27	0.49
20:W:485:CYS:O	20:W:489:LYS:N	2.44	0.49
1:A:410:ARG:NE	6:F:104:ASN:OD1	2.46	0.49
1:A:12:ARG:N	2:B:1144:GLU:O	2.41	0.49
1:A:269:ARG:HB3	1:A:285:LEU:HD23	1.94	0.49
1:A:893:LEU:HD12	1:A:1361:VAL:HG11	1.95	0.49
2:B:51:PHE:HD2	2:B:52:LEU:HD12	1.77	0.49
19:V:273:GLN:HG2	19:V:274:LYS:HB2	1.95	0.49
1:A:768:GLY:HA2	1:A:771:SER:HB3	1.95	0.49
2:B:837:GLN:N	2:B:840:GLN:OE1	2.40	0.49
18:U:220:ARG:HG2	18:U:224:TYR:HE2	1.78	0.49
2:B:217:GLN:HG3	2:B:356:VAL:HG22	1.95	0.49
5:E:93:MET:HG2	5:E:123:LEU:HD11	1.94	0.49
18:U:196:ARG:HG3	18:U:203:VAL:HG12	1.95	0.49
18:U:215:THR:OG1	21:X:24:DA:N3	2.39	0.49
1:A:910:GLY:HA2	5:E:174:GLN:HB2	1.95	0.49
1:A:1161:VAL:HG23	1:A:1275:LEU:HD13	1.95	0.49
1:A:1177:TYR:OH	1:A:1260:MET:SD	2.71	0.49
5:E:147:HIS:HE1	5:E:149:LEU:HD23	1.77	0.49
20:W:413:ARG:HE	21:X:20:DC:H4'	1.78	0.49
1:A:1031:LEU:HD23	1:A:1031:LEU:H	1.77	0.48
2:B:580:ARG:HH22	2:B:614:ILE:HD13	1.78	0.48
5:E:37:LEU:HD11	5:E:42:PHE:HB2	1.94	0.48
10:J:17:LYS:HB3	10:J:39:LEU:HD21	1.94	0.48
1:A:14:LYS:HD2	2:B:1144:GLU:HG3	1.95	0.48
1:A:911:ILE:HB	5:E:176:PRO:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1186:VAL:HB	1:A:1230:ILE:HG23	1.95	0.48
2:B:329:THR:HG22	2:B:345:LYS:HD3	1.94	0.48
14:N:307:PHE:HB3	14:N:416:ILE:HG13	1.95	0.48
15:O:129:ILE:HG21	15:O:164:ILE:HD13	1.95	0.48
2:B:338:GLU:HG3	2:B:342:PHE:CE1	2.48	0.48
8:H:93:TYR:CD2	8:H:143:LEU:HB3	2.48	0.48
16:P:263:VAL:HG12	16:P:265:LEU:H	1.78	0.48
18:U:230:ILE:O	18:U:233:VAL:HG22	2.13	0.48
1:A:57:LYS:HB3	1:A:68:ALA:HB3	1.96	0.48
1:A:545:LYS:HG3	1:A:1350:VAL:HG12	1.95	0.48
1:A:1058:GLN:HE22	8:H:135:LEU:HG	1.78	0.48
3:C:169:PHE:CE2	3:C:171:PRO:HG3	2.48	0.48
13:M:140:TRP:HD1	13:M:142:GLY:H	1.61	0.48
18:U:67:LEU:HD12	18:U:160:ILE:HG13	1.95	0.48
2:B:127:ALA:O	2:B:152:MET:N	2.46	0.48
2:B:698:ARG:NH2	2:B:952:ARG:HG2	2.28	0.48
2:B:806:ILE:HG21	2:B:829:LEU:HD22	1.94	0.48
18:U:114:LEU:HB3	18:U:122:VAL:HG13	1.94	0.48
18:U:133:LYS:HB3	18:U:137:ARG:HH22	1.79	0.48
1:A:789:ASN:ND2	1:A:791:PRO:HD2	2.29	0.48
3:C:172:GLN:HG3	3:C:173:GLY:H	1.78	0.48
18:U:197:MET:HB3	18:U:200:PRO:HD2	1.95	0.48
19:V:485:ARG:HG3	20:W:498:PHE:HB2	1.96	0.48
19:V:4:CYS:SG	19:V:5:LYS:N	2.87	0.48
20:W:311:ARG:HH22	20:W:314:ARG:NH2	2.12	0.48
1:A:583:MET:HB2	1:A:696:ARG:HG2	1.96	0.48
2:B:969:LEU:HB3	2:B:994:GLN:HG3	1.96	0.48
3:C:282:TYR:O	3:C:283:GLU:HG3	2.13	0.48
1:A:91:PHE:CE2	1:A:224:PRO:HG3	2.49	0.47
2:B:253:ILE:HA	2:B:256:VAL:HG22	1.96	0.47
2:B:347:LEU:HD21	2:B:541:ILE:HD11	1.95	0.47
2:B:614:ILE:HG23	2:B:621:ARG:HD2	1.95	0.47
4:D:20:LEU:HD11	4:D:59:THR:HG23	1.96	0.47
4:D:99:SER:OG	4:D:101:GLU:OE1	2.31	0.47
2:B:66:ASN:HD21	2:B:159:ASN:HD21	1.60	0.47
15:O:102:ARG:O	15:O:123:ASN:ND2	2.46	0.47
2:B:209:ALA:HA	2:B:215:ILE:HG22	1.96	0.47
2:B:216:VAL:HG23	2:B:234:ILE:HG22	1.96	0.47
2:B:848:PRO:HG3	2:B:866:TYR:HE1	1.79	0.47
7:G:153:GLU:HB3	7:G:196:LEU:HD13	1.96	0.47
15:O:370:LEU:HD12	15:O:371:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:88:HIS:HB2	19:V:475:LEU:HD22	1.96	0.47
20:W:367:ASN:HB3	20:W:370:GLY:O	2.15	0.47
1:A:91:PHE:CD2	1:A:224:PRO:HG3	2.49	0.47
1:A:1373:ARG:HD3	1:A:1391:LYS:HD3	1.96	0.47
2:B:971:GLY:HA3	10:J:33:GLY:HA2	1.97	0.47
4:D:129:ALA:H	4:D:157:ILE:HG12	1.80	0.47
8:H:118:PHE:HZ	8:H:142:LEU:HD13	1.78	0.47
1:A:481:HIS:CE1	1:A:483:LEU:HB2	2.49	0.47
1:A:518:ASN:OD1	1:A:518:ASN:N	2.48	0.47
13:M:105:PRO:HB2	13:M:123:ILE:HD11	1.95	0.47
1:A:398:VAL:HG23	2:B:1037:ALA:HB2	1.97	0.47
1:A:1162:GLU:HA	1:A:1278:ILE:HD11	1.97	0.47
2:B:190:THR:OG1	2:B:192:LYS:NZ	2.47	0.47
2:B:270:GLN:HE21	2:B:547:ALA:HB2	1.80	0.47
2:B:929:GLU:HB2	3:C:69:ARG:HG2	1.97	0.47
3:C:88:ASN:O	12:L:60:ARG:NH1	2.48	0.47
7:G:120:TYR:O	7:G:128:TRP:HB3	2.14	0.47
18:U:136:SER:OG	18:U:137:ARG:NH1	2.48	0.47
2:B:602:ALA:O	2:B:607:ARG:NH2	2.48	0.47
2:B:615:VAL:HG23	2:B:673:LEU:H	1.80	0.47
20:W:288:GLN:HB3	20:W:289:ILE:H	1.53	0.47
15:O:653:MET:SD	15:O:653:MET:N	2.88	0.47
16:P:236:THR:HG23	16:P:239:ASN:H	1.80	0.47
20:W:507:ASN:O	20:W:511:HIS:ND1	2.31	0.47
1:A:856:LEU:HD23	1:A:861:PHE:HA	1.96	0.47
3:C:21:PRO:HD2	11:K:82:LYS:HA	1.97	0.47
2:B:737:LYS:HE3	2:B:975:TYR:HE1	1.80	0.46
9:I:30:PRO:HB3	13:M:136:ALA:HB2	1.97	0.46
15:O:105:LYS:HB3	15:O:210:PRO:HD3	1.97	0.46
3:C:52:ALA:HB3	3:C:302:VAL:HG22	1.97	0.46
7:G:81:LEU:HD23	7:G:81:LEU:H	1.81	0.46
19:V:498:GLN:HG2	20:W:506:GLN:NE2	2.30	0.46
2:B:696:SER:OG	2:B:697:PRO:HD3	2.14	0.46
2:B:773:LEU:HB3	2:B:942:ILE:HG12	1.98	0.46
5:E:147:HIS:CE1	5:E:149:LEU:HD23	2.50	0.46
15:O:203:ILE:HG13	15:O:279:SER:O	2.16	0.46
18:U:209:SER:HB2	19:V:289:SER:HB2	1.98	0.46
19:V:165:VAL:HG23	19:V:170:ILE:HB	1.97	0.46
1:A:1122:GLY:HA2	1:A:1346:HIS:HE1	1.81	0.46
2:B:622:VAL:HG23	2:B:623:LYS:H	1.81	0.46
3:C:229:LEU:HB2	3:C:293:ARG:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:55:ARG:HH12	5:E:113:GLN:HG3	1.80	0.46
1:A:919:ASP:N	1:A:919:ASP:OD1	2.47	0.46
1:A:1083:LEU:HD21	1:A:1089:ILE:HG21	1.97	0.46
4:D:3:VAL:HG13	7:G:7:ILE:HG22	1.97	0.46
5:E:199:ILE:HG22	5:E:209:ALA:HB2	1.98	0.46
15:O:491:VAL:HG11	15:O:650:VAL:HG11	1.97	0.46
20:W:488:ILE:HA	20:W:491:ASN:HB2	1.97	0.46
1:A:217:ARG:HH22	15:O:555:ALA:HA	1.81	0.46
1:A:329:SER:HB3	1:A:355:GLN:HG3	1.98	0.46
1:A:1079:ARG:HD3	6:F:84:TYR:HE2	1.80	0.46
1:A:1320:LEU:HD23	1:A:1320:LEU:H	1.81	0.46
2:B:689:PRO:HG3	2:B:915:ARG:NH2	2.31	0.46
7:G:10:LEU:HA	7:G:69:ASN:HA	1.97	0.46
14:N:386:ALA:HA	14:N:416:ILE:HG22	1.98	0.46
14:N:394:VAL:HG23	14:N:412:VAL:HB	1.97	0.46
18:U:221:GLU:HA	18:U:224:TYR:HD2	1.81	0.46
20:W:310:LEU:HD13	20:W:313:LEU:HD21	1.97	0.46
1:A:107:CYS:N	1:A:112:ALA:O	2.43	0.46
2:B:811:VAL:HG12	2:B:816:ASP:HA	1.96	0.46
2:B:846:SER:HB3	2:B:866:TYR:HB3	1.98	0.46
6:F:136:ARG:N	6:F:144:GLU:O	2.48	0.46
9:I:5:CYS:O	9:I:9:ASN:N	2.44	0.46
15:O:152:HIS:HD2	15:O:156:VAL:HB	1.80	0.46
15:O:259:LEU:HD23	15:O:259:LEU:H	1.80	0.46
18:U:140:ALA:HA	18:U:143:ILE:HD12	1.98	0.46
19:V:80:LEU:HA	19:V:83:ALA:HB3	1.98	0.46
8:H:12:VAL:HG22	8:H:53:ASP:H	1.81	0.46
15:O:199:TYR:HA	15:O:283:ASN:HB3	1.96	0.46
16:P:102:ARG:HG2	16:P:154:GLN:HG2	1.97	0.46
2:B:860:VAL:HG23	2:B:861:ASN:H	1.80	0.45
4:D:147:GLU:CD	4:D:148:LYS:H	2.19	0.45
1:A:20:ALA:HB3	1:A:256:TYR:HE1	1.80	0.45
2:B:884:VAL:HB	2:B:898:VAL:HG23	1.97	0.45
5:E:88:VAL:HG11	5:E:110:PHE:HZ	1.81	0.45
5:E:168:TYR:HB2	5:E:170:LEU:HD22	1.97	0.45
19:V:274:LYS:HG2	19:V:275:PHE:H	1.80	0.45
21:X:28:DA:H1'	21:X:29:DA:O4'	2.17	0.45
1:A:628:ALA:O	1:A:652:VAL:HG12	2.17	0.45
11:K:58:GLY:O	11:K:113:ALA:N	2.39	0.45
13:M:227:LEU:HB2	13:M:231:LEU:HD21	1.99	0.45
18:U:73:THR:HA	18:U:122:VAL:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:GLY:O	1:A:771:SER:N	2.48	0.45
7:G:39:ILE:HD11	7:G:45:CYS:SG	2.56	0.45
15:O:294:LYS:HD2	15:O:297:ILE:HD11	1.98	0.45
2:B:534:TYR:HA	2:B:538:VAL:HG12	1.99	0.45
1:A:352:GLY:H	1:A:355:GLN:HB2	1.80	0.45
1:A:826:GLY:N	1:A:830:ARG:O	2.50	0.45
18:U:78:CYS:HB2	18:U:149:ALA:HB3	1.99	0.45
1:A:223:ASN:HB2	1:A:316:TRP:CH2	2.52	0.45
2:B:554:GLY:HA2	2:B:564:SER:HA	1.98	0.45
2:B:1101:MET:SD	2:B:1126:LYS:HG2	2.57	0.45
15:O:552:PRO:HG3	15:O:557:ARG:HE	1.81	0.45
19:V:165:VAL:HA	19:V:170:ILE:HD13	1.99	0.45
1:A:790:ALA:HB3	1:A:791:PRO:HD3	1.99	0.45
2:B:683:ALA:HB1	2:B:744:ILE:HD13	1.99	0.45
2:B:961:LEU:HD12	2:B:1022:ILE:HD11	1.99	0.44
2:B:1088:ASP:OD2	2:B:1123:TYR:N	2.50	0.44
8:H:7:ASP:OD1	8:H:58:THR:OG1	2.27	0.44
15:O:194:LEU:O	15:O:200:LEU:HD13	2.17	0.44
22:Y:76:DT:H6	22:Y:76:DT:H2'	1.66	0.44
1:A:218:CYS:HB2	15:O:551:VAL:HG12	1.98	0.44
11:K:95:HIS:HD2	11:K:97:SER:HB3	1.82	0.44
15:O:57:LEU:HD23	15:O:58:GLY:N	2.31	0.44
19:V:237:LEU:HB3	20:W:290:SER:HB3	1.99	0.44
1:A:955:LEU:HD23	1:A:1031:LEU:HD21	1.99	0.44
2:B:738:THR:O	2:B:741:ILE:HG13	2.18	0.44
2:B:913:SER:OG	2:B:914:SER:N	2.50	0.44
11:K:55:SER:OG	11:K:57:ASP:O	2.33	0.44
15:O:51:GLU:OE2	15:O:590:PHE:HA	2.17	0.44
19:V:275:PHE:HE2	19:V:279:ASP:HB2	1.82	0.44
19:V:287:PRO:HA	19:V:288:PRO:HD3	1.82	0.44
15:O:464:ASN:ND2	16:P:254:GLU:OE2	2.50	0.44
15:O:578:ARG:NH2	15:O:651:PHE:O	2.40	0.44
16:P:240:ILE:HA	16:P:243:LEU:HB2	2.00	0.44
8:H:118:PHE:CZ	8:H:142:LEU:HD13	2.52	0.44
8:H:142:LEU:HD23	8:H:144:ILE:HD11	1.99	0.44
15:O:51:GLU:HA	15:O:54:LYS:HB3	2.00	0.44
1:A:1391:LYS:HE3	1:A:1395:HIS:HE2	1.83	0.44
2:B:347:LEU:HD23	2:B:347:LEU:H	1.83	0.44
1:A:274:MET:SD	1:A:281:ASN:HB2	2.58	0.44
1:A:1145:LEU:HD11	1:A:1157:VAL:HG11	2.00	0.44
2:B:1093:ASP:OD1	2:B:1093:ASP:N	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:47:CYS:HA	5:E:54:GLN:HG3	2.00	0.44
7:G:88:TRP:HE1	7:G:145:LYS:HG2	1.83	0.44
20:W:287:GLY:O	20:W:288:GLN:HG3	2.18	0.44
1:A:89:PRO:HG2	1:A:228:LEU:HD13	2.00	0.44
1:A:153:ARG:NE	1:A:158:GLY:O	2.47	0.44
1:A:1316:THR:OG1	1:A:1317:ASN:N	2.50	0.44
3:C:103:LEU:HD23	3:C:218:LYS:HG2	2.00	0.44
1:A:203:GLU:HG3	15:O:515:LYS:HB2	2.00	0.43
1:A:555:GLN:NE2	2:B:767:ILE:O	2.50	0.43
2:B:303:GLU:HA	2:B:325:GLU:HG2	1.99	0.43
16:P:55:LEU:HD22	16:P:58:LYS:HB2	2.00	0.43
2:B:343:ARG:NE	13:M:178:GLN:OE1	2.51	0.43
2:B:660:ALA:HB2	2:B:670:MET:SD	2.58	0.43
2:B:907:GLU:HA	2:B:925:ILE:HD11	2.00	0.43
2:B:916:HIS:HD1	2:B:957:LYS:HG3	1.83	0.43
8:H:93:TYR:HD2	8:H:143:LEU:HB3	1.83	0.43
19:V:238:ARG:HA	20:W:293:PHE:HZ	1.82	0.43
19:V:275:PHE:CE2	19:V:279:ASP:HB2	2.53	0.43
1:A:422:ASN:HB3	1:A:426:VAL:HG23	2.00	0.43
1:A:482:ARG:NH1	1:A:544:PRO:HG3	2.32	0.43
2:B:296:TYR:OH	9:I:27:ARG:NH2	2.45	0.43
5:E:78:LEU:HD11	5:E:109:ILE:HG13	1.98	0.43
7:G:16:ASP:N	7:G:16:ASP:OD1	2.51	0.43
