



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 10:35 pm GMT

PDB ID : 6F44
EMDB ID : EMD-4183
Title : RNA Polymerase III closed complex CC2.
Authors : Vorlaender, M.K.; Khatter, H.; Wetzels, R.; Hagen, W.J.H.; Mueller, C.W.
Deposited on : 2017-11-29
Resolution : 4.20 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.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

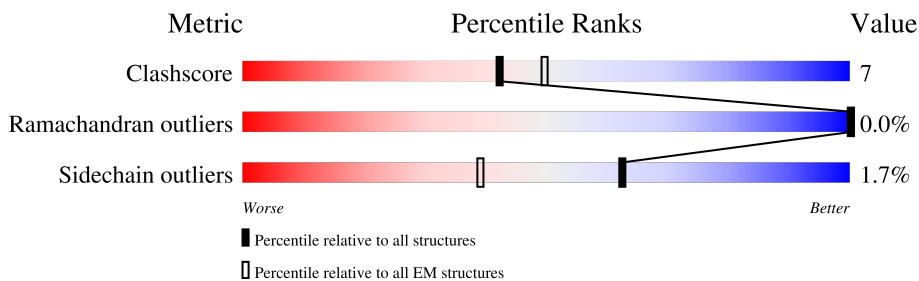
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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 $\leq 5\%$. 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	
2	B	1149	
3	C	335	
4	D	161	
5	E	215	
6	F	155	
7	G	212	
8	H	146	

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Mol	Chain	Length	Quality of chain
9	I	110	
10	J	70	
11	K	142	
12	L	70	
13	M	282	
14	N	422	
15	O	654	
16	P	317	
17	Q	251	
18	U	240	
19	V	596	
20	W	594	
21	X	81	
22	Y	81	

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 45251 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	1399	10974	6919	1936	2061	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	8784	5555	1516	1653	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	Total	C	N	O	S	0	0
			1448	950	231	261	6		

- 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	Total	C	N	O	S	0	0
			1120	703	188	224	5		

- 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	Total	C	N	O	S	0	0
			255	161	39	49	6		

- 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	Total	C	N	O	S	0	0
			549	350	95	98	6		

- 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	Total	C	N	O	S	0	0
			792	496	130	161	5		

- 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	Total	C	N	O	S	0	0
			358	221	71	62	4		

- 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	171	Total	C	N	O	S	0	0
			1387	886	239	261	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	201	PRO	ASN	conflict	UNP P36121

- 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	4290	2732	736	804	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	99	827	538	127	158	4	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	2674	1675	483	502	14	0	0

- Molecule 20 is a protein called Transcription factor TFIIB component B”.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	172	Total	C	N	O	S	0	0
			1442	920	256	259	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	44	Total	C	N	O	P	0	0
			896	433	149	270	44		

- Molecule 22 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	44	Total	C	N	O	P	0	0
			908	435	171	258	44		

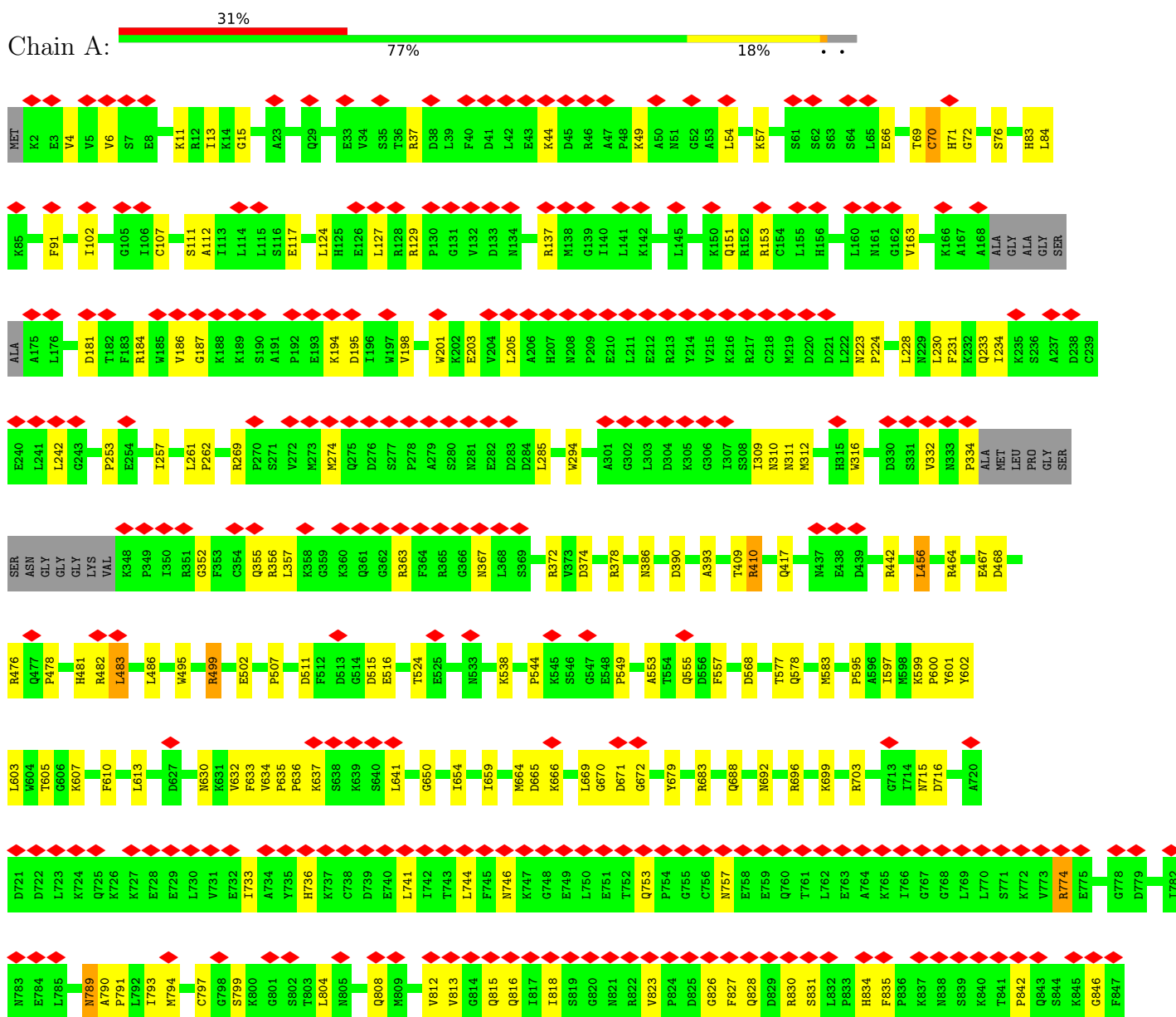
- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

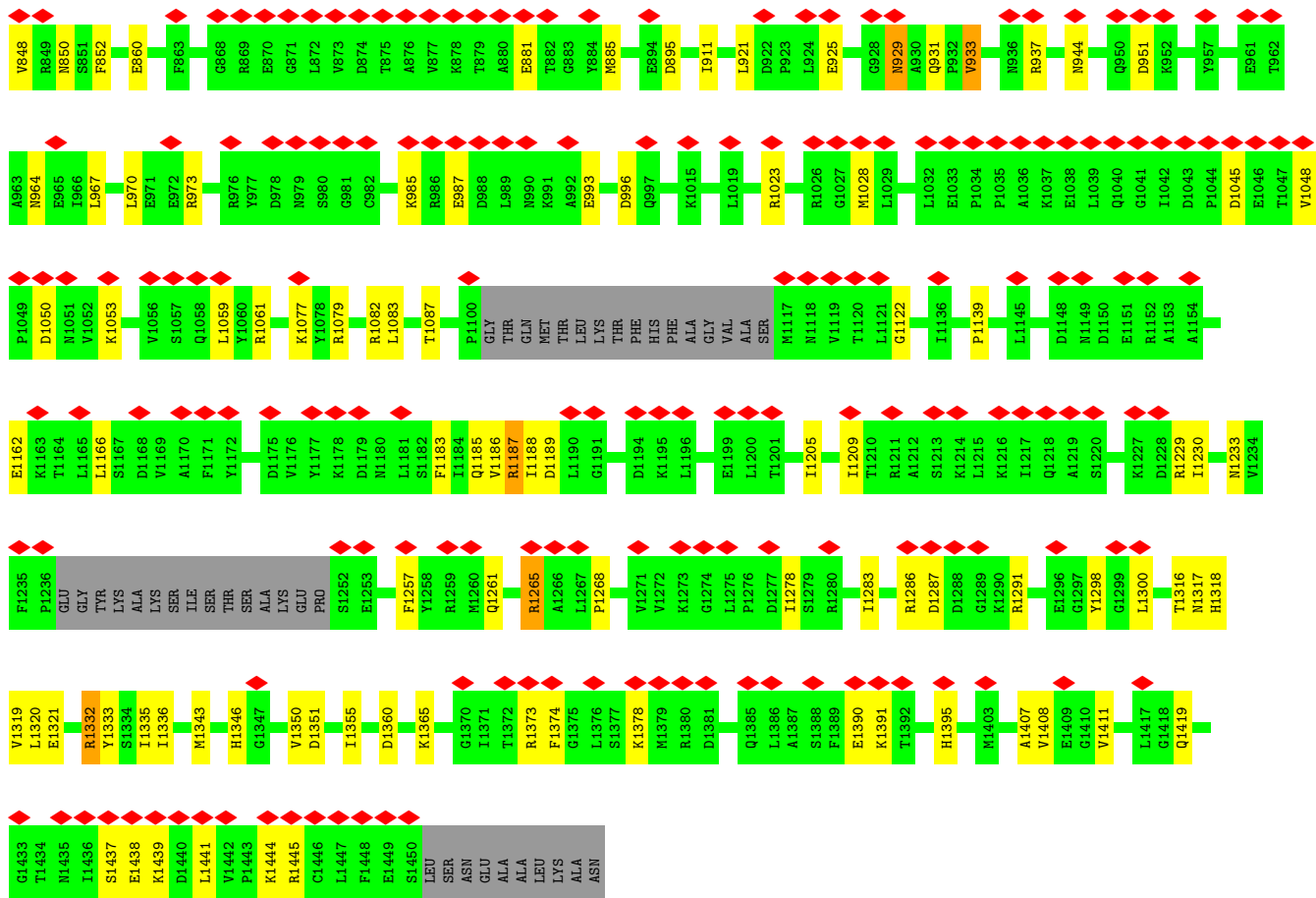
Mol	Chain	Residues	Atoms		AltConf
23	A	2	Total	Zn	0
			2	2	
23	B	1	Total	Zn	0
			1	1	
23	I	1	Total	Zn	0
			1	1	
23	J	1	Total	Zn	0
			1	1	
23	L	1	Total	Zn	0
			1	1	
23	V	1	Total	Zn	0
			1	1	

3 Residue-property plots

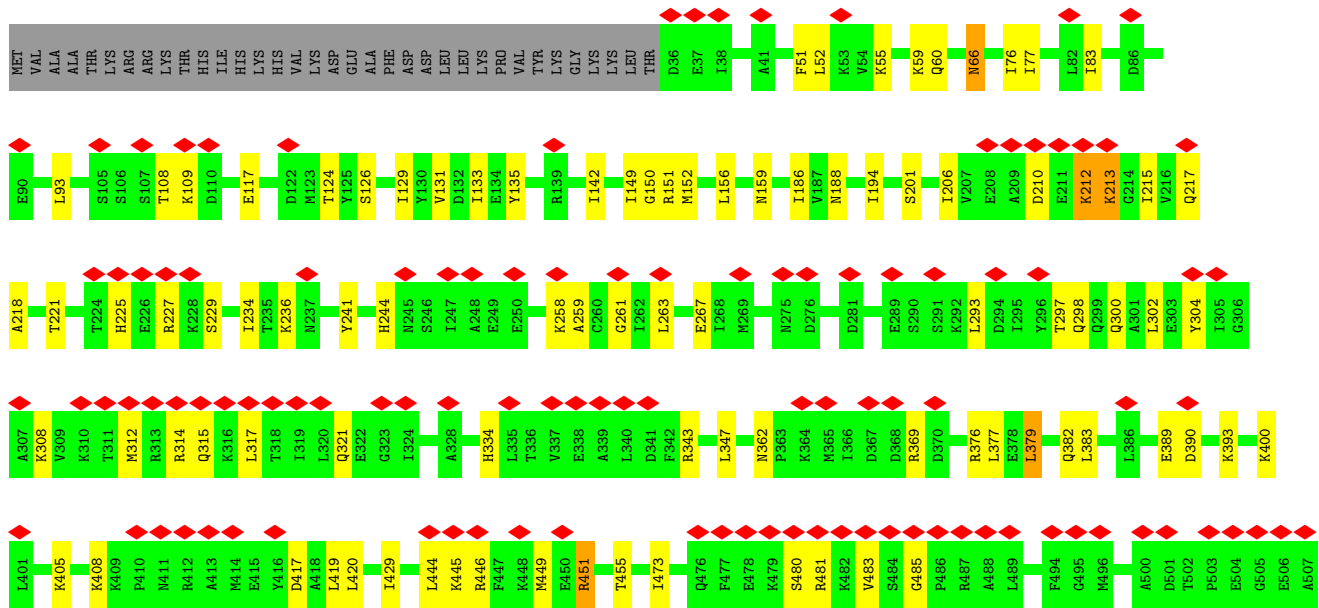
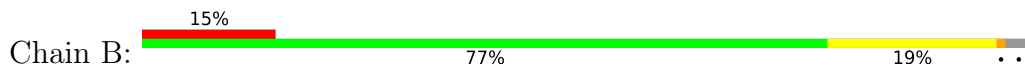
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

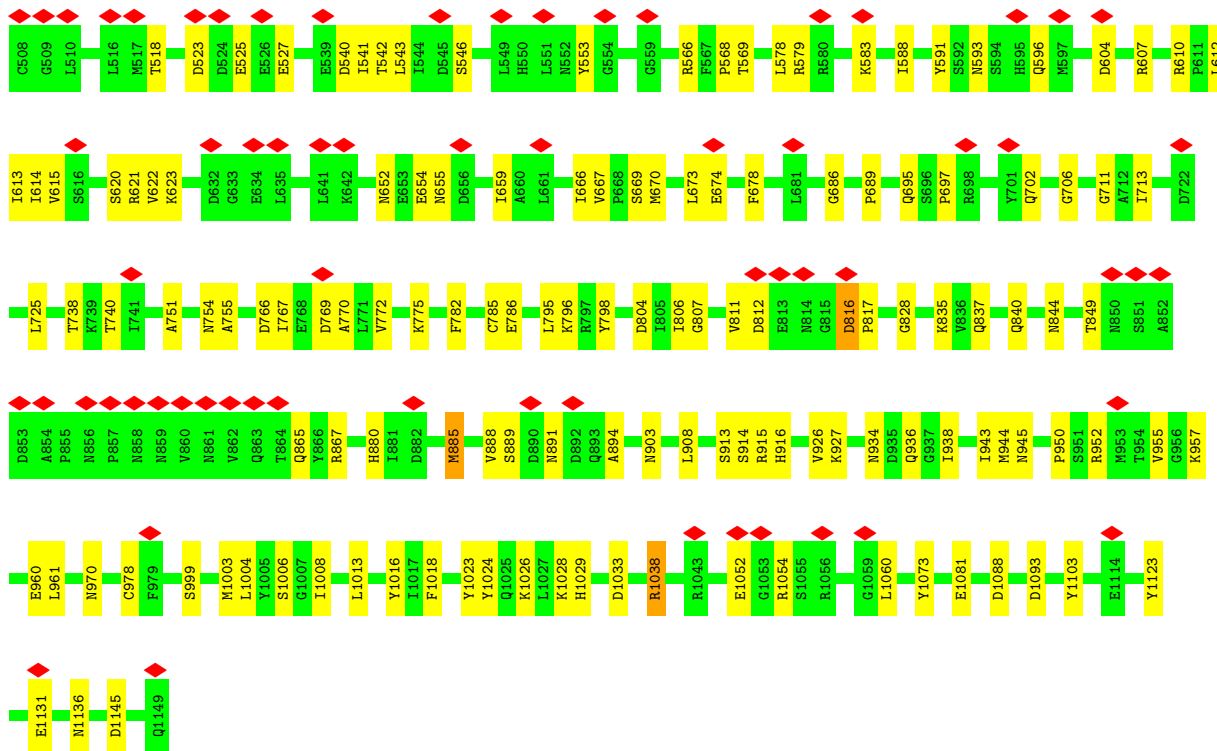
- Molecule 1: DNA-directed RNA polymerase III subunit RPC1



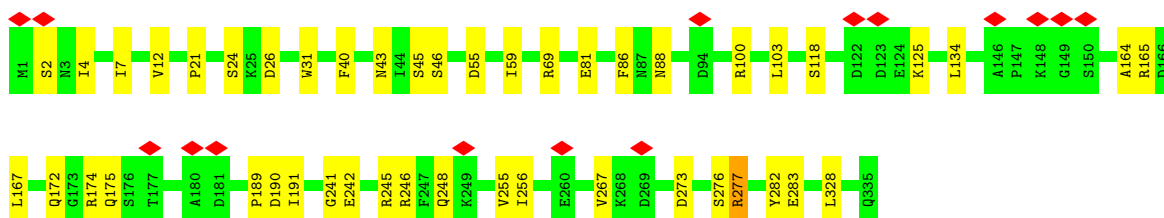
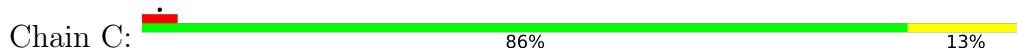


• Molecule 2: DNA-directed RNA polymerase III subunit RPC2

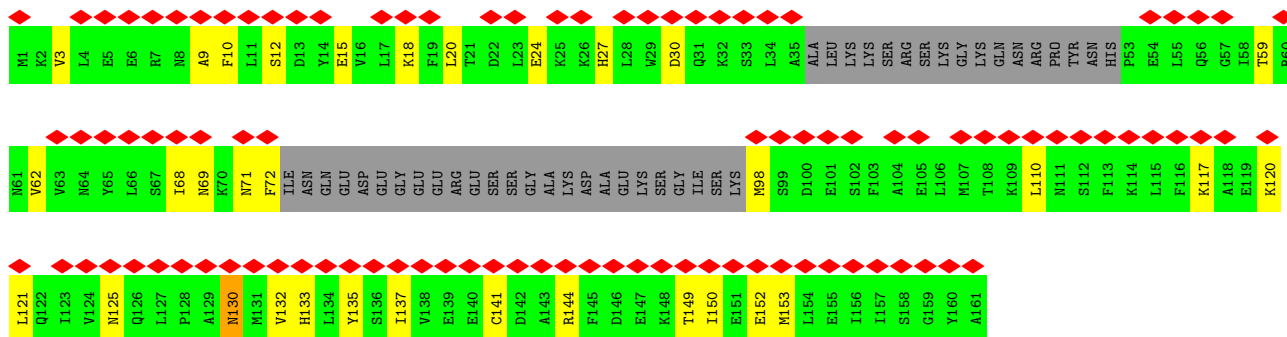




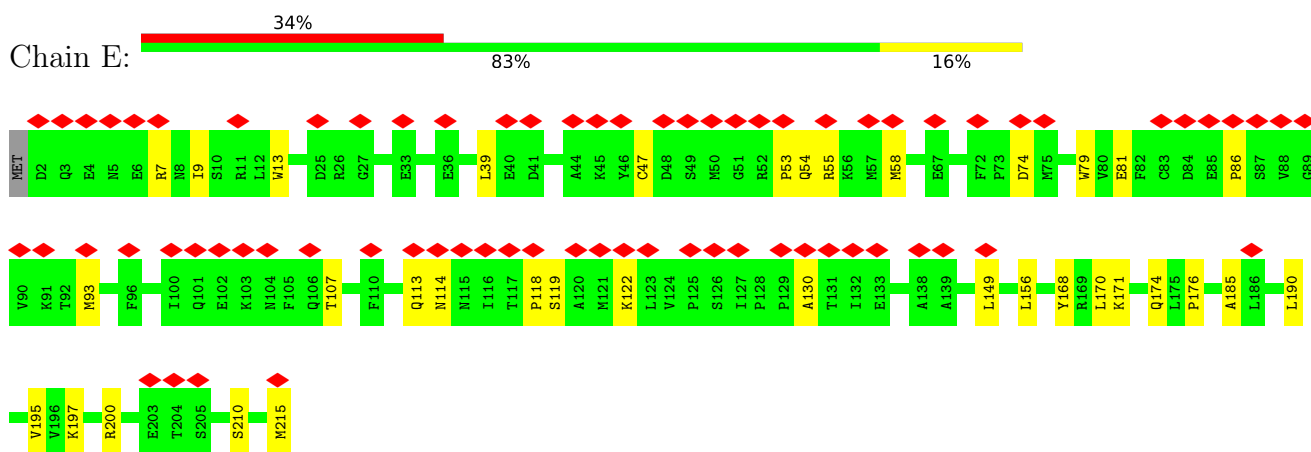
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



