



Full wwPDB EM Validation Report ⓘ

Apr 22, 2024 – 04:46 PM JST

PDB ID : 8JR0
EMDB ID : EMD-36589
Title : Cryo-EM structure of Mycobacterium tuberculosis ATP synthase in complex with TBAJ-587
Authors : Zhang, Y.; Lai, Y.; Liu, F.; Rao, Z.; Gong, H.
Deposited on : 2023-06-15
Resolution : 2.80 Å(reported)

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We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

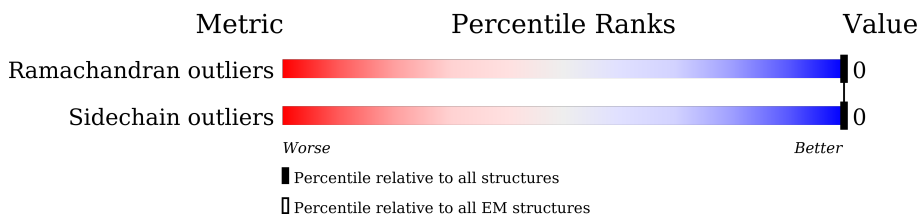
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.80 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.





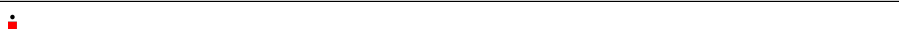
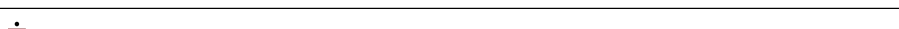
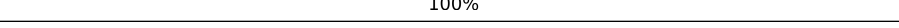
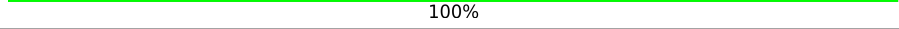


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	549	
1	B	549	
1	C	549	
2	D	486	
2	E	486	
2	F	486	
3	G	305	
4	H	121	
5	1	81	

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Mol	Chain	Length	Quality of chain
5	2	81	 100%
5	3	81	 100%
5	4	81	 100%
5	5	81	 100%
5	6	81	 100%
5	7	81	 100%
5	8	81	 100%
5	9	81	 100%
6	a	250	 11% 88% 12%
7	b	171	 5% 84% 16%
8	d	446	 19% 100%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 37460 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 alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	517	Total	C	N	O	S	0	0
			3916	2449	684	772	11		
1	B	491	Total	C	N	O	S	0	0
			3740	2341	654	734	11		
1	C	530	Total	C	N	O	S	0	0
			4033	2529	701	792	11		

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

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

- Molecule 3 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	287	Total	C	N	O	S	0	0
			2251	1415	398	430	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	119	Total	C	N	O	S	0	0
			906	562	162	181	1		

- Molecule 5 is a protein called ATP synthase subunit c.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	a	220	Total	C	N	O	S	0	0
			1706	1145	269	286	6		

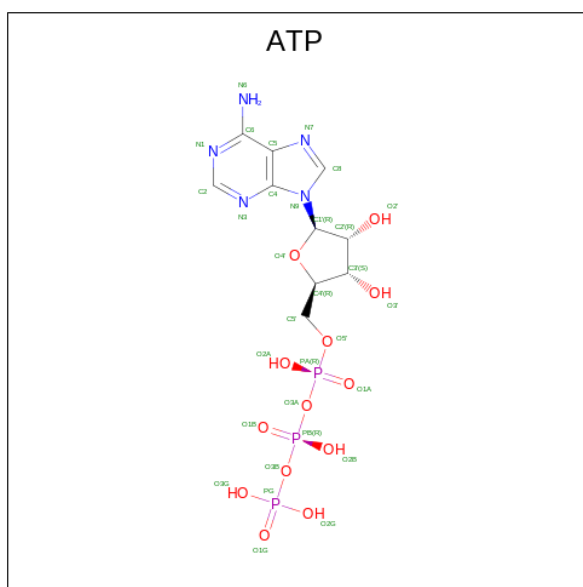
- Molecule 7 is a protein called ATP synthase subunit b.

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

- Molecule 8 is a protein called Multifunctional fusion protein.

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

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

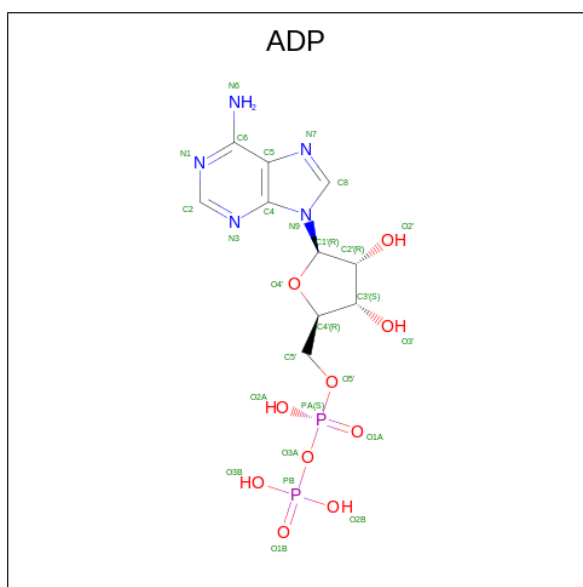


Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

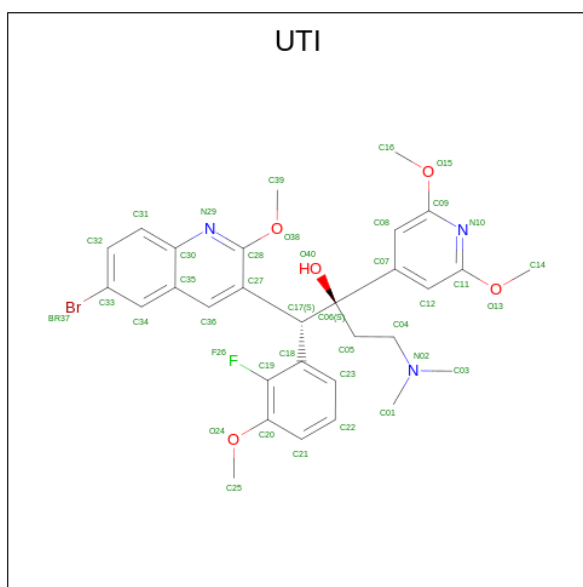
Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Mg	0
			1	1	
10	B	1	Total	Mg	0
			1	1	
10	C	1	Total	Mg	0
			1	1	
10	D	1	Total	Mg	0
			1	1	
10	F	1	Total	Mg	0
			1	1	

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
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 (1 {S},2 {S})-1-(6-bromanyl-2-methoxy-quinolin-3-yl)-2-(2,6-dimethoxypyridin-4-yl)-4-(dimethylamino)-1-(2-fluoranyl-3-methoxy-phenyl)butan-2-ol (three-letter code: UTI) (formula: C₃₀H₃₃BrFN₃O₅).



Mol	Chain	Residues	Atoms						AltConf
			Total	Br	C	F	N	O	
12	1	1	Total	Br	C	F	N	O	0
			40	1	30	1	3	5	

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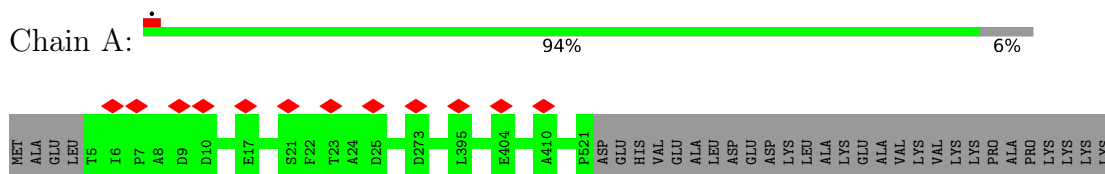
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Mol	Chain	Residues	Atoms						AltConf
			Total	Br	C	F	N	O	
12	4	1	Total 40	Br 1	C 30	F 1	N 3	O 5	0
12	5	1	Total 40	Br 1	C 30	F 1	N 3	O 5	0
12	6	1	Total 40	Br 1	C 30	F 1	N 3	O 5	0
12	7	1	Total 40	Br 1	C 30	F 1	N 3	O 5	0
12	8	1	Total 40	Br 1	C 30	F 1	N 3	O 5	0
12	9	1	Total 40	Br 1	C 30	F 1	N 3	O 5	0

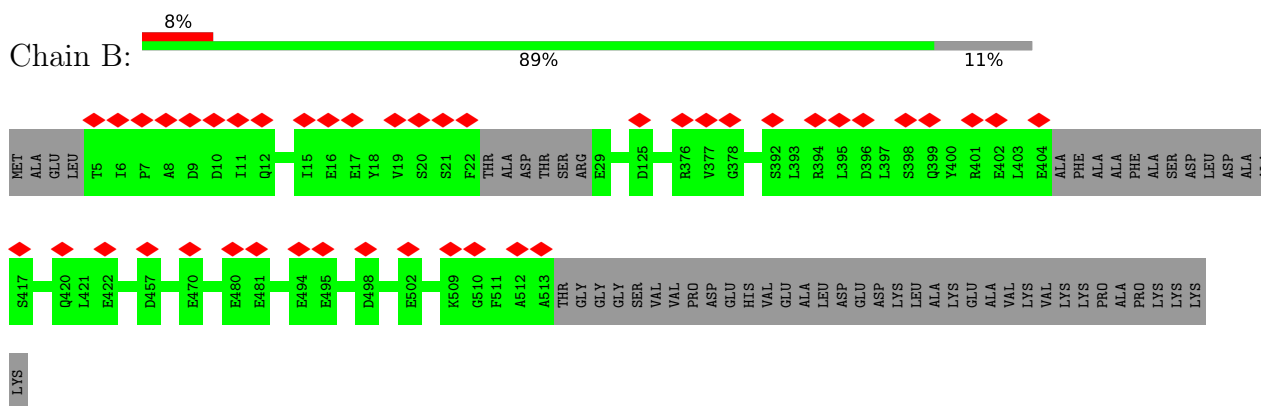
3 Residue-property plots [i](#)

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.

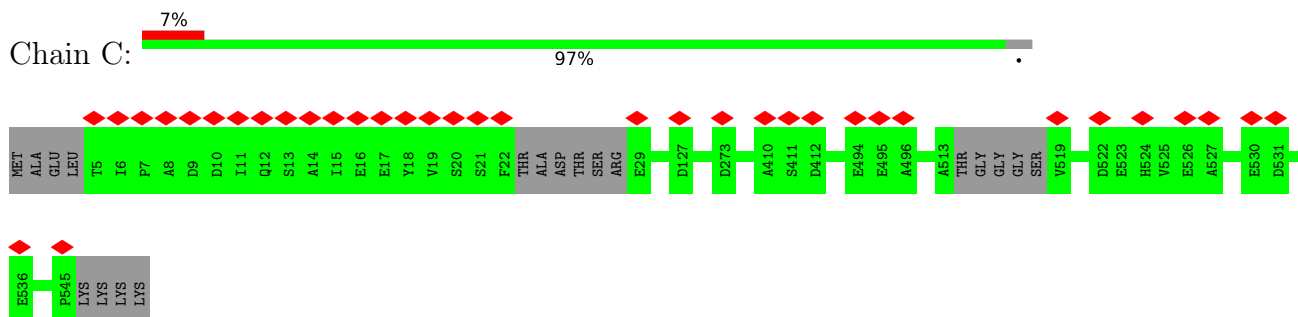
- Molecule 1: ATP synthase subunit alpha



- Molecule 1: ATP synthase subunit alpha

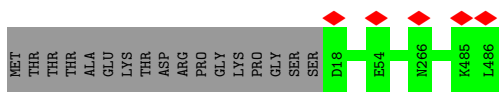


- Molecule 1: ATP synthase subunit alpha



- Molecule 2: ATP synthase subunit beta

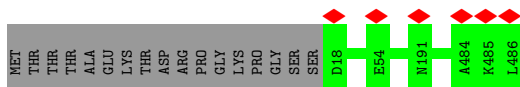




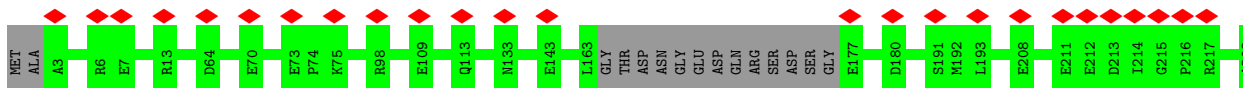
- Molecule 2: ATP synthase subunit beta



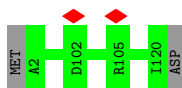
- Molecule 2: ATP synthase subunit beta



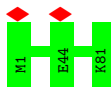
- Molecule 3: ATP synthase gamma chain



- Molecule 4: ATP synthase epsilon chain



- Molecule 5: ATP synthase subunit c



- Molecule 5: ATP synthase subunit c



There are no outlier residues recorded for this chain.

