



Full wwPDB EM Validation Report ⓘ

Aug 12, 2024 – 12:29 PM JST

PDB ID : 8JR1
EMDB ID : EMD-36590
Title : Cryo-EM structure of Mycobacterium tuberculosis ATP synthase Fo in complex with TBAJ-587
Authors : Zhang, Y.; Lai, Y.; Liu, F.; Rao, Z.; Gong, H.
Deposited on : 2023-06-15
Resolution : 3.17 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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) : 2.37.1

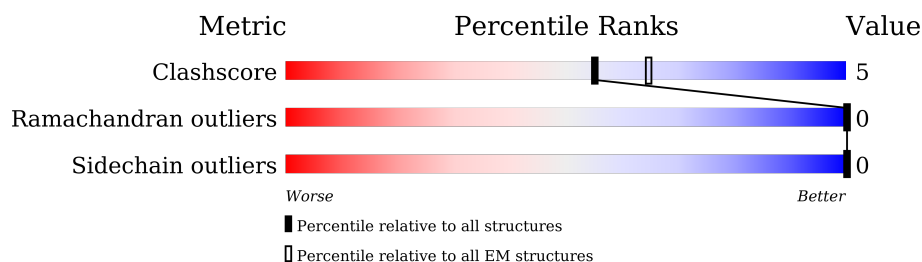
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.17 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	158937	4297
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	1	81	<div> <div>10%</div> <div>85%</div> <div>15%</div> </div>
1	2	81	<div> <div>5%</div> <div>95%</div> <div>5%</div> </div>
1	3	81	<div> <div>6%</div> <div>90%</div> <div>10%</div> </div>
1	4	81	<div> <div>•</div> <div>88%</div> <div>12%</div> </div>
1	5	81	<div> <div>7%</div> <div>86%</div> <div>14%</div> </div>
1	6	81	<div> <div>5%</div> <div>91%</div> <div>9%</div> </div>
1	7	81	<div> <div>7%</div> <div>89%</div> <div>11%</div> </div>
1	8	81	<div> <div>10%</div> <div>93%</div> <div>7%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	9	81	<div><div></div><div>11%</div><div>91%</div><div>9%</div></div>
2	a	250	<div><div></div><div>67%</div><div>88%</div><div>12%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7089 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 c.

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

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

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

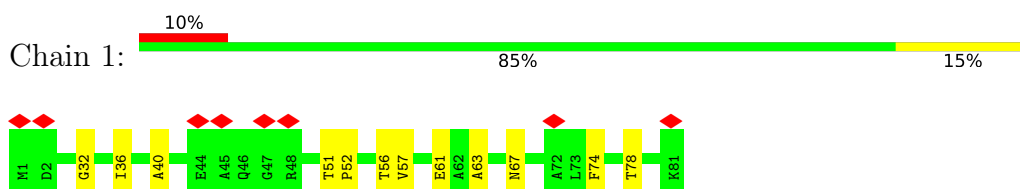
- Molecule 3 is (1 {S},2 {S})-1-(6-bromanyl-2-methoxy-quinolin-3-yl)-2-(2,6-dimethoxypyridin-4-yl)-4-(dimethylamino)-1-(2-fluoranyl-3-methoxy-phenyl)butan-2-ol (three-letter code: UTI) (formula: C₃₀H₃₃BrFN₃O₅).



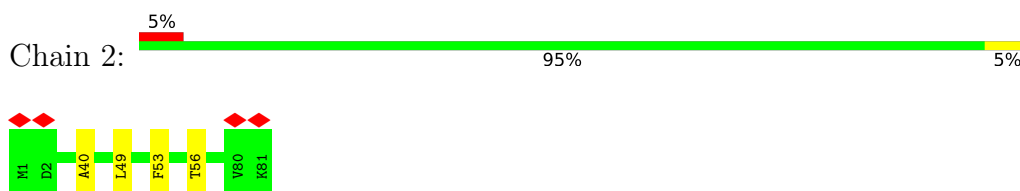
3 Residue-property plots [i](#)

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.

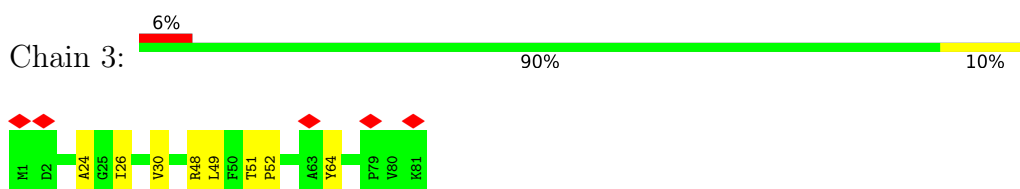
- Molecule 1: ATP synthase subunit c



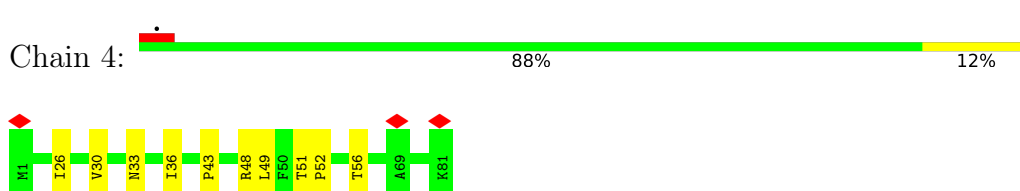
- Molecule 1: ATP synthase subunit c



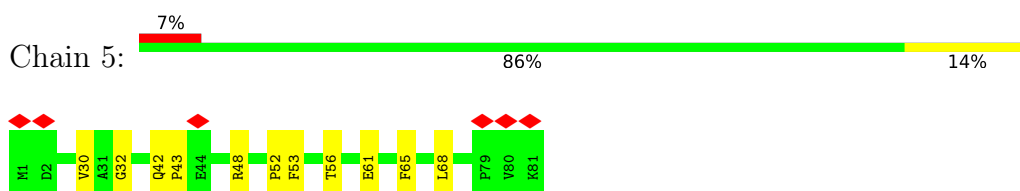
- Molecule 1: ATP synthase subunit c



- Molecule 1: ATP synthase subunit c



- Molecule 1: ATP synthase subunit c



- Chain a:
-
- 67% 88% 12%
- MET THR THR THR ILE LEU ALA Q9 I10 E11 V12 G13 E14 H15 H16 T17 A18 I19 I20 G22 G23 T24 V25 N26 T27 D28 T29 V30 L31 S32 S33 A34 I35 A36 G37 L38 I39 V40 I41 A42 A43 A44 F45 Y46 L47 R48 A49 K50 V51 T52 S53 T54 D55 V56 P57 P58 G58 G59 V60
- Q61 L62 F63 F64 E65 A66 T67 T68 Q70 M71 R72 W73 Q74 E75 E76 S77 A78 I79 G80 G81 R82 I83 A84 P85 L88 P89 V92 V96 F97 I100 S101 N102 W103 L104 A105 V106 I107 P108 V109 Q110 T111 THR ASP LYS HIS GLY THR T119 E120 L121 L122 K123 A126
- A127 D128 M130 Y131 V132 L133 A134 L137 F138 V139 F140 V141 G142 Y143 H144 T145 A146 G147 I148 W149 R150 R151 G152 ILE VAL GLY HIS PRO ILE LYS LEU LEU LYS G163 H164 Q227 V165 T166 F229 I230 L168 A169 P170 I171 M172 L173 V174 E175 E176 V177 A178 K179 P180 I181 S182 I183 L187 F188
- I191 G194 G195 I196 V198 A199 L200 I201 A202 L203 F204 P205 P206 Y207 I208 M209 W210 A211 P212 N213 I215 W216 K217 A218 F219 D220 L221 F222 V223 G224 A225 I226 Q227 A228 F229 I230 F231 Y238 F239 S240 Q241 Q242 A242 M243 L244 E244 L245 GLU GLU HIS HIS HIS HIS

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	0.741	Depositor
Minimum map value	-0.444	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.12	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1	0.48	0/578	0.70	0/784
1	2	0.51	0/578	0.75	0/784
1	3	0.53	0/578	0.76	0/784
1	4	0.50	0/578	0.68	0/784
1	5	0.46	0/578	0.63	0/784
1	6	0.53	0/578	0.78	0/784
1	7	0.57	0/578	0.84	0/784
1	8	0.57	0/578	0.80	0/784
1	9	0.53	0/578	0.74	0/784
2	a	0.57	0/1748	0.83	0/2390
All	All	0.53	0/6950	0.77	0/9446

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	1	567	0	585	10	0
1	2	567	0	585	6	0
1	3	567	0	585	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4	567	0	585	7	0
1	5	567	0	585	12	0
1	6	567	0	585	8	0
1	7	567	0	585	7	0
1	8	567	0	585	4	0
1	9	567	0	585	5	0
2	a	1706	0	1772	0	0
3	4	40	0	0	0	0
3	5	40	0	0	2	0
3	6	40	0	0	0	0
3	7	40	0	0	0	0
3	8	40	0	0	0	0
3	9	40	0	0	1	0
3	a	40	0	0	0	0
All	All	7089	0	7037	48	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 5.

All (48) 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)
1:7:51:THR:HB	1:7:52:PRO:HD3	1.66	0.77
1:1:51:THR:HB	1:1:52:PRO:HD3	1.65	0.77
1:5:61:GLU:OE2	3:5:600:UTI:N02	2.24	0.71
1:8:41:ARG:HG2	1:8:42:GLN:HG3	1.75	0.68
1:3:51:THR:HG22	1:3:52:PRO:HD3	1.77	0.66
1:3:51:THR:CG2	1:3:52:PRO:HD3	2.27	0.64
1:5:61:GLU:OE2	3:5:600:UTI:C03	2.49	0.60
1:3:48:ARG:O	1:3:51:THR:HG22	2.01	0.60
1:6:32:GLY:HA3	1:7:56:THR:HG21	1.85	0.59
1:9:17:MET:HG2	1:9:71:MET:HG3	1.84	0.58
1:1:63:ALA:O	1:1:67:ASN:ND2	2.35	0.58
1:9:61:GLU:OE1	3:9:600:UTI:N02	2.39	0.56
1:2:40:ALA:HB2	1:3:49:LEU:HD21	1.88	0.55
1:4:33:ASN:ND2	1:5:30:VAL:O	2.40	0.55
1:4:36:ILE:HD11	1:5:53:PHE:HA	1.89	0.54
1:4:48:ARG:O	1:4:51:THR:HG22	2.08	0.54
1:1:57:VAL:O	1:1:61:GLU:HG2	2.09	0.53
1:7:75:VAL:O	1:8:80:VAL:HG13	2.09	0.51
1:3:24:ALA:HB2	1:3:64:TYR:HB2	1.91	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:32:GLY:HA3	1:2:56:THR:HG21	1.92	0.50
1:8:3:PRO:O	1:8:6:ALA:HB3	2.13	0.48
1:7:45:ALA:O	1:7:48:ARG:HG2	2.13	0.48
1:1:67:ASN:HD21	1:9:21:ALA:HB2	1.79	0.48
1:5:32:GLY:CA	1:6:56:THR:HG21	2.44	0.47
1:5:43:PRO:HB3	1:6:48:ARG:NE	2.29	0.47
1:4:49:LEU:O	1:4:52:PRO:HD2	2.15	0.47
1:6:2:ASP:OD1	1:6:81:LYS:NZ	2.47	0.47
1:7:26:ILE:O	1:7:30:VAL:HG23	2.15	0.47
1:1:32:GLY:CA	1:2:56:THR:HG21	2.44	0.47
1:5:52:PRO:O	1:5:56:THR:HG23	2.16	0.46
1:1:74:PHE:O	1:1:78:THR:HG22	2.16	0.46
1:6:78:THR:O	1:6:78:THR:OG1	2.33	0.46
1:1:56:THR:HG21	1:9:32:GLY:CA	2.46	0.45
1:2:49:LEU:HD23	1:2:49:LEU:HA	1.83	0.45
1:5:42:GLN:NE2	1:5:48:ARG:HH12	2.15	0.44
1:4:26:ILE:O	1:4:30:VAL:HG23	2.17	0.44
1:7:32:GLY:HA3	1:8:56:THR:HG21	1.98	0.44
1:3:49:LEU:O	1:3:52:PRO:HD2	2.18	0.43
1:5:32:GLY:HA3	1:6:56:THR:HG21	1.99	0.43
1:4:52:PRO:O	1:4:56:THR:HG23	2.18	0.42
1:1:40:ALA:HB2	1:2:49:LEU:HD21	2.01	0.42
1:3:26:ILE:O	1:3:30:VAL:HG23	2.19	0.42
1:9:24:ALA:HB2	1:9:64:TYR:HB2	2.02	0.41
1:4:43:PRO:HG3	1:5:48:ARG:NH1	2.35	0.41
1:5:43:PRO:HD3	1:6:48:ARG:NH1	2.36	0.41
1:5:65:PHE:O	1:5:68:LEU:HB3	2.20	0.41
1:1:36:ILE:HD11	1:2:53:PHE:HA	2.02	0.41
1:6:40:ALA:O	1:7:48:ARG:NH1	2.54	0.40

There are no symmetry-related clashes.

