wwPDB EM Validation Summary Report (i)

Feb 26, 2024 – 01:02 PM JST

PDB ID	:	8X1C
EMDB ID	:	EMD-37990
Title	:	Structure of nucleosome-bound SRCAP-C in the ADP-bound state
Authors	:	Yu, J.; Wang, Q.; Yu, Z.; Li, W.; Wang, L.; Xu, Y.
Deposited on	:	2023-11-06
Resolution	:	3.20 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

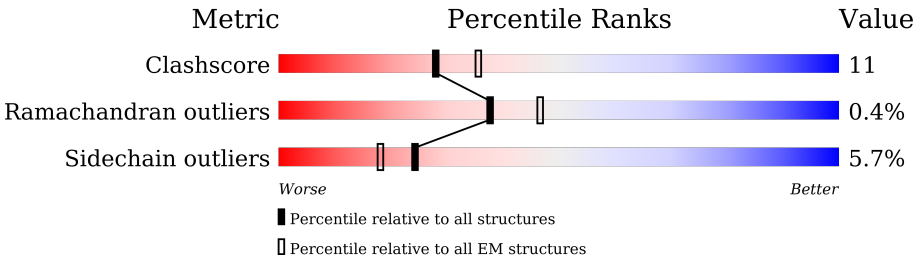
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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 <=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	130	8% 72% 17% 11%
1	E	130	68% 12% 19%
2	B	126	56% 20% 24%
2	F	126	62% 11% 25%
3	C	136	7% 53% 15% 30%
3	G	136	65% 6% 29%
4	D	103	68% 11% 21%
4	H	103	73% 5% 22%

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Mol	Chain	Length	Quality of chain
5	I	3230	20% 6% 74%
6	J	364	6% 28% 7% 63%
7	K	396	73% 24%
8	L	154	6% 55% 13% 32%
9	M	456	75% 17% 6%
9	O	456	81% 13% 5%
9	Q	456	75% 20%
10	N	463	77% 12% 10%
10	P	463	72% 19% 8%
10	R	463	72% 18% 8%
11	S	375	50% 97%
11	U	375	61% 72% 22%
12	T	429	61% 83% 10% 6%
13	V	467	42% 33% 9% 56%
14	W	227	82% 70% 11% 18%
15	X	147	10% 18% 52% 31%
16	Y	147	9% 25% 50% 25%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 56519 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 H2A type 1-C.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	116	Total 898	C 564	N 179	O 155	0	0
1	E	105	Total 808	C 510	N 158	O 140	0	0

- Molecule 2 is a protein called Histone H2B type 1-C/E/F/G/I.

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

- Molecule 3 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	95	Total 779	C 491	N 148	O 136	S 4	0	0
3	G	97	Total 801	C 505	N 155	O 137	S 4	0	0

- Molecule 4 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	81	Total 646	C 407	N 126	O 112	S 1	0	0
4	H	80	Total 638	C 401	N 125	O 111	S 1	0	0

- Molecule 5 is a protein called Helicase SRCAP.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	852	Total	C	N	O	S	0	0
			7031	4476	1299	1217	39		

- Molecule 6 is a protein called Vacuolar protein sorting-associated protein 72 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	135	Total	C	N	O	S	0	0
			1114	708	203	199	4		

- Molecule 7 is a protein called Actin-related protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	394	Total	C	N	O	S	0	0
			3209	2054	526	611	18		

- Molecule 8 is a protein called Zinc finger HIT domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	105	Total	C	N	O	S	0	0
			823	506	157	152	8		

- Molecule 9 is a protein called RuvB-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	428	Total	C	N	O	S	0	0
			3293	2075	567	635	16		
9	O	435	Total	C	N	O	S	0	0
			3339	2105	571	646	17		
9	Q	440	Total	C	N	O	S	0	0
			3368	2121	579	651	17		

- Molecule 10 is a protein called RuvB-like 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	415	Total	C	N	O	S	0	0
			3223	2016	565	627	15		
10	P	427	Total	C	N	O	S	0	0
			3287	2054	576	642	15		
10	R	424	Total	C	N	O	S	0	0
			3293	2057	578	642	16		

- Molecule 11 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	375	Total	C	N	O	S	0	0
			2925	1850	491	561	23		
11	U	359	Total	C	N	O	S	0	0
			2802	1775	468	540	19		

- Molecule 12 is a protein called Actin-like protein 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	403	Total	C	N	O	S	0	0
			3146	1988	535	599	24		

- Molecule 13 is a protein called DNA methyltransferase 1-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	V	204	Total	C	N	O	S	0	0
			1757	1117	327	309	4		

- Molecule 14 is a protein called YEATS domain-containing protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	187	Total	C	N	O	S	0	0
			1542	998	255	284	5		

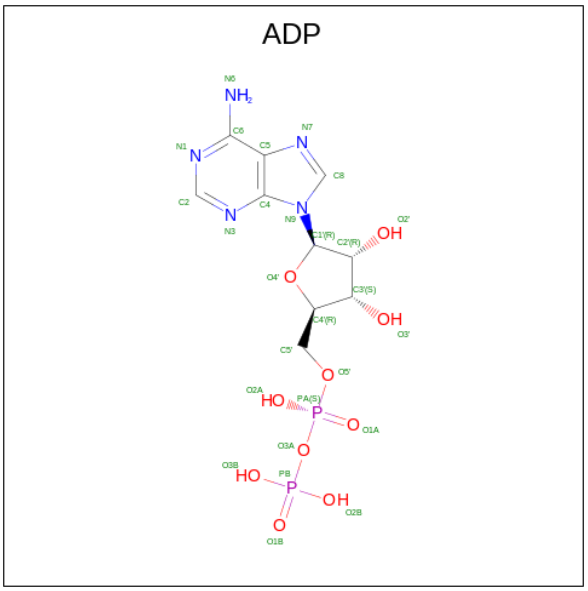
- Molecule 15 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	147	Total	C	N	O	P	0	0
			3034	1435	572	880	147		

- Molecule 16 is a DNA chain called DNA (147-MER).

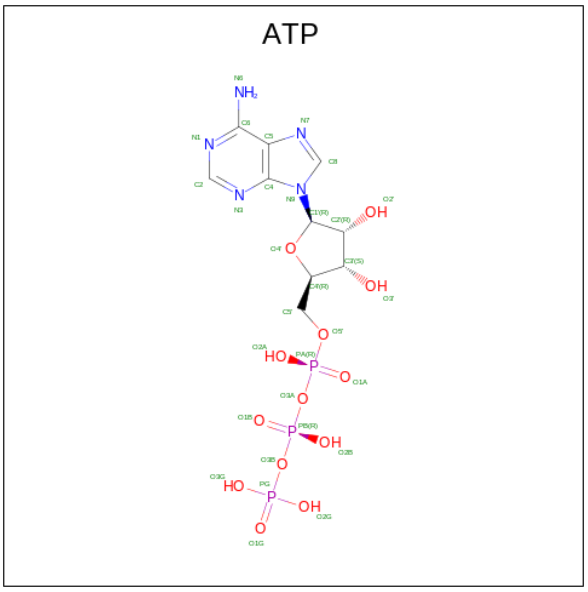
Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	147	Total	C	N	O	P	0	0
			2990	1422	540	882	146		

- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
17	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	M	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	N	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	O	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	P	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	Q	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	R	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 18 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



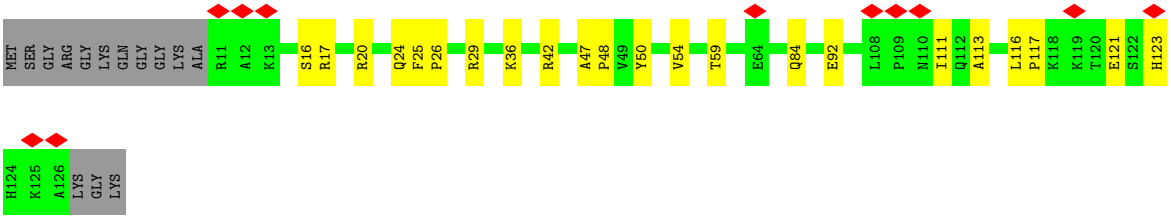
Mol	Chain	Residues	Atoms					AltConf
18	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
18	T	1	Total	C	N	O	P	0
			31	10	5	13	3	
18	U	1	Total	C	N	O	P	0
			31	10	5	13	3	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

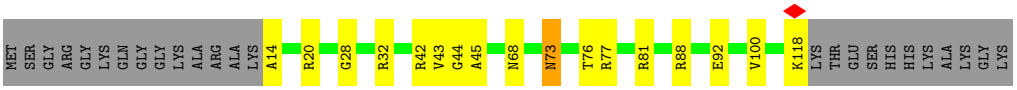
• Molecule 1: Histone H2A type 1-C

Chain A:



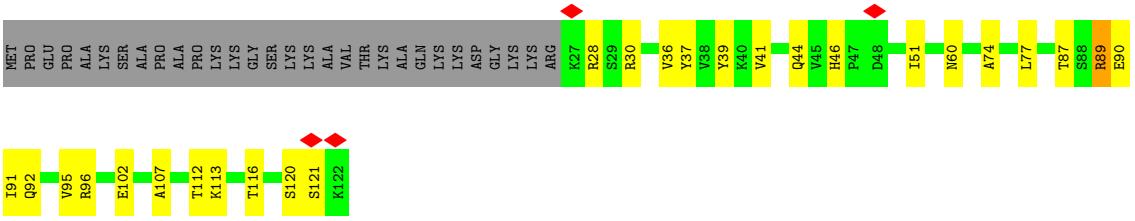
• Molecule 1: Histone H2A type 1-C

Chain E:



• Molecule 2: Histone H2B type 1-C/E/F/G/I

Chain B:

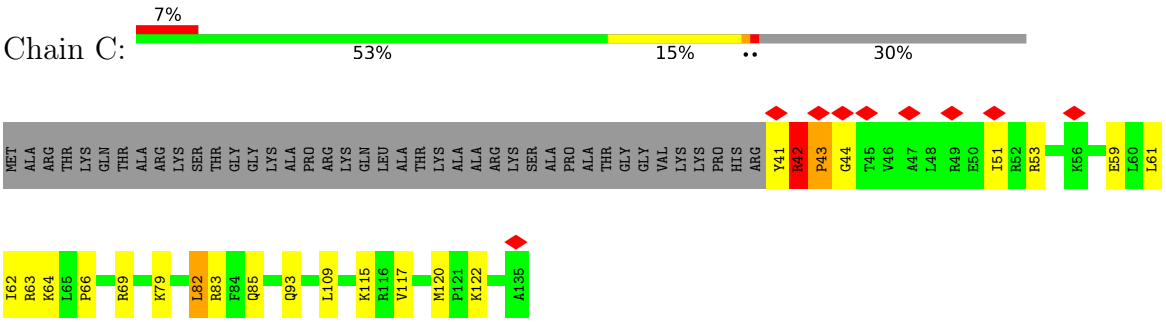


• Molecule 2: Histone H2B type 1-C/E/F/G/I

Chain F:

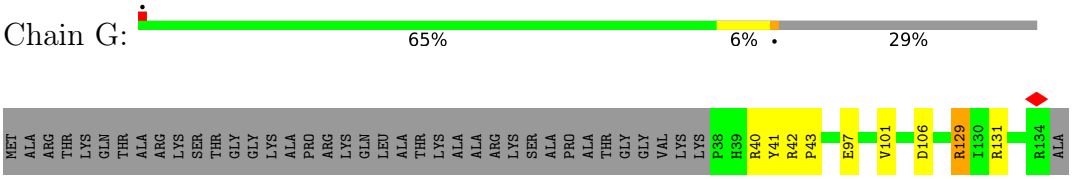
• Molecule 3: Histone H3.1

Chain C:



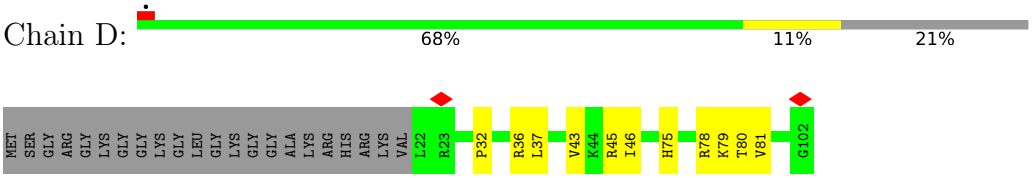
• Molecule 3: Histone H3.1

Chain G:



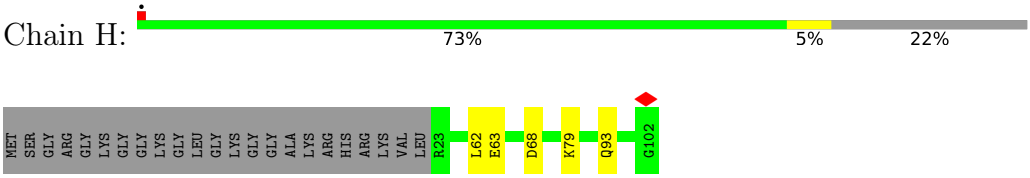
• Molecule 4: Histone H4

Chain D:



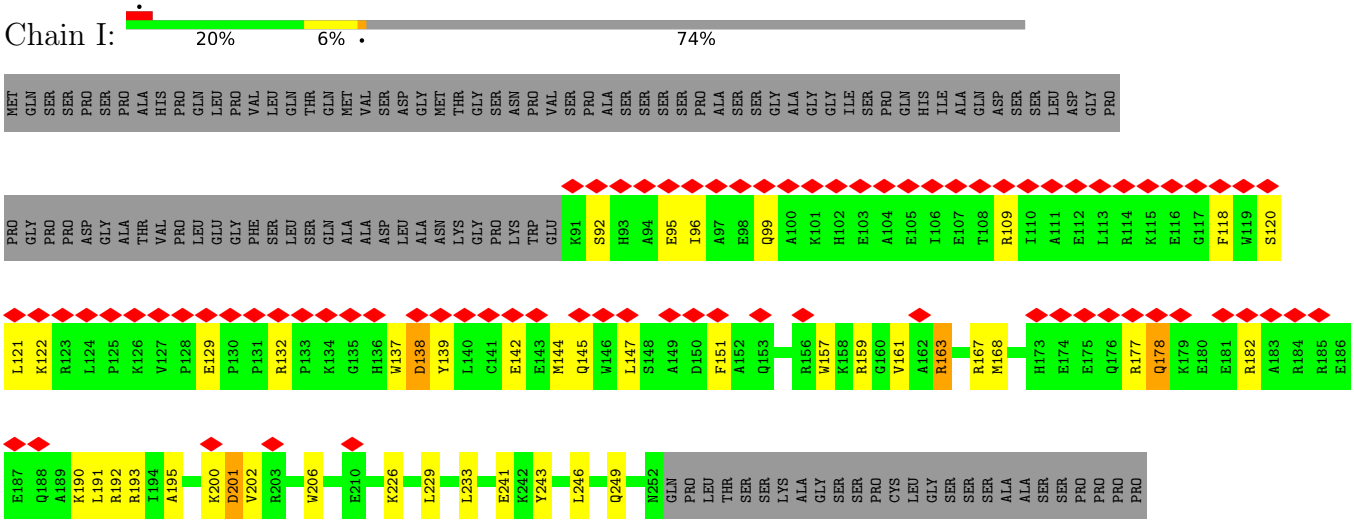
• Molecule 4: Histone H4

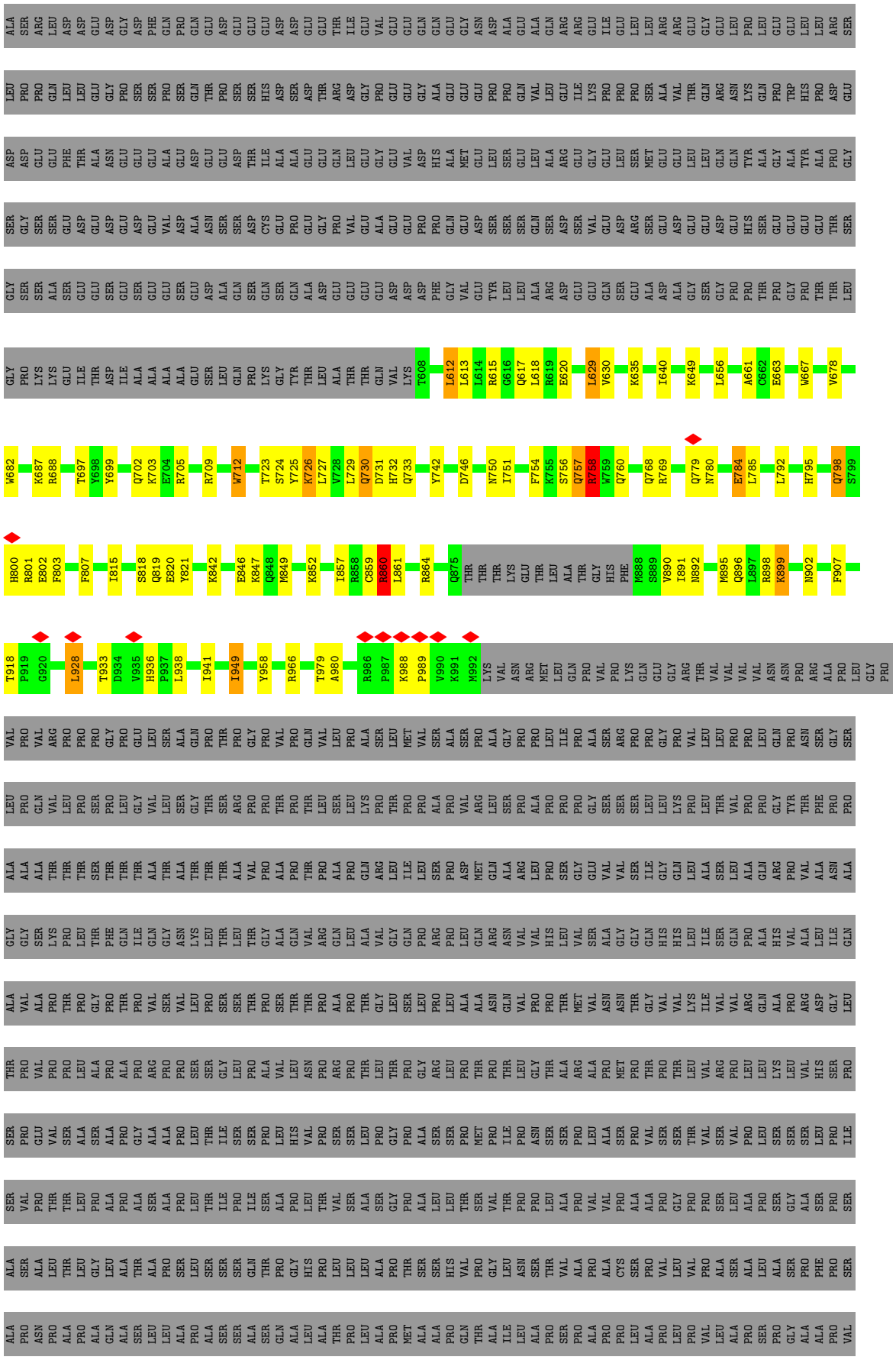
Chain H:

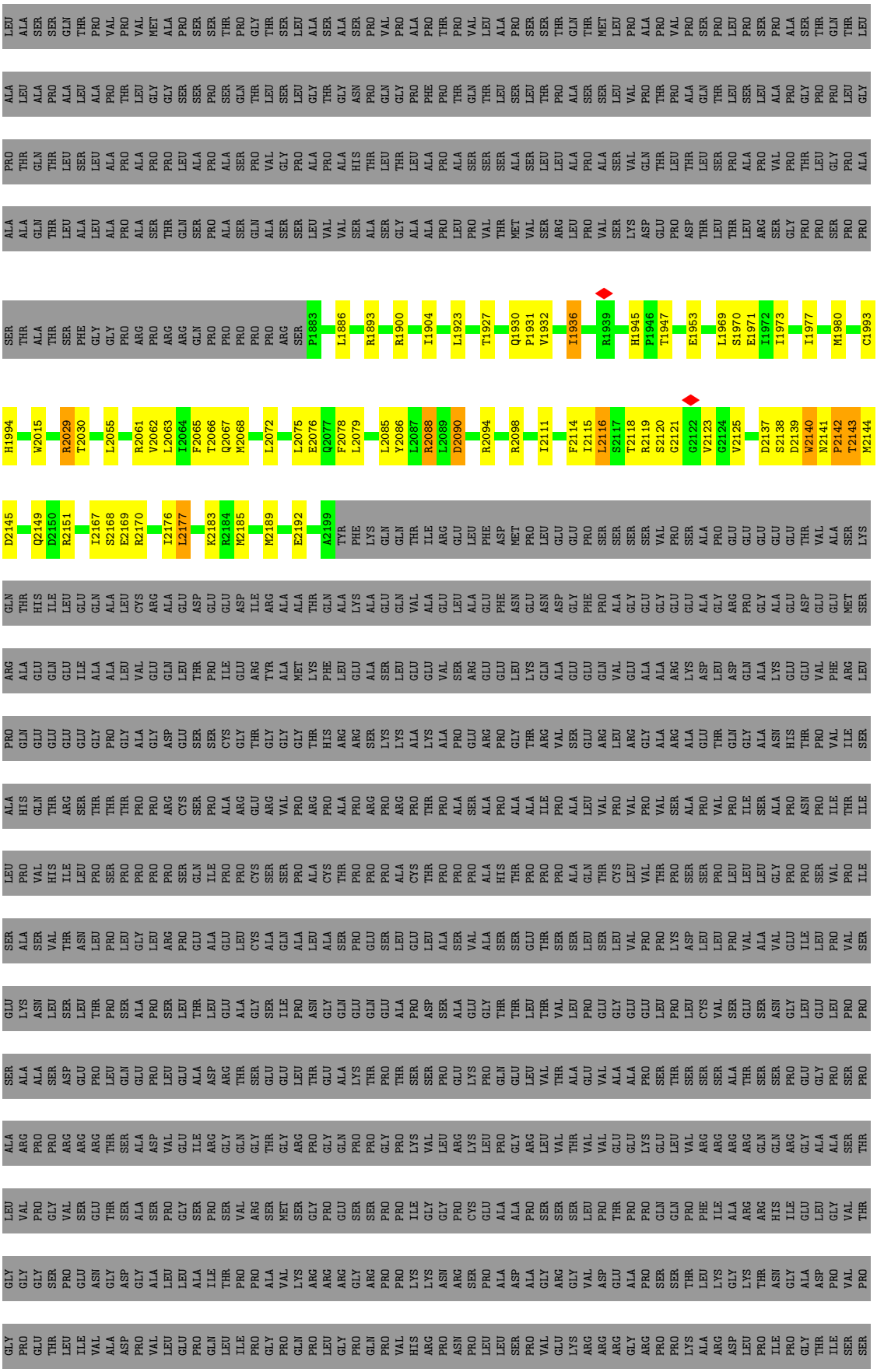


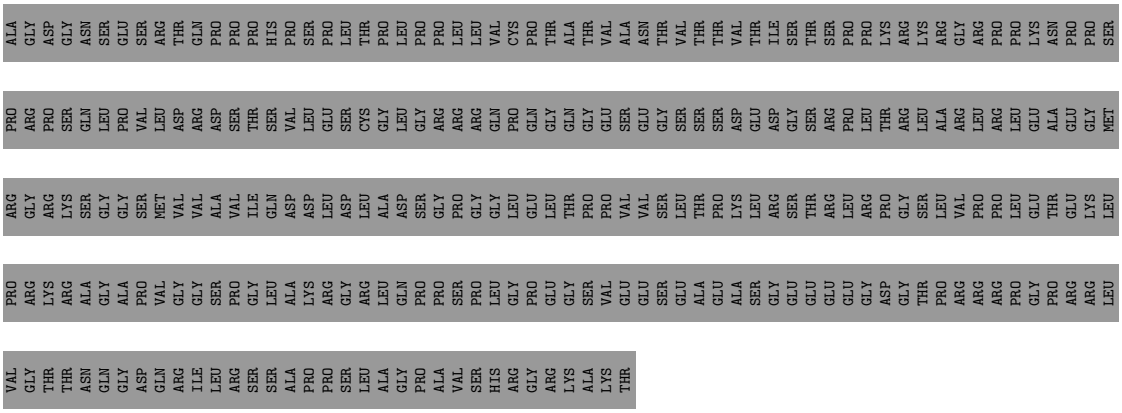
• Molecule 5: Helicase SRCAP

Chain I:



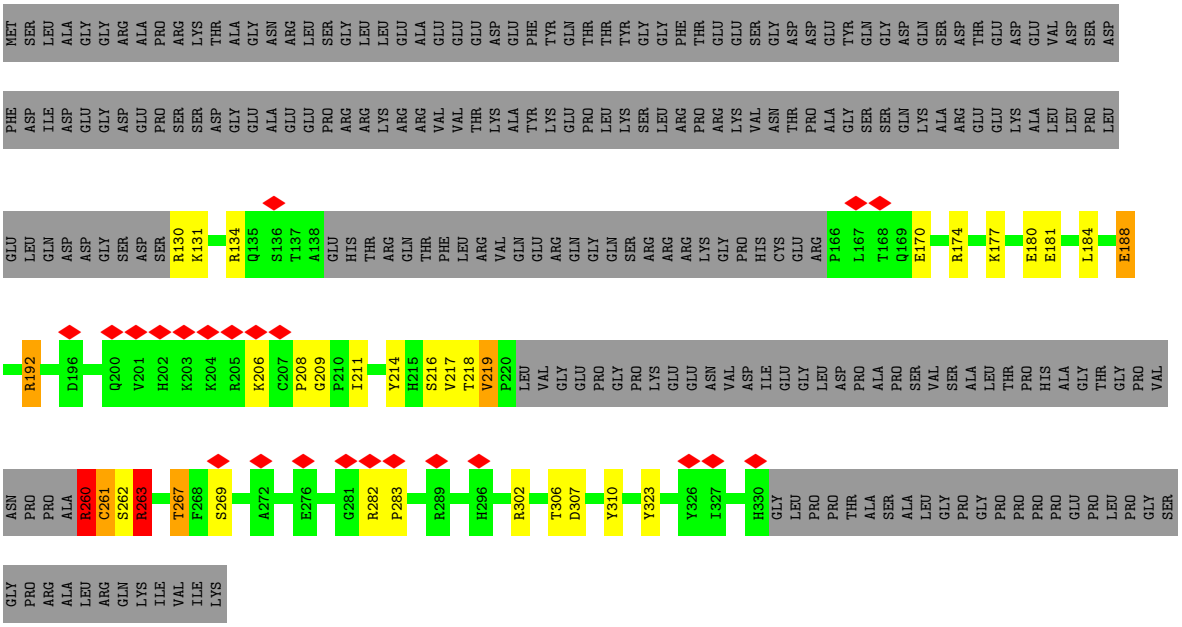

T608 L612 L613 L614 R615 G616 Q617 L618 R619 E620 L629 V630 K635 I640 K649 L656 A661 C662 E663 W667 V678
W682 K687 R688 T697 Y698 Y699 Q702 K703 E704 R705 R709 W712 T723 S724 Y725 K726 L727 V728 L729 Q730 D731 H732 Q733 Y742 D746 N750 I751 F754 K755 S756 Q757 R758 W759 Q760 Q768 R769 Q779 N780 E784 L785 L792 H795 Q798 S799
H800 R801 E802 F803 F807 I815 S818 Q819 E820 Y821 K842 E846 K847 Q848 M849 K852 I857 R858 C859 R860 L861 R864 Q875 M888 S889 V890 I891 N892 M895 Q896 L897 R898 K899 N902 F907
T918 P919 G920 L928 T933 D934 V935 H936 P937 L938 I941 I949 Y958 R966 T979 A980 R986 P987 K988 P989 V990 K991 M992


P1883 L1886 R1893 R1900 I1904 L1923 T1927 Q1930 P1931 V1932 I1936 R1939 H1945 P1946 T1947 E1963 L1969 S1970 E1971 I1972 I1973 I1977 M1980 C1993
H1994 W2015 R2029 T2030 L2055 R2061 V2062 L2063 I2064 F2065 T2066 Q2067 M2068 L2072 L2075 E2076 Q2077 F2078 L2079 L2085 Y2086 L2087 R2088 L2089 D2090 R2094 R2098 I2111 F2114 I2115 L2116 S2117 T2118 R2119 S2120 G2121 G2122 V2123 G2124 V2125 D2137 S2138 D2139 W2140 N2141 P2142 T2143 N2144
D2145 Q2149 D2150 R2151 I2167 S2168 E2169 R2170 I2176 L2177 K2183 R2184 M2185 M2189 E2192 A2199



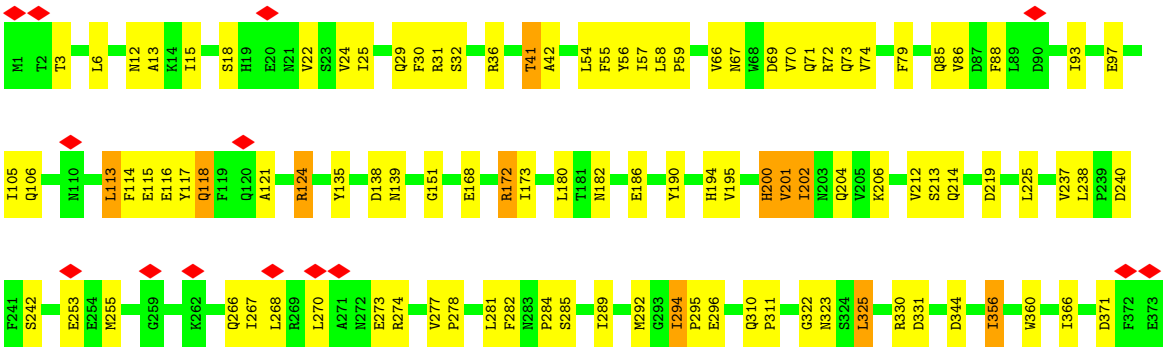
• Molecule 6: Vacuolar protein sorting-associated protein 72 homolog

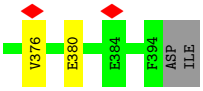
Chain J:



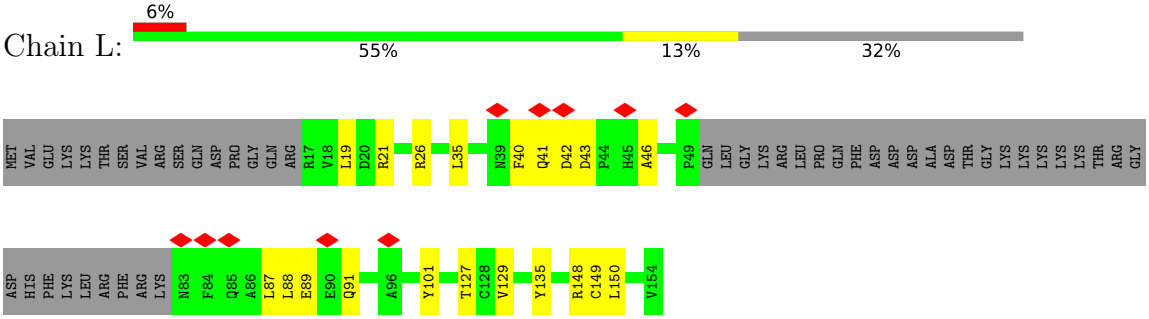
• Molecule 7: Actin-related protein 6

Chain K:

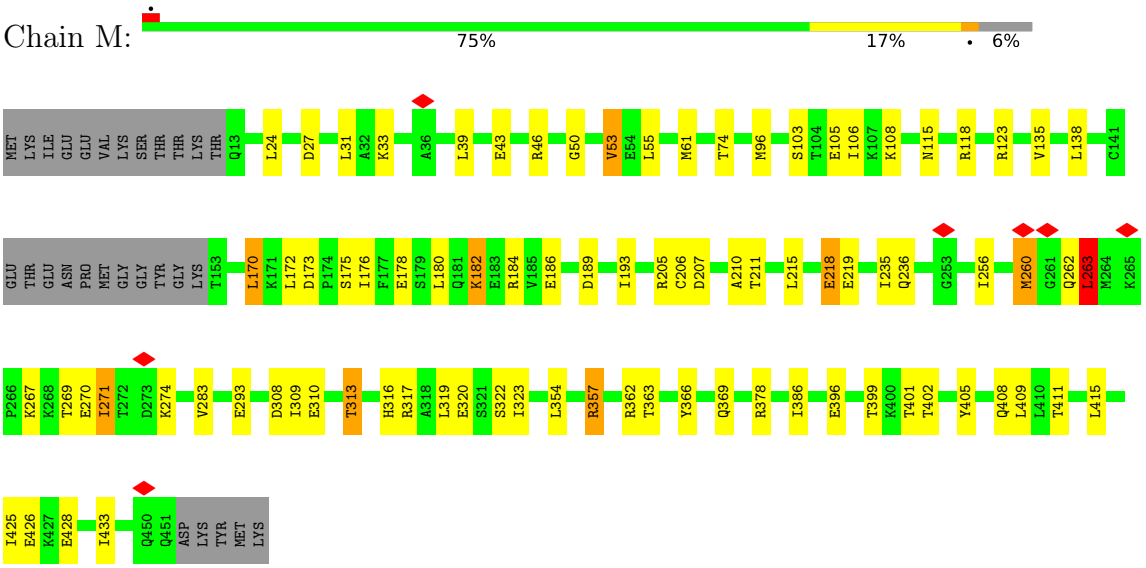




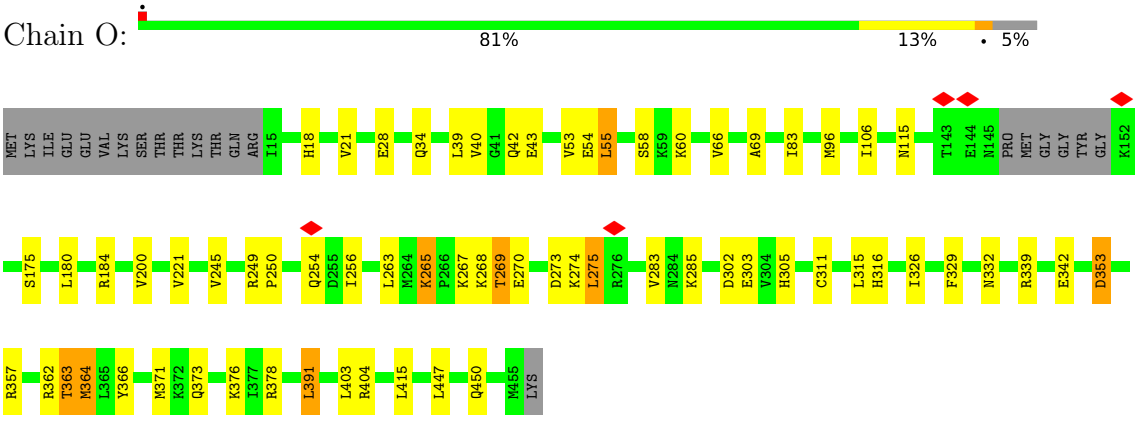
• Molecule 8: Zinc finger HIT domain-containing protein 1



