



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 08:58 AM UTC

PDB ID : 8QZ0 / pdb_00008qz0
EMDB ID : EMD-18769
Title : SWR1-hexasome-dimer complex
Authors : Jalal, A.S.B.; Wigley, D.B.
Deposited on : 2023-10-26
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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

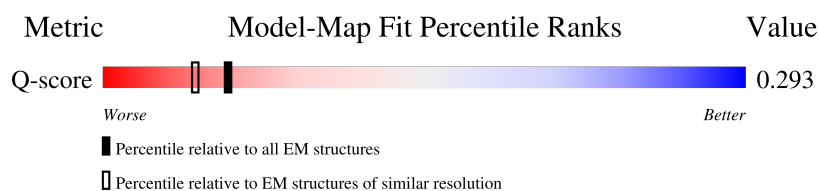
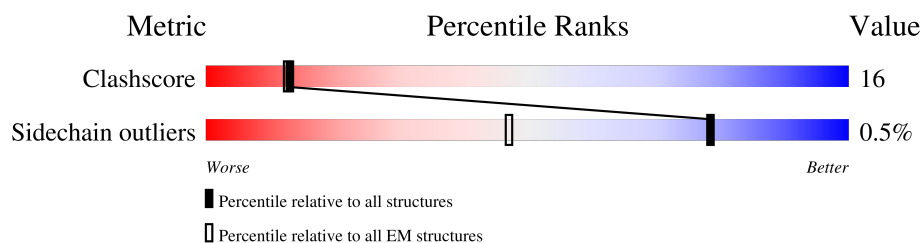
1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	
1	B	136	
2	C	103	
2	D	103	
3	E	132	

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Mol	Chain	Length	Quality of chain
4	G	131	
5	H	131	
6	I	118	
7	J	118	
8	L	134	
9	P	303	
10	R	438	
11	S	280	
12	U	471	
12	W	471	
12	Y	471	
13	T	463	
13	V	463	
13	X	463	
14	Z	795	
15	M	1514	
16	K	153	

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
18	BEF	M	1602	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 44167 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	108	Total	C	N	O	S	0	0
			864	546	165	152	1		
1	B	110	Total	C	N	O	S	0	0
			850	538	166	145	1		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	MET	GLN	engineered mutation	UNP P61830
A	121	PRO	LYS	engineered mutation	UNP P61830
A	123	GLU	ASP	conflict	UNP P61830
A	125	GLN	LYS	engineered mutation	UNP P61830
B	120	MET	GLN	engineered mutation	UNP P61830
B	121	PRO	LYS	engineered mutation	UNP P61830
B	123	GLU	ASP	conflict	UNP P61830
B	125	GLN	LYS	engineered mutation	UNP P61830

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	76	Total	C	N	O	0	0
			558	356	101	101		
2	D	71	Total	C	N	O	0	0
			527	329	103	95		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	102	Total	C	N	O	0	0
			715	454	129	132		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	88	Total	C	N	O	S	0	0
			640	396	112	131	1		

- Molecule 5 is a protein called Histone H2B.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	91	Total	C	N	O	S	0	0
			712	449	125	136	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	115	CYS	SER	engineered mutation	UNP P02293

- Molecule 6 is a DNA chain called DNA (113-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	113	Total	C	N	O	P	0	0
			2300	1090	419	678	113		

- Molecule 7 is a DNA chain called DNA (113-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	113	Total	C	N	O	P	0	0
			2333	1101	441	678	113		

- Molecule 8 is a protein called Histone H2A.Z.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	L	87	Total	C	N	O	0	0
			675	423	131	121		

- Molecule 9 is a protein called SWR1-complex protein 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	P	114	Total	C	N	O	0	0
			901	557	175	169		

- Molecule 10 is a protein called Actin-like protein ARP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	R	385	Total	C	N	O	S	0	0
			3118	2024	507	572	15		

- Molecule 11 is a protein called Vacuolar protein sorting-associated protein 71.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	188	Total	C	N	O	S	0	0
			1500	940	270	281	9		

- Molecule 12 is a protein called RuvB-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	446	Total	C	N	O	S	0	0
			3430	2143	595	680	12		
12	W	433	Total	C	N	O	S	0	0
			3307	2076	569	651	11		
12	Y	443	Total	C	N	O	S	0	0
			3342	2091	581	659	11		

- Molecule 13 is a protein called RuvB-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	V	427	Total	C	N	O	S	0	0
			3257	2058	560	629	10		
13	X	441	Total	C	N	O	S	0	0
			3371	2128	581	653	9		
13	T	439	Total	C	N	O	S	0	0
			3304	2084	574	637	9		

- Molecule 14 is a protein called Vacuolar protein sorting-associated protein 72.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Z	173	Total	C	N	O	S	0	0
			1400	875	259	262	4		

- Molecule 15 is a protein called Helicase SWR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	794	Total	C	N	O	S	0	0
			6223	3929	1098	1170	26		

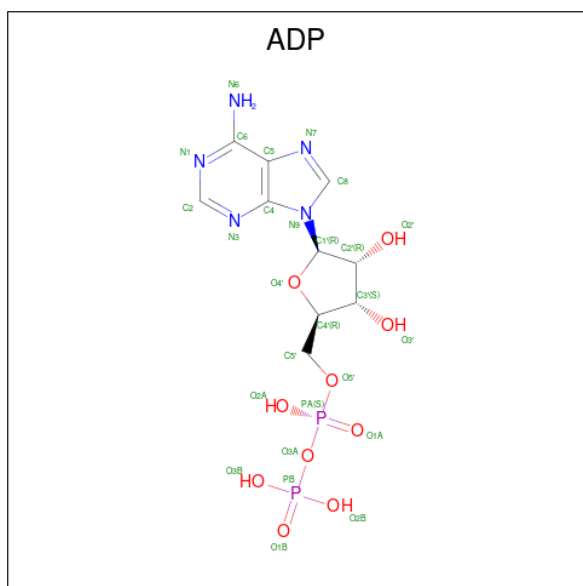
- Molecule 16 is a protein called Histone H2A.Z-specific chaperone CHZ1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	76	Total	C	N	O	S	0	0
			606	356	95	152	3		

There is a discrepancy between the modelled and reference sequences:

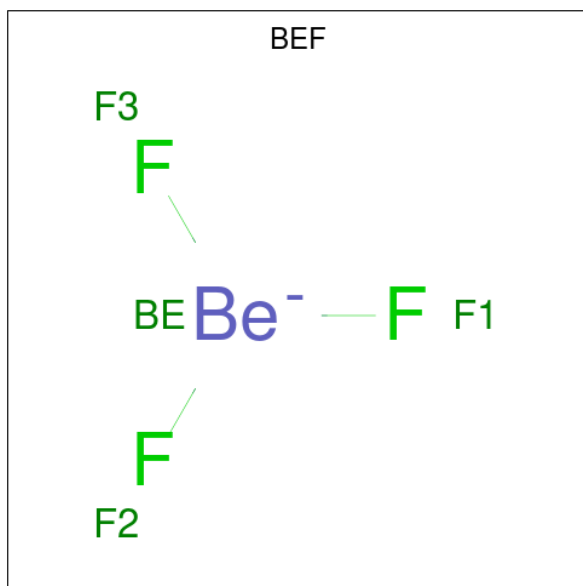
Chain	Residue	Modelled	Actual	Comment	Reference
K	98	CYS	SER	engineered mutation	UNP P40019

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



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

- Molecule 18 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



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

- Molecule 19 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

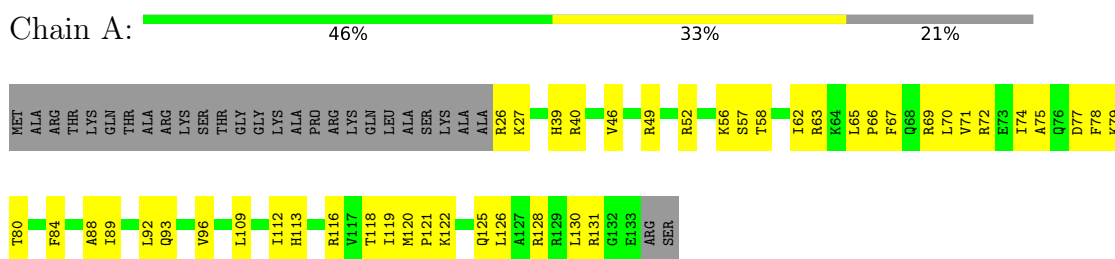
- Molecule 20 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

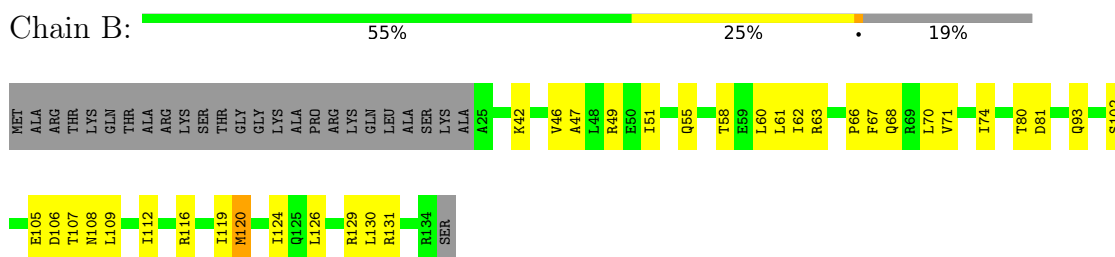
3 Residue-property plots

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.

