wwPDB EM Validation Summary Report ⓘ

May 13, 2024 – 12:26 PM JST

PDB ID	:	8J0S
EMDB ID	:	EMD-35909
Title	:	Cryo-EM structure of Mycobacterium tuberculosis ATP synthase in complex with bedaquiline(BDQ)
Authors	:	Zhang, Y.; Lai, Y.; Liu, F.; Rao, Z.; Gong, H.
Deposited on	:	2023-04-11
Resolution	:	2.58 Å(reported)

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

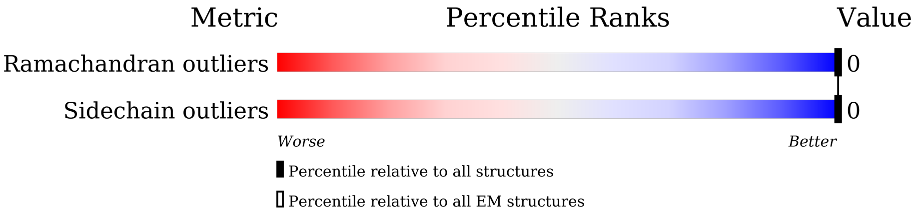
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance ⓘ

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

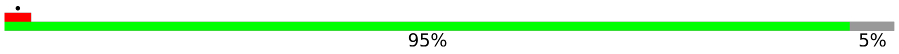
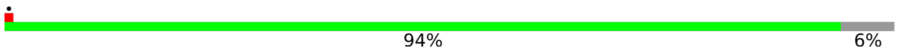
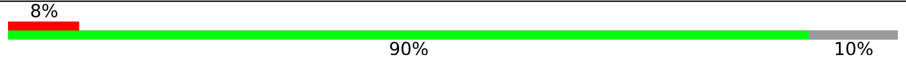
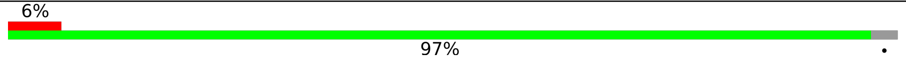
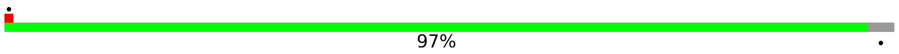
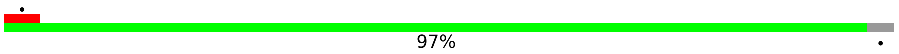
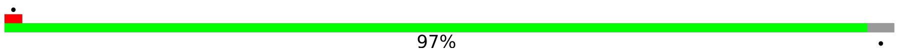
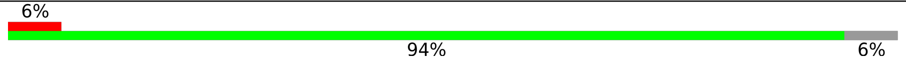
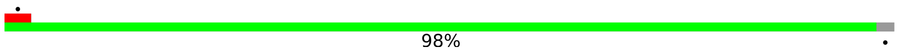
The reported resolution of this entry is 2.58 Å.

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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	250	
2	A	549	
2	B	549	
2	C	549	
3	D	486	
3	E	486	
3	F	486	
4	G	305	
5	H	121	

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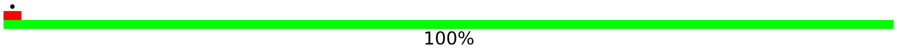
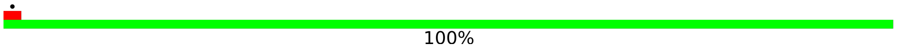
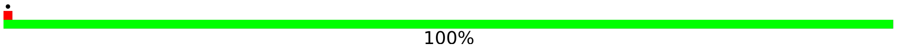
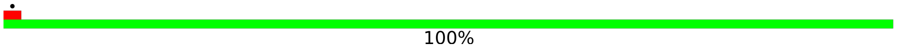
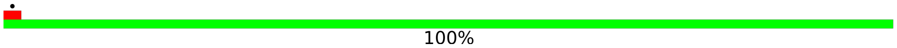
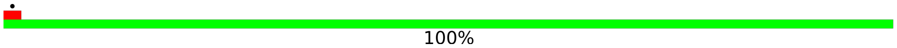
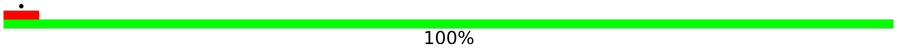
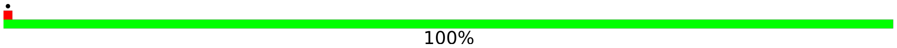
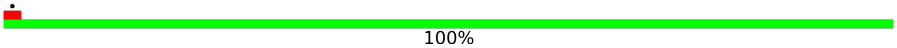
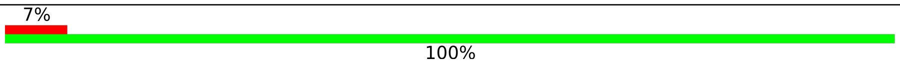
Mol	Chain	Length	Quality of chain
6	1	81	
6	2	81	
6	3	81	
6	4	81	
6	5	81	
6	6	81	
6	7	81	
6	8	81	
6	9	81	
7	b	171	
8	d	446	

2 Entry composition ⓘ

There are 12 unique types of molecules in this entry. The entry contains 37586 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 ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	a	237	1839	1231	295	307	6	0	0

- Molecule 2 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	517	3916	2449	684	772	11	0	0
2	B	492	3747	2345	655	736	11	0	0
2	C	531	4040	2533	702	794	11	0	0

- Molecule 3 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	469	3614	2279	622	701	12	0	0
3	E	469	3614	2279	622	701	12	0	0
3	F	469	3614	2279	622	701	12	0	0

- Molecule 4 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	288	2256	1418	399	431	8	0	0

- Molecule 5 is a protein called ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	118	901	559	161	180	1	0	0

- Molecule 6 is a protein called ATP synthase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	1	81	567	373	92	99	3	0	0
6	2	81	567	373	92	99	3	0	0
6	3	81	567	373	92	99	3	0	0
6	4	81	567	373	92	99	3	0	0
6	5	81	567	373	92	99	3	0	0
6	6	81	567	373	92	99	3	0	0
6	7	81	567	373	92	99	3	0	0
6	8	81	567	373	92	99	3	0	0
6	9	81	567	373	92	99	3	0	0

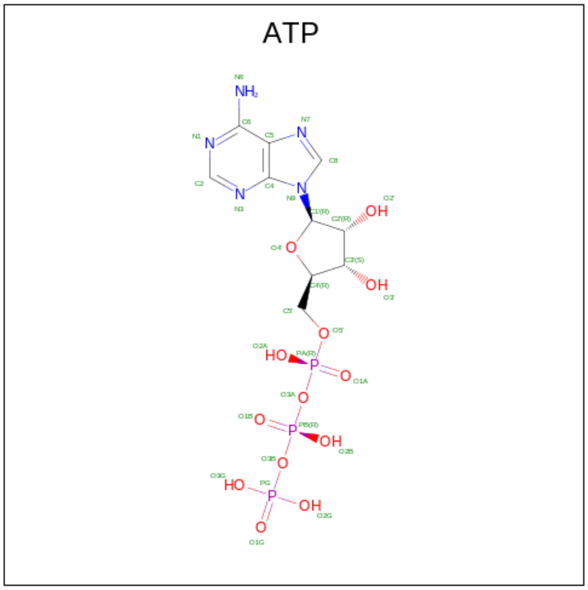
- Molecule 7 is a protein called ATP synthase subunit b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	b	144	1107	691	201	212	3	0	0

- Molecule 8 is a protein called Multifunctional fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	d	445	3424	2131	637	649	7	0	0

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

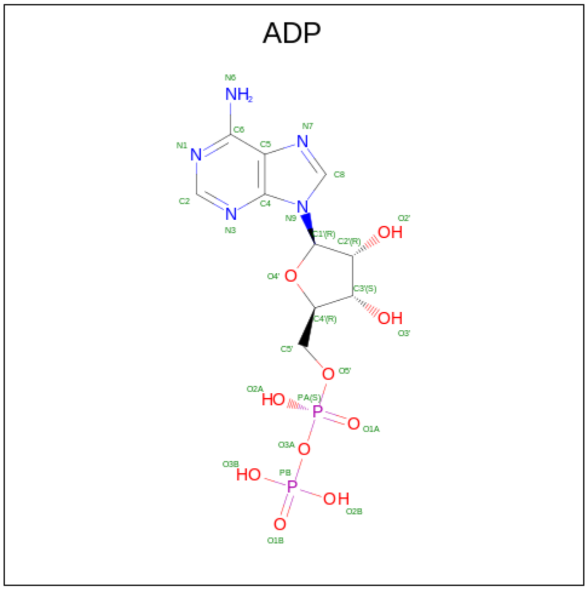


Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total C N O P 31 10 5 13 3	0
9	B	1	Total C N O P 31 10 5 13 3	0
9	C	1	Total C N O P 31 10 5 13 3	0

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

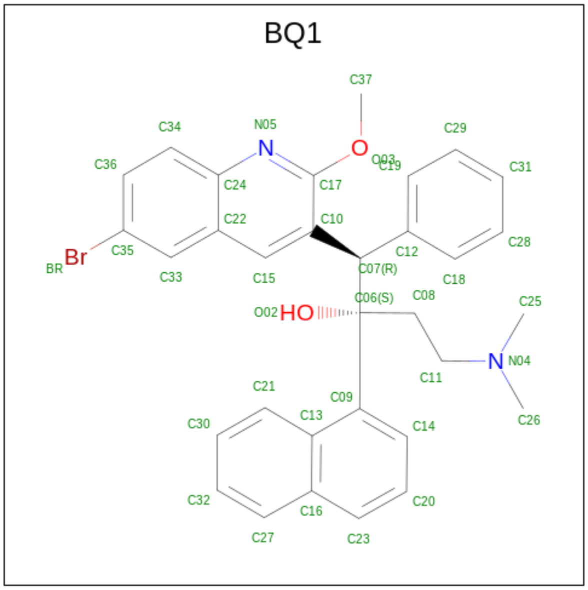
Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total Mg 1 1	0
10	B	1	Total Mg 1 1	0
10	C	1	Total Mg 1 1	0
10	D	1	Total Mg 1 1	0
10	F	1	Total Mg 1 1	0

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
11	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 12 is Bedaquiline (three-letter code: BQ1) (formula: $C_{32}H_{31}BrN_2O_2$).



Mol	Chain	Residues	Atoms					AltConf
12	1	1	Total	Br	C	N	O	0
			37	1	32	2	2	
12	4	1	Total	Br	C	N	O	0
			37	1	32	2	2	

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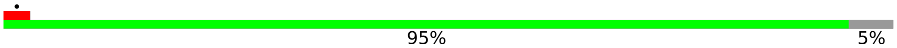
Mol	Chain	Residues	Atoms	AltConf
12	5	1	Total Br C N O 37 1 32 2 2	0
12	6	1	Total Br C N O 37 1 32 2 2	0
12	7	1	Total Br C N O 37 1 32 2 2	0
12	8	1	Total Br C N O 37 1 32 2 2	0
12	9	1	Total Br C N O 37 1 32 2 2	0

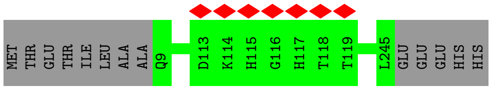
3 Residue-property plots ⓘ

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

- Molecule 1: ATP synthase subunit a

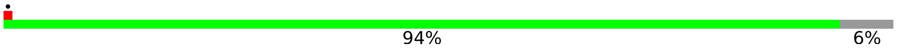
Chain a:

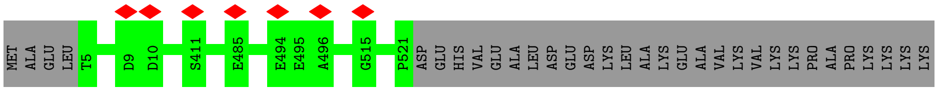




- Molecule 2: ATP synthase subunit alpha

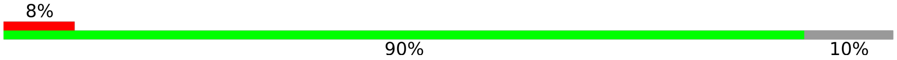
Chain A:

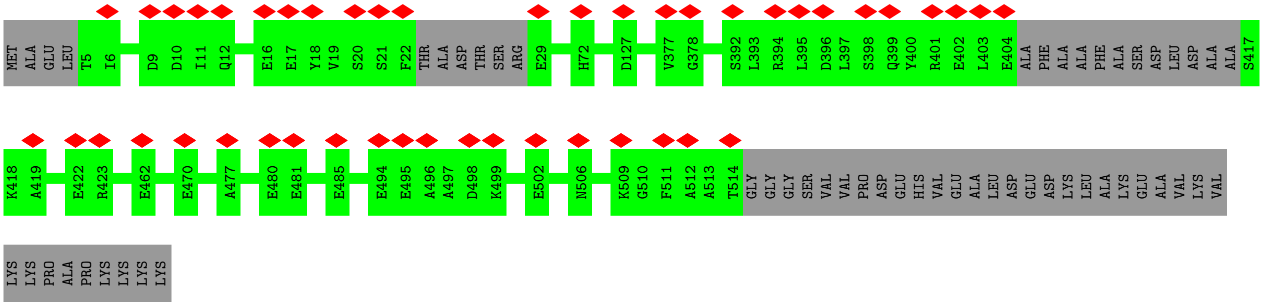




- Molecule 2: ATP synthase subunit alpha

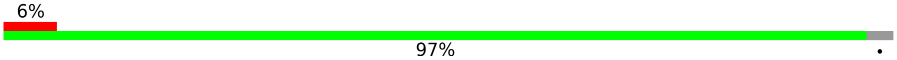
Chain B:

