



wwPDB EM Validation Summary Report ⓘ

Mar 13, 2025 – 12:41 PM JST

PDB ID : 8YCX
EMDB ID : EMD-39157
Title : CryoEM structure of M. tuberculosis ClpC1P1P2 complex bound to bortezomib, conformation 2
Authors : Zhou, B.; Zhao, H.; Gao, Y.; Chen, X.; Zhang, T.; He, J.; Xiong, X.
Deposited on : 2024-02-18
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ 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.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

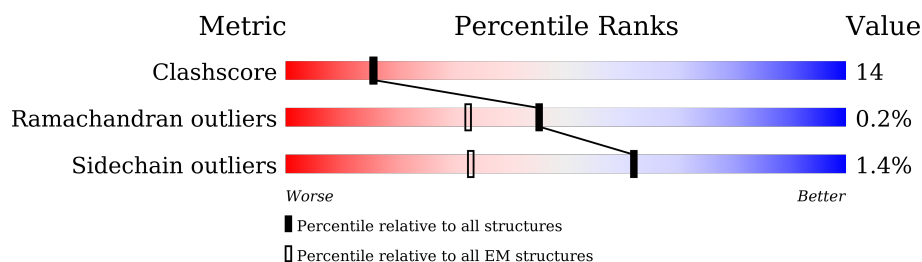
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.20 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.



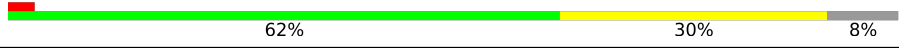
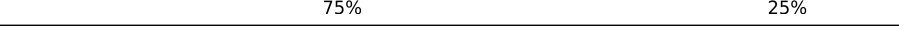
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	657	
1	B	657	
1	C	657	
1	D	657	
1	E	657	
1	F	657	
2	G	195	
2	H	195	

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Mol	Chain	Length	Quality of chain
2	I	195	
2	J	195	
2	K	195	
2	L	195	
2	M	195	
3	N	178	
3	O	178	
3	P	178	
3	Q	178	
3	R	178	
3	S	178	
3	T	178	
4	U	23	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ADP	D	901	-	-	X	-
5	ADP	F	901	-	-	X	-
6	ATP	A	902	-	-	X	-
6	ATP	A	904	-	-	X	-
6	ATP	B	902	-	-	X	-
6	ATP	B	903	-	-	X	-
6	ATP	C	902	-	-	X	-
6	ATP	E	902	-	-	X	-
7	MG	A	903	-	-	X	-
8	BO2	G	301	-	-	X	-
8	BO2	I	301	-	-	X	-
8	BO2	J	301	-	-	X	-
8	BO2	L	301	-	-	X	-
8	BO2	M	301	-	-	X	-
8	BO2	N	201	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	BO2	O	201	-	-	X	-
8	BO2	P	201	-	-	X	-
8	BO2	Q	201	-	-	X	-
8	BO2	R	201	-	-	X	-
8	BO2	S	201	-	-	X	-
8	BO2	T	201	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 46505 atoms, of which 48 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-dependent Clp protease ATP-binding subunit ClpC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	595	Total	C	N	O	S	0	0
			4652	2928	830	883	11		
1	B	595	Total	C	N	O	S	0	0
			4653	2929	830	883	11		
1	C	590	Total	C	N	O	S	0	0
			4618	2910	824	874	10		
1	D	557	Total	C	N	O	S	0	0
			4365	2753	785	816	11		
1	E	507	Total	C	N	O	S	0	0
			3986	2513	717	747	9		
1	F	517	Total	C	N	O	S	0	0
			4096	2583	737	765	11		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	288	ALA	GLU	engineered mutation	UNP P9WPC9
A	444	SER	PHE	engineered mutation	UNP P9WPC9
A	626	ALA	GLU	engineered mutation	UNP P9WPC9
B	288	ALA	GLU	engineered mutation	UNP P9WPC9
B	444	SER	PHE	engineered mutation	UNP P9WPC9
B	626	ALA	GLU	engineered mutation	UNP P9WPC9
C	288	ALA	GLU	engineered mutation	UNP P9WPC9
C	444	SER	PHE	engineered mutation	UNP P9WPC9
C	626	ALA	GLU	engineered mutation	UNP P9WPC9
D	288	ALA	GLU	engineered mutation	UNP P9WPC9
D	444	SER	PHE	engineered mutation	UNP P9WPC9
D	626	ALA	GLU	engineered mutation	UNP P9WPC9
E	288	ALA	GLU	engineered mutation	UNP P9WPC9
E	444	SER	PHE	engineered mutation	UNP P9WPC9
E	626	ALA	GLU	engineered mutation	UNP P9WPC9
F	288	ALA	GLU	engineered mutation	UNP P9WPC9
F	444	SER	PHE	engineered mutation	UNP P9WPC9
F	626	ALA	GLU	engineered mutation	UNP P9WPC9

- Molecule 2 is a protein called ATP-dependent Clp protease proteolytic subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	181	Total	C	N	O	S	0	0
			1389	869	239	273	8		
2	H	180	Total	C	N	O	S	0	0
			1383	866	238	271	8		
2	I	179	Total	C	N	O	S	0	0
			1375	862	236	269	8		
2	J	180	Total	C	N	O	S	0	0
			1383	866	238	271	8		
2	K	180	Total	C	N	O	S	0	0
			1383	866	238	271	8		
2	L	181	Total	C	N	O	S	0	0
			1389	869	239	273	8		
2	M	181	Total	C	N	O	S	0	0
			1389	869	239	273	8		

- Molecule 3 is a protein called ATP-dependent Clp protease proteolytic subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	178	Total	C	N	O	S	0	0
			1357	858	229	261	9		
3	O	178	Total	C	N	O	S	0	0
			1357	858	229	261	9		
3	P	178	Total	C	N	O	S	0	0
			1357	858	229	261	9		
3	Q	178	Total	C	N	O	S	0	0
			1357	858	229	261	9		
3	R	178	Total	C	N	O	S	0	0
			1357	858	229	261	9		
3	S	178	Total	C	N	O	S	0	0
			1357	858	229	261	9		
3	T	178	Total	C	N	O	S	0	0
			1357	858	229	261	9		

- Molecule 4 is a protein called Beta-casein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	23	Total	C	N	O	S	0	0
			173	114	28	30	1		

- Molecule 5 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).

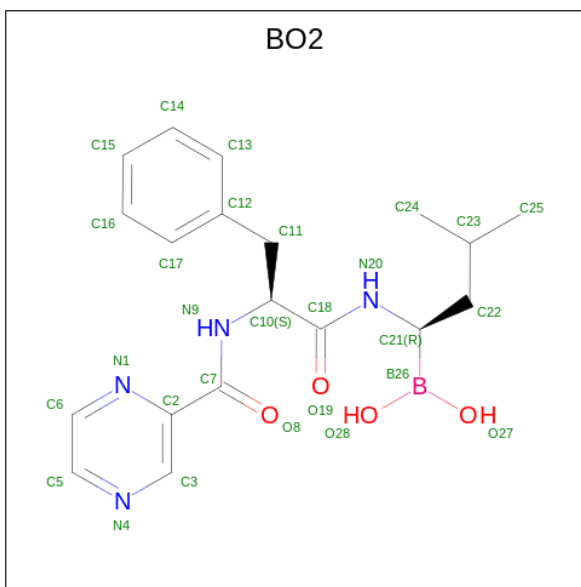


Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	E	1	Total	C	H	N	O	P
			43	10	12	5	13	3

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	A	2	Total	Mg	0
			2	2	
7	B	2	Total	Mg	0
			2	2	
7	C	2	Total	Mg	0
			2	2	
7	D	1	Total	Mg	0
			1	1	

- Molecule 8 is N-[(1R)-1-(DIHYDROXYBORYL)-3-METHYLBUTYL]-N-(PYRAZIN-2-YLCARBONYL)-L-PHENYLALANINAMIDE (three-letter code: BO2) (formula: C₁₉H₂₅BN₄O₄) (labeled as "Ligand of Interest" by depositor).

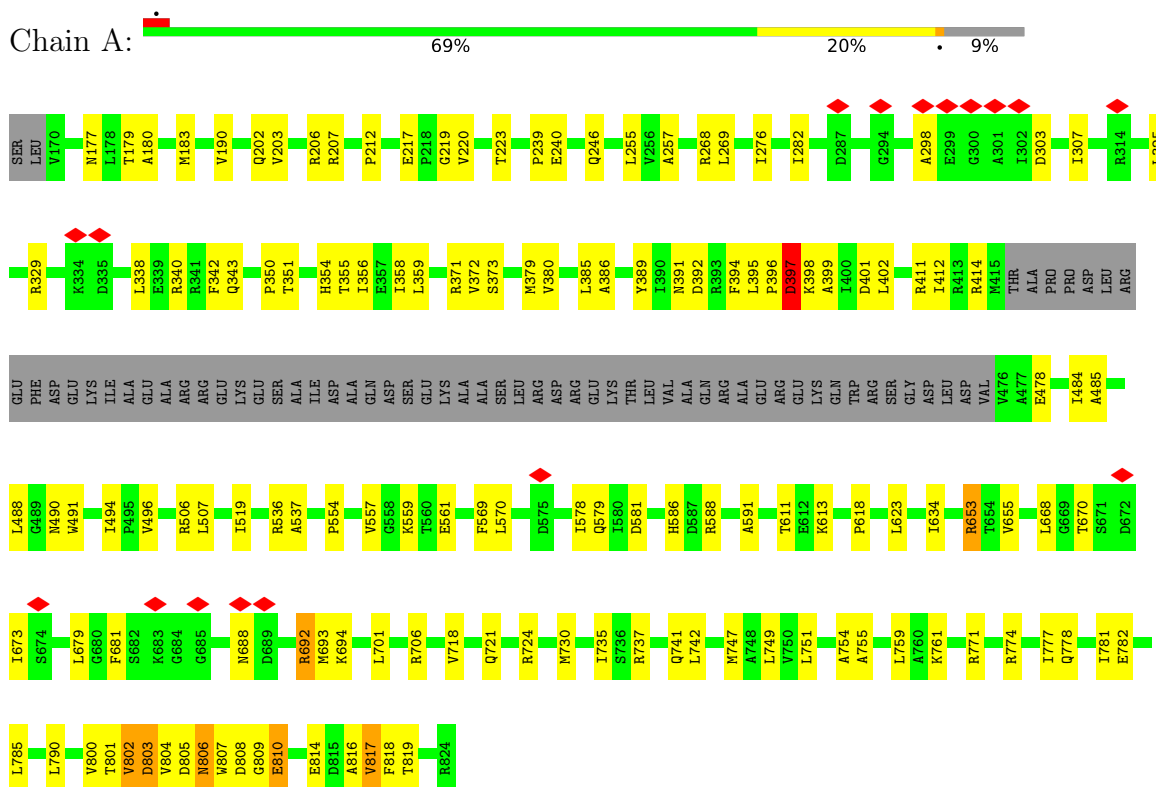


Mol	Chain	Residues	Atoms					AltConf
8	G	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	H	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	I	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	J	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	K	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	L	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	M	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	N	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	O	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	P	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	Q	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	R	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	S	1	Total	B	C	N	O	0
			28	1	19	4	4	
8	T	1	Total	B	C	N	O	0
			28	1	19	4	4	

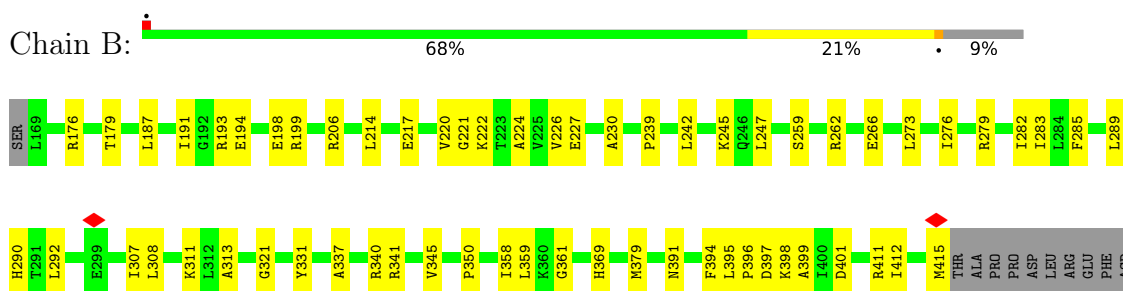
3 Residue-property plots

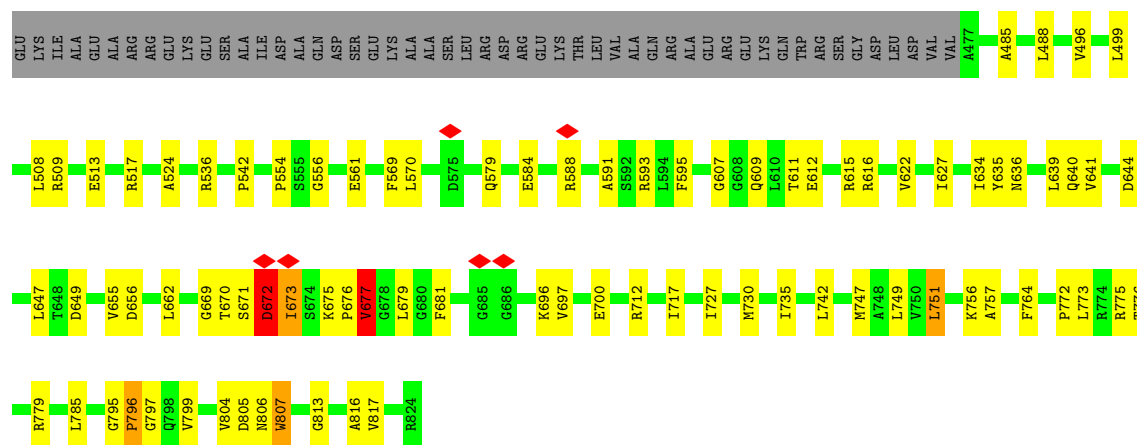
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC1



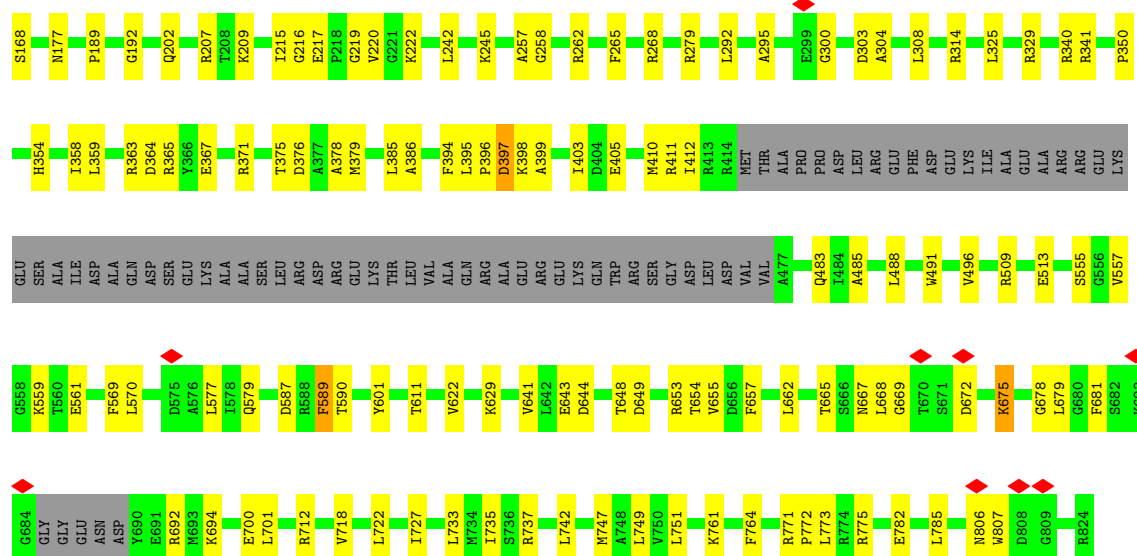
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC1





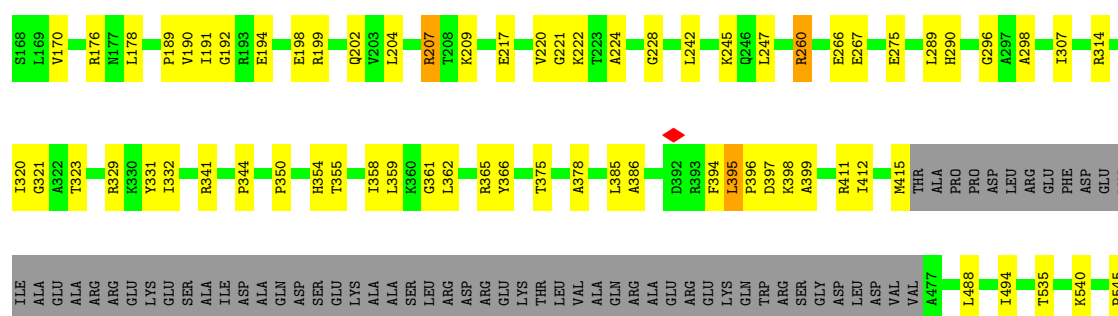
• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC1

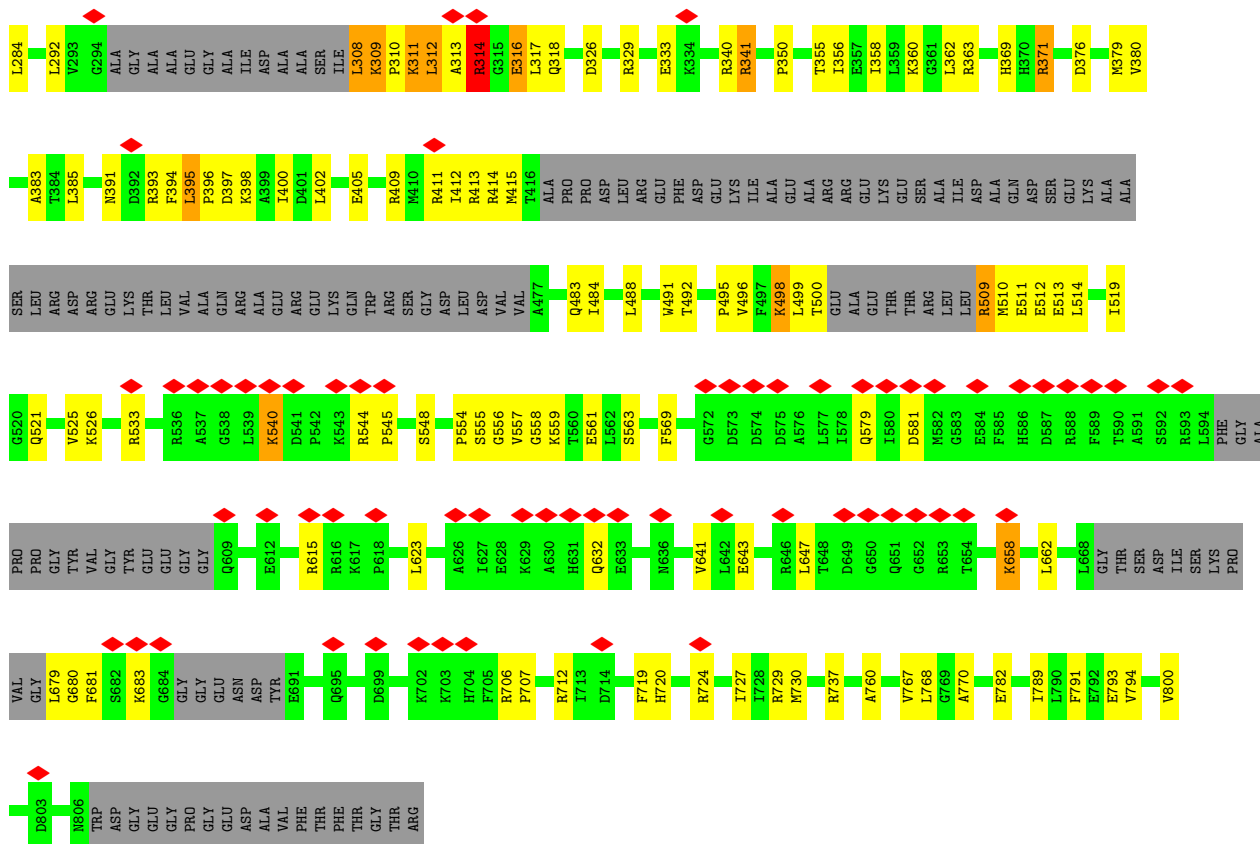
Chain C: 71% 18% 10%



• Molecule 1: ATP-dependent Clp protease ATP-binding subunit ClpC1

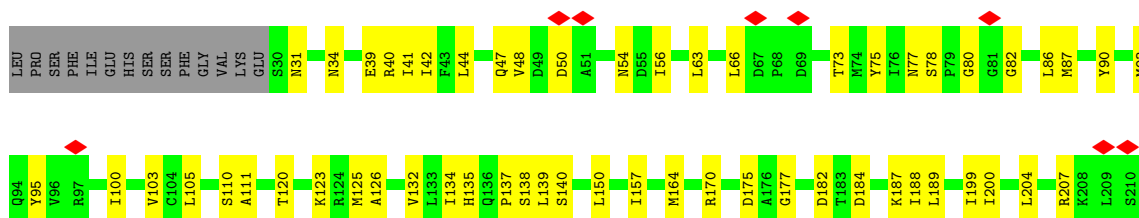
Chain D: 67% 18% 15%





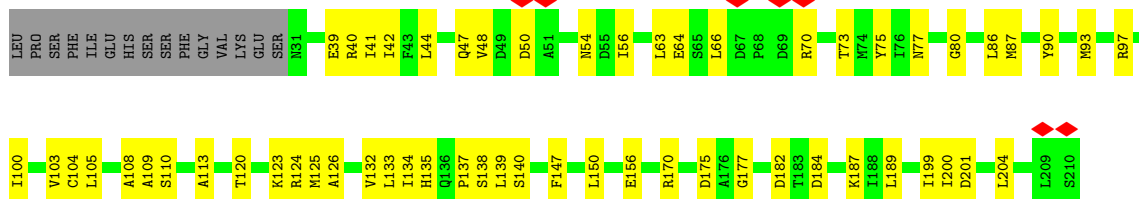
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 2