- Molecule 5: ATP synthase subunit c

Chain 3:  100%



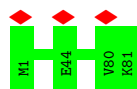
- Molecule 5: ATP synthase subunit c

Chain 4:  100%



- Molecule 5: ATP synthase subunit c

Chain 5:  100%



- Molecule 5: ATP synthase subunit c

Chain 6:  100%



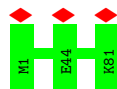
- Molecule 5: ATP synthase subunit c

Chain 7:  100%



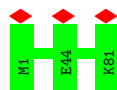
- Molecule 5: ATP synthase subunit c

Chain 8:  100%

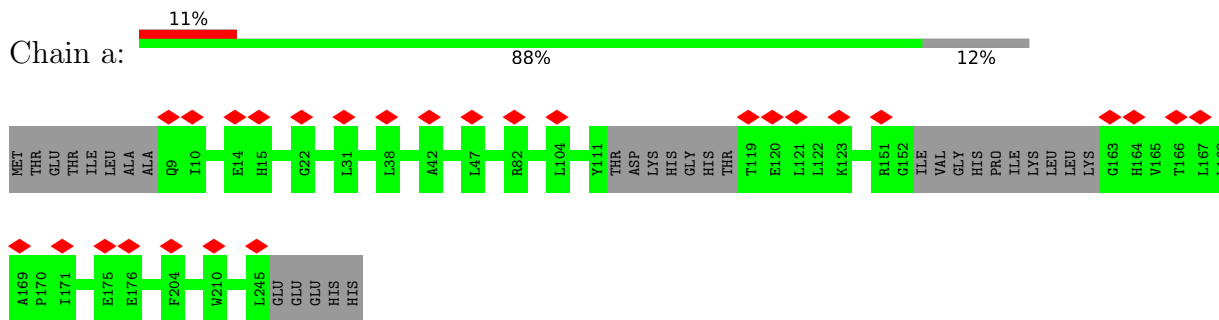


- Molecule 5: ATP synthase subunit c

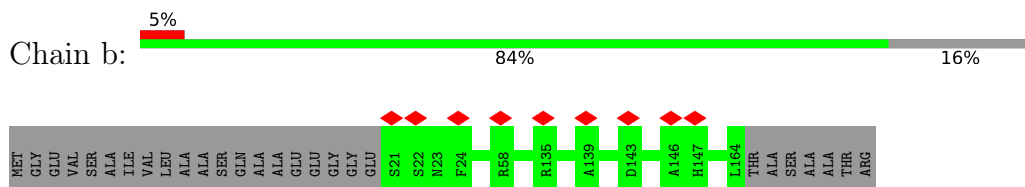
Chain 9:  100%



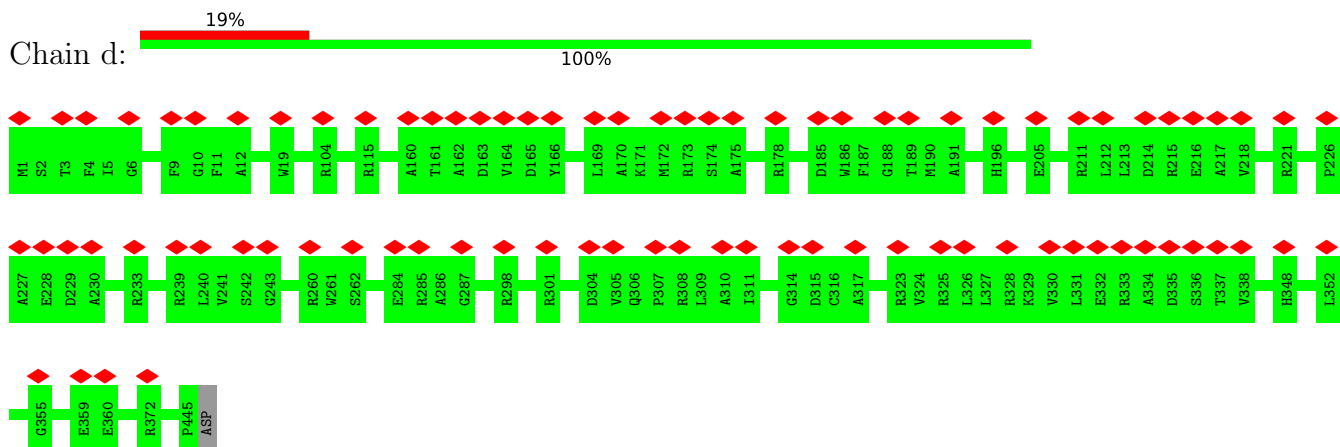
• Molecule 6: ATP synthase subunit a



• 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	81528	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	41.551	Depositor
Minimum map value	-27.483	Depositor
Average map value	0.012	Depositor
Map value standard deviation	1.107	Depositor
Recommended contour level	5.6	Depositor
Map size (\AA)	373.76, 373.76, 373.76	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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: ATP, ADP, MG, UTI

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	0.31	0/3976	0.46	0/5387
1	B	0.31	0/3795	0.44	0/5137
1	C	0.30	0/4094	0.44	0/5543
2	D	0.31	0/3680	0.45	0/4990
2	E	0.30	0/3680	0.43	0/4990
2	F	0.31	0/3680	0.45	0/4990
3	G	0.30	0/2286	0.43	0/3092
4	H	0.34	0/915	0.48	0/1237
5	1	0.32	0/578	0.45	0/784
5	2	0.33	0/578	0.44	0/784
5	3	0.35	0/578	0.44	0/784
5	4	0.34	0/578	0.45	0/784
5	5	0.34	0/578	0.43	0/784
5	6	0.34	0/578	0.44	0/784
5	7	0.34	0/578	0.46	0/784
5	8	0.32	0/578	0.43	0/784
5	9	0.31	0/578	0.44	0/784
6	a	0.29	0/1748	0.44	0/2390
7	b	0.27	0/1118	0.47	0/1512
8	d	0.28	0/3462	0.47	0/4697
All	All	0.31	0/37636	0.45	0/51021

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 [i](#)

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

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	515/549 (94%)	496 (96%)	19 (4%)	0	100	100
1	B	485/549 (88%)	471 (97%)	14 (3%)	0	100	100
1	C	524/549 (95%)	503 (96%)	21 (4%)	0	100	100
2	D	467/486 (96%)	448 (96%)	19 (4%)	0	100	100
2	E	467/486 (96%)	450 (96%)	17 (4%)	0	100	100
2	F	467/486 (96%)	455 (97%)	12 (3%)	0	100	100
3	G	283/305 (93%)	275 (97%)	8 (3%)	0	100	100
4	H	117/121 (97%)	108 (92%)	9 (8%)	0	100	100
5	1	79/81 (98%)	72 (91%)	7 (9%)	0	100	100
5	2	79/81 (98%)	76 (96%)	3 (4%)	0	100	100
5	3	79/81 (98%)	71 (90%)	8 (10%)	0	100	100
5	4	79/81 (98%)	74 (94%)	5 (6%)	0	100	100
5	5	79/81 (98%)	74 (94%)	5 (6%)	0	100	100
5	6	79/81 (98%)	76 (96%)	3 (4%)	0	100	100
5	7	79/81 (98%)	76 (96%)	3 (4%)	0	100	100
5	8	79/81 (98%)	75 (95%)	4 (5%)	0	100	100
5	9	79/81 (98%)	73 (92%)	6 (8%)	0	100	100
6	a	214/250 (86%)	203 (95%)	11 (5%)	0	100	100
7	b	142/171 (83%)	139 (98%)	3 (2%)	0	100	100
8	d	443/446 (99%)	426 (96%)	17 (4%)	0	100	100
All	All	4835/5127 (94%)	4641 (96%)	194 (4%)	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	417/444 (94%)	417 (100%)	0	100	100
1	B	400/444 (90%)	400 (100%)	0	100	100
1	C	430/444 (97%)	430 (100%)	0	100	100
2	D	389/403 (96%)	389 (100%)	0	100	100
2	E	389/403 (96%)	389 (100%)	0	100	100
2	F	389/403 (96%)	389 (100%)	0	100	100
3	G	235/248 (95%)	235 (100%)	0	100	100
4	H	94/96 (98%)	94 (100%)	0	100	100
5	1	52/52 (100%)	52 (100%)	0	100	100
5	2	52/52 (100%)	52 (100%)	0	100	100
5	3	52/52 (100%)	52 (100%)	0	100	100
5	4	52/52 (100%)	52 (100%)	0	100	100
5	5	52/52 (100%)	52 (100%)	0	100	100
5	6	52/52 (100%)	52 (100%)	0	100	100
5	7	52/52 (100%)	52 (100%)	0	100	100
5	8	52/52 (100%)	52 (100%)	0	100	100
5	9	52/52 (100%)	52 (100%)	0	100	100
6	a	178/204 (87%)	178 (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	3862/4047 (95%)	3862 (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. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	143	GLN
1	B	335	ASN
1	B	420	GLN
1	C	506	ASN
2	D	128	HIS
2	D	209	ASN
2	D	388	GLN
2	D	394	GLN
2	E	414	ASN
2	F	209	ASN
2	F	388	GLN
4	H	38	HIS
5	4	67	ASN
5	5	42	GLN
5	5	67	ASN
5	6	42	GLN
5	6	46	GLN
5	7	67	ASN
5	8	67	ASN
5	9	67	ASN
6	a	172	ASN
6	a	227	GLN
7	b	82	GLN
8	d	295	GLN
8	d	411	HIS

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 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	UTI	6	600	-	41,43,43	1.71	10 (24%)	48,62,62	1.83	11 (22%)
12	UTI	8	600	-	41,43,43	1.72	10 (24%)	48,62,62	1.89	13 (27%)
12	UTI	1	600	-	41,43,43	1.49	7 (17%)	48,62,62	2.31	13 (27%)
12	UTI	4	600	-	41,43,43	1.69	10 (24%)	48,62,62	1.83	13 (27%)
12	UTI	9	600	-	41,43,43	1.71	10 (24%)	48,62,62	1.83	12 (25%)
12	UTI	5	600	-	41,43,43	1.68	9 (21%)	48,62,62	1.83	13 (27%)
11	ADP	F	600	10	24,29,29	0.93	1 (4%)	29,45,45	1.44	4 (13%)
9	ATP	C	600	10	26,33,33	0.90	1 (3%)	31,52,52	1.52	5 (16%)
9	ATP	B	600	10	26,33,33	0.91	1 (3%)	31,52,52	1.52	5 (16%)
11	ADP	D	600	10	24,29,29	0.95	1 (4%)	29,45,45	1.40	4 (13%)
9	ATP	A	600	10	26,33,33	0.90	1 (3%)	31,52,52	1.52	5 (16%)
12	UTI	7	600	-	41,43,43	1.71	9 (21%)	48,62,62	1.79	11 (22%)

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	UTI	6	600	-	-	8/34/34/34	0/4/4/4
12	UTI	8	600	-	-	12/34/34/34	0/4/4/4
12	UTI	1	600	-	-	8/34/34/34	0/4/4/4
12	UTI	4	600	-	-	4/34/34/34	0/4/4/4
12	UTI	9	600	-	-	7/34/34/34	0/4/4/4
12	UTI	5	600	-	-	6/34/34/34	0/4/4/4
11	ADP	F	600	10	-	4/12/32/32	0/3/3/3
9	ATP	C	600	10	-	8/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ATP	B	600	10	-	8/18/38/38	0/3/3/3
11	ADP	D	600	10	-	2/12/32/32	0/3/3/3
9	ATP	A	600	10	-	8/18/38/38	0/3/3/3
12	UTI	7	600	-	-	7/34/34/34	0/4/4/4

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	6	600	UTI	O13-C11	4.13	1.41	1.35
12	8	600	UTI	O13-C11	4.10	1.41	1.35
12	5	600	UTI	O13-C11	4.09	1.41	1.35
12	7	600	UTI	O13-C11	4.07	1.41	1.35
12	9	600	UTI	O13-C11	4.07	1.41	1.35
12	4	600	UTI	O13-C11	4.04	1.41	1.35
12	1	600	UTI	C35-C30	-3.99	1.36	1.42
12	6	600	UTI	O40-C06	-3.80	1.37	1.43
12	1	600	UTI	O13-C11	3.77	1.41	1.35
12	4	600	UTI	O40-C06	-3.75	1.37	1.43
12	5	600	UTI	O40-C06	-3.73	1.37	1.43
12	1	600	UTI	O40-C06	-3.73	1.37	1.43
12	7	600	UTI	O40-C06	-3.69	1.37	1.43
12	9	600	UTI	O40-C06	-3.63	1.37	1.43
12	8	600	UTI	O15-C09	3.58	1.41	1.35
12	7	600	UTI	O15-C09	3.55	1.41	1.35
12	8	600	UTI	O40-C06	-3.54	1.37	1.43
12	9	600	UTI	O15-C09	3.51	1.40	1.35
12	6	600	UTI	O15-C09	3.51	1.40	1.35
12	5	600	UTI	O15-C09	3.47	1.40	1.35
12	4	600	UTI	O15-C09	3.44	1.40	1.35
12	5	600	UTI	C35-C30	-3.43	1.36	1.42
12	8	600	UTI	C35-C30	-3.43	1.36	1.42
12	7	600	UTI	C35-C30	-3.36	1.37	1.42
12	9	600	UTI	C35-C30	-3.32	1.37	1.42
12	4	600	UTI	C35-C30	-3.28	1.37	1.42
12	8	600	UTI	C06-C07	3.21	1.56	1.52
12	6	600	UTI	C06-C07	3.19	1.56	1.52
12	6	600	UTI	C35-C30	-3.17	1.37	1.42
12	7	600	UTI	C06-C07	3.14	1.56	1.52
12	8	600	UTI	O38-C28	3.11	1.40	1.35
12	9	600	UTI	C06-C07	3.11	1.56	1.52
12	7	600	UTI	O38-C28	3.07	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	9	600	UTI	O38-C28	3.06	1.39	1.35
12	5	600	UTI	O38-C28	3.06	1.39	1.35
12	4	600	UTI	O38-C28	3.05	1.39	1.35
12	6	600	UTI	O38-C28	3.05	1.39	1.35
12	4	600	UTI	C06-C07	3.05	1.56	1.52
12	8	600	UTI	C05-C04	3.04	1.57	1.53
12	9	600	UTI	C05-C04	2.98	1.57	1.53
12	7	600	UTI	C05-C04	2.96	1.57	1.53
12	1	600	UTI	C05-C04	2.94	1.57	1.53
12	4	600	UTI	C05-C04	2.92	1.57	1.53
12	5	600	UTI	C06-C07	2.90	1.56	1.52
12	5	600	UTI	C05-C04	2.84	1.57	1.53
12	9	600	UTI	O24-C20	2.78	1.41	1.37
12	6	600	UTI	C05-C04	2.78	1.57	1.53
12	7	600	UTI	O24-C20	2.74	1.41	1.37
12	6	600	UTI	O24-C20	2.70	1.41	1.37
12	5	600	UTI	O24-C20	2.68	1.41	1.37
12	4	600	UTI	O24-C20	2.67	1.41	1.37
12	8	600	UTI	O24-C20	2.65	1.41	1.37
12	1	600	UTI	O15-C09	2.54	1.39	1.35
12	1	600	UTI	C06-C07	2.41	1.55	1.52
12	9	600	UTI	C34-C33	2.40	1.40	1.36
12	6	600	UTI	C34-C33	2.35	1.40	1.36
12	7	600	UTI	C34-C33	2.31	1.40	1.36
12	1	600	UTI	O24-C20	2.31	1.40	1.37
11	F	600	ADP	C5-C4	2.29	1.47	1.40
9	B	600	ATP	C5-C4	2.28	1.47	1.40
9	C	600	ATP	C5-C4	2.27	1.46	1.40
9	A	600	ATP	C5-C4	2.27	1.46	1.40
12	5	600	UTI	C34-C33	2.26	1.40	1.36
12	8	600	UTI	C34-C33	2.26	1.40	1.36
12	4	600	UTI	C34-C33	2.19	1.40	1.36
11	D	600	ADP	C5-C4	2.18	1.46	1.40
12	4	600	UTI	BR37-C33	2.15	1.94	1.90
12	9	600	UTI	BR37-C33	2.12	1.94	1.90
12	6	600	UTI	BR37-C33	2.10	1.94	1.90
12	8	600	UTI	BR37-C33	2.10	1.94	1.90

