



wwPDB EM Validation Summary Report ⓘ

Mar 14, 2024 – 04:43 PM EDT

PDB ID : 8UXX
EMDB ID : EMD-42788
Title : Arp2/3 branch junction complex, BeFx state
Authors : Chavali, S.S.; Chou, S.Z.; Sindelar, C.V.
Deposited on : 2023-11-11
Resolution : 3.20 Å(reported)

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<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.dev70
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

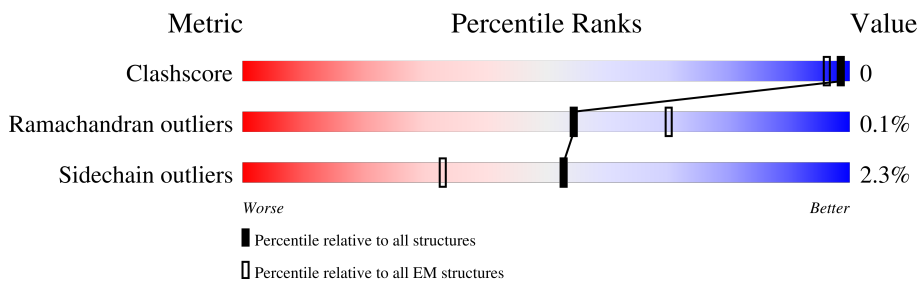
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	A	427	
2	B	390	
3	C	377	
4	D	317	
5	E	174	
6	F	168	
7	G	152	
8	H	377	

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Mol	Chain	Length	Quality of chain
8	I	377	 92% 6% ..
8	M	377	 94% ..
8	N	377	 94% ..
8	O	377	 94% ..
8	P	377	 92% 5% ..
8	Q	377	 95% ..
8	R	377	 94% ..

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 77522 atoms, of which 38460 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 Actin-related protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	400	Total	C	H	N	O	S	0	0
			6226	2002	3065	540	608	11		

- Molecule 2 is a protein called Actin-related protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	B	387	Total	C	H	N	O	S	0	0
			6153	1969	3073	530	566	15		

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	C	362	Total	C	H	N	O	S	0	0
			5576	1785	2751	501	532	7		

- Molecule 4 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	D	316	Total	C	H	N	O	S	0	0
			5153	1652	2563	445	482	11		

- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	E	172	Total	C	H	N	O	S	0	0
			2746	889	1361	237	251	8		

- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	F	168	Total	C	H	N	O	S	0	0
			2781	877	1404	234	258	8		

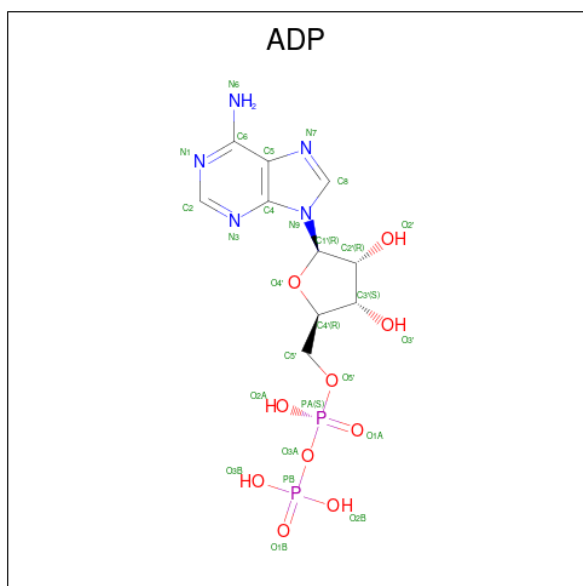
- Molecule 7 is a protein called Actin-related protein 2/3 complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	G	151	2362	746	1179	202	233	2	0	0

- Molecule 8 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	H	370	5760	1833	2867	488	551	21	0	0
8	I	370	5760	1833	2867	488	551	21	0	0
8	M	370	5760	1833	2867	488	551	21	0	0
8	N	370	5758	1833	2865	488	551	21	0	0
8	O	370	5760	1833	2867	488	551	21	0	0
8	P	370	5760	1833	2867	488	551	21	0	0
8	Q	370	5760	1833	2867	488	551	21	0	0
8	R	370	5760	1833	2867	488	551	21	0	0

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

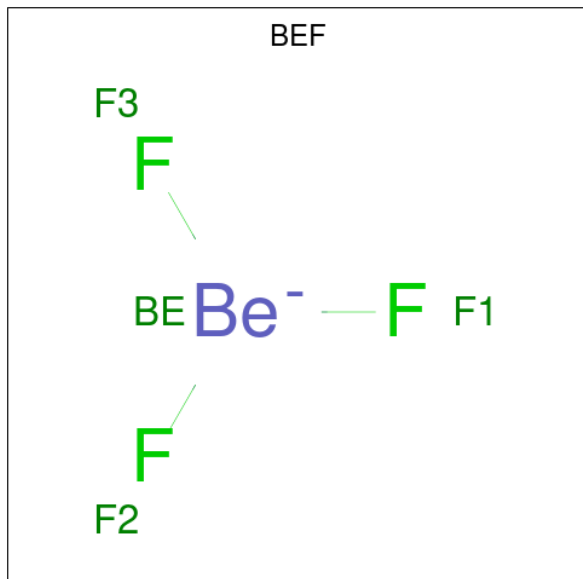


Mol	Chain	Residues	Atoms					AltConf	
9	A	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
9	H	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
9	I	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
9	M	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
9	N	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
9	O	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
9	P	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
9	Q	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
9	R	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

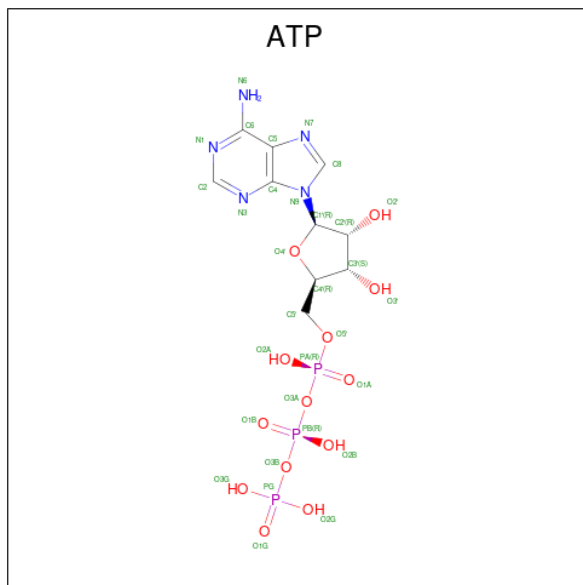
Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Mg	0
			1	1	
10	B	1	Total	Mg	0
			1	1	
10	H	1	Total	Mg	0
			1	1	
10	I	1	Total	Mg	0
			1	1	
10	M	1	Total	Mg	0
			1	1	
10	N	1	Total	Mg	0
			1	1	
10	O	1	Total	Mg	0
			1	1	
10	P	1	Total	Mg	0
			1	1	
10	Q	1	Total	Mg	0
			1	1	
10	R	1	Total	Mg	0
			1	1	

- Molecule 11 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
11	A	1	4	1	3	0
11	M	1	4	1	3	0
11	N	1	4	1	3	0
11	O	1	4	1	3	0
11	P	1	4	1	3	0
11	Q	1	4	1	3	0
11	R	1	4	1	3	0

- Molecule 12 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
12	B	1	43	10	12	5	13	3	0

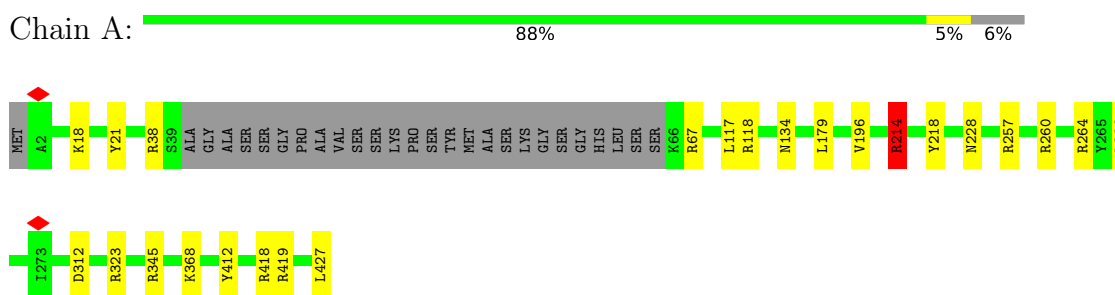
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		AltConf	
			Total	H		O
13	A	5	15	10	5	0

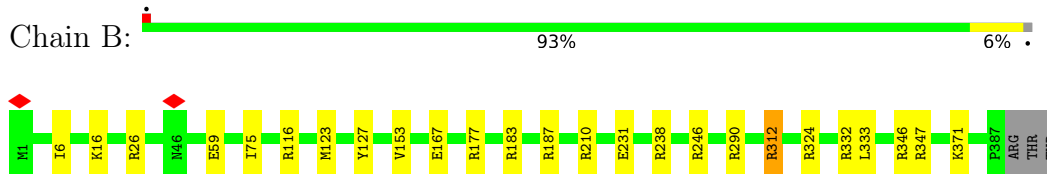
3 Residue-property plots [i](#)

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.

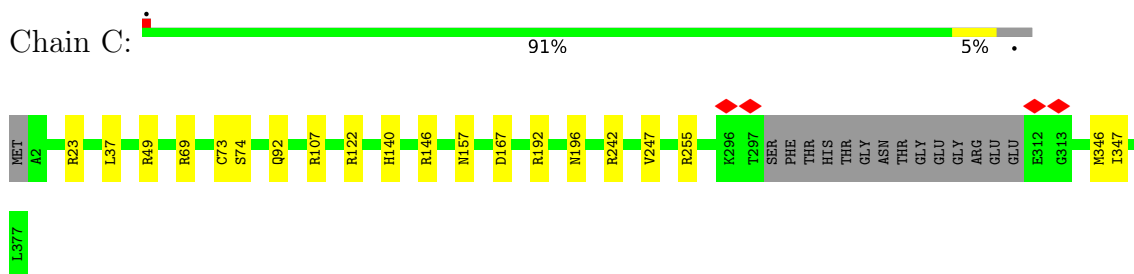
- Molecule 1: Actin-related protein 3



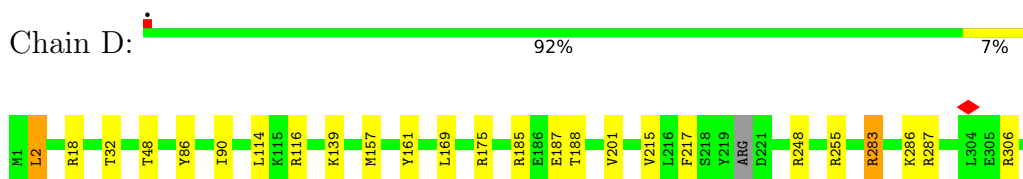
- Molecule 2: Actin-related protein 2



- Molecule 3: Actin-related protein 2/3 complex subunit 1



- Molecule 4: Actin-related protein 2/3 complex subunit 2



- Molecule 5: Actin-related protein 2/3 complex subunit 3

Chain E: 90% 8% ..



- Molecule 6: Actin-related protein 2/3 complex subunit 4

Chain F: 92% 8%



- Molecule 7: Actin-related protein 2/3 complex subunit 5

Chain G: 94% 5% ..



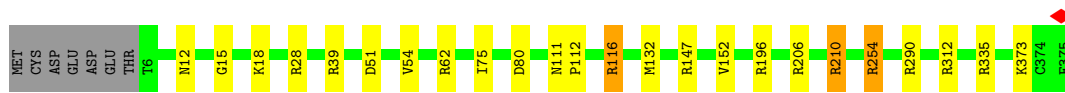
- Molecule 8: Actin, alpha skeletal muscle

Chain H: 95% ...



- Molecule 8: Actin, alpha skeletal muscle

Chain I: 92% 6% ..



- Molecule 8: Actin, alpha skeletal muscle

Chain M: 94% ..



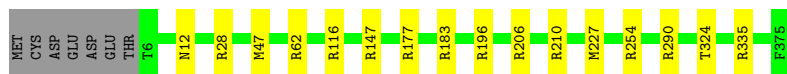
- Molecule 8: Actin, alpha skeletal muscle

Chain N: 94% ..



- Molecule 8: Actin, alpha skeletal muscle

Chain O:  94%



- Molecule 8: Actin, alpha skeletal muscle

Chain P:  92%



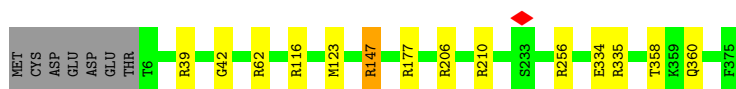
- Molecule 8: Actin, alpha skeletal muscle

Chain Q:  95%



- Molecule 8: Actin, alpha skeletal muscle

Chain R:  94%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	200000	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 ($e^-/\text{\AA}^2$)	51.4	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.244	Depositor
Minimum map value	-1.269	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.23	Depositor
Map size (\AA)	344.576, 344.576, 344.576	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.346, 1.346, 1.346	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: ADP, HIC, MG, ATP, BEF

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.64	0/3235	1.05	13/4384 (0.3%)
2	B	0.64	0/3147	1.08	13/4257 (0.3%)
3	C	0.62	0/2902	1.07	9/3963 (0.2%)
4	D	0.64	0/2647	1.02	6/3575 (0.2%)
5	E	0.67	0/1422	1.02	5/1924 (0.3%)
6	F	0.65	0/1398	1.10	7/1879 (0.4%)
7	G	0.60	0/1202	1.06	5/1640 (0.3%)
8	H	0.62	0/2943	1.01	11/3984 (0.3%)
8	I	0.65	0/2943	1.01	13/3984 (0.3%)
8	M	0.63	0/2943	0.99	11/3984 (0.3%)
8	N	0.62	0/2943	1.00	13/3984 (0.3%)
8	O	0.61	0/2943	1.07	15/3984 (0.4%)
8	P	0.61	0/2943	1.03	13/3984 (0.3%)
8	Q	0.60	0/2943	1.03	9/3984 (0.2%)
8	R	0.62	0/2943	1.04	11/3984 (0.3%)
All	All	0.63	0/39497	1.04	154/53494 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	2
3	C	0	1
4	D	0	2
6	F	0	2
8	H	0	2
8	I	0	1
8	M	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	N	0	1
8	P	0	3
8	Q	0	1
8	R	0	1
All	All	0	19

There are no bond length outliers.

