



wwPDB EM Validation Summary Report ⓘ

Jun 25, 2025 – 02:48 pm BST

PDB ID : 8QKU / pdb_00008qku
EMDB ID : EMD-18471
Title : SWR1-nucleosome complex in configuration 1
Authors : Jalal, A.S.B.; Wigley, D.B.
Deposited on : 2023-09-18
Resolution : 3.80 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.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

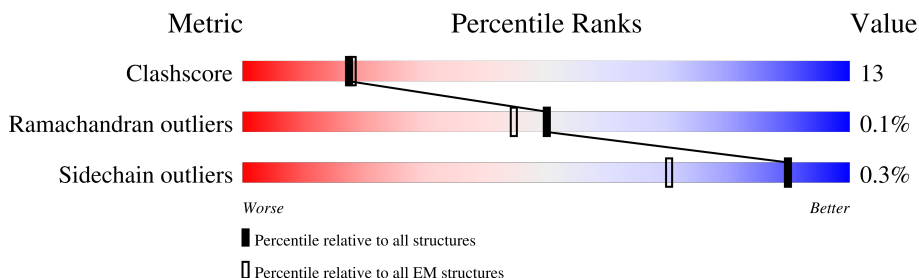
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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.




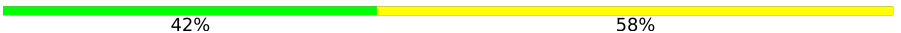










Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	136	<div> <div>46%</div> <div>25%</div> <div>29%</div> </div>
1	B	136	<div> <div>46%</div> <div>26%</div> <div>29%</div> </div>
2	C	103	<div> <div>51%</div> <div>28%</div> <div>20%</div> </div>
2	D	103	<div> <div>44%</div> <div>34%</div> <div>22%</div> </div>
3	E	158	<div> <div>37%</div> <div>28%</div> <div>35%</div> </div>
3	F	158	<div> <div>38%</div> <div>26%</div> <div>36%</div> </div>
4	G	131	<div> <div>34%</div> <div>39%</div> <div>27%</div> </div>
4	H	131	<div> <div>33%</div> <div>37%</div> <div>31%</div> </div>

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Mol	Chain	Length	Quality of chain
5	I	177	 47%53%.
6	J	177	 42%58%.
7	M	1514	 33%12%55%.
8	R	438	 65%29%6%.
9	S	280	 56%18%26%.
10	T	463	 70%25%.
10	V	463	 67%26%6%.
10	X	463	 69%27%5%.
11	U	471	 66%25%9%.
11	W	471	 69%23%8%.
11	Y	471	 74%21%5%.
12	Z	180	 65%33%..

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 45395 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Histone H3.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	97	Total	C	N	O	0	0
			796	506	152	138		
1	B	97	Total	C	N	O	0	0
			796	506	152	138		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	GLU	ASP	conflict	UNP P61830
B	123	GLU	ASP	conflict	UNP P61830

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	82	Total	C	N	O	0	0
			651	410	126	115		
2	D	80	Total	C	N	O	0	0
			638	401	124	113		

- Molecule 3 is a protein called Histone H2A.2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	103	Total	C	N	O	0	0
			795	499	156	140		
3	F	101	Total	C	N	O	0	0
			779	489	153	137		

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	127	GLU	-	expression tag	UNP P04912
E	128	VAL	-	expression tag	UNP P04912
E	129	CYS	-	expression tag	UNP P04912

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Chain	Residue	Modelled	Actual	Comment	Reference
E	130	GLN	-	expression tag	UNP P04912
E	131	ASP	-	expression tag	UNP P04912
E	132	CYS	-	expression tag	UNP P04912
E	133	GLN	-	expression tag	UNP P04912
E	134	SER	-	expression tag	UNP P04912
E	135	PHE	-	expression tag	UNP P04912
E	136	SER	-	expression tag	UNP P04912
E	137	ARG	-	expression tag	UNP P04912
E	138	THR	-	expression tag	UNP P04912
E	139	VAL	-	expression tag	UNP P04912
E	140	ARG	-	expression tag	UNP P04912
E	141	THR	-	expression tag	UNP P04912
E	142	GLU	-	expression tag	UNP P04912
E	143	LEU	-	expression tag	UNP P04912
E	144	LYS	-	expression tag	UNP P04912
E	145	ARG	-	expression tag	UNP P04912
E	146	ASN	-	expression tag	UNP P04912
E	147	LYS	-	expression tag	UNP P04912
E	148	ALA	-	expression tag	UNP P04912
E	149	ASN	-	expression tag	UNP P04912
E	150	GLN	-	expression tag	UNP P04912
E	151	THR	-	expression tag	UNP P04912
E	152	PHE	-	expression tag	UNP P04912
E	153	LEU	-	expression tag	UNP P04912
E	154	SER	-	expression tag	UNP P04912
E	155	PHE	-	expression tag	UNP P04912
E	156	GLY	-	expression tag	UNP P04912
E	157	VAL	-	expression tag	UNP P04912
F	127	GLU	-	expression tag	UNP P04912
F	128	VAL	-	expression tag	UNP P04912
F	129	CYS	-	expression tag	UNP P04912
F	130	GLN	-	expression tag	UNP P04912
F	131	ASP	-	expression tag	UNP P04912
F	132	CYS	-	expression tag	UNP P04912
F	133	GLN	-	expression tag	UNP P04912
F	134	SER	-	expression tag	UNP P04912
F	135	PHE	-	expression tag	UNP P04912
F	136	SER	-	expression tag	UNP P04912
F	137	ARG	-	expression tag	UNP P04912
F	138	THR	-	expression tag	UNP P04912
F	139	VAL	-	expression tag	UNP P04912
F	140	ARG	-	expression tag	UNP P04912

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Chain	Residue	Modelled	Actual	Comment	Reference
F	141	THR	-	expression tag	UNP P04912
F	142	GLU	-	expression tag	UNP P04912
F	143	LEU	-	expression tag	UNP P04912
F	144	LYS	-	expression tag	UNP P04912
F	145	ARG	-	expression tag	UNP P04912
F	146	ASN	-	expression tag	UNP P04912
F	147	LYS	-	expression tag	UNP P04912
F	148	ALA	-	expression tag	UNP P04912
F	149	ASN	-	expression tag	UNP P04912
F	150	GLN	-	expression tag	UNP P04912
F	151	THR	-	expression tag	UNP P04912
F	152	PHE	-	expression tag	UNP P04912
F	153	LEU	-	expression tag	UNP P04912
F	154	SER	-	expression tag	UNP P04912
F	155	PHE	-	expression tag	UNP P04912
F	156	GLY	-	expression tag	UNP P04912
F	157	VAL	-	expression tag	UNP P04912

- Molecule 4 is a protein called Histone H2B.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	96	Total	C	N	O	S	0	0
			741	465	129	146	1		
4	H	91	Total	C	N	O	S	0	0
			712	449	125	137	1		

- Molecule 5 is a DNA chain called DNA (177-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	177	Total	C	N	O	P	0	0
			3608	1713	654	1064	177		

- Molecule 6 is a DNA chain called DNA (177-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	177	Total	C	N	O	P	0	0
			3649	1726	686	1060	177		

- Molecule 7 is a protein called Helicase SWR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	688	Total	C	N	O	S	0	0
			5398	3438	960	974	26		

- Molecule 8 is a protein called Actin-like protein ARP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	411	Total	C	N	O	S	0	0
			3335	2156	544	619	16		

- Molecule 9 is a protein called Vacuolar protein sorting-associated protein 71.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	208	Total	C	N	O	S	0	0
			1695	1071	302	312	10		

- Molecule 10 is a protein called RuvB-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	T	443	Total	C	N	O	S	0	0
			3391	2140	584	657	10		
10	V	434	Total	C	N	O	S	0	0
			3336	2107	574	645	10		
10	X	442	Total	C	N	O	S	0	0
			3397	2144	584	659	10		

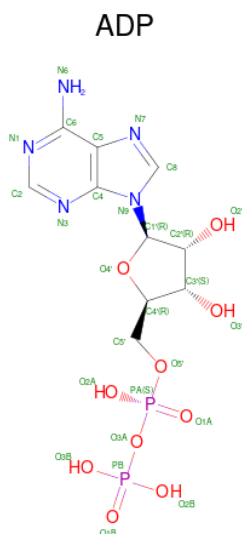
- Molecule 11 is a protein called RuvB-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	U	430	Total	C	N	O	S	0	0
			3299	2063	570	655	11		
11	W	433	Total	C	N	O	S	0	0
			3325	2085	572	657	11		
11	Y	447	Total	C	N	O	S	0	0
			3410	2133	590	675	12		

- Molecule 12 is a protein called Vacuolar protein sorting-associated protein 72.

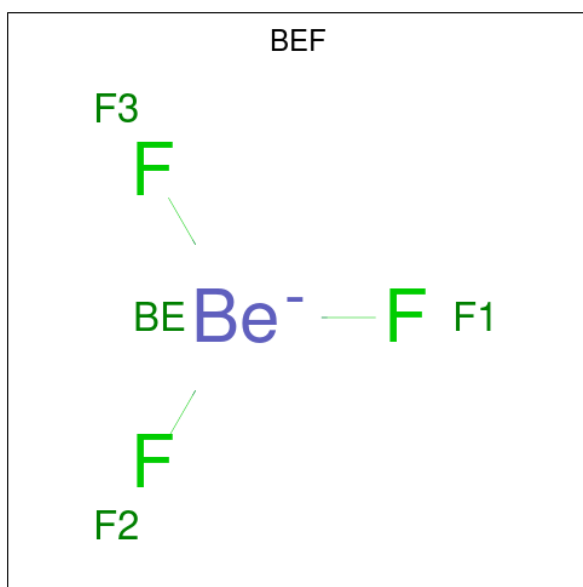
Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	180	Total	C	N	O	S	0	0
			1410	885	255	266	4		

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
13	M	1	Total 27	C 10	N 5	O 10	P 2	0
13	R	1	Total 27	C 10	N 5	O 10	P 2	0
13	T	1	Total 27	C 10	N 5	O 10	P 2	0
13	U	1	Total 27	C 10	N 5	O 10	P 2	0
13	V	1	Total 27	C 10	N 5	O 10	P 2	0
13	W	1	Total 27	C 10	N 5	O 10	P 2	0
13	X	1	Total 27	C 10	N 5	O 10	P 2	0
13	Y	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 14 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
14	M	1	Total	Be	F	0
			4	1	3	
14	R	1	Total	Be	F	0
			4	1	3	

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
15	M	1	Total	Mg	0
			1	1	
15	R	1	Total	Mg	0
			1	1	
15	U	2	Total	Mg	0
			2	2	
15	V	1	Total	Mg	0
			1	1	
15	W	1	Total	Mg	0
			1	1	
15	X	1	Total	Mg	0
			1	1	
15	Y	1	Total	Mg	0
			1	1	

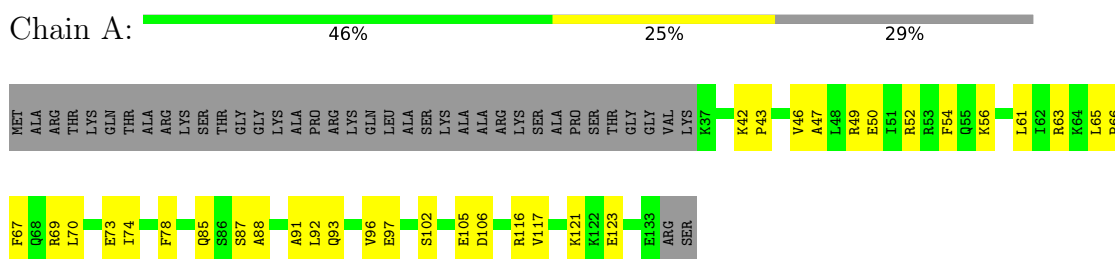
- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
16	S	2	Total	Zn	0
			2	2	

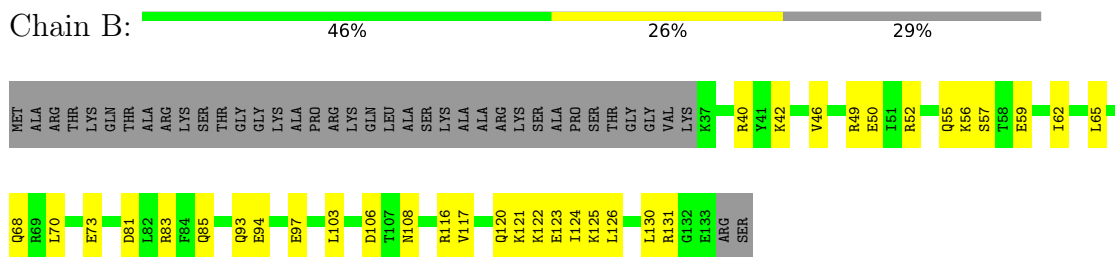
3 Residue-property plots

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

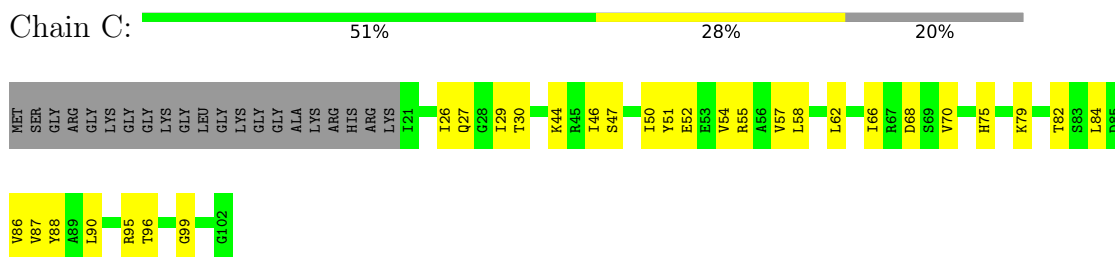
• Molecule 1: Histone H3



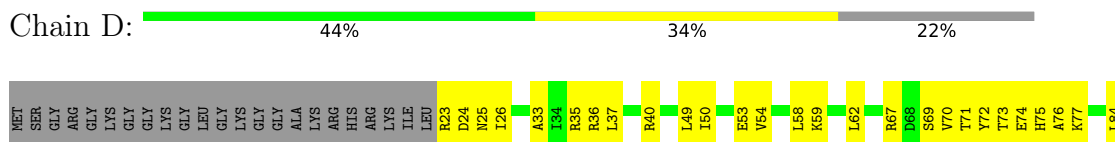
• Molecule 1: Histone H3



• Molecule 2: Histone H4



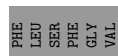
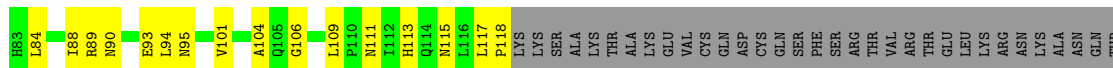
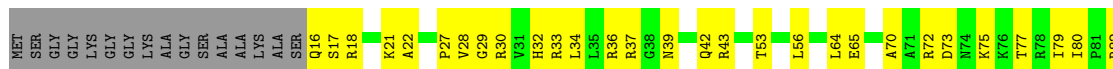
• Molecule 2: Histone H4





