



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 12:29 PM UTC

PDB ID : 7SCA / pdb_00007sca
EMDB ID : EMD-25031
Title : Synechocystis PCC 6803 Phycobilisome rod from OCP-PBS complex sample
Authors : Sauer, P.V.; Sutter, M.; Dominguez-Martin, M.A.; Kirst, H.; Kerfeld, C.A.
Deposited on : 2021-09-27
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

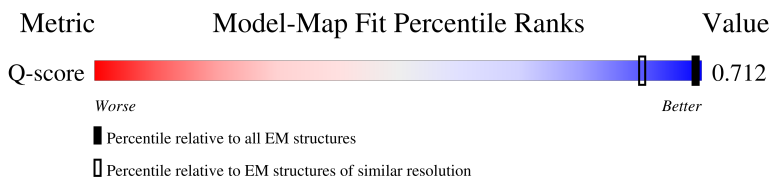
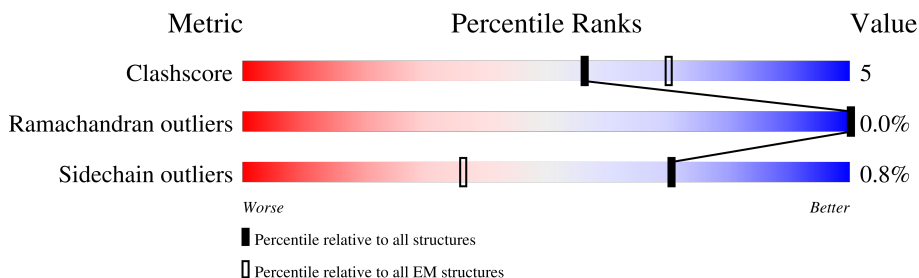
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.10 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.



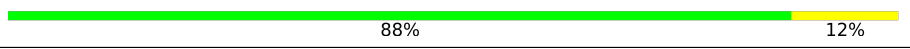
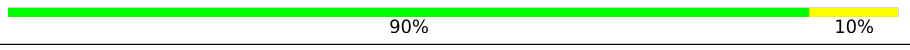
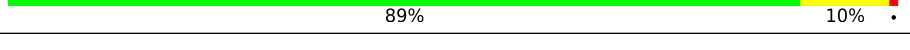
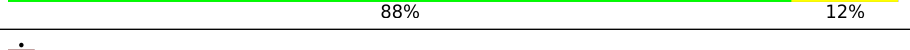
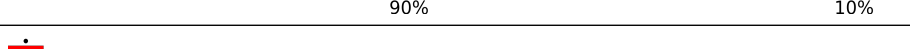
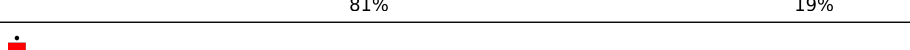
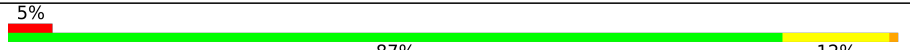
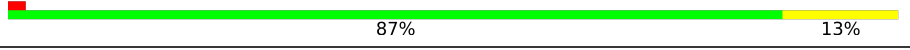
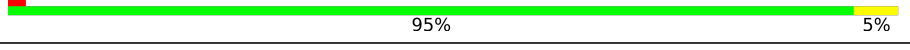
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2317 (1.60 - 2.60)

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	AA	162	
1	AC	162	
1	AE	162	
1	AG	162	

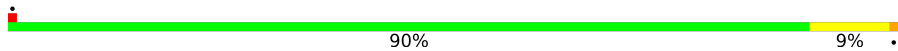
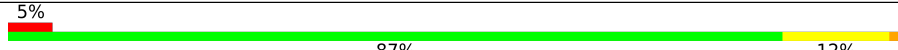
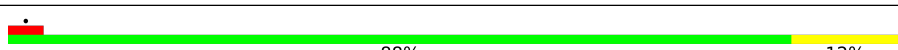
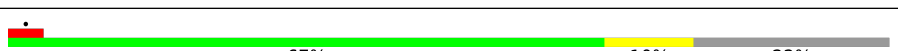
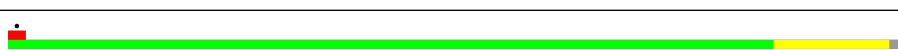
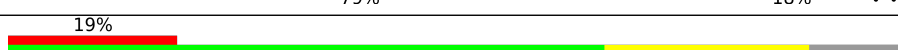
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Mol	Chain	Length	Quality of chain
1	AI	162	 90% 10%
1	AK	162	 86% 14%
1	AM	162	 88% 12%
1	AO	162	 90% 10%
1	AQ	162	 90% 10%
1	AS	162	 87% 13%
1	AU	162	 89% 10%
1	AW	162	 88% 12%
1	AY	162	 90% 10%
1	BA	162	 81% 19%
1	BC	162	 89% 10%
1	BE	162	 88% 12%
1	BG	162	 86% 13%
1	BI	162	 88% 12%
2	AB	172	 88% 12%
2	AD	172	 87% 12% 5%
2	AF	172	 91% 9%
2	AH	172	 90% 10%
2	AJ	172	 90% 10%
2	AL	172	 85% 15%
2	AN	172	 88% 12%
2	AP	172	 87% 13%
2	AR	172	 95% 5%
2	AT	172	 87% 13%
2	AV	172	 90% 10%

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Mol	Chain	Length	Quality of chain
2	AX	172	 88% 12%
2	AZ	172	 90% 9% .
2	BB	172	 82% 18%
2	BD	172	 89% 10% .
2	BF	172	 88% 12%
2	BH	172	 5% 87% 12% .
2	BJ	172	 88% 12%
3	BK	249	 67% 10% 22%
4	BL	291	 86% 13% .
5	BM	273	 79% 18% . .
6	BN	83	 19% 67% 23% 10%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 55437 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called C-phycocyanin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	AC	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	AE	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	AG	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	AI	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	AK	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	AM	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	AO	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	AQ	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	AS	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	AU	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	AW	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	AY	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	BA	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	BC	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	BE	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		
1	BG	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	BI	162	Total	C	N	O	S	0	0
			1240	775	215	247	3		

- Molecule 2 is a protein called C-phycocyanin beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	AD	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	AF	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	AH	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	AJ	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	AL	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	AN	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	AP	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	AR	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	AT	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	AV	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	AX	172	Total	C	N	O	S	0	0
			1269	784	228	250	7		
2	AZ	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	BB	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	BD	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	BF	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	BH	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		
2	BJ	172	Total	C	N	O	S	0	0
			1270	784	228	251	7		

- Molecule 3 is a protein called Phycobilisome rod-core linker polypeptide CpcG.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	BK	194	Total	C	N	O	S	0	0
			1617	1031	286	298	2		

- Molecule 4 is a protein called Phycobilisome 32.1 kDa linker polypeptide, phycocyanin-associated, rod 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	BL	289	Total	C	N	O	S	0	0
			2282	1438	408	433	3		

- Molecule 5 is a protein called Phycobilisome 32.1 kDa linker polypeptide, phycocyanin-associated, rod 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BM	266	Total	C	N	O	S	0	0
			2122	1317	393	409	3		

- Molecule 6 is a protein called Phycobilisome 8.9 kDa linker polypeptide, phycocyanin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BN	75	Total	C	N	O	S	0	0
			590	363	114	110	3		

- Molecule 7 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).