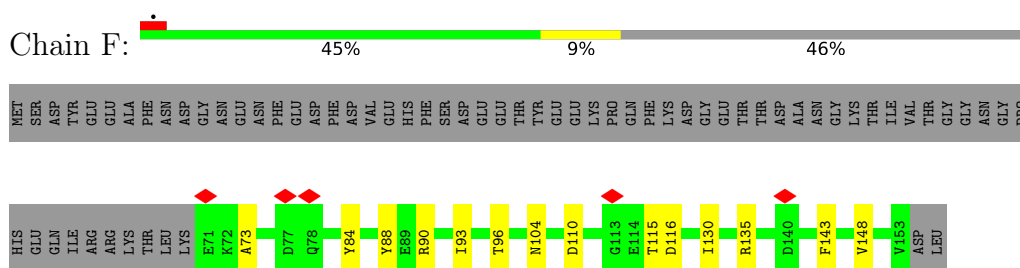
• Molecule 4: DNA-directed RNA polymerase III subunit RPC9



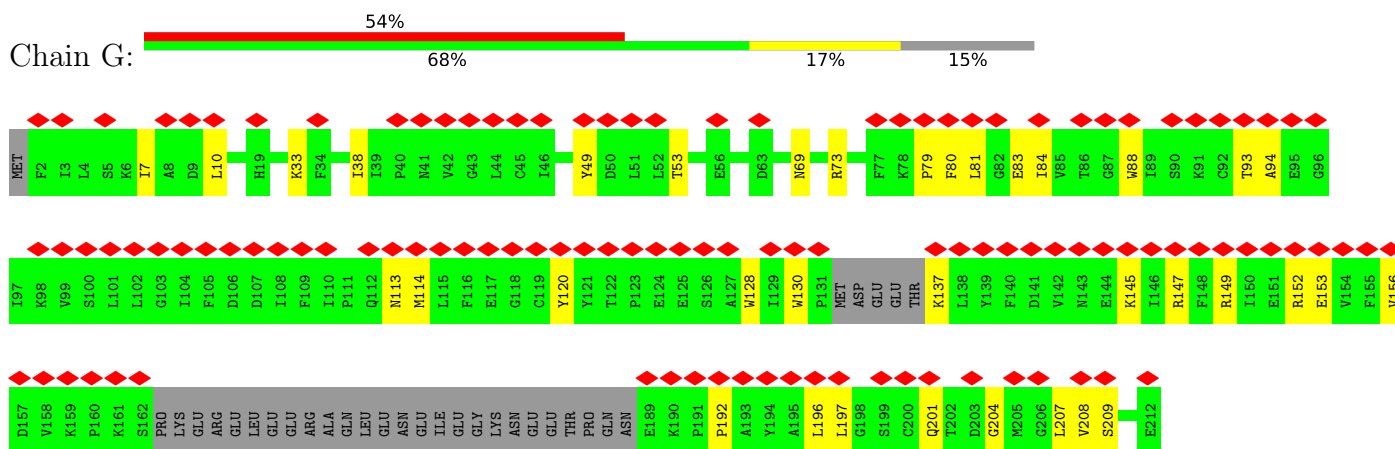
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



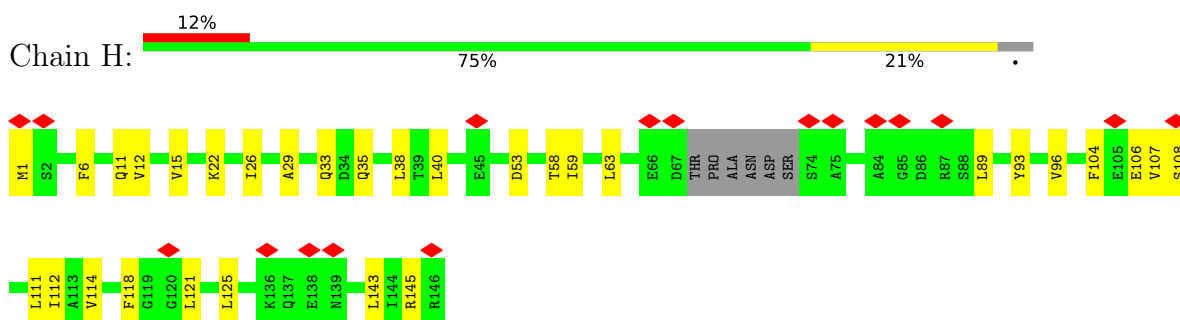
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



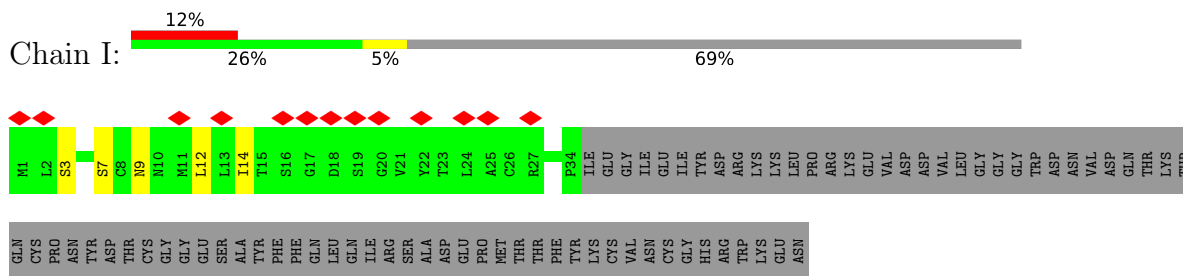
- Molecule 7: DNA-directed RNA polymerase III subunit RPC8



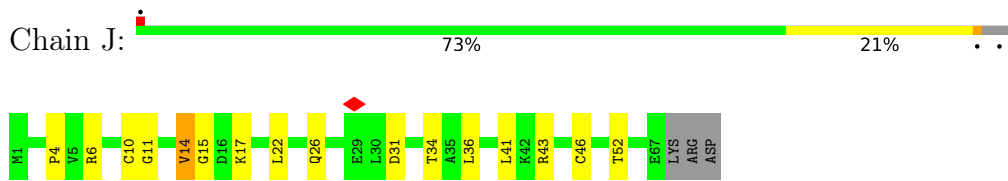
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



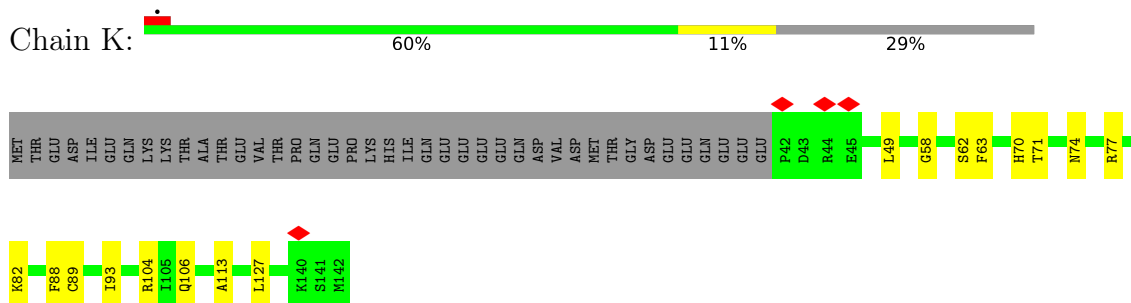
- Molecule 9: DNA-directed RNA polymerase III subunit RPC10



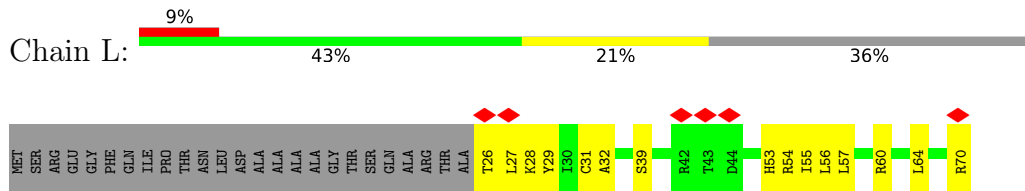
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



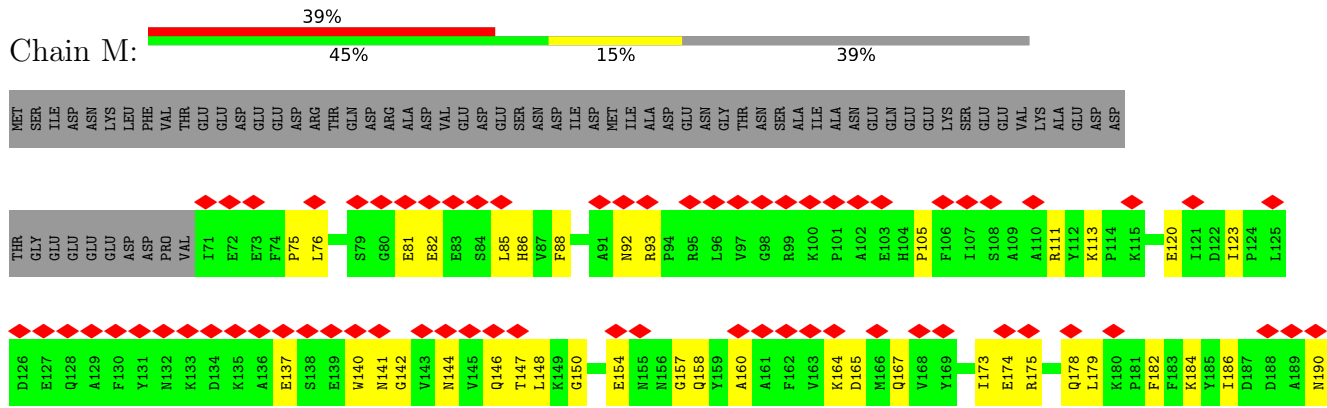
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