The worst 5 of 154 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	210	ARG	NE-CZ-NH2	11.72	126.16	120.30
8	O	183	ARG	NE-CZ-NH2	11.36	125.98	120.30
8	R	39	ARG	NE-CZ-NH2	10.76	125.68	120.30
8	R	62	ARG	NE-CZ-NH2	10.04	125.32	120.30
8	M	210	ARG	NE-CZ-NH2	9.71	125.16	120.30

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	ARG	Sidechain
1	A	412	TYR	Sidechain
2	B	127	TYR	Sidechain
2	B	312	ARG	Sidechain
3	C	122	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3161	3065	3063	1	0
2	B	3080	3073	3073	0	0
3	C	2825	2751	2747	0	0
4	D	2590	2563	2562	5	0
5	E	1385	1361	1360	2	0
6	F	1377	1404	1404	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1183	1179	1178	0	0
8	H	2893	2867	2865	0	0
8	I	2893	2867	2865	1	0
8	M	2893	2867	2865	0	0
8	N	2893	2865	2863	0	0
8	O	2893	2867	2865	0	0
8	P	2893	2867	2865	1	0
8	Q	2893	2867	2865	0	0
8	R	2893	2867	2865	0	0
9	A	27	12	12	0	0
9	H	27	12	12	0	0
9	I	27	12	12	0	0
9	M	27	12	12	0	0
9	N	27	12	12	0	0
9	O	27	12	12	0	0
9	P	27	12	12	0	0
9	Q	27	12	12	0	0
9	R	27	12	12	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	H	1	0	0	0	0
10	I	1	0	0	0	0
10	M	1	0	0	0	0
10	N	1	0	0	0	0
10	O	1	0	0	0	0
10	P	1	0	0	0	0
10	Q	1	0	0	0	0
10	R	1	0	0	0	0
11	A	4	0	0	0	0
11	M	4	0	0	0	0
11	N	4	0	0	0	0
11	O	4	0	0	0	0
11	P	4	0	0	0	0
11	Q	4	0	0	0	0
11	R	4	0	0	0	0
12	B	31	12	12	0	0
13	A	5	10	0	0	0
All	All	39062	38460	38425	9	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 0.

The worst 5 of 9 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)
4:D:201:VAL:HG21	4:D:217:PHE:HB3	1.95	0.47
1:A:21:TYR:CE1	4:D:32:THR:HG22	2.49	0.47
4:D:2:LEU:HD22	6:F:163:THR:HG21	1.98	0.45
4:D:201:VAL:HG21	4:D:217:PHE:CB	2.47	0.45
8:I:75:ILE:HD12	8:I:112:PRO:CD	2.46	0.44

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	396/427 (93%)	381 (96%)	14 (4%)	1 (0%)	41	74
2	B	385/390 (99%)	366 (95%)	19 (5%)	0	100	100
3	C	358/377 (95%)	334 (93%)	24 (7%)	0	100	100
4	D	312/317 (98%)	303 (97%)	9 (3%)	0	100	100
5	E	168/174 (97%)	160 (95%)	8 (5%)	0	100	100
6	F	166/168 (99%)	162 (98%)	3 (2%)	1 (1%)	25	64
7	G	149/152 (98%)	145 (97%)	4 (3%)	0	100	100
8	H	367/377 (97%)	347 (95%)	20 (5%)	0	100	100
8	I	367/377 (97%)	351 (96%)	15 (4%)	1 (0%)	41	74
8	M	367/377 (97%)	350 (95%)	17 (5%)	0	100	100
8	N	367/377 (97%)	354 (96%)	13 (4%)	0	100	100
8	O	367/377 (97%)	346 (94%)	21 (6%)	0	100	100
8	P	367/377 (97%)	352 (96%)	15 (4%)	0	100	100
8	Q	367/377 (97%)	355 (97%)	11 (3%)	1 (0%)	41	74
8	R	367/377 (97%)	345 (94%)	20 (5%)	2 (0%)	29	67
All	All	4870/5021 (97%)	4651 (96%)	213 (4%)	6 (0%)	54	83

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	2	SER
8	R	360	GLN
1	A	179	LEU
8	I	15	GLY
8	Q	15	GLY

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	344/364 (94%)	334 (97%)	10 (3%)	42	74
2	B	329/335 (98%)	318 (97%)	11 (3%)	38	71
3	C	305/317 (96%)	295 (97%)	10 (3%)	38	71
4	D	285/287 (99%)	271 (95%)	14 (5%)	25	61
5	E	149/150 (99%)	142 (95%)	7 (5%)	26	62
6	F	157/157 (100%)	155 (99%)	2 (1%)	69	87
7	G	133/134 (99%)	130 (98%)	3 (2%)	50	78
8	H	312/319 (98%)	309 (99%)	3 (1%)	76	90
8	I	312/319 (98%)	301 (96%)	11 (4%)	36	69
8	M	312/319 (98%)	306 (98%)	6 (2%)	57	81
8	N	312/319 (98%)	310 (99%)	2 (1%)	86	94
8	O	312/319 (98%)	308 (99%)	4 (1%)	69	87
8	P	312/319 (98%)	306 (98%)	6 (2%)	57	81
8	Q	312/319 (98%)	307 (98%)	5 (2%)	62	84
8	R	312/319 (98%)	309 (99%)	3 (1%)	76	90
All	All	4198/4296 (98%)	4101 (98%)	97 (2%)	53	78

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	283	MET
8	M	18	LYS
8	H	315	LYS
8	I	111	ASN
8	M	346	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	131	GLN
8	H	246	GLN
8	I	161	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](#)

8 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
8	HIC	R	73	8	8,11,12	0.46	0	6,14,16	0.76	0
8	HIC	H	73	8	8,11,12	0.38	0	6,14,16	0.78	0
8	HIC	O	73	8	8,11,12	0.41	0	6,14,16	0.62	0
8	HIC	N	73	8	8,11,12	0.37	0	6,14,16	0.61	0
8	HIC	I	73	8	8,11,12	0.39	0	6,14,16	0.74	0
8	HIC	M	73	8	8,11,12	0.39	0	6,14,16	0.59	0
8	HIC	Q	73	8	8,11,12	0.42	0	6,14,16	0.69	0
8	HIC	P	73	8	8,11,12	0.41	0	6,14,16	0.72	0

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
8	HIC	R	73	8	-	2/5/6/8	0/1/1/1
8	HIC	H	73	8	-	2/5/6/8	0/1/1/1
8	HIC	O	73	8	-	0/5/6/8	0/1/1/1
8	HIC	N	73	8	-	0/5/6/8	0/1/1/1
8	HIC	I	73	8	-	0/5/6/8	0/1/1/1
8	HIC	M	73	8	-	0/5/6/8	0/1/1/1
8	HIC	Q	73	8	-	2/5/6/8	0/1/1/1
8	HIC	P	73	8	-	1/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	H	73	HIC	CA-CB-CG-ND1
8	H	73	HIC	CA-CB-CG-CD2
8	Q	73	HIC	CA-CB-CG-ND1
8	R	73	HIC	CA-CB-CG-ND1
8	R	73	HIC	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 10 are monoatomic - leaving 17 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$
9	ADP	I	802	10	24,29,29	1.02	0	29,45,45	1.69	8 (27%)
9	ADP	Q	401	10	24,29,29	1.05	1 (4%)	29,45,45	1.52	6 (20%)
11	BEF	A	503	-	0,3,3	-	-	-	-	-
11	BEF	R	403	-	0,3,3	-	-	-	-	-
9	ADP	A	501	10	24,29,29	1.04	1 (4%)	29,45,45	1.64	6 (20%)
9	ADP	M	401	10,11	24,29,29	0.96	1 (4%)	29,45,45	1.64	7 (24%)
11	BEF	Q	403	-	0,3,3	-	-	-	-	-
9	ADP	N	401	10,11	24,29,29	1.05	1 (4%)	29,45,45	1.61	8 (27%)
11	BEF	M	403	9	0,3,3	-	-	-	-	-
9	ADP	H	802	10	24,29,29	1.05	1 (4%)	29,45,45	1.79	8 (27%)
9	ADP	O	401	10	24,29,29	1.02	1 (4%)	29,45,45	1.48	5 (17%)
9	ADP	R	401	10	24,29,29	0.99	1 (4%)	29,45,45	1.49	4 (13%)
11	BEF	N	403	9	0,3,3	-	-	-	-	-
12	ATP	B	902	10	26,33,33	1.10	1 (3%)	31,52,52	1.53	6 (19%)
9	ADP	P	401	10	24,29,29	1.02	1 (4%)	29,45,45	1.60	6 (20%)
11	BEF	O	403	-	0,3,3	-	-	-	-	-
11	BEF	P	403	-	0,3,3	-	-	-	-	-

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
9	ADP	I	802	10	-	0/12/32/32	0/3/3/3
9	ADP	Q	401	10	-	0/12/32/32	0/3/3/3
9	ADP	A	501	10	-	0/12/32/32	0/3/3/3
9	ADP	M	401	10,11	-	1/12/32/32	0/3/3/3
9	ADP	N	401	10,11	-	0/12/32/32	0/3/3/3
9	ADP	H	802	10	-	1/12/32/32	0/3/3/3
9	ADP	O	401	10	-	0/12/32/32	0/3/3/3
9	ADP	R	401	10	-	0/12/32/32	0/3/3/3
12	ATP	B	902	10	-	1/18/38/38	0/3/3/3
9	ADP	P	401	10	-	0/12/32/32	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	O	401	ADP	C5-C4	-2.24	1.35	1.40
9	R	401	ADP	C5-C4	-2.17	1.35	1.40
12	B	902	ATP	C5-C4	-2.17	1.35	1.40
9	A	501	ADP	C5-C4	-2.17	1.35	1.40
9	P	401	ADP	C5-C4	-2.10	1.35	1.40

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	401	ADP	C4-C5-N7	4.67	114.27	109.40
9	R	401	ADP	C4-C5-N7	4.63	114.22	109.40
9	O	401	ADP	C4-C5-N7	4.51	114.10	109.40
9	H	802	ADP	C4-C5-N7	4.50	114.09	109.40
9	M	401	ADP	C4-C5-N7	4.49	114.08	109.40

There are no chirality outliers.

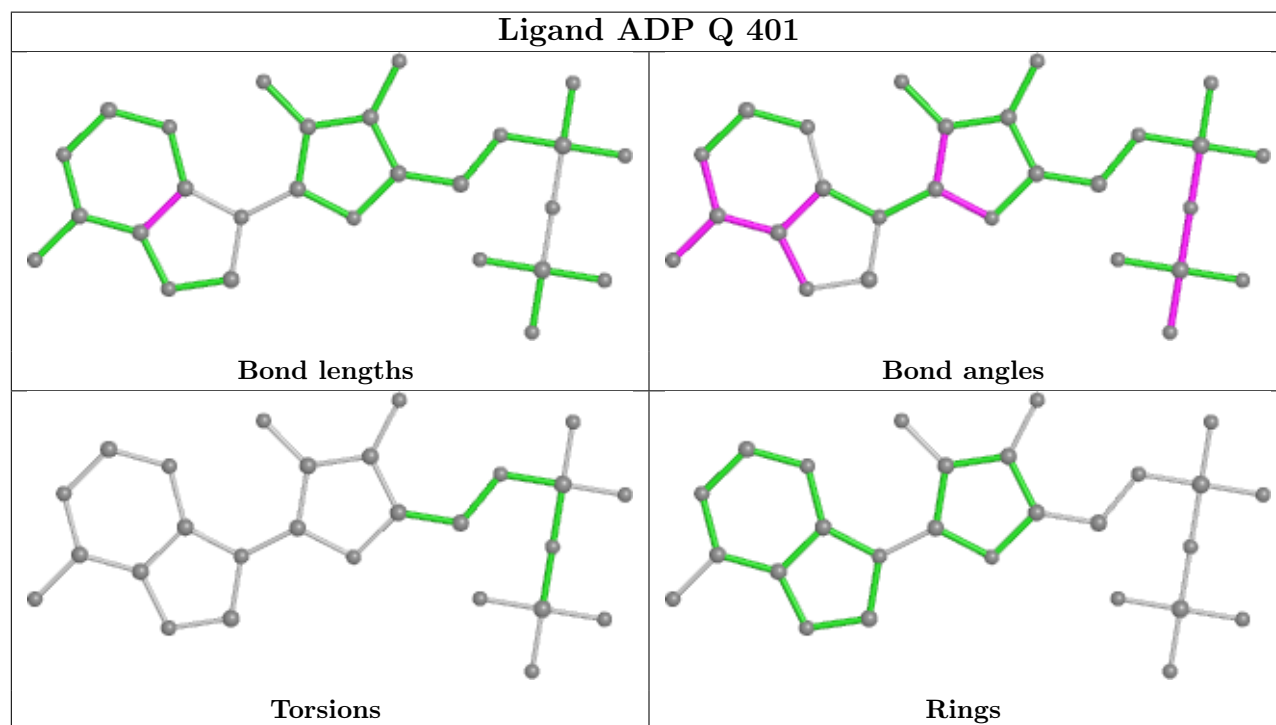
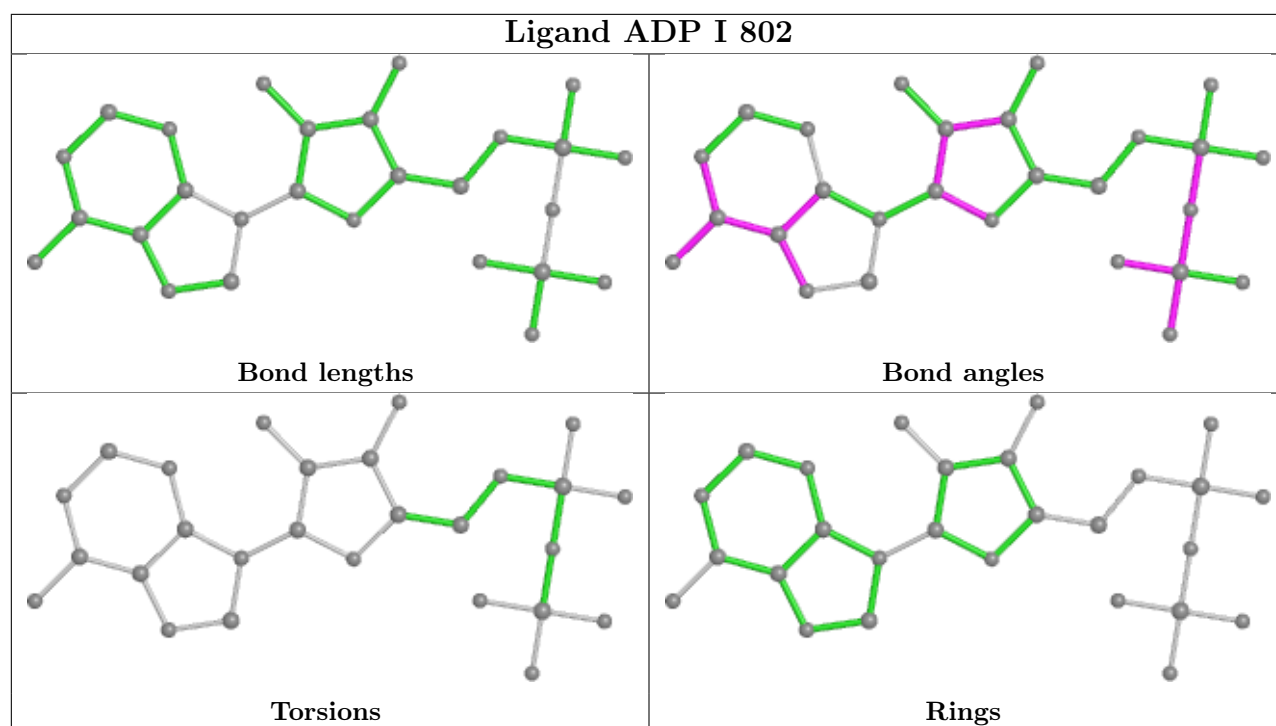
All (3) torsion outliers are listed below:

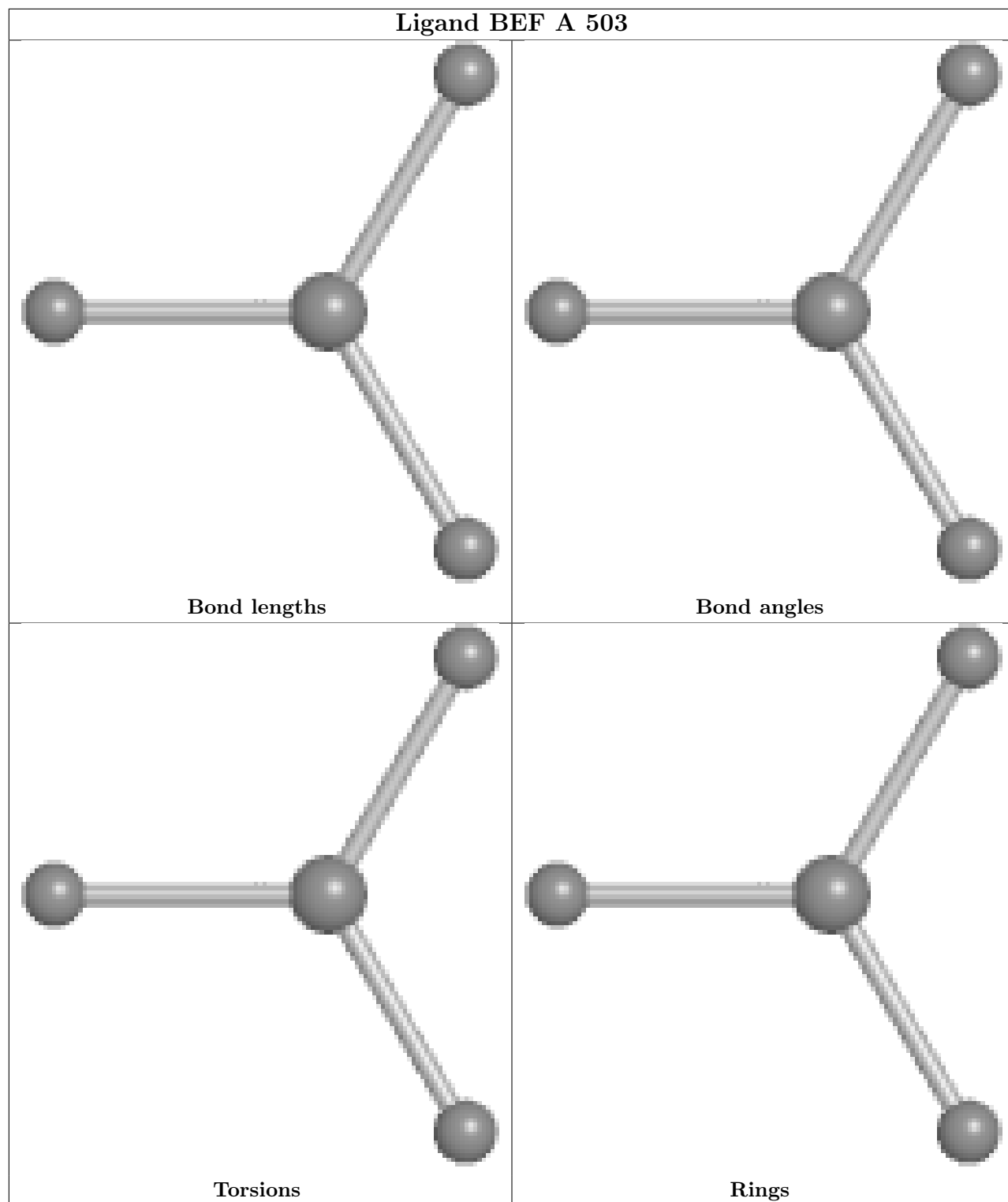
Mol	Chain	Res	Type	Atoms
9	H	802	ADP	PA-O3A-PB-O1B
9	M	401	ADP	PA-O3A-PB-O3B
12	B	902	ATP	PG-O3B-PB-O1B

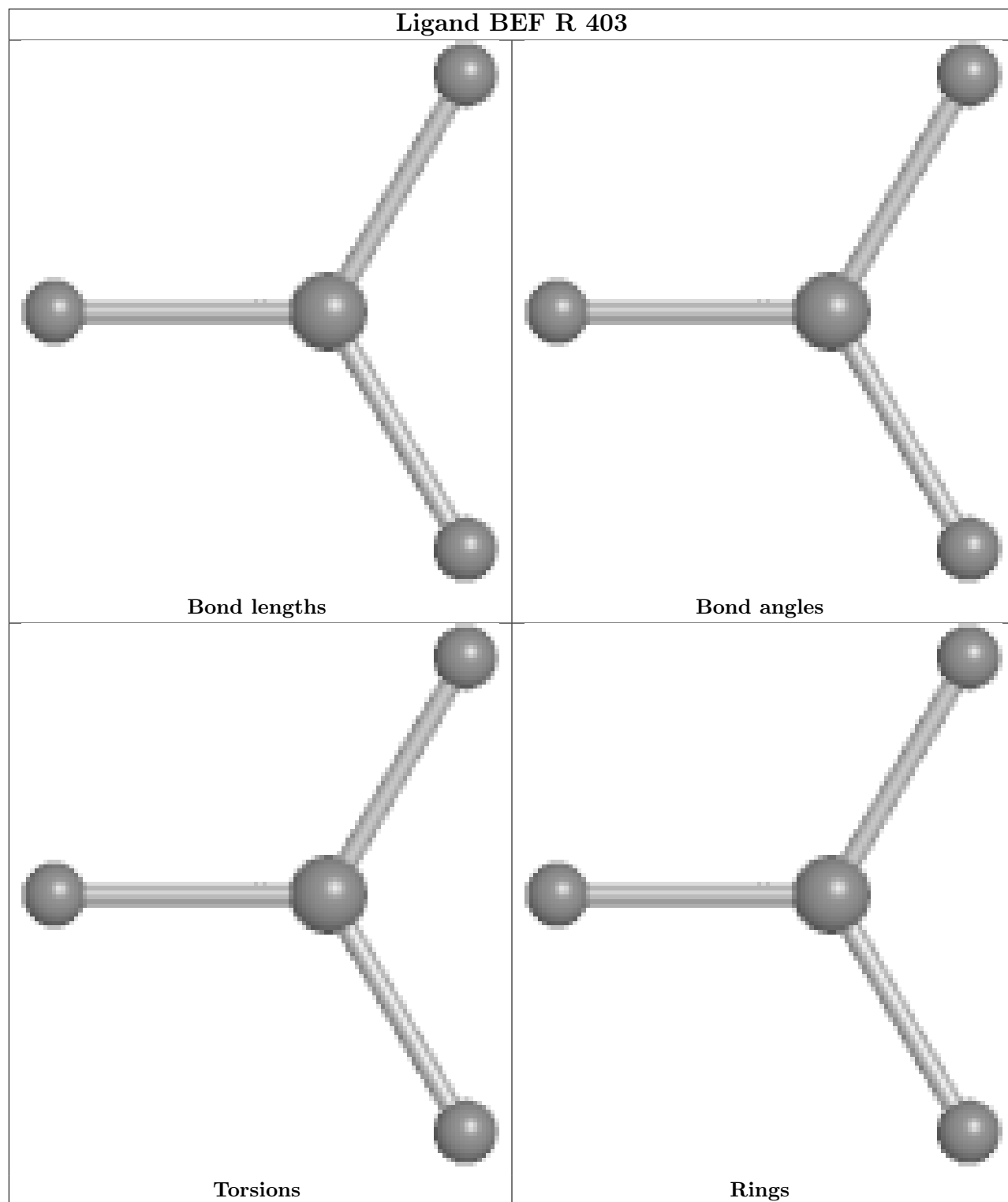
There are no ring outliers.

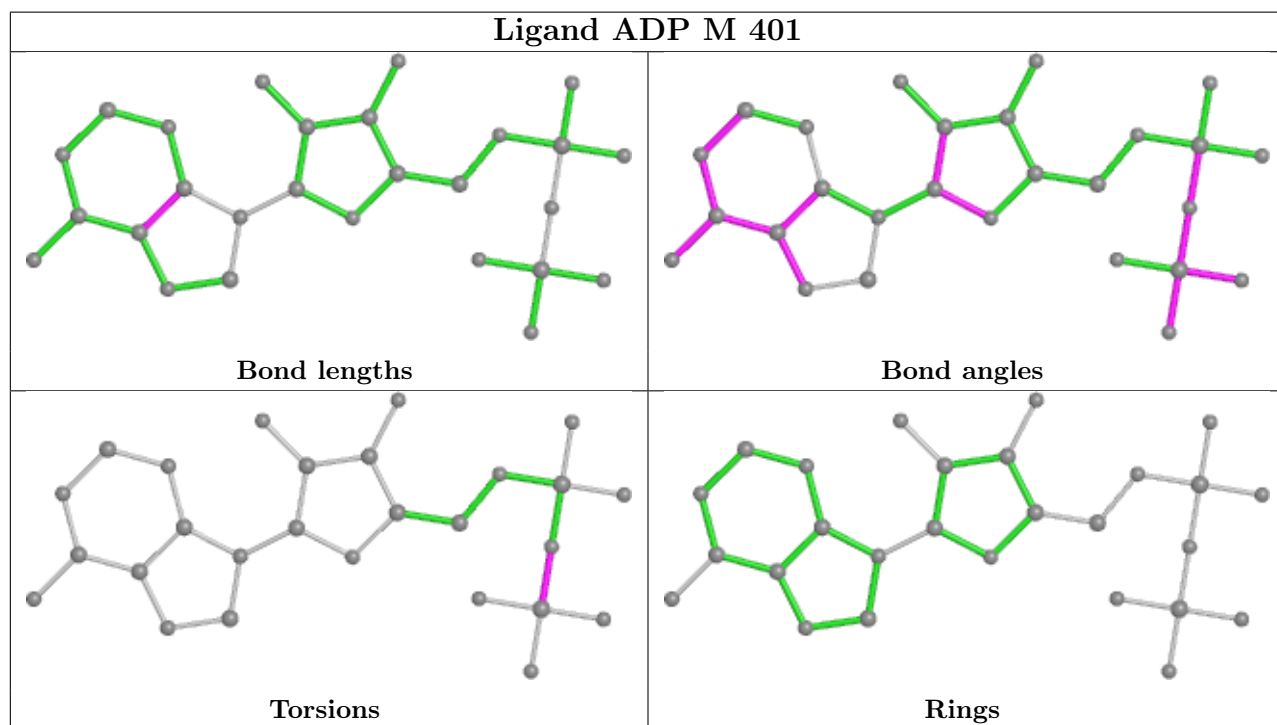
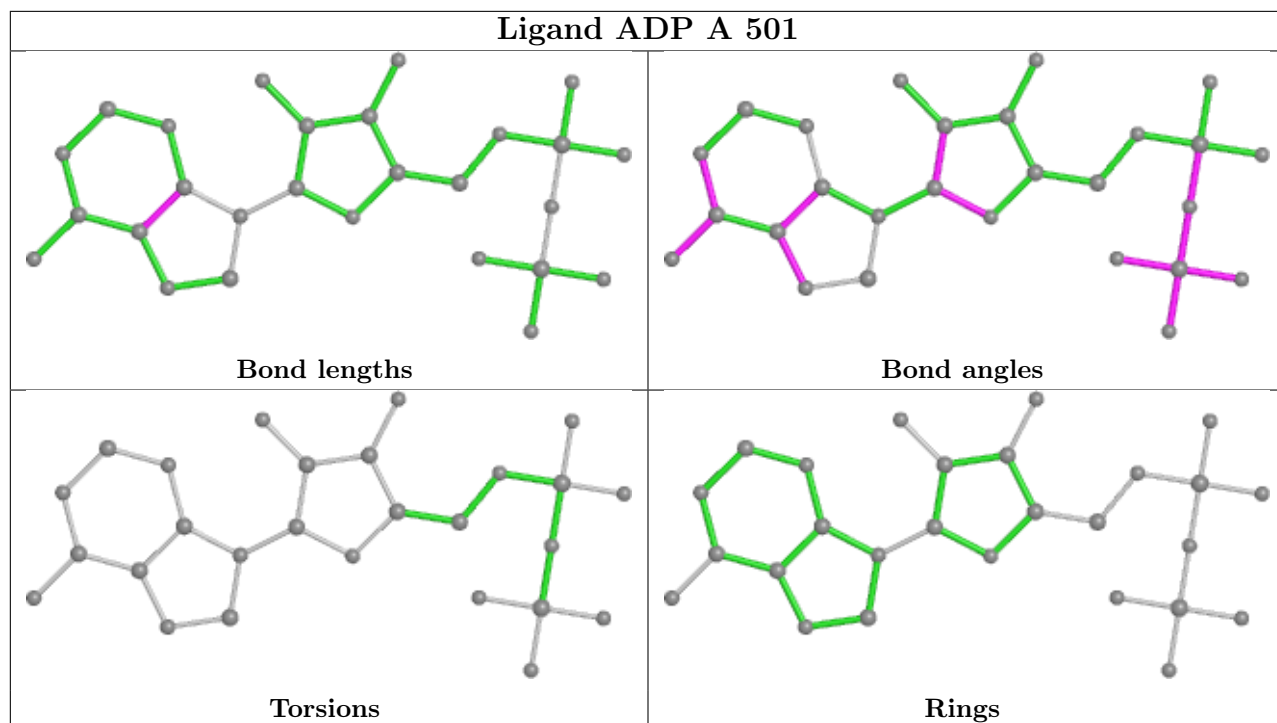
No monomer is involved in short contacts.