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	1	79/81 (98%)	76 (96%)	3 (4%)	0	100	100
1	2	79/81 (98%)	76 (96%)	3 (4%)	0	100	100
1	3	79/81 (98%)	78 (99%)	1 (1%)	0	100	100
1	4	79/81 (98%)	75 (95%)	4 (5%)	0	100	100
1	5	79/81 (98%)	75 (95%)	4 (5%)	0	100	100
1	6	79/81 (98%)	78 (99%)	1 (1%)	0	100	100
1	7	79/81 (98%)	76 (96%)	3 (4%)	0	100	100
1	8	79/81 (98%)	77 (98%)	2 (2%)	0	100	100
1	9	79/81 (98%)	77 (98%)	2 (2%)	0	100	100
2	a	214/250 (86%)	198 (92%)	16 (8%)	0	100	100
All	All	925/979 (94%)	886 (96%)	39 (4%)	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	1	52/52 (100%)	52 (100%)	0	100	100
1	2	52/52 (100%)	52 (100%)	0	100	100
1	3	52/52 (100%)	52 (100%)	0	100	100
1	4	52/52 (100%)	52 (100%)	0	100	100
1	5	52/52 (100%)	52 (100%)	0	100	100
1	6	52/52 (100%)	52 (100%)	0	100	100
1	7	52/52 (100%)	52 (100%)	0	100	100
1	8	52/52 (100%)	52 (100%)	0	100	100
1	9	52/52 (100%)	52 (100%)	0	100	100
2	a	178/204 (87%)	178 (100%)	0	100	100
All	All	646/672 (96%)	646 (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 (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	5	42	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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	$\# Z > 2$
3	UTI	4	600	-	41,43,43	1.69	10 (24%)	48,62,62	1.83	13 (27%)
3	UTI	a	600	-	41,43,43	1.50	7 (17%)	48,62,62	2.31	13 (27%)
3	UTI	8	600	-	41,43,43	1.73	10 (24%)	48,62,62	1.89	13 (27%)
3	UTI	5	600	-	41,43,43	1.68	9 (21%)	48,62,62	1.83	13 (27%)
3	UTI	6	600	-	41,43,43	1.72	10 (24%)	48,62,62	1.83	11 (22%)
3	UTI	9	600	-	41,43,43	1.71	10 (24%)	48,62,62	1.83	12 (25%)
3	UTI	7	600	-	41,43,43	1.71	9 (21%)	48,62,62	1.80	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
3	UTI	4	600	-	-	4/34/34/34	0/4/4/4
3	UTI	a	600	-	-	8/34/34/34	0/4/4/4
3	UTI	8	600	-	-	13/34/34/34	0/4/4/4
3	UTI	5	600	-	-	6/34/34/34	0/4/4/4
3	UTI	6	600	-	-	8/34/34/34	0/4/4/4
3	UTI	9	600	-	-	7/34/34/34	0/4/4/4
3	UTI	7	600	-	-	7/34/34/34	0/4/4/4

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	6	600	UTI	O13-C11	4.13	1.41	1.35
3	8	600	UTI	O13-C11	4.11	1.41	1.35
3	5	600	UTI	O13-C11	4.09	1.41	1.35
3	7	600	UTI	O13-C11	4.07	1.41	1.35
3	9	600	UTI	O13-C11	4.07	1.41	1.35
3	4	600	UTI	O13-C11	4.04	1.41	1.35
3	a	600	UTI	C35-C30	-4.03	1.35	1.42
3	6	600	UTI	O40-C06	-3.78	1.37	1.43
3	a	600	UTI	O13-C11	3.76	1.41	1.35
3	a	600	UTI	O40-C06	-3.72	1.37	1.43
3	5	600	UTI	O40-C06	-3.72	1.37	1.43
3	7	600	UTI	O40-C06	-3.71	1.37	1.43
3	4	600	UTI	O40-C06	-3.70	1.37	1.43
3	9	600	UTI	O40-C06	-3.64	1.37	1.43
3	8	600	UTI	O15-C09	3.58	1.41	1.35
3	7	600	UTI	O15-C09	3.54	1.41	1.35
3	9	600	UTI	O15-C09	3.54	1.41	1.35
3	8	600	UTI	O40-C06	-3.53	1.37	1.43
3	6	600	UTI	O15-C09	3.51	1.40	1.35
3	8	600	UTI	C35-C30	-3.44	1.36	1.42
3	5	600	UTI	C35-C30	-3.44	1.36	1.42
3	5	600	UTI	O15-C09	3.43	1.40	1.35
3	4	600	UTI	O15-C09	3.43	1.40	1.35
3	7	600	UTI	C35-C30	-3.37	1.36	1.42
3	9	600	UTI	C35-C30	-3.30	1.37	1.42
3	4	600	UTI	C35-C30	-3.28	1.37	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	6	600	UTI	C06-C07	3.24	1.56	1.52
3	8	600	UTI	C06-C07	3.23	1.56	1.52
3	6	600	UTI	C35-C30	-3.20	1.37	1.42
3	8	600	UTI	O38-C28	3.12	1.40	1.35
3	9	600	UTI	C06-C07	3.11	1.56	1.52
3	7	600	UTI	C06-C07	3.11	1.56	1.52
3	6	600	UTI	O38-C28	3.08	1.39	1.35
3	8	600	UTI	C05-C04	3.08	1.57	1.53
3	7	600	UTI	O38-C28	3.07	1.39	1.35
3	5	600	UTI	O38-C28	3.04	1.39	1.35
3	4	600	UTI	O38-C28	3.03	1.39	1.35
3	9	600	UTI	O38-C28	3.03	1.39	1.35
3	4	600	UTI	C06-C07	2.99	1.56	1.52
3	9	600	UTI	C05-C04	2.97	1.57	1.53
3	4	600	UTI	C05-C04	2.95	1.57	1.53
3	a	600	UTI	C05-C04	2.91	1.57	1.53
3	7	600	UTI	C05-C04	2.91	1.57	1.53
3	5	600	UTI	C06-C07	2.89	1.56	1.52
3	5	600	UTI	C05-C04	2.87	1.57	1.53
3	9	600	UTI	O24-C20	2.81	1.41	1.37
3	7	600	UTI	O24-C20	2.78	1.41	1.37
3	6	600	UTI	C05-C04	2.77	1.57	1.53
3	6	600	UTI	O24-C20	2.74	1.41	1.37
3	8	600	UTI	O24-C20	2.72	1.41	1.37
3	5	600	UTI	O24-C20	2.69	1.41	1.37
3	4	600	UTI	O24-C20	2.66	1.41	1.37
3	a	600	UTI	O15-C09	2.58	1.39	1.35
3	a	600	UTI	C06-C07	2.48	1.55	1.52
3	6	600	UTI	C34-C33	2.40	1.40	1.36
3	9	600	UTI	C34-C33	2.40	1.40	1.36
3	a	600	UTI	O24-C20	2.38	1.40	1.37
3	7	600	UTI	C34-C33	2.34	1.40	1.36
3	8	600	UTI	C34-C33	2.28	1.40	1.36
3	5	600	UTI	C34-C33	2.23	1.40	1.36
3	4	600	UTI	C34-C33	2.17	1.40	1.36
3	4	600	UTI	BR37-C33	2.14	1.94	1.90
3	9	600	UTI	BR37-C33	2.12	1.94	1.90
3	8	600	UTI	BR37-C33	2.09	1.94	1.90
3	6	600	UTI	BR37-C33	2.08	1.94	1.90

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	600	UTI	C39-O38-C28	-7.57	109.71	117.21
3	a	600	UTI	C09-N10-C11	6.05	121.52	115.70
3	6	600	UTI	C09-N10-C11	5.71	121.20	115.70
3	4	600	UTI	C09-N10-C11	5.69	121.18	115.70
3	7	600	UTI	C09-N10-C11	5.68	121.17	115.70
3	8	600	UTI	C09-N10-C11	5.65	121.14	115.70
3	9	600	UTI	C09-N10-C11	5.63	121.11	115.70
3	5	600	UTI	C09-N10-C11	5.52	121.01	115.70
3	6	600	UTI	O24-C20-C19	5.27	120.02	116.27
3	7	600	UTI	O24-C20-C19	5.18	119.95	116.27
3	a	600	UTI	C16-O15-C09	-5.04	109.47	117.36
3	8	600	UTI	O24-C20-C19	5.03	119.85	116.27
3	8	600	UTI	C27-C28-N29	-4.93	120.86	125.70
3	4	600	UTI	O24-C20-C19	4.88	119.74	116.27
3	9	600	UTI	O24-C20-C19	4.88	119.74	116.27
3	5	600	UTI	O24-C20-C19	4.81	119.69	116.27
3	9	600	UTI	C27-C28-N29	-4.76	121.03	125.70
3	7	600	UTI	C27-C28-N29	-4.58	121.21	125.70
3	5	600	UTI	C27-C28-N29	-4.57	121.22	125.70
3	6	600	UTI	C27-C28-N29	-4.54	121.24	125.70
3	4	600	UTI	C27-C28-N29	-4.50	121.28	125.70
3	a	600	UTI	C27-C28-N29	-4.23	121.55	125.70
3	5	600	UTI	C39-O38-C28	-3.87	113.38	117.21
3	a	600	UTI	C25-O24-C20	-3.85	111.72	117.53
3	9	600	UTI	C39-O38-C28	-3.63	113.61	117.21
3	a	600	UTI	C27-C17-C18	-3.56	103.07	111.03
3	a	600	UTI	O38-C28-C27	3.34	120.19	115.03
3	8	600	UTI	C39-O38-C28	-3.24	114.01	117.21
3	4	600	UTI	C39-O38-C28	-3.17	114.07	117.21
3	6	600	UTI	C39-O38-C28	-3.14	114.10	117.21
3	a	600	UTI	O24-C20-C19	3.02	118.42	116.27
3	9	600	UTI	O38-C28-C27	3.01	119.68	115.03
3	7	600	UTI	C39-O38-C28	-2.98	114.26	117.21
3	8	600	UTI	C25-O24-C20	-2.95	113.08	117.53
3	a	600	UTI	C12-C11-N10	-2.91	120.69	124.08
3	4	600	UTI	C25-O24-C20	-2.83	113.25	117.53
3	6	600	UTI	O24-C20-C21	-2.75	119.66	124.37
3	8	600	UTI	O38-C28-C27	2.74	119.27	115.03
3	8	600	UTI	O24-C20-C21	-2.73	119.69	124.37
3	6	600	UTI	C25-O24-C20	-2.73	113.41	117.53
3	a	600	UTI	C14-O13-C11	-2.73	113.08	117.36
3	5	600	UTI	O38-C28-C27	2.69	119.19	115.03
3	7	600	UTI	O24-C20-C21	-2.69	119.76	124.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	600	UTI	C25-O24-C20	-2.66	113.51	117.53
3	4	600	UTI	O38-C28-C27	2.65	119.11	115.03
3	5	600	UTI	C16-O15-C09	-2.63	113.23	117.36
3	8	600	UTI	C27-C17-C18	-2.61	105.18	111.03
3	7	600	UTI	O38-C28-C27	2.61	119.05	115.03
3	7	600	UTI	C14-O13-C11	-2.57	113.34	117.36
3	4	600	UTI	O24-C20-C21	-2.56	119.99	124.37
3	9	600	UTI	O24-C20-C21	-2.49	120.11	124.37
3	6	600	UTI	C16-O15-C09	-2.48	113.47	117.36
3	6	600	UTI	O38-C28-C27	2.47	118.84	115.03
3	4	600	UTI	C16-O15-C09	-2.46	113.51	117.36
3	5	600	UTI	O24-C20-C21	-2.45	120.17	124.37
3	8	600	UTI	C28-N29-C30	2.44	121.82	116.41
3	9	600	UTI	C28-N29-C30	2.41	121.75	116.41
3	8	600	UTI	C14-O13-C11	-2.41	113.58	117.36
3	5	600	UTI	C28-N29-C30	2.40	121.73	116.41
3	7	600	UTI	C28-N29-C30	2.40	121.72	116.41
3	a	600	UTI	C28-N29-C30	2.38	121.68	116.41
3	4	600	UTI	C14-O13-C11	-2.37	113.64	117.36
3	6	600	UTI	C28-N29-C30	2.36	121.64	116.41
3	7	600	UTI	C25-O24-C20	-2.34	113.99	117.53
3	6	600	UTI	C12-C11-N10	-2.32	121.37	124.08
3	5	600	UTI	C14-O13-C11	-2.31	113.74	117.36
3	8	600	UTI	C08-C09-N10	-2.30	121.39	124.08
3	4	600	UTI	C28-N29-C30	2.30	121.51	116.41
3	9	600	UTI	C16-O15-C09	-2.30	113.76	117.36
3	9	600	UTI	C12-C11-N10	-2.29	121.41	124.08
3	7	600	UTI	C08-C09-N10	-2.28	121.42	124.08
3	9	600	UTI	C25-O24-C20	-2.24	114.15	117.53
3	a	600	UTI	O24-C20-C21	-2.21	120.58	124.37
3	7	600	UTI	C12-C11-N10	-2.18	121.54	124.08
3	5	600	UTI	C23-C18-C19	2.17	119.48	116.70
3	4	600	UTI	C08-C09-N10	-2.17	121.55	124.08
3	4	600	UTI	C12-C11-N10	-2.17	121.55	124.08
3	6	600	UTI	C08-C09-N10	-2.12	121.61	124.08
3	5	600	UTI	C12-C11-N10	-2.12	121.61	124.08
3	8	600	UTI	C12-C11-N10	-2.11	121.62	124.08
3	a	600	UTI	C21-C20-C19	2.09	121.01	117.72
3	9	600	UTI	C14-O13-C11	-2.09	114.08	117.36
3	5	600	UTI	C08-C09-N10	-2.06	121.68	124.08
3	8	600	UTI	C36-C27-C28	2.04	118.70	116.37
3	4	600	UTI	C23-C18-C19	2.03	119.29	116.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	9	600	UTI	C08-C09-N10	-2.03	121.72	124.08

