Full wwPDB EM Validation Report (i)

Jun 26, 2024 – 01:57 PM JST

PDB ID	:	7Y8R
EMDB ID	:	EMD-33684
Title	:	The nucleosome-bound human PBAF complex
Authors	:	Wang, L.; Yu, J.; Yu, Z.; Wang, Q.; He, S.; Xu, Y.
Deposited on	:	2022-06-24
Resolution	:	4.40 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 (1)) were used in the production of this report:

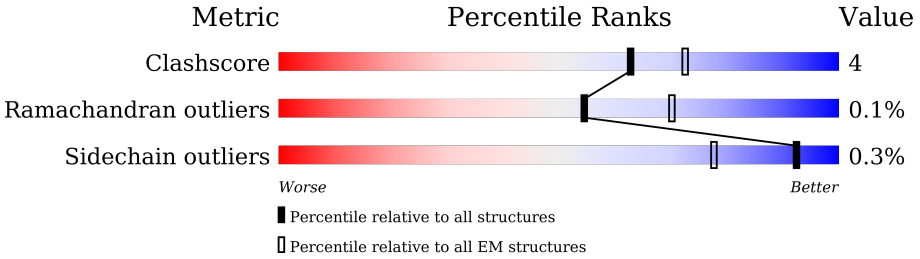
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 4.40 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	135	65% 8% 27%
1	E	135	67% 6% 27%
2	B	102	15% 89% 8%
2	F	102	83% 15%
3	C	129	76% 5% 19%
3	G	129	69% 15% 16%
4	D	125	74% 23%
4	H	125	67% 8% 25%

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Mol	Chain	Length	Quality of chain
5	Z	29	100%
6	I	1647	40% 56%
7	J	375	13% 82% 14%
8	K	429	5% 70% 12% 17%
9	L	1835	24% 72%
10	M	385	24% 83% 11% 6%
11	N	1214	19% 79%
11	O	1214	22% 76%
12	a	12	17% 100%
13	P	515	13% 68% 7% 25%
14	Q	411	5% 20% 78%
15	R	498	7% 91%
16	S	651	20% 30% 67%
17	T	22	18% 100%
18	U	1597	99%
19	V	102	19% 82% 18%
20	X	213	48% 30% 23%
21	Y	213	60% 18% 23%
22	W	24	29% 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	ADP	I	1701	-	-	X	-

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 43109 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 Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	99	815	514	158	139	4	0	0
1	E	98	806	508	156	138	4	0	0

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	94	741	465	150	125	1	0	0
2	F	87	702	442	142	117	1	0	0

- Molecule 3 is a protein called Histone H2A type 1-C.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	104	799	504	156	139	0	0
3	G	108	833	525	165	143	0	0

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	96	755	473	138	142	2	0	0
4	H	94	736	461	134	139	2	0	0

- Molecule 5 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	Z	29	141	83	29	29	0	0

- Molecule 6 is a protein called Transcription activator BRG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	I	732	6051	3831	1104	1087	29	0	0

- Molecule 7 is a protein called ACTB protein (Fragment).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	J	360	2821	1786	474	543	18	0	0

- Molecule 8 is a protein called Actin-like protein 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	K	356	2787	1767	470	529	21	0	0

- Molecule 9 is a protein called AT-rich interactive domain-containing protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	L	521	4151	2642	708	777	24	0	0

- Molecule 10 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily B member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	M	362	2918	1828	511	564	15	0	0

- Molecule 11 is a protein called SWI/SNF complex subunit SMARCC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	N	255	2085	1324	366	384	11	0	0
11	O	297	2354	1489	418	434	13	0	0

- Molecule 12 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	a	12	58	34	12	12	0	0

- Molecule 13 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily D member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	P	385	3174	2006	562	592	14	0	0

- Molecule 14 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	Q	91	739	456	145	135	3	0	0

- Molecule 15 is a protein called PHD finger protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	R	44	366	230	69	66	1	0	0

- Molecule 16 is a protein called Bromodomain-containing protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	S	213	1738	1102	288	337	11	0	0

- Molecule 17 is a protein called Unkown.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	T	22	110	66	22	22	0	0

- Molecule 18 is a protein called Protein polybromo-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	U	11	92	60	14	18	0	0

- Molecule 19 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	V	84	420	252	84	84	0	0

- Molecule 20 is a DNA chain called DNA (213-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
20	X	165	3360	1596	606	993	165	0	0

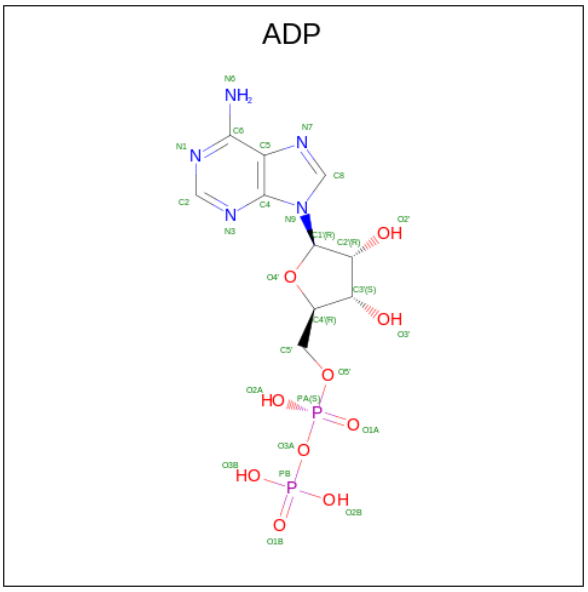
- Molecule 21 is a DNA chain called DNA (213-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
21	Y	165	3405	1610	643	987	165	0	0

- Molecule 22 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	W	24	120	72	24	24	0	0

- Molecule 23 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

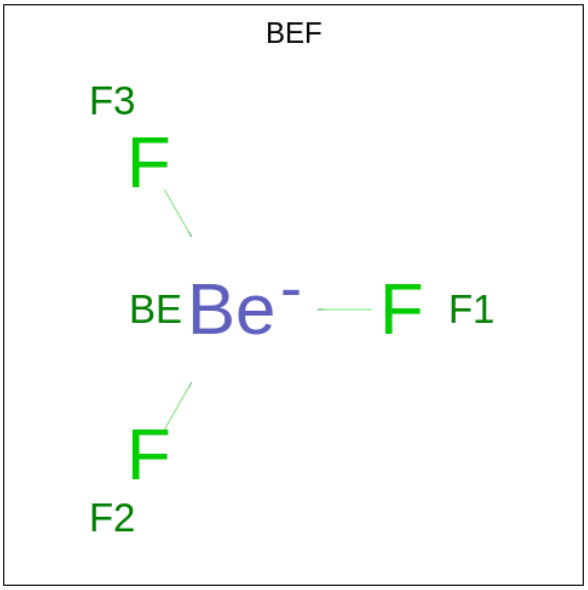


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
23	I	1	27	10	5	10	2	0

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
24	I	1	1	1	0

- Molecule 25 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



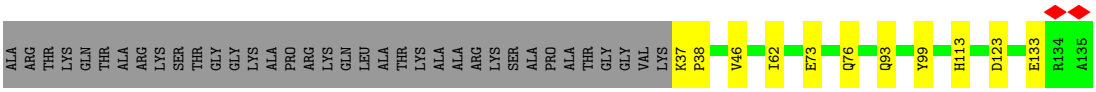
Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
25	I	1	4	1	3	0

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.

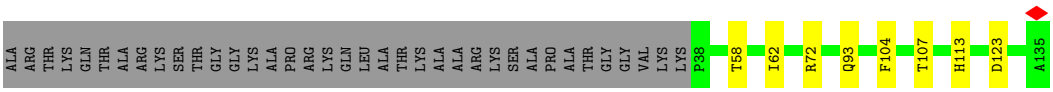
• Molecule 1: Histone H3

Chain A:



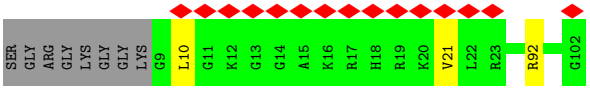
• Molecule 1: Histone H3

Chain E:



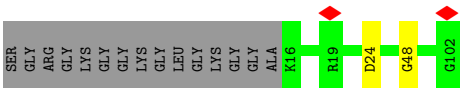
• Molecule 2: Histone H4

Chain B:



• Molecule 2: Histone H4

Chain F:

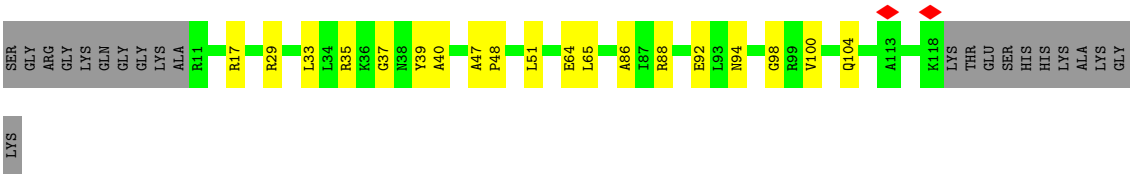


• Molecule 3: Histone H2A type 1-C

Chain C:

• Molecule 3: Histone H2A type 1-C

Chain G:

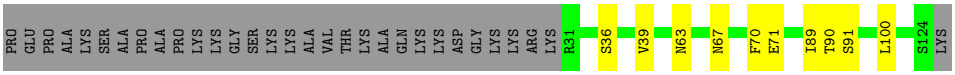


- Molecule 4: Histone H2B

Chain D:

- Molecule 4: Histone H2B

Chain H:



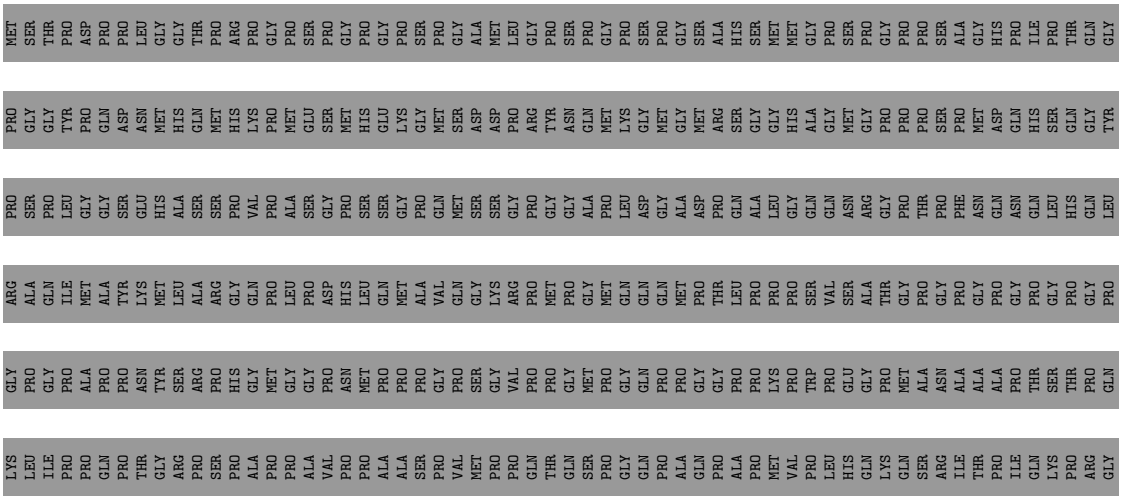
- Molecule 5: Unknown

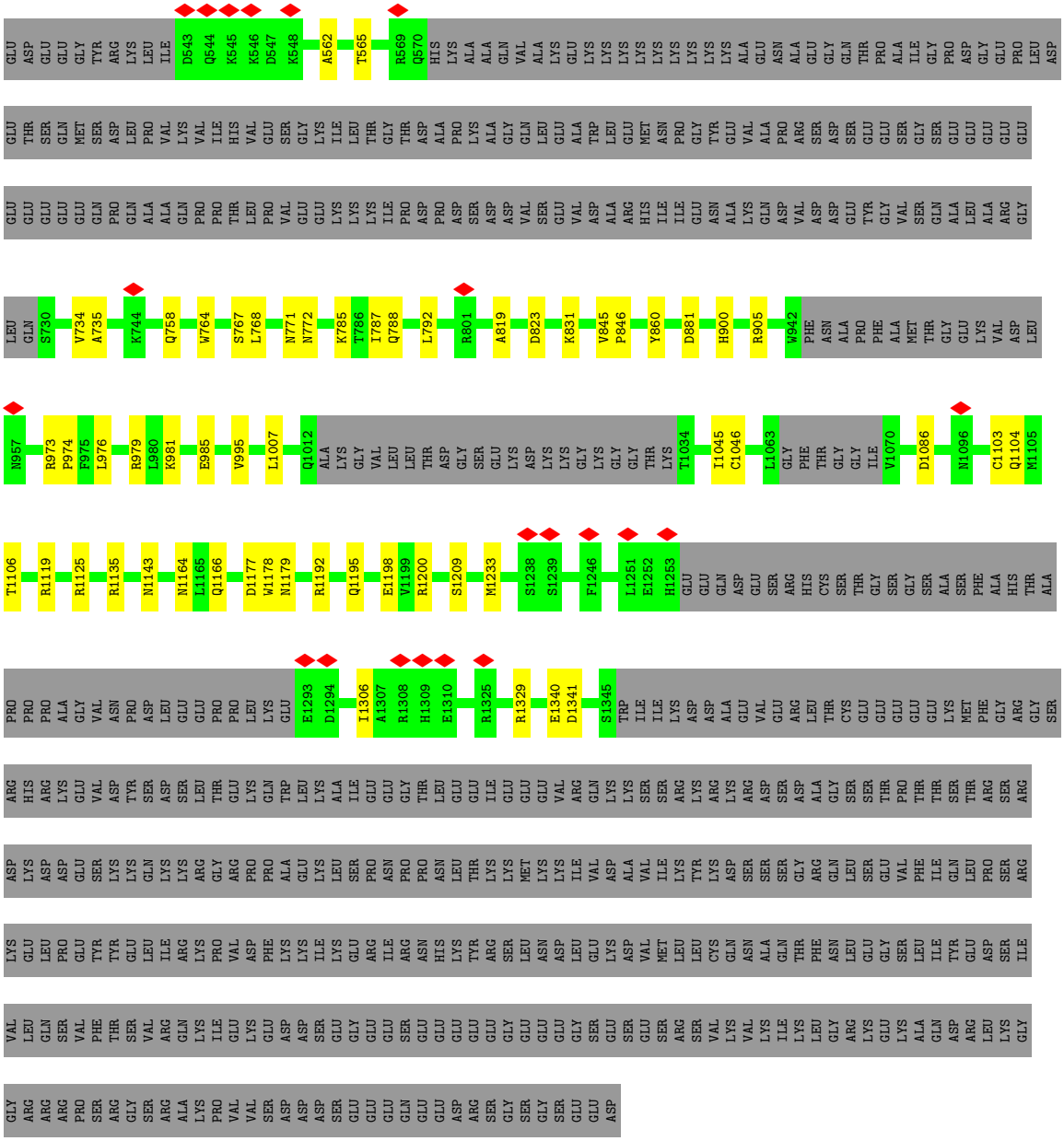
Chain Z:

There are no outlier residues recorded for this chain.

