wwPDB EM Validation Summary Report (i)

Dec 2, 2024 – 08:28 AM EST

PDB ID	:	9B1D
EMDB ID	:	EMD-44074
Title	:	Cryo-EM structure of native SWR1 bound to DNA (composite structure)
Authors	:	Louder, R.K.; Park, G.; Wu, C.
Deposited on	:	2024-03-13
Resolution	:	3.30 Å(reported)
Based on initial models	:	., 6GEJ

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:

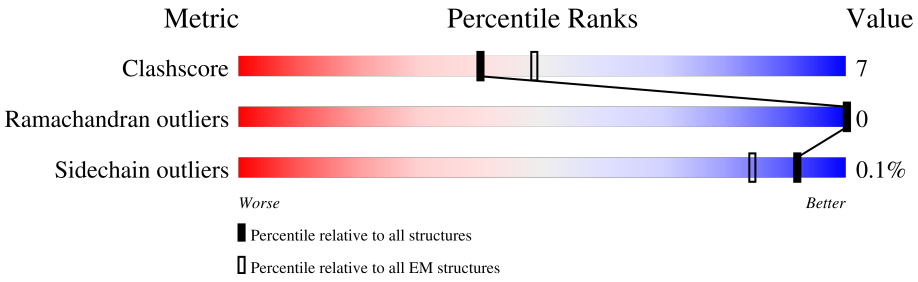
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.30 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	1544	9% 37% 9% 54%
2	B	795	6% 16% 83%
3	C	438	75% 19% 6%
4	D	280	12% 56% 10% 33%
5	E	837	42% 9% 49%
5	G	837	41% 11% 48%
5	I	837	44% 8% 48%
6	F	471	81% 13% 6%

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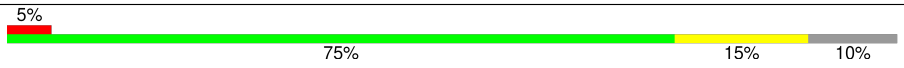
Mol	Chain	Length	Quality of chain
6	H	471	
6	J	471	
7	Y	147	
8	Z	147	

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 33147 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 Helicase SWR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	710	5827	3714	1027	1059	27	0	0

- Molecule 2 is a protein called Vacuolar protein sorting-associated protein 72.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	138	1152	740	196	212	4	0	0

- Molecule 3 is a protein called Actin-like protein ARP6.

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

- Molecule 4 is a protein called Vacuolar protein sorting-associated protein 71.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	187	1518	960	267	281	10	0	0

- Molecule 5 is a protein called RuvB-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	426	3281	2072	565	634	10	0	0
5	G	434	3334	2104	575	645	10	0	0
5	I	436	3351	2115	577	649	10	0	0

- Molecule 6 is a protein called RuvB-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	443	Total	C	N	O	S	0	0
			3410	2131	591	676	12		
6	H	441	Total	C	N	O	S	0	0
			3393	2119	588	674	12		
6	J	426	Total	C	N	O	S	0	0
			3279	2052	566	650	11		

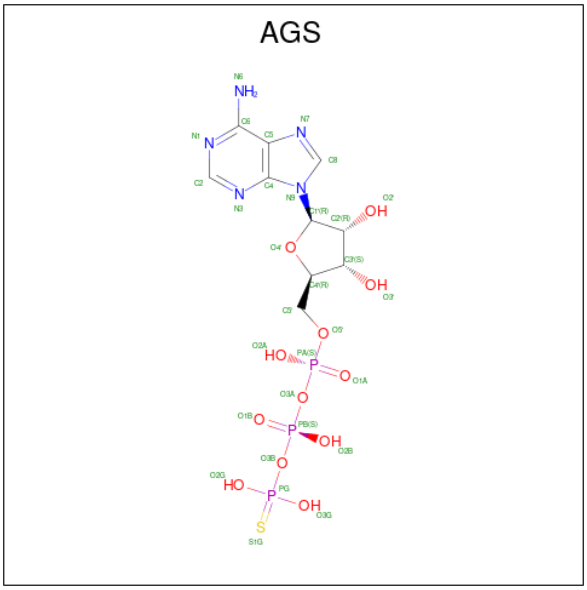
- Molecule 7 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	25	Total	C	N	O	P	0	0
			512	243	93	151	25		

- Molecule 8 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	25	Total	C	N	O	P	0	0
			513	243	96	149	25		

- Molecule 9 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						AltConf
9	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
9	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

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Mol	Chain	Residues	Atoms						AltConf
9	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
9	G	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

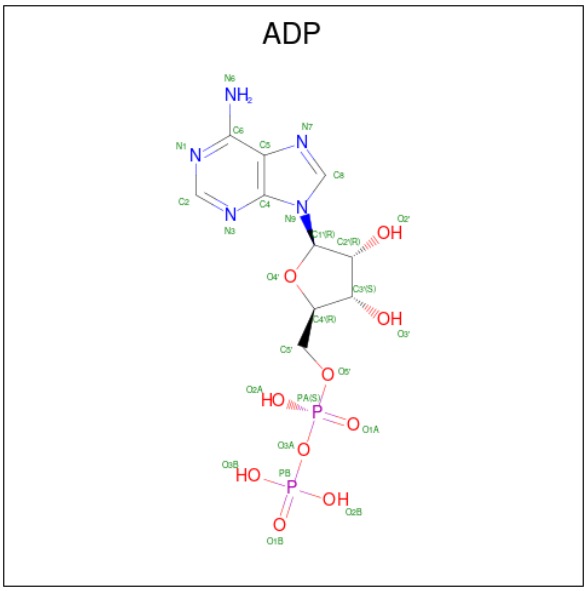
- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Mg	0
			1	1	
10	C	1	Total	Mg	0
			1	1	
10	E	1	Total	Mg	0
			1	1	
10	F	1	Total	Mg	0
			1	1	
10	G	1	Total	Mg	0
			1	1	
10	H	1	Total	Mg	0
			1	1	
10	I	1	Total	Mg	0
			1	1	
10	J	1	Total	Mg	0
			1	1	

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
11	D	2	Total	Zn	0
			2	2	

- Molecule 12 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



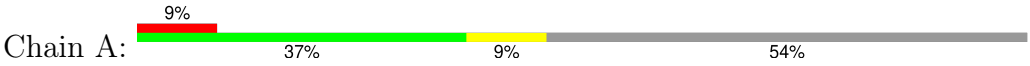
Mol	Chain	Residues	Atoms					AltConf
12	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

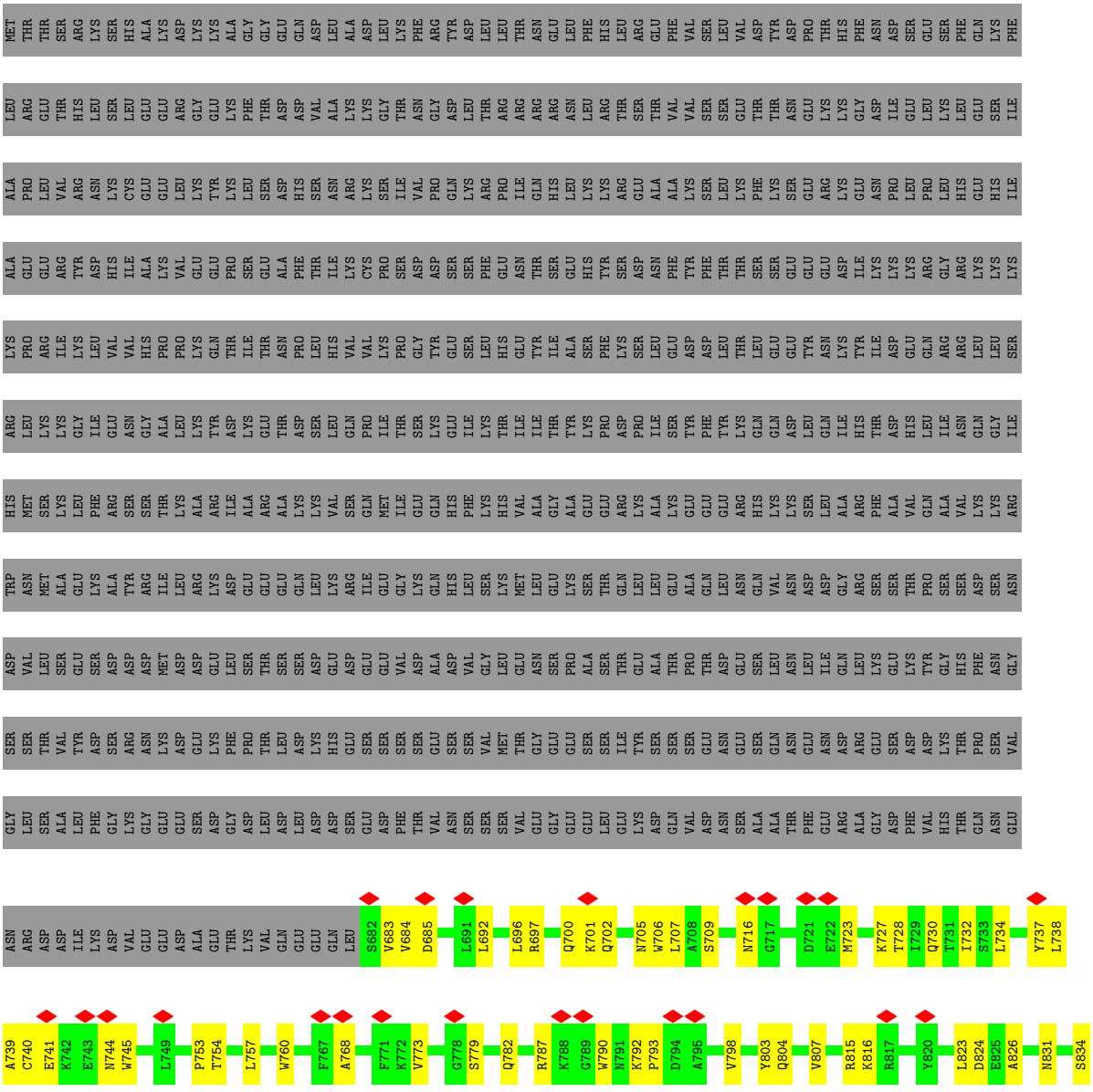
3 Residue-property plots (i)

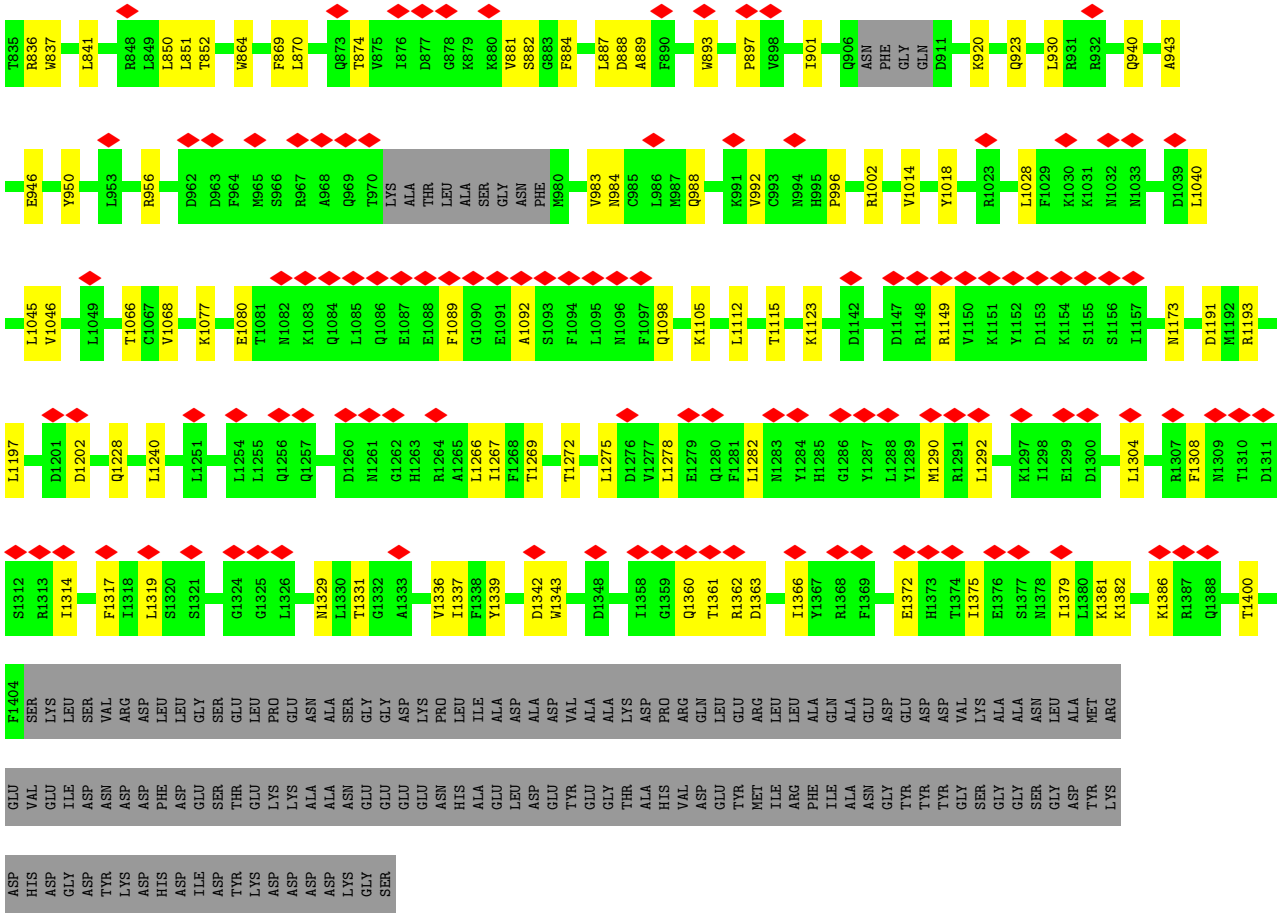
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Helicase SWR1