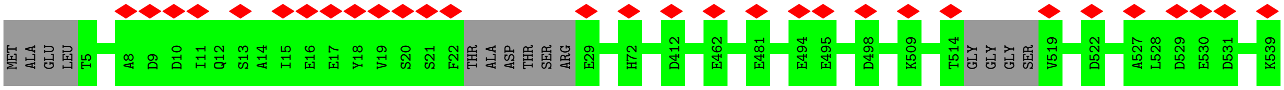


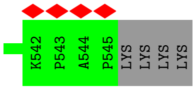


- Molecule 2: ATP synthase subunit alpha

Chain C:

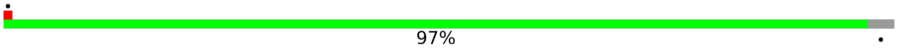


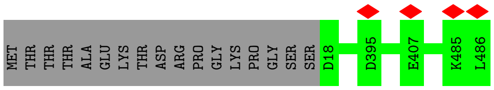




- Molecule 3: ATP synthase subunit beta

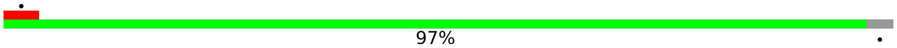
Chain D:

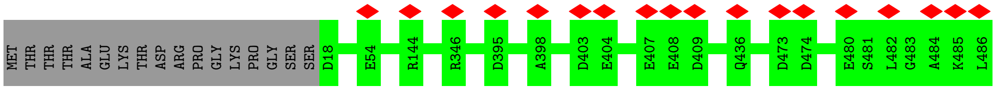




- Molecule 3: ATP synthase subunit beta

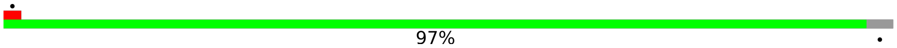
Chain E:

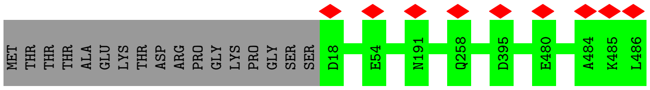




- Molecule 3: ATP synthase subunit beta

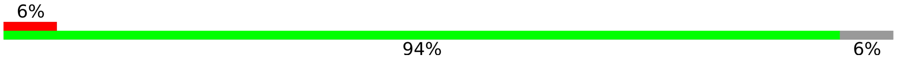
Chain F:

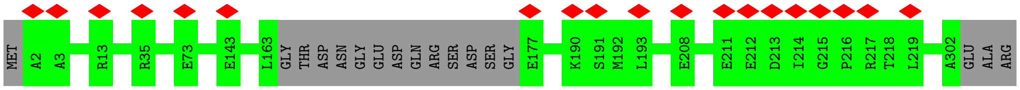




- Molecule 4: ATP synthase gamma chain

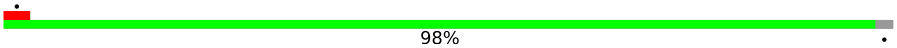
Chain G:

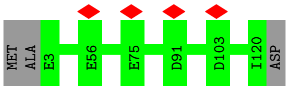




- Molecule 5: ATP synthase epsilon chain

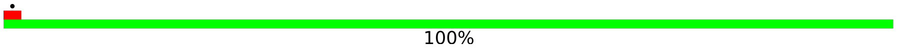
Chain H:

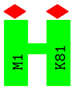




- Molecule 6: ATP synthase subunit c

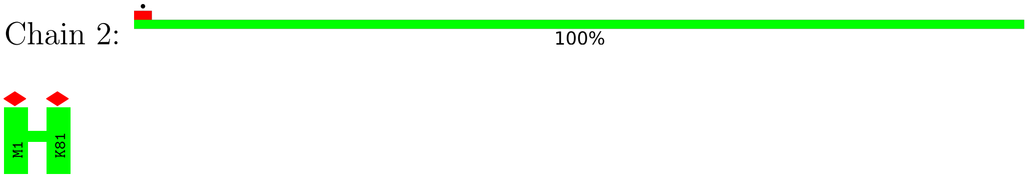
Chain 1:





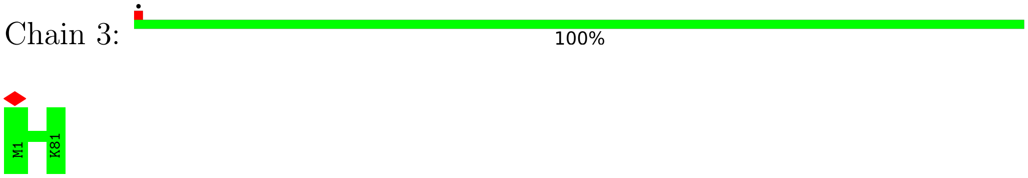
- Molecule 6: ATP synthase subunit c

Chain 2:



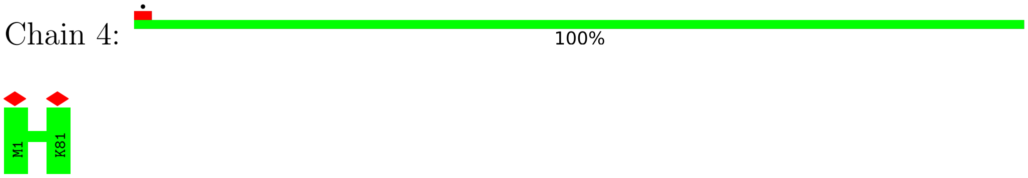
- Molecule 6: ATP synthase subunit c

Chain 3:



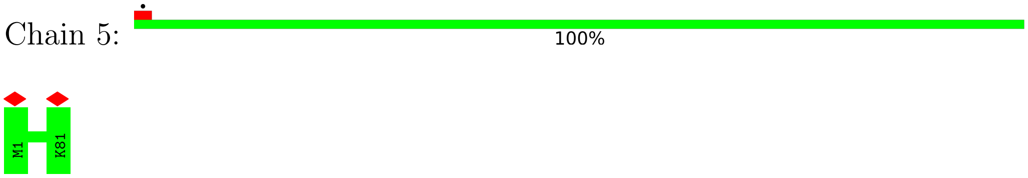
- Molecule 6: ATP synthase subunit c

Chain 4:



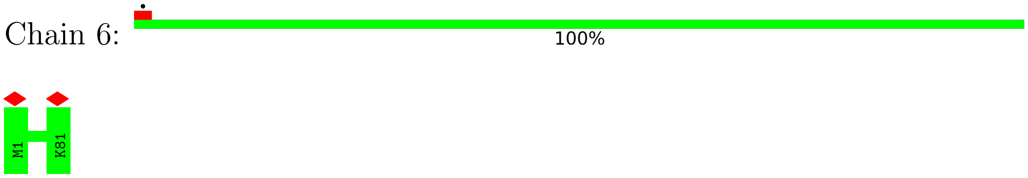
- Molecule 6: ATP synthase subunit c

Chain 5:



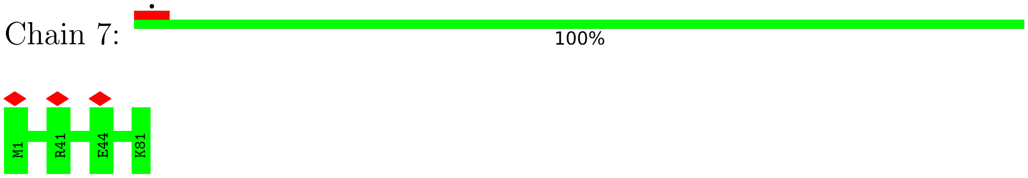
- Molecule 6: ATP synthase subunit c

Chain 6:



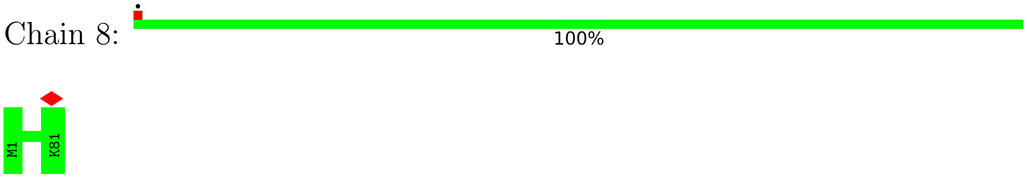
- Molecule 6: ATP synthase subunit c

Chain 7:

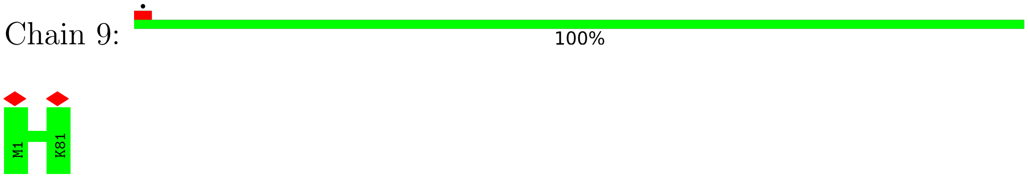


- Molecule 6: ATP synthase subunit c

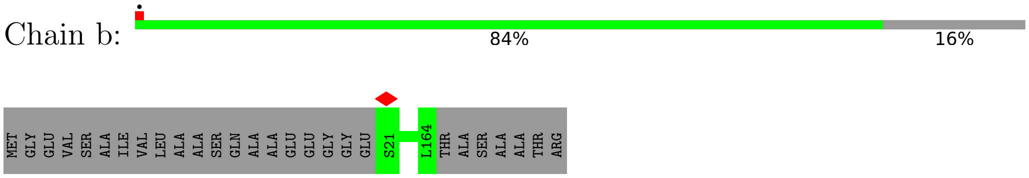
Chain 8:



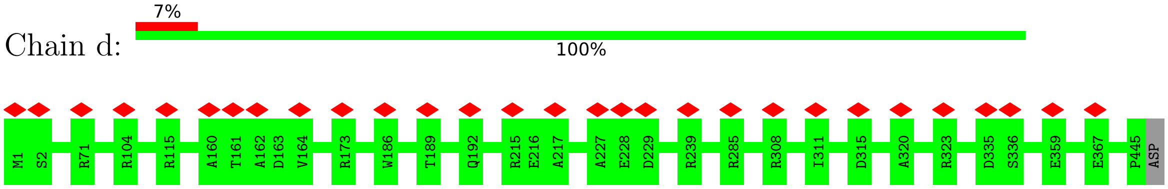
- Molecule 6: ATP synthase subunit c



- Molecule 7: ATP synthase subunit b



- Molecule 8: Multifunctional fusion protein



4 Experimental information

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96592	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	42.036	Depositor
Minimum map value	-22.616	Depositor
Average map value	0.010	Depositor
Map value standard deviation	1.115	Depositor
Recommended contour level	5.6	Depositor
Map size (Å)	373.76, 373.76, 373.76	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.73, 0.73, 0.73	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, BQ1, ATP

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	0.37	0/1887	0.53	0/2581
2	A	0.30	0/3976	0.46	0/5387
2	B	0.30	0/3802	0.45	0/5147
2	C	0.30	0/4101	0.44	0/5553
3	D	0.31	0/3680	0.46	0/4990
3	E	0.31	0/3680	0.44	0/4990
3	F	0.31	0/3680	0.46	0/4990
4	G	0.31	0/2291	0.43	0/3099
5	H	0.30	0/910	0.47	0/1230
6	1	0.34	0/578	0.45	0/784
6	2	0.34	0/578	0.47	0/784
6	3	0.36	0/578	0.47	0/784
6	4	0.33	0/578	0.43	0/784
6	5	0.34	0/578	0.45	0/784
6	6	0.35	0/578	0.44	0/784
6	7	0.33	0/578	0.43	0/784
6	8	0.32	0/578	0.44	0/784
6	9	0.33	0/578	0.45	0/784
7	b	0.28	0/1118	0.44	0/1512
8	d	0.28	0/3462	0.48	0/4697
All	All	0.31	0/37789	0.45	0/51232