- Molecule 6: Transcription activator BRG1

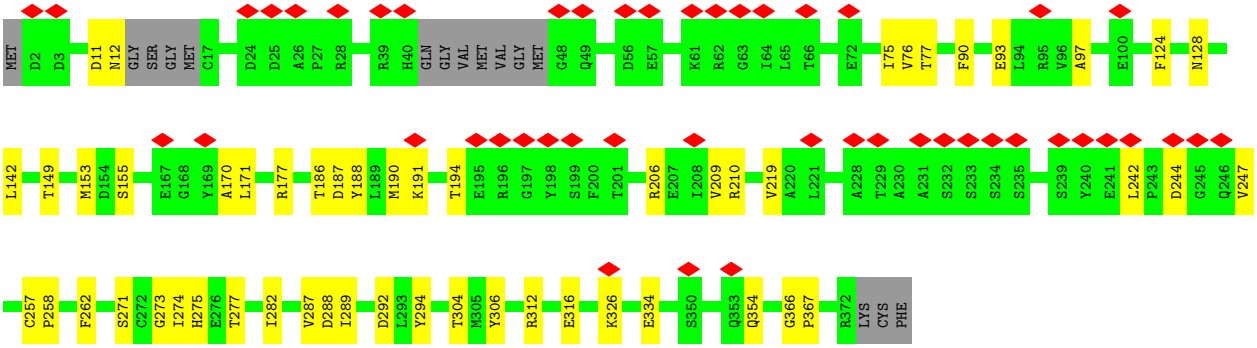
Chain I:





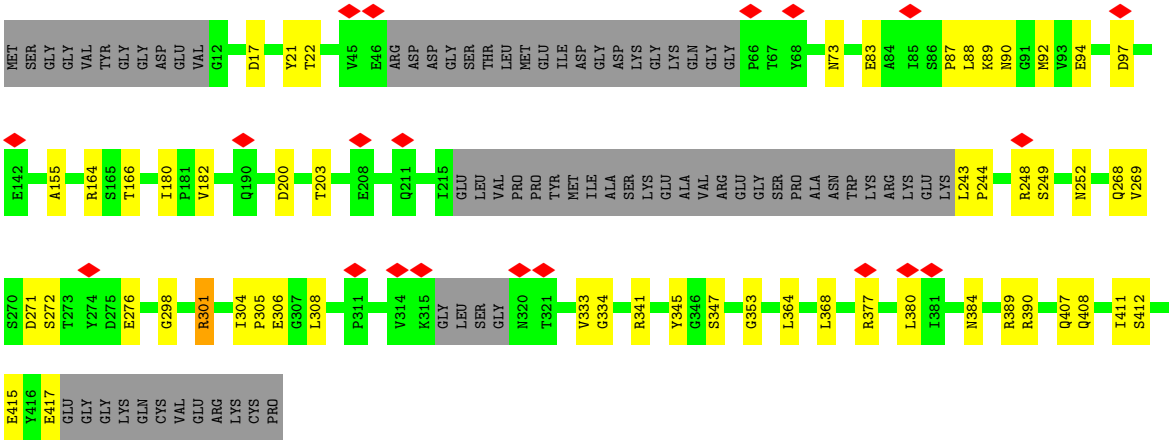
• Molecule 7: ACTB protein (Fragment)

Chain J:



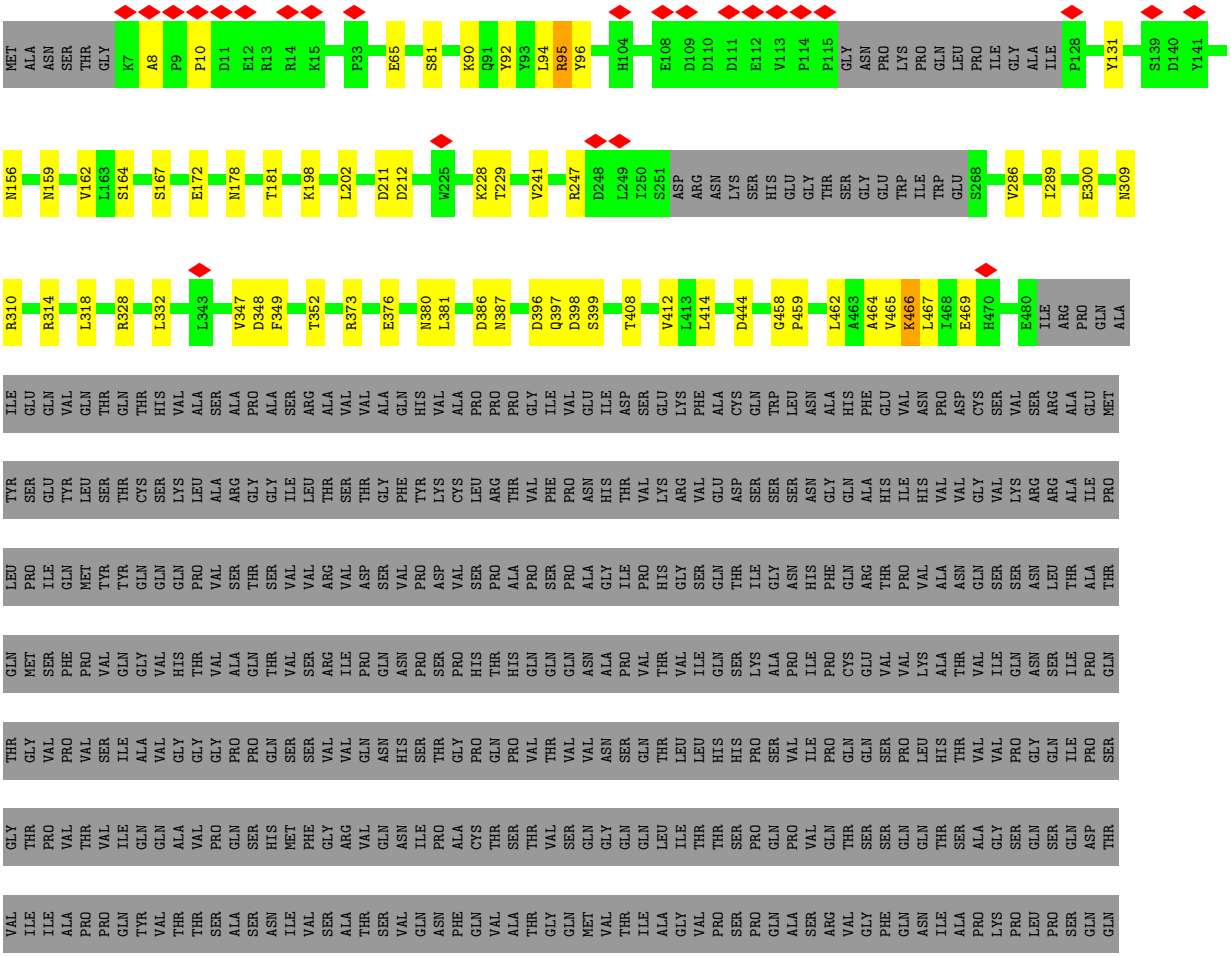
• Molecule 8: Actin-like protein 6A

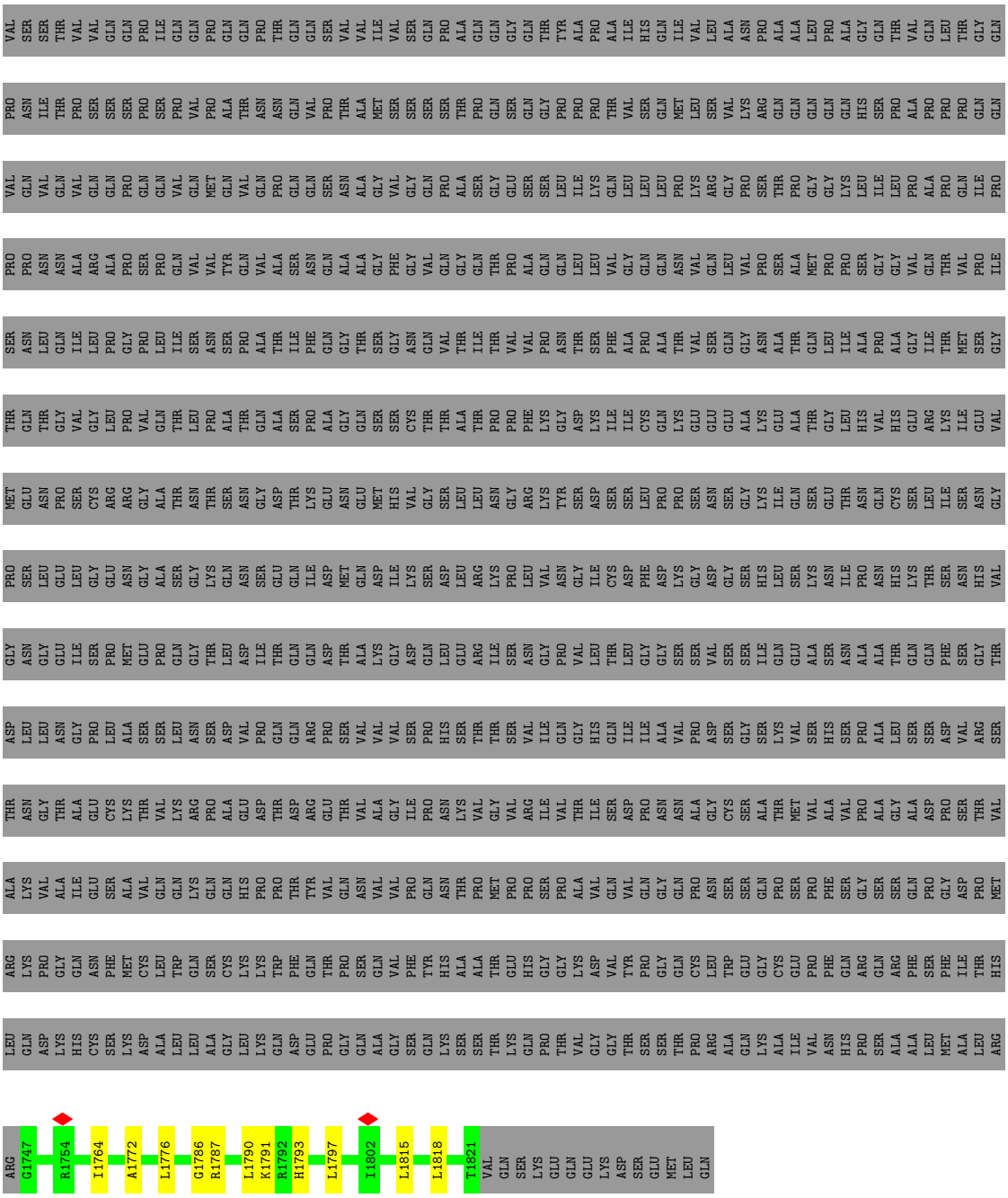
Chain K:



• Molecule 9: AT-rich interactive domain-containing protein 2

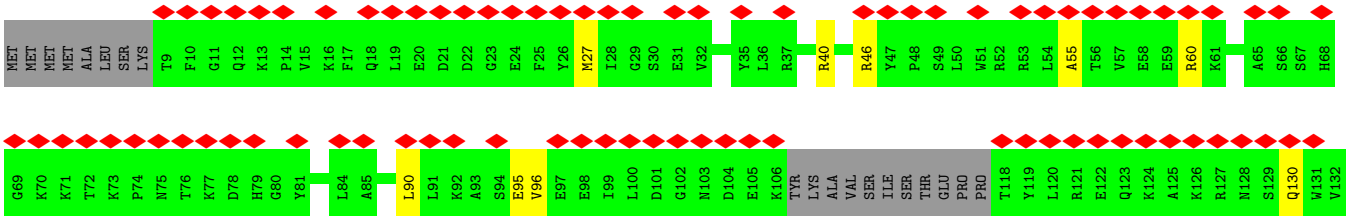
Chain L:

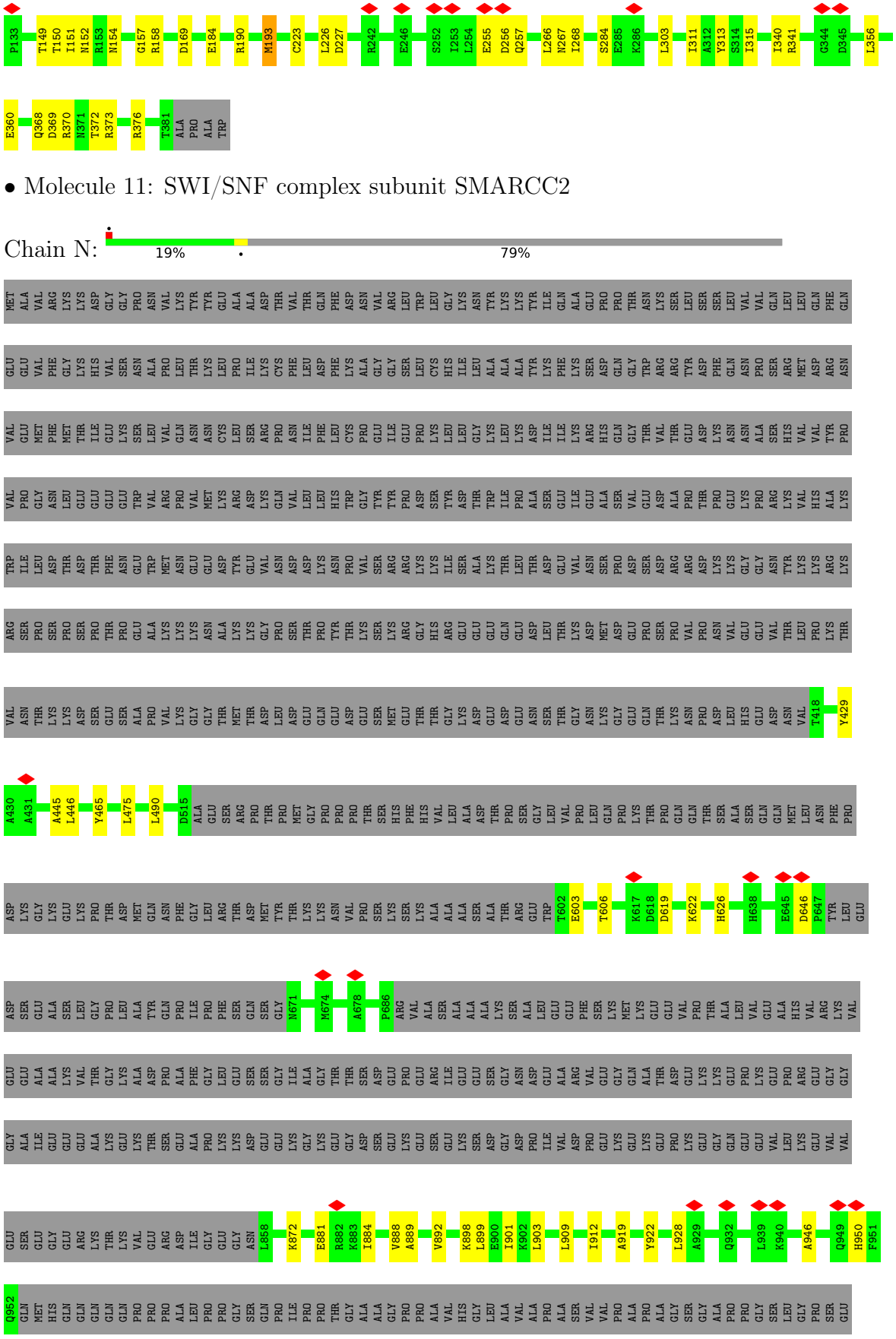


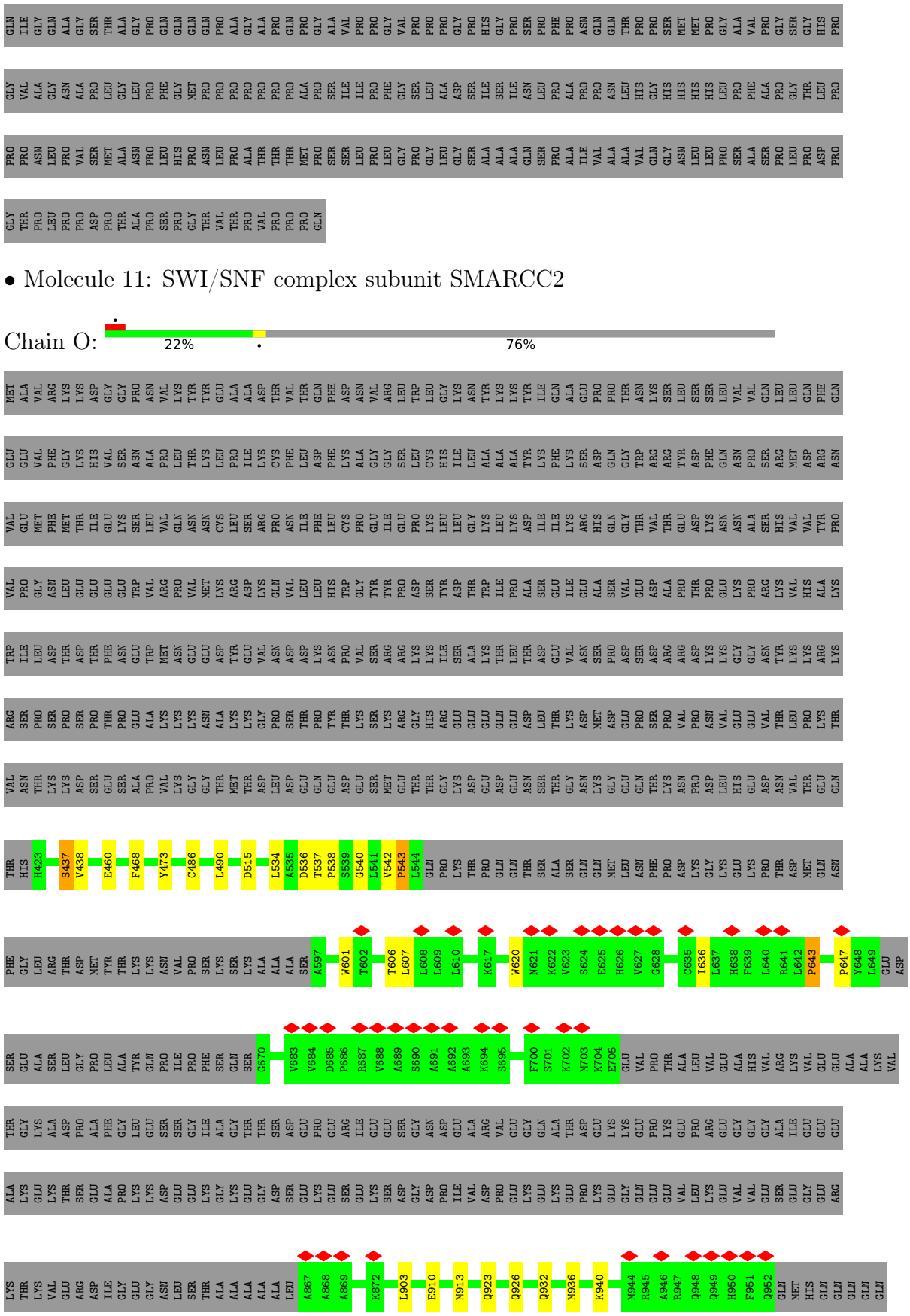


• Molecule 10: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily B member 1