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Mol	Chain	Residues	Atoms				AltConf
7	AJ	1	Total 43	C 33	N 4	O 6	0
7	AK	1	Total 43	C 33	N 4	O 6	0
7	AL	1	Total 43	C 33	N 4	O 6	0
7	AL	1	Total 43	C 33	N 4	O 6	0
7	AM	1	Total 43	C 33	N 4	O 6	0
7	AN	1	Total 43	C 33	N 4	O 6	0
7	AN	1	Total 43	C 33	N 4	O 6	0
7	AO	1	Total 43	C 33	N 4	O 6	0
7	AP	1	Total 43	C 33	N 4	O 6	0
7	AP	1	Total 43	C 33	N 4	O 6	0
7	AQ	1	Total 43	C 33	N 4	O 6	0
7	AR	1	Total 43	C 33	N 4	O 6	0
7	AR	1	Total 43	C 33	N 4	O 6	0
7	AS	1	Total 43	C 33	N 4	O 6	0
7	AT	1	Total 43	C 33	N 4	O 6	0
7	AT	1	Total 43	C 33	N 4	O 6	0
7	AU	1	Total 43	C 33	N 4	O 6	0
7	AV	1	Total 43	C 33	N 4	O 6	0
7	AV	1	Total 43	C 33	N 4	O 6	0
7	AW	1	Total 43	C 33	N 4	O 6	0
7	AX	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
7	AX	1	Total 43	C 33	N 4	O 6	0
7	AY	1	Total 43	C 33	N 4	O 6	0
7	AZ	1	Total 43	C 33	N 4	O 6	0
7	AZ	1	Total 43	C 33	N 4	O 6	0
7	BA	1	Total 43	C 33	N 4	O 6	0
7	BB	1	Total 43	C 33	N 4	O 6	0
7	BB	1	Total 43	C 33	N 4	O 6	0
7	BC	1	Total 43	C 33	N 4	O 6	0
7	BD	1	Total 43	C 33	N 4	O 6	0
7	BD	1	Total 43	C 33	N 4	O 6	0
7	BE	1	Total 43	C 33	N 4	O 6	0
7	BF	1	Total 43	C 33	N 4	O 6	0
7	BF	1	Total 43	C 33	N 4	O 6	0
7	BG	1	Total 43	C 33	N 4	O 6	0
7	BH	1	Total 43	C 33	N 4	O 6	0
7	BH	1	Total 43	C 33	N 4	O 6	0
7	BI	1	Total 43	C 33	N 4	O 6	0
7	BJ	1	Total 43	C 33	N 4	O 6	0
7	BJ	1	Total 43	C 33	N 4	O 6	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	AltConf
8	AA	17	Total O 17 17	0
8	AB	14	Total O 14 14	0
8	AC	22	Total O 22 22	0
8	AD	24	Total O 24 24	0
8	AE	19	Total O 19 19	0
8	AF	22	Total O 22 22	0
8	AG	26	Total O 26 26	0
8	AH	33	Total O 33 33	0
8	AI	24	Total O 24 24	0
8	AJ	28	Total O 28 28	0
8	AK	24	Total O 24 24	0
8	AL	31	Total O 31 31	0
8	AM	47	Total O 47 47	0
8	AN	55	Total O 55 55	0
8	AO	53	Total O 53 53	0
8	AP	32	Total O 32 32	0
8	AQ	37	Total O 37 37	0
8	AR	37	Total O 37 37	0
8	AS	39	Total O 39 39	0
8	AT	54	Total O 54 54	0
8	AU	49	Total O 49 49	0
8	AV	44	Total O 44 44	0

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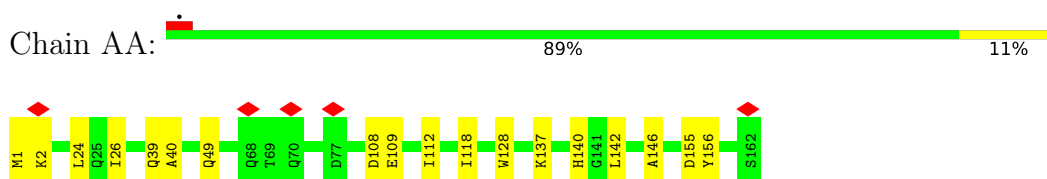
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Mol	Chain	Residues	Atoms		AltConf
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8	AX	28	Total 28	O 28	0
8	AY	29	Total 29	O 29	0
8	AZ	36	Total 36	O 36	0
8	BA	23	Total 23	O 23	0
8	BB	34	Total 34	O 34	0
8	BC	27	Total 27	O 27	0
8	BD	22	Total 22	O 22	0
8	BE	27	Total 27	O 27	0
8	BF	19	Total 19	O 19	0
8	BG	21	Total 21	O 21	0
8	BH	30	Total 30	O 30	0
8	BI	26	Total 26	O 26	0
8	BJ	18	Total 18	O 18	0
8	BK	53	Total 53	O 53	0
8	BL	79	Total 79	O 79	0
8	BM	66	Total 66	O 66	0
8	BN	9	Total 9	O 9	0

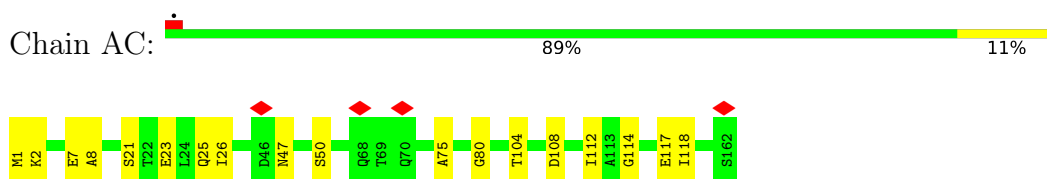
3 Residue-property plots [i](#)

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.

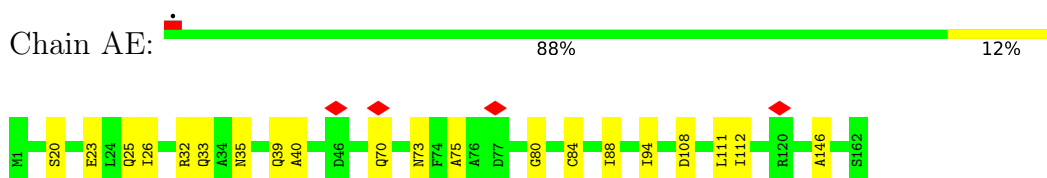
- Molecule 1: C-phycoerythrin alpha subunit



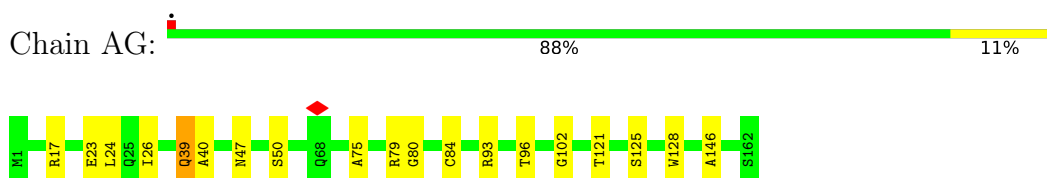
- Molecule 1: C-phycoerythrin alpha subunit



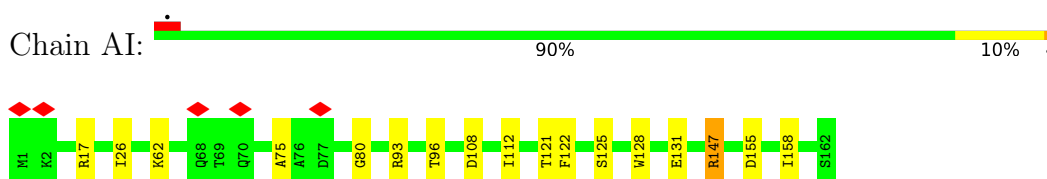
- Molecule 1: C-phycoerythrin alpha subunit



- Molecule 1: C-phycoerythrin alpha subunit

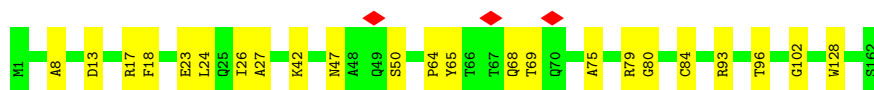


- Molecule 1: C-phycoerythrin alpha subunit



- Molecule 1: C-phycocyanin alpha subunit

Chain AK:  86% 14%



- Molecule 1: C-phycocyanin alpha subunit

Chain AM:  88% 12%



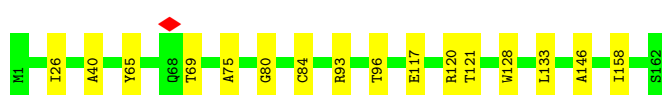
- Molecule 1: C-phycocyanin alpha subunit

Chain AO:  90% 10%



- Molecule 1: C-phycocyanin alpha subunit

Chain AQ:  90% 10%



- Molecule 1: C-phycocyanin alpha subunit

Chain AS:  87% 13%



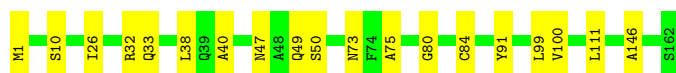
- Molecule 1: C-phycocyanin alpha subunit

Chain AU:  89% 10% .