16:P:116:LEU:HB3	16:P:120:VAL:HG13	2.00	0.43
18:U:98:ARG:NH1	22:Y:55:DA:OP1	2.49	0.43
21:X:16:DG:H2"	21:X:17:DC:OP2	2.18	0.43
1:A:17:GLU:OE2	2:B:1142:ARG:NE	2.51	0.43
1:A:175:ALA:O	1:A:176:LEU:HG	2.19	0.43
1:A:381:ILE:HG21	1:A:517:MET:HE3	2.00	0.43
1:A:1302:ASP:OD1	1:A:1302:ASP:N	2.51	0.43
2:B:58:VAL:HG12	2:B:61:HIS:HB2	2.00	0.43
7:G:91:LYS:HZ2	7:G:98:LYS:HE3	1.83	0.43
19:V:503:LEU:HD22	19:V:506:GLU:HB3	2.01	0.43
1:A:578:GLN:HE21	11:K:77:ARG:NH1	2.16	0.43
7:G:14:PRO:HA	7:G:15:PRO:HD3	1.86	0.43
15:O:210:PRO:HD2	15:O:213:ASP:OD2	2.18	0.43
19:V:154:VAL:HG11	20:W:408:TYR:HD1	1.82	0.43
1:A:482:ARG:HD3	1:A:544:PRO:HG3	2.00	0.43
1:A:495:TRP:CD2	2:B:908:LEU:HD21	2.54	0.43
1:A:556:ASP:HB3	2:B:767:ILE:HD12	2.00	0.43
1:A:959:ILE:HD11	1:A:1016:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:369:ARG:NH2	2:B:480:SER:OG	2.51	0.43
3:C:81:GLU:OE2	12:L:70:ARG:NH2	2.52	0.43
15:O:141:ILE:HD12	15:O:153:LYS:NZ	2.33	0.43
16:P:53:GLN:NE2	20:W:363:GLN:OE1	2.28	0.43
18:U:90:ARG:HB3	19:V:473:HIS:CE1	2.53	0.43
1:A:815:GLN:NE2	1:A:816:GLN:O	2.51	0.43
3:C:78:VAL:HG21	3:C:108:VAL:HG13	2.01	0.43
5:E:18:THR:HG23	5:E:143:ASN:HB3	2.01	0.43
8:H:93:TYR:CD1	8:H:145:ARG:HB3	2.54	0.43
1:A:623:VAL:HG23	1:A:656:GLY:HA2	2.00	0.43
1:A:895:ASP:OD1	1:A:895:ASP:N	2.52	0.43
2:B:81:GLN:HE21	2:B:94:LYS:HB2	1.84	0.43
2:B:240:ILE:HG12	2:B:286:ASN:HD21	1.83	0.43
6:F:77:ASP:OD1	6:F:78:GLN:N	2.49	0.43
15:O:91:VAL:O	15:O:95:LEU:N	2.48	0.43
18:U:186:GLU:OE2	18:U:188:GLU:HG2	2.19	0.43
19:V:488:ILE:HD12	19:V:491:ASN:HD22	1.83	0.43
1:A:591:ASP:OD1	1:A:591:ASP:N	2.51	0.43
1:A:955:LEU:HD22	1:A:957:TYR:HE1	1.83	0.43
1:A:997:GLN:HG3	1:A:998:TYR:CD1	2.54	0.43
2:B:464:ILE:H	2:B:464:ILE:HG13	1.65	0.43
14:N:287:HIS:HA	14:N:290:ILE:HG22	2.00	0.43
15:O:605:LYS:NZ	15:O:623:GLU:OE1	2.44	0.43
19:V:458:ASP:OD1	19:V:458:ASP:N	2.51	0.43
1:A:1391:LYS:HE3	1:A:1395:HIS:NE2	2.34	0.42
2:B:279:TYR:HD1	2:B:357:VAL:HG12	1.83	0.42
8:H:38:LEU:HB3	8:H:125:LEU:HB3	2.00	0.42
1:A:4:VAL:HA	7:G:38:ILE:HG22	2.01	0.42
1:A:482:ARG:HG3	1:A:483:LEU:HD12	2.00	0.42
1:A:429:GLY:O	1:A:465:HIS:ND1	2.52	0.42
1:A:504:VAL:O	1:A:507:PRO:HD2	2.19	0.42
15:O:602:LEU:H	15:O:602:LEU:HD23	1.84	0.42
16:P:135:LYS:HB3	16:P:151:TYR:HE1	1.83	0.42
15:O:568:CYS:SG	15:O:569:LYS:N	2.93	0.42
16:P:129:GLU:OE2	16:P:132:ARG:NH2	2.52	0.42
2:B:124:THR:HG22	2:B:188:ASN:H	1.83	0.42
2:B:1135:MET:O	2:B:1137:ILE:N	2.52	0.42
1:A:234:ILE:HD11	1:A:253:PRO:HG3	2.01	0.42
16:P:111:LYS:HG2	16:P:116:LEU:O	2.20	0.42
1:A:501:ASN:OD1	1:A:502:GLU:N	2.52	0.42
2:B:204:ARG:NH1	2:B:604:ASP:OD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:ILE:HD11	2:B:355:ARG:NH2	2.33	0.42
2:B:916:HIS:ND1	2:B:957:LYS:HG3	2.35	0.42
13:M:111:ARG:HH12	13:M:242:ASN:HA	1.85	0.42
14:N:373:VAL:HG23	14:N:381:ASP:HB2	2.00	0.42
16:P:311:TYR:HD2	17:Q:37:PRO:HG2	1.83	0.42
1:A:32:VAL:HG12	1:A:57:LYS:NZ	2.35	0.42
2:B:829:LEU:HD13	2:B:829:LEU:HA	1.93	0.42
8:H:113:ALA:HA	8:H:126:GLU:HA	2.00	0.42
20:W:418:ASP:HB3	20:W:449:ARG:NH1	2.35	0.42
3:C:26:ASP:OD1	3:C:26:ASP:N	2.52	0.42
7:G:57:GLY:HA2	7:G:68:ILE:HG13	2.02	0.42
16:P:310:VAL:HG12	17:Q:41:LEU:HD23	2.02	0.42
20:W:489:LYS:HE2	20:W:489:LYS:HB3	1.91	0.42
22:Y:63:DT:H6	22:Y:63:DT:H2'	1.71	0.42
1:A:311:ASN:O	1:A:314:GLU:HG3	2.19	0.42
2:B:412:ARG:NH2	19:V:151:GLN:OE1	2.35	0.42
3:C:134:LEU:HD12	3:C:167:LEU:HB3	2.01	0.42
7:G:6:LYS:HE3	7:G:52:LEU:HD13	2.02	0.42
1:A:1185:GLN:NE2	1:A:1229:ARG:HD2	2.35	0.41
2:B:1100:LEU:HD21	2:B:1109:THR:HG21	2.01	0.41
1:A:774:ARG:HH21	1:A:808:GLN:HE21	1.67	0.41
1:A:1165:LEU:HD11	1:A:1269:ASP:HA	2.02	0.41
2:B:59:LYS:NZ	2:B:518:THR:O	2.46	0.41
2:B:330:THR:OG1	2:B:338:GLU:OE2	2.32	0.41
5:E:100:ILE:HA	5:E:105:PHE:HD2	1.85	0.41
13:M:159:TYR:CD2	14:N:309:LEU:HD23	2.55	0.41
15:O:56:HIS:CE1	15:O:130:LEU:HD22	2.55	0.41
17:Q:48:THR:HG22	17:Q:50:LYS:H	1.84	0.41
20:W:283:ASN:ND2	21:X:13:DT:OP2	2.53	0.41
22:Y:17:DG:H2'	22:Y:18:DG:C8	2.55	0.41
2:B:580:ARG:NH2	2:B:647:GLU:OE2	2.52	0.41
2:B:620:SER:OG	2:B:621:ARG:N	2.53	0.41
8:H:17:PRO:HB3	8:H:24:CYS:HB3	2.02	0.41
15:O:511:ILE:HG12	15:O:517:VAL:HG11	2.02	0.41
1:A:163:VAL:O	1:A:181:ASP:N	2.53	0.41
1:A:716:ASP:HB2	1:A:789:ASN:ND2	2.35	0.41
1:A:1303:VAL:O	1:A:1306:THR:HG22	2.21	0.41
2:B:497:LEU:HD11	2:B:512:LYS:HD3	2.01	0.41
15:O:580:ASN:O	15:O:584:ASN:ND2	2.53	0.41
18:U:219:GLN:HB3	18:U:222:GLU:HB2	2.02	0.41
1:A:635:PRO:HA	1:A:636:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:GLN:N	1:A:757:ASN:OD1	2.54	0.41
1:A:789:ASN:HD22	1:A:790:ALA:H	1.66	0.41
1:A:951:ASP:O	1:A:1061:ARG:NH2	2.53	0.41
1:A:1161:VAL:HA	1:A:1275:LEU:HD13	2.02	0.41
2:B:580:ARG:NH2	2:B:614:ILE:HD13	2.35	0.41
2:B:961:LEU:HD21	2:B:1019:PHE:O	2.21	0.41
13:M:186:ILE:H	13:M:186:ILE:HG13	1.62	0.41
15:O:327:ARG:NE	15:O:332:GLN:HE22	2.18	0.41
1:A:443:ASN:OD1	1:A:444:LEU:N	2.53	0.41
1:A:1140:ILE:HG22	1:A:1296:GLU:HG3	2.02	0.41
2:B:284:ALA:HA	2:B:287:LEU:HD13	2.02	0.41
2:B:667:VAL:HB	2:B:670:MET:HB2	2.01	0.41
5:E:156:LEU:HD12	5:E:160:GLU:HG2	2.00	0.41
13:M:76:LEU:HD22	14:N:363:ILE:HD12	2.03	0.41
1:A:641:LEU:HD23	1:A:645:MET:HB3	2.02	0.41
2:B:159:ASN:HA	2:B:164:TYR:CG	2.55	0.41
2:B:614:ILE:HA	2:B:672:HIS:HD2	1.86	0.41
3:C:282:TYR:O	3:C:284:GLU:N	2.53	0.41
20:W:496:ALA:HB3	20:W:498:PHE:CE1	2.56	0.41
1:A:850:ASN:ND2	1:A:860:GLU:OE2	2.52	0.41
2:B:710:ILE:HD11	2:B:1026:LYS:HD3	2.02	0.41
13:M:221:ASP:HB2	16:P:115:ASN:HB3	2.03	0.41
15:O:214:LEU:HA	15:O:217:PHE:HE1	1.86	0.41
15:O:635:LEU:HD21	17:Q:52:ARG:HG3	2.02	0.41
1:A:1050:ASP:HA	1:A:1053:LYS:HE2	2.02	0.41
2:B:907:GLU:H	2:B:907:GLU:HG3	1.75	0.41
6:F:115:THR:HG22	6:F:116:ASP:N	2.36	0.41
15:O:56:HIS:HE1	15:O:130:LEU:HD22	1.85	0.41
15:O:268:LYS:O	15:O:269:THR:HG22	2.21	0.41
16:P:33:GLN:NE2	16:P:37:GLN:HB2	2.36	0.41
16:P:293:ILE:HD12	16:P:294:PHE:N	2.36	0.41
18:U:99:PHE:CE2	18:U:101:ALA:HB3	2.56	0.41
19:V:265:THR:O	19:V:286:ARG:NH2	2.54	0.41
1:A:307:ILE:O	15:O:534:ARG:HG2	2.20	0.41
2:B:529:ILE:H	2:B:529:ILE:HG13	1.68	0.41
2:B:542:THR:HG21	13:M:153:VAL:HG11	2.03	0.41
3:C:276:SER:O	3:C:277:ARG:HD2	2.21	0.41
1:A:203:GLU:HG3	15:O:515:LYS:HE2	2.03	0.40
3:C:211:GLY:HA3	3:C:219:PHE:CE2	2.56	0.40
2:B:788:ARG:HD3	2:B:899:LEU:HD21	2.04	0.40
4:D:17:LEU:HD21	4:D:66:LEU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:352:VAL:O	15:O:356:THR:OG1	2.22	0.40
2:B:464:ILE:HD13	2:B:684:VAL:HG23	2.03	0.40
2:B:553:TYR:CE2	2:B:568:PRO:HG3	2.56	0.40
2:B:774:ASN:HB3	2:B:931:MET:HG3	2.04	0.40
3:C:31:TRP:NE1	11:K:123:ASP:OD1	2.55	0.40
4:D:134:LEU:HD13	4:D:137:ILE:HD12	2.03	0.40
8:H:104:PHE:HE1	8:H:114:VAL:HG13	1.86	0.40
8:H:107:VAL:N	8:H:111:LEU:O	2.53	0.40
22:Y:61:DA:H4'	22:Y:62:DG:OP1	2.21	0.40
1:A:1045:ASP:O	1:A:1053:LYS:NZ	2.54	0.40
2:B:523:ASP:N	2:B:523:ASP:OD1	2.54	0.40
7:G:203:ASP:N	7:G:203:ASP:OD1	2.55	0.40
15:O:101:LEU:HD23	15:O:167:GLY:HA2	2.02	0.40
20:W:289:ILE:H	20:W:289:ILE:HD12	1.86	0.40
1:A:559:THR:HG21	2:B:947:HIS:CE1	2.56	0.40
2:B:420:LEU:O	19:V:149:ARG:NH1	2.54	0.40
2:B:548:SER:OG	14:N:389:THR:HB	2.22	0.40
2:B:848:PRO:HG3	2:B:866:TYR:CE1	2.56	0.40
2:B:885:MET:HB3	12:L:57:LEU:HD23	2.03	0.40
15:O:175:LEU:O	15:O:184:LYS:NZ	2.52	0.40
15:O:471:THR:OG1	15:O:472:LYS:N	2.54	0.40
15:O:471:THR:OG1	15:O:475:VAL:O	2.39	0.40
19:V:474:LEU:HD22	19:V:475:LEU:H	1.86	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	1388/1460 (95%)	1211 (87%)	176 (13%)	1 (0%)	51 83
2	B	1112/1149 (97%)	980 (88%)	131 (12%)	1 (0%)	51 83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	333/335 (99%)	296 (89%)	37 (11%)	0	100	100
4	D	113/161 (70%)	100 (88%)	13 (12%)	0	100	100
5	E	212/215 (99%)	191 (90%)	21 (10%)	0	100	100
6	F	81/155 (52%)	72 (89%)	9 (11%)	0	100	100
7	G	174/212 (82%)	152 (87%)	21 (12%)	1 (1%)	25	62
8	H	136/146 (93%)	118 (87%)	18 (13%)	0	100	100
9	I	32/110 (29%)	25 (78%)	7 (22%)	0	100	100
10	J	65/70 (93%)	60 (92%)	5 (8%)	0	100	100
11	K	99/142 (70%)	94 (95%)	5 (5%)	0	100	100
12	L	43/70 (61%)	36 (84%)	7 (16%)	0	100	100
13	M	179/282 (64%)	161 (90%)	18 (10%)	0	100	100
14	N	100/422 (24%)	84 (84%)	16 (16%)	0	100	100
15	O	528/654 (81%)	493 (93%)	35 (7%)	0	100	100
16	P	238/317 (75%)	214 (90%)	24 (10%)	0	100	100
17	Q	33/251 (13%)	29 (88%)	4 (12%)	0	100	100
18	U	178/240 (74%)	163 (92%)	15 (8%)	0	100	100
19	V	331/596 (56%)	302 (91%)	29 (9%)	0	100	100
20	W	214/594 (36%)	194 (91%)	20 (9%)	0	100	100
All	All	5589/7581 (74%)	4975 (89%)	611 (11%)	3 (0%)	54	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	769	ASP
1	A	71	HIS
7	G	79	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1214/1257 (97%)	1194 (98%)	20 (2%)	62	80
2	B	975/1006 (97%)	958 (98%)	17 (2%)	60	79
3	C	296/296 (100%)	294 (99%)	2 (1%)	84	91
4	D	110/145 (76%)	106 (96%)	4 (4%)	35	63
5	E	196/197 (100%)	193 (98%)	3 (2%)	65	81
6	F	73/137 (53%)	72 (99%)	1 (1%)	67	82
7	G	160/190 (84%)	158 (99%)	2 (1%)	69	83
8	H	123/128 (96%)	122 (99%)	1 (1%)	81	89
9	I	31/98 (32%)	31 (100%)	0	100	100
10	J	62/65 (95%)	62 (100%)	0	100	100
11	K	91/130 (70%)	90 (99%)	1 (1%)	73	85
12	L	40/57 (70%)	40 (100%)	0	100	100
13	M	160/249 (64%)	154 (96%)	6 (4%)	33	61
14	N	88/360 (24%)	86 (98%)	2 (2%)	50	71
15	O	490/593 (83%)	479 (98%)	11 (2%)	52	72
16	P	227/285 (80%)	222 (98%)	5 (2%)	52	72
17	Q	31/212 (15%)	31 (100%)	0	100	100
18	U	152/205 (74%)	147 (97%)	5 (3%)	38	64
19	V	295/513 (58%)	289 (98%)	6 (2%)	55	74
20	W	194/534 (36%)	189 (97%)	5 (3%)	46	69
All	All	5008/6657 (75%)	4917 (98%)	91 (2%)	61	77

