



wwPDB EM Validation Summary Report ⓘ

Feb 26, 2024 – 01:00 PM JST

PDB ID : 8X19
EMDB ID : EMD-37988
Title : Structure of nucleosome-bound SRCAP-C in the ADP-BeFx-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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

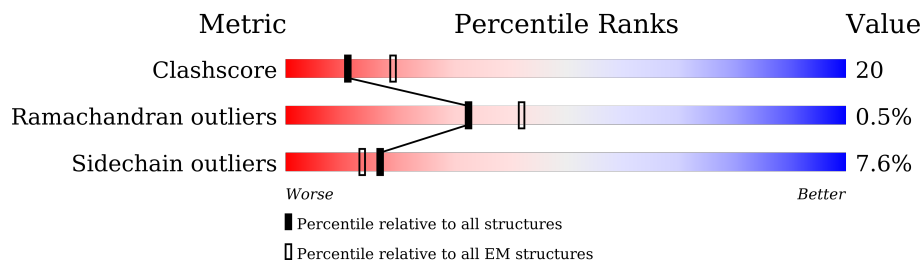
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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





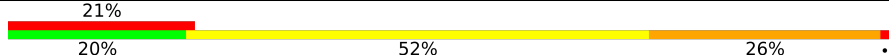
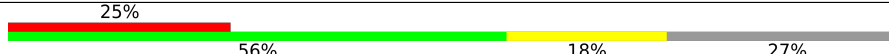
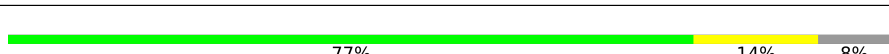
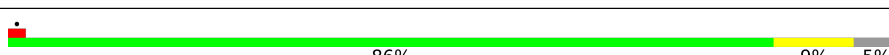
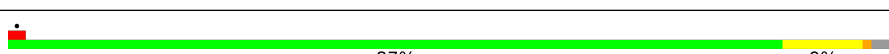
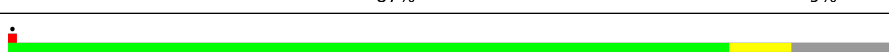

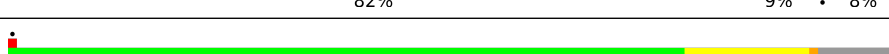
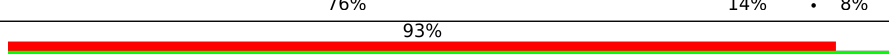
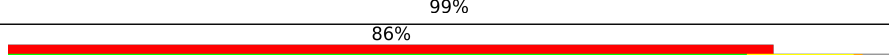

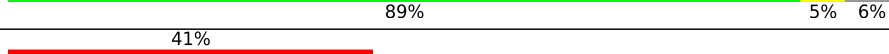


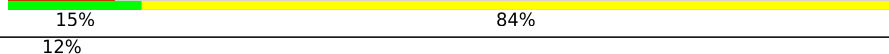
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	130	
1	E	130	
2	B	126	
2	F	126	
3	C	136	
3	G	136	
4	D	103	
4	H	103	

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Mol	Chain	Length	Quality of chain
5	I	3230	
6	J	364	
7	K	396	
8	L	154	
9	M	456	
9	O	456	
9	Q	456	
10	N	463	
10	P	463	
10	R	463	
11	S	375	
11	U	375	
12	T	429	
13	V	467	
14	W	227	
15	X	147	
16	Y	147	

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
19	BEF	I	3303	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 56704 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
			Total	C	N	O		
1	A	108	Total	C	N	O	0	0
			833	525	165	143		
1	E	105	Total	C	N	O	0	0
			808	510	158	140		

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

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

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

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

- Molecule 4 is a protein called Histone H4.

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

- Molecule 5 is a protein called Helicase SRCAP.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	864	7122	4533	1314	1236	39	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	162	1350	846	260	239	5	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	L	113	893	546	173	165	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	M	418	3213	2026	557	614	16	0	0
9	O	435	3339	2105	571	646	17	0	0
9	Q	440	3368	2121	579	651	17	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	N	411	3185	1988	560	622	15	0	0
10	P	427	3287	2054	576	642	15	0	0
10	R	424	3293	2057	578	642	16	0	0

- 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		

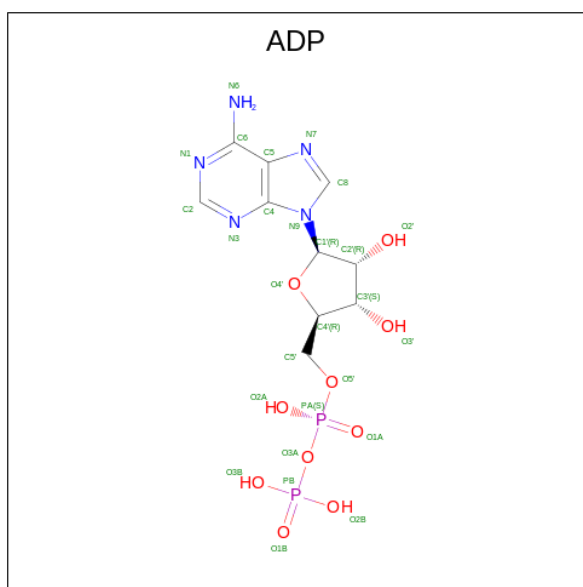
- Molecule 15 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	147	Total	C	N	O	P	0	0
			3031	1435	572	878	146		

- 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: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

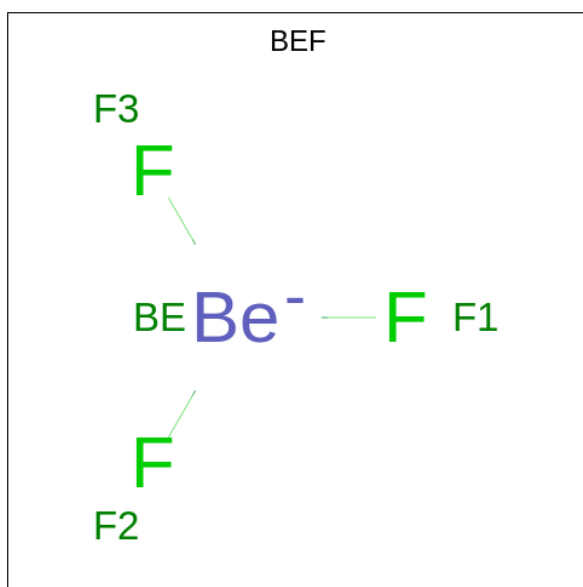


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
17	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	M	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	N	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	O	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	P	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	Q	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	R	1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

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

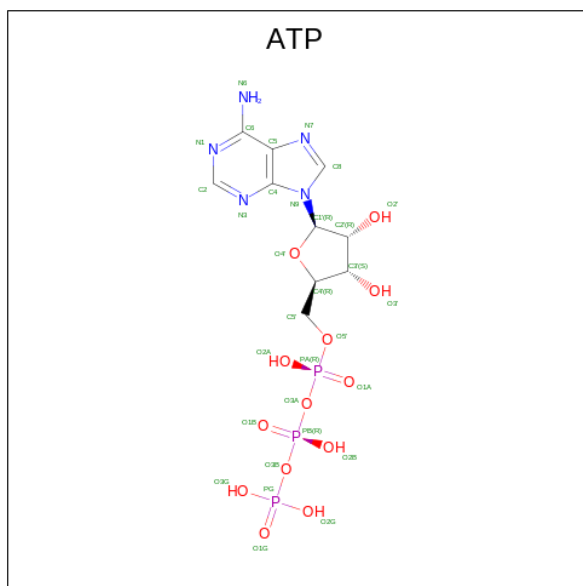
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
18	I	1	Total	Mg	0
			1	1	

- Molecule 19 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 20 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

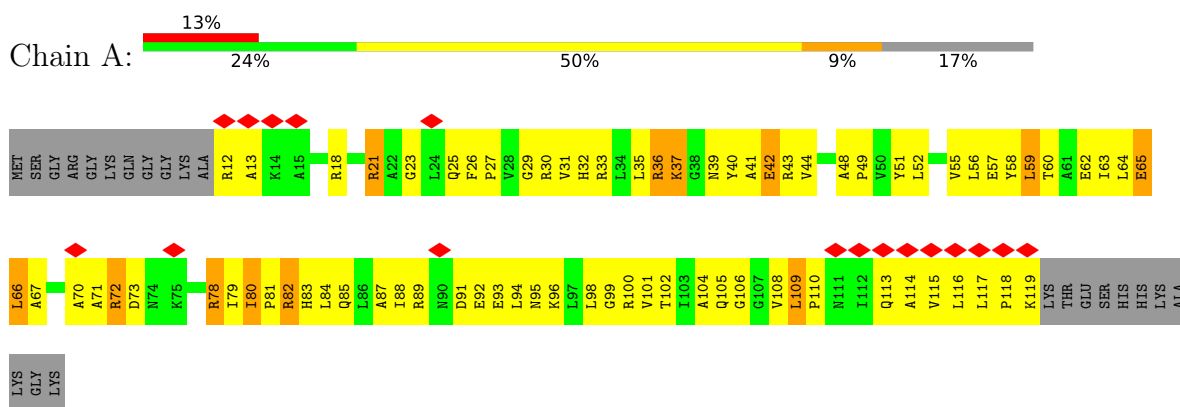


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
20	T	1	31	10	5	13	3	0
20	U	1	31	10	5	13	3	0

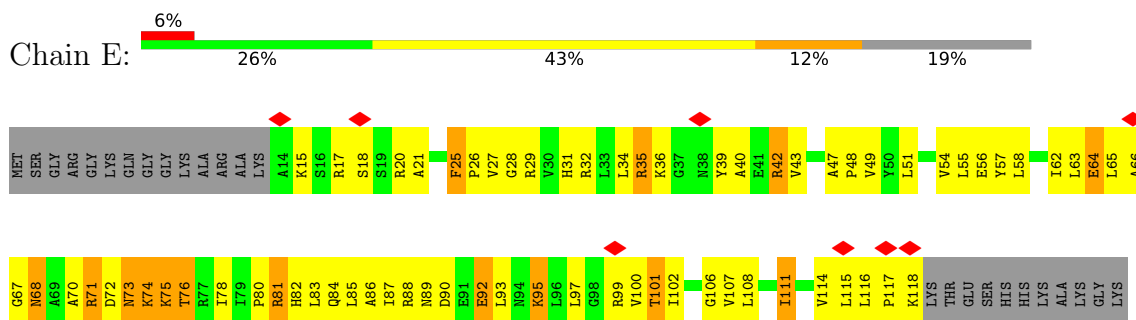
3 Residue-property plots [i](#)

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.

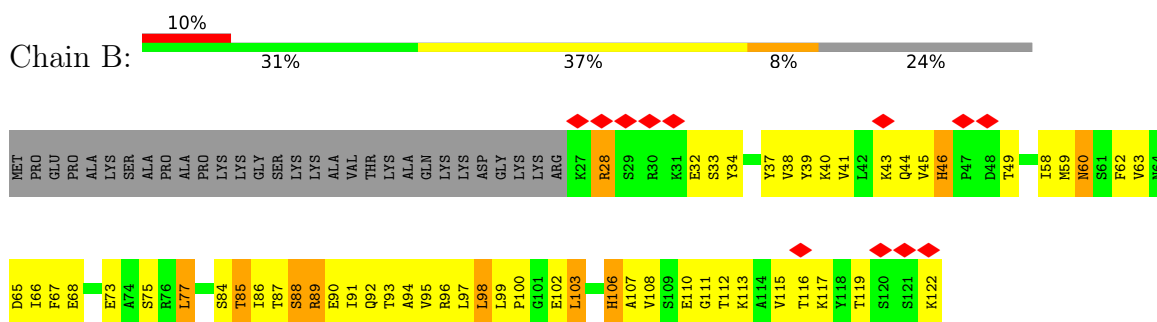
- Molecule 1: Histone H2A type 1-C



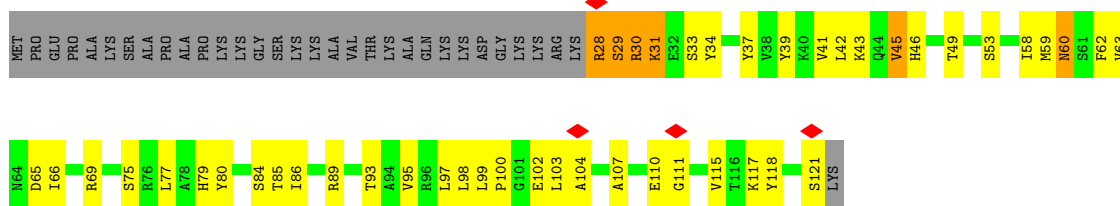
- Molecule 1: Histone H2A type 1-C



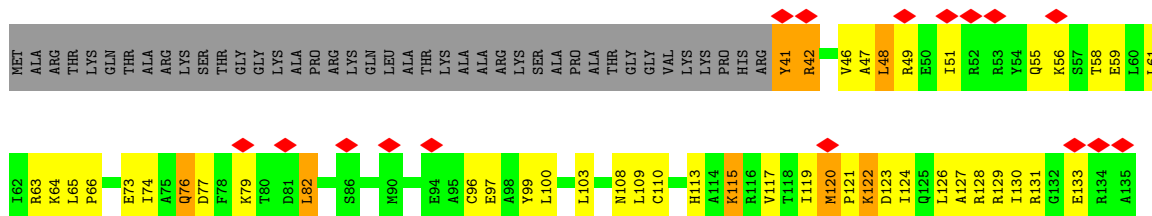
- Molecule 2: Histone H2B type 1-C/E/F/G/I



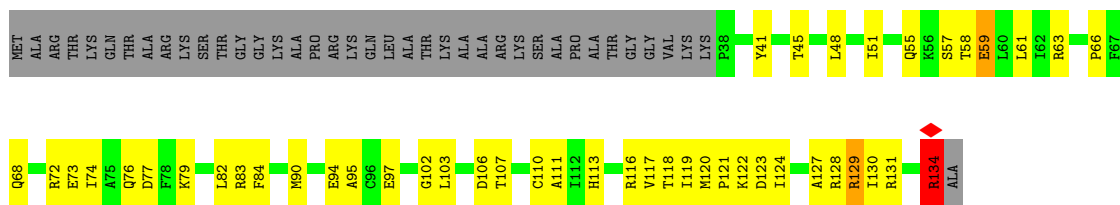
- Molecule 2: Histone H2B type 1-C/E/F/G/I