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	1	600	UTI	C39-O38-C28	-7.58	109.70	117.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	1	600	UTI	C09-N10-C11	6.08	121.55	115.70
12	6	600	UTI	C09-N10-C11	5.73	121.21	115.70
12	4	600	UTI	C09-N10-C11	5.70	121.19	115.70
12	7	600	UTI	C09-N10-C11	5.67	121.16	115.70
12	9	600	UTI	C09-N10-C11	5.65	121.14	115.70
12	8	600	UTI	C09-N10-C11	5.60	121.09	115.70
12	5	600	UTI	C09-N10-C11	5.50	120.99	115.70
12	6	600	UTI	O24-C20-C19	5.23	119.98	116.27
12	7	600	UTI	O24-C20-C19	5.14	119.92	116.27
12	8	600	UTI	O24-C20-C19	5.09	119.89	116.27
12	1	600	UTI	C16-O15-C09	-5.02	109.48	117.36
12	8	600	UTI	C27-C28-N29	-4.93	120.86	125.70
12	4	600	UTI	O24-C20-C19	4.90	119.75	116.27
12	9	600	UTI	O24-C20-C19	4.89	119.75	116.27
12	5	600	UTI	O24-C20-C19	4.83	119.70	116.27
12	9	600	UTI	C27-C28-N29	-4.75	121.04	125.70
12	6	600	UTI	C27-C28-N29	-4.54	121.24	125.70
12	7	600	UTI	C27-C28-N29	-4.53	121.26	125.70
12	5	600	UTI	C27-C28-N29	-4.50	121.29	125.70
12	4	600	UTI	C27-C28-N29	-4.47	121.31	125.70
12	1	600	UTI	C27-C28-N29	-4.23	121.55	125.70
12	1	600	UTI	C25-O24-C20	-3.86	111.70	117.53
12	5	600	UTI	C39-O38-C28	-3.86	113.39	117.21
12	9	600	UTI	C39-O38-C28	-3.64	113.60	117.21
12	1	600	UTI	C27-C17-C18	-3.55	103.10	111.03
11	F	600	ADP	C3'-C2'-C1'	3.43	106.14	100.98
9	B	600	ATP	PB-O3B-PG	-3.38	121.22	132.83
9	C	600	ATP	PA-O3A-PB	-3.38	121.23	132.83
9	C	600	ATP	PB-O3B-PG	-3.38	121.24	132.83
9	A	600	ATP	PA-O3A-PB	-3.38	121.24	132.83
9	B	600	ATP	PA-O3A-PB	-3.37	121.25	132.83
11	D	600	ADP	N3-C2-N1	-3.37	123.41	128.68
9	A	600	ATP	PB-O3B-PG	-3.37	121.27	132.83
12	1	600	UTI	O38-C28-C27	3.31	120.13	115.03
12	8	600	UTI	C39-O38-C28	-3.29	113.95	117.21
11	F	600	ADP	N3-C2-N1	-3.23	123.62	128.68
11	D	600	ADP	C3'-C2'-C1'	3.21	105.81	100.98
12	4	600	UTI	C39-O38-C28	-3.14	114.10	117.21
9	A	600	ATP	N3-C2-N1	-3.14	123.77	128.68
9	C	600	ATP	N3-C2-N1	-3.14	123.77	128.68
12	6	600	UTI	C39-O38-C28	-3.13	114.11	117.21
9	B	600	ATP	N3-C2-N1	-3.12	123.81	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	1	600	UTI	O24-C20-C19	3.08	118.46	116.27
12	9	600	UTI	O38-C28-C27	2.99	119.64	115.03
12	7	600	UTI	C39-O38-C28	-2.97	114.26	117.21
12	1	600	UTI	C12-C11-N10	-2.93	120.66	124.08
12	8	600	UTI	C25-O24-C20	-2.93	113.11	117.53
11	D	600	ADP	PA-O3A-PB	-2.90	122.89	132.83
12	4	600	UTI	C25-O24-C20	-2.86	113.22	117.53
9	B	600	ATP	C3'-C2'-C1'	2.85	105.27	100.98
9	A	600	ATP	C3'-C2'-C1'	2.84	105.25	100.98
9	C	600	ATP	C3'-C2'-C1'	2.82	105.23	100.98
11	F	600	ADP	PA-O3A-PB	-2.79	123.26	132.83
12	6	600	UTI	C25-O24-C20	-2.75	113.38	117.53
12	1	600	UTI	C14-O13-C11	-2.74	113.07	117.36
12	8	600	UTI	O24-C20-C21	-2.73	119.69	124.37
12	6	600	UTI	O24-C20-C21	-2.72	119.71	124.37
12	8	600	UTI	O38-C28-C27	2.72	119.22	115.03
12	5	600	UTI	O38-C28-C27	2.67	119.16	115.03
12	5	600	UTI	C25-O24-C20	-2.67	113.50	117.53
9	A	600	ATP	C4-C5-N7	-2.66	106.63	109.40
12	4	600	UTI	O38-C28-C27	2.66	119.13	115.03
12	7	600	UTI	O24-C20-C21	-2.65	119.82	124.37
9	B	600	ATP	C4-C5-N7	-2.64	106.65	109.40
12	5	600	UTI	C16-O15-C09	-2.62	113.25	117.36
9	C	600	ATP	C4-C5-N7	-2.62	106.67	109.40
12	8	600	UTI	C27-C17-C18	-2.62	105.17	111.03
12	7	600	UTI	O38-C28-C27	2.60	119.04	115.03
11	D	600	ADP	C4-C5-N7	-2.57	106.72	109.40
12	4	600	UTI	O24-C20-C21	-2.56	119.97	124.37
12	7	600	UTI	C14-O13-C11	-2.56	113.35	117.36
11	F	600	ADP	C4-C5-N7	-2.55	106.74	109.40
12	6	600	UTI	C16-O15-C09	-2.50	113.44	117.36
12	9	600	UTI	O24-C20-C21	-2.48	120.12	124.37
12	6	600	UTI	O38-C28-C27	2.47	118.84	115.03
12	4	600	UTI	C16-O15-C09	-2.46	113.51	117.36
12	5	600	UTI	O24-C20-C21	-2.45	120.18	124.37
12	8	600	UTI	C28-N29-C30	2.43	121.80	116.41
12	9	600	UTI	C28-N29-C30	2.41	121.75	116.41
12	8	600	UTI	C14-O13-C11	-2.41	113.59	117.36
12	1	600	UTI	C28-N29-C30	2.40	121.73	116.41
12	7	600	UTI	C28-N29-C30	2.39	121.71	116.41
12	4	600	UTI	C14-O13-C11	-2.38	113.63	117.36
12	5	600	UTI	C28-N29-C30	2.38	121.69	116.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	7	600	UTI	C25-O24-C20	-2.37	113.95	117.53
12	6	600	UTI	C28-N29-C30	2.36	121.64	116.41
12	5	600	UTI	C14-O13-C11	-2.34	113.69	117.36
12	4	600	UTI	C28-N29-C30	2.30	121.52	116.41
12	6	600	UTI	C12-C11-N10	-2.30	121.40	124.08
12	9	600	UTI	C12-C11-N10	-2.29	121.41	124.08
12	9	600	UTI	C16-O15-C09	-2.28	113.79	117.36
12	8	600	UTI	C08-C09-N10	-2.27	121.43	124.08
12	7	600	UTI	C08-C09-N10	-2.27	121.43	124.08
12	9	600	UTI	C25-O24-C20	-2.25	114.14	117.53
12	1	600	UTI	O24-C20-C21	-2.21	120.59	124.37
12	4	600	UTI	C12-C11-N10	-2.20	121.52	124.08
12	7	600	UTI	C12-C11-N10	-2.16	121.57	124.08
12	5	600	UTI	C23-C18-C19	2.15	119.45	116.70
12	4	600	UTI	C08-C09-N10	-2.15	121.57	124.08
12	5	600	UTI	C12-C11-N10	-2.12	121.60	124.08
12	6	600	UTI	C08-C09-N10	-2.12	121.61	124.08
12	9	600	UTI	C14-O13-C11	-2.09	114.08	117.36
12	8	600	UTI	C12-C11-N10	-2.09	121.64	124.08
12	8	600	UTI	C36-C27-C28	2.06	118.72	116.37
12	9	600	UTI	C08-C09-N10	-2.05	121.69	124.08
12	1	600	UTI	C21-C20-C19	2.05	120.95	117.72
12	5	600	UTI	C08-C09-N10	-2.04	121.70	124.08
12	4	600	UTI	C23-C18-C19	2.03	119.29	116.70

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	600	ATP	C5'-O5'-PA-O1A
9	B	600	ATP	C5'-O5'-PA-O1A
9	C	600	ATP	C5'-O5'-PA-O1A
11	F	600	ADP	C5'-O5'-PA-O1A
12	1	600	UTI	C18-C17-C27-C28
12	1	600	UTI	C19-C20-O24-C25
12	1	600	UTI	C27-C28-O38-C39
12	1	600	UTI	N29-C28-O38-C39
12	4	600	UTI	C19-C20-O24-C25
12	4	600	UTI	C27-C28-O38-C39
12	5	600	UTI	C19-C20-O24-C25
12	5	600	UTI	C27-C28-O38-C39
12	6	600	UTI	C19-C20-O24-C25

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Mol	Chain	Res	Type	Atoms
12	7	600	UTI	C12-C11-O13-C14
12	7	600	UTI	N10-C11-O13-C14
12	7	600	UTI	C19-C20-O24-C25
12	8	600	UTI	C12-C11-O13-C14
12	8	600	UTI	N10-C11-O13-C14
12	8	600	UTI	C06-C17-C18-C23
12	8	600	UTI	C06-C17-C18-C19
12	8	600	UTI	C19-C20-O24-C25
12	9	600	UTI	C12-C11-O13-C14
12	9	600	UTI	N10-C11-O13-C14
12	9	600	UTI	C19-C20-O24-C25
12	6	600	UTI	C12-C11-O13-C14
12	7	600	UTI	C08-C09-O15-C16
12	6	600	UTI	N10-C11-O13-C14
12	6	600	UTI	N10-C09-O15-C16
12	7	600	UTI	N10-C09-O15-C16
12	8	600	UTI	N10-C09-O15-C16
11	D	600	ADP	O4'-C4'-C5'-O5'
11	D	600	ADP	C3'-C4'-C5'-O5'
12	6	600	UTI	C21-C20-O24-C25
12	8	600	UTI	C21-C20-O24-C25
12	9	600	UTI	C21-C20-O24-C25
12	4	600	UTI	N29-C28-O38-C39
12	5	600	UTI	N29-C28-O38-C39
12	7	600	UTI	C21-C20-O24-C25
12	1	600	UTI	C05-C04-N02-C03
12	6	600	UTI	C08-C09-O15-C16
12	8	600	UTI	C08-C09-O15-C16
12	1	600	UTI	C21-C20-O24-C25
12	5	600	UTI	C21-C20-O24-C25
12	1	600	UTI	C05-C04-N02-C01
12	7	600	UTI	C05-C04-N02-C03
12	8	600	UTI	C05-C04-N02-C01
12	8	600	UTI	C05-C04-N02-C03
12	4	600	UTI	C21-C20-O24-C25
9	A	600	ATP	O4'-C4'-C5'-O5'
9	B	600	ATP	O4'-C4'-C5'-O5'
9	C	600	ATP	O4'-C4'-C5'-O5'
12	6	600	UTI	C04-C05-C06-C17
9	A	600	ATP	C3'-C4'-C5'-O5'
9	B	600	ATP	C3'-C4'-C5'-O5'
9	C	600	ATP	C3'-C4'-C5'-O5'