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	4	600	UTI	C19-C20-O24-C25
3	4	600	UTI	C27-C28-O38-C39
3	5	600	UTI	C19-C20-O24-C25
3	5	600	UTI	C27-C28-O38-C39
3	6	600	UTI	C19-C20-O24-C25
3	7	600	UTI	C12-C11-O13-C14
3	7	600	UTI	N10-C11-O13-C14
3	7	600	UTI	C19-C20-O24-C25
3	8	600	UTI	C12-C11-O13-C14
3	8	600	UTI	N10-C11-O13-C14
3	8	600	UTI	C06-C17-C18-C23
3	8	600	UTI	C06-C17-C18-C19
3	8	600	UTI	C19-C20-O24-C25
3	9	600	UTI	C12-C11-O13-C14
3	9	600	UTI	N10-C11-O13-C14
3	9	600	UTI	C19-C20-O24-C25
3	a	600	UTI	C18-C17-C27-C28
3	a	600	UTI	C19-C20-O24-C25
3	a	600	UTI	C27-C28-O38-C39
3	a	600	UTI	N29-C28-O38-C39
3	6	600	UTI	C12-C11-O13-C14
3	7	600	UTI	C08-C09-O15-C16
3	6	600	UTI	N10-C11-O13-C14
3	6	600	UTI	N10-C09-O15-C16
3	7	600	UTI	N10-C09-O15-C16
3	8	600	UTI	N10-C09-O15-C16
3	6	600	UTI	C21-C20-O24-C25
3	8	600	UTI	C21-C20-O24-C25
3	9	600	UTI	C21-C20-O24-C25
3	4	600	UTI	N29-C28-O38-C39
3	5	600	UTI	N29-C28-O38-C39
3	7	600	UTI	C21-C20-O24-C25
3	a	600	UTI	C05-C04-N02-C03
3	6	600	UTI	C08-C09-O15-C16
3	8	600	UTI	C08-C09-O15-C16
3	a	600	UTI	C21-C20-O24-C25

Continued on next page...

Continued from previous page...

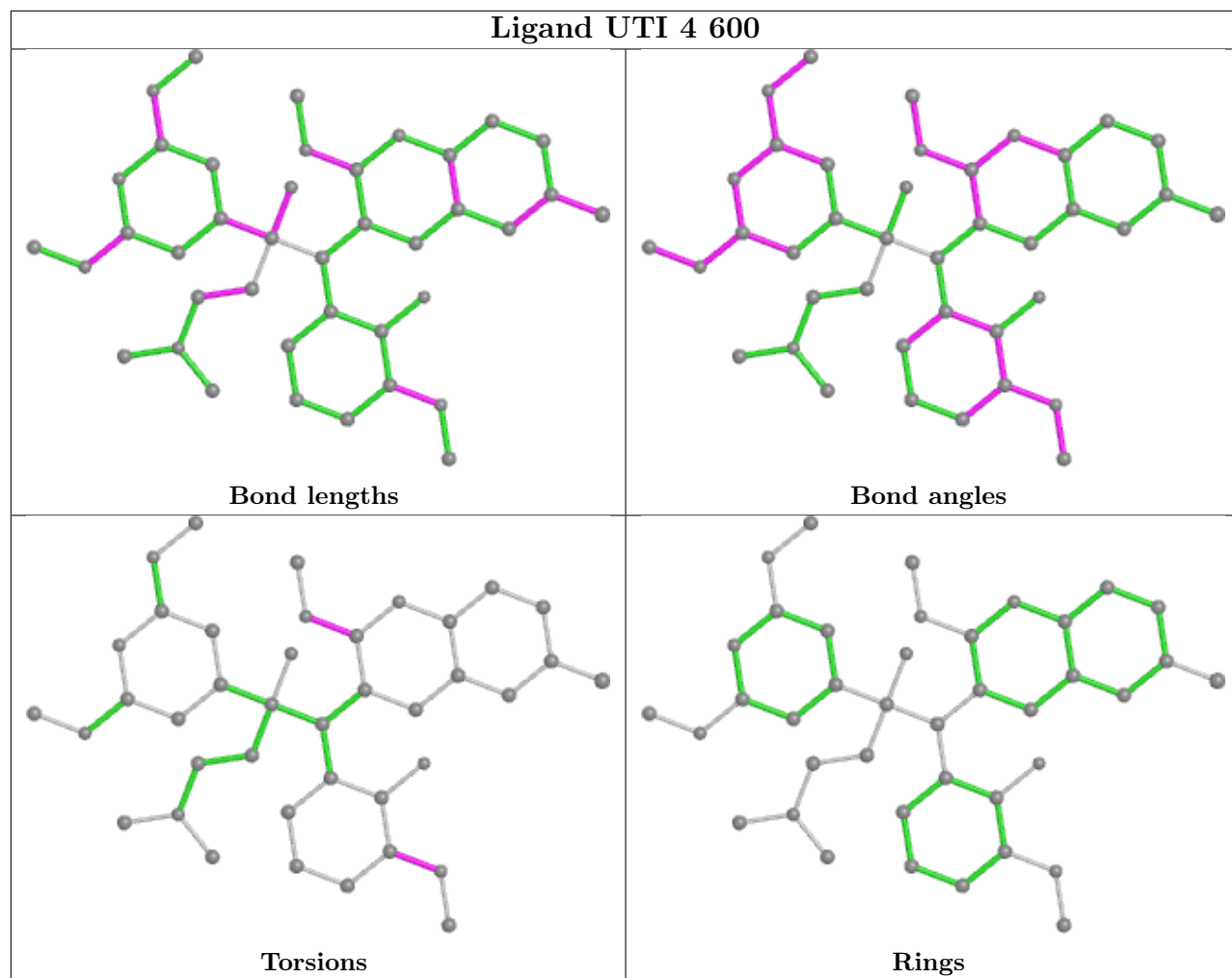
Mol	Chain	Res	Type	Atoms
3	5	600	UTI	C21-C20-O24-C25
3	7	600	UTI	C05-C04-N02-C03
3	8	600	UTI	C05-C04-N02-C01
3	8	600	UTI	C05-C04-N02-C03
3	a	600	UTI	C05-C04-N02-C01
3	4	600	UTI	C21-C20-O24-C25
3	6	600	UTI	C04-C05-C06-C17
3	8	600	UTI	C27-C17-C18-C23
3	a	600	UTI	C18-C17-C27-C36
3	6	600	UTI	C04-C05-C06-O40
3	8	600	UTI	C27-C17-C18-C19
3	9	600	UTI	N29-C28-O38-C39
3	5	600	UTI	C12-C11-O13-C14
3	9	600	UTI	C05-C04-N02-C03
3	5	600	UTI	N10-C11-O13-C14
3	8	600	UTI	C18-C17-C27-C36
3	9	600	UTI	C27-C28-O38-C39

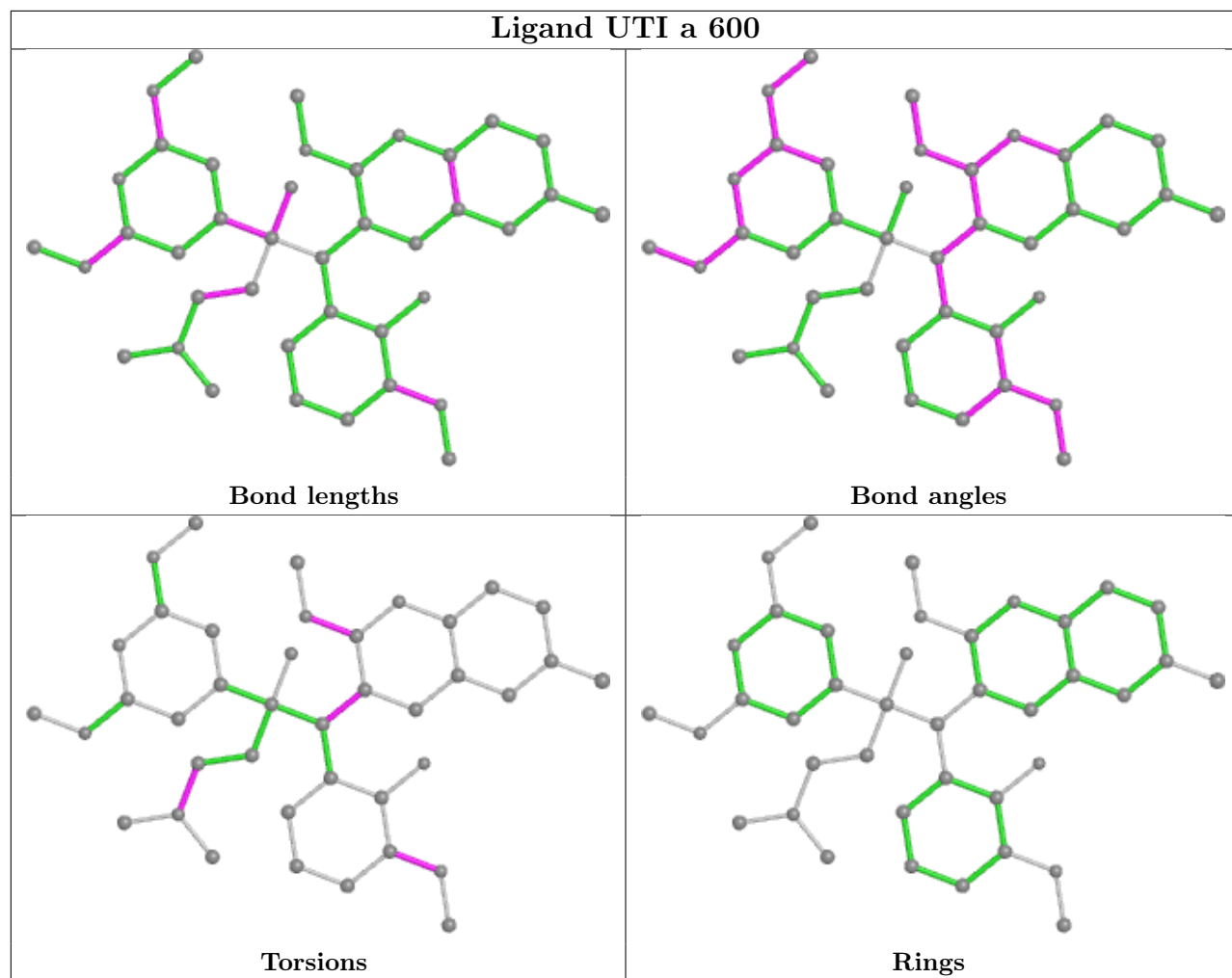
There are no ring outliers.