Chain M:

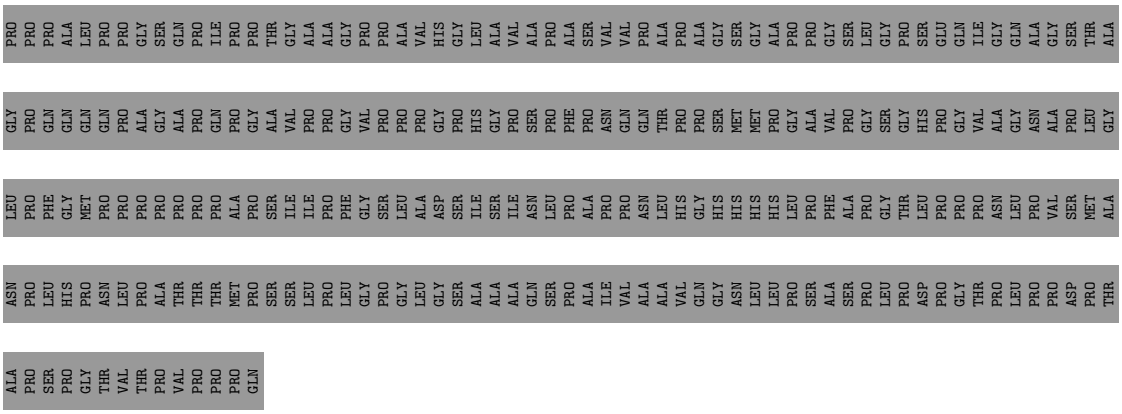



P133 T149 T150 I151 N152 R153 N154 G157 R158 D169 E184 R190 M193 C223 L226 D227 R242 E246 S252 I253 L254 E255 D256 Q257 L266 N267 I268 S284 E285 K286 L303 I311 A312 Y313 S314 I315 I340 R341 G344 D345 L356
E360 Q368 D369 R370 N371 T372 R373 R376 T381 ALA PRO ALA TRP
• Molecule 11: SWI/SNF complex subunit SMARCC2
Chain N:
19%
79%
T418 Y429
A430 A431 A445 L446 Y465 L475 L490 D515
T602 E603 T606 K617 D618 D619 K622 H626 H638 E645 D646 P647
N671 M674 A678 P686
L858 K872 E881 R882 K883 I884 V888 A889 V892 K898 L899 E900 I901 K902 L903 L909 I912 A919 Y922 L928 A929 Q932 L939 K940 A946 Q949 H950 F951
Q952



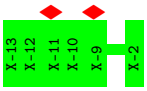
• Molecule 11: SWI/SNF complex subunit SMARCC2

Chain O: 22% 76%



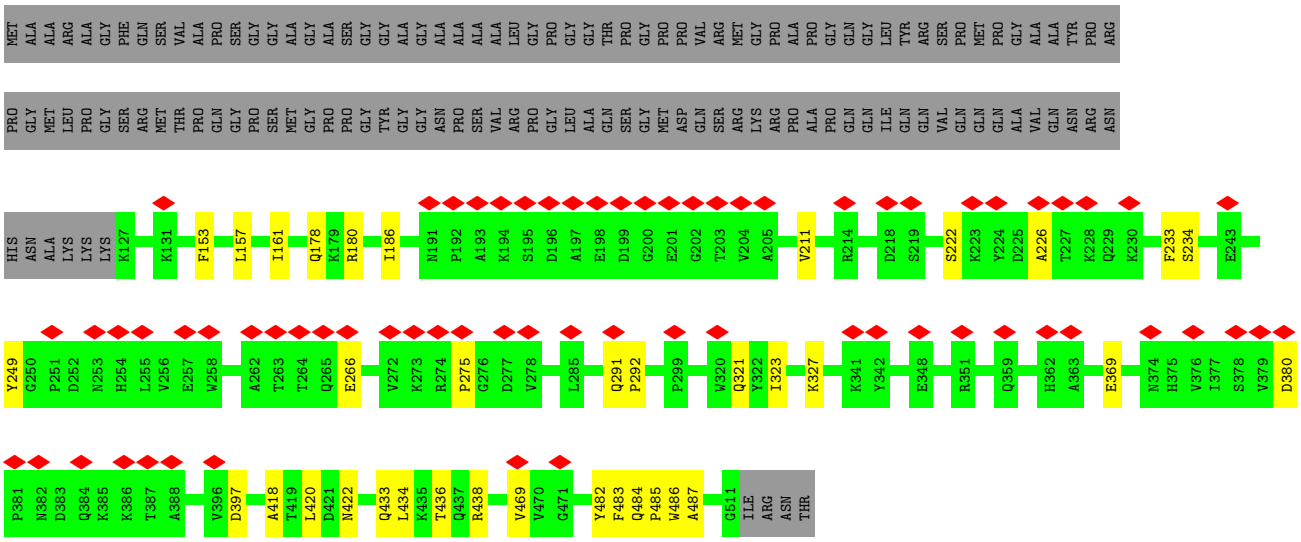
• Molecule 12: Unknown

Chain a: 17% 100%



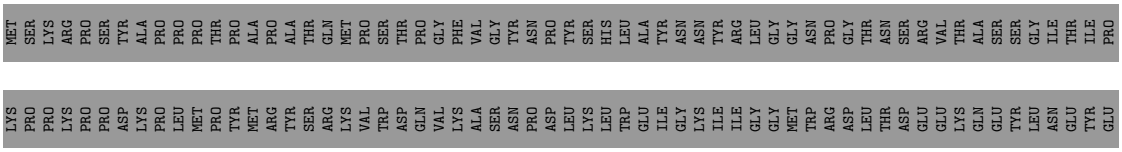
• Molecule 13: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily D member 1

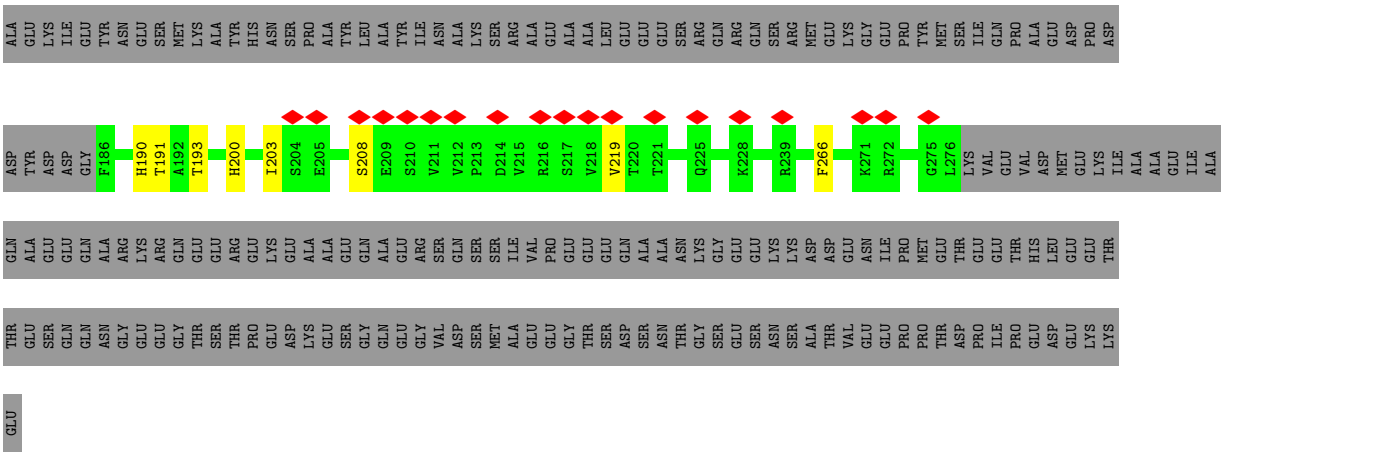
Chain P: 13% 68% 7% 25%



• Molecule 14: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1

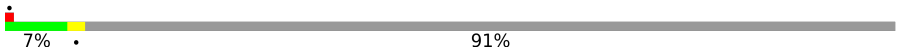
Chain Q: 5% 20% 78%

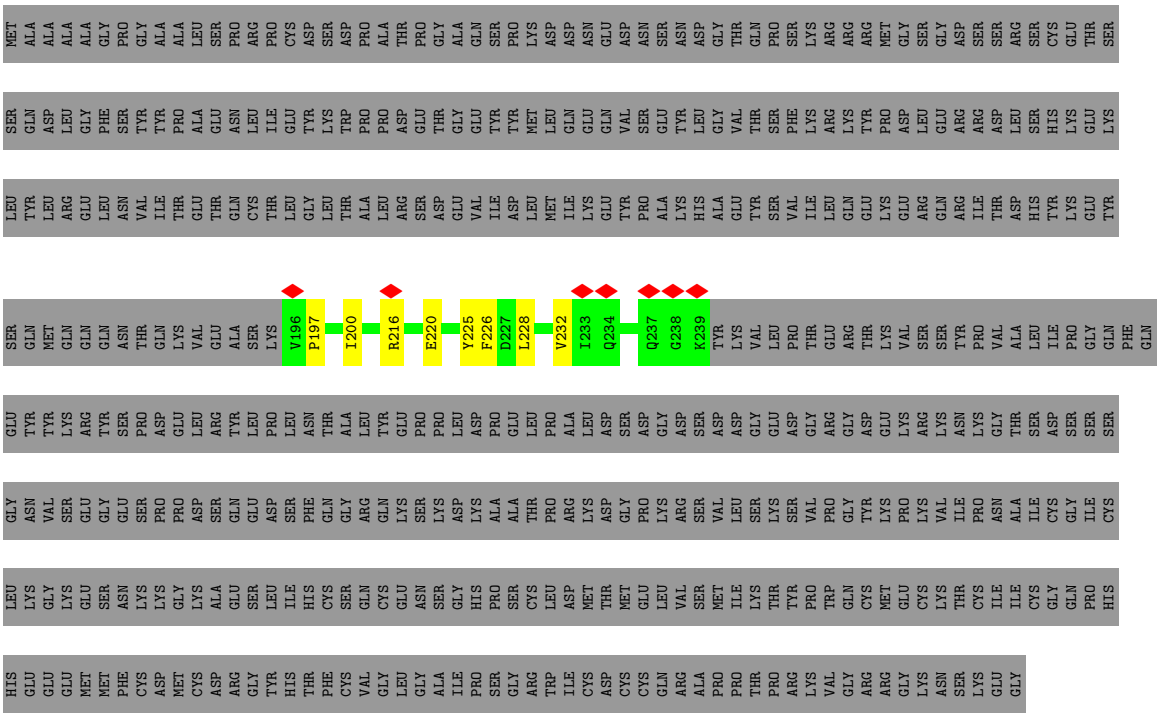




• Molecule 15: PHD finger protein 10

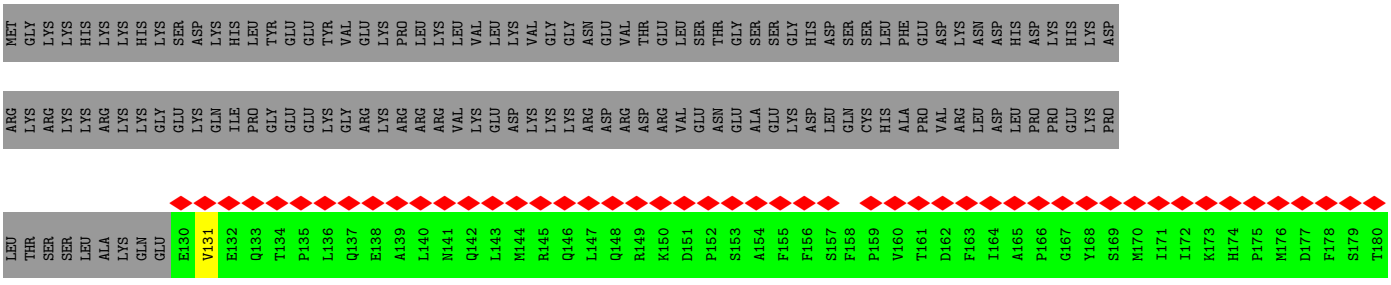
Chain R:

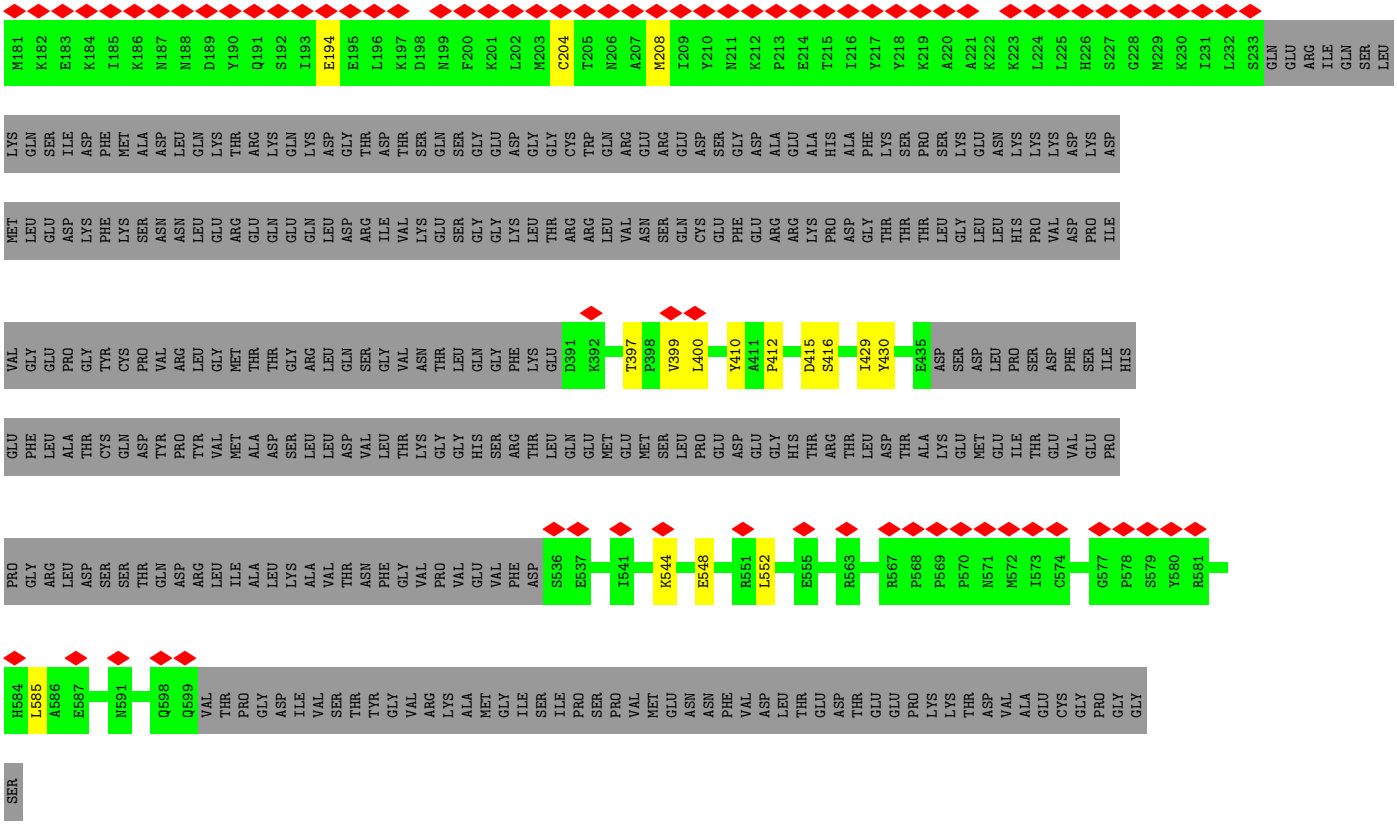




• Molecule 16: Bromodomain-containing protein 7

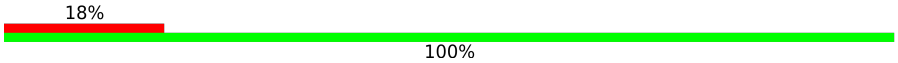
Chain S:

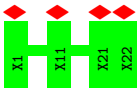




- Molecule 17: Unkown

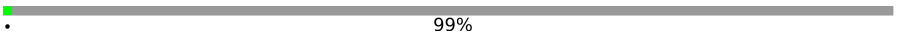
Chain T:

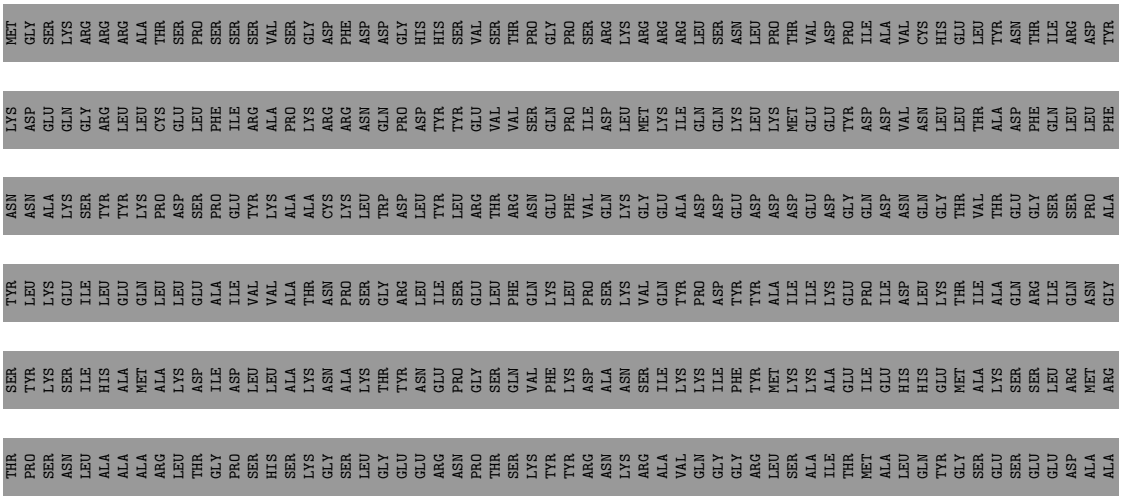




- Molecule 18: Protein polybromo-1

Chain U:

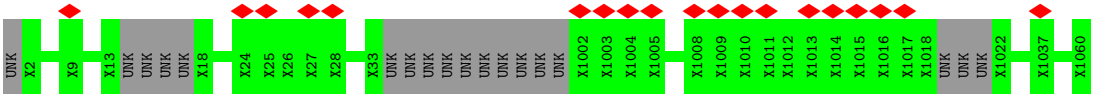




H1514
E1523
G1524

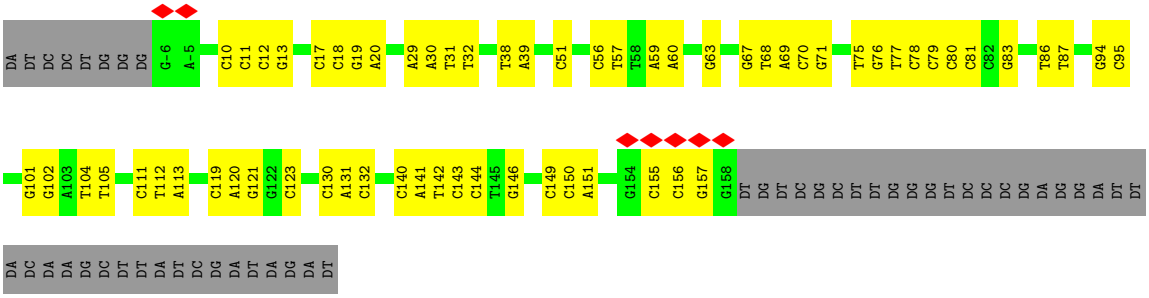
• Molecule 19: Unknown

Chain V:



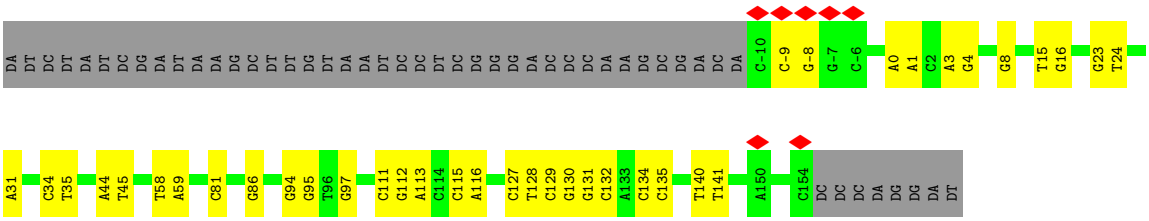
• Molecule 20: DNA (213-MER)

Chain X:



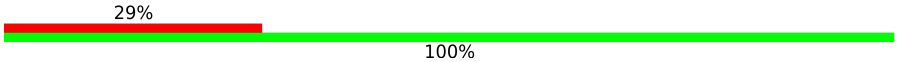
• Molecule 21: DNA (213-MER)

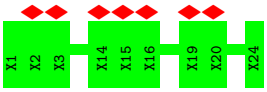
Chain Y:



• Molecule 22: Unknown

Chain W:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37528	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.472	Depositor
Minimum map value	-0.644	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.28	Depositor
Map size (Å)	480.24, 480.24, 480.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.334, 1.334, 1.334	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: BEF, MG, ADP

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	0/827	0.36	0/1109
1	E	0.23	0/818	0.36	0/1097
2	B	0.25	0/749	0.41	0/997
2	F	0.23	0/710	0.38	0/948
3	C	0.24	0/809	0.37	0/1093
3	G	0.24	0/843	0.37	0/1136
4	D	0.24	0/766	0.36	0/1026
4	H	0.24	0/747	0.35	0/1004
6	I	0.23	0/6152	0.37	0/8268
7	J	0.23	0/2881	0.41	0/3904
8	K	0.24	0/2849	0.41	0/3866
9	L	0.24	0/4229	0.38	0/5705
10	M	0.24	0/2976	0.41	0/4025
11	N	0.24	0/2125	0.37	0/2870
11	O	0.24	0/2401	0.44	3/3244 (0.1%)
13	P	0.24	0/3237	0.39	0/4369
14	Q	0.23	0/746	0.39	0/999
15	R	0.27	0/372	0.45	0/497
16	S	0.24	0/1773	0.35	0/2390
18	U	0.28	0/94	0.38	0/125
20	X	0.55	0/3763	0.90	0/5800
21	Y	0.54	0/3825	0.88	0/5907
All	All	0.31	0/43692	0.52	3/60379 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	O	543	PRO	N-CA-CB	6.97	111.67	103.30
11	O	643	PRO	N-CA-CB	6.27	110.82	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	O	647	PRO	N-CA-CB	5.99	110.49	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	815	0	856	7	0
1	E	806	0	844	7	0
2	B	741	0	796	3	0
2	F	702	0	755	2	0
3	C	799	0	851	5	0
3	G	833	0	895	14	0
4	D	755	0	782	4	0
4	H	736	0	756	8	0
5	Z	141	0	27	0	0
6	I	6051	0	6176	57	0
7	J	2821	0	2780	33	0
8	K	2787	0	2725	34	0
9	L	4151	0	4161	46	0
10	M	2918	0	2870	30	0
11	N	2085	0	2068	25	0
11	O	2354	0	2282	17	0
12	a	58	0	14	0	0
13	P	3174	0	3173	28	0
14	Q	739	0	755	7	0
15	R	366	0	369	6	0
16	S	1738	0	1718	12	0
17	T	110	0	31	0	0
18	U	92	0	84	0	0
19	V	420	0	98	0	0
20	X	3360	0	1853	45	0
21	Y	3405	0	1850	28	0
22	W	120	0	28	0	0
23	I	27	0	12	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	I	1	0	0	0	0
25	I	4	0	0	1	0
All	All	43109	0	39609	366	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 4.