Chain A:

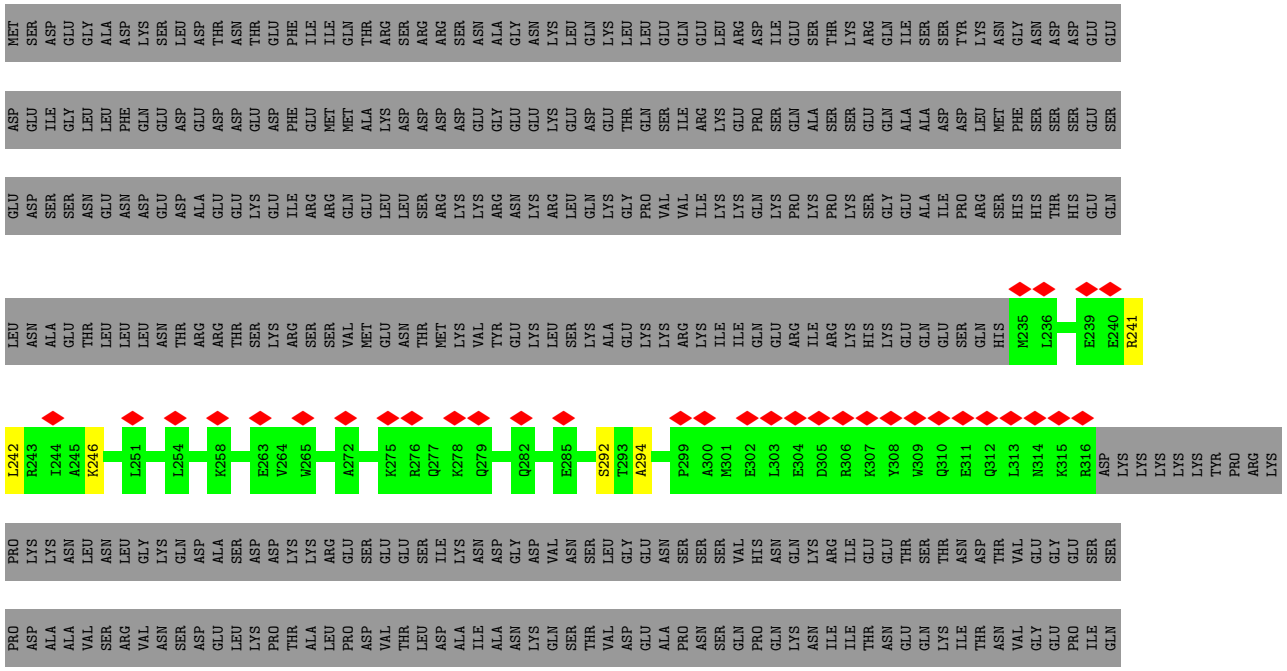


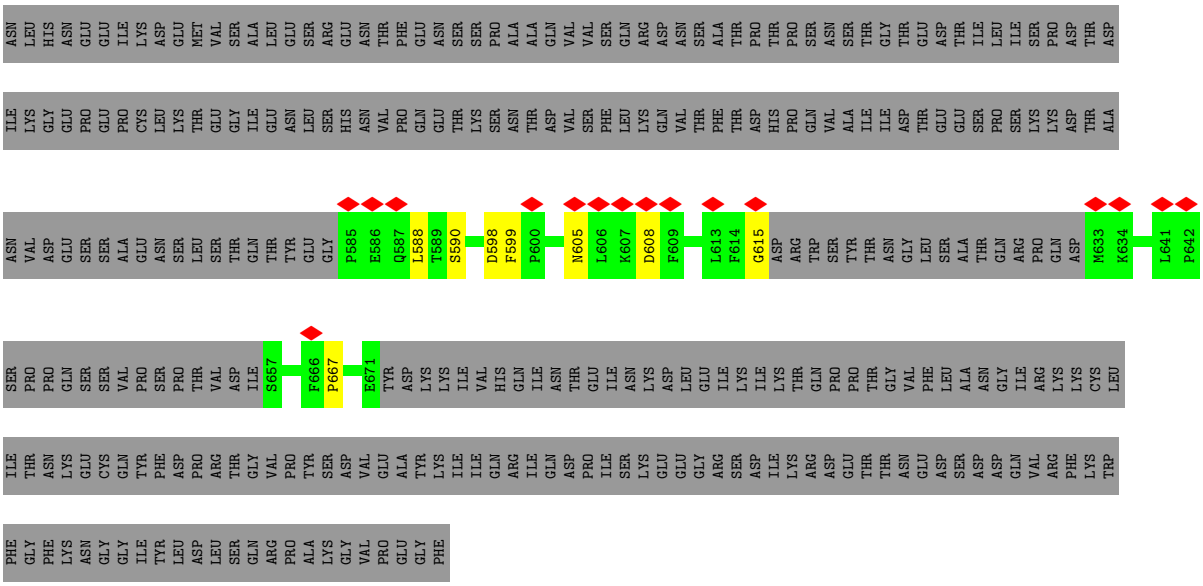




• Molecule 2: Vacuolar protein sorting-associated protein 72

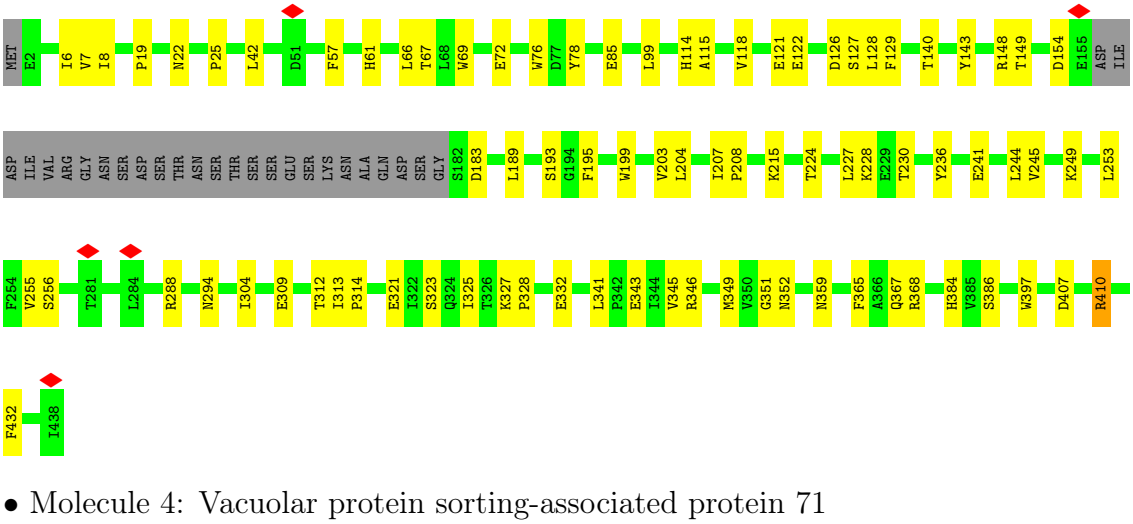
Chain B:





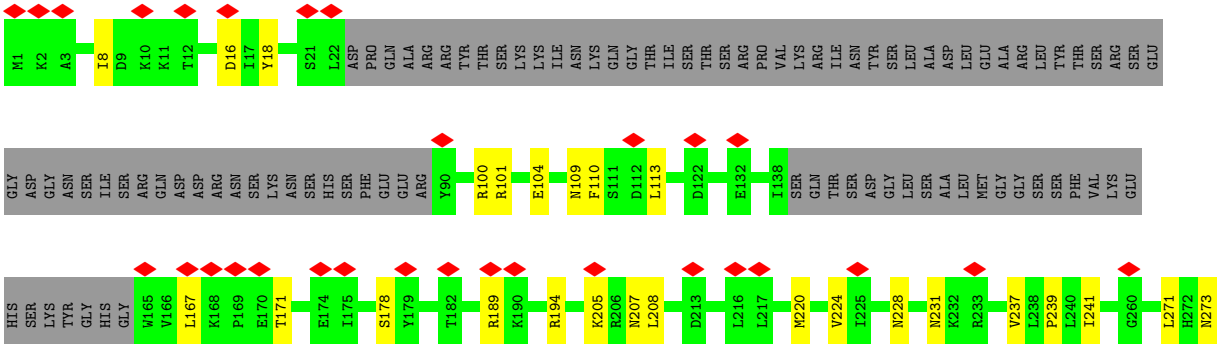
• Molecule 3: Actin-like protein ARP6

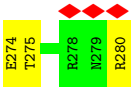
Chain C:



• Molecule 4: Vacuolar protein sorting-associated protein 71

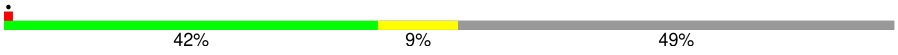
Chain D:

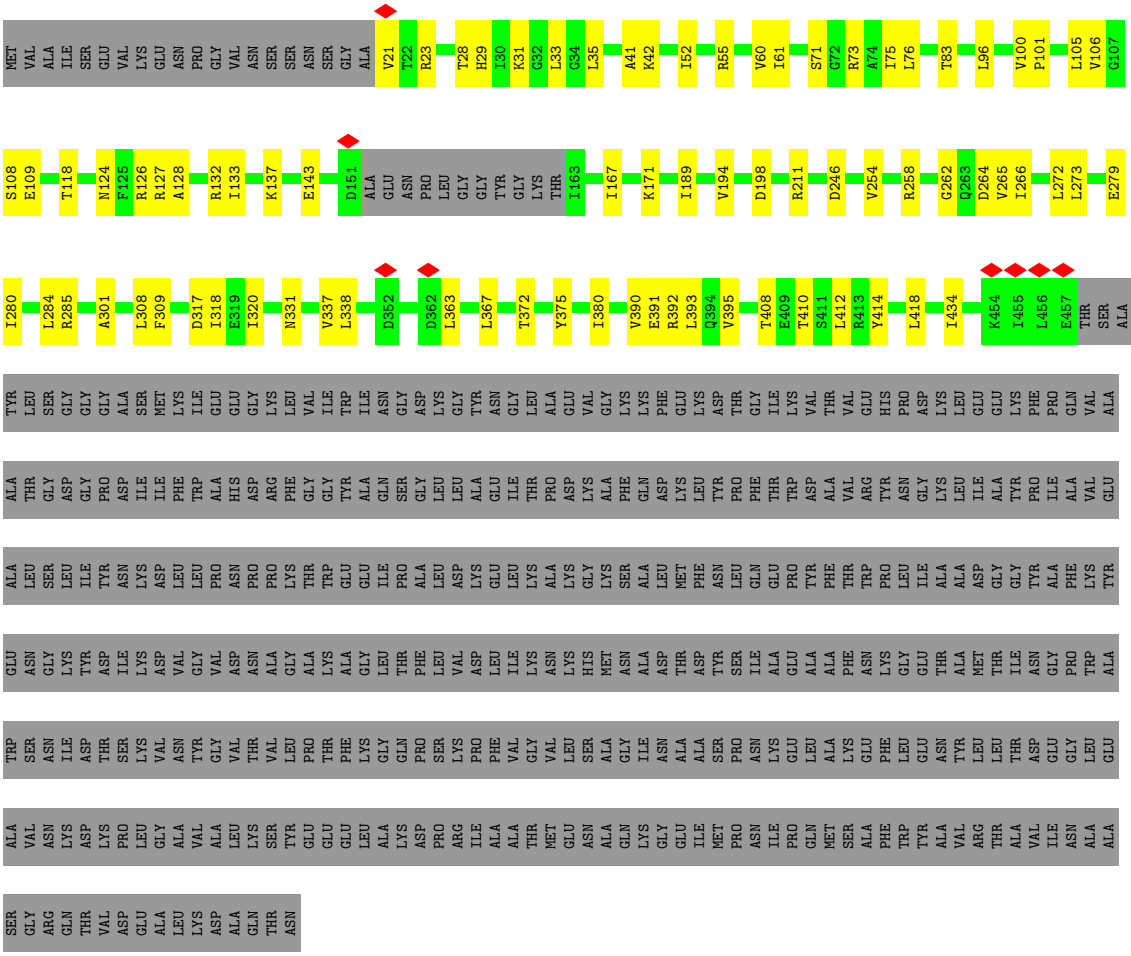




• Molecule 5: RuvB-like protein 1

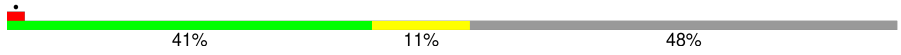
Chain E:

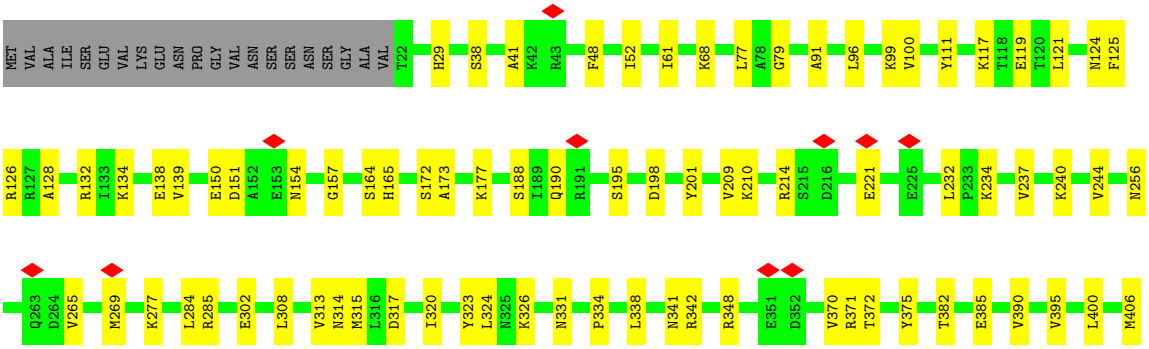


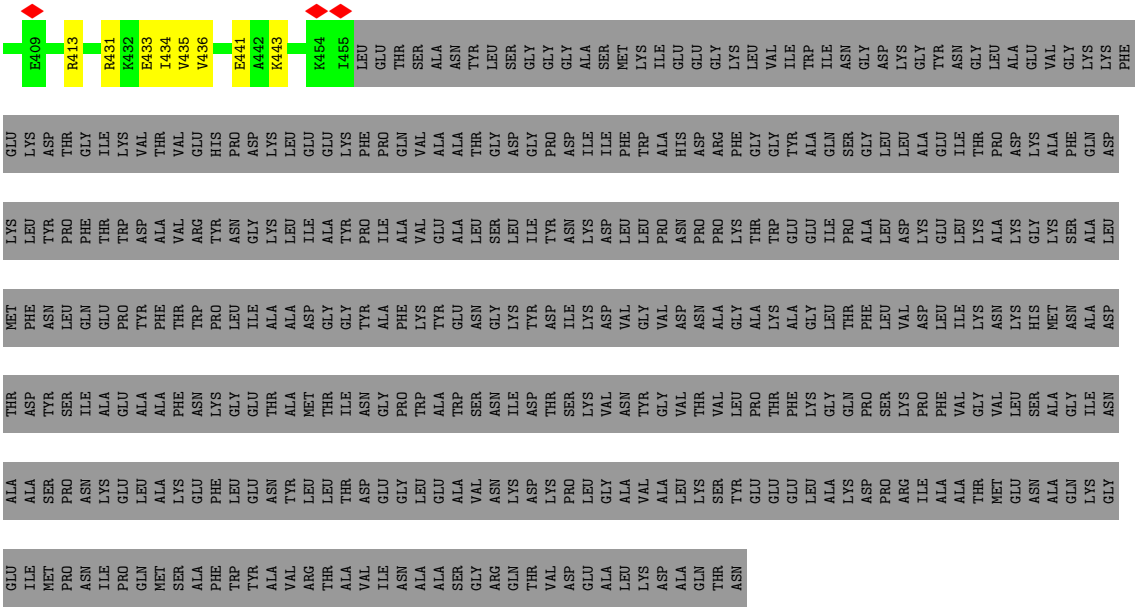


• Molecule 5: RuvB-like protein 1

Chain G:

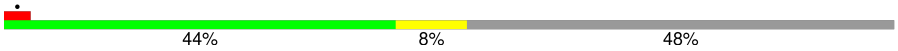


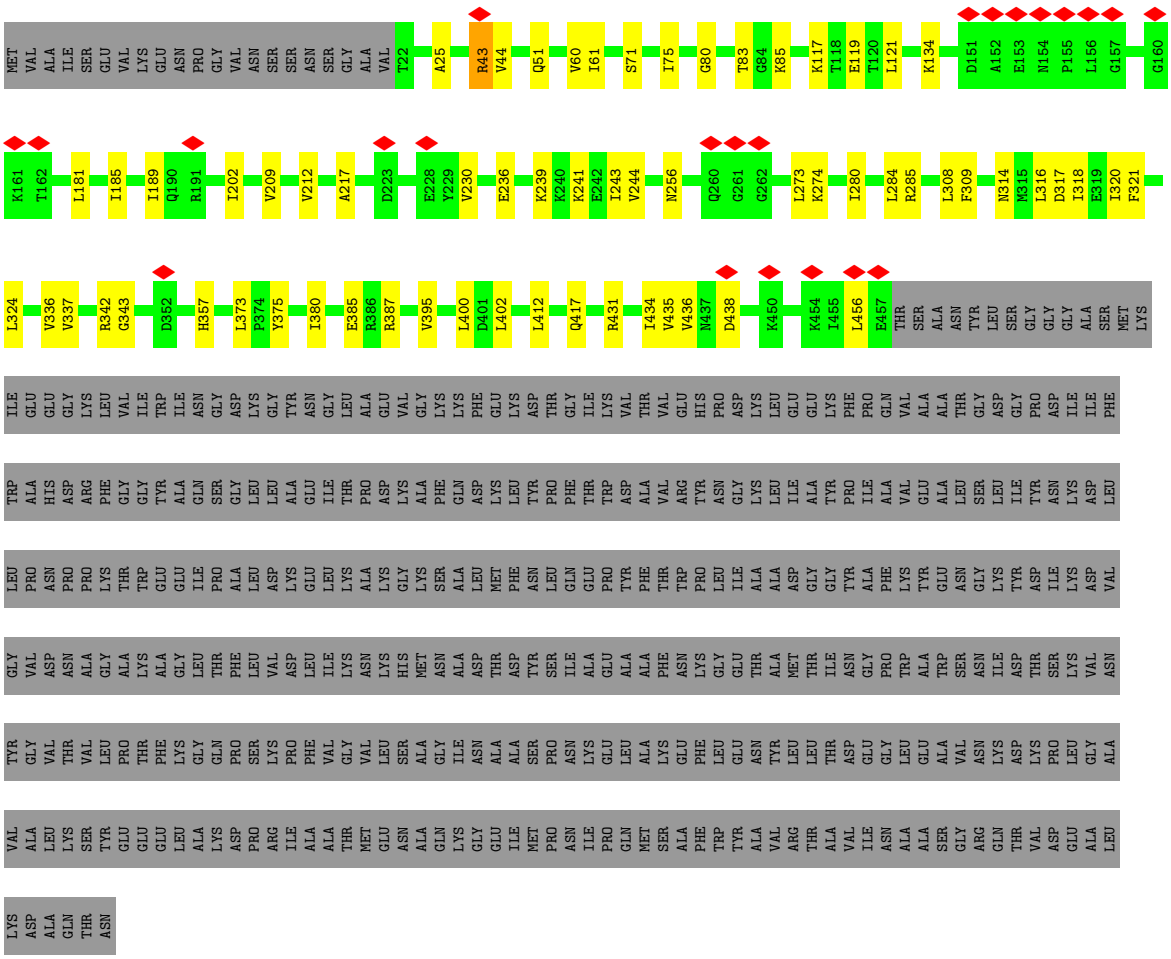




• Molecule 5: RuvB-like protein 1

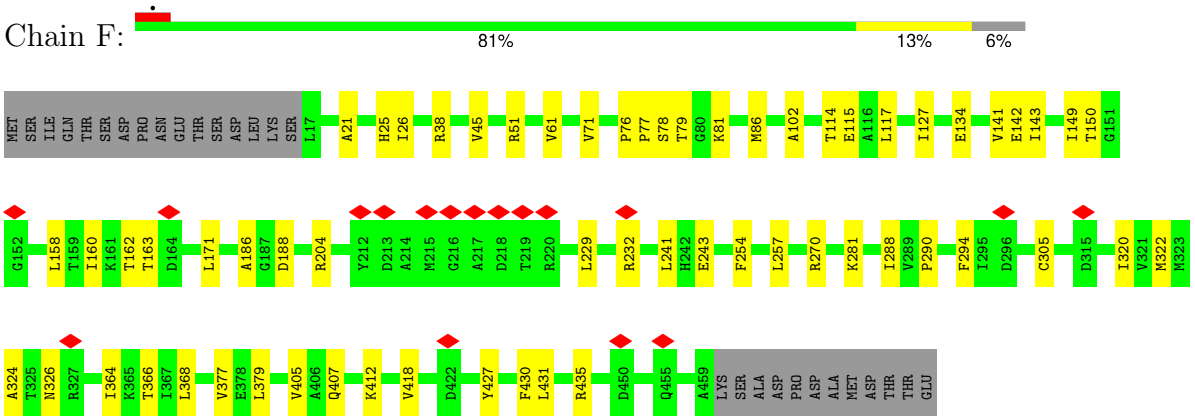
Chain I:





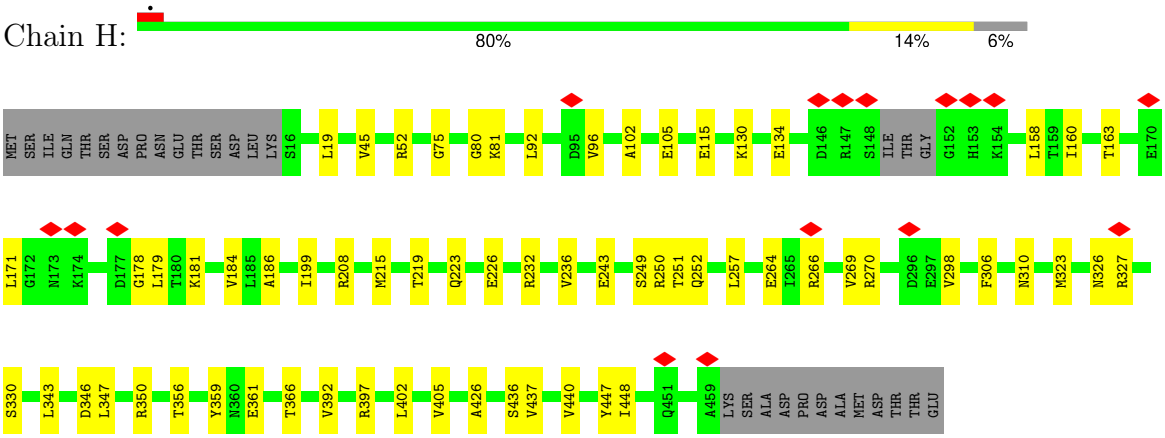
• Molecule 6: RuvB-like protein 2

Chain F:



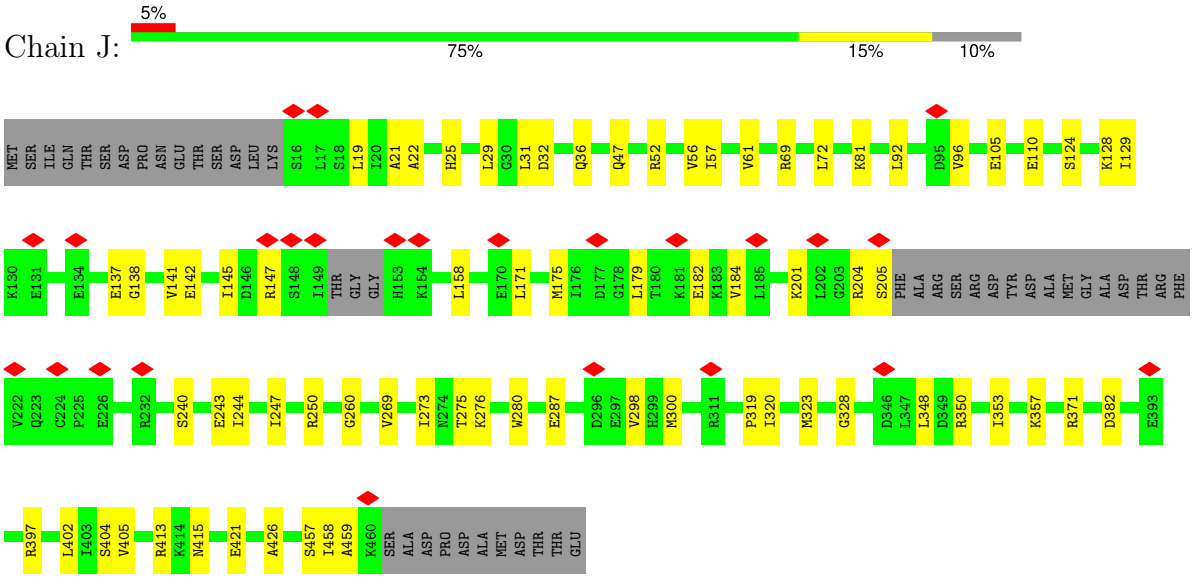
• Molecule 6: RuvB-like protein 2

Chain H:



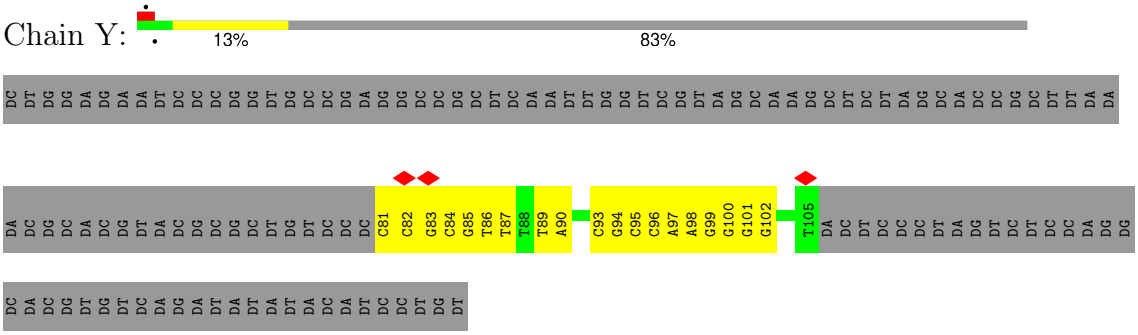
• Molecule 6: RuvB-like protein 2

Chain J:



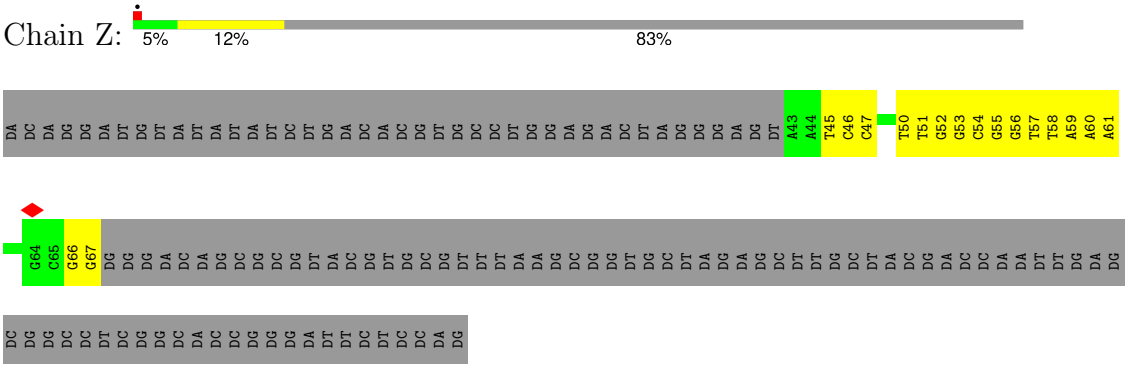
• Molecule 7: DNA (147-MER)

Chain Y:



• Molecule 8: DNA (147-MER)

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	101246	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 ($e^-/Å^2$)	54	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	48543	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.988	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	395.52, 395.52, 395.52	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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, ADP, AGS, 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	0.26	0/5938	0.47	0/8011
2	B	0.25	0/1175	0.43	0/1580
3	C	0.27	0/3429	0.46	0/4650
4	D	0.24	0/1543	0.49	0/2080
5	E	0.28	0/3319	0.49	0/4487
5	G	0.27	0/3375	0.49	0/4564
5	I	0.28	0/3392	0.49	0/4587
6	F	0.27	0/3448	0.48	0/4648
6	H	0.27	0/3430	0.48	0/4623
6	J	0.27	0/3312	0.47	0/4462
7	Y	0.59	0/573	0.95	0/882
8	Z	0.63	0/575	0.97	0/885
All	All	0.29	0/33509	0.50	0/45459

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5827	0	5905	96	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1152	0	1151	9	0
3	C	3335	0	3256	57	0
4	D	1518	0	1561	25	0
5	E	3281	0	3425	54	0
5	G	3334	0	3473	59	0
5	I	3351	0	3489	44	0
6	F	3410	0	3484	39	0
6	H	3393	0	3456	44	0
6	J	3279	0	3370	58	0
7	Y	512	0	282	15	0
8	Z	513	0	281	19	0
9	A	31	0	12	5	0
9	C	31	0	12	1	0
9	E	31	0	12	4	0
9	G	31	0	12	2	0
10	A	1	0	0	0	0
10	C	1	0	0	0	0
10	E	1	0	0	0	0
10	F	1	0	0	0	0
10	G	1	0	0	0	0
10	H	1	0	0	0	0
10	I	1	0	0	0	0
10	J	1	0	0	0	0
11	D	2	0	0	0	0
12	F	27	0	12	3	0
12	H	27	0	12	4	0
12	I	27	0	12	1	0
12	J	27	0	12	7	0
All	All	33147	0	33229	459	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 7.

The worst 5 of 459 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:H:440:VAL:HG23	6:H:447:TYR:HD2	1.48	0.78
4:D:110:PHE:HA	4:D:113:LEU:HD23	1.67	0.77
1:A:826:ALA:HB3	1:A:852:THR:HB	1.69	0.74
1:A:1272:THR:HA	1:A:1275:LEU:HD13	1.73	0.71
5:I:274:LYS:HA	6:J:250:ARG:HD3	1.72	0.70

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	704/1544 (46%)	691 (98%)	13 (2%)	0	100	100
2	B	130/795 (16%)	125 (96%)	5 (4%)	0	100	100
3	C	407/438 (93%)	394 (97%)	13 (3%)	0	100	100
4	D	181/280 (65%)	176 (97%)	5 (3%)	0	100	100
5	E	422/837 (50%)	415 (98%)	7 (2%)	0	100	100
5	G	432/837 (52%)	422 (98%)	10 (2%)	0	100	100
5	I	434/837 (52%)	423 (98%)	11 (2%)	0	100	100
6	F	441/471 (94%)	429 (97%)	12 (3%)	0	100	100
6	H	437/471 (93%)	426 (98%)	11 (2%)	0	100	100
6	J	420/471 (89%)	409 (97%)	11 (3%)	0	100	100
All	All	4008/6981 (57%)	3910 (98%)	98 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	652/1400 (47%)	649 (100%)	3 (0%)	86	91
2	B	128/732 (18%)	128 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	372/396 (94%)	371 (100%)	1 (0%)	91 94
4	D	180/261 (69%)	180 (100%)	0	100 100
5	E	363/688 (53%)	363 (100%)	0	100 100
5	G	367/688 (53%)	367 (100%)	0	100 100
5	I	369/688 (54%)	368 (100%)	1 (0%)	91 94
6	F	377/403 (94%)	377 (100%)	0	100 100
6	H	375/403 (93%)	375 (100%)	0	100 100
6	J	366/403 (91%)	366 (100%)	0	100 100
All	All	3549/6062 (58%)	3544 (100%)	5 (0%)	92 96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	815	ARG
1	A	1149	ARG
1	A	1193	ARG
3	C	410	ARG
5	I	43	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 18 ligands modelled in this entry, 10 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
12	ADP	I	901	10	24,29,29	0.82	0	29,45,45	1.21	2 (6%)
12	ADP	H	502	10	24,29,29	0.81	0	29,45,45	1.21	2 (6%)
9	AGS	A	1601	10	28,33,33	0.81	1 (3%)	31,52,52	0.98	2 (6%)
12	ADP	J	501	10	24,29,29	0.83	0	29,45,45	1.20	2 (6%)
9	AGS	C	501	10	28,33,33	0.95	2 (7%)	31,52,52	1.01	2 (6%)
12	ADP	F	502	10	24,29,29	0.83	0	29,45,45	1.23	2 (6%)
9	AGS	E	901	10	28,33,33	0.83	1 (3%)	31,52,52	0.97	2 (6%)
9	AGS	G	902	10	28,33,33	0.85	1 (3%)	31,52,52	0.98	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
12	ADP	I	901	10	-	1/12/32/32	0/3/3/3
12	ADP	H	502	10	-	2/12/32/32	0/3/3/3
9	AGS	A	1601	10	-	3/17/38/38	0/3/3/3
12	ADP	J	501	10	-	3/12/32/32	0/3/3/3
9	AGS	C	501	10	-	6/17/38/38	0/3/3/3
12	ADP	F	502	10	-	1/12/32/32	0/3/3/3
9	AGS	E	901	10	-	6/17/38/38	0/3/3/3
9	AGS	G	902	10	-	2/17/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	501	AGS	PB-O3A	-2.19	1.57	1.59
9	G	902	AGS	PG-S1G	2.16	1.95	1.90
9	A	1601	AGS	PG-S1G	2.15	1.95	1.90
9	E	901	AGS	PG-S1G	2.09	1.95	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	501	AGS	PG-S1G	2.02	1.95	1.90

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	501	AGS	PB-O3B-PG	-4.08	118.25	133.17
9	A	1601	AGS	PB-O3B-PG	-3.85	119.07	133.17
9	G	902	AGS	PB-O3B-PG	-3.85	119.10	133.17
9	E	901	AGS	PB-O3B-PG	-3.74	119.49	133.17
12	F	502	ADP	N3-C2-N1	-3.68	123.68	128.67

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	501	AGS	C5'-O5'-PA-O1A
9	C	501	AGS	C5'-O5'-PA-O3A
12	J	501	ADP	C5'-O5'-PA-O1A
12	J	501	ADP	C5'-O5'-PA-O2A
12	J	501	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

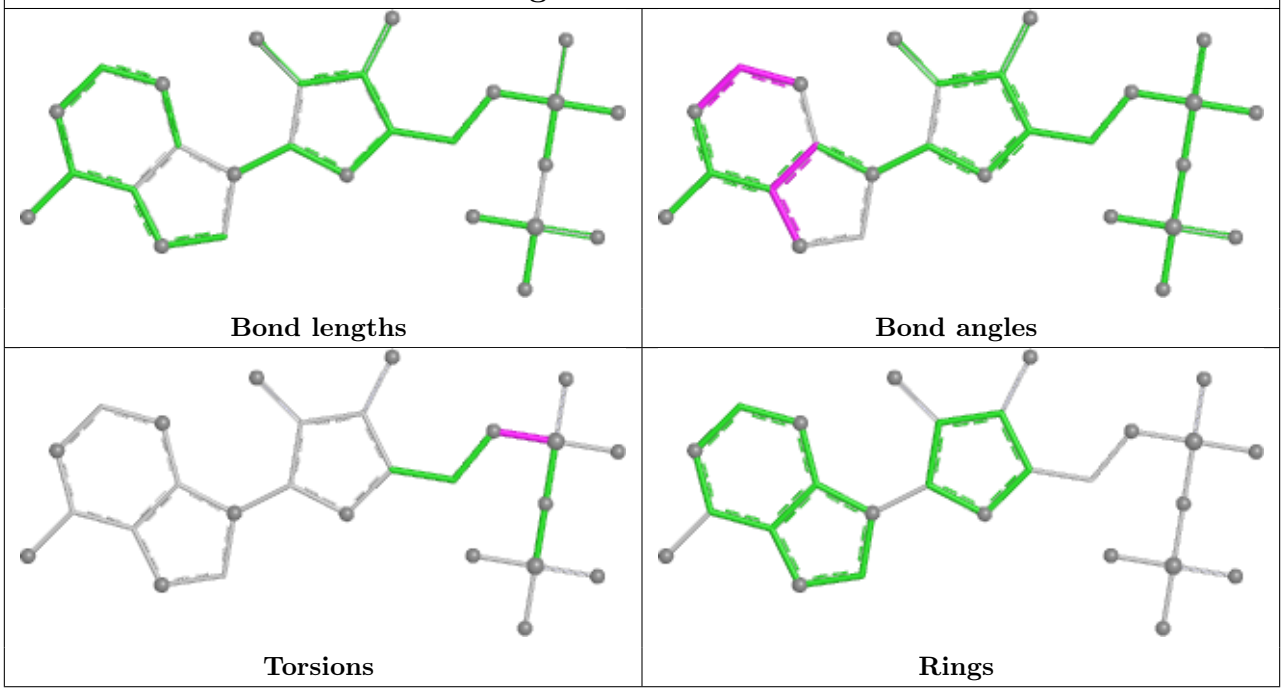
8 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	I	901	ADP	1	0
12	H	502	ADP	4	0
9	A	1601	AGS	5	0
12	J	501	ADP	7	0
9	C	501	AGS	1	0
12	F	502	ADP	3	0
9	E	901	AGS	4	0
9	G	902	AGS	2	0