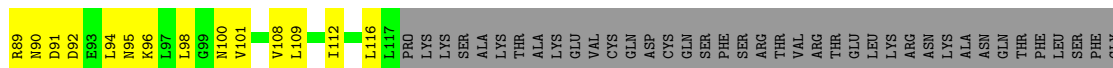
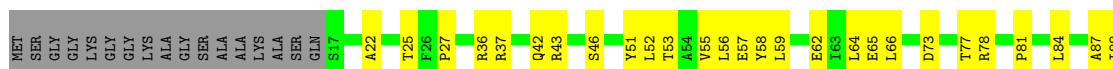
- Molecule 3: Histone H2A.2

Chain E: 37% 28% 35%



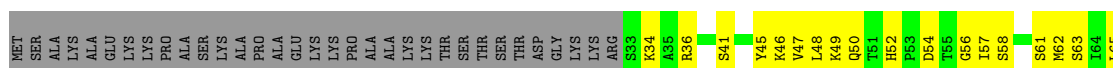
- Molecule 3: Histone H2A.2

Chain F: 38% 26% 36%



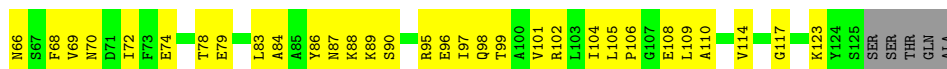
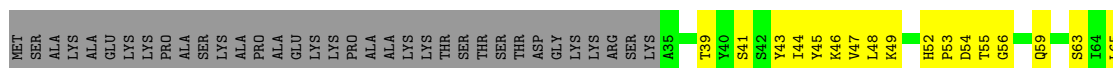
- Molecule 4: Histone H2B.1

Chain G: 34% 39% 27%



- Molecule 4: Histone H2B.1

Chain H: 33% 37% 31%



- Molecule 5: DNA (177-MER)



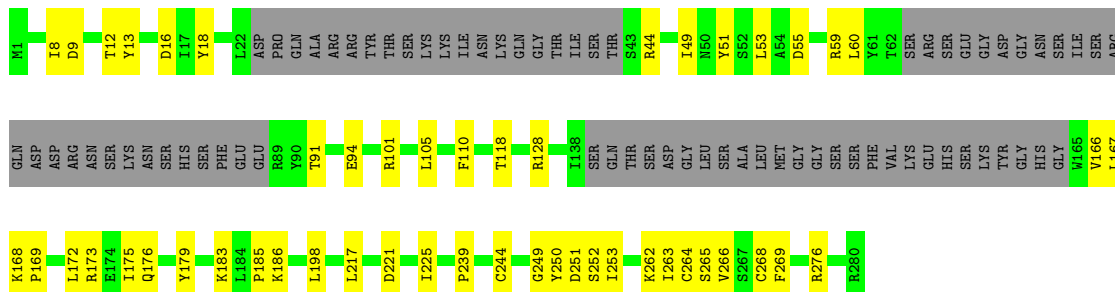


- Molecule 8: Actin-like protein ARP6



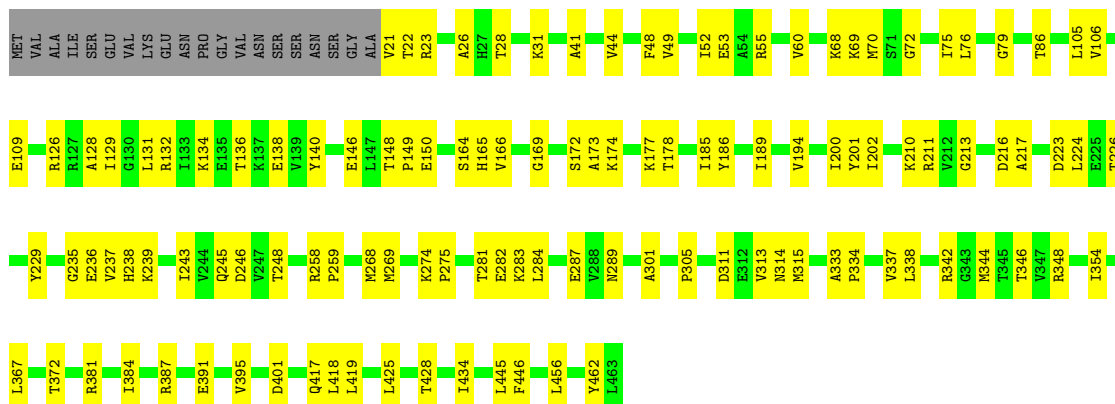
• Molecule 9: Vacuolar protein sorting-associated protein 71

Chain S: 56% 18% 26%



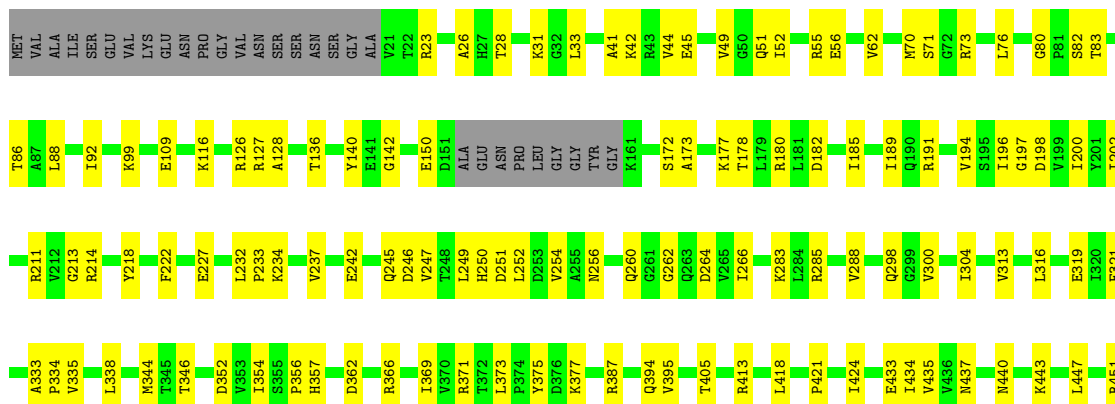
• Molecule 10: RuvB-like protein 1

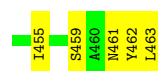
Chain T: 70% 25% .



• Molecule 10: RuvB-like protein 1

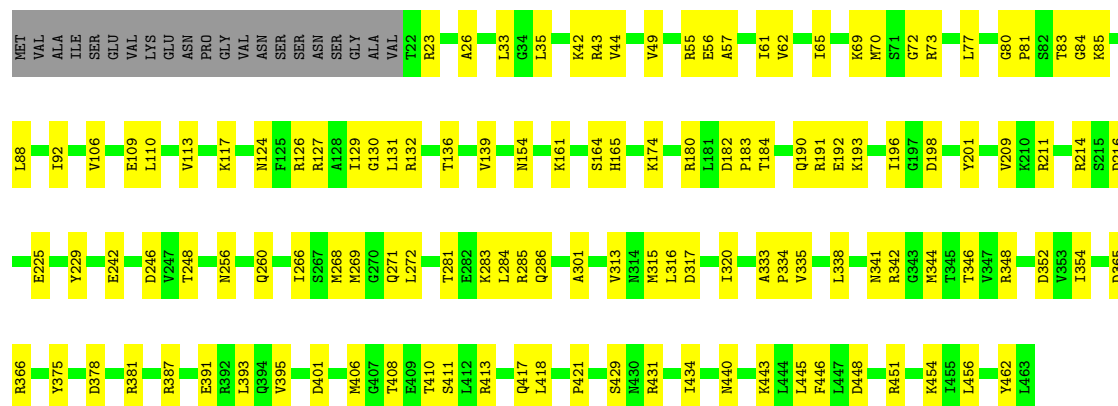
Chain V: 67% 26% 6%





• Molecule 10: RuvB-like protein 1

Chain X: 69% 27% 5%



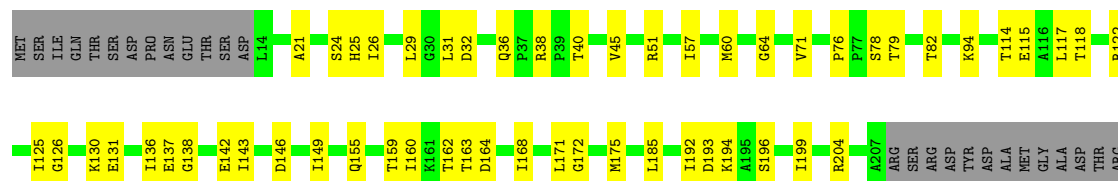
• Molecule 11: RuvB-like protein 2

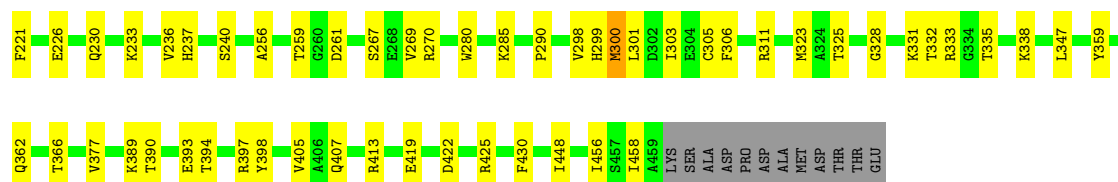
Chain U: 66% 25% 9%



• Molecule 11: RuvB-like protein 2

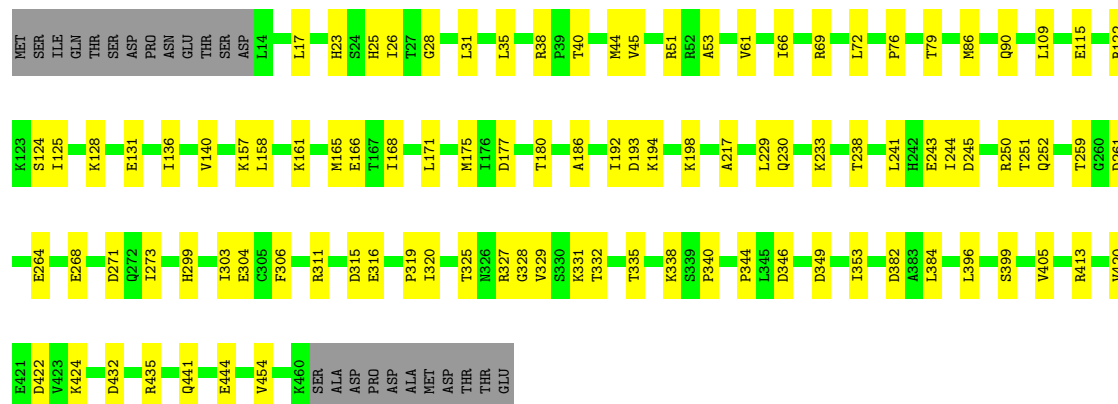
Chain W: 69% 23% 8%





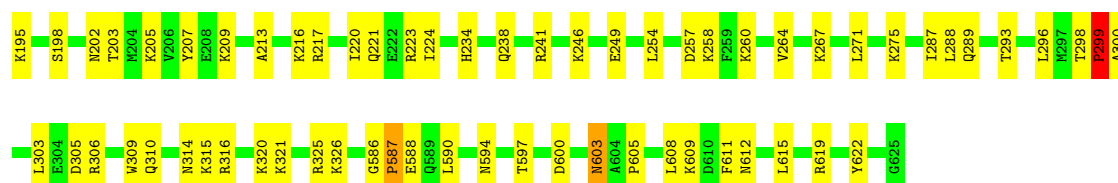
• Molecule 11: RuvB-like protein 2

Chain Y: 74% 21% 5%



• Molecule 12: Vacuolar protein sorting-associated protein 72

Chain Z: 65% 33% ::



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123591	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00197	Depositor
Map size (\AA)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	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, ADP, ZN, 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	0.16	0/807	0.44	0/1081
1	B	0.17	0/807	0.52	0/1081
2	C	0.14	0/658	0.43	0/880
2	D	0.16	0/645	0.44	0/862
3	E	0.13	0/806	0.33	0/1091
3	F	0.11	0/789	0.33	0/1067
4	G	0.18	0/750	0.51	0/1009
4	H	0.18	0/722	0.51	0/972
5	I	0.16	0/4042	0.39	2/6231 (0.0%)
6	J	0.17	0/4098	0.37	2/6328 (0.0%)
7	M	0.11	0/5495	0.30	0/7442
8	R	0.09	0/3429	0.23	0/4650
9	S	0.10	0/1722	0.28	0/2320
10	T	0.11	0/3433	0.26	0/4646
10	V	0.10	0/3375	0.25	0/4565
10	X	0.11	0/3439	0.28	0/4652
11	U	0.10	0/3333	0.26	0/4492
11	W	0.10	0/3361	0.24	0/4530
11	Y	0.10	0/3447	0.25	0/4649
12	Z	0.15	0/1431	0.52	4/1923 (0.2%)
All	All	0.12	0/46589	0.33	8/64471 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	-77	DC	OP1-P-O3'	-8.90	81.31	108.00
6	J	-77	DA	OP2-P-O3'	-8.39	82.84	108.00
6	J	-77	DA	OP1-P-O3'	-8.21	83.36	108.00
5	I	-77	DC	OP2-P-O3'	-7.75	84.75	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Z	587	PRO	CA-C-N	6.86	134.05	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	796	0	841	35	0
1	B	796	0	841	33	0
2	C	651	0	690	25	0
2	D	638	0	677	37	0
3	E	795	0	834	44	0
3	F	779	0	819	37	0
4	G	741	0	766	52	0
4	H	712	0	736	42	0
5	I	3608	0	1987	82	0
6	J	3649	0	1985	97	0
7	M	5398	0	5351	146	0
8	R	3335	0	3256	97	0
9	S	1695	0	1745	56	0
10	T	3391	0	3513	86	0
10	V	3336	0	3474	92	0
10	X	3397	0	3532	100	0
11	U	3299	0	3387	95	0
11	W	3325	0	3412	81	0
11	Y	3410	0	3465	67	0
12	Z	1410	0	1362	59	0
13	M	27	0	12	6	0
13	R	27	0	12	0	0
13	T	27	0	12	1	0
13	U	27	0	12	3	0
13	V	27	0	12	5	0
13	W	27	0	12	4	0
13	X	27	0	12	3	0
13	Y	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	M	4	0	0	1	0
14	R	4	0	0	0	0
15	M	1	0	0	0	0
15	R	1	0	0	0	0
15	U	2	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	X	1	0	0	0	0
15	Y	1	0	0	0	0
16	S	2	0	0	0	0
All	All	45395	0	42769	1165	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 13.