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	ARG
1	A	137	ARG
1	A	213	ARG
1	A	274	MET
1	A	310	ASN
1	A	367	ASN
1	A	410	ARG
1	A	436	ARG
1	A	499	ARG
1	A	774	ARG
1	A	783	ASN

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Mol	Chain	Res	Type
1	A	789	ASN
1	A	848	VAL
1	A	904	VAL
1	A	933	VAL
1	A	944	ASN
1	A	1187	ARG
1	A	1215	LEU
1	A	1332	ARG
1	A	1439	LYS
2	B	66	ASN
2	B	314	ARG
2	B	383	LEU
2	B	481	ARG
2	B	780	ARG
2	B	816	ASP
2	B	859	ASN
2	B	867	ARG
2	B	874	ARG
2	B	885	MET
2	B	908	LEU
2	B	970	ASN
2	B	1004	LEU
2	B	1038	ARG
2	B	1054	ARG
2	B	1135	MET
2	B	1136	ASN
3	C	174	ARG
3	C	277	ARG
4	D	71	ASN
4	D	98	MET
4	D	120	LYS
4	D	130	ASN
5	E	58	MET
5	E	93	MET
5	E	215	MET
6	F	90	ARG
7	G	73	ARG
7	G	113	ASN
8	H	141	TYR
11	K	74	ASN
13	M	78	ILE
13	M	111	ARG