All (366) 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)
6:I:1192:ARG:NH1	23:I:1701:ADP:O2A	1.94	0.99
6:I:1192:ARG:HD3	23:I:1701:ADP:H5'1	1.54	0.88
7:J:186:THR:OG1	7:J:206:ARG:O	1.92	0.85
6:I:1166:GLN:OE1	23:I:1701:ADP:H4'	1.78	0.82
6:I:365:GLU:OE1	14:Q:191:THR:OG1	1.97	0.82
11:O:473:TYR:OH	11:O:515:ASP:OD2	2.00	0.79
6:I:758:GLN:HE22	23:I:1701:ADP:HN61	1.30	0.76
6:I:1200:ARG:NH1	6:I:1306:ILE:O	2.19	0.76
1:A:62:ILE:O	1:A:93:GLN:NE2	2.21	0.74
3:G:39:TYR:OH	4:H:71:GLU:OE1	2.05	0.73
9:L:373:ARG:NH2	9:L:376:GLU:OE1	2.21	0.73
9:L:444:ASP:OD1	9:L:1793:HIS:NE2	2.22	0.71
10:M:158:ARG:NH1	10:M:158:ARG:O	2.24	0.71
6:I:1106:THR:OG1	6:I:1125:ARG:NH2	2.24	0.71
13:P:180:ARG:NH2	13:P:397:ASP:OD2	2.23	0.71
1:A:99:TYR:OH	1:A:133:GLU:OE1	2.09	0.70
3:G:64:GLU:OE1	10:M:376:ARG:NH1	2.23	0.70
1:A:73:GLU:OE1	1:A:76:GLN:NE2	2.24	0.70
13:P:433:GLN:O	13:P:436:THR:OG1	2.09	0.69
7:J:149:THR:OG1	7:J:292:ASP:OD2	2.07	0.69
13:P:178:GLN:OE1	13:P:180:ARG:NH1	2.25	0.69
11:N:946:ALA:O	11:N:950:HIS:ND1	2.27	0.68
6:I:788:GLN:OE1	6:I:979:ARG:NH1	2.27	0.68
3:C:17:ARG:NE	20:X:31:DT:OP1	2.27	0.67
11:N:909:LEU:HD22	13:P:161:ILE:CD1	2.25	0.67
1:E:72:ARG:NH1	20:X:51:DC:OP1	2.28	0.67
10:M:55:ALA:HB2	10:M:90:LEU:HD21	1.76	0.67
6:I:772:ASN:OD1	6:I:905:ARG:NH2	2.29	0.66
11:N:429:TYR:N	11:O:536:ASP:OD2	2.29	0.66
15:R:228:LEU:O	15:R:228:LEU:HD23	1.96	0.66
13:P:234:SER:OG	13:P:266:GLU:OE1	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:334:GLY:O	8:K:341:ARG:NH2	2.30	0.65
11:N:884:ILE:HG22	13:P:434:LEU:HD23	1.79	0.65
6:I:758:GLN:NE2	23:I:1701:ADP:HN61	1.93	0.65
8:K:298:GLY:O	8:K:301:ARG:NH1	2.30	0.65
2:B:92:ARG:NH2	4:H:100:LEU:O	2.30	0.64
3:C:20:ARG:NH1	20:X:32:DT:OP1	2.31	0.64
6:I:1192:ARG:CZ	23:I:1701:ADP:O2A	2.45	0.64
1:E:72:ARG:NH2	20:X:51:DC:OP2	2.31	0.64
8:K:155:ALA:HB2	8:K:180:ILE:HD12	1.80	0.63
9:L:164:SER:O	9:L:167:SER:OG	2.12	0.63
11:O:534:LEU:HD23	11:O:542:VAL:HA	1.81	0.63
6:I:1198:GLU:N	6:I:1198:GLU:OE1	2.31	0.63
8:K:415:GLU:OE1	8:K:417:GLU:N	2.32	0.63
8:K:407:GLN:OE1	8:K:408:GLN:NE2	2.31	0.62
2:F:48:GLY:N	21:Y:81:DC:OP1	2.30	0.62
6:I:381:ARG:NH2	11:N:646:ASP:O	2.33	0.62
9:L:408:THR:O	16:S:410:TYR:OH	2.15	0.61
13:P:418:ALA:O	13:P:422:ASN:ND2	2.33	0.61
11:O:923:GLN:OE1	11:O:926:GLN:NE2	2.32	0.61
11:N:909:LEU:HD22	13:P:161:ILE:HD13	1.83	0.61
9:L:65:GLU:OE1	9:L:65:GLU:N	2.34	0.60
15:R:216:ARG:NH1	15:R:220:GLU:OE1	2.34	0.60
10:M:368:GLN:O	10:M:372:THR:HG23	2.01	0.60
6:I:1135:ARG:NH2	20:X:56:DC:OP2	2.36	0.59
9:L:156:ASN:OD1	9:L:159:ASN:ND2	2.34	0.59
7:J:287:VAL:HG22	7:J:288:ASP:H	1.67	0.59
6:I:1192:ARG:CD	23:I:1701:ADP:H5'1	2.31	0.59
9:L:172:GLU:OE1	9:L:172:GLU:N	2.36	0.59
21:Y:127:DC:H2'	21:Y:128:DT:H72	1.83	0.59
3:C:29:ARG:NH1	4:D:36:SER:O	2.36	0.59
21:Y:44:DA:H2"	21:Y:45:DT:H71	1.85	0.58
6:I:785:LYS:N	23:I:1701:ADP:O1B	2.36	0.58
4:D:56:SER:OG	20:X:20:DA:OP2	2.13	0.58
1:A:113:HIS:NE2	1:E:123:ASP:OD1	2.33	0.58
16:S:544:LYS:NZ	16:S:548:GLU:OE2	2.37	0.58
9:L:349:PHE:O	9:L:352:THR:N	2.31	0.58
3:G:29:ARG:NH1	4:H:36:SER:O	2.37	0.57
10:M:223:CYS:O	10:M:227:ASP:N	2.38	0.57
13:P:369:GLU:N	13:P:369:GLU:OE1	2.36	0.57
21:Y:127:DC:C2'	21:Y:128:DT:H72	2.34	0.57
6:I:1103:CYS:SG	6:I:1104:GLN:N	2.78	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ASP:OD1	1:E:113:HIS:NE2	2.36	0.56
6:I:498:GLN:O	6:I:501:THR:OG1	2.20	0.56
7:J:93:GLU:O	7:J:97:ALA:N	2.33	0.56
9:L:90:LYS:O	9:L:94:LEU:HD23	2.05	0.56
4:H:63:ASN:OD1	4:H:67:ASN:ND2	2.38	0.56
6:I:1192:ARG:NH1	25:I:1703:BEF:F2	2.28	0.56
7:J:271:SER:OG	8:K:73:ASN:OD1	2.19	0.56
11:O:936:MET:SD	11:O:940:LYS:NZ	2.74	0.56
3:G:92:GLU:OE2	10:M:370:ARG:NH2	2.39	0.56
3:C:39:TYR:OH	4:D:71:GLU:OE1	2.23	0.56
9:L:398:ASP:OD1	9:L:399:SER:N	2.39	0.55
8:K:384:ASN:OD1	8:K:389:ARG:NH1	2.39	0.55
16:S:552:LEU:HD22	16:S:585:LEU:HD22	1.88	0.55
14:Q:200:HIS:HA	14:Q:203:ILE:HG22	1.86	0.55
7:J:75:ILE:HG22	7:J:77:THR:H	1.72	0.55
14:Q:191:THR:HG21	16:S:429:ILE:HD13	1.89	0.55
13:P:323:ILE:O	13:P:327:LYS:N	2.39	0.55
6:I:819:ALA:O	6:I:831:LYS:NZ	2.38	0.54
8:K:164:ARG:NH1	8:K:347:SER:OG	2.39	0.54
9:L:414:LEU:HD11	16:S:412:PRO:HG3	1.90	0.54
6:I:503:ALA:O	6:I:506:THR:OG1	2.25	0.53
11:O:620:TRP:CZ3	11:O:636:ILE:HD11	2.43	0.53
9:L:386:ASP:OD1	9:L:387:ASN:N	2.40	0.53
6:I:508:HIS:O	6:I:511:THR:OG1	2.24	0.53
6:I:995:VAL:O	6:I:995:VAL:HG13	2.07	0.53
8:K:353:GLY:O	8:K:390:ARG:NH2	2.41	0.53
10:M:95:GLU:N	10:M:95:GLU:OE1	2.41	0.53
13:P:211:VAL:HG22	13:P:233:PHE:CZ	2.43	0.53
13:P:482:TYR:O	13:P:486:TRP:NE1	2.39	0.53
3:G:33:LEU:O	3:G:37:GLY:N	2.43	0.52
8:K:249:SER:O	8:K:252:ASN:ND2	2.42	0.52
6:I:442:SER:CB	9:L:467:LEU:HD12	2.39	0.52
10:M:40:ARG:NH1	21:Y:8:DG:O6	2.43	0.52
21:Y:134:DC:N3	21:Y:135:DC:N4	2.57	0.52
7:J:273:GLY:O	7:J:277:THR:OG1	2.13	0.52
21:Y:34:DC:H2'	21:Y:35:DT:H72	1.91	0.52
10:M:149:THR:O	10:M:150:THR:OG1	2.23	0.51
8:K:89:LYS:NZ	8:K:90:ASN:OD1	2.33	0.51
11:N:872:LYS:NZ	14:Q:208:SER:O	2.26	0.51
11:O:534:LEU:CD2	11:O:542:VAL:HA	2.40	0.51
8:K:83:GLU:OE1	8:K:83:GLU:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:LEU:HD23	2:B:10:LEU:H	1.76	0.51
7:J:124:PHE:O	7:J:128:ASN:N	2.43	0.51
6:I:395:ASP:O	6:I:398:THR:OG1	2.27	0.51
10:M:154:ASN:ND2	10:M:227:ASP:OD2	2.44	0.51
13:P:483:PHE:O	13:P:487:ALA:HB2	2.11	0.50
9:L:408:THR:O	9:L:408:THR:HG23	2.11	0.50
9:L:328:ARG:O	9:L:332:LEU:HD23	2.12	0.50
11:N:881:GLU:HA	11:N:884:ILE:HG12	1.94	0.50
11:N:901:ILE:HG13	13:P:420:LEU:HD11	1.93	0.50
21:Y:34:DC:C2'	21:Y:35:DT:H72	2.42	0.50
6:I:411:ASN:O	6:I:414:ARG:NH1	2.41	0.50
11:N:884:ILE:HD13	13:P:438:ARG:HD3	1.94	0.50
6:I:1007:LEU:HD13	6:I:1045:ILE:HD11	1.94	0.49
7:J:11:ASP:OD1	7:J:12:ASN:N	2.45	0.49
6:I:787:ILE:HD13	23:I:1701:ADP:N7	2.27	0.49
20:X:146:DG:N1	21:Y:3:DA:C6	2.80	0.49
7:J:187:ASP:OD1	7:J:188:TYR:N	2.45	0.49
16:S:415:ASP:OD1	16:S:416:SER:N	2.46	0.49
7:J:312:ARG:NE	7:J:316:GLU:OE2	2.38	0.49
8:K:166:THR:OG1	8:K:182:VAL:O	2.19	0.49
6:I:1340:GLU:OE1	6:I:1340:GLU:N	2.40	0.49
8:K:268:GLN:OE1	8:K:268:GLN:N	2.45	0.49
16:S:397:THR:HG23	16:S:397:THR:O	2.13	0.49
9:L:396:ASP:OD1	9:L:397:GLN:N	2.45	0.48
4:D:93:GLU:OE1	4:D:93:GLU:N	2.45	0.48
8:K:364:LEU:HD23	8:K:368:LEU:HD23	1.95	0.48
20:X:86:DT:H2'	20:X:87:DT:H72	1.95	0.48
6:I:1046:CYS:HG	6:I:1209:SER:HG	1.54	0.48
13:P:157:LEU:O	13:P:161:ILE:HG12	2.14	0.48
8:K:411:ILE:HG22	8:K:412:SER:N	2.28	0.48
13:P:380:ASP:N	13:P:380:ASP:OD1	2.46	0.48
21:Y:23:DG:C2'	21:Y:24:DT:H72	2.43	0.48
2:B:21:VAL:HG23	2:B:21:VAL:O	2.13	0.48
11:N:898:LYS:HA	13:P:420:LEU:HD13	1.94	0.48
6:I:1166:GLN:OE1	23:I:1701:ADP:C4'	2.55	0.48
1:E:58:THR:O	3:G:104:GLN:NE2	2.47	0.48
10:M:356:LEU:HD23	10:M:360:GLU:OE1	2.13	0.47
21:Y:44:DA:C2'	21:Y:45:DT:H71	2.44	0.47
6:I:562:ALA:O	6:I:565:THR:OG1	2.29	0.47
6:I:442:SER:HB2	9:L:467:LEU:HD12	1.97	0.47
7:J:155:SER:OG	7:J:304:THR:HG21	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:23:DG:H2'	21:Y:24:DT:H72	1.94	0.47
3:G:94:ASN:O	3:G:98:GLY:N	2.47	0.47
9:L:300:GLU:N	9:L:300:GLU:OE1	2.47	0.47
8:K:248:ARG:O	8:K:249:SER:OG	2.23	0.47
6:I:1177:ASP:OD1	6:I:1178:TRP:N	2.48	0.47
16:S:204:CYS:HB3	16:S:208:MET:HE3	1.97	0.47
20:X:141:DA:H2'	20:X:142:DT:H72	1.95	0.47
6:I:392:LEU:HD13	6:I:396:LEU:HB2	1.96	0.47
21:Y:128:DT:H2"	21:Y:129:DC:C6	2.50	0.47
6:I:1086:ASP:OD2	6:I:1119:ARG:NH2	2.48	0.47
9:L:198:LYS:NZ	10:M:169:ASP:O	2.39	0.47
6:I:981:LYS:O	6:I:985:GLU:N	2.48	0.46
10:M:257:GLN:O	10:M:284:SER:OG	2.33	0.46
6:I:845:VAL:N	6:I:846:PRO:CD	2.78	0.46
6:I:418:GLN:O	6:I:422:VAL:HG23	2.15	0.46
7:J:242:LEU:HD22	7:J:244:ASP:OD1	2.16	0.46
21:Y:140:DT:H2'	21:Y:141:DT:H71	1.97	0.46
7:J:257:CYS:HB3	7:J:258:PRO:HD3	1.97	0.46
8:K:200:ASP:O	8:K:203:THR:OG1	2.27	0.46
11:N:475:LEU:HD21	15:R:232:VAL:HG23	1.97	0.46
20:X:63:DG:N1	21:Y:86:DG:O6	2.48	0.46
20:X:130:DC:O3'	20:X:131:DA:C8	2.68	0.46
6:I:764:TRP:CZ2	6:I:768:LEU:HD11	2.51	0.46
9:L:309:ASN:OD1	9:L:310:ARG:N	2.48	0.46
9:L:380:ASN:OD1	9:L:381:LEU:N	2.49	0.46
2:F:24:ASP:OD1	2:F:24:ASP:N	2.49	0.46
9:L:1772:ALA:O	9:L:1776:LEU:HD23	2.16	0.46
11:O:486:CYS:O	11:O:490:LEU:HD12	2.15	0.46
6:I:976:LEU:HD22	6:I:1233:MET:HG3	1.98	0.46
3:C:33:LEU:O	3:C:37:GLY:N	2.47	0.46
8:K:88:LEU:HD23	8:K:88:LEU:H	1.80	0.46
3:G:65:LEU:HB3	3:G:86:ALA:HB1	1.96	0.46
7:J:274:ILE:HG23	7:J:275:HIS:N	2.31	0.46
8:K:269:VAL:O	8:K:269:VAL:HG13	2.15	0.46
13:P:291:GLN:N	13:P:291:GLN:OE1	2.49	0.46
7:J:354:GLN:OE1	7:J:354:GLN:N	2.48	0.45
20:X:68:DT:H2"	20:X:69:DA:N7	2.32	0.45
21:Y:130:DG:H2'	21:Y:131:DG:C8	2.51	0.45
7:J:76:VAL:HG22	7:J:76:VAL:O	2.16	0.45
16:S:399:VAL:HG13	16:S:400:LEU:N	2.31	0.45
4:H:90:THR:OG1	4:H:91:SER:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:1166:GLN:CD	23:I:1701:ADP:H4'	2.36	0.45
9:L:347:VAL:HG12	9:L:348:ASP:N	2.31	0.45
8:K:269:VAL:HG23	8:K:306:GLU:HA	1.99	0.45
21:Y:112:DG:C2	21:Y:113:DA:C6	3.03	0.45
6:I:1007:LEU:CD1	6:I:1045:ILE:HD11	2.47	0.45
10:M:267:ASN:OD1	10:M:268:ILE:N	2.50	0.45
16:S:194:GLU:OE1	16:S:194:GLU:N	2.47	0.45
8:K:304:ILE:N	8:K:305:PRO:CD	2.79	0.45
9:L:95:ARG:NH1	9:L:96:TYR:HB2	2.31	0.45
10:M:266:LEU:HD21	10:M:315:ILE:CG1	2.47	0.45
11:N:603:GLU:O	11:N:606:THR:OG1	2.32	0.45
21:Y:58:DT:H2"	21:Y:59:DA:N7	2.32	0.45
21:Y:131:DG:C8	21:Y:132:DC:N4	2.84	0.45
8:K:276:GLU:N	8:K:276:GLU:OE1	2.50	0.45
20:X:104:DT:H2'	20:X:105:DT:H71	1.99	0.45
20:X:120:DA:H2"	20:X:121:DG:N7	2.31	0.45
20:X:150:DC:C2	20:X:151:DA:N7	2.85	0.45
11:O:468:PHE:HB3	11:O:490:LEU:HD21	1.99	0.45
9:L:228:LYS:O	9:L:229:THR:OG1	2.23	0.45
8:K:97:ASP:OD1	8:K:97:ASP:N	2.49	0.44
11:N:919:ALA:HA	11:N:922:TYR:CE2	2.53	0.44
20:X:149:DC:H2"	20:X:150:DC:C5	2.52	0.44
7:J:219:VAL:HG23	7:J:306:TYR:CG	2.53	0.44
10:M:130:GLN:O	10:M:130:GLN:HG2	2.18	0.44
11:O:601:TRP:O	11:O:607:LEU:HB2	2.18	0.44
20:X:10:DC:H2"	20:X:11:DC:C6	2.52	0.44
7:J:153:MET:SD	7:J:153:MET:N	2.91	0.44
9:L:465:VAL:O	9:L:466:LYS:HG3	2.18	0.44
20:X:75:DT:H2'	20:X:76:DG:C8	2.53	0.44
20:X:155:DC:H2"	20:X:156:DC:C5	2.53	0.44
1:E:62:ILE:O	1:E:93:GLN:NE2	2.51	0.44
7:J:191:LYS:O	7:J:194:THR:OG1	2.31	0.44
11:N:622:LYS:O	11:N:626:HIS:ND1	2.50	0.44
11:O:460:GLU:OE1	11:O:460:GLU:N	2.50	0.44
13:P:249:TYR:OH	13:P:275:PRO:O	2.29	0.44
21:Y:-9:DC:H2"	21:Y:-8:DG:N7	2.33	0.44
20:X:19:DG:H2"	20:X:20:DA:N7	2.33	0.44
20:X:80:DC:O3'	20:X:81:DC:C6	2.71	0.44
20:X:12:DC:N4	20:X:13:DG:O6	2.51	0.44
6:I:1166:GLN:O	6:I:1195:GLN:NE2	2.51	0.43
7:J:171:LEU:HG	7:J:171:LEU:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:282:ILE:HG21	7:J:294:TYR:CE1	2.53	0.43
9:L:131:TYR:CG	9:L:131:TYR:O	2.70	0.43
9:L:1787:ARG:O	9:L:1791:LYS:N	2.50	0.43
10:M:55:ALA:O	10:M:60:ARG:NH1	2.51	0.43
11:N:909:LEU:HA	11:N:912:ILE:HD12	2.00	0.43
9:L:211:ASP:OD1	9:L:212:ASP:N	2.51	0.43
11:N:899:LEU:O	11:N:903:LEU:HD23	2.18	0.43
20:X:56:DC:H2'	20:X:57:DT:H72	2.00	0.43
20:X:156:DC:H2"	20:X:157:DG:N7	2.33	0.43
9:L:81:SER:OG	15:R:220:GLU:O	2.35	0.43
9:L:1797:LEU:HD13	9:L:1815:LEU:CD1	2.48	0.43
11:N:884:ILE:HG22	13:P:434:LEU:CD2	2.46	0.43
20:X:29:DA:O3'	20:X:30:DA:C8	2.71	0.43
6:I:767:SER:O	6:I:771:ASN:ND2	2.48	0.43
9:L:412:VAL:HG13	9:L:1764:ILE:HD11	2.01	0.43
7:J:262:PHE:HB2	7:J:273:GLY:HA3	2.00	0.43
8:K:87:PRO:O	8:K:94:GLU:N	2.46	0.43
11:O:903:LEU:HB2	13:P:153:PHE:CE1	2.54	0.43
3:G:51:LEU:HD21	4:H:70:PHE:CD1	2.54	0.43
9:L:314:ARG:O	9:L:318:LEU:HD23	2.17	0.43
6:I:392:LEU:HD13	6:I:396:LEU:CB	2.49	0.43
20:X:67:DG:C8	20:X:68:DT:H72	2.54	0.43
3:G:17:ARG:NH2	21:Y:31:DA:OP2	2.52	0.43
6:I:734:VAL:HG23	6:I:735:ALA:N	2.33	0.43
10:M:255:GLU:HG2	10:M:256:ASP:H	1.84	0.43
11:N:619:ASP:N	11:N:619:ASP:OD1	2.52	0.43
20:X:69:DA:H2"	20:X:70:DC:C5	2.54	0.43
7:J:209:VAL:HG13	7:J:210:ARG:N	2.34	0.43
20:X:76:DG:H2'	20:X:77:DT:H72	2.01	0.43
20:X:143:DC:H2"	20:X:144:DC:C6	2.54	0.43
6:I:1086:ASP:OD1	6:I:1119:ARG:NH1	2.46	0.42
6:I:1179:ASN:ND2	21:Y:97:DG:OP1	2.49	0.42
8:K:308:LEU:HD23	8:K:308:LEU:H	1.84	0.42
8:K:308:LEU:O	8:K:308:LEU:HG	2.19	0.42
9:L:178:ASN:O	9:L:181:THR:OG1	2.38	0.42
11:N:889:ALA:O	11:N:892:VAL:HG12	2.19	0.42
21:Y:115:DC:N3	21:Y:116:DA:N6	2.66	0.42
6:I:860:TYR:OH	6:I:881:ASP:O	2.36	0.42
7:J:170:ALA:C	7:J:171:LEU:HD23	2.39	0.42
9:L:462:LEU:HD12	9:L:464:ALA:H	1.84	0.42
15:R:197:PRO:HA	15:R:200:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:70:DC:H1'	20:X:71:DG:C5	2.54	0.42
4:H:39:VAL:HG23	20:X:123:DC:OP2	2.20	0.42
9:L:286:VAL:HA	9:L:289:ILE:HG22	2.01	0.42
9:L:458:GLY:N	9:L:459:PRO:CD	2.82	0.42
9:L:1786:GLY:O	9:L:1790:LEU:N	2.44	0.42
11:O:536:ASP:O	11:O:540:GLY:N	2.51	0.42
20:X:12:DC:H2'	20:X:13:DG:C8	2.55	0.42
9:L:1797:LEU:HD13	9:L:1815:LEU:HD11	2.02	0.42
11:N:928:LEU:HD21	14:Q:266:PHE:HD1	1.84	0.42
13:P:291:GLN:HB2	13:P:292:PRO:HD3	2.00	0.42
6:I:823:ASP:HB2	6:I:831:LYS:HZ3	1.84	0.42
10:M:157:GLY:O	10:M:158:ARG:HB3	2.19	0.42
16:S:131:VAL:HG23	16:S:131:VAL:O	2.20	0.42
7:J:287:VAL:HG22	7:J:288:ASP:N	2.33	0.42
8:K:243:LEU:N	8:K:244:PRO:CD	2.82	0.42
8:K:271:ASP:OD1	8:K:272:SER:N	2.53	0.42
9:L:8:ALA:O	9:L:10:PRO:HD3	2.20	0.42
9:L:92:TYR:HA	9:L:95:ARG:HD3	2.02	0.42
9:L:162:VAL:HG13	9:L:202:LEU:CD1	2.49	0.42
9:L:1797:LEU:C	9:L:1797:LEU:HD12	2.39	0.42
10:M:303:LEU:HG	10:M:303:LEU:O	2.19	0.42
10:M:340:ILE:HG23	10:M:341:ARG:N	2.33	0.42
11:O:537:THR:N	11:O:538:PRO:HD2	2.35	0.42
20:X:38:DT:H2"	20:X:39:DA:N7	2.35	0.42
9:L:466:LYS:NZ	9:L:469:GLU:OE2	2.52	0.42
10:M:27:MET:SD	10:M:96:VAL:HG11	2.60	0.42
13:P:484:GLN:N	13:P:485:PRO:CD	2.82	0.42
15:R:225:TYR:O	15:R:226:PHE:HB3	2.20	0.42
11:N:465:TYR:CD1	11:N:490:LEU:HD12	2.55	0.42
16:S:399:VAL:HG11	16:S:430:TYR:OH	2.20	0.42
6:I:500:LEU:HD11	7:J:142:LEU:HD23	2.02	0.41
10:M:369:ASP:O	10:M:373:ARG:HG3	2.20	0.41
20:X:101:DG:H2"	20:X:102:DG:N7	2.34	0.41
8:K:21:TYR:CD2	8:K:22:THR:HG23	2.56	0.41
10:M:190:ARG:HB2	10:M:313:TYR:OH	2.20	0.41
10:M:193:MET:SD	10:M:193:MET:N	2.87	0.41
3:G:88:ARG:NH2	3:G:100:VAL:O	2.54	0.41
6:I:1143:ASN:ND2	6:I:1164:ASN:O	2.54	0.41
9:L:241:VAL:O	9:L:247:ARG:NH2	2.53	0.41
9:L:1790:LEU:HD23	9:L:1818:LEU:HD21	2.01	0.41
13:P:484:GLN:HG3	13:P:485:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Q:219:VAL:HG12	14:Q:219:VAL:O	2.20	0.41
6:I:792:LEU:C	6:I:792:LEU:HD23	2.41	0.41
11:N:881:GLU:O	11:N:884:ILE:HG12	2.21	0.41
13:P:222:SER:O	13:P:226:ALA:N	2.53	0.41
20:X:111:DC:H2"	20:X:112:DT:C5	2.56	0.41
3:G:35:ARG:NH2	20:X:113:DA:OP2	2.47	0.41
3:G:40:ALA:HB2	4:H:89:ILE:HD12	2.01	0.41
7:J:90:PHE:O	7:J:93:GLU:N	2.54	0.41
6:I:900:HIS:ND1	6:I:900:HIS:O	2.54	0.41
7:J:334:GLU:N	7:J:334:GLU:OE1	2.54	0.41
8:K:333:VAL:HG11	8:K:345:TYR:CZ	2.55	0.41
8:K:380:LEU:H	8:K:380:LEU:HD23	1.86	0.41
11:O:606:THR:OG1	11:O:607:LEU:N	2.53	0.41
20:X:131:DA:H2"	20:X:132:DC:C6	2.56	0.41
1:A:37:LYS:N	1:A:38:PRO:CD	2.83	0.41
6:I:973:ARG:N	6:I:974:PRO:HD2	2.36	0.41
6:I:1340:GLU:HG2	6:I:1341:ASP:N	2.36	0.41
7:J:187:ASP:O	7:J:190:MET:HG3	2.21	0.41
7:J:247:VAL:O	7:J:247:VAL:HG23	2.21	0.41
10:M:150:THR:HG22	10:M:226:LEU:HD21	2.02	0.41
10:M:184:GLU:N	10:M:184:GLU:OE1	2.54	0.41
11:N:445:ALA:C	11:N:446:LEU:HD22	2.41	0.41
13:P:186:ILE:HG23	13:P:186:ILE:O	2.20	0.41
20:X:59:DA:H1'	20:X:60:DA:C8	2.55	0.41
20:X:94:DG:H2'	20:X:95:DC:C6	2.56	0.41
21:Y:15:DT:H4'	21:Y:16:DG:OP1	2.21	0.41
1:E:104:PHE:HA	1:E:107:THR:HG22	2.03	0.41
8:K:17:ASP:OD1	8:K:17:ASP:N	2.53	0.41
11:O:932:GLN:HE22	13:P:321:GLN:HB2	1.86	0.41
3:G:47:ALA:N	3:G:48:PRO:HD2	2.36	0.40
7:J:287:VAL:HG13	7:J:289:ILE:HG12	2.03	0.40
7:J:366:GLY:N	7:J:367:PRO:CD	2.84	0.40
20:X:56:DC:C6	20:X:57:DT:H72	2.55	0.40
21:Y:111:DC:C2'	21:Y:112:DG:C8	3.04	0.40
10:M:151:ILE:HG23	10:M:152:ASN:N	2.37	0.40
10:M:266:LEU:HD23	10:M:311:ILE:HG13	2.02	0.40
20:X:119:DC:H2"	20:X:120:DA:C8	2.57	0.40
1:A:46:VAL:HB	20:X:83:DG:OP1	2.20	0.40
10:M:46:ARG:NH1	21:Y:4:DG:OP1	2.55	0.40
11:O:910:GLU:O	11:O:913:MET:HG3	2.20	0.40
20:X:140:DC:N3	20:X:141:DA:N6	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:92:MET:SD	8:K:92:MET:N	2.95	0.40
11:N:884:ILE:O	11:N:888:VAL:HG13	2.22	0.40
20:X:17:DC:O3'	20:X:18:DC:C6	2.74	0.40
20:X:78:DC:H2"	20:X:79:DC:C5	2.56	0.40
14:Q:190:HIS:O	14:Q:193:THR:OG1	2.23	0.40
21:Y:0:DA:H4'	21:Y:1:DA:OP1	2.22	0.40
21:Y:94:DG:H4'	21:Y:95:DG:OP1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	97/135 (72%)	95 (98%)	2 (2%)	0	100	100
1	E	96/135 (71%)	96 (100%)	0	0	100	100
2	B	92/102 (90%)	87 (95%)	5 (5%)	0	100	100
2	F	85/102 (83%)	84 (99%)	1 (1%)	0	100	100
3	C	102/129 (79%)	101 (99%)	1 (1%)	0	100	100
3	G	106/129 (82%)	102 (96%)	4 (4%)	0	100	100
4	D	94/125 (75%)	94 (100%)	0	0	100	100
4	H	92/125 (74%)	92 (100%)	0	0	100	100
6	I	718/1647 (44%)	693 (96%)	25 (4%)	0	100	100
7	J	354/375 (94%)	324 (92%)	30 (8%)	0	100	100
8	K	348/429 (81%)	325 (93%)	23 (7%)	0	100	100
9	L	513/1835 (28%)	474 (92%)	39 (8%)	0	100	100
10	M	358/385 (93%)	325 (91%)	33 (9%)	0	100	100
11	N	247/1214 (20%)	240 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	O	289/1214 (24%)	260 (90%)	26 (9%)	3 (1%)	15	54
13	P	383/515 (74%)	367 (96%)	15 (4%)	1 (0%)	41	76
14	Q	89/411 (22%)	88 (99%)	1 (1%)	0	100	100
15	R	42/498 (8%)	40 (95%)	2 (5%)	0	100	100
16	S	207/651 (32%)	204 (99%)	3 (1%)	0	100	100
18	U	9/1597 (1%)	8 (89%)	1 (11%)	0	100	100
All	All	4321/11753 (37%)	4099 (95%)	218 (5%)	4 (0%)	54	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	O	543	PRO
11	O	643	PRO
13	P	469	VAL
11	O	437	SER