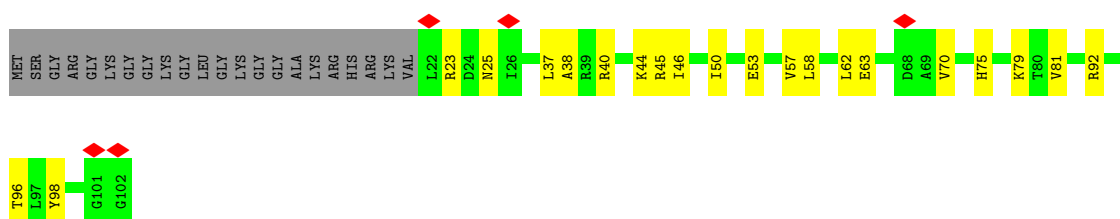
• Molecule 3: Histone H3.1



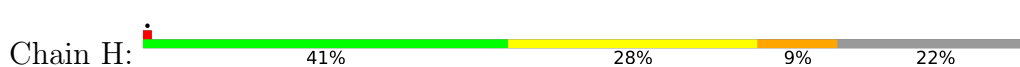
• Molecule 3: Histone H3.1

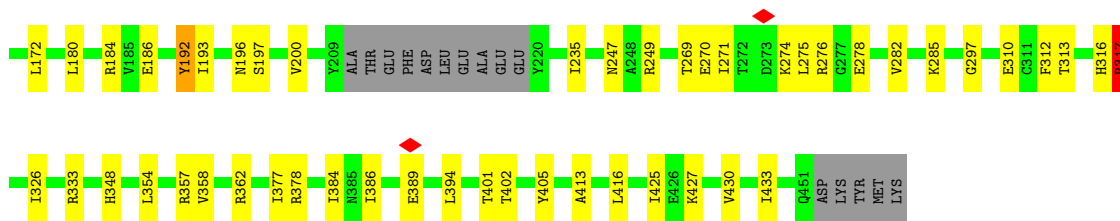


• Molecule 4: Histone H4

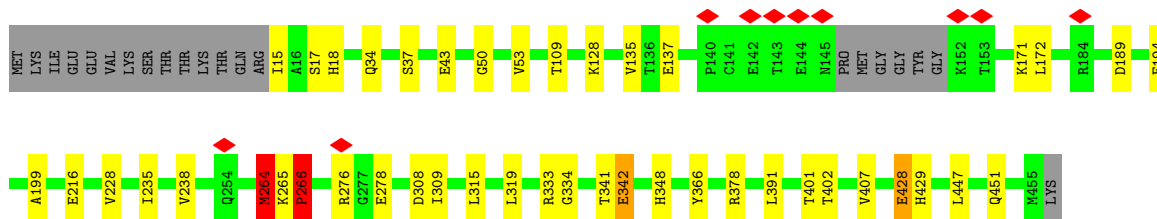
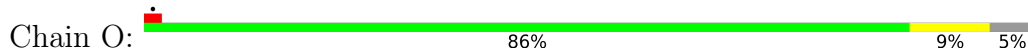


• Molecule 4: Histone H4

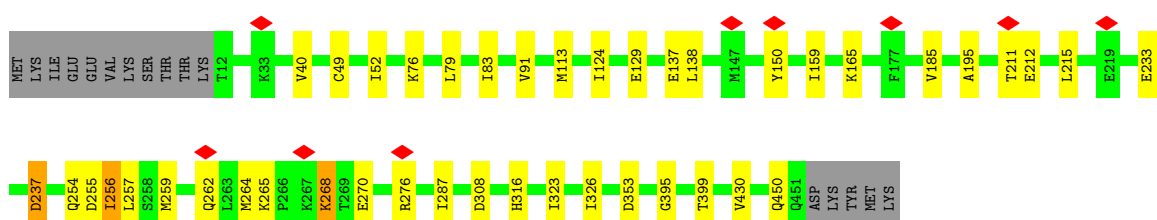
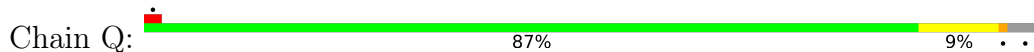




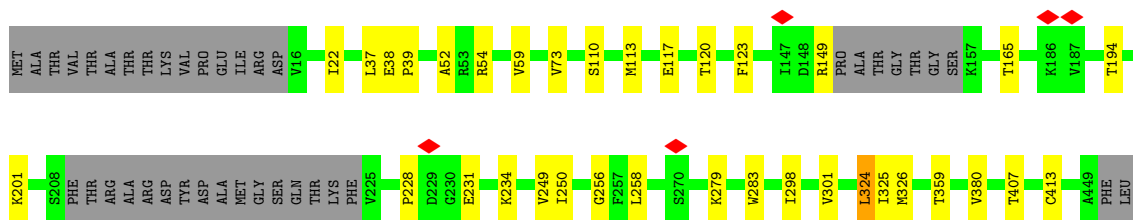
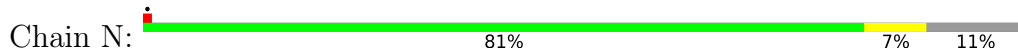
• Molecule 9: RuvB-like 1



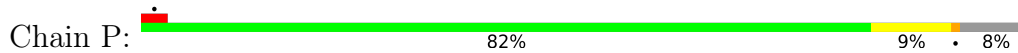
• Molecule 9: RuvB-like 1

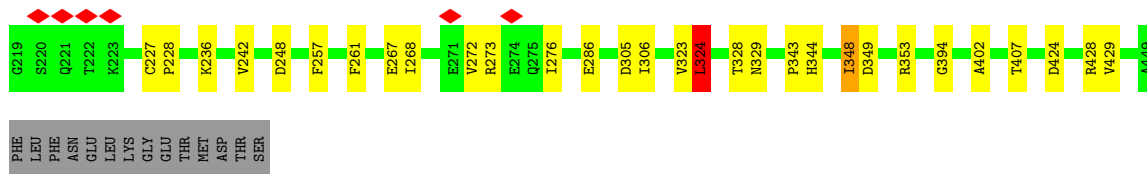


• Molecule 10: RuvB-like 2

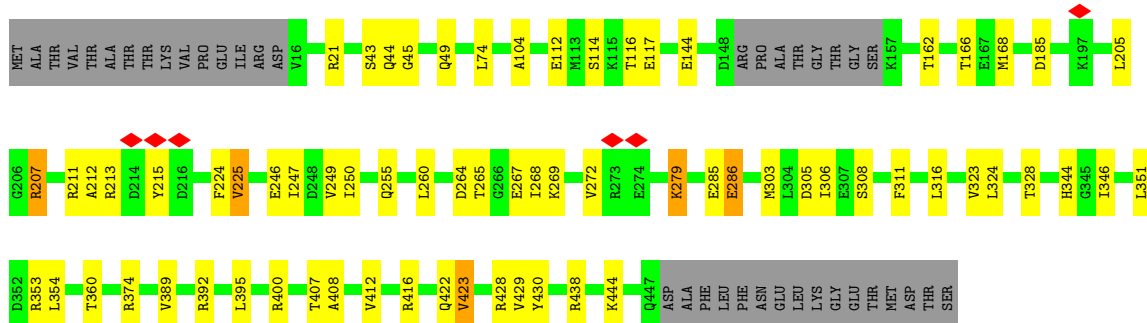
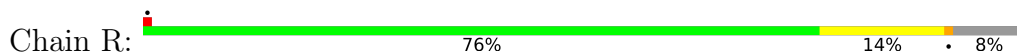