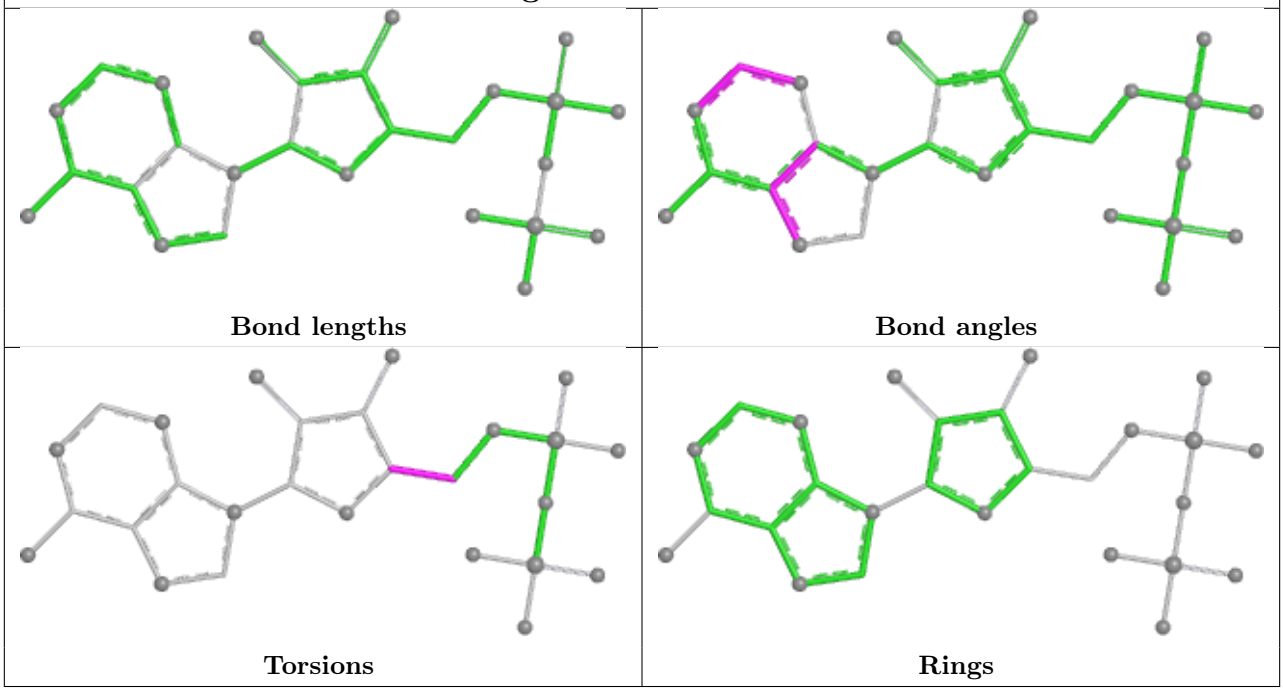
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