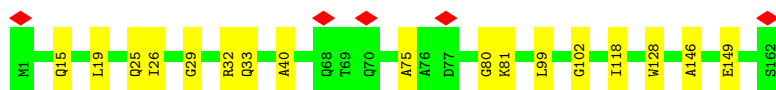
- Molecule 1: C-phycocyanin alpha subunit

Chain AW:  88% 12%



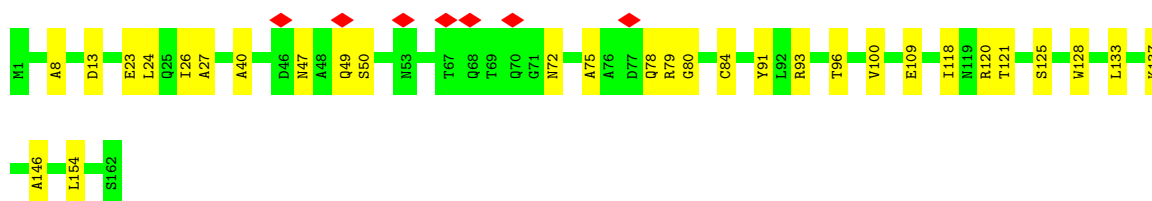
- Molecule 1: C-phycocyanin alpha subunit

Chain AY:  90% 10%



- Molecule 1: C-phycocyanin alpha subunit

Chain BA:  81% 19%



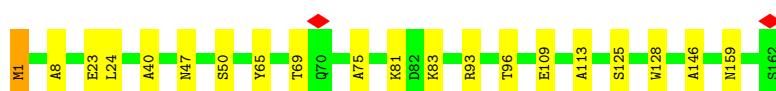
- Molecule 1: C-phycocyanin alpha subunit

Chain BC:  89% 10%



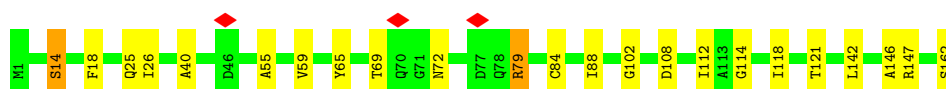
- Molecule 1: C-phycocyanin alpha subunit

Chain BE:  88% 12%



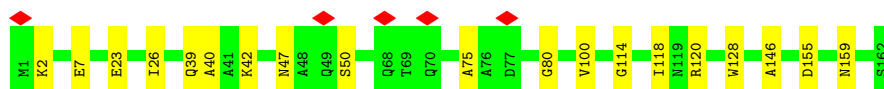
- Molecule 1: C-phycocyanin alpha subunit

Chain BG:  86% 13%



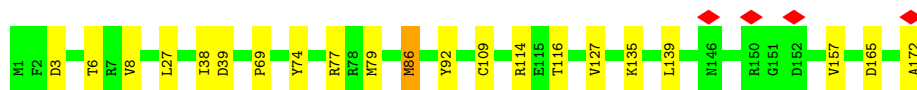
- Molecule 1: C-phycocyanin alpha subunit

Chain BI:  88% 12%



- Molecule 2: C-phycocyanin beta subunit

Chain AB:  88% 12%



• Molecule 2: C-phycoerythrin beta subunit

Chain AD:  5% 87% 12%



• Molecule 2: C-phycoerythrin beta subunit

Chain AF:  91% 9%



• Molecule 2: C-phycoerythrin beta subunit

Chain AH:  90% 10%



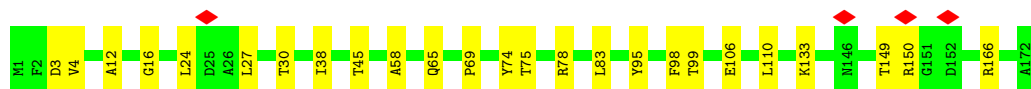
• Molecule 2: C-phycoerythrin beta subunit

Chain AJ:  90% 10%



• Molecule 2: C-phycoerythrin beta subunit

Chain AL:  85% 15%



• Molecule 2: C-phycoerythrin beta subunit

Chain AN:  88% 12%

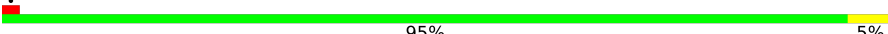


- Molecule 2: C-phycocyanin beta subunit

Chain AP:  87% 13%



- Molecule 2: C-phycocyanin beta subunit

Chain AR:  95% 5%



- Molecule 2: C-phycocyanin beta subunit

Chain AT:  87% 13%



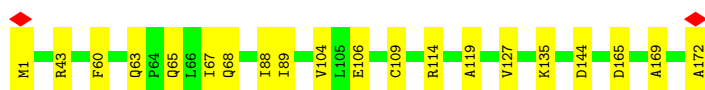
- Molecule 2: C-phycocyanin beta subunit

Chain AV:  90% 10%



- Molecule 2: C-phycocyanin beta subunit

Chain AX:  88% 12%



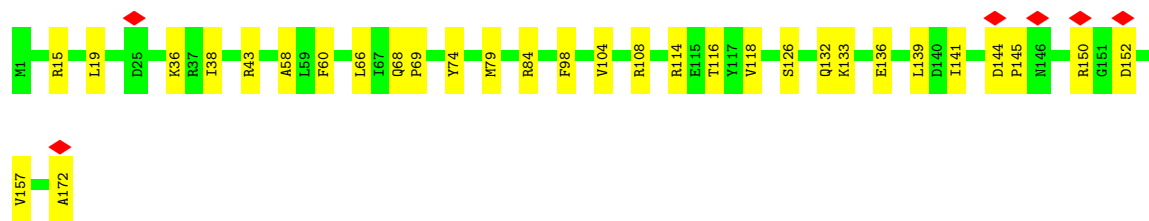
- Molecule 2: C-phycocyanin beta subunit

Chain AZ:  90% 9%

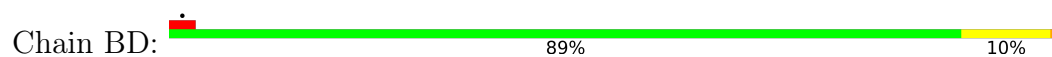


- Molecule 2: C-phycocyanin beta subunit

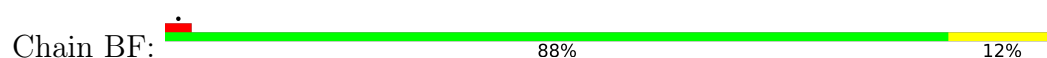
Chain BB:  82% 18%



- Molecule 2: C-phycoerythrin beta subunit



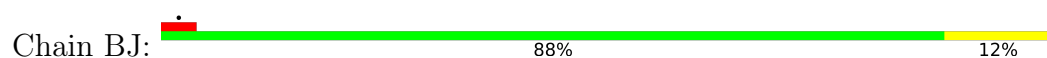
- Molecule 2: C-phycoerythrin beta subunit



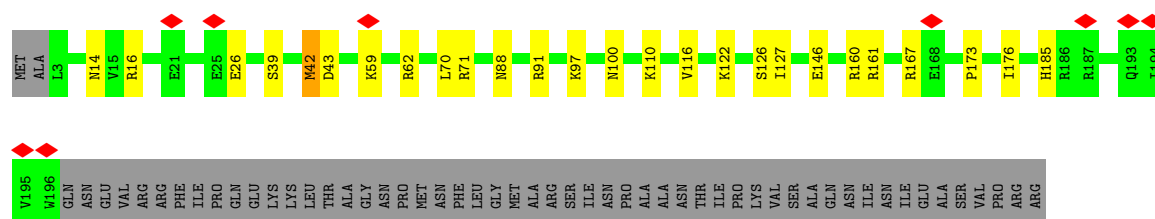
- Molecule 2: C-phycoerythrin beta subunit