Chain G: 64% 29% 7%



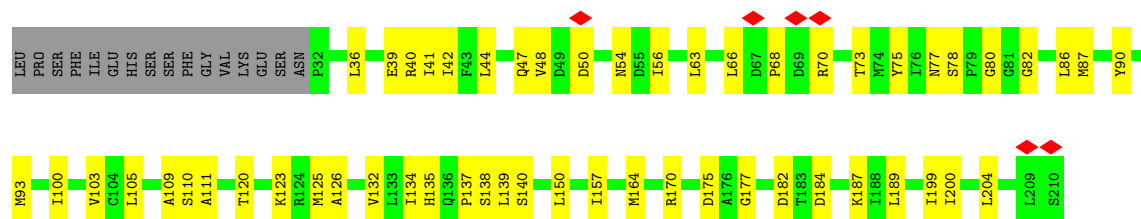
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 2

Chain H: 63% 30% 8%



- Molecule 2: ATP-dependent Clp protease proteolytic subunit 2

Chain I: 64% 28% 8%



- Molecule 2: ATP-dependent Clp protease proteolytic subunit 2

Chain J: 62% 30% 8%



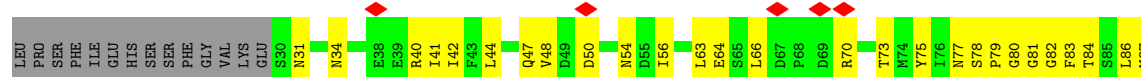
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 2

Chain K: 62% 30% 8%



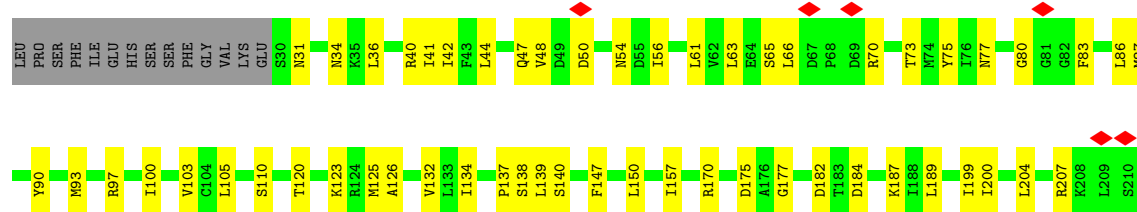
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 2

Chain L: 61% 32% 7%



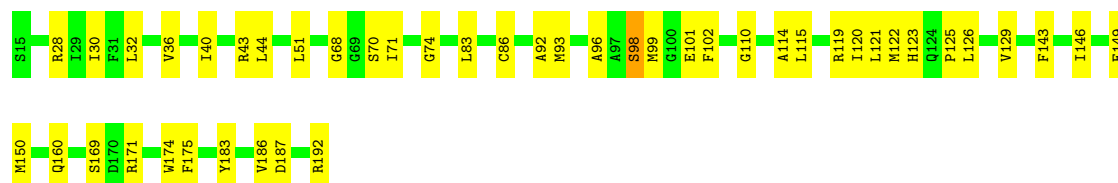
- Molecule 2: ATP-dependent Clp protease proteolytic subunit 2

Chain M: 65% 28% 7%



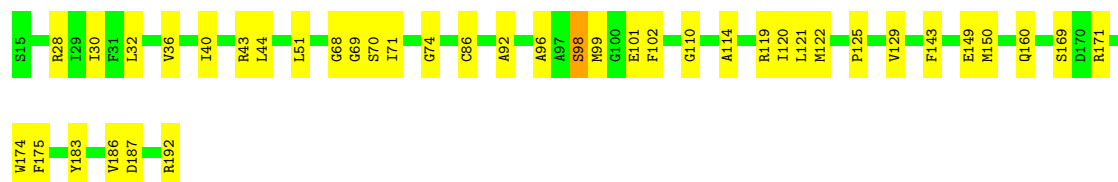
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain N: 75% 25% .



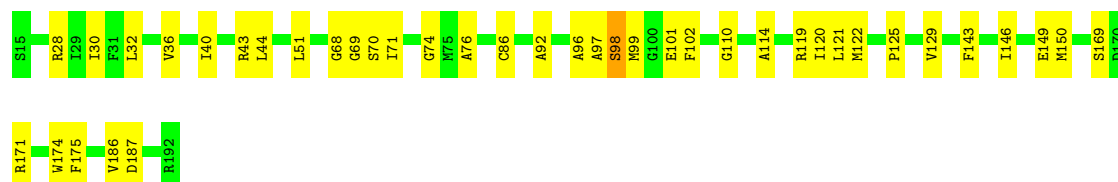
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain O: 78% 22% .



• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain P: 78% 22% .




• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain Q: 75% 25% .




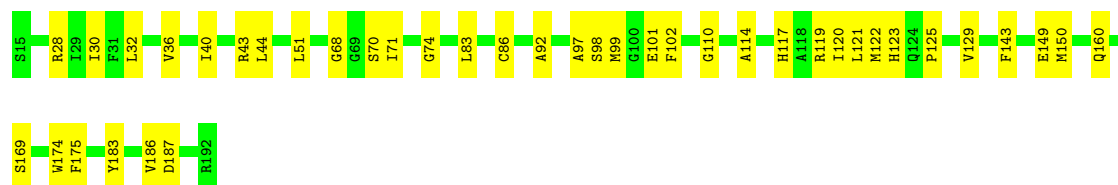
• Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain R:  77% 22%



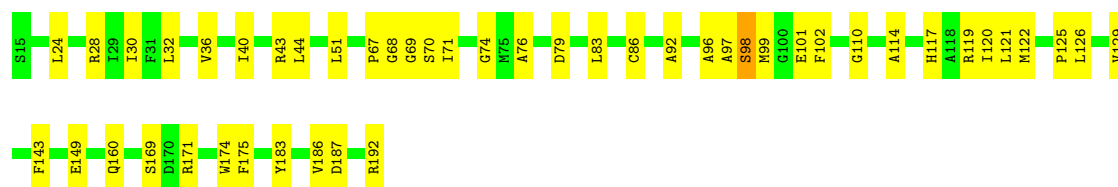
- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain S:  78% 22%




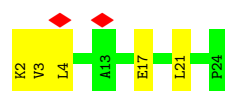
- Molecule 3: ATP-dependent Clp protease proteolytic subunit 1

Chain T:  74% 26%



- Molecule 4: Beta-casein

Chain U:  9% 78% 22%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	433061	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.699	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	363.52, 363.52, 363.52	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.71, 0.71, 0.71	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, BO2, ATP, MG

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	0.42	0/4720	0.62	0/6359
1	B	0.47	0/4721	0.61	1/6360 (0.0%)
1	C	0.47	0/4685	0.61	0/6311
1	D	0.43	0/4424	0.57	2/5950 (0.0%)
1	E	0.36	0/4037	0.58	0/5431
1	F	0.34	0/4145	0.61	0/5568
2	G	0.41	0/1406	0.58	0/1902
2	H	0.41	0/1400	0.58	0/1894
2	I	0.41	0/1392	0.58	0/1882
2	J	0.41	0/1400	0.59	0/1894
2	K	0.41	0/1400	0.58	0/1894
2	L	0.41	0/1406	0.59	0/1902
2	M	0.41	0/1406	0.58	0/1902
3	N	0.56	0/1379	0.57	0/1864
3	O	0.56	0/1379	0.57	0/1864
3	P	0.56	0/1379	0.57	0/1864
3	Q	0.56	0/1379	0.57	0/1864
3	R	0.56	0/1379	0.57	0/1864
3	S	0.56	0/1379	0.57	0/1864
3	T	0.56	0/1379	0.57	0/1864
4	U	0.39	0/173	0.73	0/235
All	All	0.45	0/46368	0.59	3/62532 (0.0%)

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	1
1	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	2
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	742	LEU	CA-CB-CG	5.61	128.19	115.30
1	D	623	LEU	CA-CB-CG	5.25	127.39	115.30
1	B	751	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	692	ARG	Sidechain
1	E	771	ARG	Sidechain
1	F	314	ARG	Sidechain
1	F	509	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	4652	0	4725	151	0
1	B	4653	0	4725	160	0
1	C	4618	0	4698	125	0
1	D	4365	0	4475	150	0
1	E	3986	0	4080	122	0
1	F	4096	0	4208	164	0
2	G	1389	0	1402	43	0
2	H	1383	0	1397	39	0
2	I	1375	0	1392	40	0
2	J	1383	0	1397	50	0
2	K	1383	0	1397	41	0
2	L	1389	0	1402	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	1389	0	1402	44	0
3	N	1357	0	1348	44	0
3	O	1357	0	1348	39	0
3	P	1357	0	1348	45	0
3	Q	1357	0	1348	43	0
3	R	1357	0	1348	38	0
3	S	1357	0	1348	39	0
3	T	1357	0	1348	45	0
4	U	173	0	196	8	0
5	A	27	12	12	8	0
5	D	27	12	12	27	0
5	E	27	0	11	7	0
5	F	27	12	11	24	0
6	A	62	0	23	36	0
6	B	62	0	24	23	0
6	C	62	0	24	29	0
6	E	31	12	12	14	0
7	A	2	0	0	2	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
7	D	1	0	0	0	0
8	G	28	0	25	10	0
8	H	28	0	25	5	0
8	I	28	0	25	11	0
8	J	28	0	25	12	0
8	K	28	0	25	6	0
8	L	28	0	25	20	0
8	M	28	0	25	11	0
8	N	28	0	25	12	0
8	O	28	0	25	11	0
8	P	28	0	25	17	0
8	Q	28	0	25	13	0
8	R	28	0	25	12	0
8	S	28	0	25	10	0
8	T	28	0	25	10	0
All	All	46457	48	46811	1343	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 14.

The worst 5 of 1343 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:F:770:ALA:CB	5:F:901:ADP:H5'2	1.38	1.49
1:F:556:GLY:CA	5:F:901:ADP:O1A	1.64	1.44
1:A:371:ARG:NH2	1:A:411:ARG:HH12	1.05	1.42
1:F:411:ARG:NH1	1:F:415:MET:HE1	1.23	1.41
1:A:371:ARG:CZ	1:A:411:ARG:NH1	1.85	1.40

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	591/657 (90%)	553 (94%)	35 (6%)	3 (0%)	25	28
1	B	591/657 (90%)	555 (94%)	31 (5%)	5 (1%)	16	16
1	C	584/657 (89%)	554 (95%)	29 (5%)	1 (0%)	44	52
1	D	549/657 (84%)	527 (96%)	21 (4%)	1 (0%)	44	52
1	E	495/657 (75%)	463 (94%)	31 (6%)	1 (0%)	44	52
1	F	501/657 (76%)	457 (91%)	44 (9%)	0	100	100
2	G	179/195 (92%)	168 (94%)	11 (6%)	0	100	100
2	H	178/195 (91%)	167 (94%)	11 (6%)	0	100	100
2	I	177/195 (91%)	166 (94%)	11 (6%)	0	100	100
2	J	178/195 (91%)	166 (93%)	11 (6%)	1 (1%)	22	23
2	K	178/195 (91%)	168 (94%)	10 (6%)	0	100	100
2	L	179/195 (92%)	167 (93%)	12 (7%)	0	100	100
2	M	179/195 (92%)	168 (94%)	11 (6%)	0	100	100
3	N	176/178 (99%)	169 (96%)	7 (4%)	0	100	100
3	O	176/178 (99%)	168 (96%)	8 (4%)	0	100	100
3	P	176/178 (99%)	168 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Q	176/178 (99%)	169 (96%)	7 (4%)	0	100	100
3	R	176/178 (99%)	169 (96%)	7 (4%)	0	100	100
3	S	176/178 (99%)	170 (97%)	6 (3%)	0	100	100
3	T	176/178 (99%)	169 (96%)	7 (4%)	0	100	100
4	U	21/23 (91%)	16 (76%)	5 (24%)	0	100	100
All	All	5812/6576 (88%)	5477 (94%)	323 (6%)	12 (0%)	45	52

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	796	PRO
1	E	772	PRO
1	A	397	ASP
1	A	806	ASN
1	B	671	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	491/543 (90%)	478 (97%)	13 (3%)	41	54
1	B	491/543 (90%)	484 (99%)	7 (1%)	62	77
1	C	488/543 (90%)	483 (99%)	5 (1%)	73	84
1	D	460/543 (85%)	454 (99%)	6 (1%)	65	78
1	E	419/543 (77%)	412 (98%)	7 (2%)	56	71
1	F	440/543 (81%)	423 (96%)	17 (4%)	27	37
2	G	149/162 (92%)	148 (99%)	1 (1%)	81	90
2	H	148/162 (91%)	147 (99%)	1 (1%)	81	90
2	I	147/162 (91%)	146 (99%)	1 (1%)	81	90
2	J	148/162 (91%)	147 (99%)	1 (1%)	81	90
2	K	148/162 (91%)	146 (99%)	2 (1%)	62	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	149/162 (92%)	148 (99%)	1 (1%)	81	90
2	M	149/162 (92%)	147 (99%)	2 (1%)	65	78
3	N	139/139 (100%)	138 (99%)	1 (1%)	81	90
3	O	139/139 (100%)	138 (99%)	1 (1%)	81	90
3	P	139/139 (100%)	138 (99%)	1 (1%)	81	90
3	Q	139/139 (100%)	139 (100%)	0	100	100
3	R	139/139 (100%)	138 (99%)	1 (1%)	81	90
3	S	139/139 (100%)	139 (100%)	0	100	100
3	T	139/139 (100%)	138 (99%)	1 (1%)	81	90
4	U	19/19 (100%)	19 (100%)	0	100	100
All	All	4819/5384 (90%)	4750 (99%)	69 (1%)	62	77

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	170	ARG
2	K	110	SER
3	O	98	SER
1	C	806	ASN
1	C	675	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	369	HIS
2	G	47	GLN
2	M	31	ASN
1	E	370	HIS
1	F	632	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 7 are monoatomic - leaving 25 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	$\# Z > 2$
6	ATP	A	904	7	26,33,33	0.69	0	31,52,52	0.80	1 (3%)
8	BO2	N	201	-	25,29,29	0.23	0	32,38,38	0.48	0
6	ATP	C	903	7	26,33,33	0.70	0	31,52,52	0.79	1 (3%)
8	BO2	H	301	-	25,29,29	0.22	0	32,38,38	0.35	0
8	BO2	M	301	-	25,29,29	0.22	0	32,38,38	0.65	1 (3%)
5	ADP	F	901	-	24,29,29	0.68	0	29,45,45	0.78	1 (3%)
8	BO2	G	301	-	25,29,29	0.21	0	32,38,38	0.30	0
8	BO2	P	201	-	25,29,29	0.23	0	32,38,38	0.42	0
5	ADP	A	901	-	24,29,29	0.67	0	29,45,45	0.76	1 (3%)
8	BO2	K	301	-	25,29,29	0.23	0	32,38,38	0.39	0
8	BO2	O	201	-	25,29,29	0.27	0	32,38,38	0.39	0
8	BO2	T	201	-	25,29,29	0.24	0	32,38,38	0.67	1 (3%)
6	ATP	B	903	7	26,33,33	0.70	0	31,52,52	0.83	1 (3%)
6	ATP	C	902	7	26,33,33	0.70	0	31,52,52	0.87	1 (3%)
5	ADP	E	901	-	24,29,29	0.73	0	29,45,45	0.88	2 (6%)
5	ADP	D	901	-	24,29,29	0.70	0	29,45,45	0.78	1 (3%)
8	BO2	I	301	-	25,29,29	0.22	0	32,38,38	0.30	0
6	ATP	E	902	7	26,33,33	0.69	0	31,52,52	0.78	1 (3%)
8	BO2	J	301	-	25,29,29	0.21	0	32,38,38	0.30	0
8	BO2	S	201	-	25,29,29	0.27	0	32,38,38	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ATP	B	902	7	26,33,33	0.72	0	31,52,52	0.77	1 (3%)
6	ATP	A	902	7	26,33,33	0.69	0	31,52,52	0.82	1 (3%)
8	BO2	L	301	-	25,29,29	0.21	0	32,38,38	0.38	0
8	BO2	R	201	-	25,29,29	0.23	0	32,38,38	0.64	1 (3%)
8	BO2	Q	201	-	25,29,29	0.27	0	32,38,38	0.49	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
6	ATP	A	904	7	-	0/18/38/38	0/3/3/3
8	BO2	N	201	-	-	13/22/28/28	0/2/2/2
6	ATP	C	903	7	-	5/18/38/38	0/3/3/3
8	BO2	H	301	-	-	9/22/28/28	0/2/2/2
8	BO2	M	301	-	-	13/22/28/28	0/2/2/2
5	ADP	F	901	-	-	1/12/32/32	0/3/3/3
8	BO2	G	301	-	-	7/22/28/28	0/2/2/2
8	BO2	P	201	-	-	12/22/28/28	0/2/2/2
5	ADP	A	901	-	-	1/12/32/32	0/3/3/3
8	BO2	K	301	-	-	8/22/28/28	0/2/2/2
8	BO2	O	201	-	-	8/22/28/28	0/2/2/2
8	BO2	T	201	-	-	10/22/28/28	0/2/2/2
6	ATP	B	903	7	-	3/18/38/38	0/3/3/3
6	ATP	C	902	7	-	4/18/38/38	0/3/3/3
5	ADP	E	901	-	-	2/12/32/32	0/3/3/3
5	ADP	D	901	-	-	3/12/32/32	0/3/3/3
8	BO2	I	301	-	-	7/22/28/28	0/2/2/2
6	ATP	E	902	7	-	2/18/38/38	0/3/3/3
8	BO2	J	301	-	-	5/22/28/28	0/2/2/2
8	BO2	S	201	-	-	7/22/28/28	0/2/2/2
6	ATP	B	902	7	-	2/18/38/38	0/3/3/3
6	ATP	A	902	7	-	1/18/38/38	0/3/3/3
8	BO2	L	301	-	-	8/22/28/28	0/2/2/2
8	BO2	R	201	-	-	14/22/28/28	0/2/2/2
8	BO2	Q	201	-	-	15/22/28/28	0/2/2/2

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	301	BO2	C21-C22-C23	3.21	119.43	115.39
8	R	201	BO2	C21-C22-C23	2.69	118.77	115.39
8	T	201	BO2	C21-C22-C23	2.63	118.69	115.39
6	A	904	ATP	C5-C6-N6	2.34	123.91	120.35
5	E	901	ADP	O2B-PB-O1B	2.28	119.60	110.68

There are no chirality outliers.