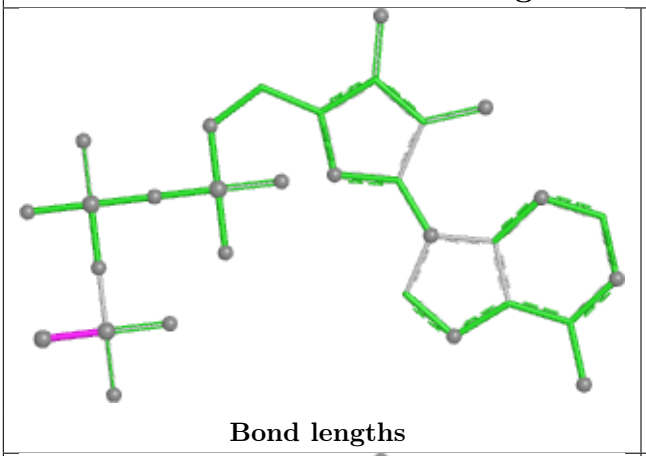
Ligand ADP I 901



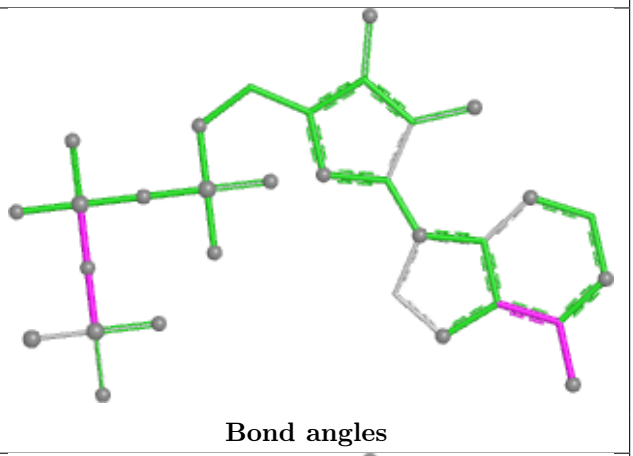
Ligand ADP H 502



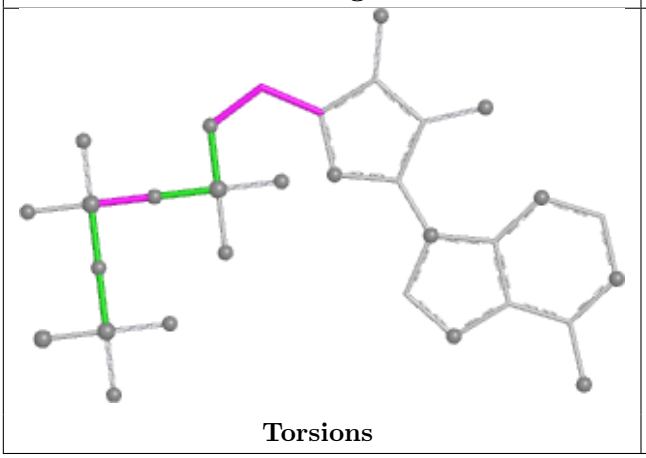
Ligand AGS A 1601



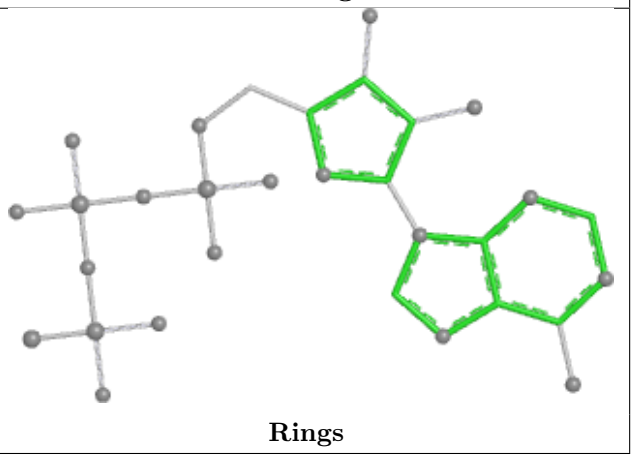
Bond lengths



Bond angles

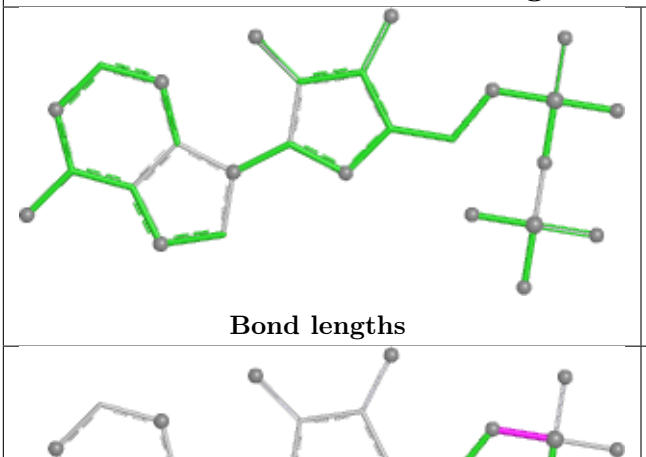


Torsions

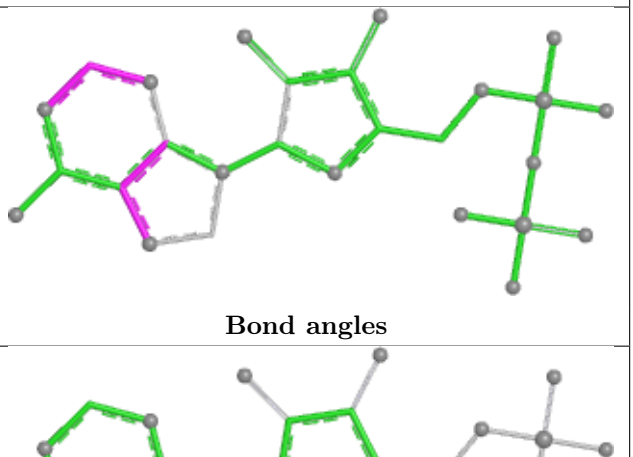


Rings

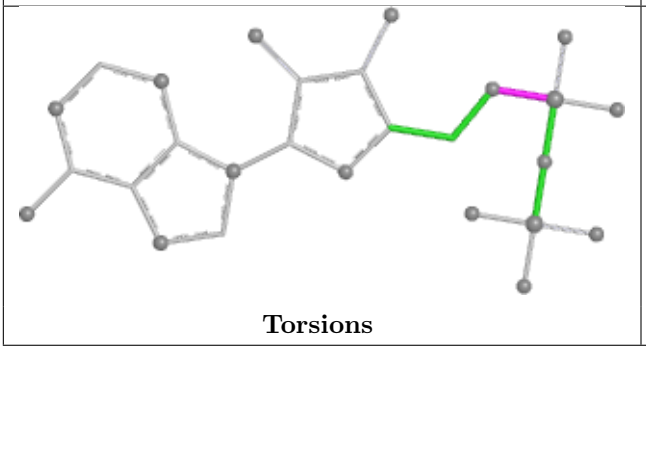
Ligand ADP J 501



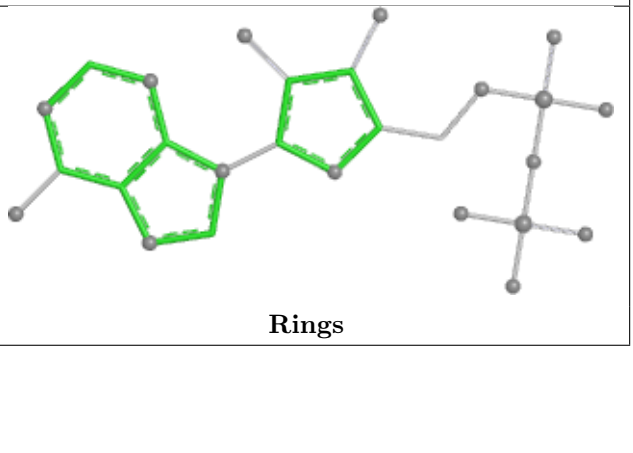
Bond lengths



Bond angles

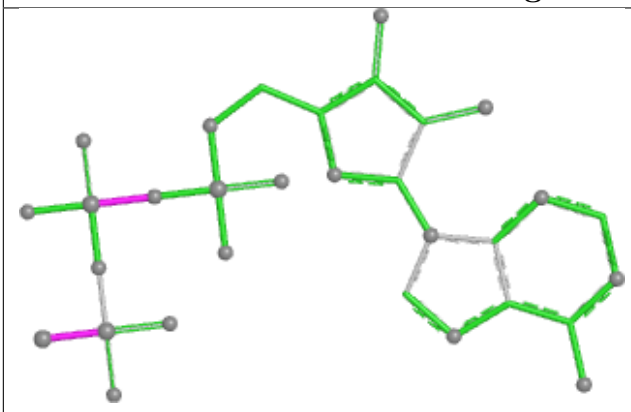


Torsions

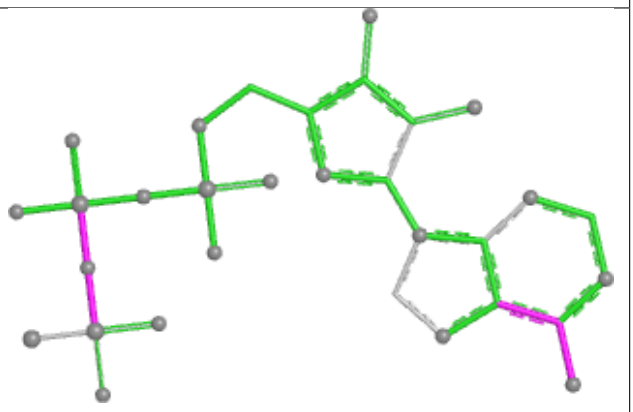


Rings

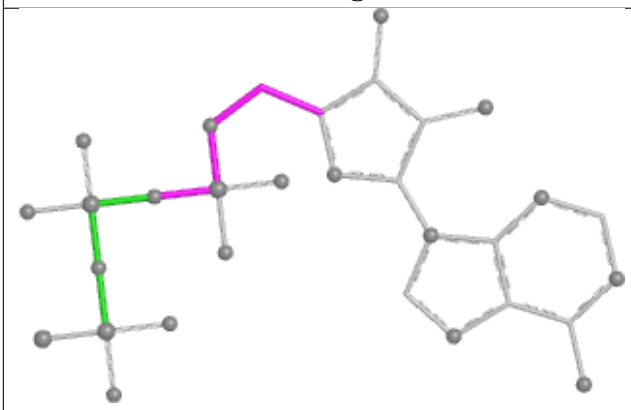
Ligand AGS C 501



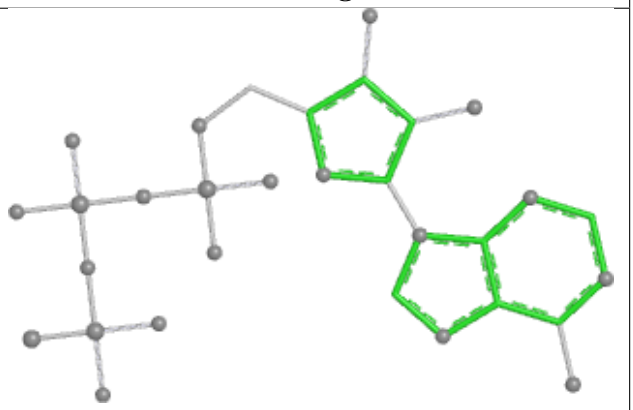
Bond lengths



Bond angles

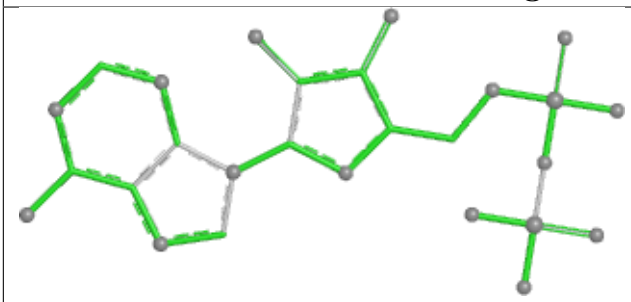


Torsions

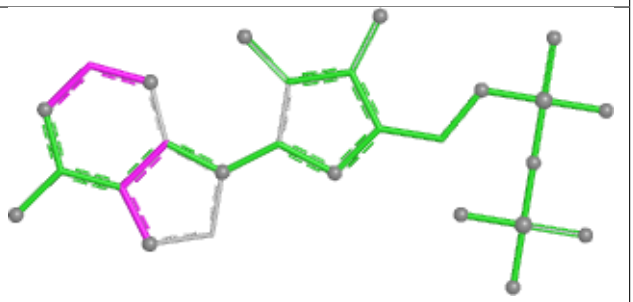


Rings

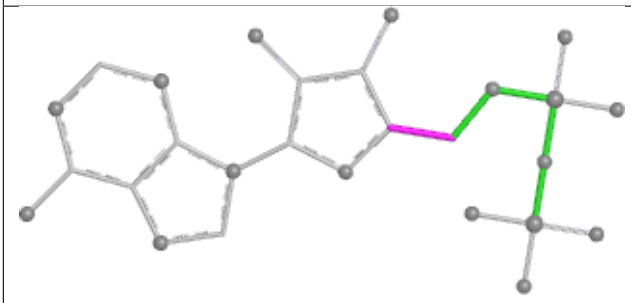
Ligand ADP F 502



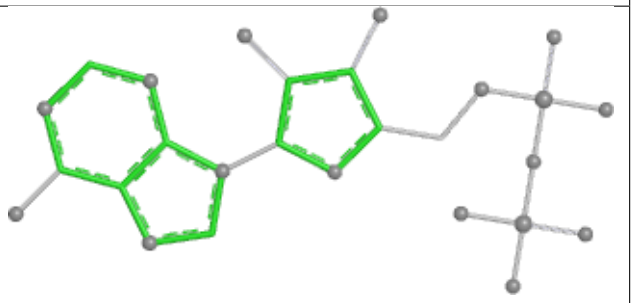
Bond lengths



Bond angles

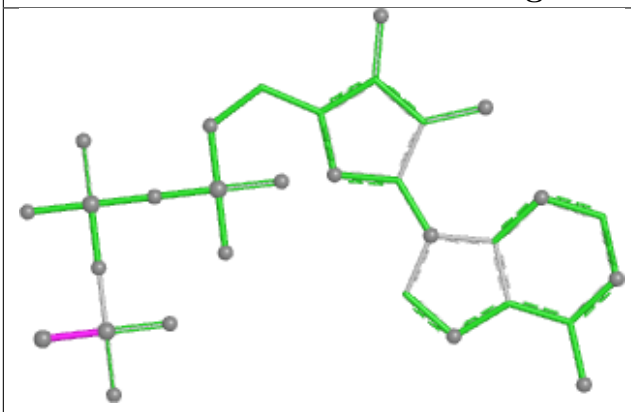


Torsions

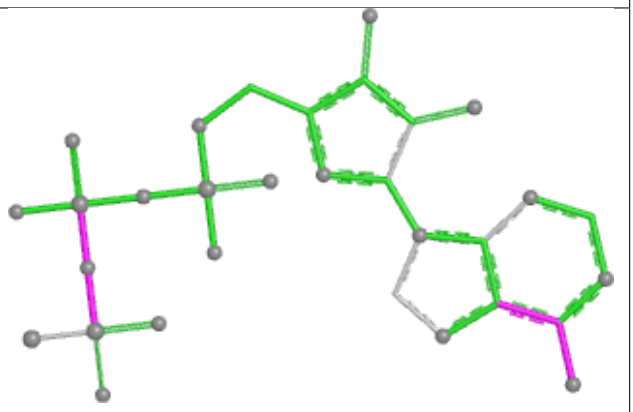


Rings

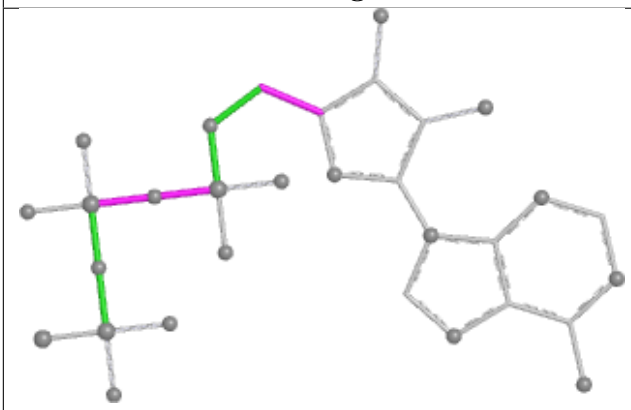
Ligand AGS E 901



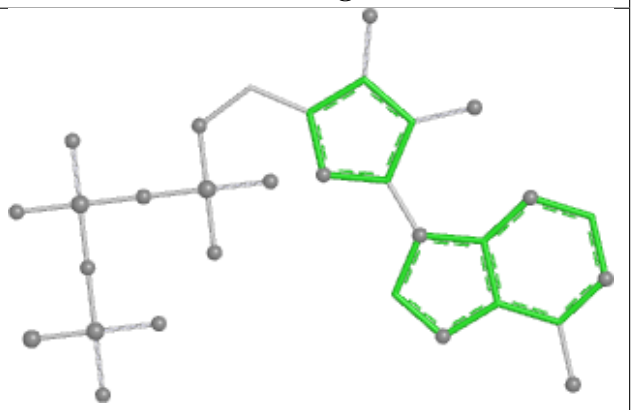
Bond lengths



Bond angles

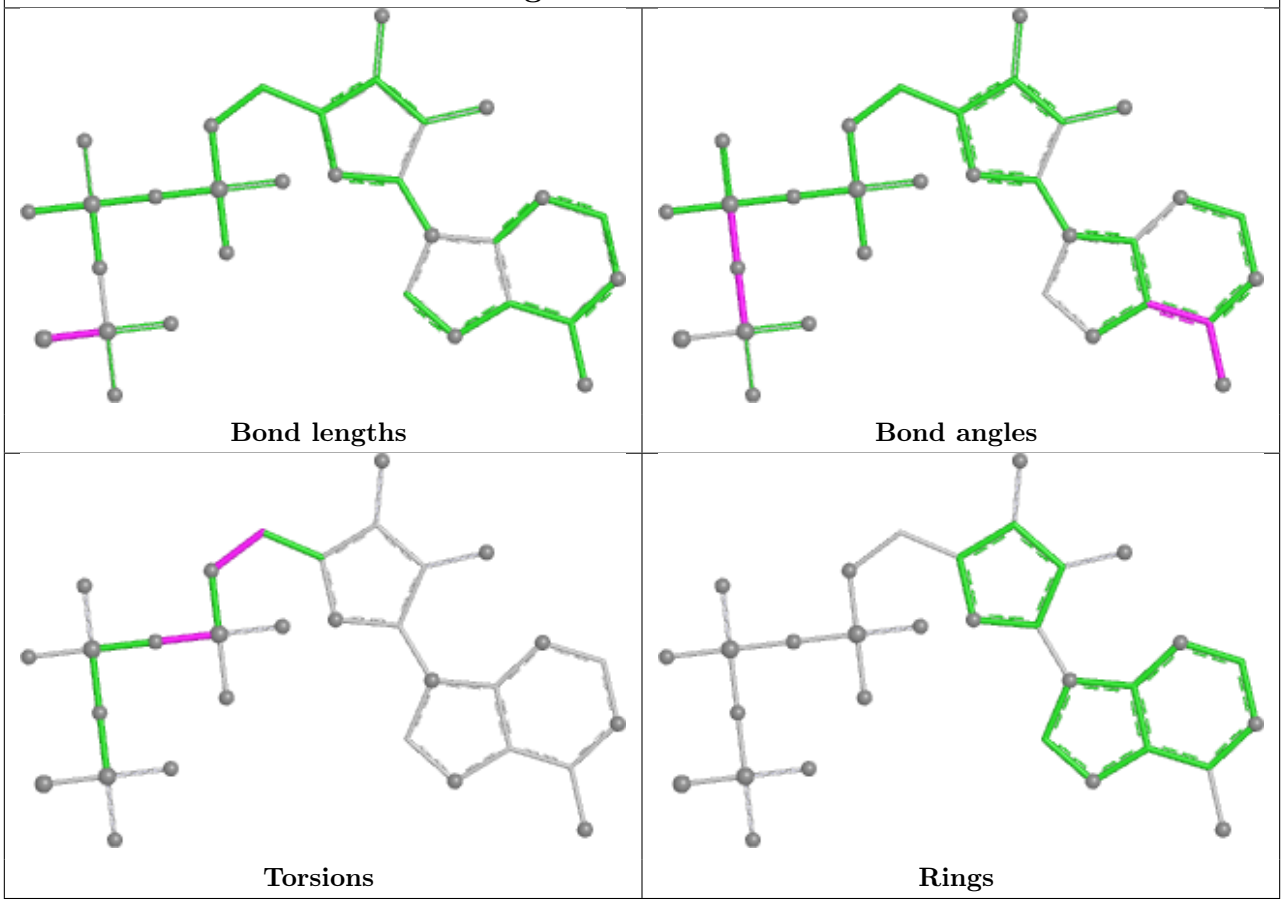


Torsions



Rings

Ligand AGS G 902



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.

