



wwPDB EM Validation Summary Report ⓘ

Aug 26, 2026 – 07:27 am BST

PDB ID : 9FBW / pdb_00009fbw
EMDB ID : EMD-50297
Title : SWR1 lacking Swc5 subunit in complex with hexasome
Authors : Jalal, A.S.B.; Wigley, D.B.
Deposited on : 2024-05-14
Resolution : 4.40 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.dev133
Mogul : 1.8.4, CSD as541be (2020)
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) : 2.50

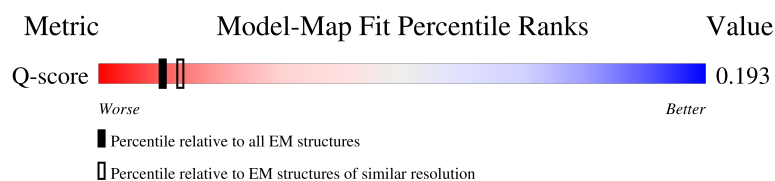
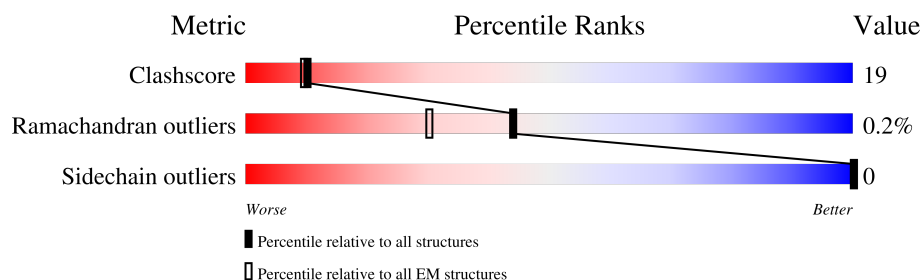
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 (3.91 - 4.90)

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	

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Mol	Chain	Length	Quality of chain
3	E	132	
4	G	131	
5	I	112	
6	J	112	
7	M	1514	
8	R	438	
9	S	280	
10	T	463	
10	V	463	
10	X	463	
11	U	471	
11	W	471	
11	Y	471	
12	Z	795	

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
14	BEF	M	1602	-	-	X	-
14	BEF	R	502	-	-	X	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 39683 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	75	Total	C	N	O	0	0
			612	390	113	109		
1	B	97	Total	C	N	O	0	0
			762	485	147	130		

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	79	Total	C	N	O	0	0
			605	383	113	109		
2	D	66	Total	C	N	O	0	0
			487	308	93	86		

- 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	67	Total	C	N	O	S	0	0
			498	311	85	101	1		

- Molecule 5 is a DNA chain called DNA (112-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	112	Total	C	N	O	P	0	0
			2281	1081	416	672	112		

- Molecule 6 is a DNA chain called DNA (112-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	112	Total	C	N	O	P	0	0
			2311	1091	436	672	112		

- Molecule 7 is a protein called Helicase SWR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	673	Total	C	N	O	S	0	0
			5248	3343	930	949	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	190	Total	C	N	O	S	0	0
			1536	971	271	285	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	T	439	Total	C	N	O	S	0	0
			3313	2090	573	640	10		
10	V	426	Total	C	N	O	S	0	0
			3245	2049	558	628	10		
10	X	441	Total	C	N	O	S	0	0
			3371	2128	581	653	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	U	446	Total	C	N	O	S	0	0
			3424	2140	592	680	12		

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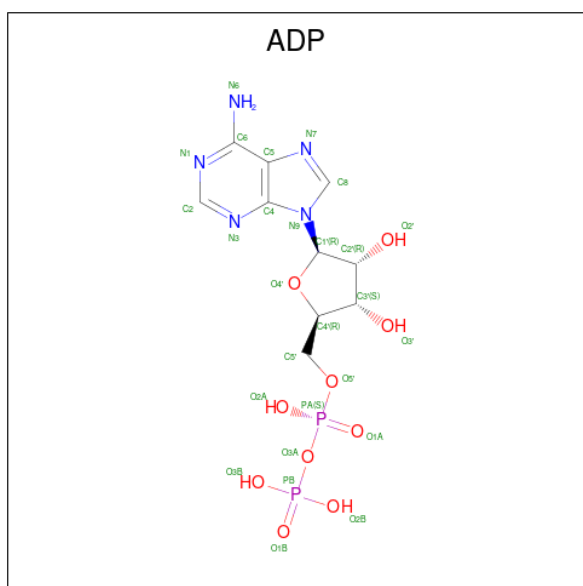
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Mol	Chain	Residues	Atoms					AltConf	Trace
11	W	433	Total	C	N	O	S	0	0
			3303	2074	569	649	11		
11	Y	443	Total	C	N	O	S	0	0
			3342	2091	581	659	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	134	Total	C	N	O	S	0	0
			1061	663	191	203	4		

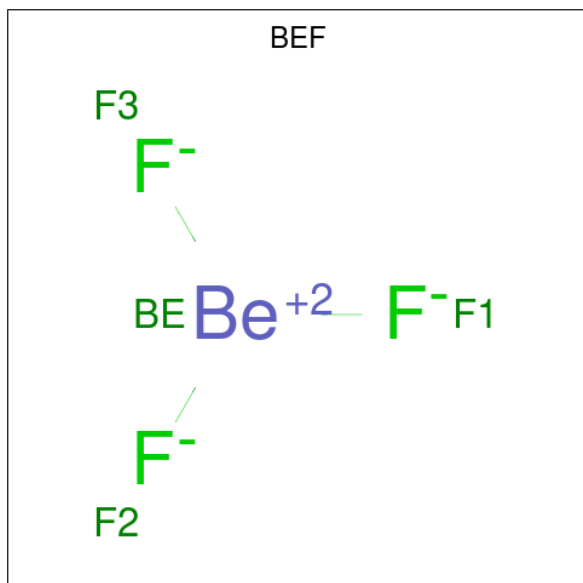
- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					AltConf
13	X	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	Y	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 14 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃) (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	

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Mol	Chain	Residues	Atoms		AltConf
15	W	1	Total 1	Mg 1	0
15	X	1	Total 1	Mg 1	0
15	Y	1	Total 1	Mg 1	0

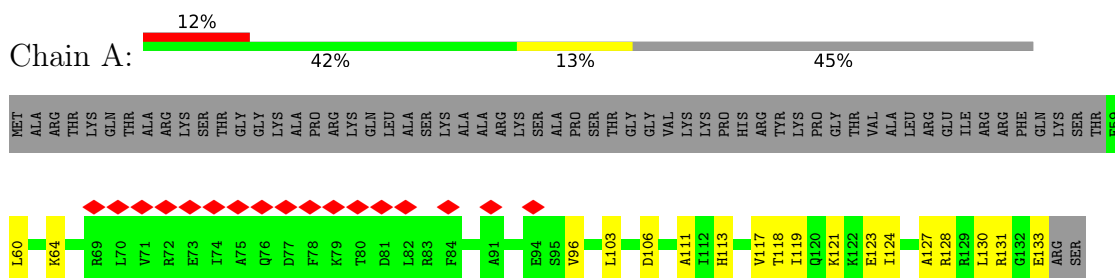
- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

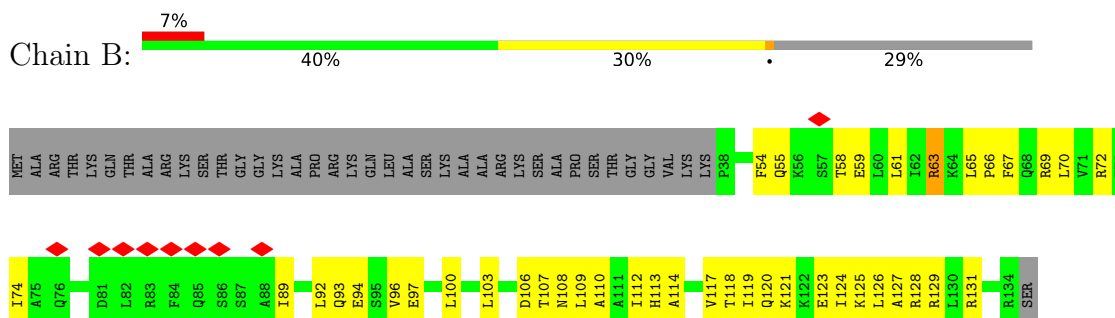
3 Residue-property plots [i](#)

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

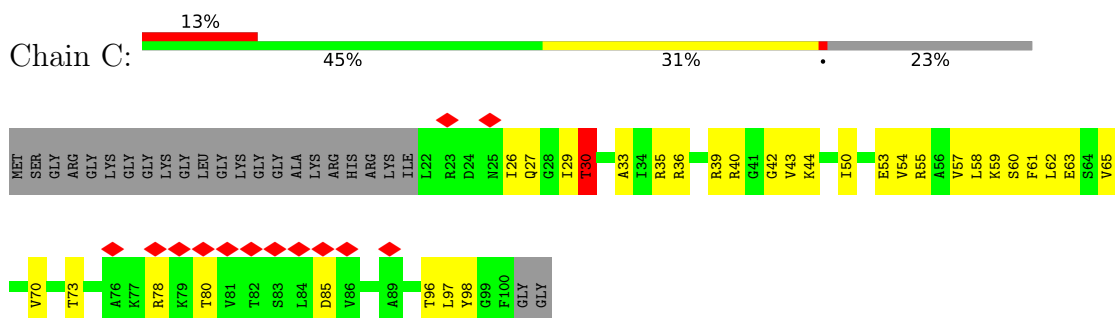
- Molecule 1: Histone H3



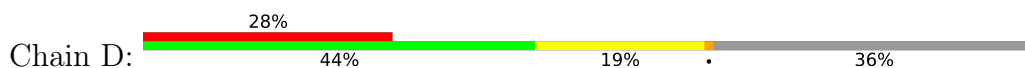
- Molecule 1: Histone H3



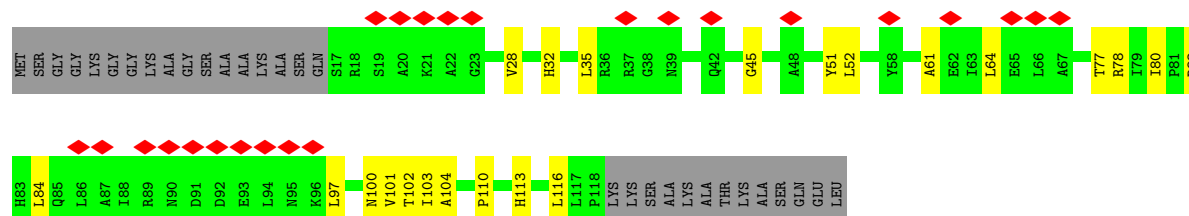
- Molecule 2: Histone H4



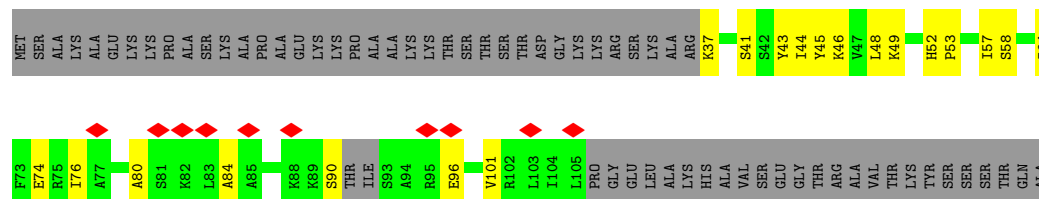
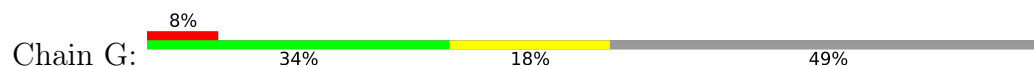
- Molecule 2: Histone H4



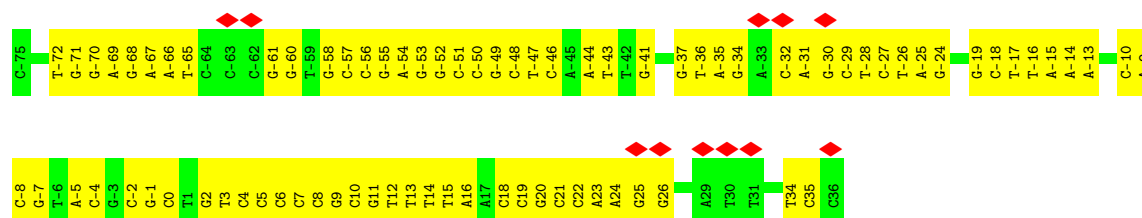
- Molecule 3: Histone H2A.1



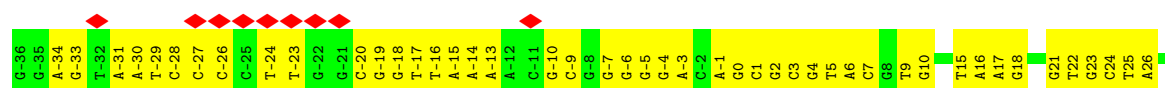
- Molecule 4: Histone H2B.1



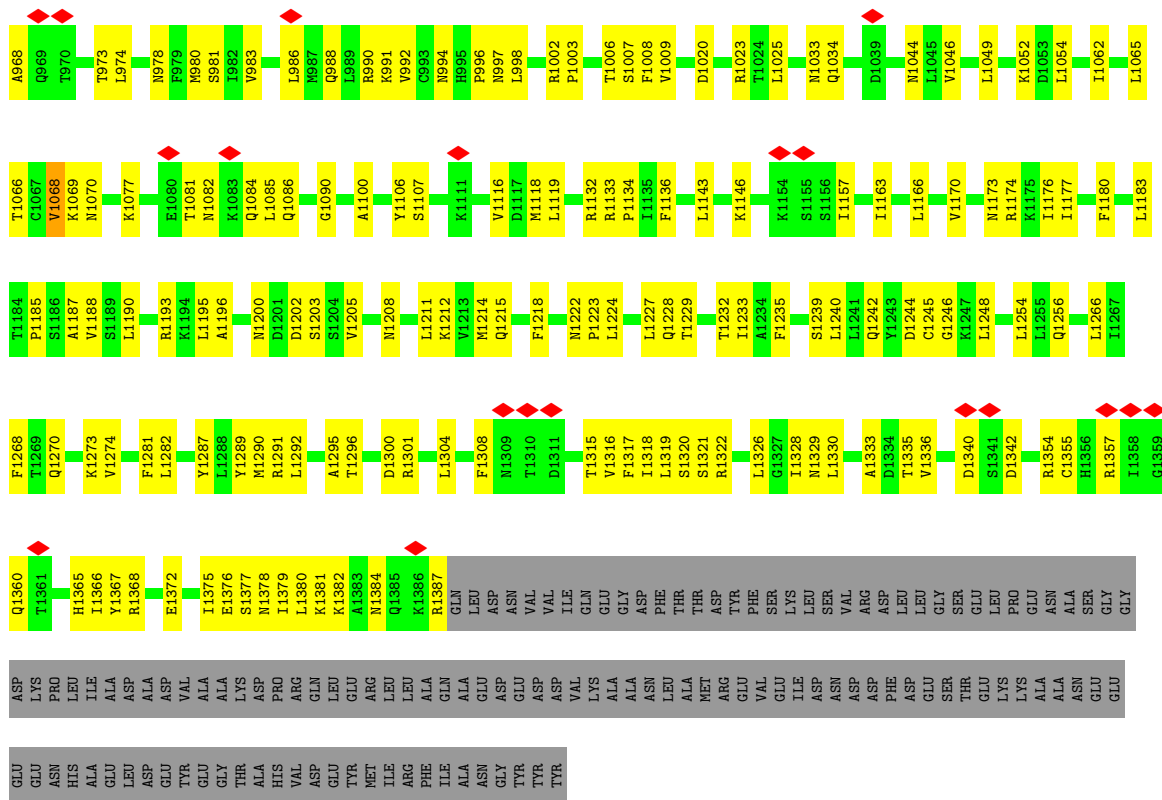
- Molecule 5: DNA (112-MER)