- Molecule 2: C-phycoerythrin beta subunit

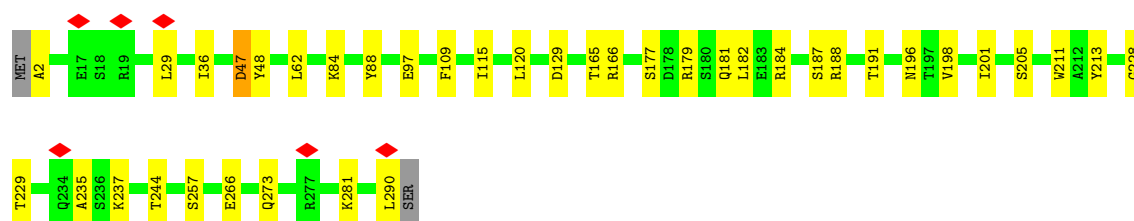


- Molecule 3: Phycobilisome rod-core linker polypeptide CpcG



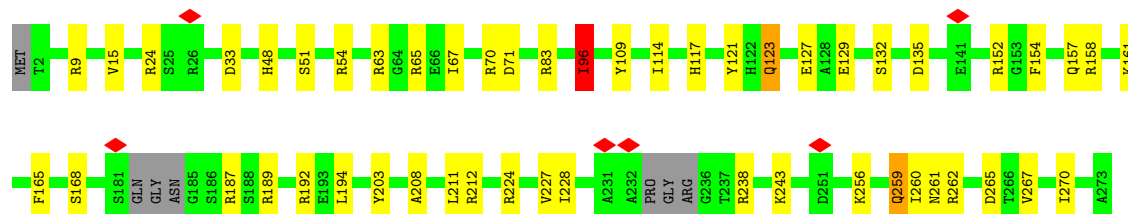
- Molecule 4: Phycobilisome 32.1 kDa linker polypeptide, phycocyanin-associated, rod 1

Chain BL:  86% 13%



- Molecule 5: Phycobilisome 32.1 kDa linker polypeptide, phycocyanin-associated, rod 2

Chain BM:  79% 18%



- Molecule 6: Phycobilisome 8.9 kDa linker polypeptide, phycocyanin-associated, rod

Chain BN:  19% 67% 23% 10%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2133253	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)	500	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.898	Depositor
Minimum map value	-3.240	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.174	Depositor
Recommended contour level	1.07	Depositor
Map size (Å)	377.99997, 377.99997, 377.99997	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CYC