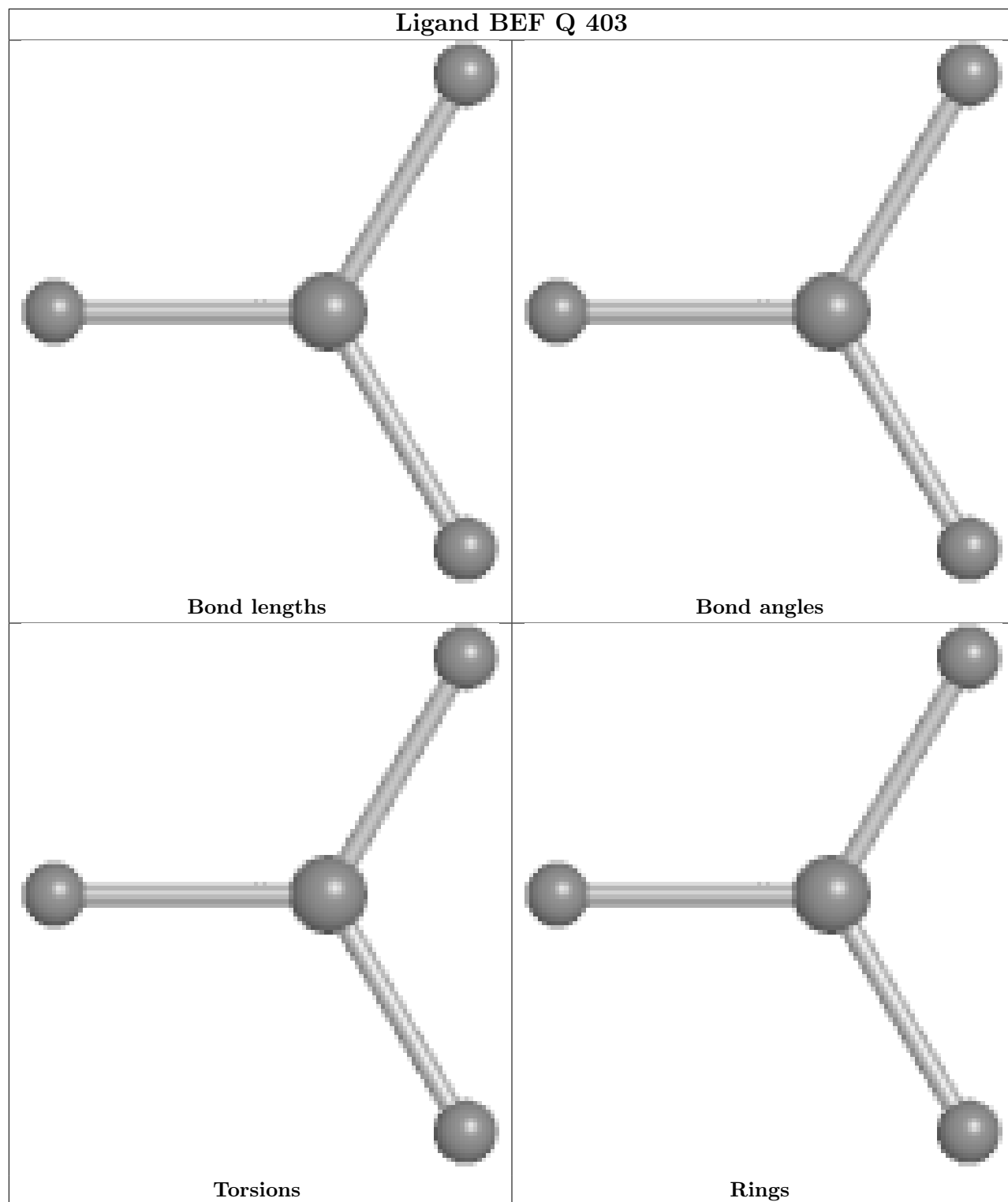
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

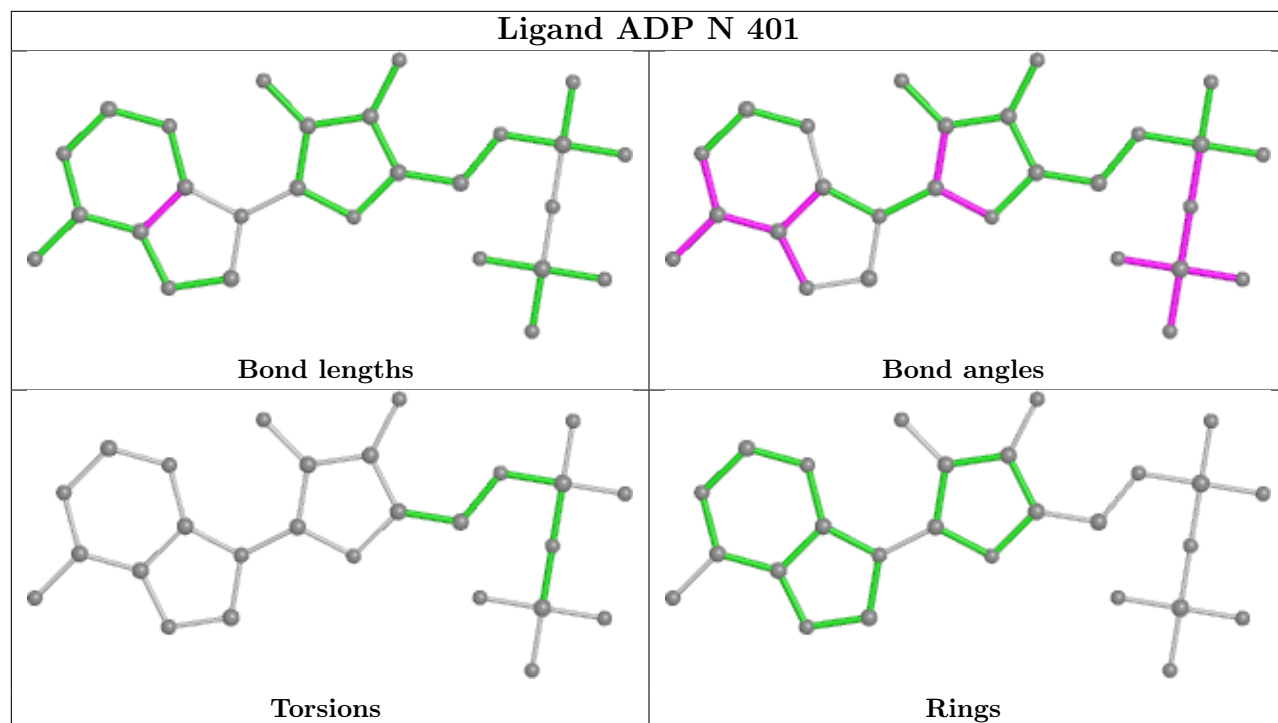


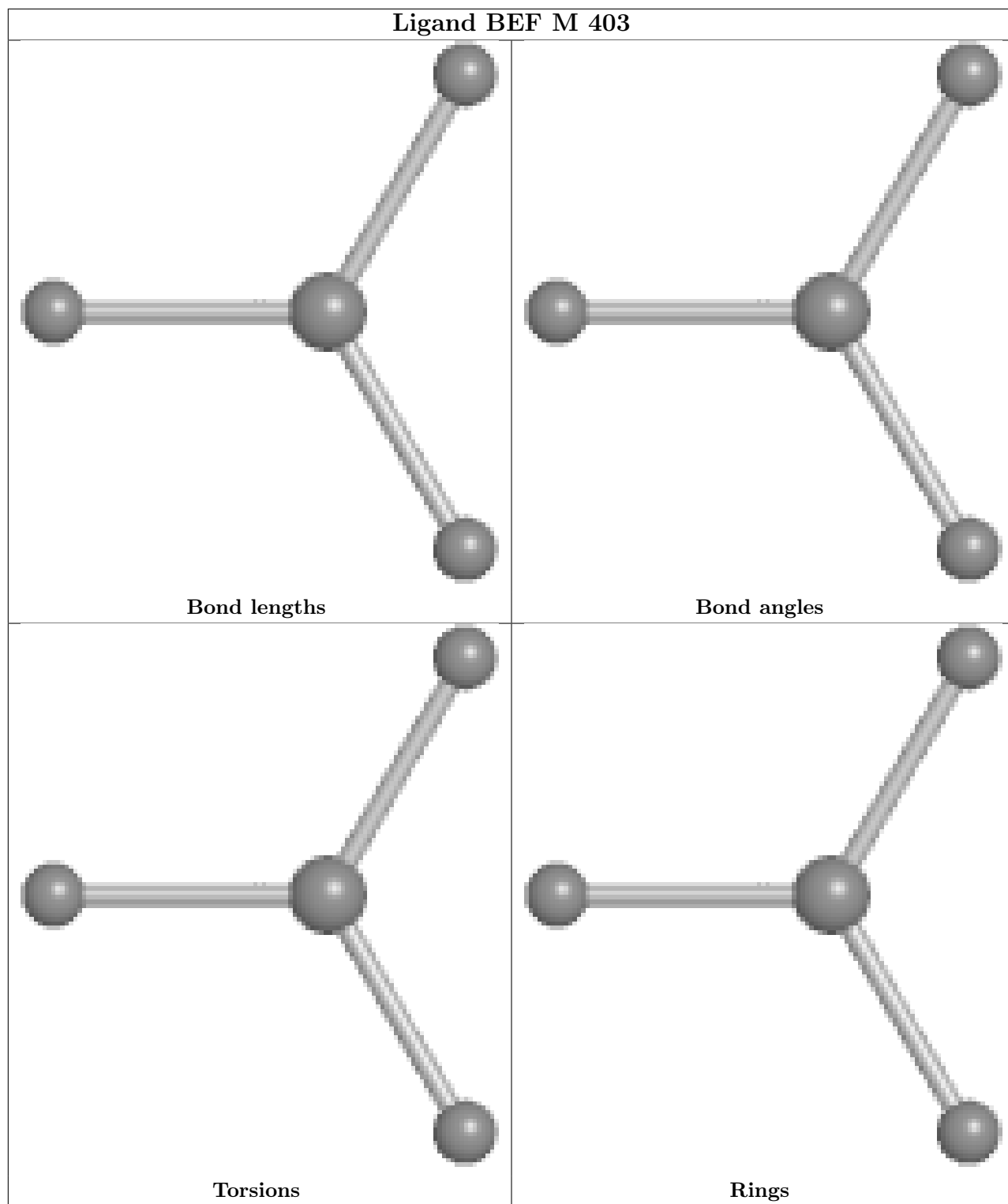


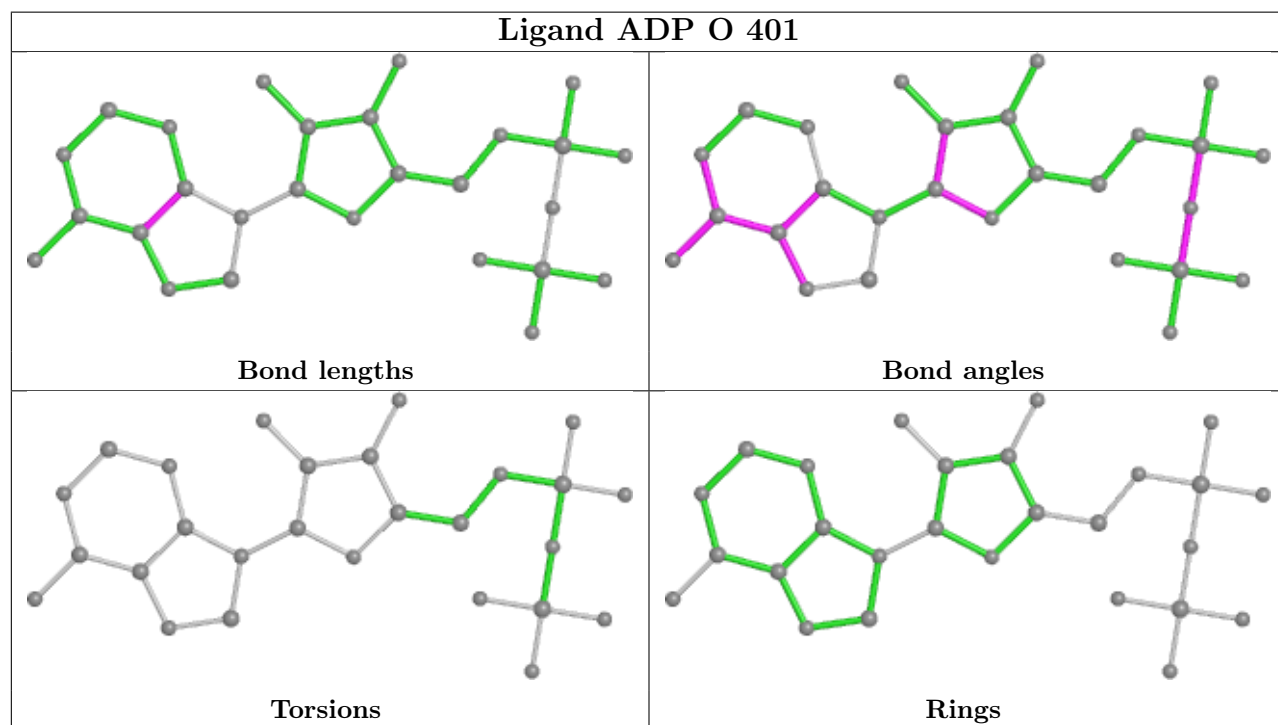
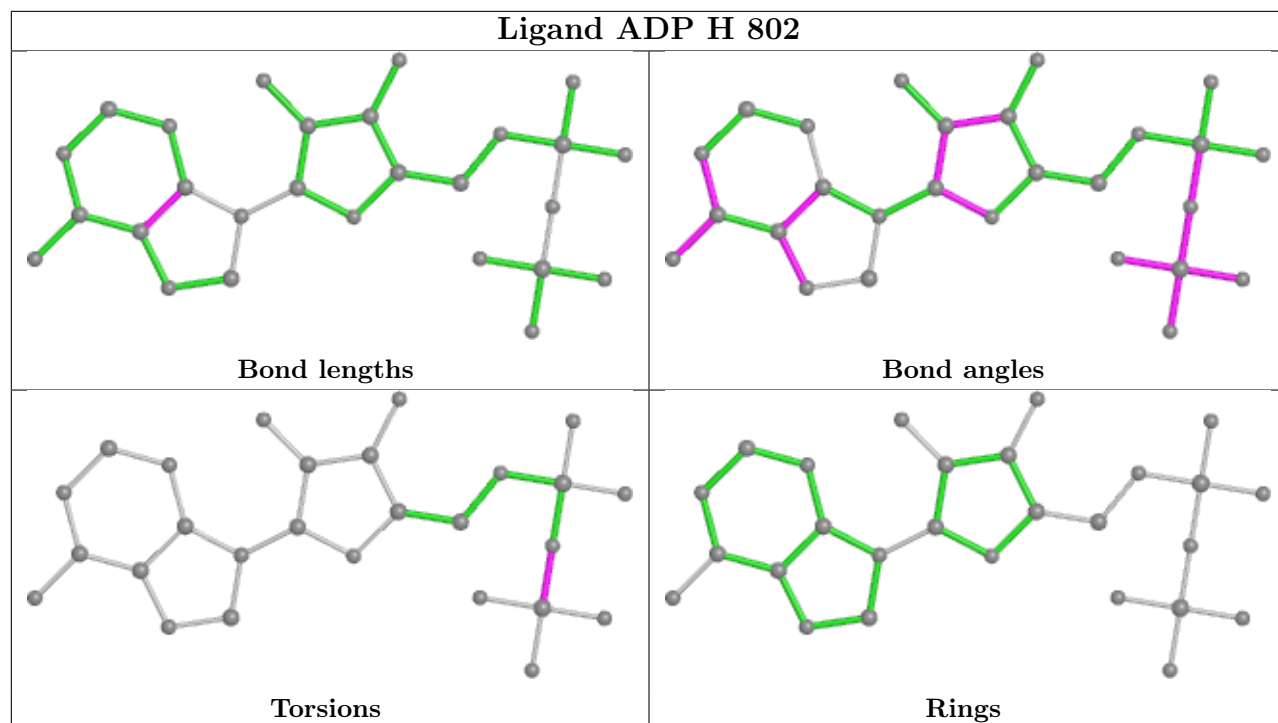