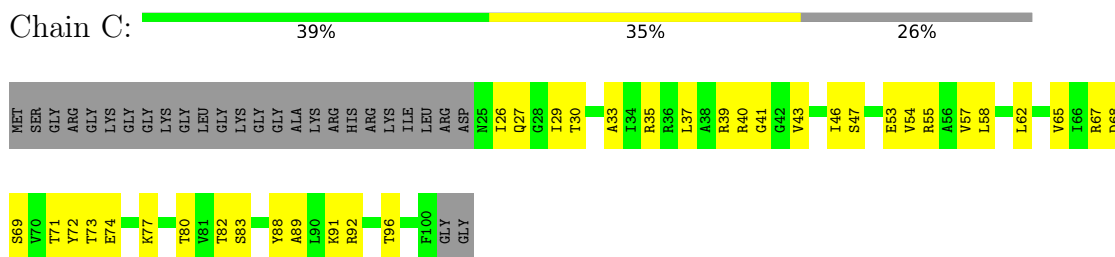
• Molecule 1: Histone H3



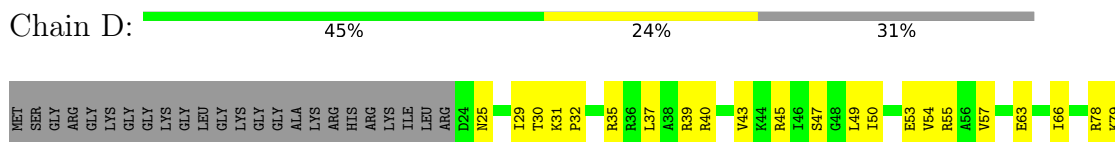
• Molecule 1: Histone H3



• Molecule 2: Histone H4

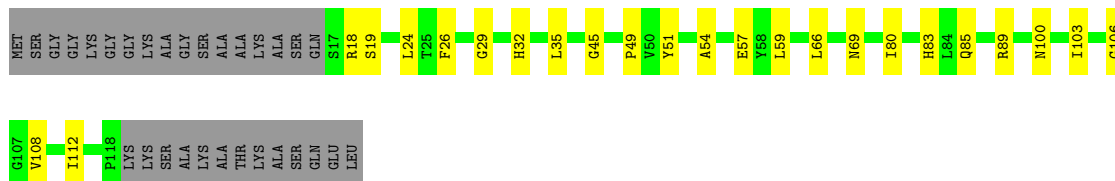


• Molecule 2: Histone H4

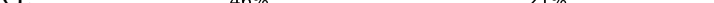


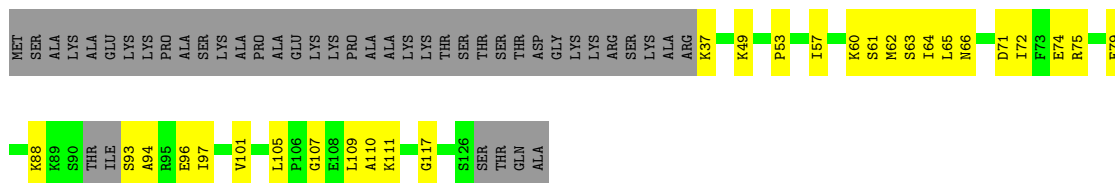
- Molecule 3: Histone H2A.1

Chain E: 59% 18% 23%

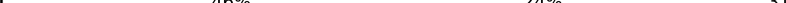


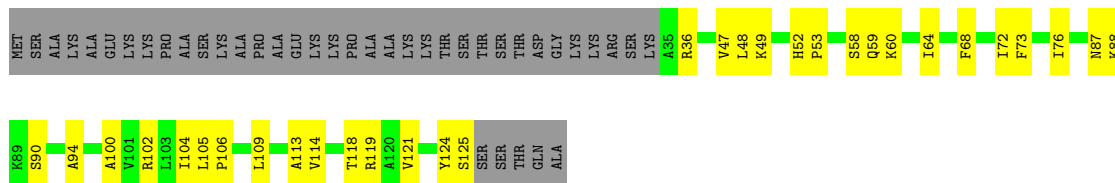
- Molecule 4: Histone H2B.1

Chain G:  46% 21% 33%



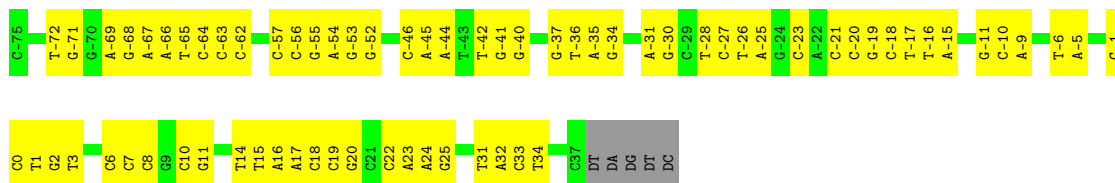
- Molecule 5: Histone H2B.1

Chain H:  46% 24% 31%



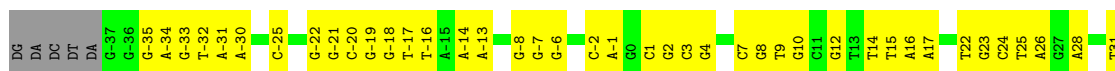
- Molecule 6: DNA (113-MER)

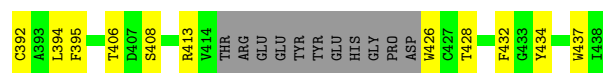
Chain I: 36% 59% .



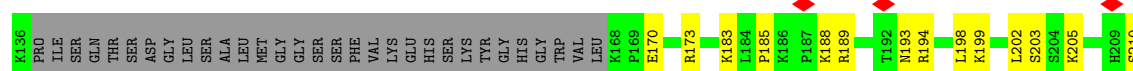
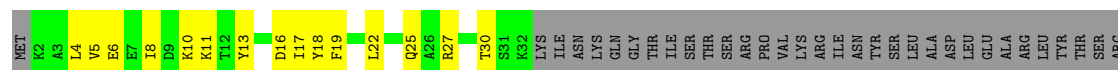
- Molecule 7: DNA (113-MER)

Chain J: 35% 61%

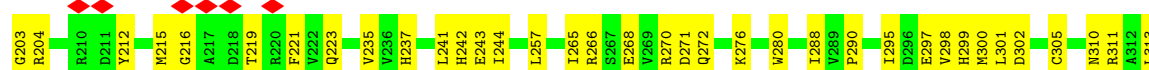
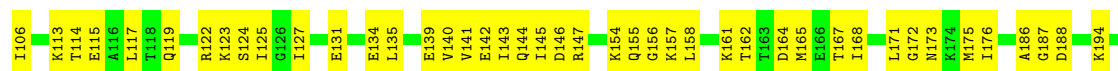




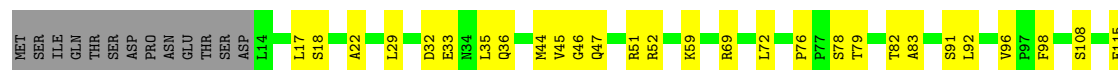
• Molecule 11: Vacuolar protein sorting-associated protein 71