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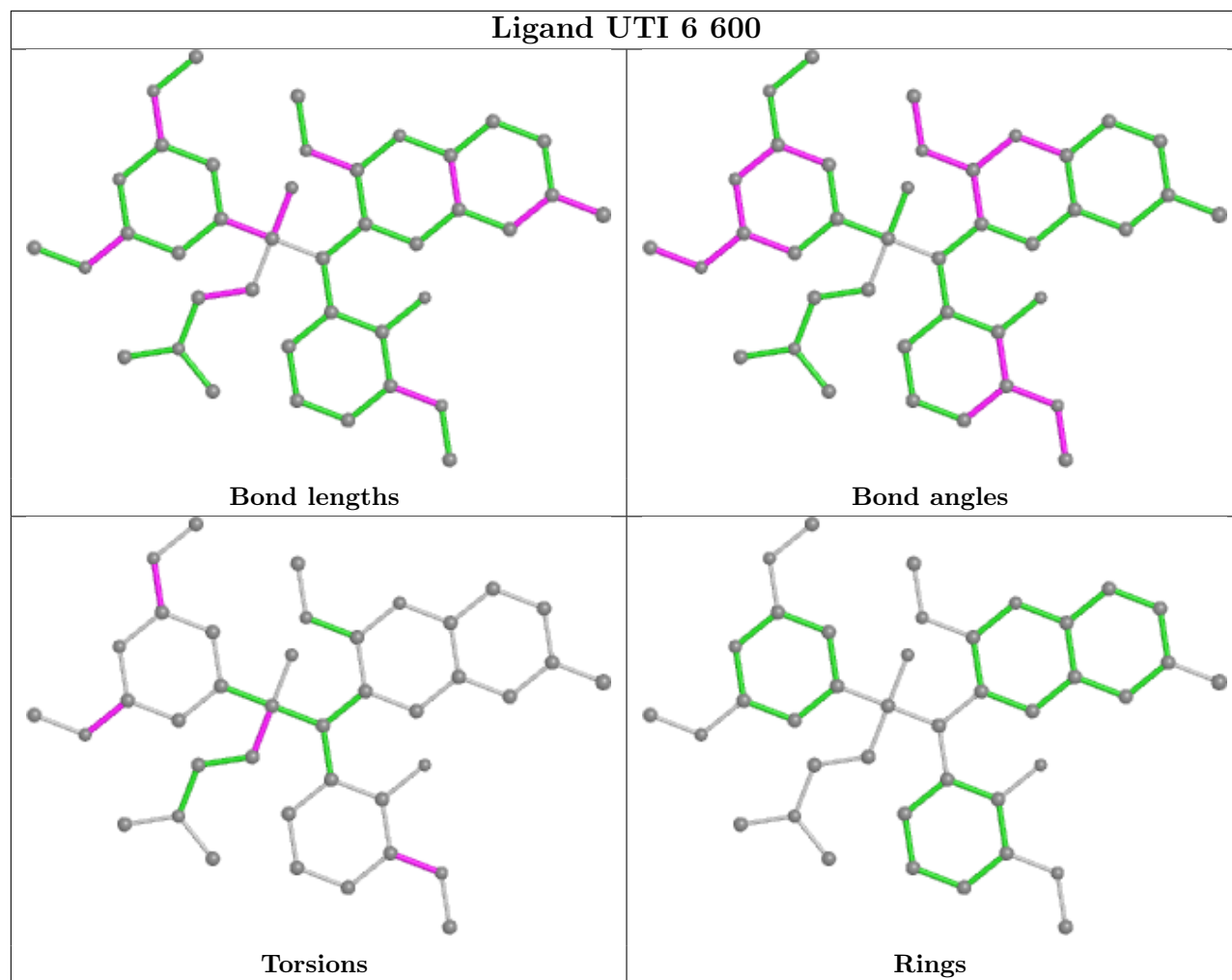
Continued from previous page...

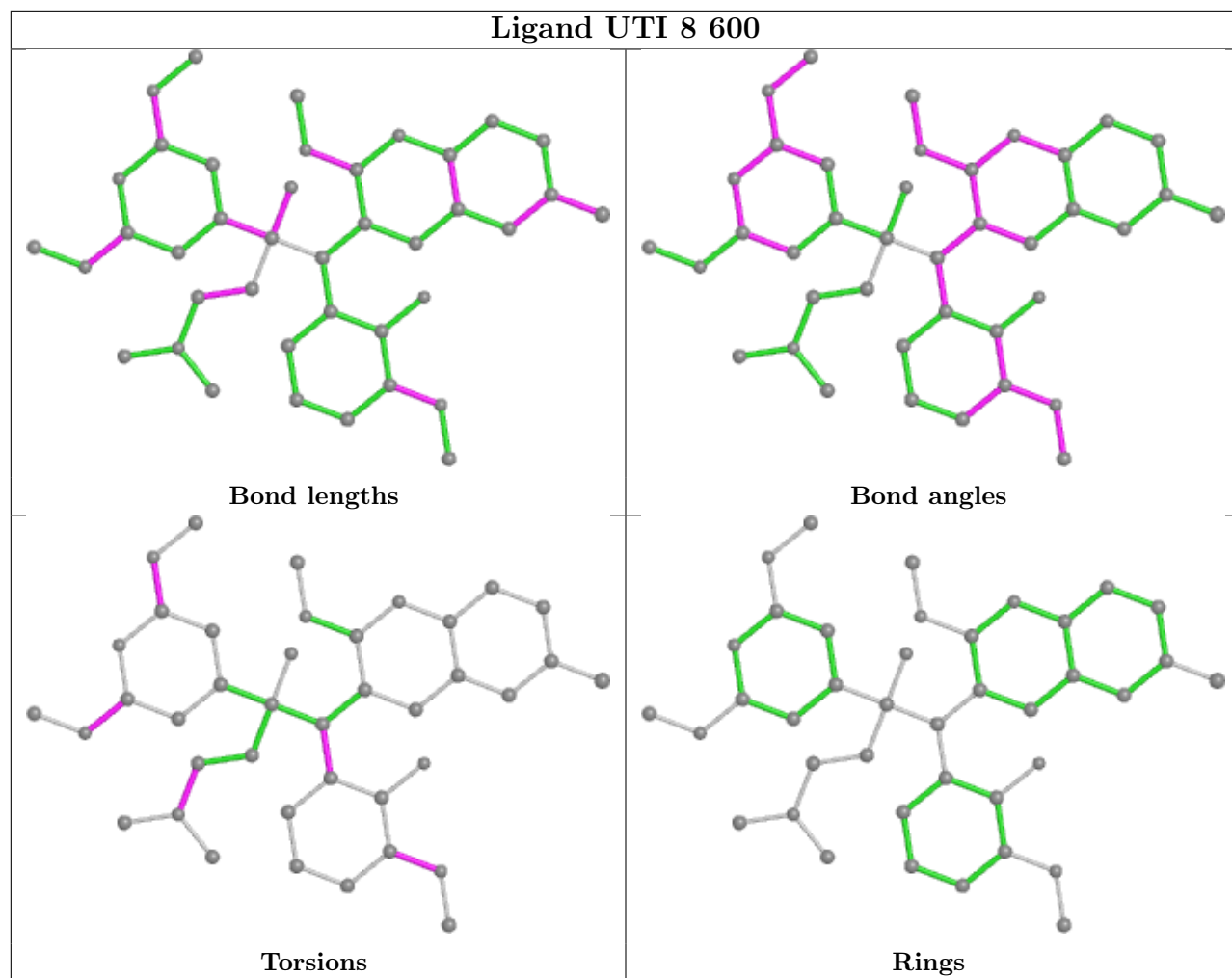
Mol	Chain	Res	Type	Atoms
9	A	600	ATP	C5'-O5'-PA-O3A
9	B	600	ATP	C5'-O5'-PA-O3A
9	C	600	ATP	C5'-O5'-PA-O3A
9	A	600	ATP	PA-O3A-PB-O1B
9	B	600	ATP	PA-O3A-PB-O1B
9	C	600	ATP	PA-O3A-PB-O1B
12	1	600	UTI	C18-C17-C27-C36
12	8	600	UTI	C27-C17-C18-C23
9	A	600	ATP	C5'-O5'-PA-O2A
9	B	600	ATP	C5'-O5'-PA-O2A
9	C	600	ATP	C5'-O5'-PA-O2A
11	F	600	ADP	C5'-O5'-PA-O2A
12	6	600	UTI	C04-C05-C06-O40
12	8	600	UTI	C27-C17-C18-C19
12	9	600	UTI	N29-C28-O38-C39
12	5	600	UTI	C12-C11-O13-C14
12	9	600	UTI	C05-C04-N02-C03
12	5	600	UTI	N10-C11-O13-C14
11	F	600	ADP	C5'-O5'-PA-O3A
9	A	600	ATP	PG-O3B-PB-O2B
9	A	600	ATP	PA-O3A-PB-O2B
9	B	600	ATP	PG-O3B-PB-O2B
9	B	600	ATP	PA-O3A-PB-O2B
9	C	600	ATP	PG-O3B-PB-O2B
9	C	600	ATP	PA-O3A-PB-O2B
11	F	600	ADP	O4'-C4'-C5'-O5'
12	9	600	UTI	C27-C28-O38-C39

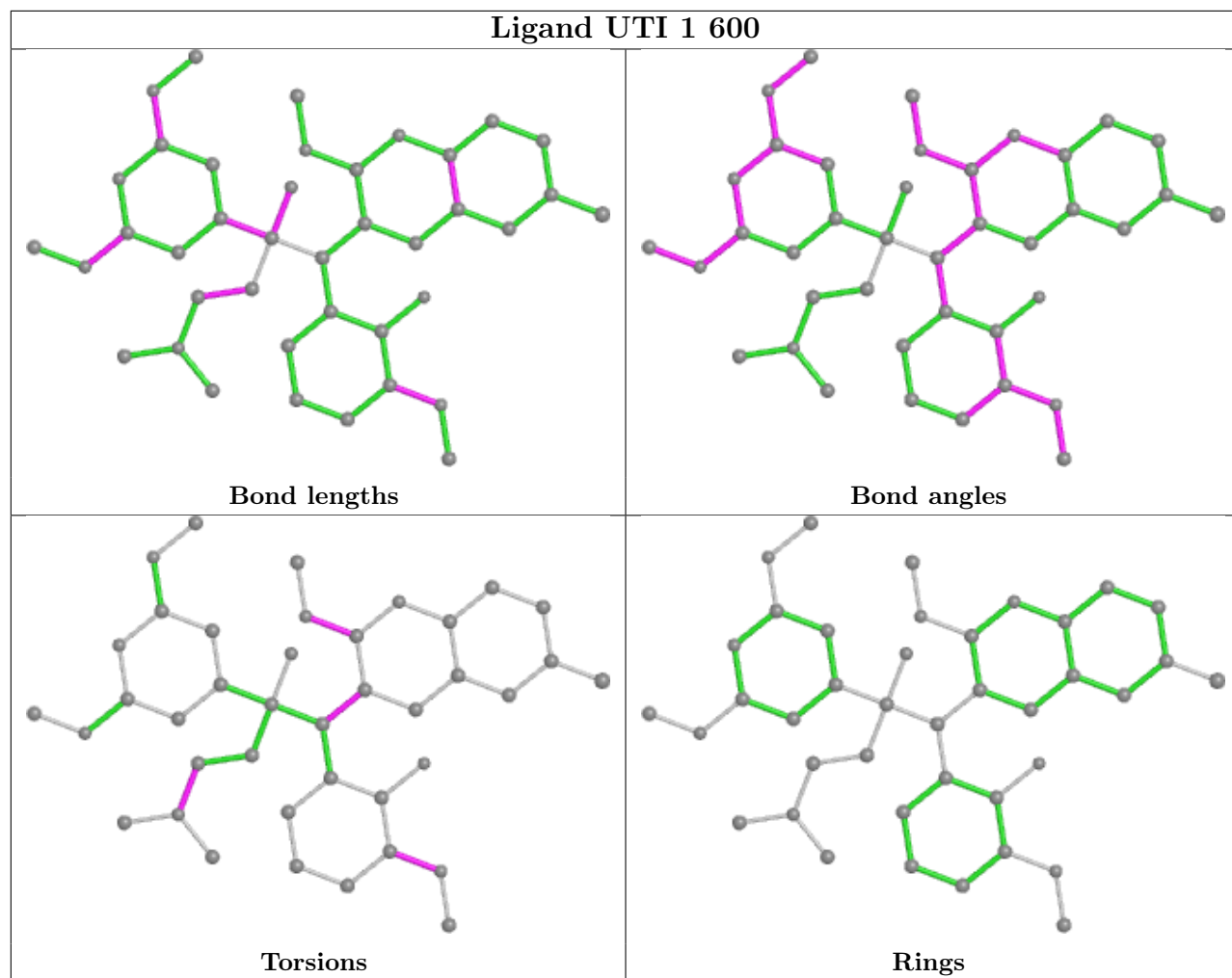
There are no ring outliers.

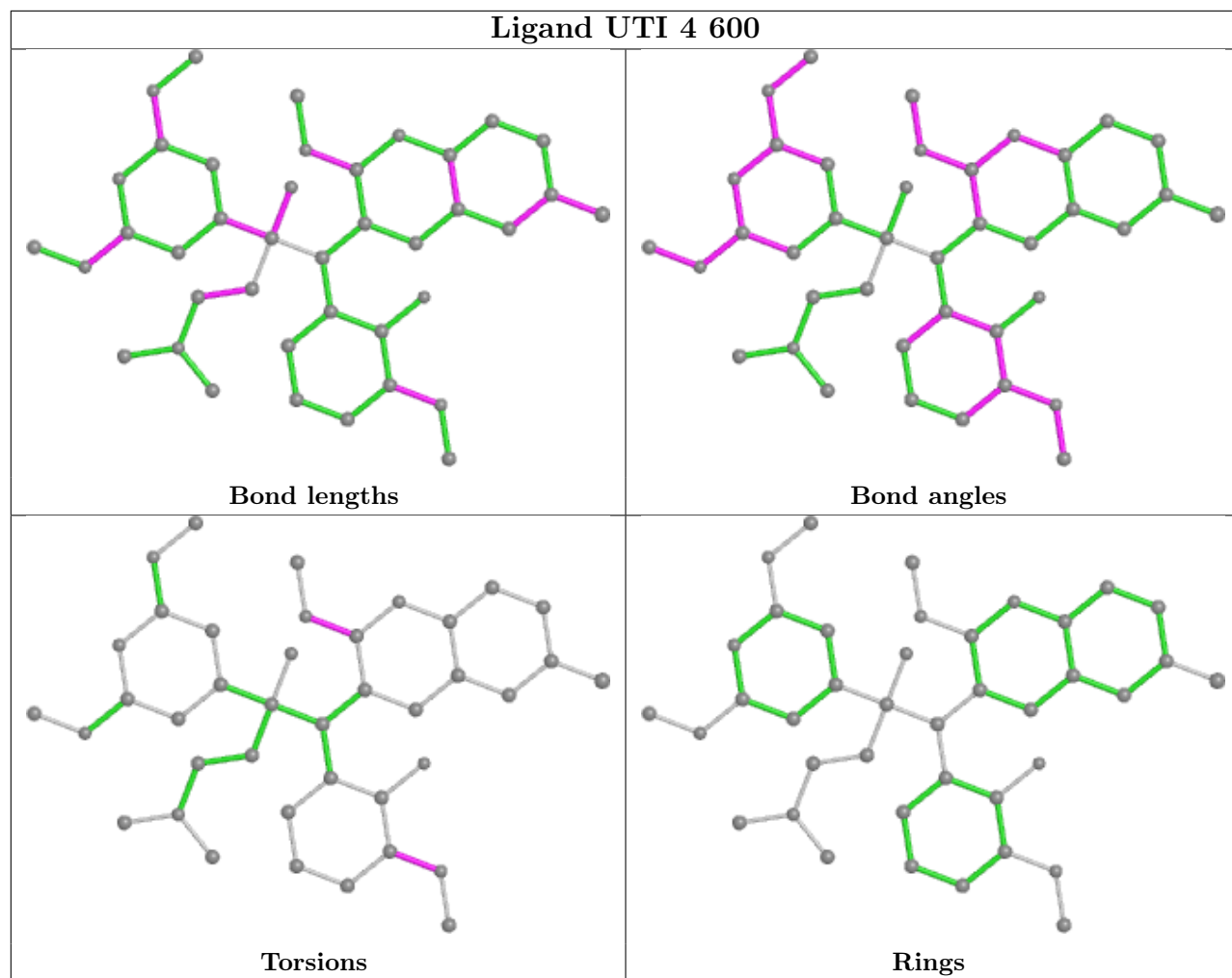
No monomer is involved in short contacts.