• Molecule 10: RuvB-like 2

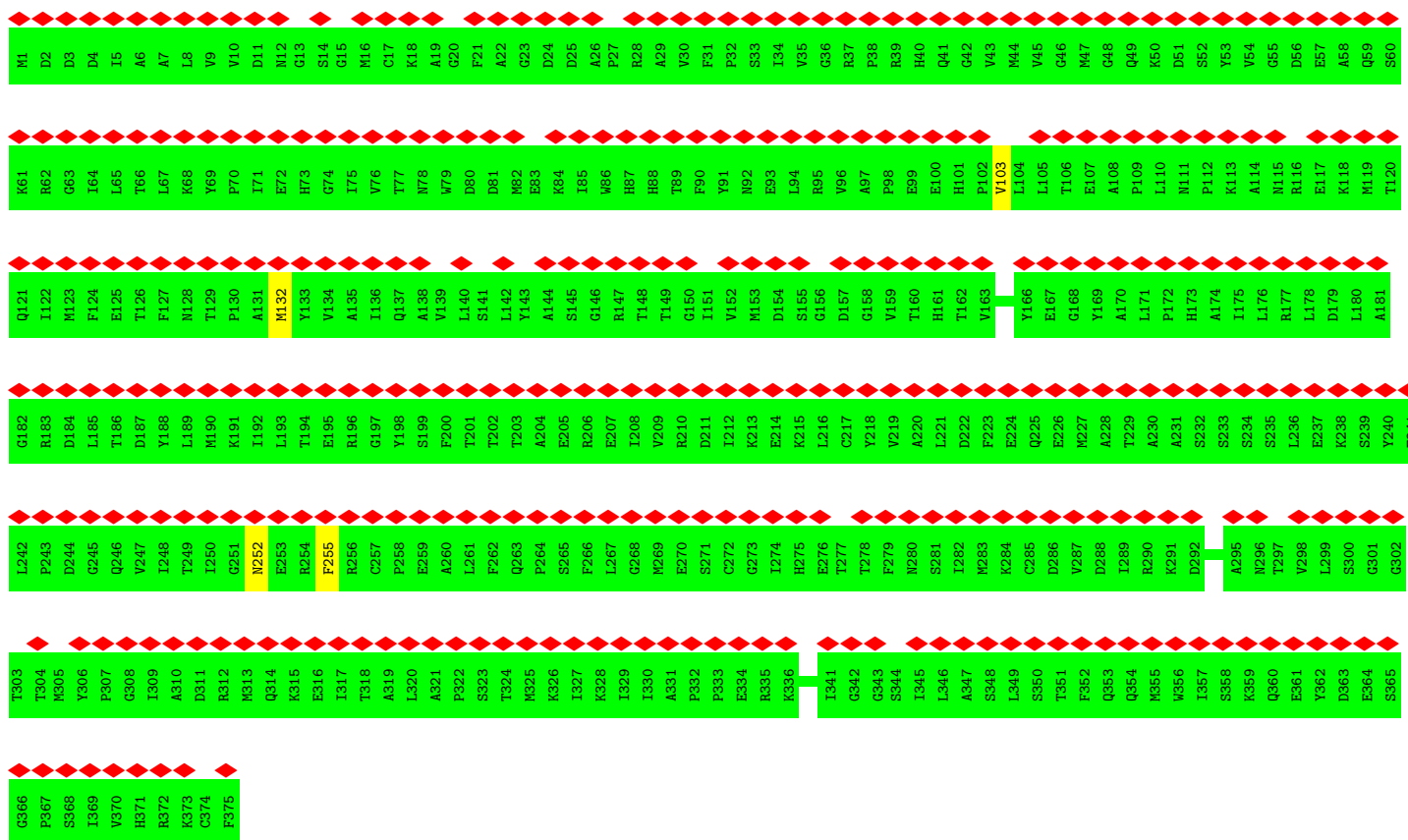




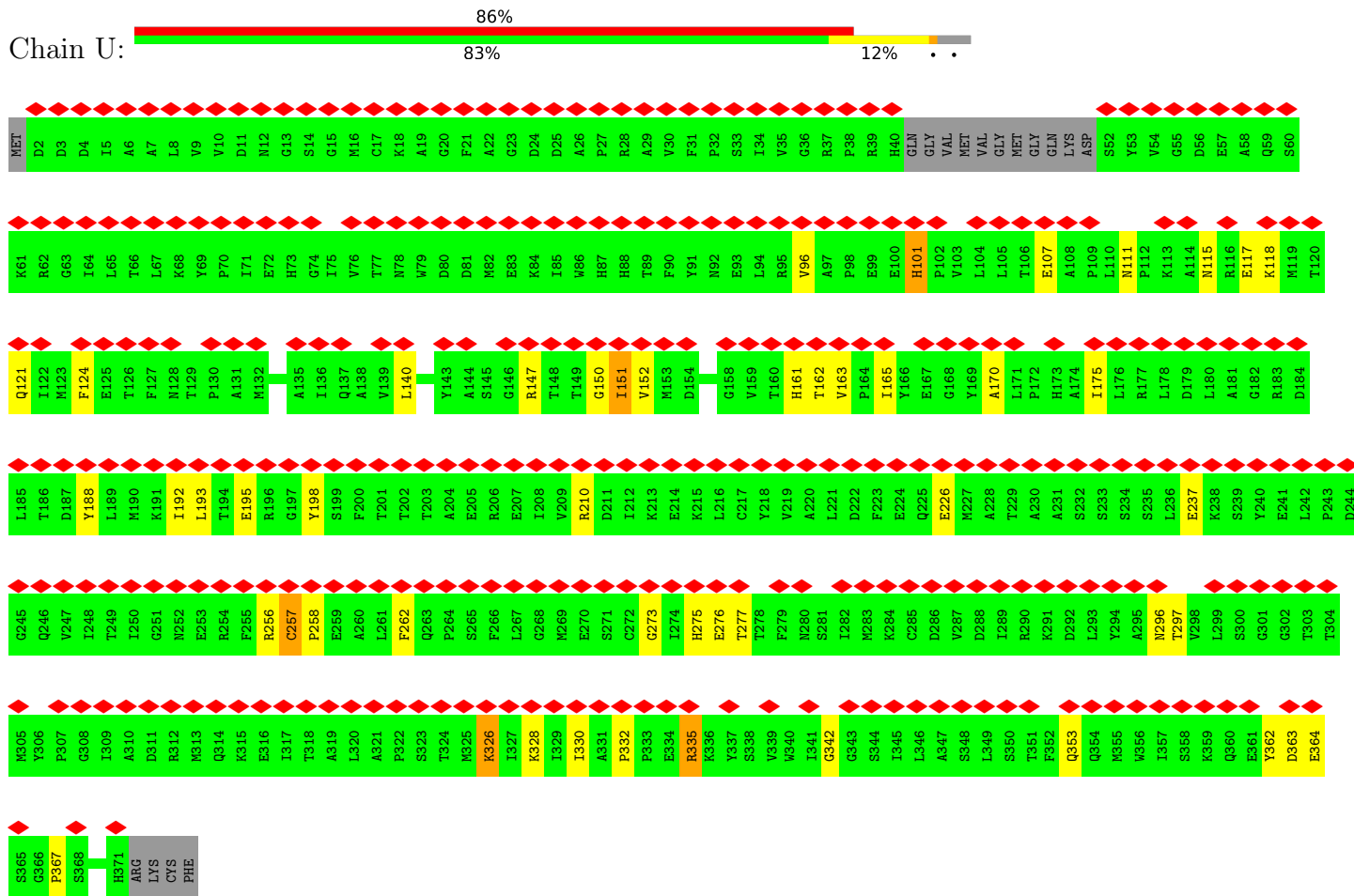
• Molecule 10: RuvB-like 2



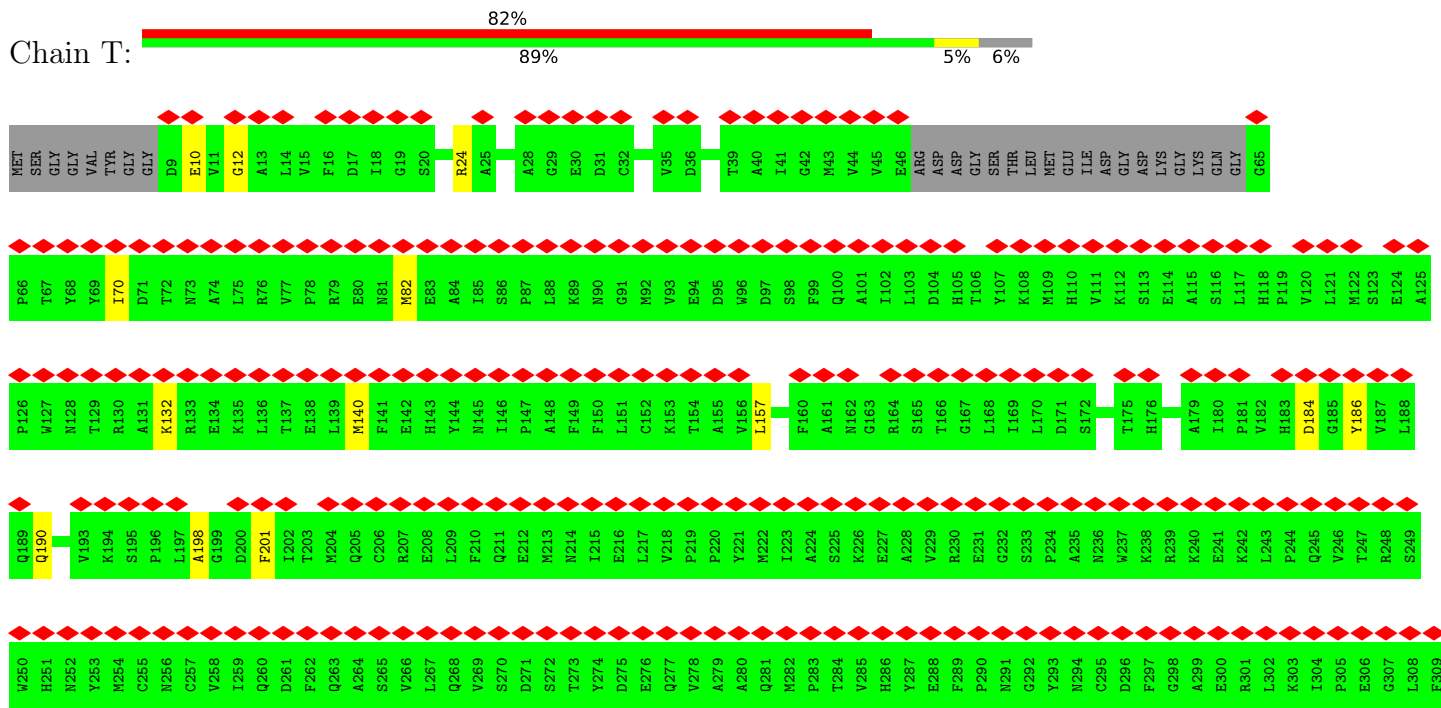
• Molecule 11: Actin, cytoplasmic 1

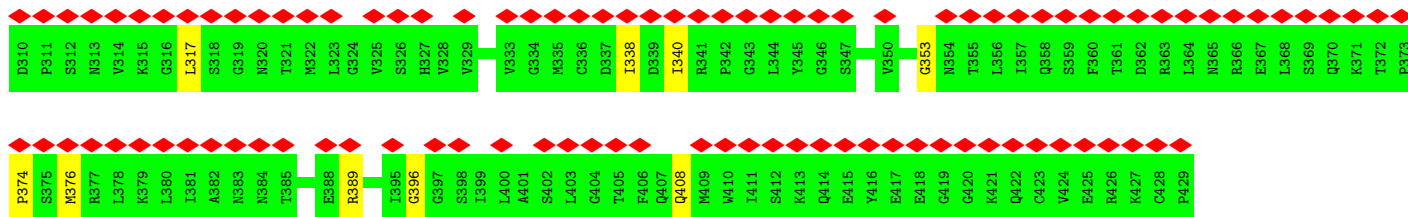


• Molecule 11: Actin, cytoplasmic 1

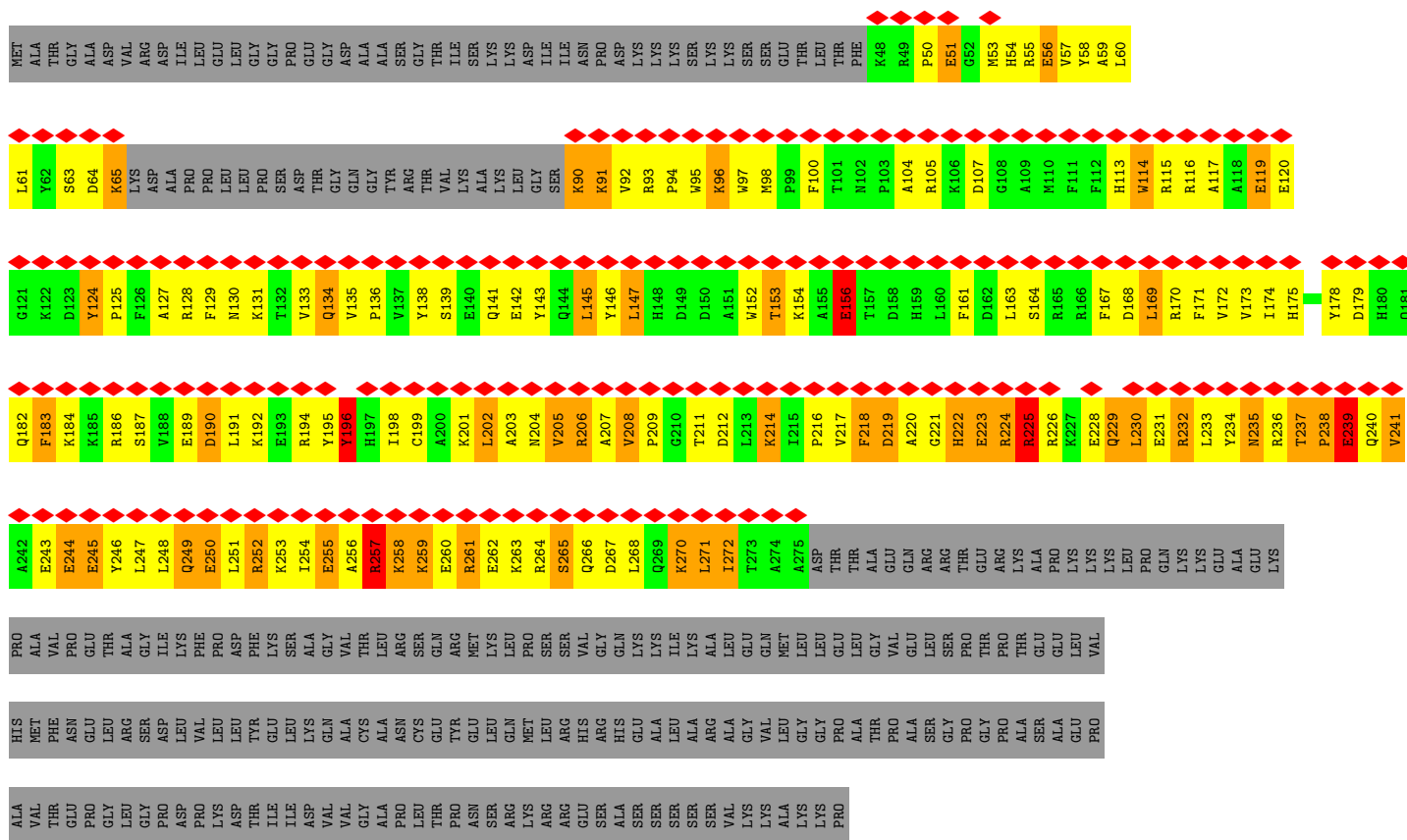
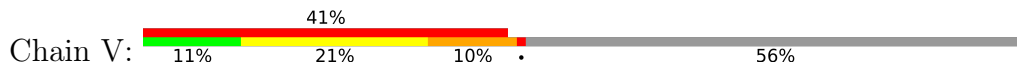


• Molecule 12: Actin-like protein 6A

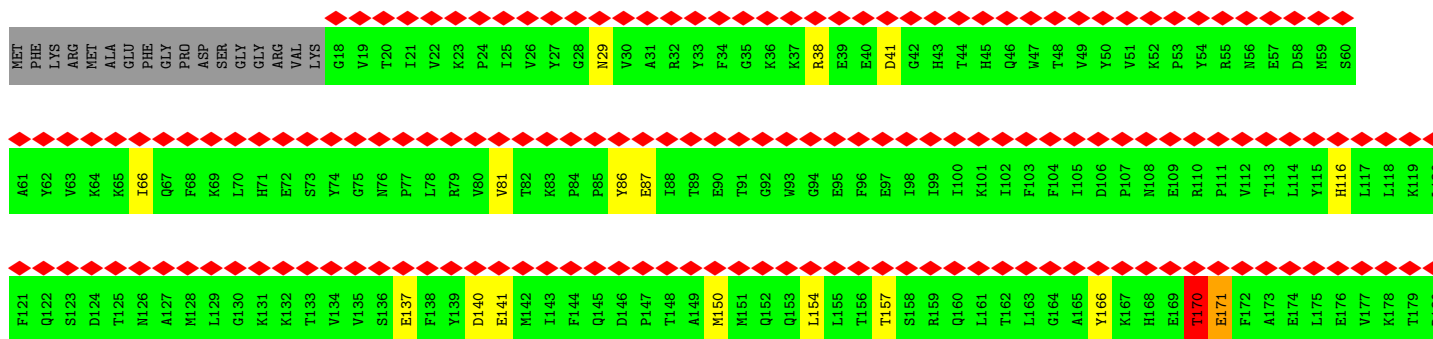
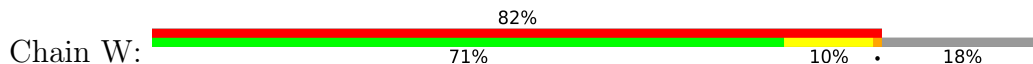


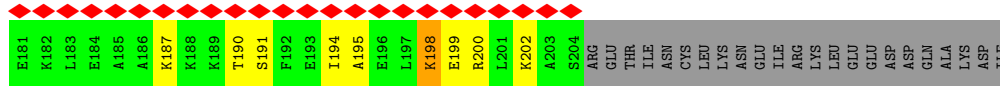


• Molecule 13: DNA methyltransferase 1-associated protein 1



• Molecule 14: YEATS domain-containing protein 4

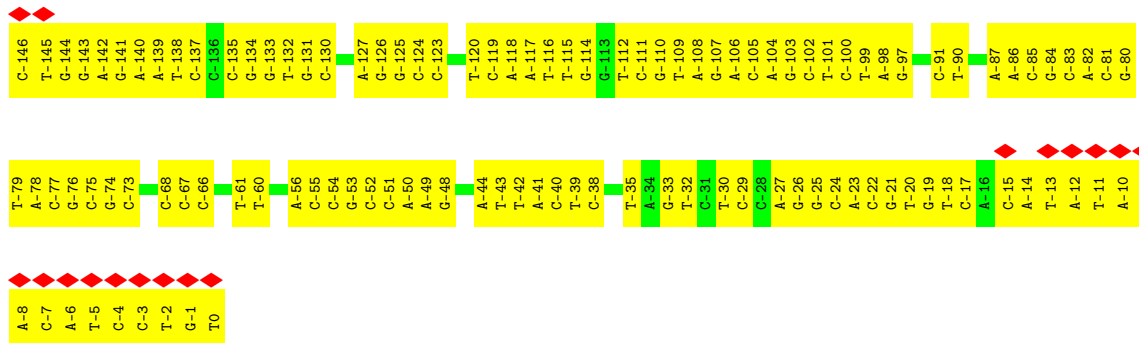




• Molecule 15: DNA (147-MER)



• Molecule 16: DNA (147-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	475617	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	0.244	Depositor
Minimum map value	-0.115	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.027	Depositor
Map size (\AA)	533.6, 533.6, 533.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.334, 1.334, 1.334	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BEF, ATP, ADP, MG

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	0.31	0/843	0.58	0/1136
1	E	0.26	0/818	0.54	0/1104
2	B	0.27	0/766	0.50	0/1026
2	F	0.27	0/747	0.50	0/1004
3	C	0.28	0/789	0.56	0/1057
3	G	0.27	0/813	0.56	0/1090
4	D	0.30	0/653	0.58	0/873
4	H	0.25	0/645	0.56	0/862
5	I	0.32	0/7296	0.62	1/9855 (0.0%)
6	J	0.34	0/1381	0.62	0/1861
7	K	0.31	0/3283	0.55	2/4445 (0.0%)
8	L	0.35	0/909	0.63	0/1227
9	M	0.31	0/3253	0.58	0/4382
9	O	0.32	0/3382	0.57	0/4559
9	Q	0.31	0/3413	0.56	1/4603 (0.0%)
10	N	0.30	0/3217	0.60	1/4328 (0.0%)
10	P	0.30	0/3324	0.60	1/4477 (0.0%)
10	R	0.30	0/3329	0.60	0/4479
11	S	0.29	0/2988	0.50	0/4045
11	U	0.31	0/2863	0.56	0/3882
12	T	0.29	0/3217	0.50	0/4362
13	V	0.57	5/1801 (0.3%)	0.67	2/2419 (0.1%)
14	W	0.37	1/1578 (0.1%)	0.53	0/2128
15	X	0.58	0/3405	0.95	2/5259 (0.0%)
16	Y	0.56	0/3349	0.93	0/5162
All	All	0.36	6/58062 (0.0%)	0.64	10/79625 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	G	0	1
5	I	0	1
9	M	0	1
10	P	0	2
10	R	0	1
13	V	0	3
14	W	0	1
All	All	0	10

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	V	156	GLU	CD-OE1	8.47	1.34	1.25
13	V	183	PHE	CD1-CE1	8.17	1.55	1.39
13	V	183	PHE	CE2-CZ	6.55	1.49	1.37
14	W	198	LYS	CD-CE	6.44	1.67	1.51
13	V	196	TYR	CD1-CE1	-5.59	1.30	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	89	LEU	CB-CG-CD2	-7.39	98.43	111.00
7	K	89	LEU	CA-CB-CG	6.25	129.68	115.30
15	X	89	DA	O4'-C1'-N9	6.19	112.33	108.00
13	V	156	GLU	CG-CD-OE2	-6.15	106.01	118.30
9	Q	79	LEU	CA-CB-CG	5.68	128.36	115.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	134	ARG	Sidechain
5	I	2029	ARG	Sidechain
9	M	317	ARG	Sidechain
10	P	18	ARG	Sidechain
10	P	21	ARG	Sidechain

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	833	0	895	184	0
1	E	808	0	864	118	0
2	B	755	0	782	136	0
2	F	736	0	756	68	0
3	C	779	0	816	72	0
3	G	801	0	839	93	0
4	D	646	0	687	36	0
4	H	638	0	676	63	0
5	I	7122	0	7212	309	0
6	J	1350	0	1370	28	0
7	K	3209	0	3132	518	0
8	L	893	0	880	52	0
9	M	3213	0	3331	90	0
9	O	3339	0	3425	28	0
9	Q	3368	0	3453	33	0
10	N	3185	0	3269	44	0
10	P	3287	0	3335	22	0
10	R	3293	0	3373	41	0
11	S	2925	0	2891	2	0
11	U	2802	0	2760	34	0
12	T	3146	0	3086	20	0
13	V	1757	0	1736	326	0
14	W	1542	0	1556	70	0
15	X	3031	0	1650	241	0
16	Y	2990	0	1652	182	0
17	I	27	0	12	6	0
17	M	27	0	12	0	0
17	N	27	0	12	0	0
17	O	27	0	12	1	0
17	P	27	0	12	0	0
17	Q	27	0	12	1	0
17	R	27	0	12	0	0
18	I	1	0	0	0	0
19	I	4	0	0	3	0
20	T	31	0	12	1	0
20	U	31	0	12	0	0
All	All	56704	0	54534	2263	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 20.