The worst 5 of 1165 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)
1:A:74:ILE:O	1:A:78:PHE:HB2	1.62	0.98
11:Y:171:LEU:HD12	11:Y:175:MET:HG2	1.54	0.89
6:J:65:DA:H4'	12:Z:223:ARG:HH22	1.43	0.82
5:I:48:DG:N2	6:J:-48:DC:O2	2.12	0.82
5:I:48:DG:N1	6:J:-48:DC:N3	2.26	0.82

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	95/136 (70%)	89 (94%)	6 (6%)	0	100	100
1	B	95/136 (70%)	92 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	80/103 (78%)	79 (99%)	1 (1%)	0	100	100
2	D	78/103 (76%)	73 (94%)	5 (6%)	0	100	100
3	E	101/158 (64%)	101 (100%)	0	0	100	100
3	F	99/158 (63%)	99 (100%)	0	0	100	100
4	G	94/131 (72%)	89 (95%)	5 (5%)	0	100	100
4	H	89/131 (68%)	86 (97%)	3 (3%)	0	100	100
7	M	684/1514 (45%)	628 (92%)	56 (8%)	0	100	100
8	R	407/438 (93%)	398 (98%)	9 (2%)	0	100	100
9	S	200/280 (71%)	196 (98%)	4 (2%)	0	100	100
10	T	441/463 (95%)	424 (96%)	17 (4%)	0	100	100
10	V	430/463 (93%)	418 (97%)	12 (3%)	0	100	100
10	X	440/463 (95%)	425 (97%)	15 (3%)	0	100	100
11	U	426/471 (90%)	408 (96%)	18 (4%)	0	100	100
11	W	429/471 (91%)	420 (98%)	9 (2%)	0	100	100
11	Y	445/471 (94%)	430 (97%)	15 (3%)	0	100	100
12	Z	176/180 (98%)	153 (87%)	20 (11%)	3 (2%)	7	34
All	All	4809/6270 (77%)	4608 (96%)	198 (4%)	3 (0%)	50	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	Z	325	ARG
12	Z	299	PRO
12	Z	326	LYS

5.3.2 Protein sidechains ⓘ

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	84/113 (74%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	84/113 (74%)	83 (99%)	1 (1%)	67	77
2	C	68/81 (84%)	67 (98%)	1 (2%)	60	74
2	D	67/81 (83%)	67 (100%)	0	100	100
3	E	82/124 (66%)	81 (99%)	1 (1%)	67	77
3	F	80/124 (64%)	80 (100%)	0	100	100
4	G	82/109 (75%)	81 (99%)	1 (1%)	67	77
4	H	78/109 (72%)	77 (99%)	1 (1%)	65	76
7	M	574/1376 (42%)	573 (100%)	1 (0%)	92	94
8	R	372/396 (94%)	371 (100%)	1 (0%)	91	92
9	S	199/261 (76%)	198 (100%)	1 (0%)	86	90
10	T	371/391 (95%)	370 (100%)	1 (0%)	91	92
10	V	368/391 (94%)	367 (100%)	1 (0%)	91	92
10	X	374/391 (96%)	374 (100%)	0	100	100
11	U	367/403 (91%)	366 (100%)	1 (0%)	91	92
11	W	369/403 (92%)	368 (100%)	1 (0%)	91	92
11	Y	372/403 (92%)	372 (100%)	0	100	100
12	Z	143/171 (84%)	142 (99%)	1 (1%)	81	86
All	All	4134/5440 (76%)	4121 (100%)	13 (0%)	90	92

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	S	13	TYR
10	T	462	TYR
12	Z	603	ASN
10	V	304	ILE
11	W	300	MET

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

Mol	Chain	Res	Type
10	V	51	GLN
11	W	453	ASN
10	V	205	ASN
11	W	173	ASN

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Mol	Chain	Res	Type
10	X	440	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 10 are 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$
13	ADP	X	501	15	24,29,29	0.96	1 (4%)	29,45,45	1.51	4 (13%)
13	ADP	T	501	15	24,29,29	0.94	1 (4%)	29,45,45	1.51	4 (13%)
13	ADP	M	1601	15	24,29,29	0.97	1 (4%)	29,45,45	1.44	4 (13%)
13	ADP	R	501	14,15	24,29,29	0.94	1 (4%)	29,45,45	1.48	4 (13%)
14	BEF	R	502	13	0,3,3	-	-	-	-	-
14	BEF	M	1602	-	0,3,3	-	-	-	-	-
13	ADP	U	502	15	24,29,29	0.95	1 (4%)	29,45,45	1.51	4 (13%)
13	ADP	W	501	15	24,29,29	0.96	1 (4%)	29,45,45	1.40	4 (13%)
13	ADP	Y	501	15	24,29,29	0.96	1 (4%)	29,45,45	1.51	4 (13%)
13	ADP	V	501	15	24,29,29	0.96	1 (4%)	29,45,45	1.41	4 (13%)

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
13	ADP	X	501	15	-	3/12/32/32	0/3/3/3
13	ADP	T	501	15	-	5/12/32/32	0/3/3/3
13	ADP	M	1601	15	-	5/12/32/32	0/3/3/3
13	ADP	R	501	14,15	-	4/12/32/32	0/3/3/3
13	ADP	U	502	15	-	2/12/32/32	0/3/3/3
13	ADP	W	501	15	-	4/12/32/32	0/3/3/3
13	ADP	Y	501	15	-	2/12/32/32	0/3/3/3
13	ADP	V	501	15	-	5/12/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	1601	ADP	C5-C4	2.49	1.47	1.40
13	W	501	ADP	C5-C4	2.48	1.47	1.40
13	Y	501	ADP	C5-C4	2.48	1.47	1.40
13	X	501	ADP	C5-C4	2.47	1.47	1.40
13	V	501	ADP	C5-C4	2.46	1.47	1.40

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	501	ADP	PA-O3A-PB	-4.14	118.62	132.83
13	Y	501	ADP	PA-O3A-PB	-3.97	119.22	132.83
13	R	501	ADP	PA-O3A-PB	-3.84	119.65	132.83
13	X	501	ADP	PA-O3A-PB	-3.80	119.77	132.83
13	U	502	ADP	PA-O3A-PB	-3.65	120.29	132.83

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

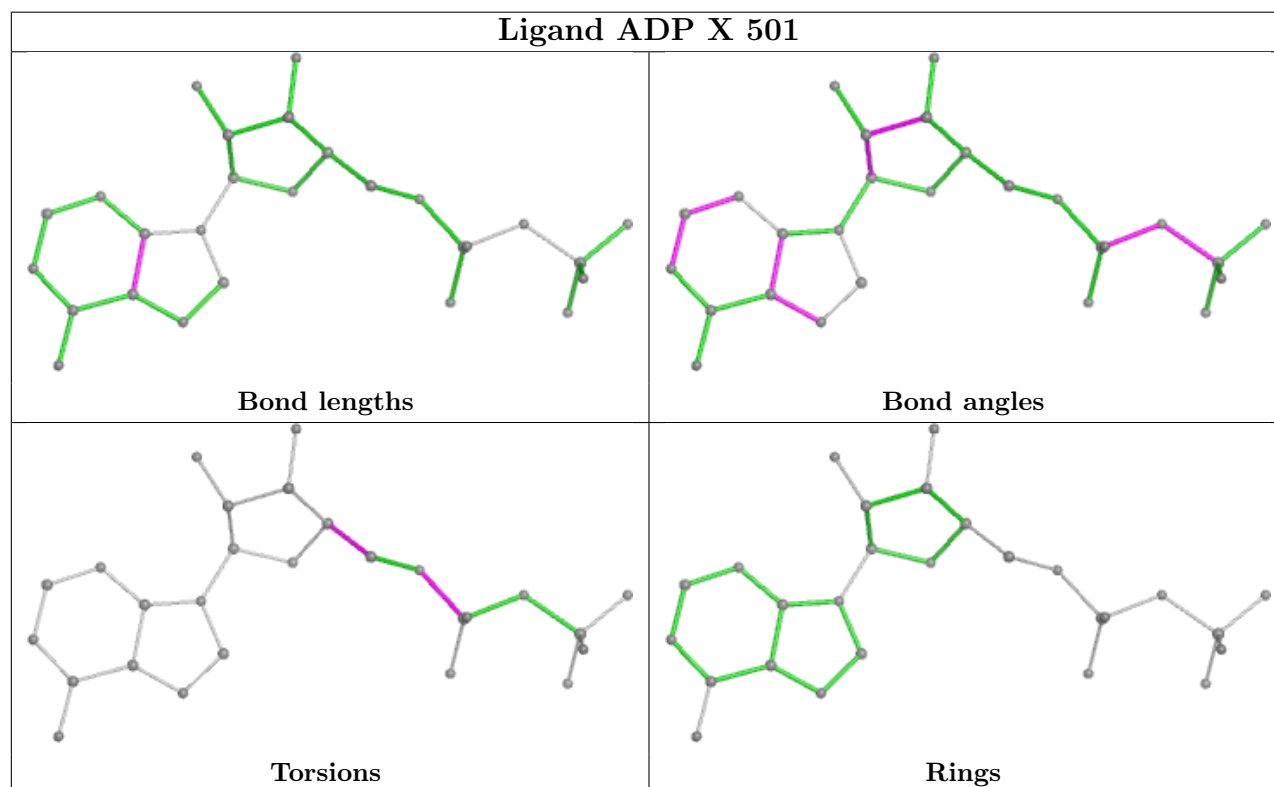
Mol	Chain	Res	Type	Atoms
13	M	1601	ADP	PB-O3A-PA-O5'
13	M	1601	ADP	C5'-O5'-PA-O2A
13	R	501	ADP	C5'-O5'-PA-O3A
13	R	501	ADP	C3'-C4'-C5'-O5'
13	T	501	ADP	C5'-O5'-PA-O2A