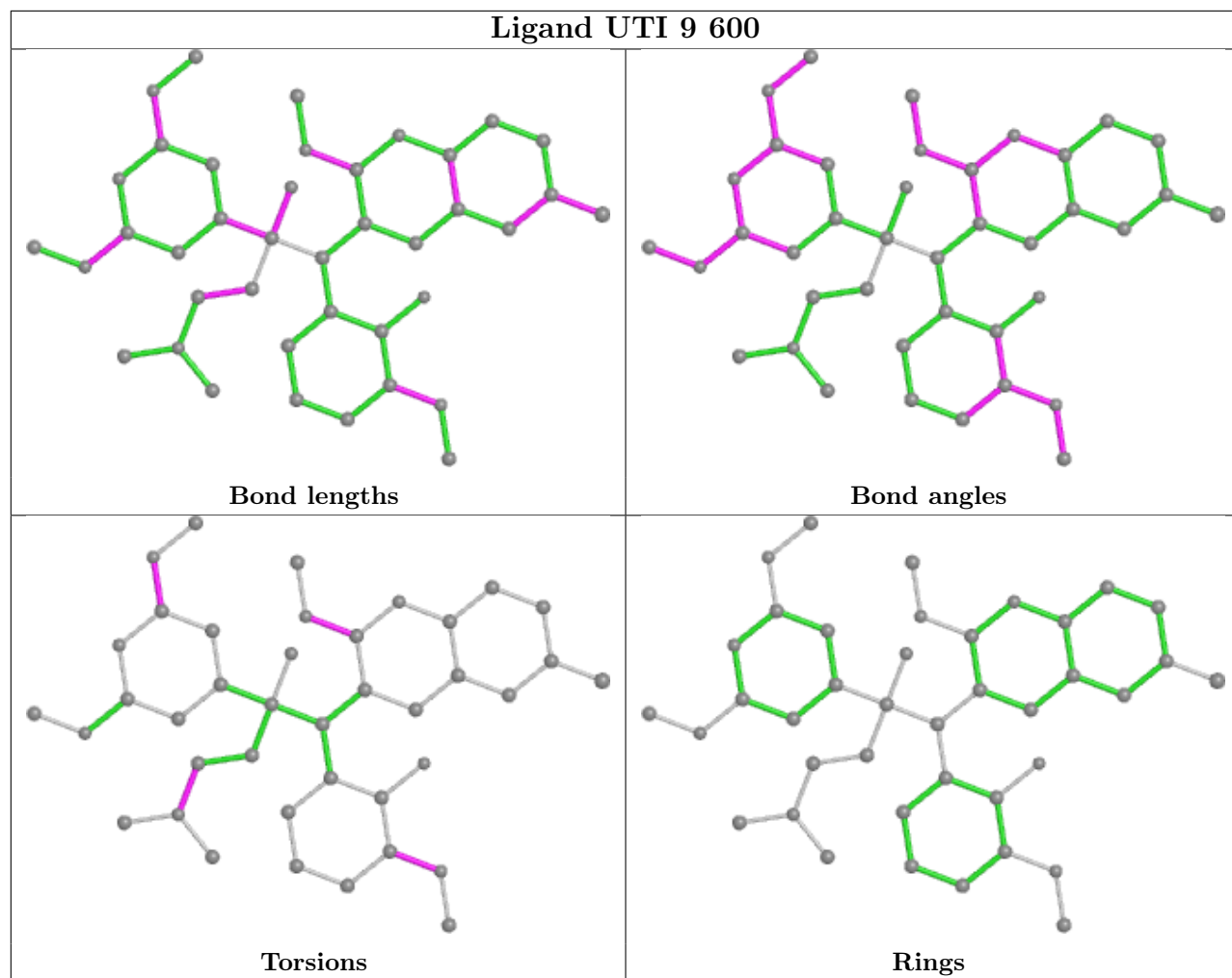
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

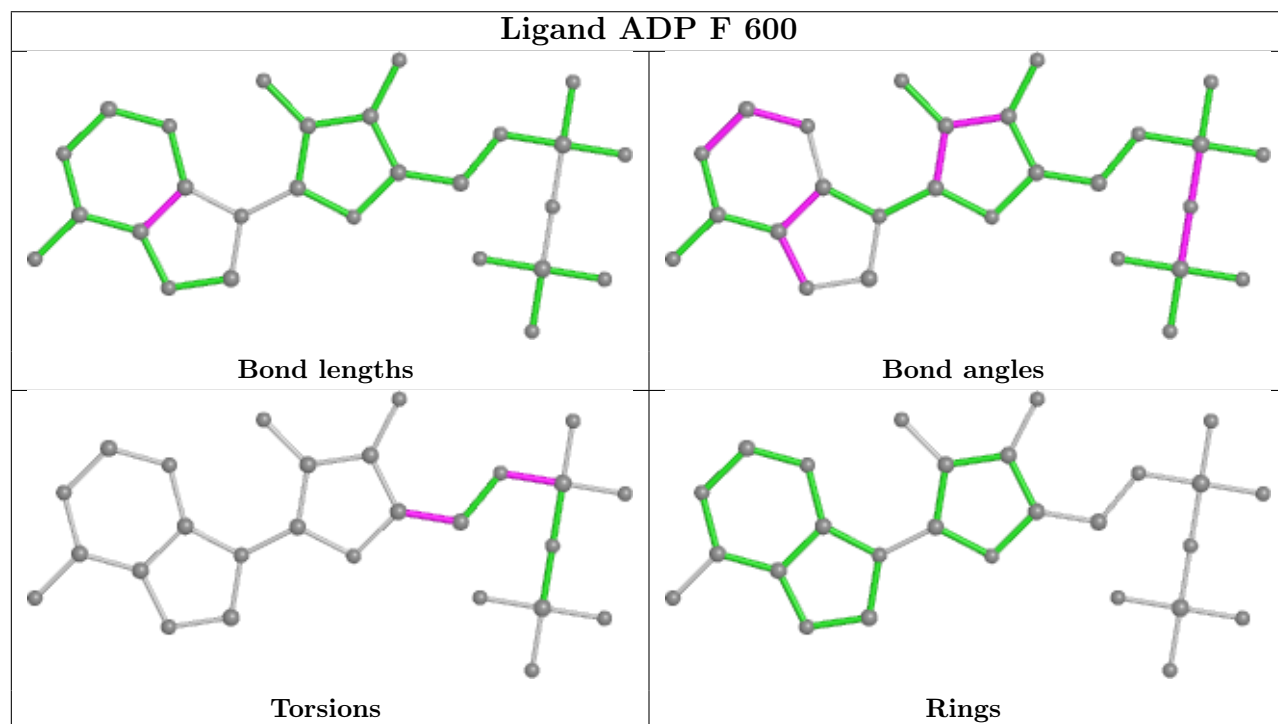
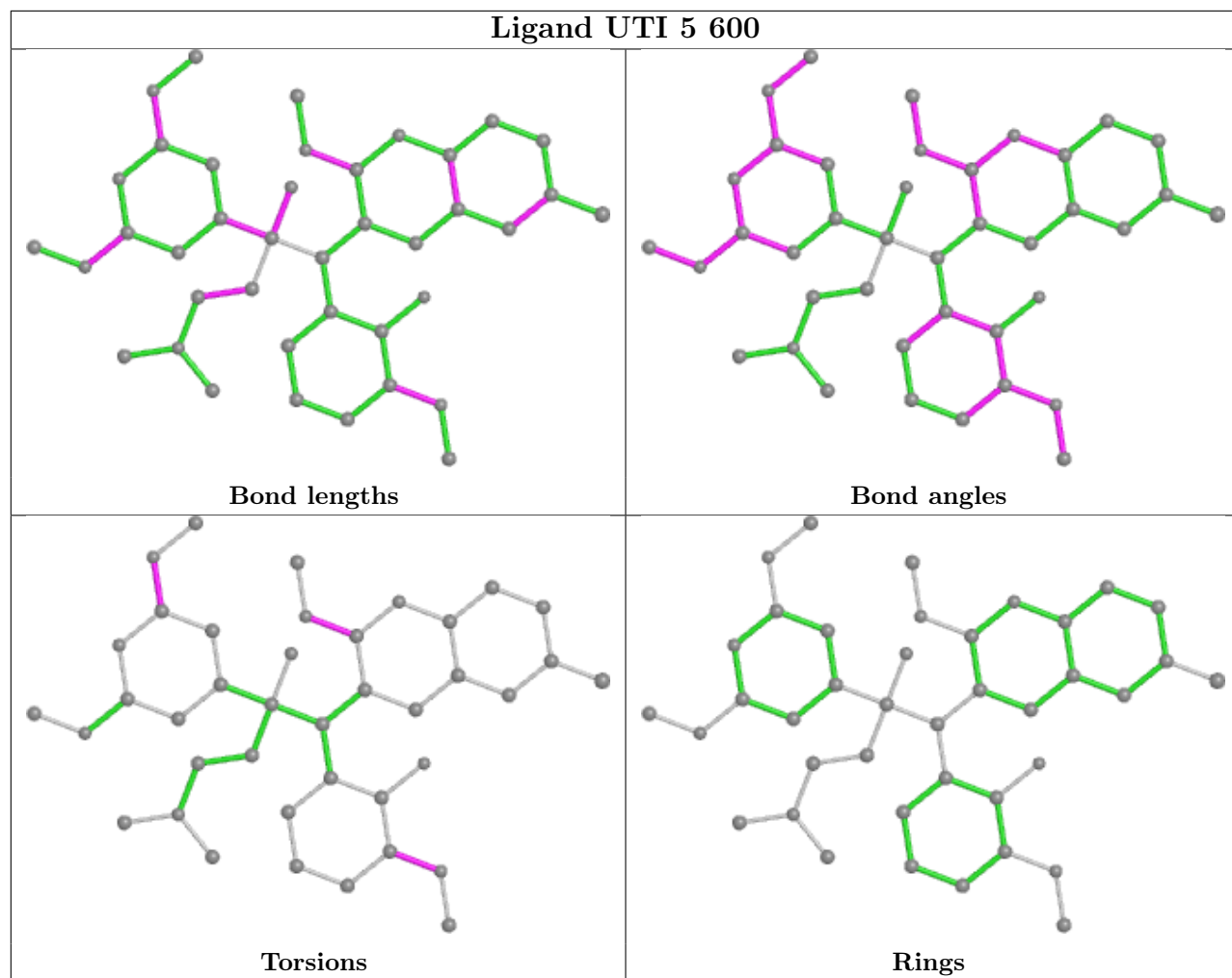