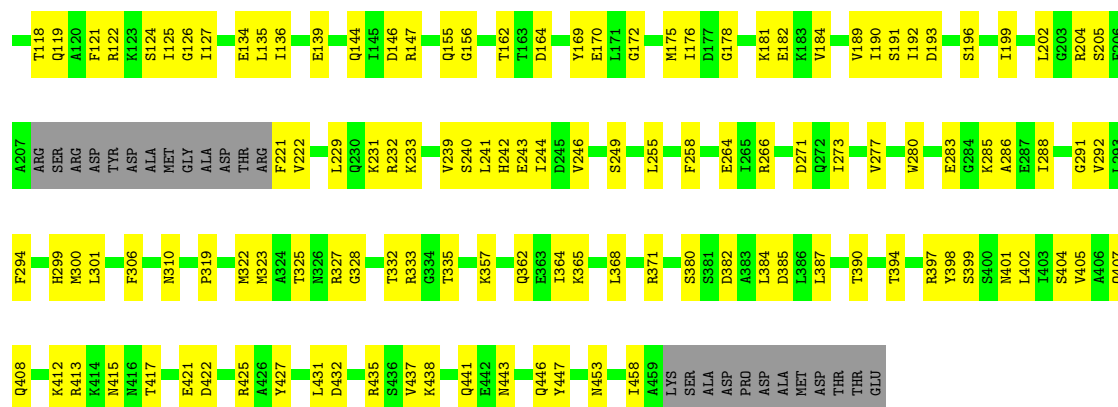


• Molecule 12: RuvB-like protein 2



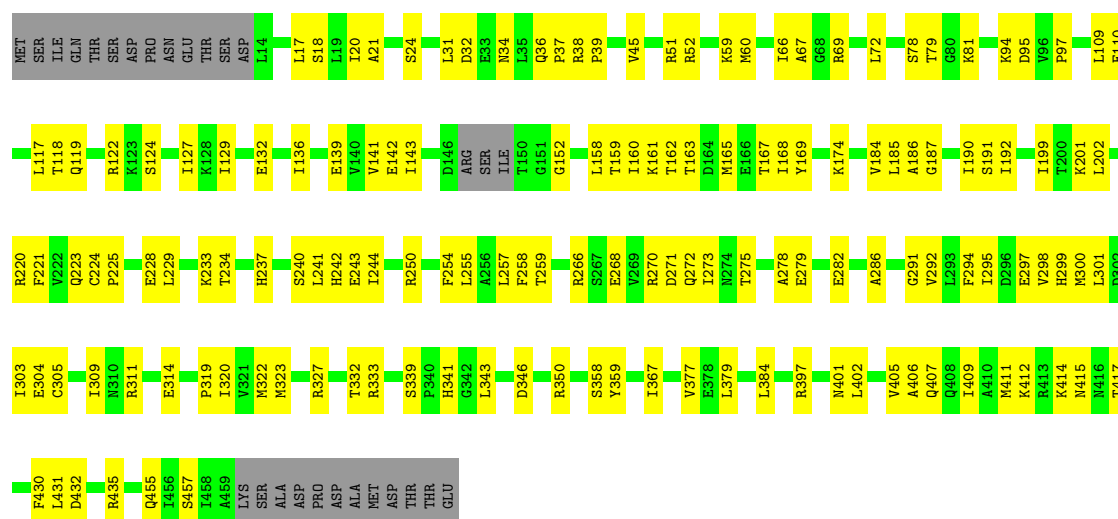
• Molecule 12: RuvB-like protein 2





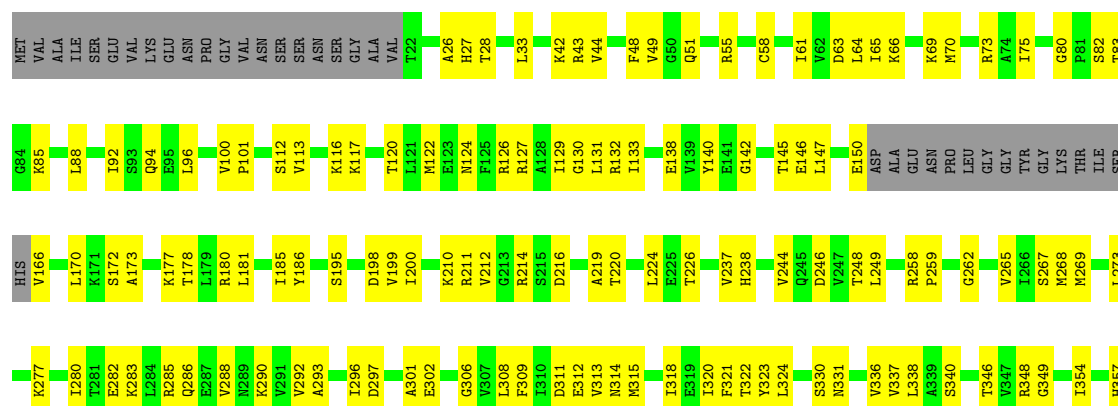
• Molecule 12: RuvB-like protein 2

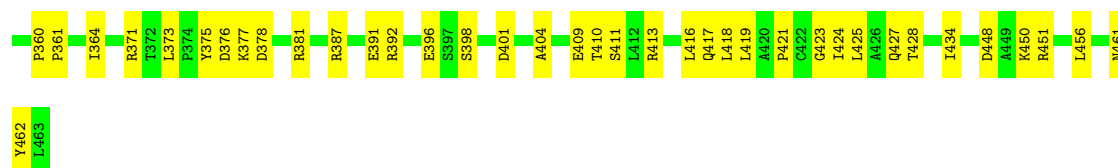
Chain Y: 63% 31% 6%



• Molecule 13: RuvB-like protein 1

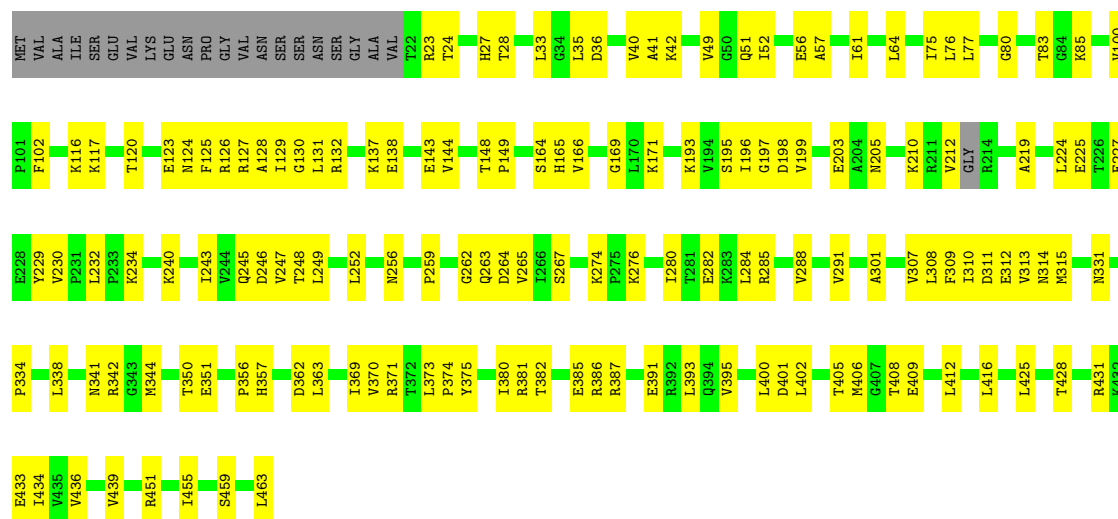
Chain V: 56% 36% 8%





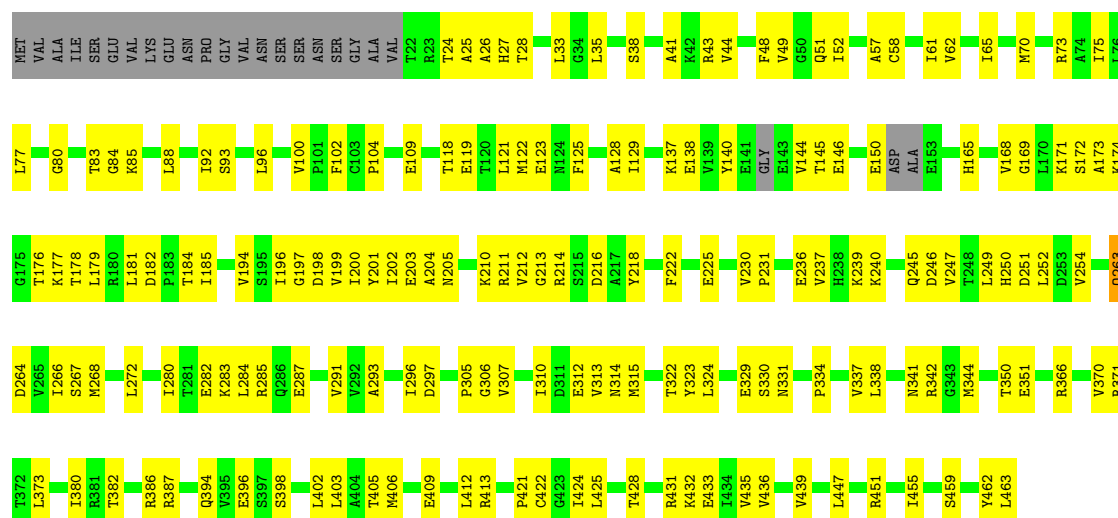
• Molecule 13: RuvB-like protein 1

Chain X: 63% 32% 5%



• Molecule 13: RuvB-like protein 1

Chain T: 57% 37% 5%



• Molecule 14: Vacuolar protein sorting-associated protein 72

Chain Z: 16% 5% 78%

- Molecule 16: Histone H2A.Z-specific chaperone CHZ1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23503	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.030	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00126	Depositor
Map size (Å)	408.0, 408.0, 408.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.13	0/877	0.42	0/1178
1	B	0.12	0/862	0.38	0/1159
2	C	0.16	0/564	0.41	0/763
2	D	0.13	0/531	0.35	0/716
3	E	0.12	0/725	0.32	0/992
4	G	0.10	0/646	0.28	0/873
5	H	0.13	0/722	0.35	0/972
6	I	0.18	0/2576	0.39	0/3969
7	J	0.17	0/2620	0.33	0/4046
8	L	0.09	0/682	0.24	0/917
9	P	0.16	0/914	0.58	2/1232 (0.2%)
10	R	0.15	0/3206	0.39	2/4351 (0.0%)
11	S	0.17	0/1521	0.46	0/2047
12	U	0.12	0/3468	0.34	0/4674
12	W	0.12	0/3343	0.30	0/4508
12	Y	0.10	0/3378	0.30	0/4561
13	T	0.14	0/3342	0.36	0/4527
13	V	0.11	0/3294	0.30	0/4458
13	X	0.11	0/3412	0.32	0/4618
14	Z	0.12	0/1419	0.38	2/1899 (0.1%)
15	M	0.11	0/6330	0.34	0/8561
16	K	0.12	0/606	0.40	0/806
All	All	0.13	0/45038	0.35	6/61827 (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
10	R	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
15	M	0	2
All	All	0	3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	233	PRO	CA-C-N	7.76	136.36	121.54
9	P	233	PRO	C-N-CA	7.76	136.36	121.54
14	Z	299	PRO	CA-C-N	6.01	132.51	121.70
14	Z	299	PRO	C-N-CA	6.01	132.51	121.70
10	R	264	PHE	CA-C-N	-5.06	112.82	122.53

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	M	1159	ASP	Peptide
15	M	871	MET	Peptide
10	R	220	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	864	0	903	41	0
1	B	850	0	878	36	0
2	C	558	0	542	36	0
2	D	527	0	536	27	0
3	E	715	0	692	24	0
4	G	640	0	617	23	0
5	H	712	0	736	35	0
6	I	2300	0	1266	78	0
7	J	2333	0	1266	84	0
8	L	675	0	718	38	0
9	P	901	0	898	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	R	3118	0	3058	107	0
11	S	1500	0	1537	68	0
12	U	3430	0	3505	137	0
12	W	3307	0	3388	119	0
12	Y	3342	0	3364	112	0
13	T	3304	0	3389	137	0
13	V	3257	0	3385	127	0
13	X	3371	0	3487	109	0
14	Z	1400	0	1393	35	0
15	M	6223	0	6066	209	0
16	K	606	0	536	20	0
17	M	27	0	10	2	0
17	R	27	0	11	5	0
17	T	27	0	12	4	0
17	U	27	0	12	2	0
17	V	27	0	12	5	0
17	W	27	0	10	4	0
17	X	27	0	12	4	0
17	Y	27	0	11	1	0
18	M	4	0	0	2	0
18	R	4	0	0	1	0
19	M	1	0	0	0	0
19	R	1	0	0	0	0
19	T	1	0	0	0	0
19	U	1	0	0	0	0
19	V	1	0	0	0	0
19	W	1	0	0	0	0
19	X	1	0	0	0	0
19	Y	1	0	0	0	0
20	S	2	0	0	0	0
All	All	44167	0	42250	1417	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 16.

The worst 5 of 1417 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:-55:DG:N2	7:J:55:DC:O2	1.97	0.95
10:R:220:GLY:O	10:R:222:PHE:N	2.01	0.93
10:R:374:GLN:HE22	13:T:174:LYS:HA	1.34	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:58:CYS:HB3	13:T:92:ILE:HD11	1.53	0.87
8:L:34:VAL:HA	8:L:60:THR:HG21	1.60	0.84

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	77/113 (68%)	77 (100%)	0	100	100
1	B	80/113 (71%)	79 (99%)	1 (1%)	61	71
2	C	50/81 (62%)	50 (100%)	0	100	100
2	D	52/81 (64%)	52 (100%)	0	100	100
3	E	65/99 (66%)	65 (100%)	0	100	100
4	G	66/109 (61%)	66 (100%)	0	100	100
5	H	78/109 (72%)	78 (100%)	0	100	100
8	L	69/103 (67%)	68 (99%)	1 (1%)	59	70
9	P	93/262 (36%)	93 (100%)	0	100	100
10	R	349/396 (88%)	348 (100%)	1 (0%)	86	84
11	S	176/261 (67%)	174 (99%)	2 (1%)	65	73
12	U	379/403 (94%)	378 (100%)	1 (0%)	86	84
12	W	365/403 (91%)	365 (100%)	0	100	100
12	Y	359/403 (89%)	356 (99%)	3 (1%)	73	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	T	344/391 (88%)	342 (99%)	2 (1%)	78	79
13	V	356/391 (91%)	356 (100%)	0	100	100
13	X	368/391 (94%)	365 (99%)	3 (1%)	73	76
14	Z	148/732 (20%)	148 (100%)	0	100	100
15	M	662/1376 (48%)	657 (99%)	5 (1%)	73	76
16	K	67/136 (49%)	67 (100%)	0	100	100
All	All	4203/6353 (66%)	4184 (100%)	19 (0%)	78	81

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	M	723	MET
15	M	1139	ASN
15	M	1214	MET
15	M	811	HIS
13	X	308	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
12	Y	326	ASN
15	M	1222	ASN
13	T	286	GLN
15	M	1280	GLN
15	M	1036	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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$
17	ADP	R	501	19	28,29,29	1.44	4 (14%)	43,45,45	1.90	11 (25%)
17	ADP	W	501	19	28,29,29	1.43	4 (14%)	43,45,45	1.80	9 (20%)
17	ADP	X	501	19	28,29,29	1.40	4 (14%)	43,45,45	1.87	8 (18%)
17	ADP	M	1601	-	28,29,29	1.41	4 (14%)	43,45,45	1.84	10 (23%)
17	ADP	T	501	19	28,29,29	1.40	4 (14%)	43,45,45	1.86	8 (18%)
17	ADP	V	501	19	28,29,29	1.39	4 (14%)	43,45,45	1.83	9 (20%)
18	BEF	R	502	-	0,3,3	-	-	-	-	-
17	ADP	Y	501	-	28,29,29	1.41	4 (14%)	43,45,45	1.85	9 (20%)
18	BEF	M	1602	-	0,3,3	-	-	-	-	-
17	ADP	U	501	19	28,29,29	1.40	4 (14%)	43,45,45	1.87	8 (18%)

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
17	ADP	R	501	19	-	0/16/32/32	0/3/3/3
17	ADP	W	501	19	-	1/16/32/32	0/3/3/3
17	ADP	X	501	19	-	3/16/32/32	0/3/3/3
17	ADP	M	1601	-	-	6/16/32/32	0/3/3/3
17	ADP	T	501	19	-	2/16/32/32	0/3/3/3
17	ADP	V	501	19	-	7/16/32/32	0/3/3/3
17	ADP	Y	501	-	-	3/16/32/32	0/3/3/3
17	ADP	U	501	19	-	2/16/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	R	501	ADP	C5-C4	4.82	1.47	1.39
17	W	501	ADP	C5-C4	4.78	1.47	1.39
17	T	501	ADP	C5-C4	4.73	1.47	1.39
17	X	501	ADP	C5-C4	4.72	1.47	1.39
17	Y	501	ADP	C5-C4	4.71	1.47	1.39

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	X	501	ADP	C5-C4-N3	-6.08	118.34	126.72
17	U	501	ADP	C5-C4-N3	-6.06	118.37	126.72
17	T	501	ADP	C5-C4-N3	-6.01	118.45	126.72
17	Y	501	ADP	C5-C4-N3	-5.95	118.52	126.72
17	R	501	ADP	C5-C4-N3	-5.94	118.54	126.72

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	U	501	ADP	C5'-O5'-PA-O3A
17	V	501	ADP	C5'-O5'-PA-O1A
17	V	501	ADP	C5'-O5'-PA-O2A
17	V	501	ADP	C5'-O5'-PA-O3A
17	W	501	ADP	C5'-O5'-PA-O1A

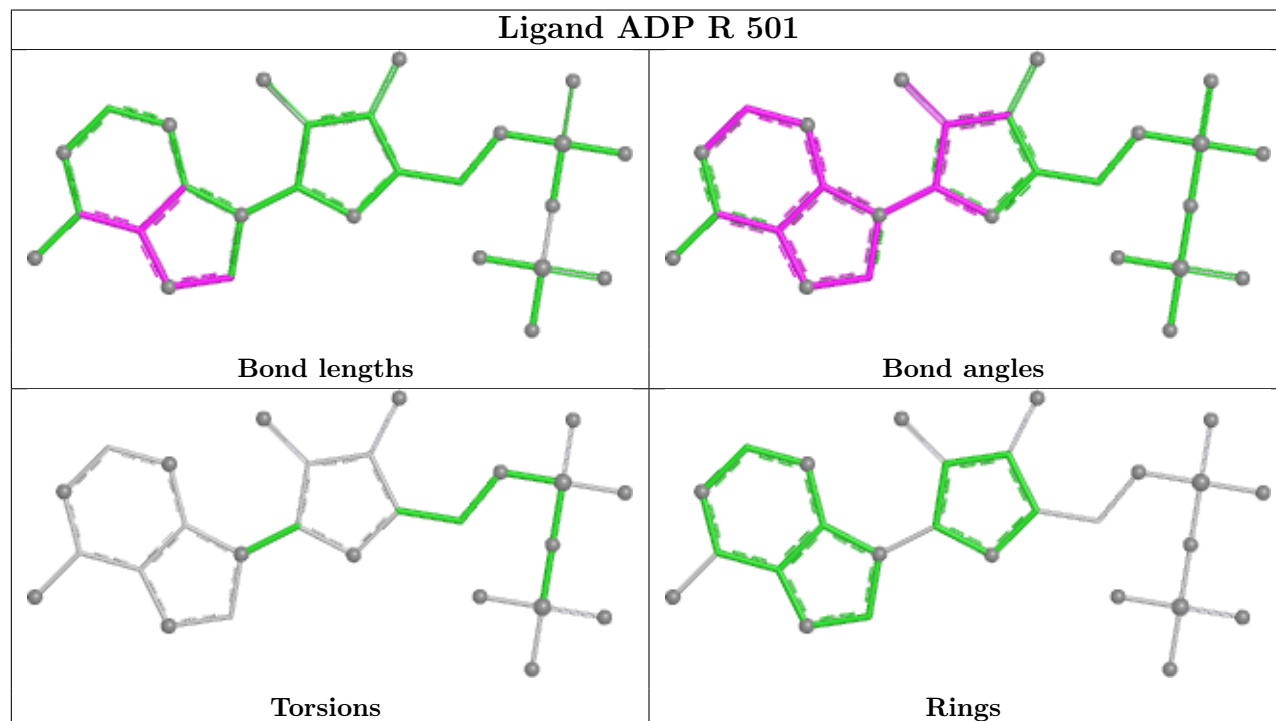
There are no ring outliers.