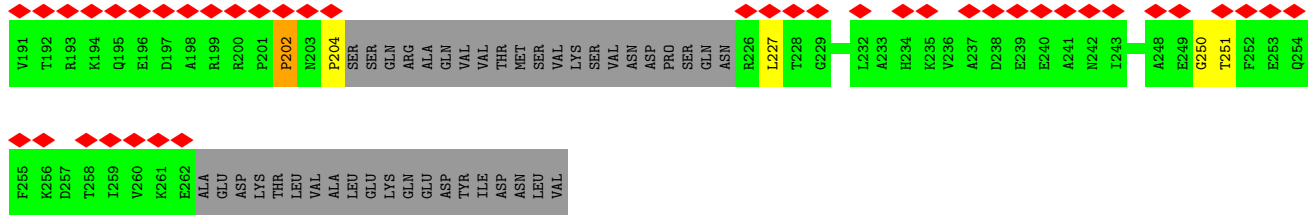


- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

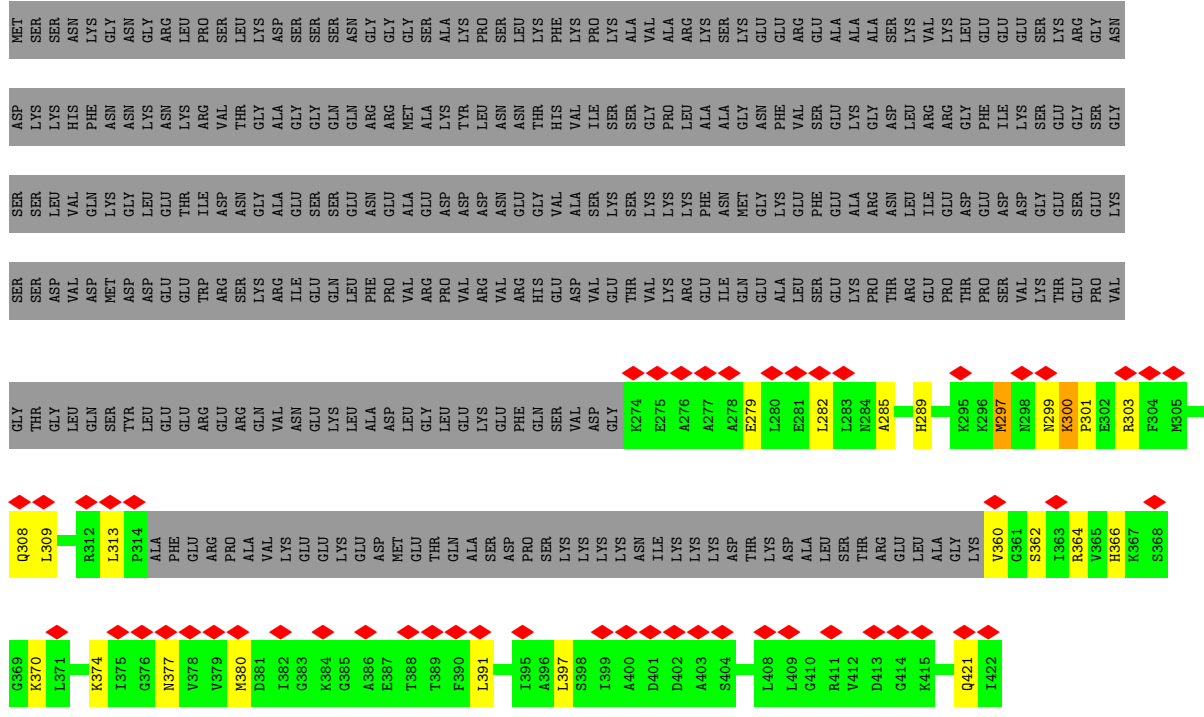


- Molecule 13: DNA-directed RNA polymerase III subunit RPC5

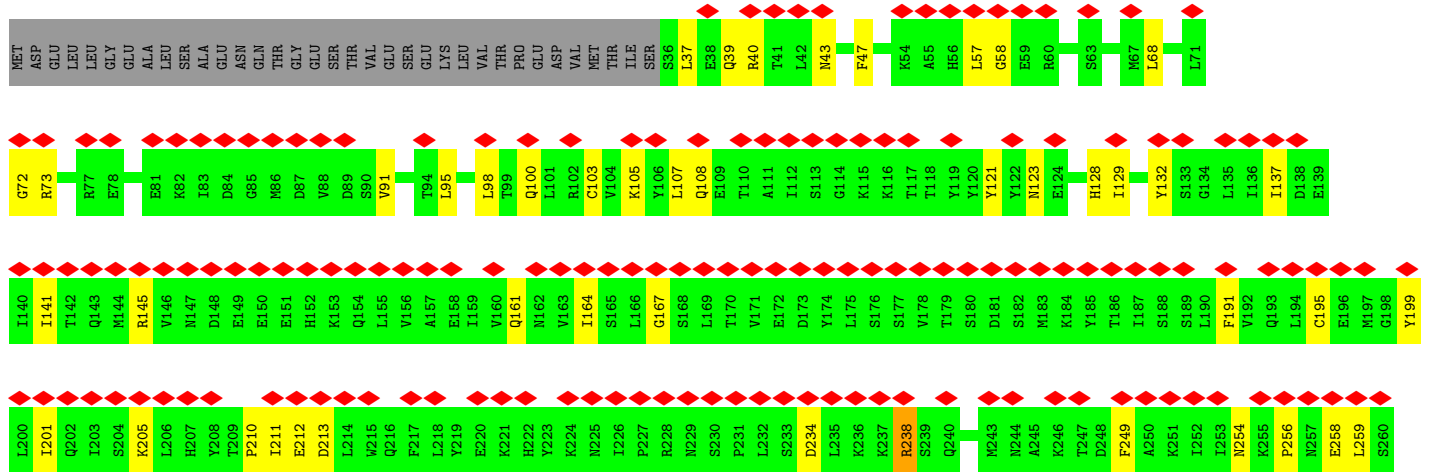


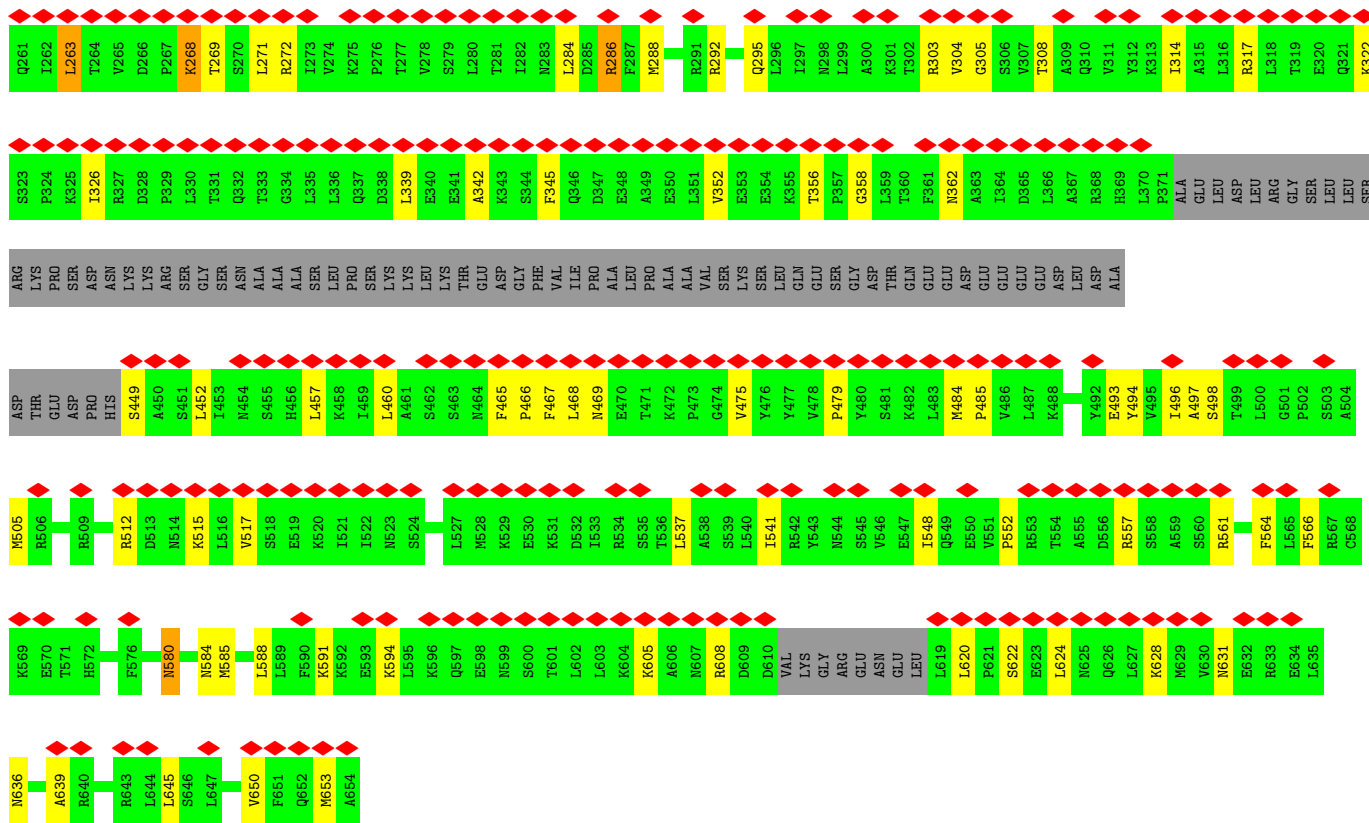


• Molecule 14: DNA-directed RNA polymerase III subunit RPC4

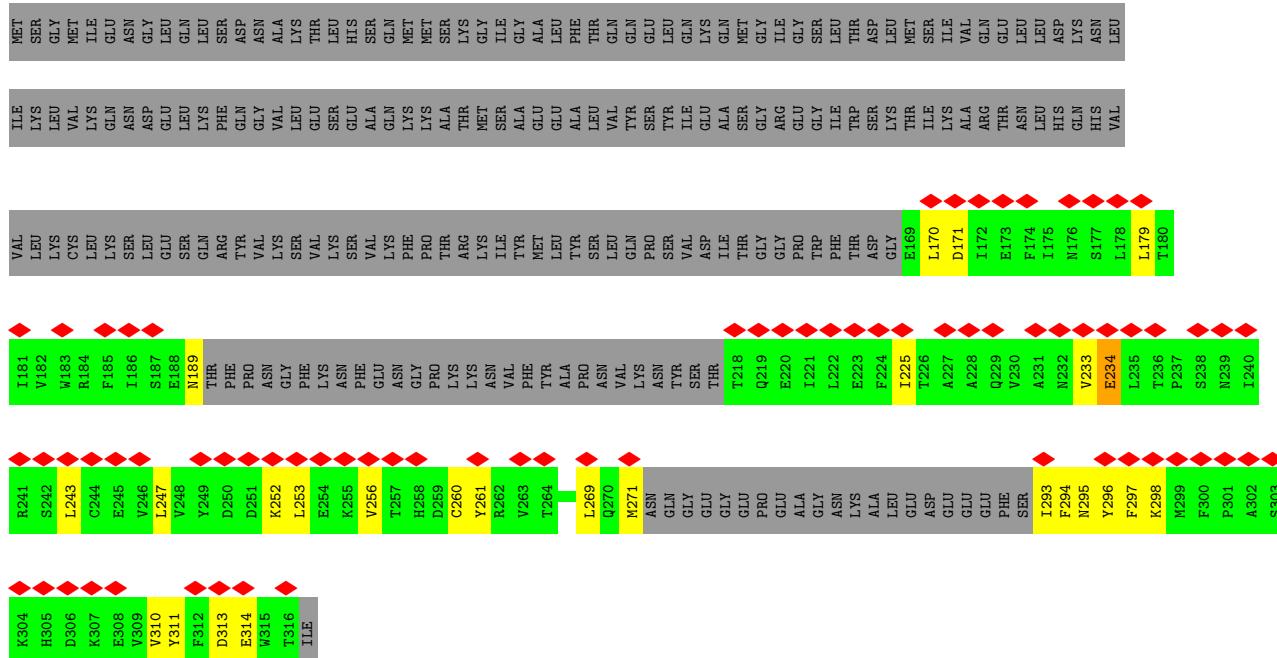


• Molecule 15: DNA-directed RNA polymerase III subunit RPC3

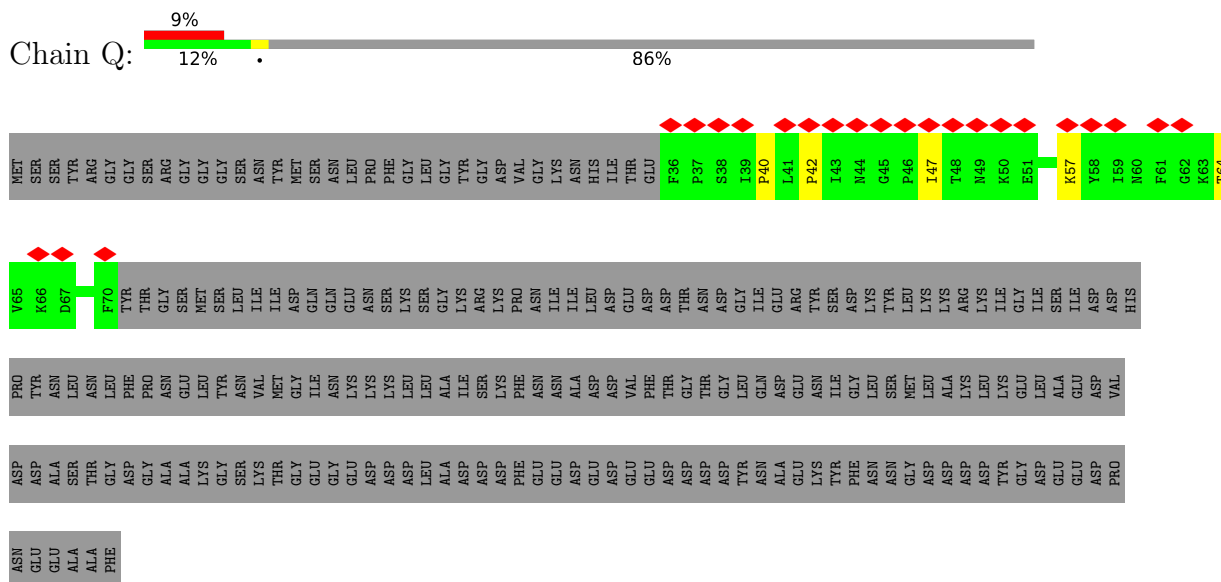




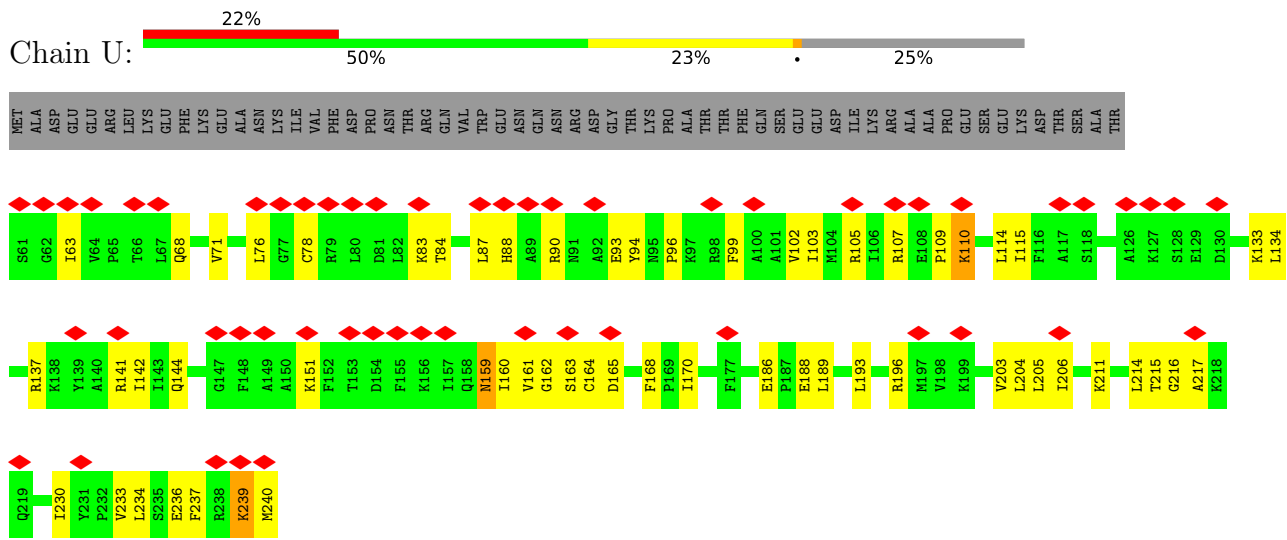
• Molecule 16: DNA-directed RNA polymerase III subunit RPC6



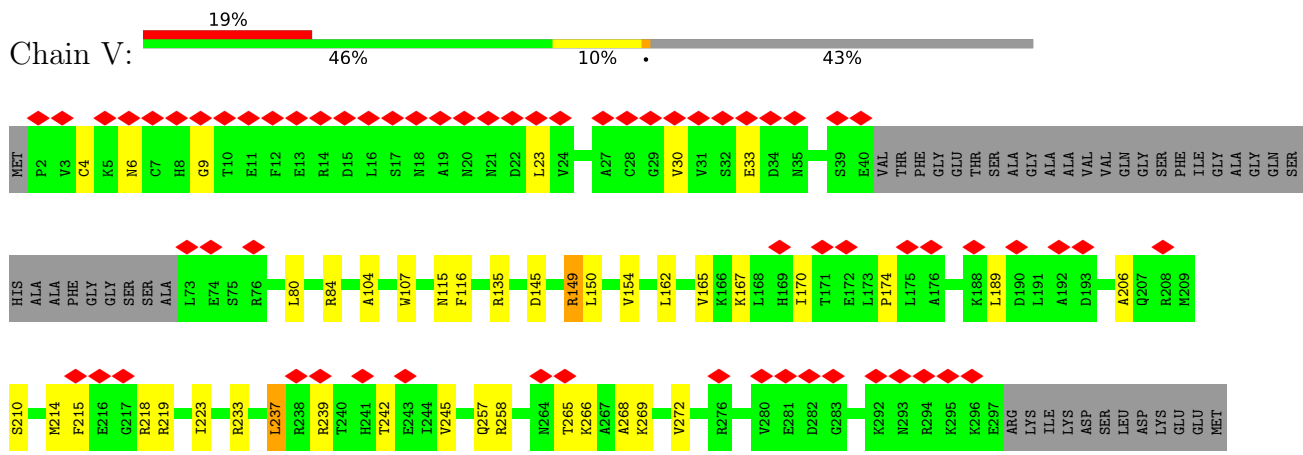
• Molecule 17: DNA-directed RNA polymerase III subunit RPC7

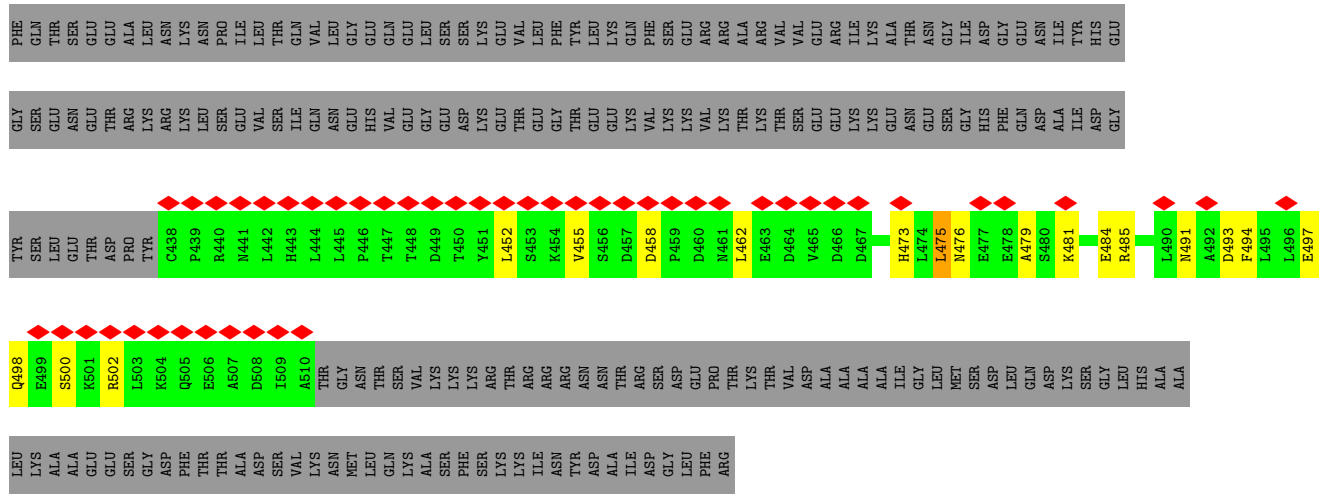


• Molecule 18: TATA-box-binding protein

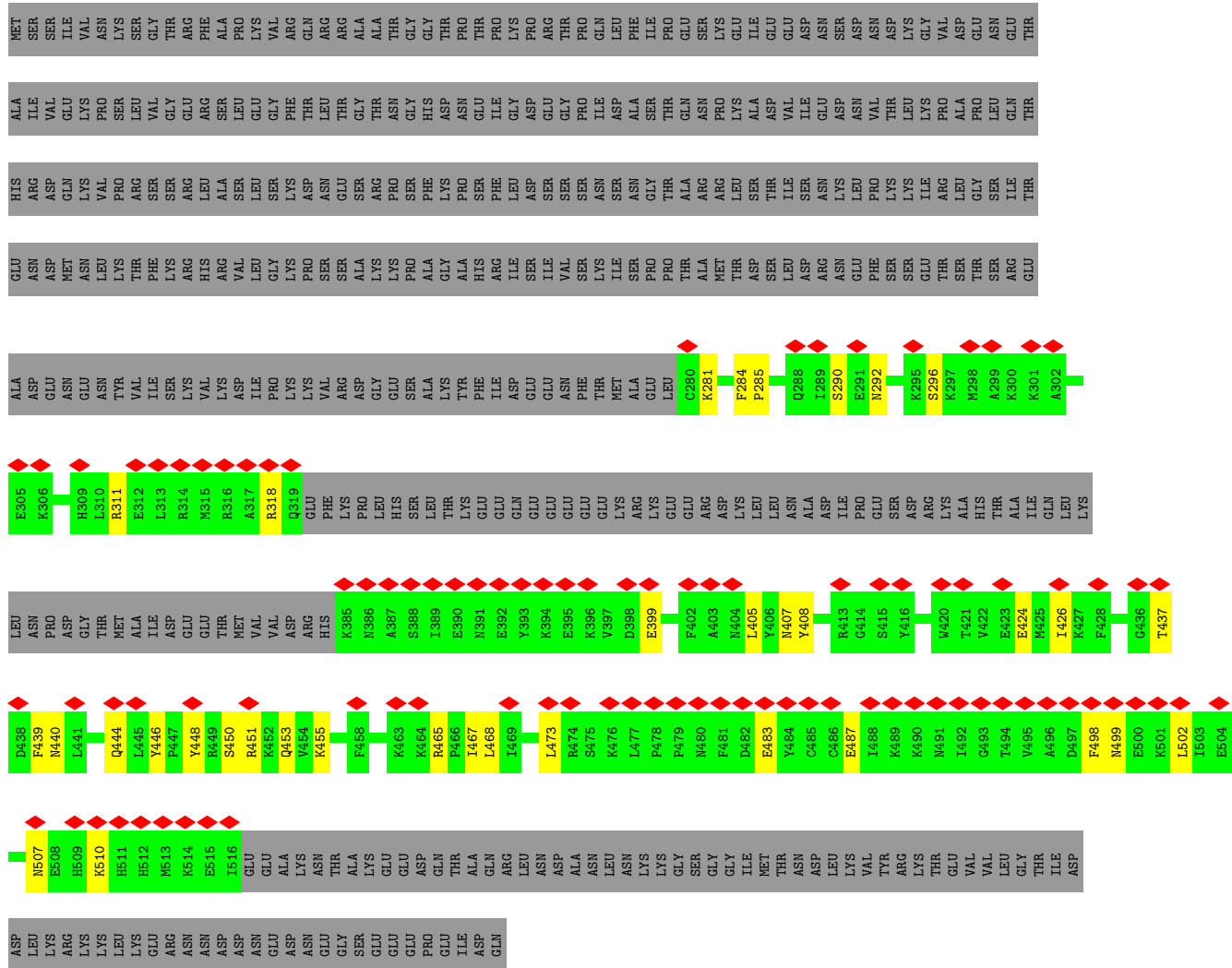


• Molecule 19: Transcription factor IIIB 70 kDa subunit

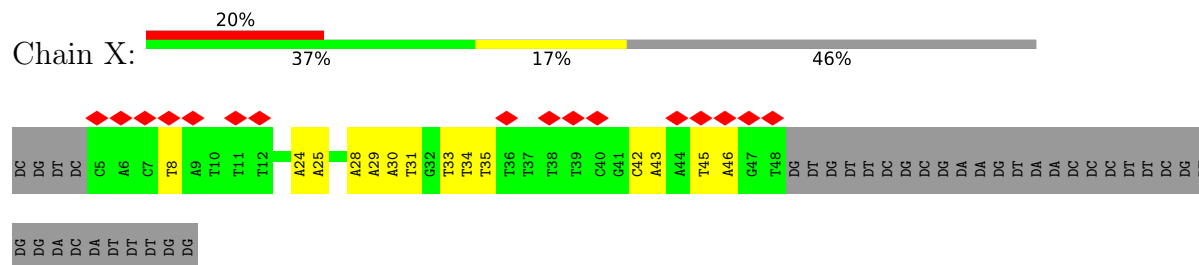




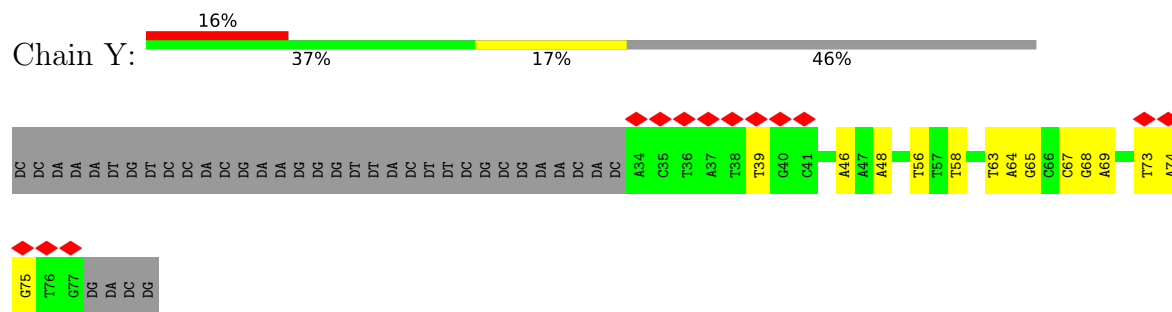
• Molecule 20: Transcription factor TFIIB component B''