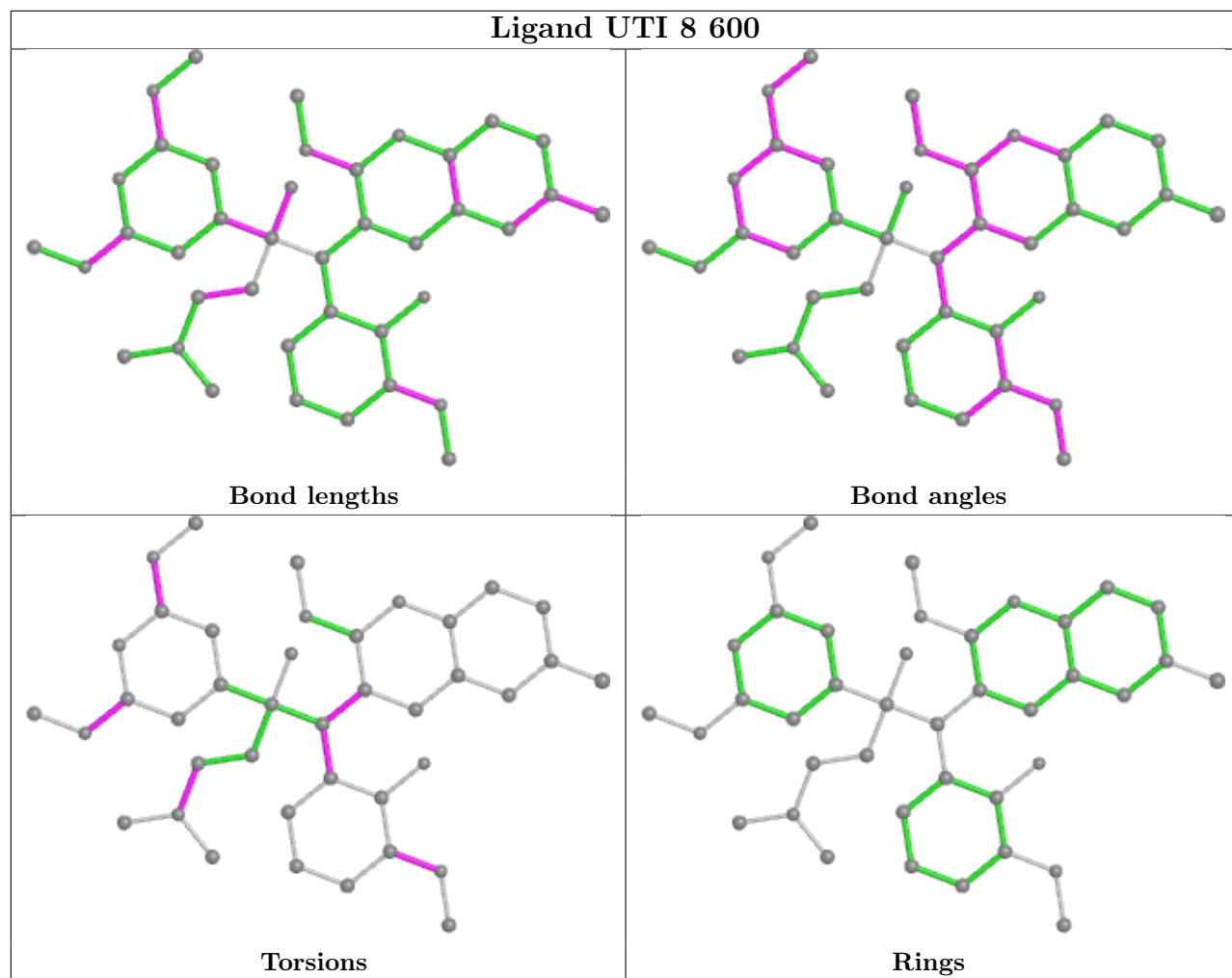
2 monomers are involved in 3 short contacts:

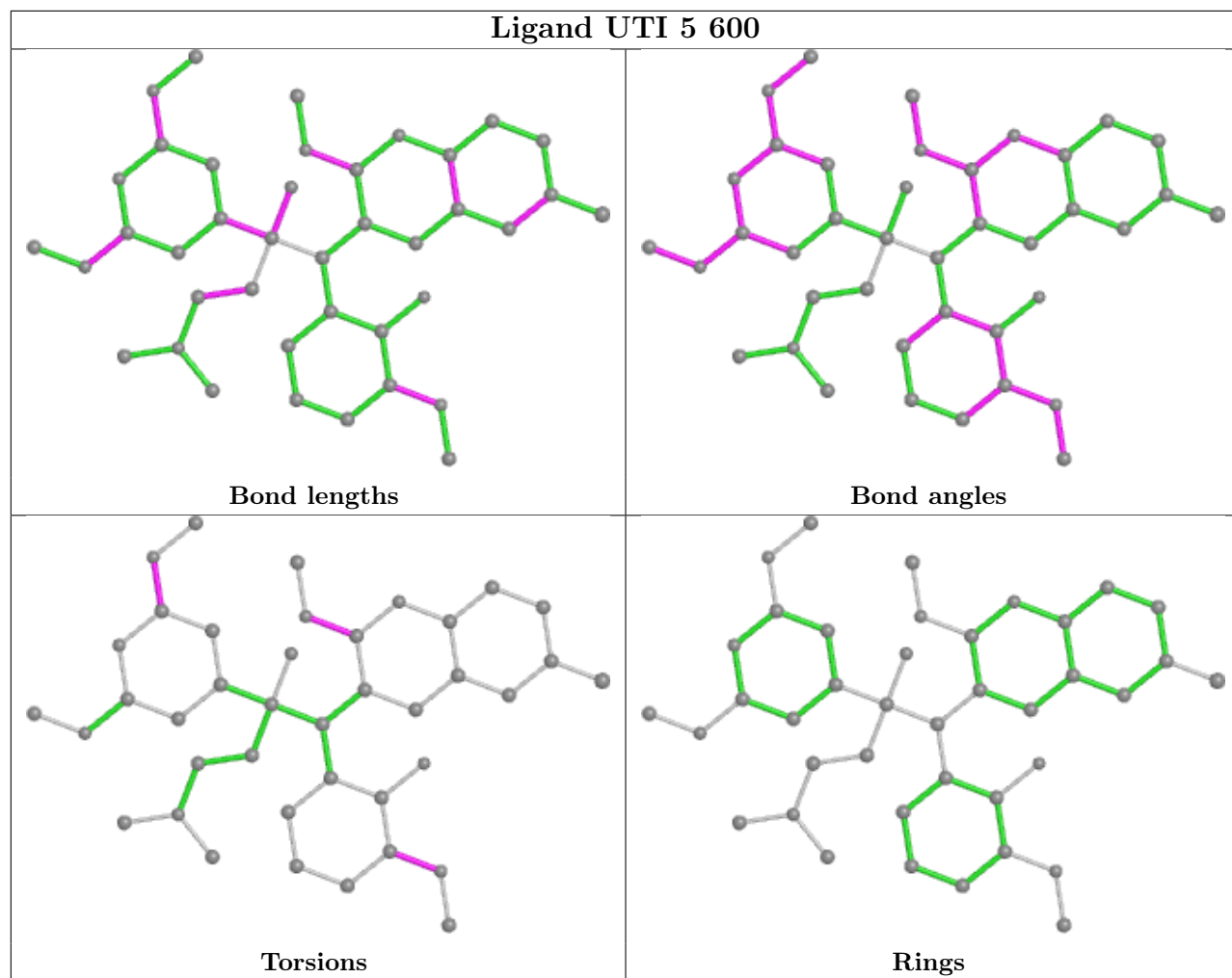
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	5	600	UTI	2	0
3	9	600	UTI	1	0

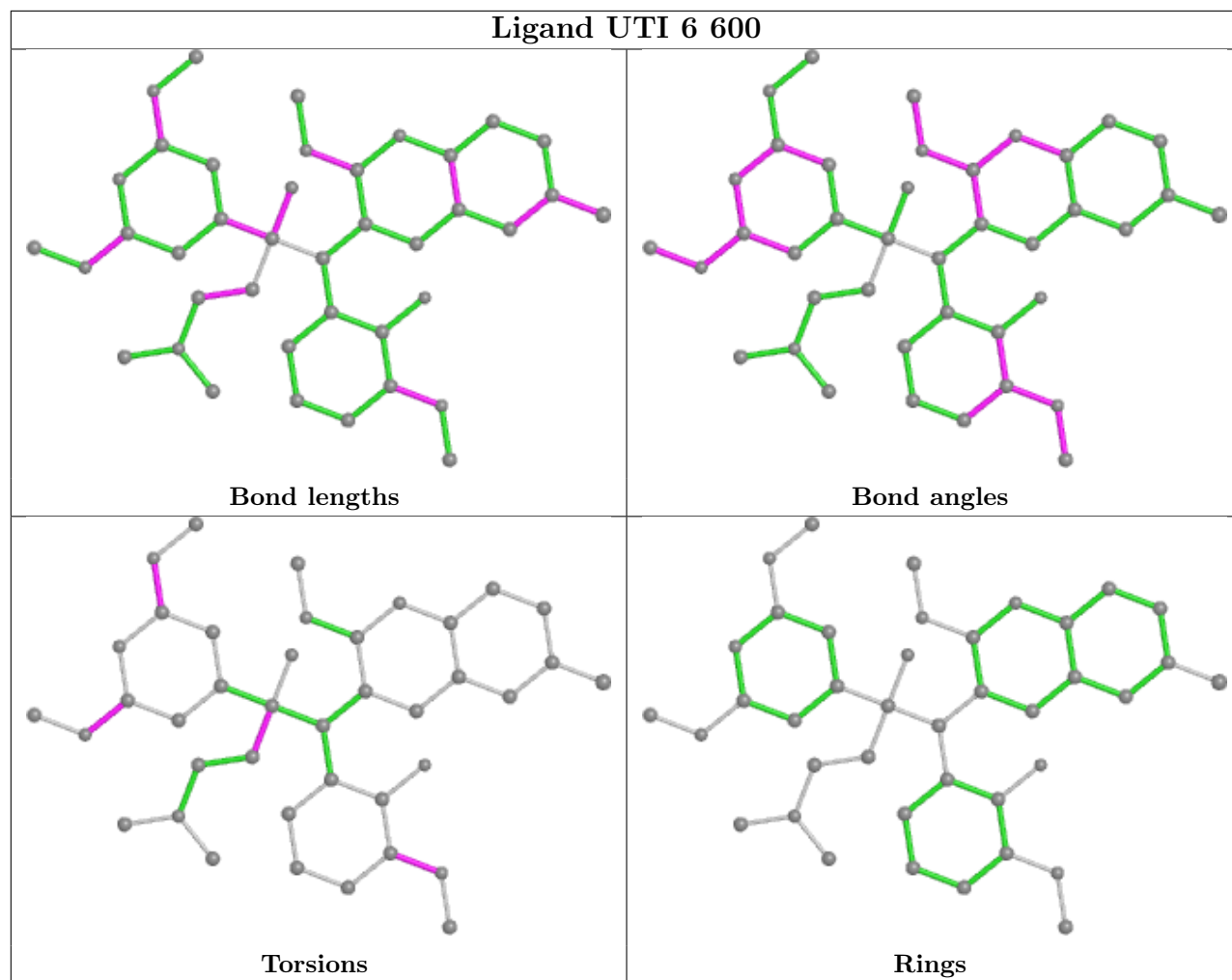
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