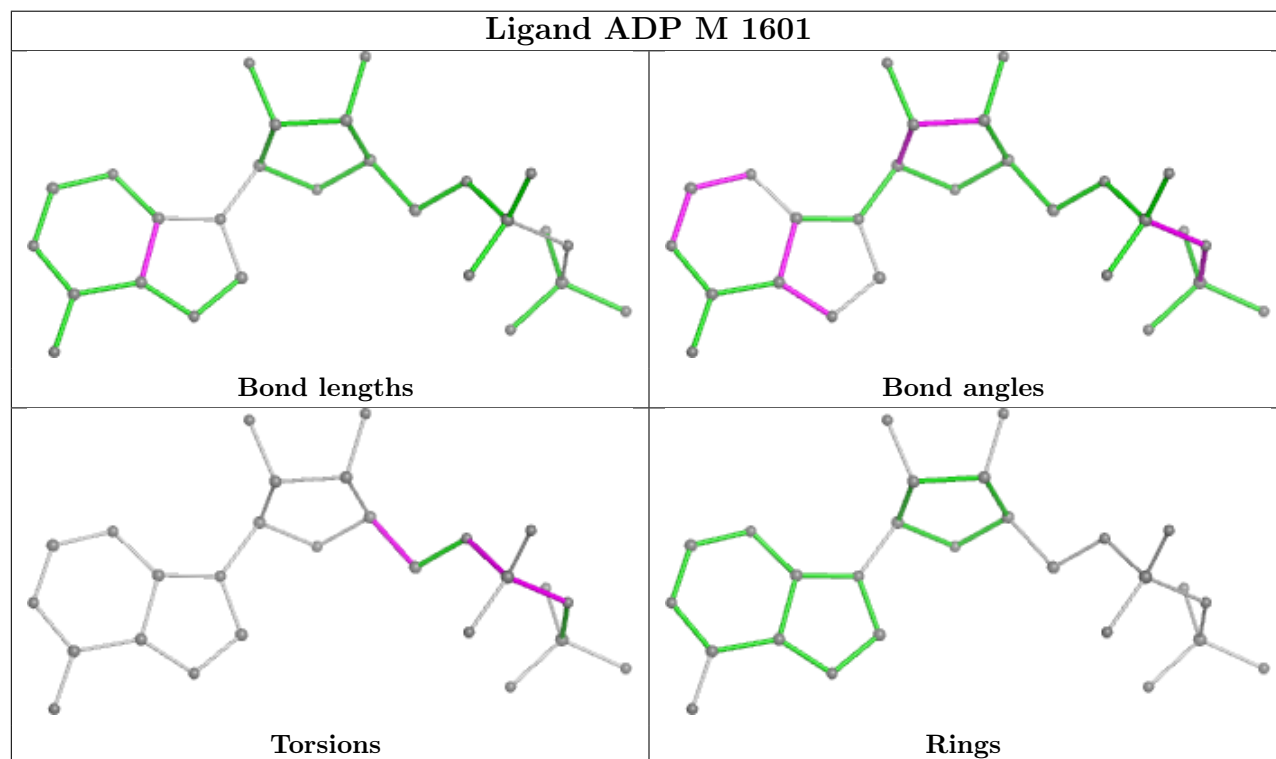
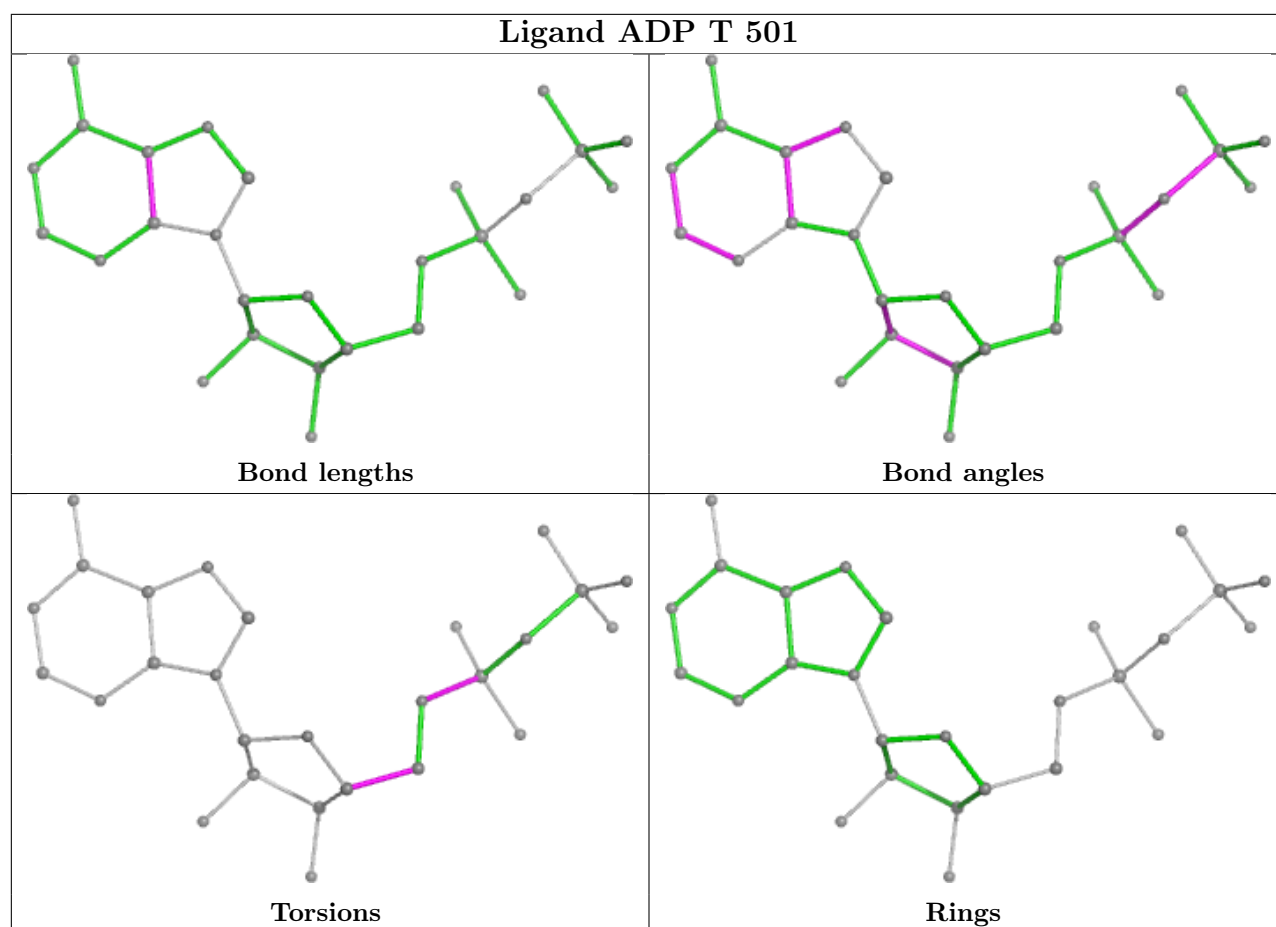
There are no ring outliers.

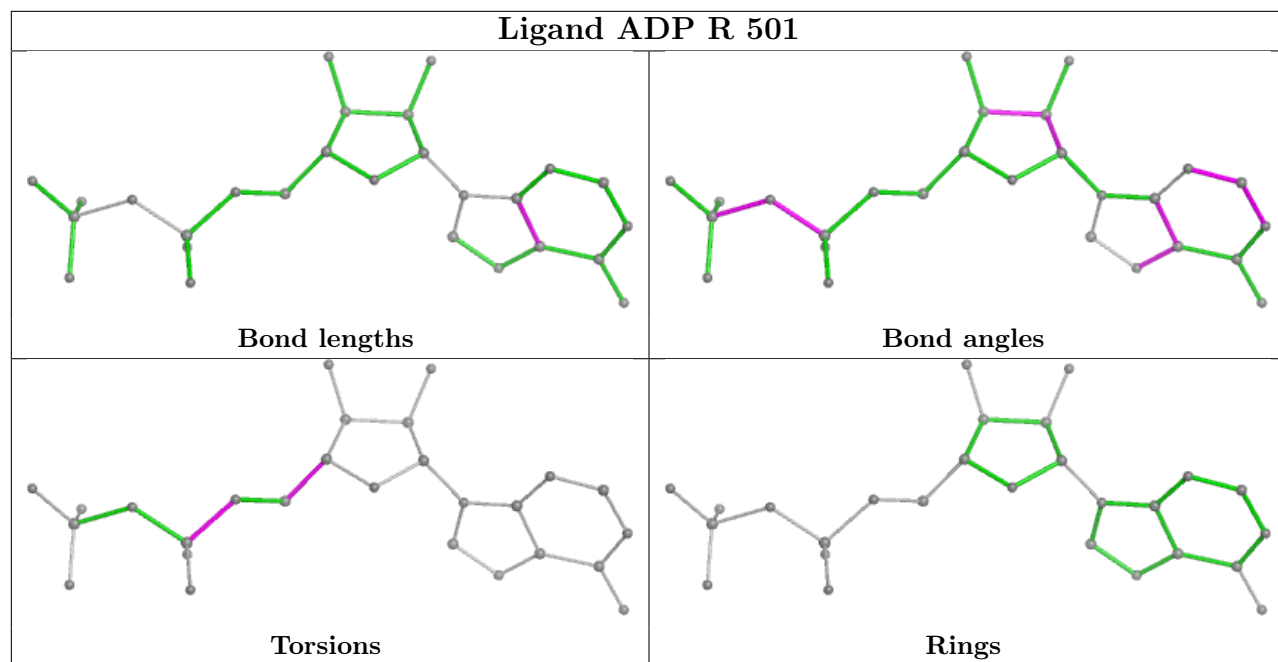
8 monomers are involved in 23 short contacts:

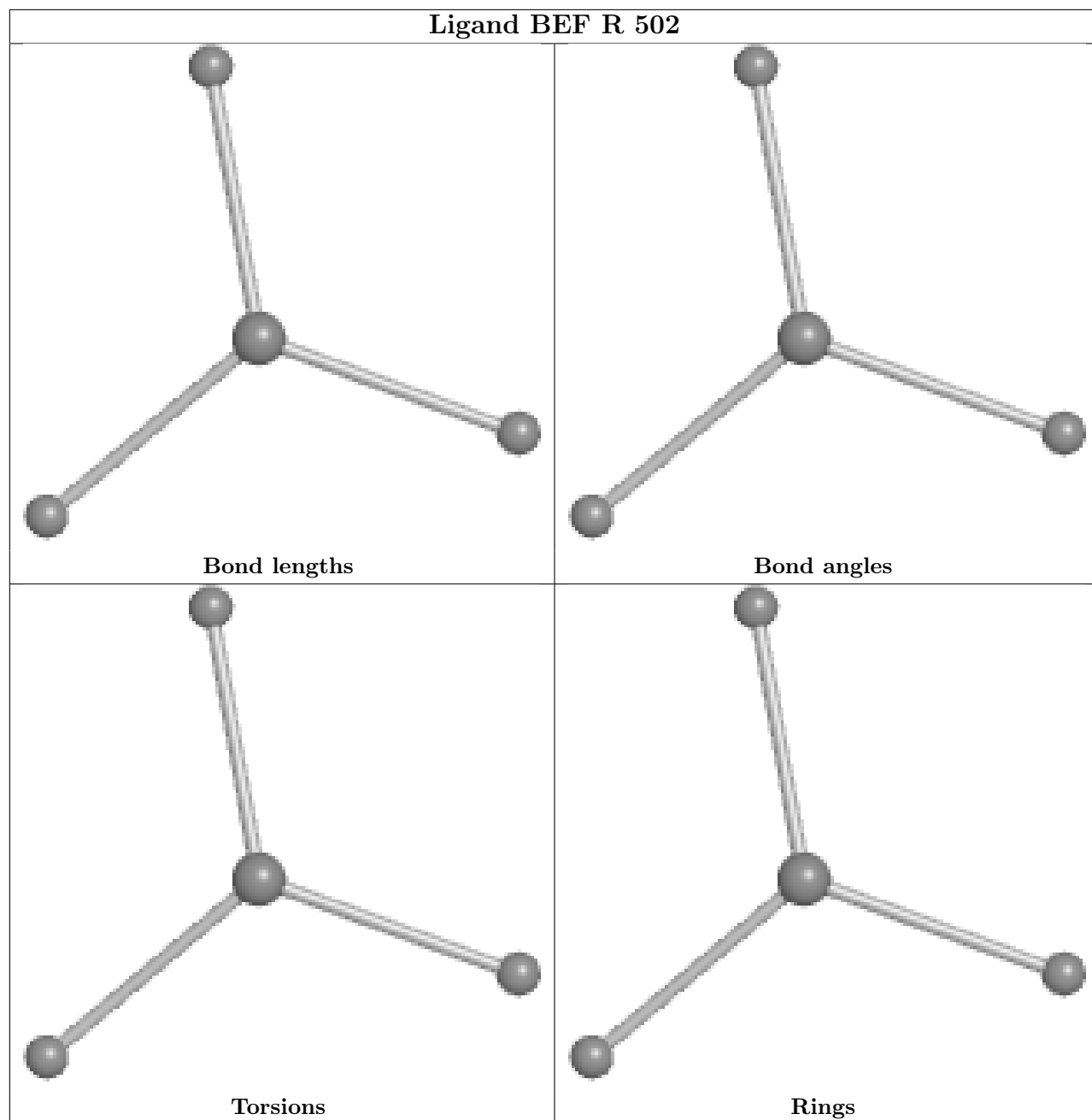
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	X	501	ADP	3	0
13	T	501	ADP	1	0
13	M	1601	ADP	6	0
14	M	1602	BEF	1	0
13	U	502	ADP	3	0
13	W	501	ADP	4	0
13	Y	501	ADP	1	0
13	V	501	ADP	5	0

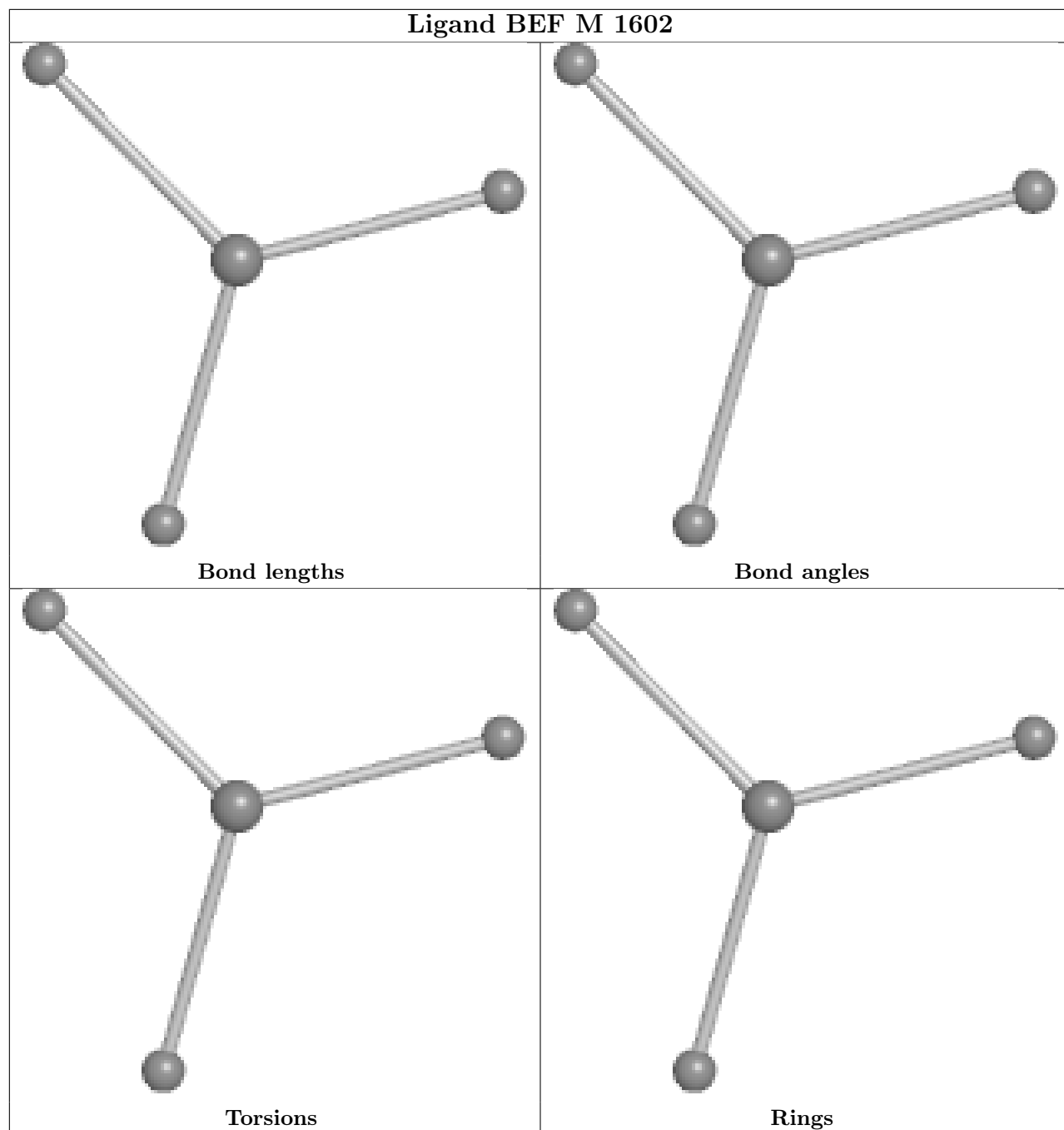
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