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	AA	0.40	0/1261	0.61	1/1709 (0.1%)
1	AC	0.38	0/1261	0.52	0/1709
1	AE	0.39	0/1261	0.51	0/1709
1	AG	0.40	0/1261	0.59	0/1709
1	AI	0.41	0/1261	0.58	1/1709 (0.1%)
1	AK	0.42	0/1261	0.62	0/1709
1	AM	0.49	0/1261	0.62	0/1709
1	AO	0.45	0/1261	0.60	0/1709
1	AQ	0.46	0/1261	0.67	0/1709
1	AS	0.49	0/1261	0.60	0/1709
1	AU	0.47	0/1261	0.62	2/1709 (0.1%)
1	AW	0.45	0/1261	0.57	0/1709
1	AY	0.38	0/1261	0.57	0/1709
1	BA	0.40	0/1261	0.59	0/1709
1	BC	0.43	0/1261	0.60	1/1709 (0.1%)
1	BE	0.41	0/1261	0.57	0/1709
1	BG	0.43	0/1261	0.61	0/1709
1	BI	0.40	0/1261	0.63	1/1709 (0.1%)
2	AB	0.40	0/1284	0.57	0/1739
2	AD	0.43	0/1284	0.64	1/1739 (0.1%)
2	AF	0.38	0/1284	0.60	0/1739
2	AH	0.40	0/1284	0.61	1/1739 (0.1%)
2	AJ	0.42	0/1284	0.56	0/1739
2	AL	0.43	0/1284	0.65	0/1739
2	AN	0.49	0/1284	0.66	0/1739
2	AP	0.47	0/1284	0.65	0/1739
2	AR	0.46	0/1284	0.66	0/1739
2	AT	0.46	0/1284	0.65	0/1739
2	AV	0.47	0/1284	0.62	0/1739
2	AX	0.50	0/1283	0.65	0/1737
2	AZ	0.43	0/1284	0.64	1/1739 (0.1%)
2	BB	0.44	0/1284	0.67	1/1739 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	BD	0.44	0/1284	0.69	2/1739 (0.1%)
2	BF	0.40	0/1284	0.65	0/1739
2	BH	0.41	0/1284	0.63	0/1739
2	BJ	0.41	0/1284	0.60	0/1739
3	BK	0.41	0/1656	0.59	0/2240
4	BL	0.45	0/2327	0.64	0/3149
5	BM	0.46	0/2156	0.66	3/2907 (0.1%)
6	BN	0.38	0/598	0.72	1/804 (0.1%)
All	All	0.43	0/52546	0.62	16/71162 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BI	120	ARG	CD-NE-CZ	-10.75	109.36	124.40
2	BD	114	ARG	CB-CA-C	-8.03	98.27	110.88
1	BC	134	LYS	CG-CD-CE	-6.36	96.67	111.30
5	BM	259	GLN	CA-CB-CG	6.35	126.81	114.10
1	AU	15	GLN	N-CA-CB	-6.18	100.98	110.44
1	AU	15	GLN	CA-CB-CG	5.86	125.83	114.10
2	BB	15	ARG	N-CA-CB	-5.69	100.85	110.41
1	AI	147	ARG	CB-CA-C	-5.57	101.54	110.79
2	AH	132	GLN	CA-CB-CG	5.48	125.05	114.10
1	AA	39	GLN	CA-CB-CG	5.47	125.04	114.10
2	BD	114	ARG	CB-CG-CD	5.44	123.81	111.30
5	BM	123	GLN	CA-CB-CG	5.31	124.71	114.10
6	BN	73	ARG	N-CA-CB	5.27	120.50	110.49
5	BM	96	ILE	CB-CG1-CD1	-5.11	103.08	113.80
2	AZ	135	LYS	CB-CG-CD	5.04	122.89	111.30
2	AD	134	MET	CB-CG-SD	-5.02	97.65	112.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	1240	0	1206	12	0
1	AC	1240	0	1206	13	0
1	AE	1240	0	1206	12	0
1	AG	1240	0	1206	15	0
1	AI	1240	0	1206	14	0
1	AK	1240	0	1206	18	0
1	AM	1240	0	1206	12	0
1	AO	1240	0	1206	13	0
1	AQ	1240	0	1206	10	0
1	AS	1240	0	1206	14	0
1	AU	1240	0	1206	14	0
1	AW	1240	0	1206	12	0
1	AY	1240	0	1206	14	0
1	BA	1240	0	1206	21	0
1	BC	1240	0	1206	10	0
1	BE	1240	0	1206	14	0
1	BG	1240	0	1206	19	0
1	BI	1240	0	1206	11	0
2	AB	1270	0	1261	13	0
2	AD	1270	0	1261	16	0
2	AF	1270	0	1261	10	0
2	AH	1270	0	1261	12	0
2	AJ	1270	0	1261	10	0
2	AL	1270	0	1261	17	0
2	AN	1270	0	1261	18	0
2	AP	1270	0	1261	15	0
2	AR	1270	0	1261	5	0
2	AT	1270	0	1261	16	0
2	AV	1270	0	1261	12	0
2	AX	1269	0	1261	13	0
2	AZ	1270	0	1261	13	0
2	BB	1270	0	1261	24	0
2	BD	1270	0	1261	13	0
2	BF	1270	0	1261	14	0
2	BH	1270	0	1261	16	0
2	BJ	1270	0	1261	13	0
3	BK	1617	0	1576	18	0
4	BL	2282	0	2261	27	0
5	BM	2122	0	2076	38	0
6	BN	590	0	590	16	0
7	AA	43	0	37	2	0
7	AB	86	0	74	2	0
7	AC	43	0	37	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	AD	86	0	74	5	0
7	AE	43	0	37	2	0
7	AF	86	0	74	1	0
7	AG	43	0	37	3	0
7	AH	86	0	74	1	0
7	AI	43	0	37	2	0
7	AJ	86	0	74	4	0
7	AK	43	0	37	4	0
7	AL	86	0	74	1	0
7	AM	43	0	37	4	0
7	AN	86	0	74	1	0
7	AO	43	0	37	4	0
7	AP	86	0	74	1	0
7	AQ	43	0	37	2	0
7	AR	86	0	74	1	0
7	AS	43	0	37	2	0
7	AT	86	0	74	1	0
7	AU	43	0	37	6	0
7	AV	86	0	74	2	0
7	AW	43	0	37	3	0
7	AX	86	0	74	5	0
7	AY	43	0	37	2	0
7	AZ	86	0	74	2	0
7	BA	43	0	37	3	0
7	BB	86	0	74	3	0
7	BC	43	0	37	1	0
7	BD	86	0	74	2	0
7	BE	43	0	37	2	0
7	BF	86	0	74	4	0
7	BG	43	0	37	3	0
7	BH	86	0	74	5	0
7	BI	43	0	37	2	0
7	BJ	86	0	74	3	0
8	AA	17	0	0	0	0
8	AB	14	0	0	0	0
8	AC	22	0	0	0	0
8	AD	24	0	0	0	0
8	AE	19	0	0	0	0
8	AF	22	0	0	0	0
8	AG	26	0	0	0	0
8	AH	33	0	0	0	0
8	AI	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	AJ	28	0	0	1	0
8	AK	24	0	0	0	0
8	AL	31	0	0	0	0
8	AM	47	0	0	1	0
8	AN	55	0	0	0	0
8	AO	53	0	0	1	0
8	AP	32	0	0	0	0
8	AQ	37	0	0	0	0
8	AR	37	0	0	0	0
8	AS	39	0	0	0	0
8	AT	54	0	0	0	0
8	AU	49	0	0	1	0
8	AV	44	0	0	1	0
8	AW	47	0	0	2	0
8	AX	28	0	0	0	0
8	AY	29	0	0	1	0
8	AZ	36	0	0	0	0
8	BA	23	0	0	0	0
8	BB	34	0	0	0	0
8	BC	27	0	0	0	0
8	BD	22	0	0	1	0
8	BE	27	0	0	1	0
8	BF	19	0	0	0	0
8	BG	21	0	0	0	0
8	BH	30	0	0	1	0
8	BI	26	0	0	0	0
8	BJ	18	0	0	1	0
8	BK	53	0	0	1	0
8	BL	79	0	0	0	0
8	BM	66	0	0	1	0
8	BN	9	0	0	0	0
All	All	55437	0	52907	524	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (524) 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)
2:BD:114:ARG:NH1	2:BD:172:ALA:O	2.06	0.88
1:AU:15:GLN:HE21	1:AU:17:ARG:HD3	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BM:96:ILE:HD11	5:BM:114:ILE:HD13	1.66	0.77
1:AC:8:ALA:HB1	1:AC:23:GLU:HG3	1.66	0.76
2:BD:107:ASP:OD1	4:BL:281:LYS:NZ	2.24	0.71
1:BI:47:ASN:ND2	1:BI:50:SER:OG	2.24	0.70