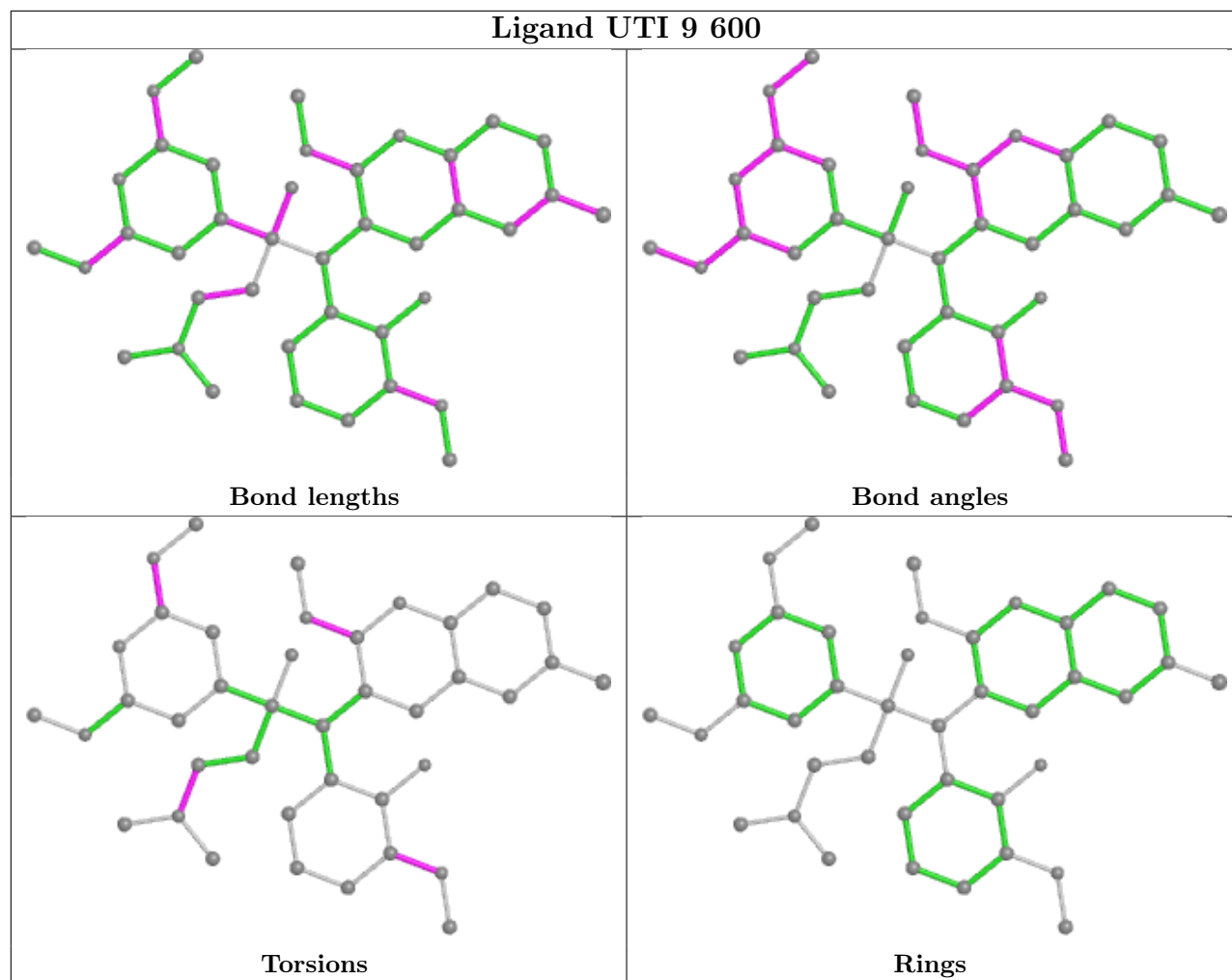


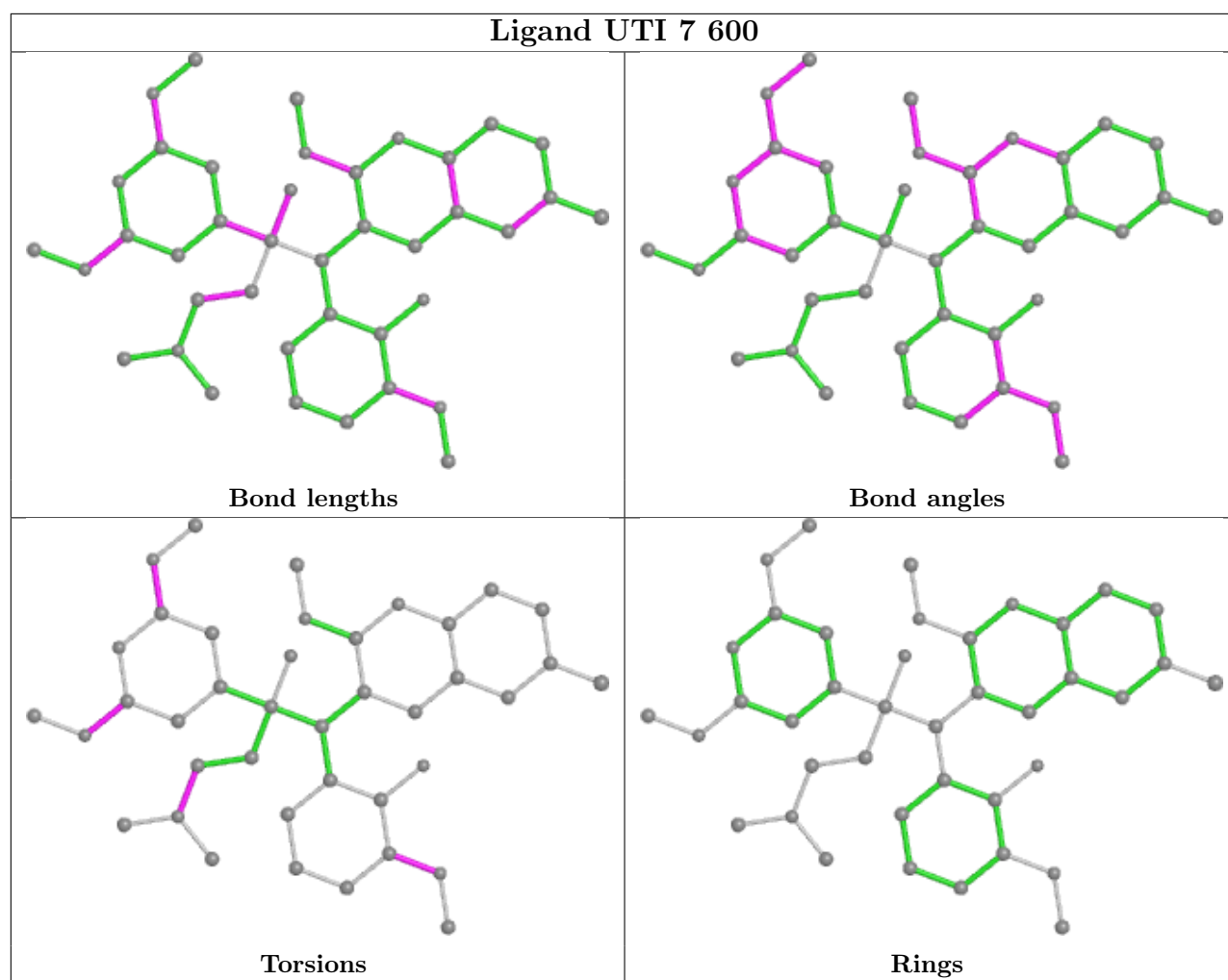












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

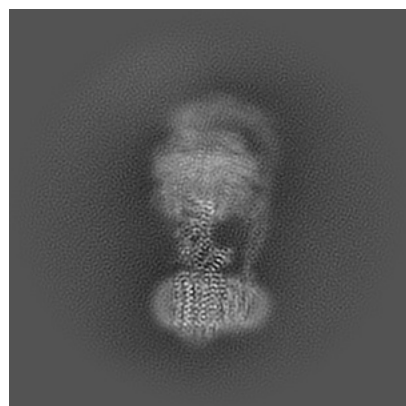
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36590. These allow visual inspection of the internal detail of the map and identification of artifacts.

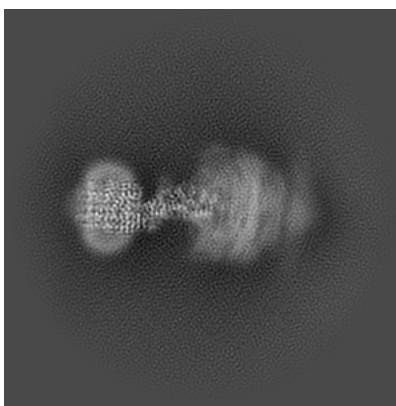
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

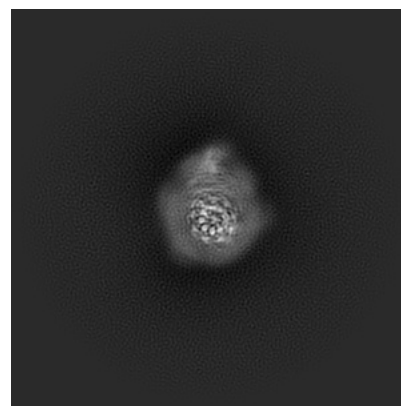
6.1.1 Primary map



X

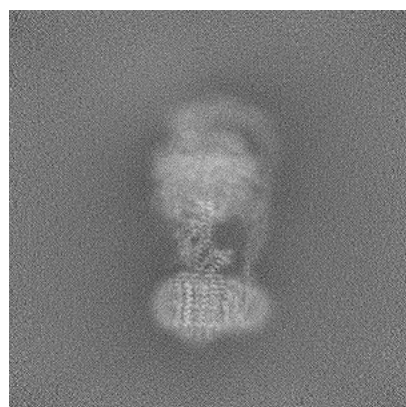


Y

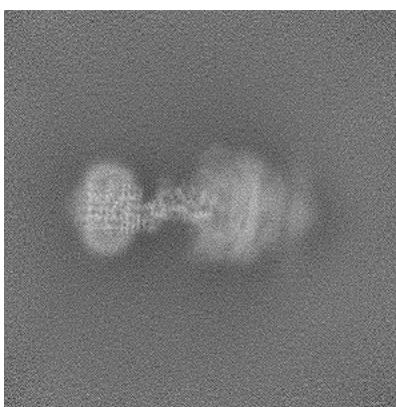


Z

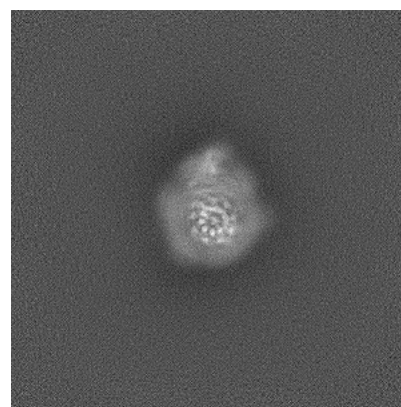
6.1.2 Raw map



X



Y

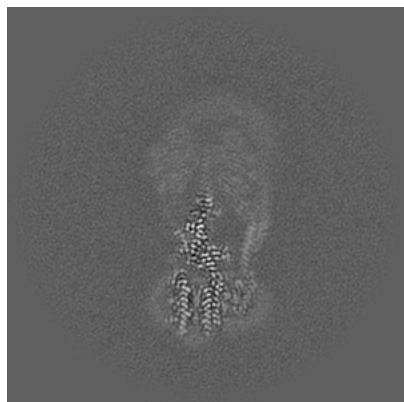


Z

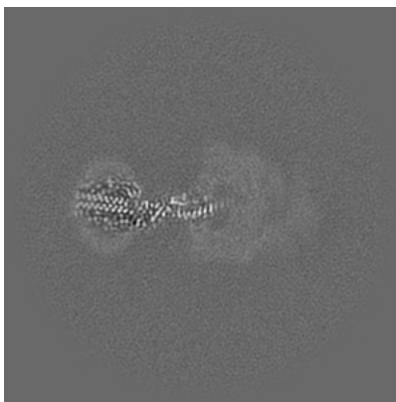
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