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	86/110 (78%)	86 (100%)	0	100	100
1	E	85/110 (77%)	85 (100%)	0	100	100
2	B	74/78 (95%)	74 (100%)	0	100	100
2	F	72/78 (92%)	72 (100%)	0	100	100
3	C	81/98 (83%)	81 (100%)	0	100	100
3	G	84/98 (86%)	84 (100%)	0	100	100
4	D	83/105 (79%)	83 (100%)	0	100	100
4	H	81/105 (77%)	81 (100%)	0	100	100
6	I	655/1422 (46%)	654 (100%)	1 (0%)	93	96
7	J	307/318 (96%)	305 (99%)	2 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	K	308/364 (85%)	306 (99%)	2 (1%)	86	92
9	L	465/1587 (29%)	463 (100%)	2 (0%)	91	94
10	M	325/346 (94%)	324 (100%)	1 (0%)	92	95
11	N	221/1030 (22%)	221 (100%)	0	100	100
11	O	241/1030 (23%)	239 (99%)	2 (1%)	81	89
13	P	351/442 (79%)	351 (100%)	0	100	100
14	Q	82/361 (23%)	82 (100%)	0	100	100
15	R	38/437 (9%)	38 (100%)	0	100	100
16	S	196/586 (33%)	196 (100%)	0	100	100
18	U	9/1433 (1%)	9 (100%)	0	100	100
All	All	3844/10138 (38%)	3834 (100%)	10 (0%)	92	95

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

Mol	Chain	Res	Type
6	I	1329	ARG
7	J	177	ARG
7	J	326	LYS
8	K	301	ARG
8	K	377	ARG
9	L	95	ARG
9	L	466	LYS
10	M	193	MET
11	O	437	SER
11	O	438	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
3	G	104	GLN
6	I	510	ASN
6	I	888	ASN
8	K	105	HIS
8	K	263	GLN
8	K	294	ASN
9	L	159	ASN
9	L	406	HIS

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Mol	Chain	Res	Type
9	L	1795	ASN
10	M	123	GLN
10	M	318	GLN
10	M	322	HIS
13	P	326	HIS
14	Q	199	ASN
16	S	206	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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	ADP	I	1701	-	24,29,29	0.96	1 (4%)	29,45,45	1.48	4 (13%)
25	BEF	I	1703	-	0,3,3	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	ADP	I	1701	-	-	2/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	I	1701	ADP	C5-C4	2.51	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	I	1701	ADP	PA-O3A-PB	-3.85	119.63	132.83
23	I	1701	ADP	C3'-C2'-C1'	3.19	105.79	100.98
23	I	1701	ADP	N3-C2-N1	-3.19	123.70	128.68
23	I	1701	ADP	C4-C5-N7	-2.66	106.62	109.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	I	1701	ADP	C5'-O5'-PA-O1A
23	I	1701	ADP	C5'-O5'-PA-O3A

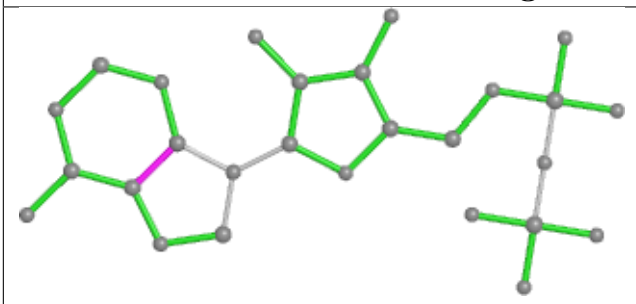
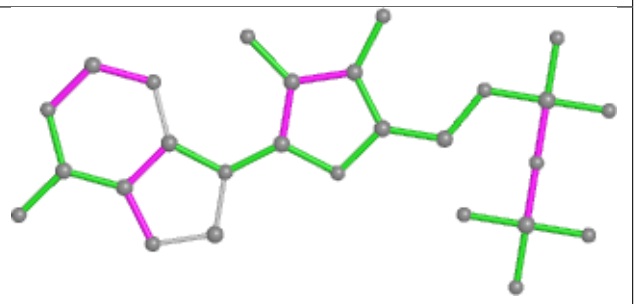
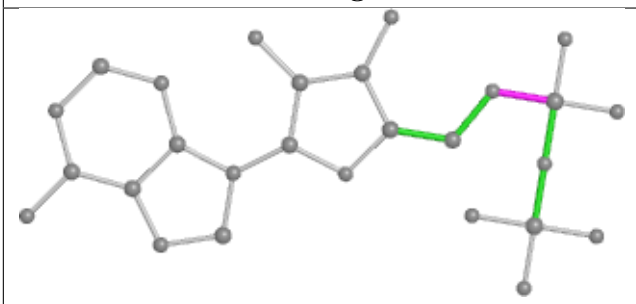
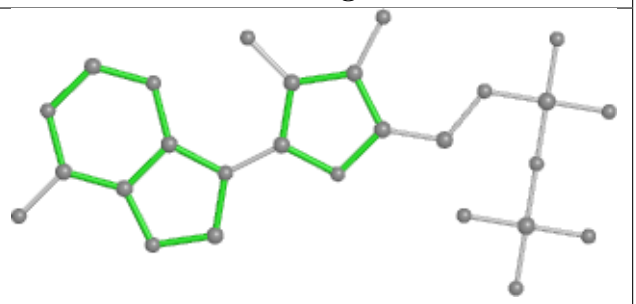
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	I	1701	ADP	11	0
25	I	1703	BEF	1	0

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

equivalents in the CSD to analyse the geometry.

Ligand ADP I 1701	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

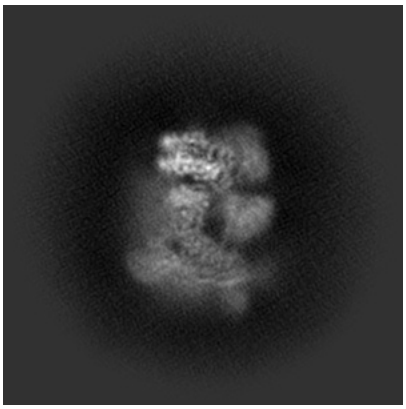
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-33684. These allow visual inspection of the internal detail of the map and identification of artifacts.

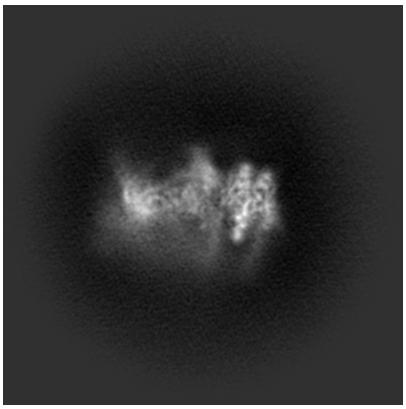
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

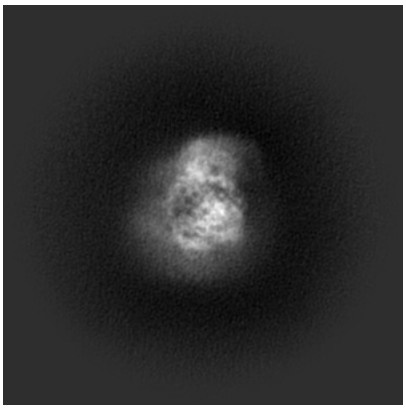
6.1.1 Primary map



X

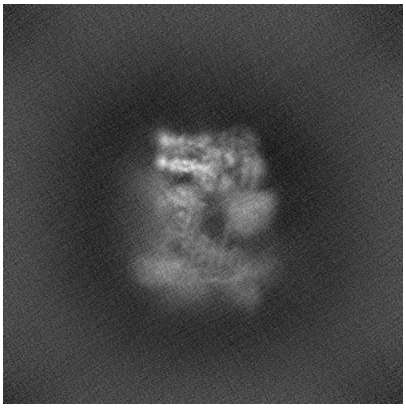


Y

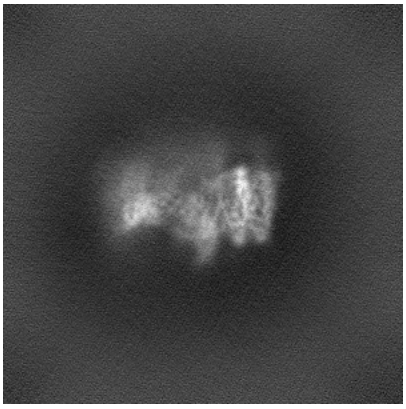


Z

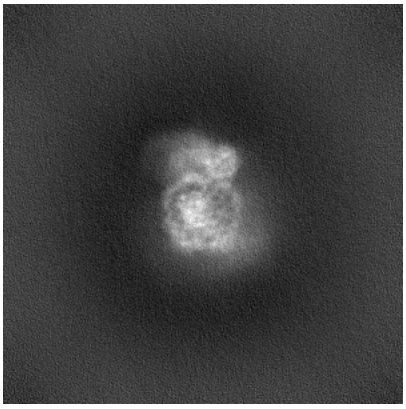
6.1.2 Raw map



X



Y

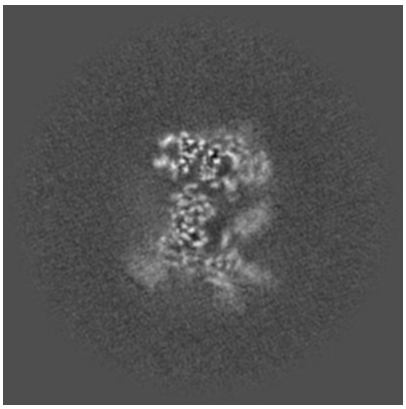


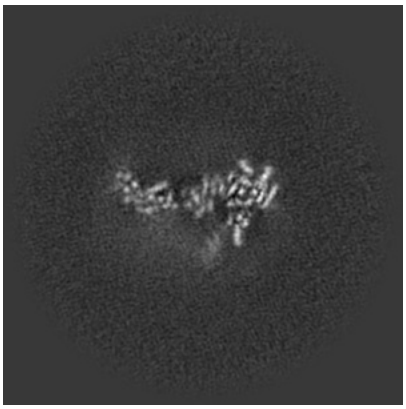
Z

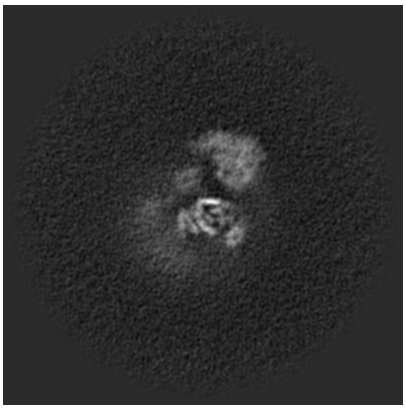
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