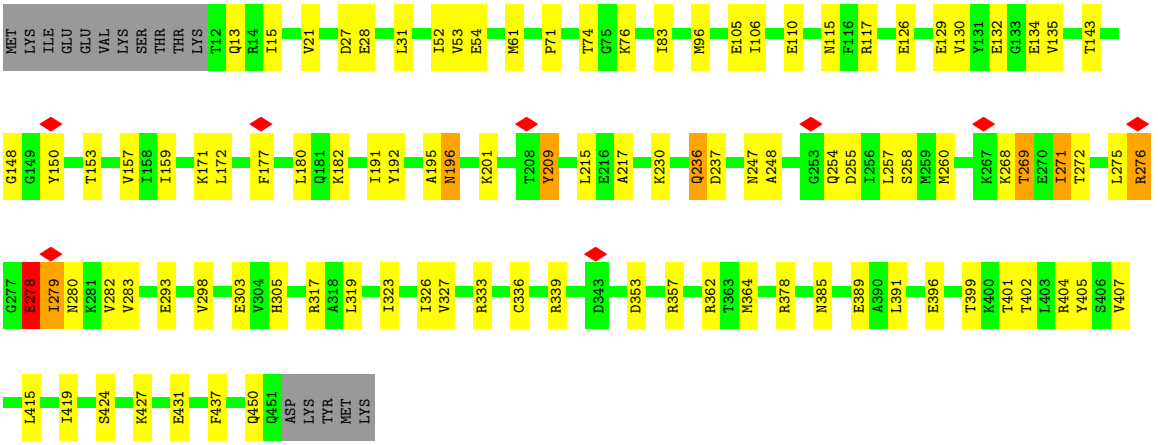
• Molecule 9: RuvB-like 1



• Molecule 9: RuvB-like 1

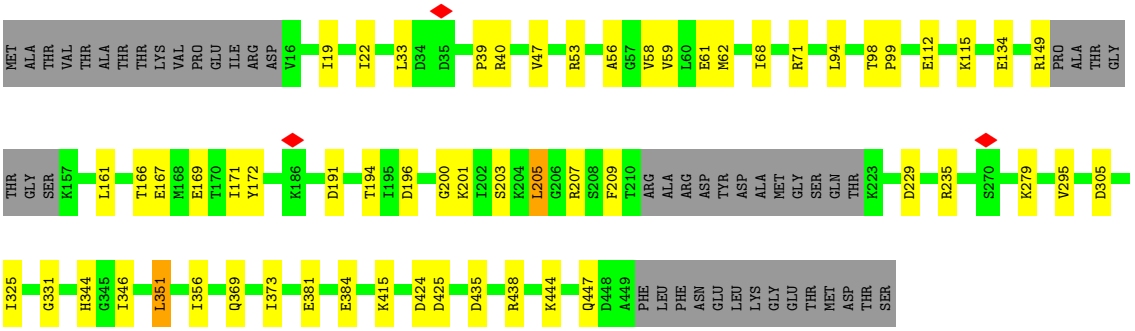


• Molecule 9: RuvB-like 1



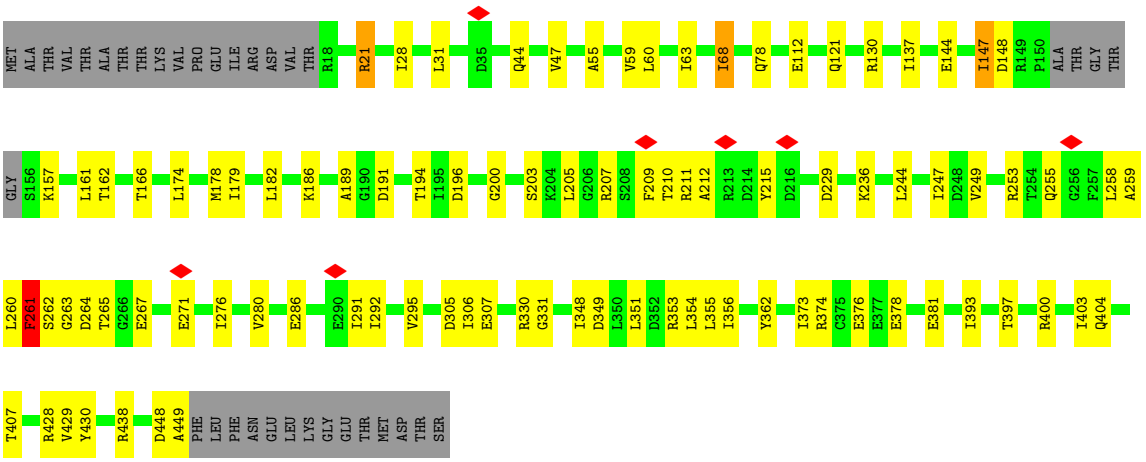
• Molecule 10: RuvB-like 2

Chain N:



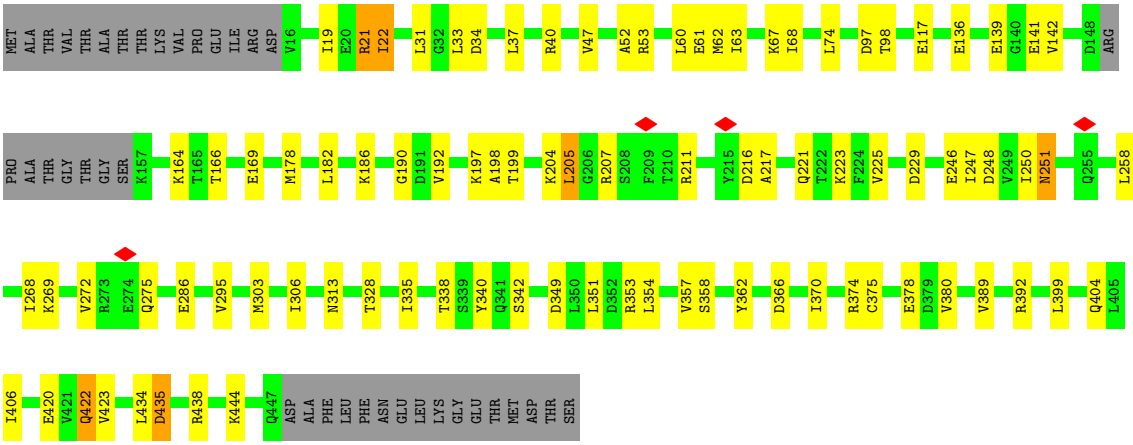
• Molecule 10: RuvB-like 2

Chain P:



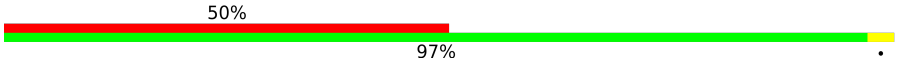
• Molecule 10: RuvB-like 2

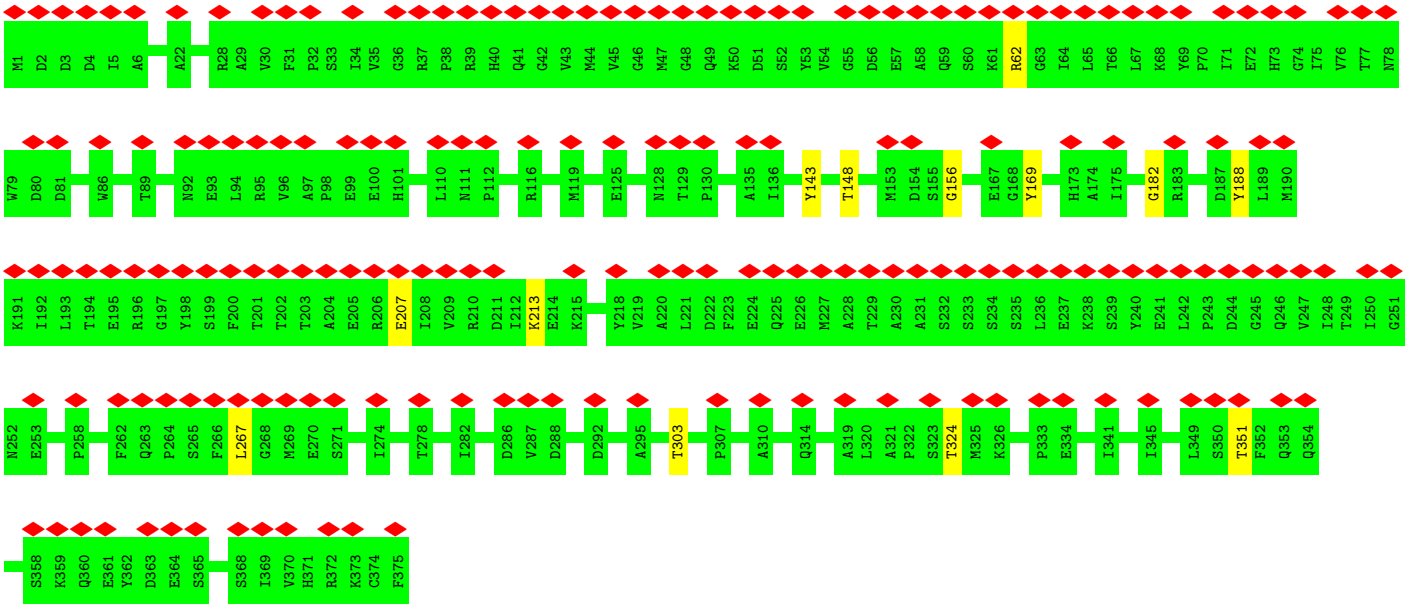
Chain R:



• Molecule 11: Actin, cytoplasmic 1

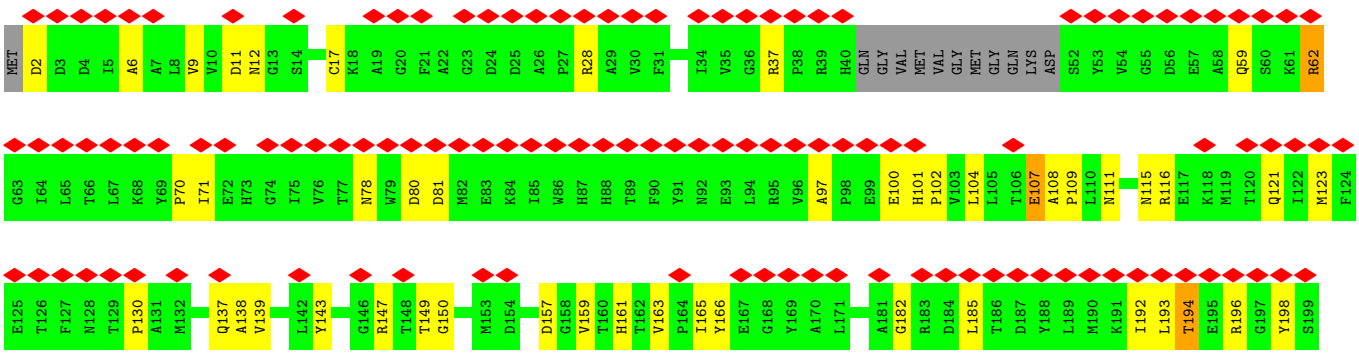
Chain S:

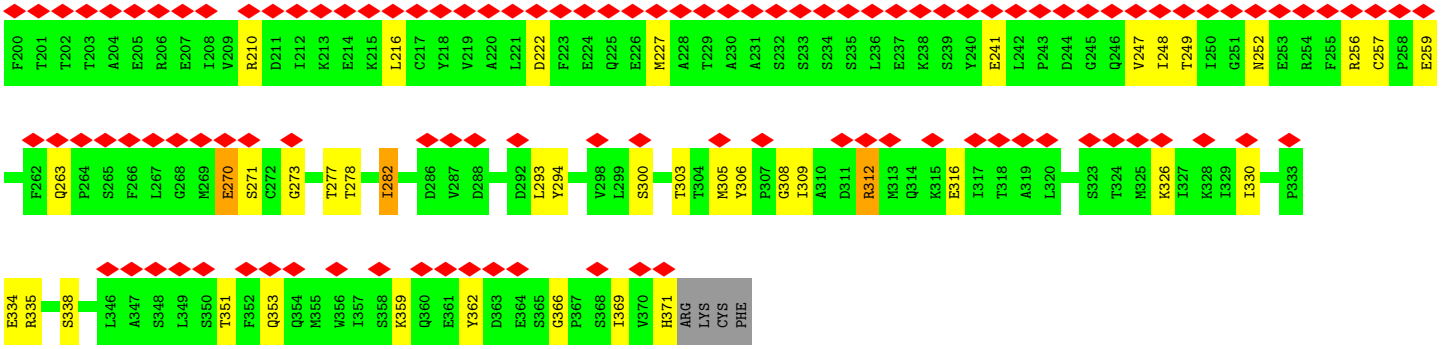




• Molecule 11: Actin, cytoplasmic 1

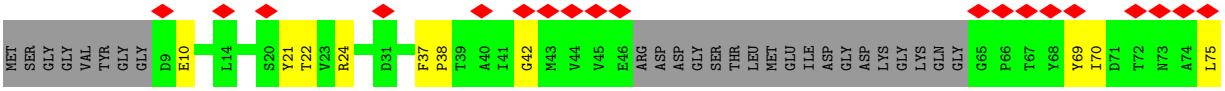
Chain U:

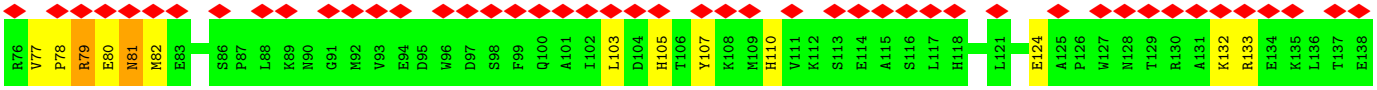


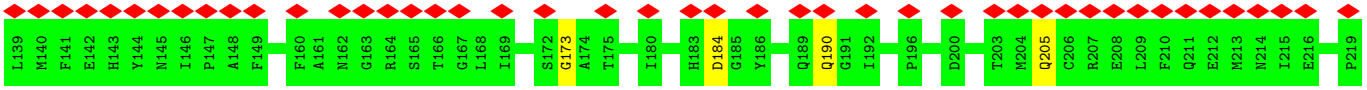


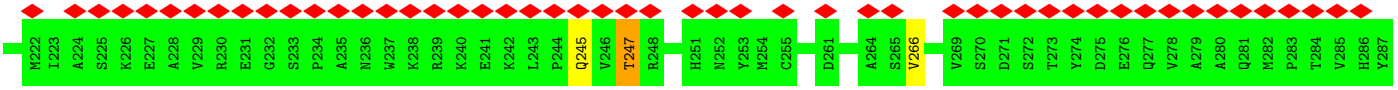
• Molecule 12: Actin-like protein 6A

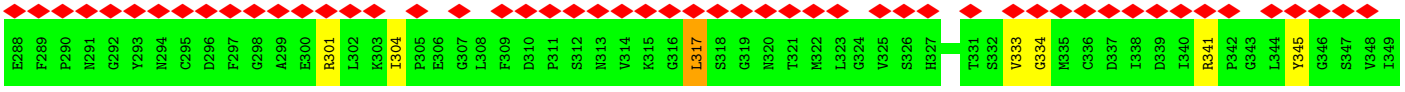
Chain T:

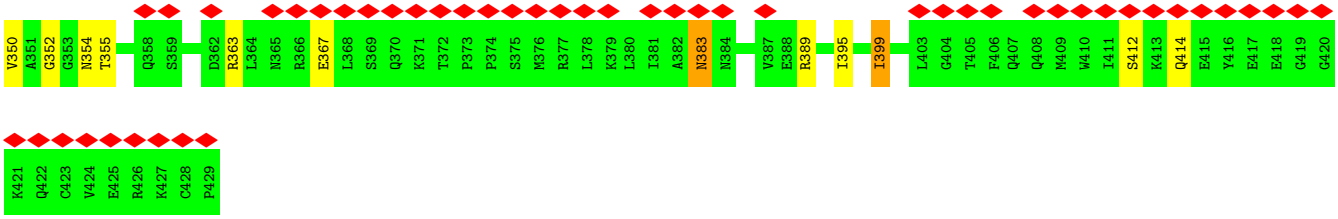






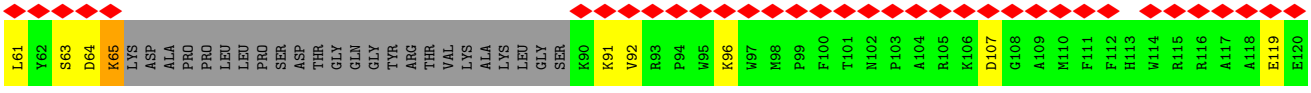


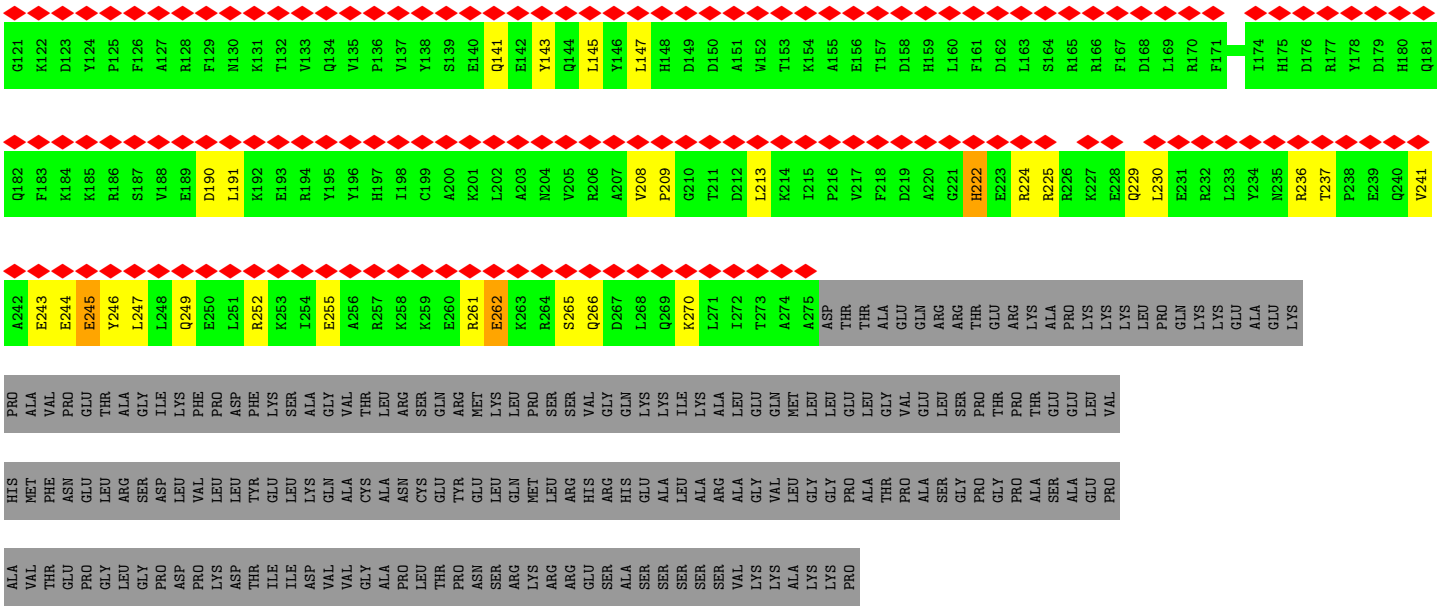




• Molecule 13: DNA methyltransferase 1-associated protein 1

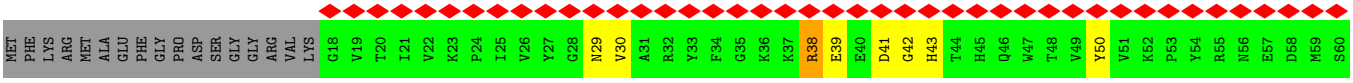
Chain V:

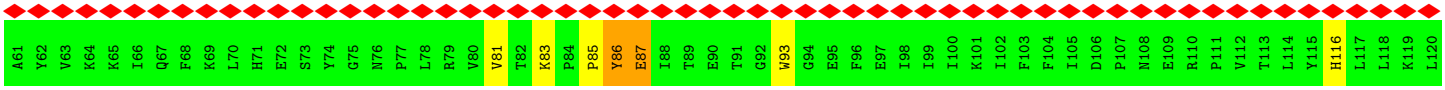


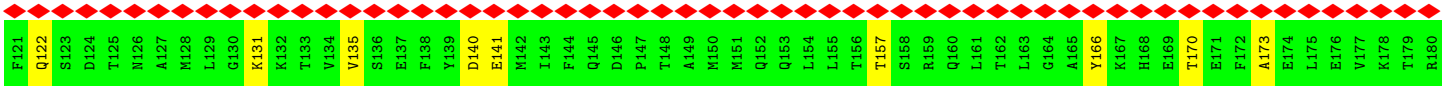


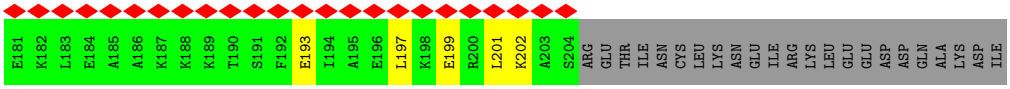
• Molecule 14: YEATS domain-containing protein 4

Chain W:



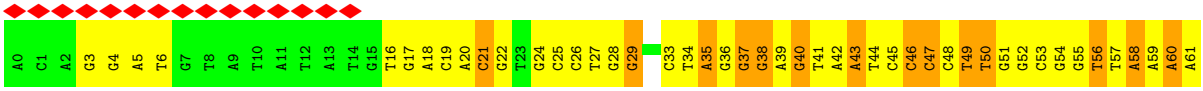


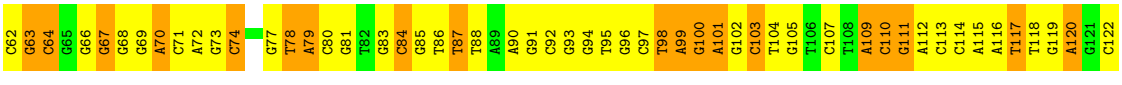




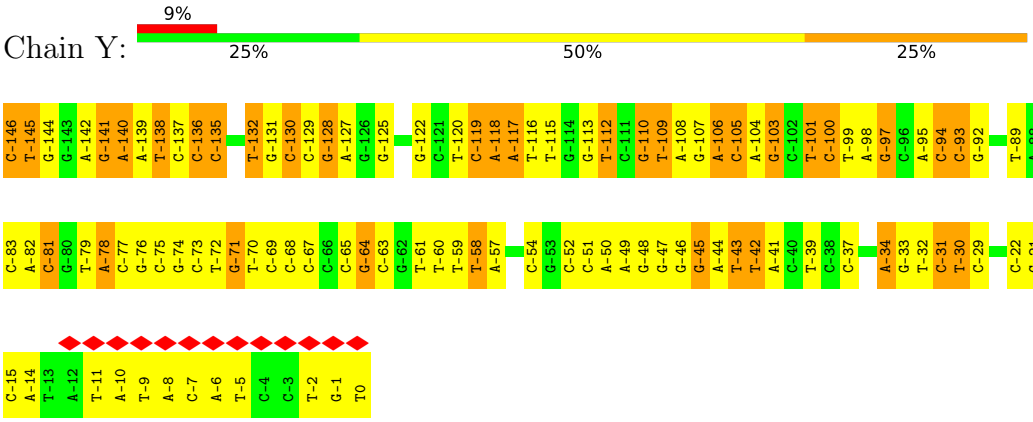
• Molecule 15: DNA (147-MER)

Chain X:





• Molecule 16: DNA (147-MER)



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	555303	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)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.222	Depositor
Minimum map value	-0.080	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.026	Depositor
Map size (Å)	533.6, 533.6, 533.6	wwPDB
Map dimensions	400, 400, 400	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: ATP, 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	0.23	0/910	0.39	0/1225
1	E	0.24	0/818	0.38	0/1104
2	B	0.29	0/766	0.41	0/1026
2	F	0.24	0/747	0.37	0/1004
3	C	0.24	0/789	0.39	0/1057
3	G	0.23	0/813	0.39	0/1090
4	D	0.24	0/653	0.41	0/873
4	H	0.24	0/645	0.42	0/862
5	I	0.25	0/7202	0.41	0/9725
6	J	0.29	0/1140	0.42	0/1539
7	K	0.24	0/3283	0.42	0/4445
8	L	0.24	0/841	0.41	0/1141
9	M	0.24	0/3335	0.43	0/4495
9	O	0.24	0/3382	0.41	0/4559
9	Q	0.24	0/3413	0.42	0/4603
10	N	0.24	0/3257	0.41	0/4381
10	P	0.24	0/3324	0.43	0/4477
10	R	0.24	0/3329	0.42	0/4479
11	S	0.24	0/2988	0.39	0/4045
11	U	0.25	0/2863	0.43	0/3882
12	T	0.24	0/3217	0.40	0/4362
13	V	0.24	0/1801	0.39	0/2419
14	W	0.26	0/1578	0.44	0/2128
15	X	0.96	8/3408 (0.2%)	1.38	62/5263 (1.2%)
16	Y	0.81	6/3349 (0.2%)	1.35	42/5162 (0.8%)
All	All	0.38	14/57851 (0.0%)	0.63	104/79346 (0.1%)

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
5	I	0	2
6	J	0	2
9	M	0	1
9	Q	0	1
11	U	0	1
All	All	0	7

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	X	21	DC	C3'-C2'	27.13	1.84	1.52
15	X	60	DA	O3'-P	-14.98	1.43	1.61
15	X	130	DG	C1'-N9	-8.87	1.34	1.47
16	Y	-45	DG	C1'-N9	-7.60	1.36	1.47
16	Y	-71	DG	C1'-N9	-7.59	1.36	1.47

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Y	-78	DA	O5'-P-OP2	-19.21	87.64	110.70
16	Y	-78	DA	O5'-P-OP1	18.91	133.39	110.70
15	X	21	DC	C3'-C2'-C1'	-11.27	88.98	102.50
15	X	141	DC	P-O3'-C3'	-10.40	107.22	119.70
16	Y	-110	DG	P-O3'-C3'	-10.24	107.41	119.70

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	I	2029	ARG	Sidechain
5	I	860	ARG	Sidechain
6	J	260	ARG	Sidechain
6	J	263	ARG	Sidechain
9	M	263	LEU	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	898	0	958	35	0
1	E	808	0	863	22	0
2	B	755	0	782	39	0
2	F	736	0	755	15	0
3	C	779	0	816	63	0
3	G	801	0	839	20	0
4	D	646	0	686	31	0
4	H	638	0	676	3	0
5	I	7031	0	7121	218	0
6	J	1114	0	1136	27	0
7	K	3209	0	3132	66	0
8	L	823	0	793	11	0
9	M	3293	0	3397	65	0
9	O	3339	0	3425	41	0
9	Q	3368	0	3453	82	0
10	N	3223	0	3309	41	0
10	P	3287	0	3335	61	0
10	R	3293	0	3373	58	0
11	S	2925	0	2891	17	0
11	U	2802	0	2760	51	0
12	T	3146	0	3086	35	0
13	V	1757	0	1736	43	0
14	W	1542	0	1553	53	0
15	X	3034	0	1648	227	0
16	Y	2990	0	1651	207	0
17	I	27	0	12	0	0
17	M	27	0	12	1	0
17	N	27	0	12	0	0
17	O	27	0	12	2	0
17	P	27	0	12	2	0
17	Q	27	0	12	0	0
17	R	27	0	12	2	0
18	K	31	0	12	1	0
18	T	31	0	12	0	0
18	U	31	0	12	1	0
All	All	56519	0	54294	1168	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 11.

The worst 5 of 1168 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)
5:I:898:ARG:CZ	5:I:2140:TRP:CH2	1.82	1.59
3:C:43:PRO:HG2	16:Y:-78:DA:C4'	1.33	1.54
15:X:21:DC:N4	16:Y:-21:DG:N1	1.63	1.47
15:X:21:DC:C2'	15:X:21:DC:C3'	1.84	1.43
3:C:42:ARG:HH22	15:X:81:DG:C1'	1.33	1.39

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	114/130 (88%)	110 (96%)	4 (4%)	0	100	100
1	E	103/130 (79%)	102 (99%)	1 (1%)	0	100	100
2	B	94/126 (75%)	93 (99%)	1 (1%)	0	100	100
2	F	92/126 (73%)	86 (94%)	4 (4%)	2 (2%)	6	35
3	C	93/136 (68%)	88 (95%)	2 (2%)	3 (3%)	4	26
3	G	95/136 (70%)	93 (98%)	2 (2%)	0	100	100
4	D	79/103 (77%)	78 (99%)	1 (1%)	0	100	100
4	H	78/103 (76%)	75 (96%)	3 (4%)	0	100	100
5	I	844/3230 (26%)	808 (96%)	32 (4%)	4 (0%)	29	67
6	J	129/364 (35%)	120 (93%)	8 (6%)	1 (1%)	19	58
7	K	392/396 (99%)	353 (90%)	36 (9%)	3 (1%)	19	58
8	L	101/154 (66%)	95 (94%)	5 (5%)	1 (1%)	15	54
9	M	424/456 (93%)	406 (96%)	17 (4%)	1 (0%)	47	79
9	O	431/456 (94%)	417 (97%)	14 (3%)	0	100	100
9	Q	438/456 (96%)	409 (93%)	26 (6%)	3 (1%)	22	61
10	N	409/463 (88%)	394 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	P	423/463 (91%)	401 (95%)	20 (5%)	2 (0%)	29 67
10	R	420/463 (91%)	406 (97%)	14 (3%)	0	100 100
11	S	373/375 (100%)	370 (99%)	3 (1%)	0	100 100
11	U	355/375 (95%)	311 (88%)	44 (12%)	0	100 100
12	T	399/429 (93%)	387 (97%)	11 (3%)	1 (0%)	41 74
13	V	200/467 (43%)	190 (95%)	10 (5%)	0	100 100
14	W	185/227 (82%)	177 (96%)	6 (3%)	2 (1%)	14 51
All	All	6271/9764 (64%)	5969 (95%)	279 (4%)	23 (0%)	38 69

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	P	261	PHE
9	Q	278	GLU
9	Q	279	ILE
7	K	201	VAL
9	M	263	LEU

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	91/99 (92%)	87 (96%)	4 (4%)	28 64
1	E	82/99 (83%)	77 (94%)	5 (6%)	18 54
2	B	83/106 (78%)	76 (92%)	7 (8%)	11 39
2	F	81/106 (76%)	78 (96%)	3 (4%)	34 68
3	C	82/111 (74%)	74 (90%)	8 (10%)	8 31
3	G	85/111 (77%)	84 (99%)	1 (1%)	71 88
4	D	66/79 (84%)	66 (100%)	0	100 100
4	H	65/79 (82%)	65 (100%)	0	100 100
5	I	765/2721 (28%)	691 (90%)	74 (10%)	8 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	J	123/312 (39%)	105 (85%)	18 (15%)	3 15
7	K	359/361 (99%)	336 (94%)	23 (6%)	17 52
8	L	89/133 (67%)	83 (93%)	6 (7%)	16 50
9	M	361/387 (93%)	342 (95%)	19 (5%)	22 58
9	O	364/387 (94%)	342 (94%)	22 (6%)	19 54
9	Q	366/387 (95%)	349 (95%)	17 (5%)	27 63
10	N	351/390 (90%)	343 (98%)	8 (2%)	50 78
10	P	352/390 (90%)	334 (95%)	18 (5%)	24 60
10	R	358/390 (92%)	339 (95%)	19 (5%)	22 58
11	S	318/318 (100%)	318 (100%)	0	100 100
11	U	305/318 (96%)	281 (92%)	24 (8%)	12 43
12	T	346/364 (95%)	336 (97%)	10 (3%)	42 74
13	V	183/400 (46%)	162 (88%)	21 (12%)	5 24
14	W	168/203 (83%)	163 (97%)	5 (3%)	41 73
All	All	5443/8251 (66%)	5131 (94%)	312 (6%)	24 56

5 of 312 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	Q	427	LYS
13	V	51	GLU
10	R	207	ARG
12	T	383	ASN
13	V	245	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
9	O	408	GLN
12	T	143	HIS
9	O	451	GLN
10	P	121	GLN
12	T	383	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)

10 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
18	ATP	K	401	-	26,33,33	0.92	1 (3%)	31,52,52	1.59	6 (19%)
17	ADP	N	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.55	4 (13%)
17	ADP	M	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.53	5 (17%)
18	ATP	U	401	-	26,33,33	0.93	1 (3%)	31,52,52	1.61	6 (19%)
17	ADP	O	501	-	24,29,29	0.94	1 (4%)	29,45,45	1.54	5 (17%)
17	ADP	I	3301	-	24,29,29	0.96	1 (4%)	29,45,45	1.45	4 (13%)
17	ADP	Q	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.46	5 (17%)
17	ADP	R	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.49	4 (13%)
18	ATP	T	501	-	26,33,33	0.93	1 (3%)	31,52,52	1.62	6 (19%)
17	ADP	P	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.56	5 (17%)

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
18	ATP	K	401	-	-	4/18/38/38	0/3/3/3
17	ADP	N	501	-	-	4/12/32/32	0/3/3/3
17	ADP	M	501	-	-	3/12/32/32	0/3/3/3
18	ATP	U	401	-	-	4/18/38/38	0/3/3/3
17	ADP	O	501	-	-	5/12/32/32	0/3/3/3
17	ADP	I	3301	-	-	6/12/32/32	0/3/3/3
17	ADP	Q	501	-	-	5/12/32/32	0/3/3/3
17	ADP	R	501	-	-	1/12/32/32	0/3/3/3
18	ATP	T	501	-	-	3/18/38/38	0/3/3/3
17	ADP	P	501	-	-	4/12/32/32	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	R	501	ADP	C5-C4	2.47	1.47	1.40
17	I	3301	ADP	C5-C4	2.45	1.47	1.40
17	Q	501	ADP	C5-C4	2.45	1.47	1.40
18	T	501	ATP	C5-C4	2.44	1.47	1.40
18	U	401	ATP	C5-C4	2.44	1.47	1.40

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	P	501	ADP	PA-O3A-PB	-3.85	119.60	132.83
18	U	401	ATP	PB-O3B-PG	-3.73	120.03	132.83
17	N	501	ADP	PA-O3A-PB	-3.70	120.13	132.83
17	P	501	ADP	N3-C2-N1	-3.70	122.90	128.68
17	O	501	ADP	PA-O3A-PB	-3.69	120.15	132.83

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	I	3301	ADP	C5'-O5'-PA-O3A
17	M	501	ADP	PA-O3A-PB-O2B
17	M	501	ADP	PA-O3A-PB-O3B
17	N	501	ADP	C5'-O5'-PA-O1A
17	N	501	ADP	C5'-O5'-PA-O2A