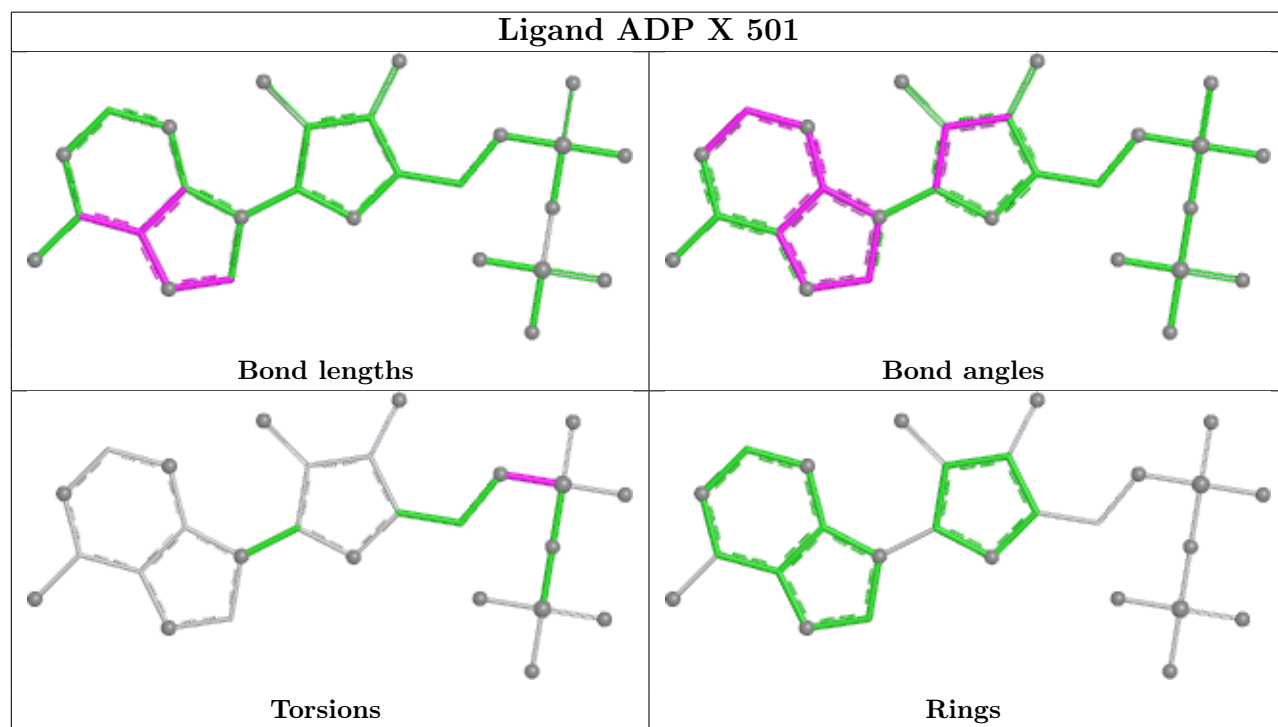
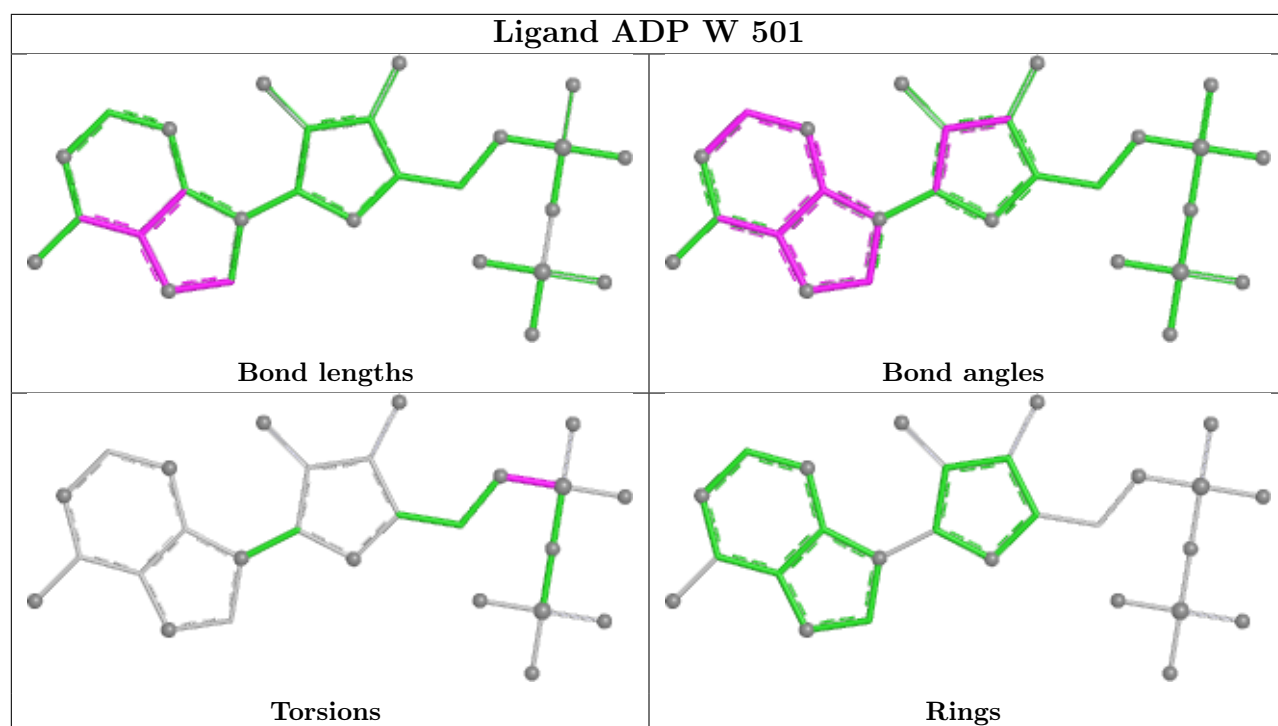
10 monomers are involved in 28 short contacts:

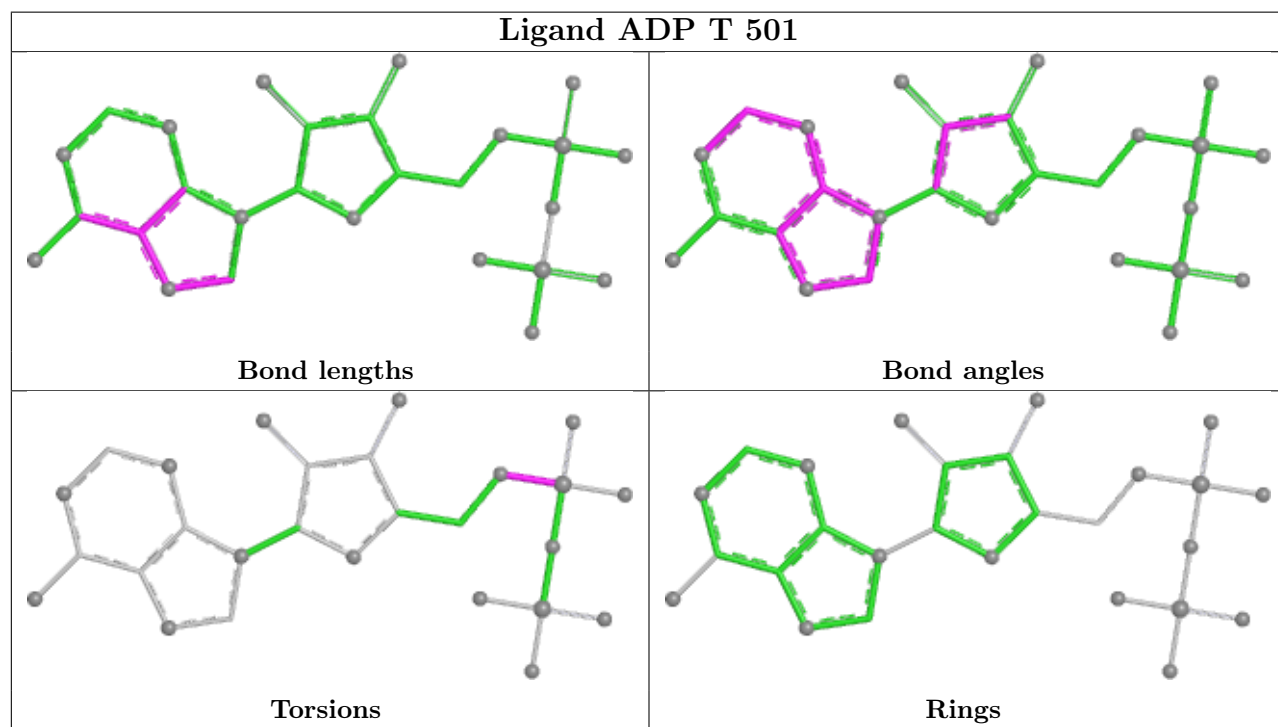
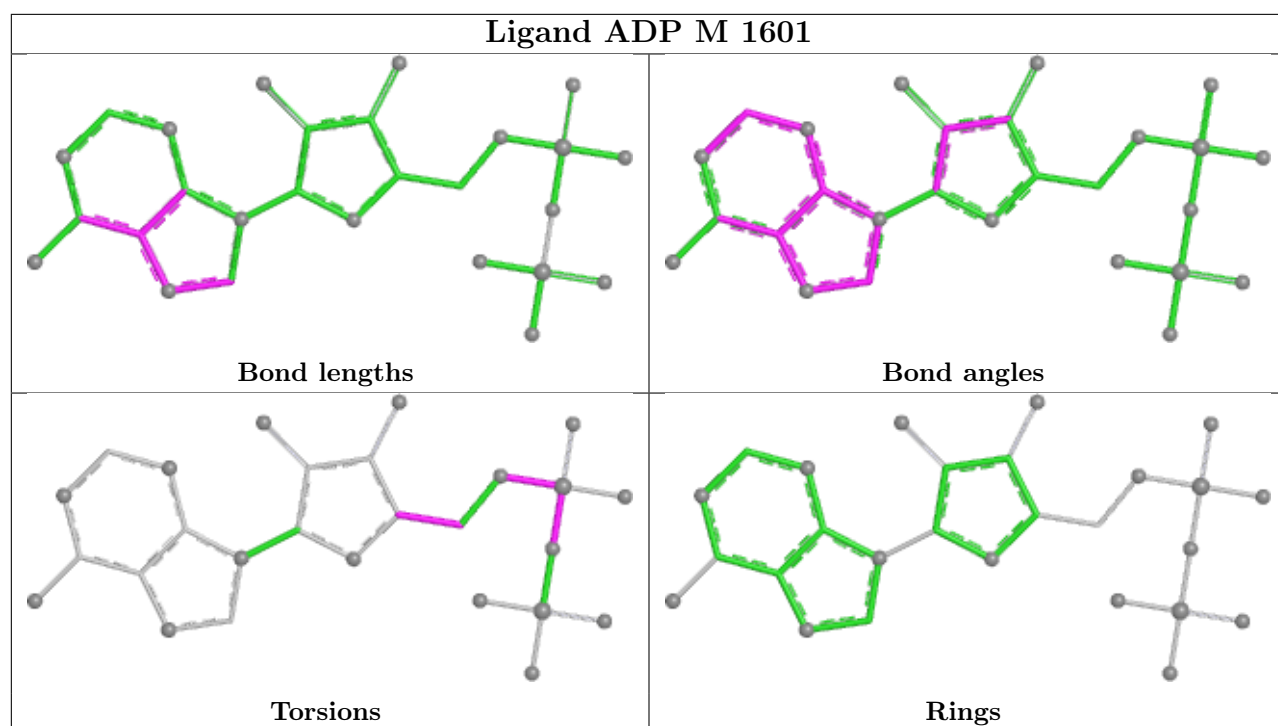
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	R	501	ADP	5	0
17	W	501	ADP	4	0
17	X	501	ADP	4	0
17	M	1601	ADP	2	0
17	T	501	ADP	4	0
17	V	501	ADP	5	0
18	R	502	BEF	1	0
17	Y	501	ADP	1	0
18	M	1602	BEF	2	0
17	U	501	ADP	2	0