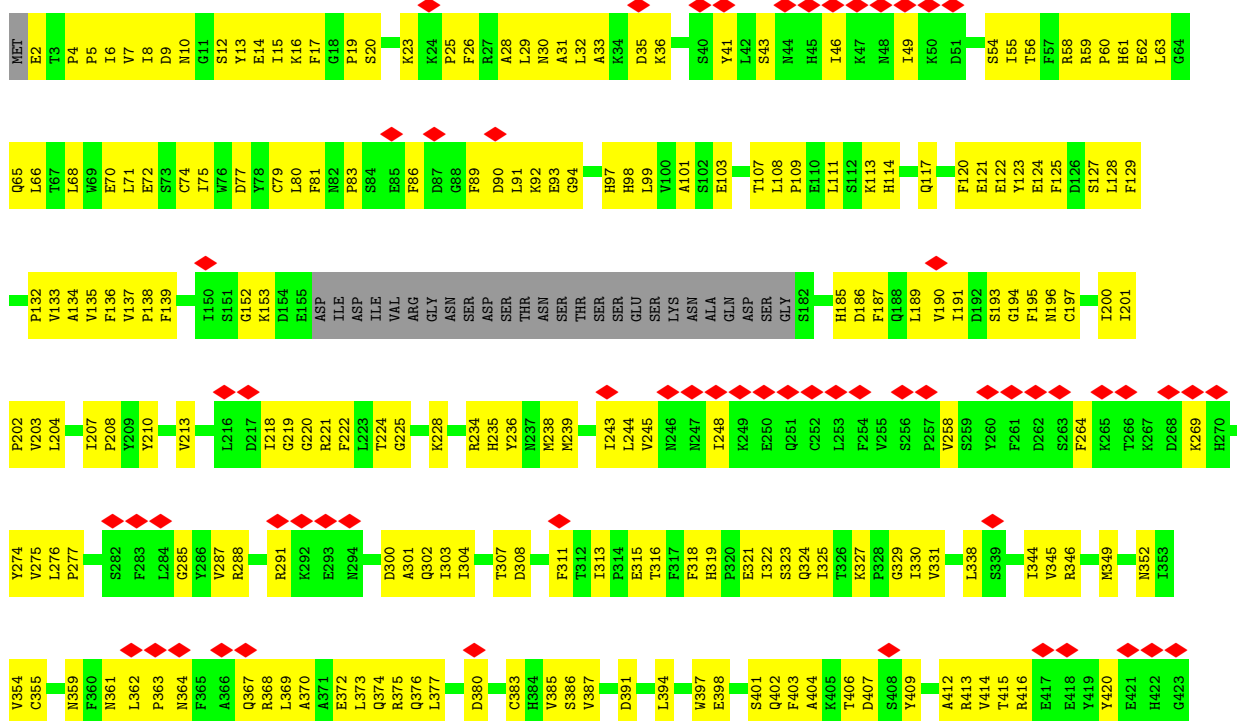
- Molecule 6: DNA (112-MER)



PHE	W818	A739	ASN	GLY	SER	ASP	TRP	HIS	ARG	LYS	ALA	ALA	LEU	MET
GLY	Q819	C740	ARG	SER	THR	VAL	ASN	MET	LEU	ARG	GLU	PRO	GLU	THR
ARG	E741	E740	ASP	THR	THR	LEU	MET	LEU	VAL	GLY	LEU	LEU	GLU	ARG
PRO	M821	C742	ILE	ALA	VAL	SER	ALA	LYS	GLY	LYS	TYR	VAL	THR	ARG
VAL	W822	E743	ILE	LEU	TYR	SER	GLU	LEU	GLY	ILE	LEU	ASN	LEU	HIS
ASP	L823	W744	LYS	PHE	ASP	SER	LYS	PHE	ILE	LEU	ASP	ASN	LEU	LYS
L824	D824	W745	ASP	GLY	SER	ASP	ALA	ARG	GLU	GLY	HIS	SER	SER	LYS
LYS	D825	E825	VAL	LYS	ARG	ASP	ASP	SER	ASN	VAL	ILE	CYS	LEU	SER
ILE	E825	E825	VAL	GLY	ARG	ASP	ASP	ARG	ASN	VAL	ILE	CYS	LEU	SER
ILE	A826	L749	GLY	GLY	ASN	ASP	ARG	LYS	GLY	HIS	ALA	GLU	GLU	ALA
THR	H827	L750	GLU	GLU	GLY	MET	ILE	THR	ALA	PRO	LYS	GLU	GLU	GLU
GLY	W828	W751	ASP	GLU	ASP	ASP	ARG	LYS	LEU	PRO	VAL	ARG	GLY	LYS
GLN	L829	E752	ALA	SER	GLU	ASP	ARG	ALA	LEU	LYS	GLU	LYS	GLY	LYS
ASN	E832	P753	GLY	ASP	LYS	GLU	LYS	ARG	TYR	GLN	GLU	TYR	GLU	LYS
ASN	R833	L757	THR	GLY	PHE	LEU	ASP	ILE	ASP	THR	PRO	GLU	GLU	ALA
PHE	R833	L758	LYS	ASP	PRO	LEU	GLU	ALA	LYS	ILE	GLU	GLU	PHE	LYS
GLY	E836	L759	VAL	ASP	THR	THR	GLU	ARG	GLU	THR	GLU	THR	THR	GLY
GLN	R836	E836	GLN	ASP	LEU	SER	GLN	ALA	THR	ASN	ALA	ASP	THR	ASP
ASP	E836	E836	GLY	LEU	ASP	SER	LEU	LYS	ASP	PRO	PHE	HIS	ASP	GLY
LYS	L840	E763	GLY	ASP	LYS	ASP	LEU	LYS	SER	LEU	THR	SER	VAL	ASP
E913	E840	E764	GLN	ASP	HIS	GLU	LYS	VAL	LEU	HIS	ILE	ASN	ALA	ASP
L921	F843	C785	LEU	SER	GLY	ASP	GLY	SER	GLN	VAL	CYS	ARG	LYS	ALA
H922	H844	R766	GLU	GLY	SER	GLU	GLY	MET	ILE	PRO	LYS	VAL	GLY	LYS
L925	Q846	F767	ASP	PHE	SER	VAL	GLY	ILE	THR	SER	PRO	ILE	THR	LYS
L926	R847	A768	SER	THR	SER	ASP	LYS	GLY	SER	GLY	ASP	VAL	ASN	PHE
P927	R848	C769	LEU	VAL	ASN	ALA	HIS	GLN	GLY	TYR	GLU	PRO	GLY	THR
Y928	L849	F769	LEU	GLY	SER	VAL	ASN	PHE	ILE	SER	SER	LEU	ASP	GLY
L850	L850	G770	ARG	SER	VAL	GLY	SER	LYS	ILE	LEU	PHE	ARG	THR	LEU
L929	L851	L851	GLY	SER	VAL	LEU	LYS	HIS	THR	HIS	GLU	PRO	ARG	LEU
L930	T852	L774	ASN	VAL	THR	GLU	MET	VAL	ILE	GLY	ASN	ILE	ARG	THR
R931	G853	T775	GLY	GLY	GLY	ASN	LEU	VAL	ILE	GLY	ASN	ILE	ARG	THR
R932	G853	T776	GLY	GLY	GLY	ASN	LEU	VAL	ILE	GLY	ASN	ILE	ARG	THR
L933	G853	T777	GLY	GLY	GLY	SER	GLY	ALA	THR	ILE	ASN	ILE	ARG	THR
K934	M859	G778	GLY	GLY	GLY	PRO	LYS	ALA	TYR	ALA	ALA	ASN	LEU	ASN
A935	E862	S779	GLY	GLY	SER	ALA	SER	GLY	LYS	SER	PHE	LYS	LEU	PHE
D936	L863	P780	LEU	LEU	SER	SER	THR	GLY	PRO	PHE	HIS	LYS	ARG	HIS
P937	L863	Q781	GLY	GLY	THR	THR	GLN	GLY	ASP	GLY	SER	LYS	THR	ARG
E938	E868	R783	LYS	LYS	TYR	GLU	LEU	LYS	PRO	SER	SER	ASN	THR	ARG
K939	F869	C784	GLN	GLN	SER	THR	GLU	LYS	SER	GLY	PHE	ALA	VAL	PHE
Q940	T874	E785	VAL	VAL	SER	PRO	ALA	GLY	TYR	ASP	LYS	VAL	VAL	VAL
Q940	T874	E786	ASP	ASP	GLU	THR	GLN	GLY	PHE	ASP	ASP	SER	SER	SER
Q940	W875	R787	ASN	ASN	GLU	ASP	GLN	GLY	TYR	ASP	ASP	SER	SER	SER
A943	E875	K788	SER	SER	GLU	ASN	ASN	GLY	TYR	THR	THR	LEU	SER	VAL
E946	D877	F796	ALA	ALA	GLM	LEU	VAL	HIS	GLN	LYS	PHE	LYS	GLU	GLU
Y950	K879	E878	THR	THR	THR	ASN	ASN	LYS	GLN	GLY	GLY	ASN	ASN	GLY
C951	E878	D877	ASN	ASN	ASN	ASN	ASN	LYS	GLN	GLY	GLY	ASN	ASN	GLY
K952	K879	A720	GLY	GLY	GLY	ILE	ASP	SER	LEU	TYR	GLU	GLU	GLU	GLY
L953	E880	D721	ARG	ARG	ASN	ILE	ASP	LEU	GLN	ASN	GLU	GLU	GLU	GLY
E881	E803	S802	ALA	ALA	ASP	GLY	GLY	LEU	ILE	LYS	ILE	LYS	LYS	LYS
R851	Q804	R804	GLY	GLY	GLU	GLY	LEU	ARG	ALA	HIS	ILE	ILE	ILE	GLY
S852	L805	T728	THR	THR	SER	LYS	SER	SER	PHE	THR	ILE	LYS	LYS	GLY
C883	W806	T729	ASP	PHE	ASP	GLY	GLY	SER	GLY	ASP	LYS	LYS	LYS	GLY
F884	R807	Q807	VAL	VAL	ASP	THR	LYS	THR	TYR	GLY	GLY	GLY	GLY	GLY
A885	Q808	Q808	HIS	HIS	ASP	ASP	LYS	VAL	GLM	GLY	GLY	GLY	GLY	GLY
ASP	LEU	ASP	THR	THR	THR	THR	HIS	VAL	GLN	GLY	GLY	GLY	GLY	GLY
LEU	ASP	F813	GLN	GLN	PRO	PHE	ASP	GLN	GLN	GLY	GLY	GLY	GLY	GLY
ASP	ASP	K814	ASN	ASN	THR	THR	ASN	LYS	GLY	LEU	LEU	LEU	LEU	LEU
ALA	E914	R815	GLY	GLY	VAL	GLY	ASN	ARG	THR	SER	SER	SER	SER	SER
E964	E964	E964	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR

