wwPDB EM Validation Summary Report (i)

Dec 31, 2024 – 11:46 PM EST

PDB ID	:	8QZ0
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 (i) symbol.

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

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

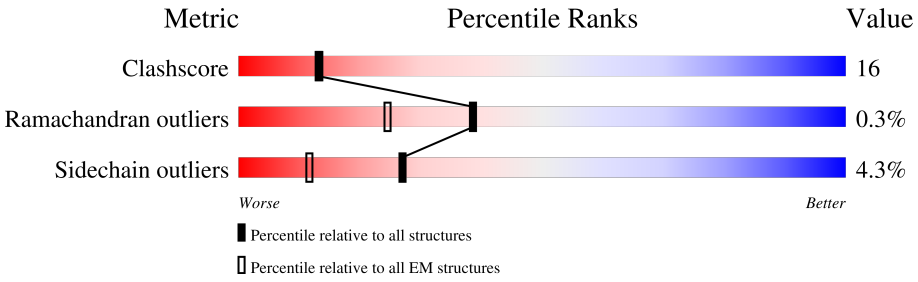
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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 <=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	46% 30% · 21%
1	B	136	54% 26% · 19%
2	C	103	37% 33% · 26%
2	D	103	44% 23% · 31%
3	E	132	60% 16% · 23%
4	G	131	43% 23% · 33%
5	H	131	45% 24% 31%
6	I	118	36% 59% ·

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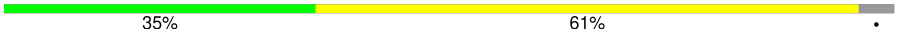
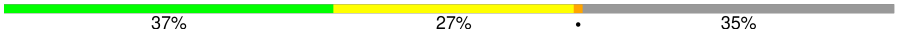
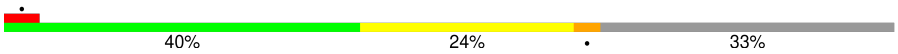
Mol	Chain	Length	Quality of chain
7	J	118	
8	L	134	
9	P	303	
10	R	438	
11	S	280	
12	U	471	
12	W	471	
12	Y	471	
13	T	463	
13	V	463	
13	X	463	
14	Z	795	
15	M	1514	
16	K	153	

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 (i)

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 864	C 546	N 165	O 152	S 1	0	0
1	B	110	Total 850	C 538	N 166	O 145	S 1	0	0

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 558	C 356	N 101	O 101	0	0
2	D	71	Total 527	C 329	N 103	O 95	0	0

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

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

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

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

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

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

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 2300	C 1090	N 419	O 678	P 113	0	0

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

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

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

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

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

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

- 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		

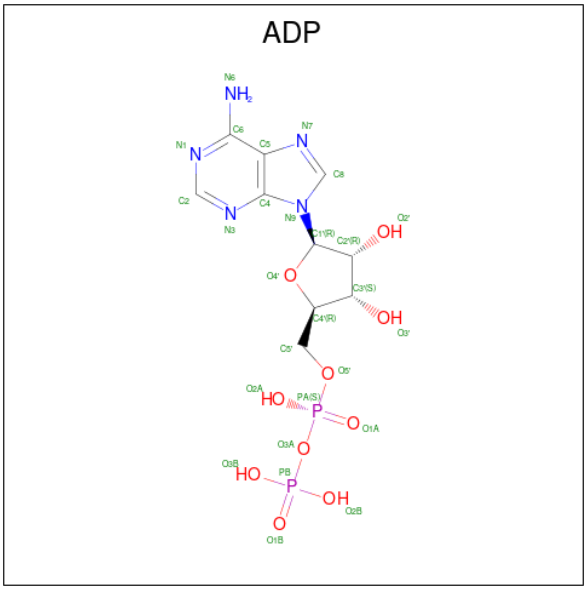
- Molecule 16 is a protein called Histone H2A.Z-specific chaperone CHZ1.

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:

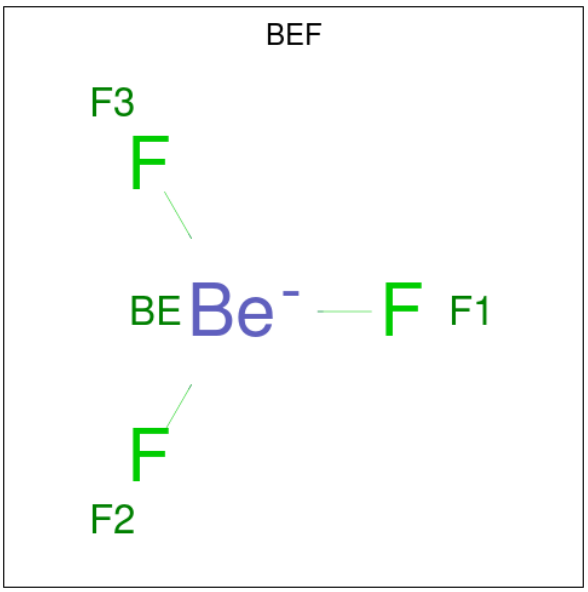
Chain	Residue	Modelled	Actual	Comment	Reference
K	98	CYS	SER	engineered mutation	UNP P40019

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



Mol	Chain	Residues	Atoms					AltConf
17	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 (three-letter code: BEF) (formula: BeF_3).



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

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

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

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

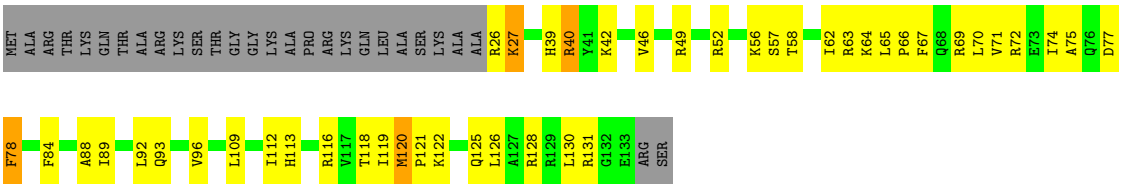
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
20	S	2	2	2	0

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.

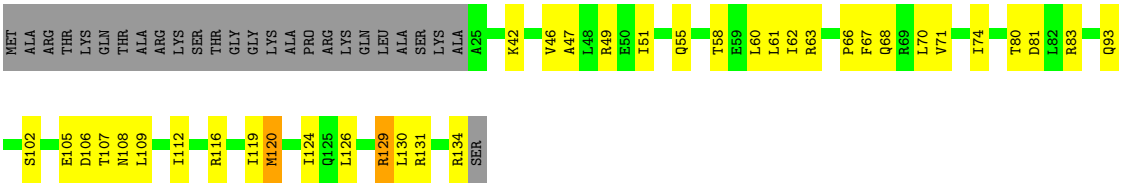
• Molecule 1: Histone H3

Chain A:



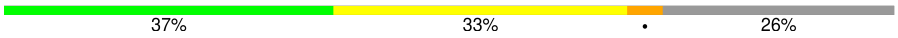
• Molecule 1: Histone H3

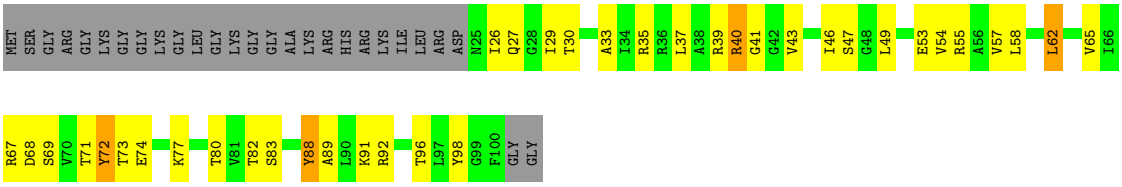
Chain B:



• Molecule 2: Histone H4

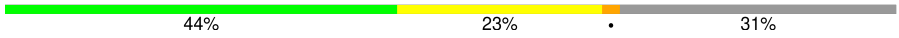
Chain C:

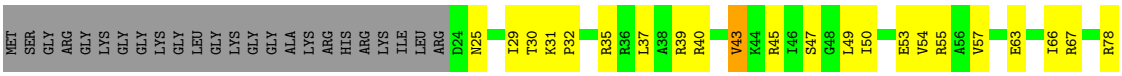


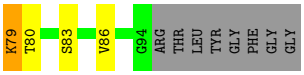


• Molecule 2: Histone H4

Chain D:

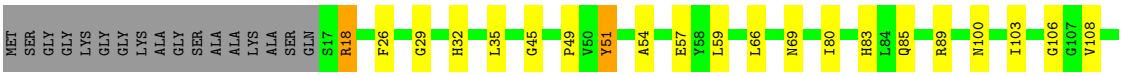


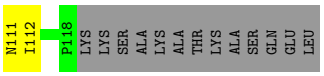




• Molecule 3: Histone H2A.1

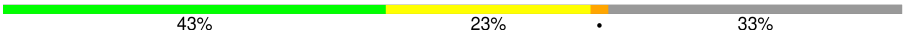
Chain E:

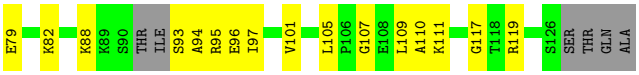




• Molecule 4: Histone H2B.1

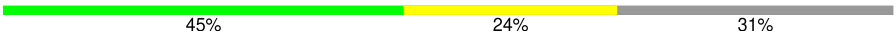
Chain G:





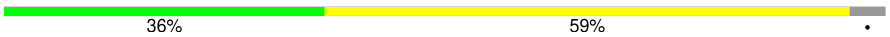
• Molecule 5: Histone H2B.1

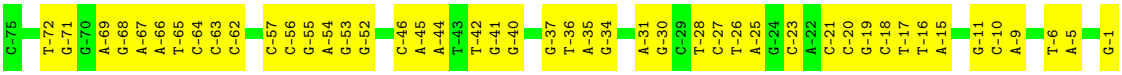
Chain H:

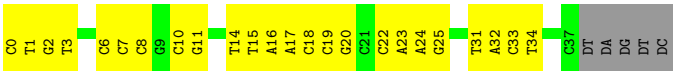


• Molecule 6: DNA (113-MER)

Chain I:

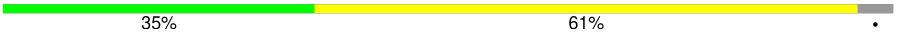


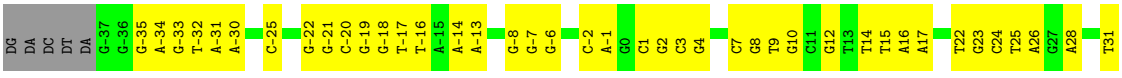


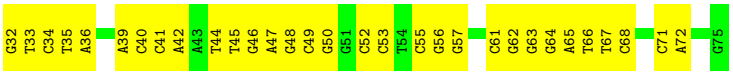


• Molecule 7: DNA (113-MER)

Chain J:

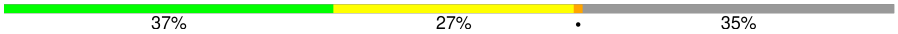


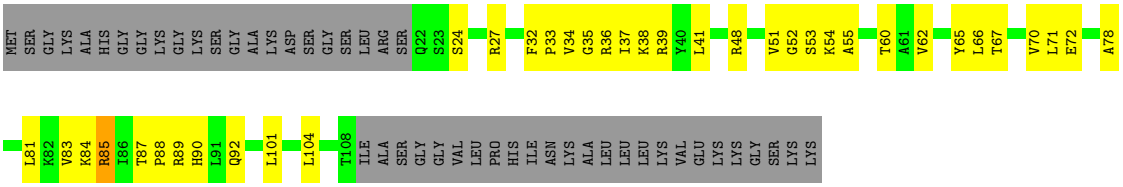




• Molecule 8: Histone H2A.Z

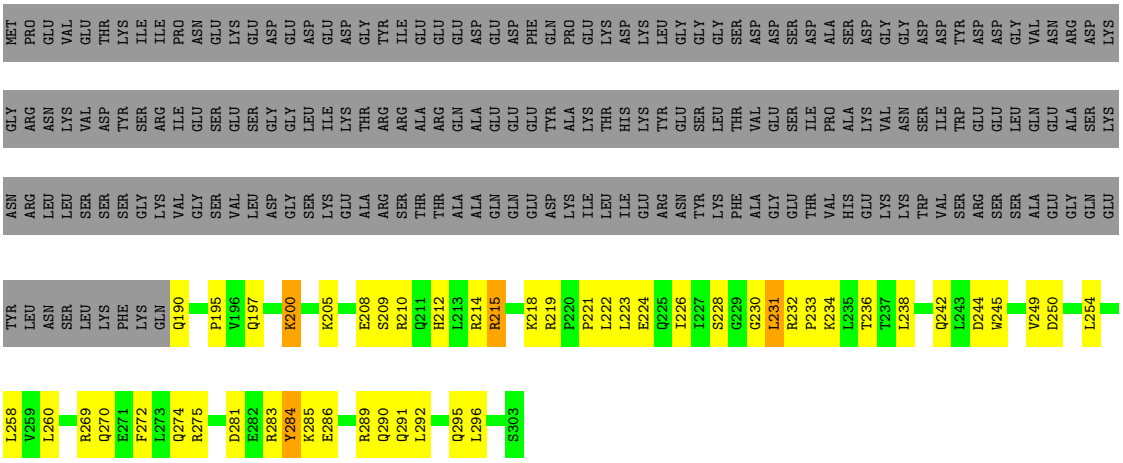
Chain L:





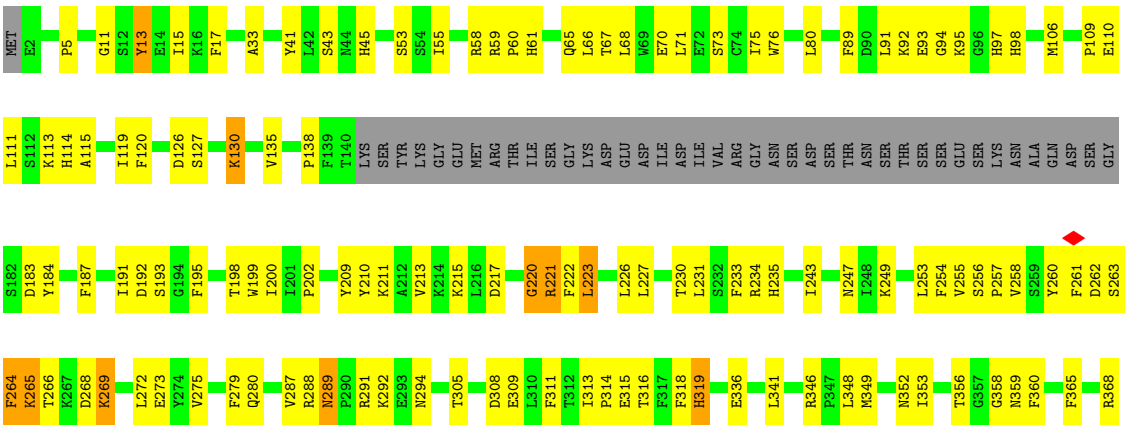
• Molecule 9: SWR1-complex protein 5

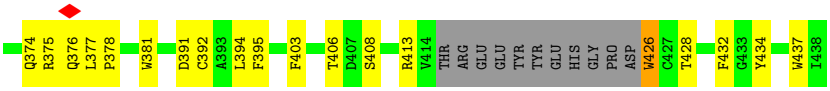
Chain P:



• Molecule 10: Actin-like protein ARP6

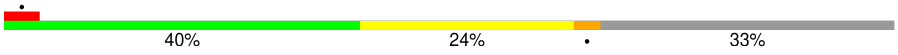
Chain R:

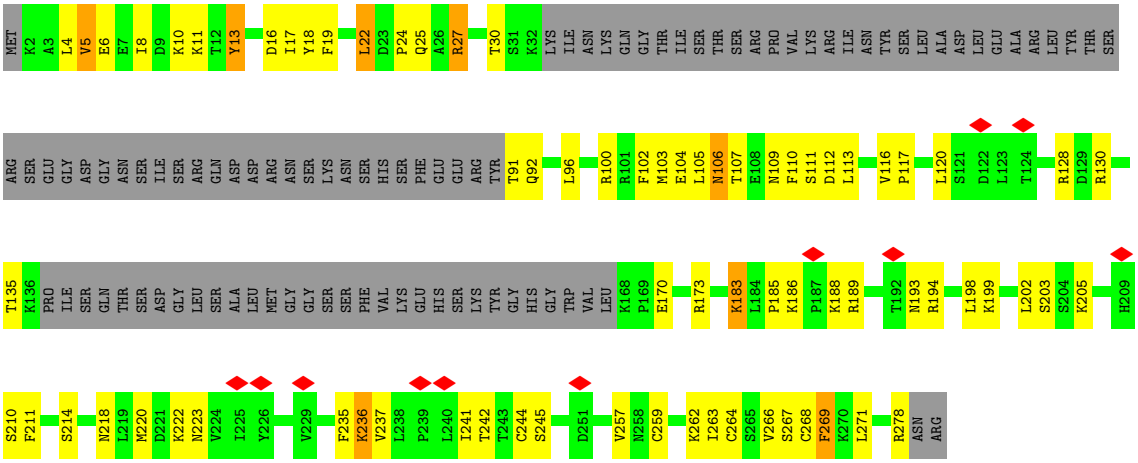




• Molecule 11: Vacuolar protein sorting-associated protein 71

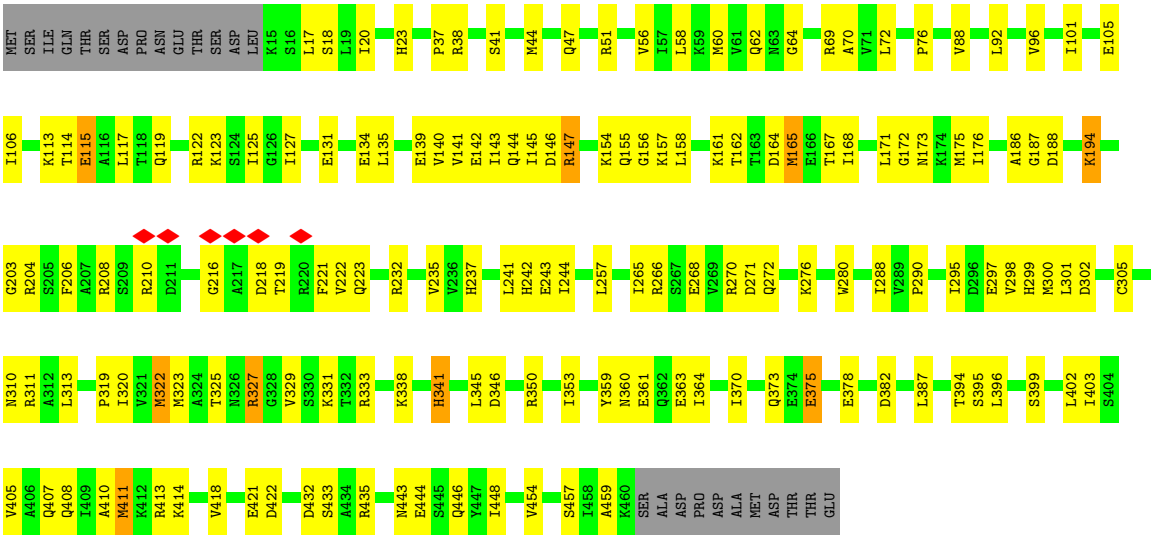
Chain S:





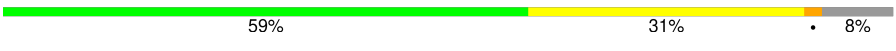
• Molecule 12: RuvB-like protein 2

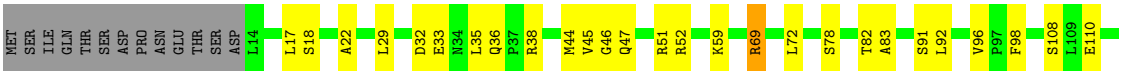
Chain U:

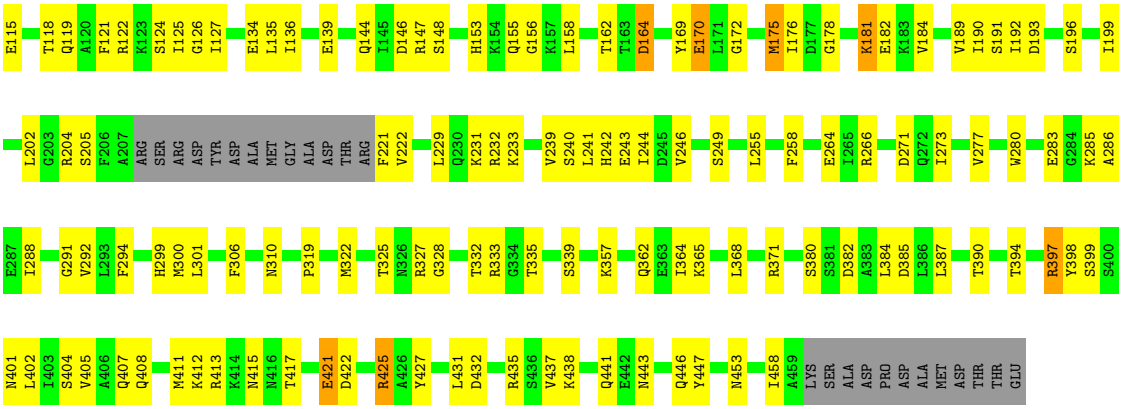


• Molecule 12: RuvB-like protein 2

Chain W:

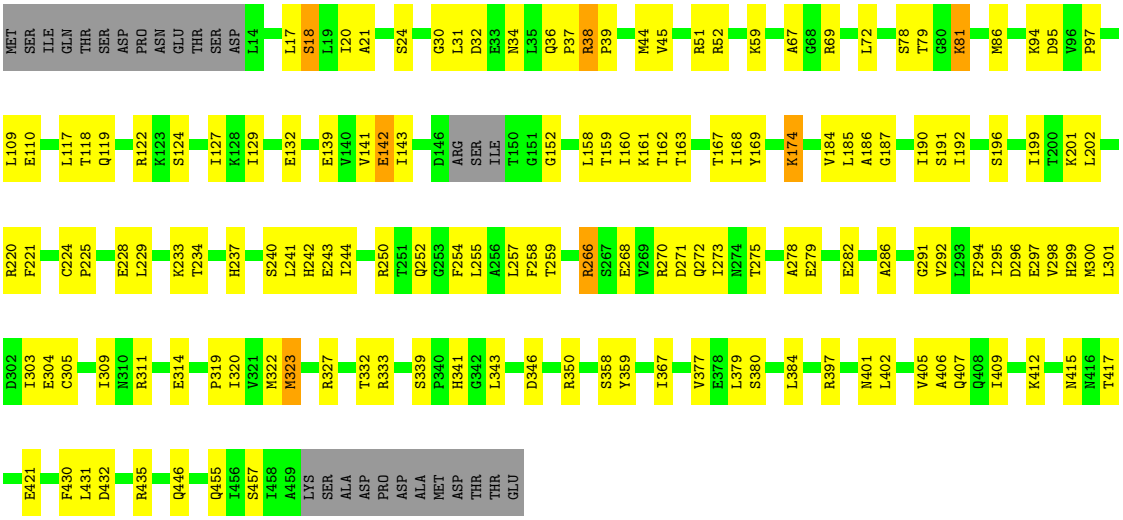






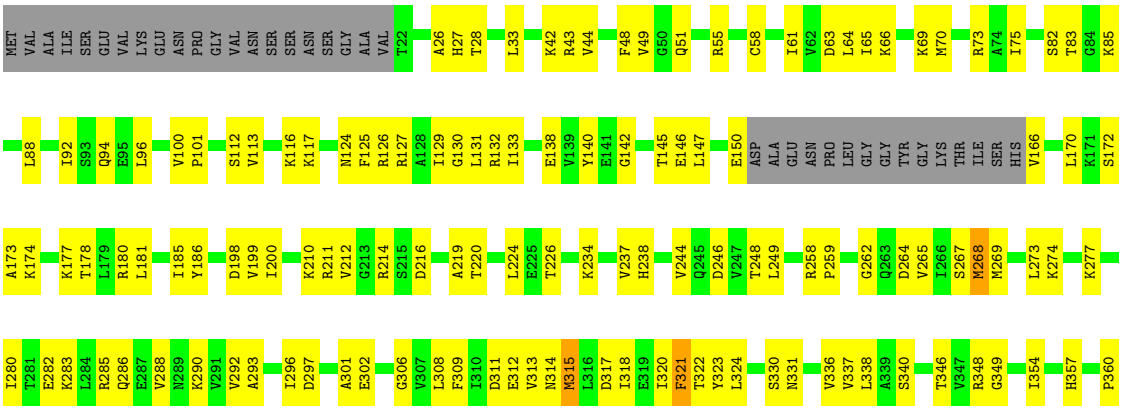
• Molecule 12: RuvB-like protein 2

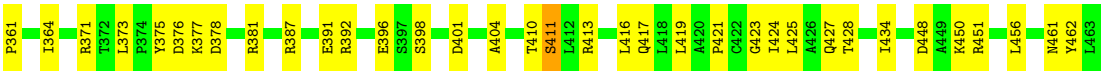
Chain Y:



• Molecule 13: RuvB-like protein 1

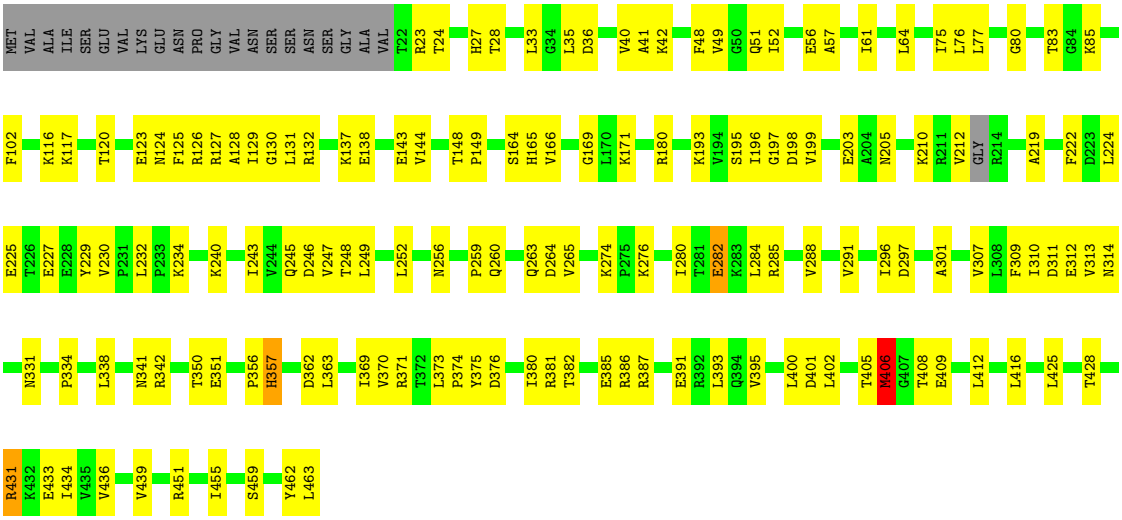
Chain V:





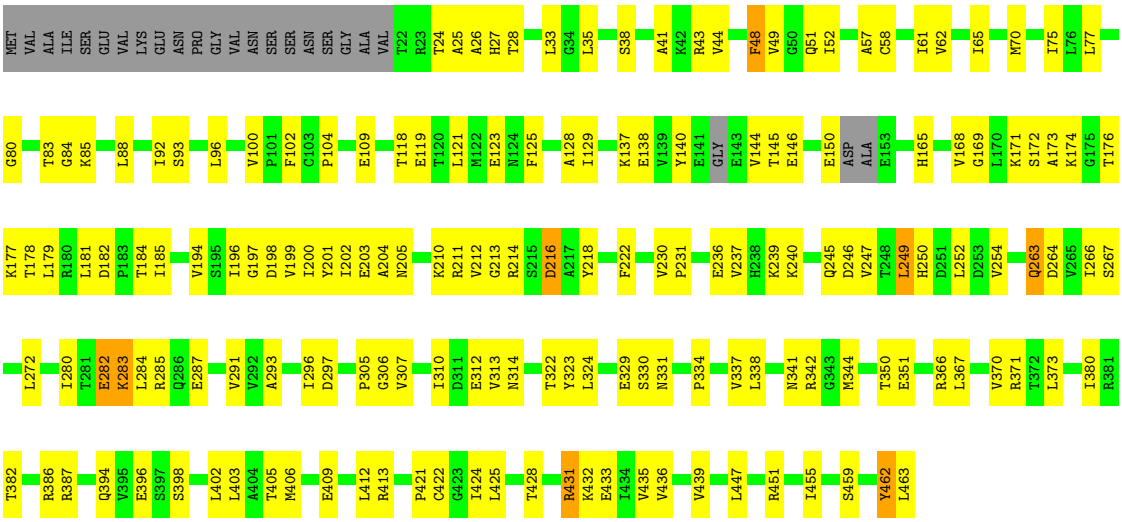
• Molecule 13: RuvB-like protein 1

Chain X:



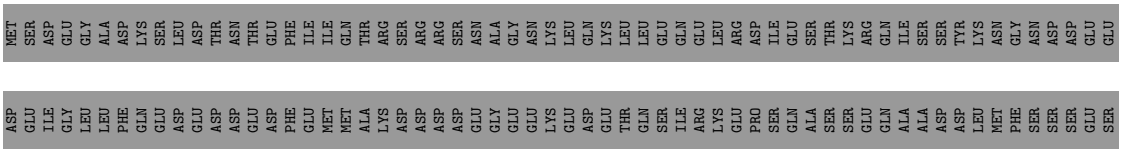
• Molecule 13: RuvB-like protein 1

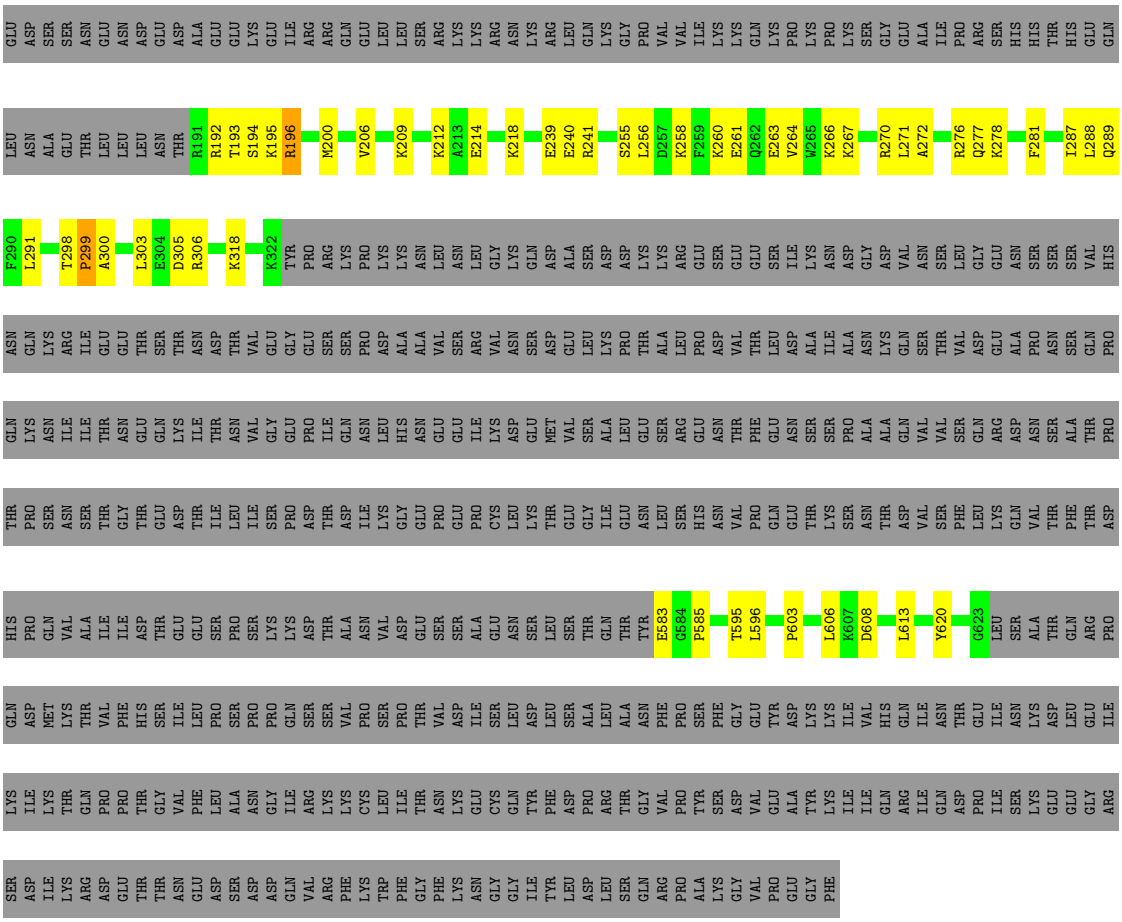
Chain T:



• Molecule 14: Vacuolar protein sorting-associated protein 72

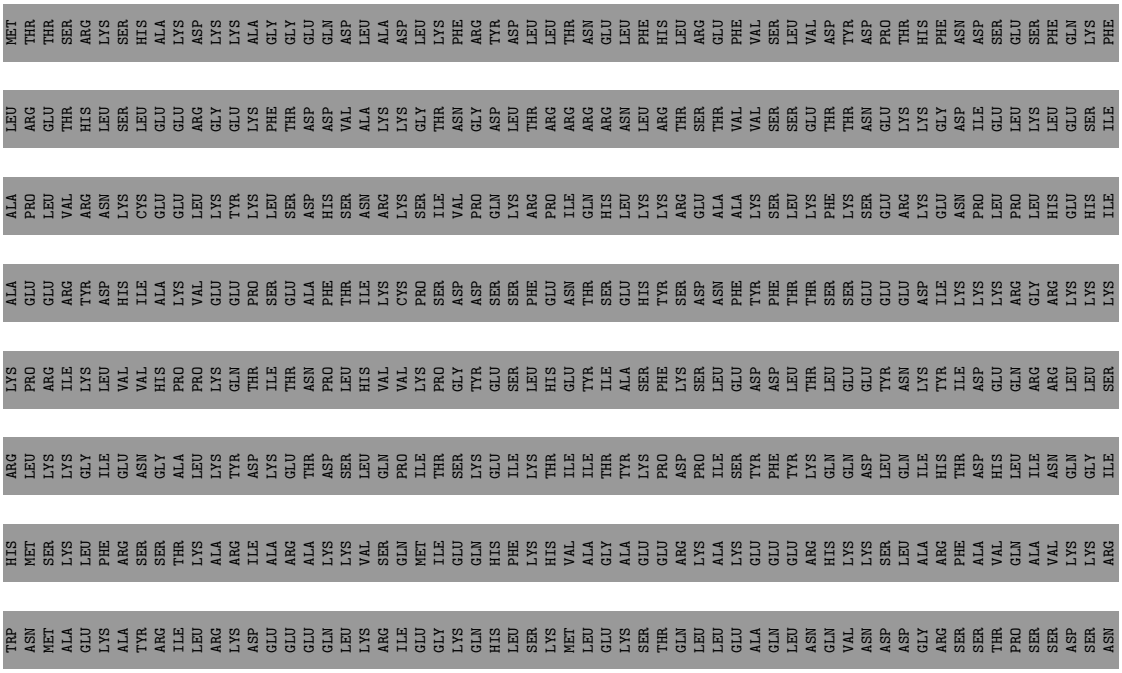
Chain Z:

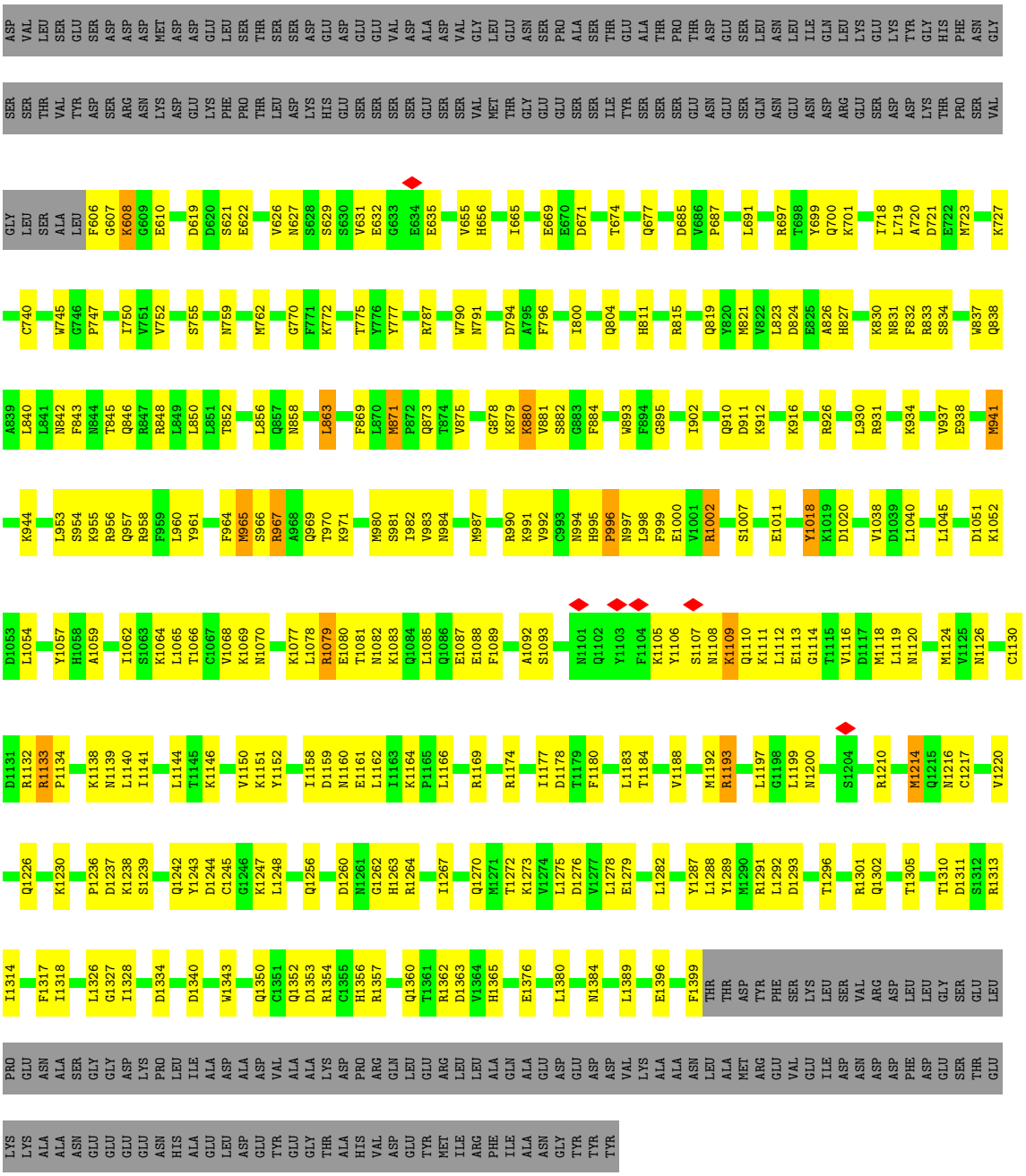




• Molecule 15: Helicase SWR1

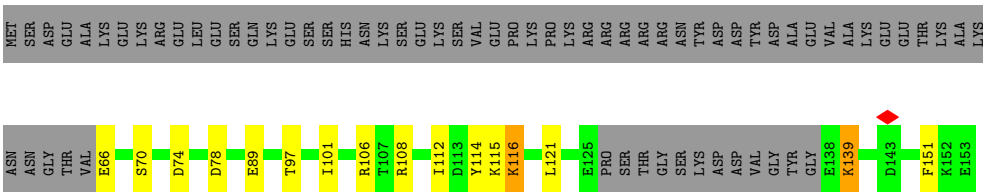
Chain M:





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

Chain K:



4 Experimental information (i)

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 ($e^-/Å^2$)	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: MG, ZN, ADP, 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	0.24	0/877	0.61	0/1178
1	B	0.25	0/862	0.61	0/1159
2	C	0.30	0/564	0.59	0/763
2	D	0.26	0/531	0.58	0/716
3	E	0.24	0/725	0.53	0/992
4	G	0.23	0/646	0.46	0/873
5	H	0.25	0/722	0.53	0/972
6	I	0.52	0/2576	0.92	0/3969
7	J	0.50	0/2620	0.87	0/4046
8	L	0.23	0/682	0.53	0/917
9	P	0.26	0/914	0.68	3/1232 (0.2%)
10	R	0.27	0/3206	0.51	0/4351
11	S	0.27	0/1521	0.57	0/2047
12	U	0.25	0/3468	0.53	0/4674
12	W	0.25	0/3343	0.50	0/4508
12	Y	0.24	0/3378	0.51	1/4561 (0.0%)
13	T	0.26	0/3342	0.55	0/4527
13	V	0.24	0/3294	0.52	0/4458
13	X	0.24	0/3412	0.52	1/4618 (0.0%)
14	Z	0.23	0/1419	0.53	0/1899
15	M	0.24	0/6330	0.50	0/8561
16	K	0.25	0/606	0.54	0/806
All	All	0.29	0/45038	0.59	5/61827 (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.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	P	231	LEU	CA-CB-CG	6.27	129.72	115.30
9	P	233	PRO	C-N-CA	5.86	136.36	121.70
9	P	254	LEU	CA-CB-CG	5.62	128.22	115.30
12	Y	346	ASP	CB-CG-OD2	5.47	123.22	118.30
13	X	406	MET	CA-CB-CG	5.42	122.52	113.30

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	39	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	23	0
4	G	640	0	617	23	0
5	H	712	0	736	34	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	104	0
11	S	1500	0	1537	67	0
12	U	3430	0	3505	132	0
12	W	3307	0	3388	117	0
12	Y	3342	0	3364	106	0
13	T	3304	0	3389	132	0
13	V	3257	0	3385	121	0
13	X	3371	0	3487	105	0
14	Z	1400	0	1393	35	0
15	M	6223	0	6066	205	0
16	K	606	0	536	17	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	1379	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 1379 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)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	106/136 (78%)	93 (88%)	10 (9%)	3 (3%)	4 27
1	B	108/136 (79%)	98 (91%)	10 (9%)	0	100 100
2	C	74/103 (72%)	73 (99%)	1 (1%)	0	100 100
2	D	69/103 (67%)	67 (97%)	1 (1%)	1 (1%)	9 37
3	E	100/132 (76%)	96 (96%)	4 (4%)	0	100 100
4	G	84/131 (64%)	81 (96%)	3 (4%)	0	100 100
5	H	89/131 (68%)	84 (94%)	5 (6%)	0	100 100
8	L	85/134 (63%)	85 (100%)	0	0	100 100
9	P	112/303 (37%)	93 (83%)	18 (16%)	1 (1%)	14 45
10	R	379/438 (86%)	349 (92%)	29 (8%)	1 (0%)	37 69
11	S	182/280 (65%)	155 (85%)	25 (14%)	2 (1%)	12 42
12	U	444/471 (94%)	415 (94%)	27 (6%)	2 (0%)	25 58
12	W	429/471 (91%)	414 (96%)	15 (4%)	0	100 100
12	Y	439/471 (93%)	422 (96%)	16 (4%)	1 (0%)	44 74
13	T	433/463 (94%)	413 (95%)	20 (5%)	0	100 100
13	V	423/463 (91%)	407 (96%)	16 (4%)	0	100 100
13	X	437/463 (94%)	410 (94%)	27 (6%)	0	100 100
14	Z	169/795 (21%)	153 (90%)	15 (9%)	1 (1%)	22 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	M	792/1514 (52%)	732 (92%)	56 (7%)	4 (0%)	25 58
16	K	72/153 (47%)	62 (86%)	9 (12%)	1 (1%)	9 37
All	All	5026/7291 (69%)	4702 (94%)	307 (6%)	17 (0%)	38 69

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	LYS
9	P	205	LYS
10	R	221	ARG
11	S	24	PRO
15	M	881	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	91/113 (80%)	88 (97%)	3 (3%)	33 56
1	B	84/113 (74%)	80 (95%)	4 (5%)	21 46
2	C	50/81 (62%)	44 (88%)	6 (12%)	4 19
2	D	52/81 (64%)	50 (96%)	2 (4%)	28 52
3	E	65/99 (66%)	62 (95%)	3 (5%)	23 47
4	G	66/109 (61%)	60 (91%)	6 (9%)	7 28
5	H	78/109 (72%)	76 (97%)	2 (3%)	41 61
8	L	69/103 (67%)	66 (96%)	3 (4%)	25 49
9	P	93/262 (36%)	88 (95%)	5 (5%)	18 43
10	R	349/396 (88%)	327 (94%)	22 (6%)	15 40
11	S	176/261 (67%)	164 (93%)	12 (7%)	13 38
12	U	379/403 (94%)	365 (96%)	14 (4%)	29 53
12	W	365/403 (91%)	352 (96%)	13 (4%)	30 54
12	Y	359/403 (89%)	344 (96%)	15 (4%)	25 49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	T	354/391 (90%)	345 (98%)	9 (2%)	42	62
13	V	356/391 (91%)	347 (98%)	9 (2%)	42	62
13	X	368/391 (94%)	357 (97%)	11 (3%)	36	58
14	Z	148/732 (20%)	141 (95%)	7 (5%)	22	46
15	M	662/1376 (48%)	628 (95%)	34 (5%)	20	45
16	K	67/136 (49%)	65 (97%)	2 (3%)	36	58
All	All	4231/6353 (67%)	4049 (96%)	182 (4%)	27	49

5 of 182 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	Y	18	SER
13	T	367	LEU
12	Y	86	MET
14	Z	196	ARG
15	M	790	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	984	ASN
15	M	1082	ASN
15	M	1280	GLN
11	S	223	ASN
10	R	374	GLN

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	$\#\|Z\| > 2$
17	ADP	M	1601	-	24,29,29	0.90	0	29,45,45	1.21	2 (6%)
17	ADP	Y	501	-	24,29,29	0.90	0	29,45,45	1.16	2 (6%)
18	BEF	M	1602	-	0,3,3	-	-	-		
17	ADP	U	501	19	24,29,29	0.90	0	29,45,45	1.25	3 (10%)
18	BEF	R	502	-	0,3,3	-	-	-		
17	ADP	V	501	19	24,29,29	0.87	0	29,45,45	1.18	2 (6%)
17	ADP	R	501	19	24,29,29	0.93	1 (4%)	29,45,45	1.41	4 (13%)
17	ADP	X	501	19	24,29,29	0.90	0	29,45,45	1.24	2 (6%)
17	ADP	T	501	19	24,29,29	0.89	0	29,45,45	1.23	2 (6%)
17	ADP	W	501	19	24,29,29	0.91	0	29,45,45	1.24	2 (6%)

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	M	1601	-	-	6/12/32/32	0/3/3/3
17	ADP	Y	501	-	-	3/12/32/32	0/3/3/3
17	ADP	U	501	19	-	2/12/32/32	0/3/3/3
17	ADP	V	501	19	-	7/12/32/32	0/3/3/3
17	ADP	R	501	19	-	0/12/32/32	0/3/3/3
17	ADP	X	501	19	-	3/12/32/32	0/3/3/3
17	ADP	T	501	19	-	2/12/32/32	0/3/3/3
17	ADP	W	501	19	-	1/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	R	501	ADP	O4'-C1'	2.12	1.43	1.40

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	R	501	ADP	N3-C2-N1	-3.71	123.63	128.67
17	M	1601	ADP	N3-C2-N1	-3.70	123.65	128.67
17	W	501	ADP	N3-C2-N1	-3.66	123.70	128.67
17	X	501	ADP	N3-C2-N1	-3.66	123.71	128.67
17	T	501	ADP	N3-C2-N1	-3.62	123.76	128.67

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.

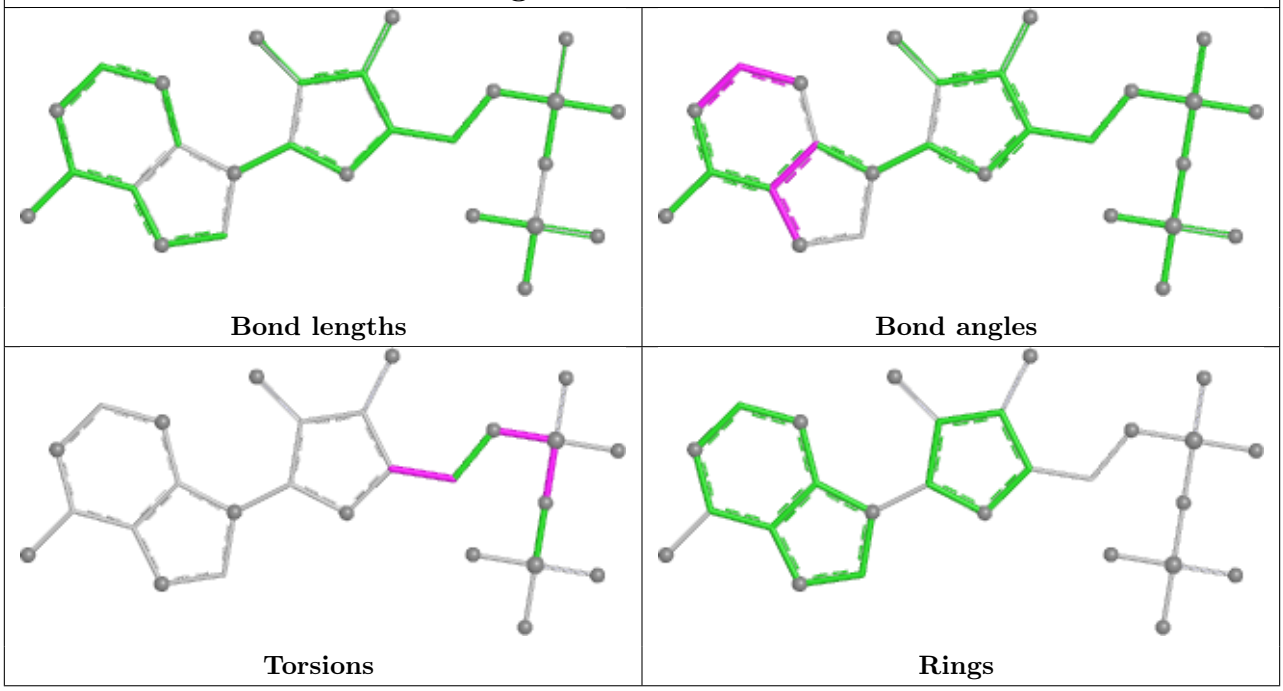
10 monomers are involved in 28 short contacts:

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

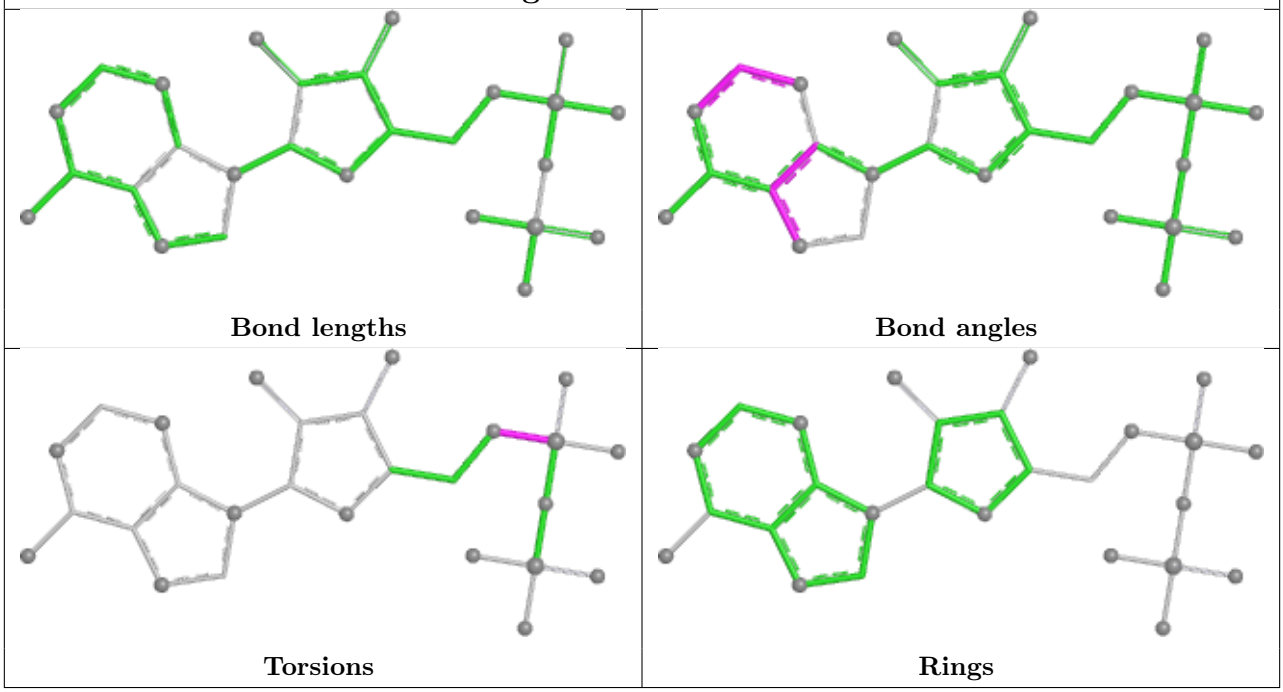
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