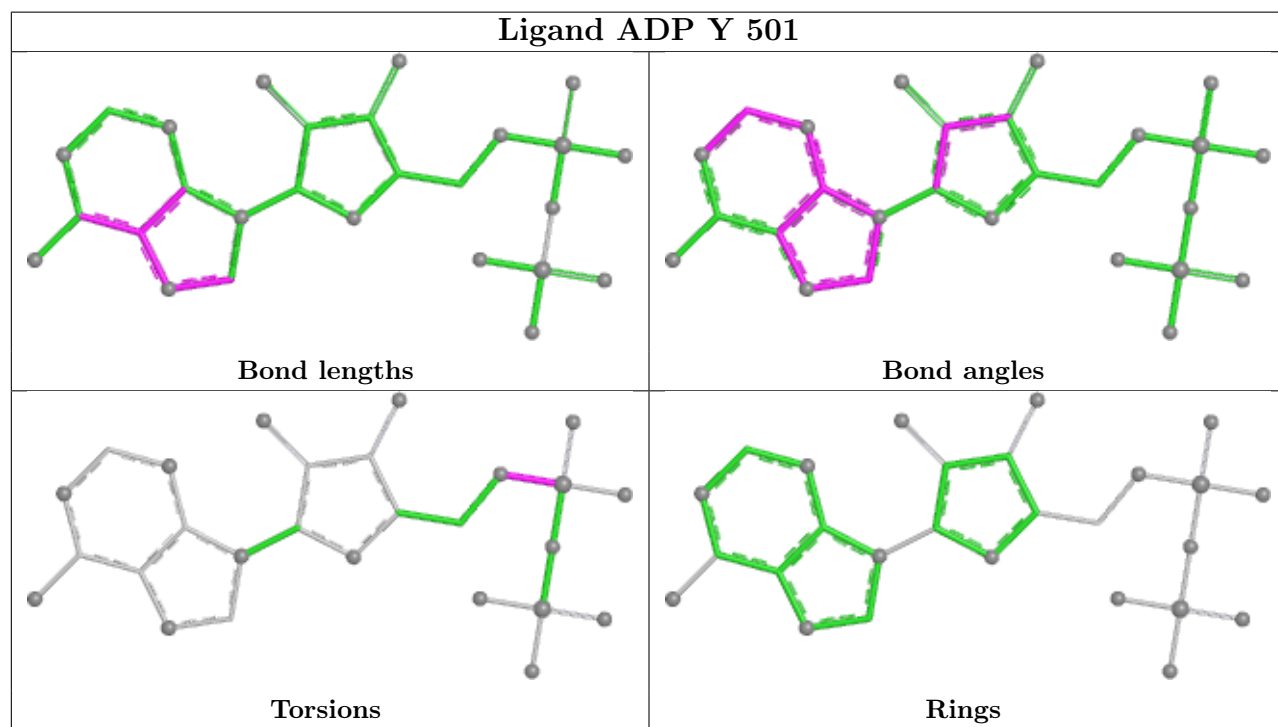
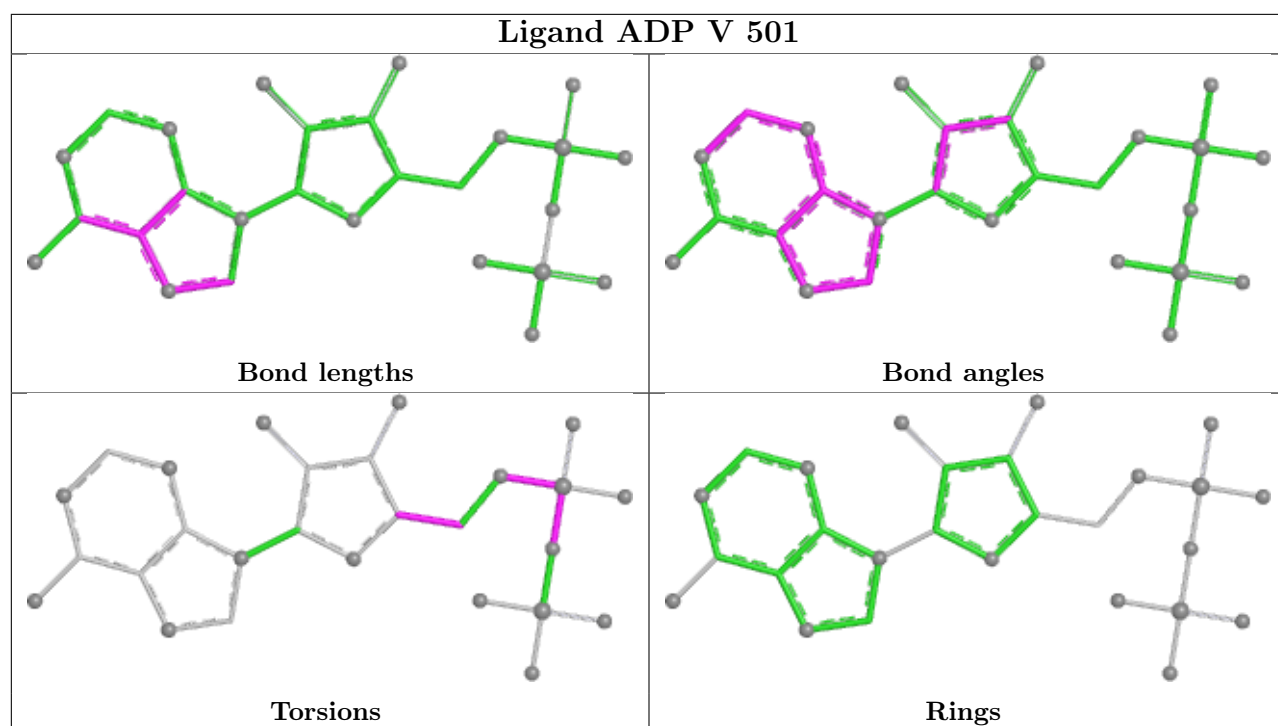
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

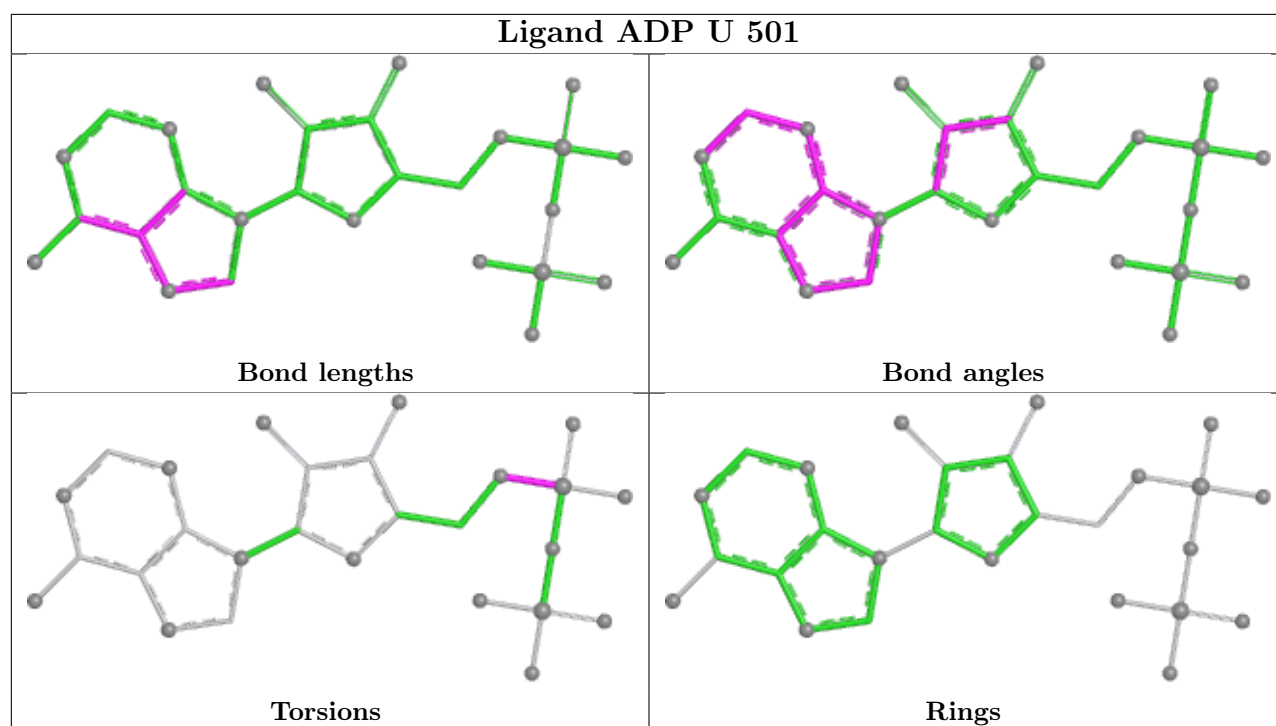
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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](#)

There are no chain breaks in this entry.

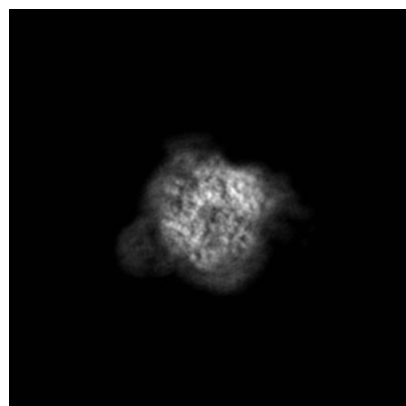
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18769. These allow visual inspection of the internal detail of the map and identification of artifacts.