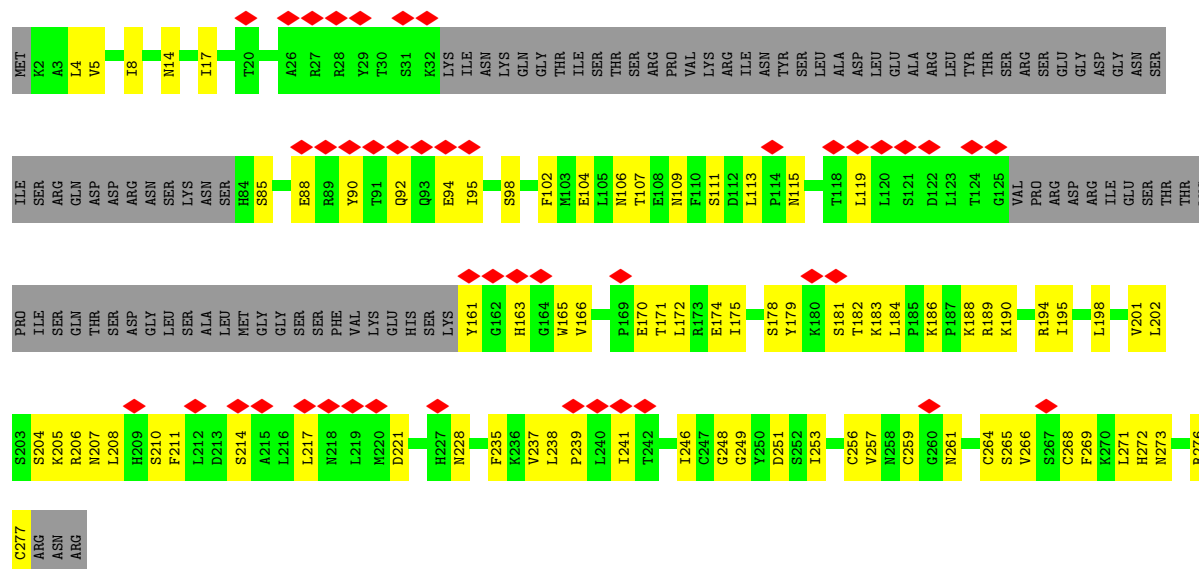


• Molecule 8: Actin-like protein ARP6

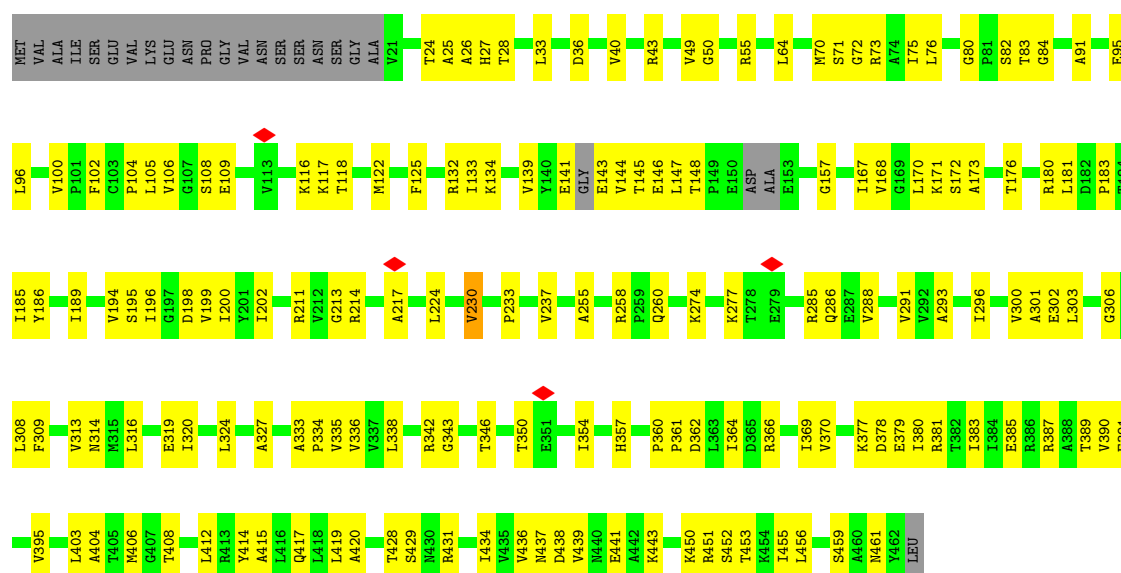




• Molecule 9: Vacuolar protein sorting-associated protein 71

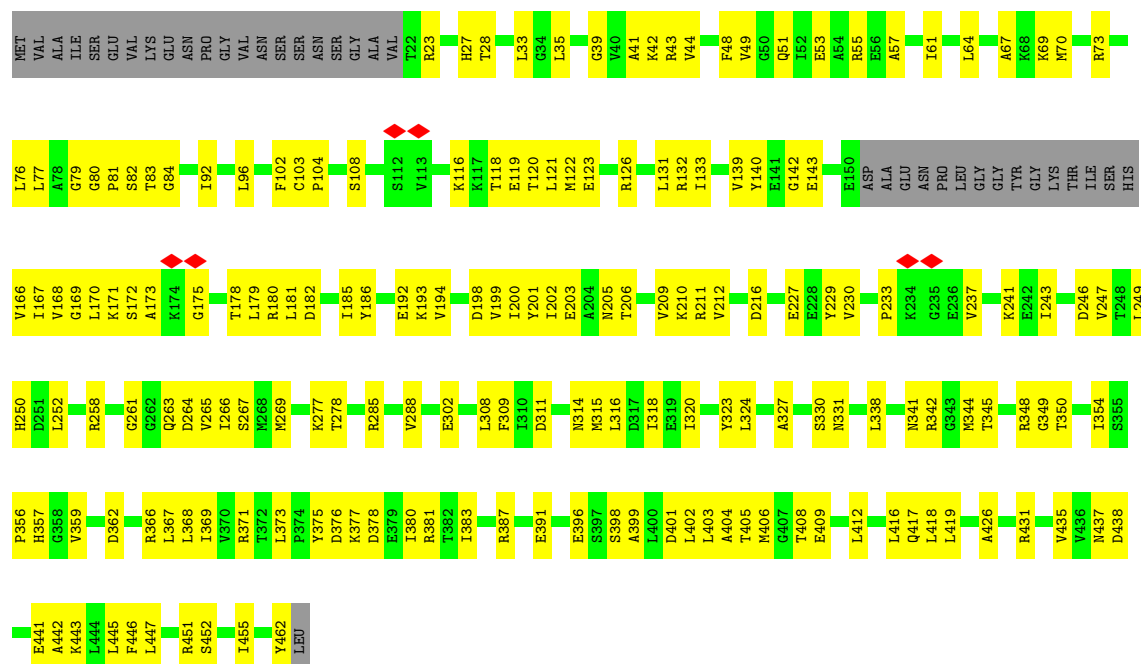


• Molecule 10: RuvB-like protein 1

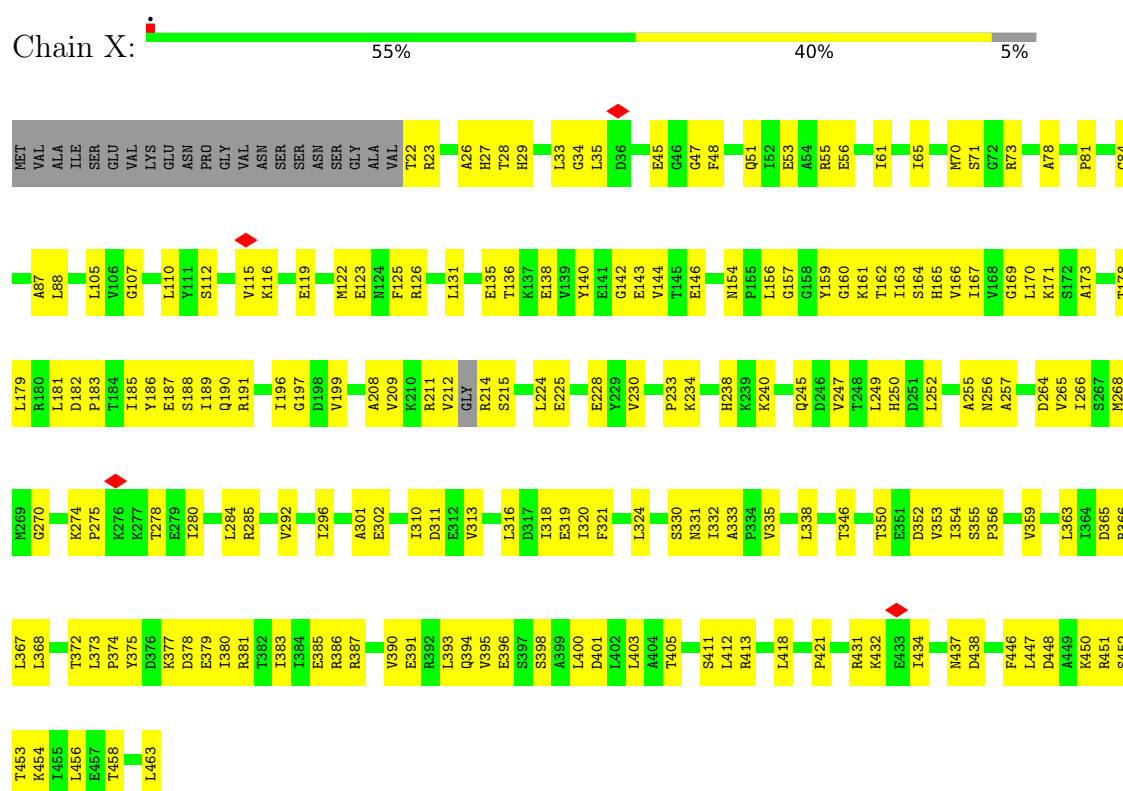


• Molecule 10: RuvB-like protein 1



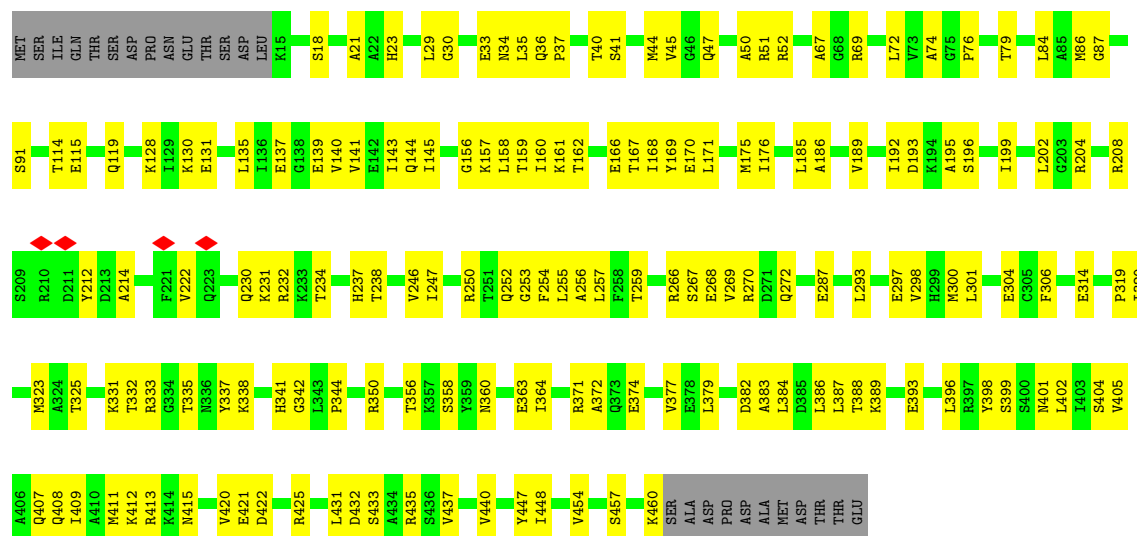


- Molecule 10: RuvB-like protein 1



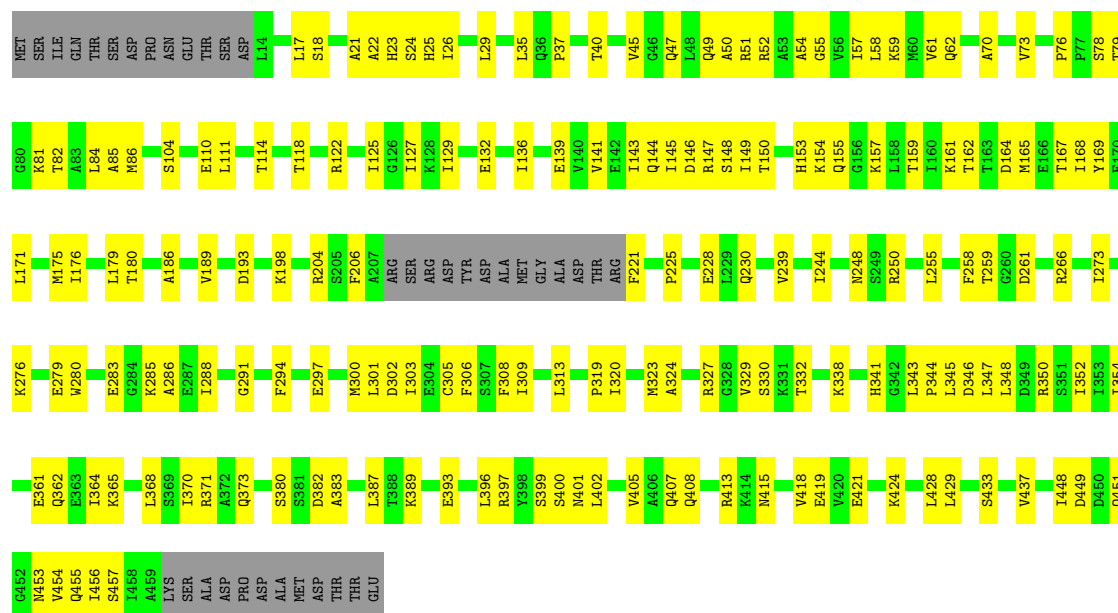
- Molecule 11: RuvB-like protein 2





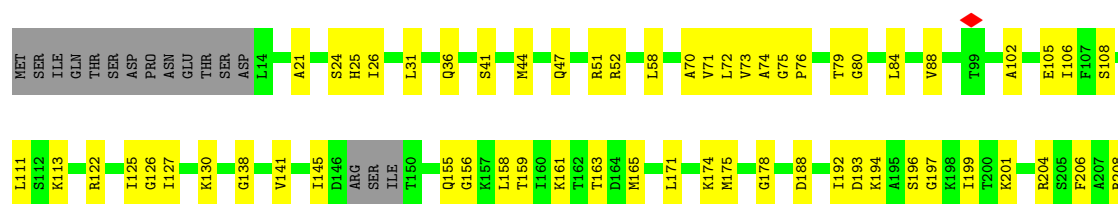
• Molecule 11: RuvB-like protein 2

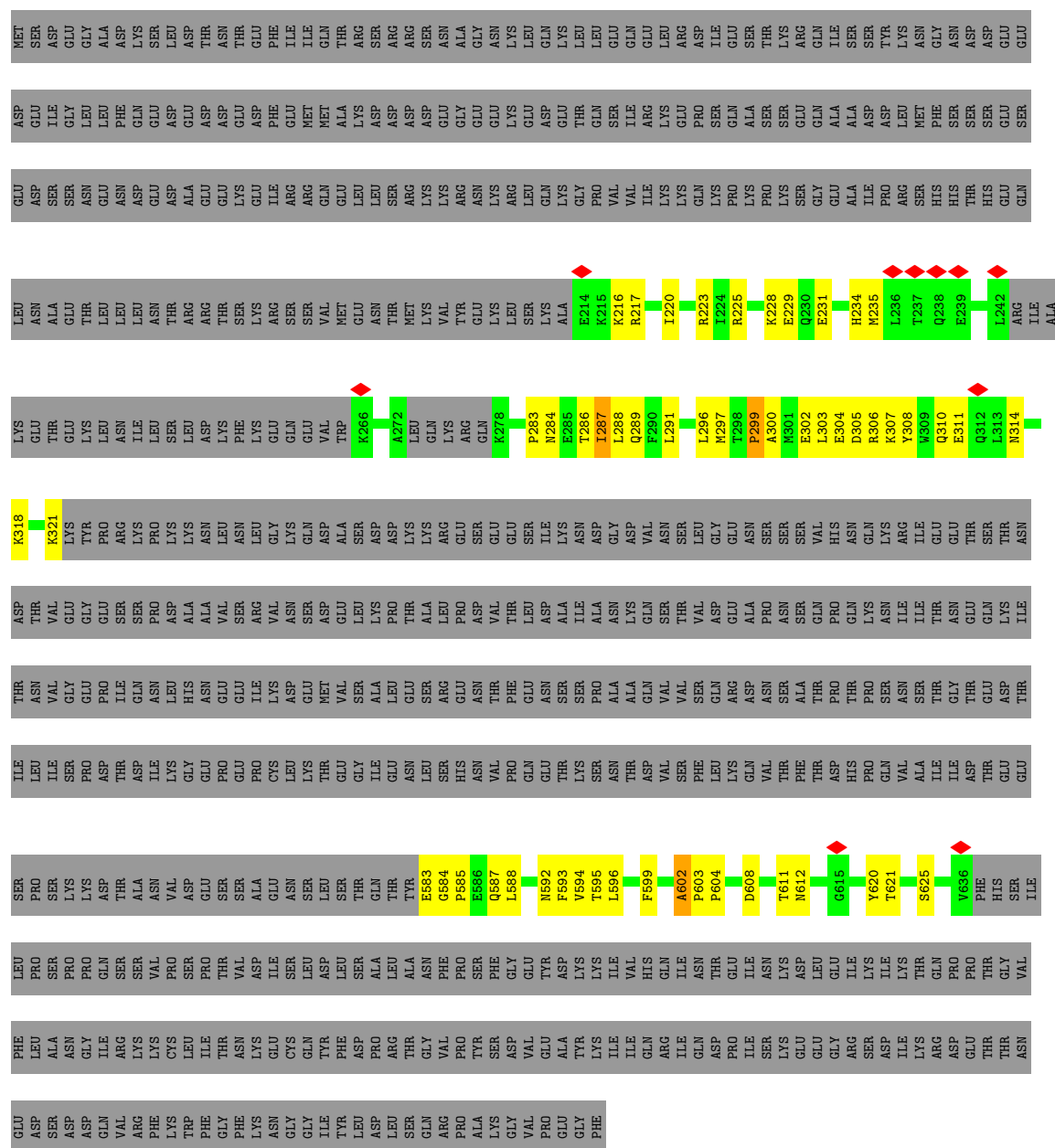
Chain W: 55% 37% 8%



• Molecule 11: RuvB-like protein 2

Chain Y: 62% 32% 6%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57997	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.016	Depositor
Minimum map value	-0.008	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.0011	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, BEF, MG, ZN

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	0.11	0/618	0.29	0/827
1	B	0.13	0/772	0.37	0/1037
2	C	0.15	0/611	0.42	0/823
2	D	0.16	0/491	0.48	0/663
3	E	0.12	0/725	0.35	0/992
4	G	0.12	0/502	0.33	0/677
5	I	0.21	0/2555	0.45	0/3937
6	J	0.21	0/2595	0.39	0/4007
7	M	0.13	0/5342	0.38	0/7236
8	R	0.13	0/3429	0.35	0/4650
9	S	0.12	0/1564	0.40	2/2107 (0.1%)
10	T	0.13	0/3351	0.33	0/4537
10	V	0.13	0/3282	0.34	0/4443
10	X	0.11	0/3412	0.33	0/4618
11	U	0.12	0/3462	0.33	0/4667
11	W	0.12	0/3339	0.34	0/4503
11	Y	0.11	0/3378	0.31	0/4561
12	Z	0.15	0/1076	0.46	0/1446
All	All	0.14	0/40504	0.36	2/55731 (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
1	B	0	1
2	C	0	1
2	D	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
9	S	115	ASN	CA-C-N	5.54	123.73	120.24
9	S	115	ASN	C-N-CA	5.54	123.73	120.24

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	63	ARG	Peptide
2	C	30	THR	Peptide
2	D	40	ARG	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	612	0	650	20	0
1	B	762	0	783	54	0
2	C	605	0	617	50	0
2	D	487	0	502	21	0
3	E	715	0	692	24	0
4	G	498	0	482	21	0
5	I	2281	0	1255	99	0
6	J	2311	0	1255	99	0
7	M	5248	0	5168	223	0
8	R	3335	0	3255	196	0
9	S	1536	0	1547	83	0
10	T	3313	0	3406	119	0
10	V	3245	0	3364	158	0
10	X	3371	0	3486	161	0
11	U	3424	0	3494	141	0
11	W	3303	0	3384	139	0
11	Y	3342	0	3369	118	0
12	Z	1061	0	1014	47	0
13	M	27	0	12	0	0
13	R	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	T	27	0	12	3	0
13	U	27	0	12	1	0
13	V	27	0	12	4	0
13	W	27	0	12	2	0
13	X	27	0	11	3	0
13	Y	27	0	12	4	0
14	M	4	0	0	2	0
14	R	4	0	0	2	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	39683	0	37818	1481	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 19.