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Mol	Chain	Res	Type
13	M	144	ASN
13	M	166	MET
13	M	203	ASN
13	M	220	ASN
14	N	297	MET
14	N	300	LYS
15	O	60	ARG
15	O	73	ARG
15	O	98	LEU
15	O	205	LYS
15	O	243	MET
15	O	268	LYS
15	O	286	ARG
15	O	484	MET
15	O	580	ASN
15	O	631	ASN
15	O	636	ASN
16	P	83	LYS
16	P	189	ASN
16	P	239	ASN
16	P	271	MET
16	P	298	LYS
18	U	104	MET
18	U	110	LYS
18	U	141	ARG
18	U	159	ASN
18	U	239	LYS
19	V	115	ASN
19	V	183	GLN
19	V	237	LEU
19	V	269	LYS
19	V	286	ARG
19	V	481	LYS
20	W	292	ASN
20	W	413	ARG
20	W	451	ARG
20	W	521	ASN
20	W	532	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	310	ASN
1	A	367	ASN
1	A	437	ASN
1	A	477	GLN
1	A	520	HIS
1	A	578	GLN
1	A	630	ASN
1	A	688	GLN
1	A	760	GLN
1	A	783	ASN
1	A	789	ASN
1	A	808	GLN
1	A	815	GLN
1	A	834	HIS
1	A	1058	GLN
1	A	1318	HIS
1	A	1346	HIS
1	A	1354	HIS
1	A	1419	GLN
2	B	66	ASN
2	B	81	GLN
2	B	203	ASN
2	B	270	GLN
2	B	382	GLN
2	B	577	HIS
2	B	600	HIS
2	B	655	ASN
2	B	859	ASN
2	B	893	GLN
2	B	1136	ASN
3	C	175	GLN
3	C	207	HIS
3	C	296	ASN
3	C	297	HIS
4	D	71	ASN
4	D	130	ASN
5	E	3	GLN
5	E	174	GLN
7	G	113	ASN
8	H	139	ASN
10	J	26	GLN
11	K	74	ASN
12	L	53	HIS