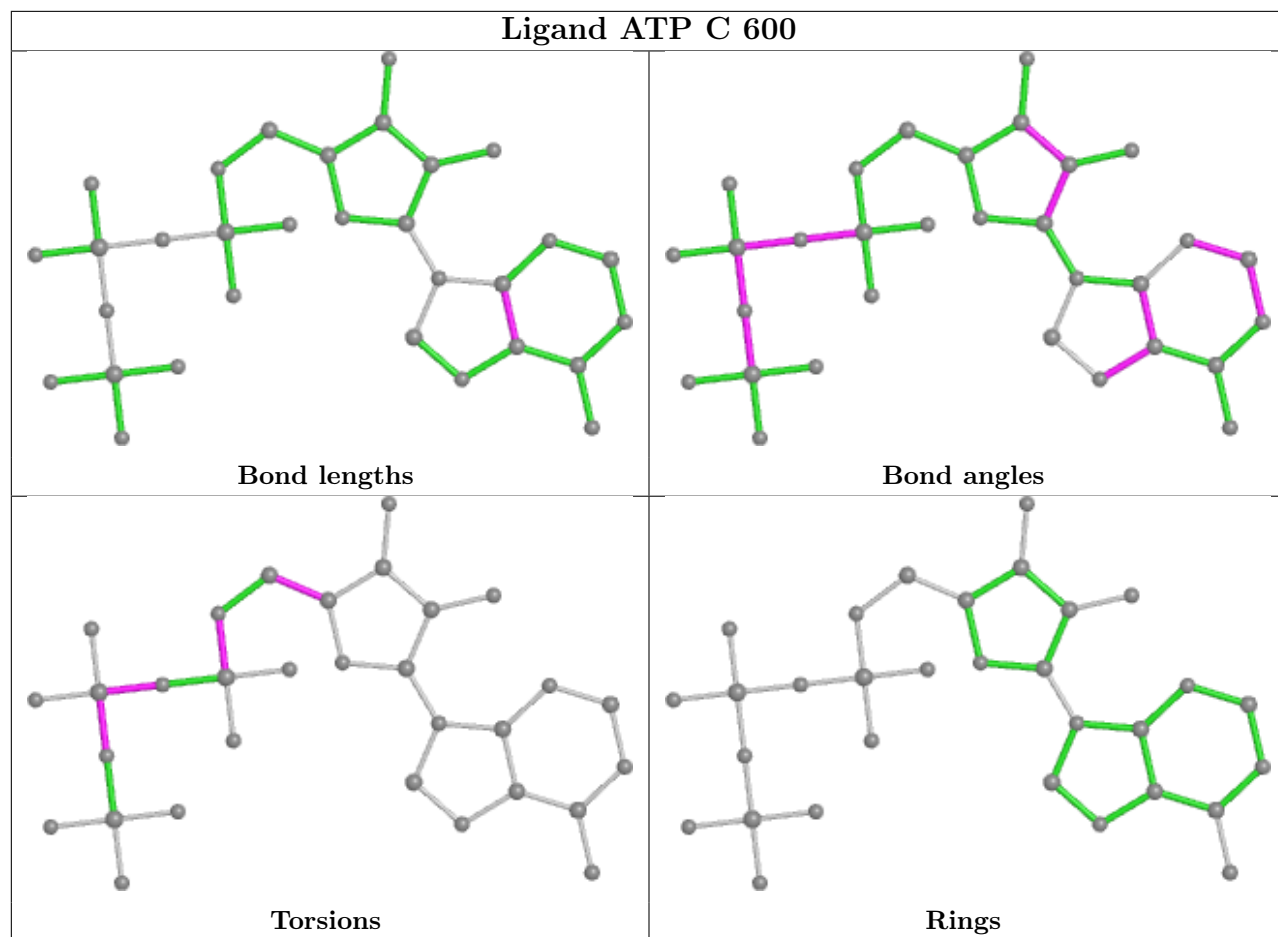


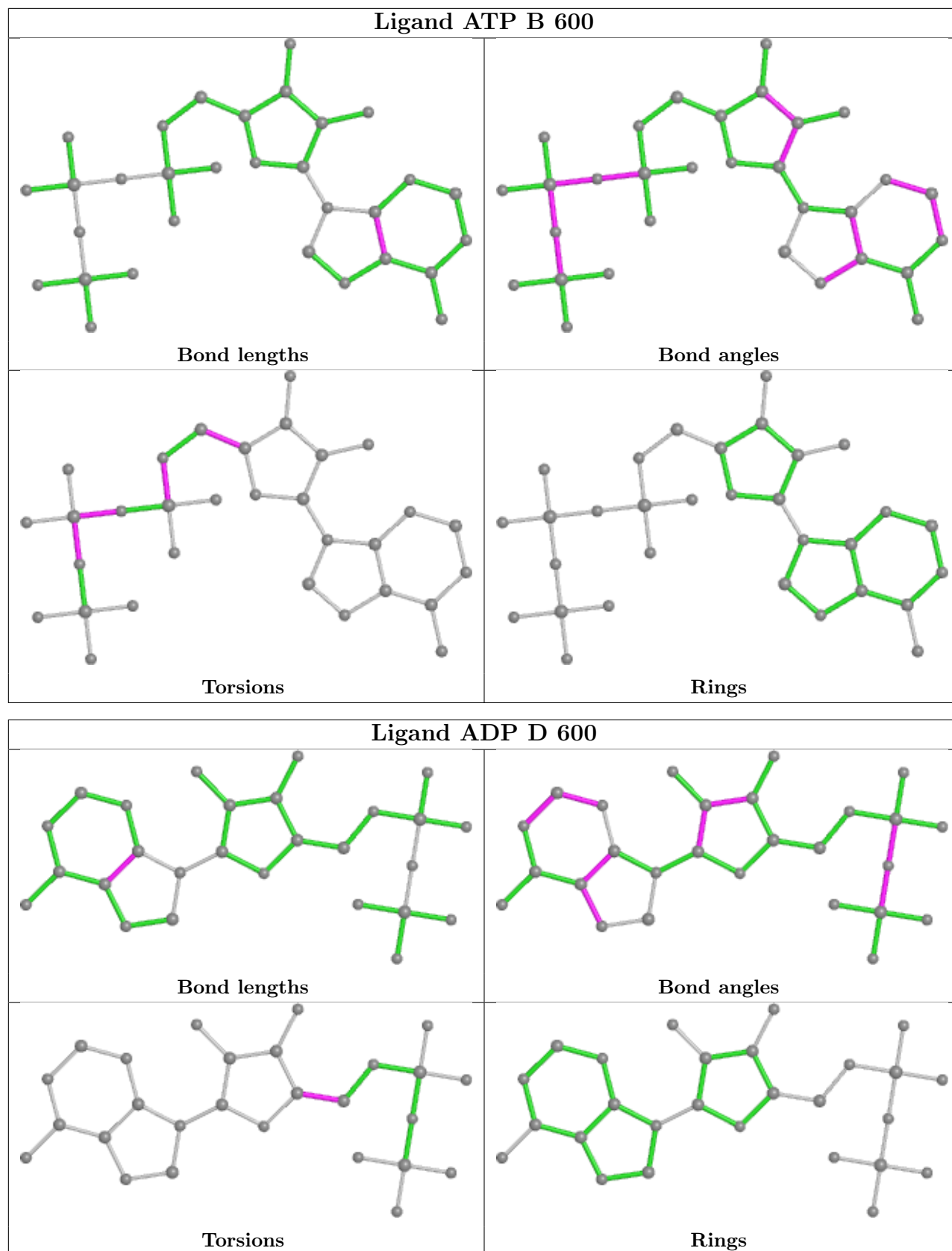


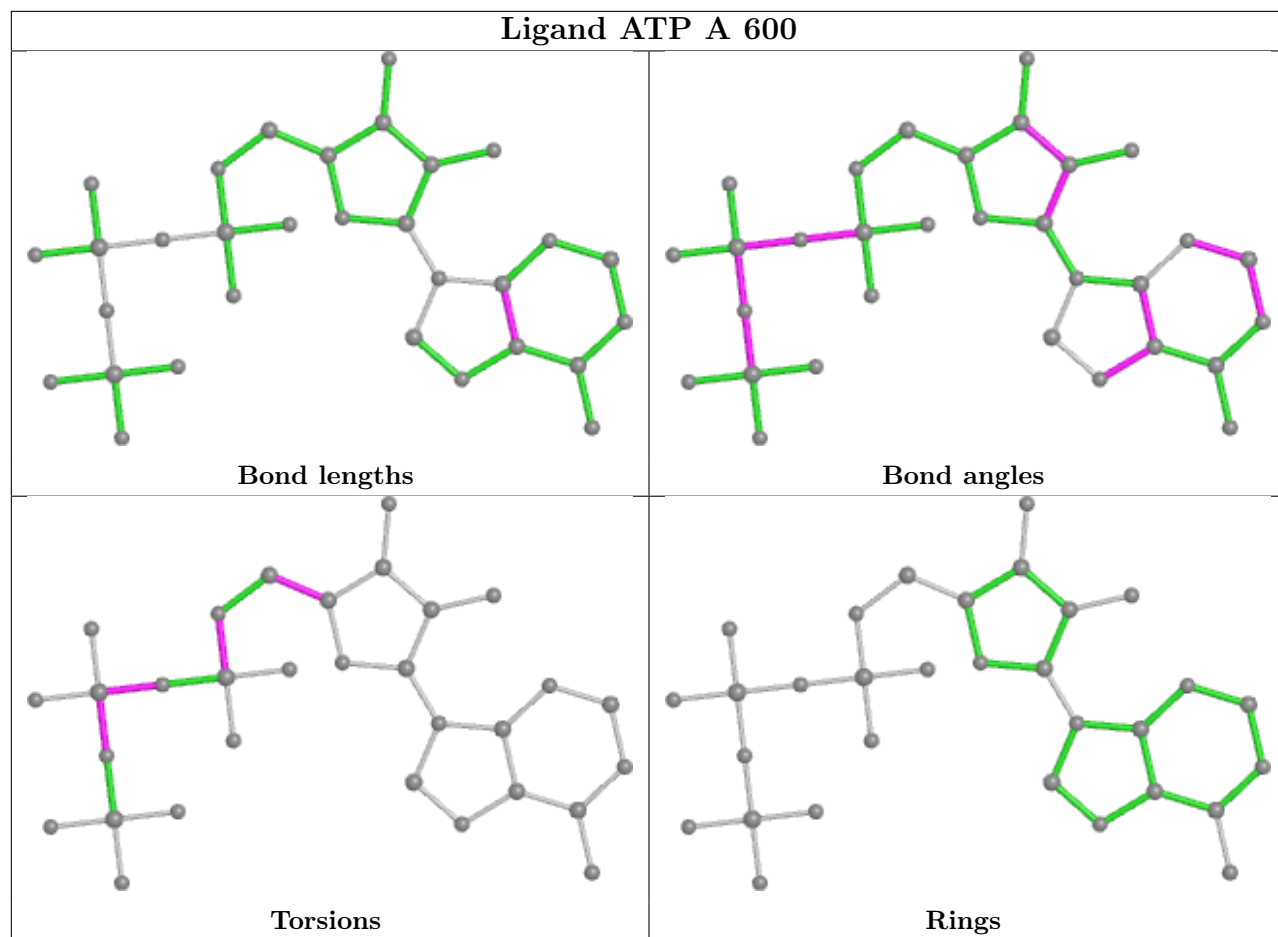


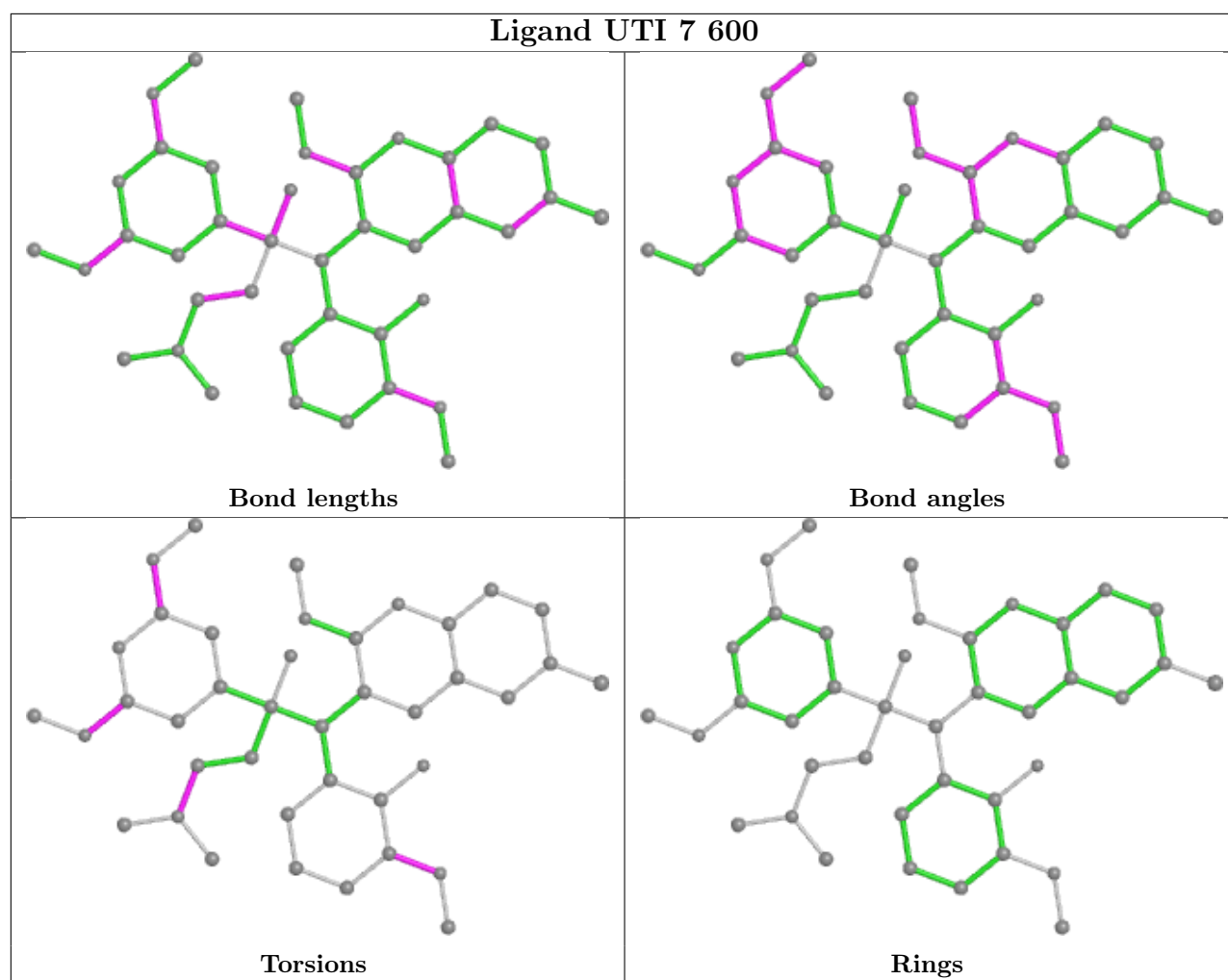












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

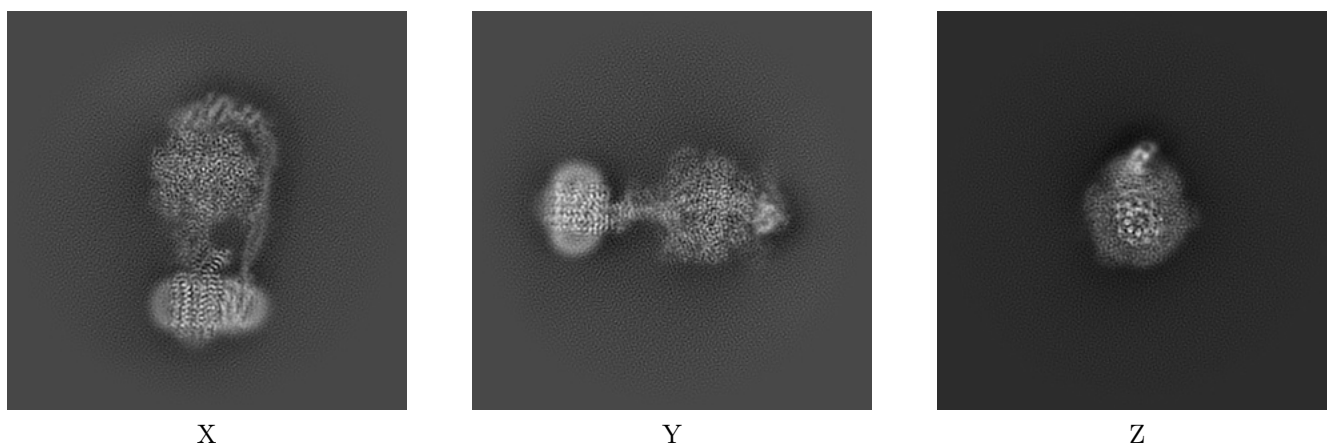
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36589. 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](#)