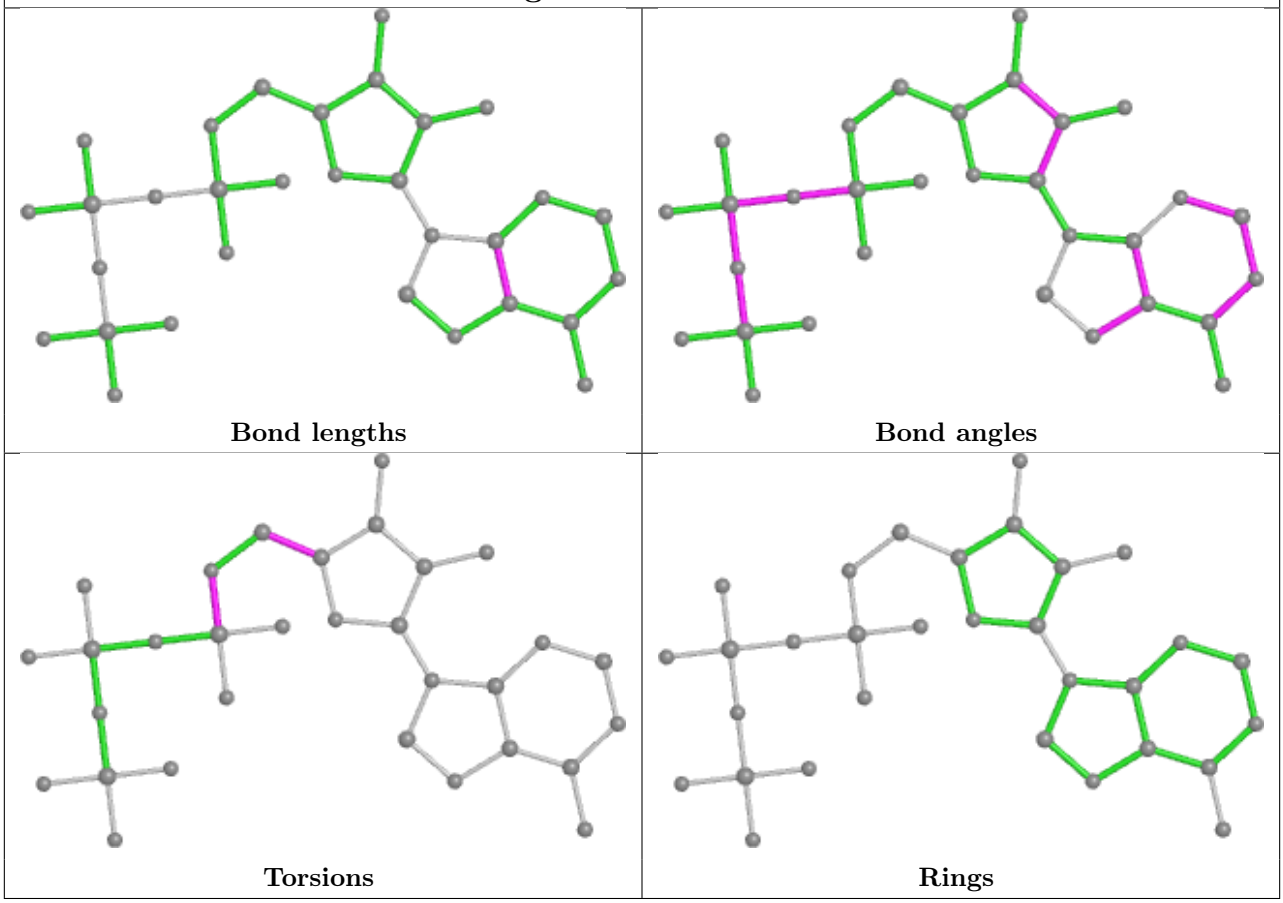
There are no ring outliers.

6 monomers are involved in 9 short contacts:

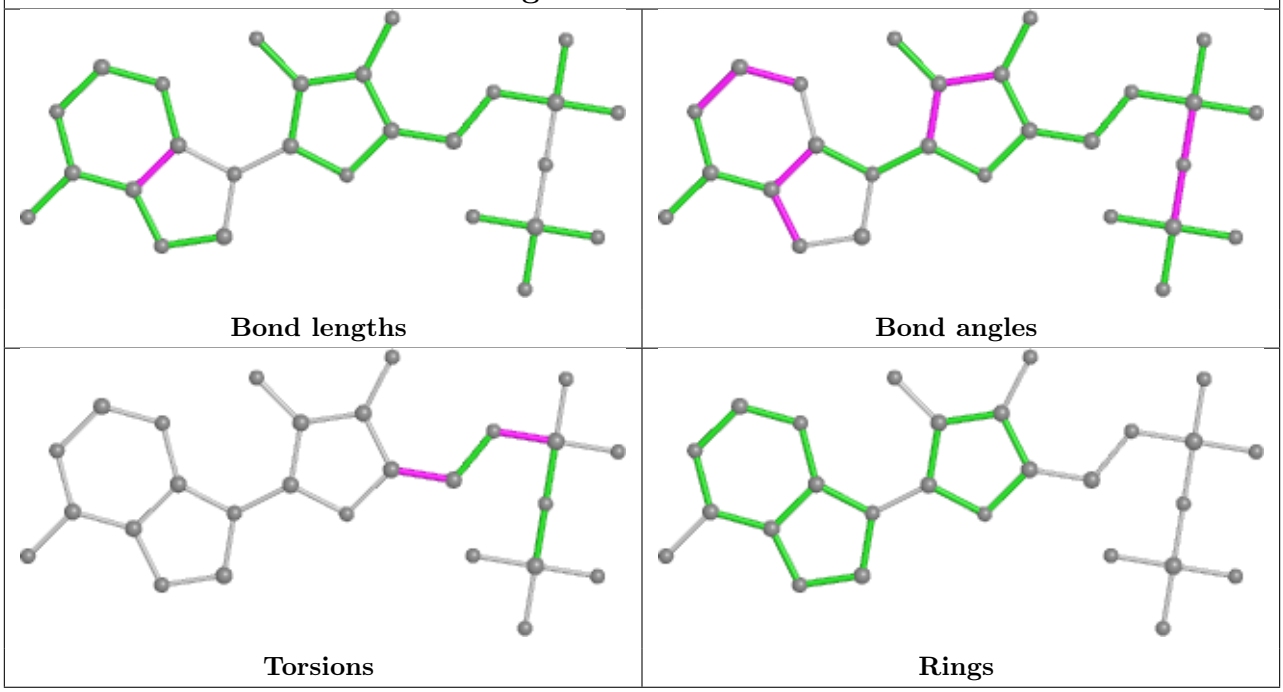
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	K	401	ATP	1	0
17	M	501	ADP	1	0
18	U	401	ATP	1	0
17	O	501	ADP	2	0
17	R	501	ADP	2	0
17	P	501	ADP	2	0

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.