2:BJ:145:PRO:O	2:BJ:150:ARG:NH2	2.25	0.69
2:AH:83:LEU:HD13	1:AI:121:THR:HG21	1.73	0.69
3:BK:116:VAL:HG21	3:BK:122:LYS:HG3	1.75	0.69
4:BL:181:GLN:HB2	4:BL:188:ARG:HH21	1.57	0.68
5:BM:33:ASP:OD1	5:BM:63:ARG:NH2	2.26	0.68
2:AZ:63:GLN:HB3	2:AZ:65:GLN:HE22	1.60	0.67
2:AD:150:ARG:NH1	7:AD:202:CYC:OC	2.26	0.67
2:AJ:120:LEU:HD11	7:AJ:201:CYC:HAA2	1.77	0.67
2:AT:114:ARG:NH1	2:AT:172:ALA:O	2.27	0.67
1:AW:47:ASN:ND2	1:AW:50:SER:OG	2.28	0.67
1:AA:137:LYS:NZ	1:AA:155:ASP:OD1	2.25	0.66
2:BB:114:ARG:NH1	2:BB:172:ALA:O	2.29	0.66
2:AN:145:PRO:HB2	2:AN:150:ARG:HH21	1.61	0.66
2:BH:84:ARG:NH1	2:BH:85:ASP:OD1	2.28	0.66
2:BB:145:PRO:O	2:BB:150:ARG:NH2	2.28	0.66
1:BG:72:ASN:O	1:BG:79:ARG:NH2	2.27	0.66
2:AN:15:ARG:NH1	2:AN:17:GLU:OE2	2.29	0.65
2:AB:114:ARG:NH1	2:AB:172:ALA:OXT	2.29	0.65
2:BF:114:ARG:NH1	2:BF:172:ALA:O	2.29	0.65
2:AX:114:ARG:NH2	2:AX:169:ALA:O	2.29	0.65
2:AF:114:ARG:NH1	2:AF:172:ALA:OXT	2.28	0.64
5:BM:256:LYS:HD2	5:BM:259:GLN:HE21	1.63	0.64
1:AK:8:ALA:HB1	1:AK:23:GLU:HG3	1.78	0.64
2:AP:83:LEU:HD13	1:AQ:121:THR:HG21	1.80	0.64
7:BF:201:CYC:HB	7:BF:201:CYC:HMA3	1.60	0.64
2:AP:139:LEU:HD22	2:AP:157:VAL:HG13	1.79	0.64
2:AZ:83:LEU:HD13	1:BA:121:THR:HG21	1.79	0.63
2:AH:145:PRO:O	2:AH:150:ARG:NH2	2.29	0.63
7:AD:201:CYC:HBB2	6:BN:59:MET:HE2	1.79	0.63
2:AN:114:ARG:NH2	2:AN:169:ALA:O	2.32	0.62
2:AN:86:MET:HE3	2:AN:134:MET:HE2	1.80	0.62
1:AU:40:ALA:HB2	1:AU:146:ALA:HB1	1.80	0.62
1:AO:79:ARG:NH2	7:AO:201:CYC:O2D	2.33	0.62
1:BG:88:ILE:HD11	7:BG:201:CYC:HBC1	1.82	0.61
5:BM:109:TYR:HB3	5:BM:161:LYS:HD3	1.81	0.61
2:AX:88:ILE:HG21	7:AX:201:CYC:HAB2	1.82	0.61
5:BM:208:ALA:O	5:BM:224:ARG:NH2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AJ:65:GLN:NE2	8:AJ:304:HOH:O	2.33	0.60
1:AK:64:PRO:O	1:AK:68:GLN:NE2	2.35	0.60
7:BB:201:CYC:HB	7:BB:201:CYC:HMA3	1.64	0.60
1:BA:47:ASN:OD1	1:BA:50:SER:OG	2.19	0.60
3:BK:59:LYS:HA	3:BK:62:ARG:HG2	1.82	0.59
3:BK:16:ARG:NH2	8:BK:304:HOH:O	2.34	0.59
1:AK:47:ASN:OD1	1:AK:50:SER:OG	2.20	0.59
1:AU:2:LYS:NZ	8:AU:305:HOH:O	2.35	0.59
5:BM:260:ILE:HG23	5:BM:265:ASP:HB2	1.85	0.59
2:AH:43:ARG:HB3	2:AH:141:ILE:HG22	1.85	0.59
1:BA:120:ARG:NH1	1:BG:162:SER:O	2.35	0.59
2:AD:114:ARG:NH1	2:AD:172:ALA:O	2.35	0.59
2:AF:139:LEU:HD22	2:AF:157:VAL:HG13	1.84	0.59
1:AS:79:ARG:NH2	7:AS:201:CYC:O2D	2.30	0.59
2:AB:79:MET:HG3	1:AC:118:ILE:HD12	1.86	0.58
1:AW:32:ARG:NH2	1:AW:33:GLN:OE1	2.35	0.58
2:AD:139:LEU:HD11	2:AD:161:ALA:HB2	1.86	0.58
7:BD:201:CYC:O1D	8:BD:301:HOH:O	2.17	0.58
1:AO:47:ASN:OD1	1:AO:50:SER:OG	2.21	0.58
1:AQ:40:ALA:HB2	1:AQ:146:ALA:HB1	1.86	0.57
1:AK:24:LEU:HD22	2:AL:38:ILE:HG23	1.86	0.57
1:AE:26:ILE:HG12	1:AK:26:ILE:HG12	1.86	0.57
2:BF:1:MET:N	3:BK:26:GLU:OE2	2.35	0.57
2:AX:135:LYS:NZ	2:AX:165:ASP:OD2	2.29	0.57
2:AZ:60:PHE:HB3	2:AZ:67:ILE:HD13	1.86	0.57
2:BH:79:MET:HE3	7:BI:201:CYC:HBA1	1.86	0.56
1:BI:40:ALA:HB2	1:BI:146:ALA:HB1	1.87	0.56
1:AY:26:ILE:HG12	1:BG:26:ILE:HG12	1.87	0.56
2:BD:72:ASN:ND2	2:BD:122:VAL:HA	2.20	0.56
4:BL:177:SER:OG	4:BL:177:SER:O	2.17	0.56
2:AX:1:MET:HE3	2:AX:104:VAL:HB	1.87	0.56
2:AP:132:GLN:O	2:AP:135:LYS:HB3	2.06	0.56
2:AN:76:SER:OG	1:AO:113:ALA:O	2.18	0.56
7:AB:201:CYC:O2A	6:BN:29:GLN:NE2	2.39	0.56
2:BH:114:ARG:NH1	2:BH:172:ALA:O	2.39	0.56
2:AR:39:ASP:OD2	7:AR:202:CYC:ND	2.37	0.55
1:AY:15:GLN:HG2	3:BK:88:ASN:HB2	1.88	0.55
1:BE:40:ALA:HB2	1:BE:146:ALA:HB1	1.88	0.55
1:BE:83:LYS:NZ	7:BE:201:CYC:O2A	2.35	0.55
1:AM:40:ALA:HB2	1:AM:146:ALA:HB1	1.88	0.55
2:AV:15:ARG:NH2	8:AV:304:HOH:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AX:114:ARG:NH2	2:AX:172:ALA:O	2.39	0.55
1:AE:32:ARG:NH2	1:AE:33:GLN:OE1	2.38	0.55
1:BC:38:LEU:HD23	1:BC:100:VAL:HG12	1.89	0.54
1:AC:108:ASP:HA	1:AC:112:ILE:HB	1.89	0.54
1:AS:1:MET:HG2	1:AS:109:GLU:HG3	1.89	0.54
1:AA:1:MET:HE2	1:AA:109:GLU:HG2	1.89	0.54
1:AK:13:ASP:O	5:BM:121:TYR:OH	2.25	0.54
2:AT:139:LEU:HD22	2:AT:157:VAL:HG13	1.89	0.54
2:BJ:139:LEU:HD22	2:BJ:157:VAL:HG13	1.89	0.54
2:AF:106:GLU:HA	2:AF:110:LEU:HB2	1.90	0.54
1:BI:100:VAL:HG21	2:BJ:19:LEU:HD12	1.90	0.54
1:AG:24:LEU:HD22	2:AH:38:ILE:HG23	1.88	0.54
1:AU:79:ARG:NH2	7:AU:201:CYC:O2D	2.37	0.54
2:BD:77:ARG:NH1	7:BD:201:CYC:O2D	2.25	0.54
2:AP:114:ARG:NH2	2:AP:172:ALA:O	2.37	0.54
1:AM:79:ARG:NH2	7:AM:201:CYC:O2D	2.37	0.54
2:AN:114:ARG:NH1	5:BM:187:ARG:HH22	2.06	0.54
5:BM:189:ARG:NH2	8:BM:312:HOH:O	2.41	0.54
5:BM:227:VAL:HG11	5:BM:260:ILE:HD13	1.89	0.54
1:AC:26:ILE:HG12	1:AG:26:ILE:HG12	1.89	0.53
1:AG:47:ASN:OD1	1:AG:50:SER:OG	2.26	0.53
3:BK:43:ASP:OD1	3:BK:71:ARG:NH2	2.29	0.53
2:AD:77:ARG:NH1	7:AD:201:CYC:O2D	2.35	0.53
2:AP:127:VAL:HG22	7:AP:201:CYC:H3C	1.89	0.53
4:BL:237:LYS:HG3	4:BL:290:LEU:HD13	1.90	0.53
2:AX:127:VAL:HG22	7:AX:201:CYC:H3C	1.89	0.53
2:AB:116:THR:HG23	6:BN:43:SER:HB2	1.91	0.53
2:AJ:15:ARG:NE	2:AJ:17:GLU:OE2	2.38	0.53
1:BC:125:SER:HB3	1:BC:128:TRP:CE2	2.43	0.53
1:AE:94:ILE:HD12	1:AE:111:LEU:HD12	1.90	0.53
1:AG:121:THR:HG21	2:AL:83:LEU:HD13	1.91	0.53
2:AN:108:ARG:HA	5:BM:261:ASN:HB3	1.90	0.53