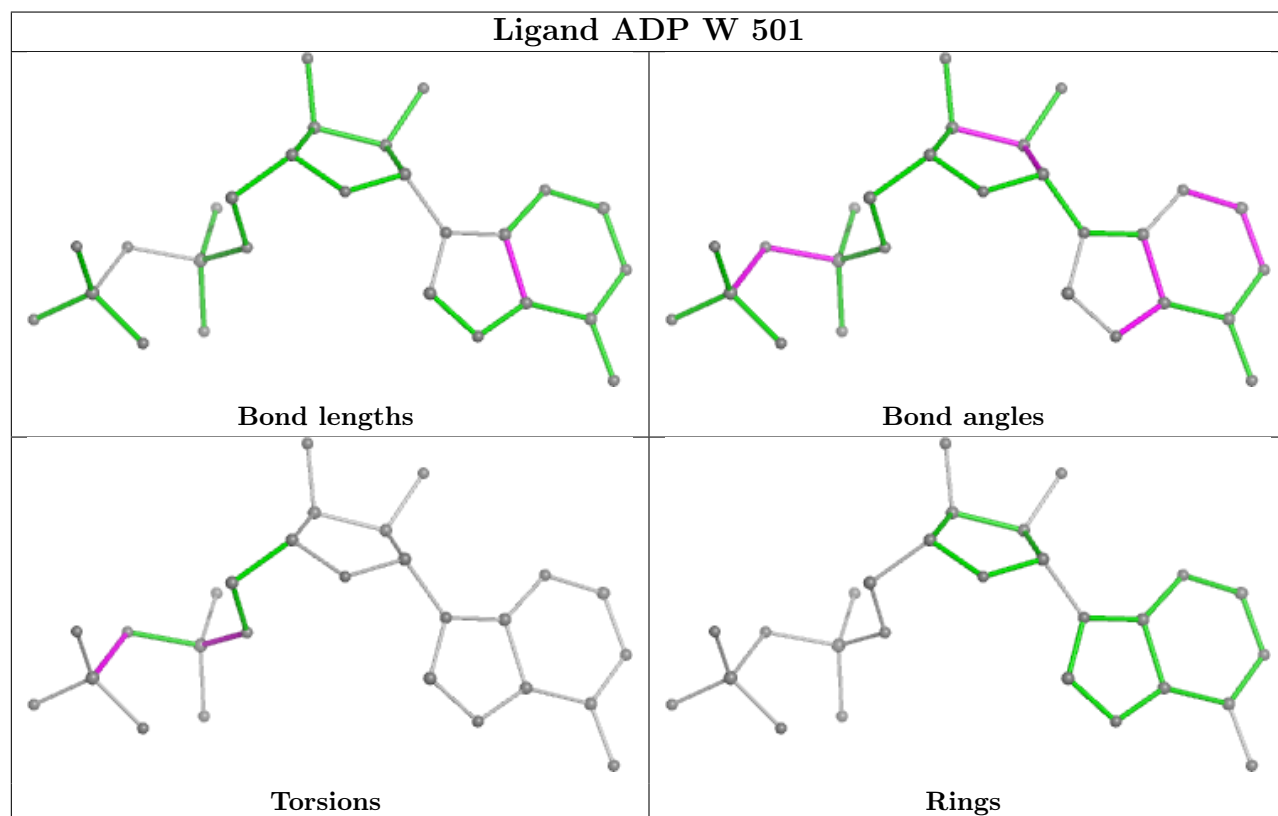
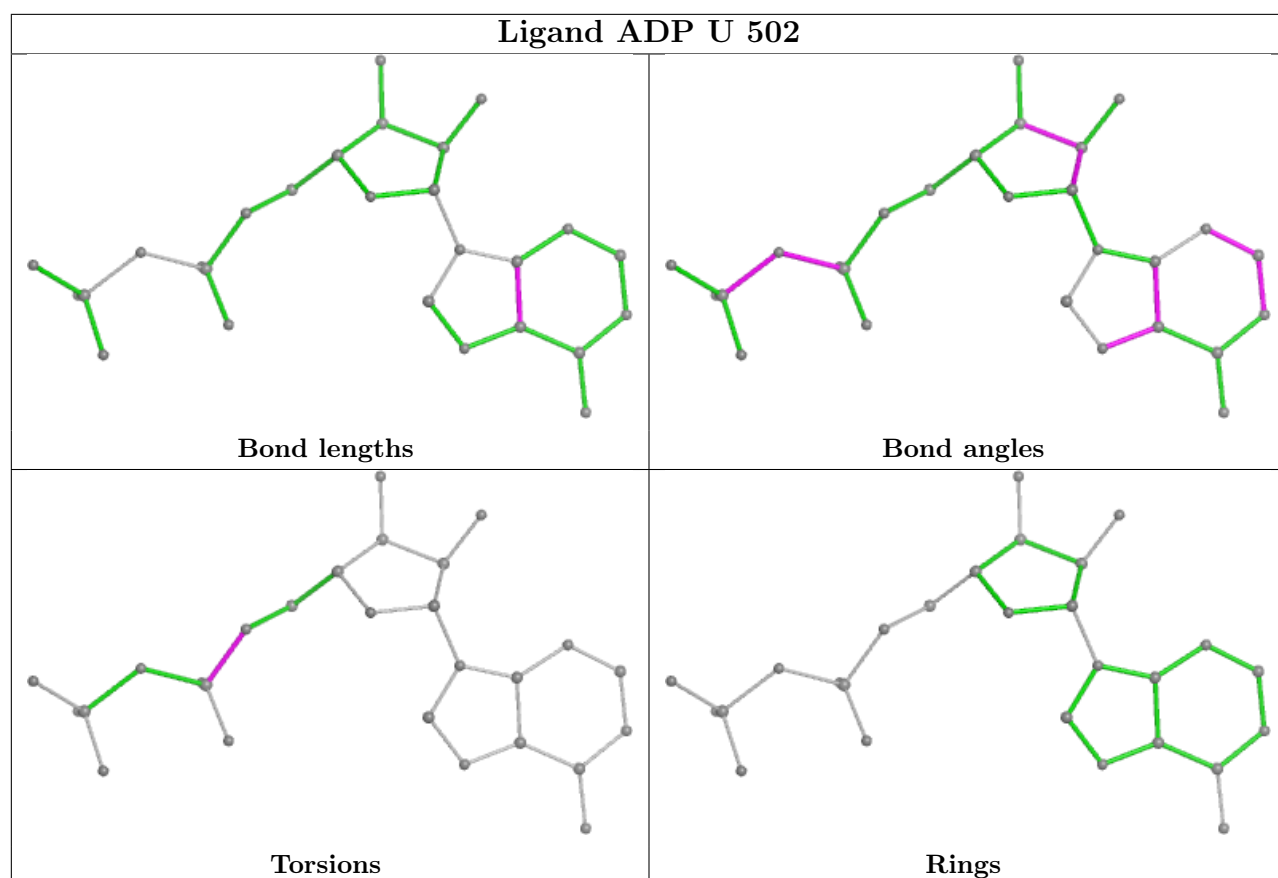


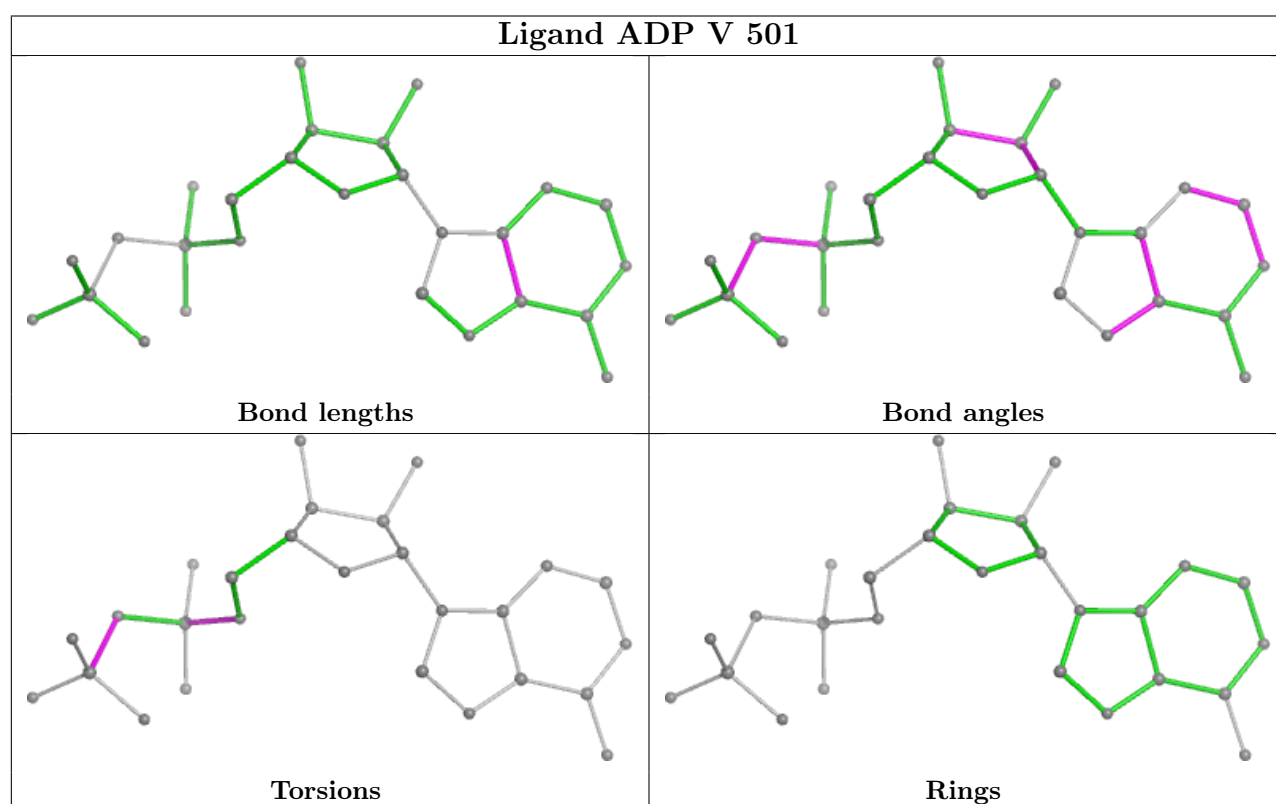
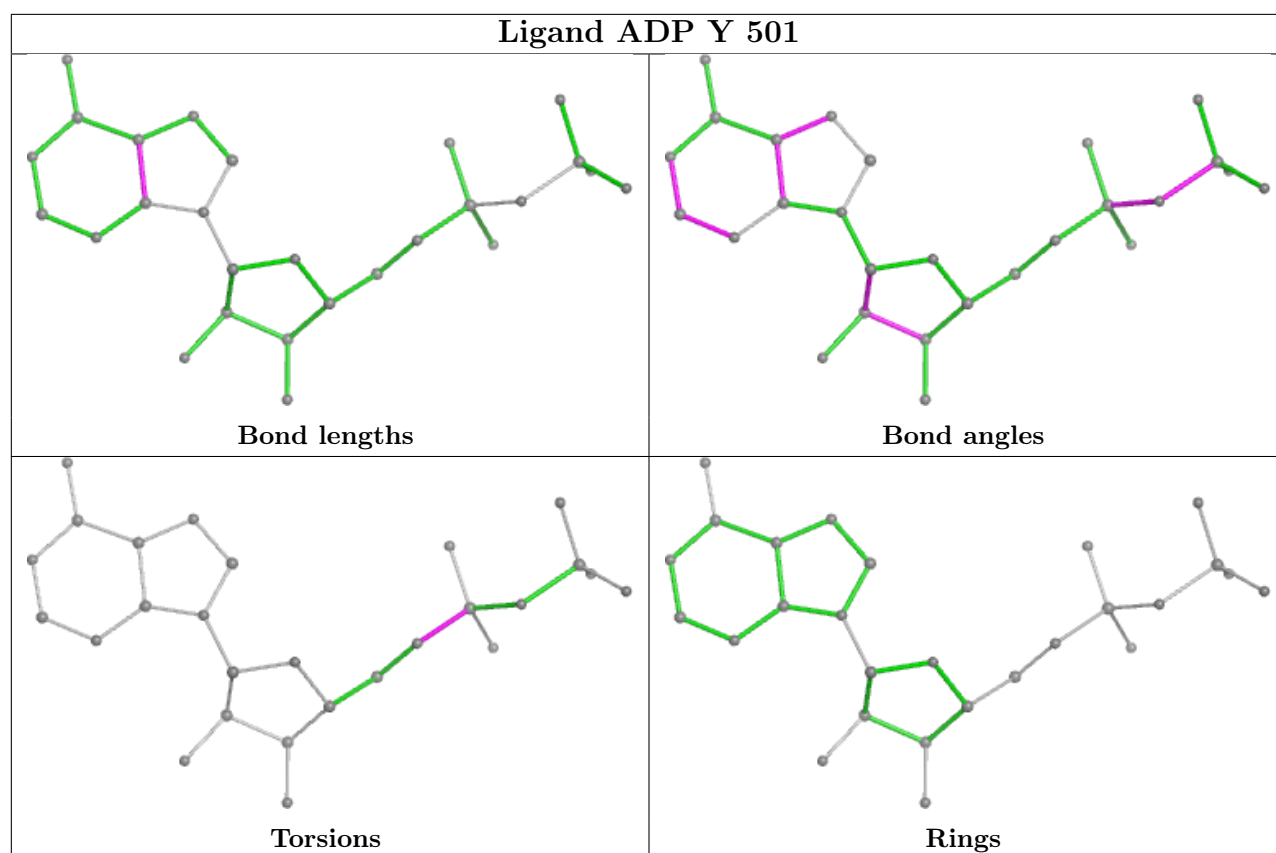












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
12	Z	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	329:LYS	C	581:THR	N	65.95

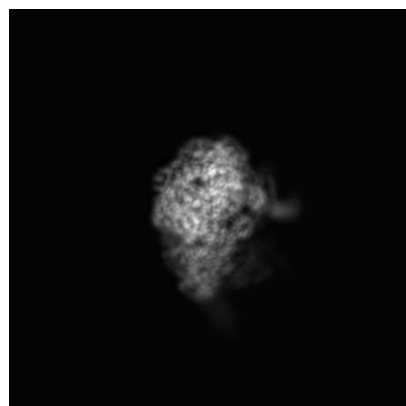
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18471. These allow visual inspection of the internal detail of the map and identification of artifacts.