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Mol	Chain	Res	Type
13	M	92	ASN
13	M	128	GLN
13	M	144	ASN
13	M	203	ASN
13	M	220	ASN
14	N	298	ASN
15	O	152	HIS
15	O	161	GLN
15	O	225	ASN
15	O	332	GLN
15	O	523	ASN
15	O	549	GLN
15	O	572	HIS
15	O	580	ASN
15	O	631	ASN
15	O	636	ASN
16	P	14	ASN
16	P	119	HIS
16	P	189	ASN
16	P	239	ASN
18	U	68	GLN
18	U	91	ASN
18	U	159	ASN
19	V	6	ASN
19	V	20	ASN
19	V	35	ASN
19	V	115	ASN
19	V	140	HIS
19	V	249	HIS
19	V	473	HIS
20	W	292	ASN
20	W	506	GLN
20	W	521	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

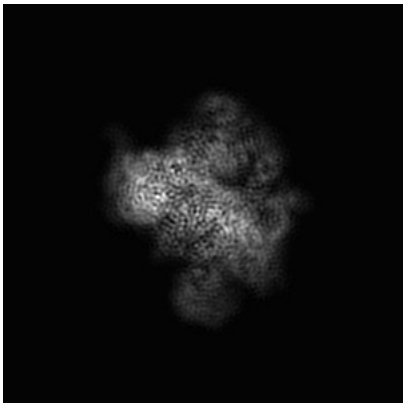
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4180. These allow visual inspection of the internal detail of the map and identification of artifacts.

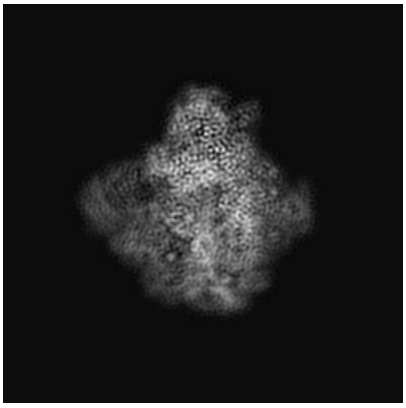
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

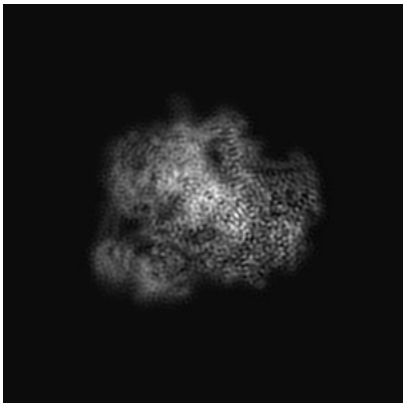
6.1.1 Primary map



X



Y

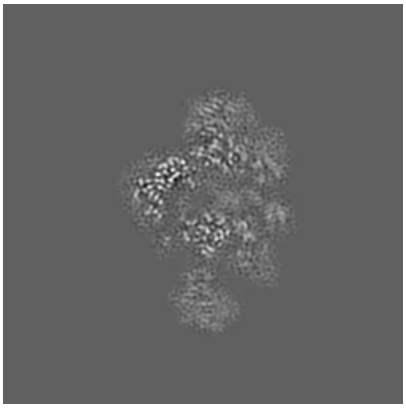


Z

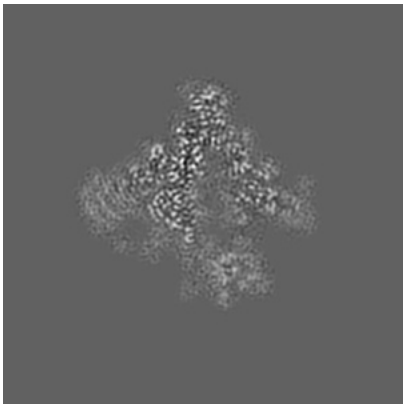
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

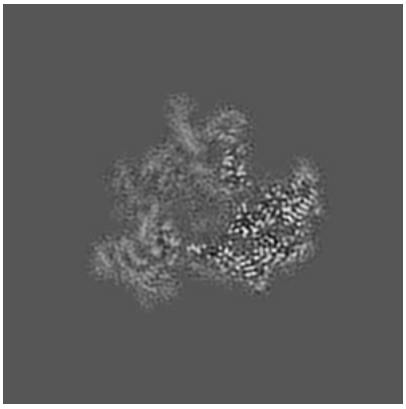
6.2.1 Primary map



X Index: 120



Y Index: 120

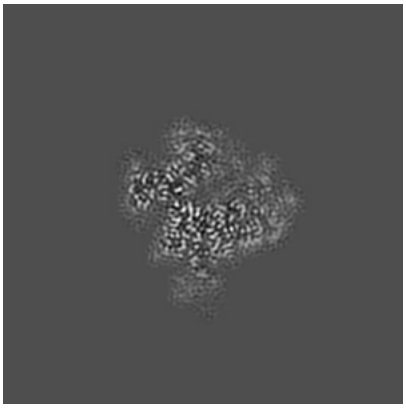


Z Index: 120

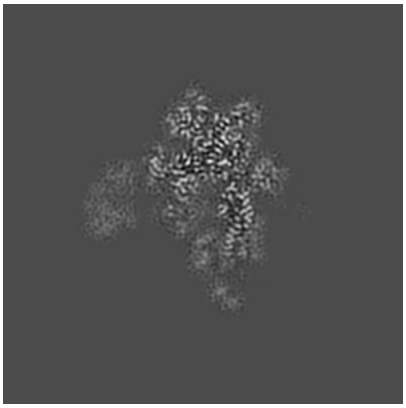
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

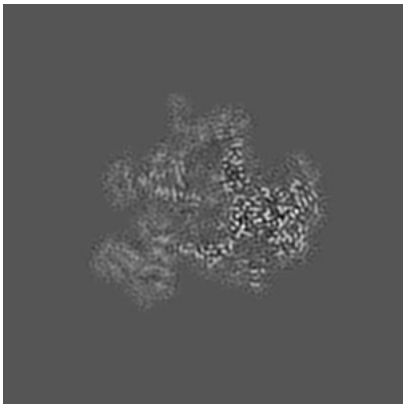
6.3.1 Primary map



X Index: 140



Y Index: 107



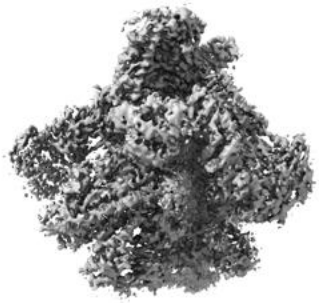
Z Index: 116

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 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