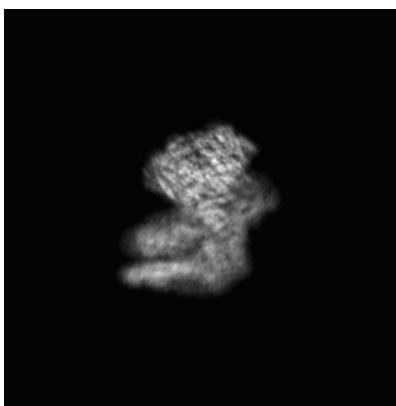
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

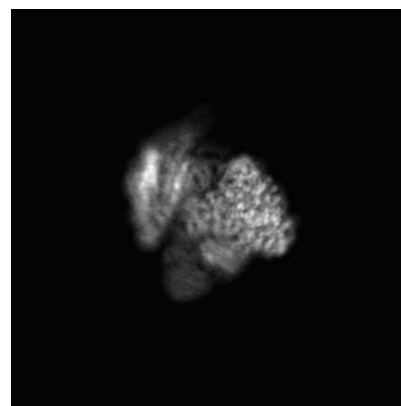
6.1.1 Primary map



X

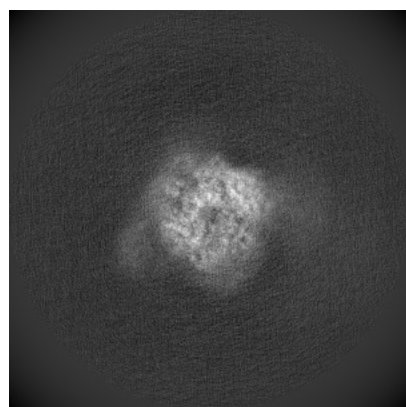


Y

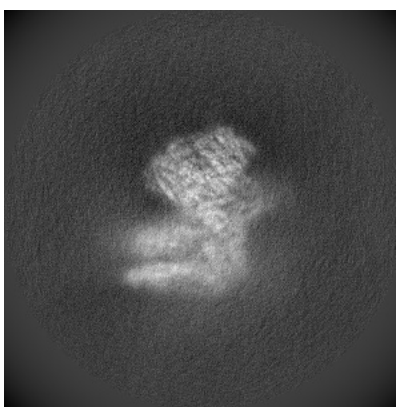


Z

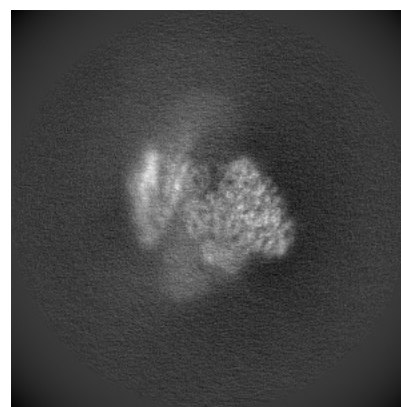
6.1.2 Raw map



X



Y

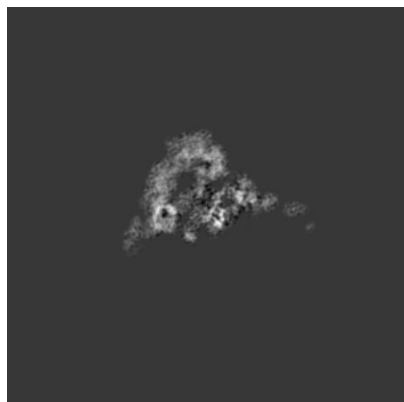


Z

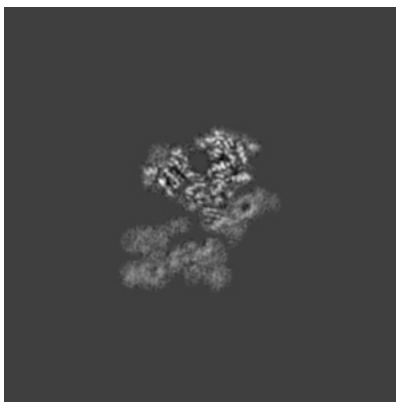
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

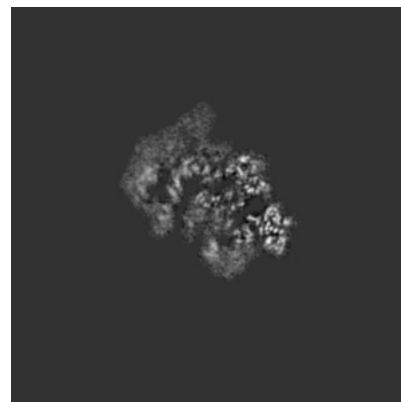
6.2.1 Primary map



X Index: 240

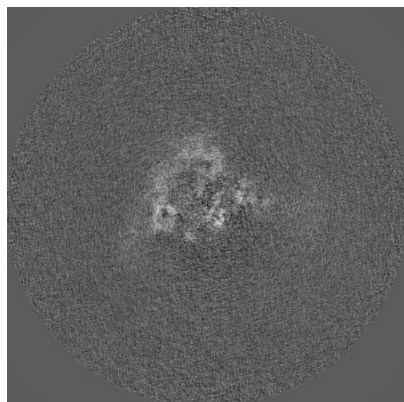


Y Index: 240

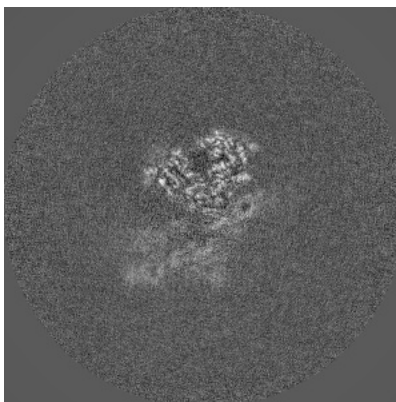


Z Index: 240

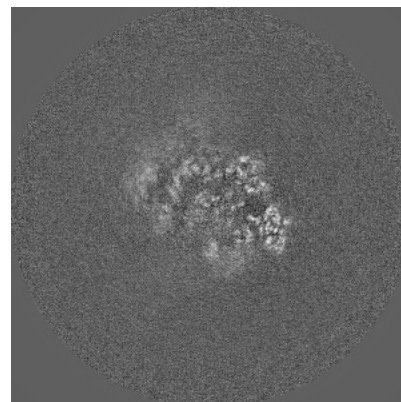
6.2.2 Raw map



X Index: 240



Y Index: 240

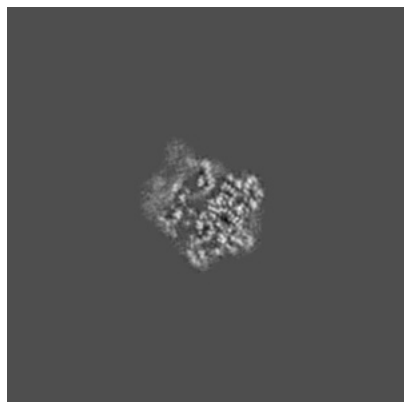


Z Index: 240

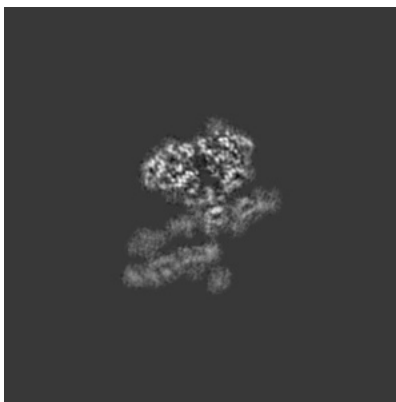
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

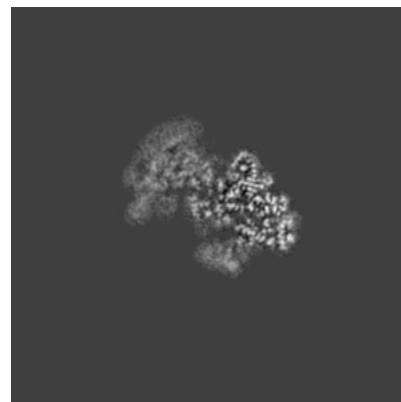
6.3.1 Primary map



X Index: 276

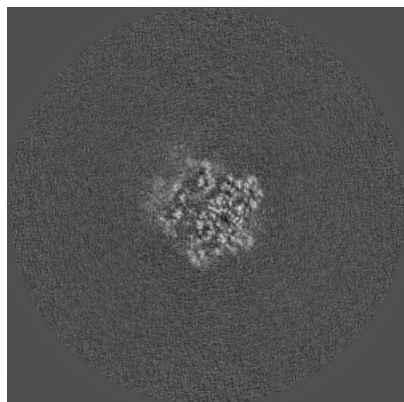


Y Index: 231

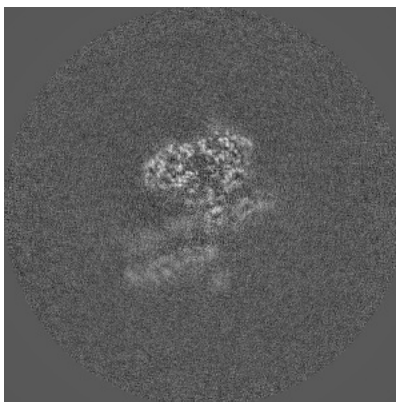


Z Index: 258

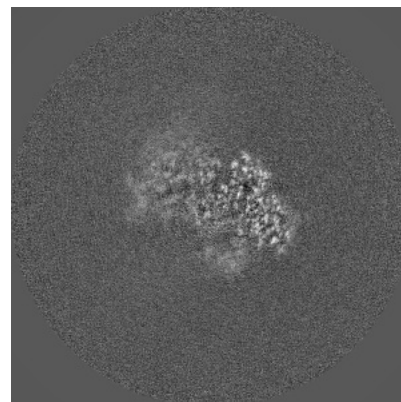
6.3.2 Raw map



X Index: 276



Y Index: 231

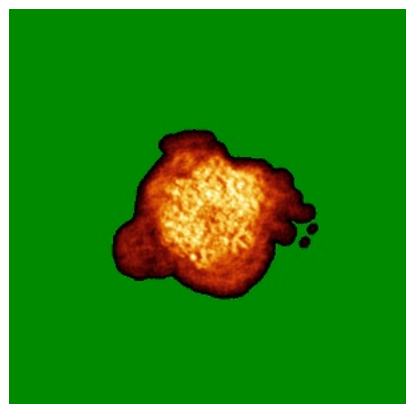


Z Index: 252

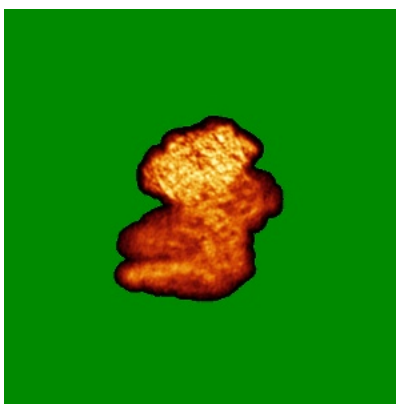
The images above show the largest variance slices of the map in three orthogonal directions.