The worst 5 of 1481 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:-30:DG:N2	6:J:30:DC:C2	2.37	0.92
5:I:-4:DC:O2	6:J:4:DG:N2	2.03	0.91
9:S:259:CYS:SG	9:S:272:HIS:CE1	2.66	0.88
7:M:778:GLY:HA3	7:M:782:GLN:HB3	1.56	0.87
10:X:131:LEU:HD11	10:X:301:ALA:HB1	1.56	0.86

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	73/136 (54%)	71 (97%)	2 (3%)	0	100	100
1	B	95/136 (70%)	89 (94%)	6 (6%)	0	100	100
2	C	77/103 (75%)	66 (86%)	10 (13%)	1 (1%)	9	41
2	D	64/103 (62%)	54 (84%)	9 (14%)	1 (2%)	7	36
3	E	100/132 (76%)	95 (95%)	5 (5%)	0	100	100
4	G	63/131 (48%)	58 (92%)	5 (8%)	0	100	100
7	M	667/1514 (44%)	589 (88%)	77 (12%)	1 (0%)	48	83
8	R	407/438 (93%)	375 (92%)	32 (8%)	0	100	100
9	S	184/280 (66%)	163 (89%)	21 (11%)	0	100	100
10	T	433/463 (94%)	407 (94%)	25 (6%)	1 (0%)	43	77
10	V	422/463 (91%)	403 (96%)	19 (4%)	0	100	100
10	X	437/463 (94%)	415 (95%)	21 (5%)	1 (0%)	43	77
11	U	444/471 (94%)	412 (93%)	32 (7%)	0	100	100
11	W	429/471 (91%)	410 (96%)	19 (4%)	0	100	100
11	Y	439/471 (93%)	407 (93%)	32 (7%)	0	100	100
12	Z	126/795 (16%)	106 (84%)	16 (13%)	4 (3%)	3	21
All	All	4460/6570 (68%)	4120 (92%)	331 (7%)	9 (0%)	44	77

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	30	THR
7	M	1068	VAL
10	X	208	ALA
12	Z	602	ALA
12	Z	287	ILE

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	65/113 (58%)	65 (100%)	0	100	100
1	B	75/113 (66%)	75 (100%)	0	100	100
2	C	60/81 (74%)	60 (100%)	0	100	100
2	D	48/81 (59%)	48 (100%)	0	100	100
3	E	65/99 (66%)	65 (100%)	0	100	100
4	G	52/109 (48%)	52 (100%)	0	100	100
7	M	553/1376 (40%)	553 (100%)	0	100	100
8	R	372/396 (94%)	372 (100%)	0	100	100
9	S	178/261 (68%)	178 (100%)	0	100	100
10	T	357/391 (91%)	357 (100%)	0	100	100
10	V	354/391 (90%)	354 (100%)	0	100	100
10	X	368/391 (94%)	368 (100%)	0	100	100
11	U	378/403 (94%)	378 (100%)	0	100	100
11	W	364/403 (90%)	364 (100%)	0	100	100
11	Y	359/403 (89%)	359 (100%)	0	100	100
12	Z	110/732 (15%)	110 (100%)	0	100	100
All	All	3758/5743 (65%)	3758 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
11	Y	341	HIS
11	Y	441	GLN
12	Z	592	ASN
8	R	235	HIS
7	M	1378	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 [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	U	502	15	27,29,29	1.36	4 (14%)	42,45,45	1.99	10 (23%)
13	ADP	R	501	8	27,29,29	1.36	4 (14%)	42,45,45	1.94	11 (26%)
13	ADP	M	1601	7,15	27,29,29	1.36	4 (14%)	42,45,45	1.95	11 (26%)
13	ADP	Y	501	15	27,29,29	1.35	4 (14%)	42,45,45	2.02	9 (21%)
13	ADP	W	501	11,15	27,29,29	1.37	4 (14%)	42,45,45	1.98	9 (21%)
13	ADP	V	501	15	27,29,29	1.36	4 (14%)	42,45,45	1.97	10 (23%)
13	ADP	T	501	10	27,29,29	1.36	4 (14%)	42,45,45	2.04	11 (26%)
14	BEF	R	502	-	0,3,3	-	-	-	-	-
13	ADP	X	501	10	27,29,29	1.36	4 (14%)	42,45,45	2.03	9 (21%)
14	BEF	M	1602	-	0,3,3	-	-	-	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	ADP	U	502	15	-	4/16/32/32	0/3/3/3
13	ADP	R	501	8	-	5/16/32/32	0/3/3/3
13	ADP	M	1601	7,15	-	5/16/32/32	0/3/3/3
13	ADP	Y	501	15	-	3/16/32/32	0/3/3/3
13	ADP	W	501	11,15	-	5/16/32/32	0/3/3/3
13	ADP	V	501	15	-	4/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	ADP	T	501	10	-	2/16/32/32	0/3/3/3
13	ADP	X	501	10	-	4/16/32/32	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)
13	X	501	ADP	C5-C4	4.67	1.47	1.39
13	W	501	ADP	C5-C4	4.65	1.47	1.39
13	Y	501	ADP	C5-C4	4.59	1.47	1.39
13	V	501	ADP	C5-C4	4.58	1.47	1.39
13	M	1601	ADP	C5-C4	4.58	1.47	1.39

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	X	501	ADP	C5-C4-N3	-6.44	118.34	126.75
13	Y	501	ADP	C5-C4-N3	-6.41	118.38	126.75
13	W	501	ADP	C5-C4-N3	-6.39	118.41	126.75
13	T	501	ADP	C5-C4-N3	-6.27	118.57	126.75
13	M	1601	ADP	C5-C4-N3	-6.26	118.59	126.75

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	M	1601	ADP	C5'-O5'-PA-O2A
13	R	501	ADP	C5'-O5'-PA-O1A
13	R	501	ADP	C5'-O5'-PA-O2A
13	R	501	ADP	C3'-C4'-C5'-O5'
13	T	501	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

9 monomers are involved in 21 short contacts:

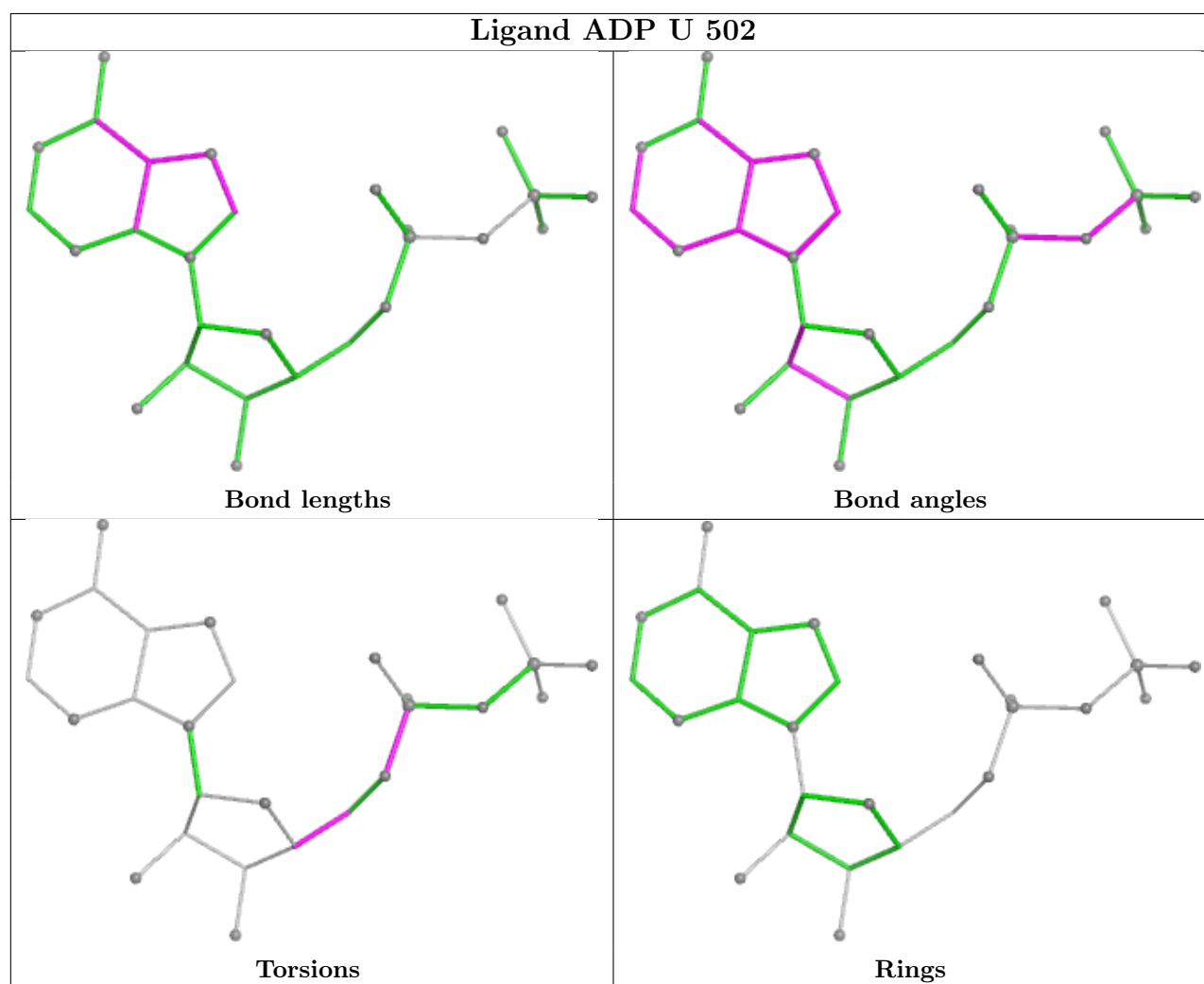
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	U	502	ADP	1	0
13	R	501	ADP	1	0
13	Y	501	ADP	4	0
13	W	501	ADP	2	0
13	V	501	ADP	4	0