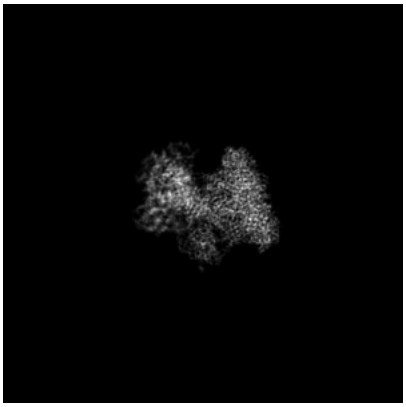
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44074. These allow visual inspection of the internal detail of the map and identification of artifacts.

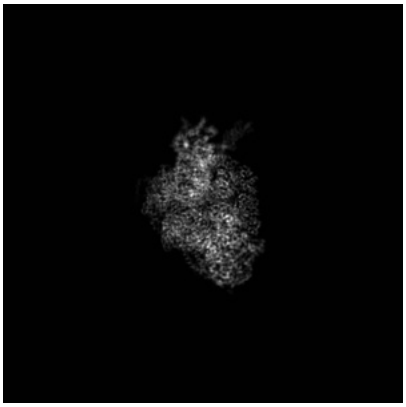
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

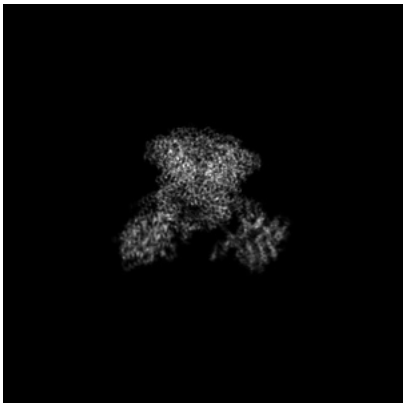
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 192

Y Index: 192

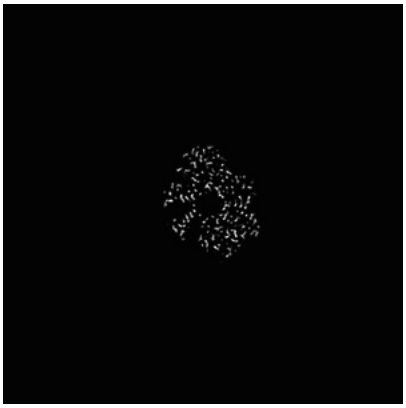
Z Index: 192

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

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 159



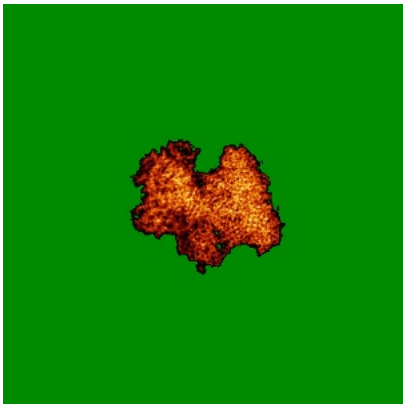
Y Index: 231

Z Index: 196

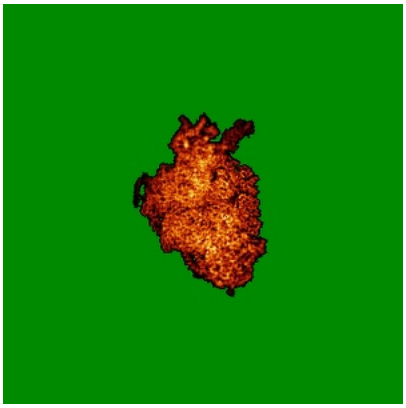
The images above show the largest variance slices of the map in three orthogonal directions.

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

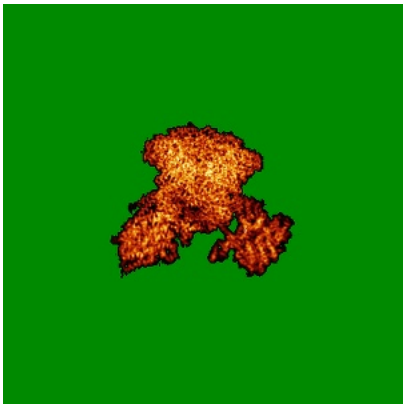
6.4.1 Primary map



X



Y



Z

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 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

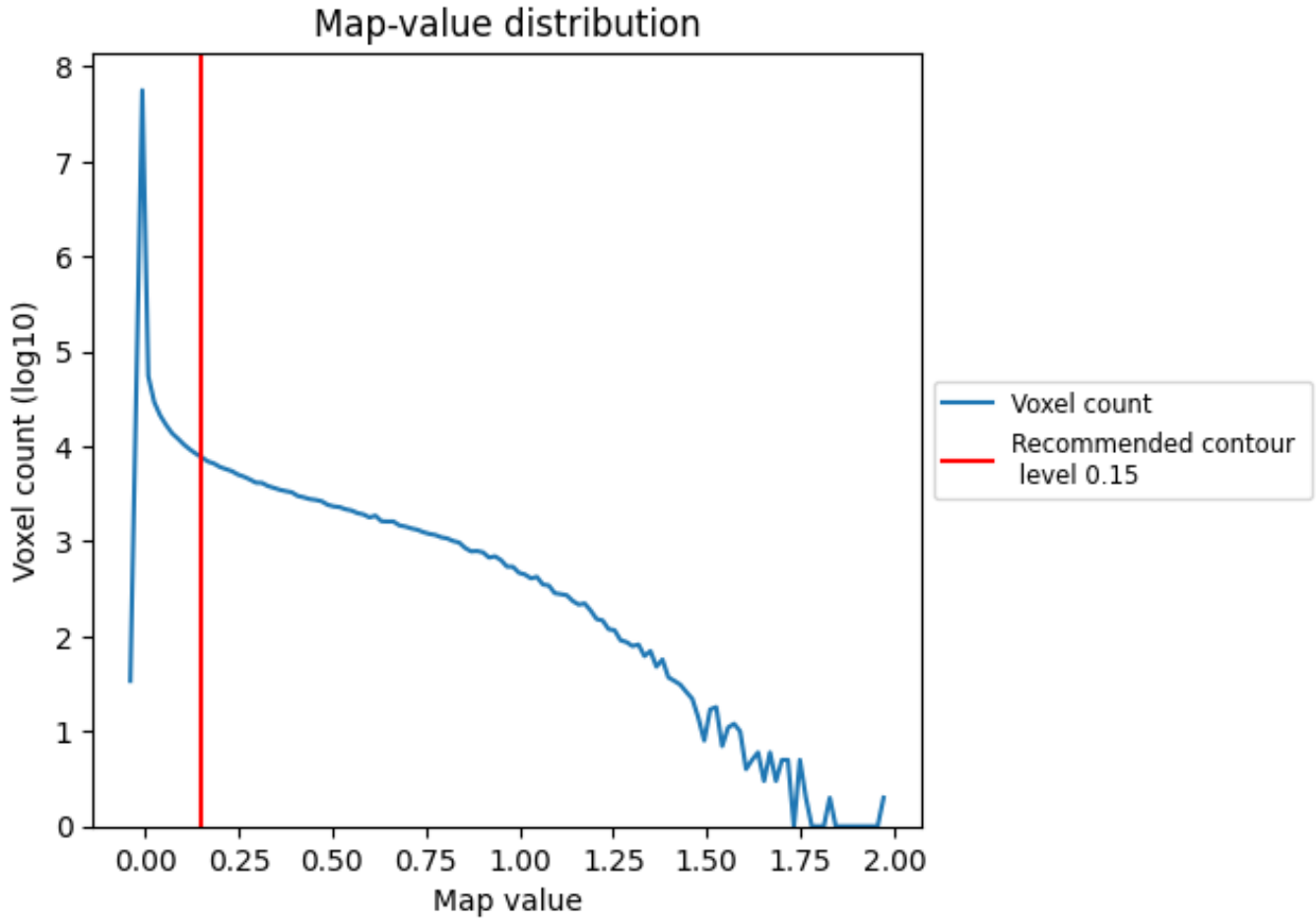
6.6 Mask visualisation (i)

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

7 Map analysis

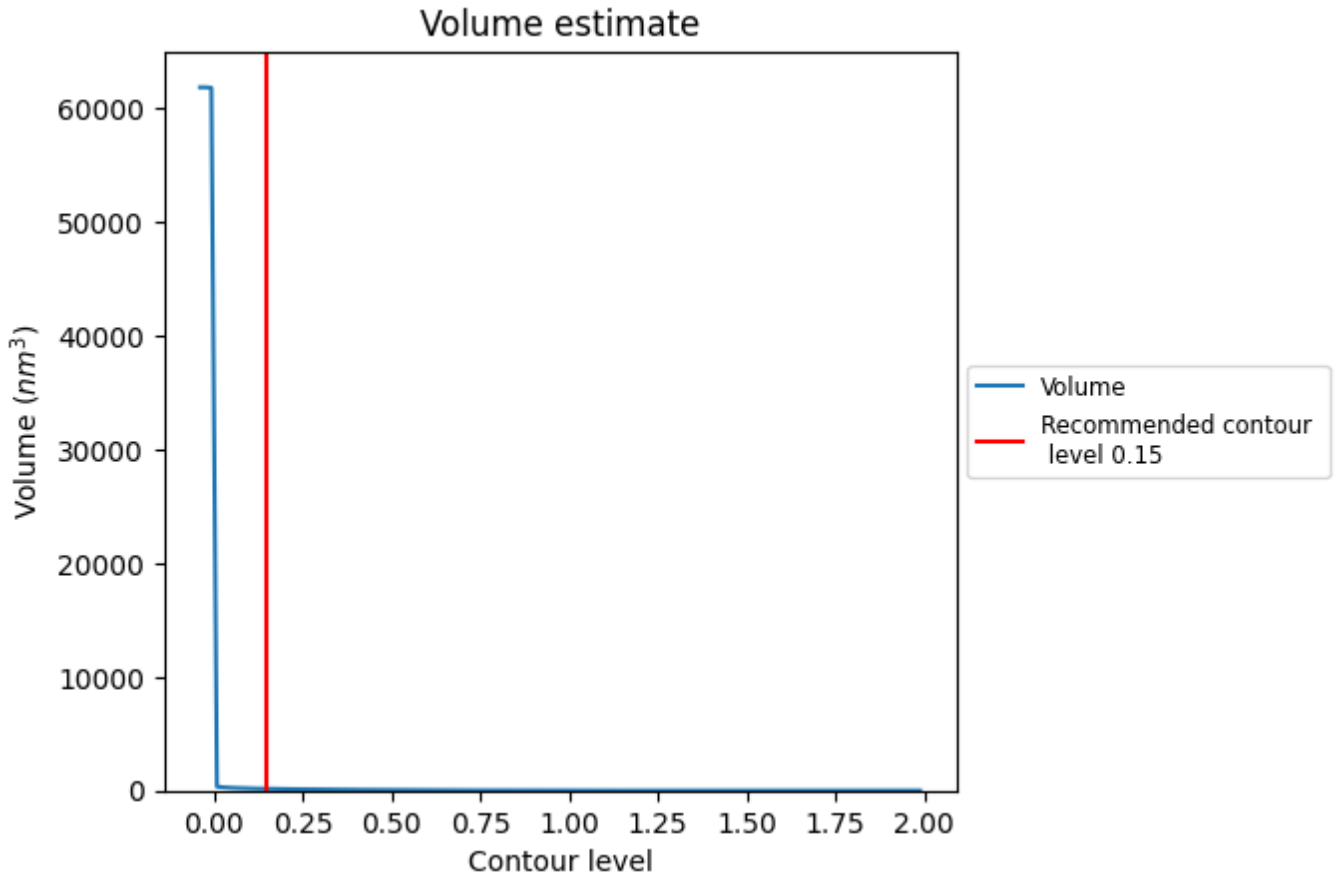
This section contains the results of statistical analysis of the map.

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.