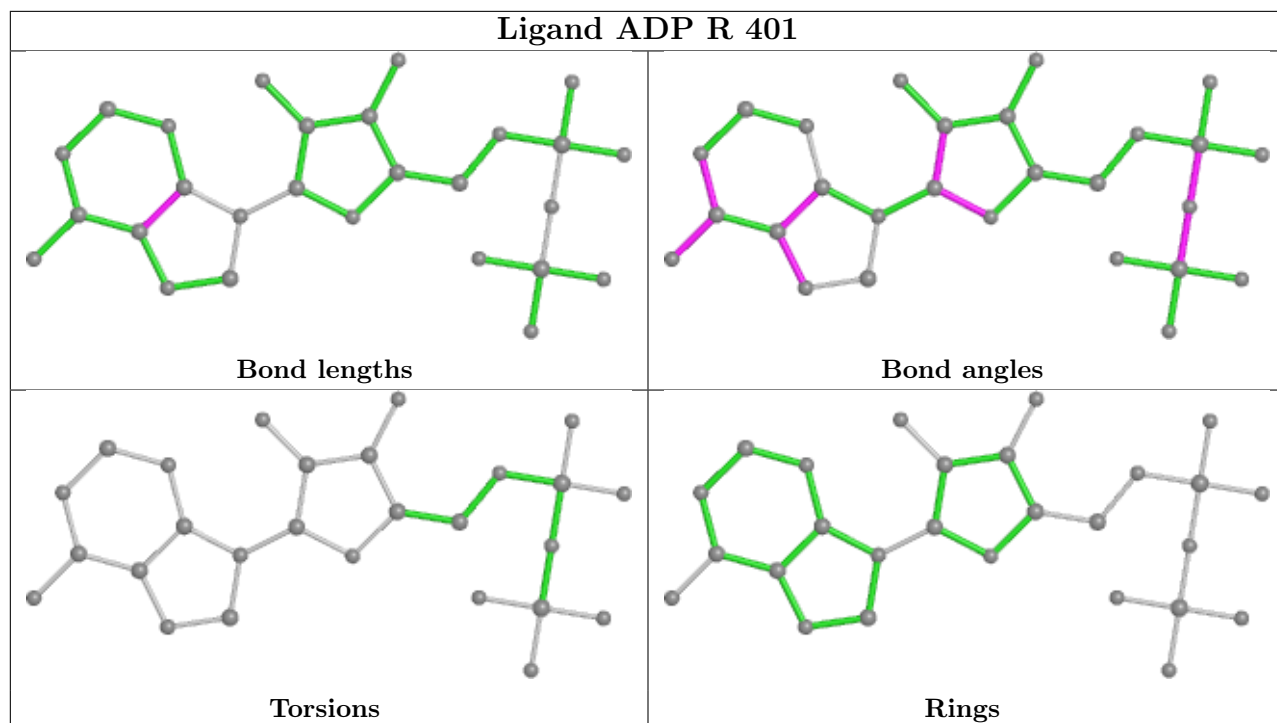


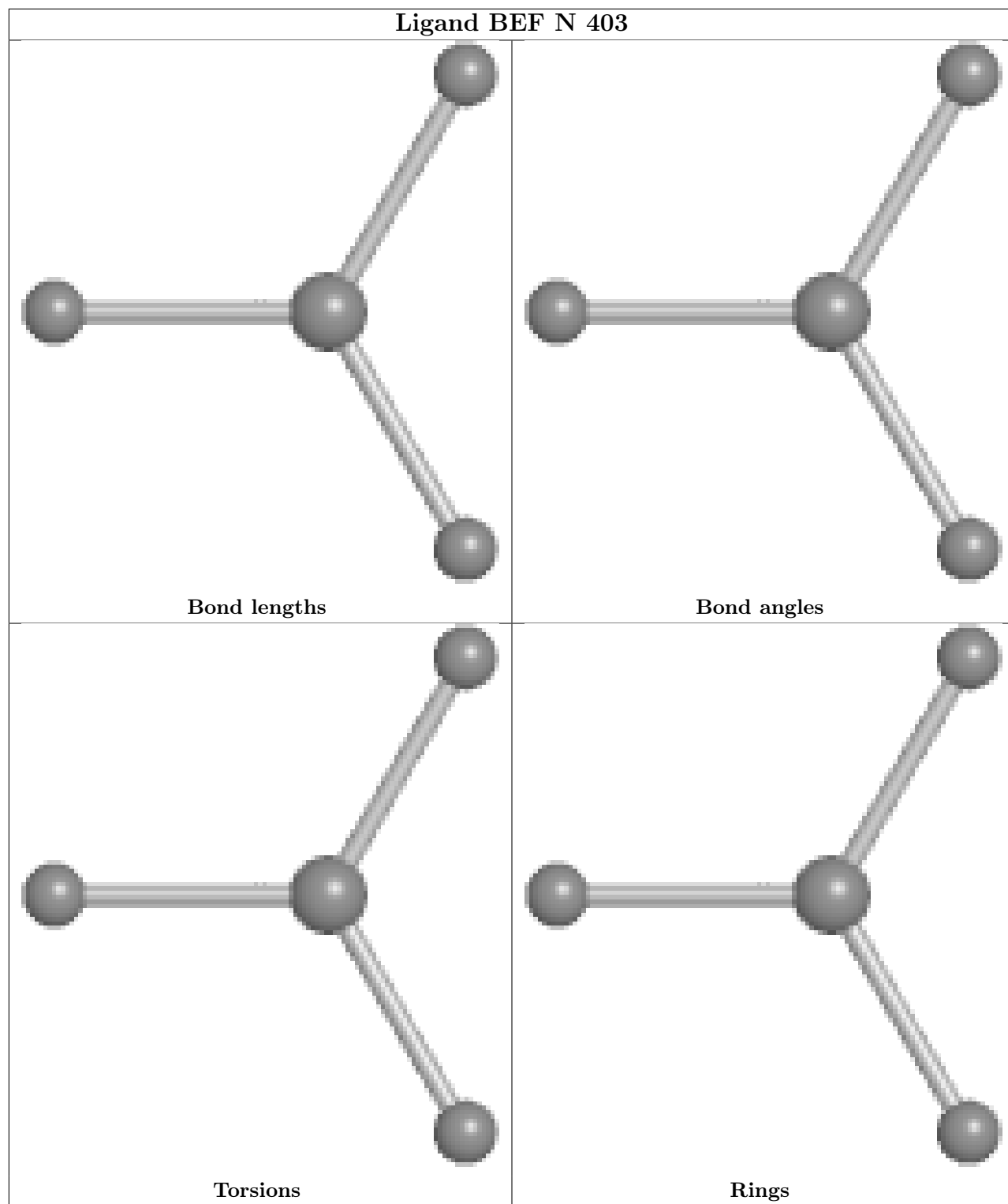


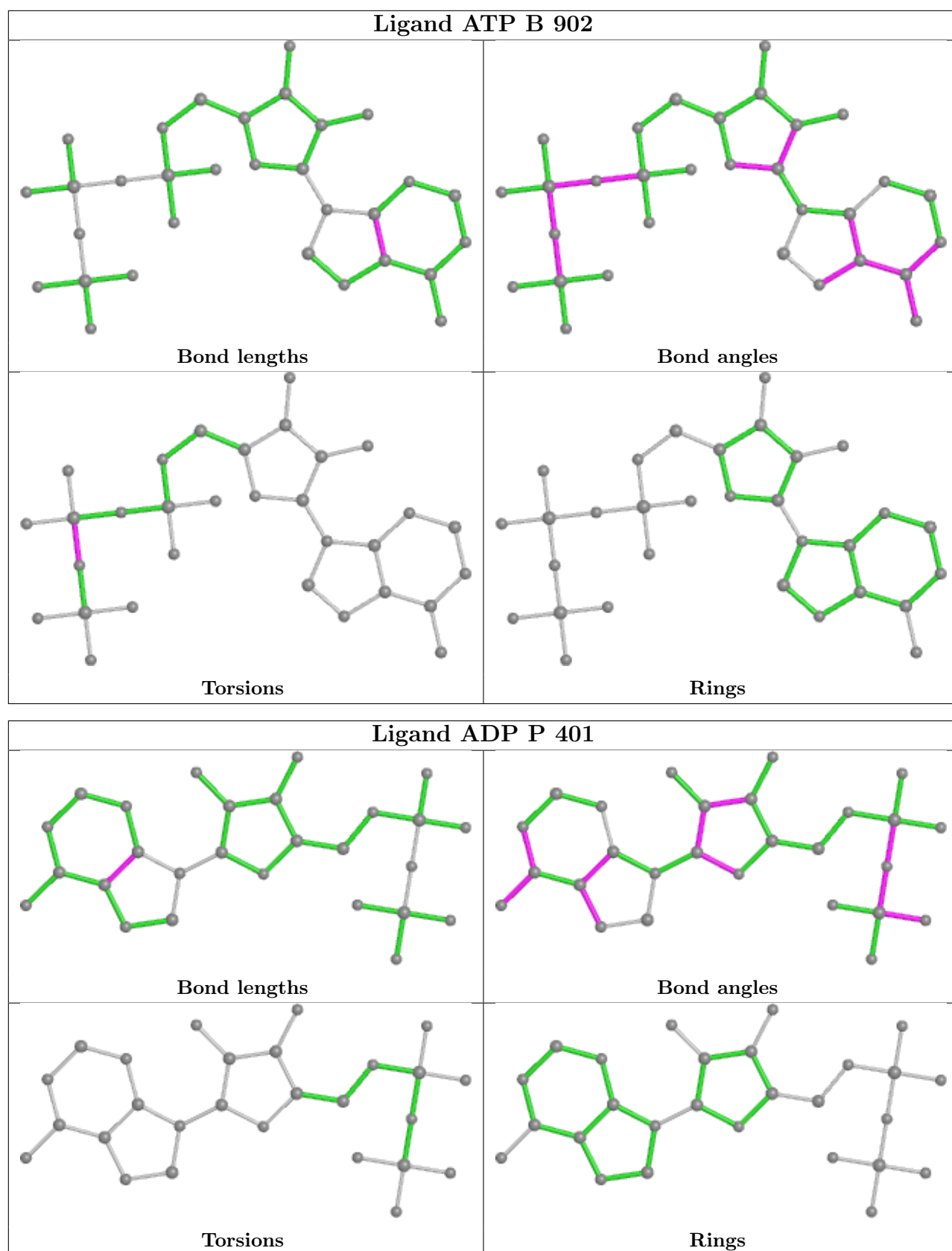


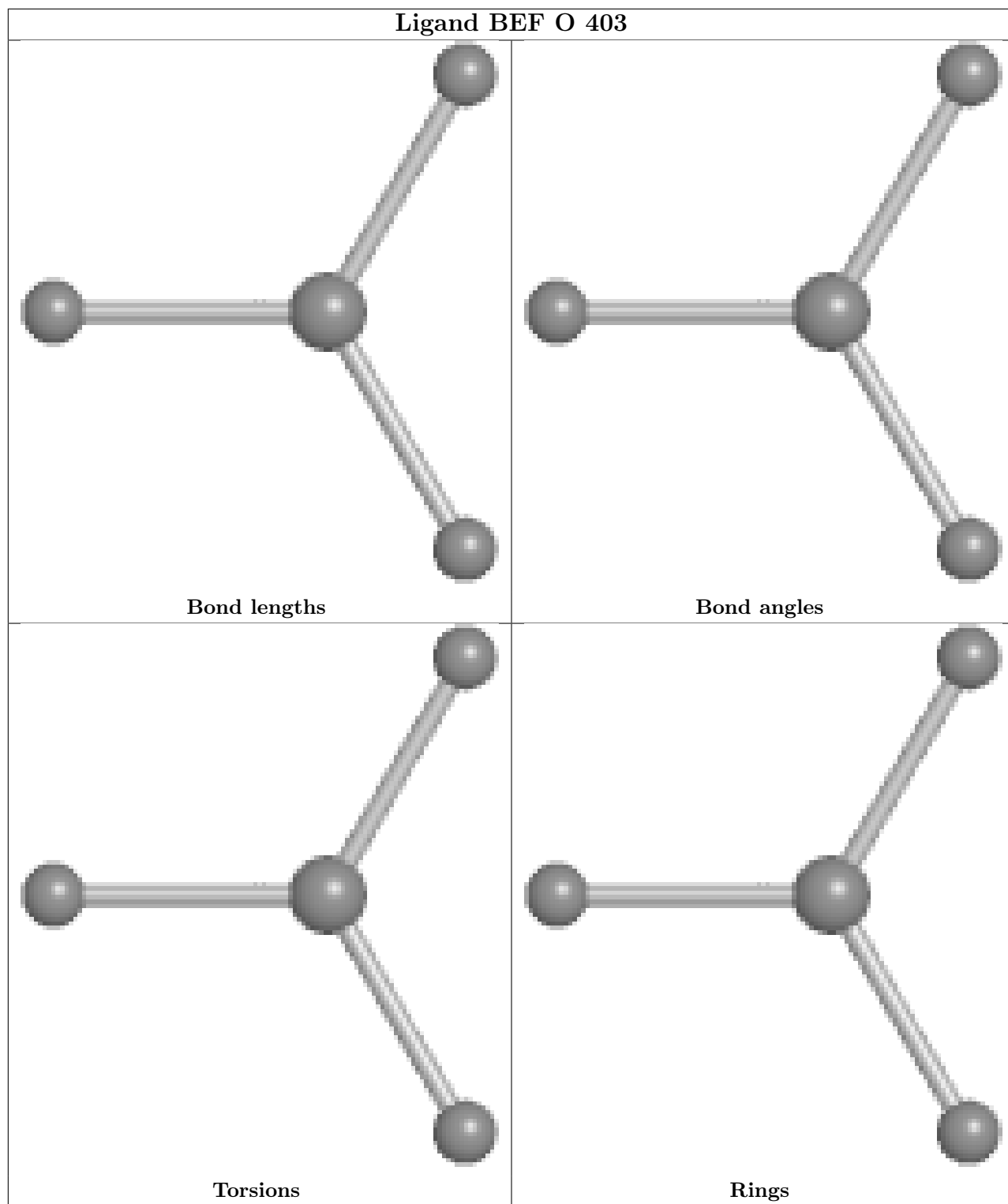


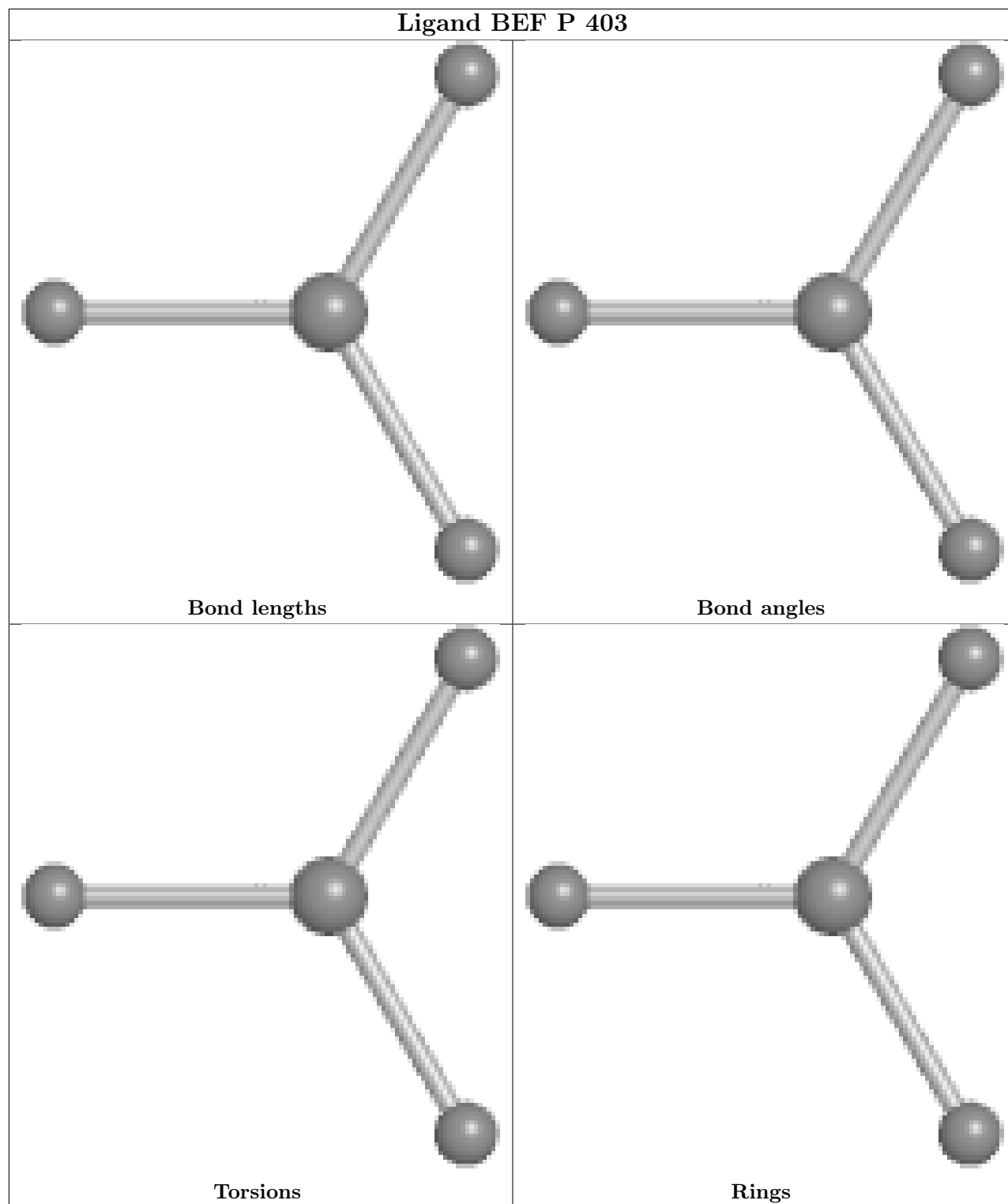












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

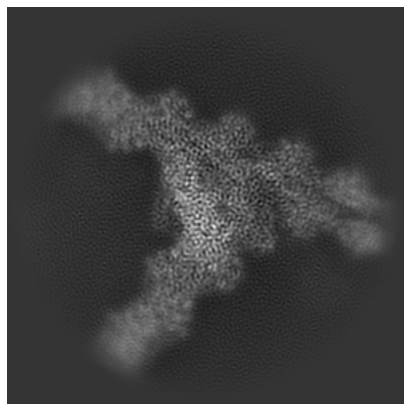
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42788. These allow visual inspection of the internal detail of the map and identification of artifacts.

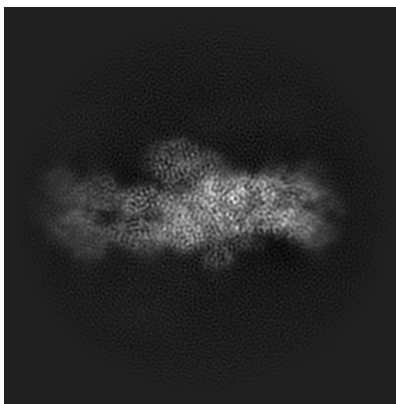
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

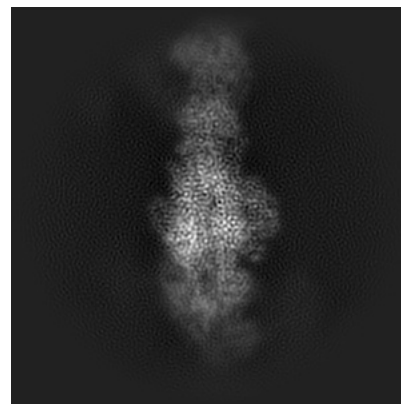
6.1.1 Primary map



X

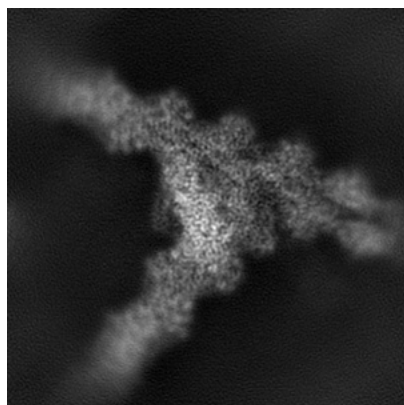


Y

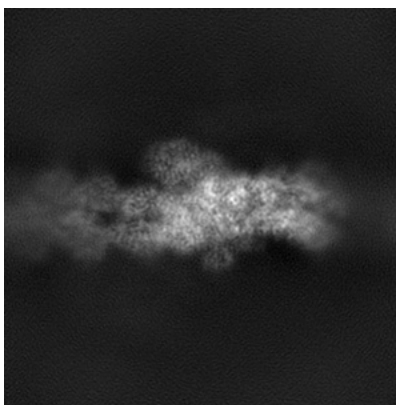


Z

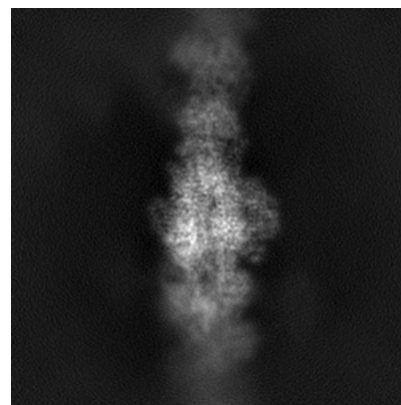
6.1.2 Raw map



X



Y

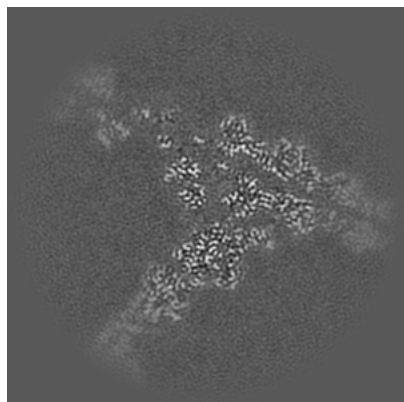


Z

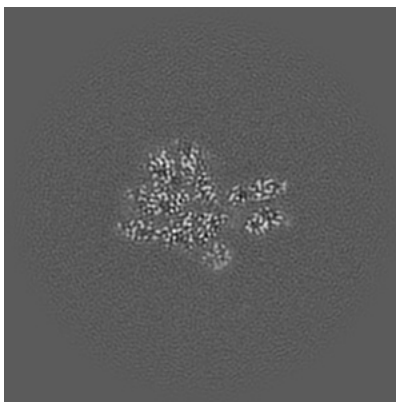
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