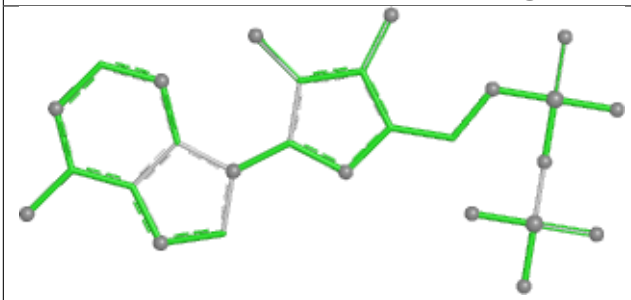
Ligand ADP M 1601



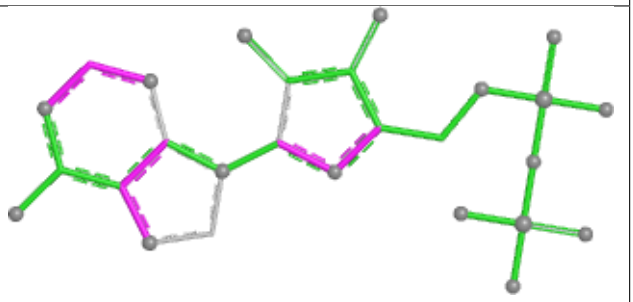
Ligand ADP Y 501



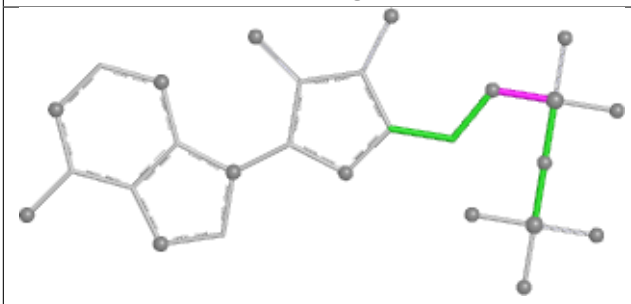
Ligand ADP U 501



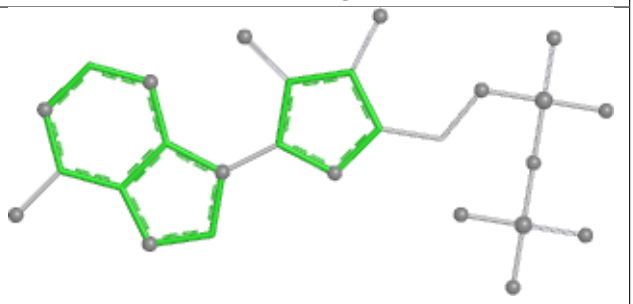
Bond lengths



Bond angles

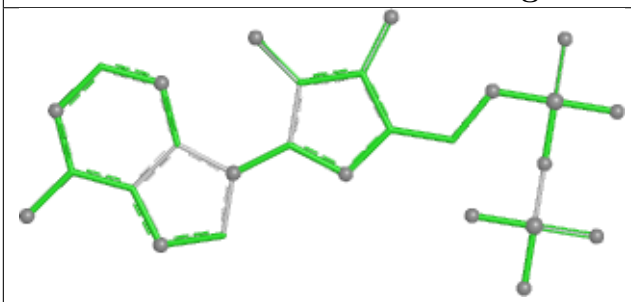


Torsions

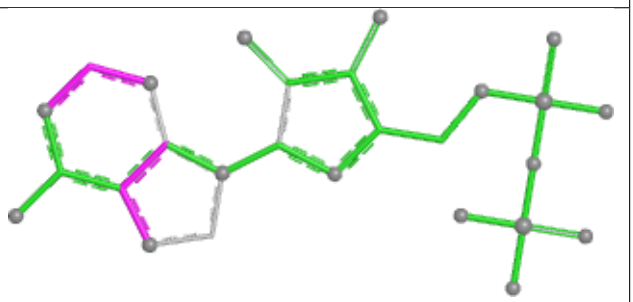


Rings

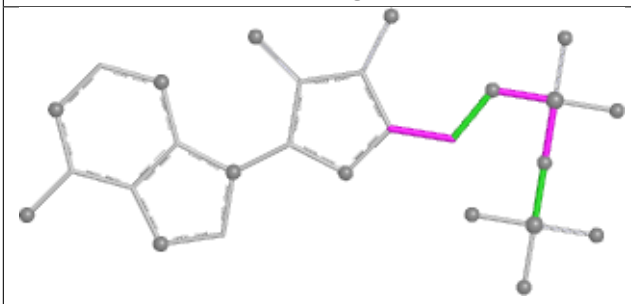
Ligand ADP V 501



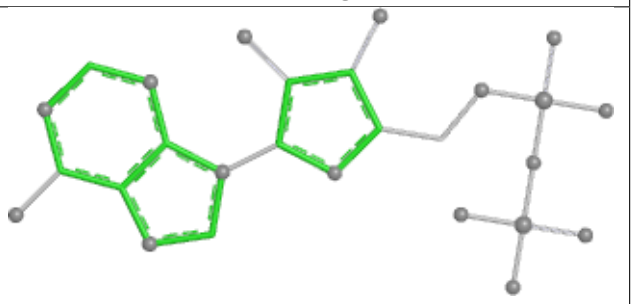
Bond lengths



Bond angles

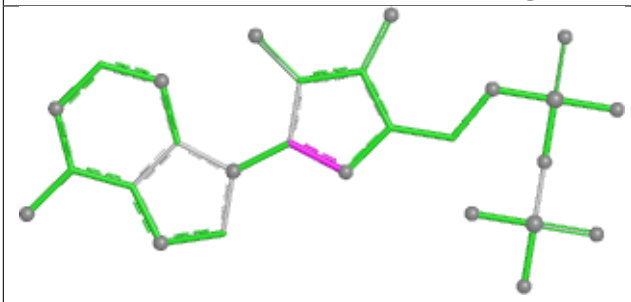


Torsions

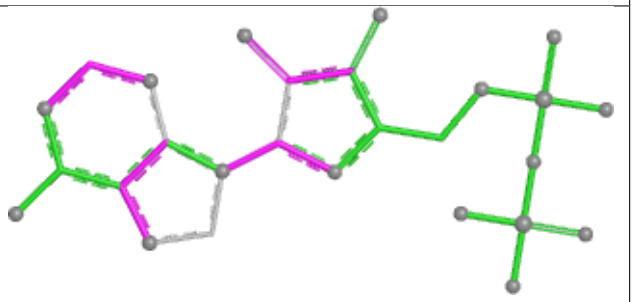


Rings

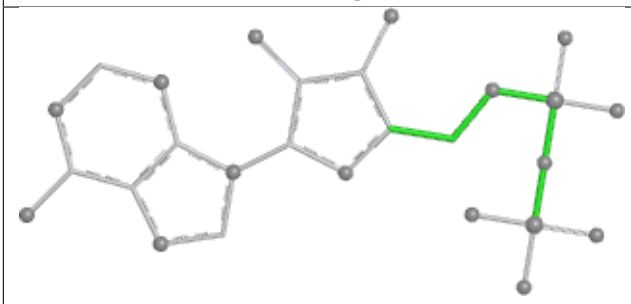
Ligand ADP R 501



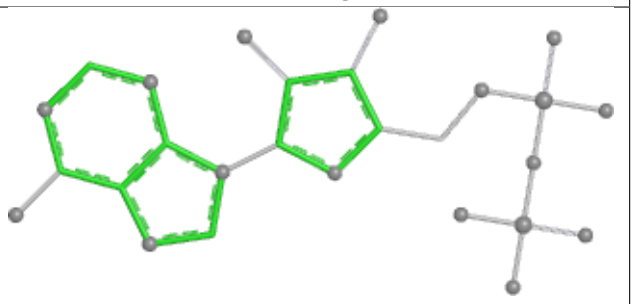
Bond lengths



Bond angles

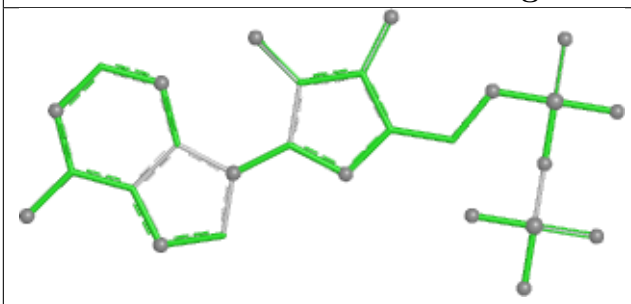


Torsions

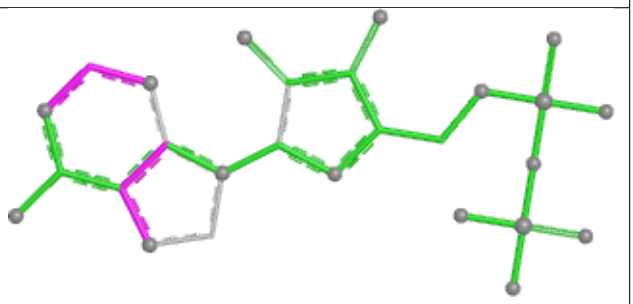


Rings

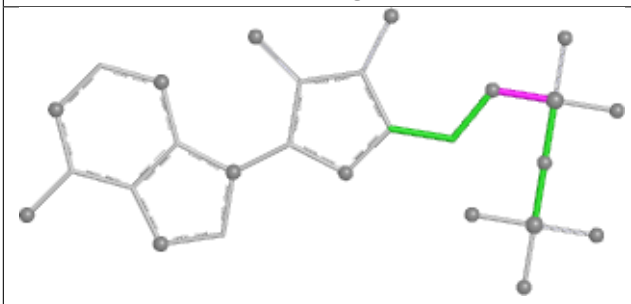
Ligand ADP X 501



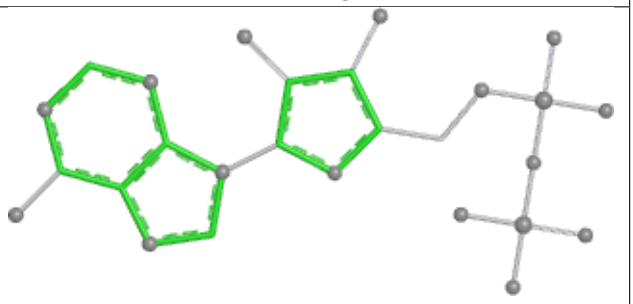
Bond lengths



Bond angles

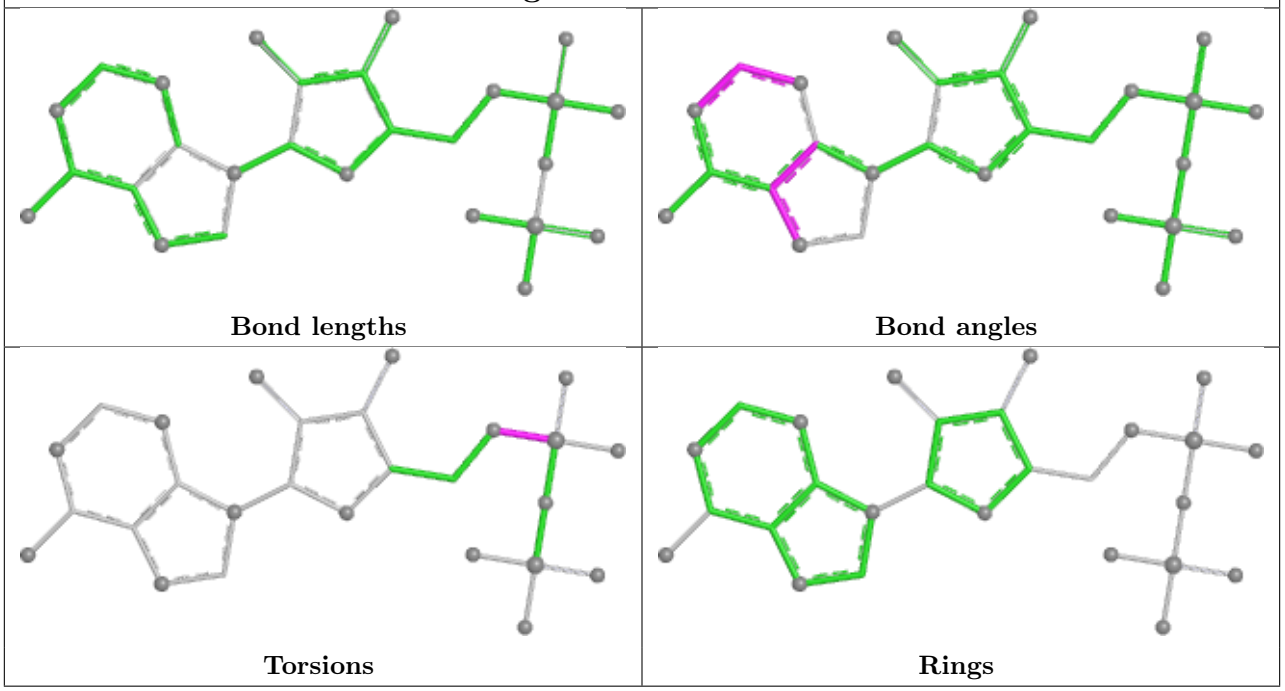


Torsions

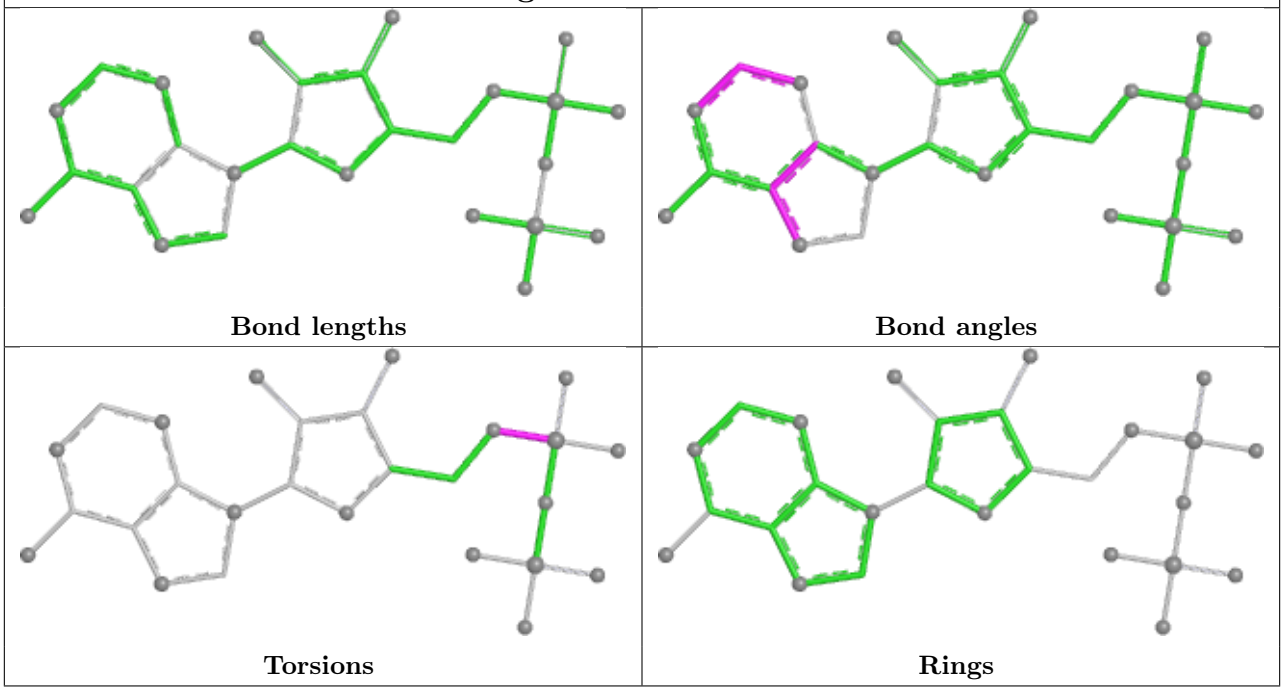


Rings

Ligand ADP T 501