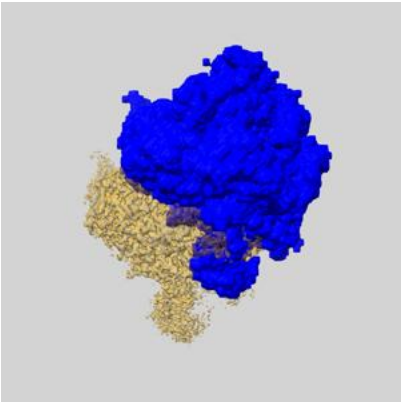
6.5 Mask visualisation (i)

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

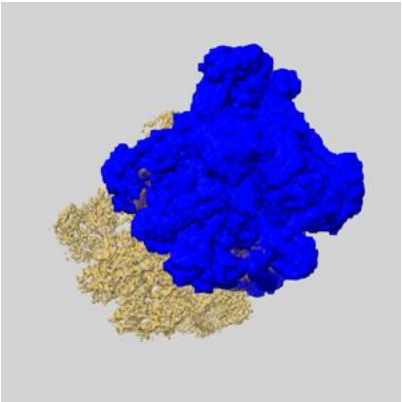
A mask typically either:

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

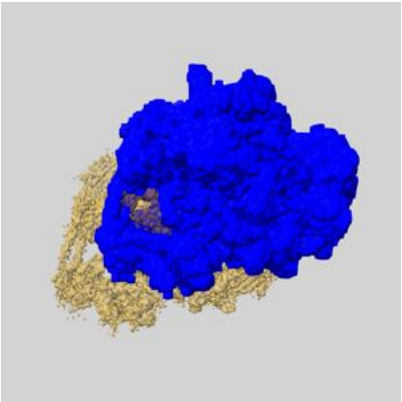
6.5.1 emd_4180_msk_1.map (i)



X



Y

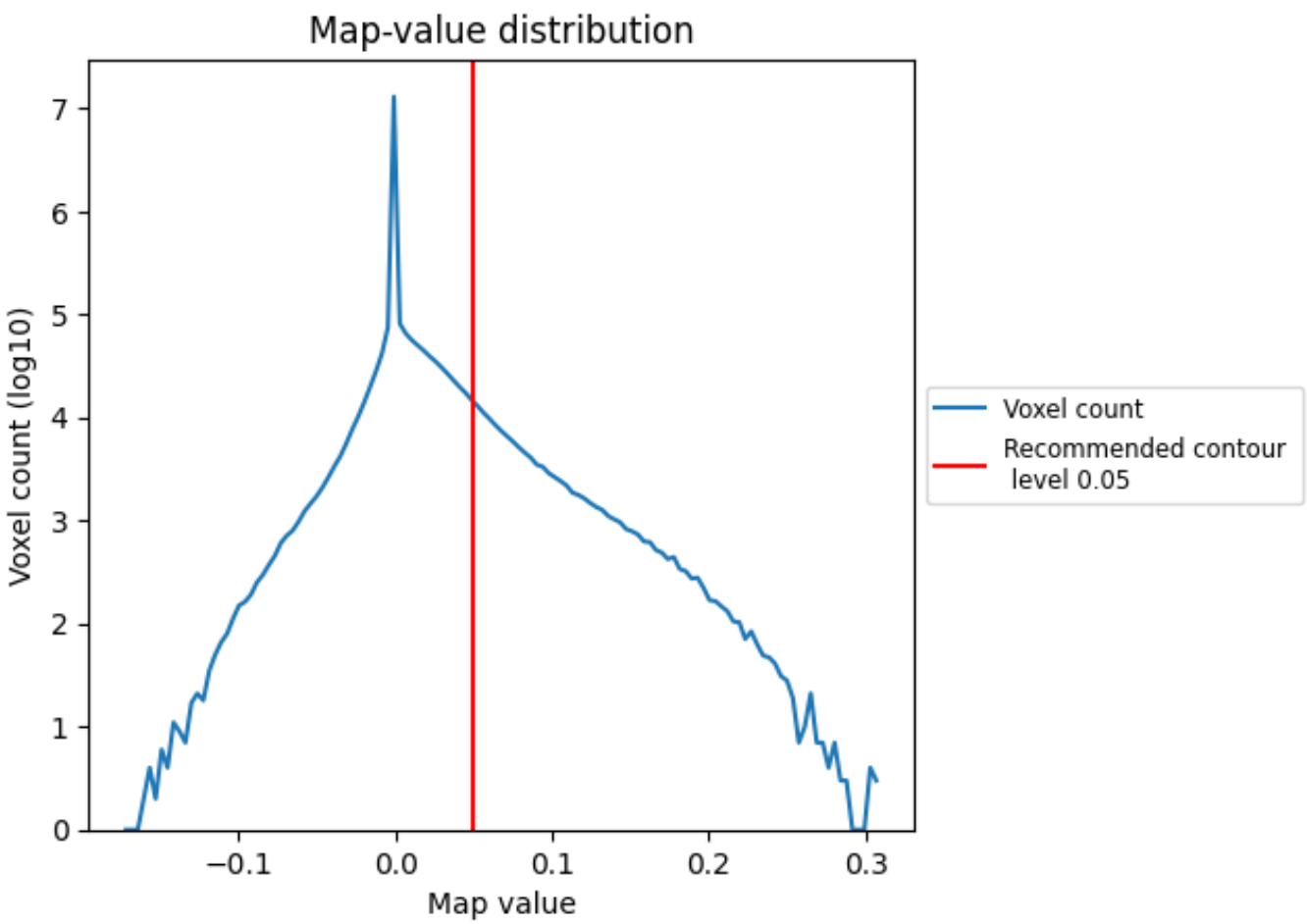


Z

7 Map analysis (i)

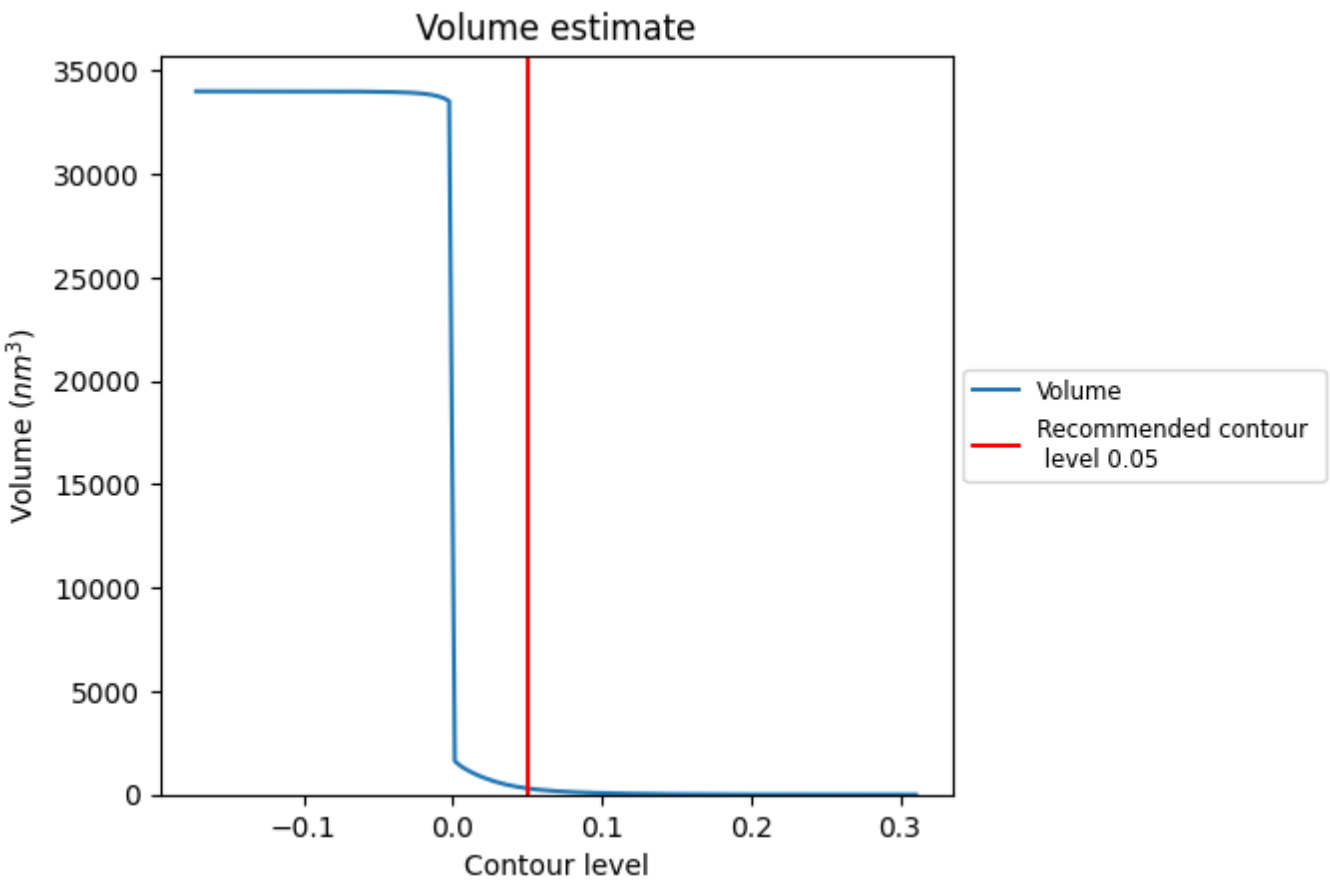
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