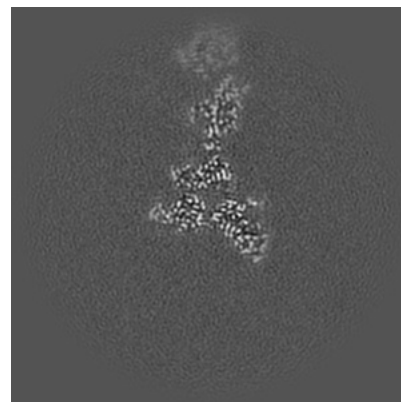
6.2.1 Primary map



X Index: 128

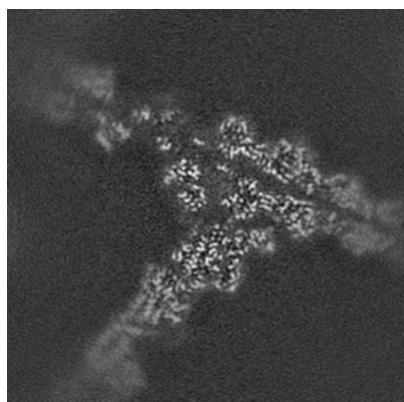


Y Index: 128

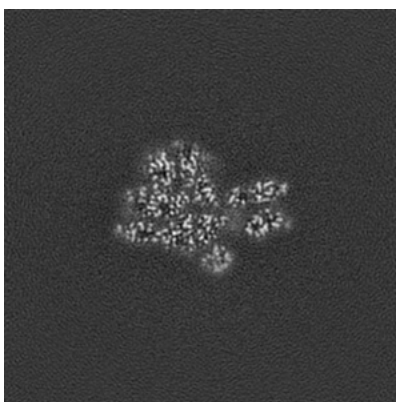


Z Index: 128

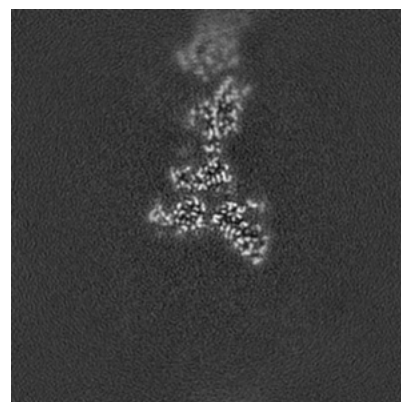
6.2.2 Raw map



X Index: 128



Y Index: 128

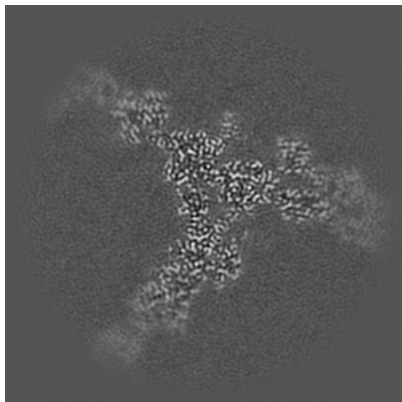


Z Index: 128

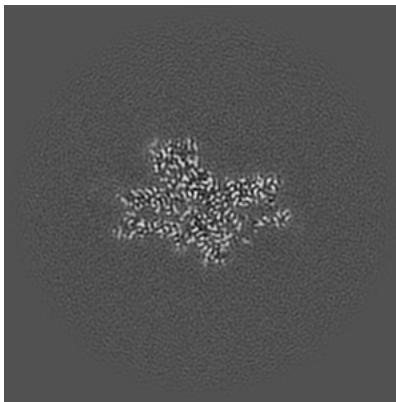
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

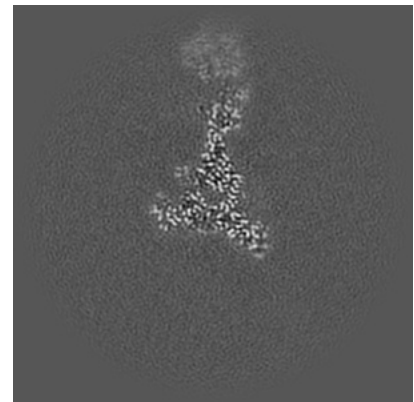
6.3.1 Primary map



X Index: 134

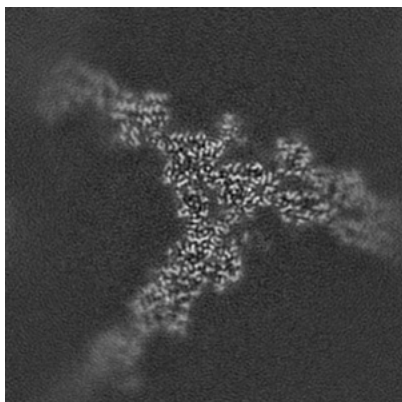


Y Index: 121

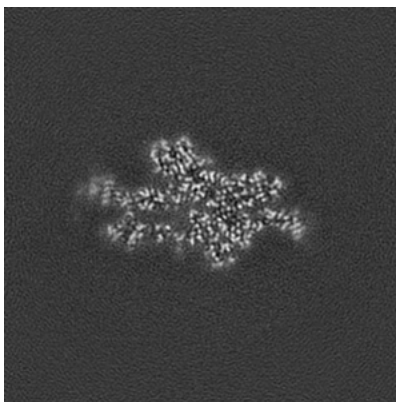


Z Index: 132

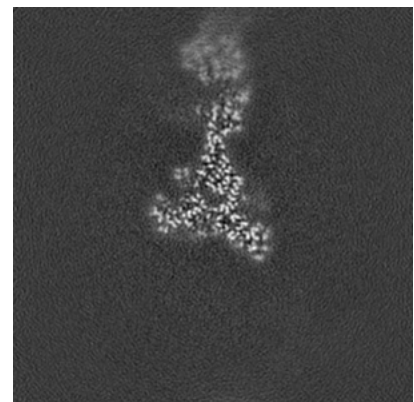
6.3.2 Raw map



X Index: 134



Y Index: 117

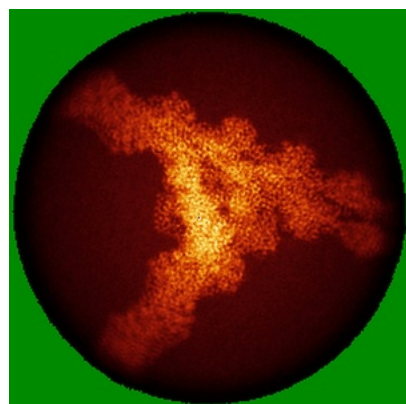


Z Index: 132

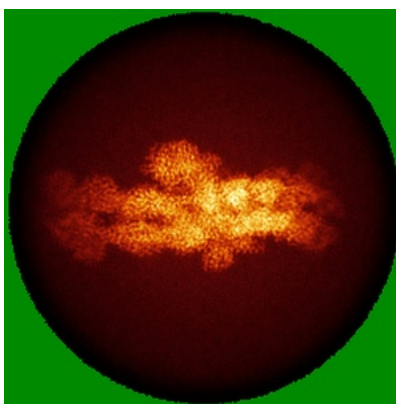
The images above show the largest variance slices of the map in three orthogonal directions.