Ligand ADP W 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

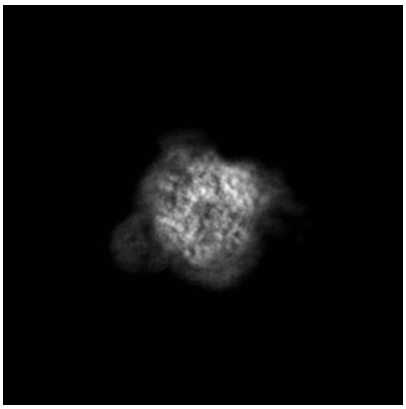
6 Map visualisation

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

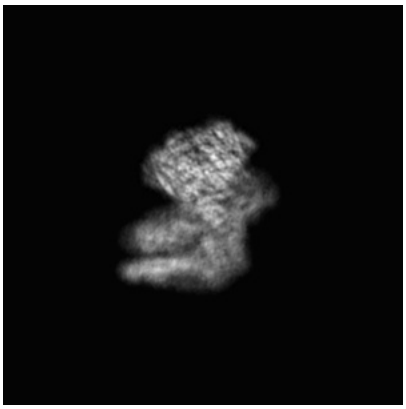
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

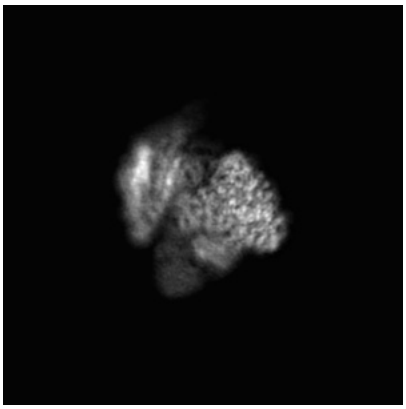
6.1.1 Primary map



X

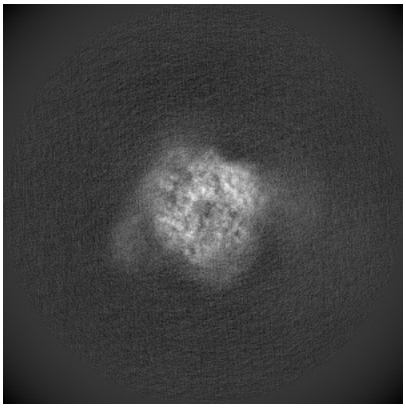


Y

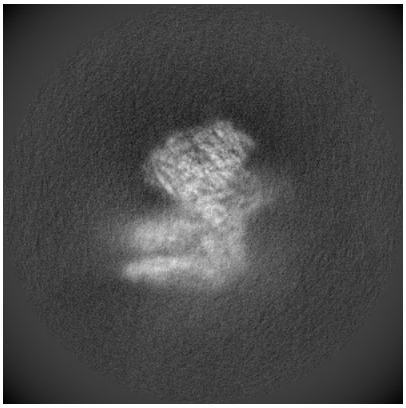


Z

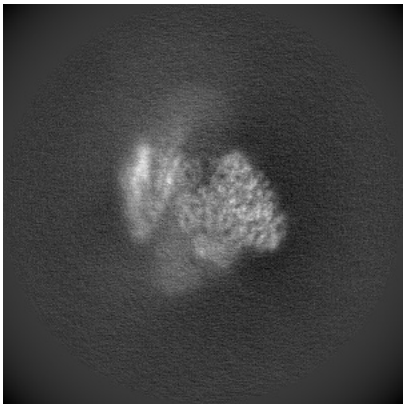
6.1.2 Raw map



X



Y

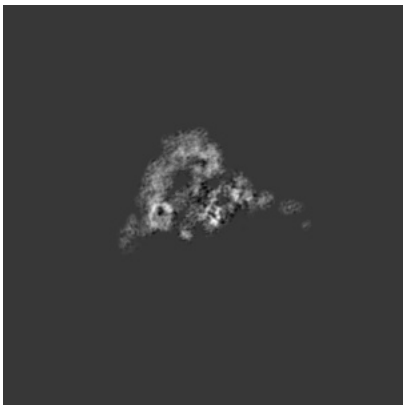


Z

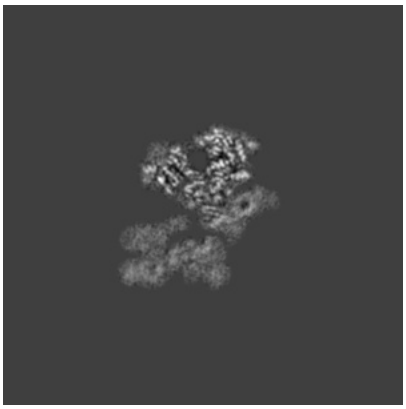
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

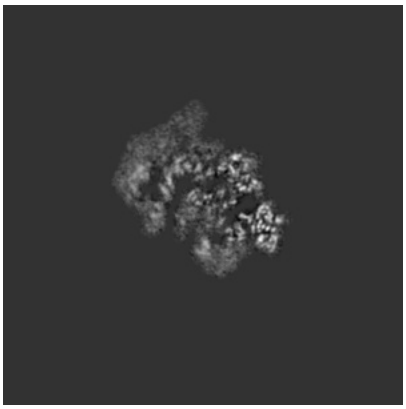
6.2.1 Primary map



X Index: 240

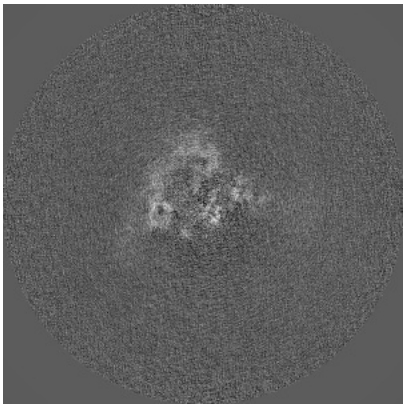


Y Index: 240

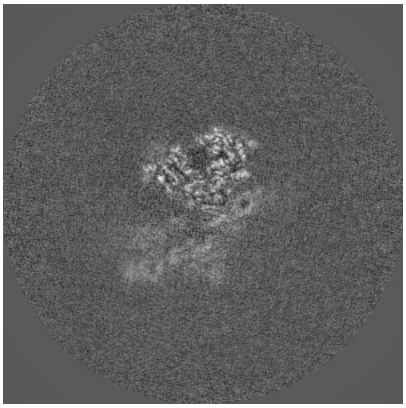


Z Index: 240

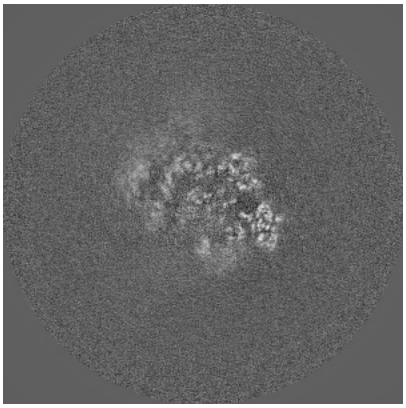
6.2.2 Raw map



X Index: 240



Y Index: 240

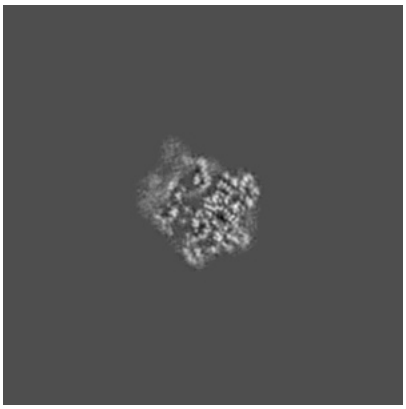


Z Index: 240

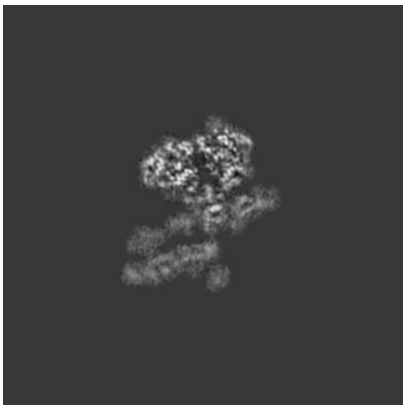
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