5 of 160 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	901	ADP	C5'-O5'-PA-O1A
6	A	902	ATP	O4'-C4'-C5'-O5'
6	B	903	ATP	O4'-C4'-C5'-O5'
6	C	902	ATP	O4'-C4'-C5'-O5'
6	C	902	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

25 monomers are involved in 328 short contacts:

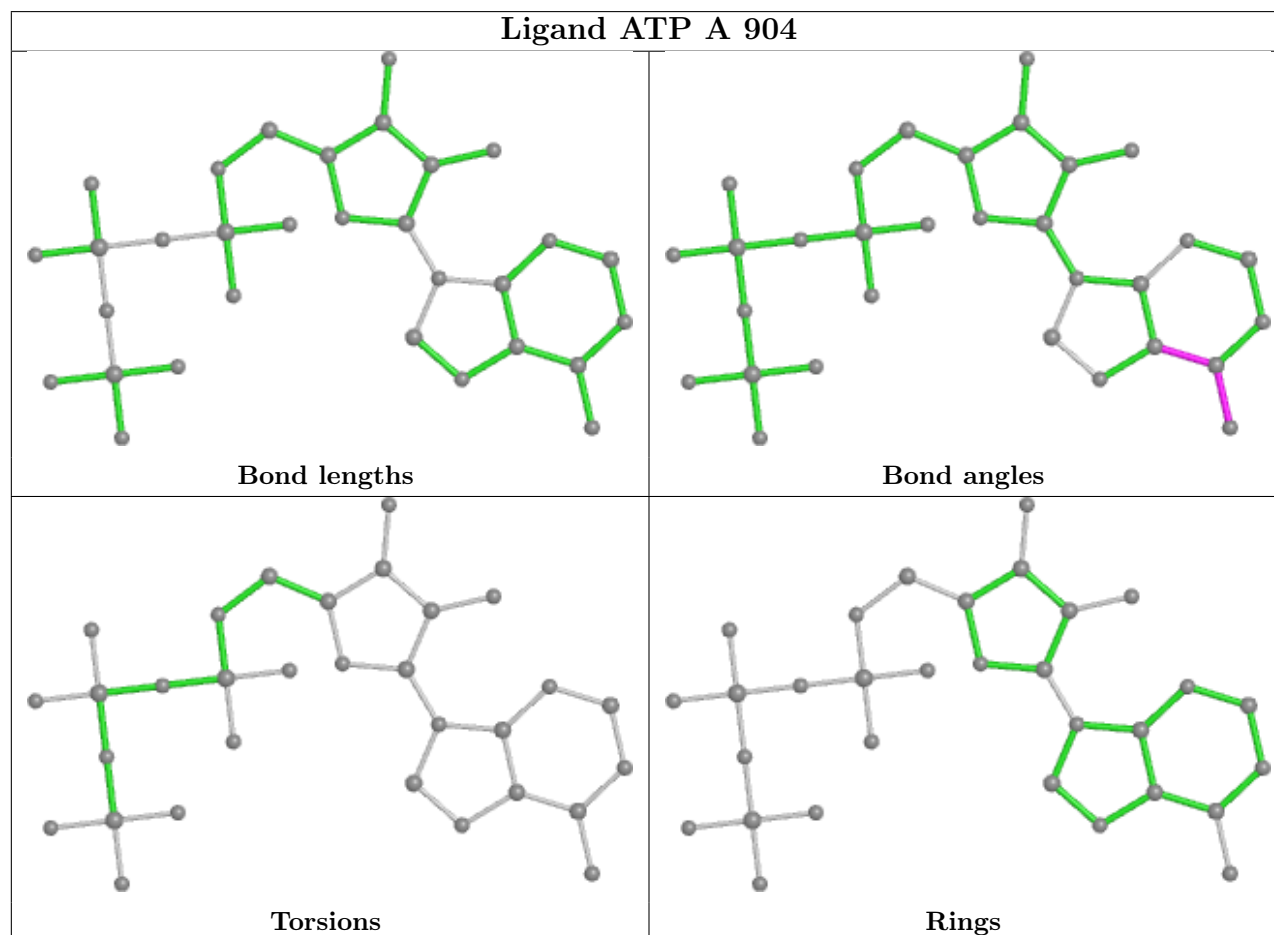
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	904	ATP	24	0
8	N	201	BO2	12	0
6	C	903	ATP	6	0
8	H	301	BO2	5	0
8	M	301	BO2	11	0
5	F	901	ADP	24	0
8	G	301	BO2	10	0
8	P	201	BO2	17	0
5	A	901	ADP	8	0
8	K	301	BO2	6	0
8	O	201	BO2	11	0
8	T	201	BO2	10	0
6	B	903	ATP	12	0
6	C	902	ATP	23	0
5	E	901	ADP	7	0
5	D	901	ADP	27	0
8	I	301	BO2	11	0
6	E	902	ATP	14	0
8	J	301	BO2	12	0

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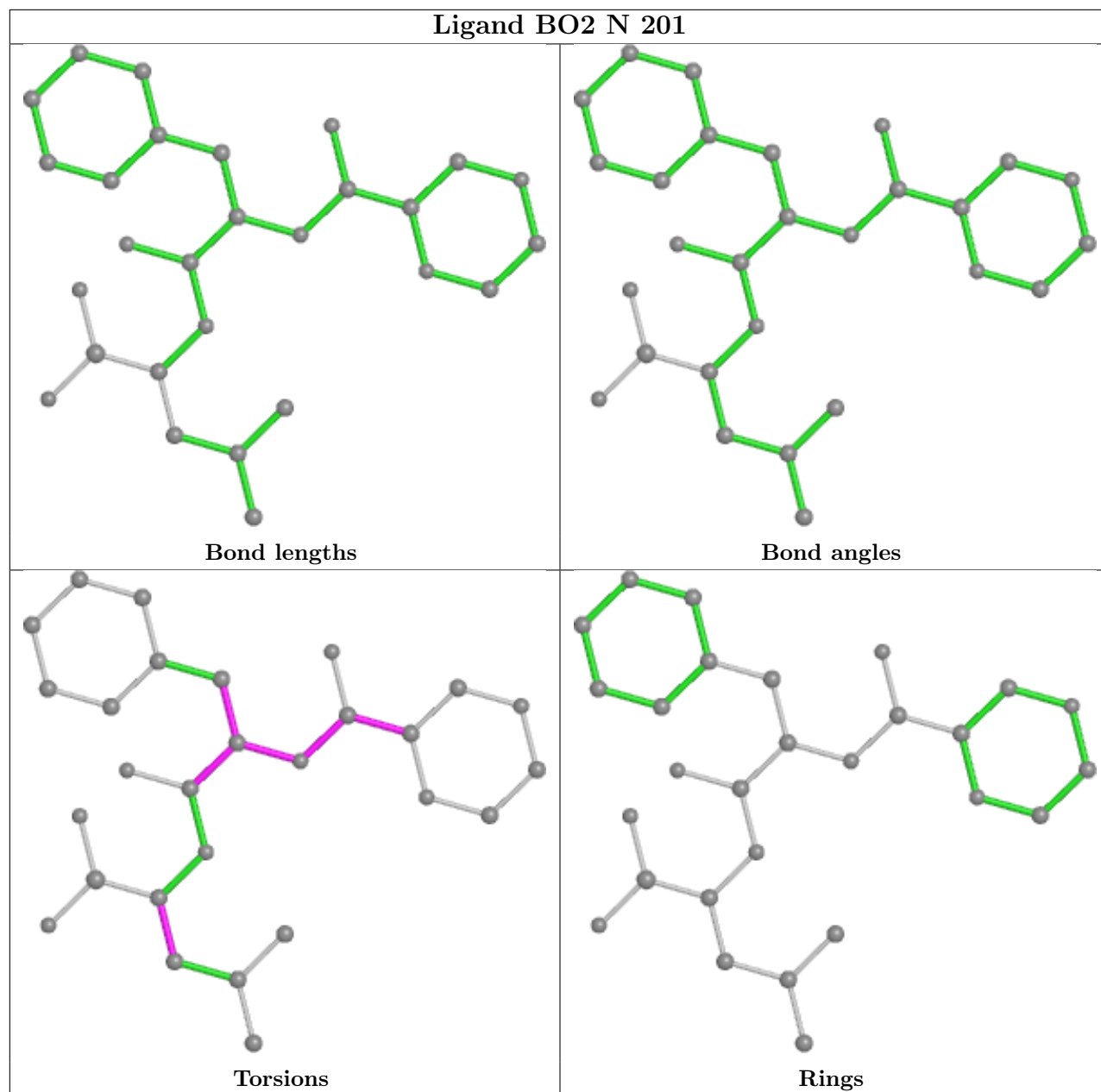
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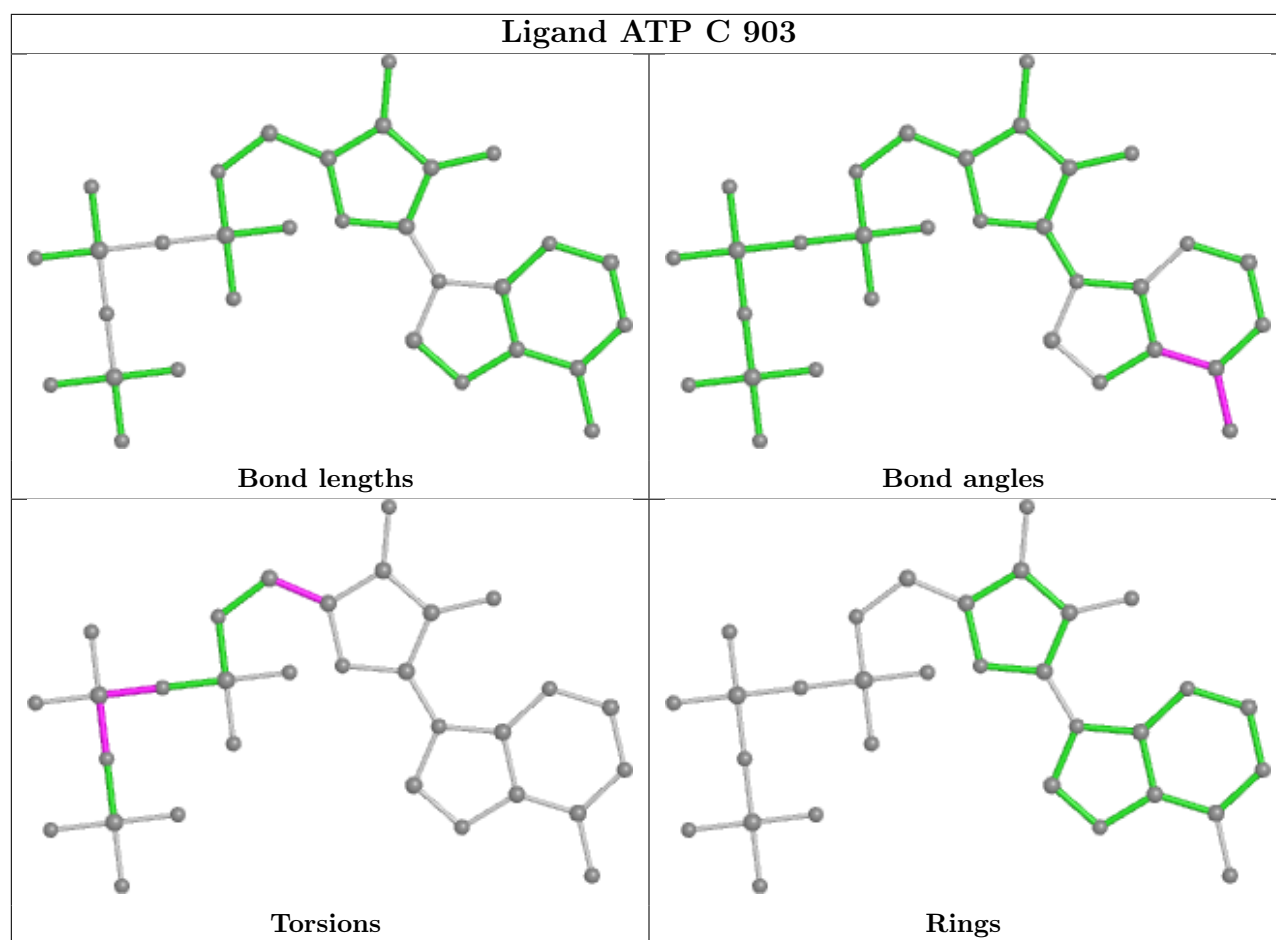
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	S	201	BO2	10	0
6	B	902	ATP	11	0
6	A	902	ATP	12	0
8	L	301	BO2	20	0
8	R	201	BO2	12	0
8	Q	201	BO2	13	0

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.