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 ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	235/250 (94%)	225 (96%)	10 (4%)	0	100	100
2	A	515/549 (94%)	504 (98%)	11 (2%)	0	100	100
2	B	486/549 (88%)	475 (98%)	11 (2%)	0	100	100
2	C	525/549 (96%)	507 (97%)	18 (3%)	0	100	100
3	D	467/486 (96%)	455 (97%)	12 (3%)	0	100	100
3	E	467/486 (96%)	459 (98%)	8 (2%)	0	100	100
3	F	467/486 (96%)	453 (97%)	14 (3%)	0	100	100
4	G	284/305 (93%)	274 (96%)	10 (4%)	0	100	100
5	H	116/121 (96%)	112 (97%)	4 (3%)	0	100	100
6	1	79/81 (98%)	74 (94%)	5 (6%)	0	100	100
6	2	79/81 (98%)	73 (92%)	6 (8%)	0	100	100
6	3	79/81 (98%)	77 (98%)	2 (2%)	0	100	100
6	4	79/81 (98%)	77 (98%)	2 (2%)	0	100	100
6	5	79/81 (98%)	77 (98%)	2 (2%)	0	100	100
6	6	79/81 (98%)	77 (98%)	2 (2%)	0	100	100
6	7	79/81 (98%)	78 (99%)	1 (1%)	0	100	100
6	8	79/81 (98%)	76 (96%)	3 (4%)	0	100	100
6	9	79/81 (98%)	74 (94%)	5 (6%)	0	100	100
7	b	142/171 (83%)	138 (97%)	4 (3%)	0	100	100
8	d	443/446 (99%)	426 (96%)	17 (4%)	0	100	100
All	All	4858/5127 (95%)	4711 (97%)	147 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	193/204 (95%)	193 (100%)	0	100	100
2	A	417/444 (94%)	417 (100%)	0	100	100
2	B	401/444 (90%)	401 (100%)	0	100	100
2	C	431/444 (97%)	431 (100%)	0	100	100
3	D	389/403 (96%)	389 (100%)	0	100	100
3	E	389/403 (96%)	389 (100%)	0	100	100
3	F	389/403 (96%)	389 (100%)	0	100	100
4	G	235/248 (95%)	235 (100%)	0	100	100
5	H	94/96 (98%)	94 (100%)	0	100	100
6	1	52/52 (100%)	52 (100%)	0	100	100
6	2	52/52 (100%)	52 (100%)	0	100	100
6	3	52/52 (100%)	52 (100%)	0	100	100
6	4	52/52 (100%)	52 (100%)	0	100	100
6	5	52/52 (100%)	52 (100%)	0	100	100
6	6	52/52 (100%)	52 (100%)	0	100	100
6	7	52/52 (100%)	52 (100%)	0	100	100
6	8	52/52 (100%)	52 (100%)	0	100	100
6	9	52/52 (100%)	52 (100%)	0	100	100
7	b	117/133 (88%)	117 (100%)	0	100	100
8	d	356/357 (100%)	356 (100%)	0	100	100
All	All	3879/4047 (96%)	3879 (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 14 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	376	HIS
6	2	67	ASN
8	d	277	GLN
8	d	128	GLN
8	d	140	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 5 are monoatomic - leaving 12 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	BQ1	9	600	-	39,41,41	1.07	3 (7%)	50,59,59	1.35	8 (16%)
11	ADP	D	600	10	24,29,29	0.93	1 (4%)	29,45,45	1.38	4 (13%)
12	BQ1	4	600	-	39,41,41	1.07	2 (5%)	50,59,59	1.30	5 (10%)
12	BQ1	7	600	-	39,41,41	1.07	2 (5%)	50,59,59	1.29	5 (10%)
12	BQ1	8	600	-	39,41,41	1.09	2 (5%)	50,59,59	1.26	7 (14%)
11	ADP	F	600	10	24,29,29	0.66	0	29,45,45	0.72	1 (3%)
12	BQ1	1	600	-	39,41,41	1.10	4 (10%)	50,59,59	1.38	7 (14%)
9	ATP	A	600	10	26,33,33	0.89	1 (3%)	31,52,52	1.43	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
9	ATP	C	600	10	26,33,33	0.91	1 (3%)	31,52,52	1.43	5 (16%)
12	BQ1	5	600	-	39,41,41	1.07	3 (7%)	50,59,59	1.26	6 (12%)
9	ATP	B	600	10	26,33,33	0.91	1 (3%)	31,52,52	1.47	5 (16%)
12	BQ1	6	600	-	39,41,41	1.06	2 (5%)	50,59,59	1.28	5 (10%)

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	BQ1	9	600	-	-	0/28/28/28	0/5/5/5
11	ADP	D	600	10	-	4/12/32/32	0/3/3/3
12	BQ1	4	600	-	-	1/28/28/28	0/5/5/5
12	BQ1	7	600	-	-	0/28/28/28	0/5/5/5
12	BQ1	8	600	-	-	0/28/28/28	0/5/5/5
11	ADP	F	600	10	-	2/12/32/32	0/3/3/3
12	BQ1	1	600	-	-	2/28/28/28	0/5/5/5
9	ATP	A	600	10	-	2/18/38/38	0/3/3/3
9	ATP	C	600	10	-	3/18/38/38	0/3/3/3
12	BQ1	5	600	-	-	0/28/28/28	0/5/5/5
9	ATP	B	600	10	-	2/18/38/38	0/3/3/3
12	BQ1	6	600	-	-	0/28/28/28	0/5/5/5

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	9	600	BQ1	O03-C17	3.32	1.40	1.35
12	8	600	BQ1	O03-C17	3.28	1.40	1.35
12	5	600	BQ1	O03-C17	3.28	1.40	1.35
12	4	600	BQ1	O03-C17	3.18	1.40	1.35
12	7	600	BQ1	O03-C17	3.18	1.40	1.35

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	9	600	BQ1	C10-C17-N05	-4.24	121.54	125.70
12	7	600	BQ1	C10-C17-N05	-4.16	121.62	125.70
12	6	600	BQ1	C10-C17-N05	-4.13	121.65	125.70
12	1	600	BQ1	C10-C17-N05	-4.03	121.75	125.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	1	600	BQ1	C37-O03-C17	-4.03	113.22	117.21

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

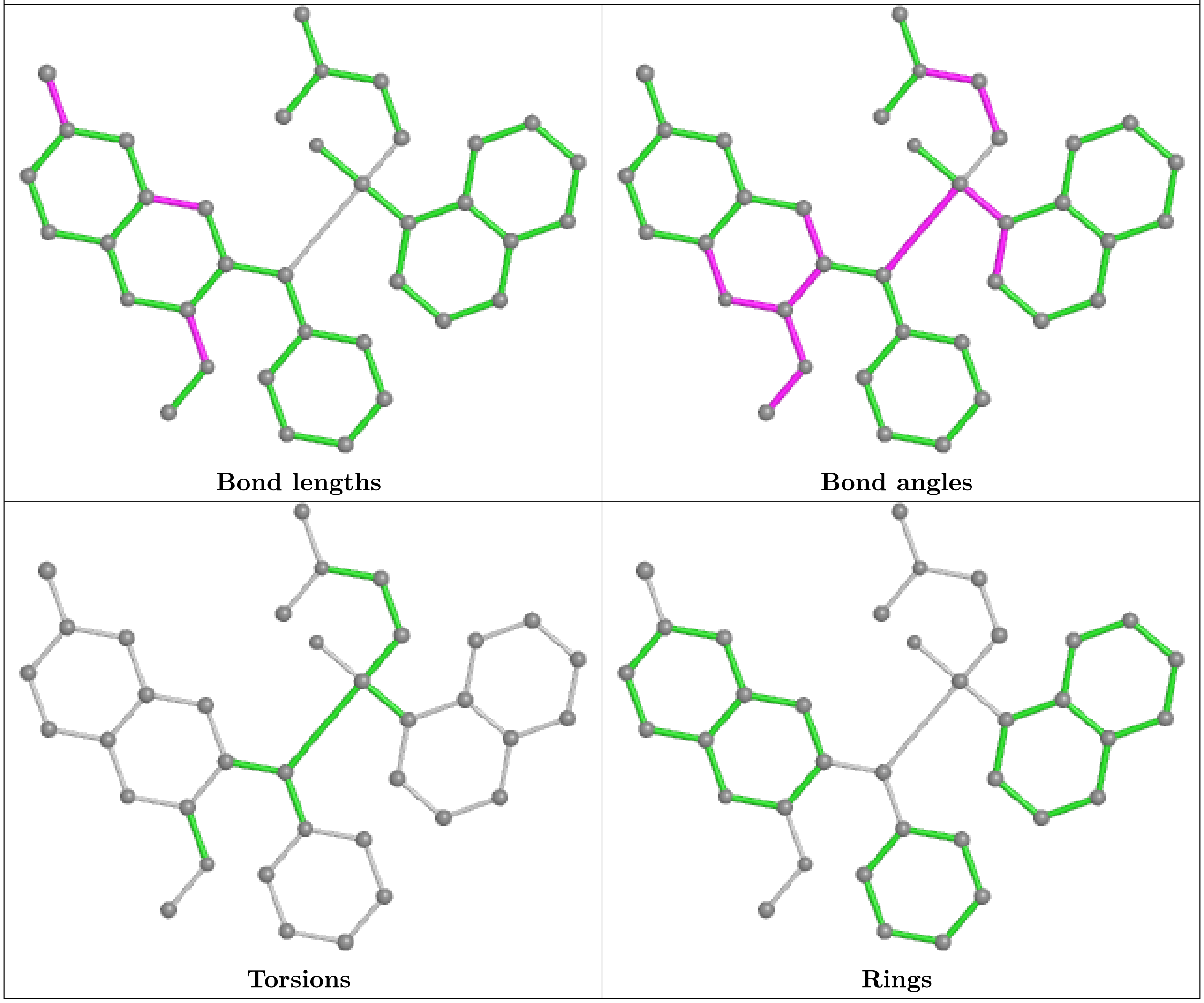
Mol	Chain	Res	Type	Atoms
11	D	600	ADP	C5'-O5'-PA-O2A
11	D	600	ADP	O4'-C4'-C5'-O5'
11	F	600	ADP	PA-O3A-PB-O2B
11	D	600	ADP	C5'-O5'-PA-O3A
9	A	600	ATP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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 BQ1 9 600