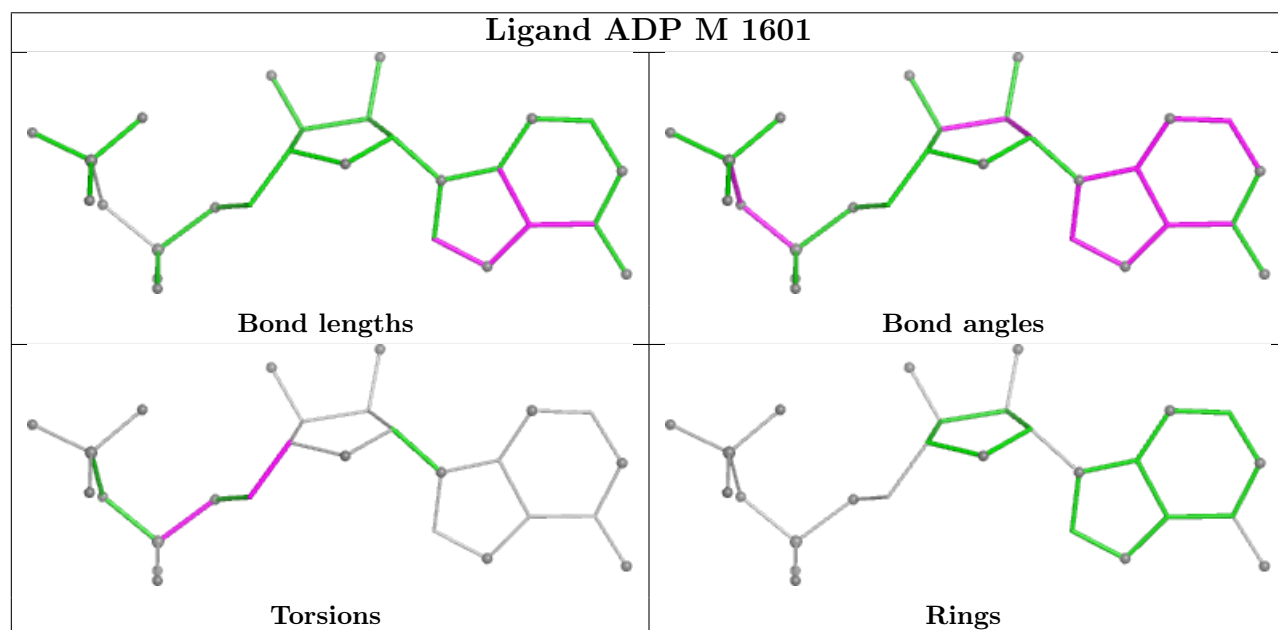
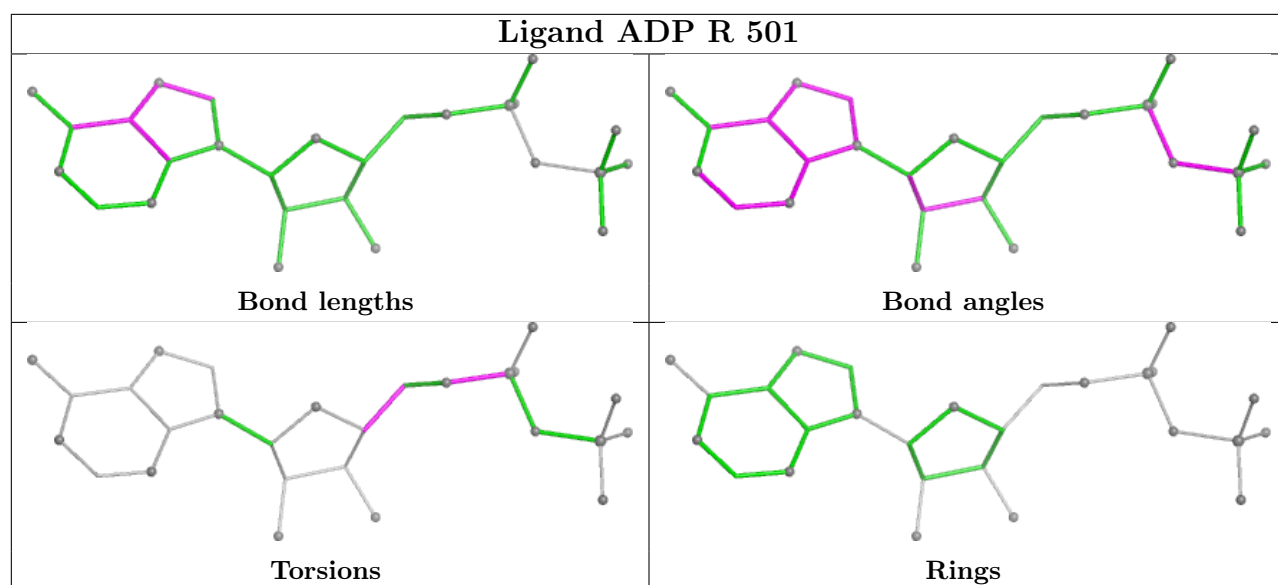
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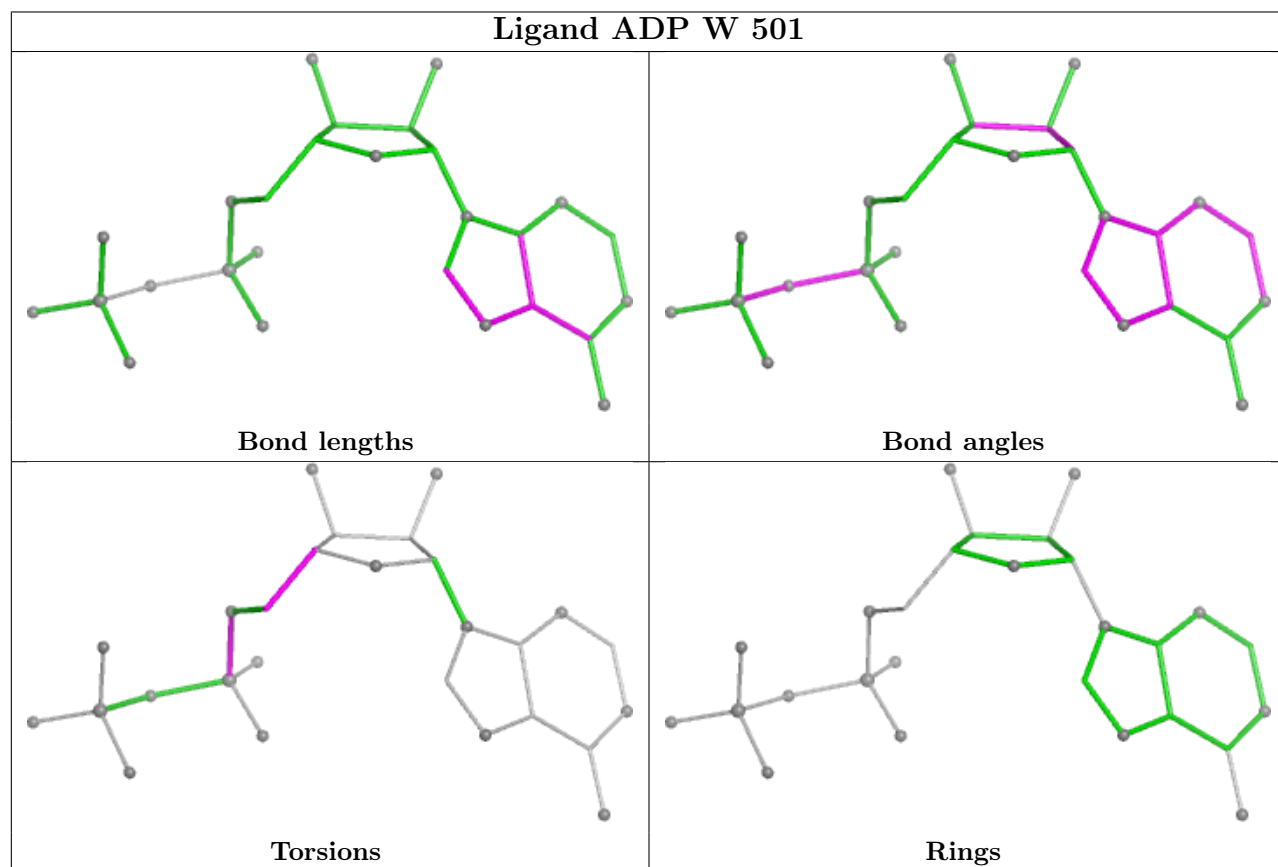
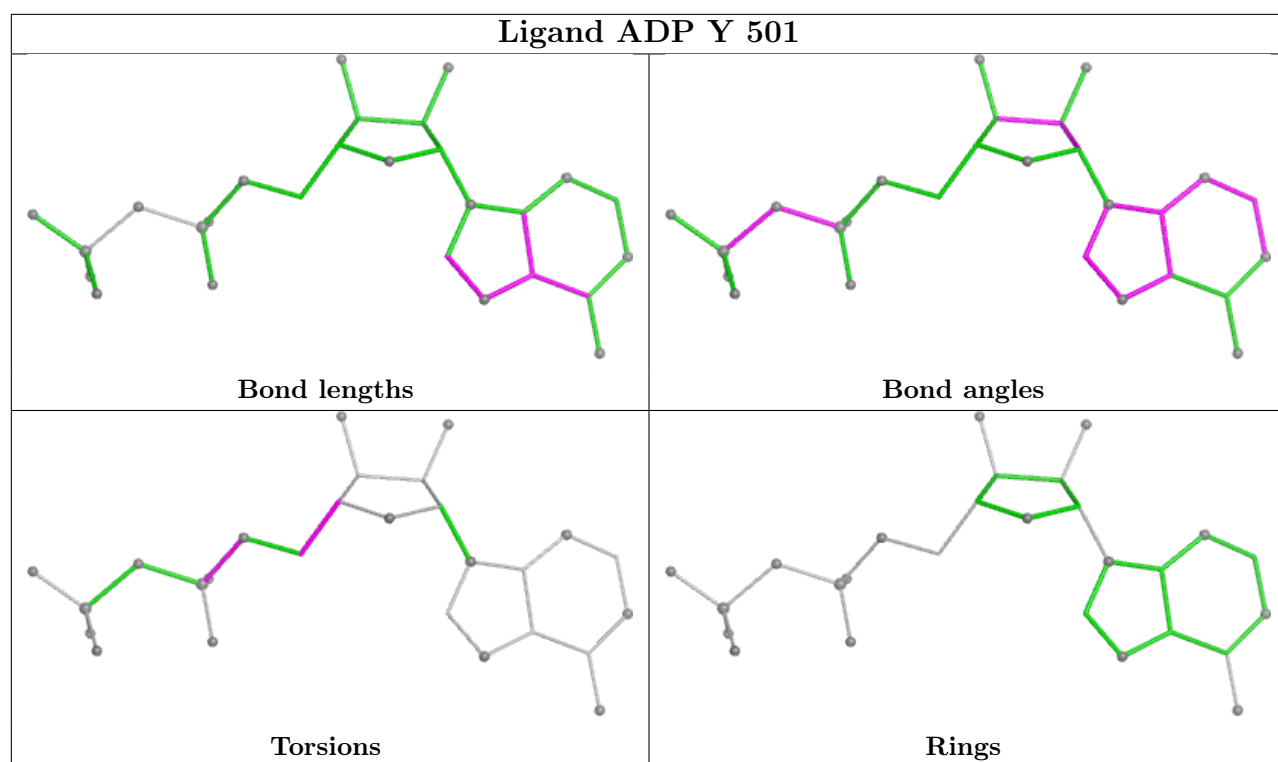
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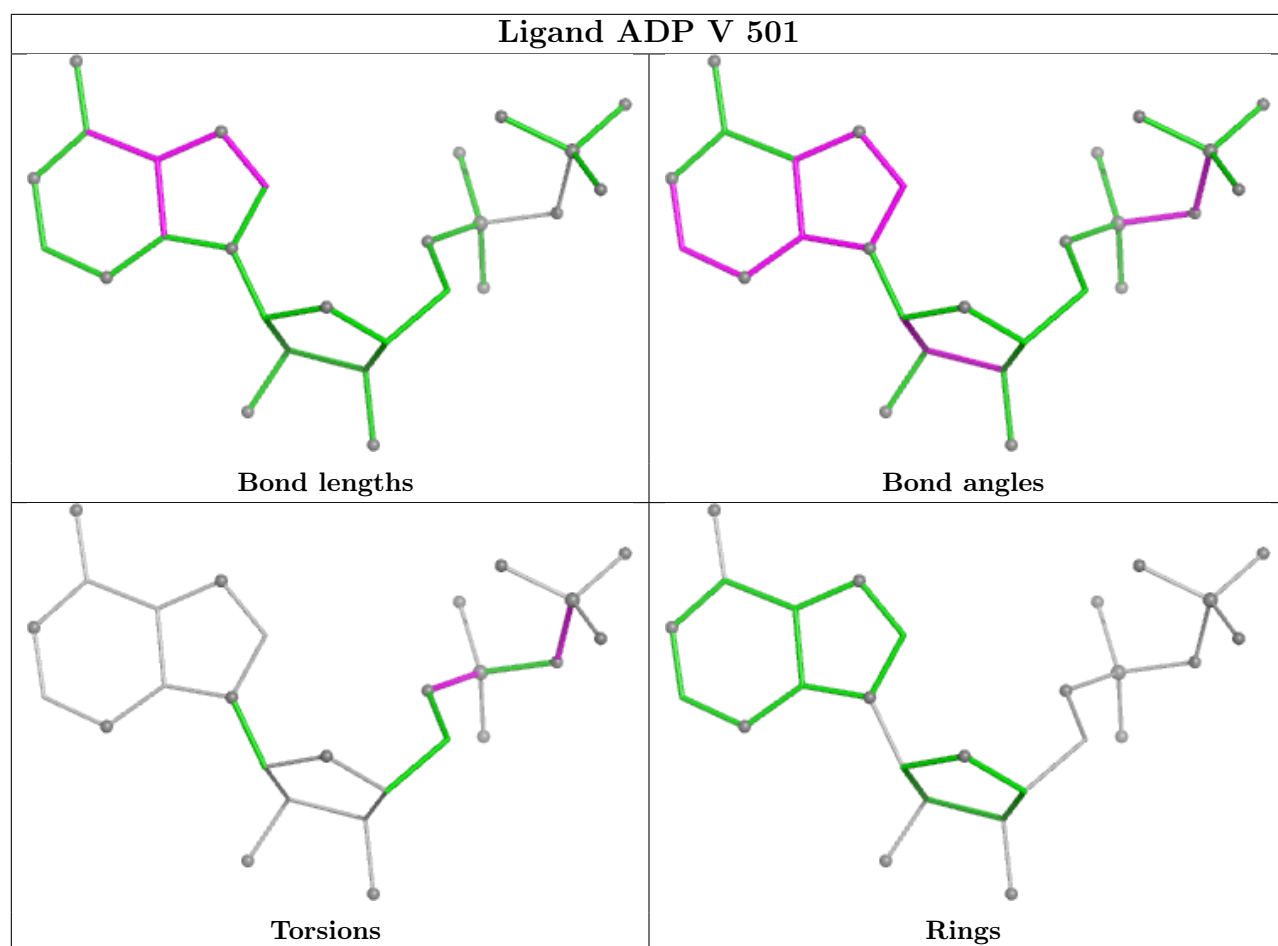
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	T	501	ADP	3	0
14	R	502	BEF	2	0
13	X	501	ADP	3	0
14	M	1602	BEF	2	0

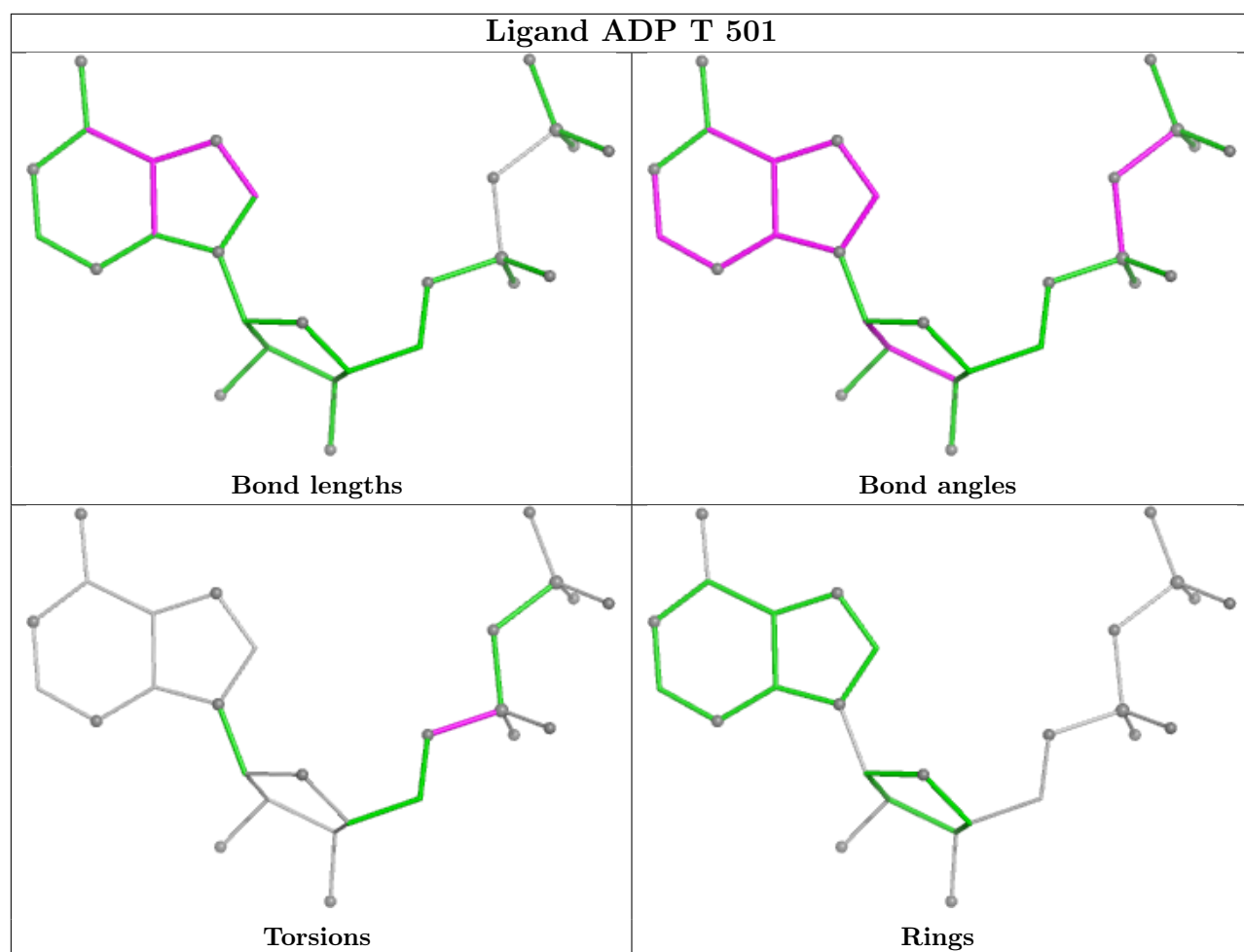
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