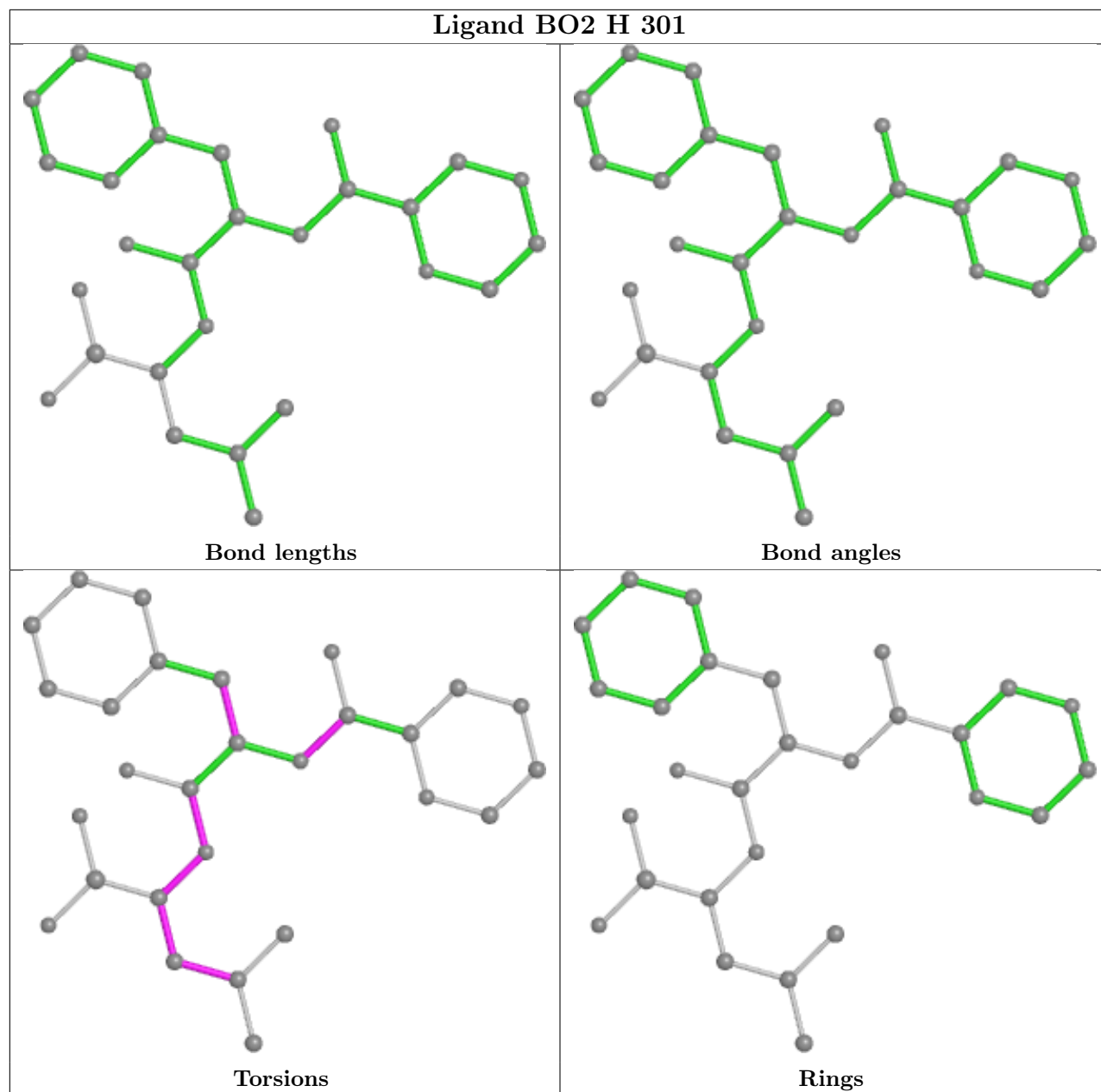


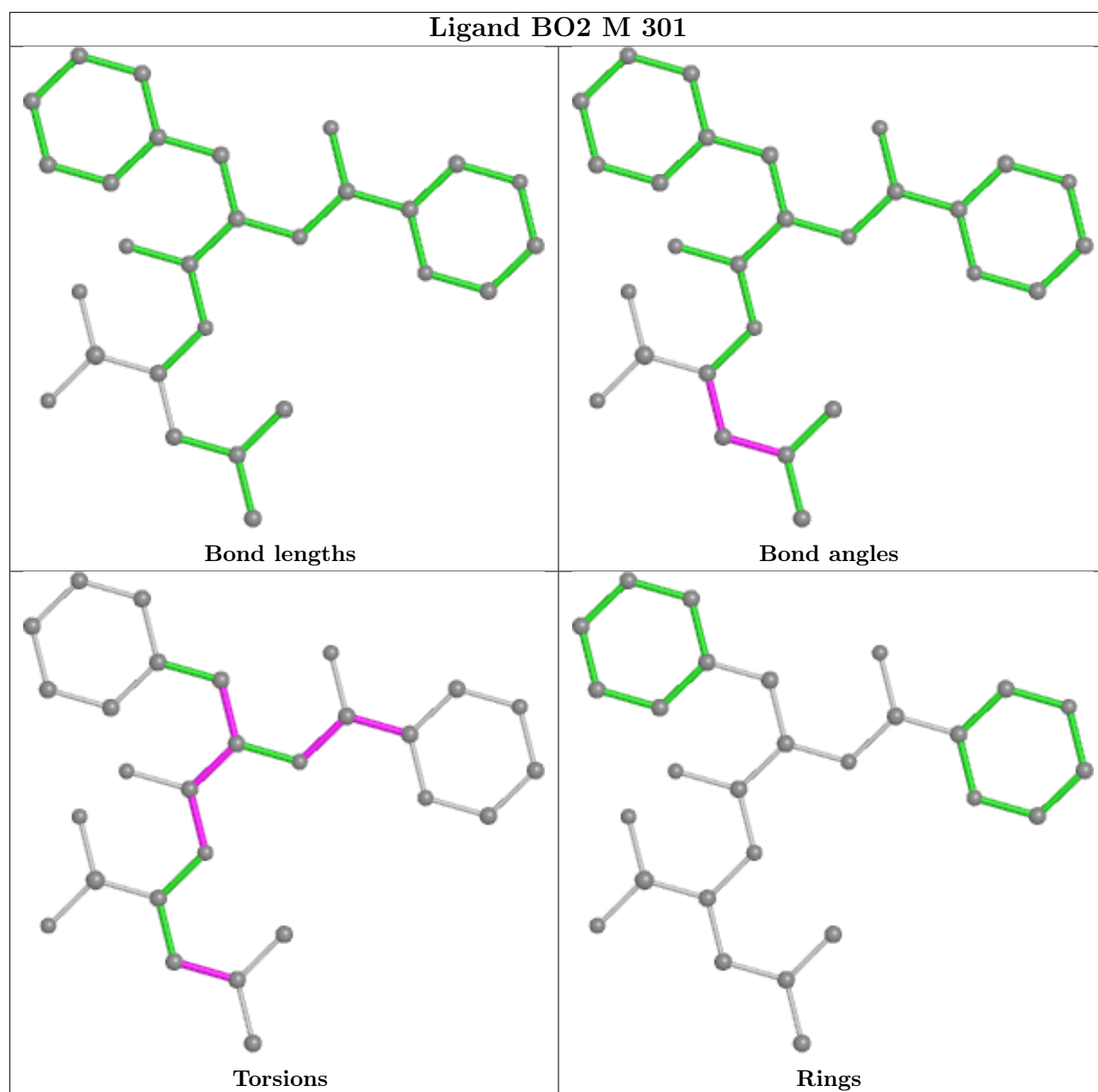
Ligand BO2 N 201

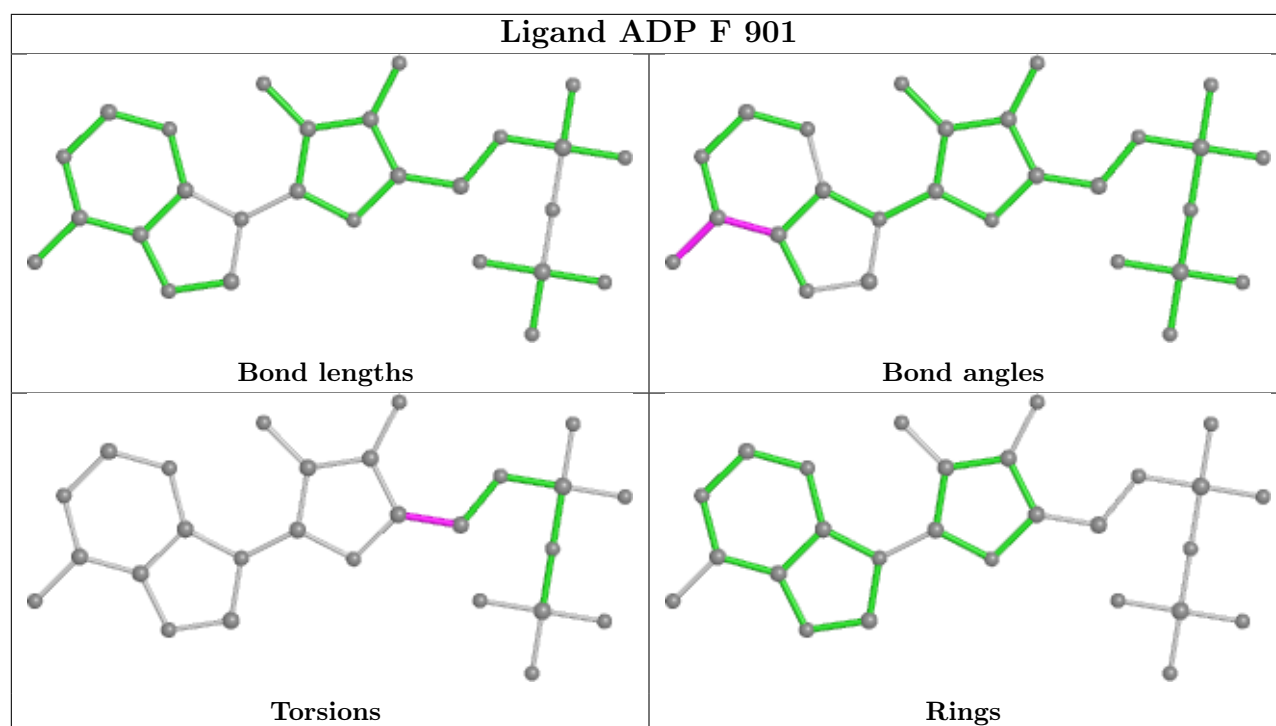




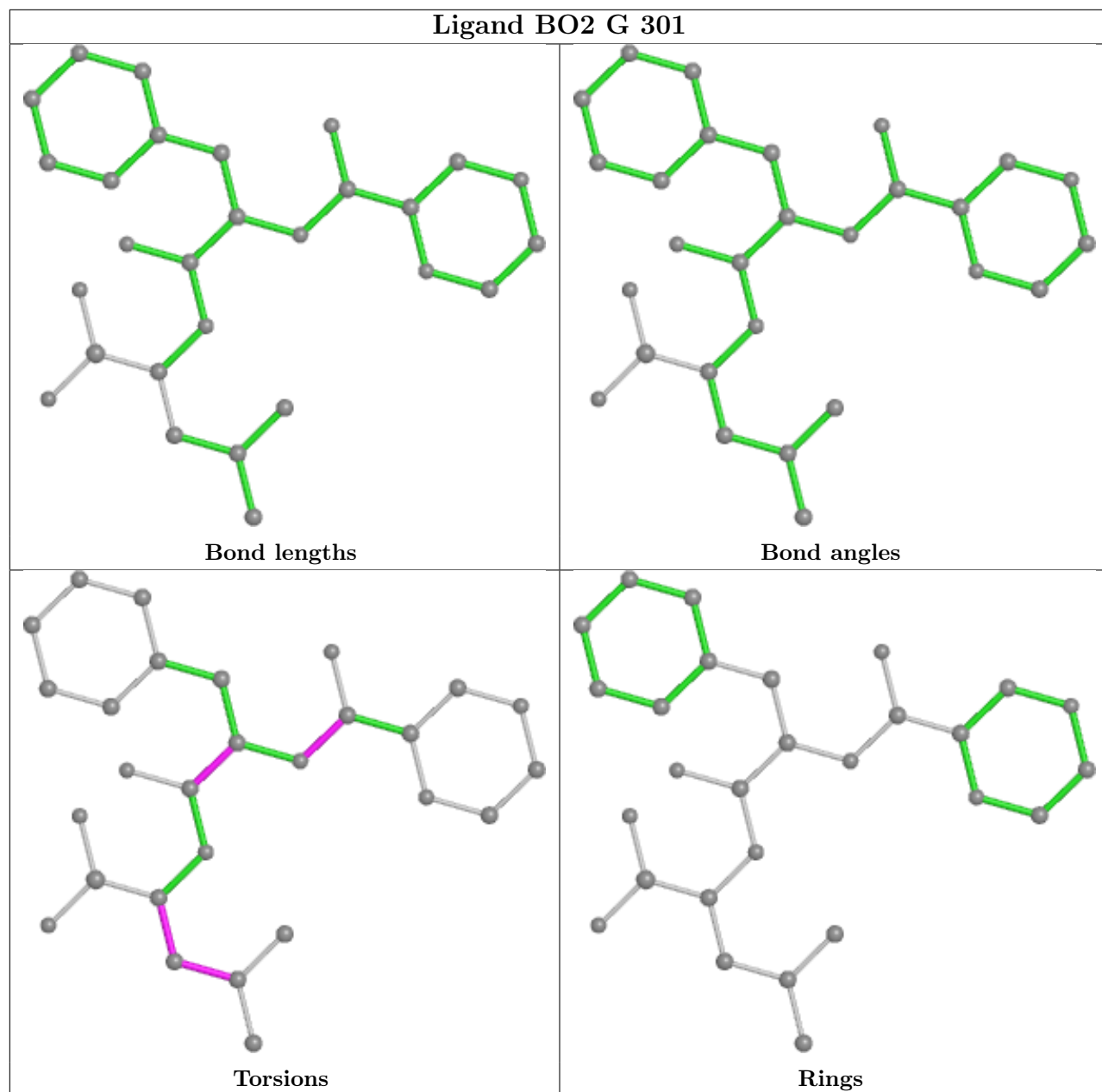
Ligand BO2 H 301



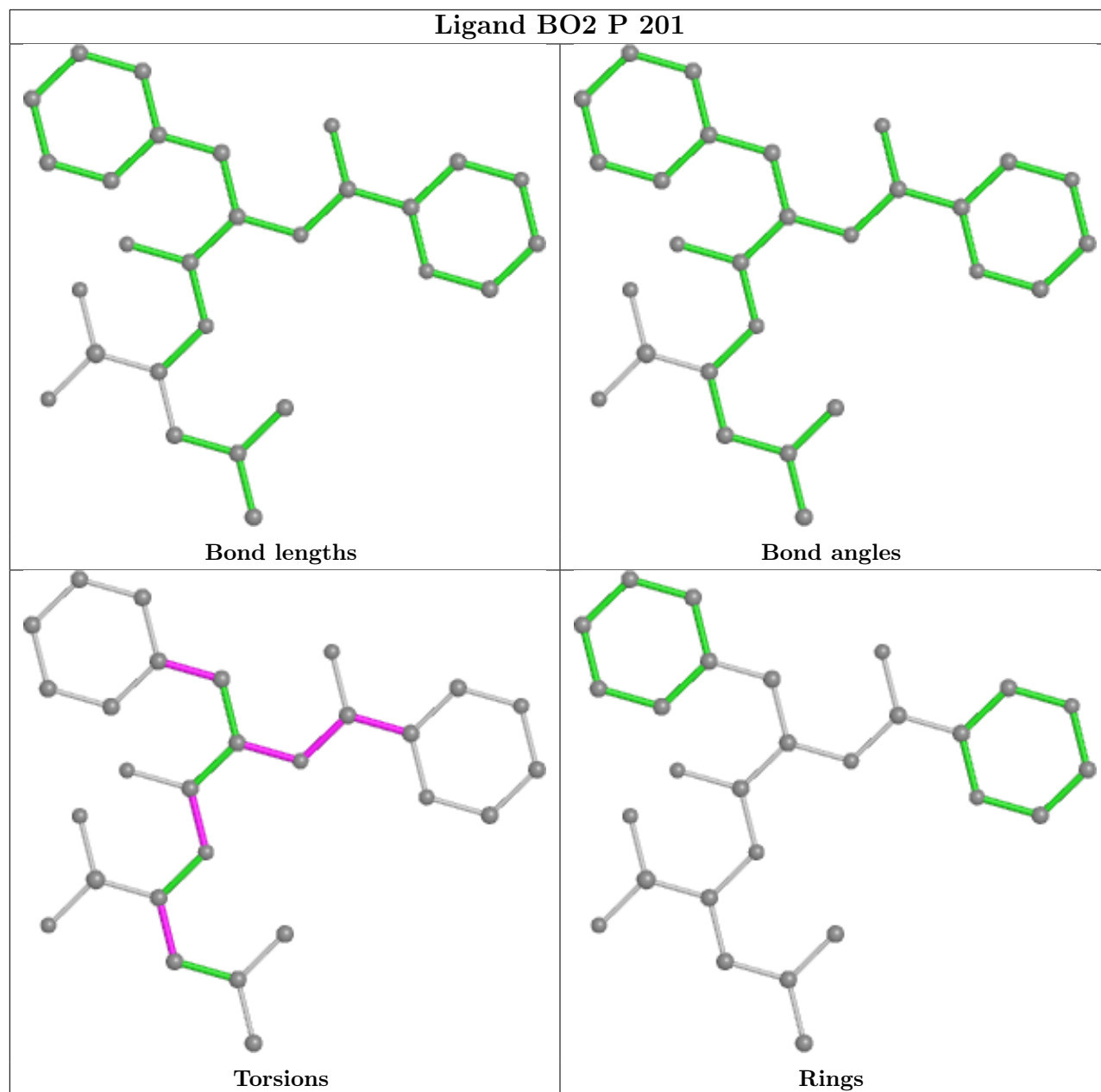


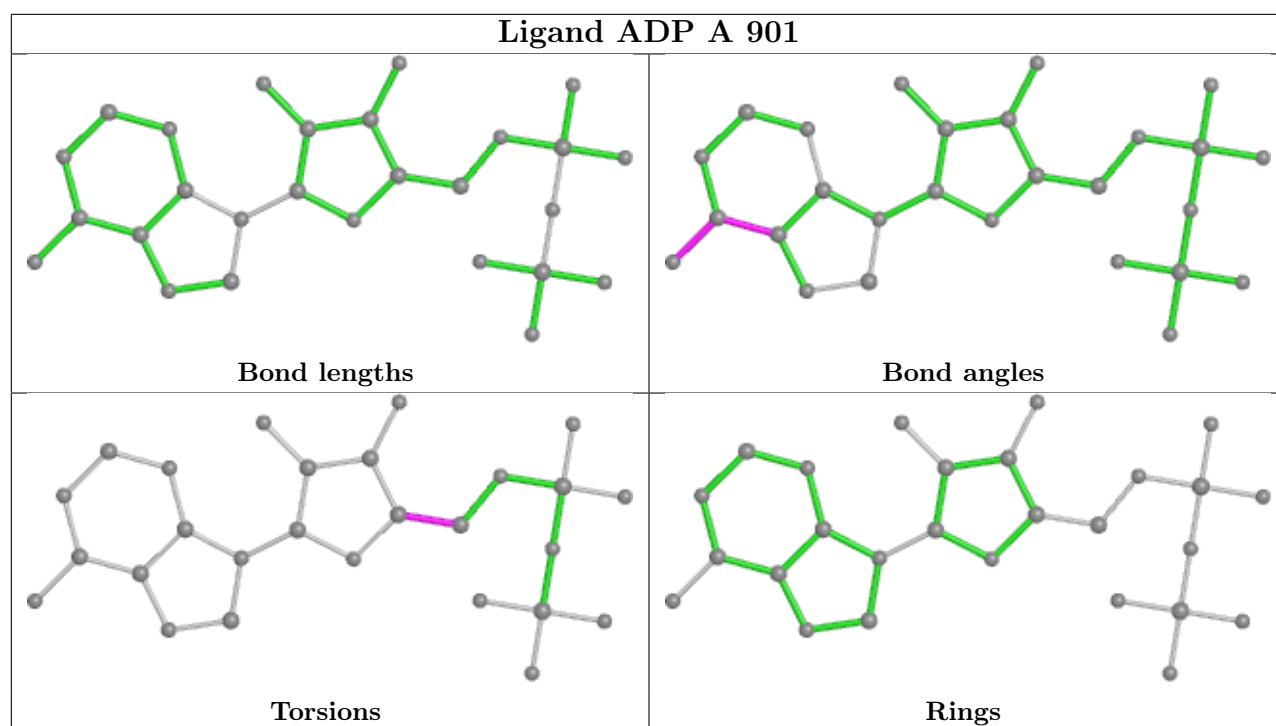


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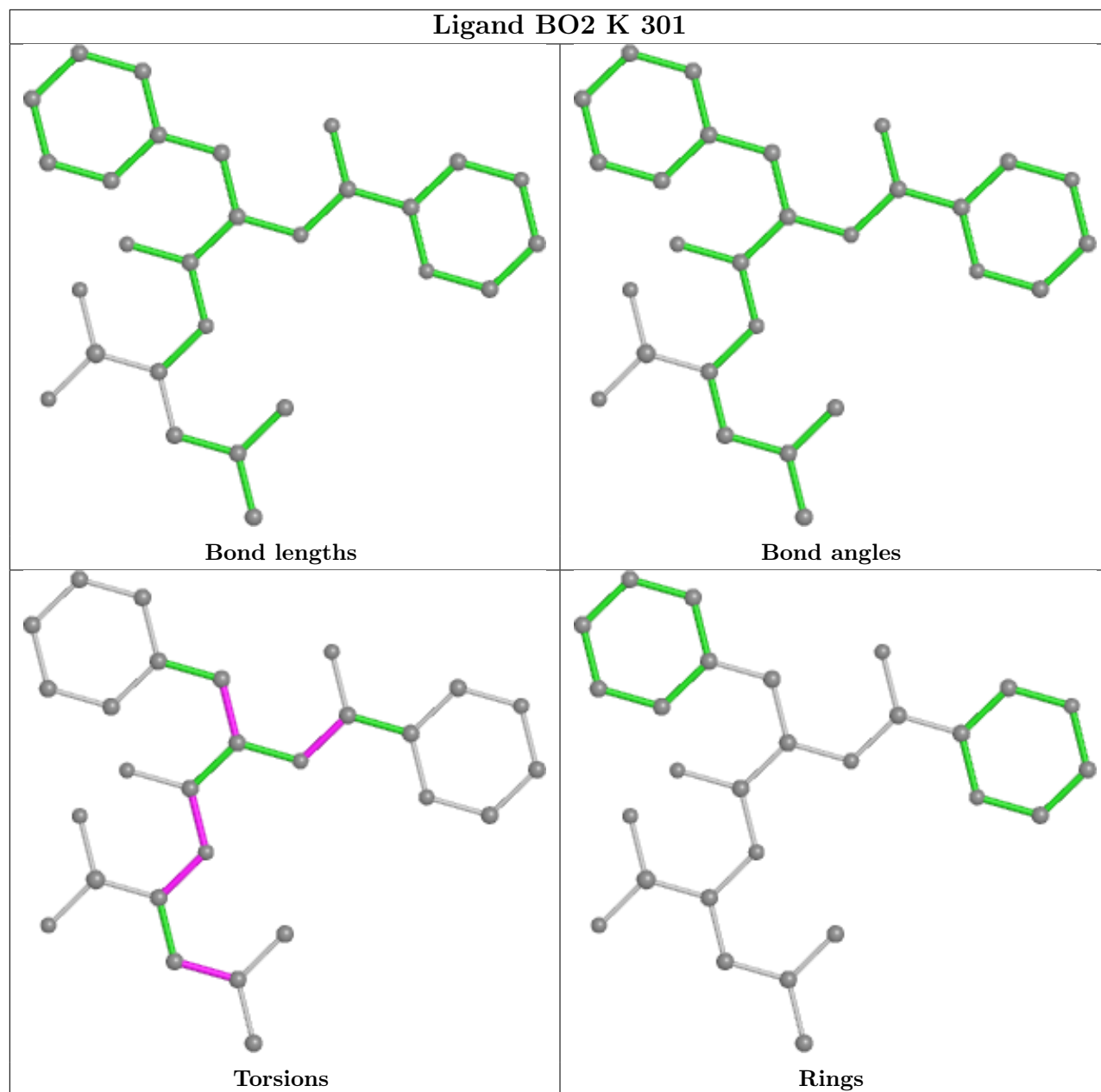


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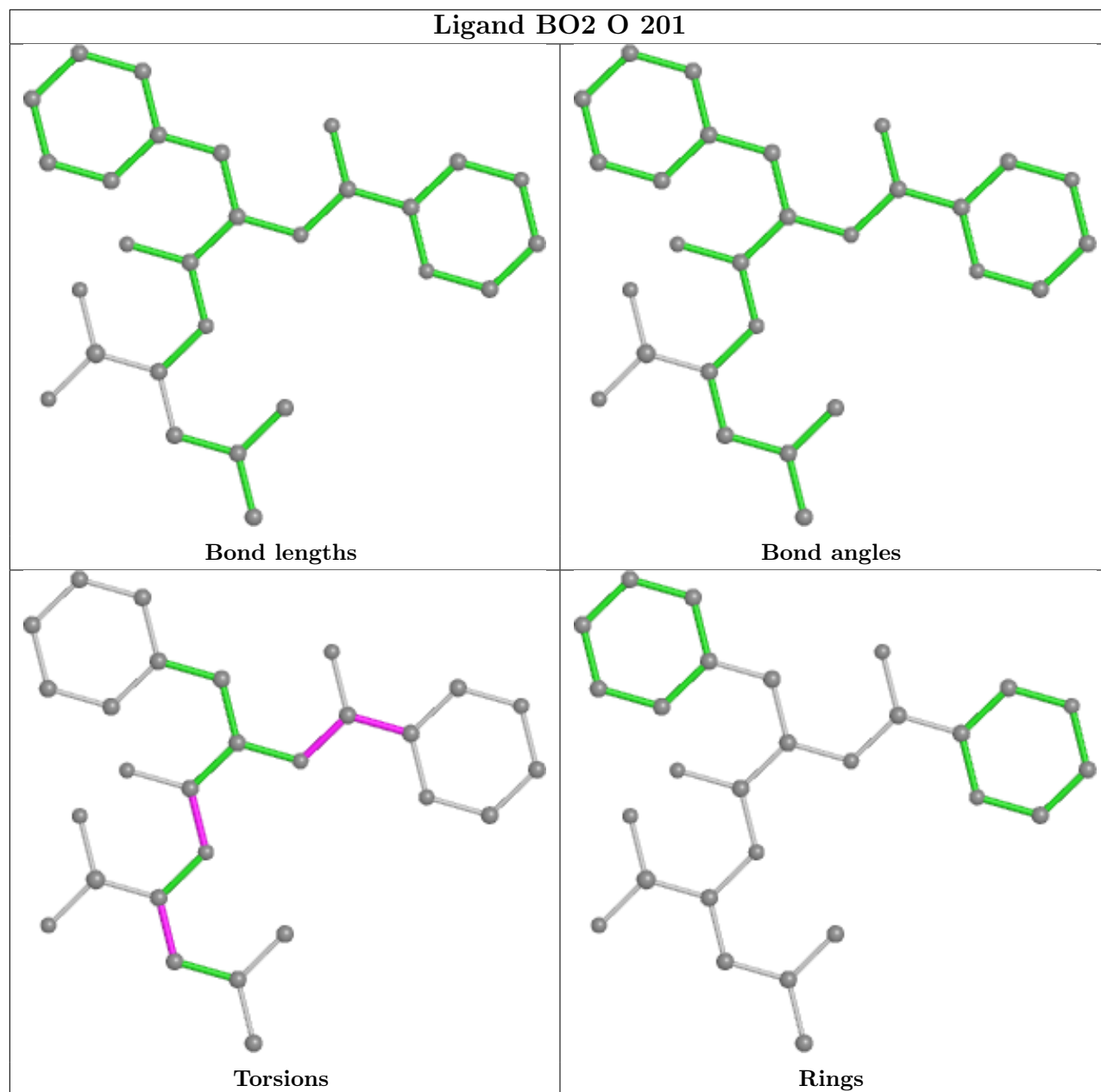




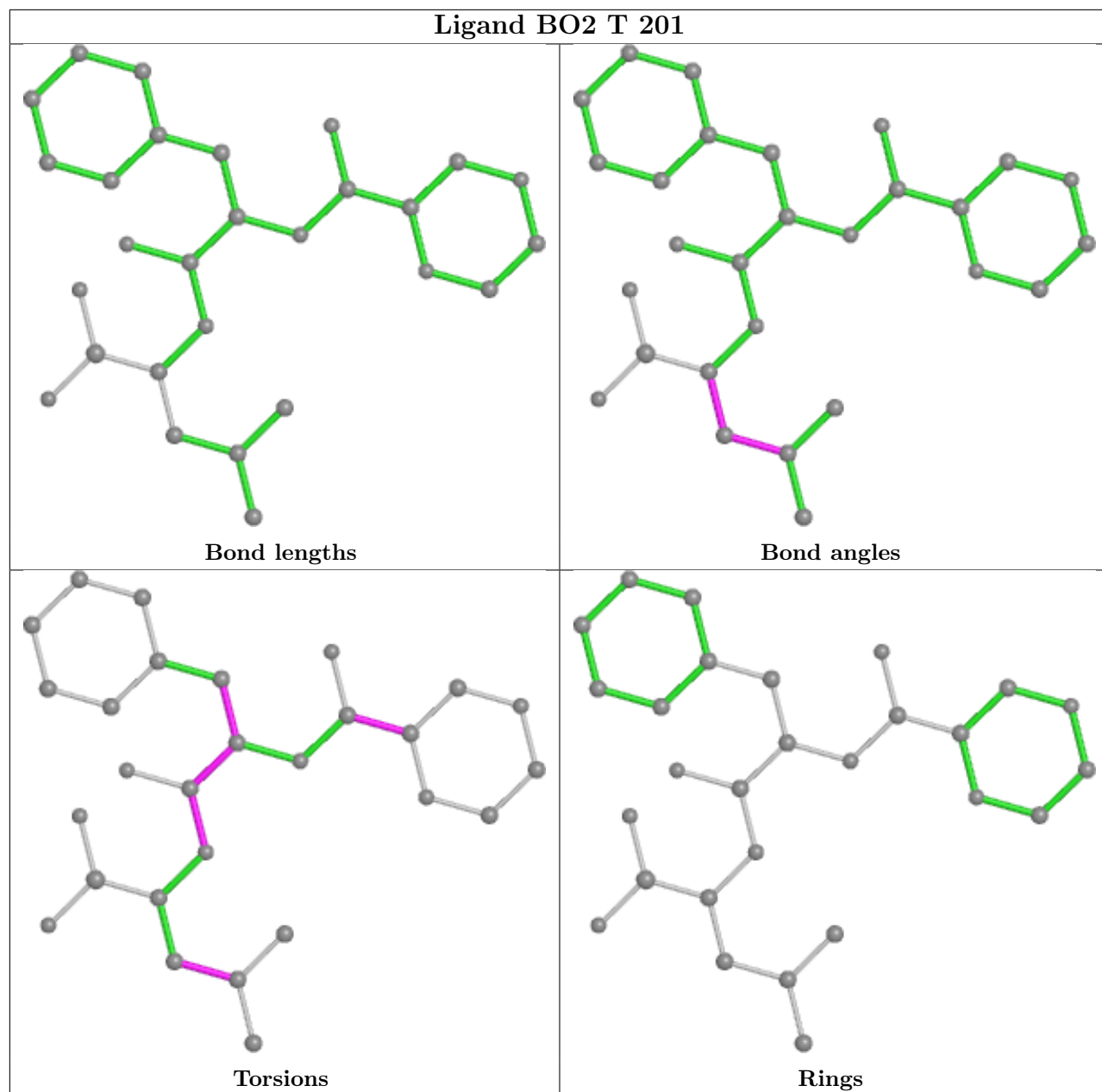
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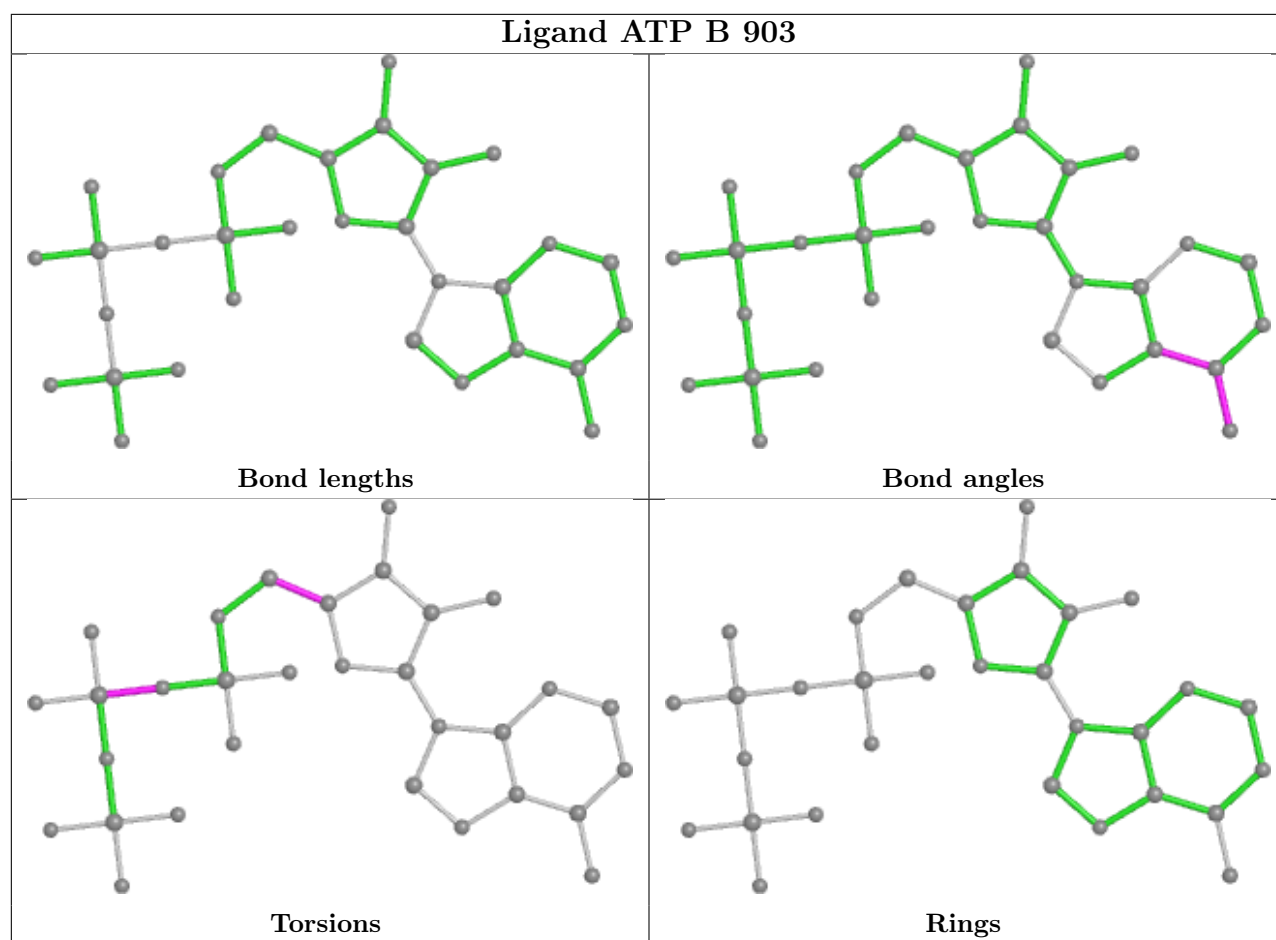