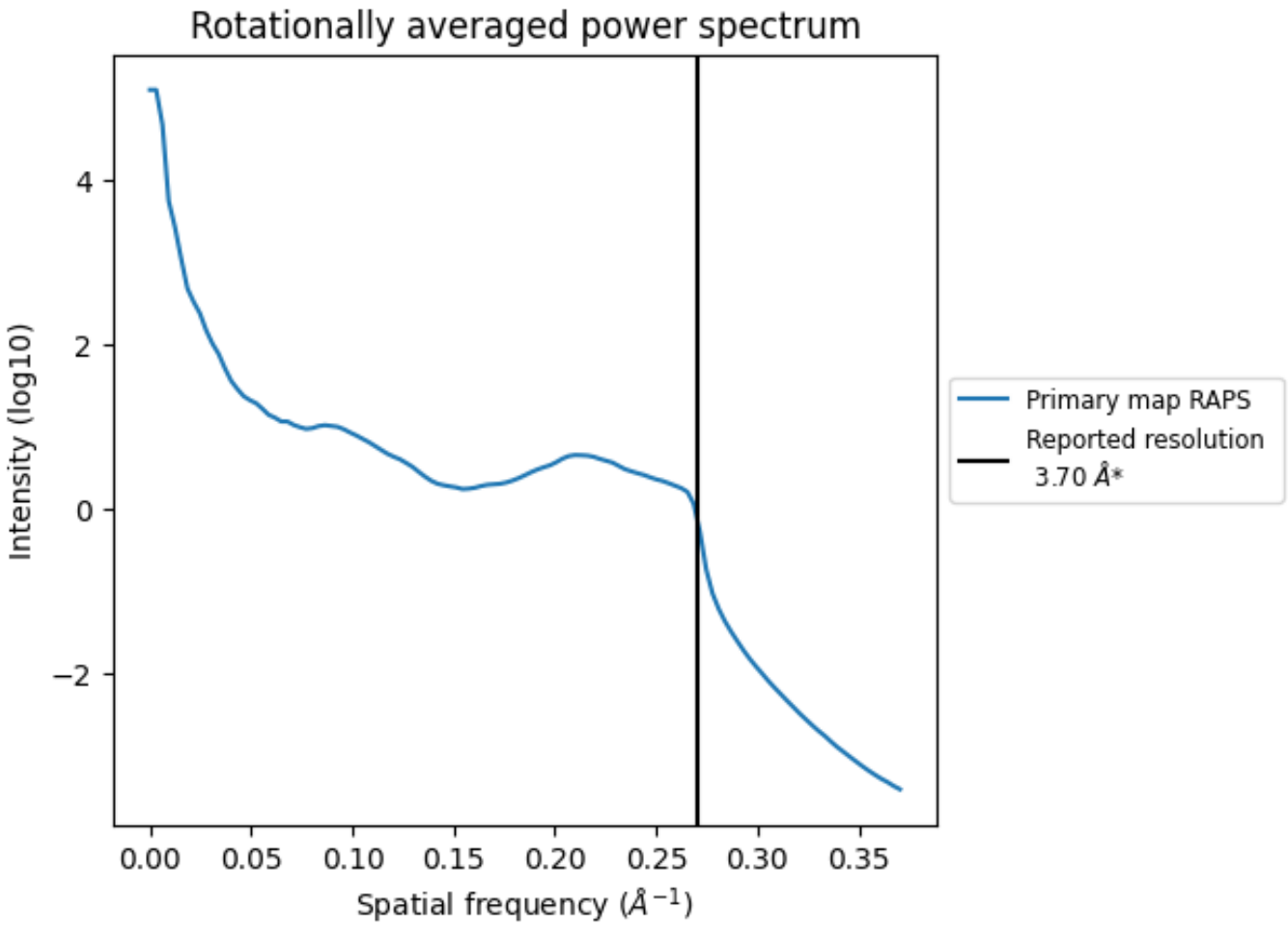
7.2 Volume estimate (i)



The volume at the recommended contour level is 301 nm^3; this corresponds to an approximate mass of 272 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)

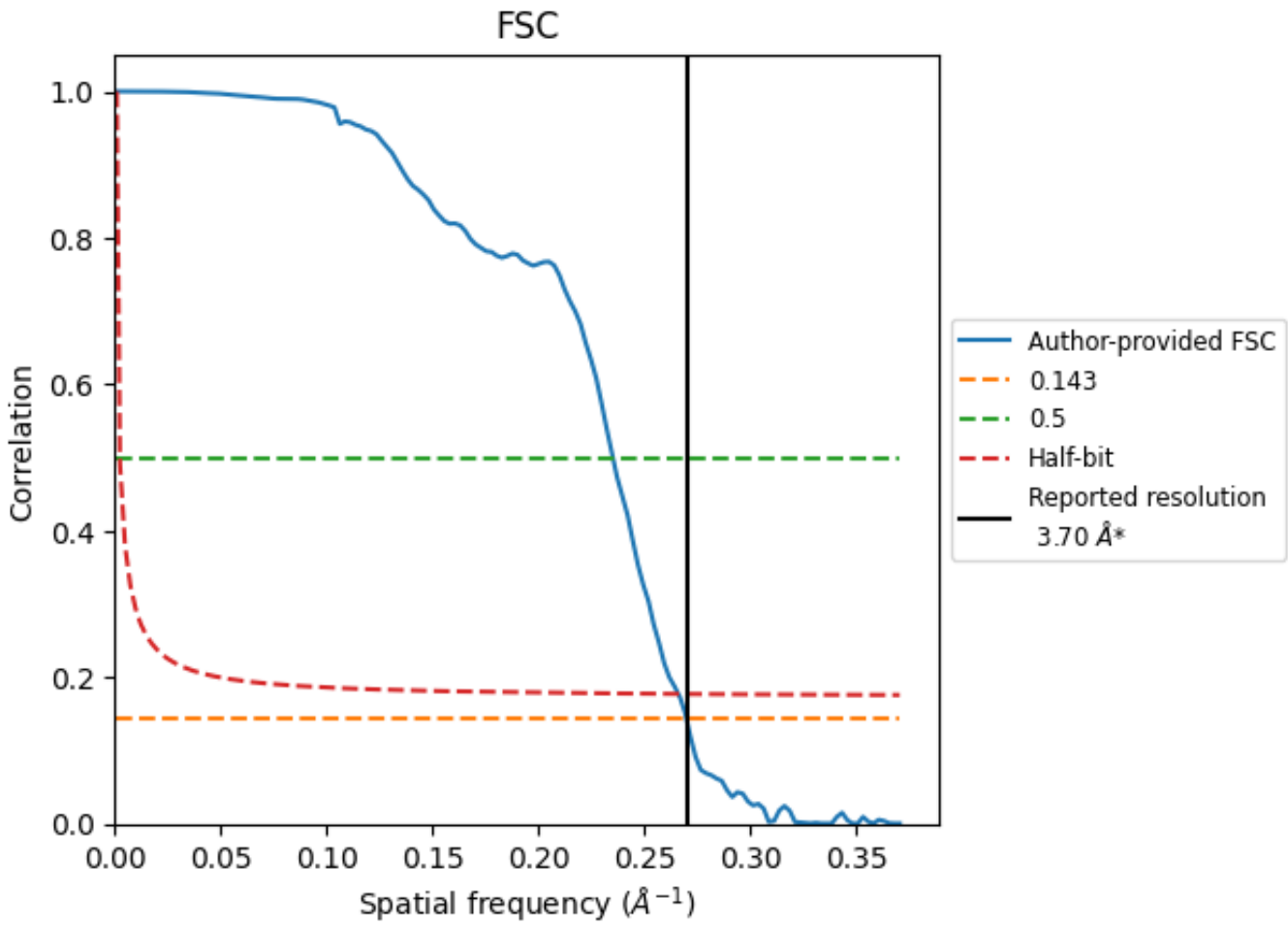


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates (i)

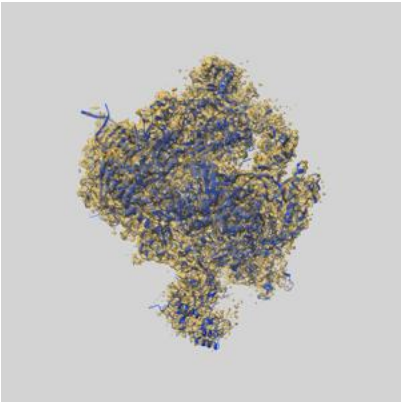
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.71	4.26	3.76
Unmasked-calculated*	-	-	-

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

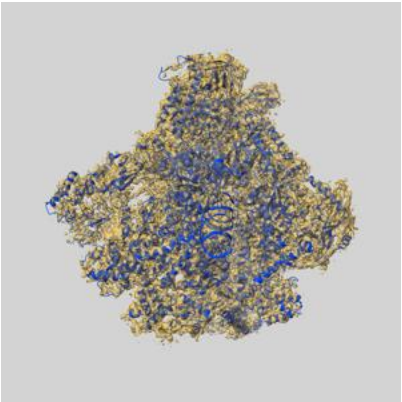
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4180 and PDB model 6F40. Per-residue inclusion information can be found in section 3 on page 8.