The worst 5 of 2263 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)
9:M:313:THR:HA	9:M:316:HIS:CE1	1.28	1.63
1:A:13:ALA:HB2	5:I:164:LYS:CD	1.25	1.61
9:M:413:ALA:HA	9:M:433:ILE:CD1	1.35	1.53
5:I:936:HIS:CE1	10:N:279:LYS:HZ3	1.29	1.48
5:I:936:HIS:HE1	10:N:279:LYS:NZ	1.08	1.47

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	106/130 (82%)	97 (92%)	9 (8%)	0	100	100
1	E	103/130 (79%)	93 (90%)	10 (10%)	0	100	100
2	B	94/126 (75%)	87 (93%)	7 (7%)	0	100	100
2	F	92/126 (73%)	88 (96%)	2 (2%)	2 (2%)	6	35
3	C	93/136 (68%)	91 (98%)	2 (2%)	0	100	100
3	G	95/136 (70%)	91 (96%)	4 (4%)	0	100	100
4	D	79/103 (77%)	78 (99%)	1 (1%)	0	100	100
4	H	78/103 (76%)	72 (92%)	6 (8%)	0	100	100
5	I	858/3230 (27%)	792 (92%)	63 (7%)	3 (0%)	41	74
6	J	158/364 (43%)	145 (92%)	13 (8%)	0	100	100
7	K	392/396 (99%)	295 (75%)	84 (21%)	13 (3%)	4	25
8	L	109/154 (71%)	96 (88%)	13 (12%)	0	100	100
9	M	412/456 (90%)	395 (96%)	16 (4%)	1 (0%)	47	79
9	O	431/456 (94%)	409 (95%)	19 (4%)	3 (1%)	22	61
9	Q	438/456 (96%)	417 (95%)	20 (5%)	1 (0%)	47	79
10	N	405/463 (88%)	386 (95%)	19 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	P	423/463 (91%)	396 (94%)	26 (6%)	1 (0%)	47	79
10	R	420/463 (91%)	393 (94%)	26 (6%)	1 (0%)	47	79
11	S	373/375 (100%)	366 (98%)	7 (2%)	0	100	100
11	U	355/375 (95%)	325 (92%)	29 (8%)	1 (0%)	41	74
12	T	399/429 (93%)	381 (96%)	18 (4%)	0	100	100
13	V	200/467 (43%)	178 (89%)	19 (10%)	3 (2%)	10	44
14	W	185/227 (82%)	182 (98%)	2 (1%)	1 (0%)	29	67
All	All	6298/9764 (64%)	5853 (93%)	415 (7%)	30 (0%)	32	67

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	I	820	GLU
7	K	89	LEU
7	K	103	THR
7	K	120	GLN
7	K	376	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/99 (85%)	64 (76%)	20 (24%)	0	3
1	E	82/99 (83%)	64 (78%)	18 (22%)	1	5
2	B	83/106 (78%)	71 (86%)	12 (14%)	3	15
2	F	81/106 (76%)	73 (90%)	8 (10%)	8	30
3	C	82/111 (74%)	68 (83%)	14 (17%)	2	10
3	G	85/111 (77%)	80 (94%)	5 (6%)	19	54
4	D	66/79 (84%)	66 (100%)	0	100	100
4	H	65/79 (82%)	54 (83%)	11 (17%)	2	10
5	I	775/2721 (28%)	759 (98%)	16 (2%)	53	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	J	148/312 (47%)	147 (99%)	1 (1%)	84	94
7	K	359/361 (99%)	238 (66%)	121 (34%)	0	0
8	L	98/133 (74%)	96 (98%)	2 (2%)	55	80
9	M	353/387 (91%)	346 (98%)	7 (2%)	55	80
9	O	364/387 (94%)	344 (94%)	20 (6%)	21	57
9	Q	366/387 (95%)	344 (94%)	22 (6%)	19	54
10	N	347/390 (89%)	340 (98%)	7 (2%)	55	80
10	P	352/390 (90%)	331 (94%)	21 (6%)	19	54
10	R	358/390 (92%)	329 (92%)	29 (8%)	11	42
11	S	318/318 (100%)	318 (100%)	0	100	100
11	U	305/318 (96%)	291 (95%)	14 (5%)	27	63
12	T	346/364 (95%)	338 (98%)	8 (2%)	50	78
13	V	183/400 (46%)	129 (70%)	54 (30%)	0	1
14	W	168/203 (83%)	164 (98%)	4 (2%)	49	77
All	All	5468/8251 (66%)	5054 (92%)	414 (8%)	17	45

5 of 414 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	M	192	TYR
9	Q	113	MET
13	V	252	ARG
10	N	283	TRP
9	O	428	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
9	Q	284	ASN
12	T	143	HIS
13	V	269	GLN
6	J	162	HIS
5	I	2060	HIS

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 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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
17	ADP	N	501	-	24,29,29	0.97	1 (4%)	29,45,45	1.33	4 (13%)
20	ATP	T	501	-	26,33,33	0.62	1 (3%)	31,52,52	1.12	4 (12%)
20	ATP	U	401	-	26,33,33	0.63	1 (3%)	31,52,52	1.06	2 (6%)
17	ADP	R	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.40	5 (17%)
17	ADP	I	3301	-	24,29,29	0.90	1 (4%)	29,45,45	1.64	5 (17%)
19	BEF	I	3303	-	0,3,3	-	-	-	-	-
17	ADP	O	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.47	5 (17%)
17	ADP	P	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.57	6 (20%)
17	ADP	Q	501	-	24,29,29	0.94	1 (4%)	29,45,45	1.48	5 (17%)
17	ADP	M	501	-	24,29,29	0.98	1 (4%)	29,45,45	1.42	3 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	ADP	N	501	-	-	4/12/32/32	0/3/3/3
20	ATP	T	501	-	-	1/18/38/38	0/3/3/3
20	ATP	U	401	-	-	2/18/38/38	0/3/3/3
17	ADP	R	501	-	-	1/12/32/32	0/3/3/3
17	ADP	I	3301	-	-	5/12/32/32	0/3/3/3
17	ADP	O	501	-	-	6/12/32/32	0/3/3/3
17	ADP	P	501	-	-	2/12/32/32	0/3/3/3
17	ADP	Q	501	-	-	3/12/32/32	0/3/3/3
17	ADP	M	501	-	-	2/12/32/32	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	O	501	ADP	C5-C4	2.67	1.48	1.40
17	R	501	ADP	C5-C4	2.60	1.47	1.40
17	P	501	ADP	C5-C4	2.60	1.47	1.40
17	Q	501	ADP	C5-C4	2.59	1.47	1.40
17	M	501	ADP	C5-C4	2.58	1.47	1.40

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	I	3301	ADP	PA-O3A-PB	-4.37	117.84	132.83
17	P	501	ADP	C3'-C2'-C1'	3.73	106.60	100.98
17	Q	501	ADP	PA-O3A-PB	-3.64	120.34	132.83
17	I	3301	ADP	N3-C2-N1	-3.53	123.16	128.68
17	M	501	ADP	PA-O3A-PB	-3.51	120.79	132.83

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

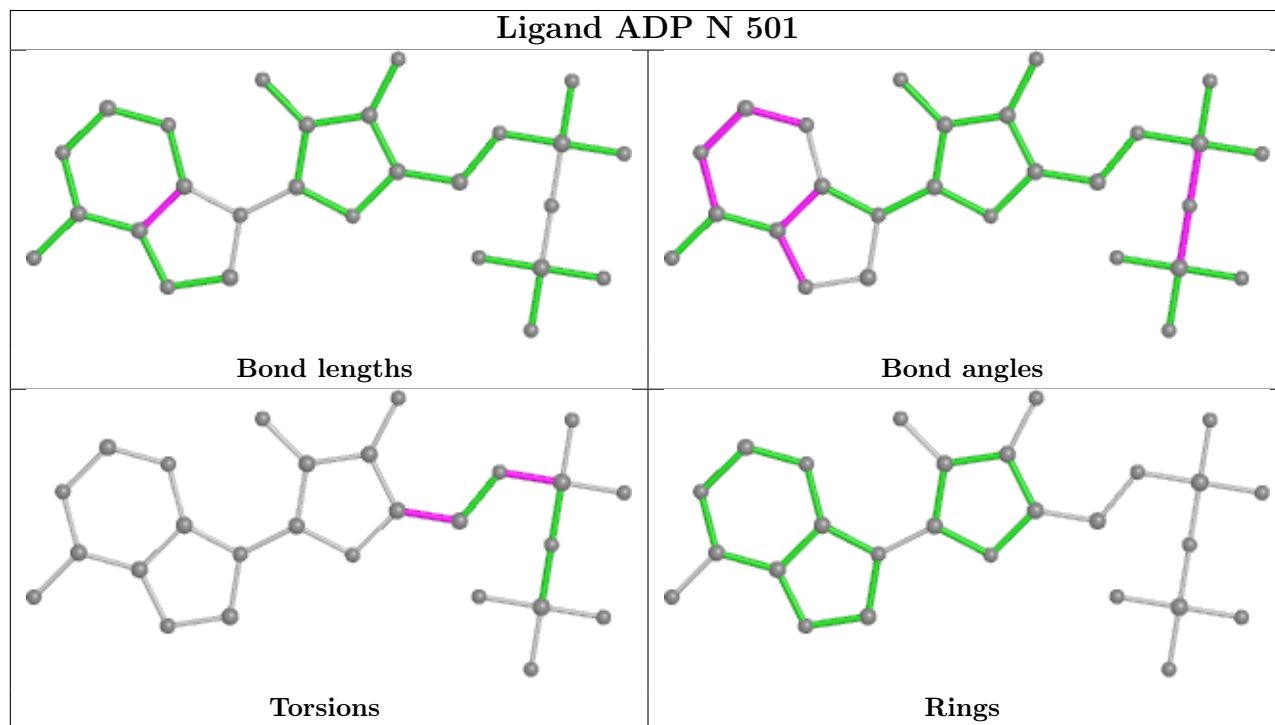
Mol	Chain	Res	Type	Atoms
17	I	3301	ADP	C5'-O5'-PA-O2A
17	N	501	ADP	C5'-O5'-PA-O1A
17	N	501	ADP	O4'-C4'-C5'-O5'
17	O	501	ADP	C5'-O5'-PA-O2A
17	P	501	ADP	PA-O3A-PB-O2B

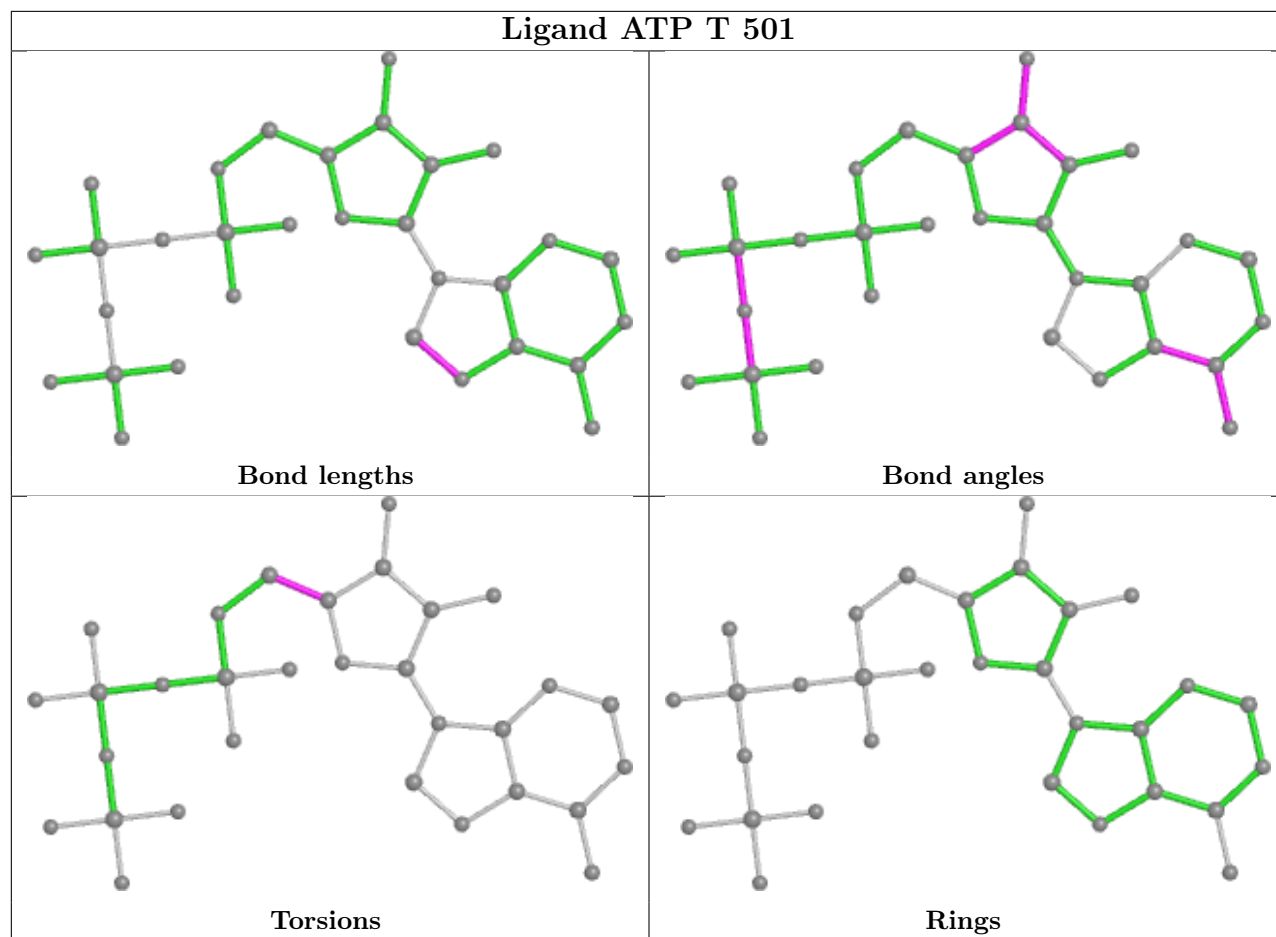
There are no ring outliers.