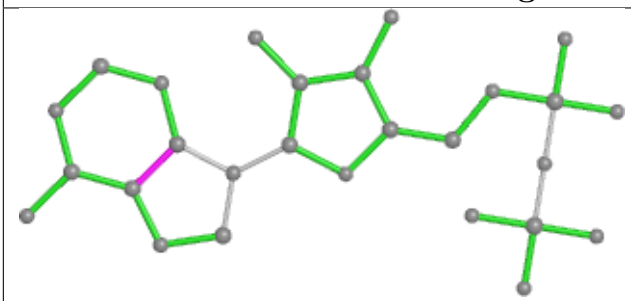
Ligand ATP K 401



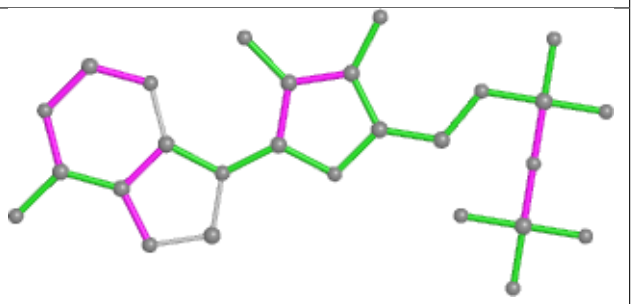
Ligand ADP N 501



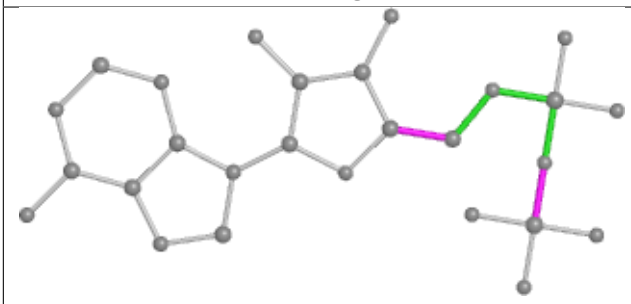
Ligand ADP M 501



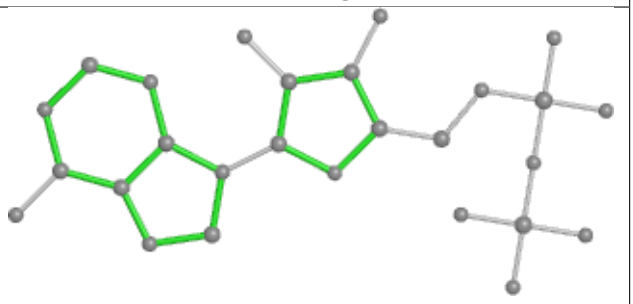
Bond lengths



Bond angles

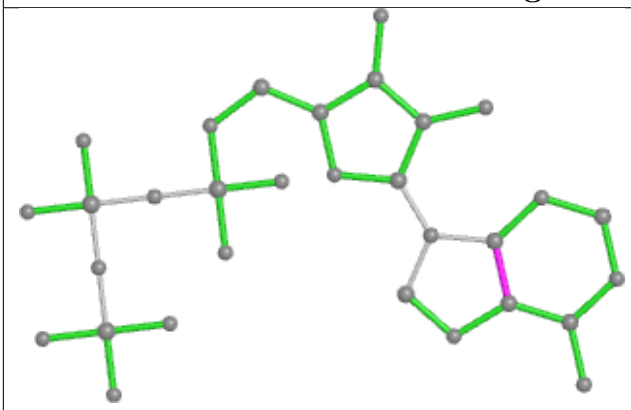


Torsions

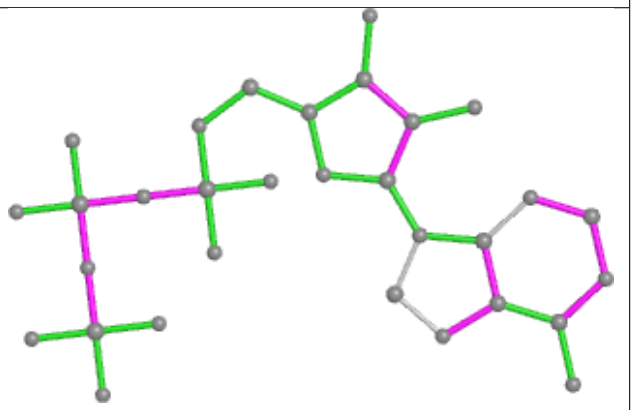


Rings

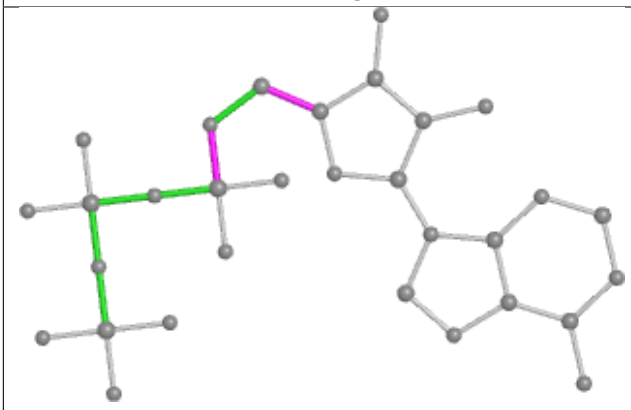
Ligand ATP U 401



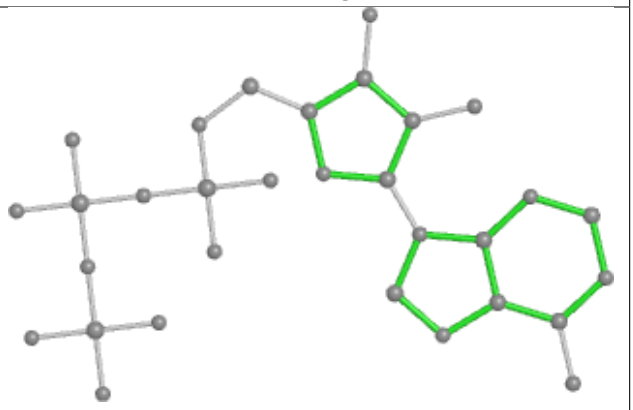
Bond lengths



Bond angles

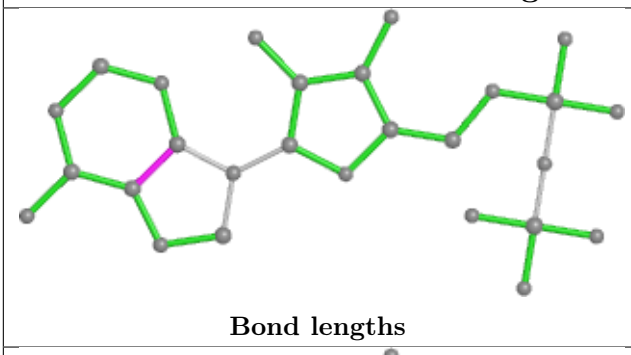


Torsions

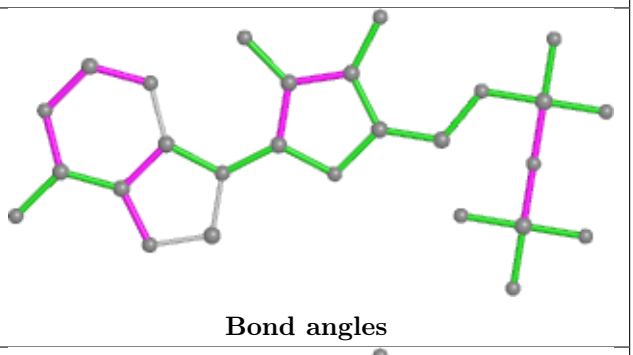


Rings

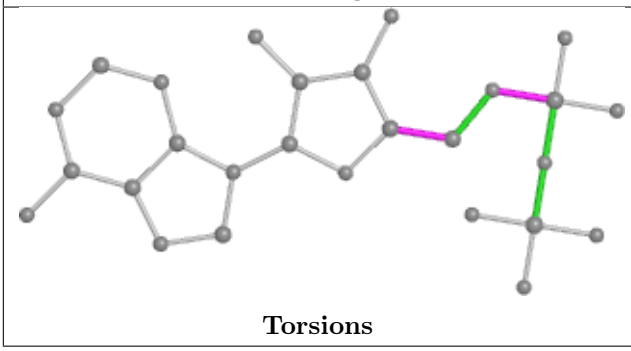
Ligand ADP O 501



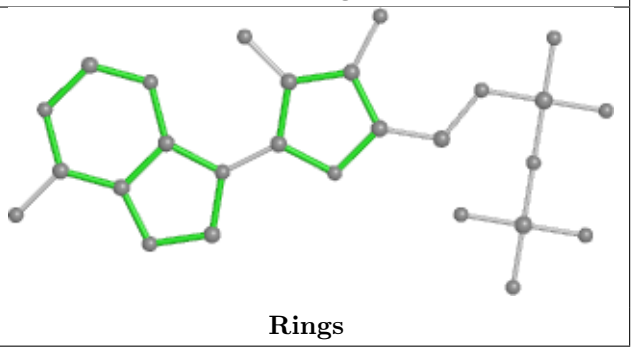
Bond lengths



Bond angles

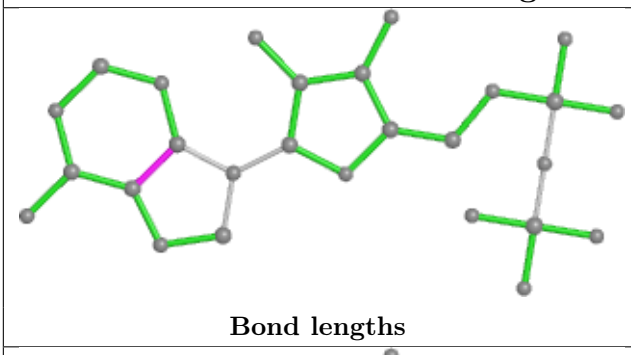


Torsions

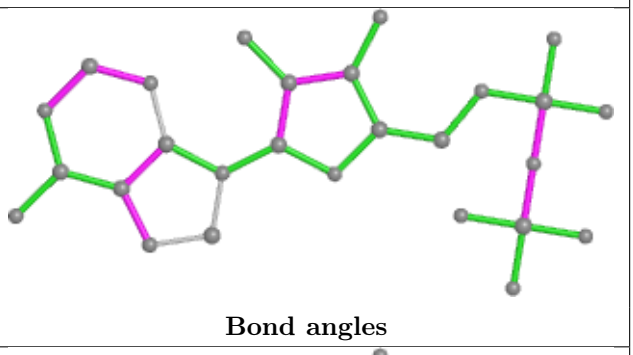


Rings

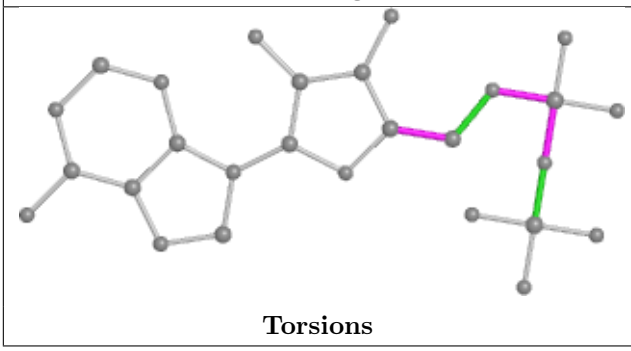
Ligand ADP I 3301



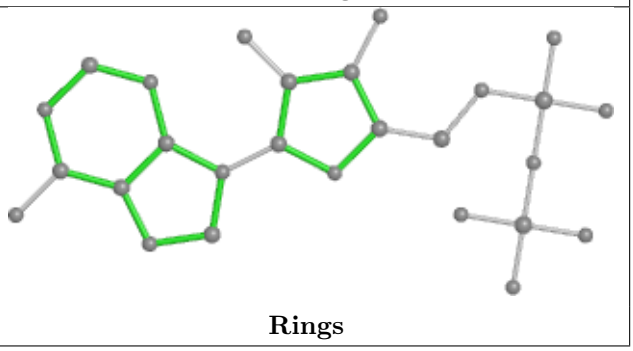
Bond lengths



Bond angles

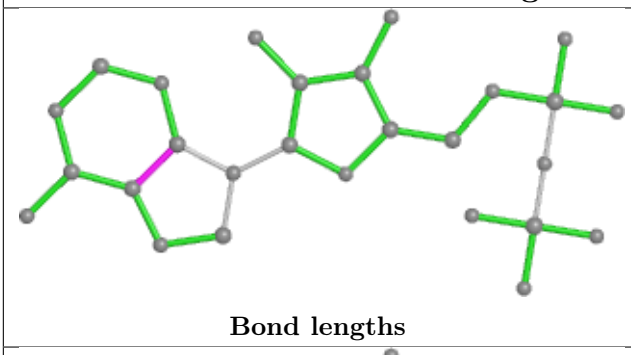


Torsions

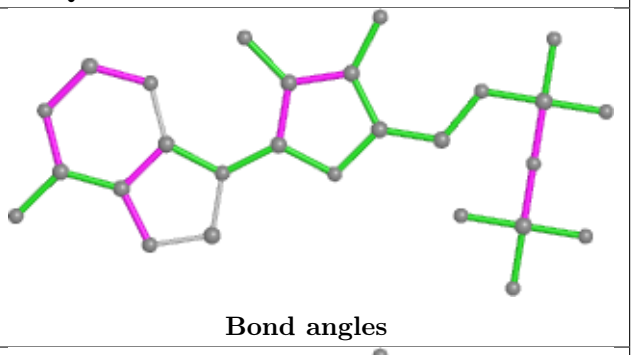


Rings

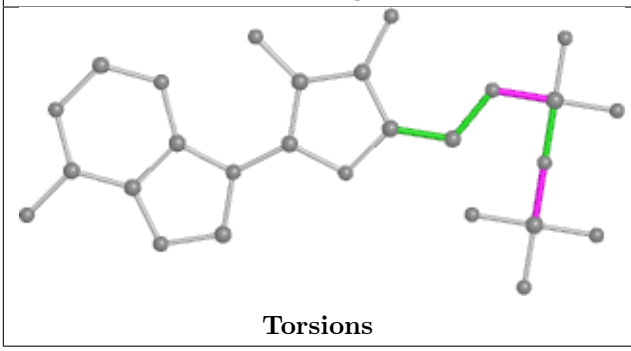
Ligand ADP Q 501



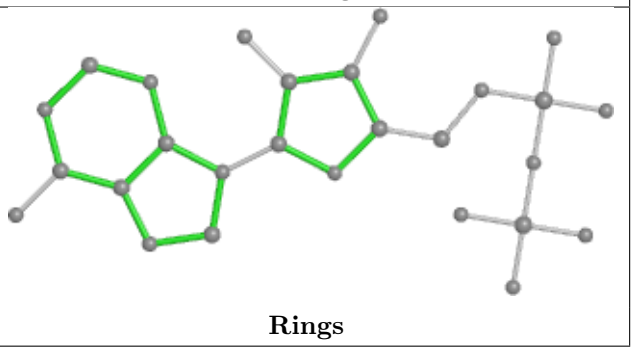
Bond lengths



Bond angles

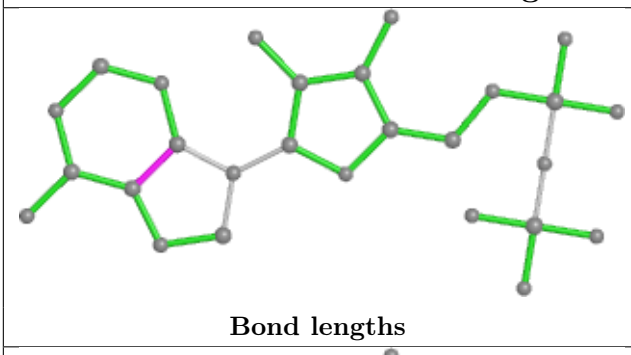


Torsions

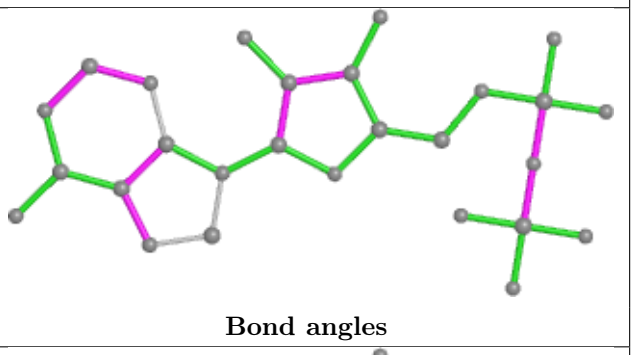


Rings

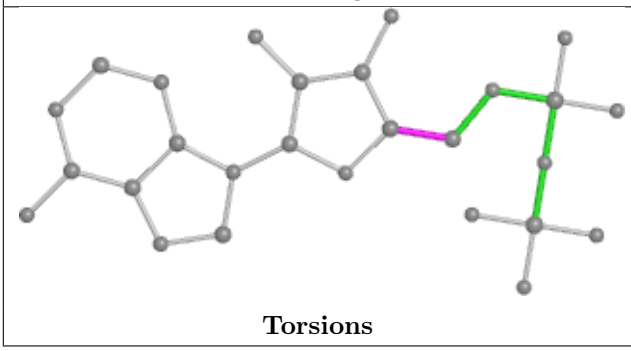
Ligand ADP R 501



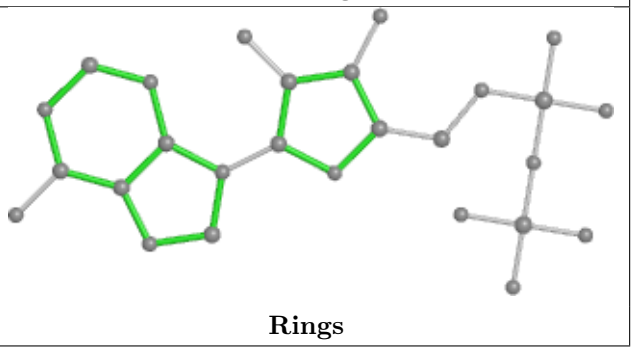
Bond lengths



Bond angles

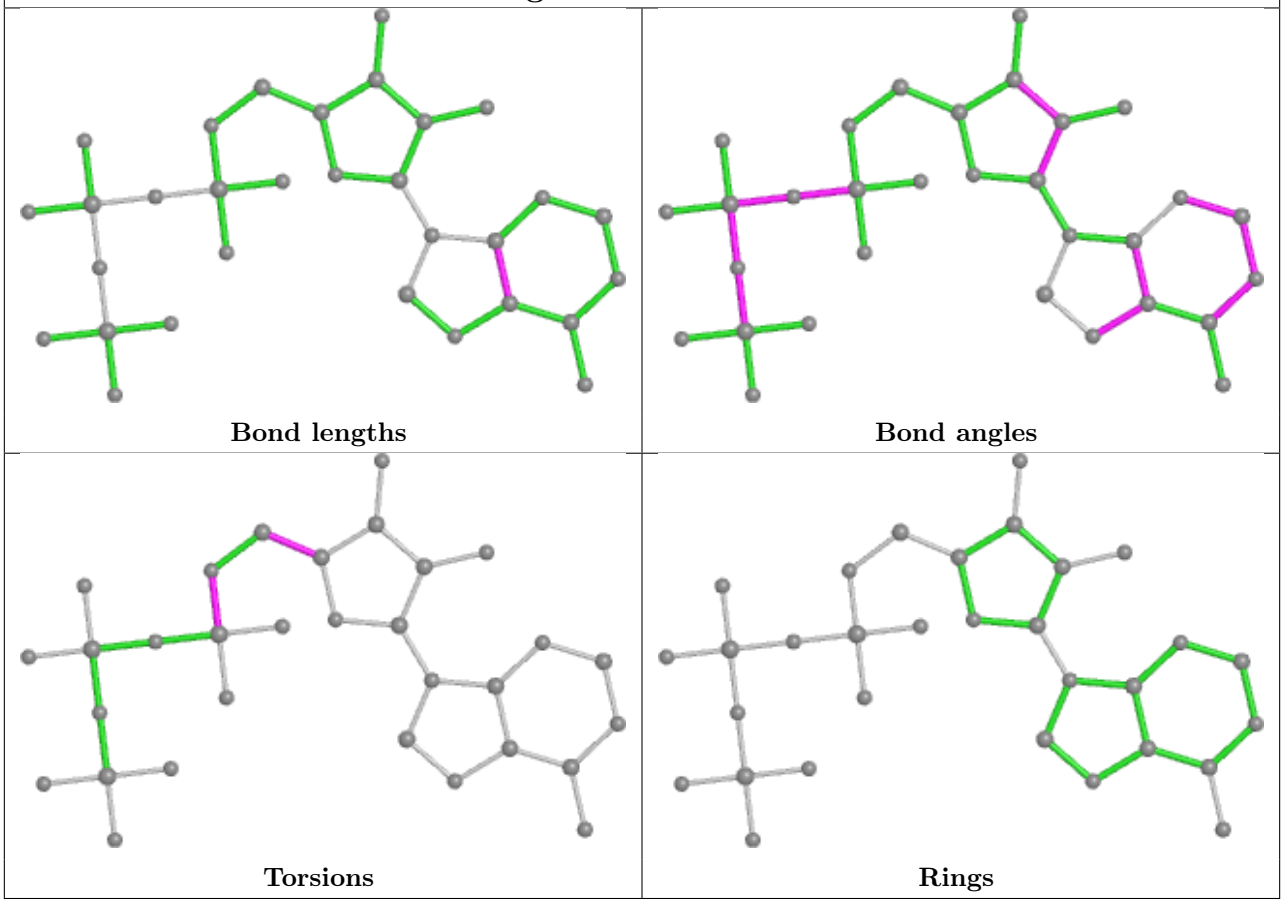


Torsions

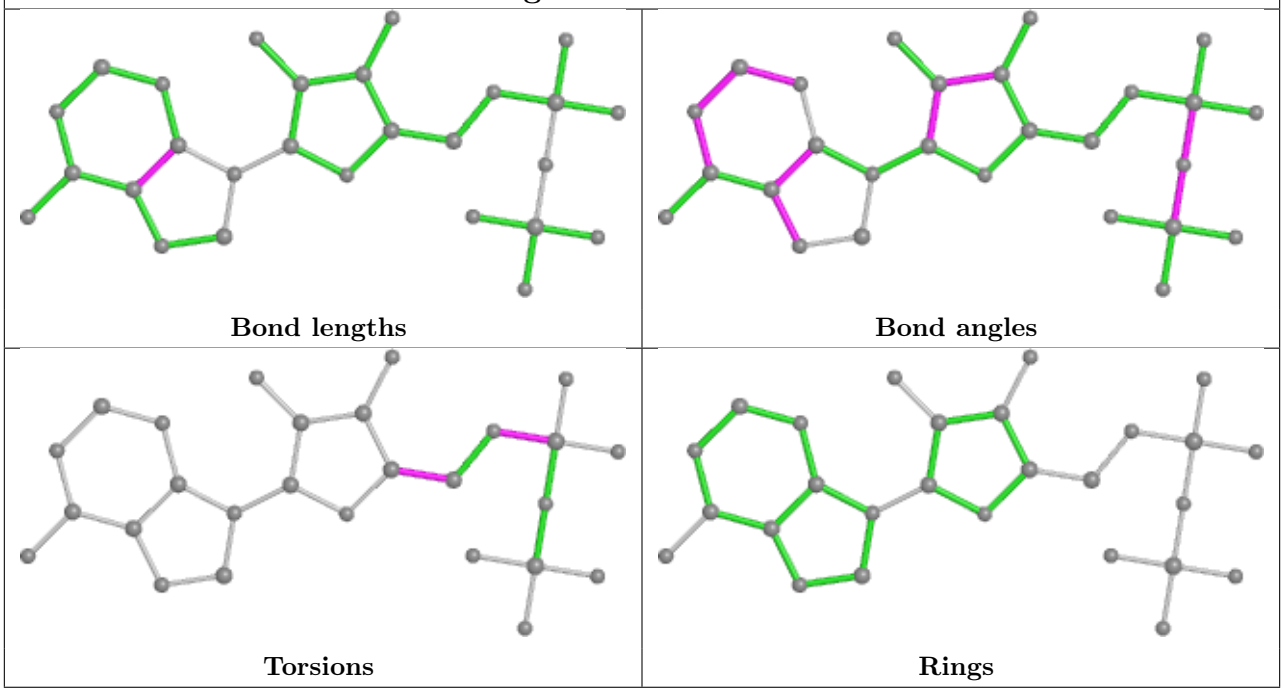


Rings

Ligand ATP T 501



Ligand ADP P 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

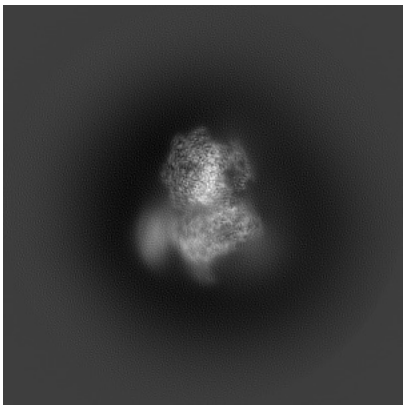
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37990. These allow visual inspection of the internal detail of the map and identification of artifacts.

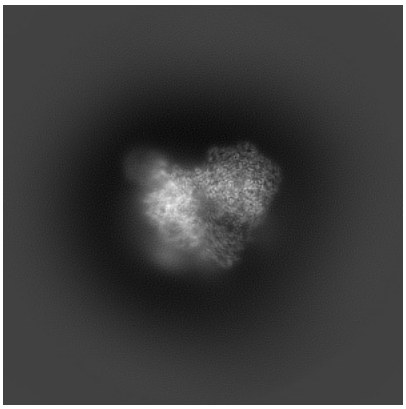
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

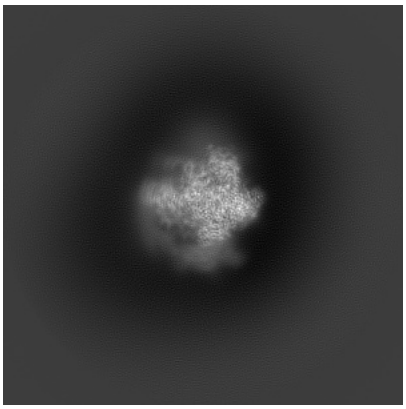
6.1.1 Primary map



X

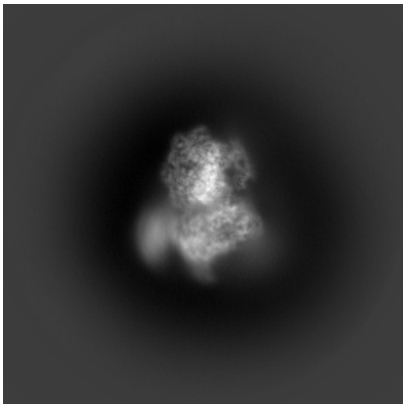


Y

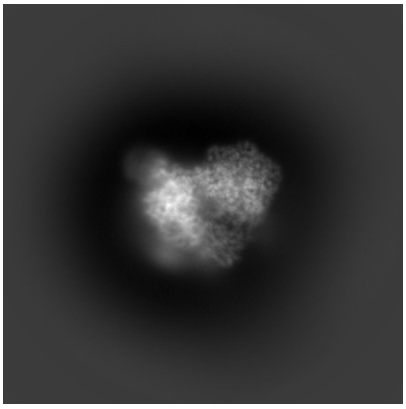


Z

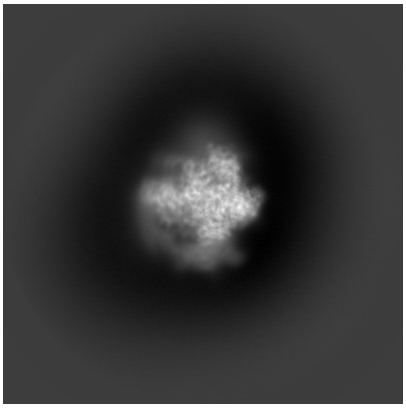
6.1.2 Raw map



X



Y

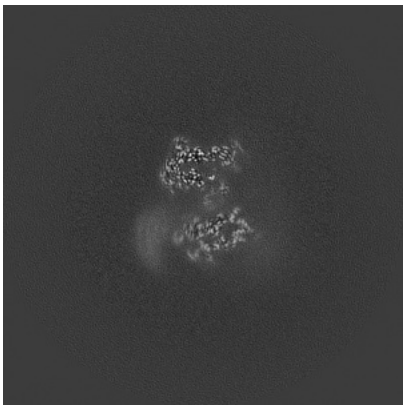


Z

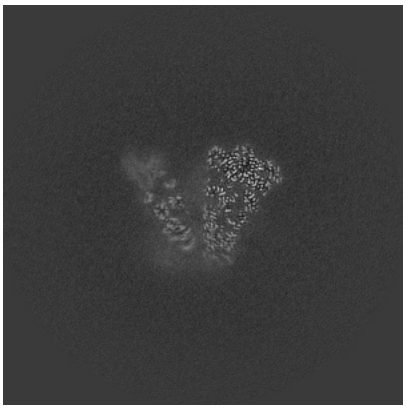
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