• Molecule 21: Non-template DNA



● Molecule 22: Template DNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	34176	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 ($e^-/\text{\AA}^2$)	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	0.141	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.045	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	0.23	0/11170	0.46	1/15090 (0.0%)
2	B	0.24	0/8939	0.47	0/12063
3	C	0.25	0/2711	0.45	0/3676
4	D	0.23	0/991	0.41	0/1328
5	E	0.23	0/1787	0.43	0/2406
6	F	0.23	0/683	0.42	0/923
7	G	0.24	0/1486	0.44	0/2017
8	H	0.24	0/1138	0.50	0/1540
9	I	0.25	0/261	0.56	0/354
10	J	0.23	0/558	0.41	0/750
11	K	0.23	0/803	0.42	0/1083
12	L	0.22	0/360	0.45	0/478
13	M	0.24	0/1419	0.50	2/1919 (0.1%)
14	N	0.23	0/805	0.49	0/1081
15	O	0.23	0/4355	0.44	0/5875
16	P	0.24	0/843	0.47	0/1142
17	Q	0.25	0/281	0.42	0/381
18	U	0.24	0/1443	0.46	0/1942
19	V	0.23	0/2716	0.43	0/3660
20	W	0.24	0/1473	0.41	0/1970
21	X	0.54	0/1001	1.10	0/1542
22	Y	0.56	0/1021	1.04	0/1574
All	All	0.26	0/46244	0.50	3/62794 (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	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
16	P	0	1
20	W	0	1
All	All	0	6