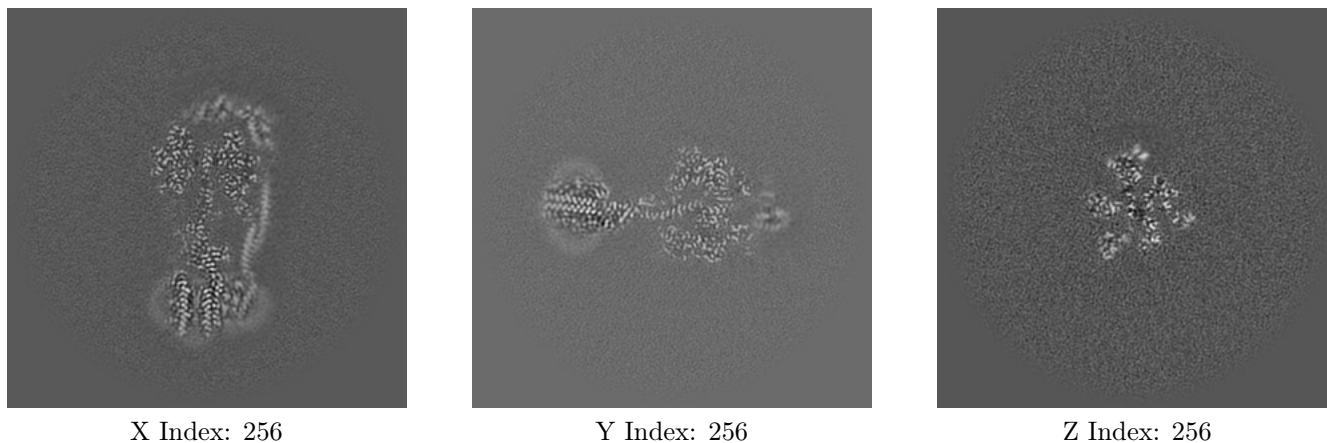
6.1.1 Primary map



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

6.2 Central slices [i](#)

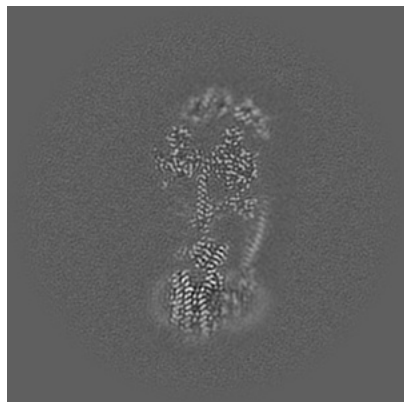
6.2.1 Primary map



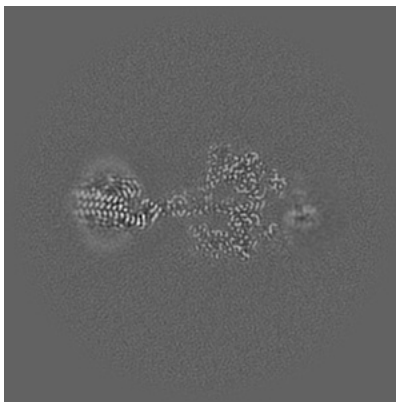
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

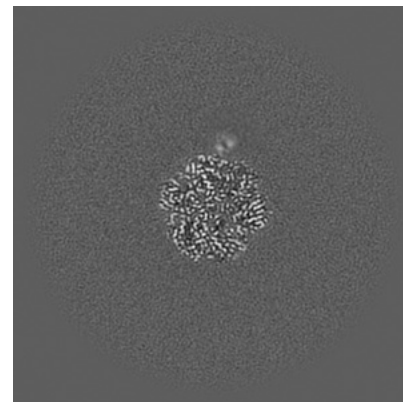
6.3.1 Primary map



X Index: 249



Y Index: 254

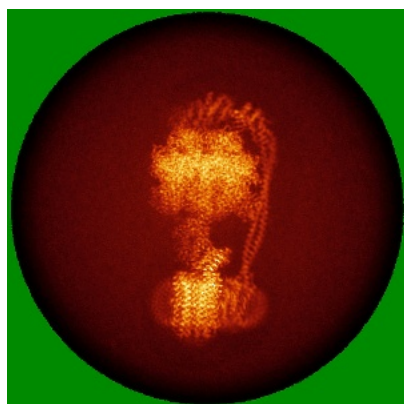


Z Index: 313

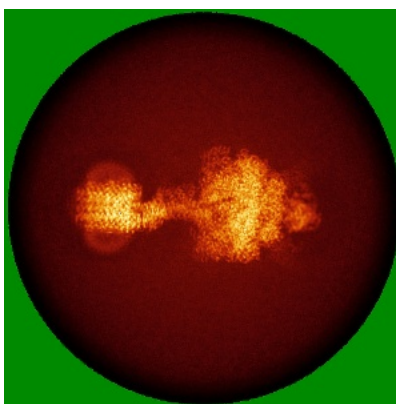
The images above show the largest variance slices of the map in three orthogonal directions.

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

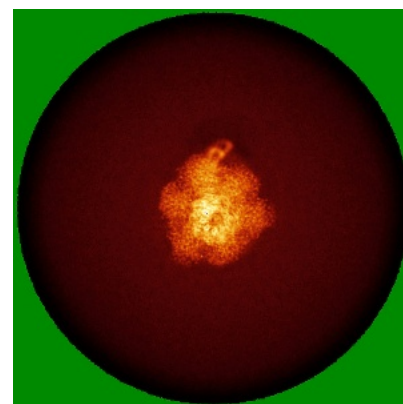
6.4.1 Primary map



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

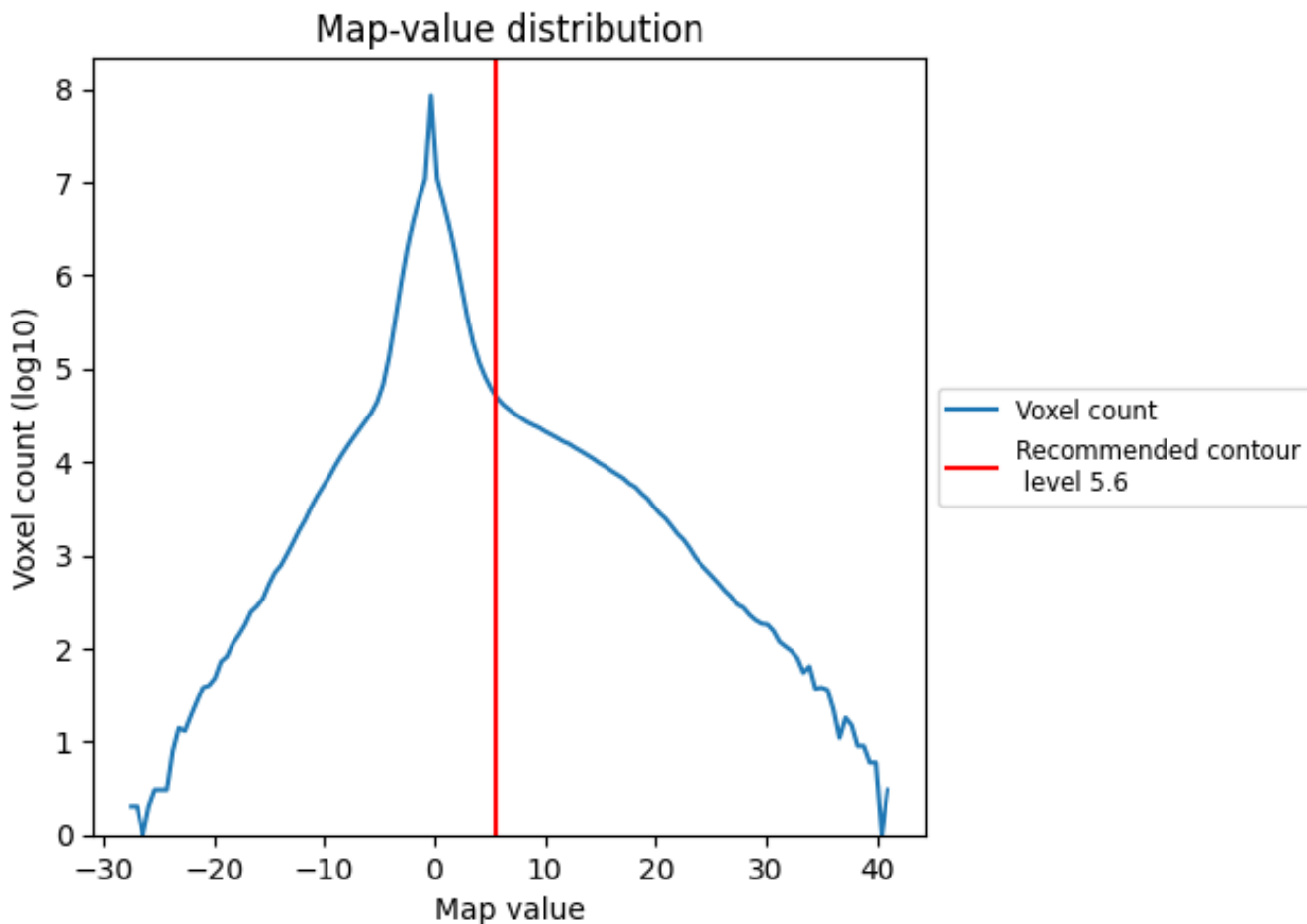
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

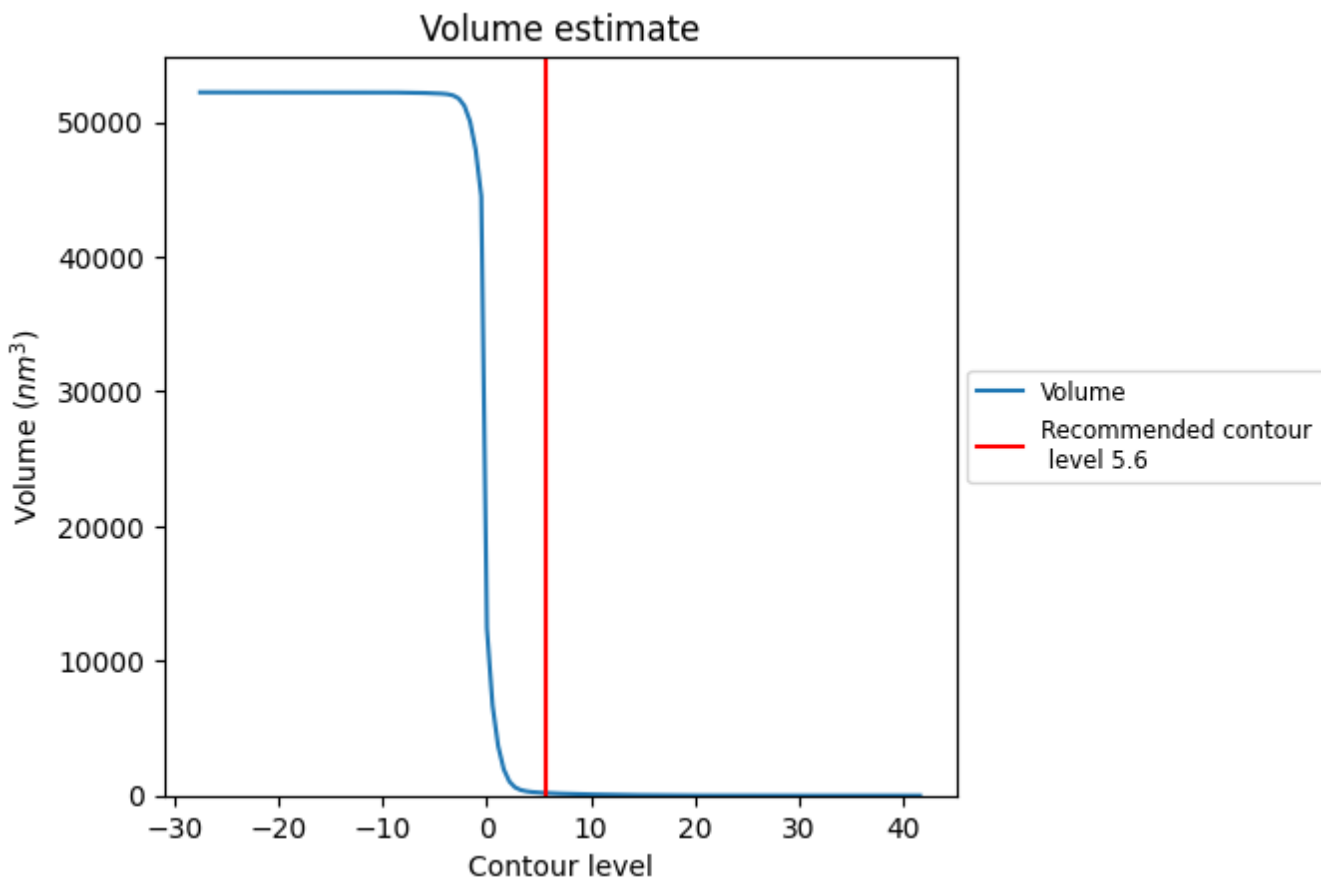
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