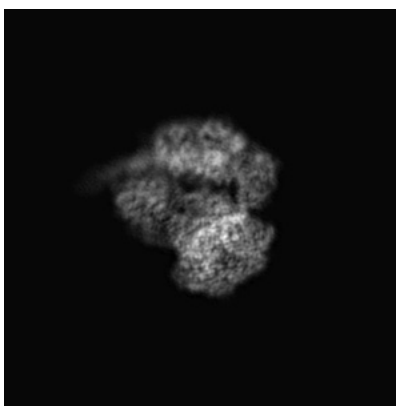
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

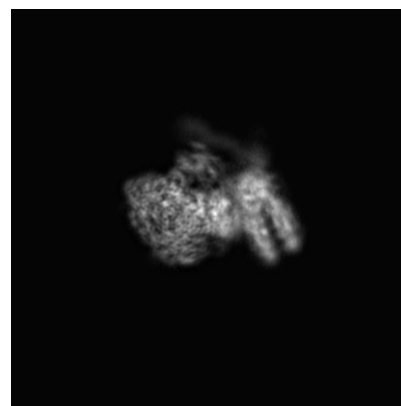
6.1.1 Primary map



X

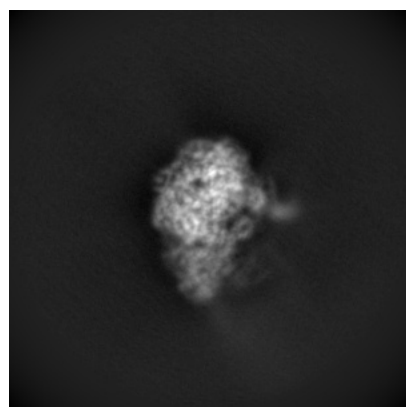


Y

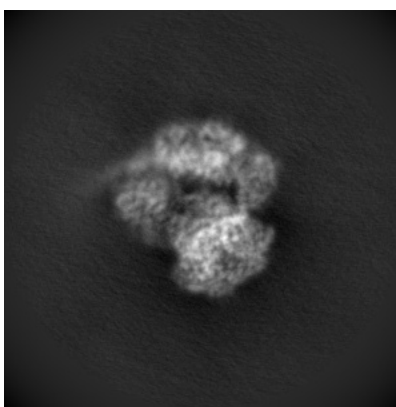


Z

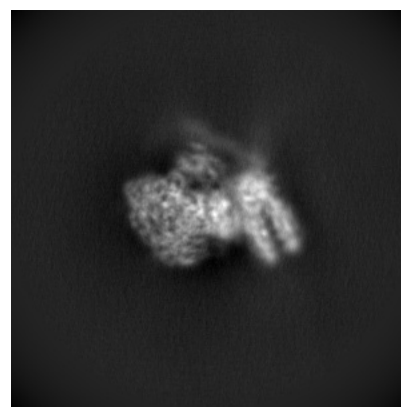
6.1.2 Raw map



X



Y

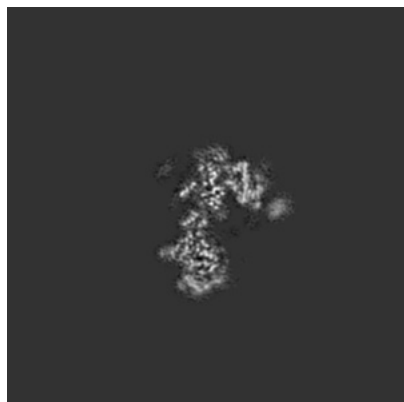


Z

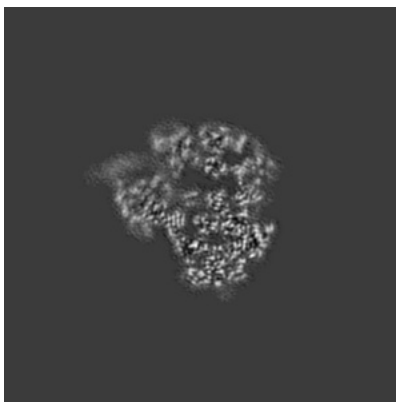
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

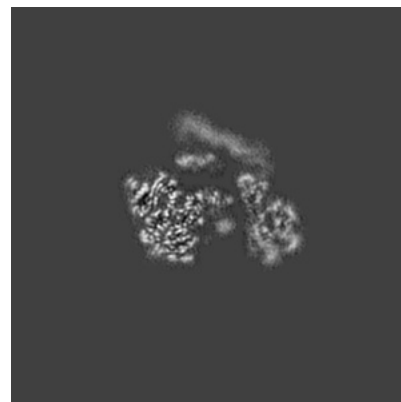
6.2.1 Primary map



X Index: 192

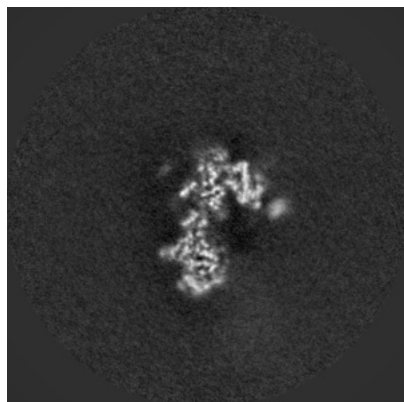


Y Index: 192

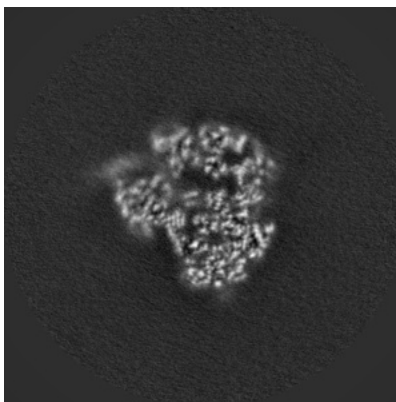


Z Index: 192

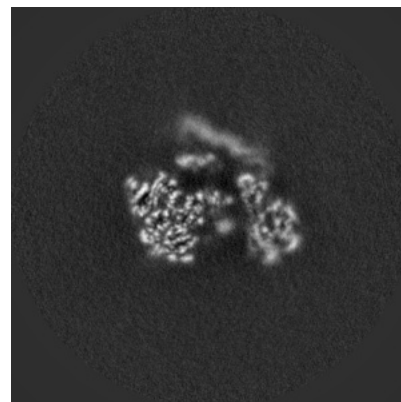
6.2.2 Raw map



X Index: 192



Y Index: 192

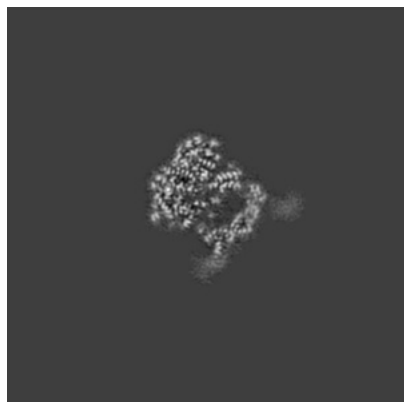


Z Index: 192

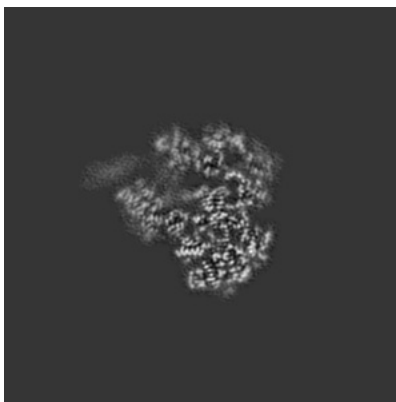
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

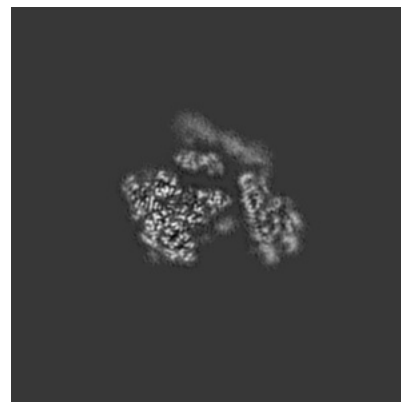
6.3.1 Primary map



X Index: 165

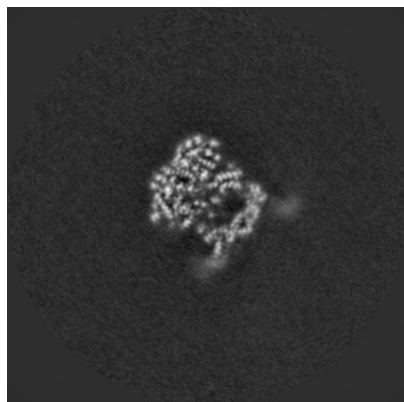


Y Index: 197

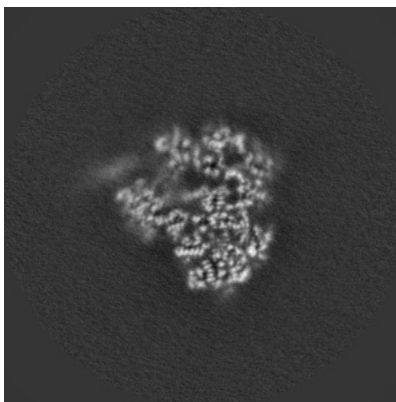


Z Index: 195

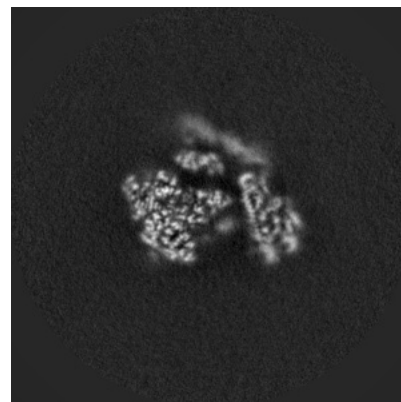
6.3.2 Raw map



X Index: 165



Y Index: 196

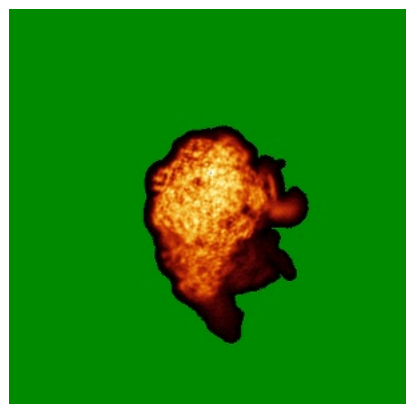


Z Index: 195

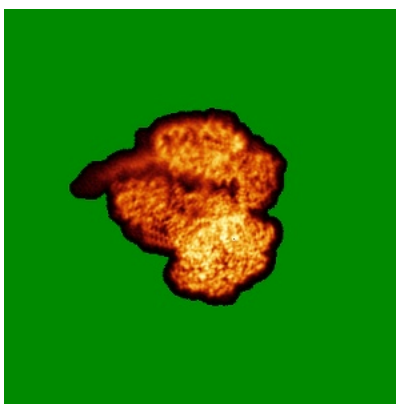
The images above show the largest variance slices of the map in three orthogonal directions.