1:AW:73:ASN:HA	7:AW:201:CYC:HBD2	1.91	0.53
1:AY:102:GLY:O	1:BG:25:GLN:NE2	2.40	0.53
2:AZ:84:ARG:NH2	7:AZ:201:CYC:O1A	2.41	0.53
1:AA:40:ALA:HB2	1:AA:146:ALA:HB1	1.91	0.52
1:AS:128:TRP:CD2	7:AS:201:CYC:HMC3	2.45	0.52
2:AT:8:VAL:HG21	2:AT:27:LEU:HD11	1.91	0.52
1:AO:49:GLN:HG2	1:AO:50:SER:N	2.25	0.52
2:AV:139:LEU:HD22	2:AV:157:VAL:HG13	1.92	0.52
2:AB:77:ARG:NH2	6:BN:34:GLU:OE1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AG:79:ARG:NH2	7:AG:201:CYC:O2D	2.43	0.52
2:AT:77:ARG:HD3	4:BL:2:ALA:HB3	1.90	0.52
7:AX:201:CYC:HB	7:AX:201:CYC:HMA3	1.74	0.52
1:BC:155:ASP:HA	1:BC:158:ILE:HB	1.92	0.52
4:BL:165:THR:HA	4:BL:201:ILE:HD11	1.92	0.52
2:AH:106:GLU:HA	2:AH:110:LEU:HB2	1.91	0.52
1:AU:128:TRP:CD2	7:AU:201:CYC:HMC3	2.45	0.52
1:AW:99:LEU:O	8:AW:301:HOH:O	2.19	0.52
1:AY:40:ALA:HB2	1:AY:146:ALA:HB1	1.90	0.52
2:BB:116:THR:HG23	4:BL:257:SER:HB2	1.91	0.52
2:BD:145:PRO:HB2	2:BD:150:ARG:HH12	1.74	0.52
1:BE:47:ASN:OD1	1:BE:50:SER:OG	2.28	0.52
4:BL:213:TYR:HB2	4:BL:244:THR:HB	1.91	0.52
3:BK:14:ASN:O	3:BK:161:ARG:NH1	2.43	0.52
2:AB:127:VAL:HG22	7:AB:201:CYC:H3C	1.91	0.51
2:BB:139:LEU:HD22	2:BB:157:VAL:HG13	1.92	0.51
7:BJ:201:CYC:O1D	3:BK:167:ARG:NH1	2.43	0.51
1:AA:128:TRP:CD2	7:AA:201:CYC:HMC3	2.45	0.51
1:AO:100:VAL:HG21	2:AP:19:LEU:HD12	1.91	0.51
2:AV:127:VAL:HG22	7:AV:201:CYC:H3C	1.93	0.51
2:BD:72:ASN:HD21	2:BD:122:VAL:HG22	1.76	0.51
2:AB:3:ASP:H	2:AB:6:THR:HG1	1.57	0.51
5:BM:24:ARG:O	5:BM:65:ARG:NH2	2.44	0.51
4:BL:109:PHE:O	4:BL:166:ARG:NH1	2.43	0.51
2:AD:43:ARG:O	2:AD:47:ASN:ND2	2.40	0.51
2:AD:84:ARG:NH1	6:BN:56:ASN:HD21	2.09	0.51
2:AF:72:ASN:ND2	2:AF:122:VAL:HA	2.26	0.51
1:BC:130:VAL:O	1:BC:134:LYS:HG2	2.11	0.51
5:BM:158:ARG:NH1	6:BN:35:ASN:HB2	2.25	0.51
1:AE:84:CYS:O	1:AE:88:ILE:HG12	2.11	0.51
2:AF:72:ASN:HD21	2:AF:122:VAL:HG22	1.76	0.51
1:BE:75:ALA:O	1:BE:81:LYS:NZ	2.44	0.51
2:AN:86:MET:SD	7:AN:201:CYC:HBC1	2.50	0.51
2:AJ:43:ARG:NH1	2:AJ:144:ASP:O	2.42	0.51
2:AJ:69:PRO:HA	2:AJ:74:TYR:CG	2.46	0.50
1:BA:93:ARG:O	1:BA:96:THR:OG1	2.24	0.50
5:BM:267:VAL:HG11	5:BM:270:ILE:HD11	1.93	0.50
1:AM:73:ASN:HA	7:AM:201:CYC:HBD2	1.94	0.50
1:BC:26:ILE:HG12	1:BI:26:ILE:HG12	1.93	0.50
2:AZ:132:GLN:O	2:AZ:135:LYS:HB3	2.11	0.50
2:BJ:108:ARG:NH1	8:BJ:306:HOH:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AI:93:ARG:O	1:AI:96:THR:OG1	2.28	0.50
1:AO:26:ILE:HG12	1:AW:26:ILE:HG12	1.94	0.50
2:AP:43:ARG:NH1	2:AP:144:ASP:O	2.42	0.50
2:AD:108:ARG:HA	6:BN:63:SER:HB3	1.94	0.50
1:AY:75:ALA:HA	1:AY:80:GLY:HA3	1.94	0.50
1:BA:8:ALA:HB2	1:BA:26:ILE:HG21	1.94	0.50
2:BB:104:VAL:HG23	2:BB:108:ARG:HD2	1.93	0.50
1:BA:49:GLN:HG2	1:BA:50:SER:N	2.27	0.49
2:BF:3:ASP:H	2:BF:6:THR:HG1	1.58	0.49
1:AK:18:PHE:HB3	2:AL:45:THR:HG23	1.94	0.49
1:BE:24:LEU:HD22	2:BF:38:ILE:HG23	1.94	0.49
2:AH:119:ALA:O	5:BM:9:ARG:NH2	2.45	0.49
1:AM:75:ALA:HA	1:AM:80:GLY:HA3	1.93	0.49
1:AW:40:ALA:HB2	1:AW:146:ALA:HB1	1.94	0.49
1:BA:75:ALA:HA	1:BA:80:GLY:HA3	1.94	0.49
2:AN:139:LEU:HD22	2:AN:157:VAL:HG13	1.94	0.49
1:AQ:75:ALA:HA	1:AQ:80:GLY:HA3	1.94	0.49
1:BE:1:MET:N	1:BE:109:GLU:OE1	2.45	0.49
2:BF:39:ASP:OD1	7:BF:202:CYC:ND	2.46	0.49
2:BJ:56:ALA:HB2	2:BJ:86:MET:HE1	1.95	0.49
4:BL:181:GLN:HB2	4:BL:188:ARG:NH2	2.26	0.49
1:AC:104:THR:OG1	1:AG:17:ARG:NH2	2.45	0.49
2:AL:149:THR:O	7:AL:202:CYC:NC	2.41	0.49
1:AQ:65:TYR:O	1:AQ:69:THR:HG22	2.12	0.49
1:BG:14:SER:HB2	3:BK:91:ARG:HH12	1.77	0.49
5:BM:15:VAL:HG11	5:BM:154:PHE:HD2	1.77	0.49
1:AA:156:TYR:OH	1:AI:17:ARG:NH2	2.45	0.49
1:AE:108:ASP:HA	1:AE:112:ILE:HB	1.95	0.49
1:AG:125:SER:HB3	1:AG:128:TRP:CE2	2.48	0.49
1:AA:26:ILE:HG12	1:AI:26:ILE:HG12	1.94	0.49
1:AC:114:GLY:O	1:AC:118:ILE:HG12	2.13	0.49
2:BH:12:ALA:O	2:BH:16:GLY:N	2.46	0.49
1:BA:24:LEU:HD22	2:BB:38:ILE:HG23	1.94	0.48
1:BC:75:ALA:HA	1:BC:80:GLY:HA3	1.95	0.48
2:BH:39:ASP:OD2	7:BH:202:CYC:ND	2.39	0.48
5:BM:129:GLU:O	5:BM:132:SER:OG	2.27	0.48
1:AE:73:ASN:HA	7:AE:201:CYC:HBD2	1.95	0.48
2:AL:74:TYR:O	2:AL:78:ARG:HB2	2.13	0.48
2:AV:145:PRO:HA	2:AV:150:ARG:HH22	1.77	0.48
1:BC:128:TRP:CD2	7:BC:201:CYC:HMC3	2.48	0.48
2:BD:33:GLU:HG3	2:BD:36:LYS:HE3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AP:60:PHE:CE2	2:AP:79:MET:HE1	2.48	0.48
5:BM:259:GLN:HA	5:BM:262:ARG:HG2	1.95	0.48
2:AV:60:PHE:HB3	2:AV:67:ILE:HD13	1.95	0.48
1:BA:109:GLU:OE2	3:BK:39:SER:OG	2.31	0.48
2:BB:60:PHE:HE2	2:BB:79:MET:HE1	1.78	0.48
2:BH:139:LEU:HD22	2:BH:157:VAL:HG13	1.96	0.48
1:BI:2:LYS:NZ	1:BI:7:GLU:OE2	2.40	0.48
1:AC:75:ALA:HA	1:AC:80:GLY:HA3	1.94	0.48
2:AF:145:PRO:HB2	2:AF:150:ARG:NH1	2.29	0.48
3:BK:42:MET:HE1	3:BK:70:LEU:HG	1.95	0.48
5:BM:127:GLU:OE2	6:BN:11:SER:N	2.46	0.48
2:AL:3:ASP:HA	2:AL:99:THR:HB	1.96	0.48
2:AX:63:GLN:HB3	2:AX:65:GLN:NE2	2.29	0.48
2:AD:86:MET:O	2:AD:134:MET:HE1	2.14	0.48
2:AD:151:GLY:HA3	7:AD:202:CYC:HMD2	1.95	0.48
1:AQ:128:TRP:CD2	7:AQ:201:CYC:HMC3	2.49	0.48
1:AQ:93:ARG:O	1:AQ:96:THR:OG1	2.24	0.48
2:AZ:139:LEU:HD22	2:AZ:157:VAL:HG13	1.95	0.48
2:BF:106:GLU:HA	2:BF:110:LEU:HB2	1.95	0.48