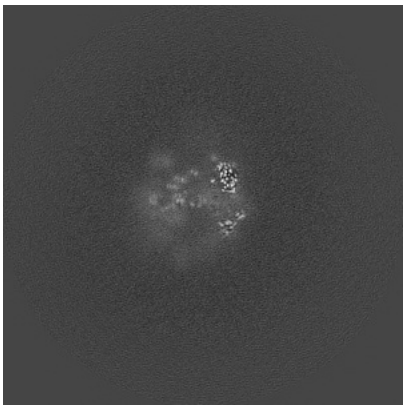
6.2.1 Primary map



X Index: 200

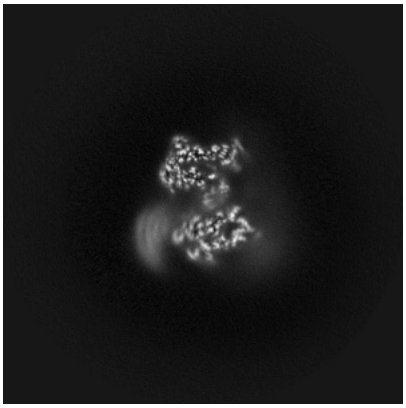


Y Index: 200

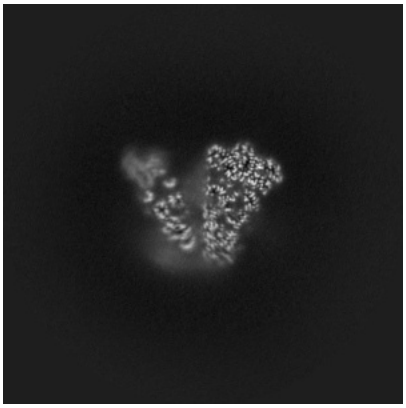


Z Index: 200

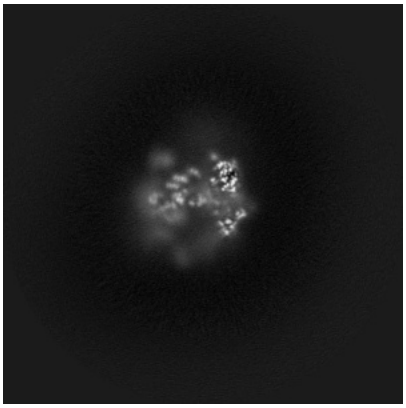
6.2.2 Raw map



X Index: 200



Y Index: 200

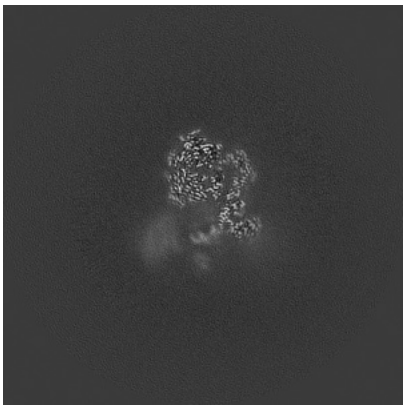


Z Index: 200

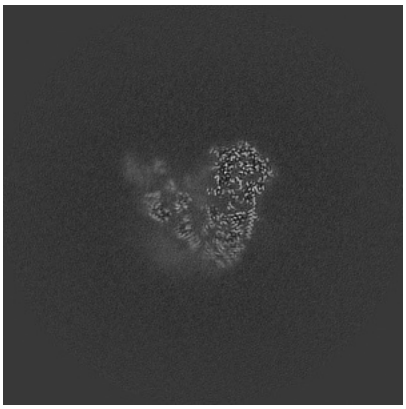
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

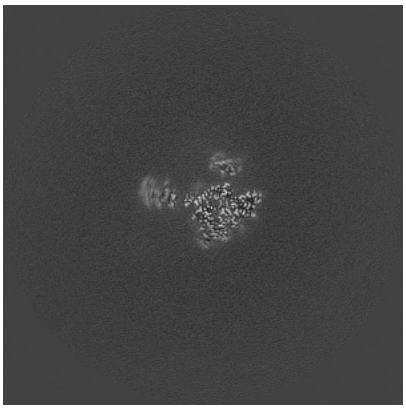
6.3.1 Primary map



X Index: 218

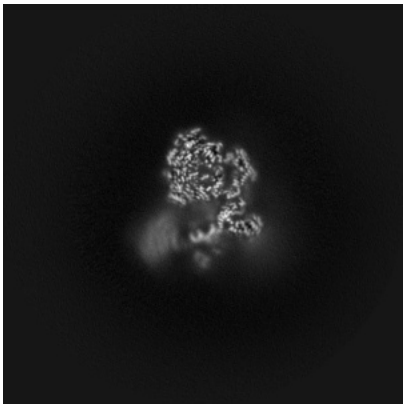


Y Index: 206

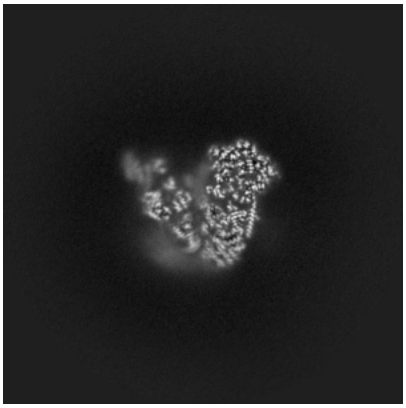


Z Index: 226

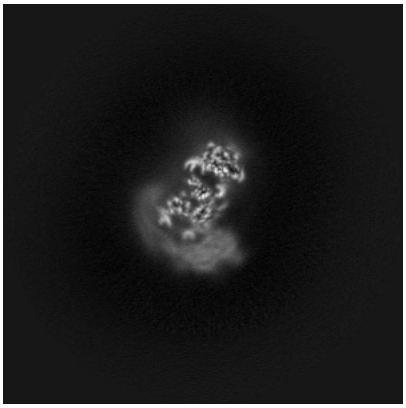
6.3.2 Raw map



X Index: 217



Y Index: 205

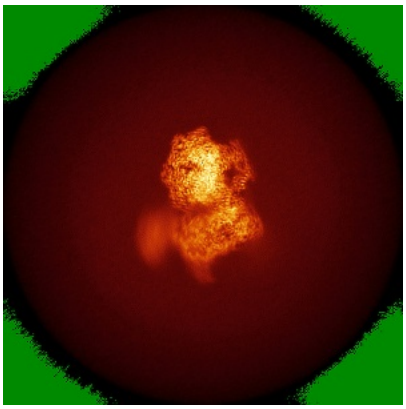


Z Index: 173

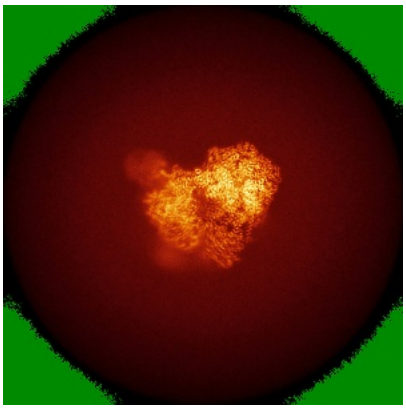
The images above show the largest variance slices of the map in three orthogonal directions.

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

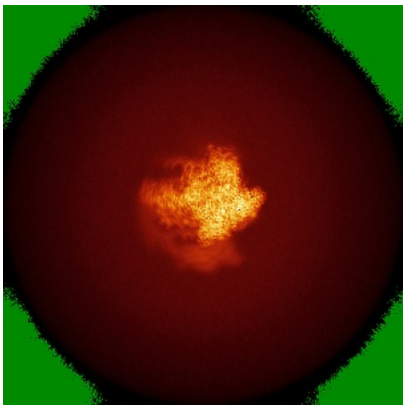
6.4.1 Primary map



X

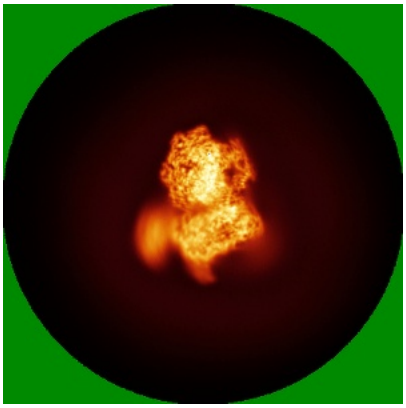


Y

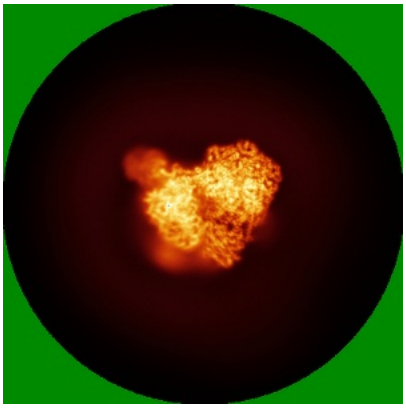


Z

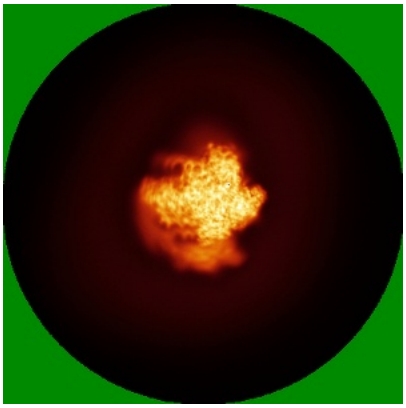
6.4.2 Raw map



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.

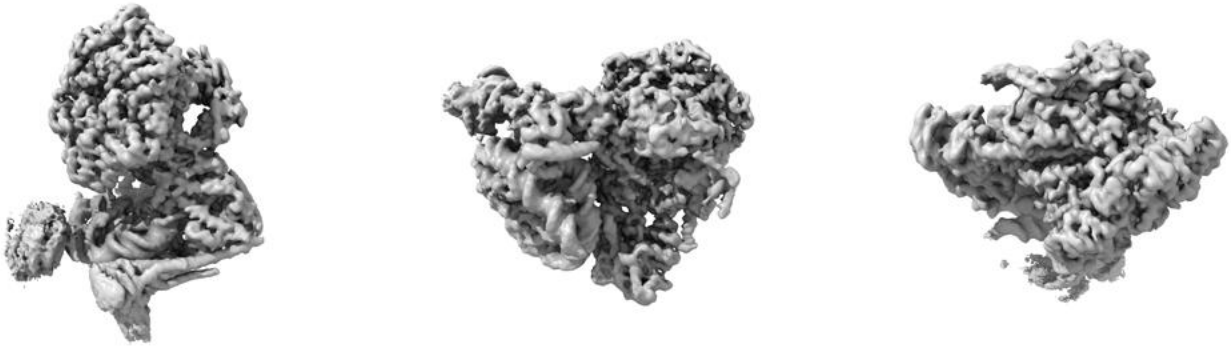
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.026. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

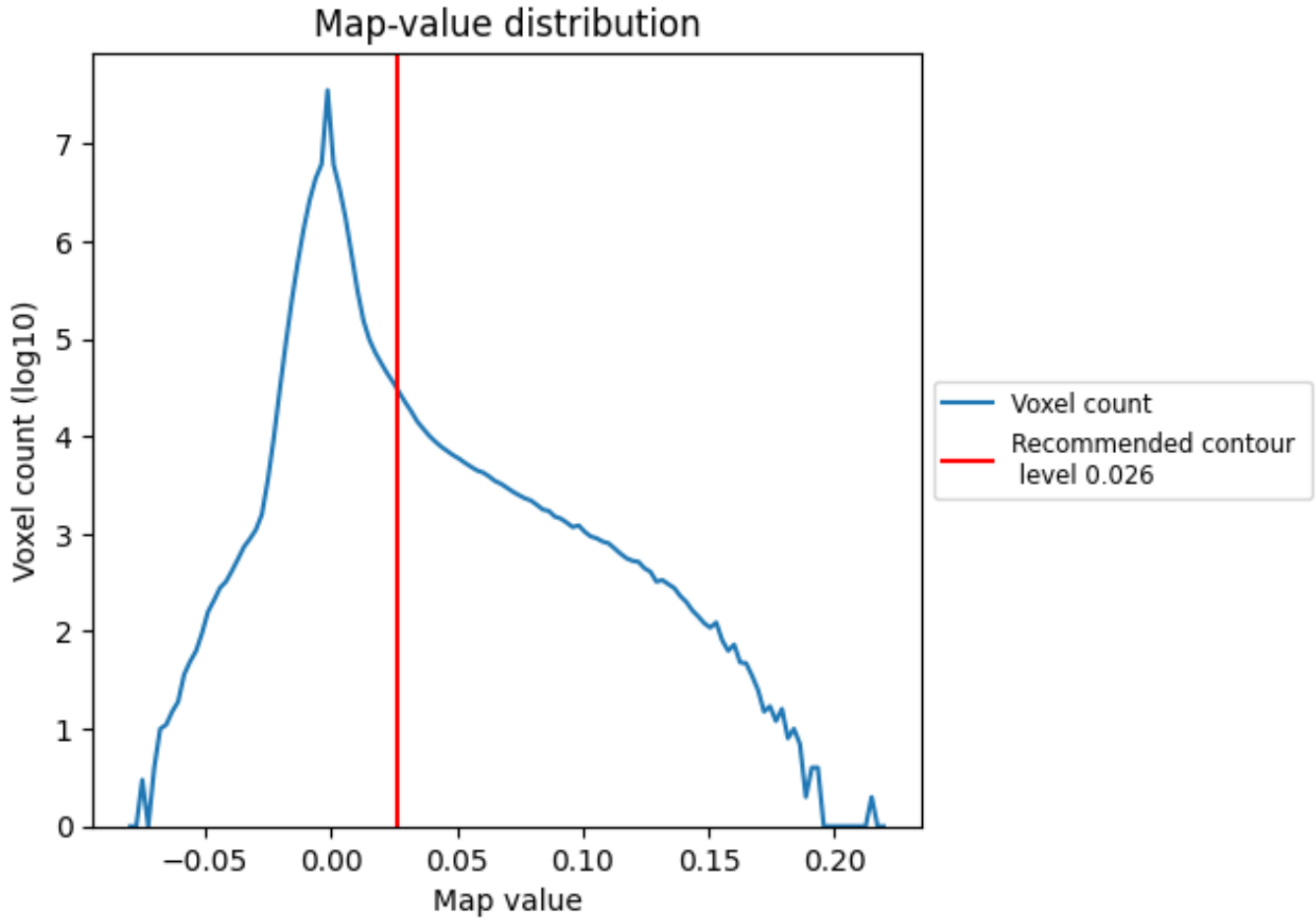
6.6 Mask visualisation (i)

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

7 Map analysis

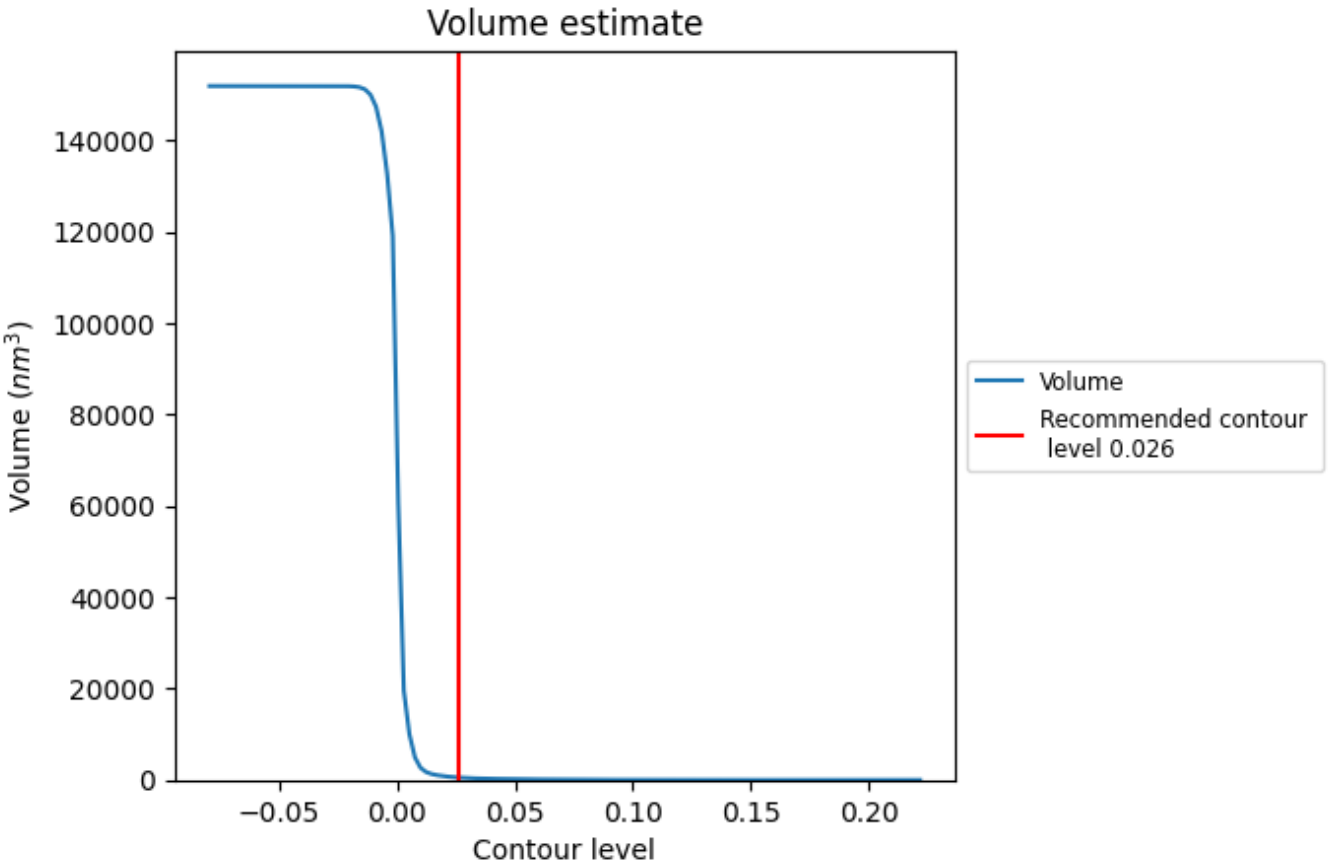
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