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

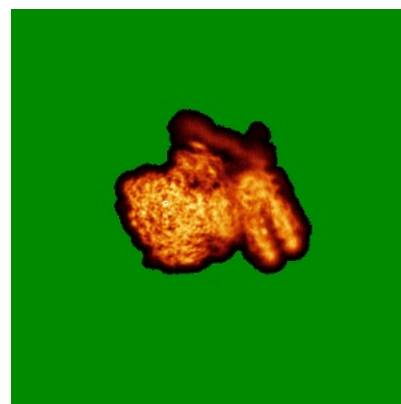
6.4.1 Primary map



X

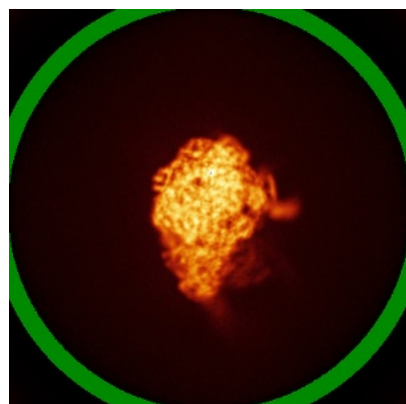


Y

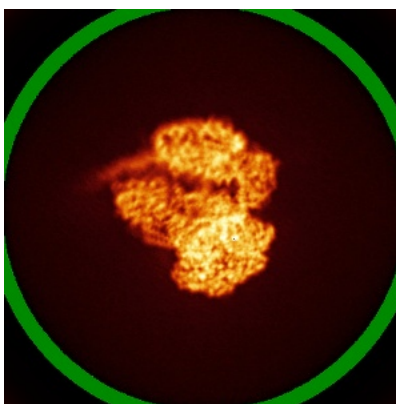


Z

6.4.2 Raw map



X



Y

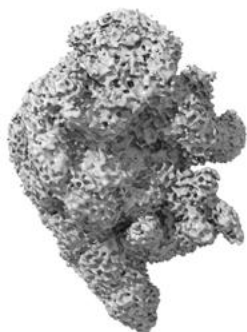


Z

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



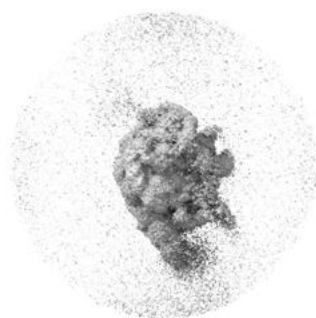
Y



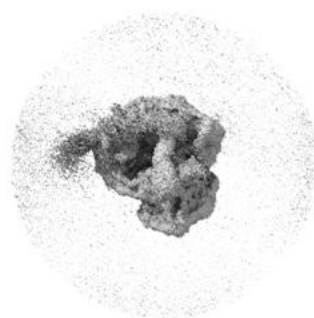
Z

The images above show the 3D surface view of the map at the recommended contour level 0.00197. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

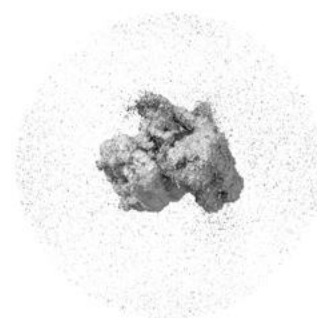
6.5.2 Raw map



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.

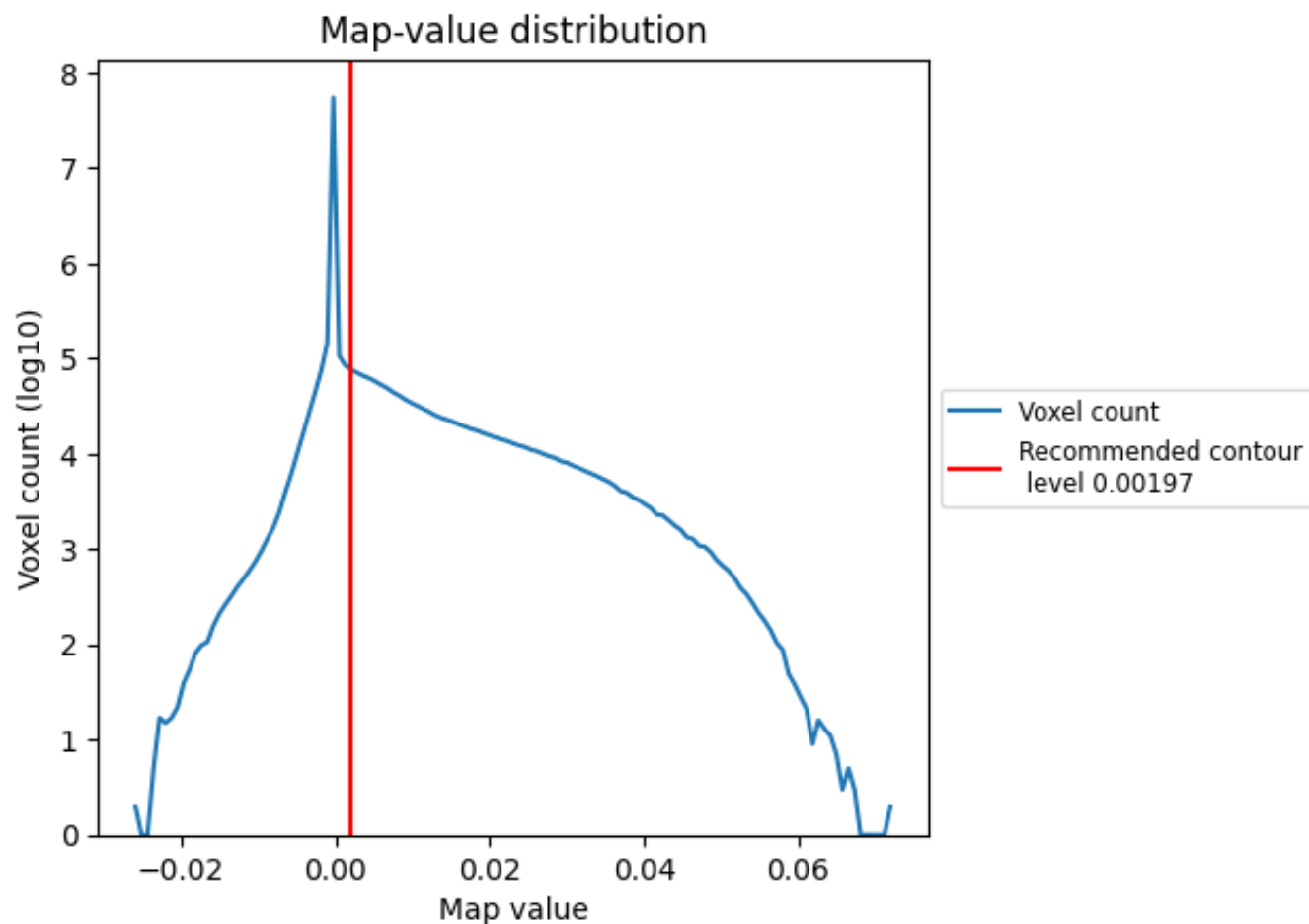
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

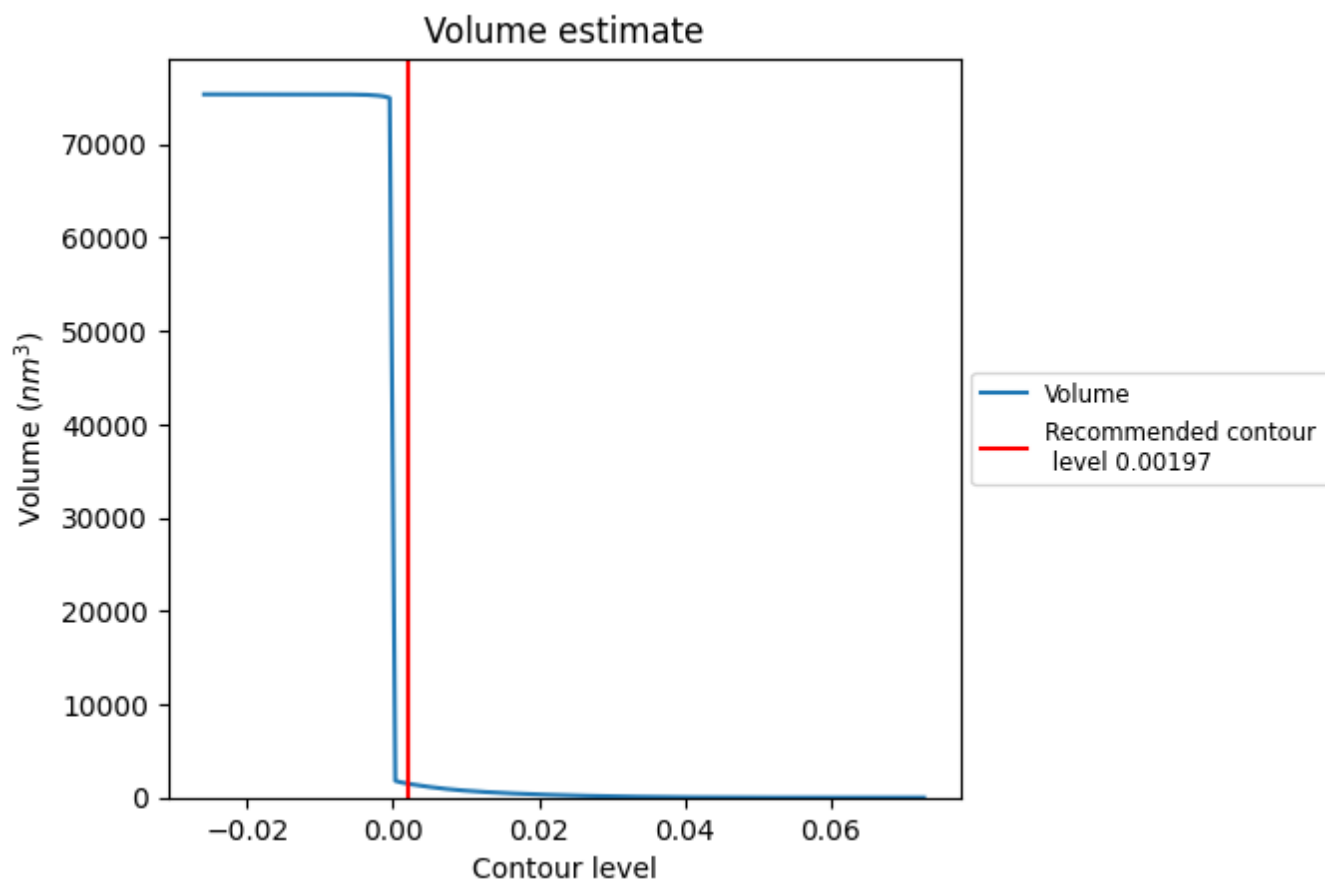
This section contains the results of statistical analysis of the map.

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.

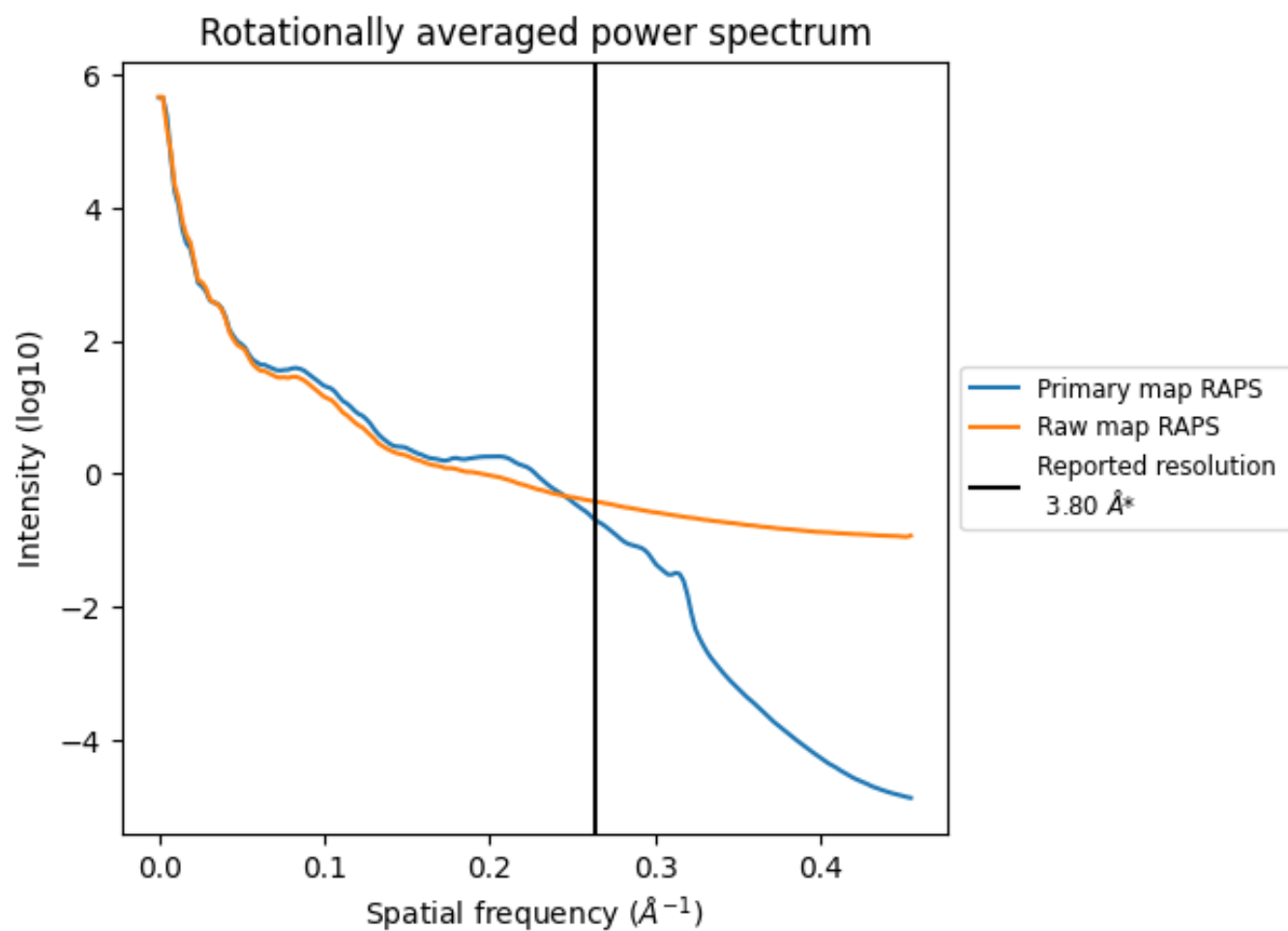
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1501 nm³; this corresponds to an approximate mass of 1356 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 ⓘ