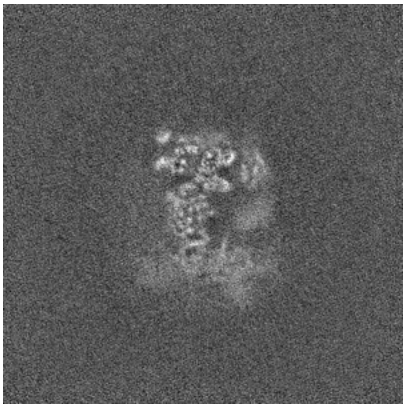
6.2.1 Primary map

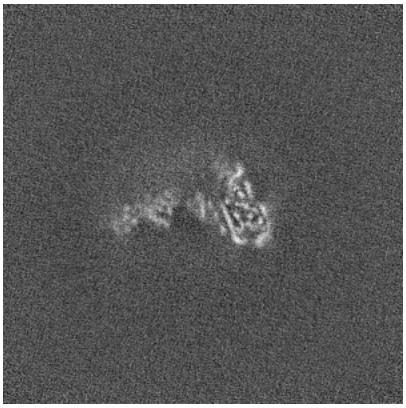

X Index: 180

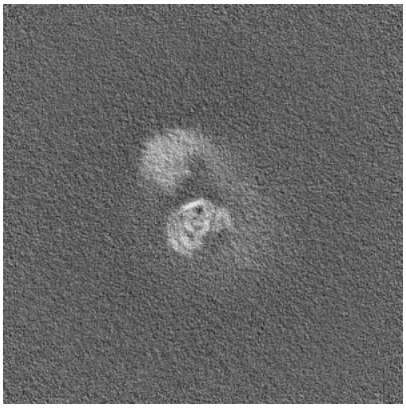

Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180

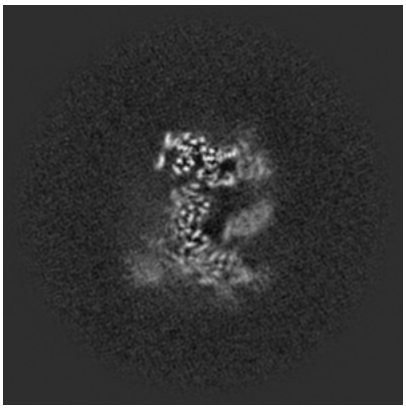

Y Index: 180


Z Index: 180

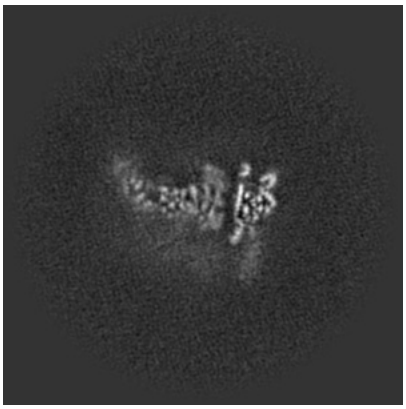
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

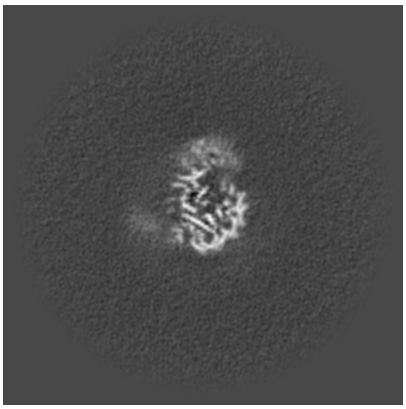
6.3.1 Primary map



X Index: 184

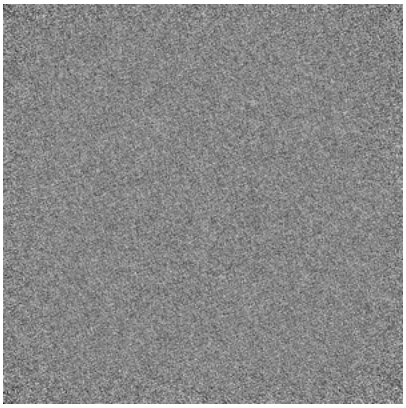


Y Index: 164

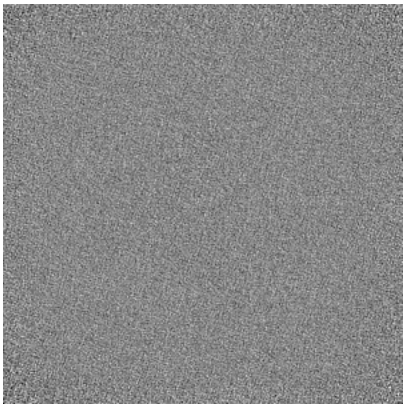


Z Index: 218

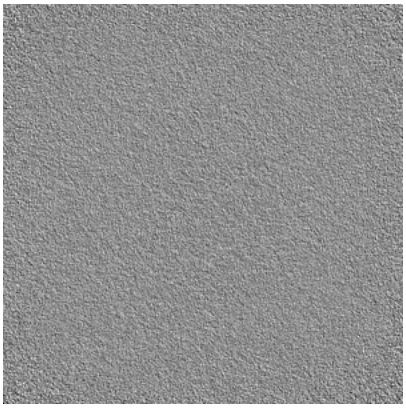
6.3.2 Raw map



X Index: 0



Y Index: 0

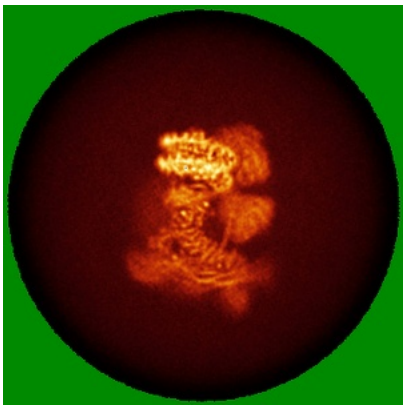


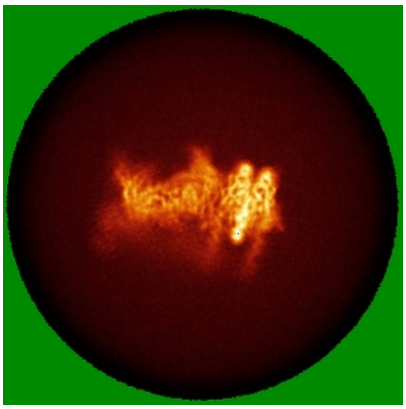
Z Index: 0

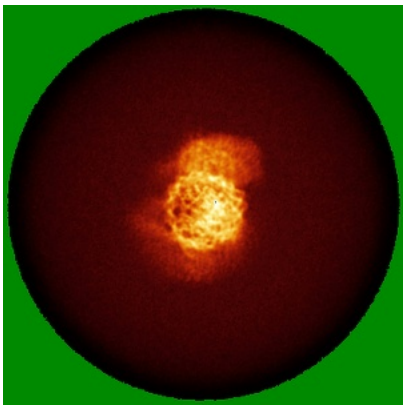
The images above show the largest variance slices of the map in three orthogonal directions.

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

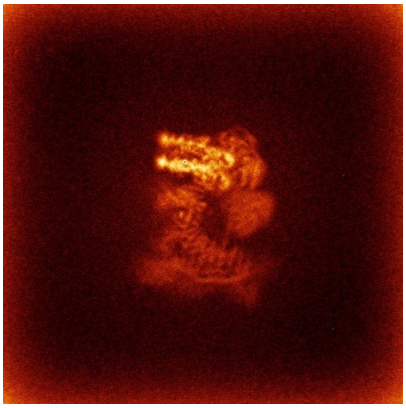
6.4.1 Primary map

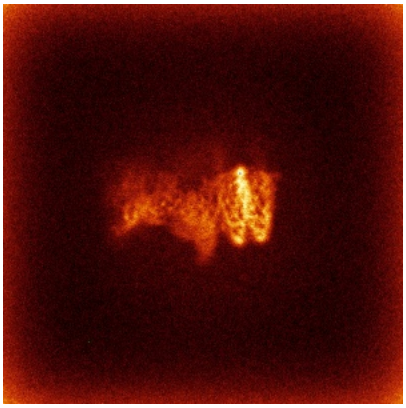

X

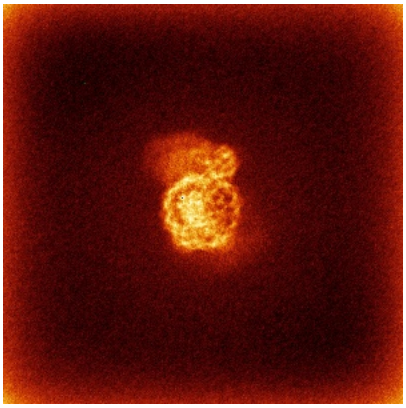

Y


Z

6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.28. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

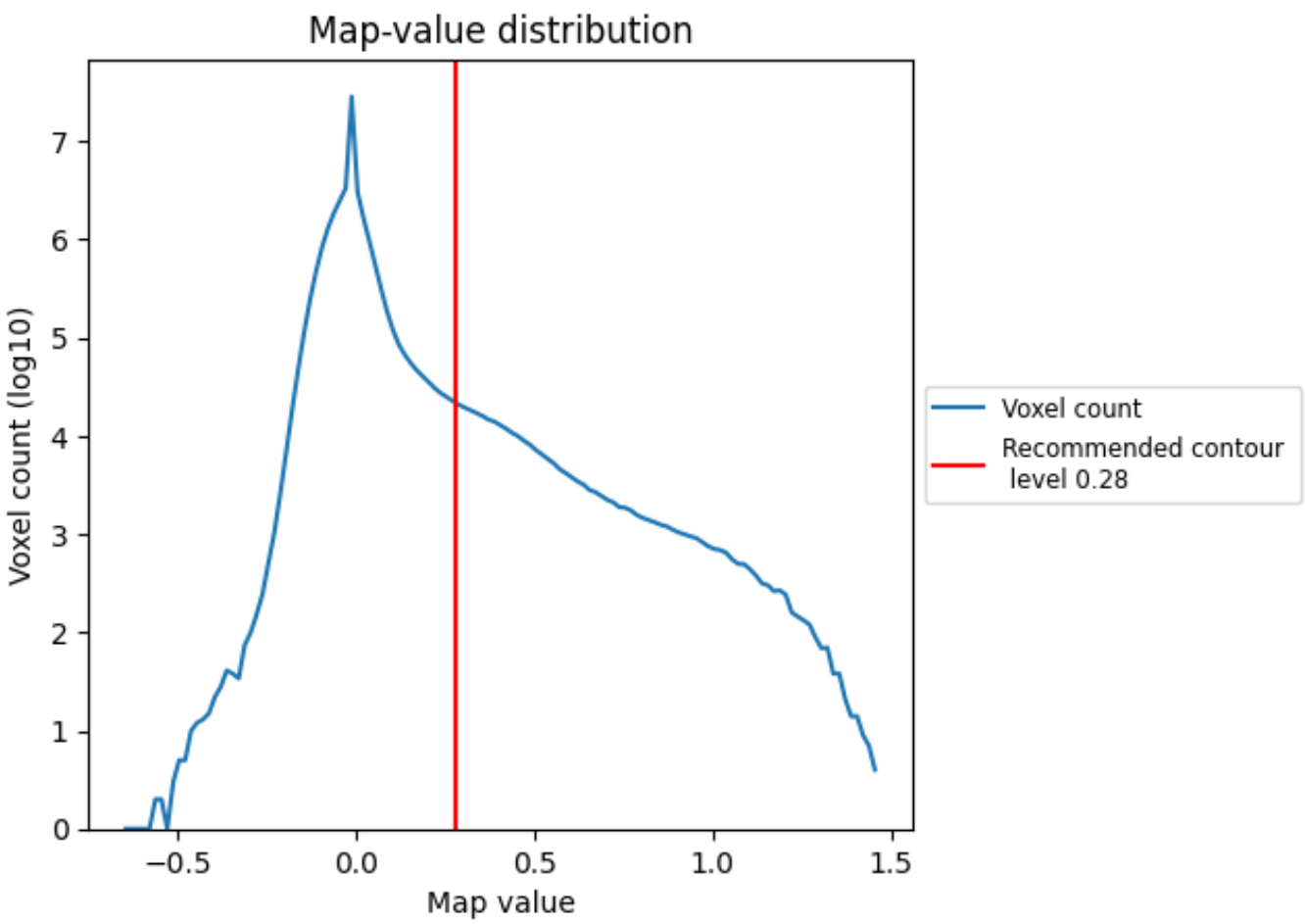
6.6 Mask visualisation (i)

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

7 Map analysis (i)

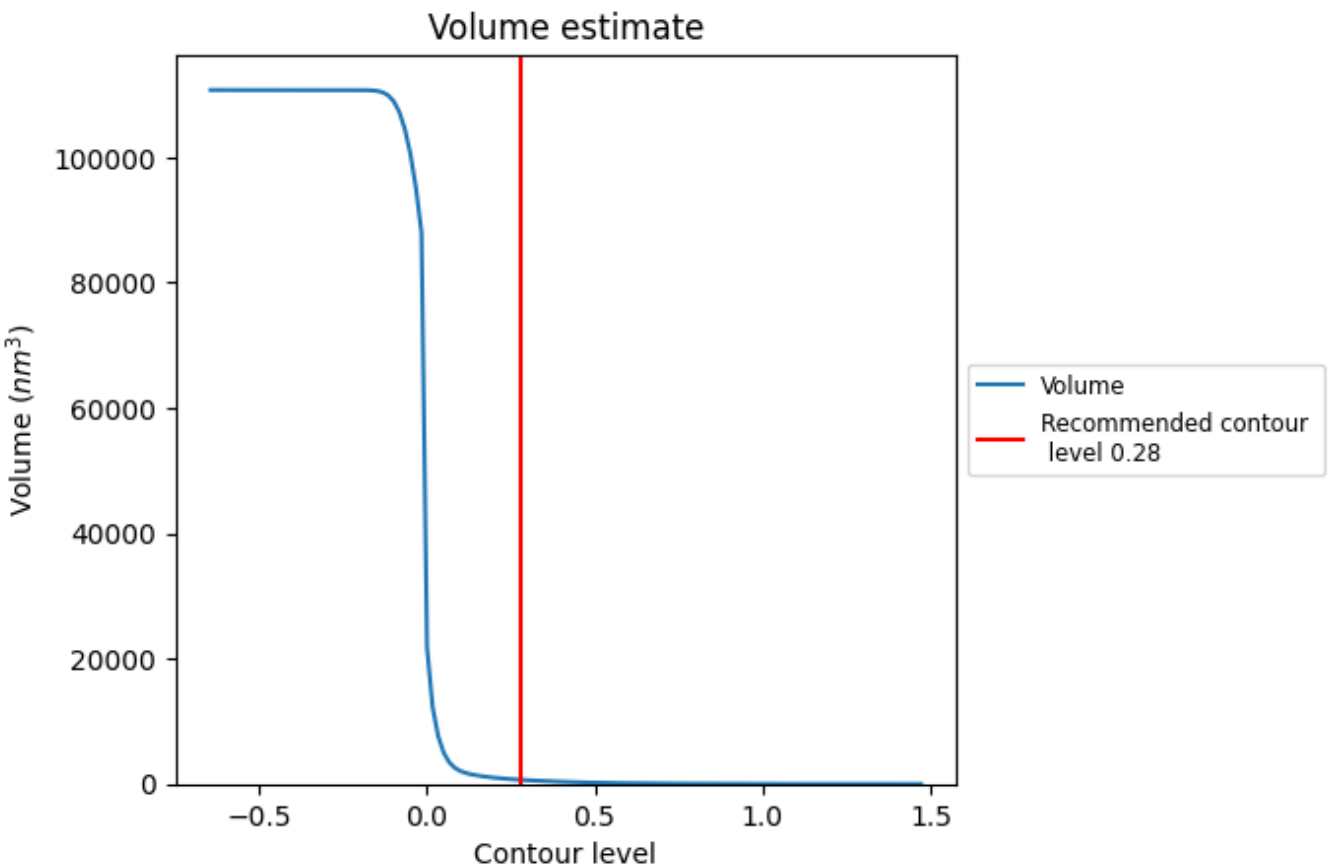
This section contains the results of statistical analysis of the map.