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	204	PRO	N-CA-CB	5.94	110.42	103.30
13	M	202	PRO	N-CA-CB	5.92	110.40	103.30
1	A	456	LEU	CA-CB-CG	5.09	127.01	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	44	LYS	Peptide
1	A	70	CYS	Peptide
1	A	842	PRO	Peptide
2	B	1103	TYR	Peptide
16	P	234	GLU	Peptide
20	W	284	PHE	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	10974	0	11096	179	0
2	B	8784	0	8892	146	0
3	C	2655	0	2628	30	0
4	D	977	0	983	18	0
5	E	1751	0	1776	20	0
6	F	671	0	692	9	0
7	G	1448	0	1446	21	0
8	H	1120	0	1089	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	255	0	244	4	0
10	J	549	0	563	11	0
11	K	792	0	790	11	0
12	L	358	0	383	13	0
13	M	1387	0	1347	29	0
14	N	797	0	846	17	0
15	O	4290	0	4454	71	0
16	P	827	0	809	15	0
17	Q	273	0	285	5	0
18	U	1416	0	1493	41	0
19	V	2674	0	2687	43	0
20	W	1442	0	1448	27	0
21	X	896	0	504	10	0
22	Y	908	0	498	11	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	1	0
23	L	1	0	0	0	0
23	V	1	0	0	0	0
All	All	45251	0	44953	646	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 (646) 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)
10:J:46:CYS:SG	23:J:2000:ZN:ZN	1.04	1.42
2:B:695:GLN:HG2	2:B:697:PRO:HD2	1.59	0.85
2:B:667:VAL:HG12	2:B:669:SER:H	1.45	0.82
2:B:55:LYS:HG2	2:B:59:LYS:HD3	1.66	0.78
2:B:229:SER:HG	2:B:244:HIS:HE2	1.30	0.75
2:B:754:ASN:HD21	10:J:52:THR:HG21	1.52	0.75
8:H:33:GLN:HG3	8:H:35:GLN:H	1.52	0.74
1:A:664:MET:HB3	1:A:669:LEU:HD22	1.69	0.73
1:A:555:GLN:NE2	2:B:767:ILE:O	2.23	0.72
2:B:379:LEU:H	2:B:382:GLN:HE21	1.37	0.71
19:V:237:LEU:HB3	20:W:290:SER:HB3	1.71	0.71
2:B:769:ASP:OD2	2:B:952:ARG:NH2	2.24	0.71
1:A:153:ARG:HH12	15:O:339:LEU:HB3	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774:ARG:HE	1:A:804:LEU:HD21	1.55	0.70
2:B:93:LEU:HD23	2:B:135:TYR:HB3	1.72	0.70
1:A:228:LEU:HB3	1:A:257:ILE:HD11	1.75	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	1.74	0.68
3:C:191:ILE:HG23	10:J:15:GLY:HA3	1.76	0.68
1:A:630:ASN:ND2	1:A:650:GLY:O	2.27	0.68
19:V:145:ASP:O	19:V:149:ARG:NH1	2.26	0.68
7:G:80:PHE:HB3	7:G:83:GLU:HB2	1.76	0.67
3:C:43:ASN:HB2	3:C:55:ASP:HB2	1.76	0.67
1:A:390:ASP:OD2	1:A:538:LYS:NZ	2.27	0.67
1:A:549:PRO:HG3	1:A:679:TYR:HB2	1.78	0.66
1:A:683:ARG:NH1	1:A:925:GLU:OE2	2.28	0.66
19:V:485:ARG:HG3	20:W:498:PHE:HB2	1.76	0.66
2:B:444:LEU:HD13	2:B:451:ARG:HH12	1.61	0.66
2:B:483:VAL:HG12	2:B:485:GLY:H	1.59	0.66
16:P:233:VAL:HG22	16:P:234:GLU:HG3	1.76	0.66
11:K:88:PHE:HB3	11:K:106:GLN:HB3	1.78	0.66
1:A:482:ARG:HH11	1:A:544:PRO:HG3	1.59	0.66
15:O:268:LYS:HD2	15:O:269:THR:HG22	1.77	0.66
18:U:94:TYR:HB2	18:U:102:VAL:HG22	1.79	0.65
3:C:165:ARG:NH2	3:C:190:ASP:OD1	2.30	0.65
1:A:502:GLU:HG3	2:B:767:ILE:HG13	1.77	0.65
1:A:599:LYS:HB2	8:H:96:VAL:HG22	1.79	0.65
15:O:620:LEU:HD23	15:O:622:SER:H	1.62	0.65
1:A:417:GLN:HG2	1:A:456:LEU:HD21	1.79	0.64
15:O:498:SER:HB2	17:Q:42:PRO:HG3	1.78	0.64
21:X:34:DT:H3	22:Y:48:DA:H61	1.44	0.64
2:B:816:ASP:OD1	2:B:816:ASP:N	2.32	0.63
20:W:450:SER:H	20:W:453:GLN:HE22	1.46	0.63
1:A:203:GLU:HG3	15:O:515:LYS:HE2	1.79	0.63
18:U:160:ILE:HB	18:U:217:ALA:HB3	1.81	0.63
1:A:1048:VAL:O	1:A:1053:LYS:NZ	2.32	0.62
18:U:84:THR:O	18:U:88:HIS:NE2	2.32	0.62
1:A:568:ASP:O	8:H:22:LYS:NZ	2.30	0.62
2:B:772:VAL:HB	2:B:943:ILE:HB	1.81	0.62
1:A:482:ARG:HD3	1:A:544:PRO:HG3	1.82	0.62
19:V:484:GLU:OE2	20:W:499:ASN:ND2	2.32	0.62
5:E:168:TYR:HB2	5:E:170:LEU:HD22	1.80	0.62
1:A:1079:ARG:HG2	1:A:1082:ARG:HH12	1.65	0.62
2:B:210:ASP:H	2:B:215:ILE:HG22	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:713:ILE:HG13	2:B:725:LEU:HD11	1.82	0.61
15:O:352:VAL:O	15:O:356:THR:OG1	2.17	0.61
1:A:72:GLY:HA3	1:A:76:SER:HB2	1.80	0.61
1:A:372:ARG:NH1	2:B:1052:GLU:OE1	2.33	0.61
2:B:221:THR:HG21	2:B:334:HIS:H	1.66	0.61
1:A:409:THR:HG22	1:A:410:ARG:HD2	1.83	0.61
15:O:129:ILE:HG21	15:O:164:ILE:HD13	1.82	0.61
1:A:665:ASP:HB2	1:A:797:CYS:HA	1.83	0.61
2:B:83:ILE:HD11	2:B:400:LYS:HB3	1.82	0.60
4:D:117:LYS:HB2	4:D:120:LYS:HE2	1.83	0.60
2:B:579:ARG:NH1	2:B:588:ILE:O	2.34	0.60
2:B:915:ARG:NH2	2:B:960:GLU:OE2	2.33	0.60
15:O:314:ILE:HG13	15:O:317:ARG:HH21	1.66	0.60
15:O:484:MET:HG3	15:O:653:MET:HB3	1.83	0.60
1:A:482:ARG:HH21	2:B:1073:TYR:HA	1.66	0.60
1:A:597:ILE:HB	1:A:603:LEU:HB2	1.84	0.60
1:A:1050:ASP:HA	1:A:1053:LYS:HE2	1.83	0.60
20:W:311:ARG:NH2	22:Y:67:DC:OP1	2.35	0.60
16:P:253:LEU:HD21	16:P:261:TYR:HB3	1.84	0.60
5:E:185:ALA:HA	5:E:190:LEU:HD13	1.84	0.60
10:J:36:LEU:HB2	10:J:41:LEU:HD12	1.83	0.60
19:V:6:ASN:HD22	19:V:30:VAL:HG21	1.67	0.60
2:B:314:ARG:NH2	2:B:317:LEU:O	2.35	0.59
18:U:68:GLN:HG2	22:Y:58:DT:H4'	1.84	0.59
9:I:3:SER:HB2	9:I:12:LEU:HB2	1.84	0.59
1:A:151:GLN:NE2	1:A:153:ARG:O	2.31	0.59
1:A:970:LEU:HD13	1:A:973:ARG:HH12	1.67	0.59
15:O:234:ASP:O	15:O:238:ARG:NH1	2.36	0.59
19:V:165:VAL:HG23	19:V:170:ILE:HB	1.84	0.59
2:B:449:MET:SD	2:B:451:ARG:NH1	2.76	0.59
2:B:1028:LYS:HG2	2:B:1029:HIS:H	1.68	0.59
1:A:442:ARG:HG2	19:V:30:VAL:HG22	1.84	0.59
3:C:255:VAL:HG21	3:C:273:ASP:HB2	1.85	0.58
2:B:666:ILE:HD11	2:B:673:LEU:HD12	1.84	0.58
2:B:93:LEU:HD21	2:B:133:ILE:HB	1.85	0.58
19:V:476:ASN:HB3	19:V:479:ALA:HB3	1.84	0.58
1:A:363:ARG:HD2	1:A:367:ASN:HD22	1.69	0.58
1:A:1187:ARG:NH1	1:A:1189:ASP:OD1	2.36	0.58
5:E:170:LEU:HB2	5:E:174:GLN:HE21	1.67	0.58
19:V:104:ALA:HA	19:V:107:TRP:HD1	1.69	0.58
1:A:84:LEU:HD12	1:A:261:LEU:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1162:GLU:HA	1:A:1278:ILE:HD11	1.85	0.58
1:A:703:ARG:NH2	11:K:93:ILE:O	2.37	0.58
2:B:766:ASP:HA	2:B:770:ALA:HB3	1.84	0.58
2:B:343:ARG:NH1	13:M:178:GLN:OE1	2.37	0.58
18:U:188:GLU:O	19:V:219:ARG:NH2	2.36	0.57
7:G:156:VAL:HG23	7:G:192:PRO:HB2	1.86	0.57
10:J:22:LEU:O	10:J:26:GLN:NE2	2.37	0.57
1:A:464:ARG:NH1	1:A:467:GLU:OE2	2.37	0.57
2:B:738:THR:HG22	2:B:740:THR:H	1.69	0.57
3:C:100:ARG:HH12	10:J:4:PRO:HA	1.69	0.57
6:F:73:ALA:HA	6:F:143:PHE:HB2	1.87	0.57
14:N:364:ARG:NH2	14:N:380:MET:SD	2.71	0.57
15:O:303:ARG:HD2	15:O:465:PHE:HE2	1.70	0.57
1:A:1185:GLN:HE21	1:A:1229:ARG:HG3	1.70	0.57
18:U:133:LYS:NZ	19:V:452:LEU:O	2.38	0.57
1:A:789:ASN:ND2	1:A:791:PRO:HD2	2.20	0.56
2:B:405:LYS:HA	2:B:408:LYS:HE2	1.86	0.56
3:C:40:PHE:HE1	3:C:59:ILE:HD11	1.69	0.56
18:U:93:GLU:OE2	20:W:439:PHE:N	2.38	0.56
18:U:170:ILE:HG21	18:U:234:LEU:HD11	1.87	0.56
1:A:102:ILE:HG22	1:A:242:LEU:HB2	1.86	0.56
1:A:828:GLN:NE2	2:B:655:ASN:O	2.32	0.56
2:B:225:HIS:O	2:B:227:ARG:NH1	2.38	0.56
4:D:141:CYS:SG	4:D:144:ARG:NH2	2.79	0.56
1:A:1023:ARG:NH2	1:A:1028:MET:SD	2.79	0.56
14:N:285:ALA:O	14:N:289:HIS:ND1	2.38	0.56
1:A:985:LYS:HE2	1:A:987:GLU:HB2	1.87	0.56
2:B:889:SER:OG	2:B:891:ASN:OD1	2.23	0.56
13:M:105:PRO:HB2	13:M:123:ILE:HD11	1.87	0.56
1:A:830:ARG:NH1	1:A:835:PHE:O	2.39	0.56
2:B:390:ASP:HA	2:B:393:LYS:HE3	1.86	0.56
2:B:540:ASP:HB3	2:B:543:LEU:HD13	1.87	0.56
1:A:107:CYS:HB3	1:A:112:ALA:H	1.70	0.56
8:H:15:VAL:HG22	8:H:26:ILE:HG22	1.86	0.56
15:O:588:LEU:HD21	16:P:310:VAL:HG22	1.87	0.56
7:G:207:LEU:HG	7:G:209:SER:H	1.70	0.56
1:A:6:VAL:O	7:G:33:LYS:NZ	2.39	0.56
2:B:934:ASN:HA	2:B:1004:LEU:HB2	1.88	0.56
2:B:837:GLN:N	2:B:840:GLN:OE1	2.37	0.55
15:O:263:LEU:HD13	15:O:272:ARG:HH22	1.70	0.55
2:B:377:LEU:HD11	2:B:473:ILE:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1003:MET:HB3	2:B:1016:TYR:HD1	1.71	0.55
6:F:115:THR:HG22	6:F:116:ASP:H	1.71	0.55
2:B:593:ASN:HD21	2:B:596:GLN:HE21	1.55	0.55
4:D:69:ASN:ND2	4:D:125:ASN:O	2.39	0.55
1:A:632:VAL:HG23	1:A:633:PHE:H	1.70	0.55
1:A:1373:ARG:HH21	1:A:1390:GLU:HB3	1.71	0.55
13:M:75:PRO:HA	14:N:362:SER:HA	1.88	0.55
15:O:484:MET:SD	15:O:485:PRO:HD3	2.47	0.55
3:C:256:ILE:HG22	3:C:267:VAL:HA	1.88	0.55
19:V:491:ASN:HD21	19:V:494:PHE:HB2	1.72	0.55
2:B:806:ILE:HG22	2:B:828:GLY:HA3	1.89	0.55
15:O:100:GLN:HG3	15:O:167:GLY:HA3	1.89	0.55
15:O:580:ASN:O	15:O:584:ASN:ND2	2.40	0.55
1:A:1166:LEU:HD21	1:A:1268:PRO:HA	1.89	0.55
19:V:245:VAL:HG12	20:W:405:LEU:HD21	1.89	0.55
8:H:106:GLU:HA	8:H:112:ILE:HA	1.88	0.55
19:V:257:GLN:OE1	19:V:258:ARG:NH1	2.40	0.55
2:B:807:GLY:O	2:B:844:ASN:ND2	2.40	0.54
13:M:76:LEU:O	14:N:360:VAL:N	2.40	0.54
13:M:123:ILE:HG22	13:M:146:GLN:HB3	1.88	0.54
18:U:71:VAL:HG22	18:U:159:ASN:HB3	1.88	0.54
1:A:83:HIS:HA	1:A:262:PRO:HA	1.88	0.54
1:A:1045:ASP:O	1:A:1053:LYS:NZ	2.40	0.54
1:A:483:LEU:HD22	1:A:486:LEU:HD11	1.90	0.54
9:I:9:ASN:ND2	13:M:92:ASN:OD1	2.40	0.54
12:L:29:TYR:HB3	12:L:56:LEU:HD13	1.90	0.54
1:A:1122:GLY:HA2	1:A:1346:HIS:HE1	1.72	0.54
2:B:76:ILE:HD12	2:B:389:GLU:HB3	1.88	0.54
16:P:293:ILE:HD12	16:P:295:ASN:H	1.72	0.54
8:H:58:THR:HB	8:H:143:LEU:HB2	1.88	0.54
19:V:233:ARG:NH2	20:W:281:LYS:O	2.41	0.54
2:B:686:GLY:HA3	2:B:740:THR:HG21	1.89	0.54
3:C:103:LEU:HD12	10:J:6:ARG:HD2	1.89	0.54
5:E:107:THR:HB	5:E:130:ALA:HB3	1.90	0.54
1:A:601:TYR:HD1	3:C:24:SER:HB2	1.72	0.53
13:M:250:GLY:O	13:M:251:THR:HG22	2.08	0.53
5:E:118:PRO:O	5:E:122:LYS:NZ	2.37	0.53
1:A:715:ASN:OD1	2:B:999:SER:OG	2.20	0.53
2:B:1088:ASP:OD2	2:B:1123:TYR:N	2.42	0.53
1:A:1332:ARG:NH1	1:A:1360:ASP:OD1	2.41	0.53
7:G:130:TRP:HE3	7:G:137:LYS:HB3	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:31:CYS:SG	12:L:32:ALA:N	2.82	0.53
13:M:158:GLN:H	14:N:308:GLN:HA	1.74	0.53
15:O:460:LEU:HG	15:O:467:PHE:HE2	1.74	0.53
2:B:369:ARG:NH2	2:B:480:SER:OG	2.42	0.53
4:D:59:THR:HA	4:D:62:VAL:HG12	1.91	0.53
2:B:525:GLU:HG2	2:B:527:GLU:H	1.73	0.52
14:N:308:GLN:NE2	14:N:309:LEU:O	2.42	0.52
2:B:849:THR:HG22	2:B:865:GLN:HB2	1.91	0.52
5:E:47:CYS:HB2	5:E:53:PRO:HA	1.90	0.52
13:M:148:LEU:HA	13:M:182:PHE:H	1.74	0.52
15:O:304:VAL:HG22	15:O:305:GLY:H	1.74	0.52
18:U:162:GLY:O	18:U:214:LEU:N	2.42	0.52
1:A:815:GLN:NE2	1:A:816:GLN:O	2.42	0.52
1:A:1187:ARG:NH1	1:A:1188:ILE:O	2.42	0.52
1:A:1365:LYS:NZ	1:A:1378:LYS:O	2.32	0.52
15:O:561:ARG:HH22	22:Y:39:DT:H5''	1.73	0.52
20:W:507:ASN:HA	20:W:510:LYS:HG2	1.90	0.52
1:A:15:GLY:HA2	1:A:1408:VAL:HG22	1.92	0.52
11:K:62:SER:HB3	11:K:104:ARG:HH11	1.73	0.52
13:M:81:GLU:O	13:M:82:GLU:HG3	2.10	0.52
18:U:107:ARG:HB3	20:W:473:LEU:HD22	1.92	0.52
2:B:614:ILE:HG23	2:B:621:ARG:HD2	1.91	0.52
1:A:929:ASN:O	1:A:931:GLN:NE2	2.42	0.52
15:O:132:TYR:HE1	15:O:645:LEU:HD11	1.74	0.52
2:B:591:TYR:HB2	2:B:652:ASN:HB3	1.92	0.52
14:N:374:LYS:NZ	14:N:377:ASN:O	2.37	0.52
15:O:128:HIS:HB2	15:O:284:LEU:HD11	1.92	0.52
13:M:111:ARG:HE	13:M:113:LYS:HE3	1.74	0.52
16:P:179:LEU:HB3	16:P:243:LEU:HD21	1.91	0.52
19:V:206:ALA:O	19:V:210:SER:N	2.43	0.52
1:A:107:CYS:N	1:A:112:ALA:O	2.41	0.51
3:C:31:TRP:HH2	11:K:127:LEU:HD13	1.76	0.51
19:V:239:ARG:HH22	20:W:285:PRO:HD2	1.75	0.51
2:B:234:ILE:HD12	2:B:236:LYS:HE2	1.93	0.51
7:G:88:TRP:HE1	7:G:145:LYS:HG2	1.75	0.51
2:B:754:ASN:HA	2:B:1023:TYR:HA	1.92	0.51
1:A:234:ILE:HD11	1:A:253:PRO:HG3	1.93	0.51
2:B:767:ILE:O	2:B:945:ASN:ND2	2.43	0.51
10:J:10:CYS:SG	10:J:11:GLY:N	2.84	0.51
15:O:552:PRO:HG3	15:O:557:ARG:HG3	1.93	0.51
1:A:524:THR:HG23	2:B:1081:GLU:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:785:CYS:SG	2:B:1026:LYS:NZ	2.77	0.51
3:C:282:TYR:O	3:C:283:GLU:HG3	2.10	0.51
8:H:38:LEU:HB3	8:H:125:LEU:HB3	1.92	0.51
1:A:70:CYS:SG	1:A:71:HIS:N	2.83	0.51
2:B:131:VAL:HG22	2:B:149:ILE:HD11	1.93	0.51
2:B:678:PHE:HB2	2:B:978:CYS:HB3	1.93	0.51
10:J:31:ASP:HB3	10:J:34:THR:HG22	1.93	0.51
1:A:741:LEU:HD12	1:A:744:LEU:HD21	1.93	0.51
2:B:51:PHE:HD2	2:B:52:LEU:HD12	1.76	0.51
2:B:213:LYS:H	2:B:213:LYS:HD2	1.76	0.51
13:M:120:GLU:OE1	13:M:147:THR:OG1	2.25	0.51
15:O:43:ASN:HB3	15:O:47:PHE:HB2	1.93	0.51
2:B:126:SER:HG	2:B:151:ARG:HE	1.59	0.51
2:B:944:MET:SD	2:B:1024:TYR:OH	2.69	0.51
1:A:1139:PRO:HG3	1:A:1298:TYR:CZ	2.46	0.50
2:B:206:ILE:HD11	2:B:218:ALA:HB3	1.93	0.50
4:D:15:GLU:HA	4:D:18:LYS:HB3	1.94	0.50
5:E:86:PRO:HB3	5:E:114:ASN:HD22	1.75	0.50
13:M:174:GLU:HG3	13:M:175:ARG:HG3	1.91	0.50
15:O:497:ALA:HB2	15:O:505:MET:HB2	1.91	0.50
21:X:28:DA:H2''	21:X:29:DA:N7	2.26	0.50
1:A:91:PHE:CE2	1:A:224:PRO:HG3	2.46	0.50
1:A:378:ARG:HD2	2:B:1060:LEU:HD21	1.92	0.50
19:V:4:CYS:HB3	19:V:9:GLY:H	1.77	0.50
1:A:49:LYS:HE2	1:A:54:LEU:HB2	1.94	0.50
1:A:410:ARG:NE	6:F:104:ASN:OD1	2.43	0.50
21:X:35:DT:O4	22:Y:46:DA:N6	2.45	0.50
1:A:476:ARG:HG3	1:A:478:PRO:HD2	1.92	0.50
2:B:1093:ASP:OD1	2:B:1093:ASP:N	2.42	0.50
18:U:88:HIS:HB2	19:V:475:LEU:HD13	1.93	0.50
19:V:458:ASP:OD1	19:V:458:ASP:N	2.45	0.50
1:A:578:GLN:HE21	11:K:77:ARG:NH1	2.10	0.50
2:B:888:VAL:HG11	12:L:54:ARG:HH21	1.76	0.50
13:M:137:GLU:O	13:M:141:ASN:ND2	2.45	0.50
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.94	0.50
1:A:834:HIS:HD2	2:B:659:ILE:HB	1.77	0.49
13:M:150:GLY:HA3	13:M:179:LEU:HD23	1.93	0.49
15:O:98:LEU:HB2	15:O:103:CYS:HB2	1.93	0.49
18:U:164:CYS:SG	18:U:165:ASP:N	2.86	0.49
19:V:214:MET:O	19:V:218:ARG:NH1	2.41	0.49
1:A:733:ILE:HA	1:A:736:HIS:CE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:THR:HG22	2:B:188:ASN:H	1.77	0.49
2:B:934:ASN:OD1	2:B:938:ILE:N	2.43	0.49
15:O:141:ILE:O	15:O:145:ARG:NE	2.44	0.49
18:U:161:VAL:HG12	18:U:216:GLY:H	1.77	0.49
1:A:1059:LEU:HD11	8:H:112:ILE:HG21	1.94	0.49
1:A:1286:ARG:HG2	1:A:1287:ASP:H	1.76	0.49
1:A:1350:VAL:HG23	1:A:1351:ASP:H	1.77	0.49
2:B:258:LYS:HG2	2:B:263:LEU:HA	1.94	0.49
4:D:20:LEU:O	4:D:24:GLU:N	2.43	0.49
14:N:299:ASN:C	14:N:300:LYS:HD2	2.33	0.49
1:A:181:ASP:OD2	1:A:184:ARG:NH2	2.46	0.49
1:A:186:VAL:HG13	1:A:187:GLY:H	1.77	0.49
19:V:135:ARG:HG2	19:V:174:PRO:HD2	1.94	0.49
20:W:455:LYS:NZ	22:Y:56:DT:OP2	2.40	0.49
3:C:81:GLU:OE2	12:L:70:ARG:NH2	2.44	0.49
8:H:63:LEU:HG	8:H:89:LEU:HD23	1.95	0.49
15:O:254:ASN:O	15:O:258:GLU:N	2.46	0.49
2:B:66:ASN:HD21	2:B:159:ASN:HD21	1.61	0.49
2:B:775:LYS:N	2:B:926:VAL:O	2.44	0.49
2:B:835:LYS:HB3	2:B:880:HIS:CE1	2.47	0.49
2:B:59:LYS:NZ	2:B:518:THR:O	2.41	0.49
2:B:60:GLN:HB2	2:B:379:LEU:HD11	1.94	0.49
2:B:604:ASP:OD1	2:B:607:ARG:NH1	2.45	0.49
1:A:827:PHE:HD2	1:A:828:GLN:HG2	1.78	0.49
20:W:450:SER:H	20:W:453:GLN:NE2	2.09	0.49
1:A:828:GLN:HE21	1:A:830:ARG:NE	2.10	0.49
2:B:420:LEU:HB3	19:V:149:ARG:HB2	1.94	0.49
3:C:26:ASP:OD1	3:C:26:ASP:N	2.45	0.49
18:U:168:PHE:HB2	18:U:239:LYS:NZ	2.28	0.49
18:U:236:GLU:HG3	18:U:237:PHE:CD1	2.48	0.48
2:B:711:GLY:HA3	2:B:751:ALA:HA	1.96	0.48
2:B:888:VAL:HG11	12:L:54:ARG:HE	1.78	0.48
15:O:288:MET:HG3	15:O:326:ILE:HD13	1.94	0.48
15:O:548:ILE:HD11	15:O:564:PHE:HB2	1.94	0.48
8:H:118:PHE:HB2	8:H:121:LEU:HB2	1.96	0.48
2:B:795:LEU:HD22	2:B:804:ASP:HB2	1.95	0.48
4:D:15:GLU:HG3	4:D:18:LYS:HE3	1.94	0.48
18:U:99:PHE:HE2	18:U:114:LEU:HD21	1.78	0.48
21:X:42:DC:H2"	21:X:43:DA:C8	2.48	0.48
1:A:1087:THR:HG22	6:F:88:TYR:HE2	1.79	0.48
19:V:265:THR:HG23	19:V:266:LYS:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:X:30:DA:H2'	21:X:31:DT:H2'	1.95	0.48
1:A:826:GLY:H	1:A:831:SER:HA	1.78	0.48
1:A:1205:ILE:O	1:A:1209:ILE:HD12	2.14	0.48
5:E:55:ARG:HH12	5:E:113:GLN:HG3	1.79	0.48
15:O:121:TYR:HD2	15:O:210:PRO:HG2	1.79	0.48
19:V:80:LEU:O	19:V:84:ARG:N	2.43	0.48
1:A:852:PHE:HB3	2:B:955:VAL:HG21	1.96	0.48
1:A:1343:MET:HE3	1:A:1350:VAL:H	1.79	0.48
15:O:322:LYS:HE2	15:O:358:GLY:HA3	1.96	0.48
18:U:76:LEU:HG	18:U:78:CYS:H	1.78	0.48
18:U:96:PRO:HG3	19:V:494:PHE:CZ	2.49	0.48
2:B:227:ARG:HD3	2:B:334:HIS:CE1	2.49	0.48
20:W:465:ARG:HB3	20:W:468:LEU:HD13	1.96	0.48
1:A:1283:ILE:HD11	1:A:1291:ARG:HD3	1.96	0.48
2:B:612:LEU:HD22	2:B:674:GLU:HA	1.95	0.48
15:O:68:LEU:O	15:O:72:GLY:N	2.46	0.48
2:B:129:ILE:HD11	2:B:152:MET:HB2	1.94	0.47
1:A:11:LYS:HA	2:B:1145:ASP:HA	1.95	0.47
1:A:269:ARG:HB3	1:A:285:LEU:HD12	1.95	0.47
8:H:12:VAL:HG22	8:H:53:ASP:H	1.78	0.47
13:M:86:HIS:CD2	13:M:175:ARG:HB2	2.49	0.47
15:O:201:ILE:HG21	15:O:256:PRO:HB3	1.96	0.47
1:A:223:ASN:HB2	1:A:316:TRP:CH2	2.49	0.47
1:A:332:VAL:HG13	1:A:334:PRO:HD3	1.96	0.47
1:A:789:ASN:HD22	1:A:791:PRO:HD2	1.79	0.47
2:B:156:LEU:HD11	2:B:186:ILE:HD11	1.96	0.47
2:B:217:GLN:NE2	2:B:218:ALA:O	2.47	0.47
2:B:1008:ILE:HD11	11:K:70:HIS:CD2	2.49	0.47
4:D:3:VAL:HA	7:G:7:ILE:HG22	1.96	0.47
7:G:84:ILE:HD13	7:G:149:ARG:HB3	1.96	0.47
1:A:815:GLN:HE21	1:A:846:GLY:HA3	1.79	0.47
2:B:566:ARG:HH22	14:N:282:LEU:HD11	1.80	0.47
2:B:610:ARG:NH2	2:B:654:GLU:OE2	2.48	0.47