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

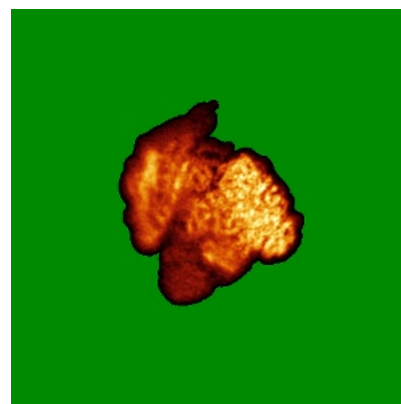
6.4.1 Primary map



X

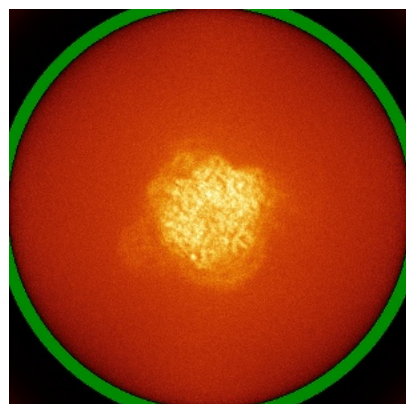


Y

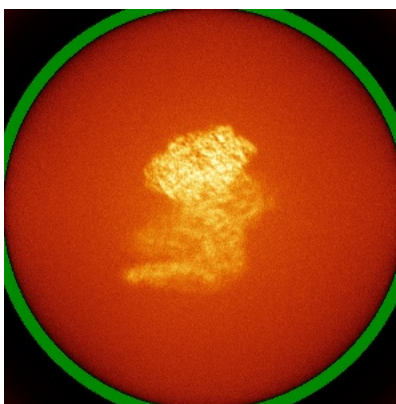


Z

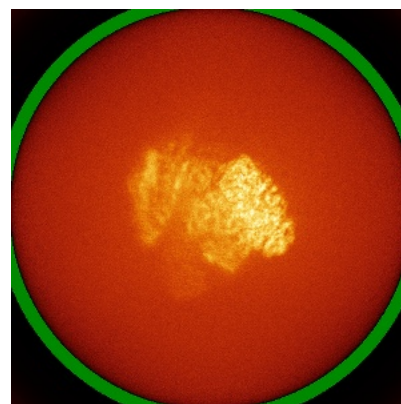
6.4.2 Raw map



X



Y

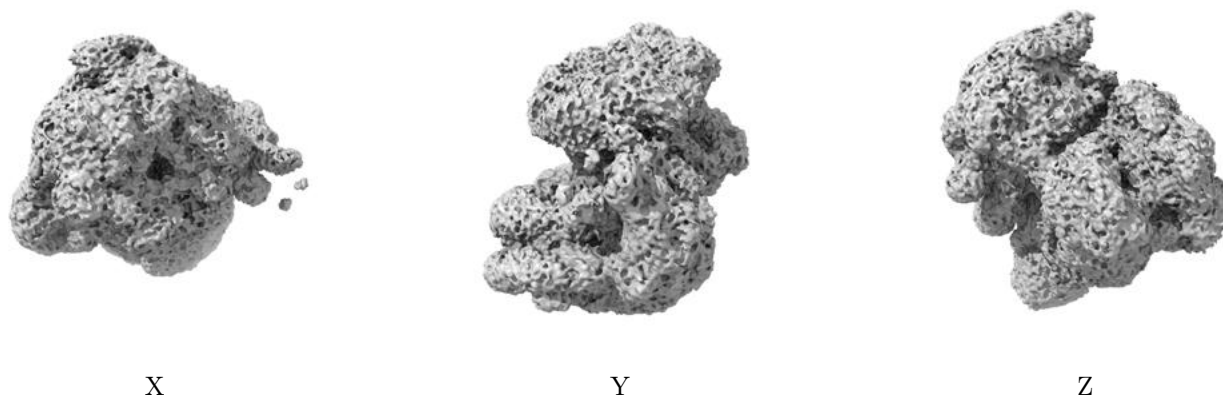


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.00126. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

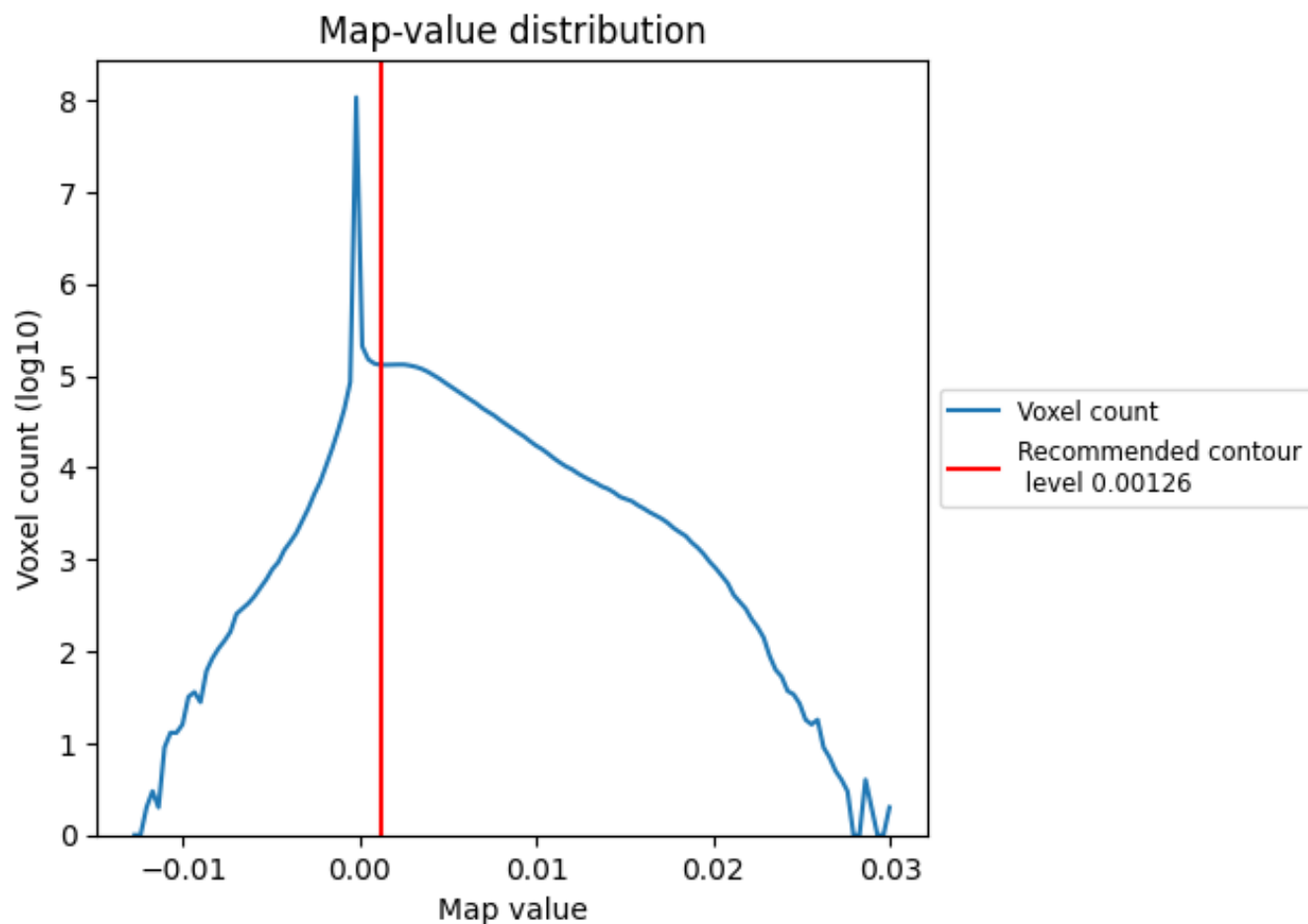
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

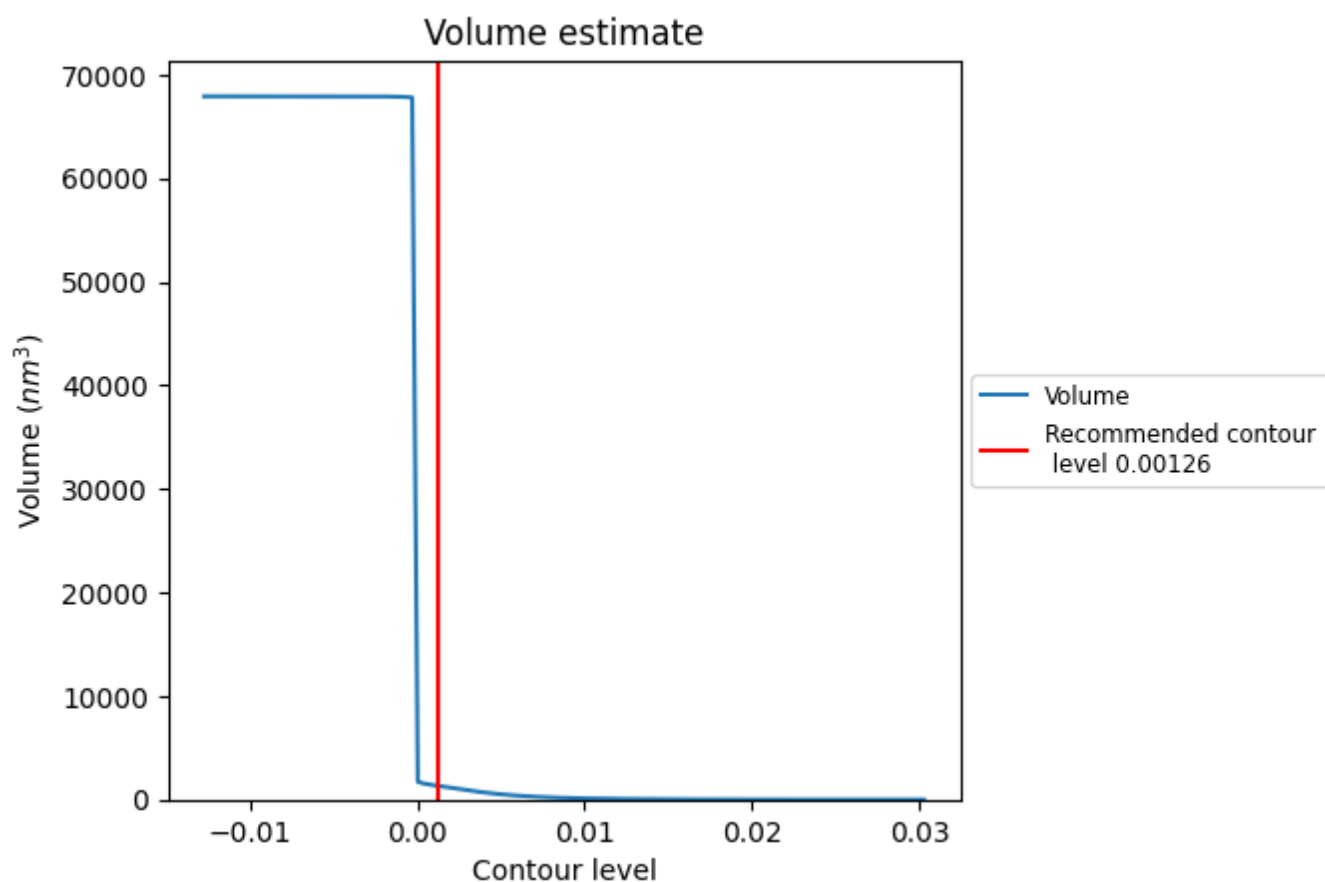
This section contains the results of statistical analysis of the map.

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.

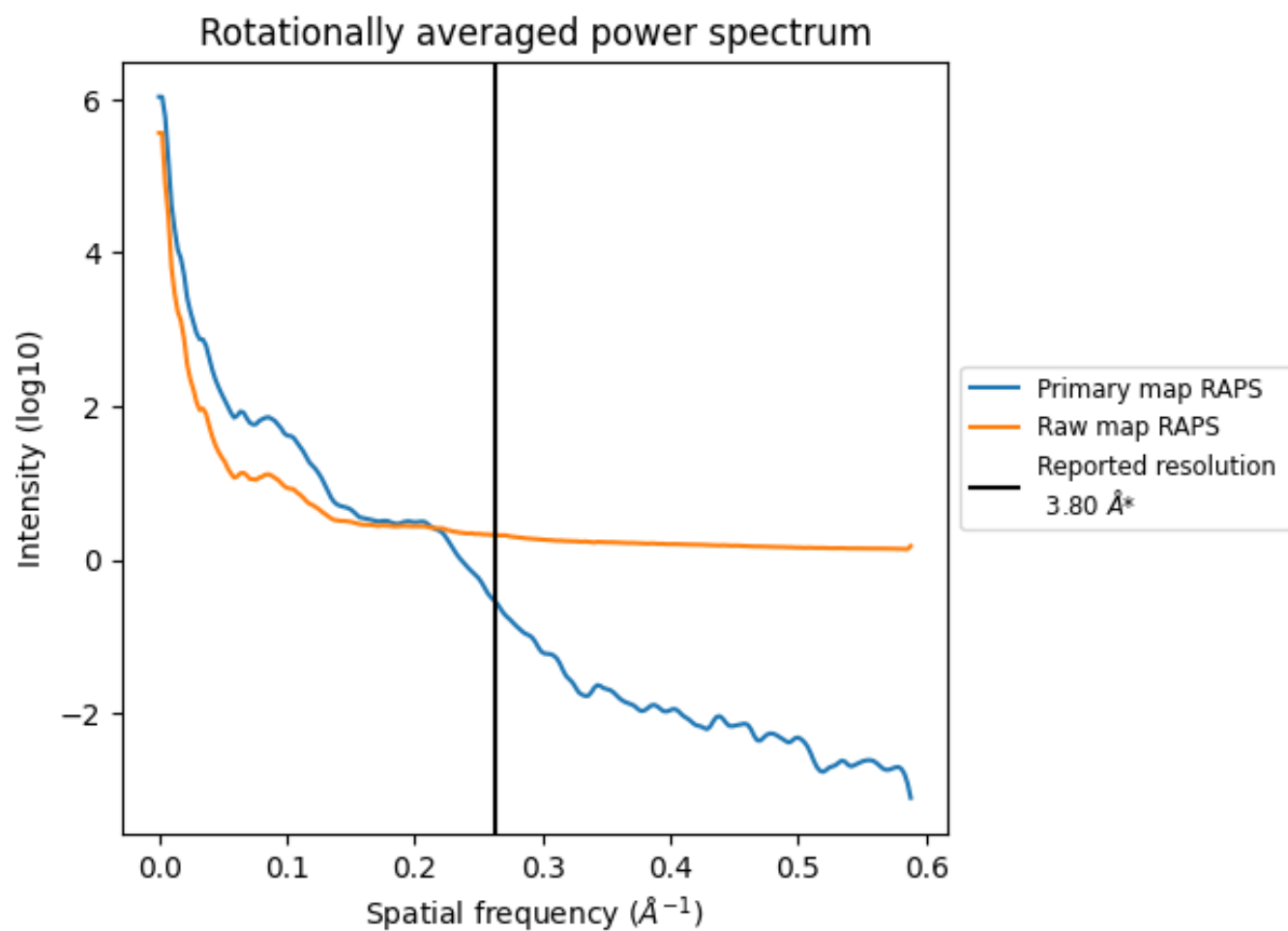
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1321 nm³; this corresponds to an approximate mass of 1193 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 ⓘ