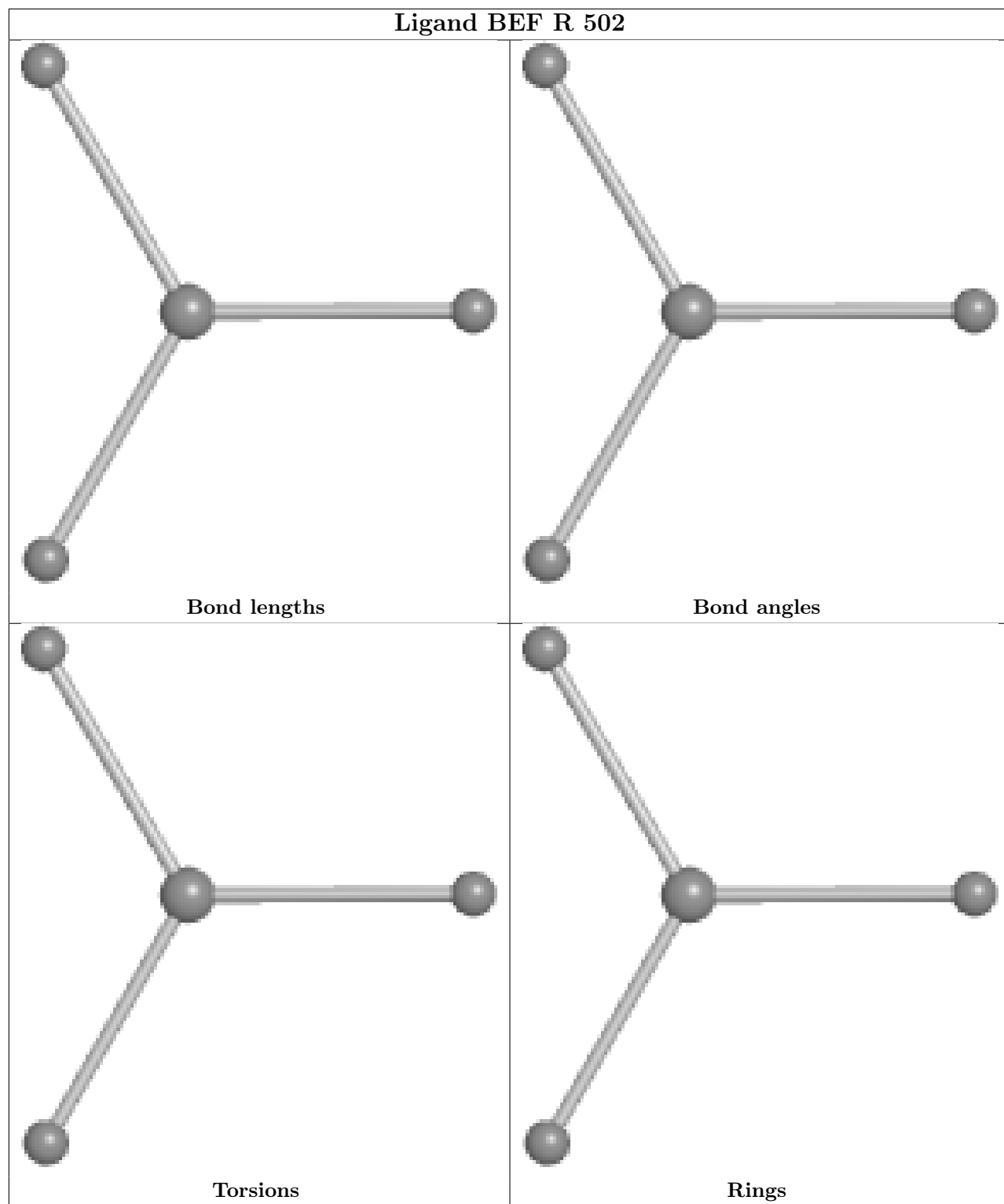


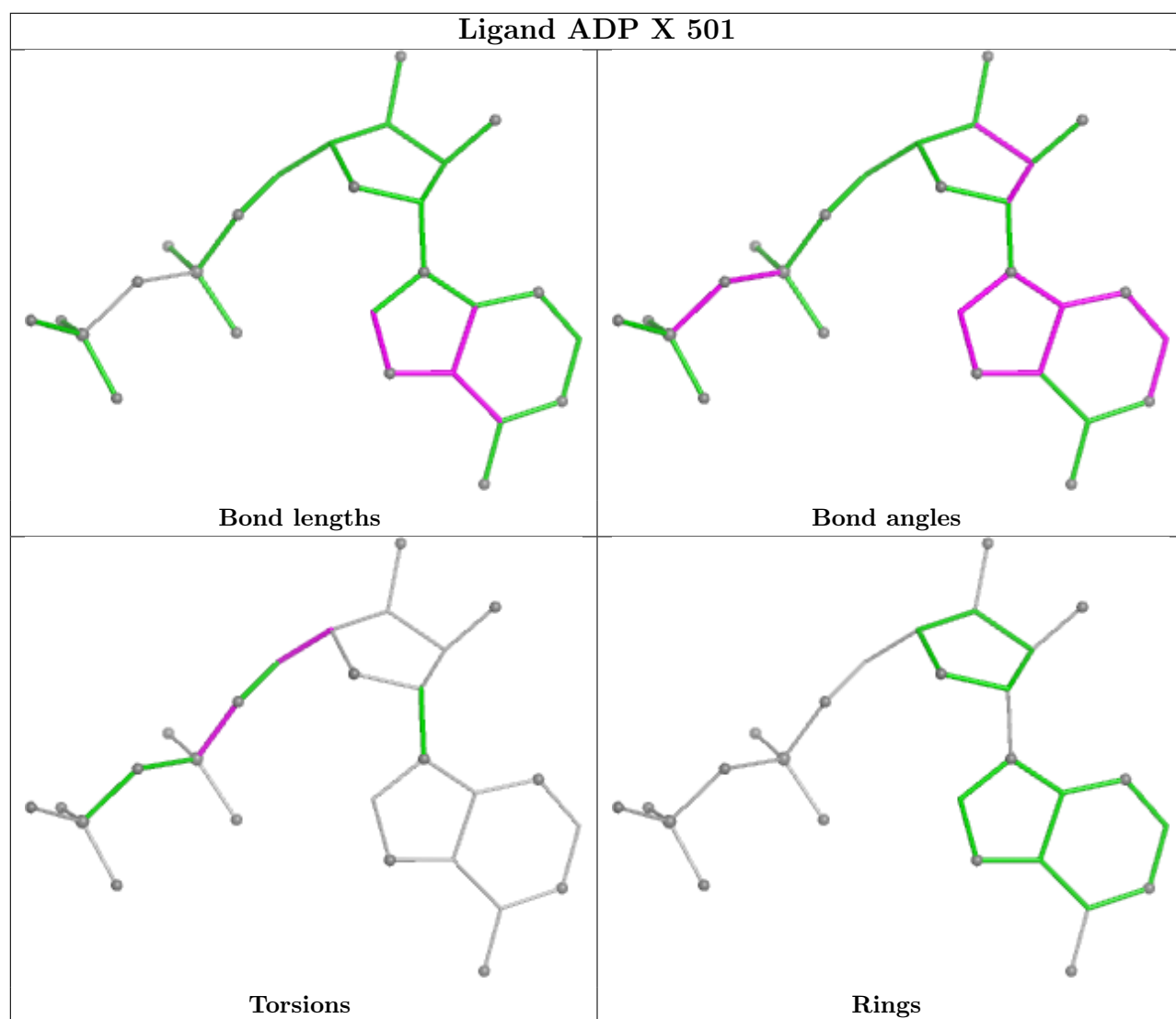


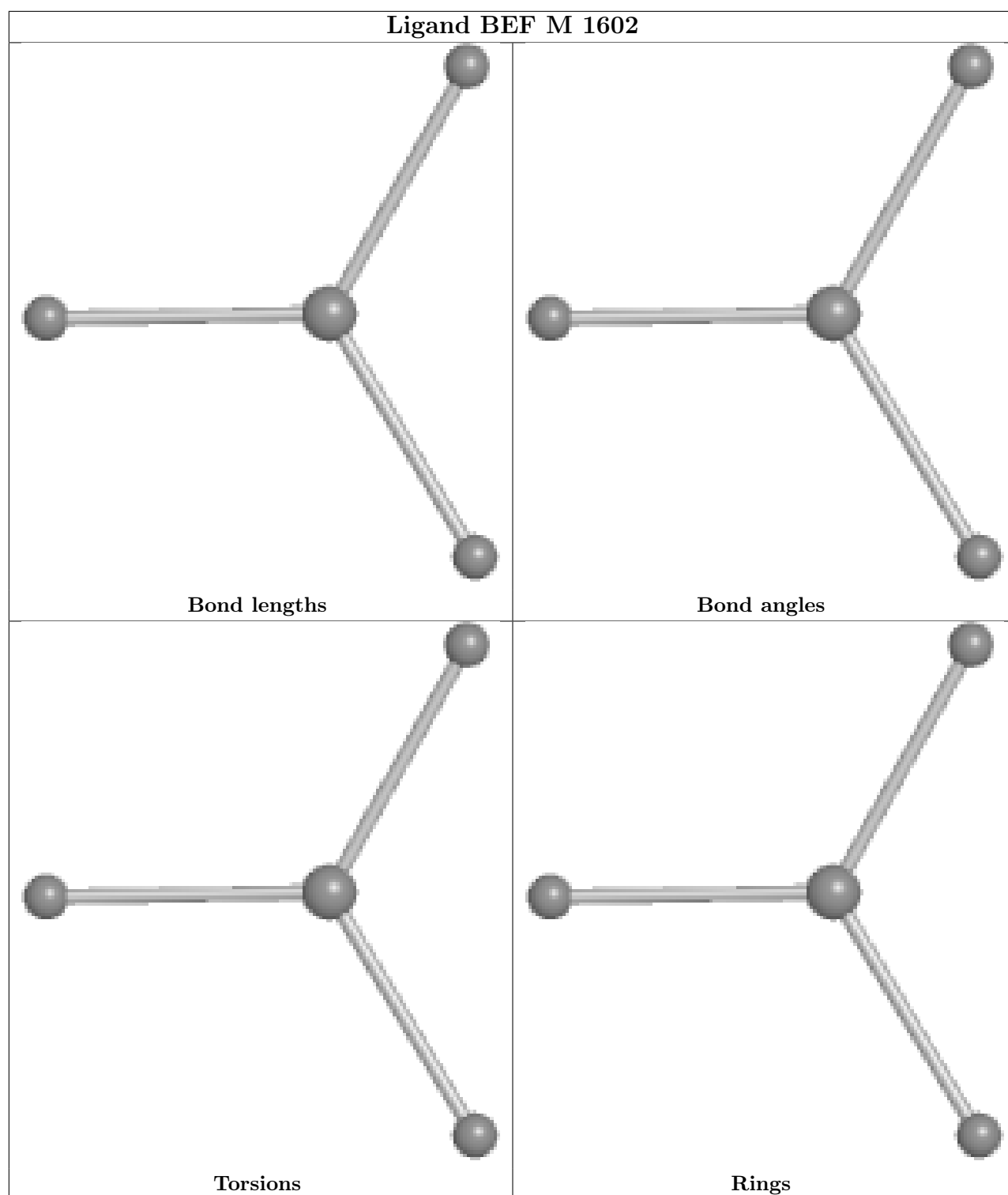












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

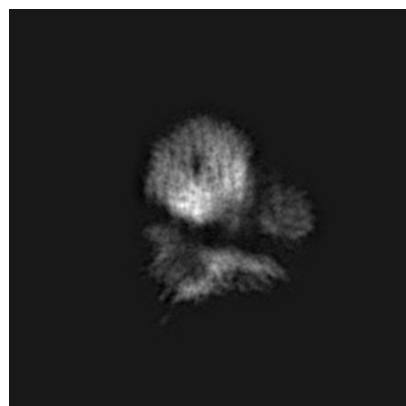
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50297. These allow visual inspection of the internal detail of the map and identification of artifacts.

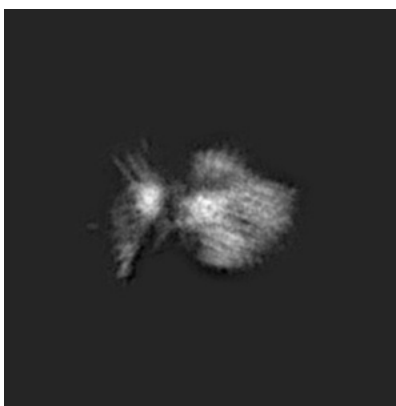
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

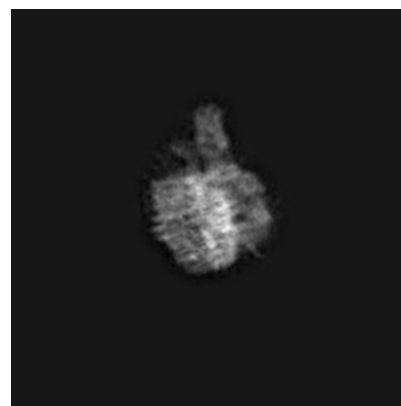
6.1.1 Primary map



X

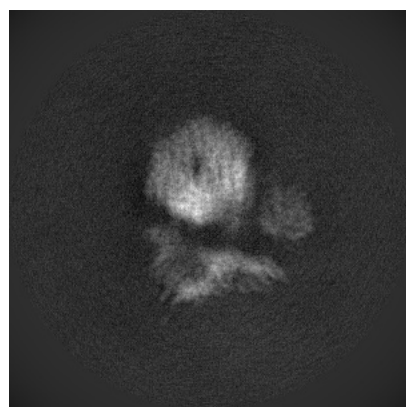


Y

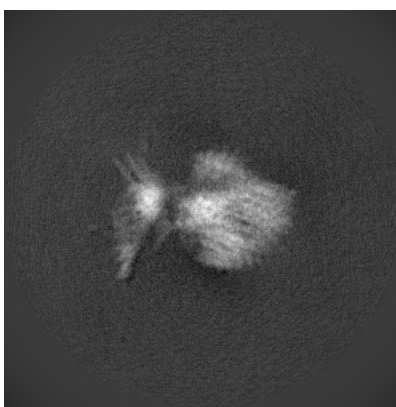


Z

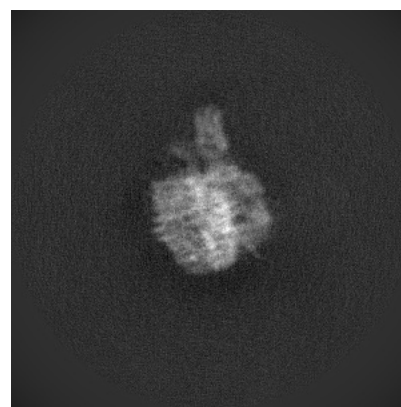
6.1.2 Raw map



X



Y

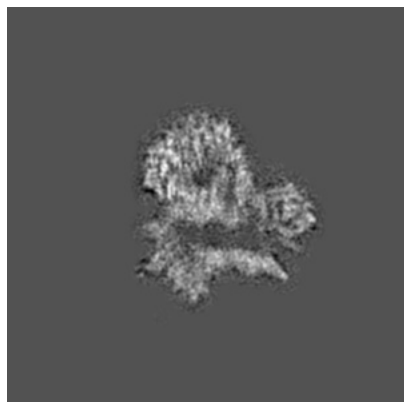


Z

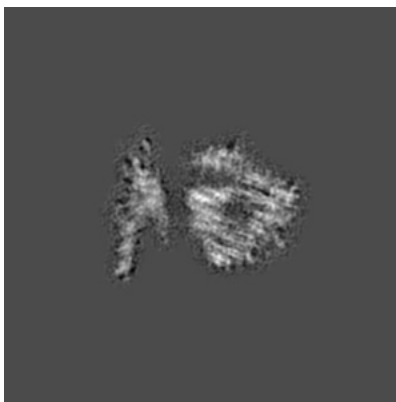
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

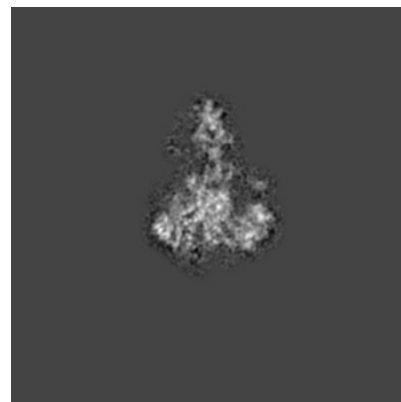
6.2.1 Primary map



X Index: 240

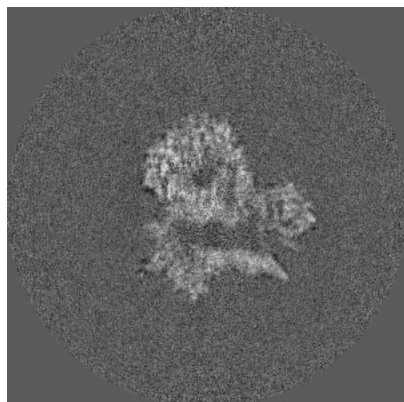


Y Index: 240

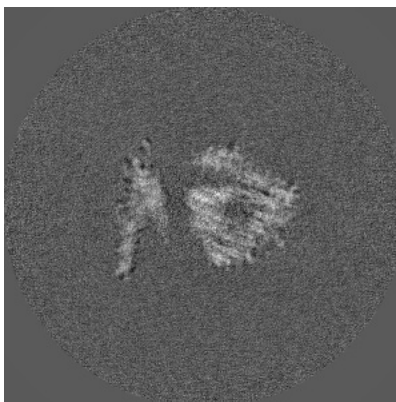


Z Index: 240

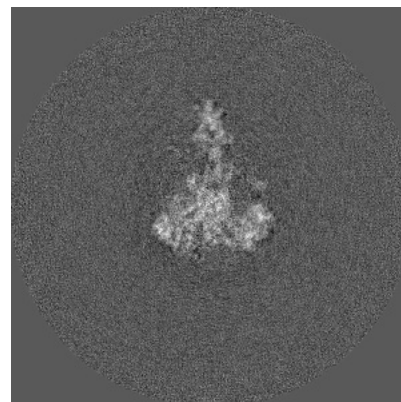
6.2.2 Raw map



X Index: 240



Y Index: 240

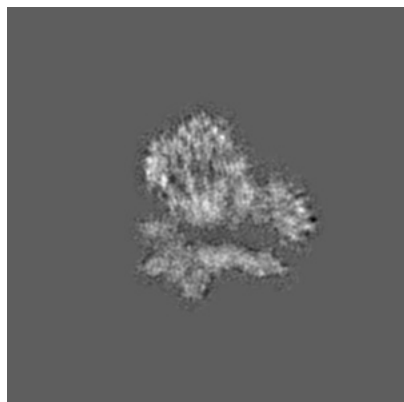


Z Index: 240

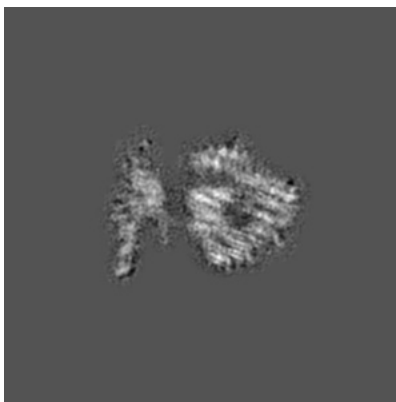
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

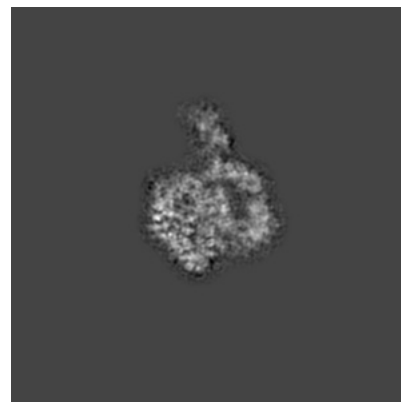
6.3.1 Primary map



X Index: 247

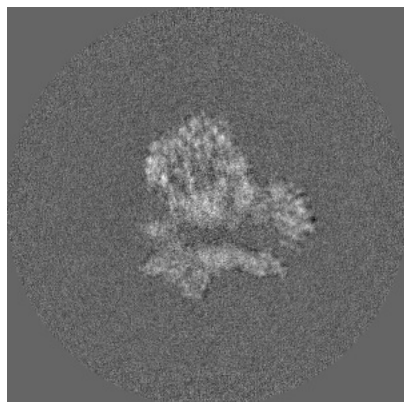


Y Index: 238

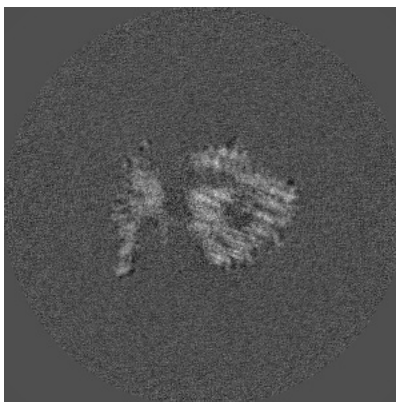


Z Index: 257

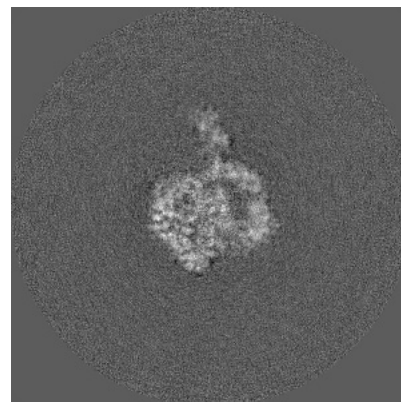
6.3.2 Raw map



X Index: 246



Y Index: 238

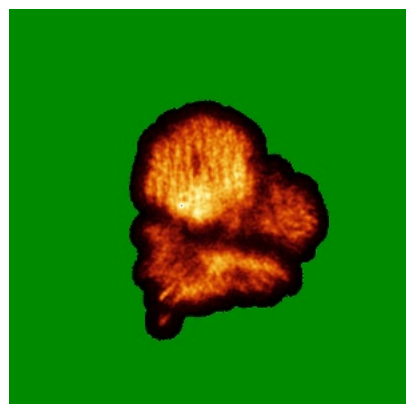


Z Index: 257

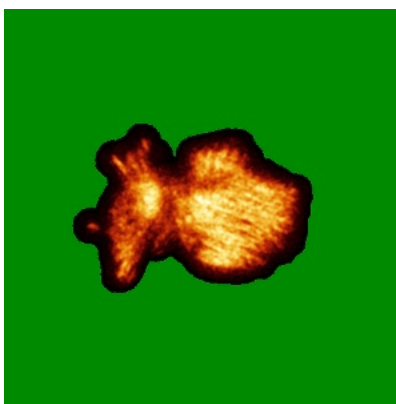
The images above show the largest variance slices of the map in three orthogonal directions.