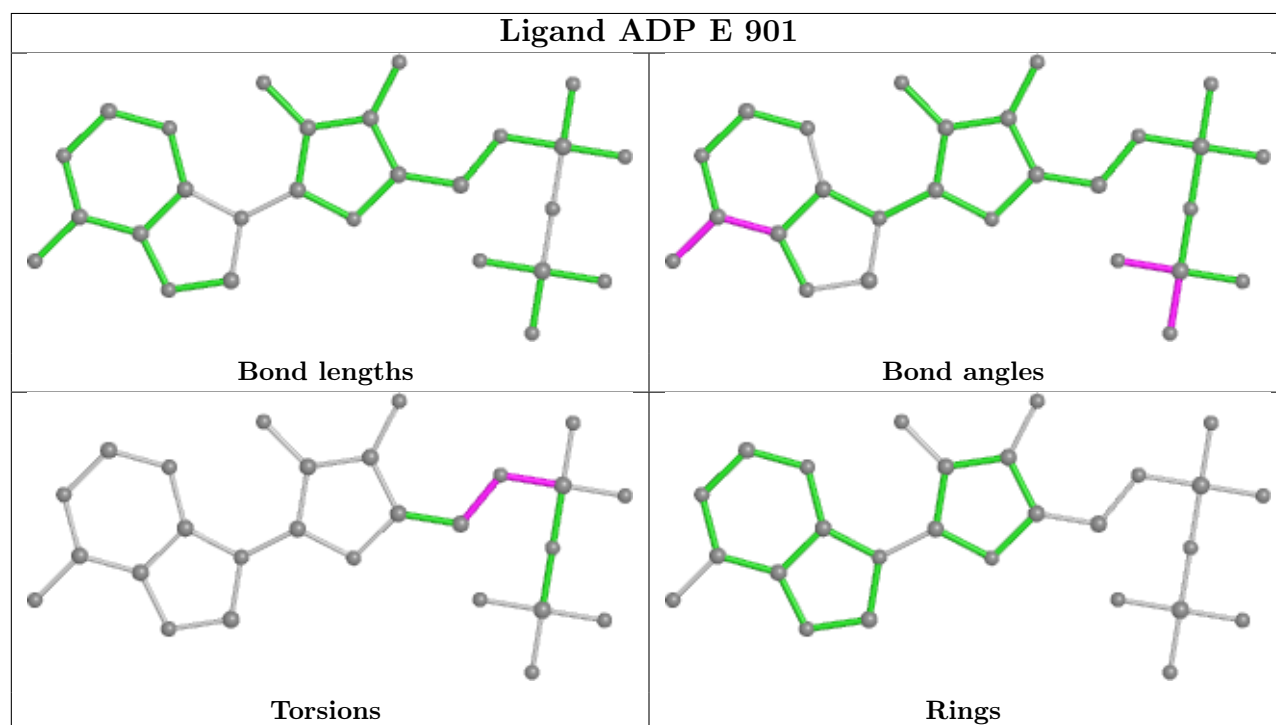
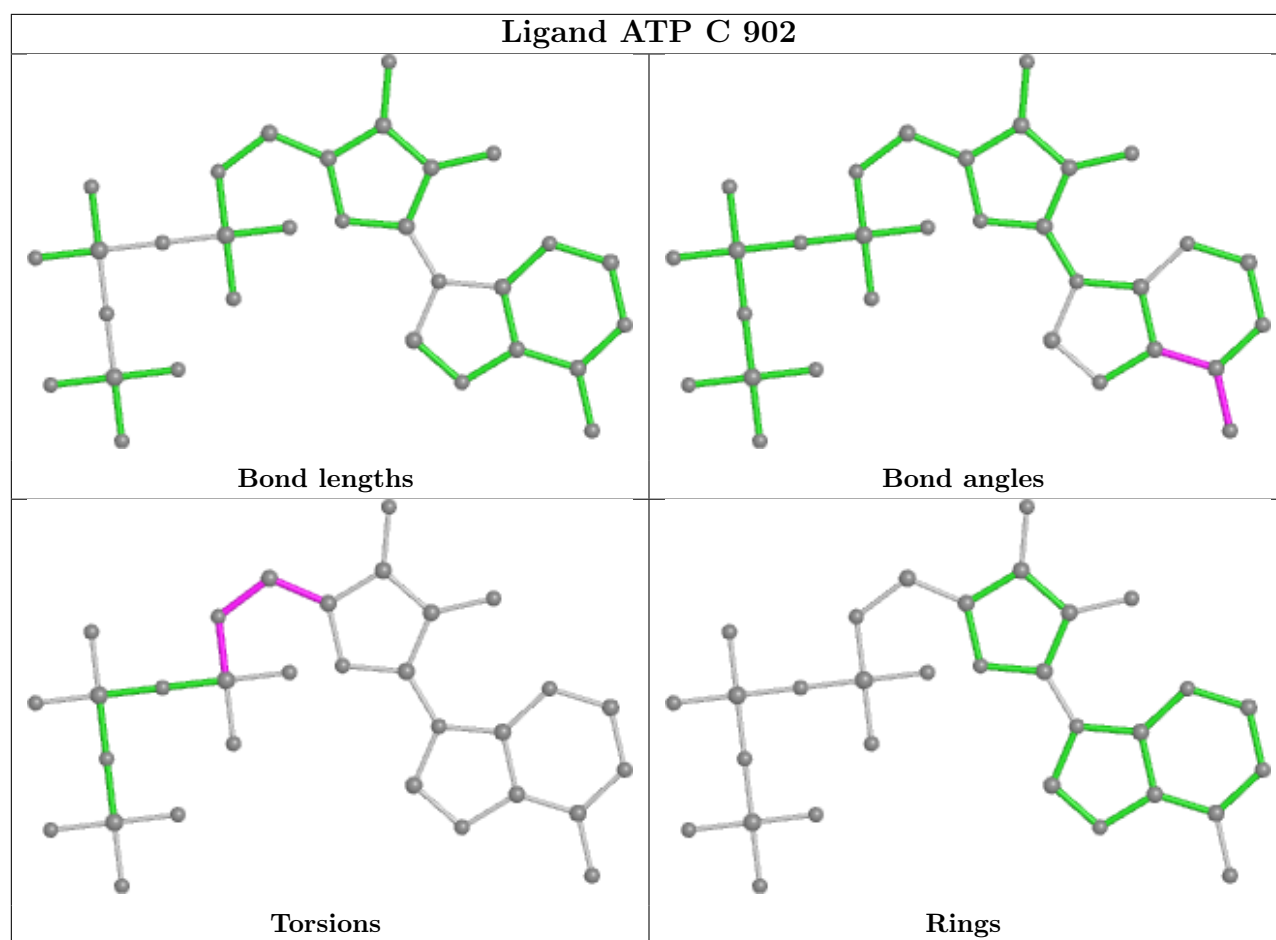
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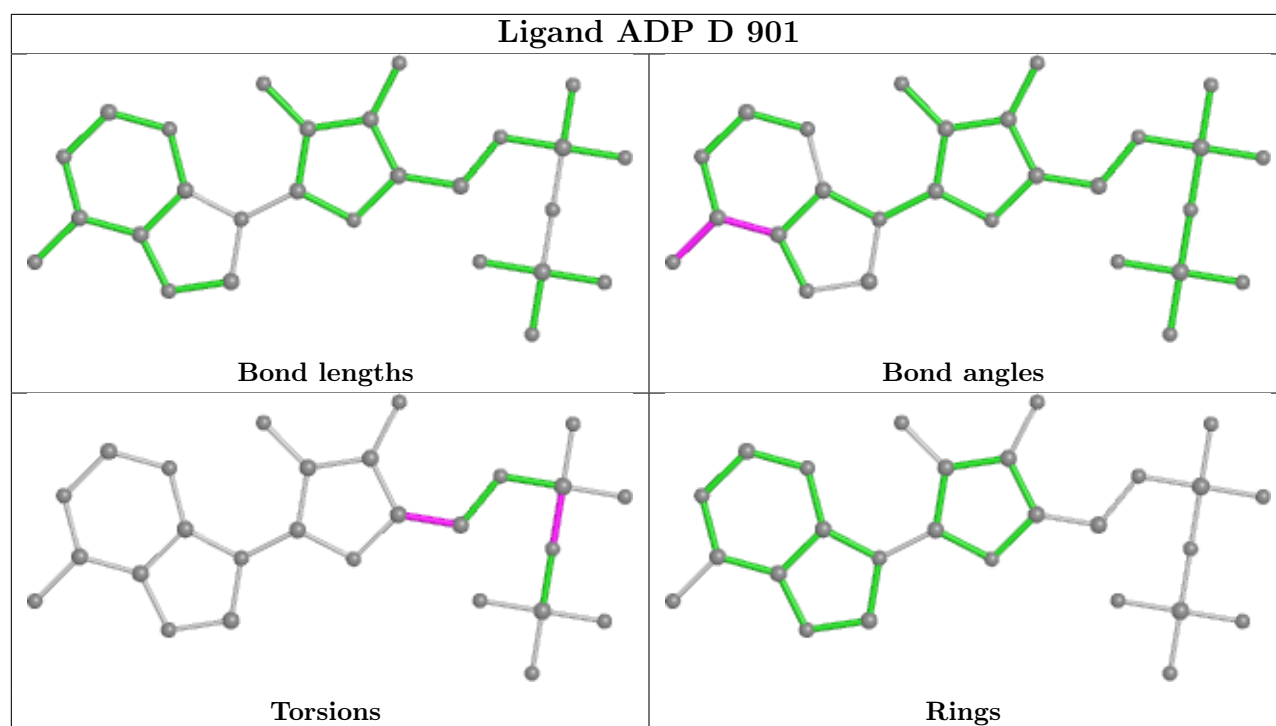