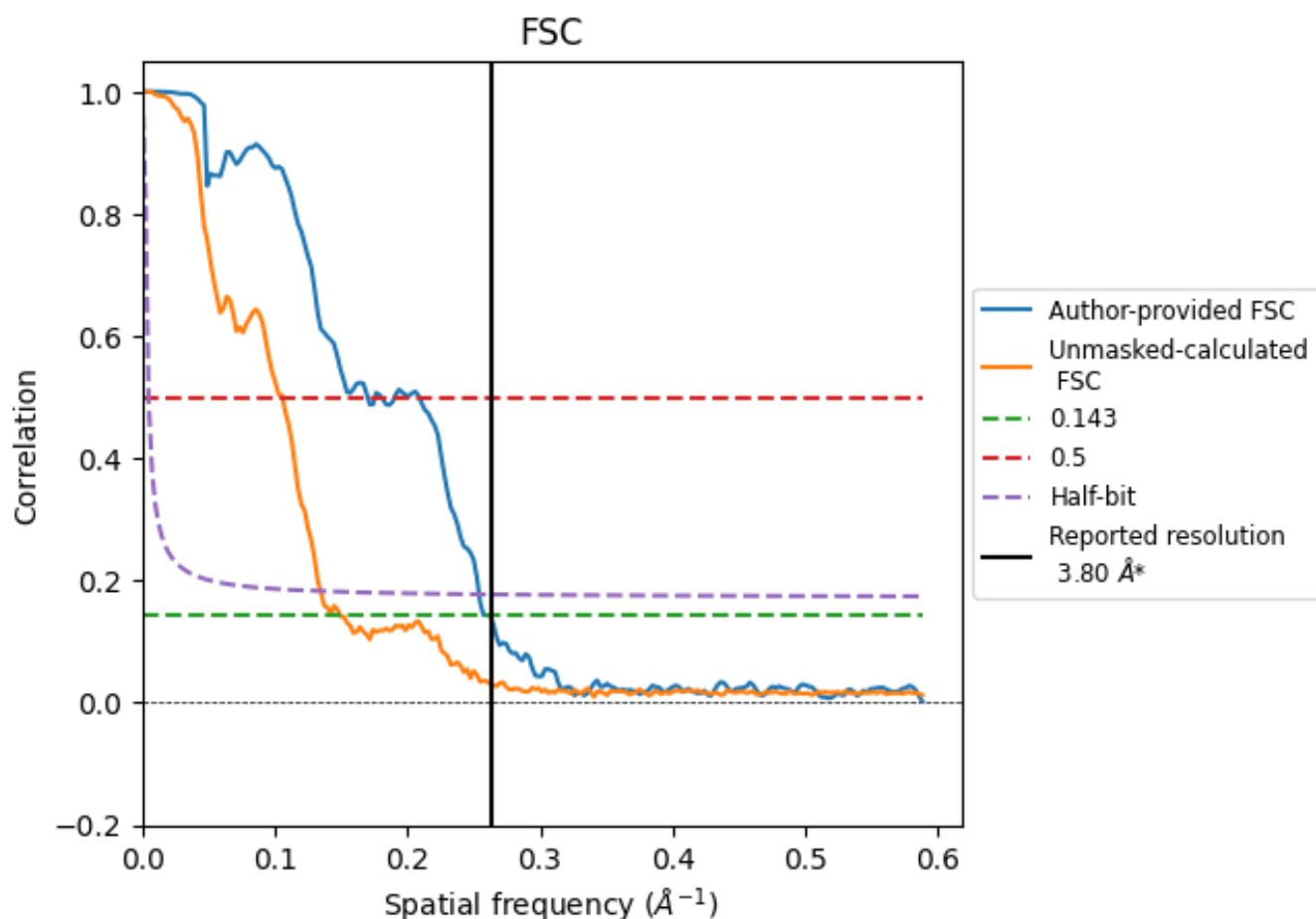


*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

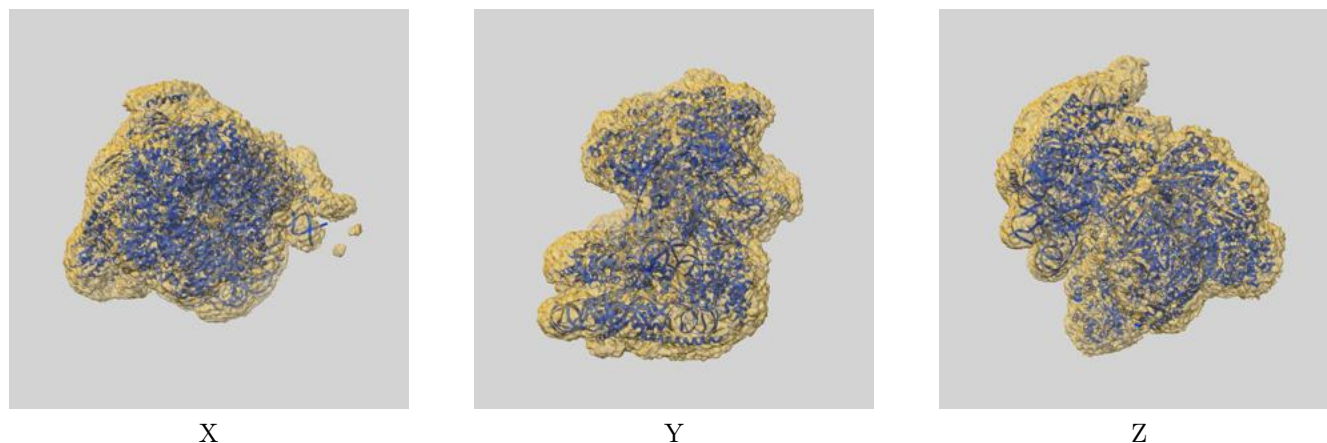
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.81	5.88	3.94
Unmasked-calculated*	6.71	9.46	7.43

*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 6.71 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-18769 and PDB model 8QZ0. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.00126 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](#)



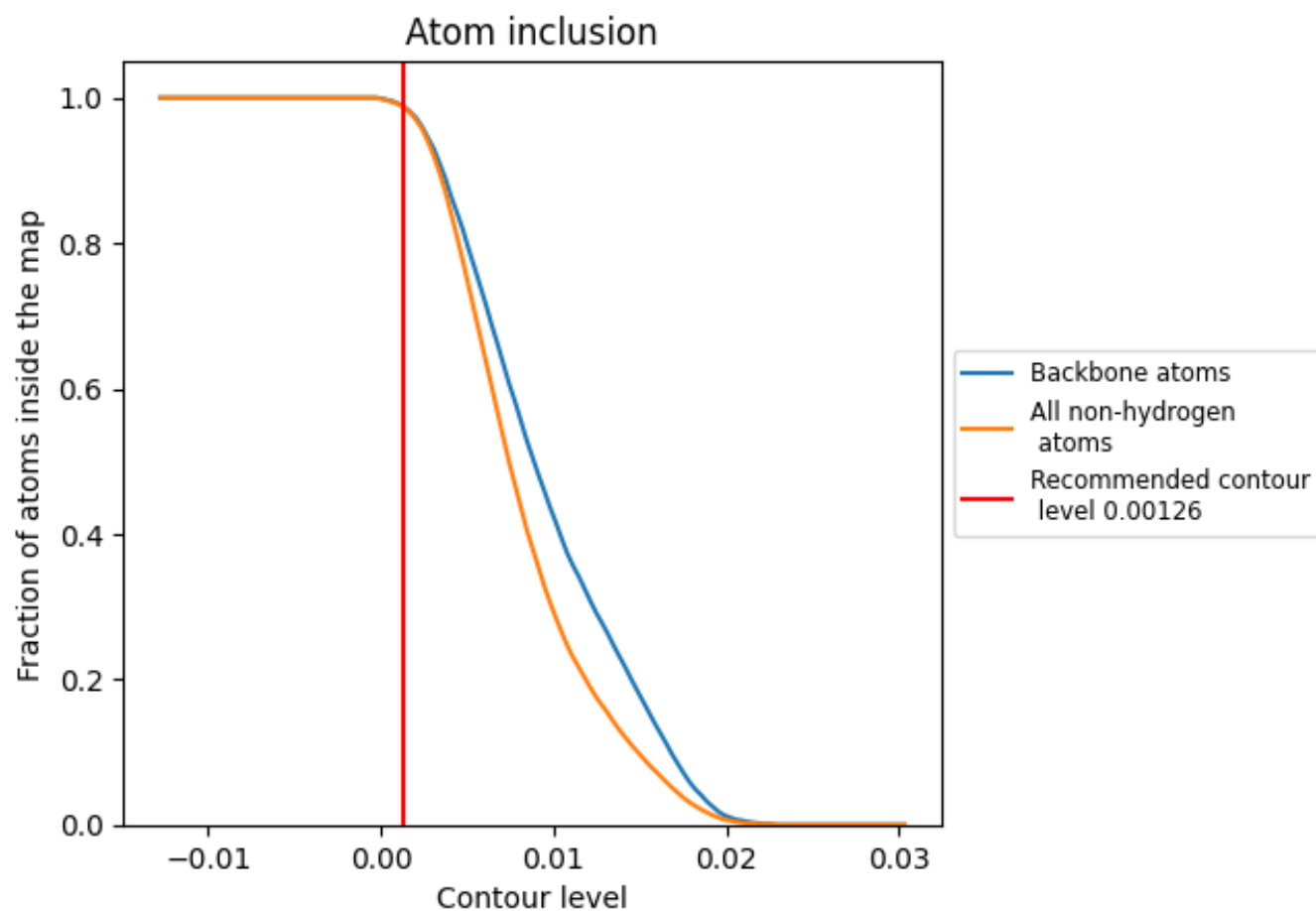
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00126).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.00126) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9880	 0.2930
A	 0.9810	 0.1980
B	 0.9790	 0.2680
C	 0.9910	 0.2440
D	 0.9980	 0.1990
E	 1.0000	 0.2110
G	 1.0000	 0.2280
H	 0.9930	 0.1740
I	 0.9900	 0.1960
J	 0.9880	 0.1900
K	 0.9480	 0.1350
L	 0.9880	 0.1420
M	 0.9880	 0.2750
P	 0.9790	 0.2670
R	 0.9620	 0.1580
S	 0.9060	 0.1520
T	 0.9990	 0.3730
U	 0.9860	 0.3760
V	 1.0000	 0.4200
W	 1.0000	 0.3980
X	 1.0000	 0.3790
Y	 0.9990	 0.3840
Z	 0.9990	 0.2230