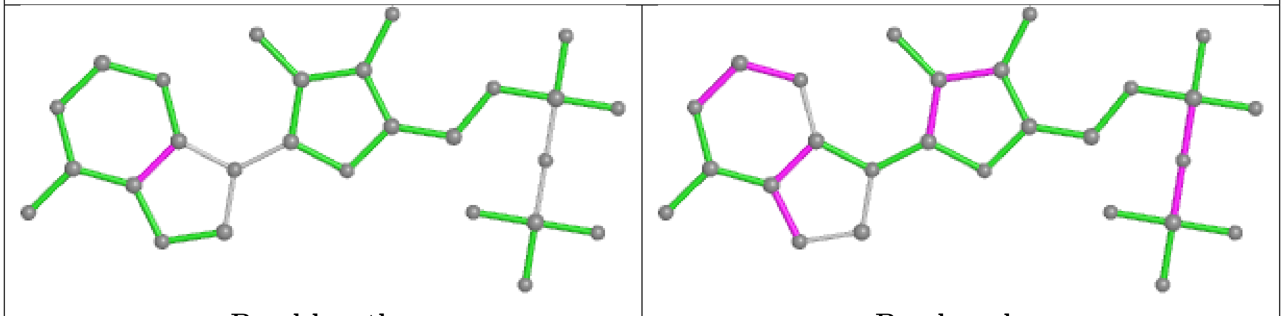
Bond lengths

Bond angles

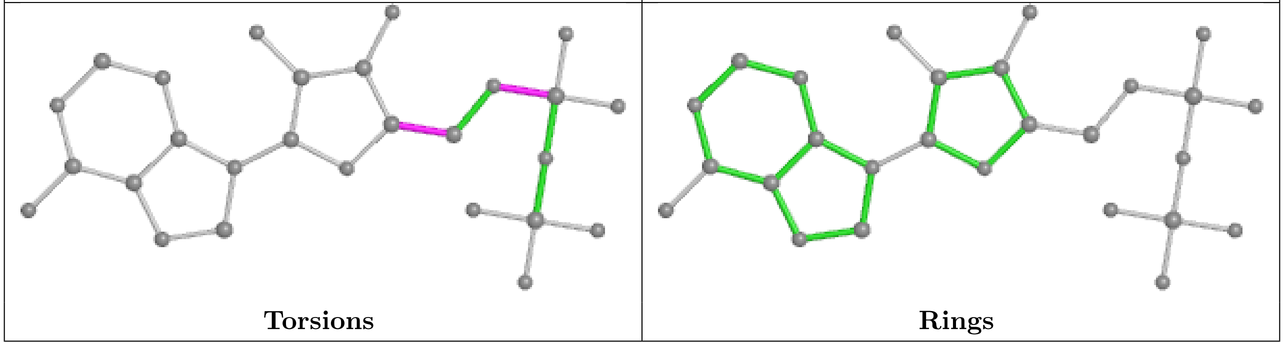
Torsions

Rings

Ligand ADP D 600

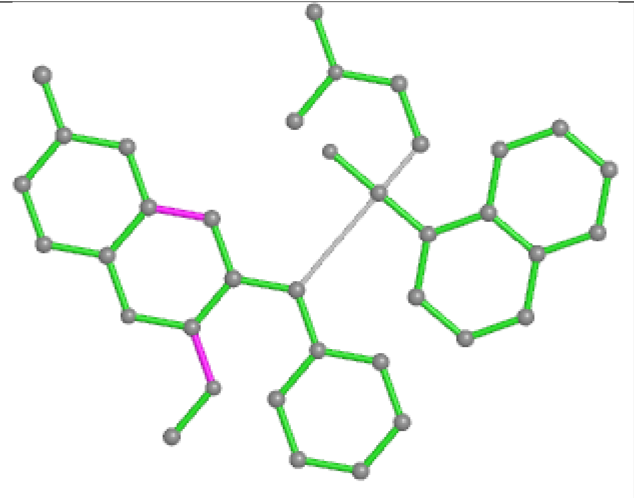


Bond lengths Bond angles

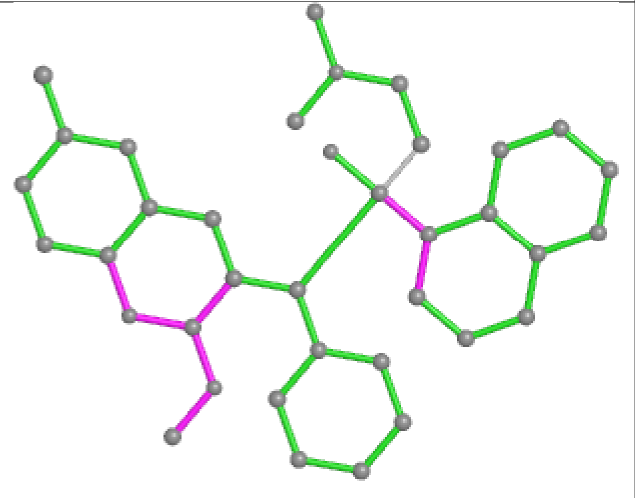


Torsions Rings

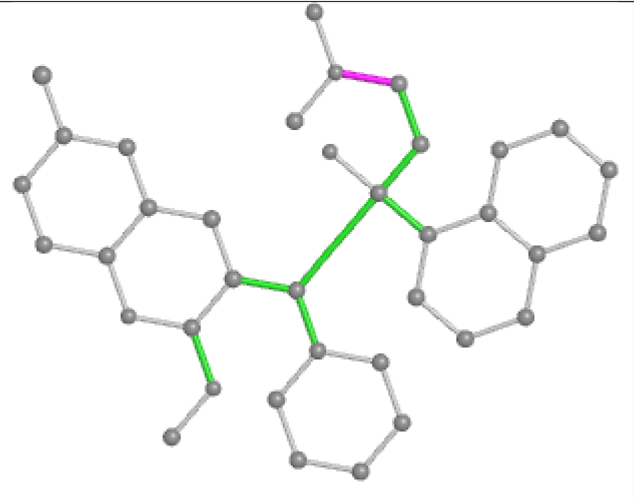
Ligand BQ1 4 600



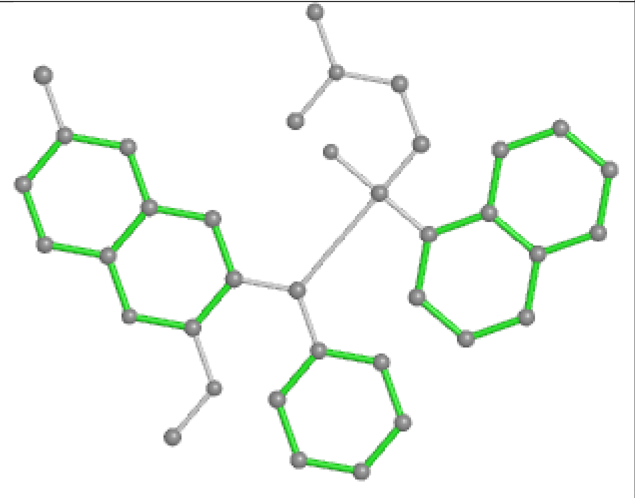
Bond lengths



Bond angles

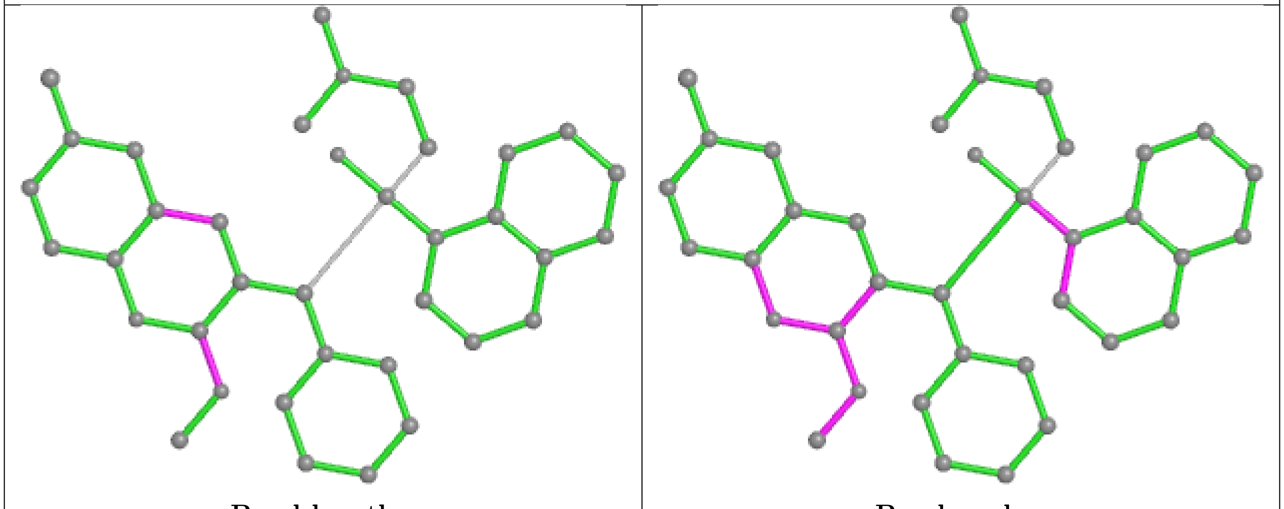


Torsions



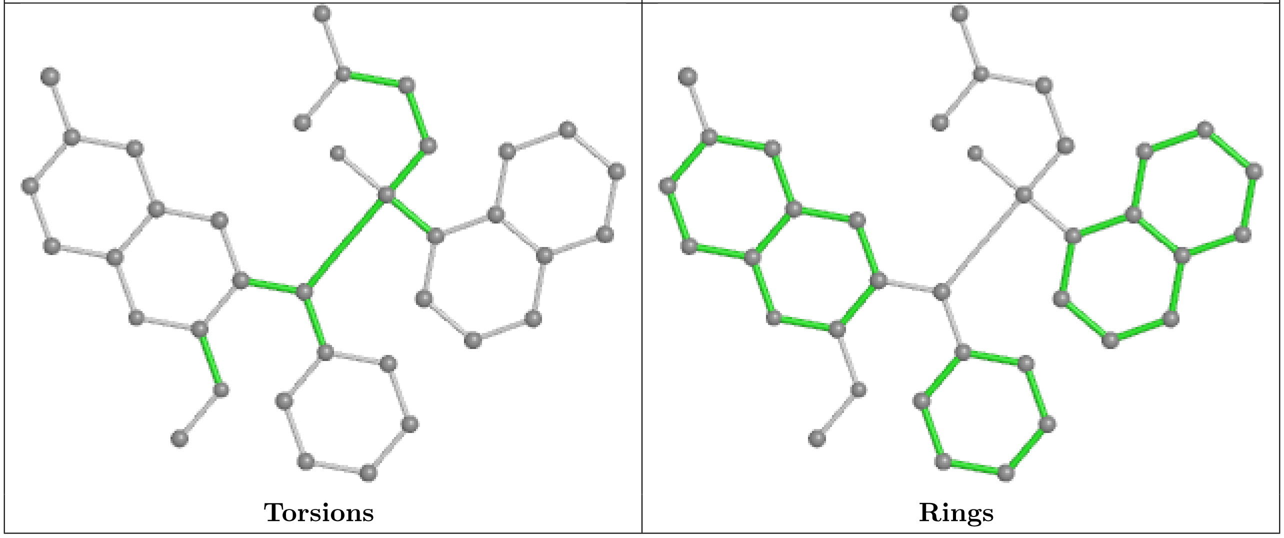
Rings

Ligand BQ1 7 600



Bond lengths

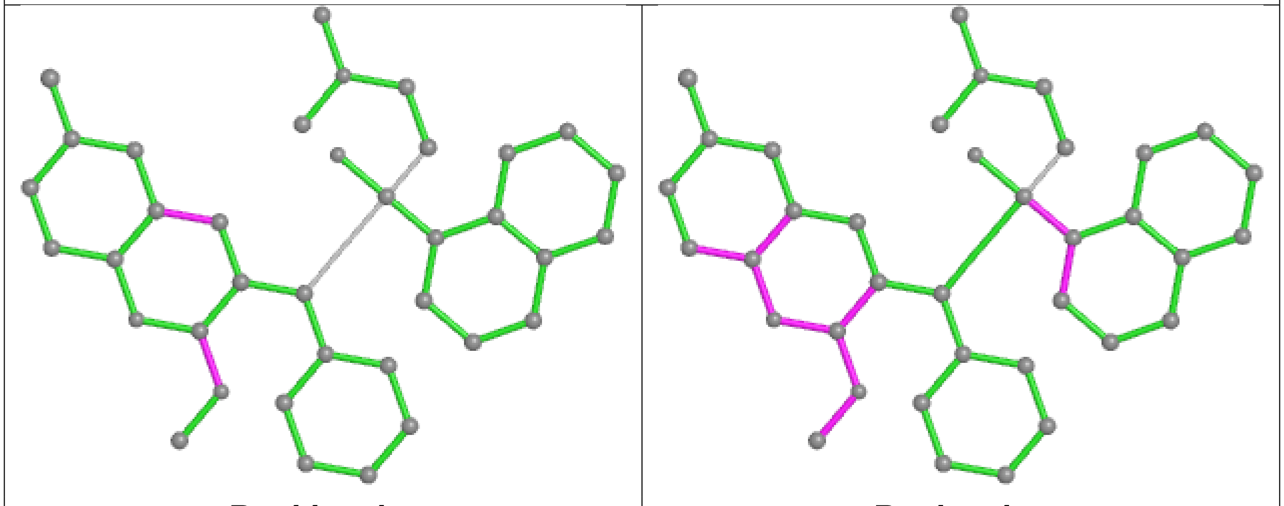
Bond angles