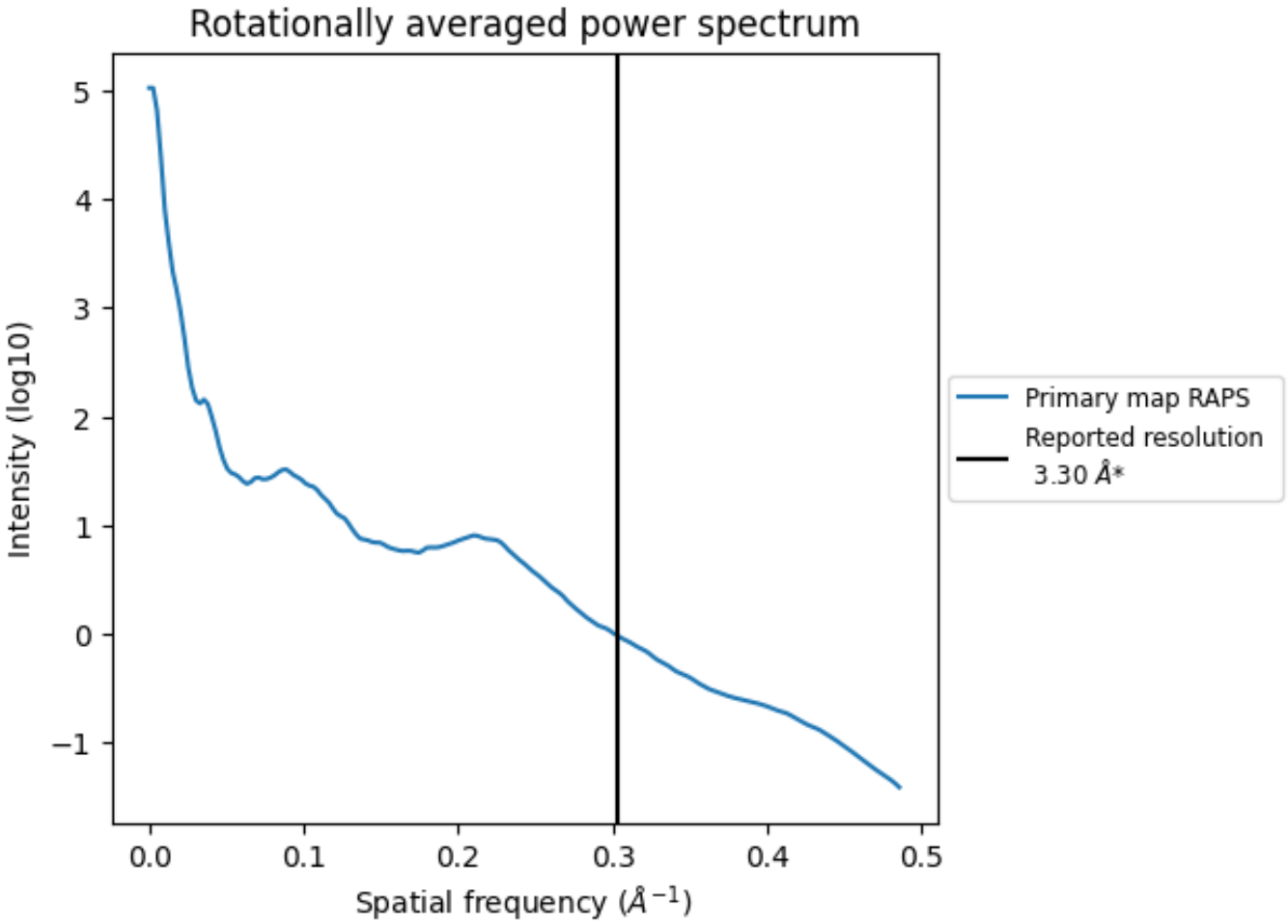
7.2 Volume estimate (i)



The volume at the recommended contour level is 156 nm^3; this corresponds to an approximate mass of 141 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 0.303 Å^{-1}

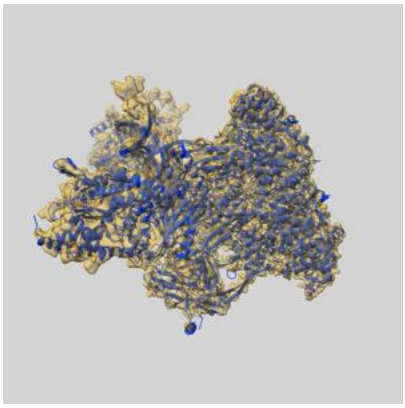
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

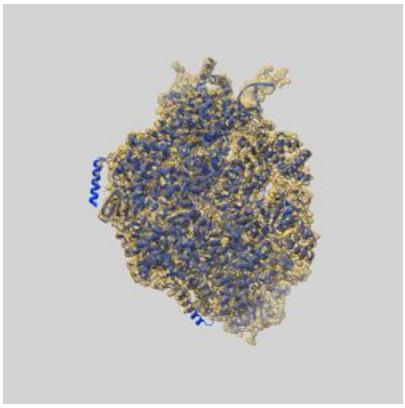
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44074 and PDB model 9B1D. Per-residue inclusion information can be found in section 3 on page 8.

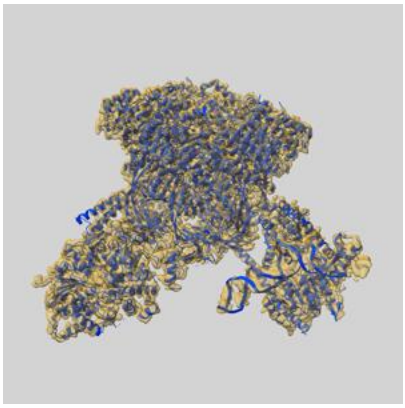
9.1 Map-model overlay



X



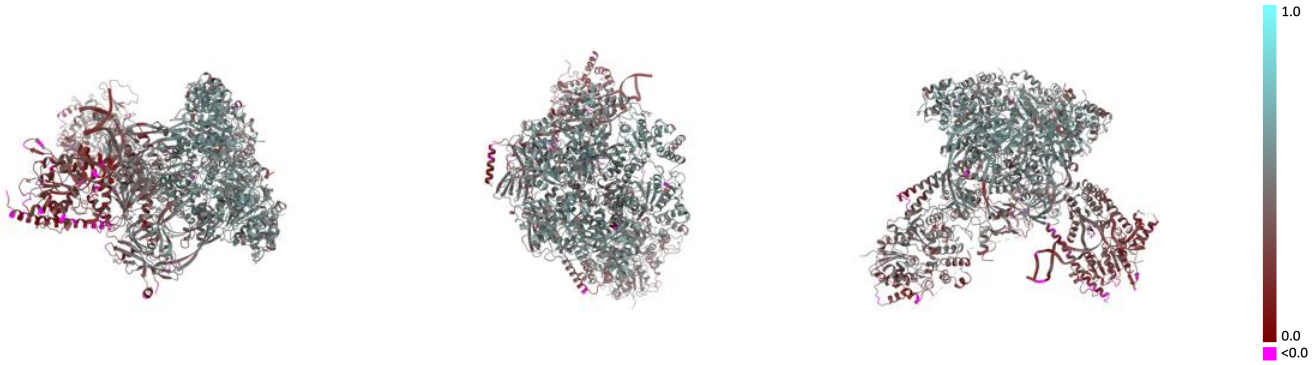
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

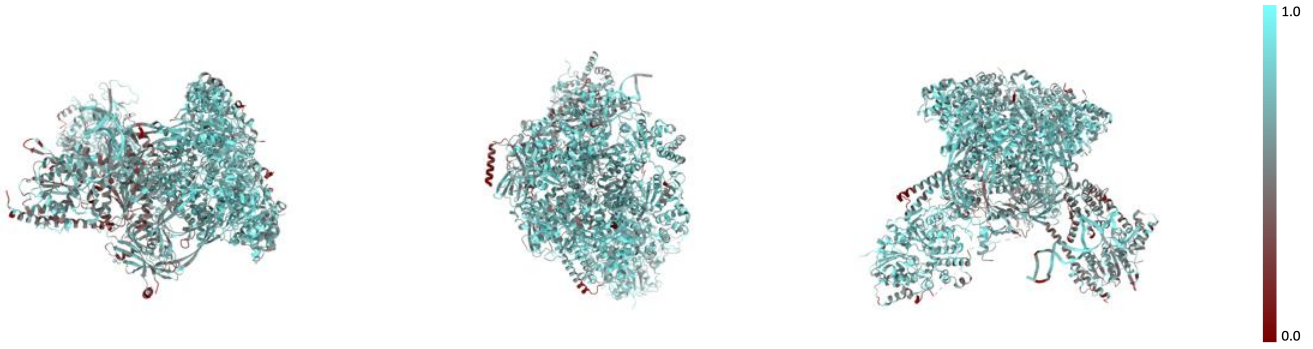
9.2 Q-score mapped to coordinate model



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.

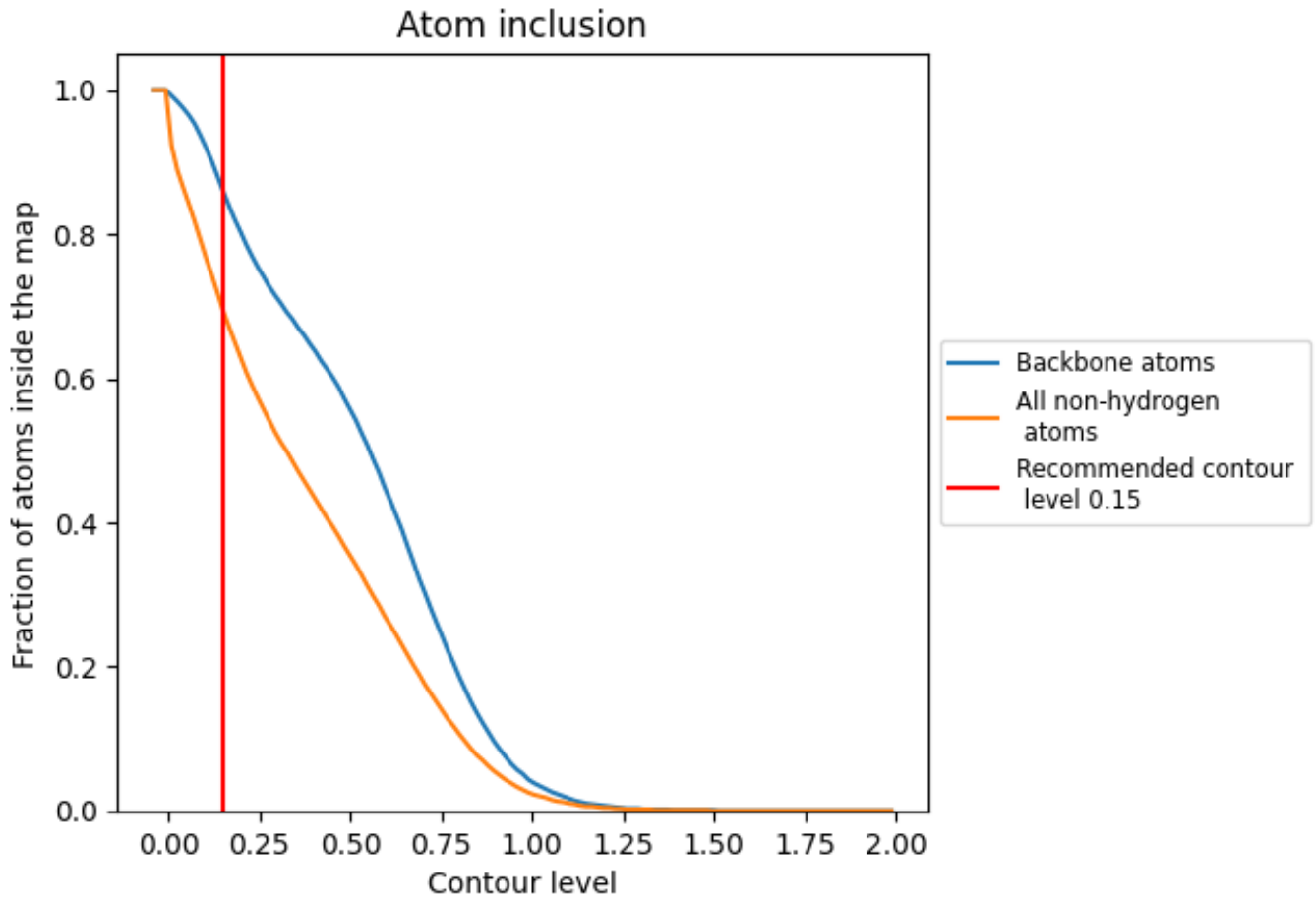
9.3 Atom inclusion mapped to coordinate model



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 (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 70% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6950	0.4350
A	0.5910	0.3360
B	0.4450	0.2230
C	0.7570	0.4170
D	0.5970	0.3130
E	0.7620	0.5090
F	0.7270	0.4980
G	0.7190	0.4860
H	0.7380	0.4990
I	0.7510	0.5070
J	0.7170	0.4850
Y	0.7050	0.2430
Z	0.7170	0.2760