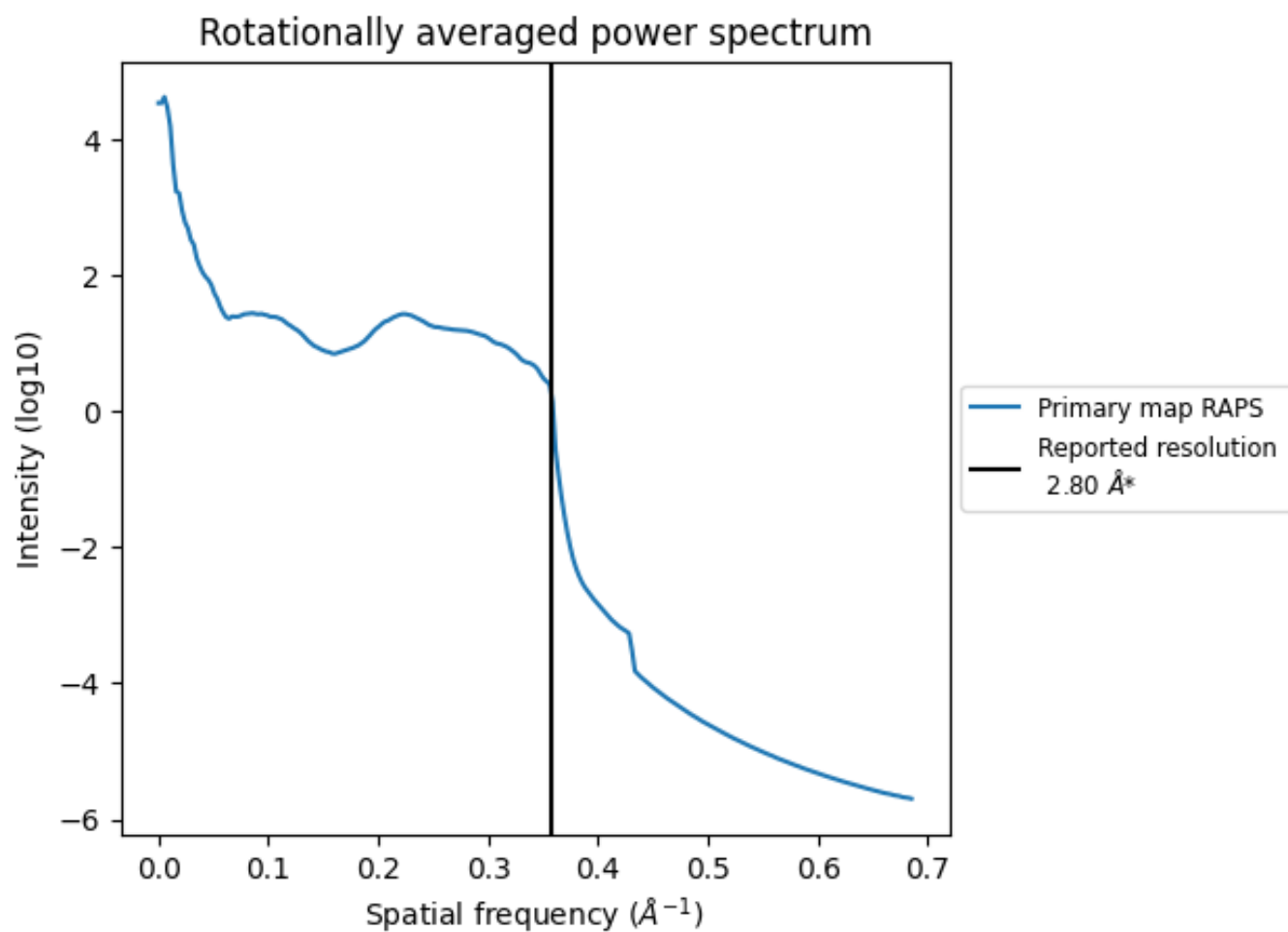
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 192 nm^3 ; this corresponds to an approximate mass of 174 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 0.357 Å⁻¹

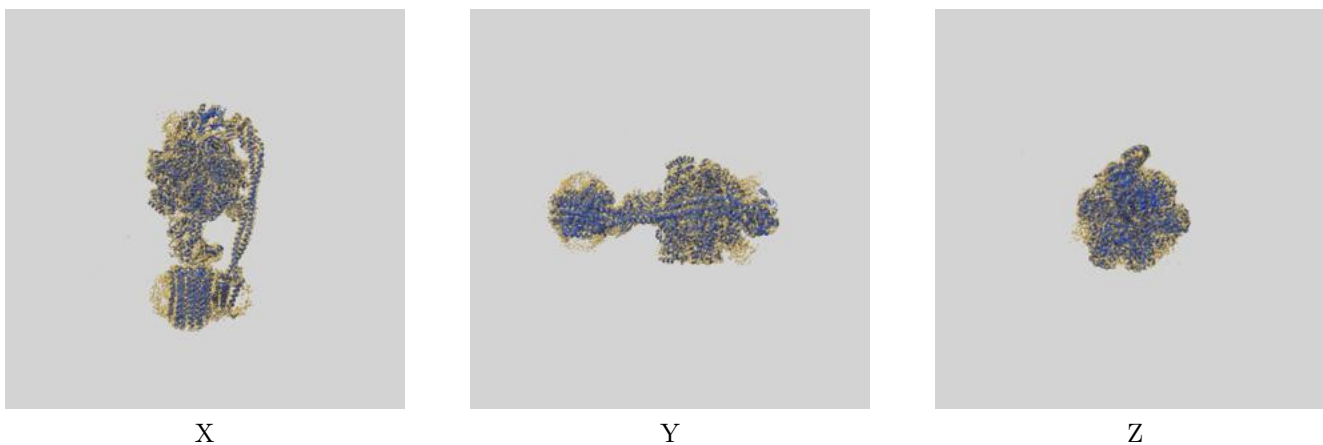
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

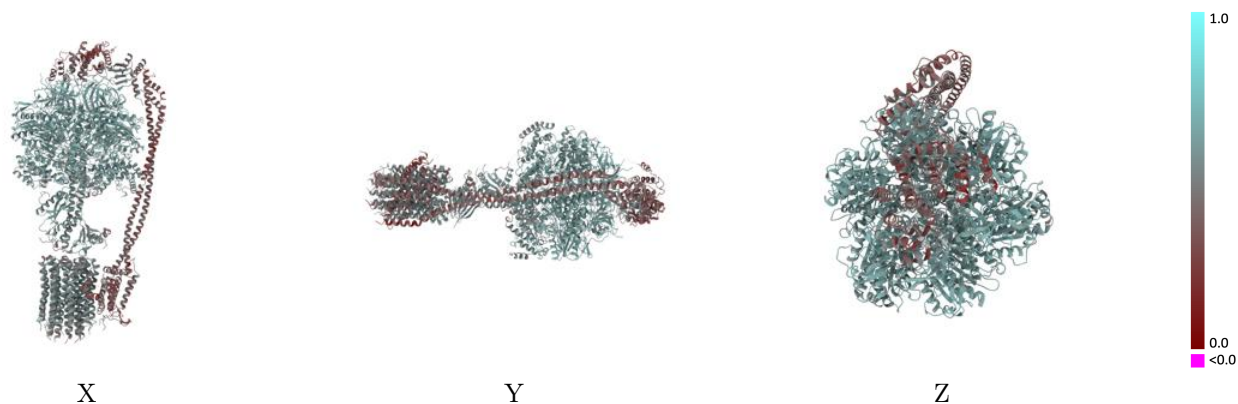
This section contains information regarding the fit between EMDB map EMD-36589 and PDB model 8JR0. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



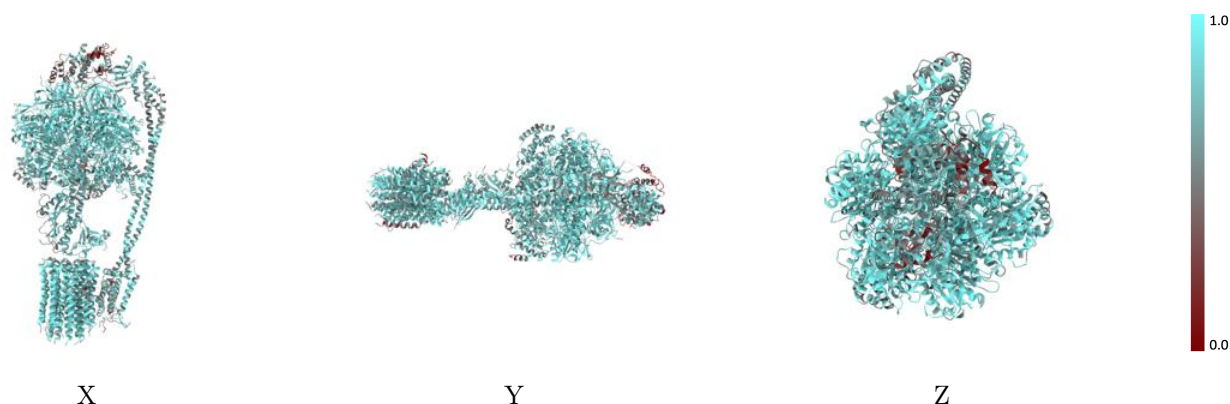
The images above show the 3D surface view of the map at the recommended contour level 5.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



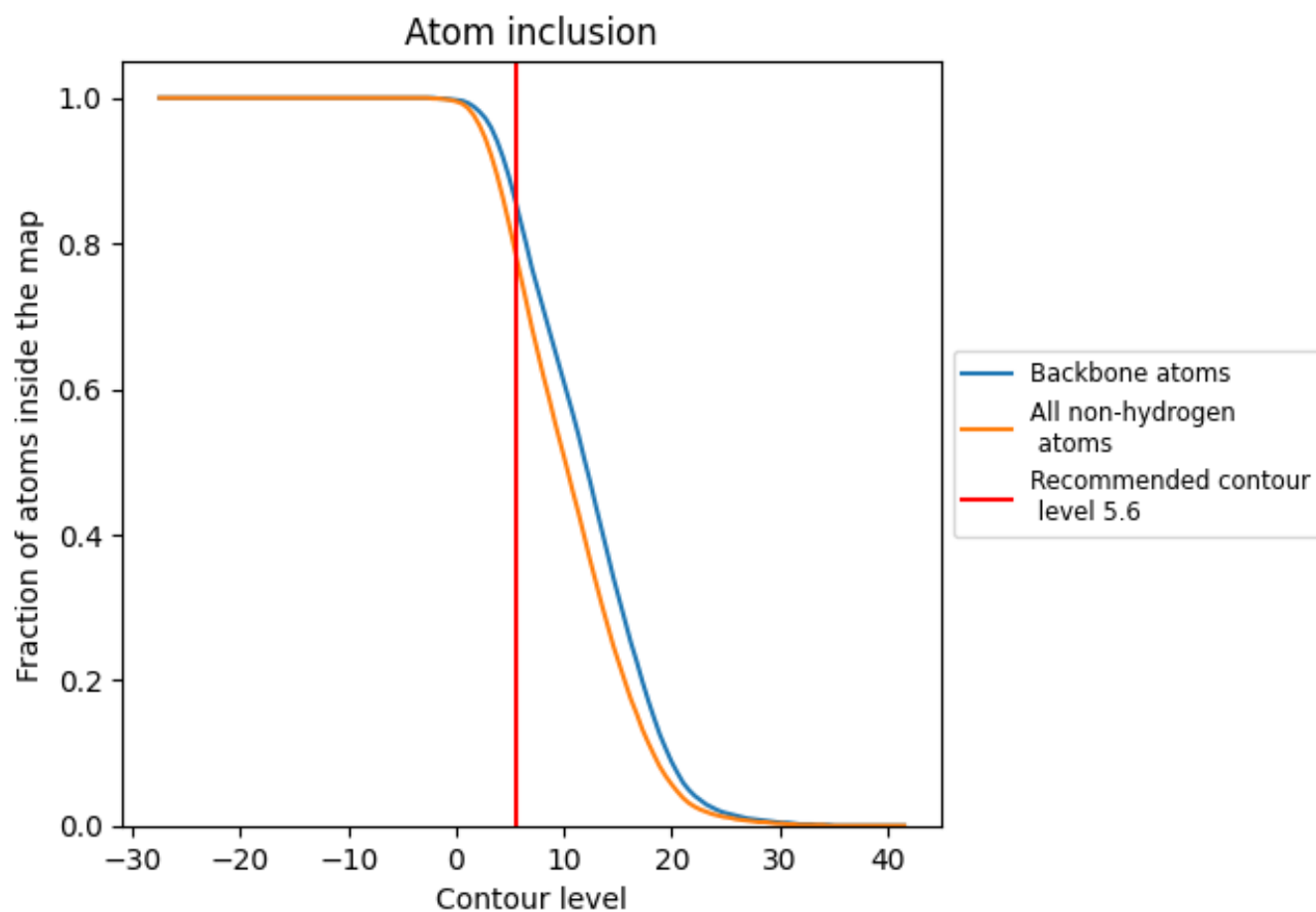
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5.6).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 78% 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	 0.7810	 0.5450
1	 0.8320	 0.5090
2	 0.8580	 0.5230
3	 0.8580	 0.5310
4	 0.8390	 0.5270
5	 0.8440	 0.5340
6	 0.8320	 0.5250
7	 0.8260	 0.5200
8	 0.8370	 0.5160
9	 0.8120	 0.5080
A	 0.8340	 0.5950
B	 0.7810	 0.5890
C	 0.7770	 0.5930
D	 0.8350	 0.6110
E	 0.8170	 0.6060
F	 0.8390	 0.6130
G	 0.7210	 0.5560
H	 0.8090	 0.5330
a	 0.6510	 0.3610
b	 0.6890	 0.3570
d	 0.6020	 0.3600