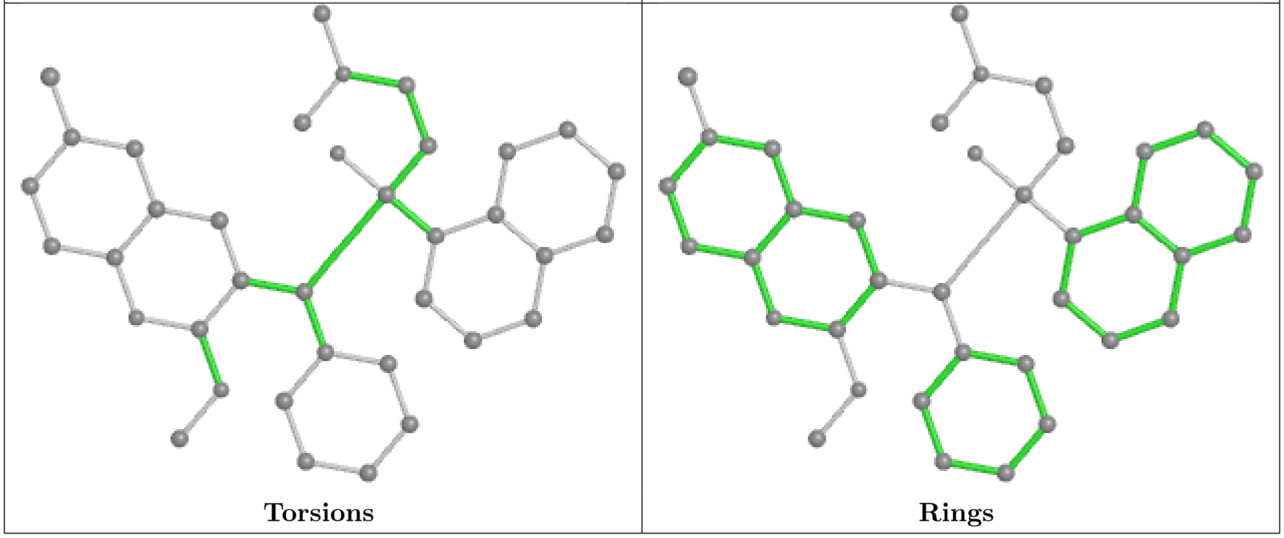
Torsions

Rings

Ligand BQ1 8 600

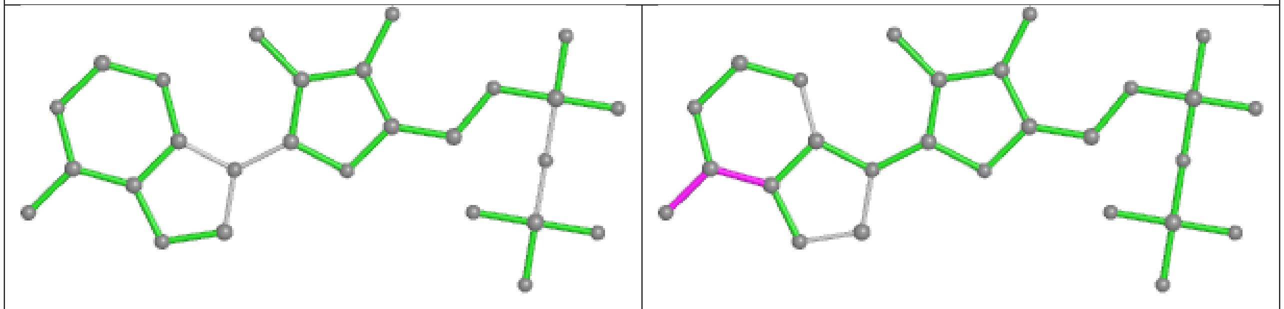


Bond lengths **Bond angles**



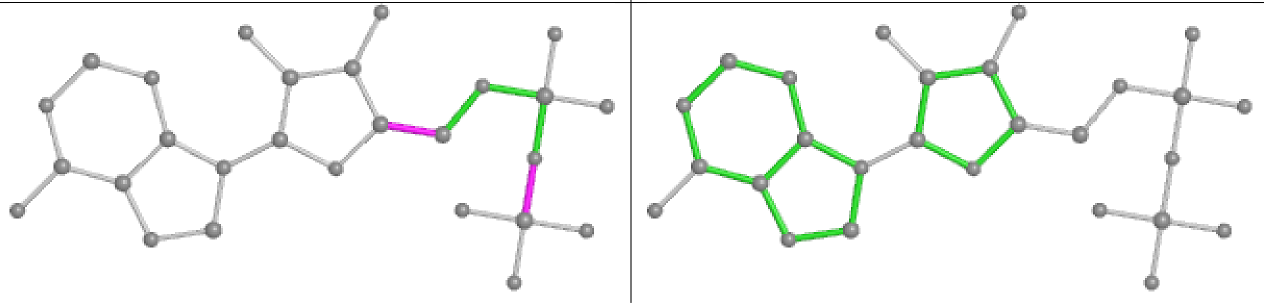
Torsions **Rings**

Ligand ADP F 600



Bond lengths

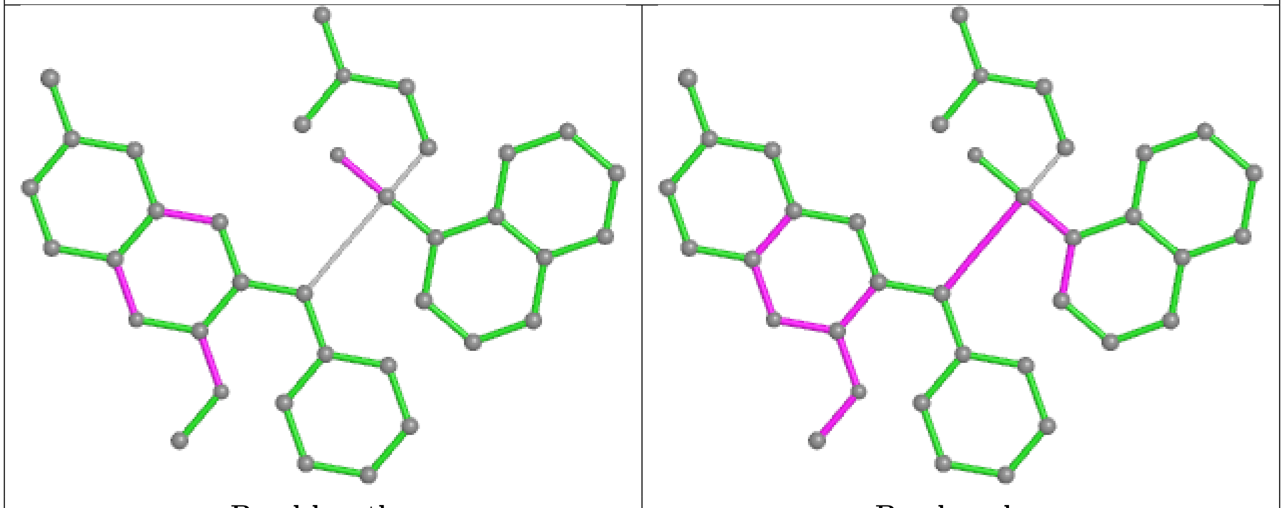
Bond angles



Torsions

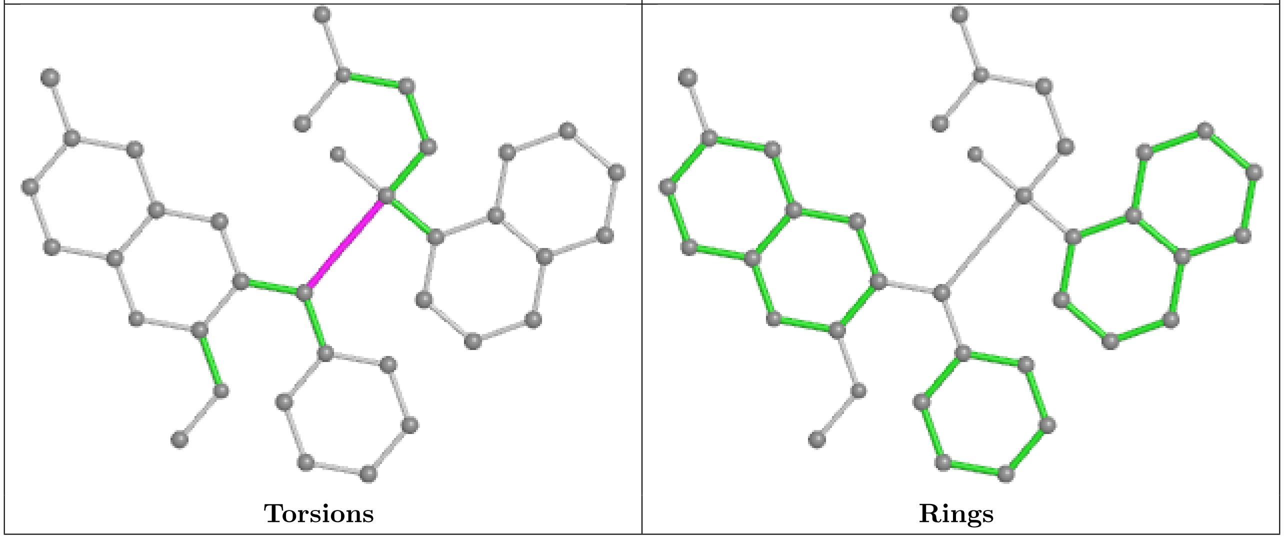
Rings

Ligand BQ1 1 600



Bond lengths

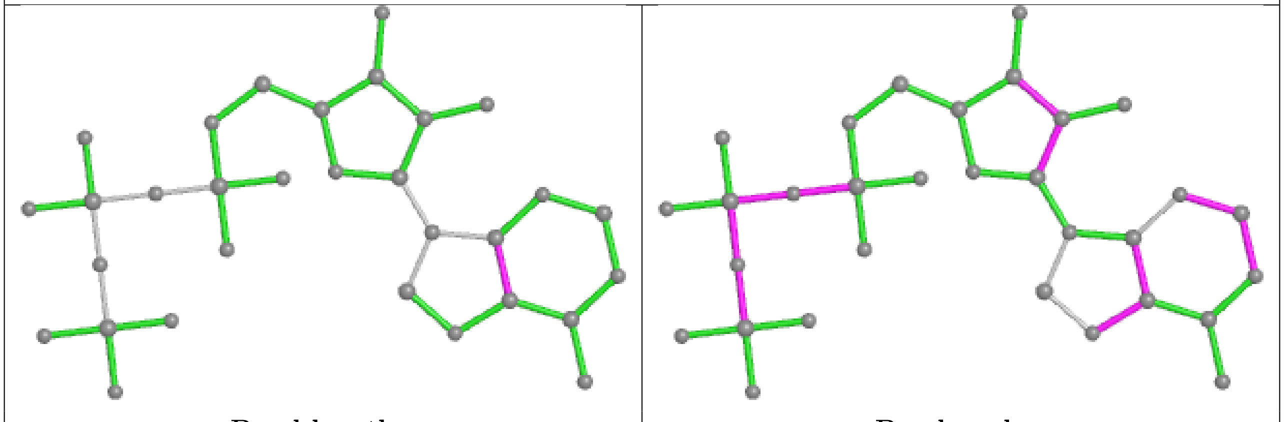
Bond angles



Torsions

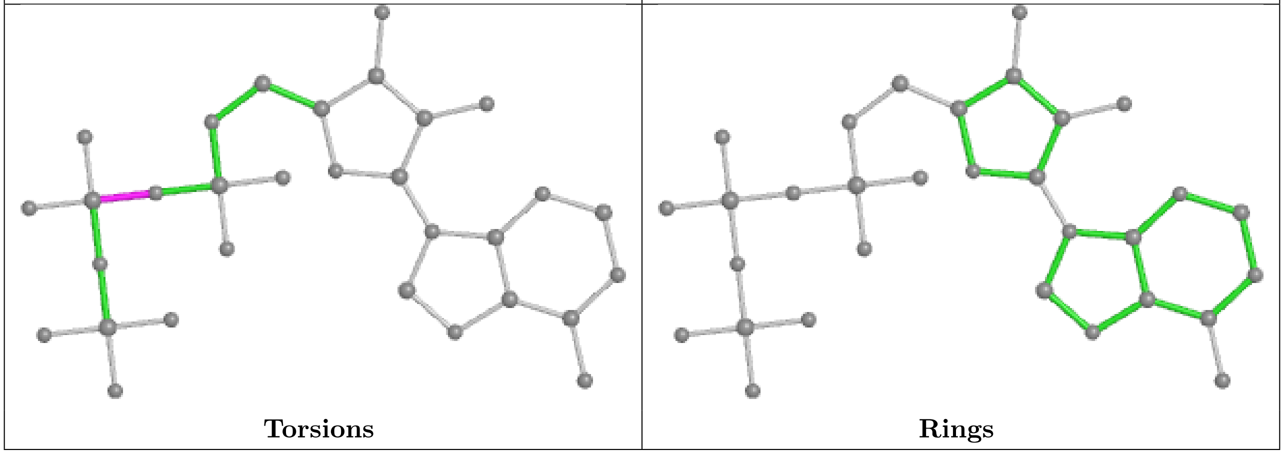
Rings

Ligand ATP A 600



Bond lengths

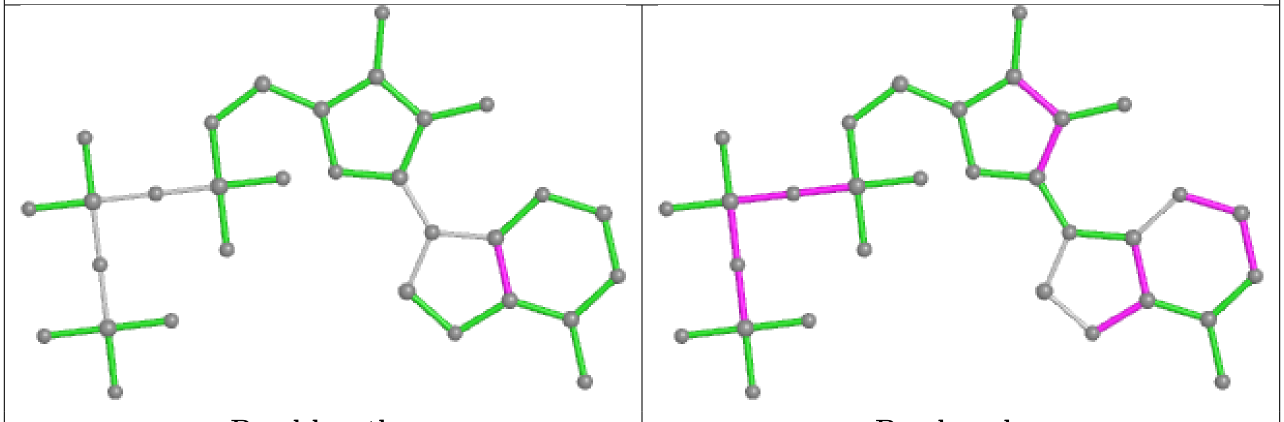
Bond angles