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

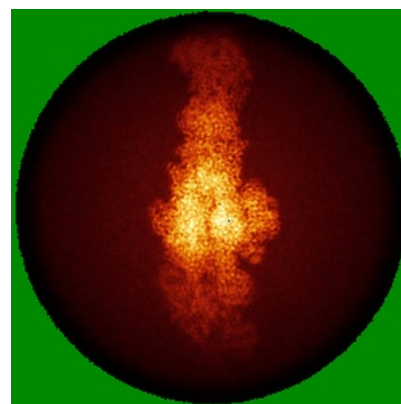
6.4.1 Primary map



X

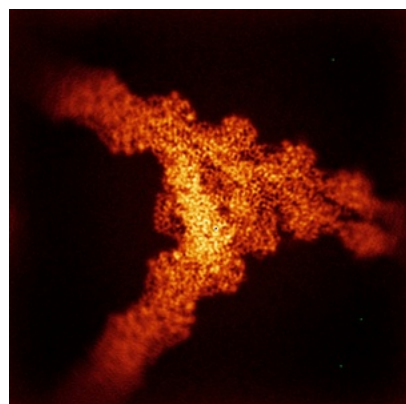


Y

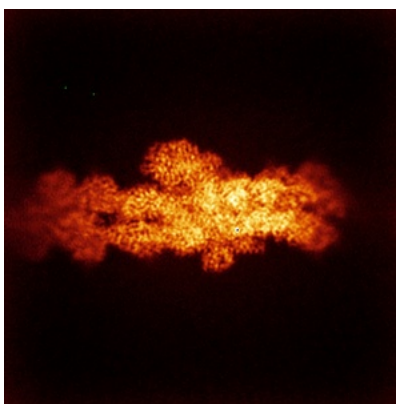


Z

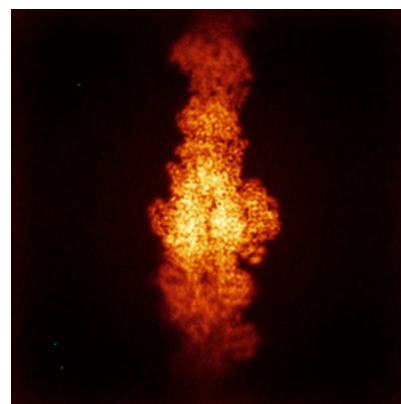
6.4.2 Raw map



X



Y

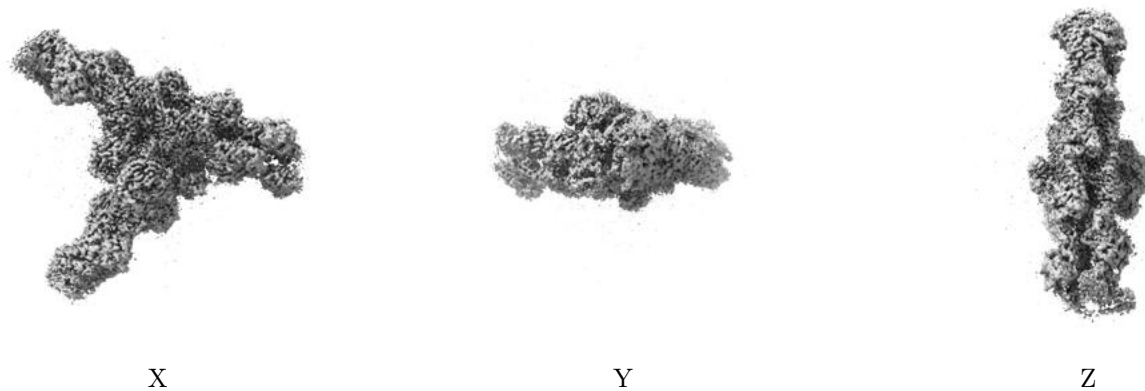


Z

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.

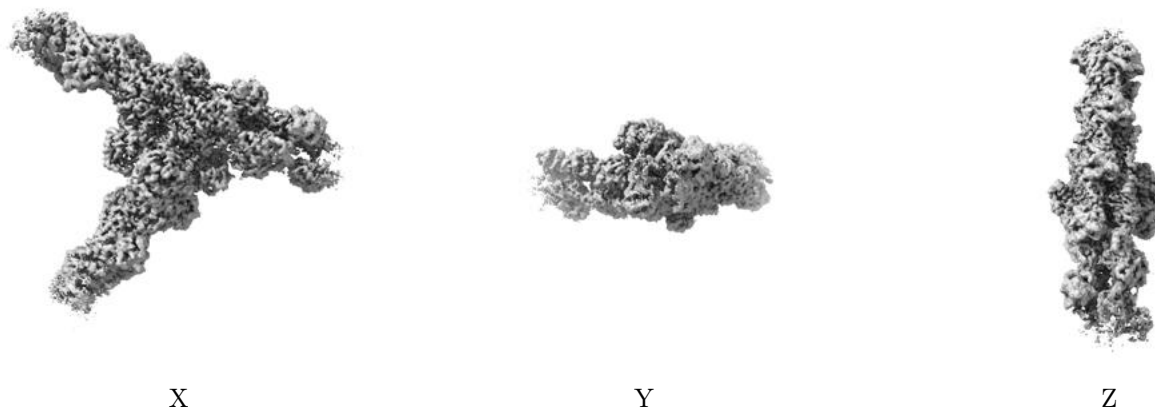
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.23. 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.

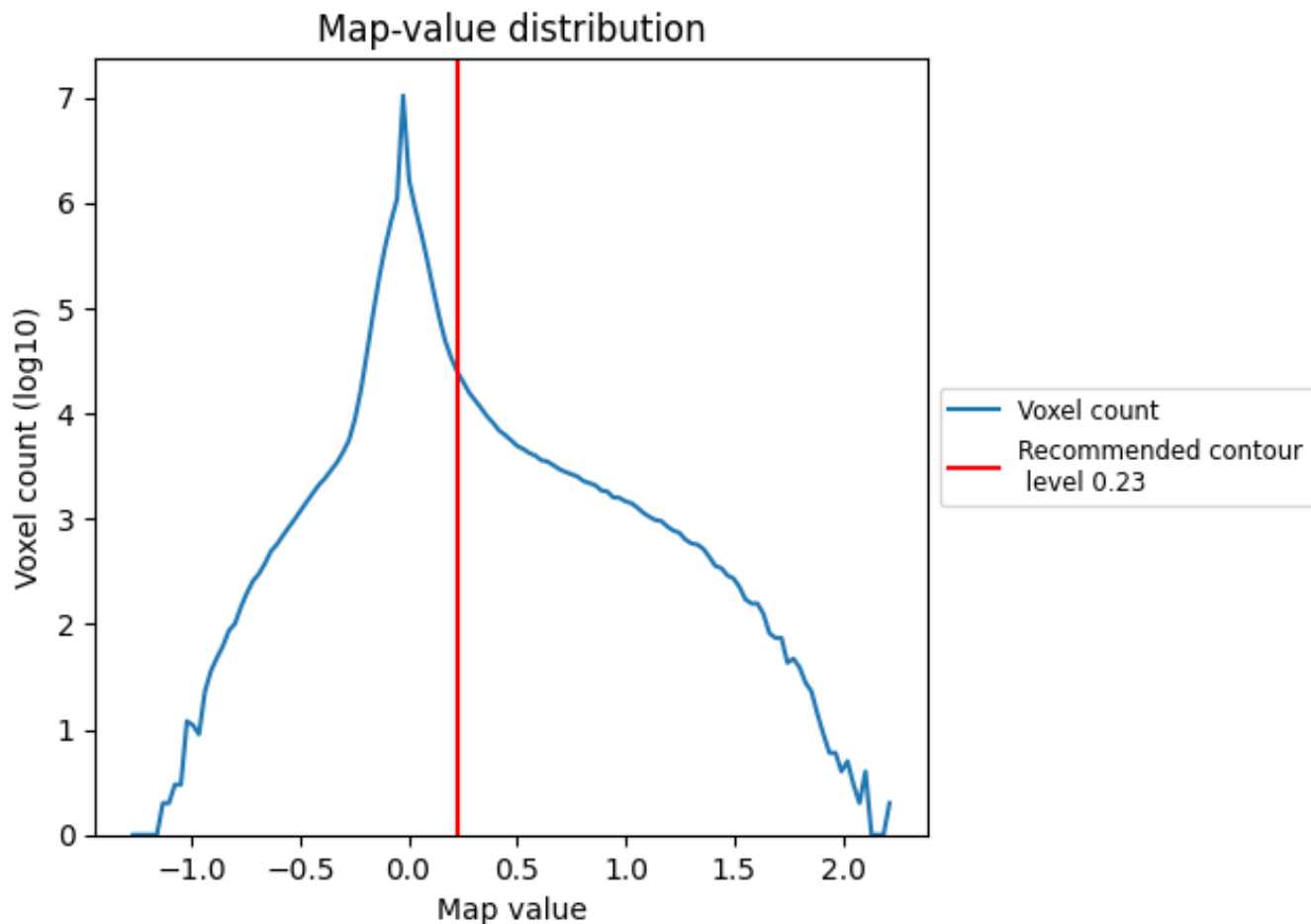
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

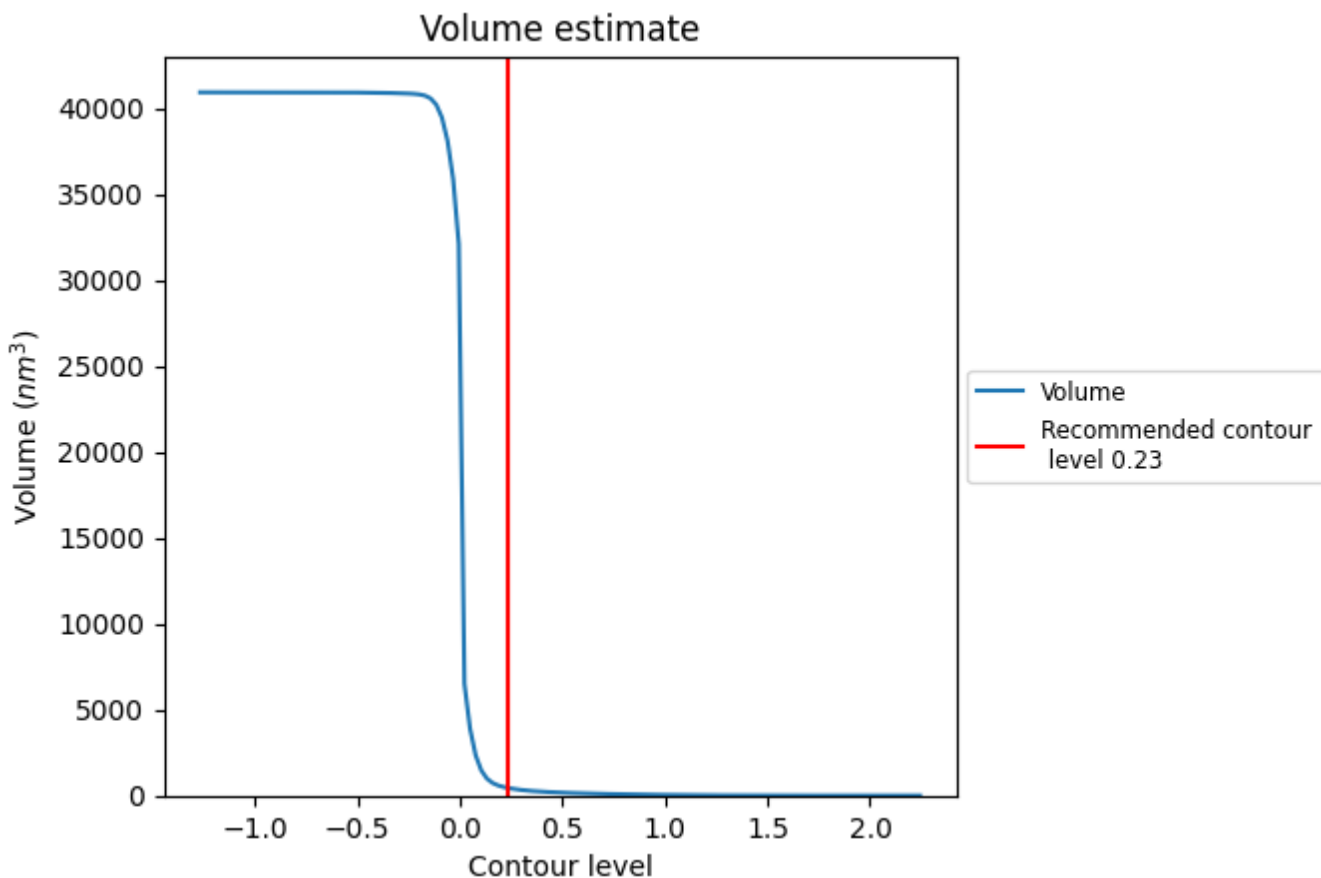
This section contains the results of statistical analysis of the map.

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.

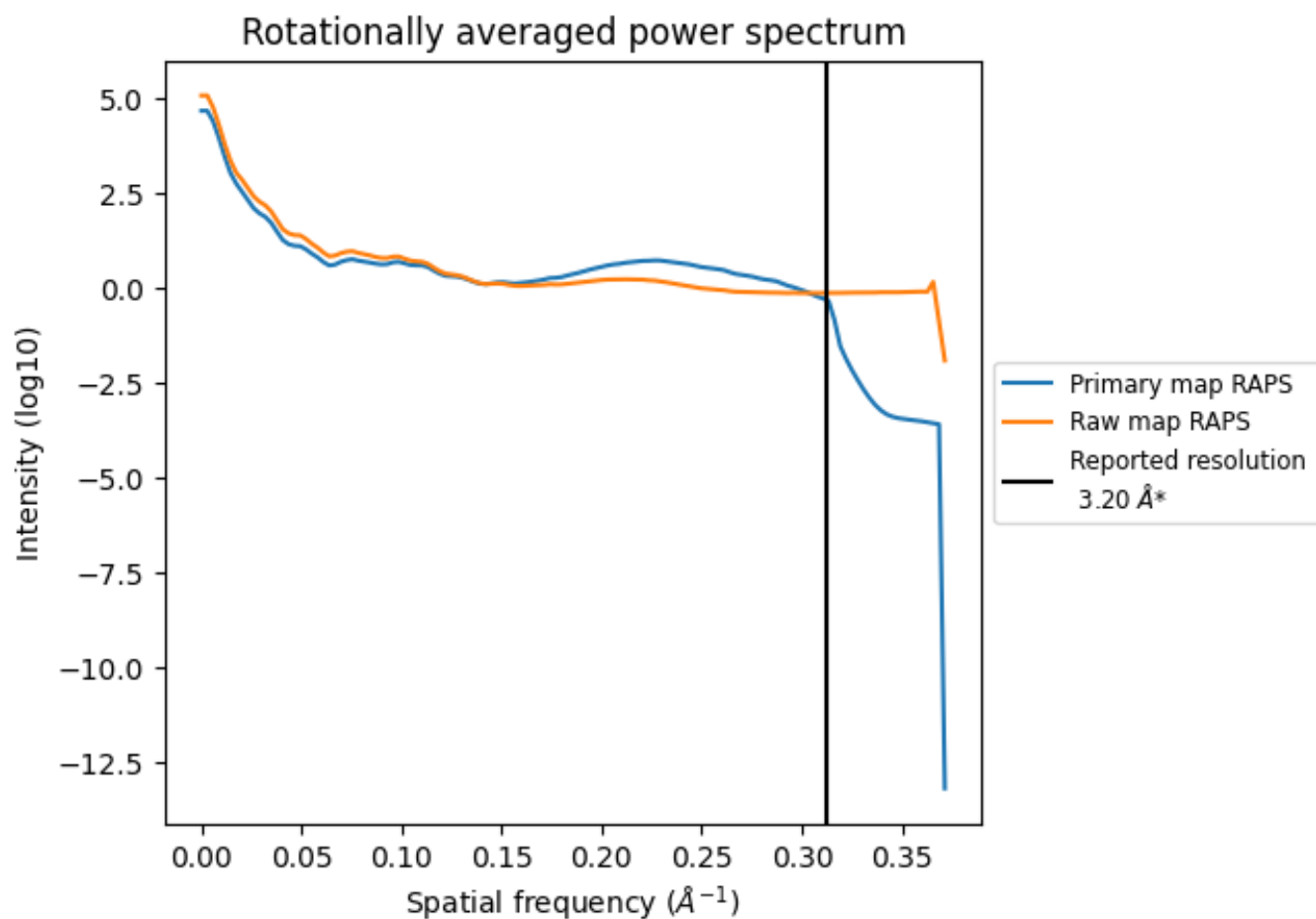
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 452 nm^3 ; this corresponds to an approximate mass of 408 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