Ligand BO2 T 201

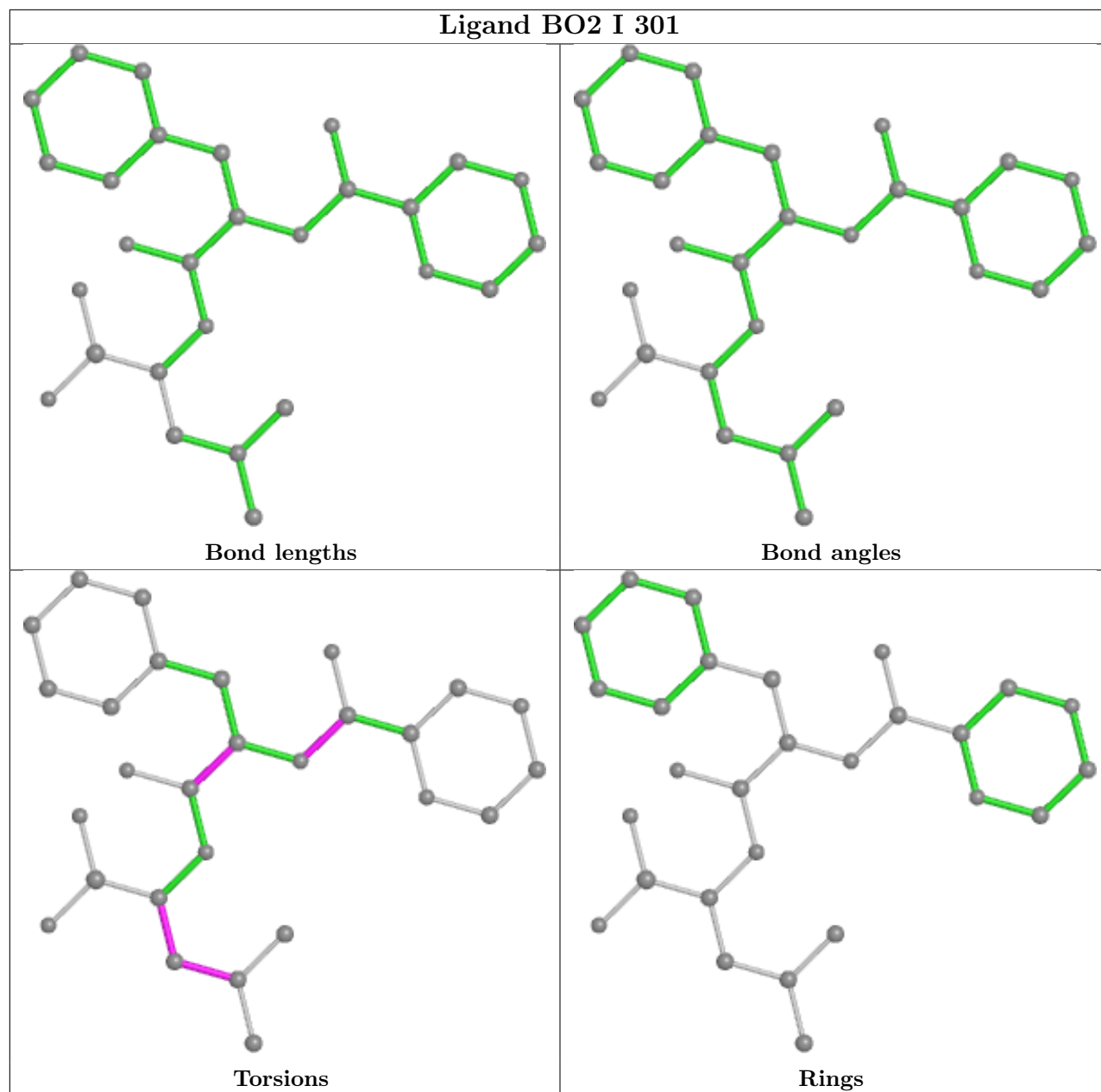


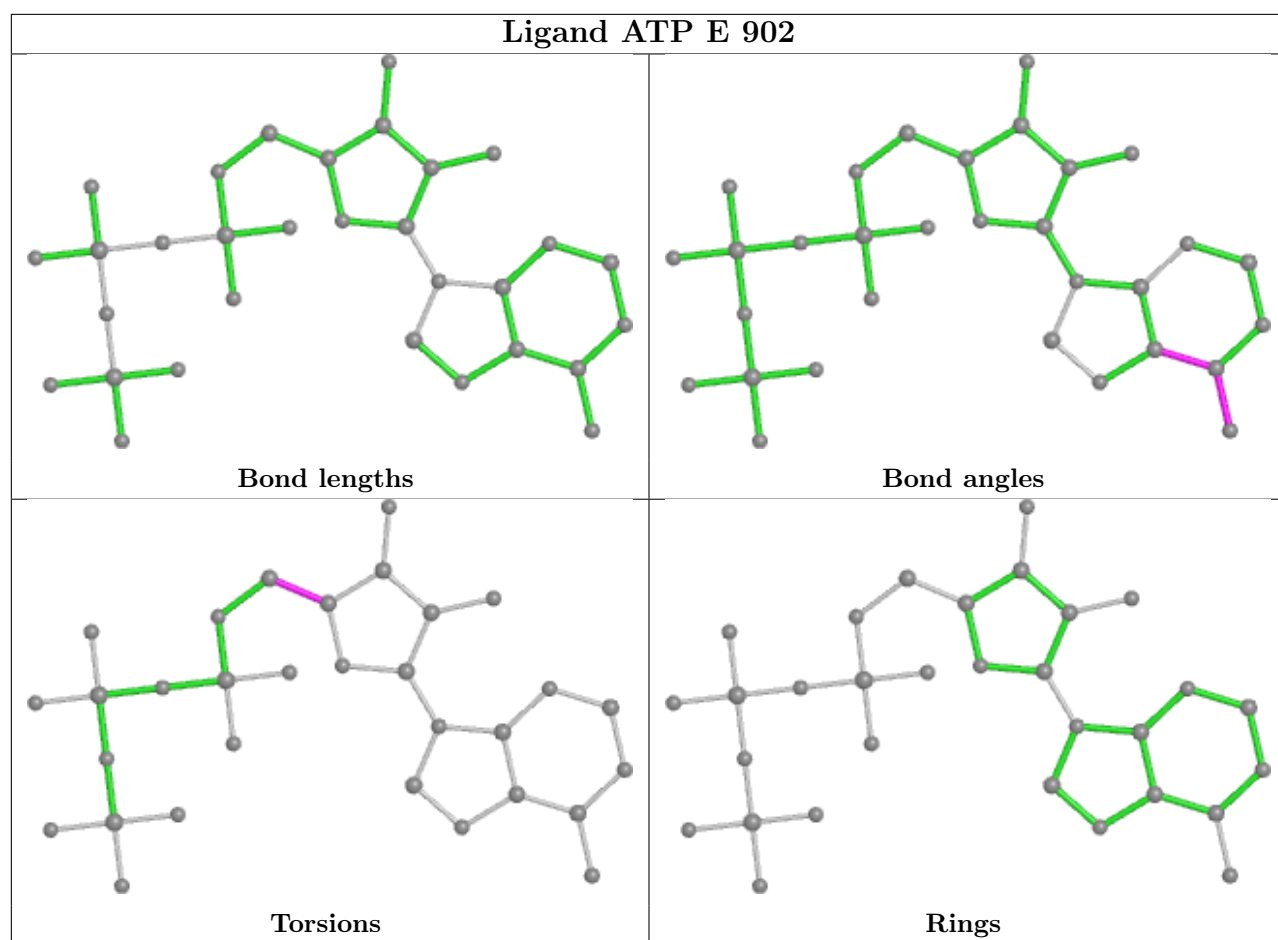




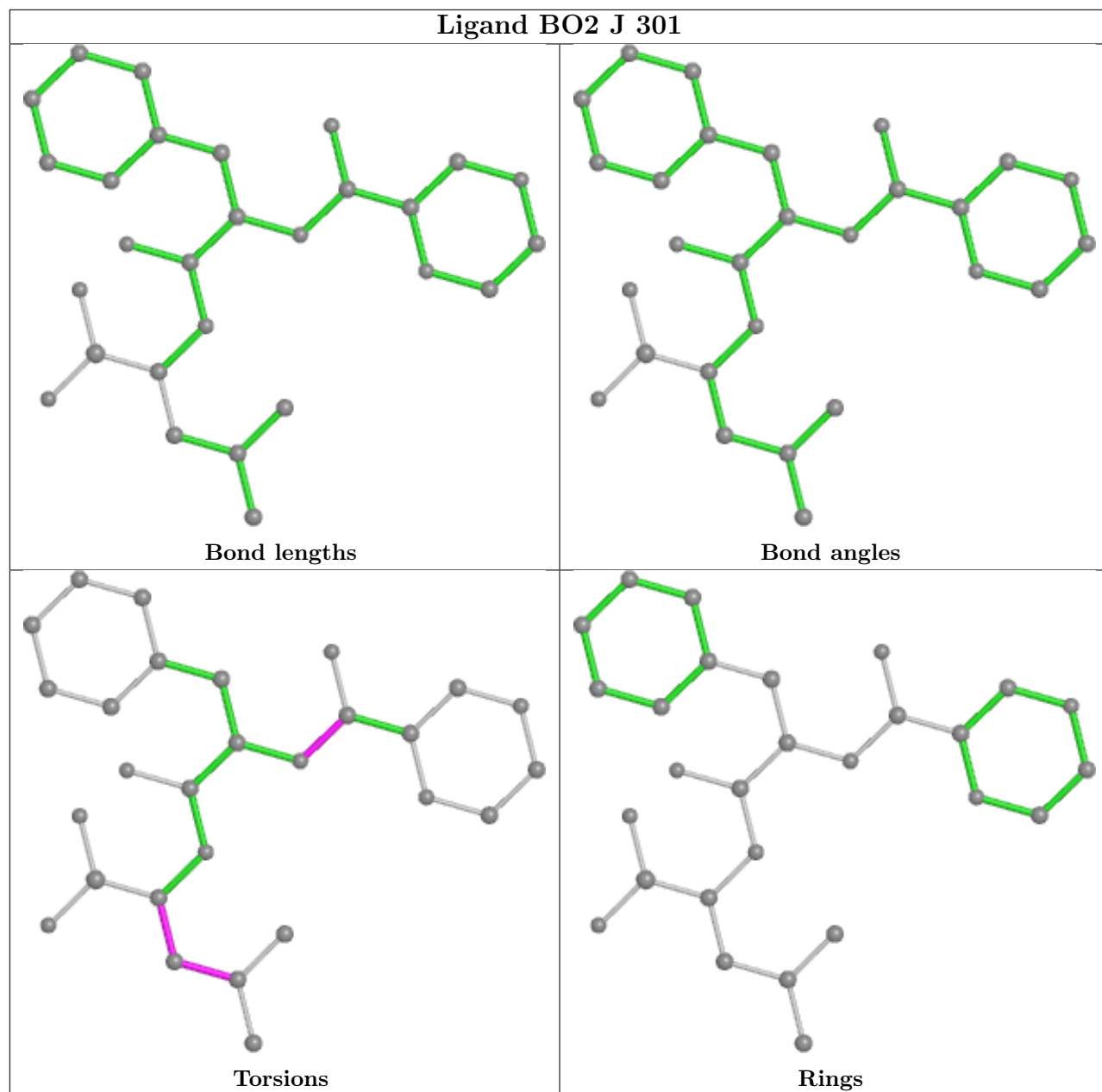


Ligand BO2 I 301

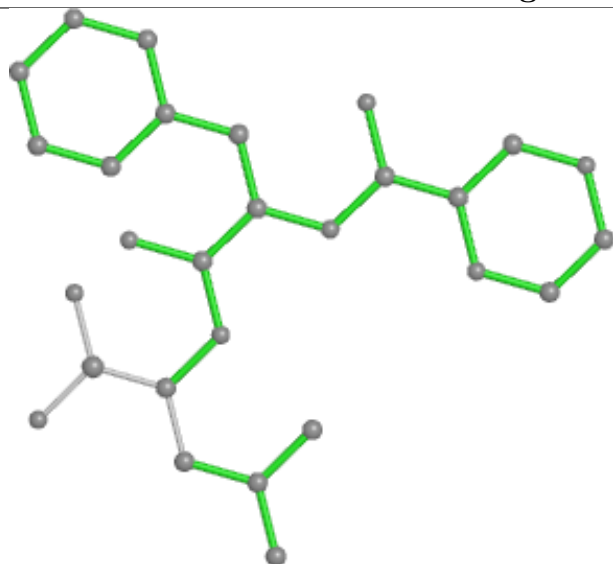




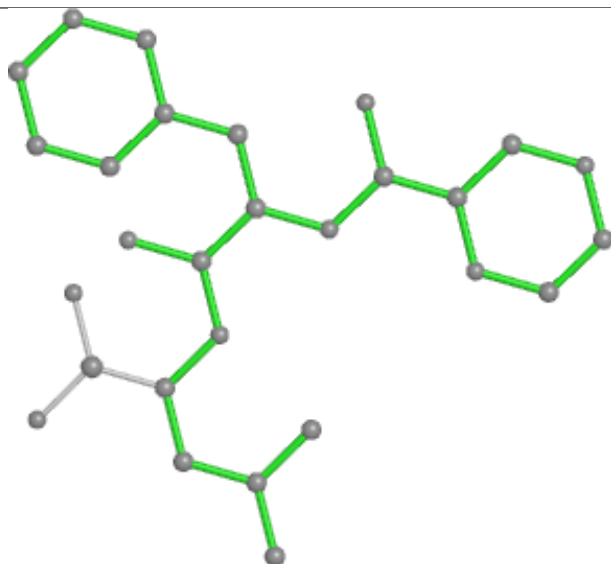
Ligand BO2 J 301



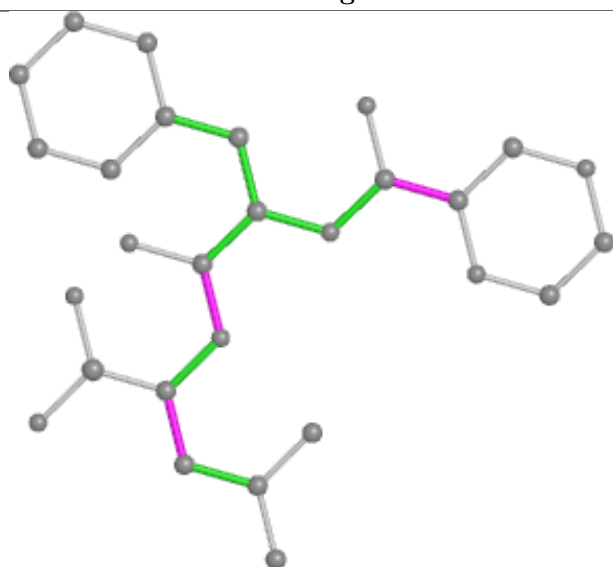
Ligand BO2 S 201



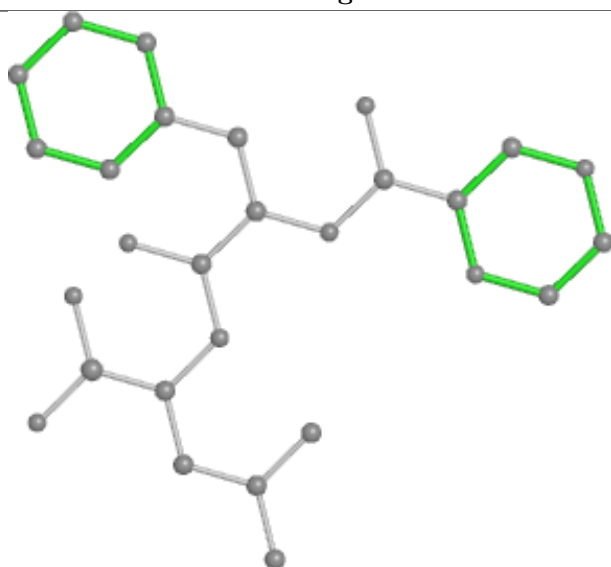
Bond lengths



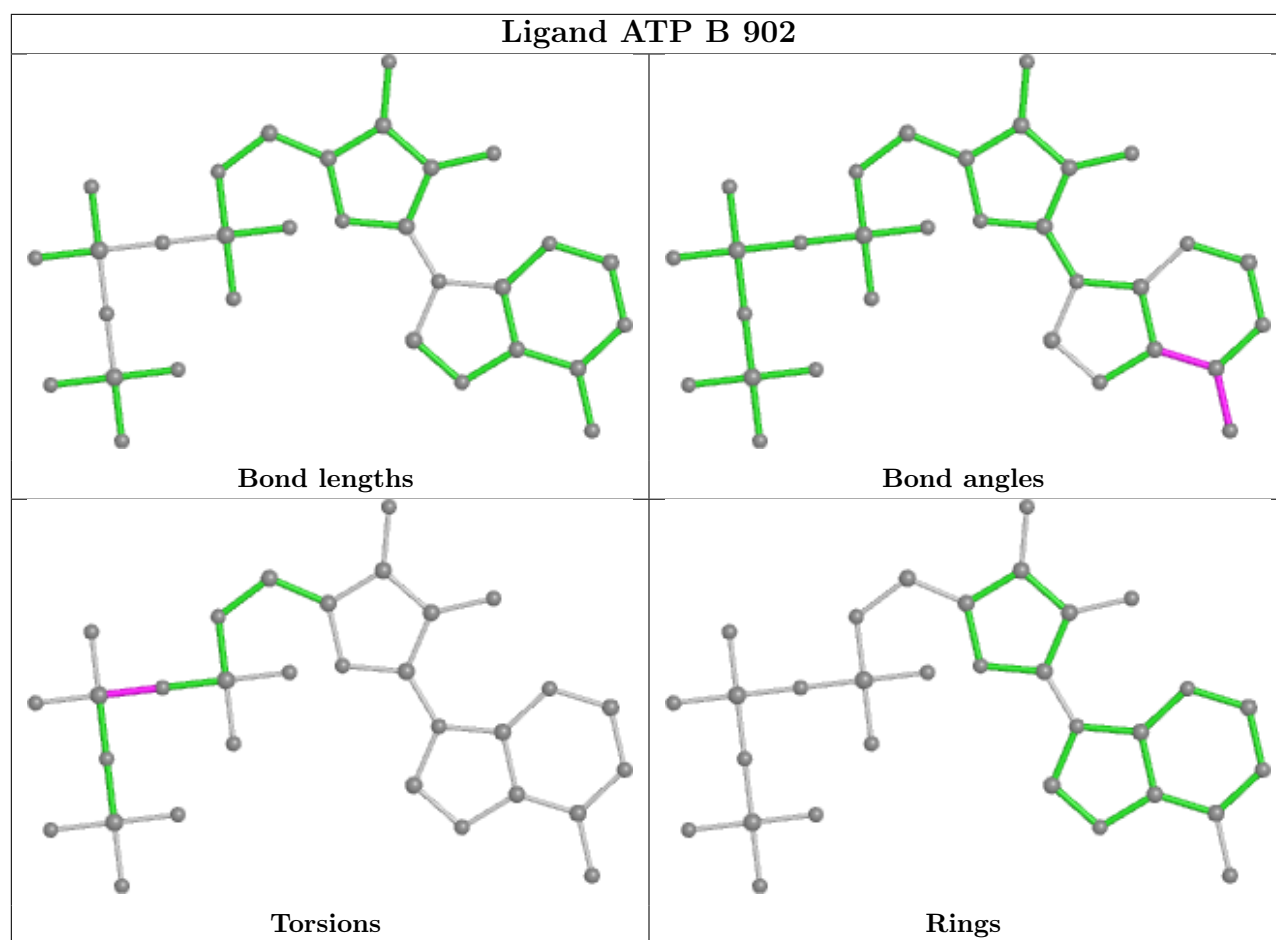
Bond angles

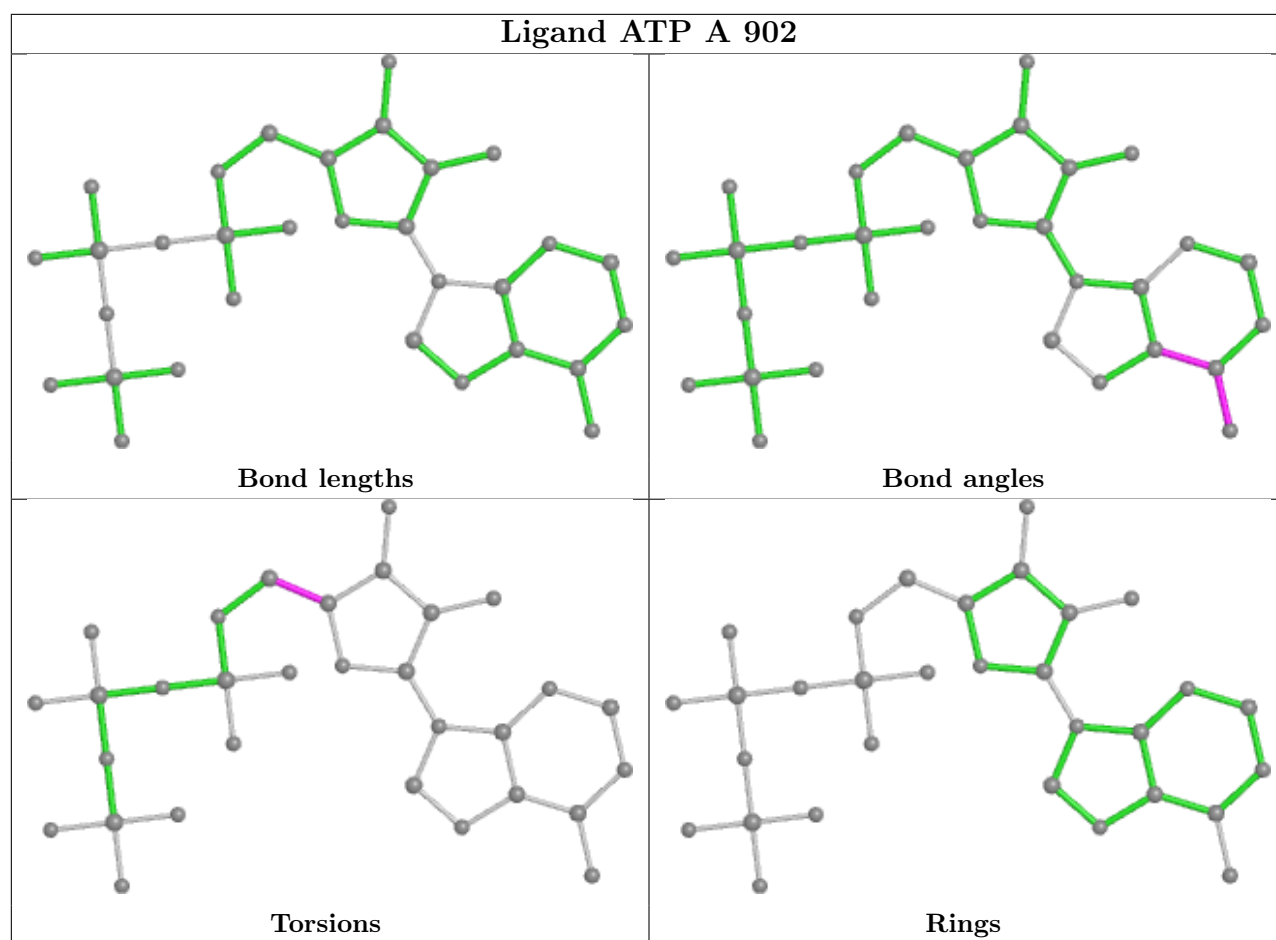


Torsions

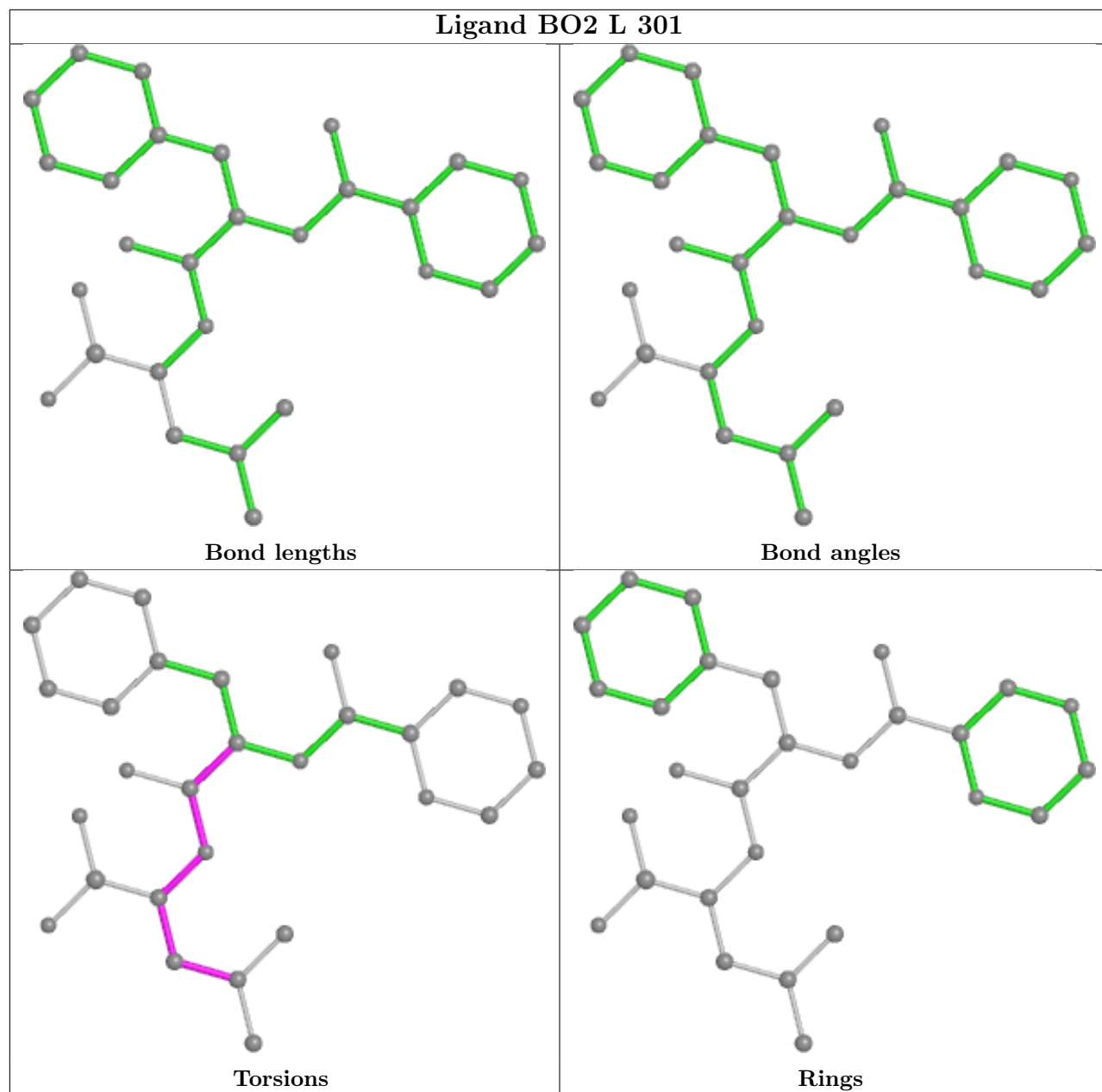


Rings

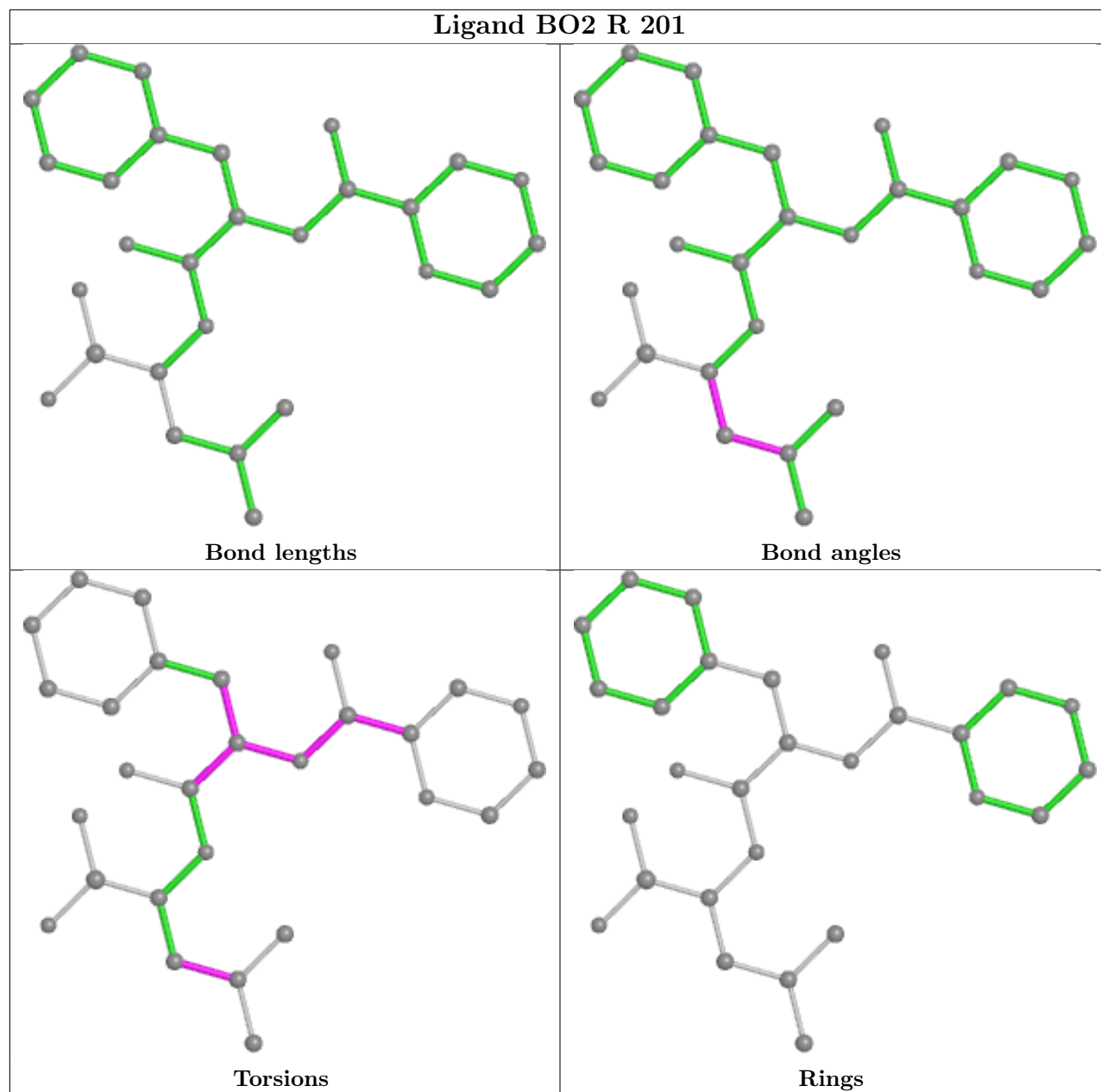


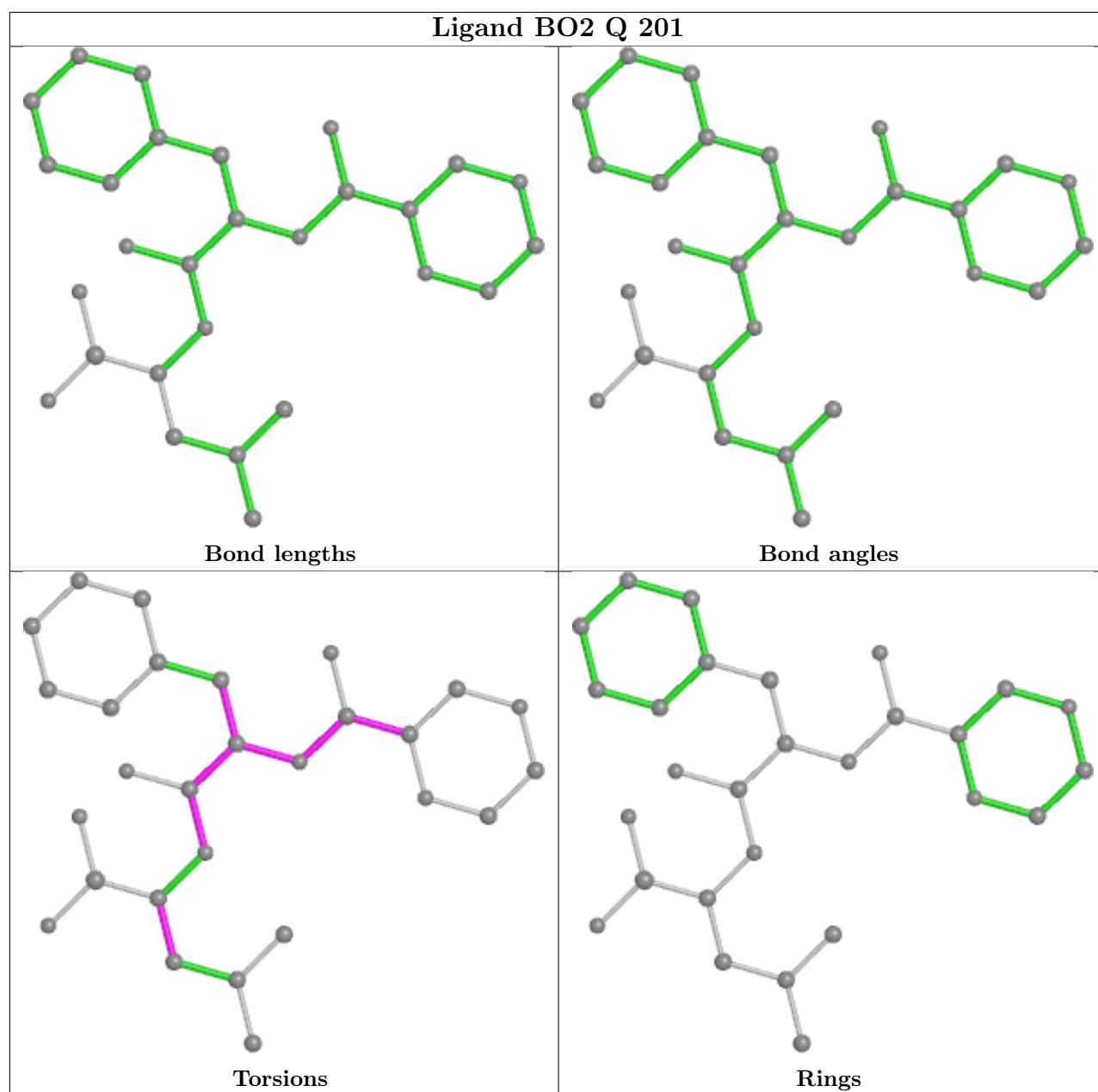


Ligand BO2 L 301



Ligand BO2 R 201





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.