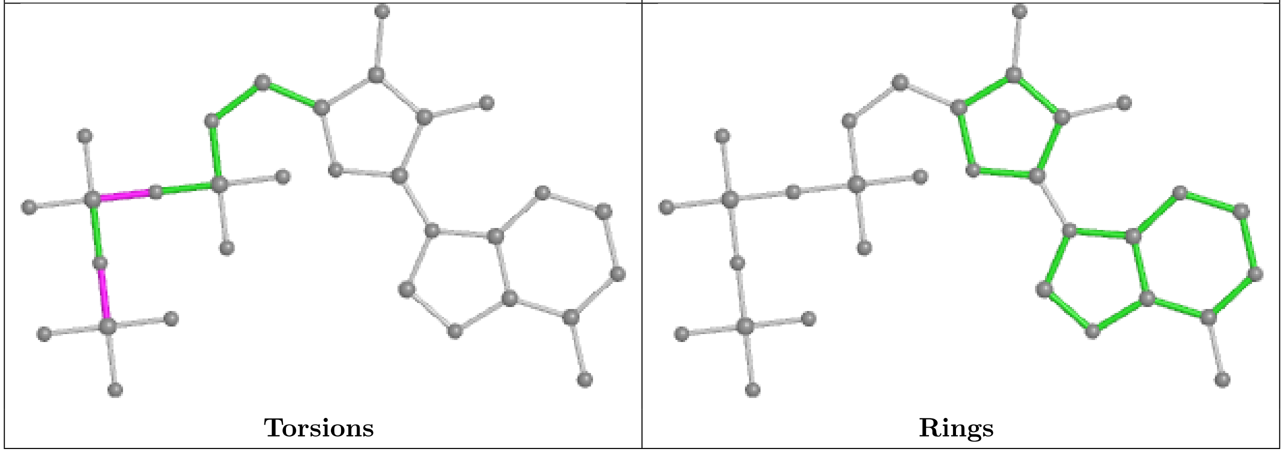
Torsions

Rings

Ligand ATP C 600

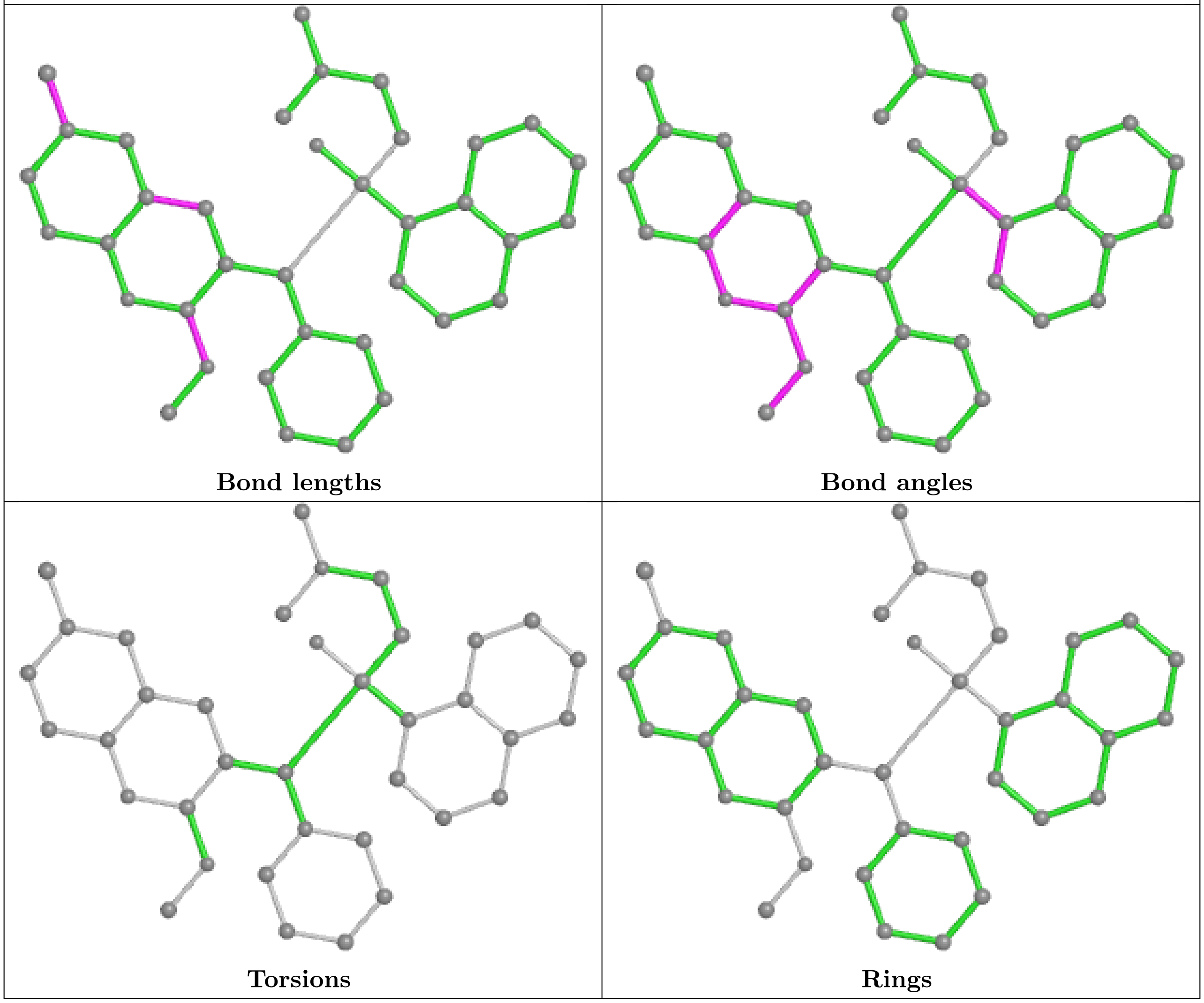


Bond lengths **Bond angles**



Torsions **Rings**

Ligand BQ1 5 600



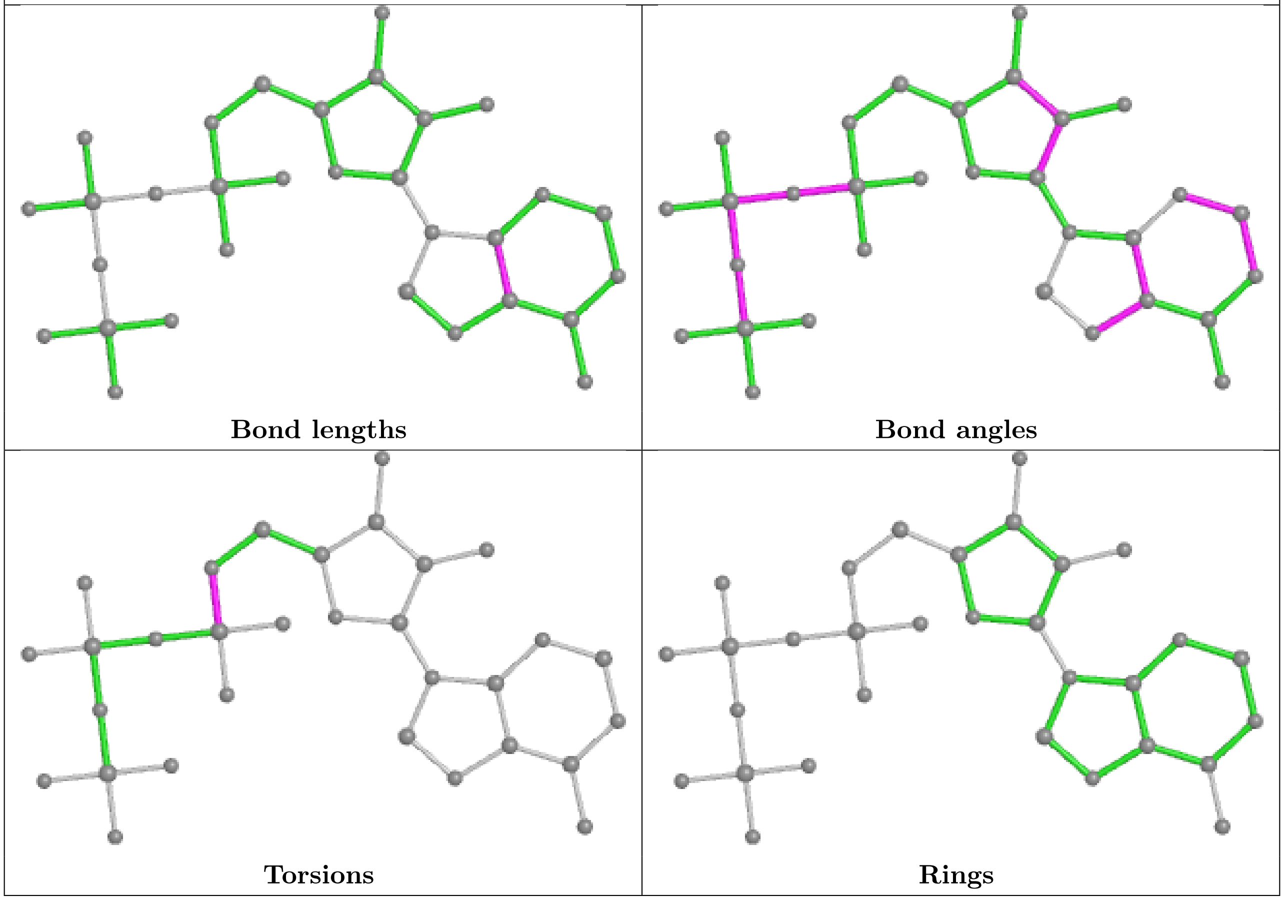
Bond lengths

Bond angles

Torsions

Rings

Ligand ATP B 600



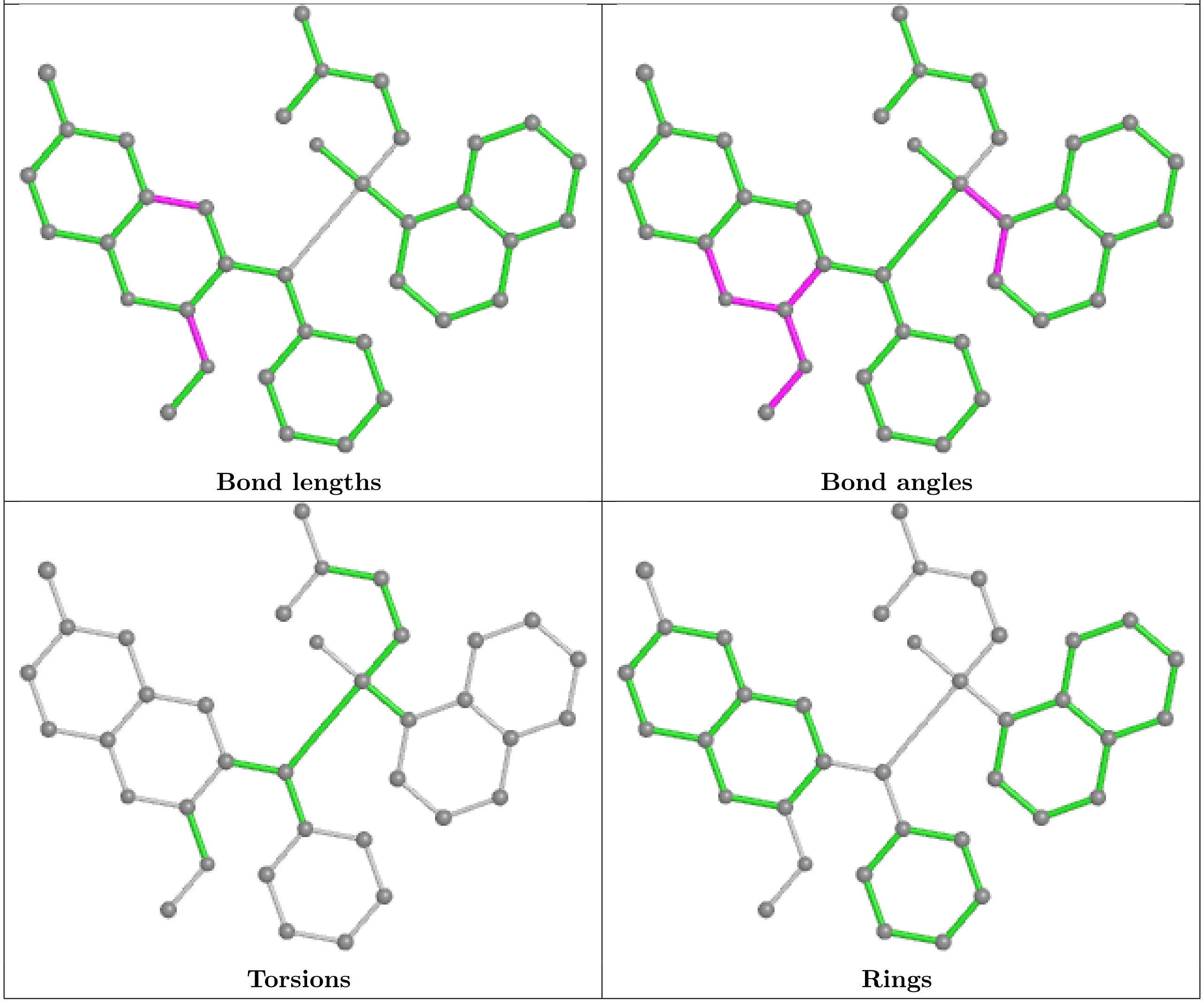
Bond lengths

Bond angles

Torsions

Rings

Ligand BQ1 6 600



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

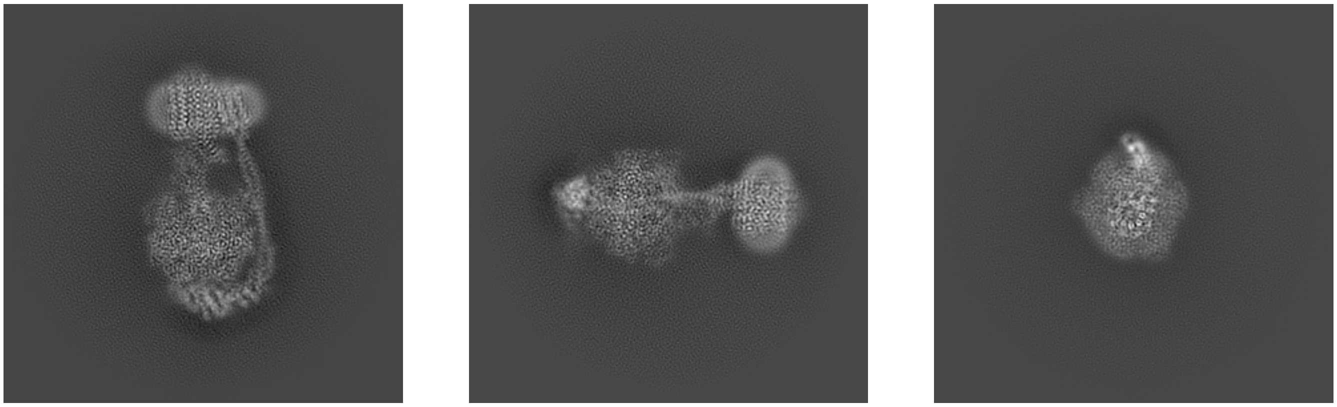
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-35909. 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 (i)