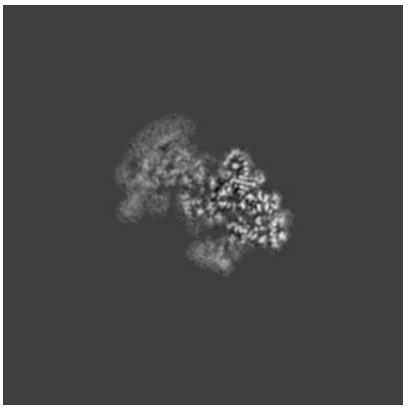
6.3.1 Primary map



X Index: 276

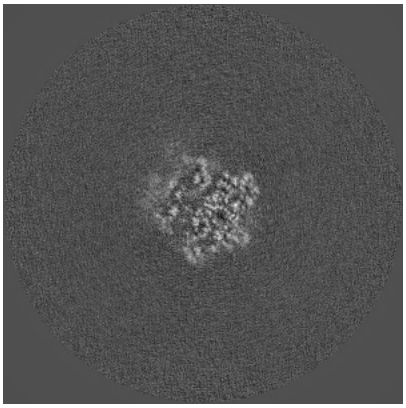


Y Index: 231

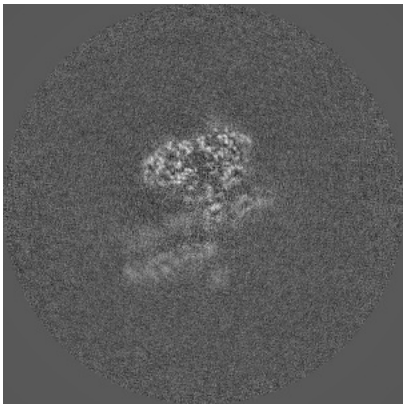


Z Index: 258

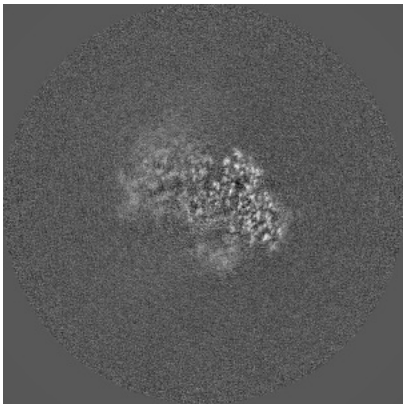
6.3.2 Raw map



X Index: 276



Y Index: 231

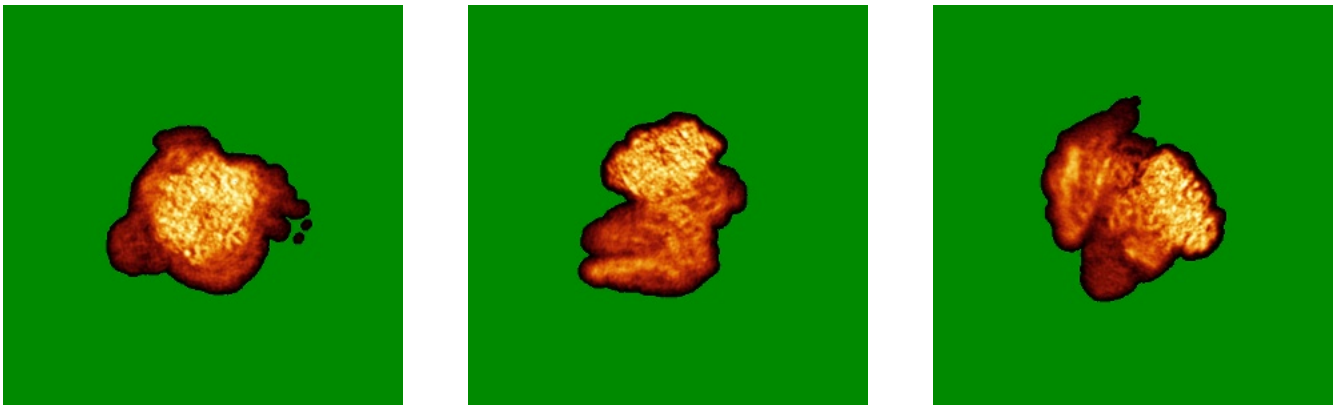


Z Index: 252

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

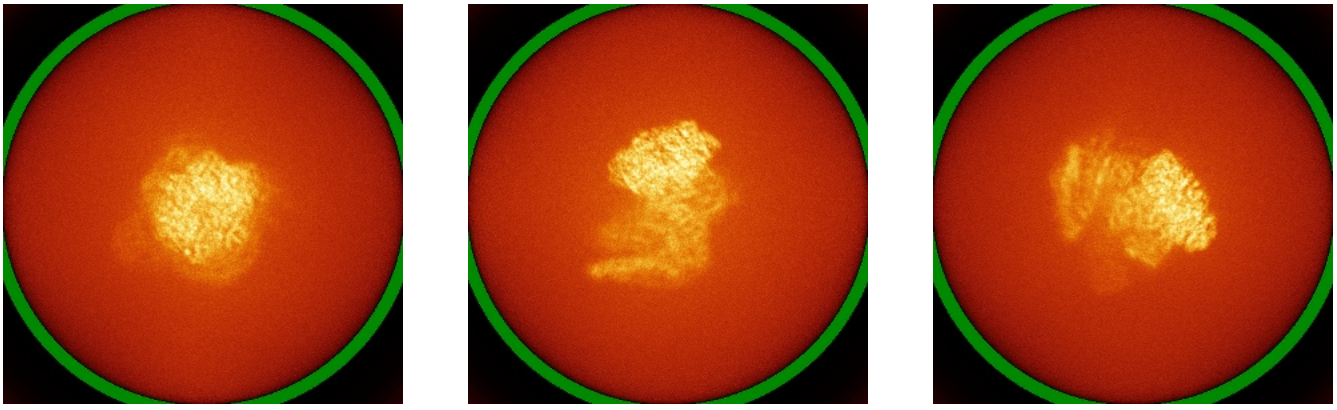
6.4 Orthogonal standard-deviation projections (False-color) (i)

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.

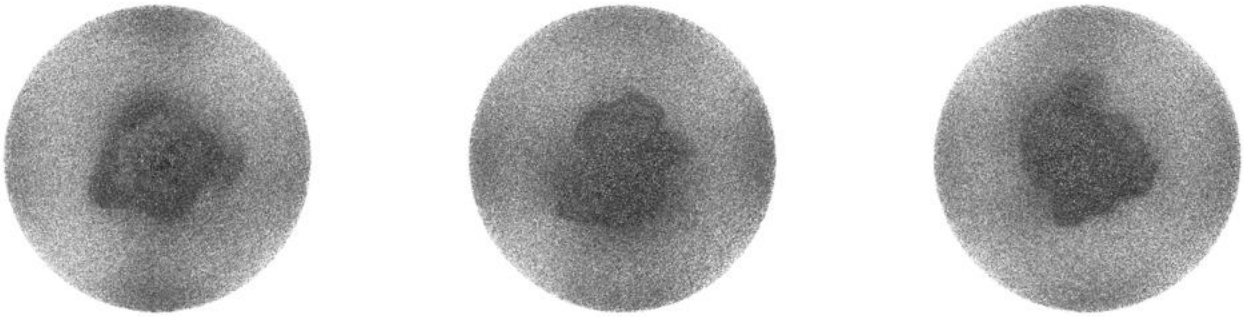
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

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.

6.5.2 Raw map



X Y Z

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

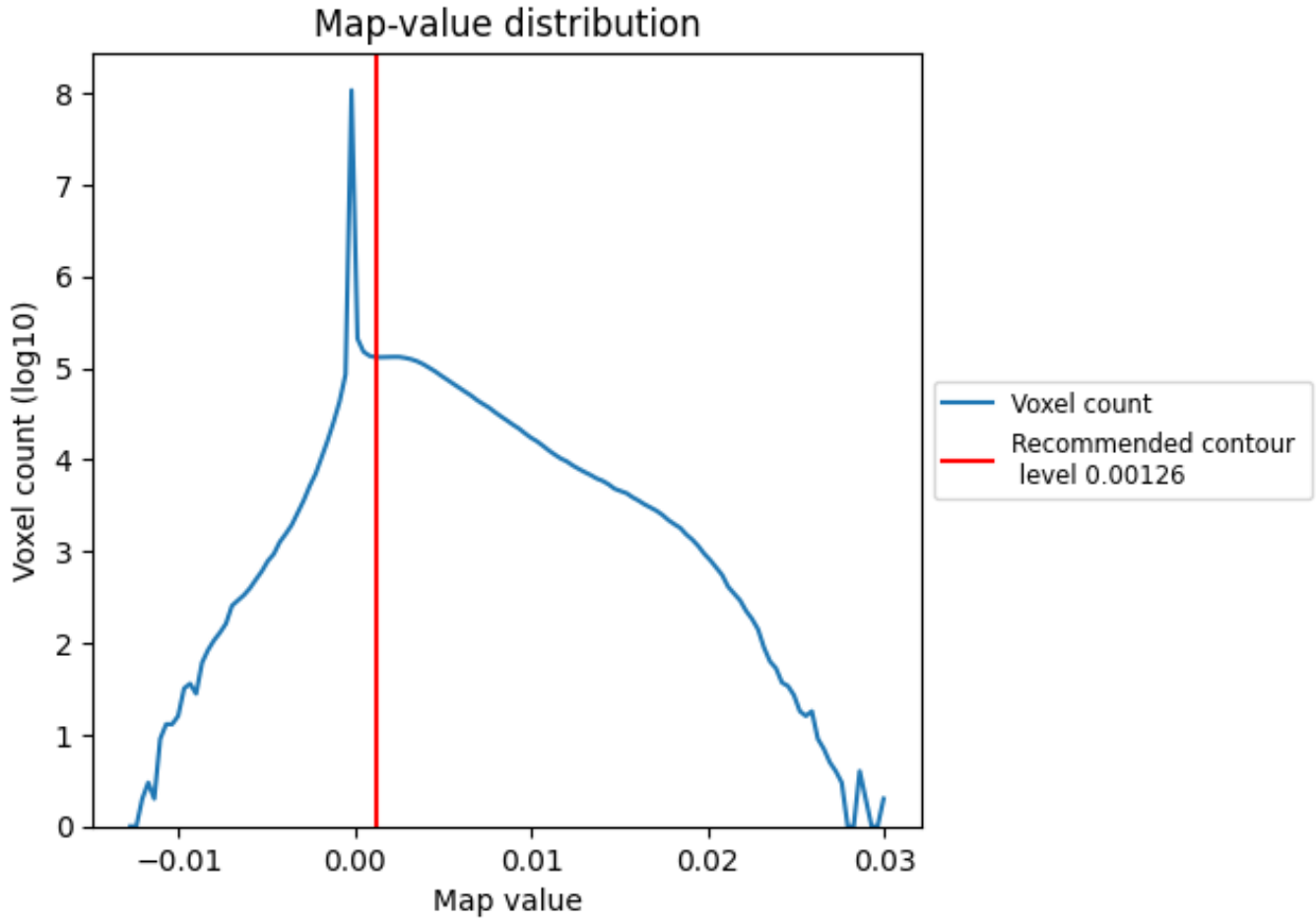
6.6 Mask visualisation (i)

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

7 Map analysis

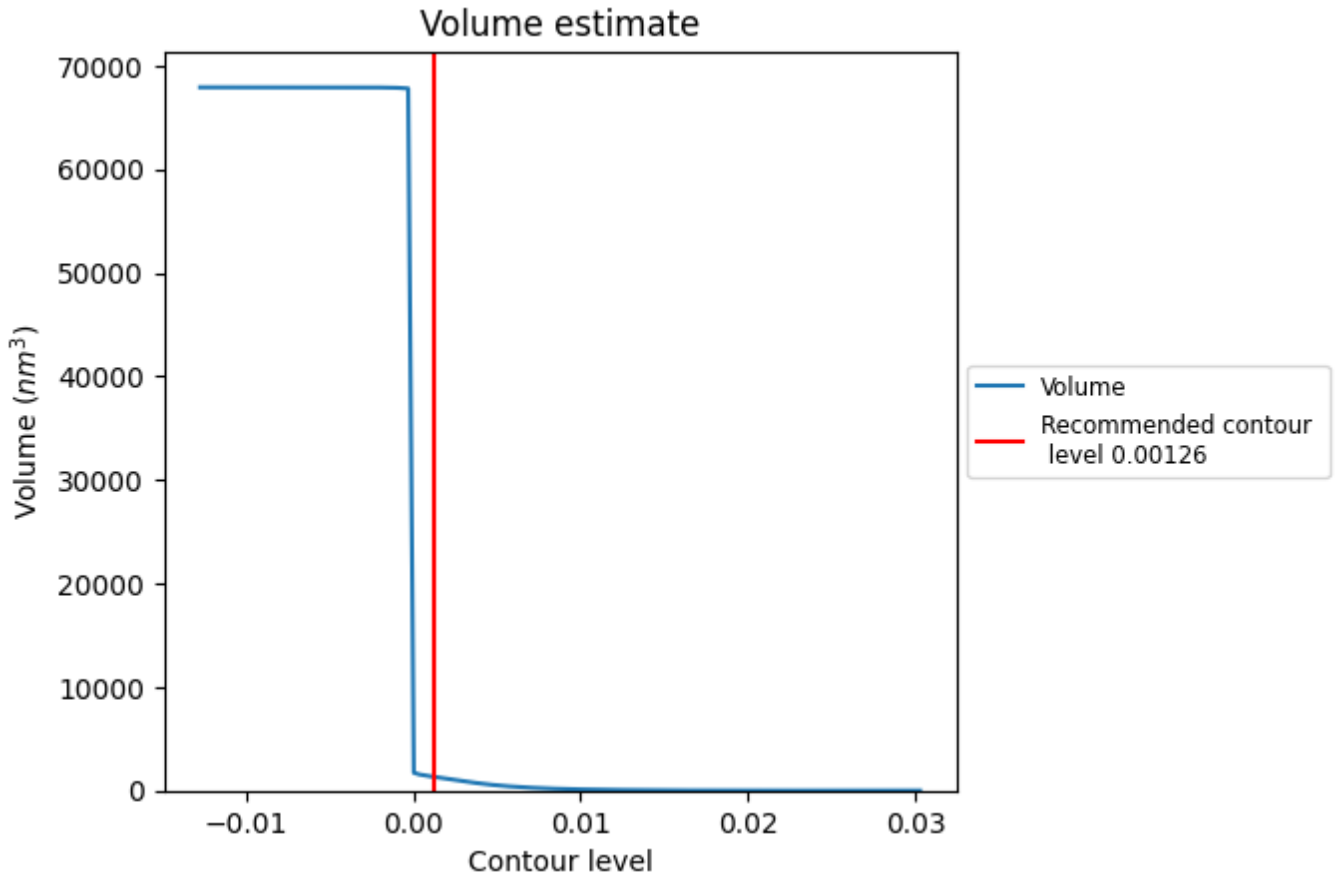
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