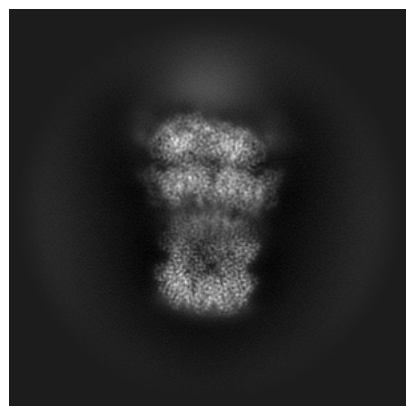
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39157. These allow visual inspection of the internal detail of the map and identification of artifacts.

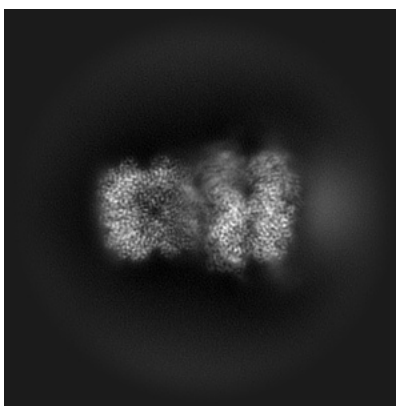
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

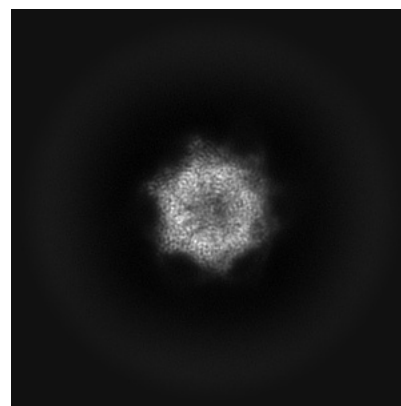
6.1.1 Primary map



X

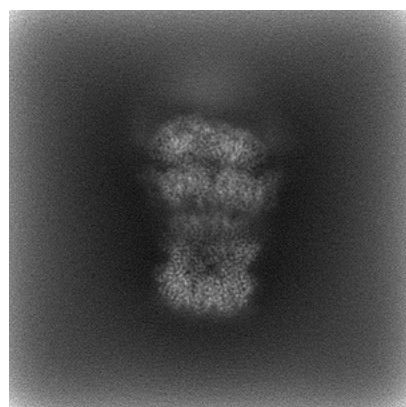


Y

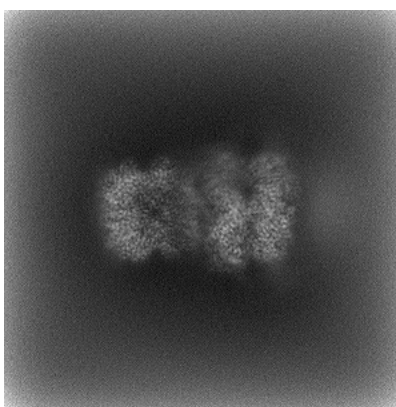


Z

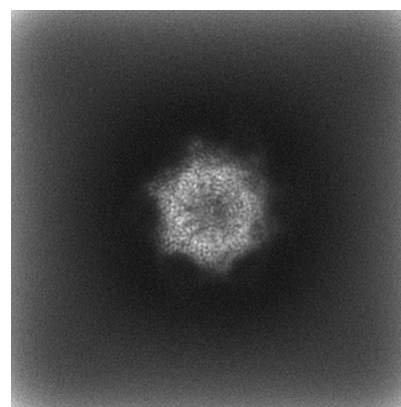
6.1.2 Raw map



X



Y

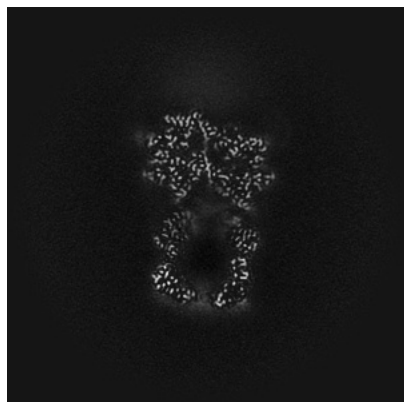


Z

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

6.2 Central slices [i](#)

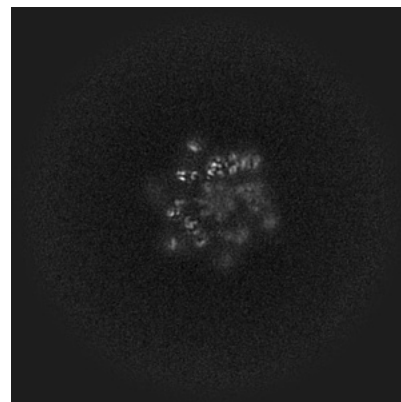
6.2.1 Primary map



X Index: 256

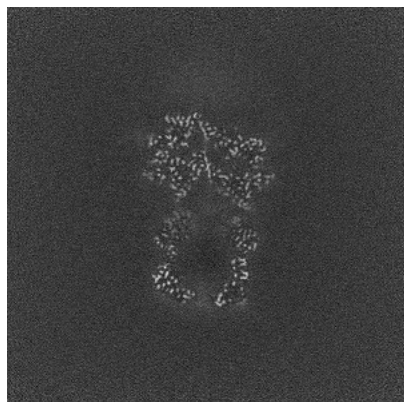


Y Index: 256

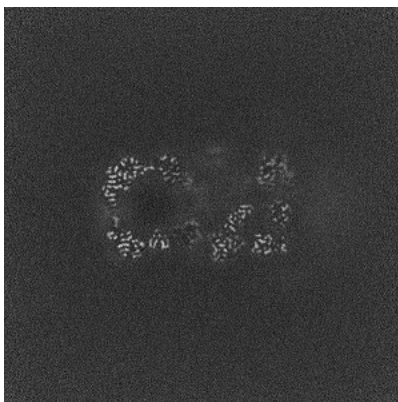


Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256

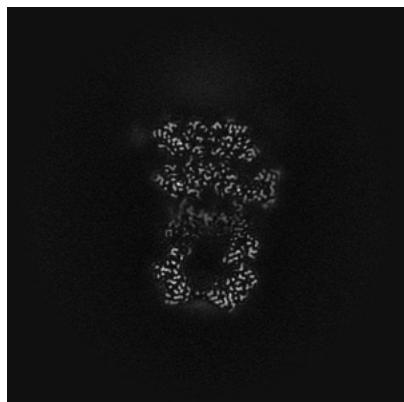


Z Index: 256

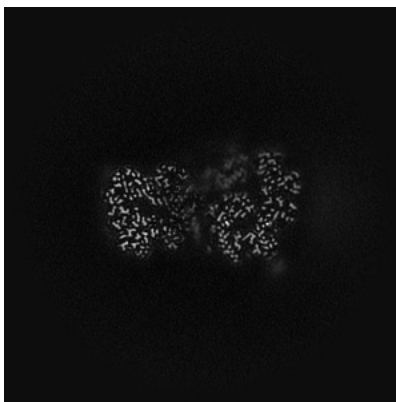
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

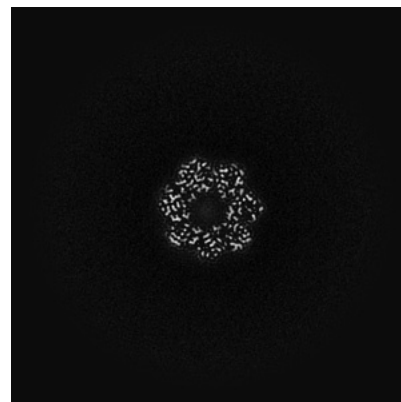
6.3.1 Primary map



X Index: 235

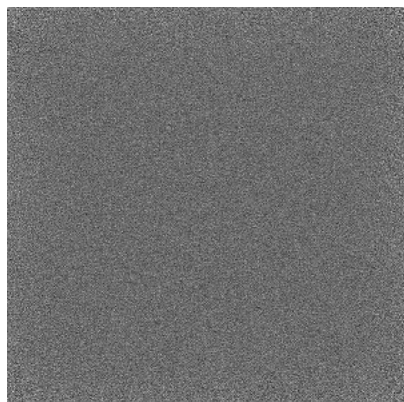


Y Index: 219

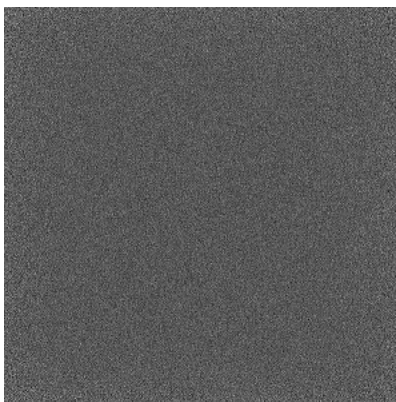


Z Index: 158

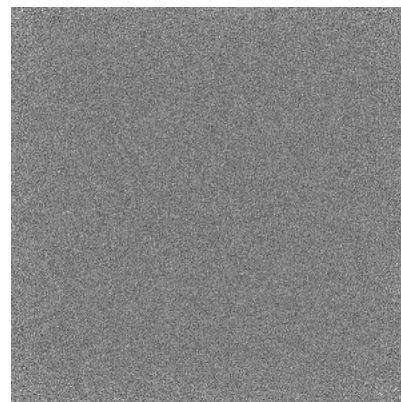
6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 0

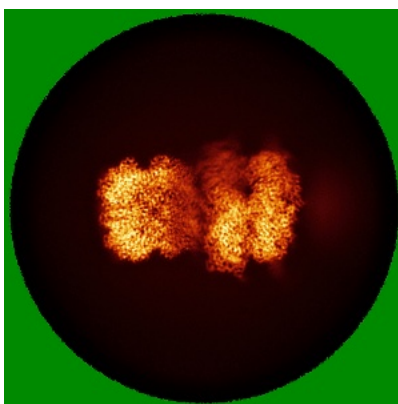
The images above show the largest variance slices of the map in three orthogonal directions.

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

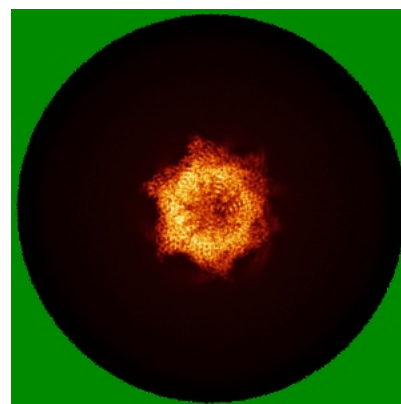
6.4.1 Primary map



X

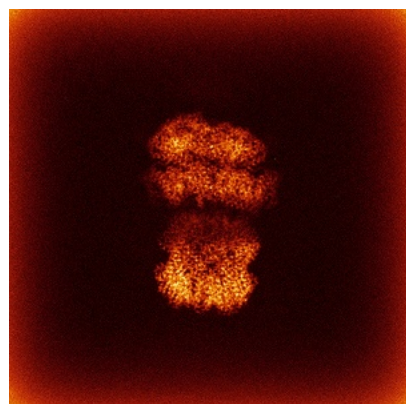


Y

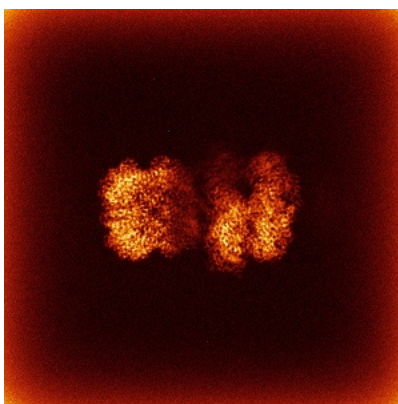


Z

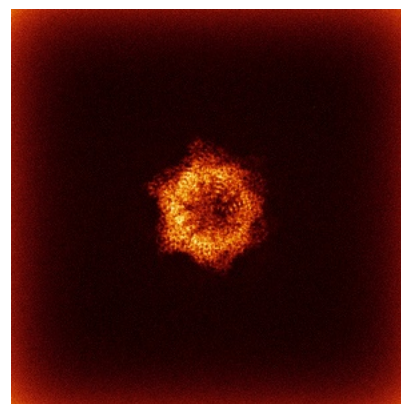
6.4.2 Raw map



X



Y

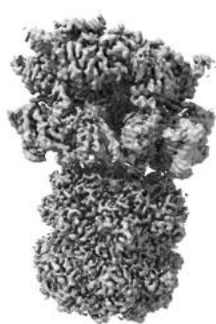


Z

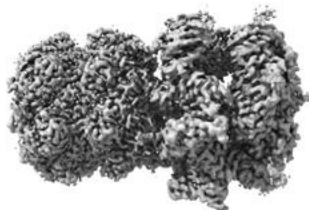
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

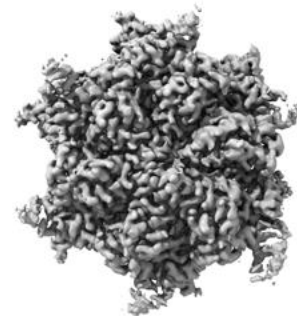
6.5.1 Primary map



X



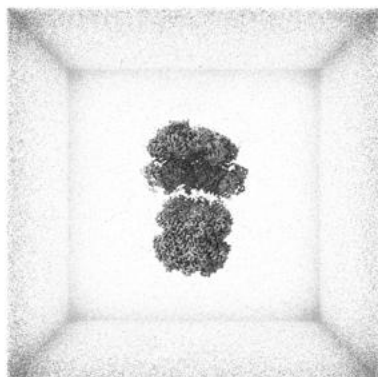
Y



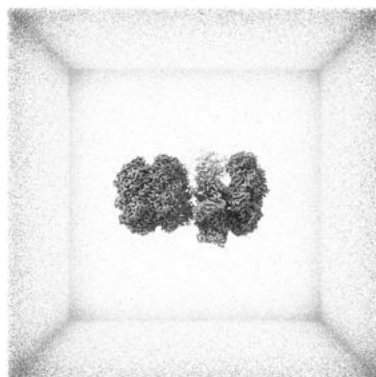
Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

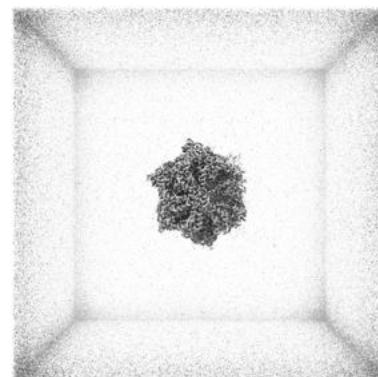
6.5.2 Raw map



X



Y



Z

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.

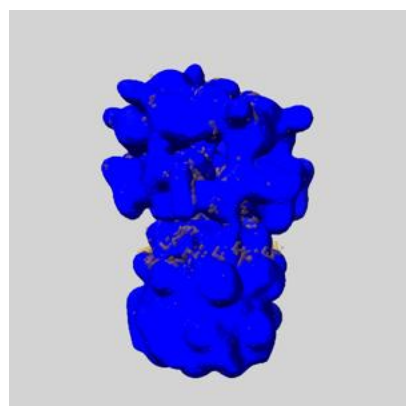
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

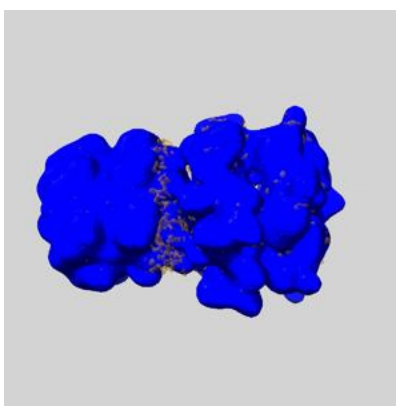
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

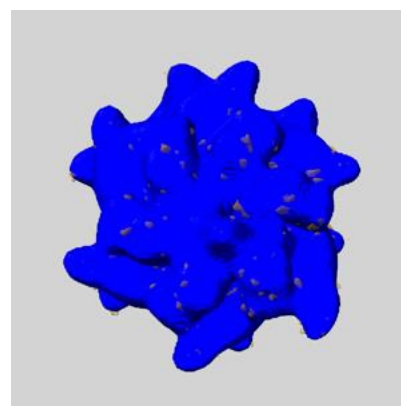
6.6.1 emd_39157_msk_1.map [i](#)