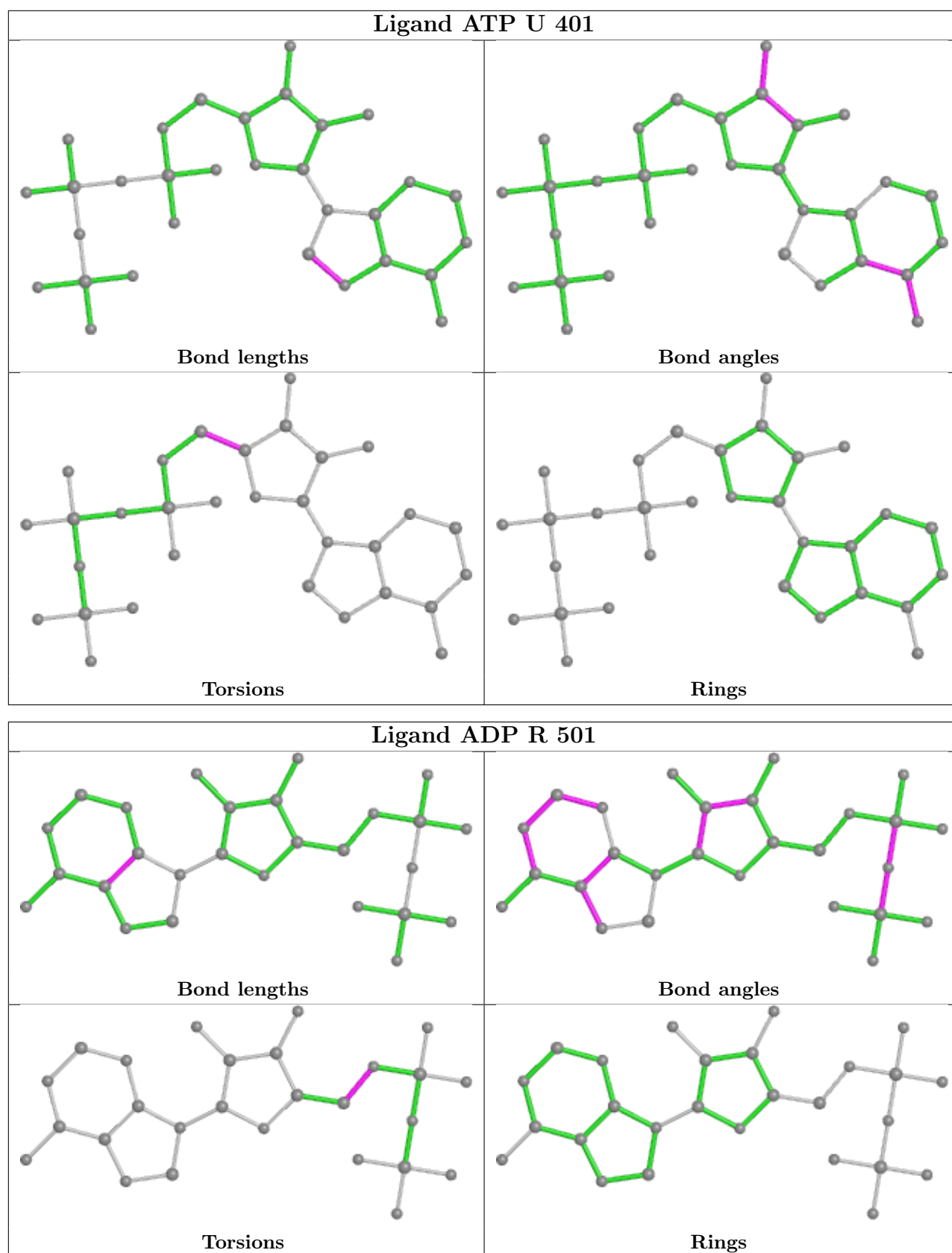
5 monomers are involved in 11 short contacts:

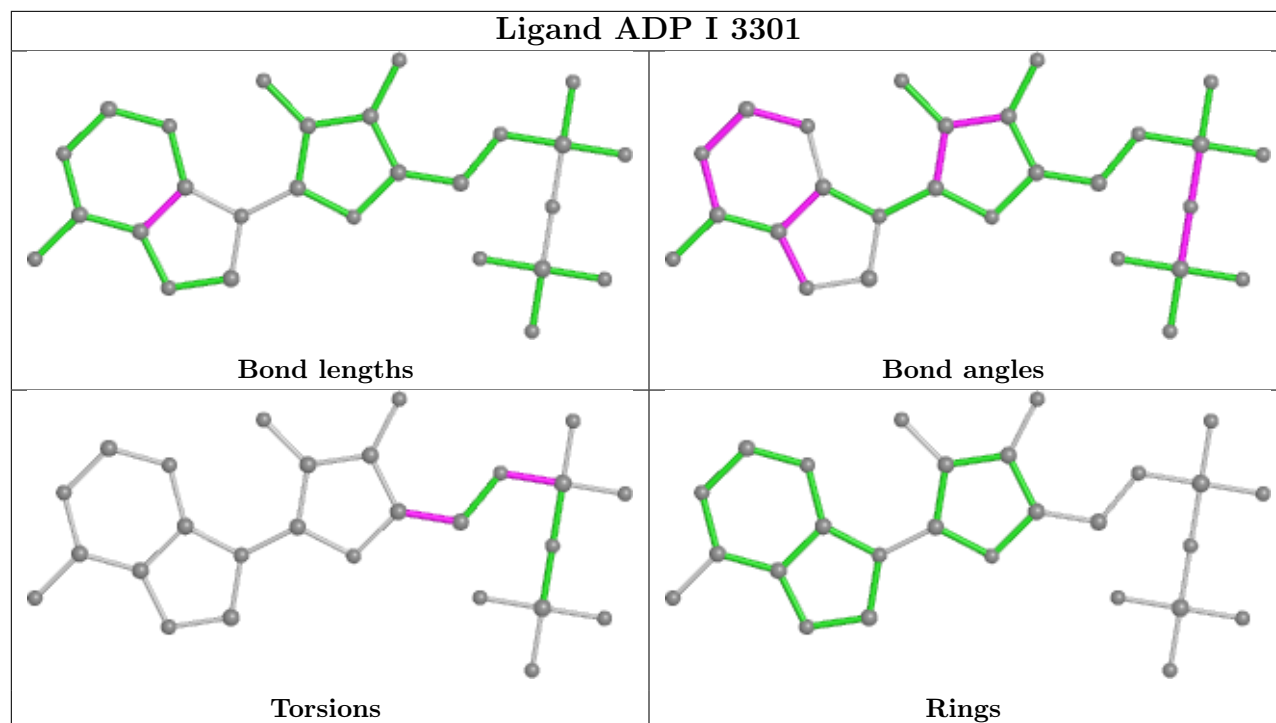
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	T	501	ATP	1	0
17	I	3301	ADP	6	0
19	I	3303	BEF	3	0
17	O	501	ADP	1	0
17	Q	501	ADP	1	0

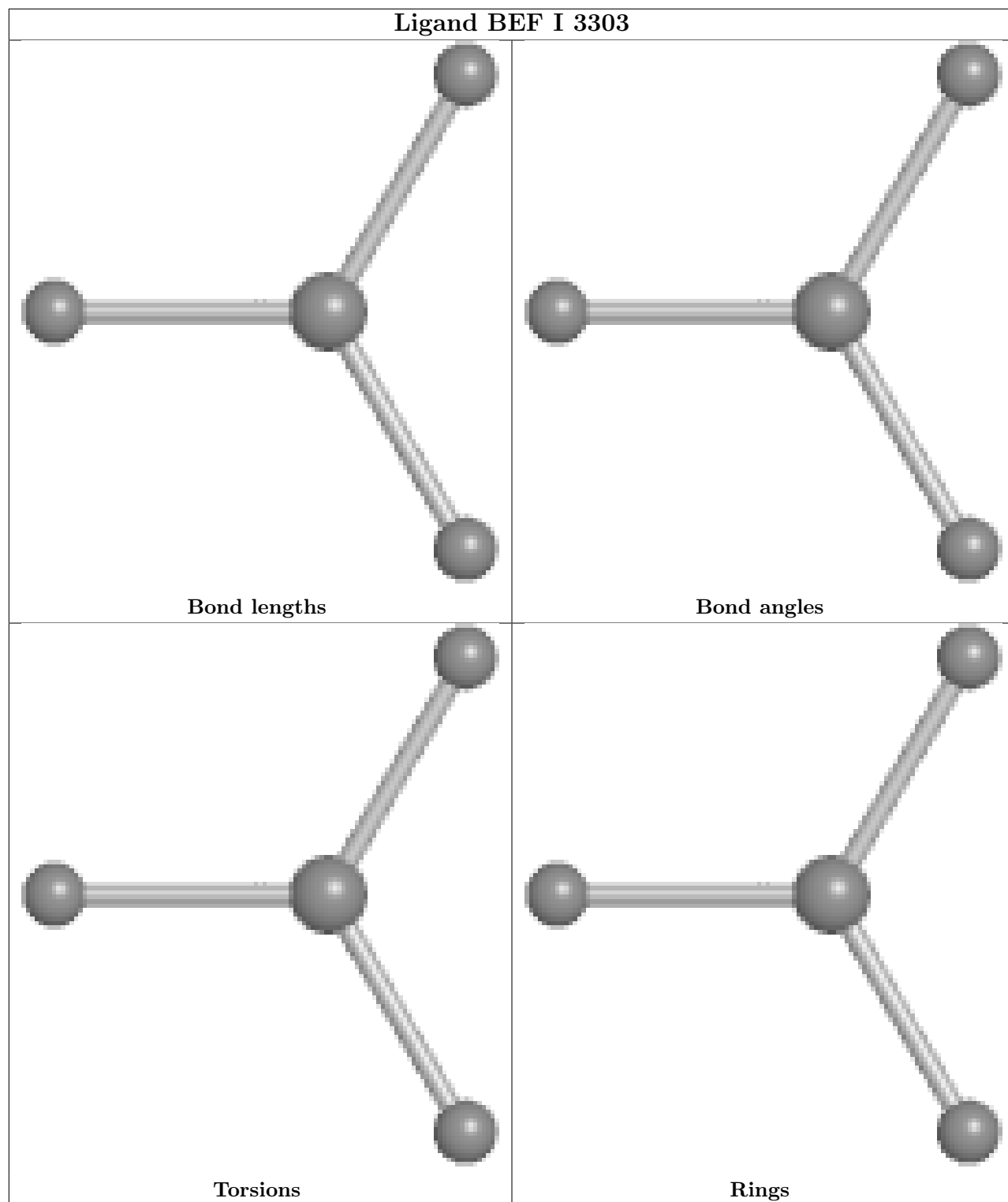
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

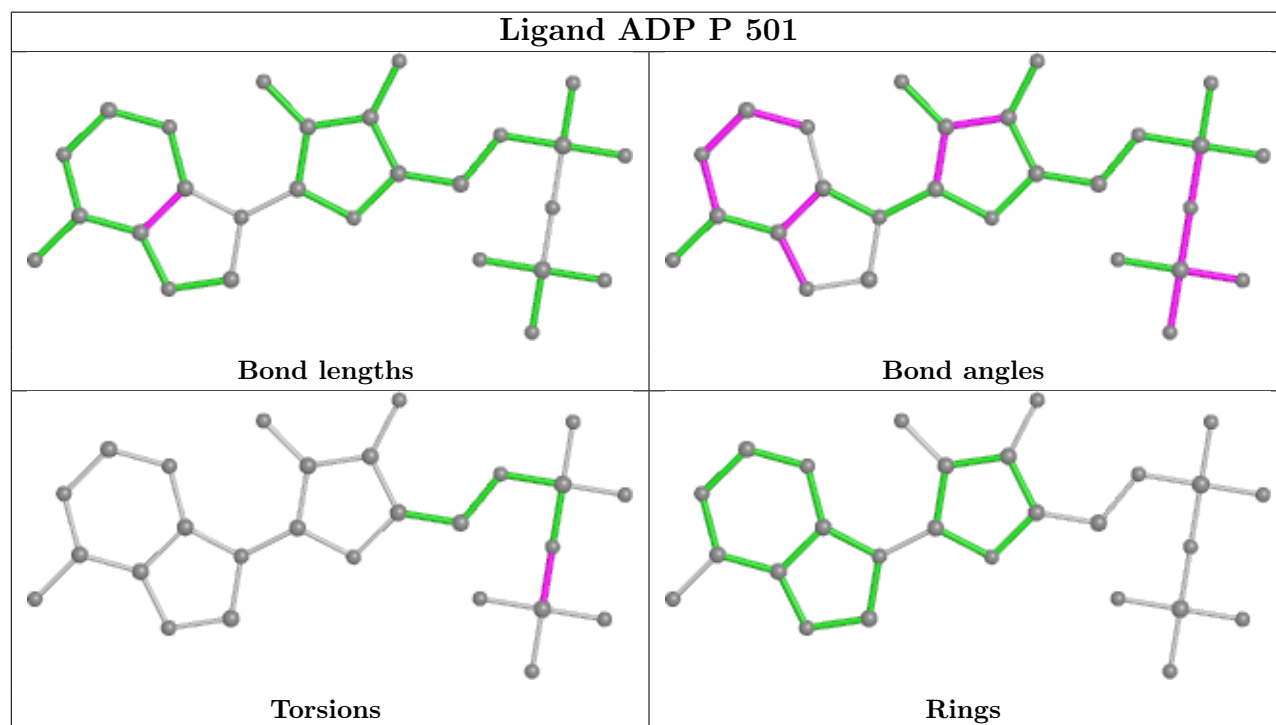
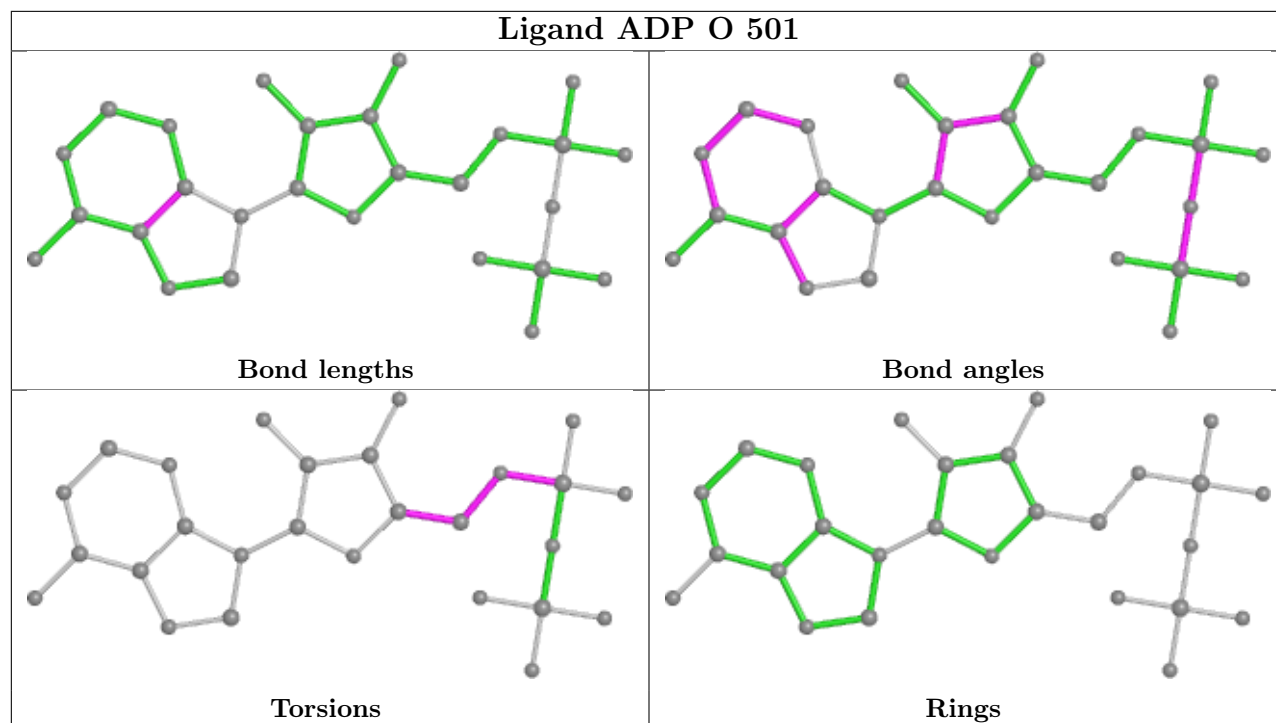