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

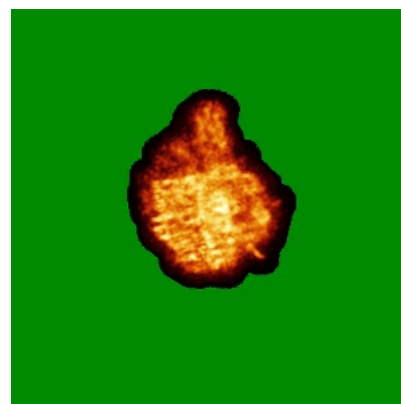
6.4.1 Primary map



X

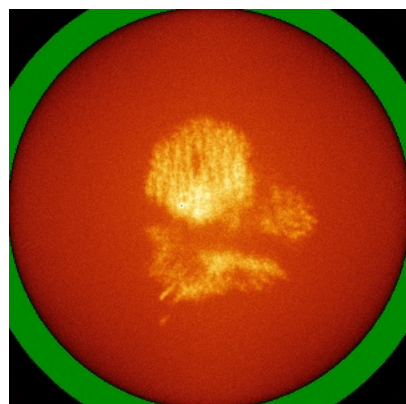


Y

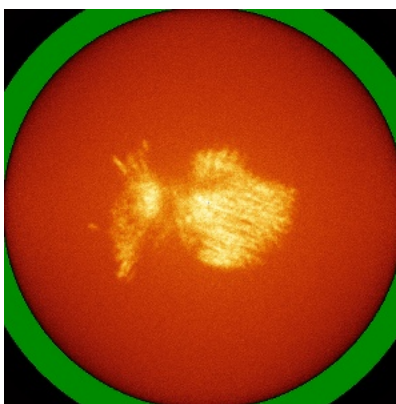


Z

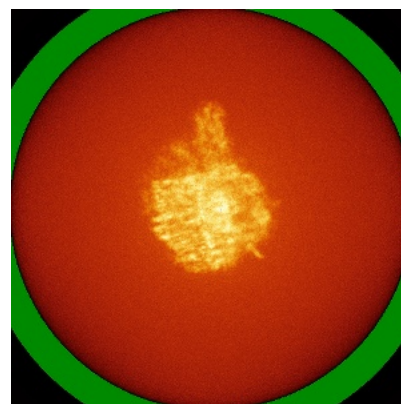
6.4.2 Raw map



X



Y

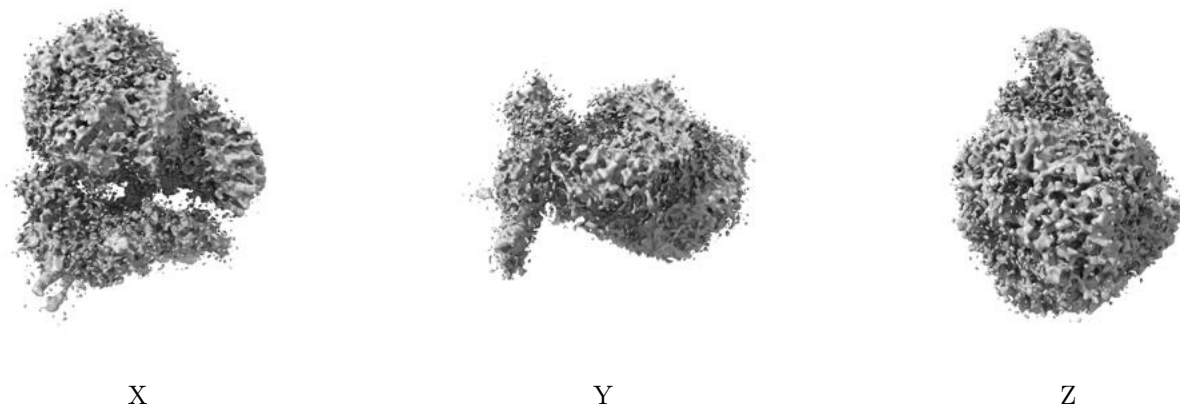


Z

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.

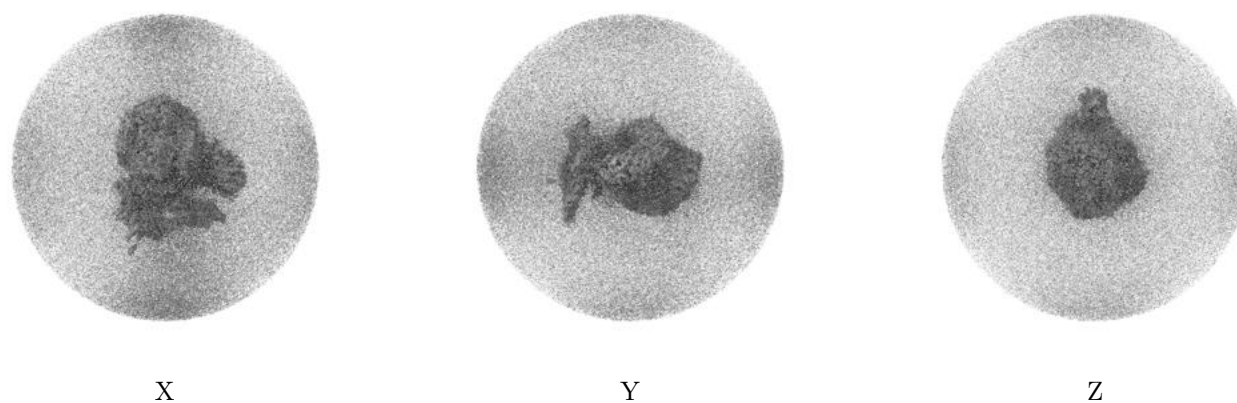
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0011. 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



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.

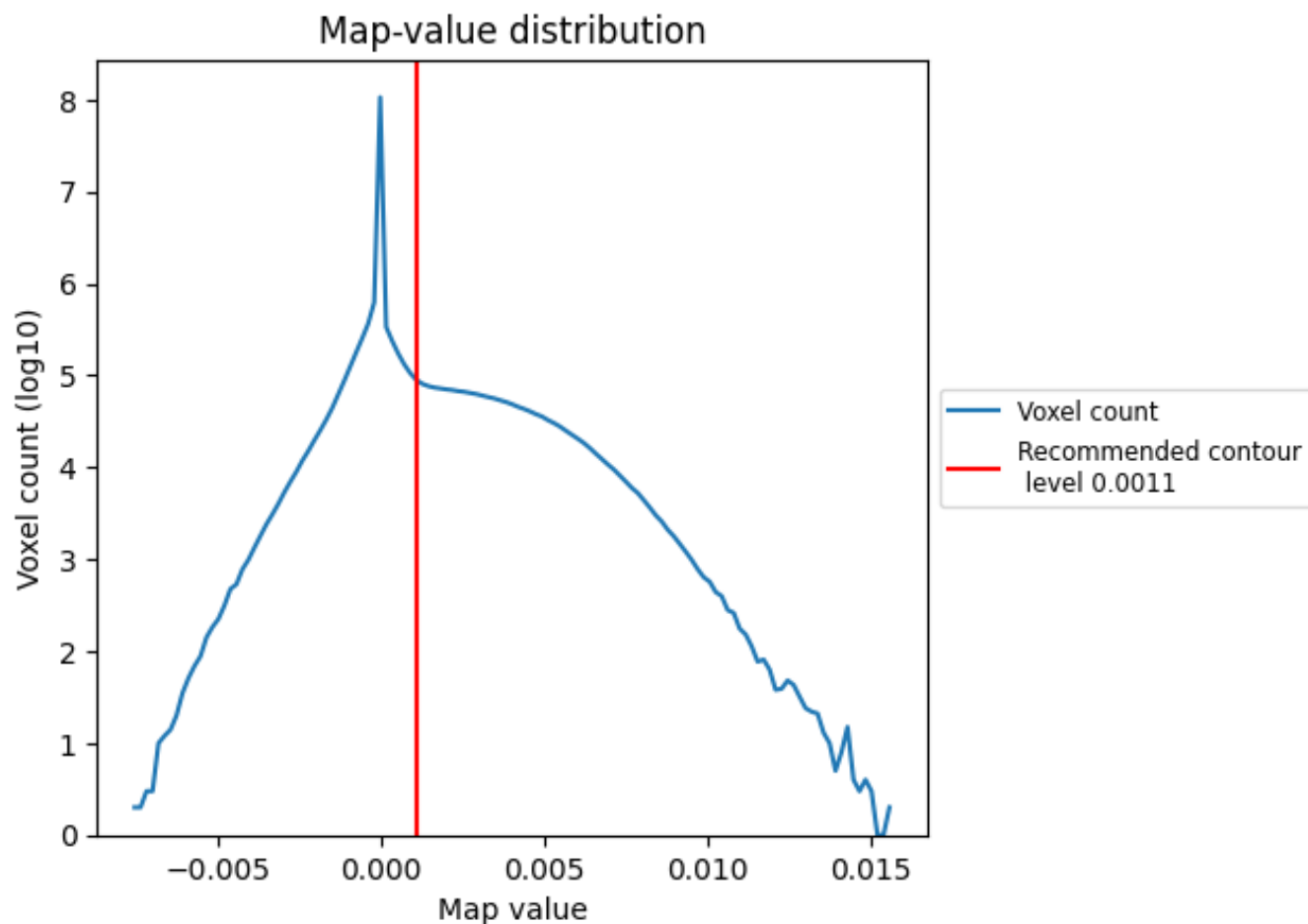
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

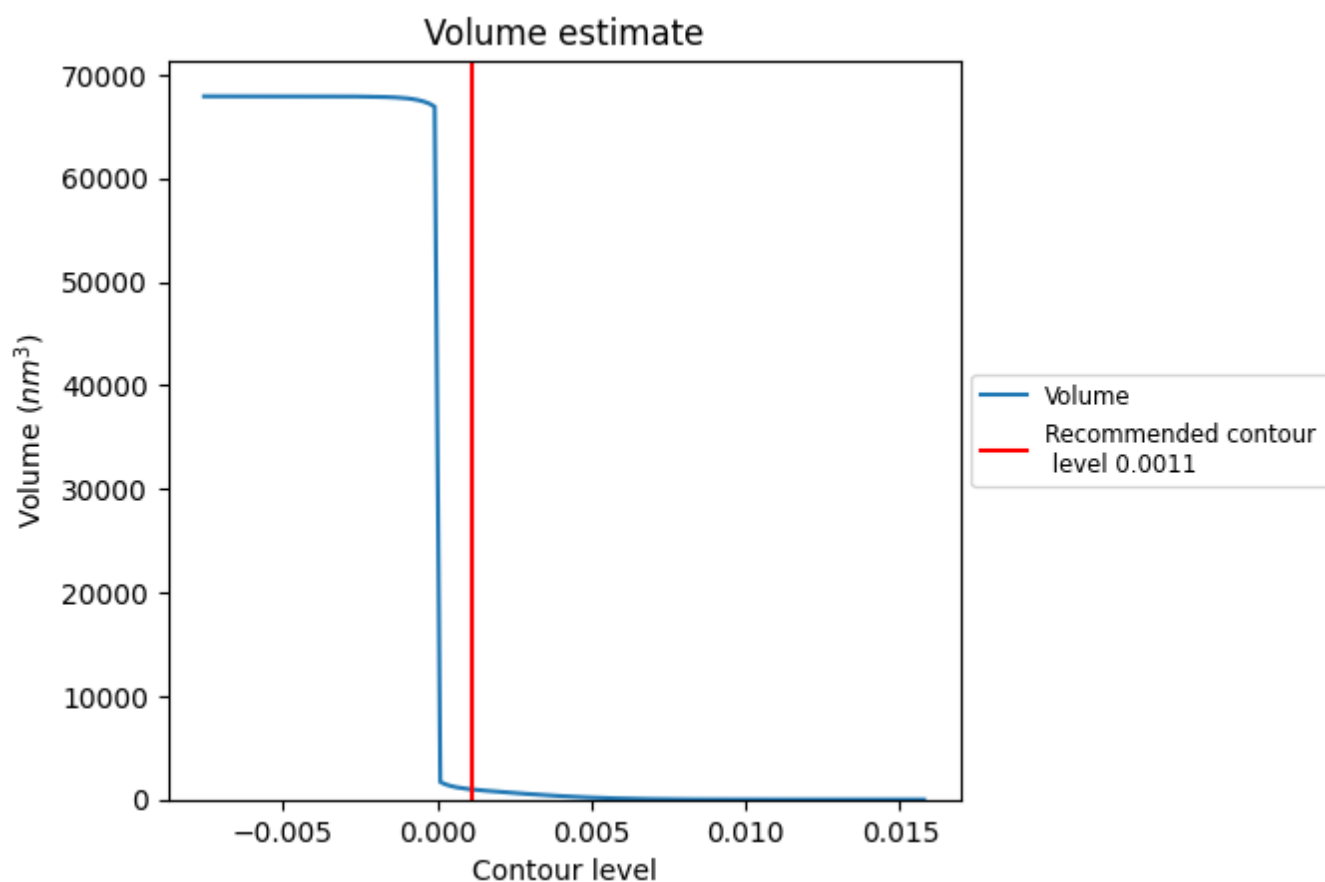
This section contains the results of statistical analysis of the map.

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.