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.

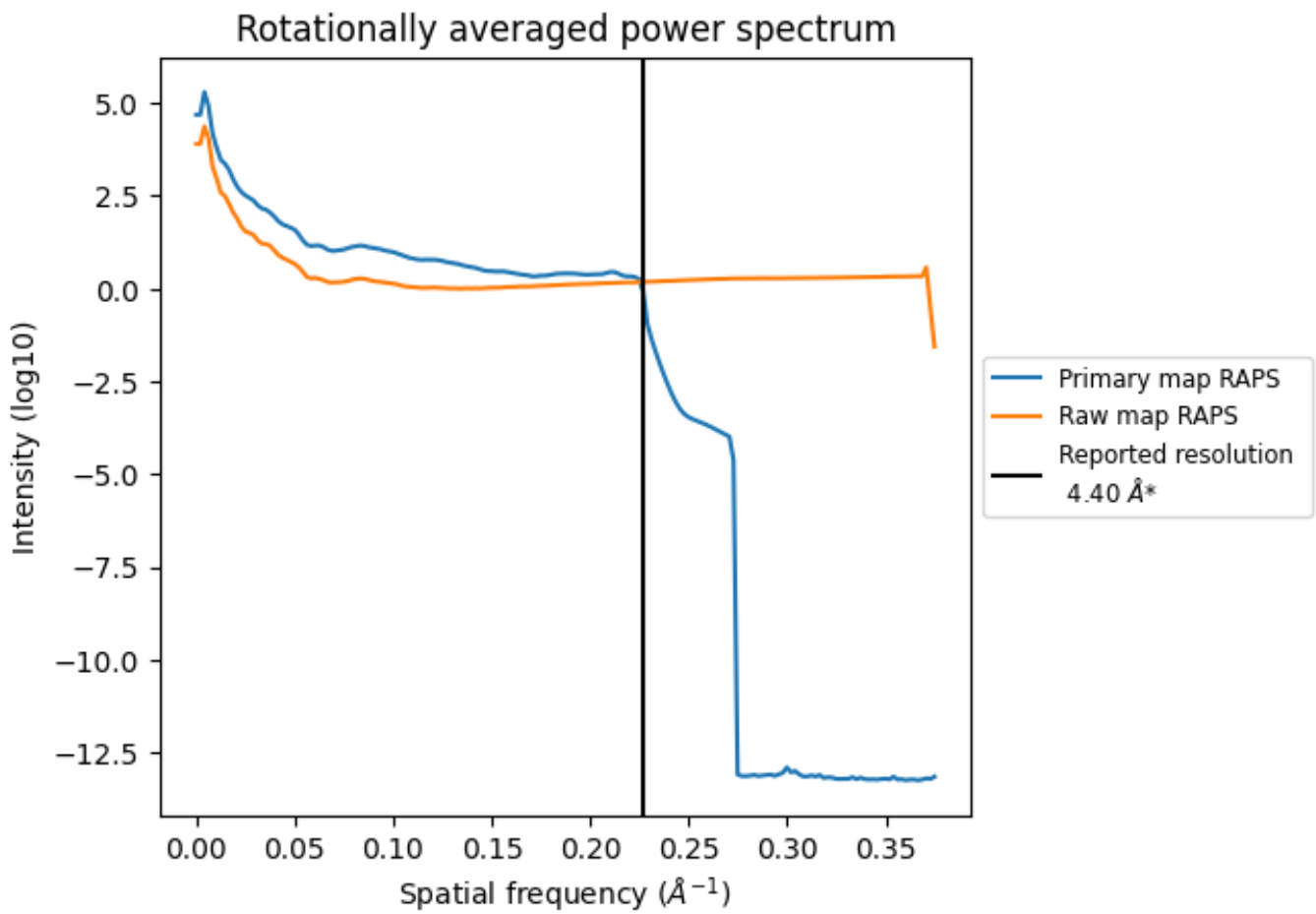
7.2 Volume estimate (i)



The volume at the recommended contour level is 660 nm^3; this corresponds to an approximate mass of 596 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)

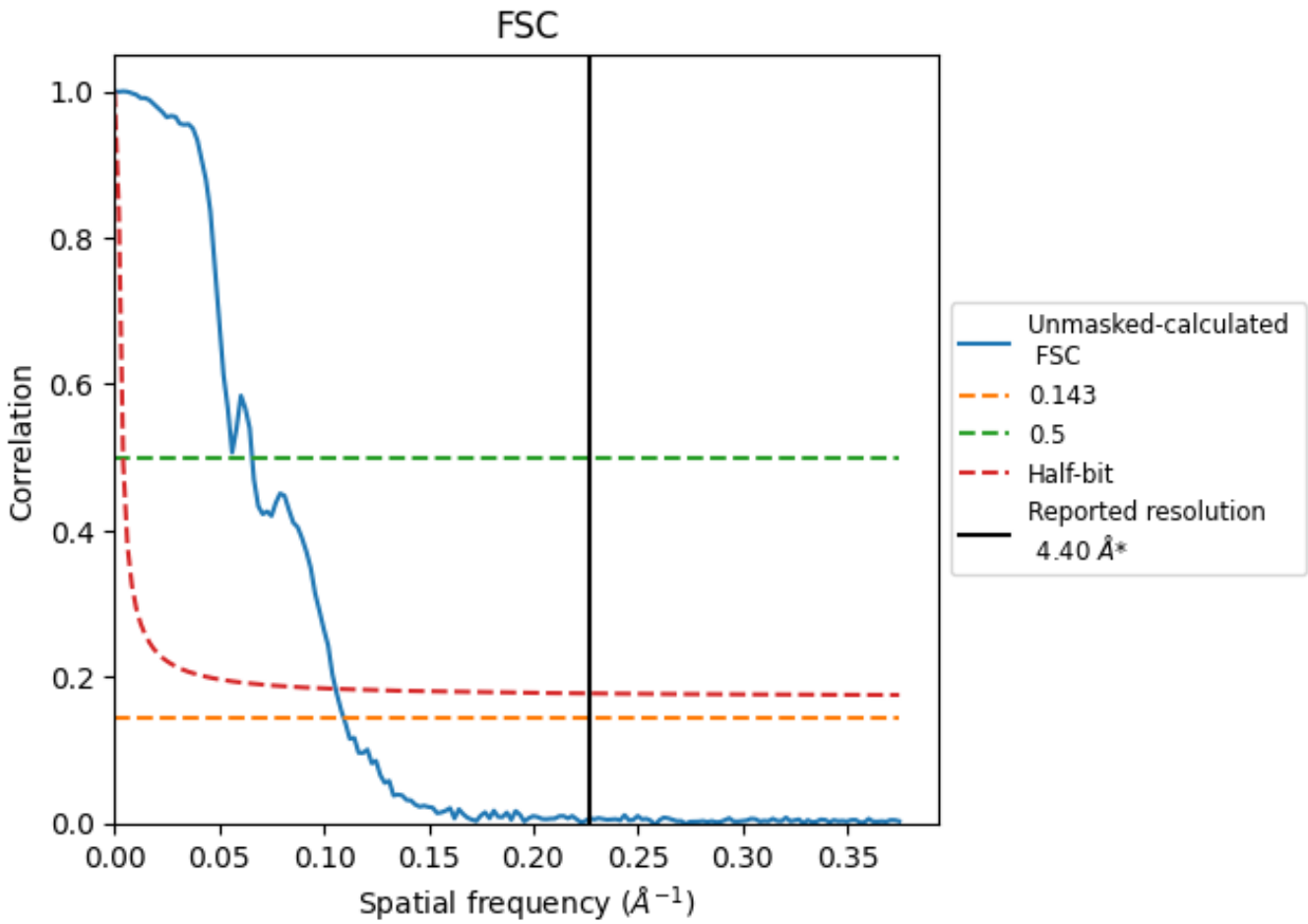


*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

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 0.227 Å^{-1}

8.2 Resolution estimates (i)

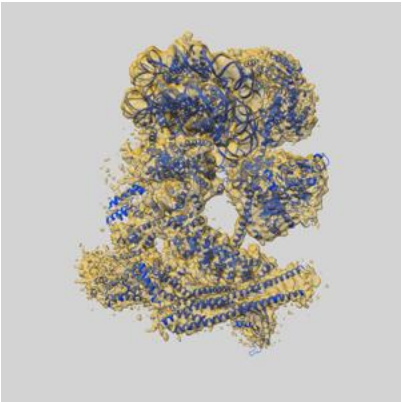
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.13	15.22	9.46

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.13 differs from the reported value 4.4 by more than 10 %

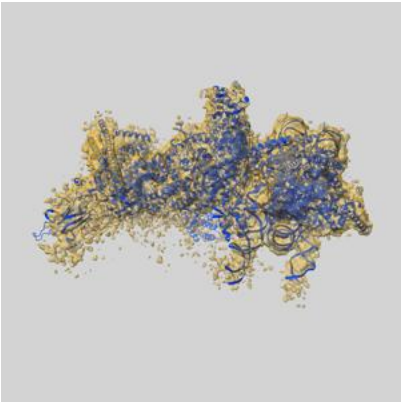
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-33684 and PDB model 7Y8R. Per-residue inclusion information can be found in section 3 on page 9.

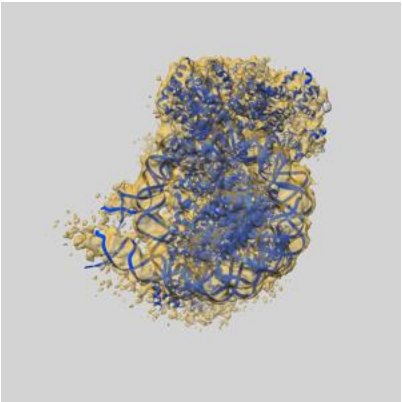
9.1 Map-model overlay (i)



X



Y



Z

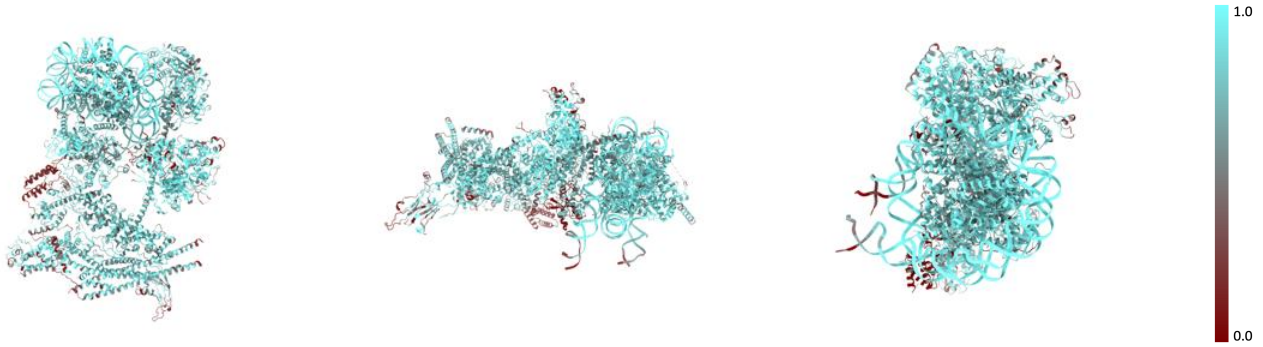
The images above show the 3D surface view of the map at the recommended contour level 0.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

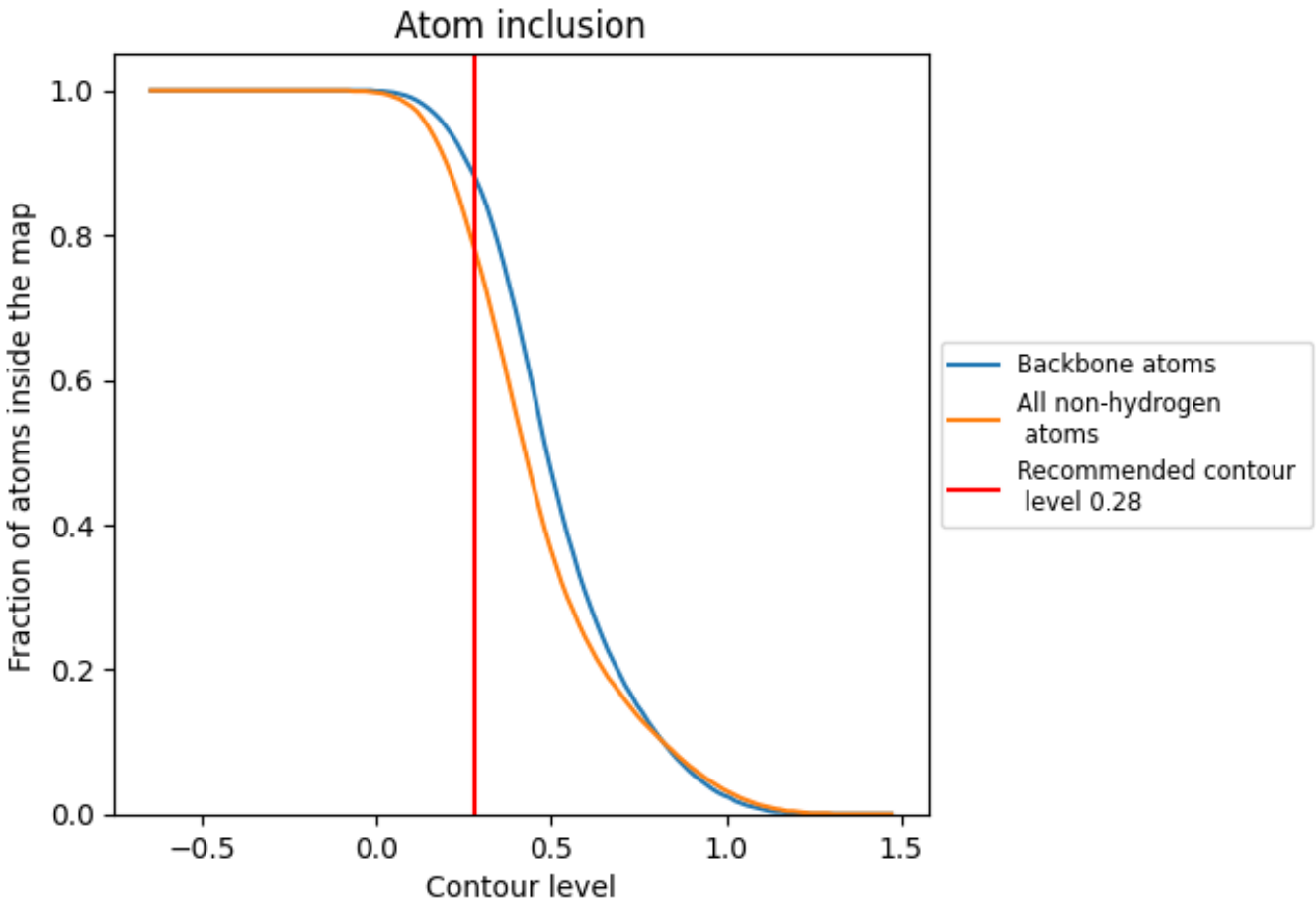
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.28).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 78% 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 (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7820	0.1720
A	0.8330	0.2410
B	0.7150	0.2210
C	0.8750	0.2650
D	0.8860	0.2630
E	0.8430	0.2570
F	0.8450	0.2740
G	0.8160	0.2600
H	0.8420	0.2620
I	0.8120	0.1630
J	0.7990	0.1100
K	0.8520	0.1160
L	0.7760	0.1940
M	0.6240	0.1630
N	0.7980	0.1570
O	0.7590	0.1110
P	0.6950	0.1030
Q	0.6720	0.1420
R	0.7420	0.1190
S	0.3800	0.0810
T	0.7910	0.1600
U	0.6440	0.1980
V	0.7360	0.1920
W	0.6670	0.1900
X	0.8970	0.2220
Y	0.9190	0.2380
Z	0.9720	0.1290
a	0.7070	0.1670