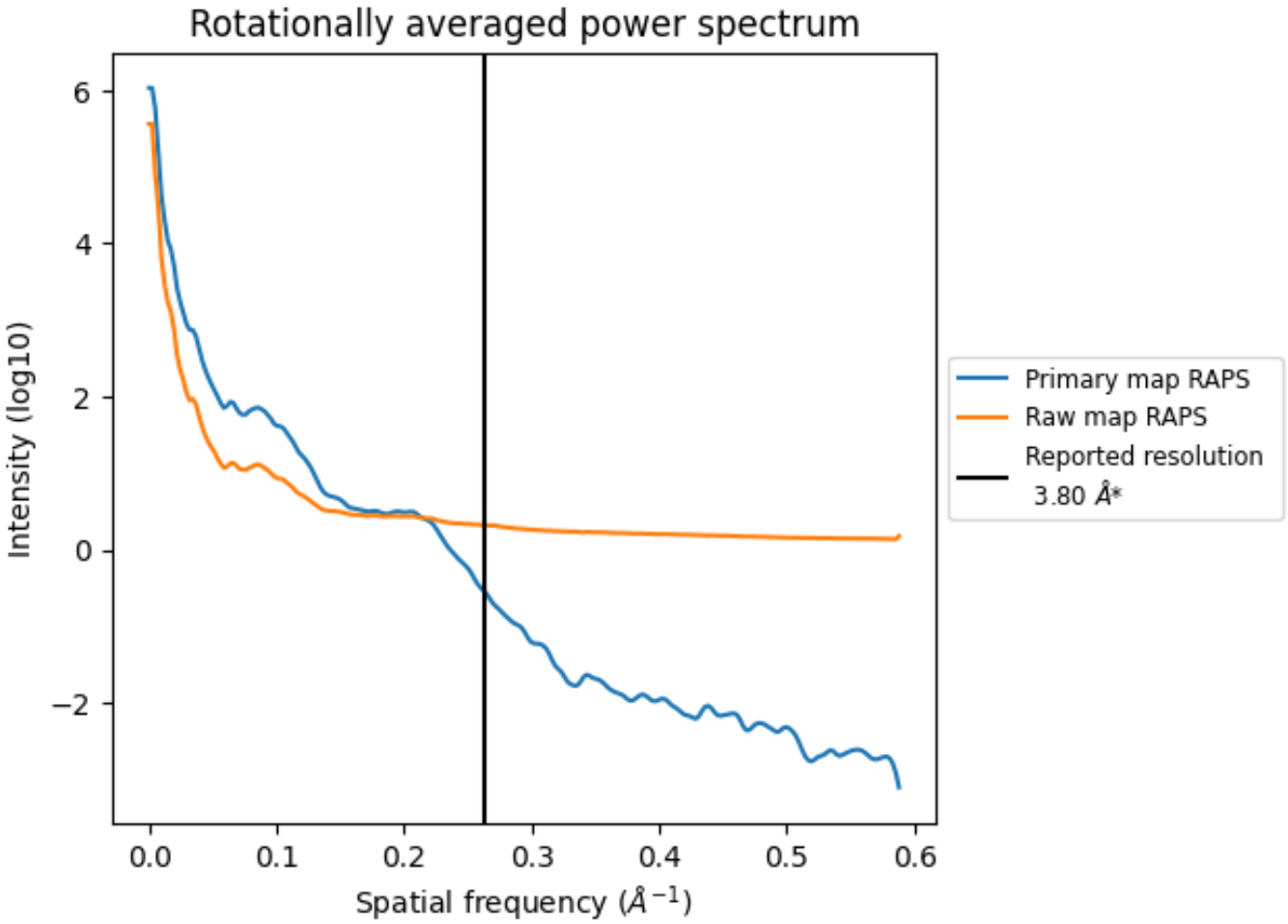
7.2 Volume estimate (i)



The volume at the recommended contour level is 1321 nm^3; 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 (i)

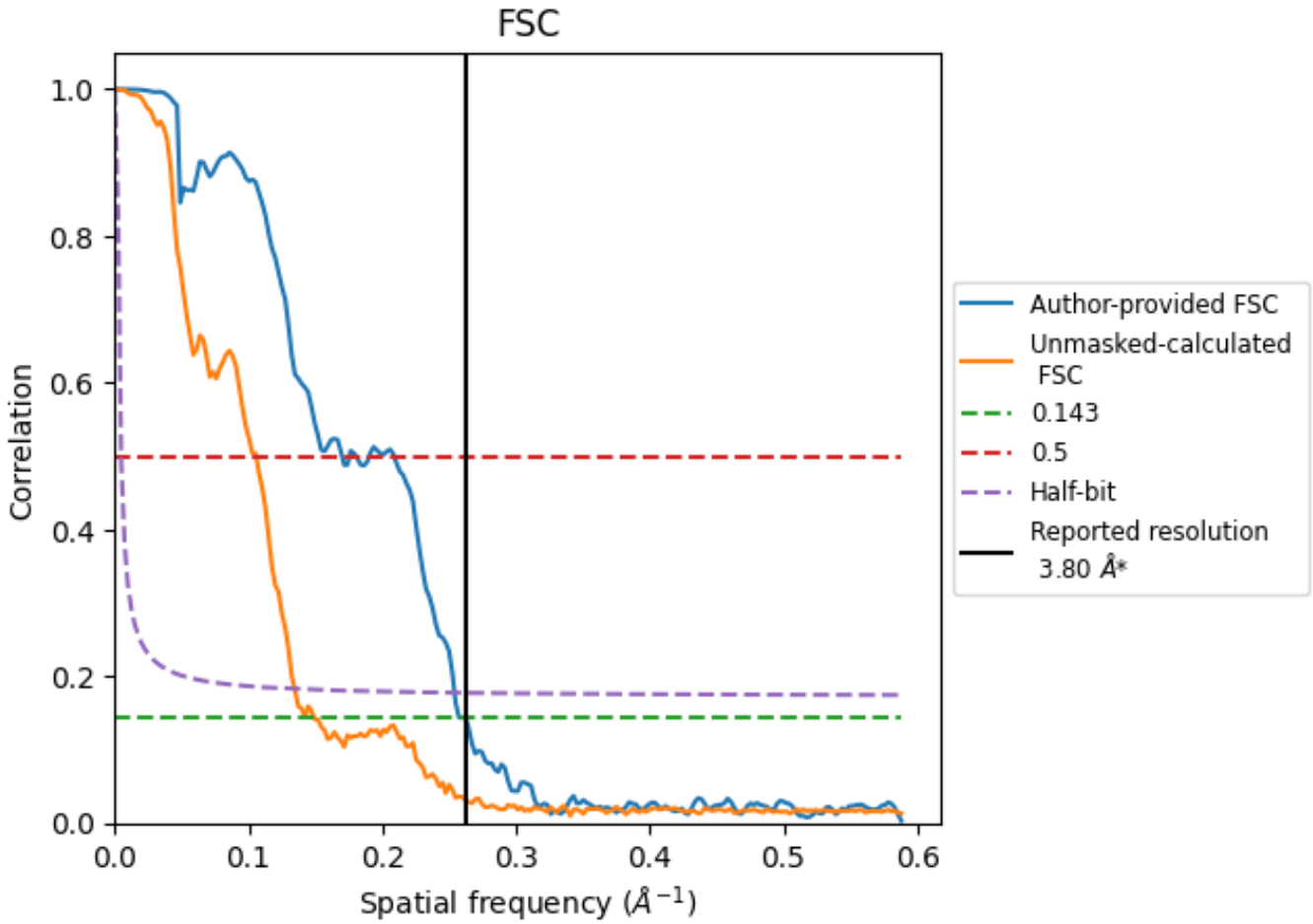


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8.2 Resolution estimates (i)

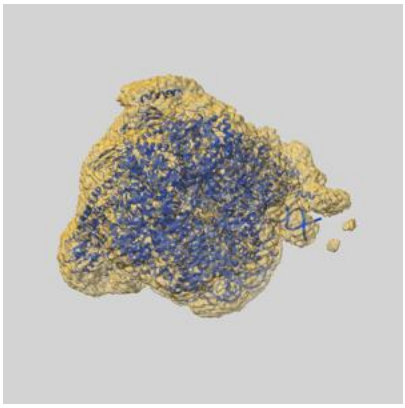
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.81	5.88	3.94
Unmasked-calculated*	6.71	9.46	7.43

*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 %

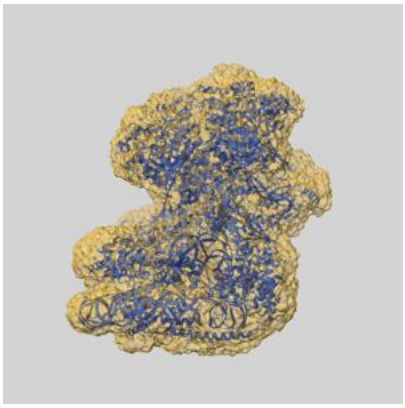
9 Map-model fit

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.

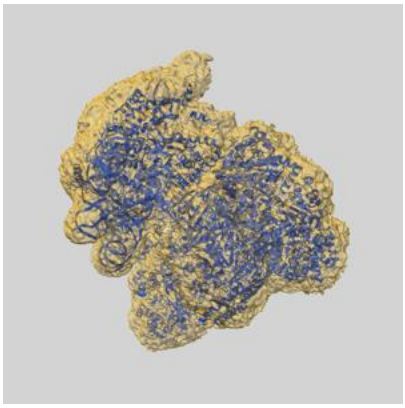
9.1 Map-model overlay



X



Y



Z

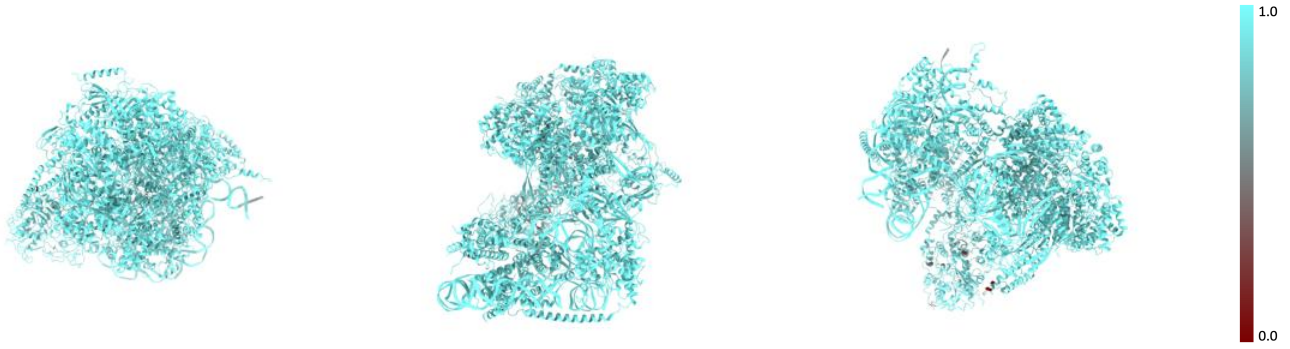
The images above show the 3D surface view of the map at the recommended contour level 0.00126 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

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

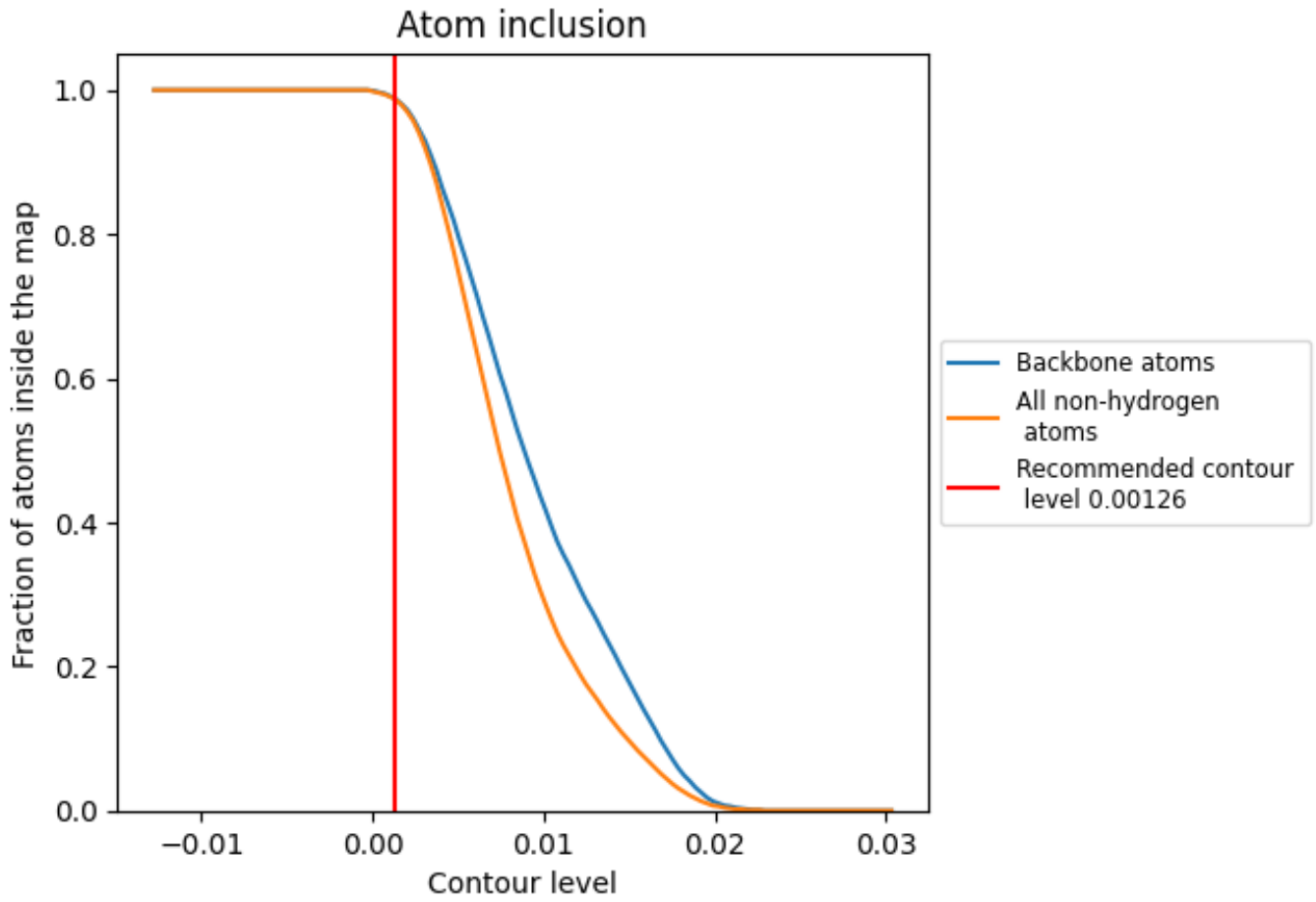
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00126).

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