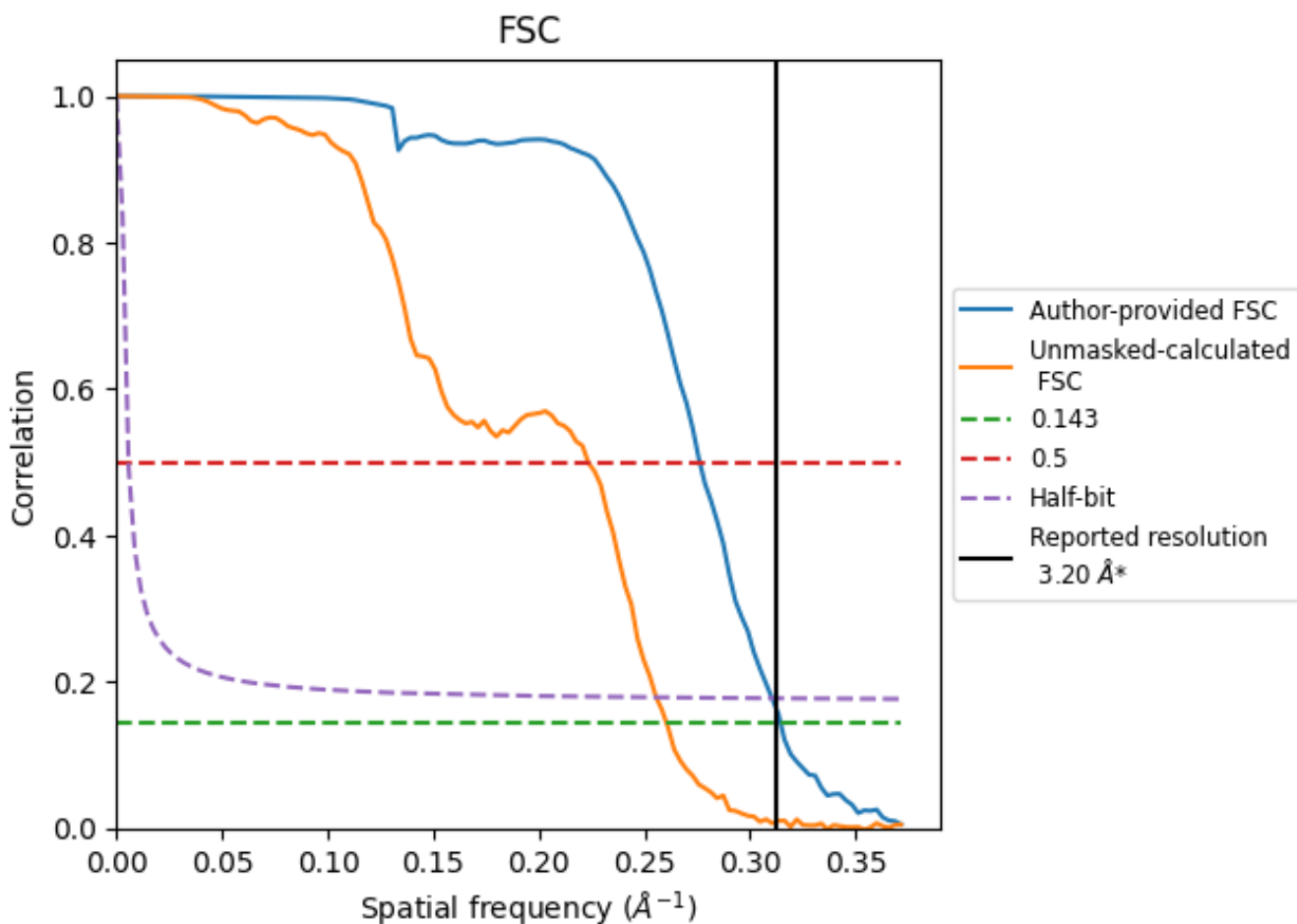


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

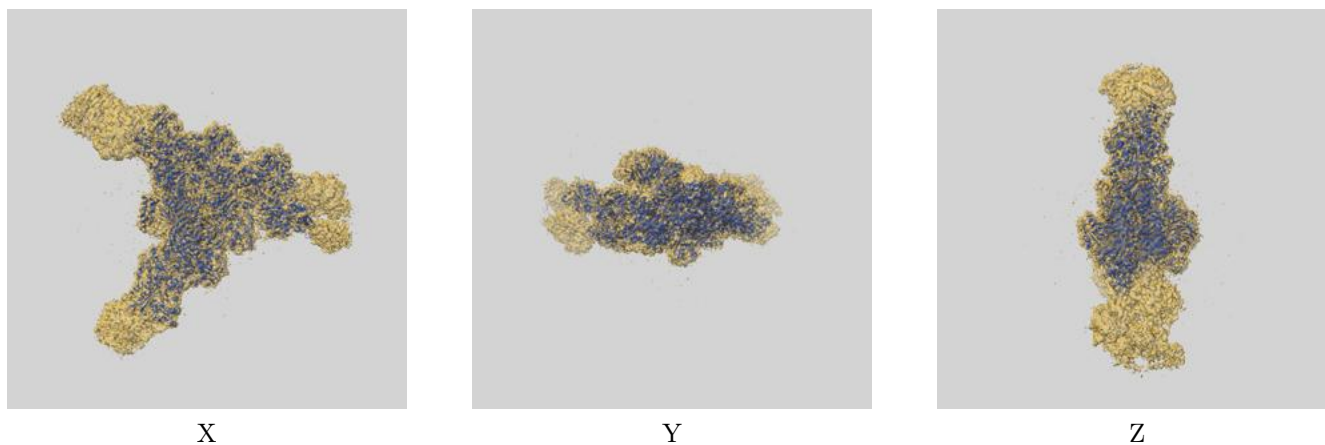
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.18	3.62	3.22
Unmasked-calculated*	3.84	4.48	3.91

*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 3.84 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

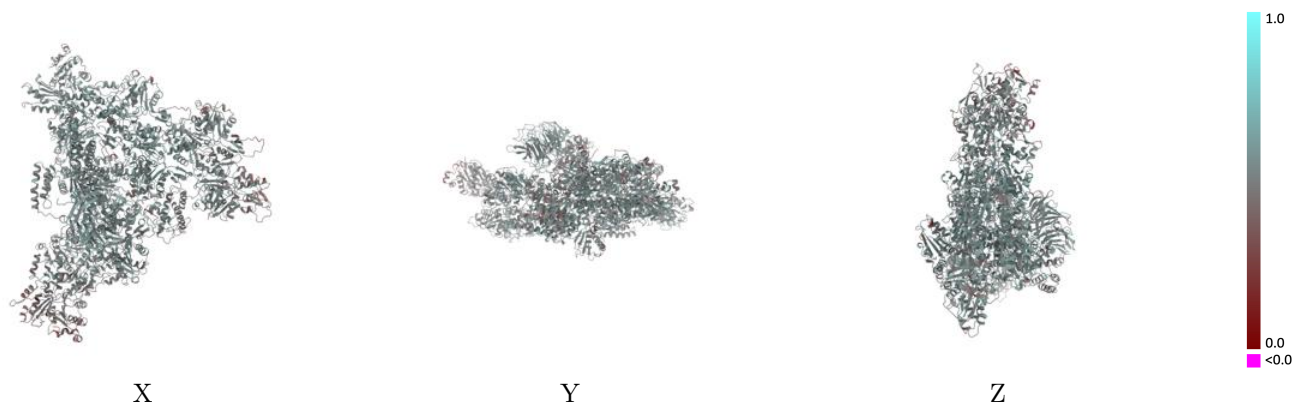
This section contains information regarding the fit between EMDB map EMD-42788 and PDB model 8UXX. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



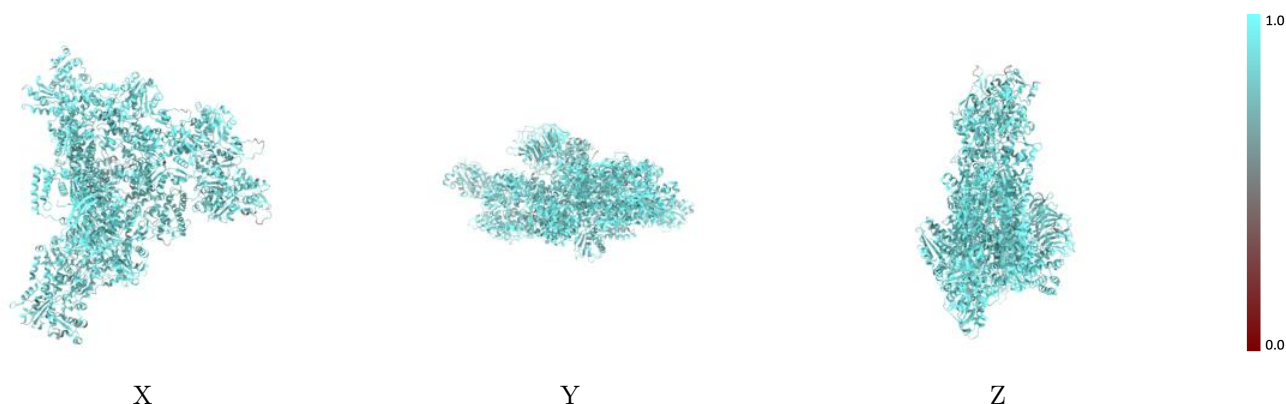
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



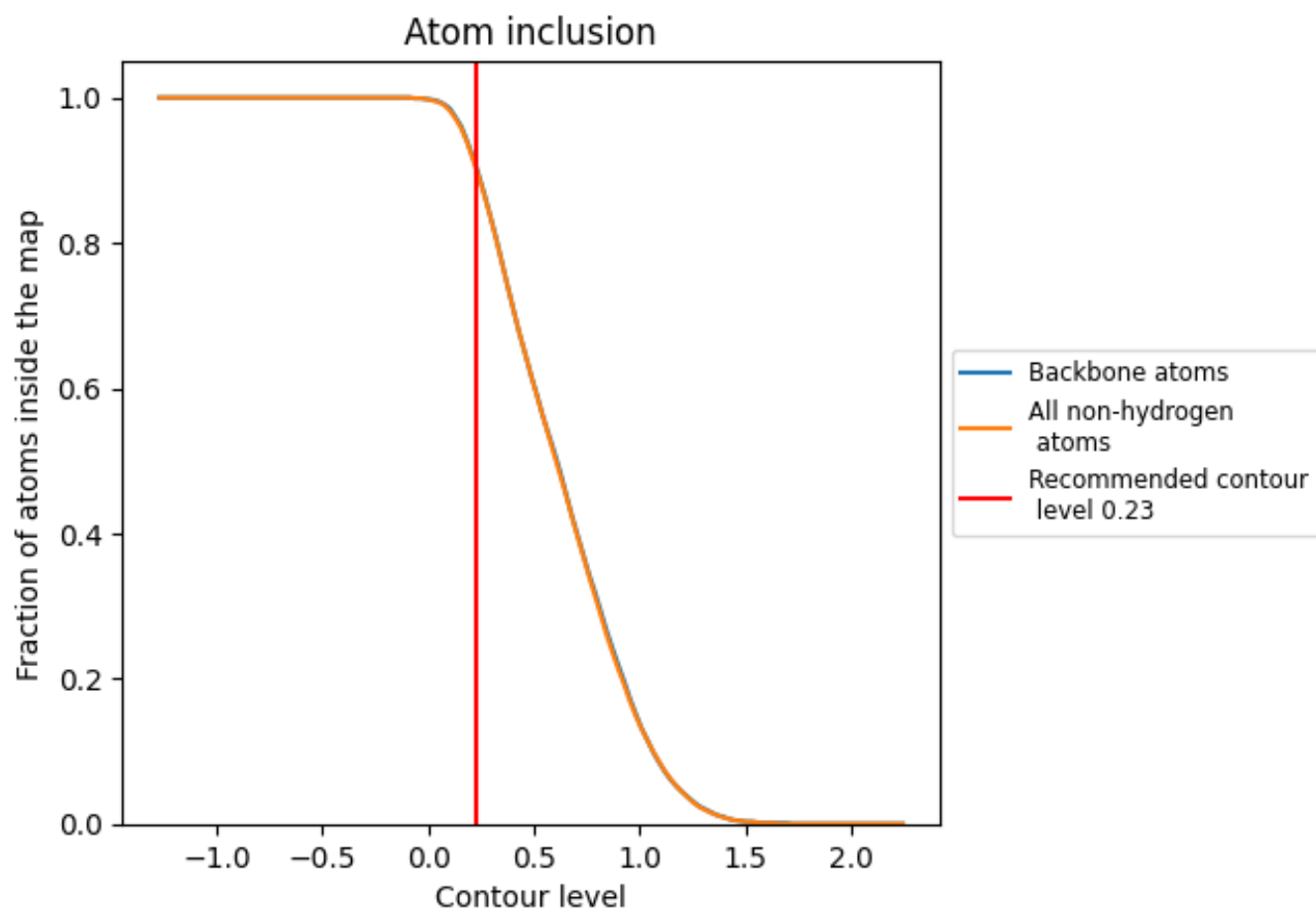
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.23).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 90% 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 (0.23) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9000	 0.5190
A	 0.9220	 0.5380
B	 0.9230	 0.5350
C	 0.9160	 0.5310
D	 0.9040	 0.5180
E	 0.8990	 0.5060
F	 0.9350	 0.5490
G	 0.8970	 0.4990
H	 0.9020	 0.5110
I	 0.8360	 0.4500
M	 0.8510	 0.4830
N	 0.8910	 0.5020
O	 0.9290	 0.5480
P	 0.9280	 0.5360
Q	 0.9370	 0.5470
R	 0.9060	 0.5190