6.1.1 Primary map

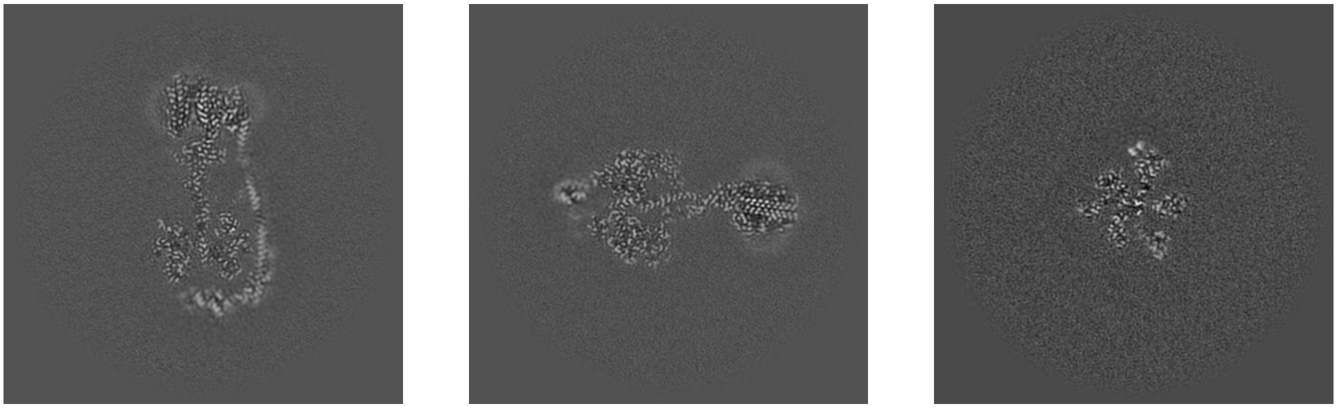


X Y Z

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

6.2 Central slices (i)

6.2.1 Primary map

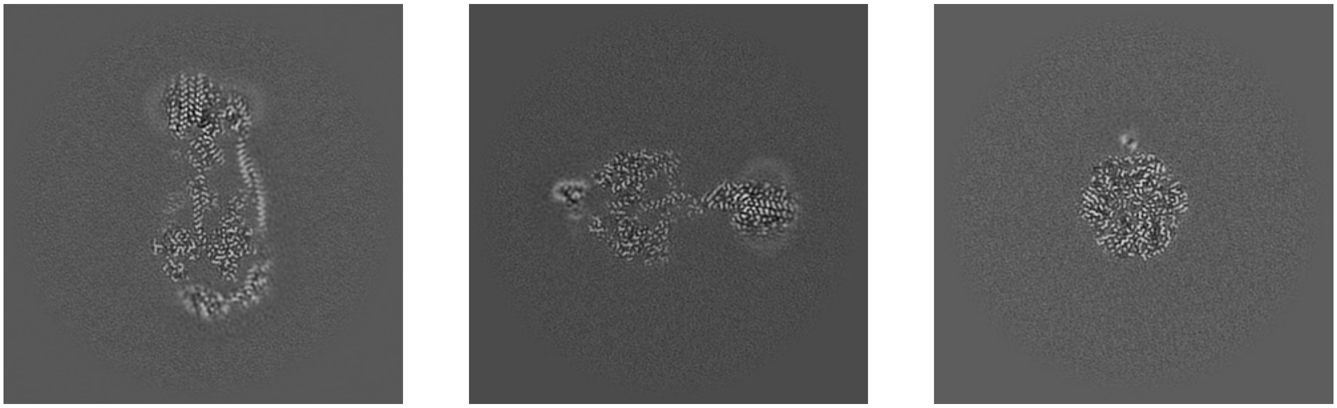


X Index: 256 Y Index: 256 Z Index: 256

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map

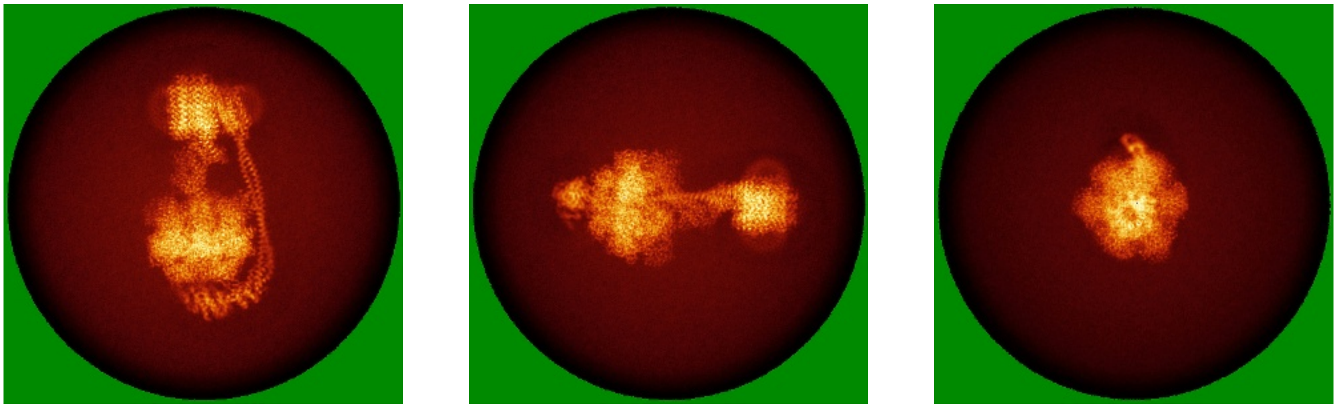


X Index: 263 Y Index: 258 Z Index: 200

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

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

6.4.1 Primary map

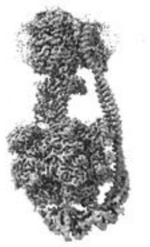


X Y Z

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

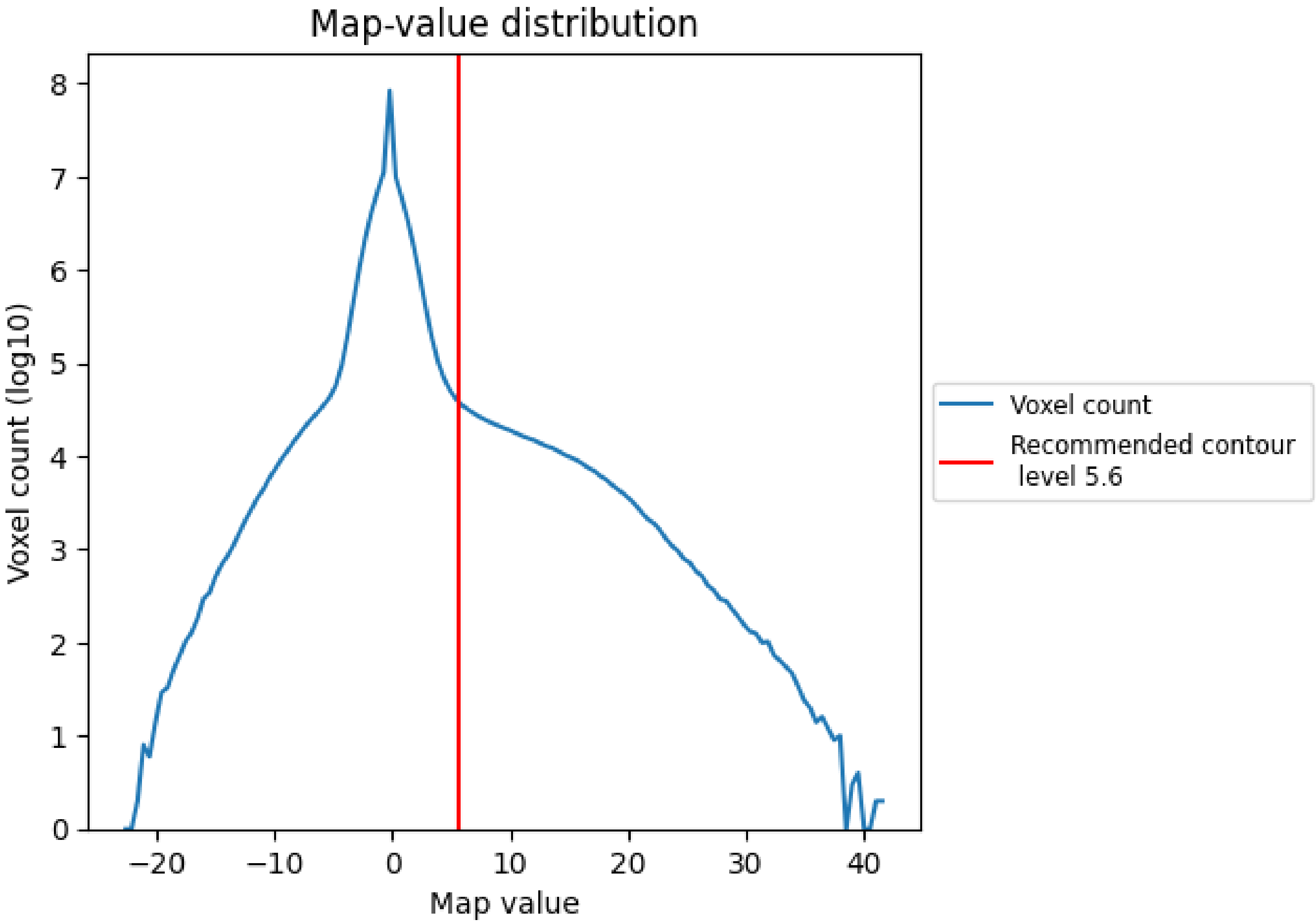
6.6 Mask visualisation (i)

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

7 Map analysis

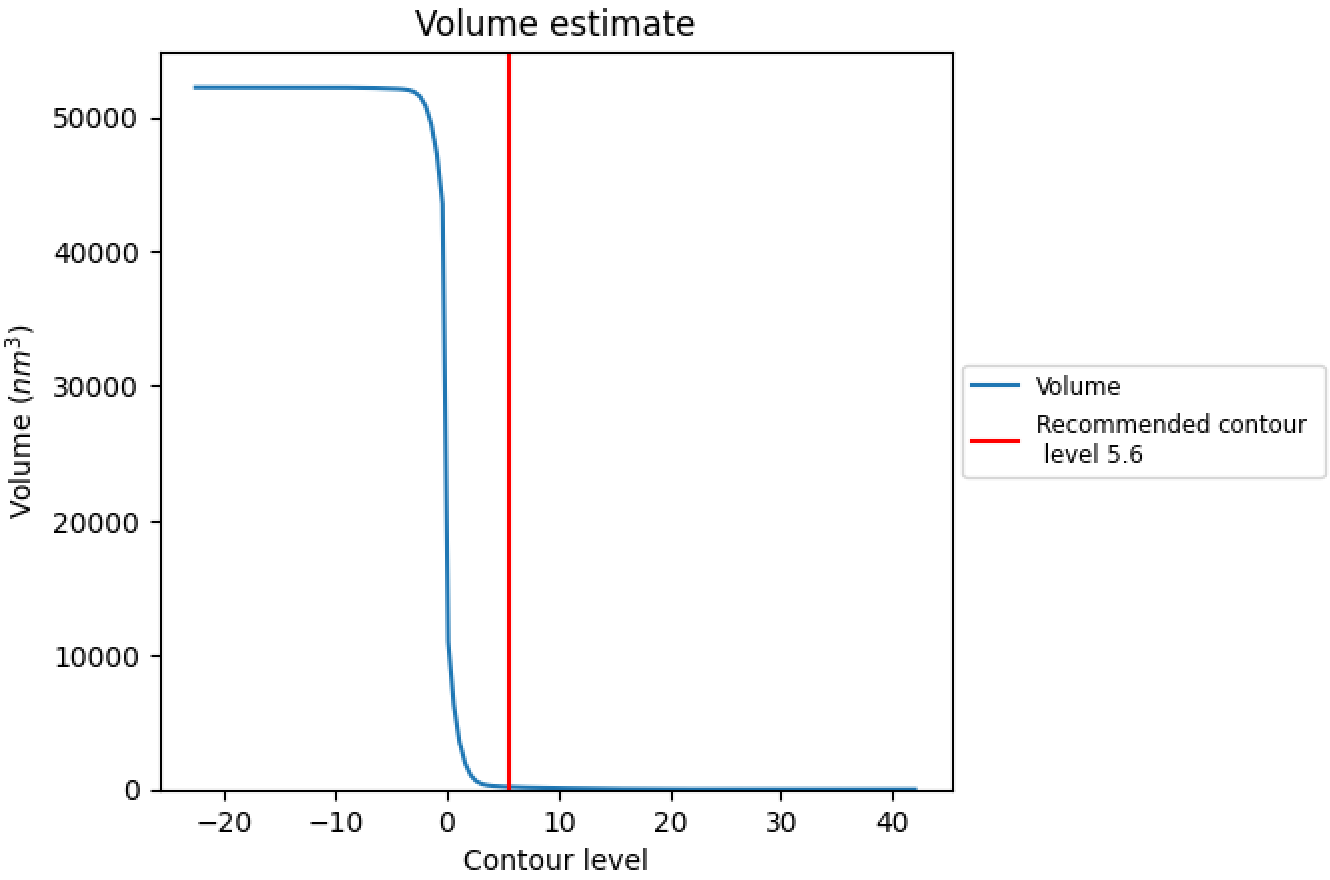
This section contains the results of statistical analysis of the map.

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.