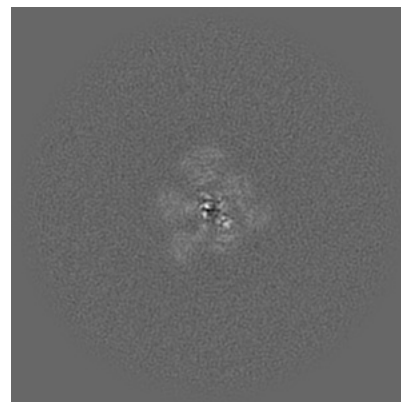
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

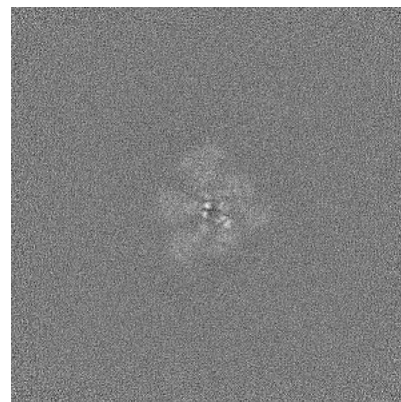
6.2.2 Raw map



X Index: 256



Y Index: 256

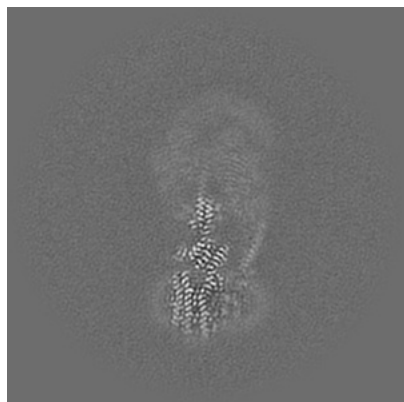


Z Index: 256

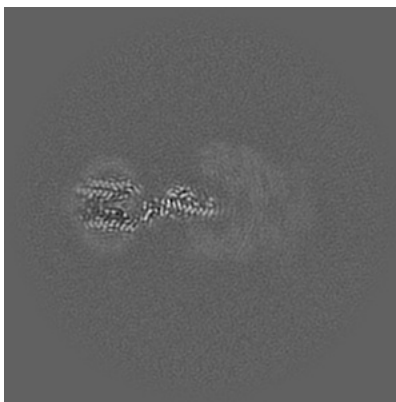
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

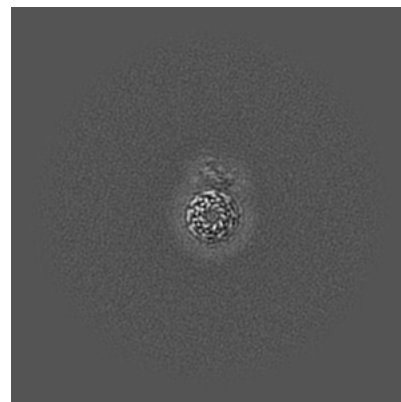
6.3.1 Primary map



X Index: 249

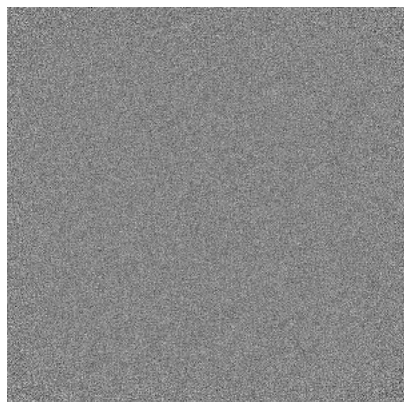


Y Index: 246

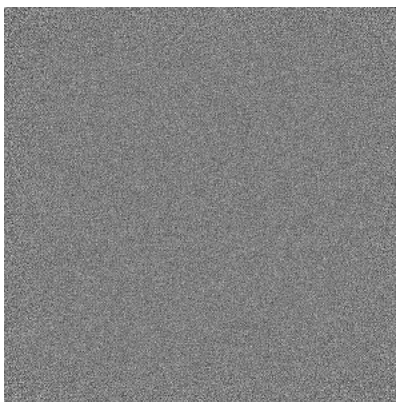


Z Index: 157

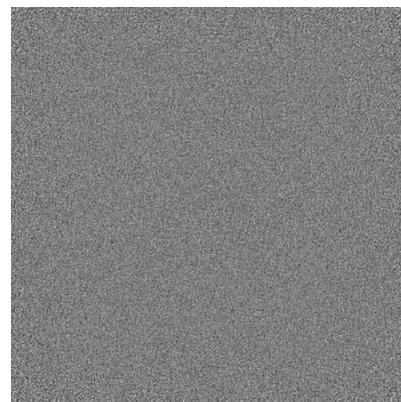
6.3.2 Raw map



X Index: 0



Y Index: 0

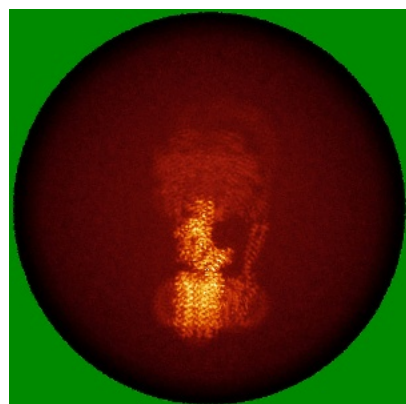


Z Index: 0

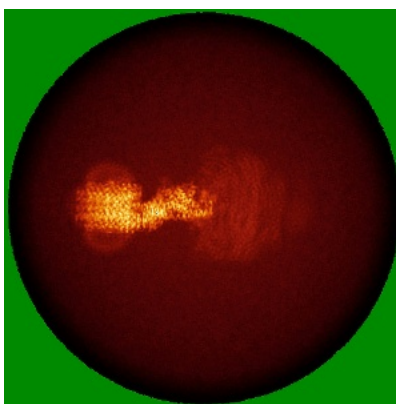
The images above show the largest variance slices of the map in three orthogonal directions.

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

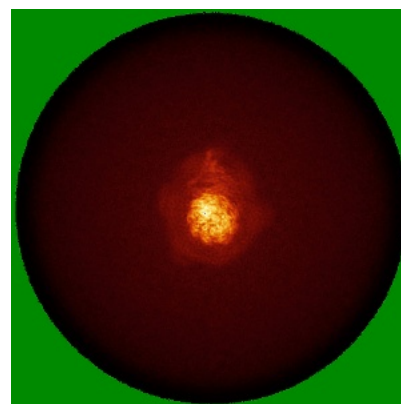
6.4.1 Primary map



X

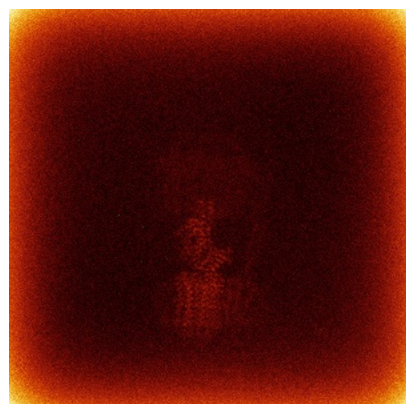


Y

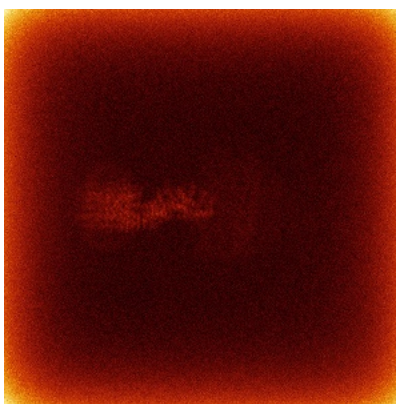


Z

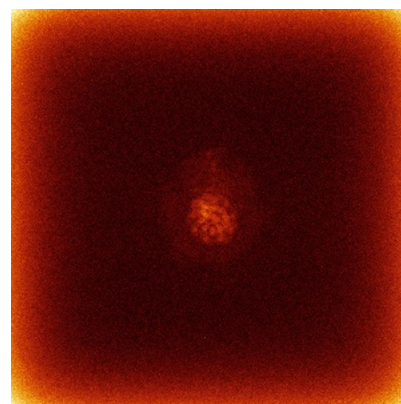
6.4.2 Raw map



X



Y

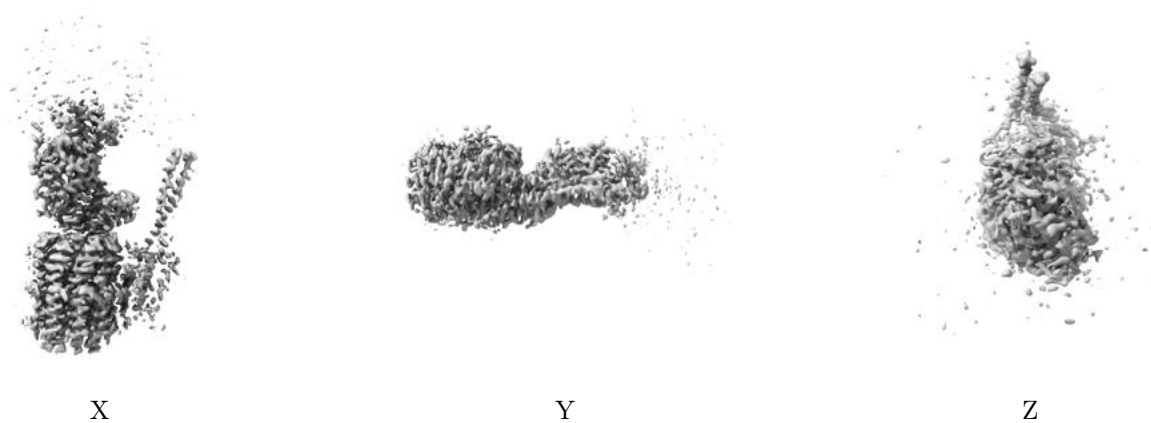


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

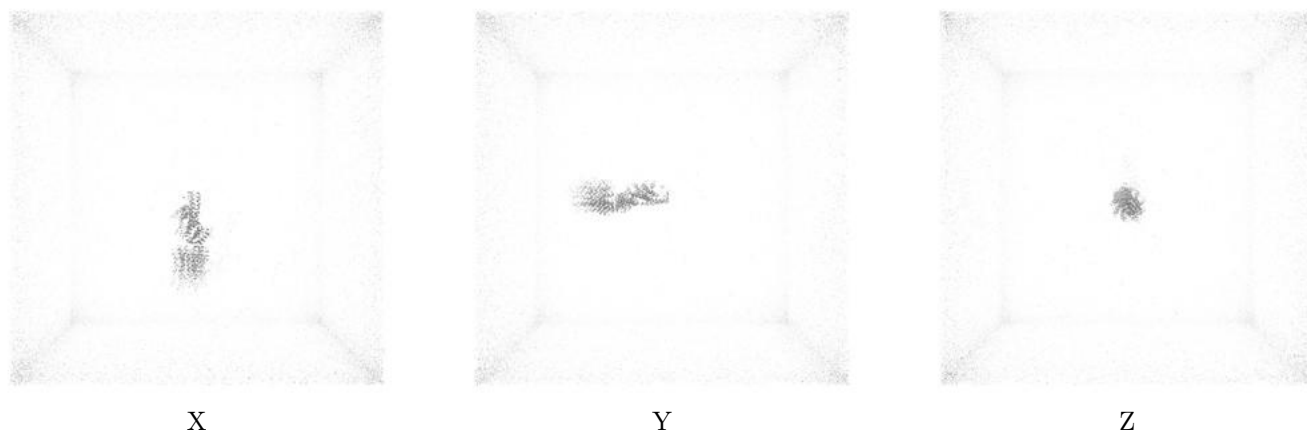
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