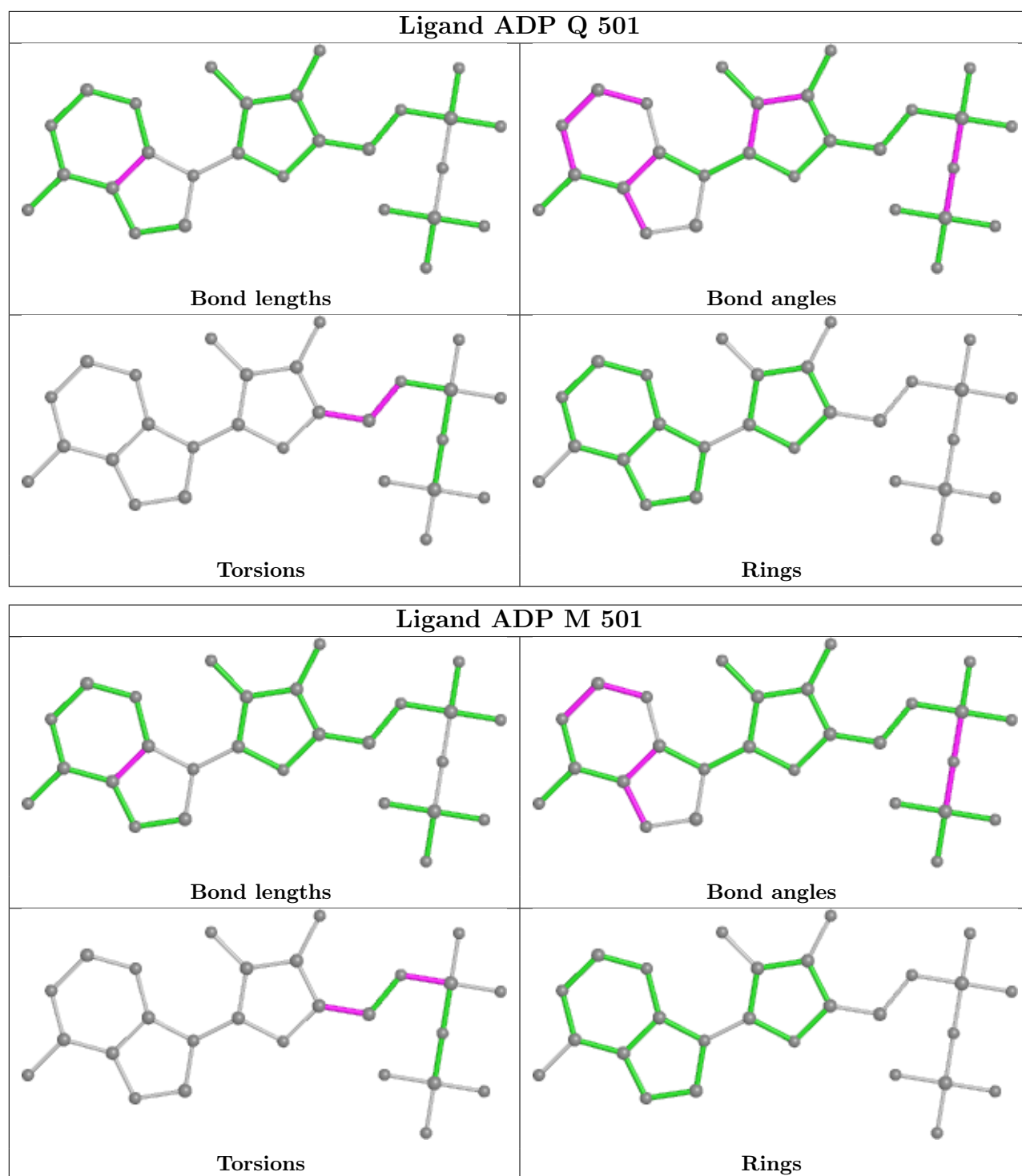












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

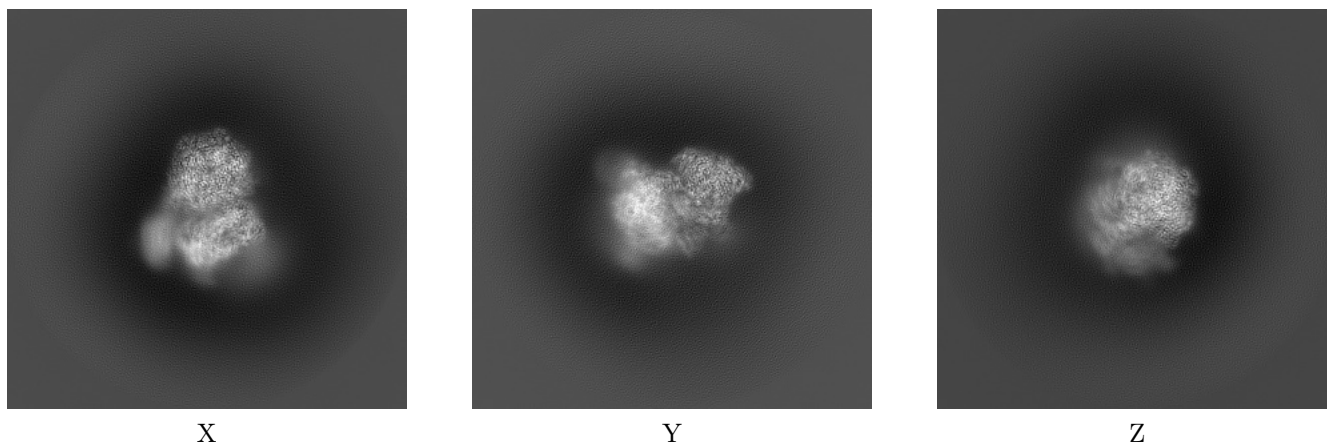
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37988. These allow visual inspection of the internal detail of the map and identification of artifacts.

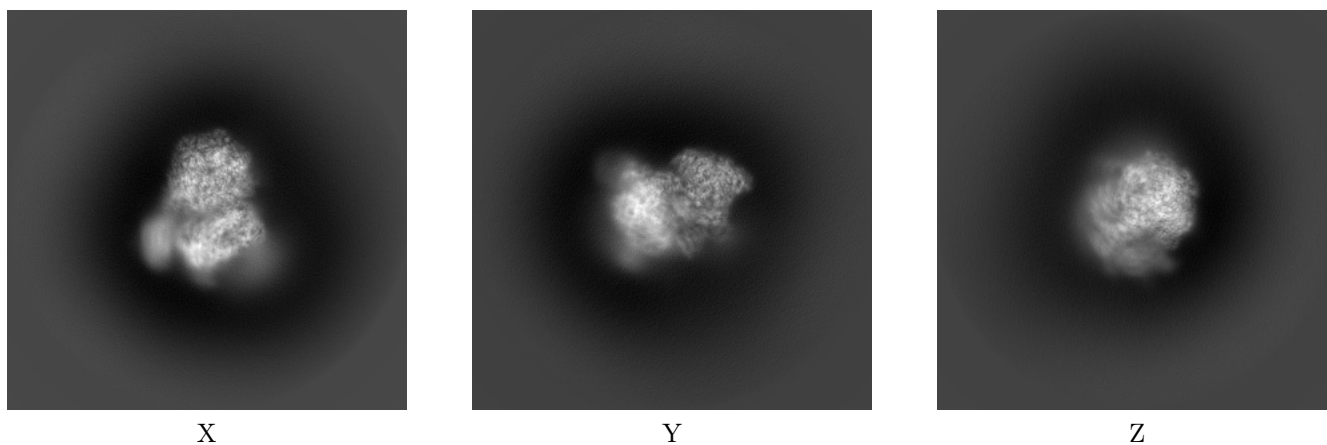
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



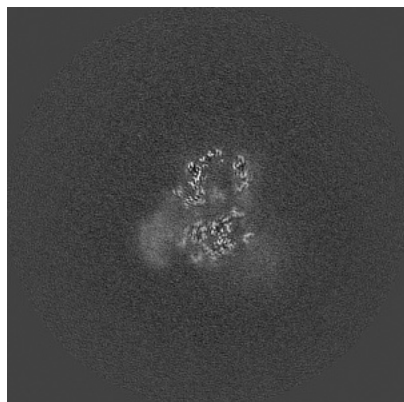
6.1.2 Raw map



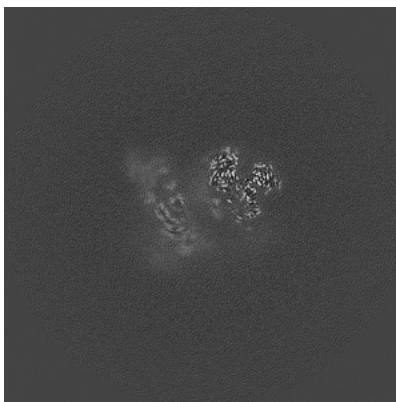
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

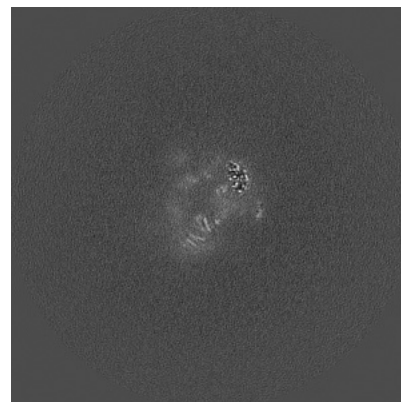
6.2.1 Primary map



X Index: 200

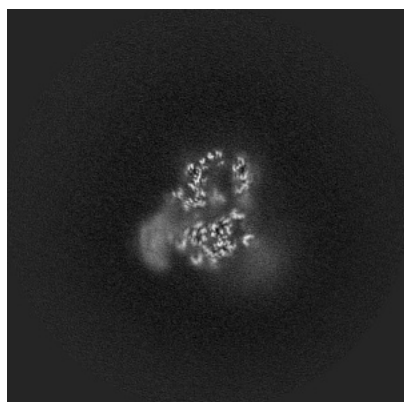


Y Index: 200

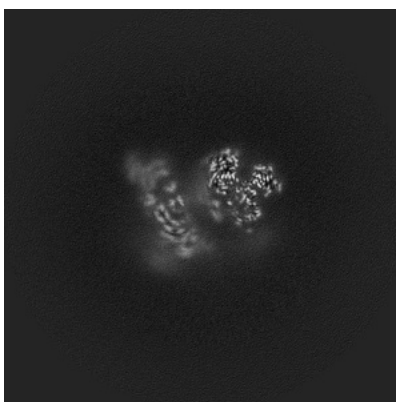


Z Index: 200

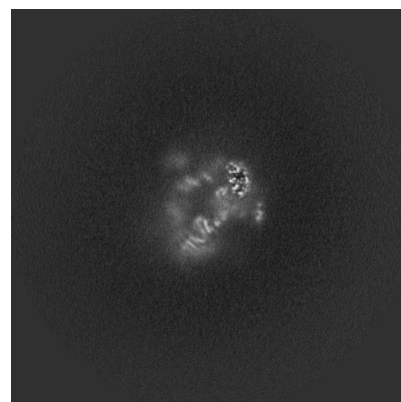
6.2.2 Raw map



X Index: 200



Y Index: 200

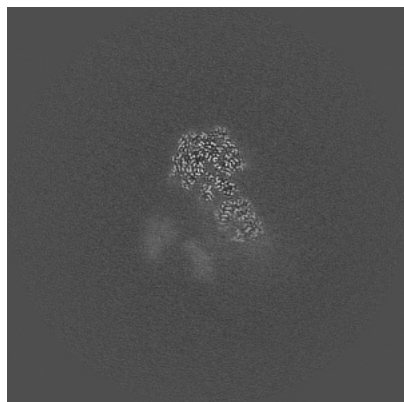


Z Index: 200

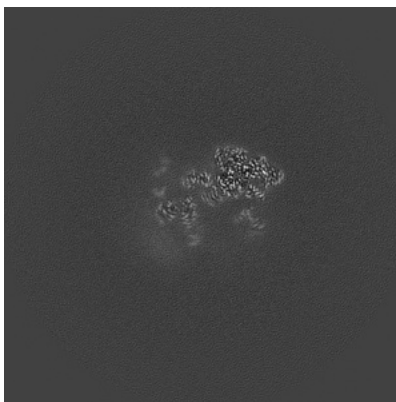
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