5:E:156:LEU:HD21	5:E:195:VAL:HG13	1.95	0.47
15:O:605:LYS:HA	15:O:608:ARG:HE	1.79	0.47
1:A:117:GLU:HG3	15:O:212:GLU:HG2	1.96	0.47
13:M:157:GLY:HA3	14:N:308:GLN:HG2	1.97	0.47
15:O:591:LYS:HA	15:O:594:LYS:HE3	1.96	0.47
1:A:393:ALA:HB3	1:A:499:ARG:HB2	1.95	0.47
1:A:911:ILE:HB	5:E:176:PRO:HD3	1.96	0.47
2:B:194:ILE:HG12	2:B:455:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:58:GLY:O	11:K:113:ALA:N	2.39	0.47
21:X:8:DT:O2	22:Y:75:DG:N2	2.47	0.47
1:A:352:GLY:H	1:A:355:GLN:HB2	1.80	0.47
1:A:481:HIS:CE1	1:A:483:LEU:HB3	2.50	0.47
1:A:607:LYS:HB3	1:A:659:ILE:HB	1.96	0.47
1:A:881:GLU:O	1:A:885:MET:N	2.39	0.47
1:A:1445:ARG:HH21	4:D:9:ALA:HB1	1.79	0.47
2:B:347:LEU:HD11	2:B:541:ILE:HD11	1.96	0.47
2:B:811:VAL:HG12	2:B:816:ASP:HA	1.95	0.47
3:C:2:SER:O	3:C:4:ILE:HG13	2.14	0.47
14:N:297:MET:HG3	14:N:303:ARG:HG3	1.97	0.47
19:V:239:ARG:NH2	20:W:285:PRO:HD2	2.30	0.47
1:A:111:SER:HB2	1:A:234:ILE:HG22	1.97	0.47
12:L:53:HIS:HE1	12:L:55:ILE:HB	1.79	0.47
18:U:68:GLN:NE2	18:U:163:SER:OG	2.48	0.47
20:W:318:ARG:NH1	20:W:448:TYR:HB2	2.30	0.47
1:A:13:ILE:H	1:A:1419:GLN:HE22	1.61	0.47
1:A:511:ASP:OD1	1:A:511:ASP:N	2.44	0.47
1:A:993:GLU:O	5:E:197:LYS:NZ	2.42	0.47
2:B:210:ASP:HB3	2:B:213:LYS:HD3	1.96	0.47
18:U:142:ILE:HG12	19:V:473:HIS:HD2	1.80	0.47
18:U:230:ILE:HD12	18:U:233:VAL:HB	1.97	0.47
1:A:124:LEU:HA	1:A:127:LEU:HD23	1.96	0.47
18:U:165:ASP:HA	18:U:211:LYS:HG2	1.97	0.47
19:V:116:PHE:HD1	19:V:167:LYS:HD3	1.80	0.47
1:A:654:ILE:HG22	1:A:659:ILE:HA	1.97	0.46
13:M:182:PHE:HE2	13:M:184:LYS:HD3	1.81	0.46
15:O:271:LEU:HG	15:O:272:ARG:H	1.79	0.46
20:W:407:ASN:ND2	22:Y:65:DG:OP1	2.40	0.46
1:A:790:ALA:HA	1:A:793:ILE:HG22	1.97	0.46
3:C:45:SER:OG	3:C:46:SER:N	2.48	0.46
8:H:6:PHE:HB3	8:H:59:ILE:HB	1.96	0.46
14:N:301:PRO:HG2	14:N:303:ARG:HG2	1.97	0.46
15:O:211:ILE:HD11	15:O:249:PHE:HZ	1.80	0.46
15:O:238:ARG:H	15:O:238:ARG:HD2	1.80	0.46
19:V:493:ASP:O	19:V:497:GLU:N	2.45	0.46
2:B:212:LYS:H	2:B:212:LYS:HD2	1.80	0.46
12:L:53:HIS:CE1	12:L:55:ILE:HB	2.51	0.46
18:U:186:GLU:OE2	18:U:188:GLU:HG2	2.15	0.46
19:V:162:LEU:HA	19:V:165:VAL:HG12	1.98	0.46
15:O:161:GLN:NE2	17:Q:64:THR:OG1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:LEU:HD13	1:A:507:PRO:HB3	1.97	0.46
2:B:142:ILE:HD11	20:W:399:GLU:HB2	1.97	0.46
4:D:27:HIS:ND1	4:D:30:ASP:OD2	2.48	0.46
7:G:114:MET:SD	7:G:114:MET:N	2.88	0.46
18:U:90:ARG:HB3	19:V:473:HIS:CE1	2.50	0.46
2:B:766:ASP:OD1	2:B:766:ASP:N	2.49	0.46
16:P:170:LEU:HD13	16:P:171:ASP:N	2.31	0.46
2:B:234:ILE:HG13	2:B:241:TYR:HB2	1.98	0.46
12:L:26:THR:OG1	12:L:27:LEU:N	2.48	0.46
16:P:297:PHE:O	16:P:298:LYS:HG2	2.16	0.46
16:P:311:TYR:HA	17:Q:40:PRO:HA	1.98	0.46
1:A:4:VAL:HA	7:G:38:ILE:HG22	1.97	0.46
1:A:194:LYS:O	1:A:198:VAL:N	2.42	0.46
1:A:666:LYS:HD2	1:A:670:GLY:HA3	1.97	0.46
3:C:241:GLY:O	3:C:245:ARG:NH1	2.48	0.46
5:E:200:ARG:NH1	5:E:210:SER:OG	2.47	0.46
2:B:312:MET:SD	2:B:315:GLN:N	2.80	0.46
3:C:7:ILE:HG22	3:C:12:VAL:HG12	1.98	0.46
7:G:153:GLU:HB3	7:G:196:LEU:HD13	1.98	0.46
15:O:191:PHE:O	15:O:195:CYS:N	2.48	0.46
19:V:145:ASP:N	19:V:145:ASP:OD1	2.47	0.46
1:A:15:GLY:HA3	1:A:1407:ALA:HA	1.98	0.46
1:A:37:ARG:HG3	1:A:294:TRP:HB2	1.97	0.46
3:C:69:ARG:HE	11:K:71:THR:HG22	1.80	0.46
8:H:93:TYR:HE1	8:H:145:ARG:HH21	1.62	0.45
13:M:154:GLU:HB3	13:M:175:ARG:HG2	1.98	0.45
15:O:362:ASN:HA	15:O:475:VAL:HG23	1.98	0.45
1:A:515:ASP:N	1:A:515:ASP:OD1	2.48	0.45
1:A:577:THR:HG21	11:K:89:CYS:H	1.81	0.45
1:A:1186:VAL:HB	1:A:1230:ILE:HG23	1.98	0.45
1:A:1300:LEU:HD11	1:A:1316:THR:HG21	1.98	0.45
14:N:380:MET:HB3	14:N:421:GLN:HE22	1.81	0.45
1:A:230:LEU:HA	1:A:233:GLN:HE22	1.81	0.45
1:A:818:ILE:HD12	1:A:823:VAL:HA	1.98	0.45
2:B:578:LEU:HD21	2:B:583:LYS:HD3	1.97	0.45
15:O:37:LEU:HD23	15:O:40:ARG:NH1	2.31	0.45
15:O:271:LEU:HD23	15:O:271:LEU:H	1.81	0.45
15:O:342:ALA:HA	15:O:345:PHE:HD2	1.80	0.45
15:O:468:LEU:H	15:O:479:PRO:HD2	1.80	0.45
1:A:951:ASP:O	1:A:1061:ARG:NH2	2.49	0.45
2:B:261:GLY:HA2	2:B:298:GLN:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:466:PRO:HA	15:O:469:ASN:HD22	1.80	0.45
1:A:1445:ARG:NH2	4:D:10:PHE:O	2.48	0.45
2:B:786:GLU:HA	2:B:903:ASN:HA	1.99	0.45
8:H:11:GLN:O	8:H:29:ALA:N	2.50	0.45
15:O:498:SER:HB3	16:P:296:TYR:CZ	2.51	0.45
1:A:309:ILE:HA	1:A:312:MET:HG3	1.98	0.45
1:A:374:ASP:OD1	2:B:1038:ARG:NE	2.49	0.45
1:A:468:ASP:OD1	1:A:468:ASP:N	2.50	0.45
13:M:227:LEU:HD23	13:M:227:LEU:H	1.82	0.45
1:A:1373:ARG:HD3	1:A:1391:LYS:HD3	1.98	0.45
1:A:1391:LYS:HE3	1:A:1395:HIS:CE1	2.52	0.45
2:B:622:VAL:HG23	2:B:623:LYS:H	1.81	0.45
2:B:816:ASP:OD1	2:B:817:PRO:HD3	2.16	0.45
3:C:242:GLU:OE1	3:C:246:ARG:NH2	2.49	0.45
1:A:808:GLN:HG2	1:A:813:VAL:HA	1.97	0.45
1:A:1079:ARG:HD3	6:F:84:TYR:HE2	1.81	0.45
2:B:553:TYR:HD2	2:B:568:PRO:HG3	1.81	0.45
18:U:144:GLN:HG3	19:V:462:LEU:HD11	1.98	0.45
1:A:1320:LEU:HD23	1:A:1320:LEU:H	1.81	0.45
5:E:9:ILE:O	5:E:13:TRP:N	2.49	0.45
18:U:196:ARG:HG3	18:U:203:VAL:HG12	1.98	0.45
1:A:357:LEU:HA	1:A:363:ARG:HB2	1.99	0.45
2:B:523:ASP:OD1	2:B:523:ASP:N	2.50	0.45
2:B:553:TYR:CD2	2:B:568:PRO:HG3	2.52	0.45
3:C:21:PRO:HD2	11:K:82:LYS:HA	1.98	0.45
3:C:86:PHE:HE1	12:L:64:LEU:HD12	1.81	0.45
8:H:93:TYR:CE2	8:H:143:LEU:HB3	2.52	0.45
19:V:268:ALA:O	19:V:272:VAL:HG23	2.17	0.45
2:B:615:VAL:HG13	2:B:620:SER:HA	1.98	0.44
2:B:795:LEU:HD21	2:B:806:ILE:HD11	1.99	0.44
15:O:292:ARG:HD3	15:O:326:ILE:HD12	1.98	0.44
1:A:1319:VAL:HG11	1:A:1335:ILE:HG13	1.99	0.44
1:A:1444:LYS:O	7:G:49:TYR:OH	2.32	0.44
4:D:133:HIS:CE1	4:D:137:ILE:HD11	2.51	0.44
7:G:120:TYR:O	7:G:128:TRP:HB3	2.17	0.44
8:H:107:VAL:N	8:H:111:LEU:O	2.48	0.44
1:A:794:MET:SD	2:B:950:PRO:HG2	2.58	0.44
1:A:895:ASP:OD1	1:A:895:ASP:N	2.50	0.44
3:C:164:ALA:HB3	3:C:189:PRO:HA	1.99	0.44
15:O:304:VAL:HG11	15:O:308:THR:HB	1.99	0.44
15:O:639:ALA:HB2	17:Q:47:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:247:LEU:HD12	16:P:252:LYS:HB2	1.99	0.44
19:V:242:THR:OG1	20:W:296:SER:OG	2.25	0.44
15:O:494:TYR:CE2	16:P:294:PHE:HA	2.53	0.44
20:W:483:GLU:O	20:W:487:GLU:N	2.51	0.44
1:A:610:PHE:CD1	1:A:613:LEU:HD21	2.53	0.44
7:G:93:THR:HG22	7:G:94:ALA:H	1.83	0.44
7:G:149:ARG:HH21	7:G:201:GLN:HG2	1.83	0.44
15:O:137:ILE:HG21	17:Q:57:LYS:HG2	2.00	0.44
2:B:569:THR:OG1	14:N:279:GLU:OE2	2.28	0.44
3:C:88:ASN:HB3	12:L:60:ARG:NH1	2.33	0.44
9:I:7:SER:H	13:M:93:ARG:HH12	1.64	0.44
13:M:160:ALA:HB2	13:M:173:ILE:HD11	1.98	0.44
15:O:295:GLN:HG2	15:O:650:VAL:HG22	2.00	0.44
1:A:716:ASP:HB2	1:A:789:ASN:ND2	2.33	0.43
1:A:808:GLN:HA	1:A:812:VAL:O	2.18	0.43
1:A:1183:PHE:HB3	1:A:1233:ASN:HB3	2.00	0.43
5:E:171:LYS:H	5:E:174:GLN:NE2	2.15	0.43
19:V:498:GLN:OE1	19:V:502:ARG:NH1	2.50	0.43
1:A:595:PRO:HG3	1:A:602:TYR:HB3	1.99	0.43
1:A:850:ASN:ND2	1:A:860:GLU:OE2	2.45	0.43
1:A:1261:GLN:O	1:A:1265:ARG:NH1	2.50	0.43
2:B:126:SER:OG	2:B:151:ARG:NE	2.45	0.43
2:B:667:VAL:HB	2:B:670:MET:HB2	1.99	0.43
5:E:47:CYS:HA	5:E:54:GLN:HG3	2.00	0.43
7:G:147:ARG:NH2	7:G:204:GLY:O	2.51	0.43
18:U:103:ILE:HG22	18:U:114:LEU:HD23	1.99	0.43
1:A:671:ASP:OD1	1:A:672:GLY:N	2.50	0.43
12:L:28:LYS:HB2	12:L:39:SER:HA	2.00	0.43
13:M:111:ARG:HD3	13:M:120:GLU:HB2	2.00	0.43
2:B:417:ASP:OD2	2:B:419:LEU:HD23	2.18	0.43
3:C:276:SER:C	3:C:277:ARG:HD2	2.39	0.43
15:O:57:LEU:HD23	15:O:58:GLY:N	2.34	0.43
15:O:466:PRO:HA	15:O:469:ASN:ND2	2.34	0.43
15:O:493:GLU:OE2	15:O:512:ARG:NH2	2.51	0.43
15:O:493:GLU:HA	15:O:496:ILE:HD12	2.00	0.43
1:A:553:ALA:HB1	1:A:557:PHE:HB2	2.00	0.43
13:M:164:LYS:HB3	13:M:167:GLN:HB2	1.99	0.43
16:P:313:ASP:O	16:P:314:GLU:HG3	2.17	0.43
1:A:774:ARG:HH21	1:A:804:LEU:HD11	1.83	0.43
2:B:775:LYS:HE2	2:B:927:LYS:HE2	2.01	0.43
15:O:107:LEU:HD22	15:O:108:GLN:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ARG:NE	2:B:1131:GLU:OE2	2.45	0.43
1:A:753:GLN:N	1:A:757:ASN:OD1	2.51	0.43
1:A:1257:PHE:HB2	9:I:14:ILE:HB	2.00	0.43
1:A:1316:THR:OG1	1:A:1317:ASN:N	2.51	0.43
8:H:93:TYR:CD1	8:H:145:ARG:HB3	2.53	0.43
1:A:495:TRP:HB3	2:B:908:LEU:HD21	2.00	0.43
1:A:583:MET:HB2	1:A:696:ARG:HG2	2.00	0.43
2:B:812:ASP:OD1	2:B:812:ASP:N	2.52	0.43
5:E:119:SER:HA	5:E:122:LYS:HD3	2.01	0.43
8:H:26:ILE:HG13	8:H:40:LEU:O	2.19	0.43
18:U:137:ARG:HH12	19:V:455:VAL:HB	1.84	0.43
6:F:135:ARG:HD3	6:F:143:PHE:HD1	1.84	0.43
2:B:259:ALA:HB1	2:B:302:LEU:HD13	2.01	0.42
2:B:343:ARG:HG2	2:B:542:THR:HG22	2.00	0.42
2:B:445:LYS:HE3	2:B:446:ARG:HH22	1.83	0.42
7:G:10:LEU:HA	7:G:69:ASN:HA	2.00	0.42
13:M:140:TRP:HD1	13:M:142:GLY:H	1.66	0.42
15:O:73:ARG:HG3	15:O:121:TYR:CE1	2.54	0.42
1:A:635:PRO:HA	1:A:636:PRO:HD3	1.95	0.42
5:E:74:ASP:OD1	5:E:74:ASP:N	2.49	0.42
15:O:537:LEU:O	15:O:541:ILE:HD12	2.18	0.42
16:P:269:LEU:HG	16:P:297:PHE:HE1	1.84	0.42
18:U:109:PRO:O	18:U:110:LYS:HG3	2.20	0.42
21:X:24:DA:H4'	21:X:25:DA:OP1	2.19	0.42
1:A:605:THR:HG23	1:A:607:LYS:H	1.84	0.42
1:A:1374:PHE:O	1:A:1378:LYS:NZ	2.44	0.42
2:B:304:TYR:O	2:B:308:LYS:NZ	2.42	0.42
2:B:1033:ASP:OD1	2:B:1033:ASP:N	2.48	0.42
18:U:63:ILE:H	18:U:63:ILE:HG13	1.66	0.42
1:A:84:LEU:HB2	1:A:261:LEU:HG	2.02	0.42
7:G:145:LYS:HE3	7:G:208:VAL:HG11	2.00	0.42
13:M:88:PHE:CE2	14:N:397:LEU:HD21	2.54	0.42
1:A:921:LEU:HA	1:A:1083:LEU:H	1.84	0.42
3:C:172:GLN:H	3:C:175:GLN:HE21	1.67	0.42
4:D:135:TYR:HE1	4:D:150:ILE:HD11	1.84	0.42
6:F:110:ASP:N	6:F:110:ASP:OD1	2.52	0.42
15:O:91:VAL:O	15:O:95:LEU:N	2.44	0.42
15:O:199:TYR:CD1	15:O:286:ARG:HD2	2.55	0.42
15:O:449:SER:HB3	15:O:452:LEU:HD13	2.02	0.42
1:A:66:GLU:OE2	1:A:72:GLY:N	2.42	0.42
1:A:223:ASN:HB2	1:A:316:TRP:HH2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:689:PRO:HG3	2:B:915:ARG:NH2	2.34	0.42
2:B:1006:SER:HB2	2:B:1013:LEU:HD21	2.01	0.42
3:C:276:SER:O	3:C:277:ARG:HD2	2.19	0.42
1:A:568:ASP:HB2	8:H:22:LYS:HB3	2.02	0.42
2:B:702:GLN:O	2:B:706:GLY:N	2.49	0.42
3:C:134:LEU:HD12	3:C:167:LEU:HB3	2.00	0.42
7:G:152:ARG:H	7:G:197:LEU:HB2	1.83	0.42
19:V:23:LEU:HB3	19:V:33:GLU:HG2	2.02	0.42
2:B:297:THR:HG23	2:B:300:GLN:H	1.84	0.42
8:H:104:PHE:HE1	8:H:114:VAL:HG13	1.85	0.42
13:M:85:LEU:HD11	13:M:173:ILE:HG12	2.02	0.42
20:W:440:ASN:O	20:W:444:GLN:NE2	2.52	0.42
2:B:961:LEU:HD23	2:B:1018:PHE:CE2	2.55	0.42
5:E:79:TRP:NE1	5:E:81:GLU:OE2	2.53	0.42
6:F:93:ILE:HA	6:F:96:THR:HG22	2.01	0.42
15:O:457:LEU:HG	15:O:460:LEU:HD22	2.02	0.42
1:A:163:VAL:O	1:A:181:ASP:N	2.53	0.41
1:A:688:GLN:O	1:A:692:ASN:ND2	2.53	0.41
2:B:108:THR:HG22	2:B:109:LYS:H	1.84	0.41
3:C:118:SER:HA	3:C:125:LYS:HD2	2.02	0.41
15:O:624:LEU:HD13	15:O:628:LYS:HE3	2.02	0.41
20:W:426:ILE:H	20:W:426:ILE:HG13	1.71	0.41
1:A:1318:HIS:O	1:A:1321:GLU:HG2	2.19	0.41
2:B:755:ALA:HB2	2:B:782:PHE:CE1	2.55	0.41
2:B:916:HIS:HD1	2:B:957:LYS:HG3	1.85	0.41
4:D:12:SER:HA	4:D:121:LEU:HD21	2.02	0.41
15:O:259:LEU:H	15:O:259:LEU:HD23	1.85	0.41
18:U:68:GLN:HE22	18:U:163:SER:H	1.68	0.41
18:U:83:LYS:HD3	18:U:87:LEU:HD23	2.01	0.41
13:M:186:ILE:O	13:M:190:ASN:ND2	2.53	0.41
1:A:931:GLN:HB3	1:A:933:VAL:HG22	2.01	0.41
2:B:914:SER:OG	2:B:957:LYS:HD3	2.20	0.41
3:C:248:GLN:HA	3:C:256:ILE:HD11	2.02	0.41
4:D:110:LEU:HD21	4:D:153:MET:HG3	2.03	0.41
16:P:256:VAL:HG13	16:P:260:CYS:HB3	2.02	0.41
22:Y:63:DT:H1'	22:Y:64:DA:H5'	2.02	0.41
2:B:796:LYS:HE3	2:B:798:TYR:HE1	1.84	0.41
2:B:885:MET:HB3	12:L:57:LEU:HD13	2.02	0.41
1:A:599:LYS:HB3	1:A:600:PRO:HD3	2.03	0.41
1:A:964:ASN:HA	1:A:967:LEU:HD23	2.01	0.41
1:A:996:ASP:OD1	1:A:996:ASP:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:GLY:HA3	2:B:429:ILE:HD11	2.01	0.41
2:B:201:SER:HA	2:B:376:ARG:HG2	2.02	0.41
7:G:81:LEU:HD23	7:G:81:LEU:H	1.86	0.41
21:X:33:DT:H2''	21:X:34:DT:OP1	2.19	0.41
1:A:634:VAL:HA	1:A:635:PRO:HD3	1.86	0.41
2:B:795:LEU:HD12	2:B:894:ALA:HB3	2.02	0.41
3:C:328:LEU:H	3:C:328:LEU:HD23	1.86	0.41
18:U:134:LEU:HD22	18:U:137:ARG:HH21	1.84	0.41
18:U:186:GLU:OE1	18:U:189:LEU:N	2.50	0.41
19:V:268:ALA:O	19:V:272:VAL:N	2.54	0.41
22:Y:73:DT:H2''	22:Y:74:DA:C8	2.56	0.41
1:A:195:ASP:OD1	1:A:195:ASP:N	2.53	0.41
1:A:378:ARG:NE	1:A:516:GLU:OE2	2.45	0.41
1:A:386:ASN:O	1:A:699:LYS:NZ	2.53	0.41
2:B:77:ILE:H	2:B:77:ILE:HG13	1.70	0.41
2:B:613:ILE:HD11	2:B:673:LEU:HD22	2.03	0.41
2:B:936:GLN:O	10:J:43:ARG:NH1	2.36	0.41
1:A:201:TRP:CD1	1:A:205:LEU:HD11	2.55	0.41
1:A:555:GLN:O	1:A:799:SER:HB2	2.21	0.41
1:A:1333:TYR:HD2	5:E:149:LEU:HD13	1.86	0.41
1:A:1336:ILE:HD13	1:A:1355:ILE:HG22	2.03	0.41
1:A:1437:SER:OG	1:A:1438:GLU:N	2.53	0.41
2:B:267:GLU:OE2	2:B:546:SER:HB3	2.20	0.41
10:J:14:VAL:HG12	10:J:17:LYS:HD2	2.03	0.41
15:O:105:LYS:HE2	15:O:123:ASN:HA	2.03	0.41
15:O:213:ASP:N	15:O:213:ASP:OD1	2.54	0.41
18:U:102:VAL:H	18:U:115:ILE:HD11	1.86	0.41
18:U:105:ARG:NH2	20:W:437:THR:OG1	2.53	0.41
19:V:215:PHE:HB3	19:V:223:ILE:HG21	2.02	0.41
20:W:467:ILE:HG13	20:W:468:LEU:HD12	2.01	0.41
22:Y:68:DG:H2''	22:Y:69:DA:H5'	2.03	0.41
1:A:57:LYS:O	1:A:69:THR:OG1	2.37	0.41
1:A:895:ASP:HB3	1:A:1411:VAL:HG23	2.03	0.41
4:D:130:ASN:ND2	4:D:132:VAL:HG12	2.36	0.41
14:N:313:LEU:H	14:N:313:LEU:HD23	1.86	0.41
19:V:154:VAL:HG11	20:W:408:TYR:HD1	1.86	0.41
19:V:497:GLU:O	19:V:500:SER:OG	2.28	0.41
21:X:45:DT:H2''	21:X:46:DA:C8	2.55	0.41
2:B:117:GLU:HG2	12:L:55:ILE:HD12	2.02	0.40
13:M:165:ASP:OD1	13:M:165:ASP:N	2.54	0.40
16:P:225:ILE:H	16:P:225:ILE:HG13	1.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:49:LEU:HD12	11:K:63:PHE:CZ	2.57	0.40
1:A:937:ARG:HH22	1:A:1077:LYS:NZ	2.19	0.40
2:B:913:SER:OG	2:B:914:SER:N	2.54	0.40
5:E:13:TRP:CD2	5:E:39:LEU:HD23	2.56	0.40
8:H:108:SER:OG	8:H:111:LEU:HD12	2.21	0.40
18:U:193:LEU:HB3	18:U:206:ILE:HG13	2.04	0.40
18:U:215:THR:OG1	21:X:24:DA:N3	2.44	0.40
4:D:68:ILE:O	4:D:72:PHE:N	2.46	0.40
15:O:517:VAL:HG12	15:O:566:PHE:HB2	2.04	0.40
18:U:230:ILE:O	18:U:234:LEU:N	2.52	0.40
1:A:231:PHE:O	1:A:234:ILE:HG12	2.22	0.40
1:A:637:LYS:HB2	1:A:641:LEU:HD13	2.04	0.40
2:B:362:ASN:OD1	2:B:362:ASN:N	2.55	0.40
4:D:149:THR:HA	4:D:152:GLU:HB3	2.04	0.40
15:O:39:GLN:HA	15:O:43:ASN:ND2	2.35	0.40
18:U:204:LEU:HD13	18:U:214:LEU:HD13	2.03	0.40
20:W:318:ARG:HH11	20:W:448:TYR:HB2	1.87	0.40
20:W:424:GLU:O	20:W:446:TYR:OH	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1389/1460 (95%)	1251 (90%)	138 (10%)	0	100	100
2	B	1112/1149 (97%)	995 (90%)	117 (10%)	0	100	100
3	C	333/335 (99%)	304 (91%)	29 (9%)	0	100	100
4	D	113/161 (70%)	103 (91%)	10 (9%)	0	100	100
5	E	212/215 (99%)	195 (92%)	17 (8%)	0	100	100
6	F	81/155 (52%)	72 (89%)	9 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	174/212 (82%)	154 (88%)	19 (11%)	1 (1%)	25	64
8	H	136/146 (93%)	124 (91%)	12 (9%)	0	100	100
9	I	32/110 (29%)	26 (81%)	6 (19%)	0	100	100
10	J	65/70 (93%)	57 (88%)	8 (12%)	0	100	100
11	K	99/142 (70%)	94 (95%)	5 (5%)	0	100	100
12	L	43/70 (61%)	38 (88%)	5 (12%)	0	100	100
13	M	167/282 (59%)	150 (90%)	16 (10%)	1 (1%)	25	64
14	N	100/422 (24%)	87 (87%)	13 (13%)	0	100	100
15	O	528/654 (81%)	491 (93%)	37 (7%)	0	100	100
16	P	93/317 (29%)	83 (89%)	10 (11%)	0	100	100
17	Q	33/251 (13%)	29 (88%)	4 (12%)	0	100	100
18	U	178/240 (74%)	166 (93%)	12 (7%)	0	100	100
19	V	331/596 (56%)	300 (91%)	31 (9%)	0	100	100
20	W	168/594 (28%)	154 (92%)	14 (8%)	0	100	100
All	All	5387/7581 (71%)	4873 (90%)	512 (10%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	M	202	PRO
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%)	1195 (98%)	19 (2%)	62	79
2	B	973/1006 (97%)	957 (98%)	16 (2%)	62	79
3	C	296/296 (100%)	294 (99%)	2 (1%)	84	90
4	D	110/145 (76%)	107 (97%)	3 (3%)	44	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	196/197 (100%)	192 (98%)	4 (2%)	55	73
6	F	73/137 (53%)	72 (99%)	1 (1%)	67	80
7	G	160/190 (84%)	158 (99%)	2 (1%)	69	82
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%)	61 (98%)	1 (2%)	62	79
11	K	91/130 (70%)	90 (99%)	1 (1%)	73	84
12	L	40/57 (70%)	40 (100%)	0	100	100
13	M	145/249 (58%)	144 (99%)	1 (1%)	84	90
14	N	88/360 (24%)	85 (97%)	3 (3%)	37	61
15	O	489/593 (82%)	480 (98%)	9 (2%)	59	76
16	P	95/285 (33%)	93 (98%)	2 (2%)	53	71
17	Q	31/212 (15%)	31 (100%)	0	100	100
18	U	152/205 (74%)	145 (95%)	7 (5%)	27	54
19	V	293/513 (57%)	285 (97%)	8 (3%)	44	66
20	W	155/534 (29%)	152 (98%)	3 (2%)	57	74
All	All	4817/6657 (72%)	4734 (98%)	83 (2%)	62	78