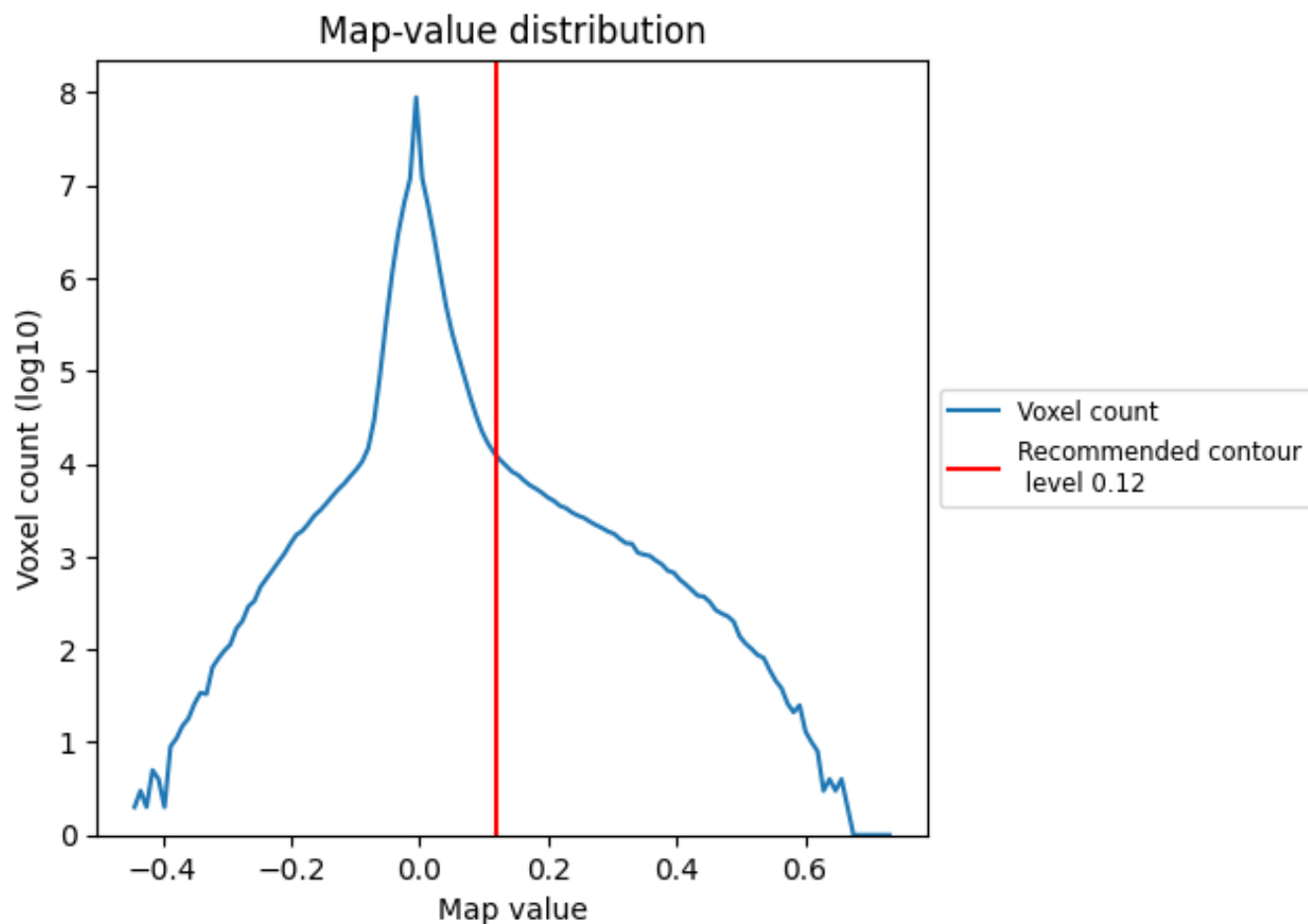
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

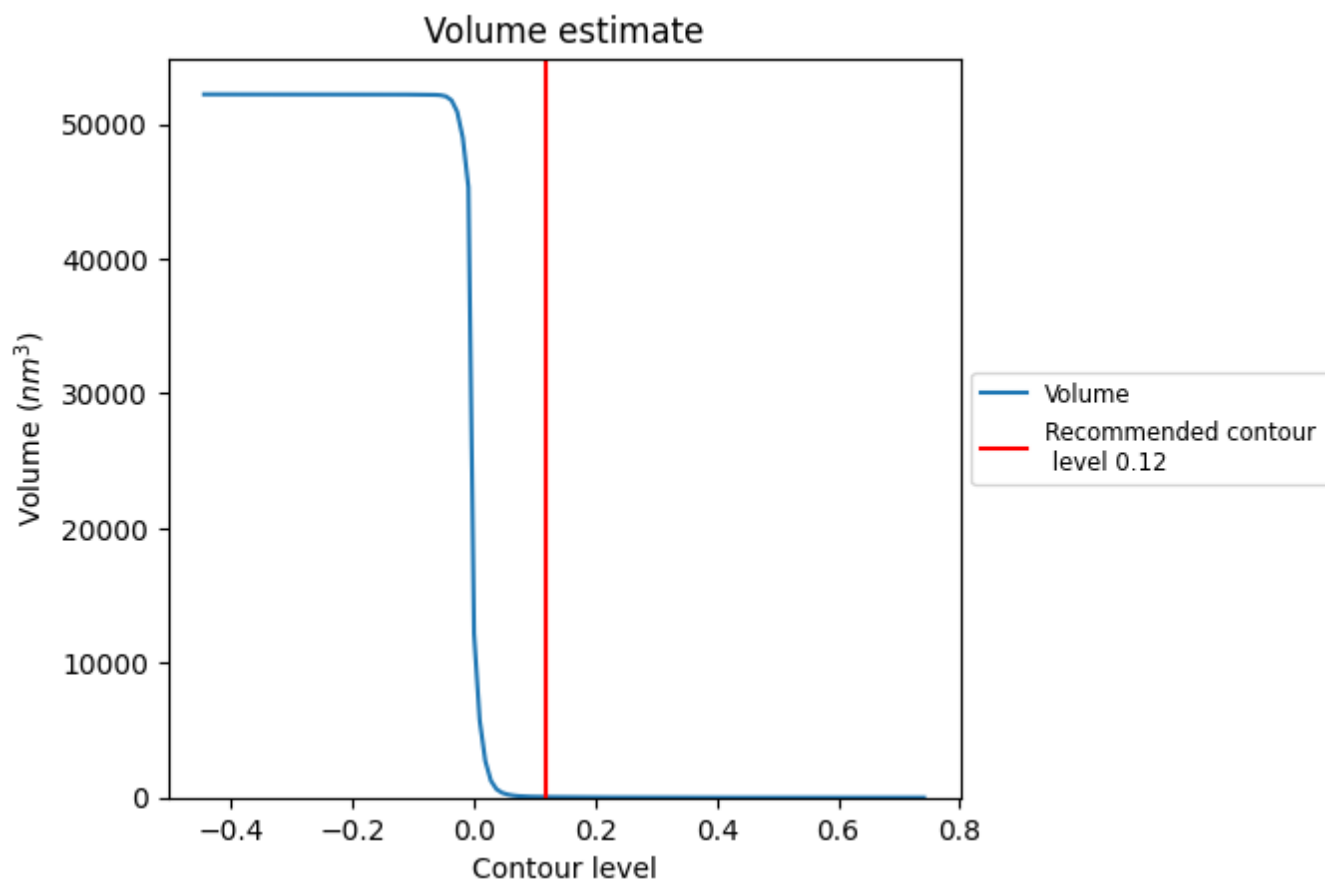
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

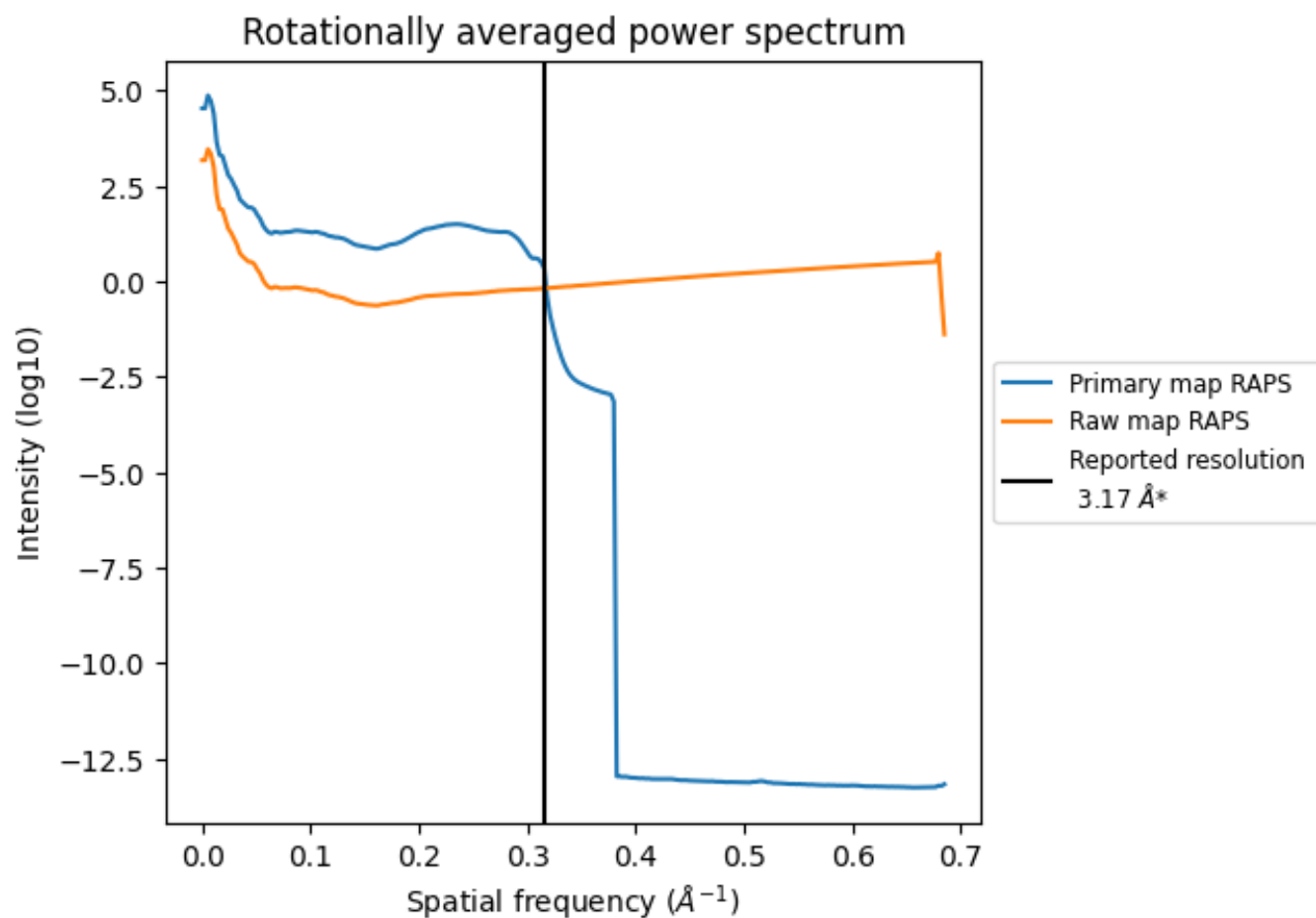
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 45 nm^3 ; this corresponds to an approximate mass of 40 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 ⓘ