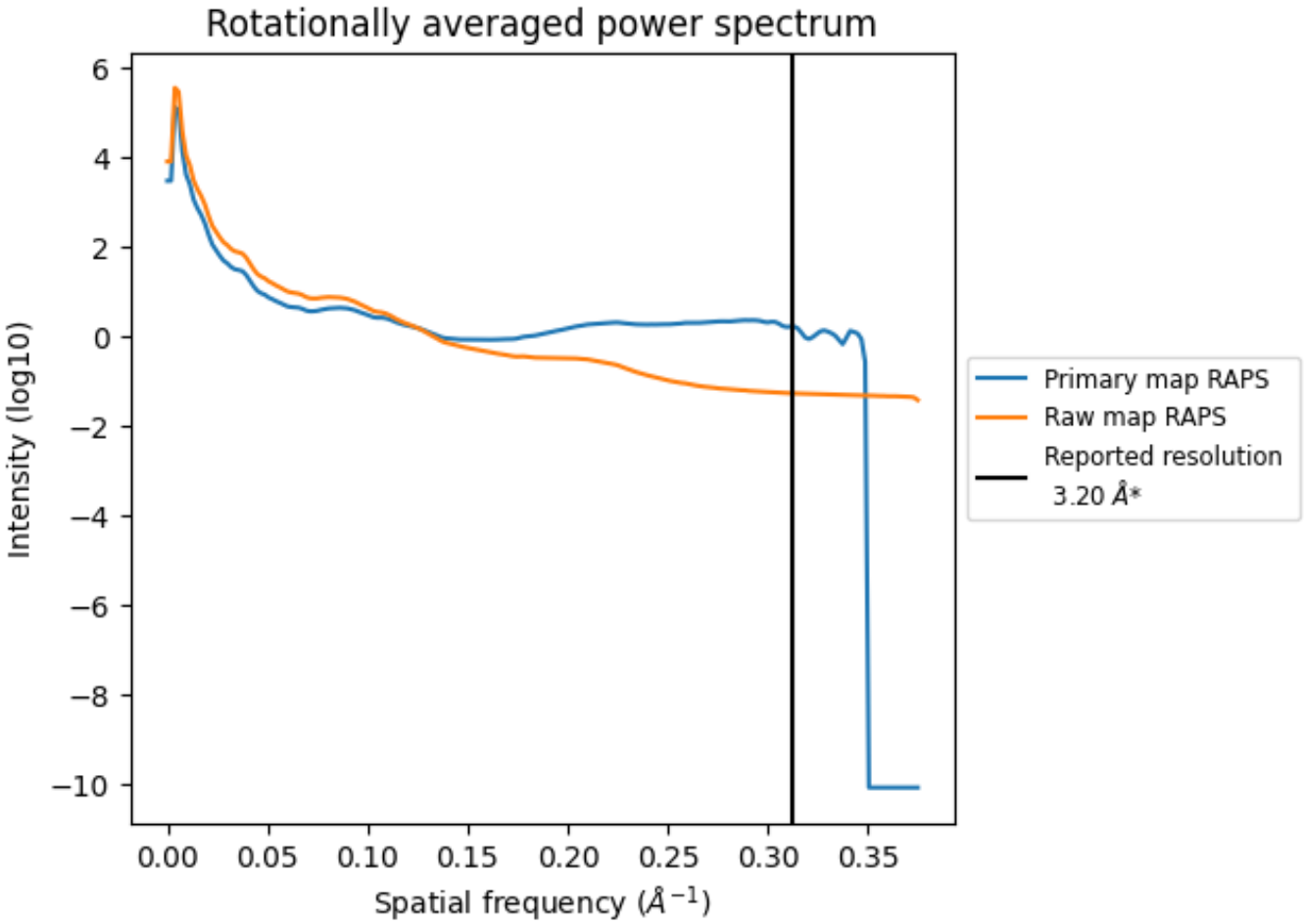
7.2 Volume estimate (i)



The volume at the recommended contour level is 528 nm^3; this corresponds to an approximate mass of 477 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)

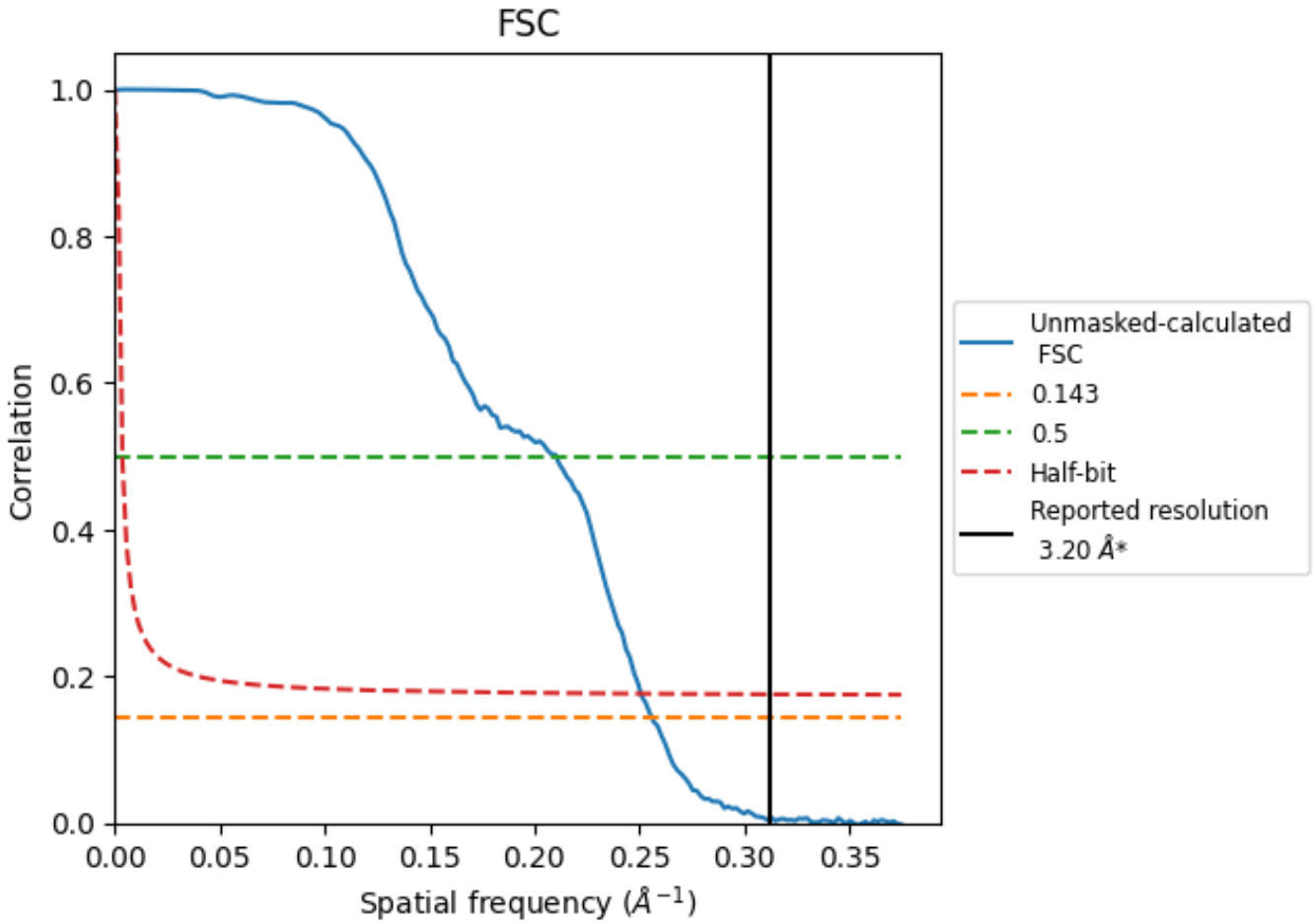


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

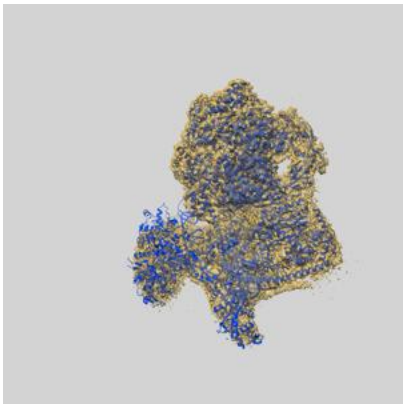
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.91	4.76	3.99

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.91 differs from the reported value 3.2 by more than 10 %

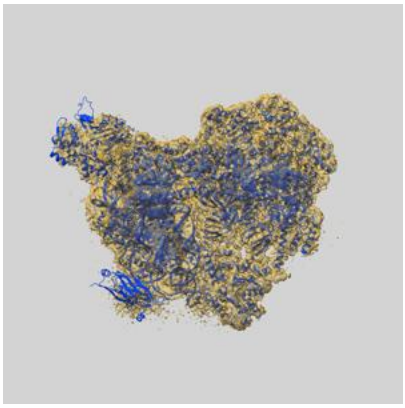
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37990 and PDB model 8X1C. Per-residue inclusion information can be found in section 3 on page 9.

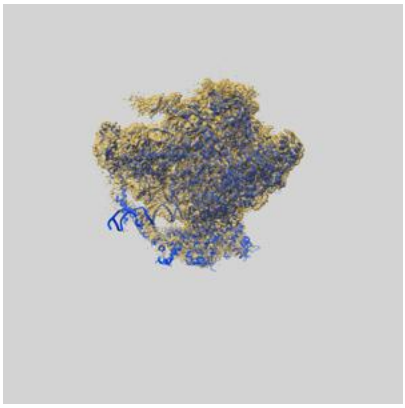
9.1 Map-model overlay



X



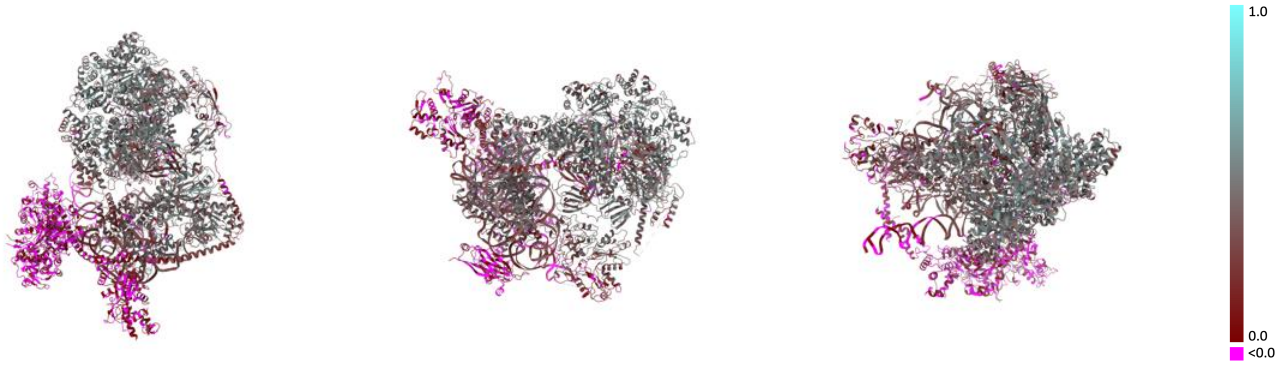
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.026 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.

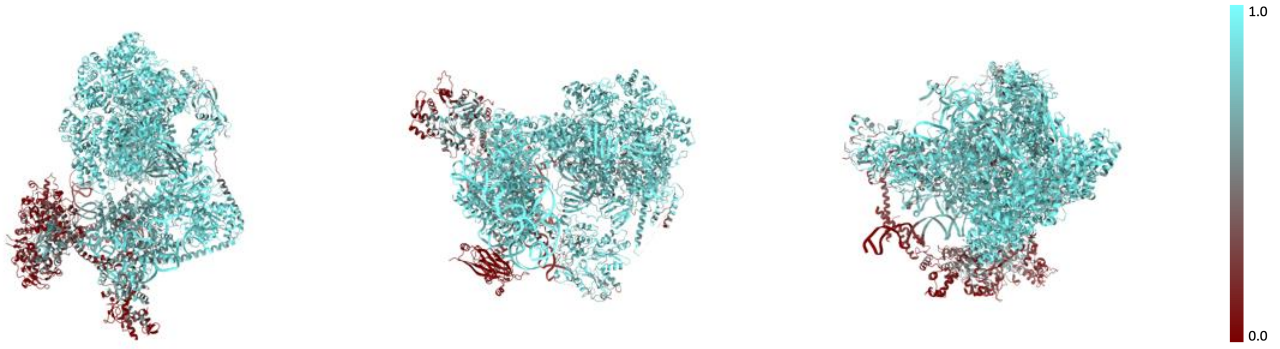
9.2 Q-score mapped to coordinate model



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.

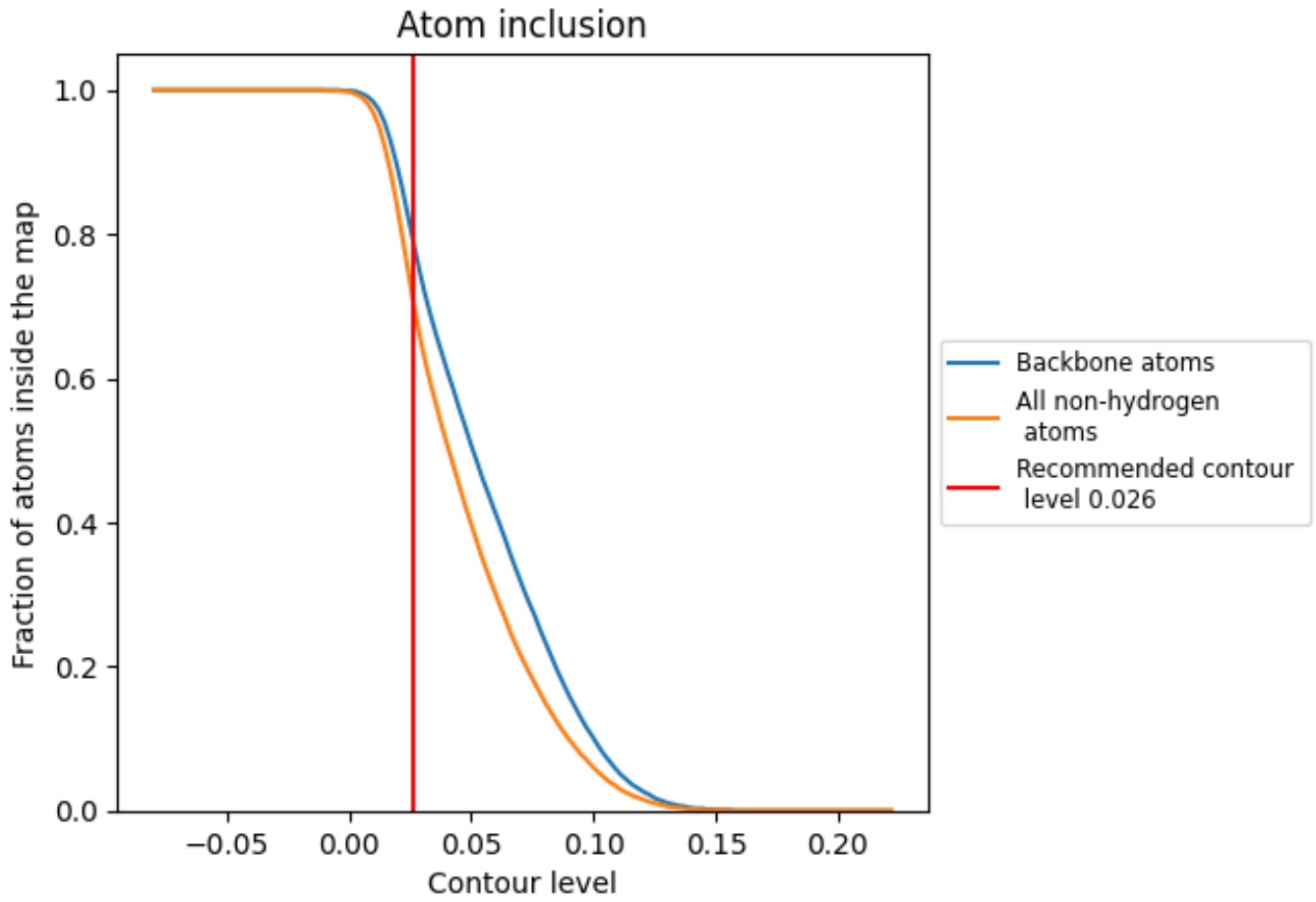
9.3 Atom inclusion mapped to coordinate model



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 (0.026).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 71% 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 (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7110	0.2970
A	0.7730	0.2670
B	0.8080	0.3070
C	0.7840	0.3120
D	0.8610	0.3610
E	0.8790	0.4280
F	0.8790	0.4090
G	0.8930	0.4450
H	0.8840	0.4420
I	0.7900	0.3700
J	0.6860	0.2640
K	0.7880	0.2910
L	0.7790	0.2790
M	0.8560	0.4210
N	0.8710	0.4260
O	0.8390	0.3980
P	0.8630	0.4380
Q	0.8590	0.4330
R	0.8660	0.4580
S	0.4050	0.0600
T	0.3090	0.0010
U	0.3030	0.0140
V	0.0750	0.0230
W	0.0190	-0.0010
X	0.8550	0.2750
Y	0.8720	0.2790