X



Y

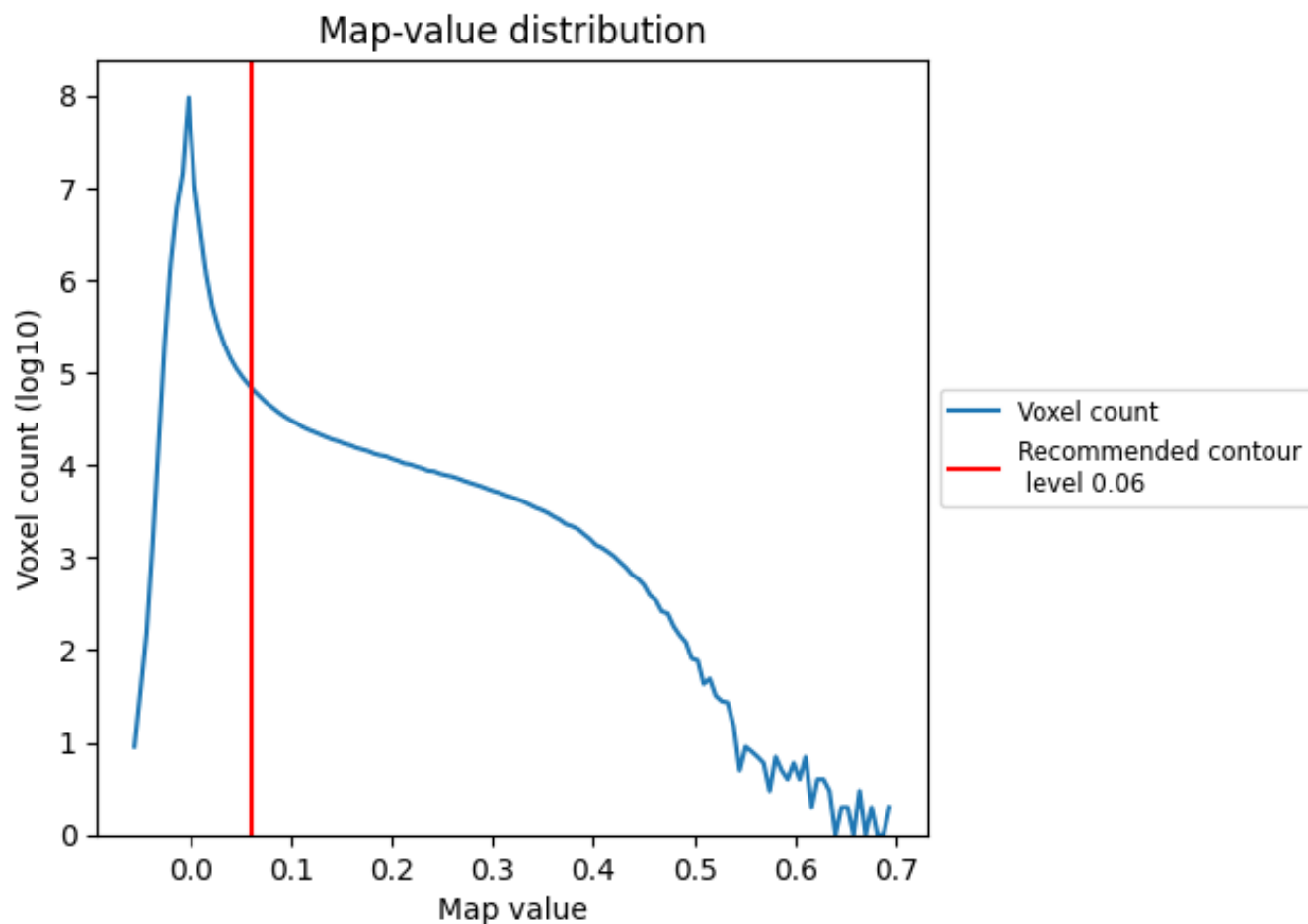


Z

7 Map analysis [i](#)

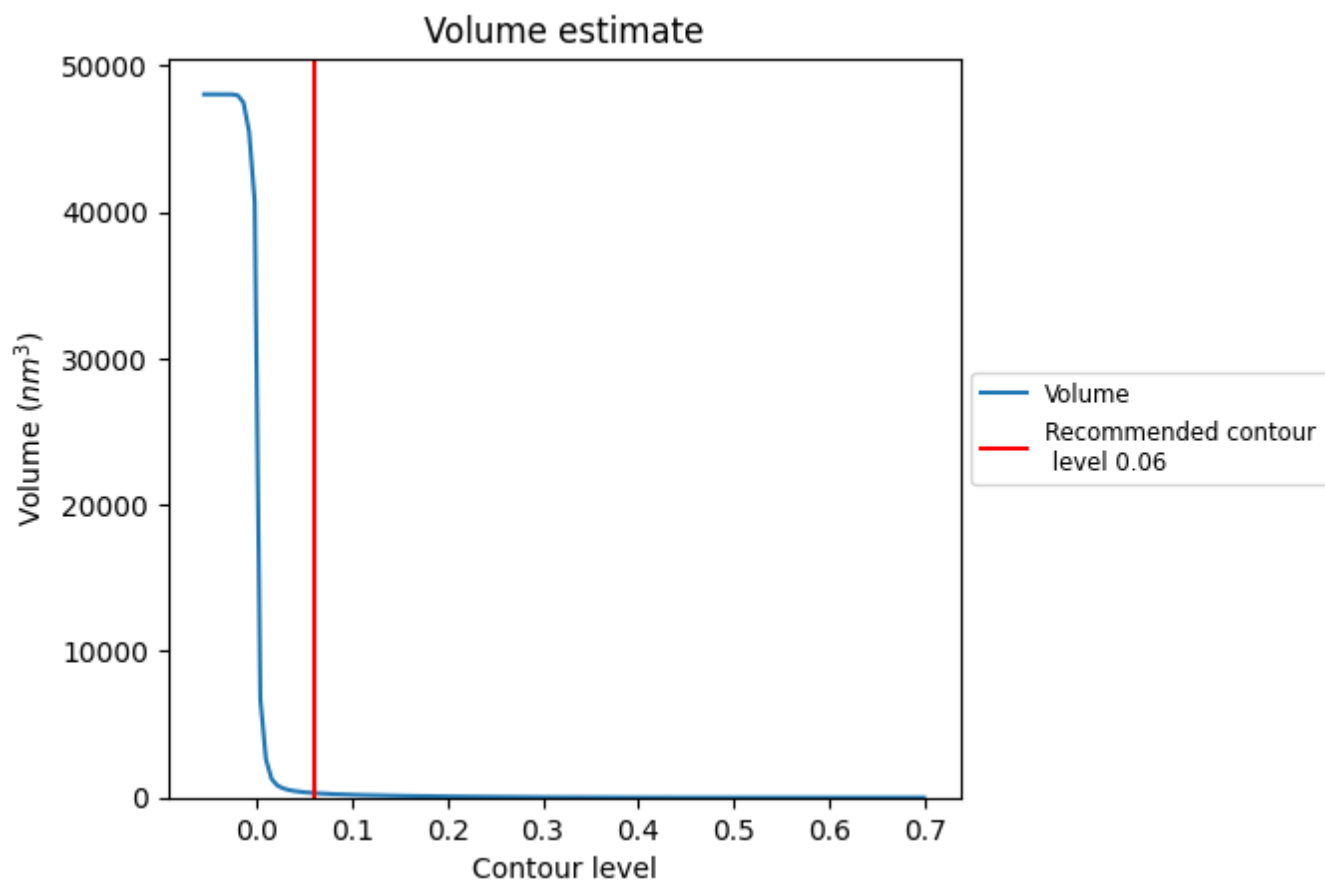
This section contains the results of statistical analysis of the map.

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.

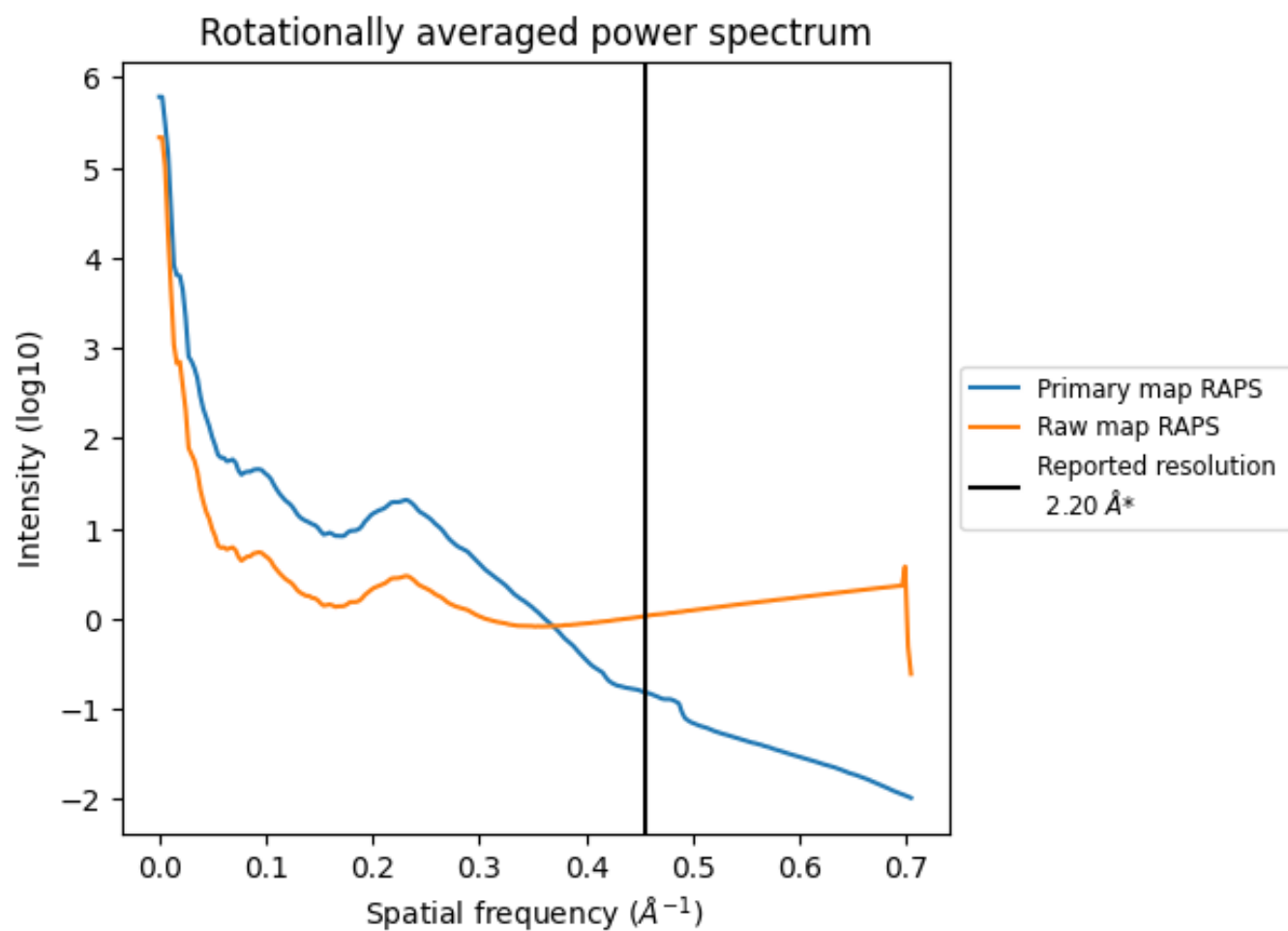
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 308 nm³; this corresponds to an approximate mass of 278 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 ⓘ

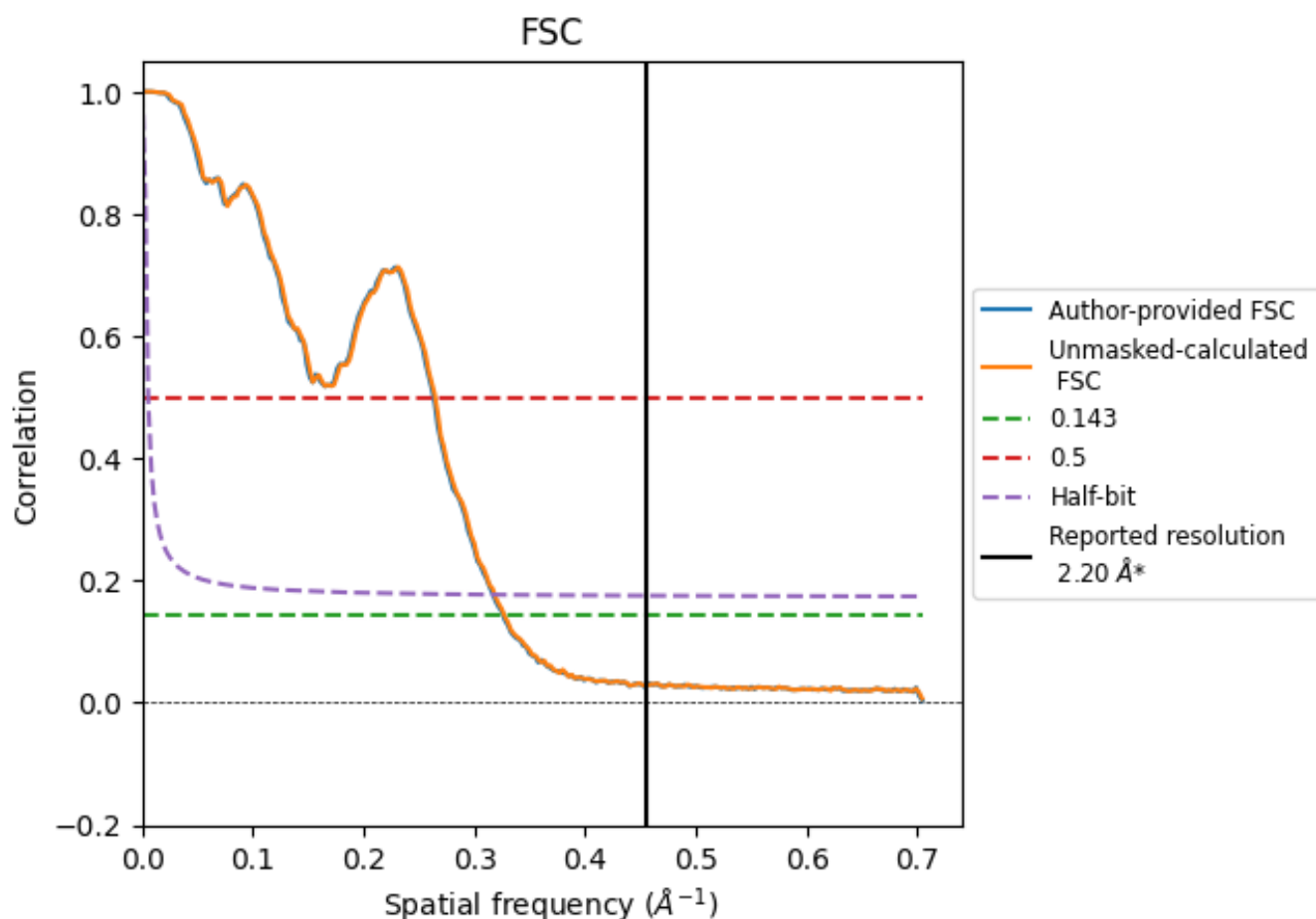


*Reported resolution corresponds to spatial frequency of 0.455 \AA^{-1}

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 0.455 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	3.07	3.80	3.16
Unmasked-calculated*	3.06	3.78	3.14

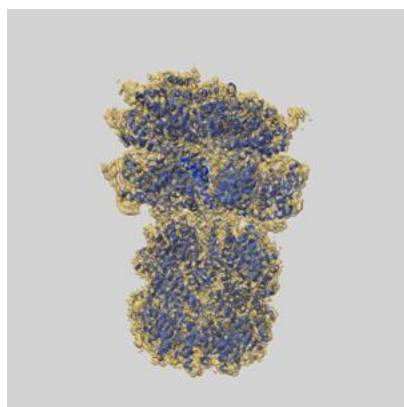
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.07 differs from the reported value 2.2 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.06 differs from the reported value 2.2 by more than 10 %

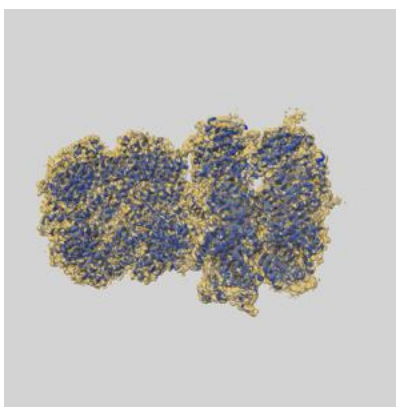
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39157 and PDB model 8YCX. Per-residue inclusion information can be found in section [3](#) on page [10](#).

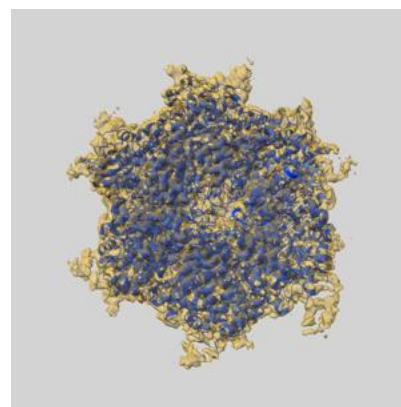
9.1 Map-model overlay [i](#)



X



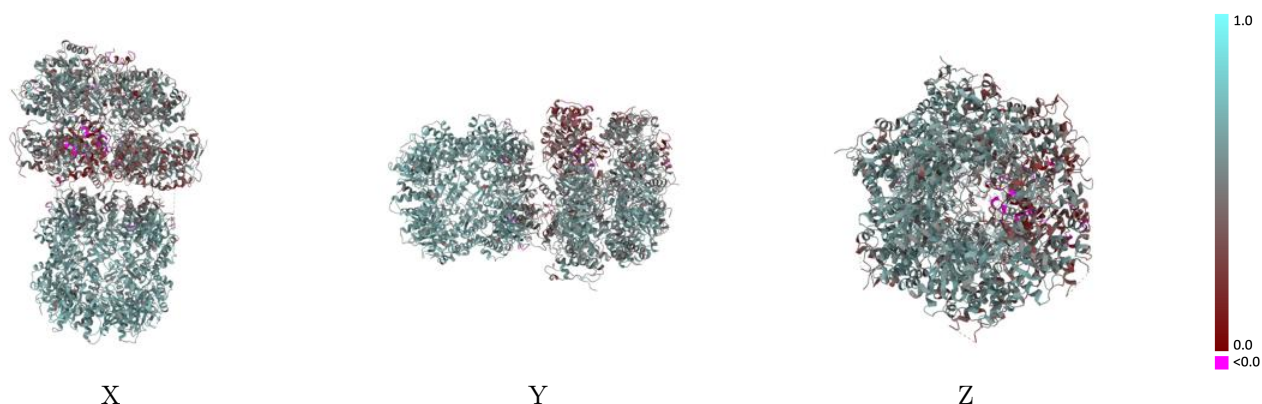
Y



Z

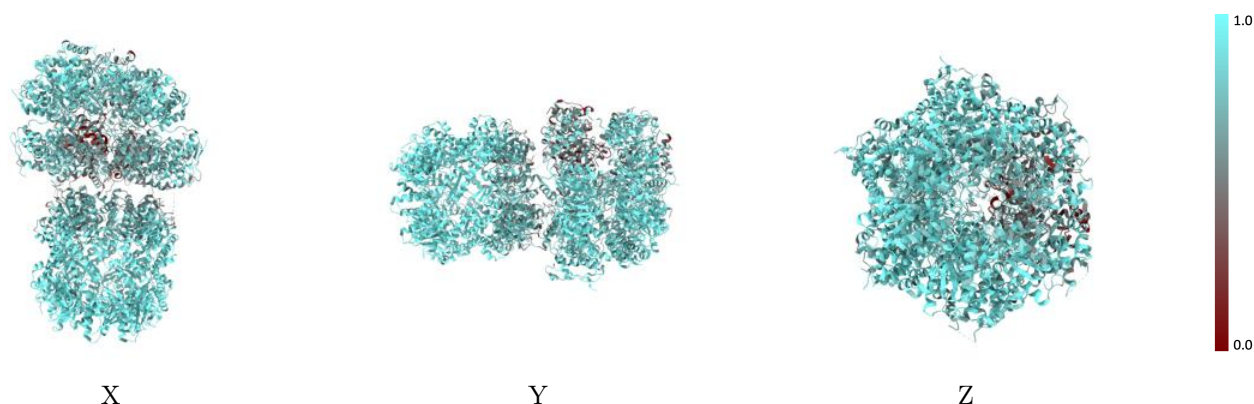
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



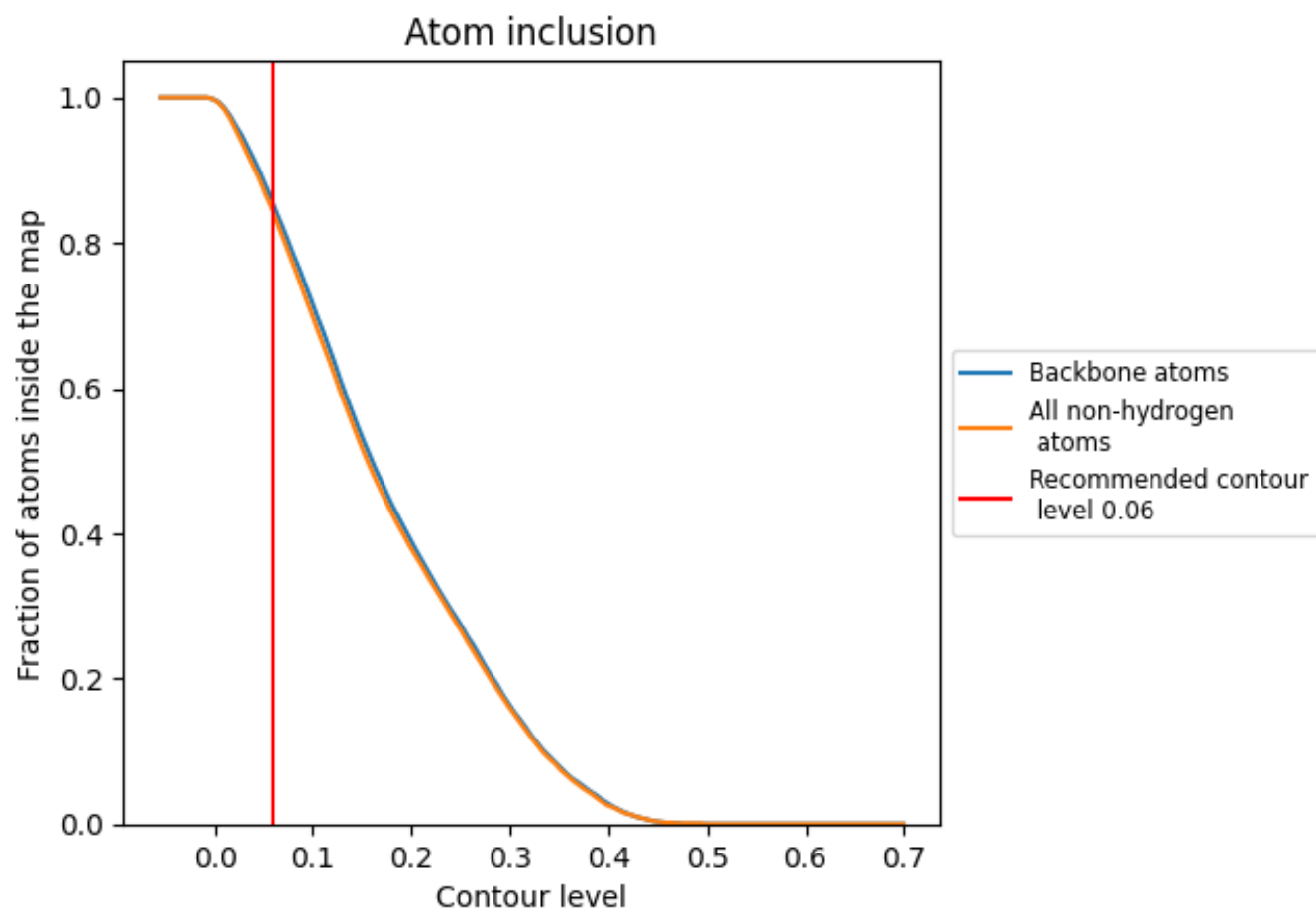
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 84% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8410	 0.5260
A	 0.8500	 0.5090
B	 0.8960	 0.5540
C	 0.8890	 0.5460
D	 0.8510	 0.5040
E	 0.6690	 0.3900
F	 0.6800	 0.3460
G	 0.8080	 0.5570
H	 0.8280	 0.5660
I	 0.8570	 0.5690
J	 0.8620	 0.5680
K	 0.8480	 0.5660
L	 0.8300	 0.5610
M	 0.8130	 0.5520
N	 0.9570	 0.6180
O	 0.9570	 0.6220
P	 0.9600	 0.6180
Q	 0.9600	 0.6190
R	 0.9560	 0.6190
S	 0.9570	 0.6230
T	 0.9570	 0.6200
U	 0.7020	 0.3840