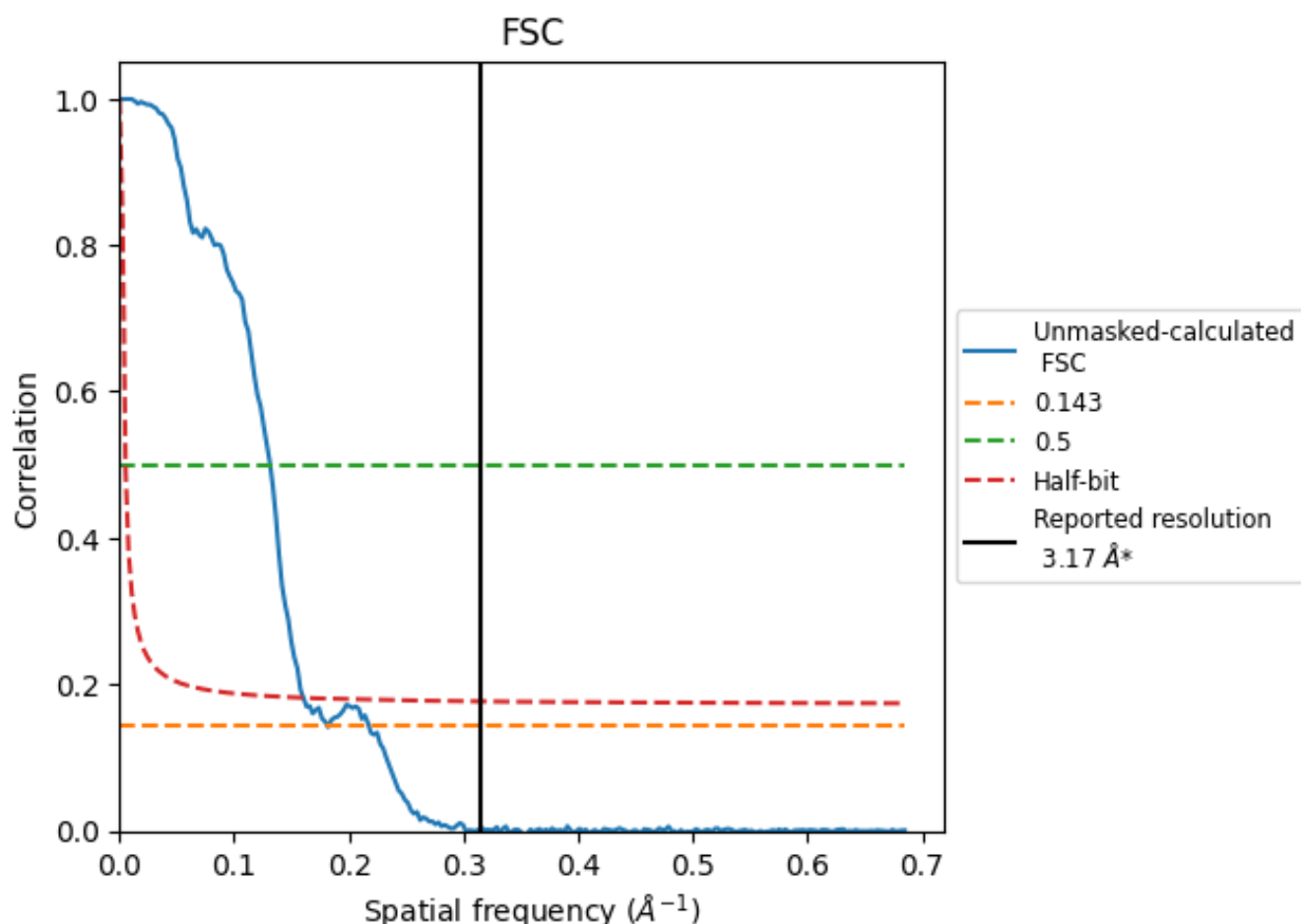


*Reported resolution corresponds to spatial frequency of 0.315 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.315 \AA^{-1}

8.2 Resolution estimates [i](#)

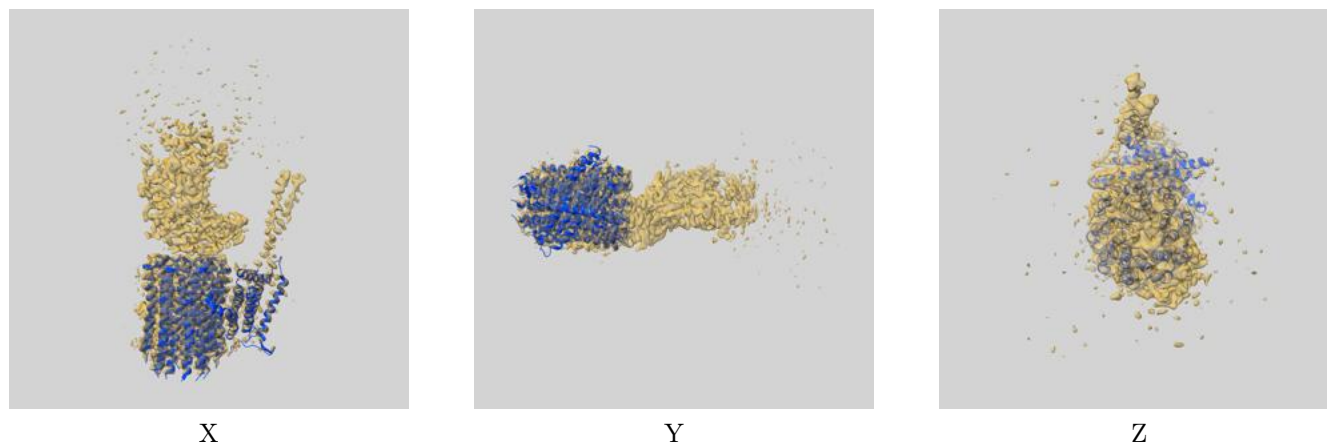
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.17	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.51	7.61	6.23

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.51 differs from the reported value 3.17 by more than 10 %

9 Map-model fit [i](#)

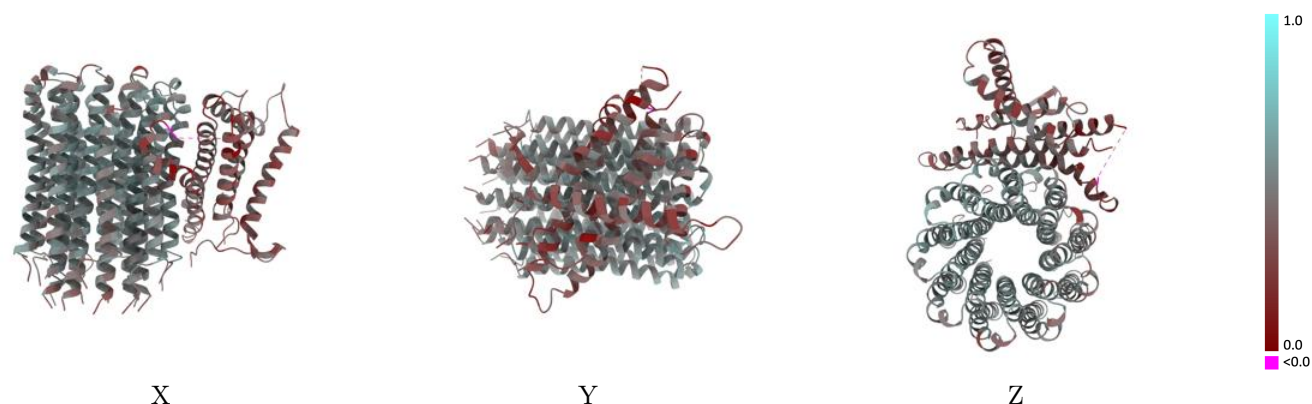
This section contains information regarding the fit between EMDB map EMD-36590 and PDB model 8JR1. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



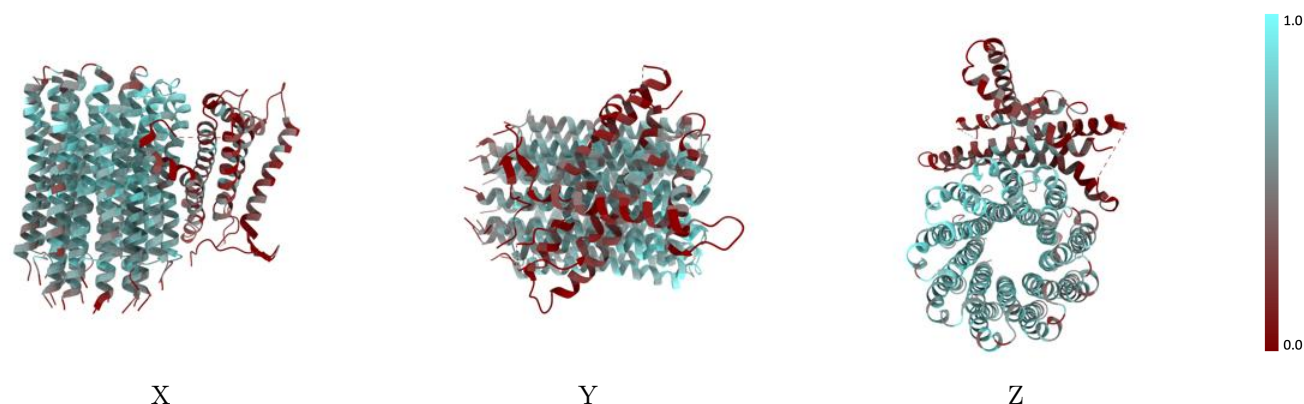
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



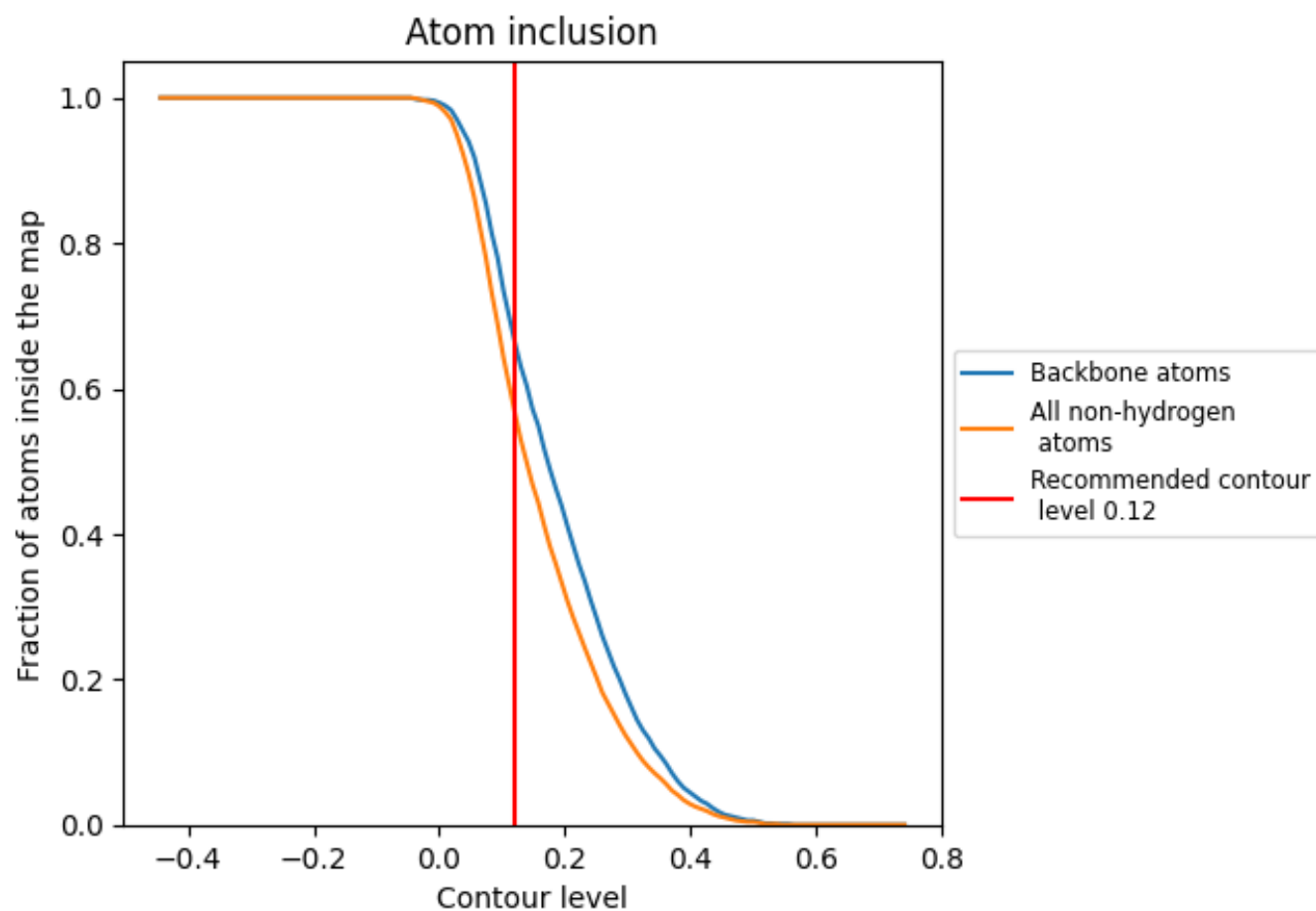
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 57% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5690	<div></div> 0.4630
1	<div></div> 0.6410	<div></div> 0.4760
2	<div></div> 0.6980	<div></div> 0.5100
3	<div></div> 0.7120	<div></div> 0.5240
4	<div></div> 0.7190	<div></div> 0.5260
5	<div></div> 0.7140	<div></div> 0.5250
6	<div></div> 0.6730	<div></div> 0.5090
7	<div></div> 0.6590	<div></div> 0.5040
8	<div></div> 0.6430	<div></div> 0.4980
9	<div></div> 0.6130	<div></div> 0.4900
a	<div></div> 0.2430	<div></div> 0.3260

1.0
0.0
<0.0