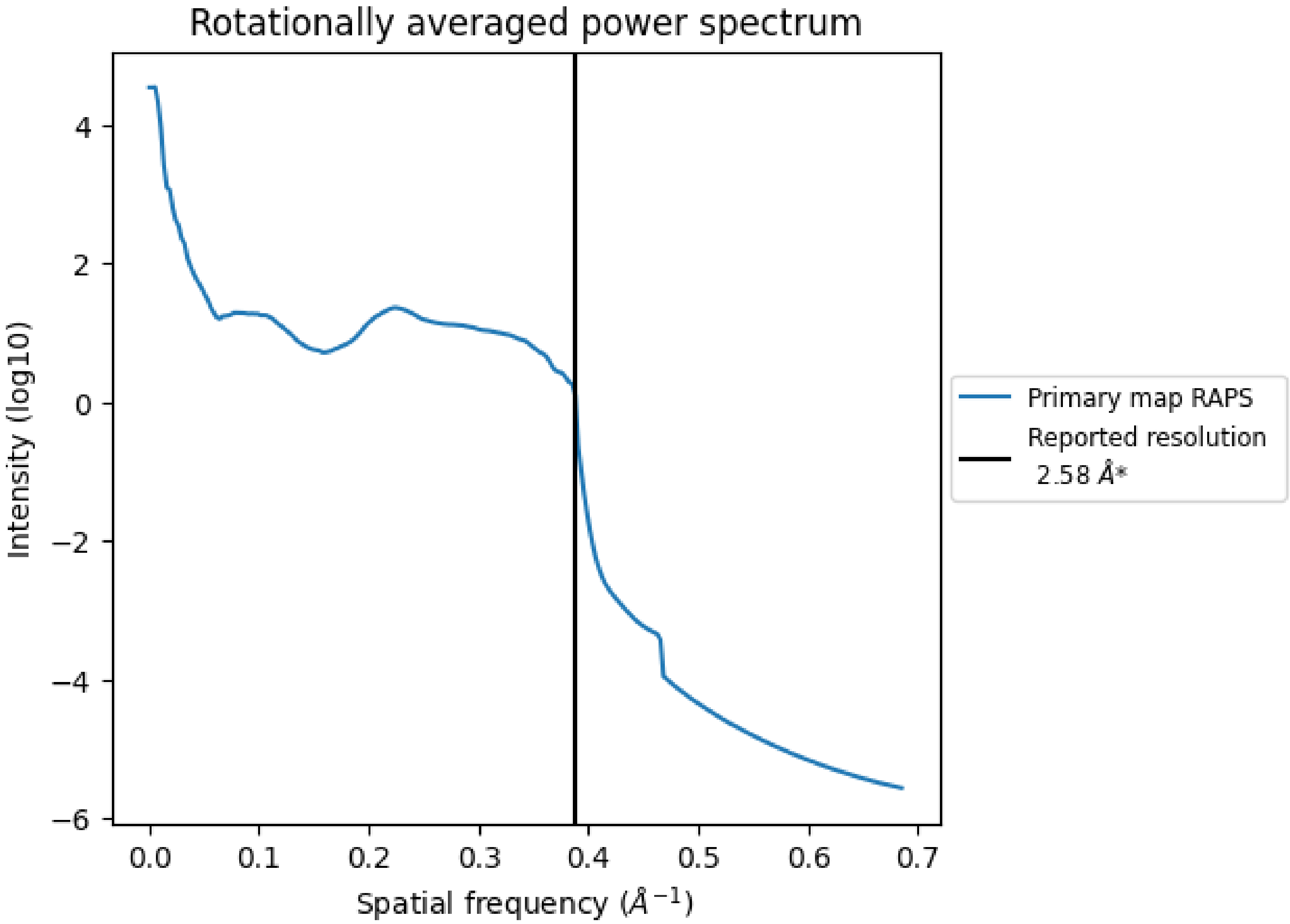
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 183 nm^3; this corresponds to an approximate mass of 165 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 0.388 $Å^{-1}$

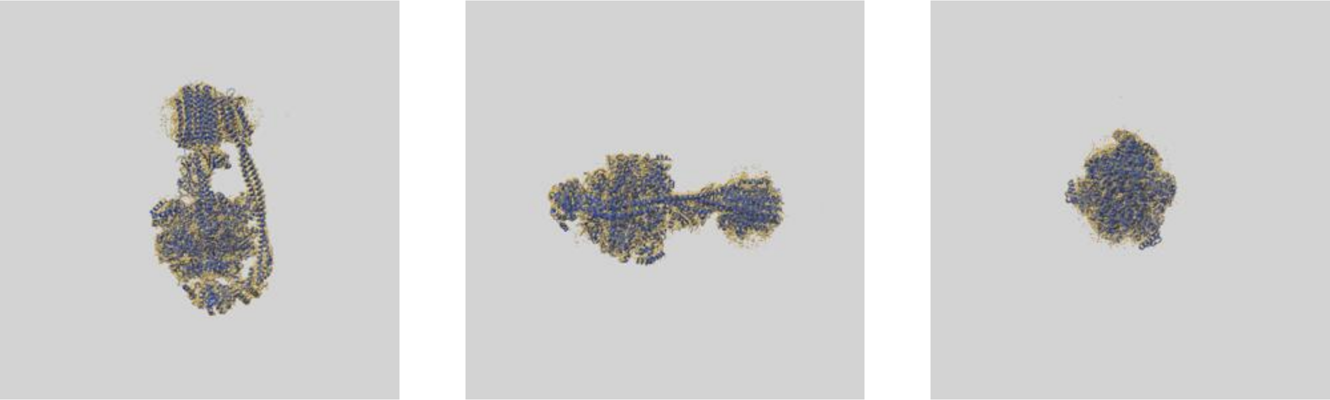
8 Fourier-Shell correlation ⓘ

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-35909 and PDB model 8J0S. Per-residue inclusion information can be found in section 3 on page 9.

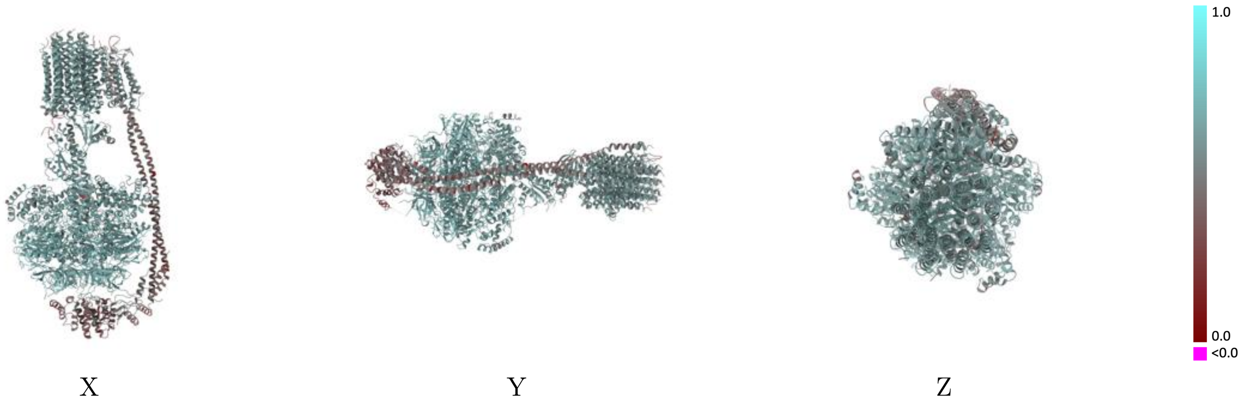
9.1 Map-model overlay ⓘ



X Y Z

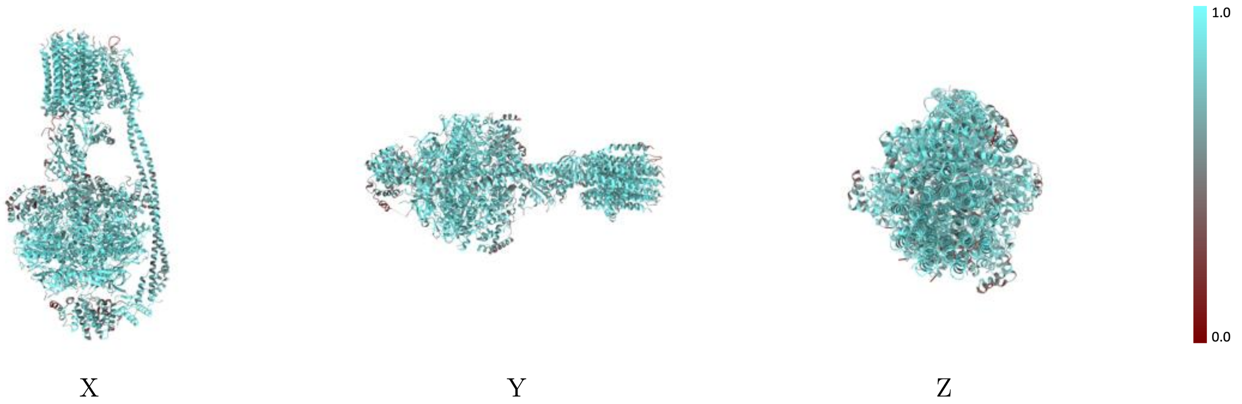
The images above show the 3D surface view of the map at the recommended contour level 5.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



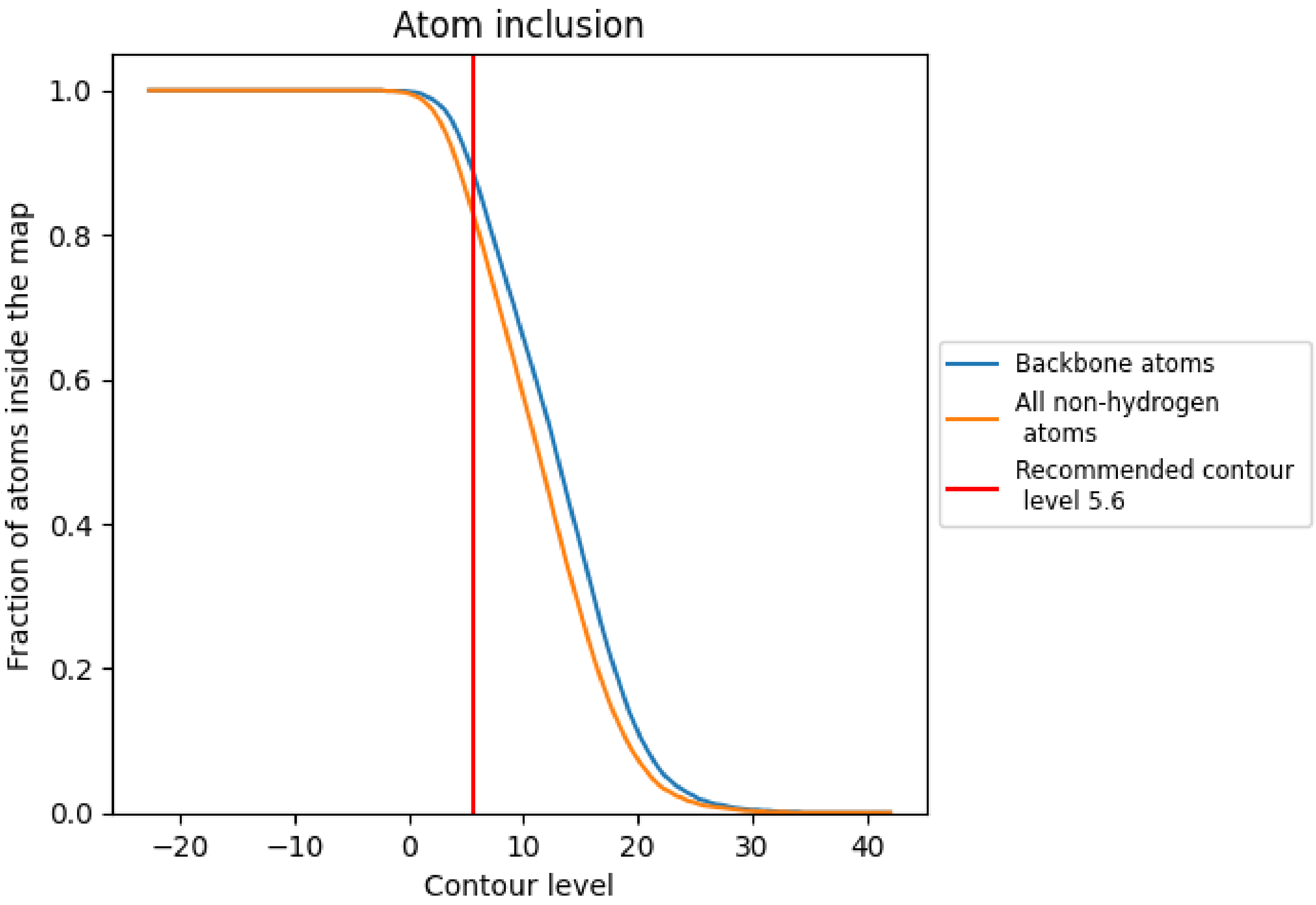
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (5.6).

9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 83% 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 (5.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	▬ 0.8310	▬ 0.5920
1	▬ 0.8580	▬ 0.5850
2	▬ 0.8740	▬ 0.5940
3	▬ 0.8770	▬ 0.5840
4	▬ 0.8830	▬ 0.5930
5	▬ 0.8700	▬ 0.5910
6	▬ 0.8630	▬ 0.5890
7	▬ 0.8530	▬ 0.5810
8	▬ 0.8500	▬ 0.5820
9	▬ 0.8680	▬ 0.5850
A	▬ 0.8670	▬ 0.6310
B	▬ 0.8060	▬ 0.6170
C	▬ 0.8250	▬ 0.6250
D	▬ 0.8820	▬ 0.6460
E	▬ 0.8470	▬ 0.6380
F	▬ 0.8940	▬ 0.6460
G	▬ 0.7620	▬ 0.5950
H	▬ 0.7860	▬ 0.5850
a	▬ 0.7970	▬ 0.5510
b	▬ 0.7800	▬ 0.4350
d	▬ 0.7260	▬ 0.4000