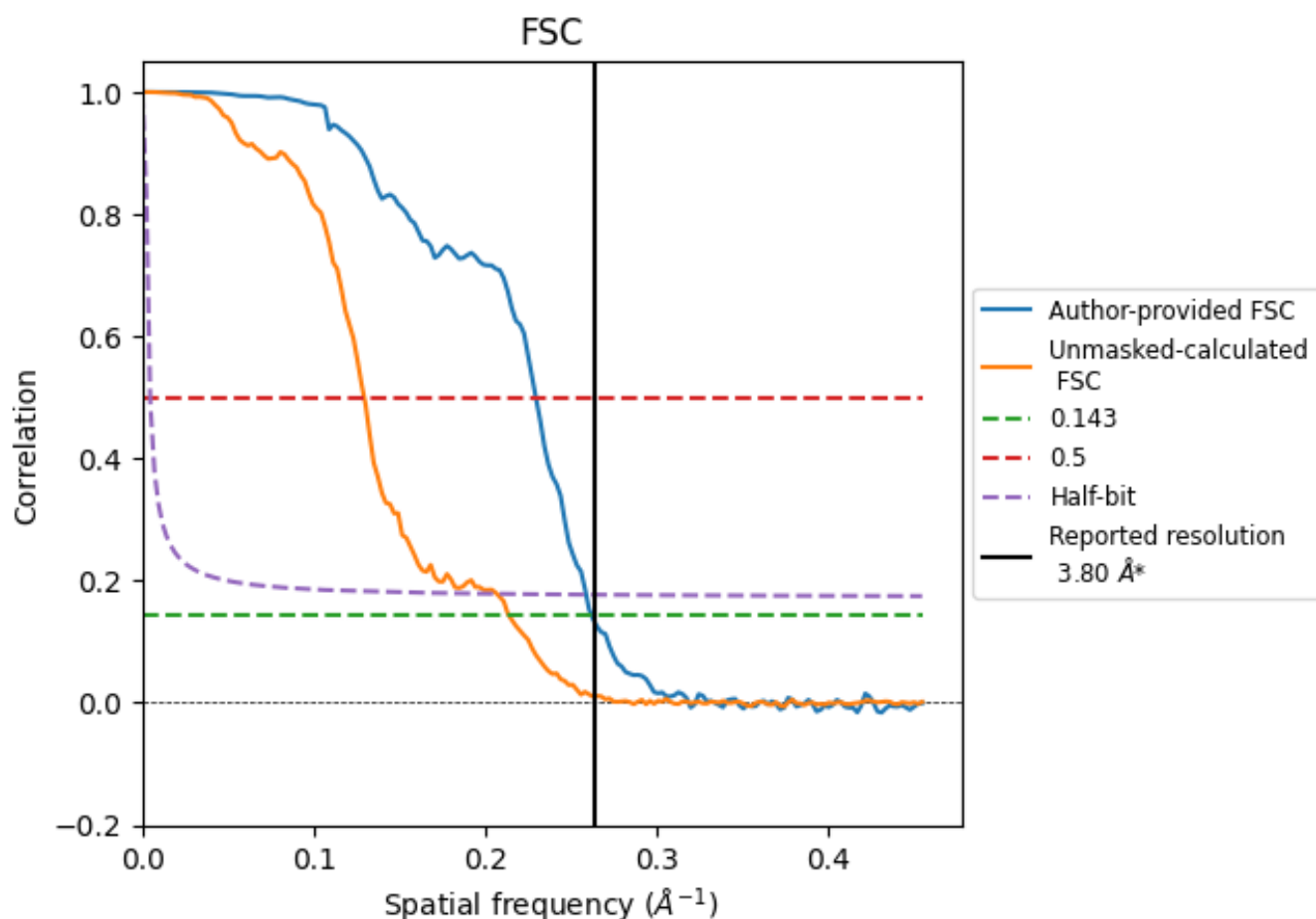


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 \AA^{-1}

8.2 Resolution estimates [i](#)

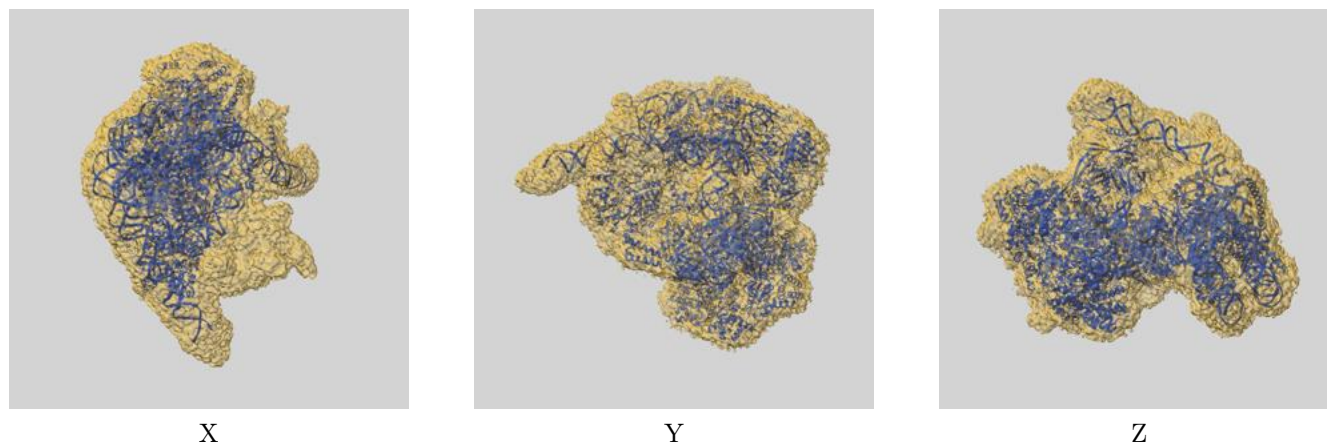
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.82	4.36	3.86
Unmasked-calculated*	4.68	7.73	4.84

*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 4.68 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

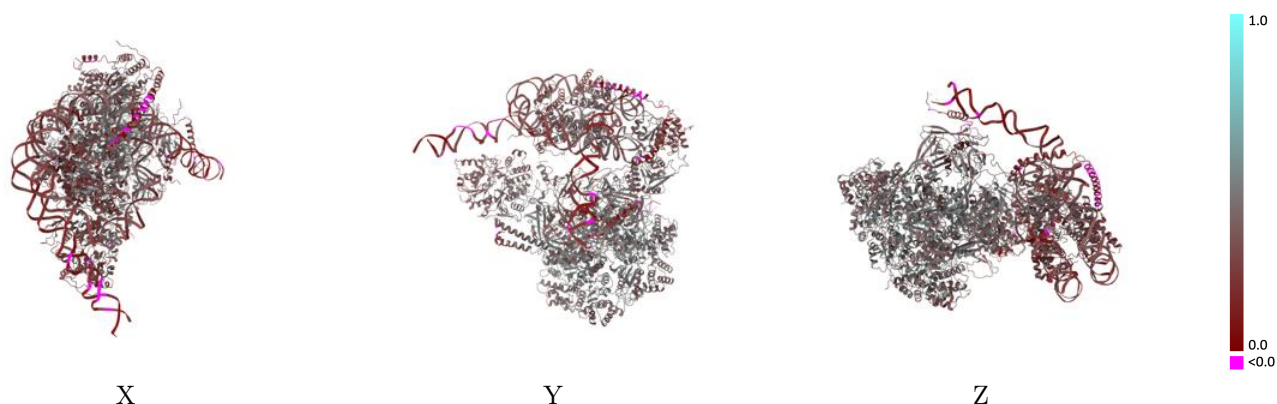
This section contains information regarding the fit between EMDB map EMD-18471 and PDB model 8QKU. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



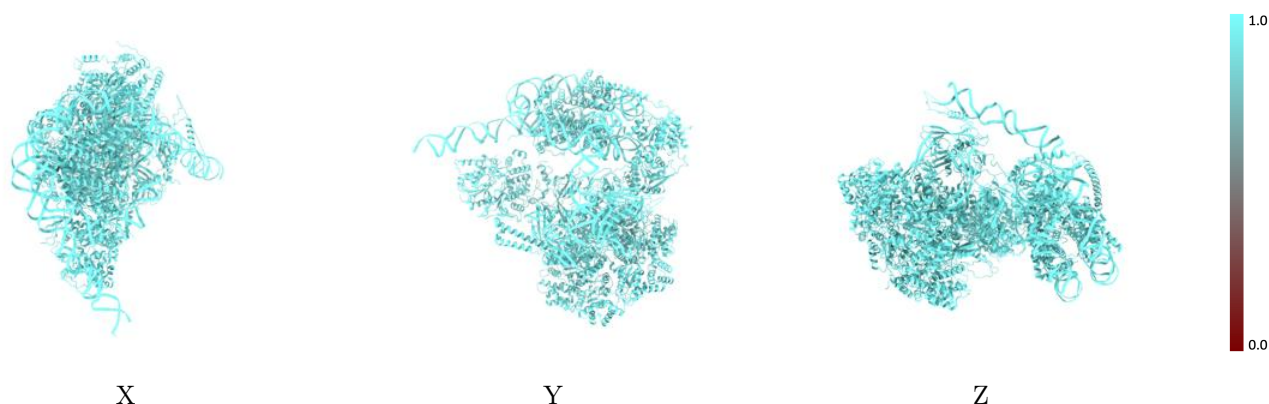
The images above show the 3D surface view of the map at the recommended contour level 0.00197 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



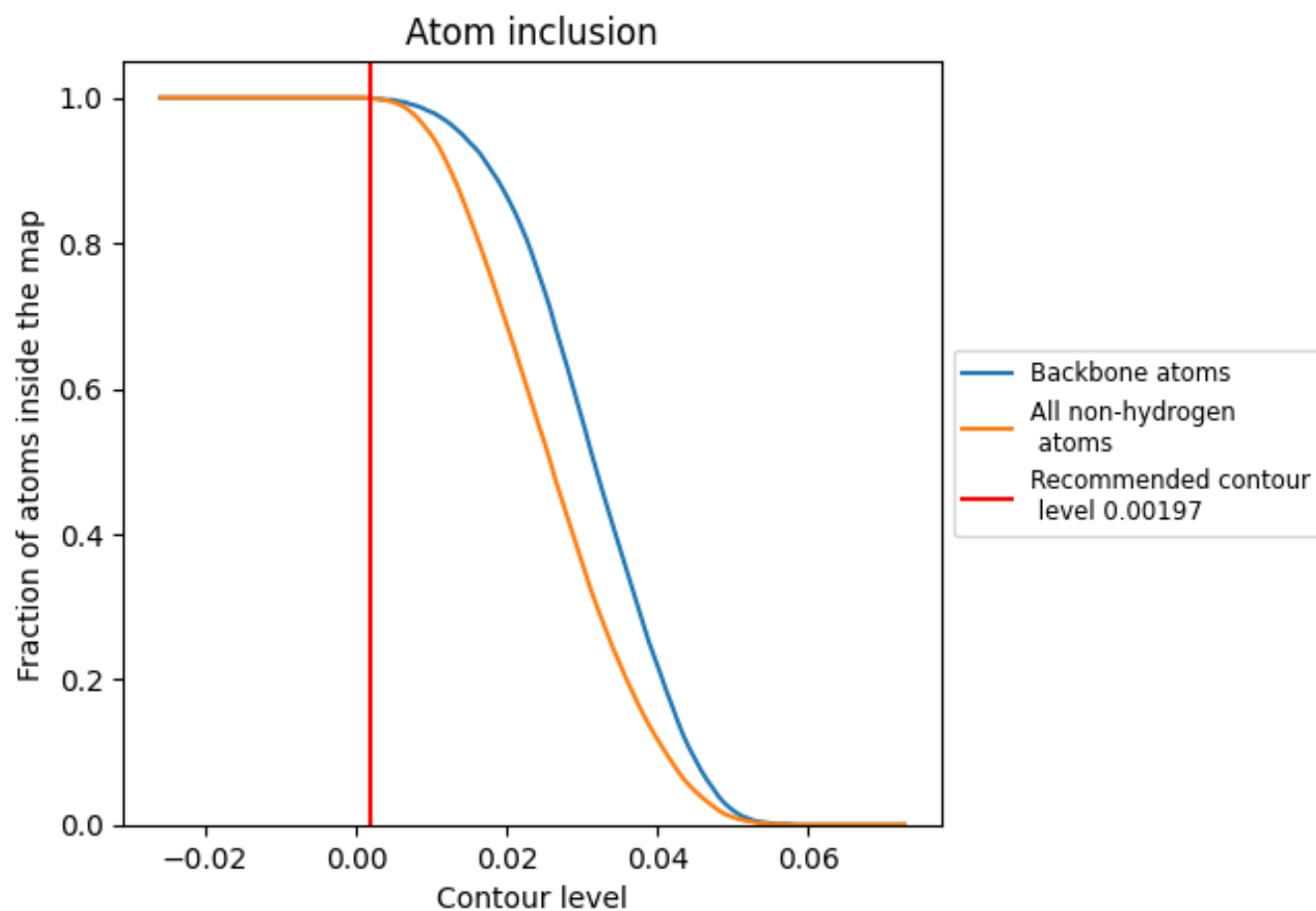
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00197).











































9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.00197) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9990	 0.3630
A	 1.0000	 0.3070
B	 0.9990	 0.3810
C	 0.9980	 0.3840
D	 0.9980	 0.2990
E	 1.0000	 0.3460
F	 1.0000	 0.3070
G	 1.0000	 0.3020
H	 1.0000	 0.2980
I	 0.9990	 0.2310
J	 1.0000	 0.2340
M	 0.9990	 0.3800
R	 0.9990	 0.3510
S	 1.0000	 0.3260
T	 1.0000	 0.4390
U	 1.0000	 0.4230
V	 1.0000	 0.4400
W	 1.0000	 0.4380
X	 1.0000	 0.4250
Y	 1.0000	 0.4310
Z	 0.9810	 0.1900