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	ARG
1	A	137	ARG
1	A	274	MET
1	A	310	ASN
1	A	311	ASN
1	A	410	ARG
1	A	483	LEU
1	A	499	ARG
1	A	746	ASN
1	A	774	ARG
1	A	789	ASN
1	A	848	VAL
1	A	929	ASN
1	A	933	VAL
1	A	944	ASN

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Mol	Chain	Res	Type
1	A	1187	ARG
1	A	1265	ARG
1	A	1332	ARG
1	A	1439	LYS
2	B	66	ASN
2	B	212	LYS
2	B	213	LYS
2	B	293	LEU
2	B	321	GLN
2	B	379	LEU
2	B	383	LEU
2	B	451	ARG
2	B	481	ARG
2	B	816	ASP
2	B	867	ARG
2	B	885	MET
2	B	970	ASN
2	B	1038	ARG
2	B	1054	ARG
2	B	1136	ASN
3	C	174	ARG
3	C	277	ARG
4	D	71	ASN
4	D	98	MET
4	D	130	ASN
5	E	7	ARG
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	1	MET
10	J	14	VAL
11	K	74	ASN
13	M	144	ASN
14	N	297	MET
14	N	300	LYS
14	N	391	LEU
15	O	205	LYS
15	O	238	ARG
15	O	263	LEU

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Mol	Chain	Res	Type
15	O	268	LYS
15	O	286	ARG
15	O	580	ASN
15	O	585	MET
15	O	631	ASN
15	O	636	ASN
16	P	189	ASN
16	P	271	MET
18	U	110	LYS
18	U	141	ARG
18	U	151	LYS
18	U	159	ASN
18	U	205	LEU
18	U	239	LYS
18	U	240	MET
19	V	115	ASN
19	V	149	ARG
19	V	150	LEU
19	V	189	LEU
19	V	237	LEU
19	V	269	LYS
19	V	475	LEU
19	V	481	LYS
20	W	292	ASN
20	W	451	ARG
20	W	502	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	A	208	ASN
1	A	229	ASN
1	A	310	ASN
1	A	311	ASN
1	A	367	ASN
1	A	520	HIS
1	A	578	GLN
1	A	630	ASN
1	A	688	GLN
1	A	692	ASN
1	A	746	ASN

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Mol	Chain	Res	Type
1	A	760	GLN
1	A	789	ASN
1	A	815	GLN
1	A	834	HIS
1	A	929	ASN
1	A	1058	GLN
1	A	1131	ASN
1	A	1185	GLN
1	A	1318	HIS
1	A	1419	GLN
2	B	61	HIS
2	B	66	ASN
2	B	203	ASN
2	B	217	GLN
2	B	382	GLN
2	B	574	GLN
2	B	577	HIS
2	B	596	GLN
2	B	600	HIS
2	B	655	ASN
2	B	693	HIS
2	B	821	HIS
2	B	844	ASN
2	B	947	HIS
2	B	970	ASN
2	B	1136	ASN
3	C	175	GLN
3	C	234	ASN
4	D	71	ASN
4	D	130	ASN
5	E	174	GLN
7	G	31	ASN
7	G	113	ASN
9	I	9	ASN
10	J	26	GLN
10	J	53	HIS
11	K	95	HIS
12	L	53	HIS
13	M	92	ASN
13	M	141	ASN
13	M	144	ASN
13	M	190	ASN

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Mol	Chain	Res	Type
15	O	43	ASN
15	O	161	GLN
15	O	207	HIS
15	O	244	ASN
15	O	332	GLN
15	O	544	ASN
15	O	572	HIS
15	O	580	ASN
15	O	584	ASN
15	O	631	ASN
15	O	636	ASN
16	P	189	ASN
18	U	68	GLN
18	U	91	ASN
18	U	144	GLN
18	U	159	ASN
18	U	219	GLN
19	V	6	ASN
19	V	20	ASN
19	V	115	ASN
19	V	140	HIS
19	V	184	HIS
19	V	473	HIS
20	W	292	ASN
20	W	391	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

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

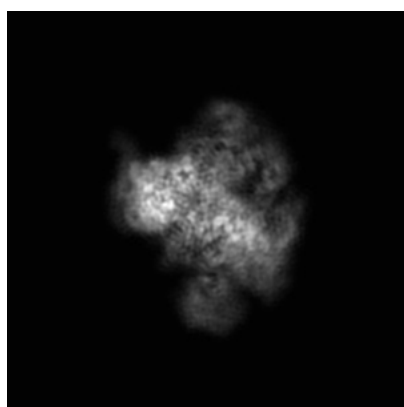
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4183. These allow visual inspection of the internal detail of the map and identification of artifacts.

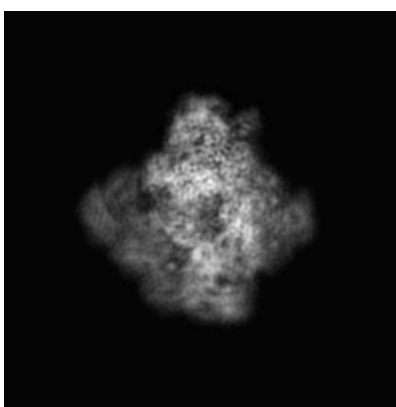
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

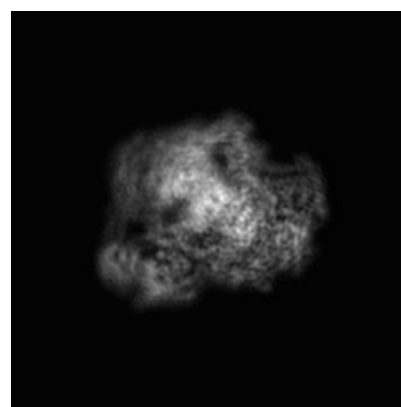
6.1.1 Primary map



X



Y

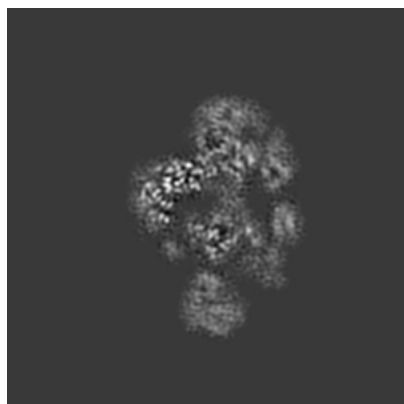


Z

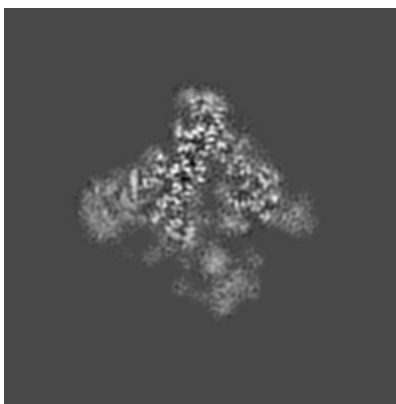
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

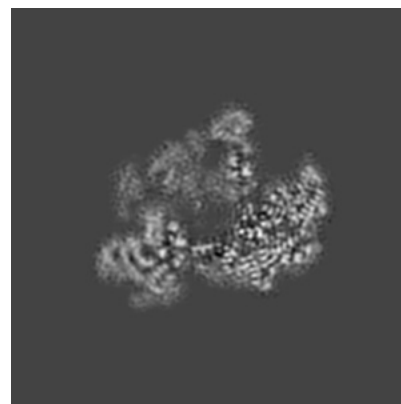
6.2.1 Primary map



X Index: 120



Y Index: 120

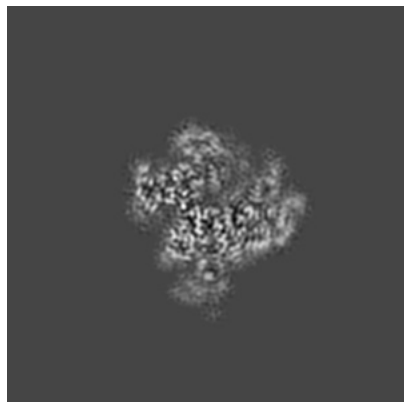


Z Index: 120

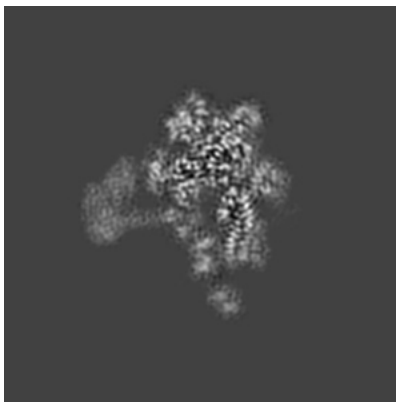
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

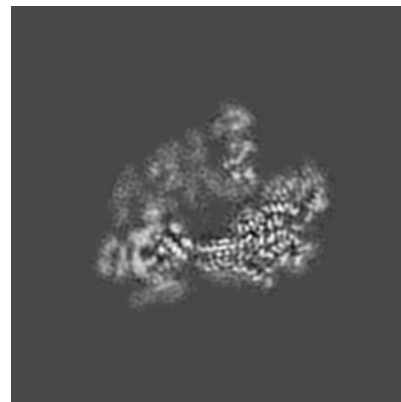
6.3.1 Primary map



X Index: 138



Y Index: 109

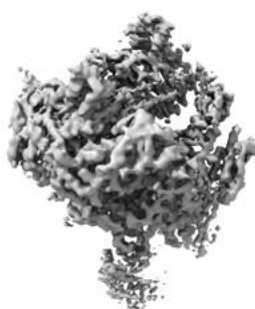


Z Index: 123

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

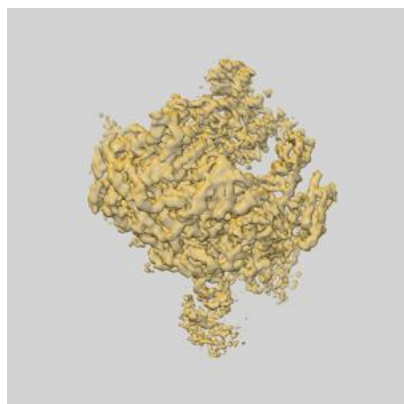
6.5 Mask visualisation [i](#)

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

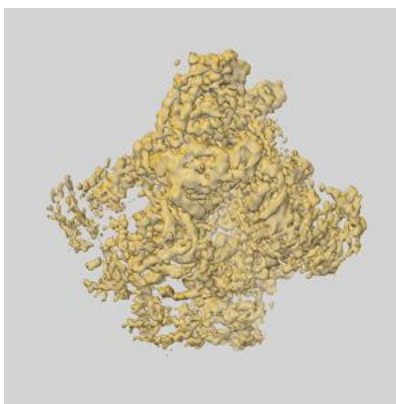
A mask typically either:

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

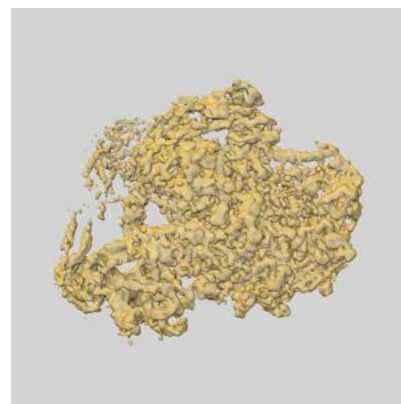
6.5.1 emd_4183_msk_1.map [i](#)



X



Y

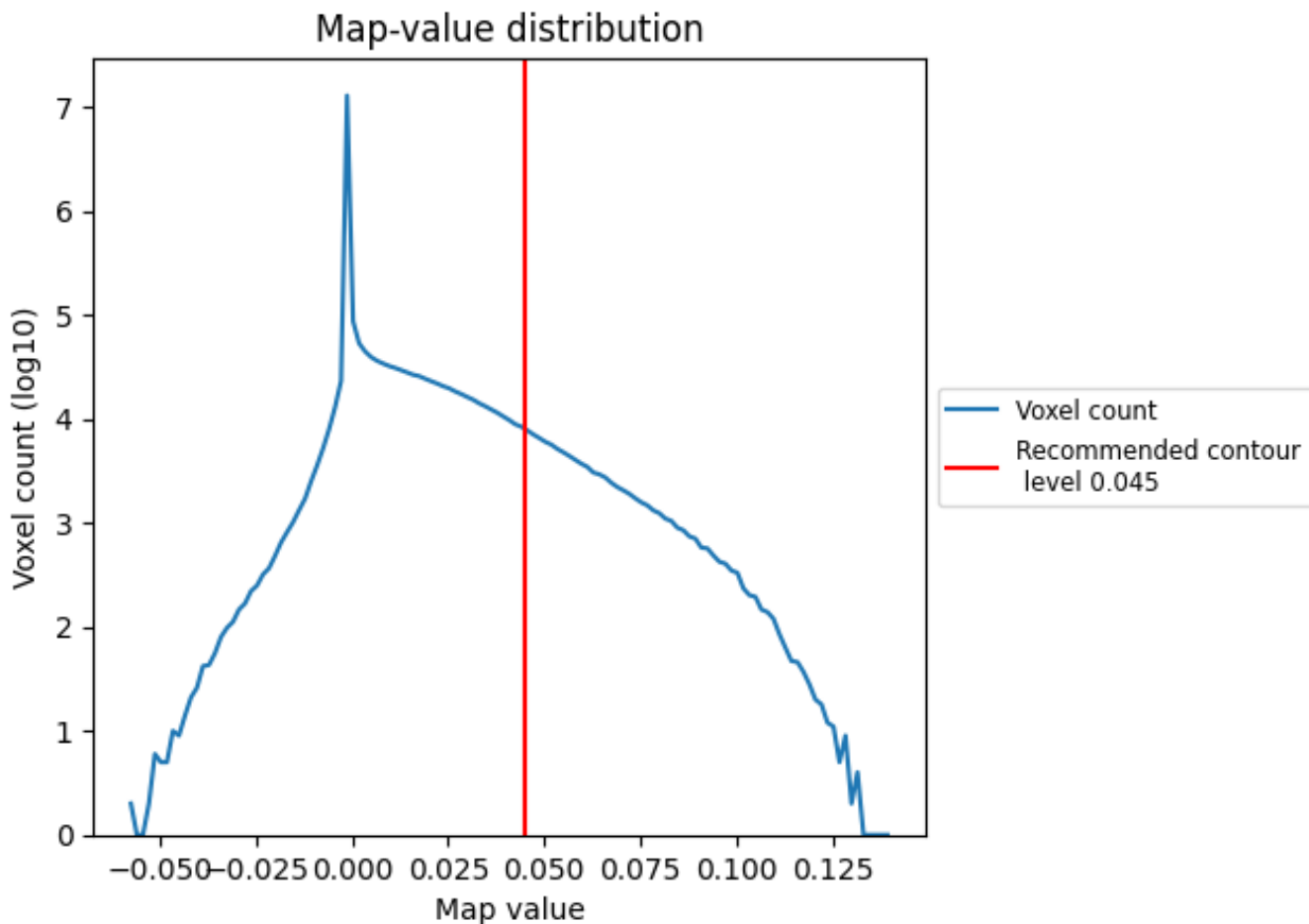


Z

7 Map analysis [i](#)

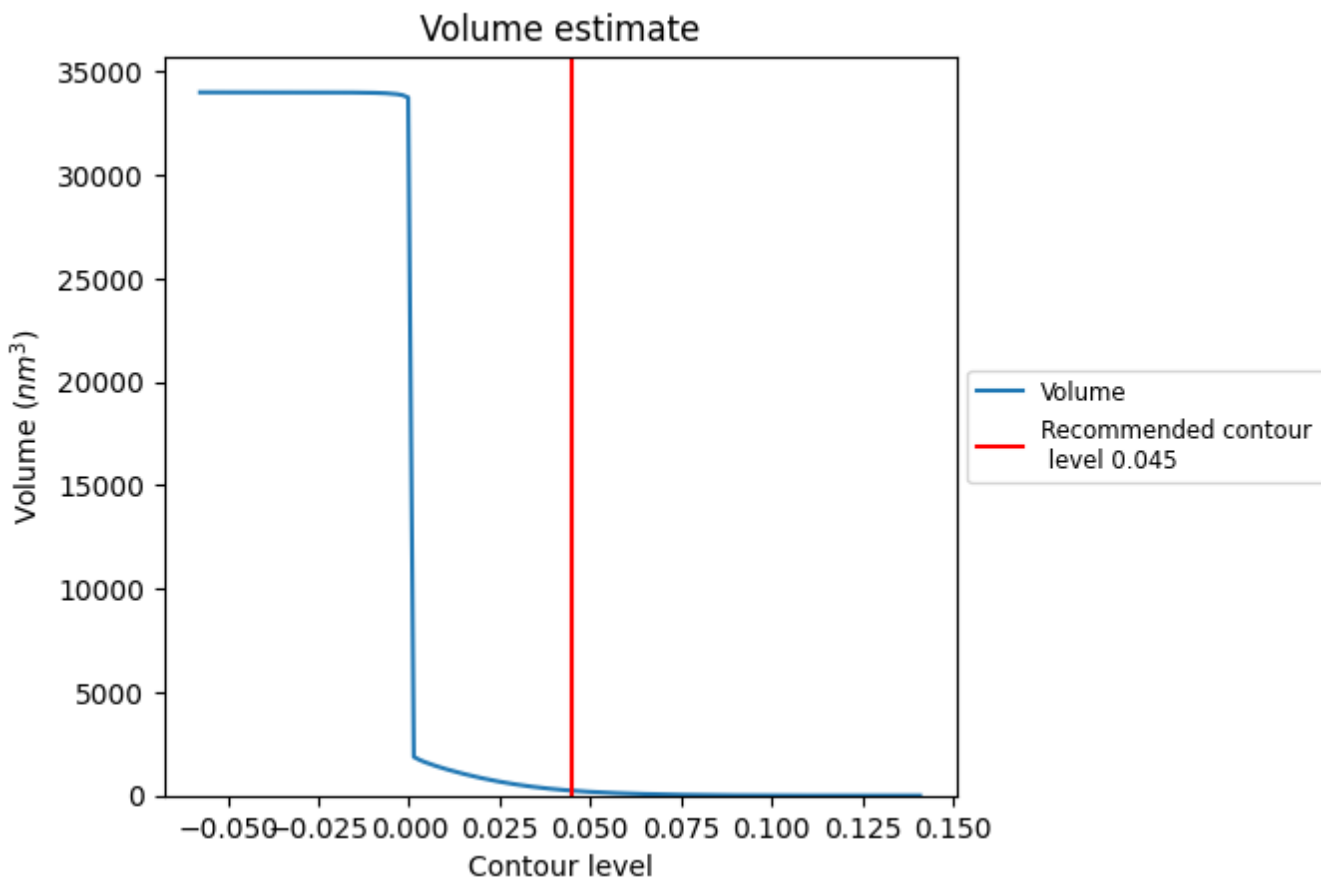
This section contains the results of statistical analysis of the map.