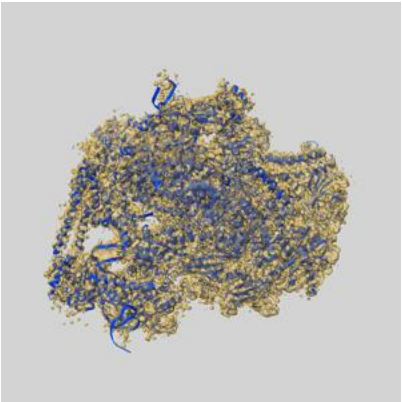
9.1 Map-model overlay (i)



X



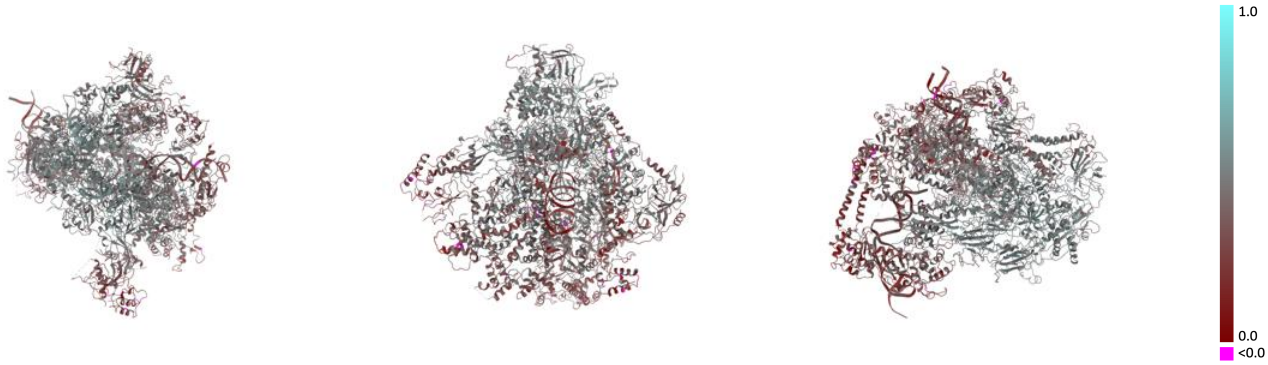
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

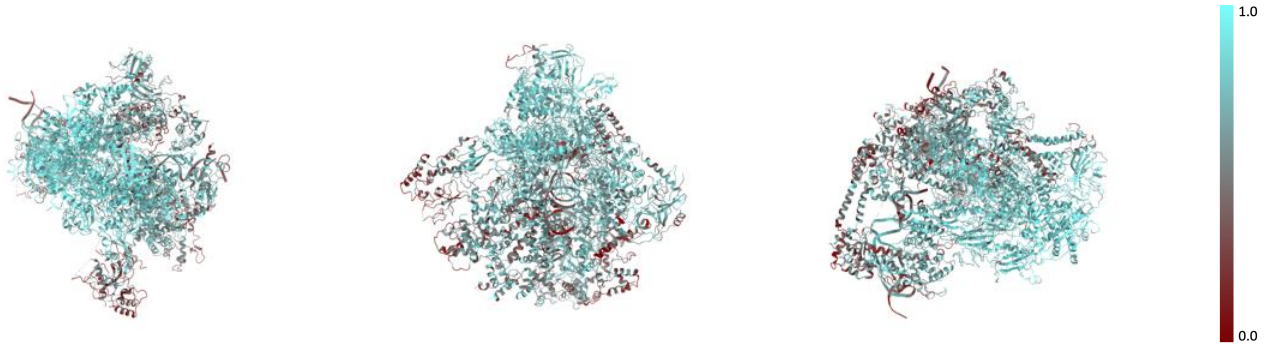
9.2 Q-score mapped to coordinate model (i)



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.

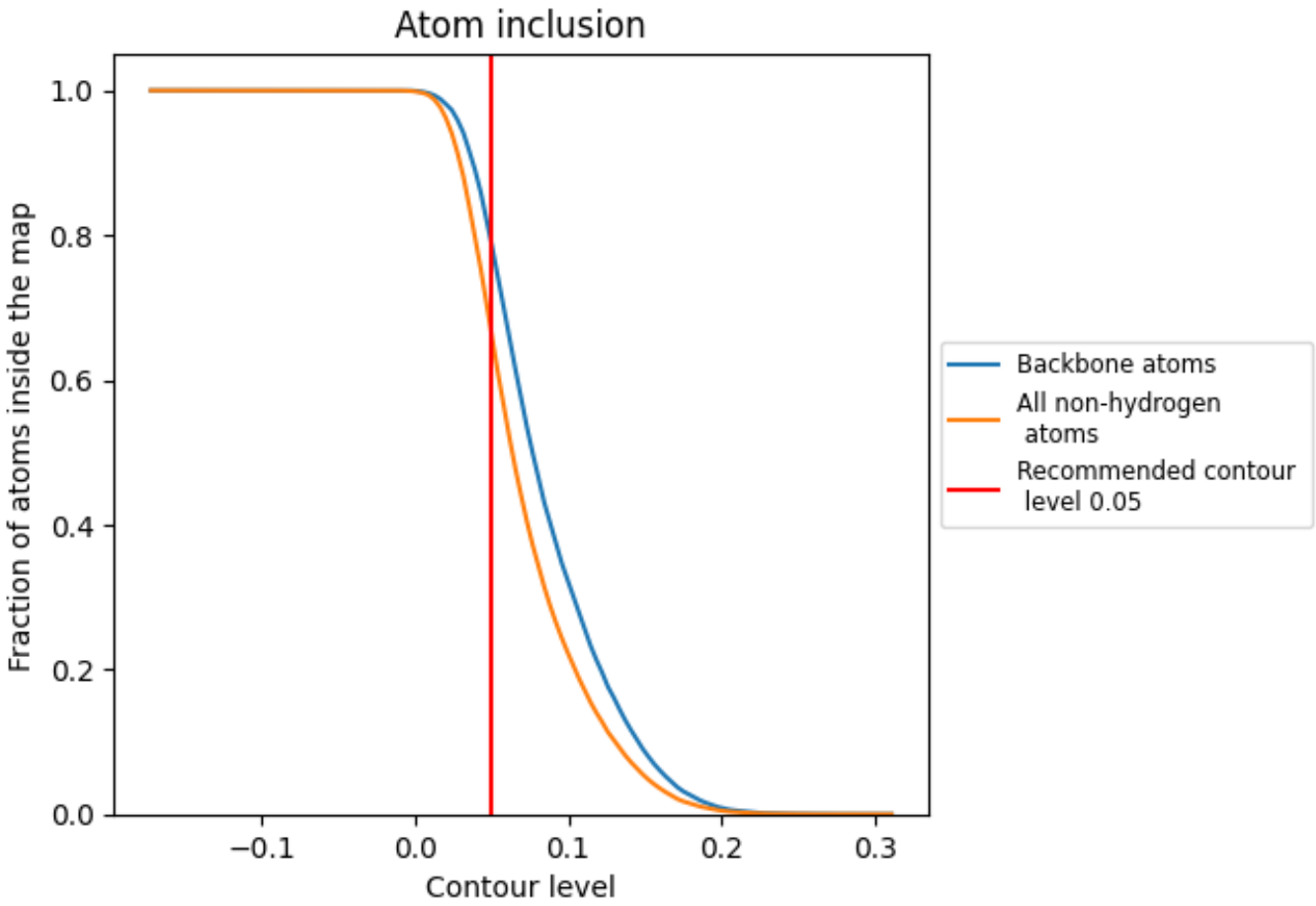
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6633	0.4120
A	0.7108	0.4550
B	0.7771	0.4790
C	0.8455	0.4900
D	0.3230	0.2780
E	0.6575	0.3930
F	0.8377	0.4850
G	0.4618	0.3390
H	0.7848	0.4680
I	0.6548	0.3580
J	0.8521	0.5140
K	0.8378	0.4940
L	0.7890	0.4700
M	0.5456	0.3720
N	0.5947	0.3700
O	0.5407	0.3720
P	0.5779	0.3300
Q	0.6926	0.3880
U	0.5288	0.3050
V	0.5991	0.3650
W	0.4503	0.3050
X	0.5356	0.2480
Y	0.5895	0.2780