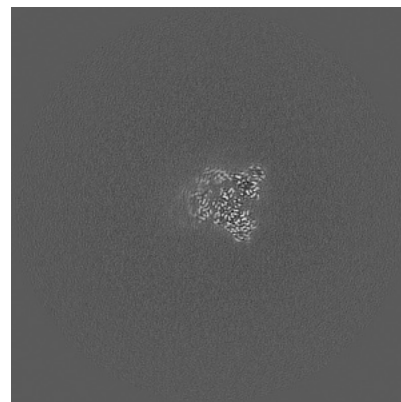
6.3.1 Primary map



X Index: 228

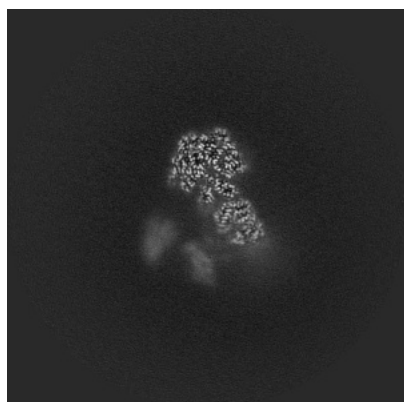


Y Index: 217

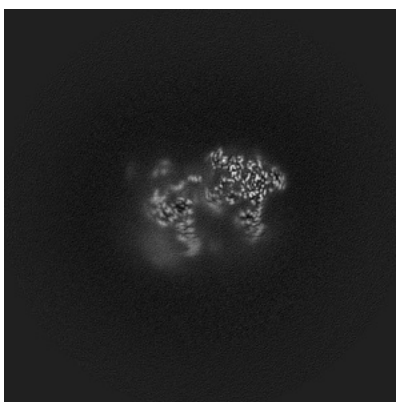


Z Index: 246

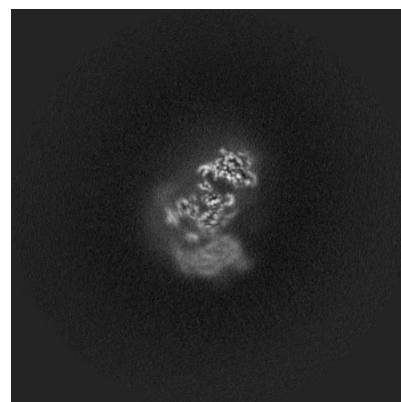
6.3.2 Raw map



X Index: 228



Y Index: 210

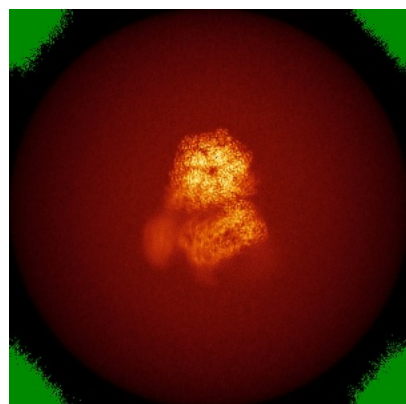


Z Index: 173

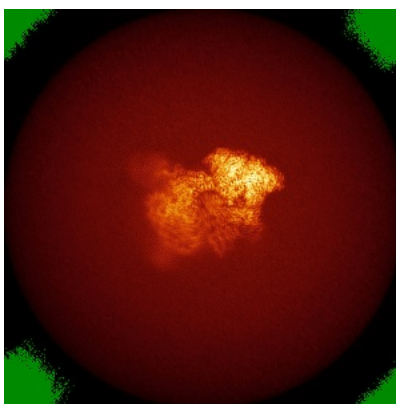
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

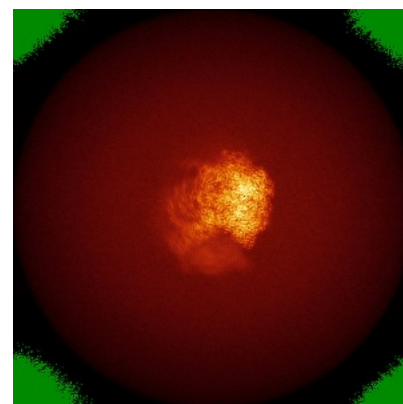
6.4.1 Primary map



X

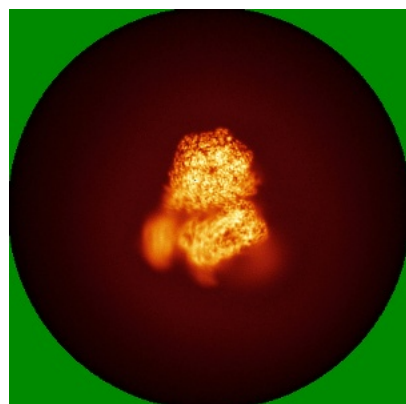


Y

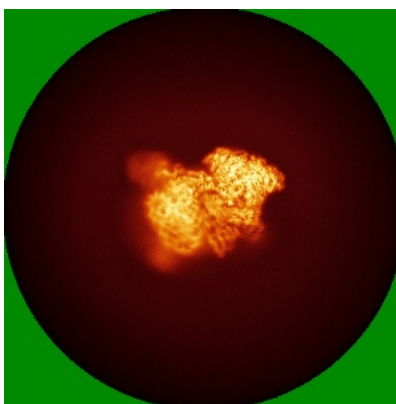


Z

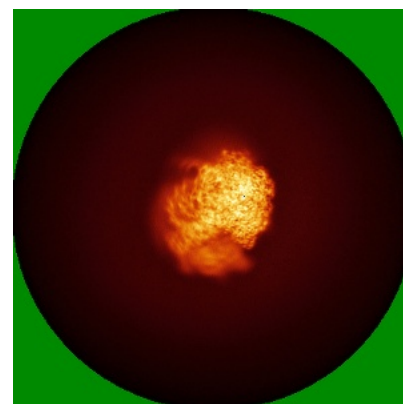
6.4.2 Raw map



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



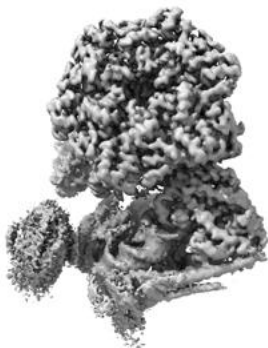
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

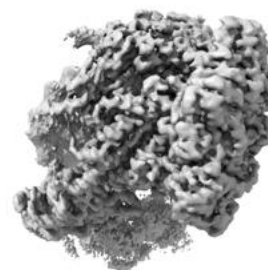
6.5.2 Raw map



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.

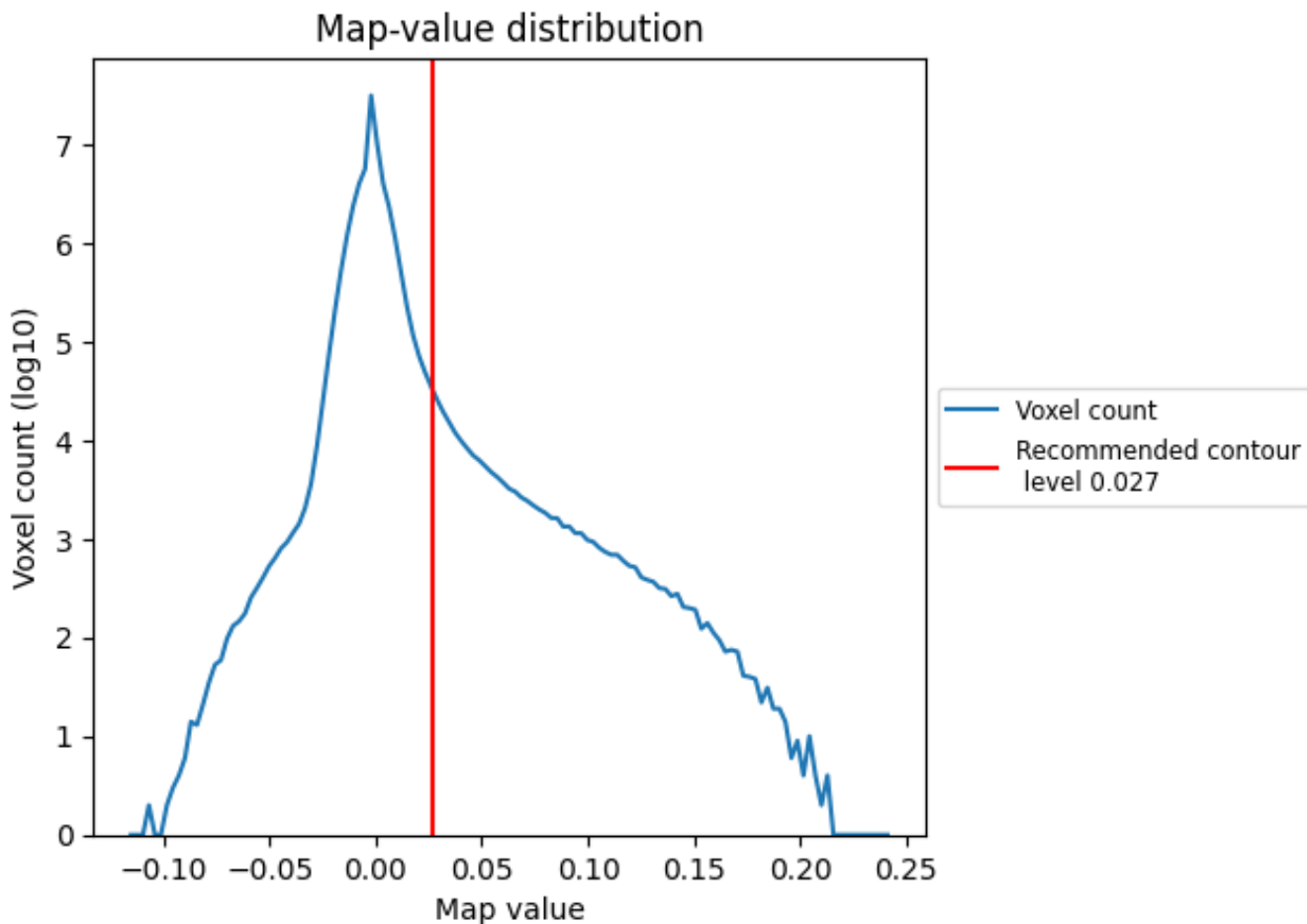
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

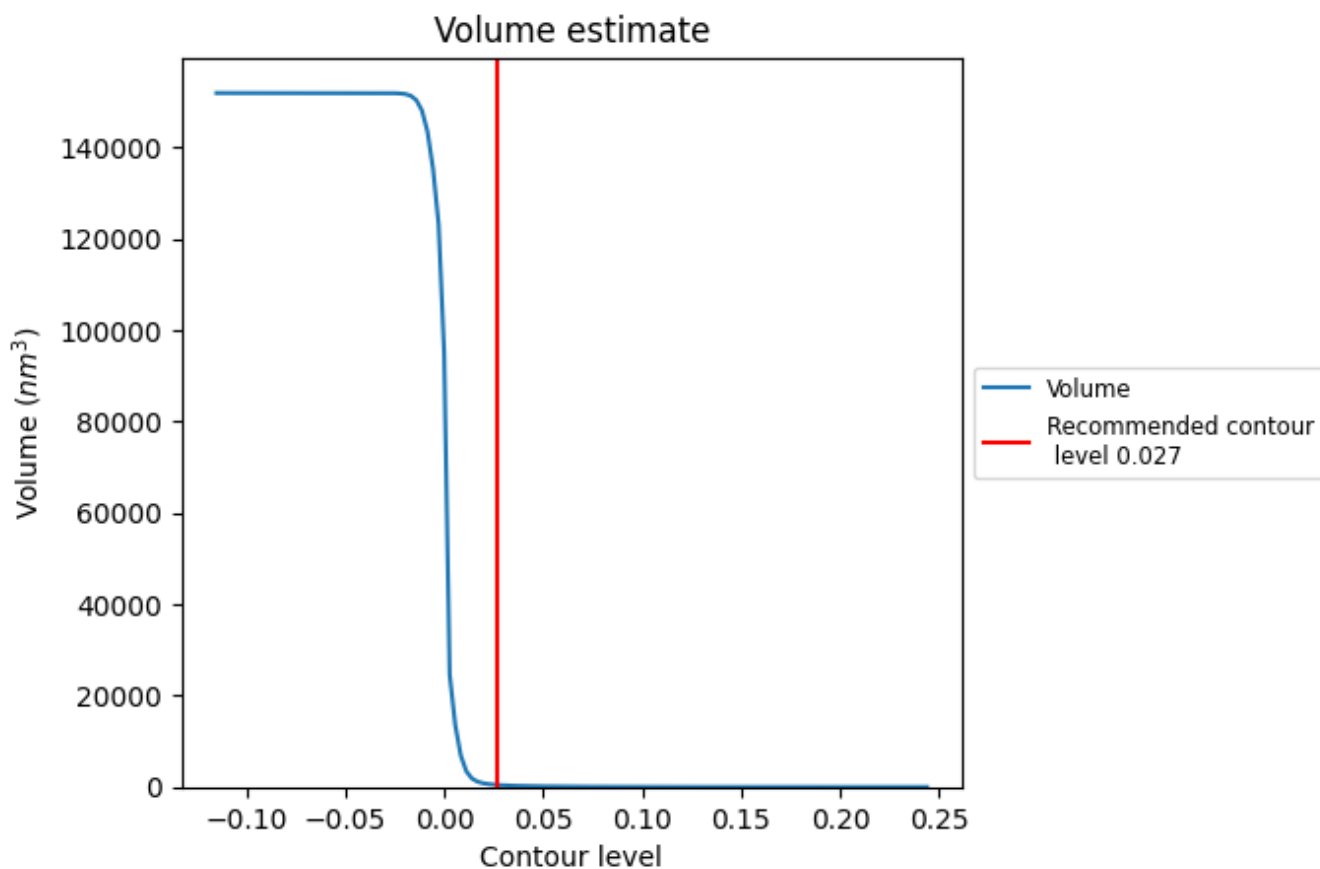
This section contains the results of statistical analysis of the map.

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.

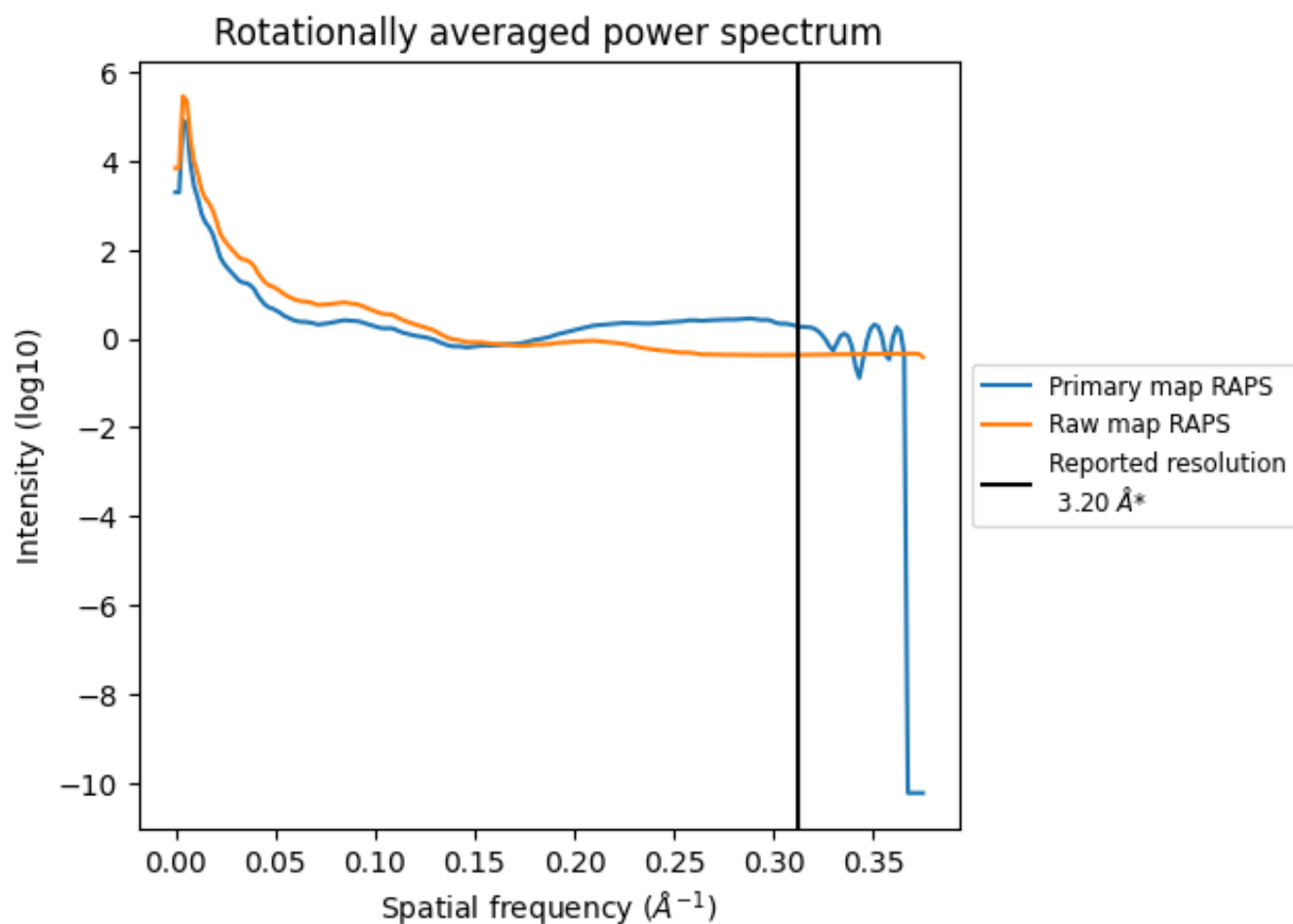
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 435 nm³; this corresponds to an approximate mass of 393 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