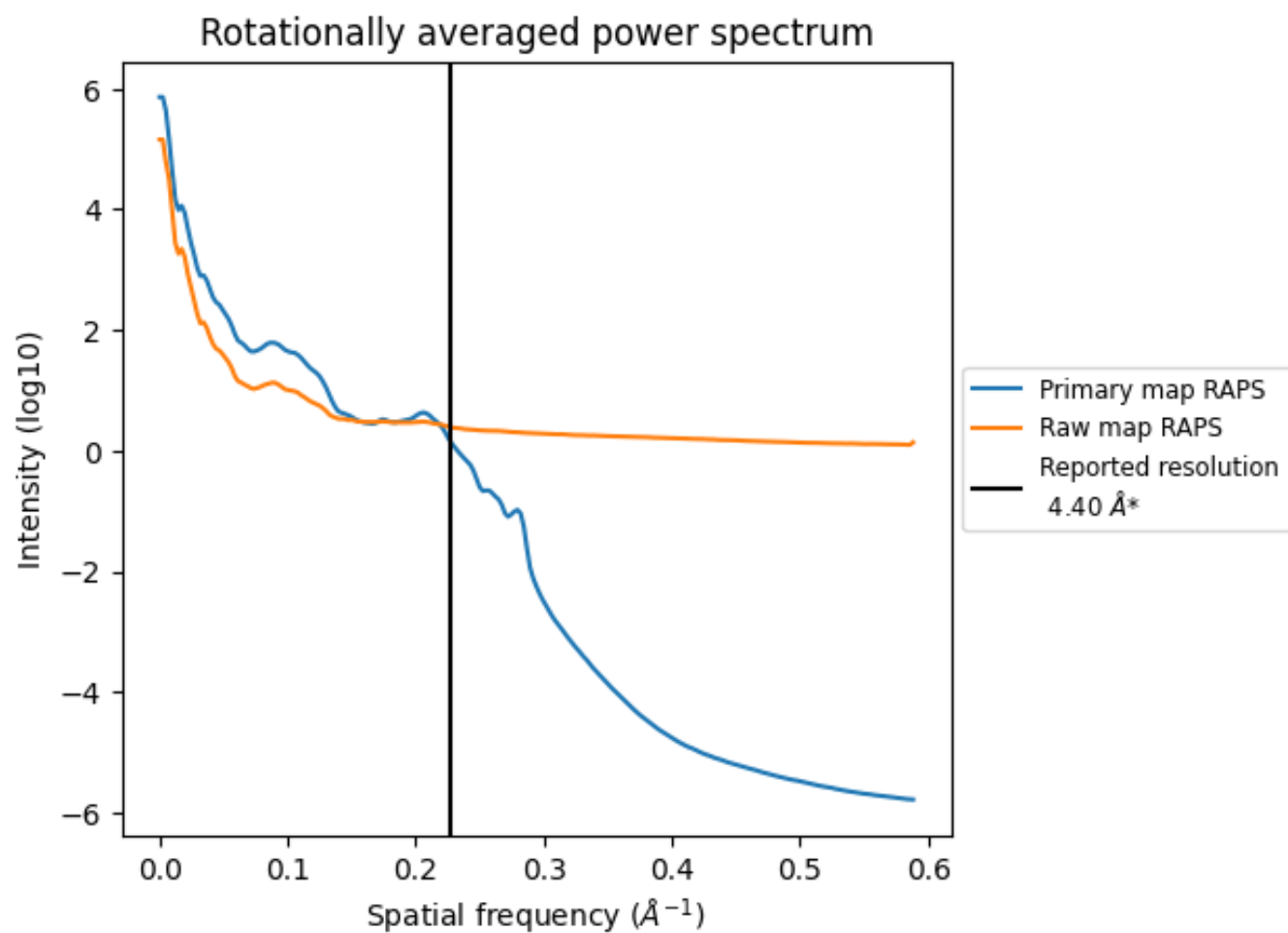
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 986 nm³; this corresponds to an approximate mass of 891 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 ⓘ

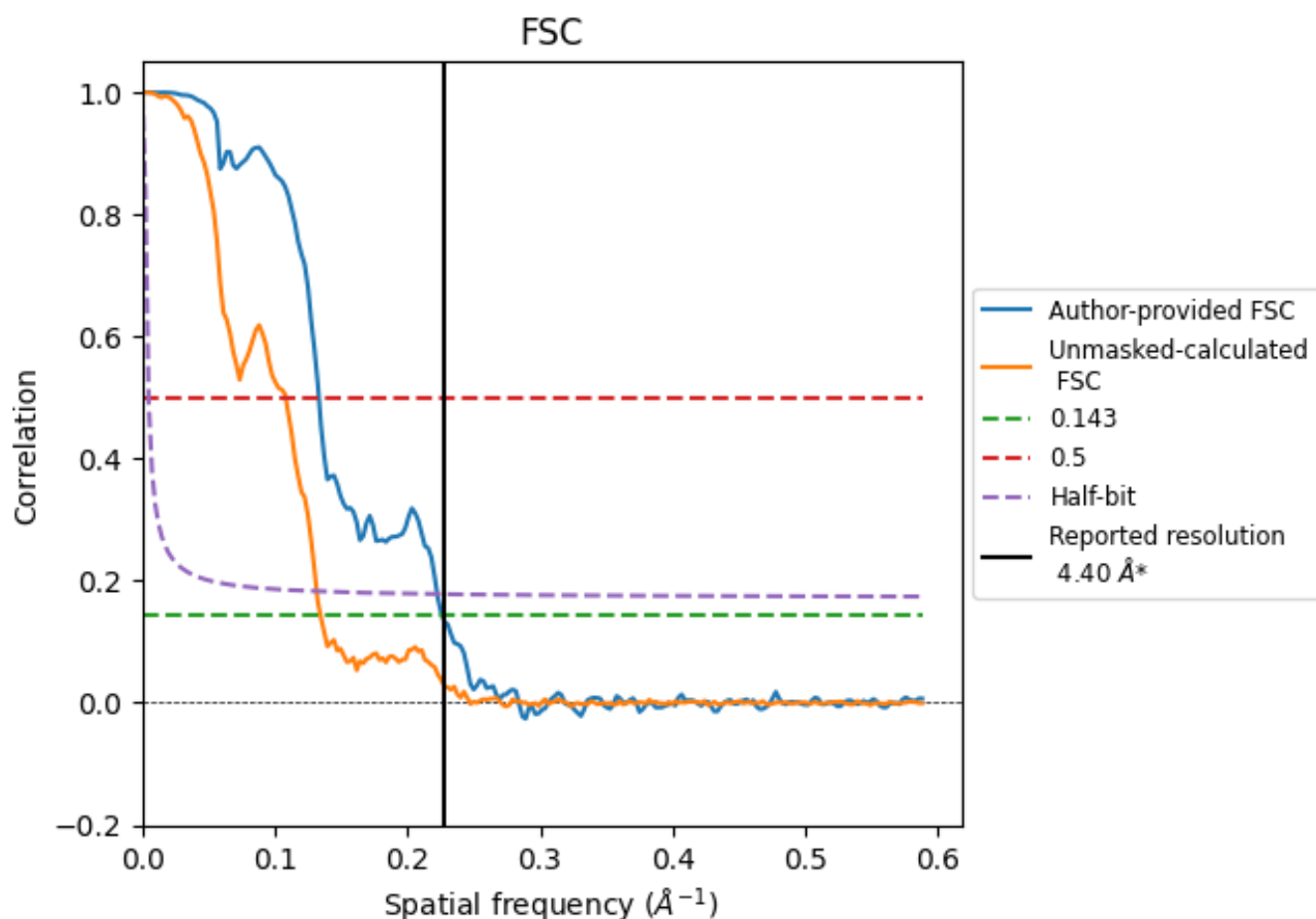


*Reported resolution corresponds to spatial frequency of 0.227 $\text{\AA}^{-1}$

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 $0.227 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

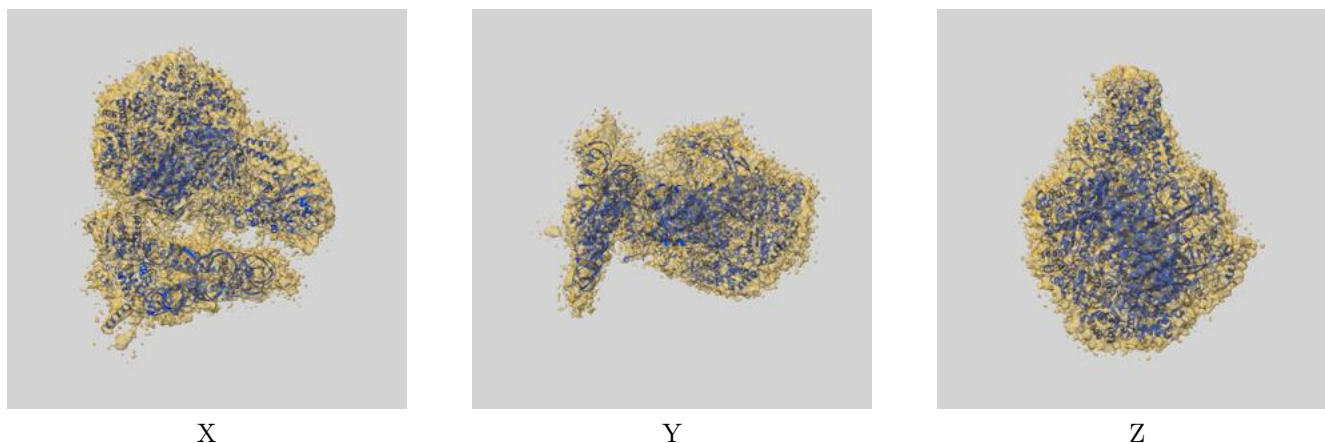
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.42	7.51	4.49
Unmasked-calculated*	7.43	9.24	7.60

*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 7.43 differs from the reported value 4.4 by more than 10 %

9 Map-model fit [i](#)

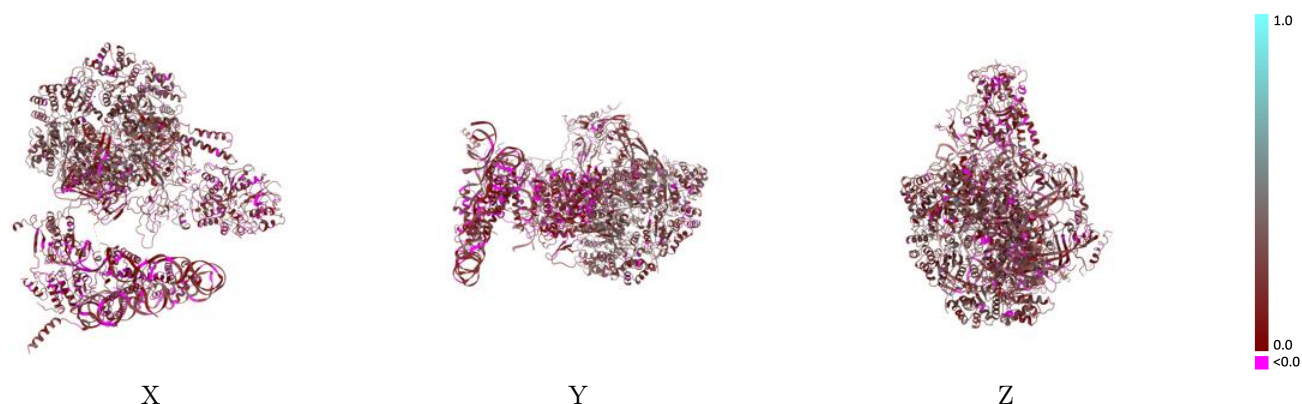
This section contains information regarding the fit between EMDB map EMD-50297 and PDB model 9FBW. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



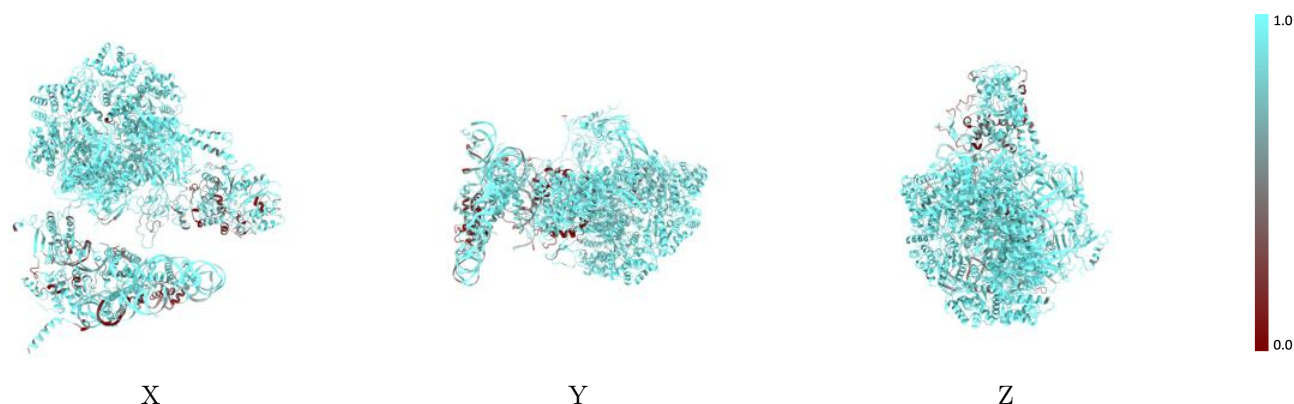
The images above show the 3D surface view of the map at the recommended contour level 0.0011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



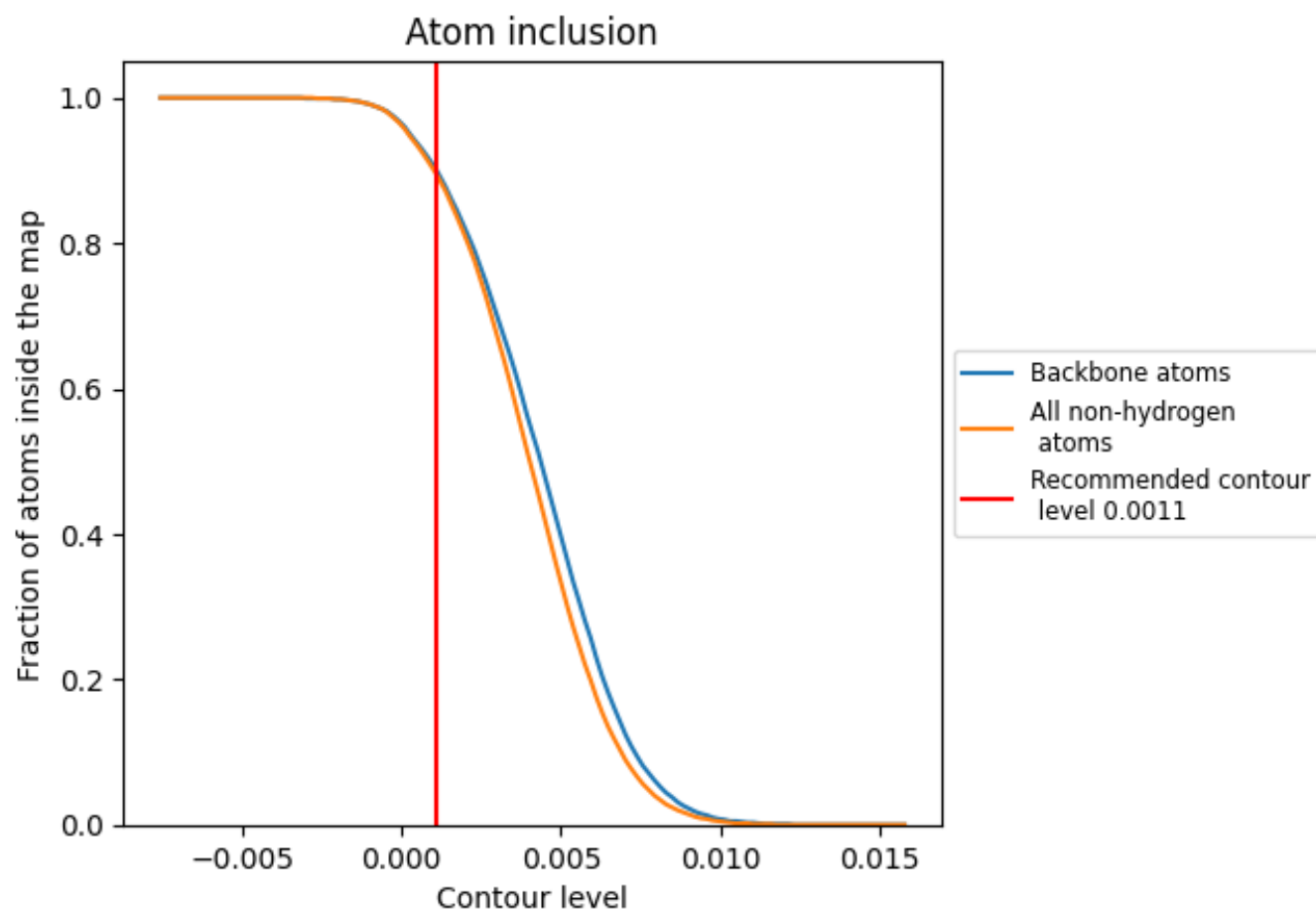
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0011).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 89% 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 (0.0011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8940	 0.1930
A	 0.6820	 0.1120
B	 0.8900	 0.1410
C	 0.7960	 0.0930
D	 0.5480	 0.1270
E	 0.7370	 0.1230
G	 0.7940	 0.1430
I	 0.8070	 0.1120
J	 0.8090	 0.1170
M	 0.8690	 0.1760
R	 0.7950	 0.1430
S	 0.7140	 0.1470
T	 0.9760	 0.2490
U	 0.9740	 0.2450
V	 0.9790	 0.2280
W	 0.9900	 0.2500
X	 0.9750	 0.2290
Y	 0.9680	 0.2330
Z	 0.8800	 0.2110