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.

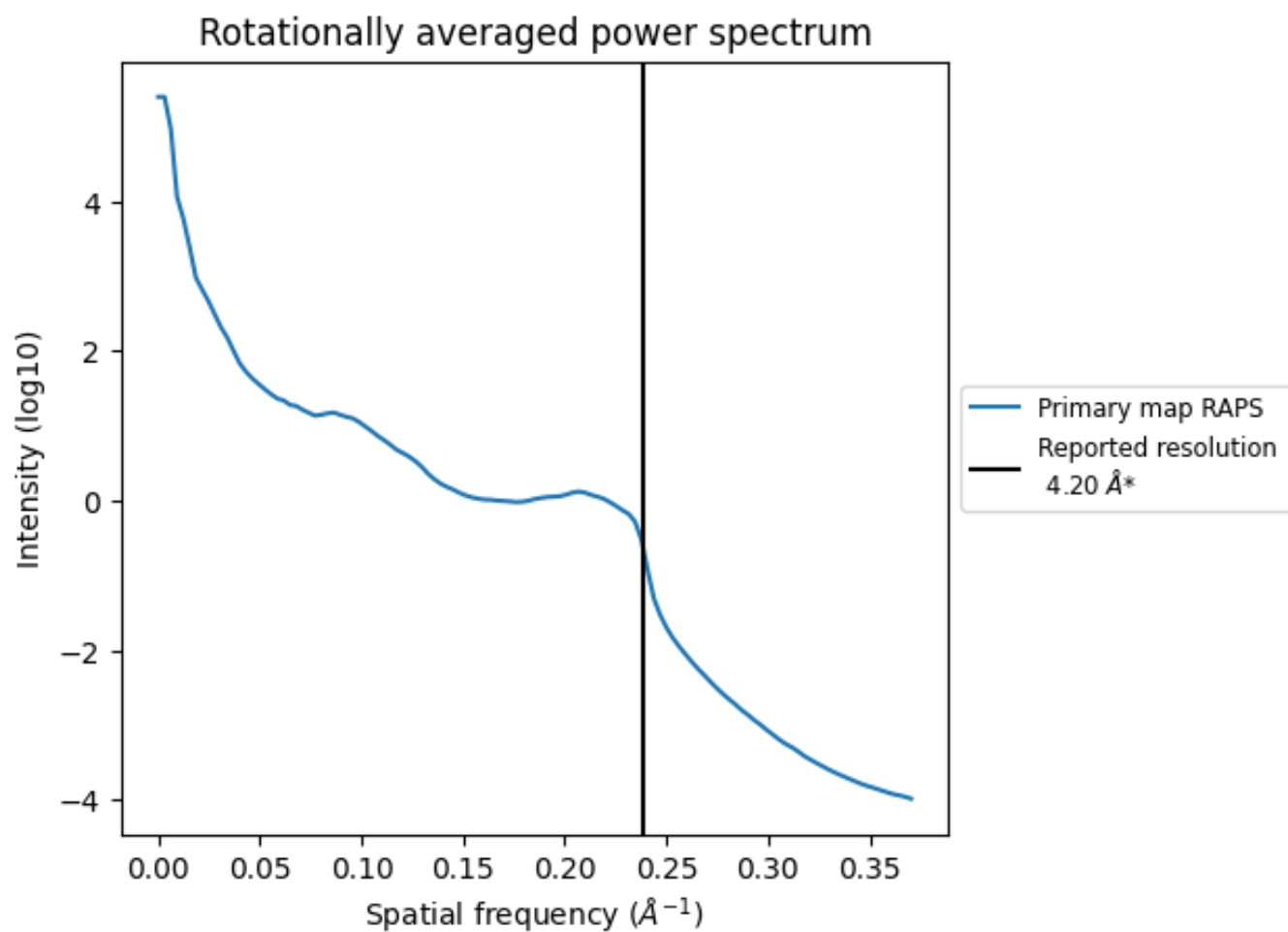
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 237 nm³; this corresponds to an approximate mass of 214 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](#)

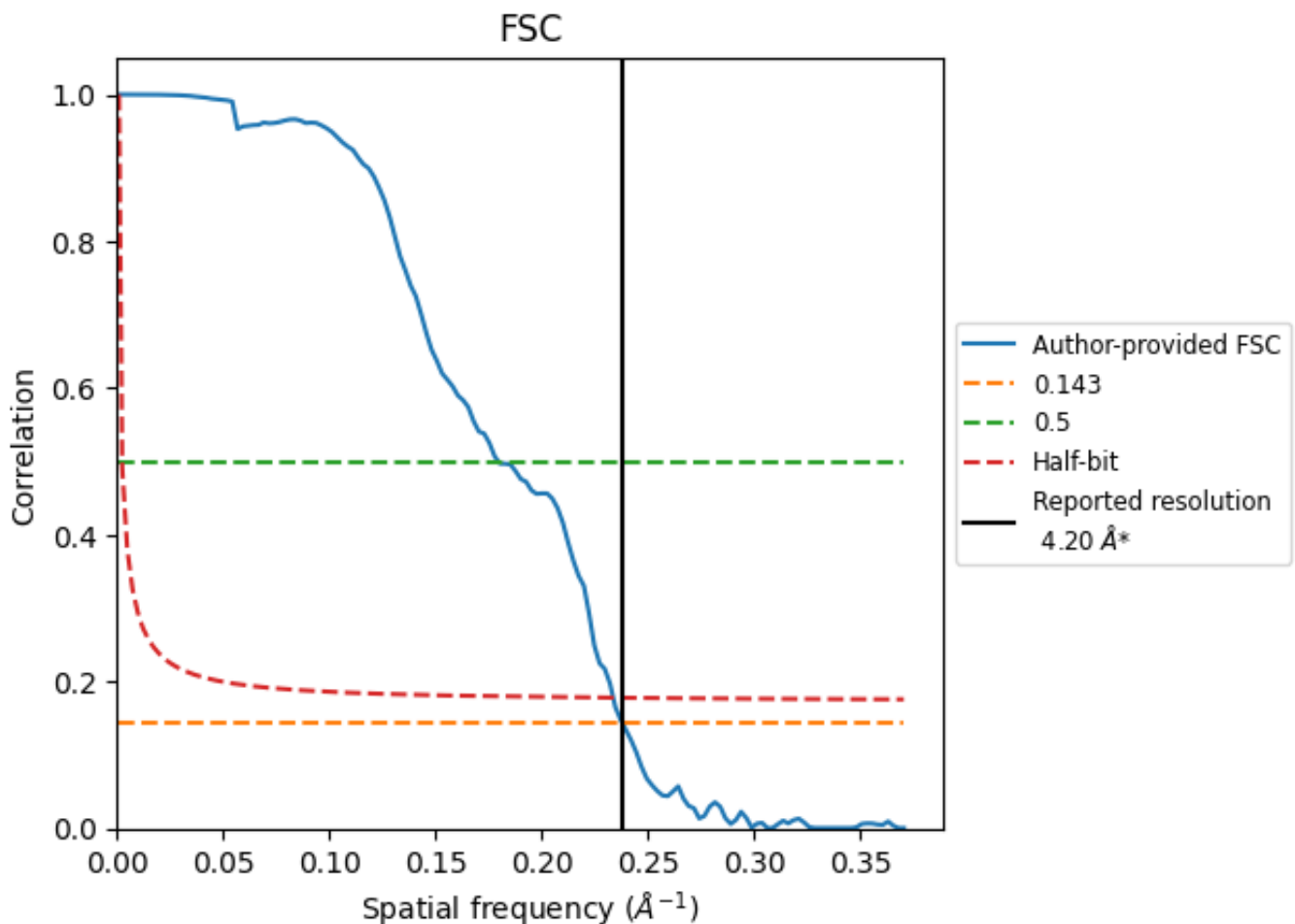


*Reported resolution corresponds to spatial frequency of 0.238\AA^{-1}

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 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

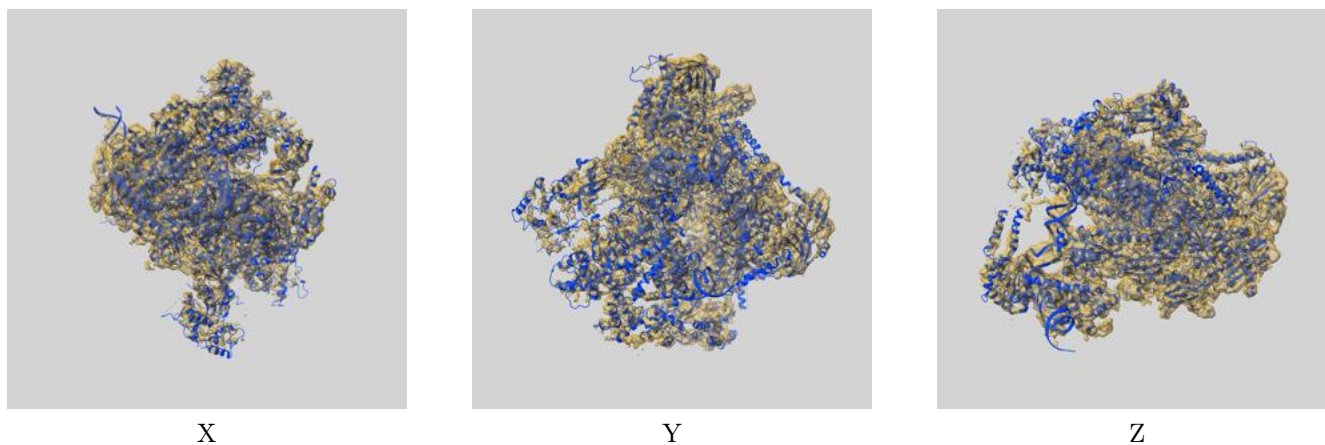
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.20	5.57	4.28
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

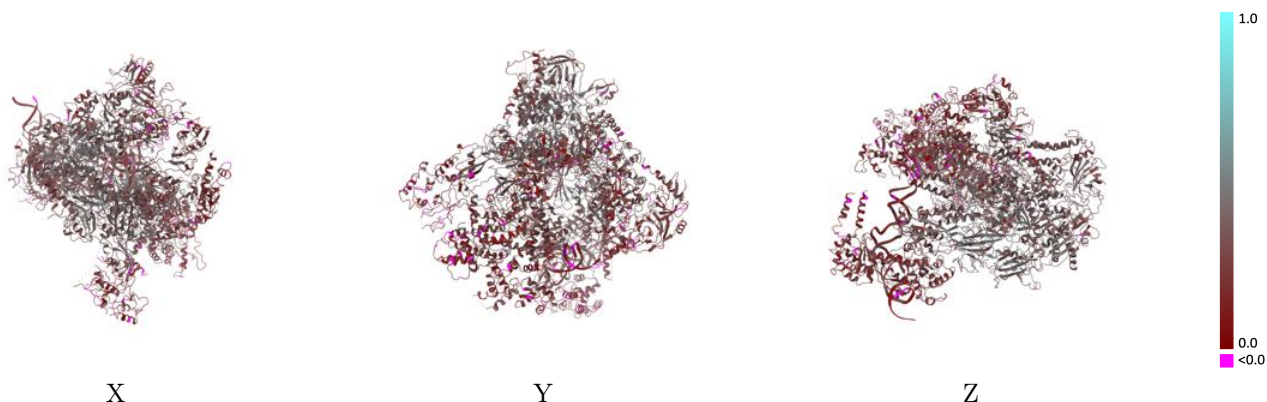
This section contains information regarding the fit between EMDB map EMD-4183 and PDB model 6F44. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



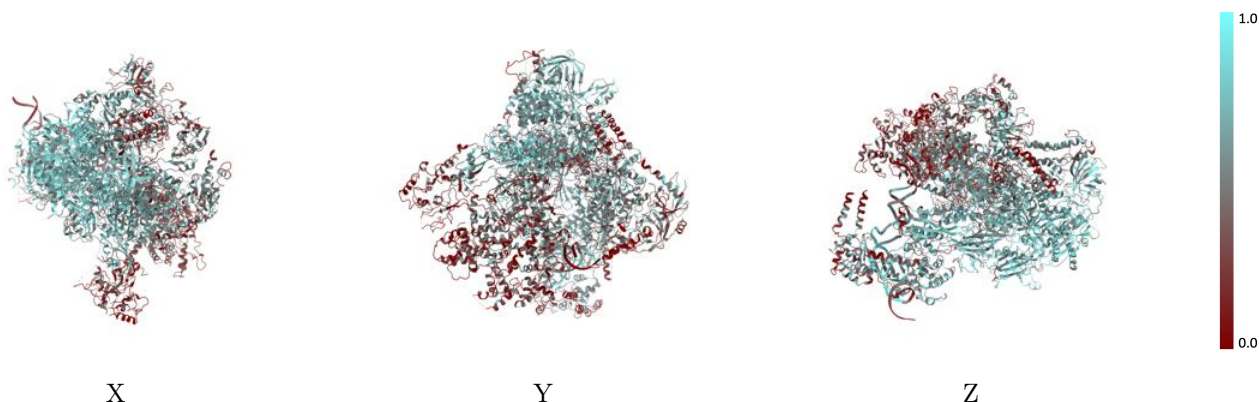
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



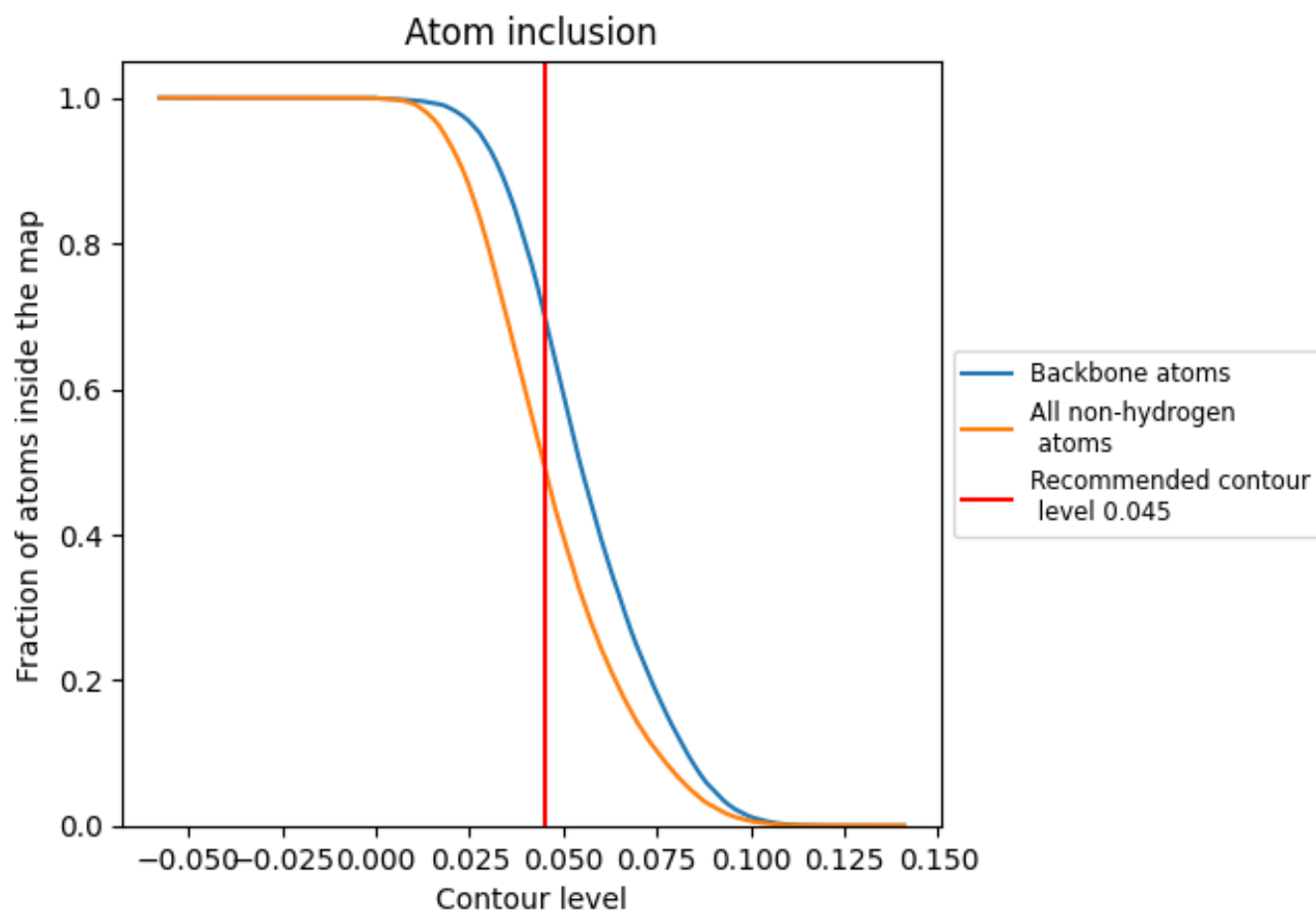
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.045).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 49% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4922	 0.3030
A	 0.4995	 0.3360
B	 0.6028	 0.3740
C	 0.7178	 0.3760
D	 0.1687	 0.1900
E	 0.5006	 0.2660
F	 0.6830	 0.3710
G	 0.3004	 0.2240
H	 0.6264	 0.3500
I	 0.4365	 0.2480
J	 0.7509	 0.3910
K	 0.7088	 0.3800
L	 0.6416	 0.3720
M	 0.2978	 0.2330
N	 0.3685	 0.2570
O	 0.2532	 0.2260
P	 0.2442	 0.2220
Q	 0.3296	 0.2410
U	 0.5173	 0.2120
V	 0.4882	 0.2610
W	 0.3634	 0.2300
X	 0.5692	 0.1800
Y	 0.5319	 0.1930