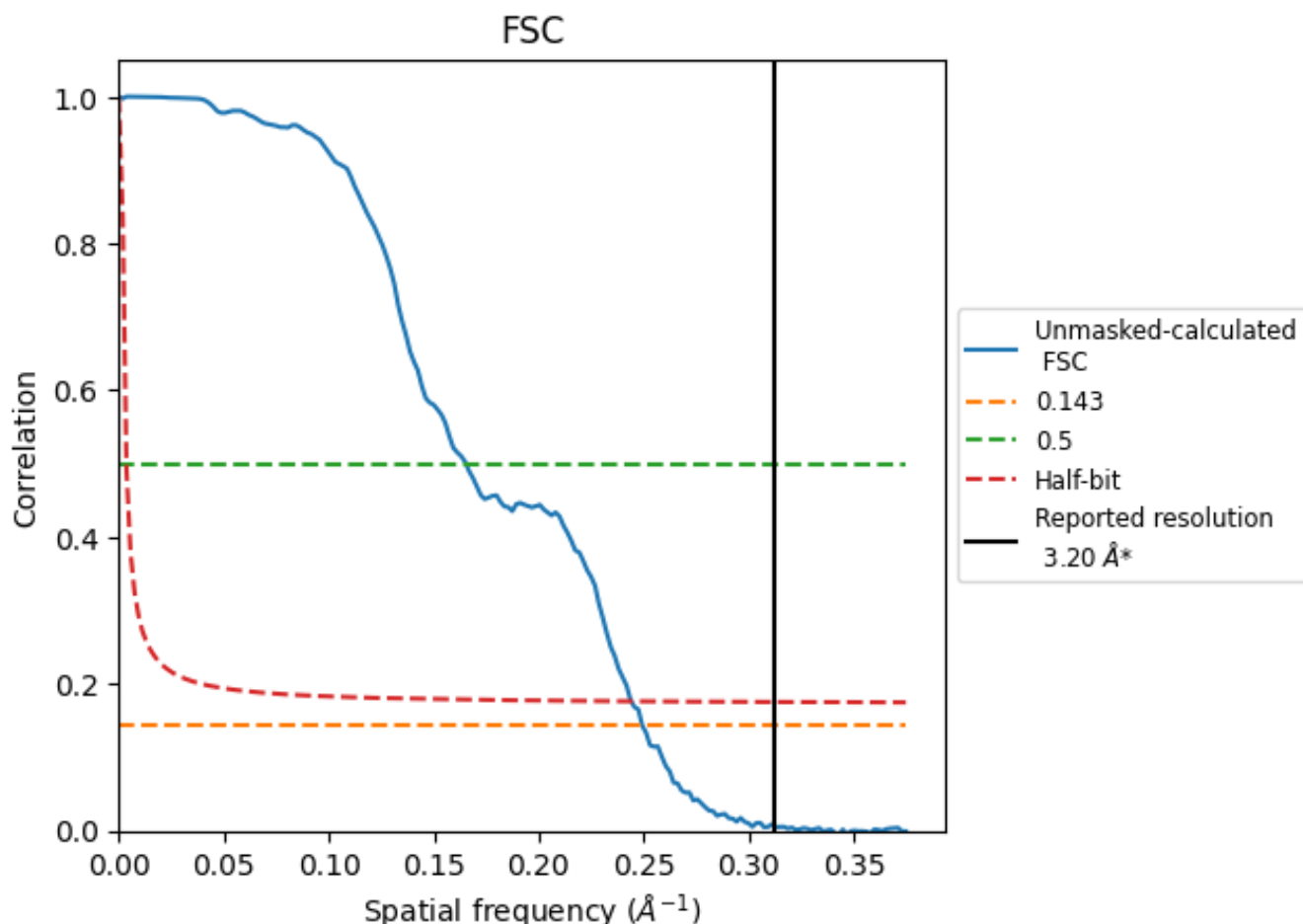


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

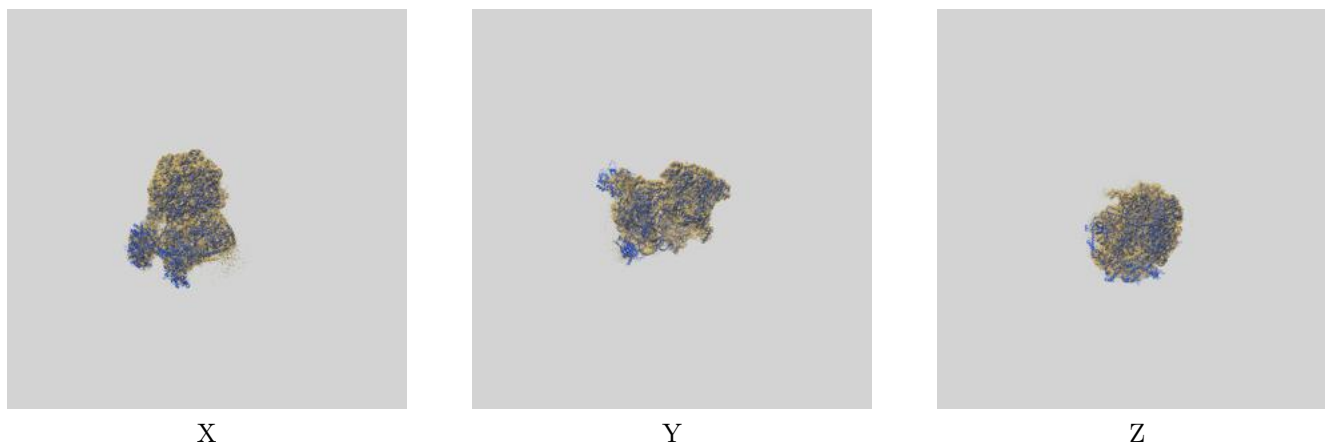
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.01	6.05	4.10

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.01 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

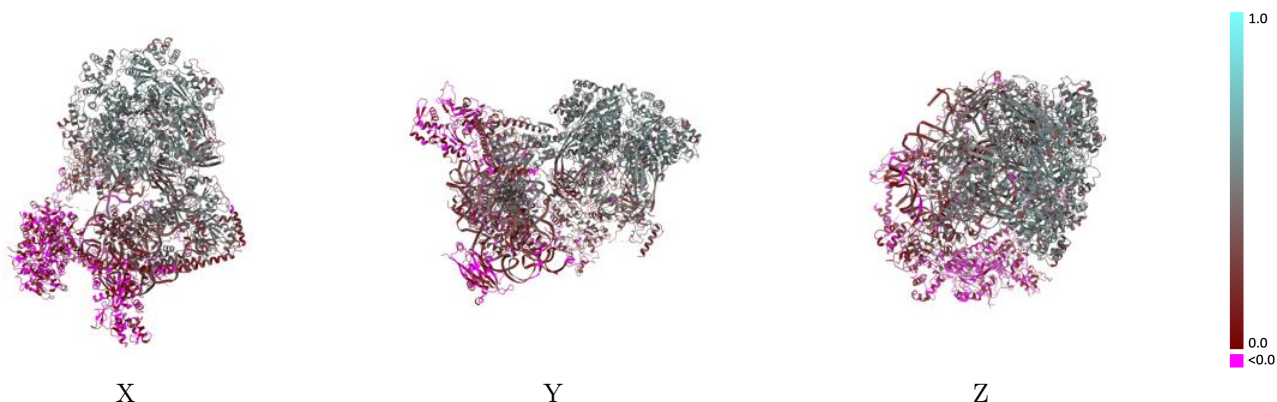
This section contains information regarding the fit between EMDB map EMD-37988 and PDB model 8X19. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



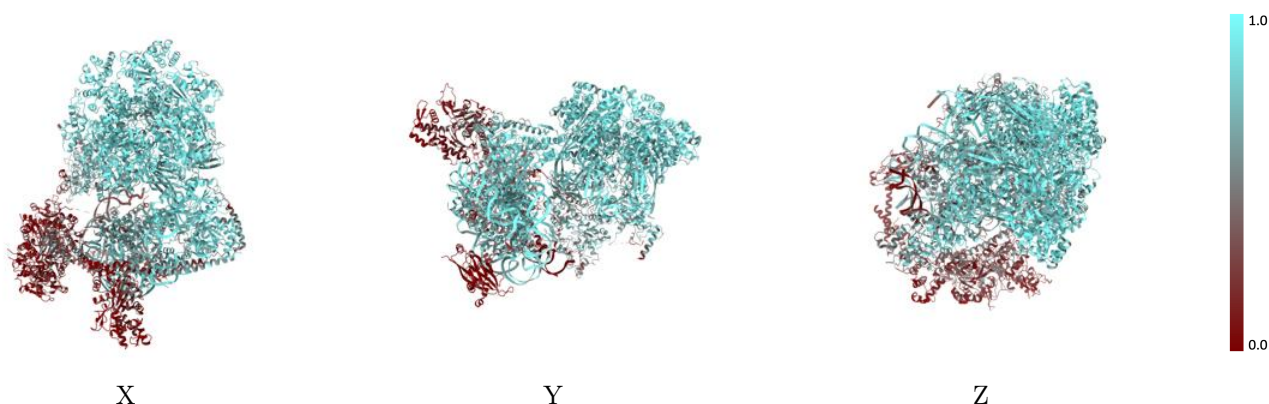
The images above show the 3D surface view of the map at the recommended contour level 0.027 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



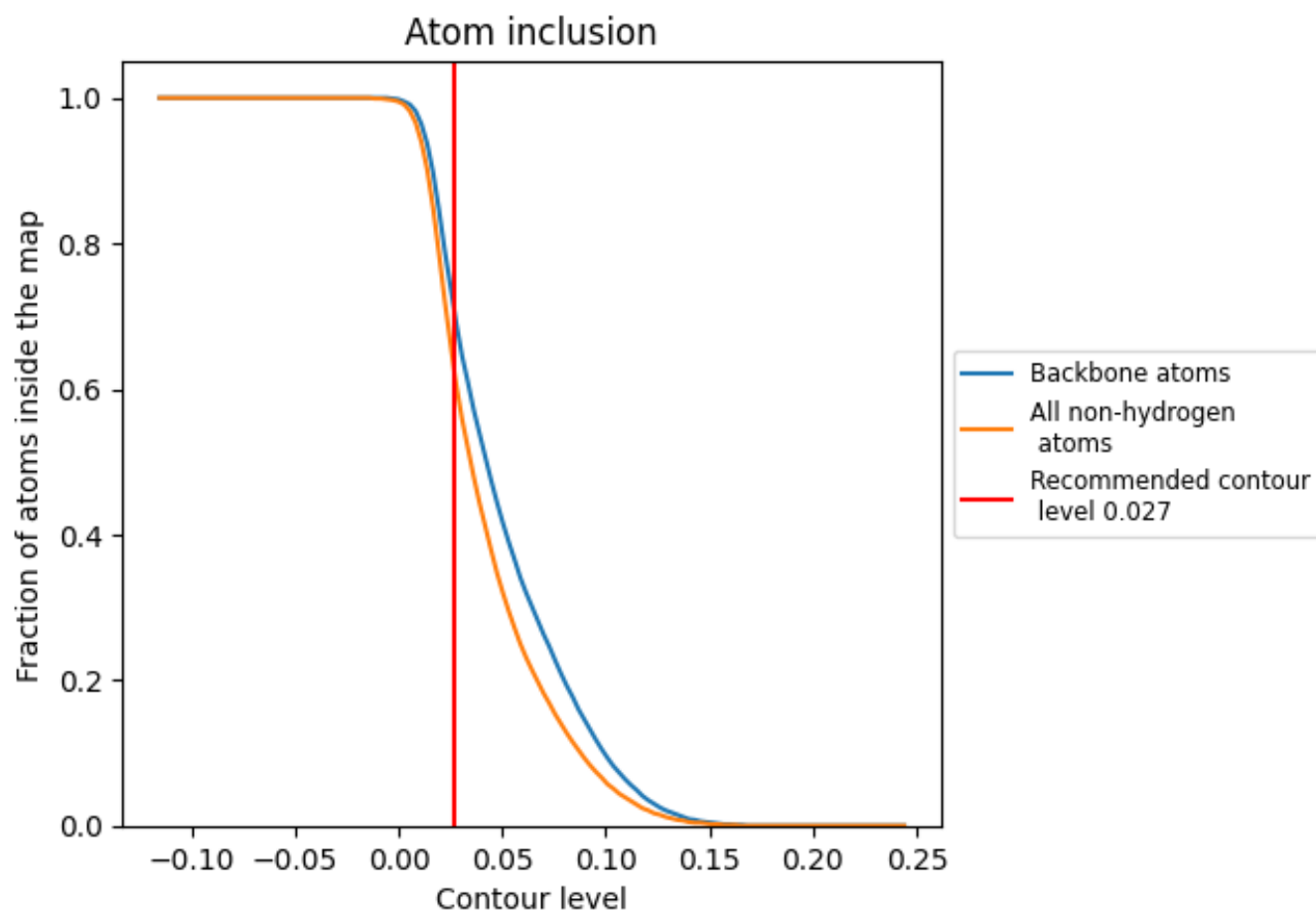
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.027).





















































9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 62% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6220	 0.2920
A	 0.6500	 0.2420
B	 0.6660	 0.2500
C	 0.6640	 0.2180
D	 0.7370	 0.2590
E	 0.7430	 0.3420
F	 0.7460	 0.3170
G	 0.8160	 0.3950
H	 0.8380	 0.4060
I	 0.7210	 0.3600
J	 0.4800	 0.2110
K	 0.6010	 0.2190
L	 0.5320	 0.1960
M	 0.8670	 0.4860
N	 0.8400	 0.4560
O	 0.8280	 0.4490
P	 0.8460	 0.4690
Q	 0.8370	 0.4600
R	 0.8400	 0.4790
S	 0.1210	 0.0340
T	 0.1710	 0.0240
U	 0.1460	 0.0250
V	 0.1000	 0.0420
W	 0.0160	 0.0120
X	 0.7320	 0.2290
Y	 0.7400	 0.2360