4:BL:229:THR:HB	4:BL:235:ALA:HB3	1.96	0.48
2:AT:15:ARG:NH2	2:AT:17:GLU:OE2	2.47	0.48
2:BH:109:CYS:HA	7:BH:201:CYC:HAB2	1.95	0.48
7:AJ:201:CYC:HBA2	7:AJ:201:CYC:HHA	1.95	0.48
2:AT:127:VAL:HG22	7:AT:201:CYC:H3C	1.96	0.48
3:BK:100:ASN:HB3	3:BK:126:SER:HB2	1.95	0.48
2:AH:102:ALA:O	2:AH:106:GLU:HG2	2.14	0.47
1:AQ:26:ILE:HG12	1:AU:26:ILE:HG12	1.95	0.47
8:AW:347:HOH:O	2:AX:1:MET:SD	2.61	0.47
1:BG:79:ARG:HH22	7:BG:201:CYC:HAD1	1.79	0.47
7:BH:201:CYC:HB	7:BH:201:CYC:HMA1	1.79	0.47
1:AE:25:GLN:NE2	1:AK:102:GLY:O	2.45	0.47
2:AH:148:ILE:HG21	7:AH:202:CYC:HMC3	1.96	0.47
1:AW:10:SER:HB2	4:BL:88:TYR:CZ	2.49	0.47
1:AE:75:ALA:HA	1:AE:80:GLY:HA3	1.96	0.47
1:AK:27:ALA:HB2	2:AL:98:PHE:CZ	2.49	0.47
1:BA:118:ILE:HD13	7:BA:201:CYC:HMA3	1.95	0.47
1:AC:47:ASN:OD1	1:AC:50:SER:OG	2.31	0.47
1:AS:75:ALA:HA	1:AS:80:GLY:HA3	1.96	0.47
2:AV:135:LYS:NZ	2:AV:165:ASP:OD1	2.40	0.47
2:AZ:63:GLN:HB3	2:AZ:65:GLN:NE2	2.29	0.47
2:BD:91:ARG:O	2:BD:94:THR:OG1	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AF:112:GLY:HA3	6:BN:1:MET:O	2.14	0.47
2:AN:8:VAL:HG21	2:AN:27:LEU:HD11	1.96	0.47
2:BD:145:PRO:HB2	2:BD:150:ARG:NH1	2.29	0.47
1:BI:75:ALA:HA	1:BI:80:GLY:HA3	1.97	0.47
3:BK:97:LYS:HD3	3:BK:185:HIS:CD2	2.50	0.47
5:BM:70:ARG:HH21	5:BM:135:ASP:HA	1.80	0.47
2:BF:127:VAL:HG22	7:BF:201:CYC:H3C	1.96	0.47
2:AJ:6:THR:HA	2:AJ:9:VAL:HB	1.97	0.47
1:AE:40:ALA:HB2	1:AE:146:ALA:HB1	1.97	0.46
2:AH:69:PRO:HA	2:AH:74:TYR:CG	2.51	0.46
1:BC:40:ALA:HB2	1:BC:146:ALA:HB1	1.97	0.46
2:BF:88:ILE:HG21	7:BF:201:CYC:HAB2	1.97	0.46
2:AV:120:LEU:HD13	7:AV:201:CYC:HBD1	1.96	0.46
1:BA:128:TRP:CD2	7:BA:201:CYC:HMC3	2.51	0.46
2:BD:43:ARG:NH1	2:BD:144:ASP:O	2.44	0.46
2:BH:145:PRO:O	2:BH:150:ARG:NH1	2.46	0.46
2:BJ:127:VAL:HG22	7:BJ:201:CYC:H3C	1.96	0.46
2:AH:106:GLU:OE2	2:AH:166:ARG:HD3	2.15	0.46
1:AK:65:TYR:O	1:AK:69:THR:HG22	2.15	0.46
1:AK:79:ARG:NH2	7:AK:201:CYC:O2D	2.39	0.46
1:BA:137:LYS:HG2	1:BA:154:LEU:HD13	1.98	0.46
4:BL:47:ASP:OD2	4:BL:177:SER:OG	2.34	0.46
1:AM:64:PRO:O	1:AM:68:GLN:HG3	2.16	0.46
1:AO:128:TRP:CD2	7:AO:201:CYC:HMC3	2.50	0.46
2:BF:15:ARG:NH1	2:BF:17:GLU:OE1	2.47	0.46
6:BN:52:TYR:HA	6:BN:55:MET:SD	2.55	0.46
2:AT:57:ARG:NE	7:AU:201:CYC:O1D	2.37	0.46
2:AZ:166:ARG:O	2:AZ:166:ARG:NH1	2.49	0.46
2:AH:108:ARG:HA	5:BM:161:LYS:HG2	1.97	0.46
1:AY:118:ILE:HD13	7:AY:201:CYC:HMA3	1.97	0.46
2:AZ:127:VAL:HG22	7:AZ:201:CYC:H3C	1.97	0.46
2:BB:118:VAL:HB	4:BL:182:LEU:HD22	1.98	0.46
5:BM:228:ILE:HG12	5:BM:243:LYS:HE2	1.97	0.46
2:AB:69:PRO:HA	2:AB:74:TYR:CG	2.51	0.46
1:AO:90:TYR:O	1:AO:94:ILE:HG12	2.16	0.46
1:AK:42:LYS:HB2	2:AL:24:LEU:HD13	1.98	0.46
2:BF:83:LEU:HD13	1:BG:121:THR:HG21	1.98	0.46
1:BG:18:PHE:HB3	2:BH:45:THR:HG23	1.98	0.46
1:AK:17:ARG:O	2:AL:95:TYR:OH	2.28	0.45
1:AM:125:SER:HB3	1:AM:128:TRP:CE2	2.51	0.45
2:BF:139:LEU:O	2:BF:143:ASN:ND2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BM:114:ILE:HD11	5:BM:194:LEU:HD13	1.97	0.45
1:AO:73:ASN:HA	7:AO:201:CYC:HBD2	1.98	0.45
2:AR:128:ALA:O	2:AR:132:GLN:HG2	2.17	0.45
1:AS:90:TYR:O	1:AS:94:ILE:HG12	2.16	0.45
1:AY:118:ILE:HD11	2:BD:79:MET:HB3	1.98	0.45
2:AF:127:VAL:HG23	7:AF:201:CYC:HBC3	1.98	0.45
2:AL:4:VAL:HG21	2:AL:30:THR:HG21	1.98	0.45
1:AI:147:ARG:HE	1:AI:147:ARG:HB3	1.47	0.45
1:AI:75:ALA:HA	1:AI:80:GLY:HA3	1.98	0.45
2:AZ:58:ALA:HB3	2:AZ:133:LYS:HD3	1.99	0.45
2:BB:36:LYS:HE2	2:BB:152:ASP:O	2.16	0.45
1:AE:20:SER:N	1:AE:23:GLU:OE1	2.45	0.45
1:AG:128:TRP:CD2	7:AG:201:CYC:HMC3	2.52	0.45
2:AB:139:LEU:HD22	2:AB:157:VAL:HG13	1.99	0.45
1:AI:108:ASP:HA	1:AI:112:ILE:HB	1.99	0.45
7:AJ:201:CYC:CGA	5:BM:48:HIS:H	2.29	0.45
2:AT:112:GLY:HA2	4:BL:198:VAL:HG21	1.98	0.45
2:AV:69:PRO:HA	2:AV:74:TYR:CG	2.51	0.45
1:AY:75:ALA:HB1	1:AY:81:LYS:HG2	1.98	0.45
2:BJ:4:VAL:HG11	2:BJ:30:THR:HG21	1.98	0.45
2:AF:8:VAL:HG21	2:AF:27:LEU:HD11	1.98	0.45
1:AO:24:LEU:HD22	2:AP:38:ILE:HG23	1.98	0.45
2:BF:152:ASP:OD2	2:BF:154:SER:OG	2.30	0.45
2:BH:106:GLU:CD	2:BH:166:ARG:HH11	2.24	0.45
1:AM:26:ILE:HG12	1:AS:26:ILE:HG12	1.99	0.45
2:AP:115:GLU:OE1	5:BM:9:ARG:NH1	2.49	0.45
1:AS:15:GLN:HG3	1:AS:17:ARG:HD3	1.98	0.45
2:AZ:33:GLU:HG2	2:AZ:156:ILE:HD11	1.99	0.45
1:AG:23:GLU:HA	1:AG:26:ILE:HD12	1.99	0.44
1:AK:128:TRP:CD2	7:AK:201:CYC:HMC3	2.52	0.44
2:AN:114:ARG:NH1	5:BM:187:ARG:HH12	2.14	0.44
2:BB:43:ARG:NH1	2:BB:144:ASP:O	2.48	0.44
2:BB:69:PRO:HA	2:BB:74:TYR:CG	2.52	0.44
1:AI:128:TRP:CD2	7:AI:201:CYC:HMC3	2.52	0.44
3:BK:110:LYS:HB3	3:BK:110:LYS:HE2	1.73	0.44
4:BL:205:SER:HA	4:BL:211:TRP:CG	2.52	0.44
1:AG:93:ARG:O	1:AG:96:THR:OG1	2.32	0.44
1:BE:128:TRP:CD2	7:BE:201:CYC:HMC3	2.53	0.44
2:AB:8:VAL:HG21	2:AB:27:LEU:HD11	1.99	0.44
1:AS:17:ARG:O	2:AT:95:TYR:OH	2.24	0.44
1:BA:100:VAL:HG21	2:BB:19:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BN:1:MET:SD	6:BN:49:LYS:HE3	2.58	0.44
1:AE:88:ILE:HD11	7:AE:201:CYC:HBC1	2.00	0.44
1:AO:79:ARG:NH1	8:AO:308:HOH:O	2.44	0.44
2:AP:6:THR:HA	2:AP:9:VAL:HB	1.98	0.44
1:BC:93:ARG:O	1:BC:96:THR:OG1	2.32	0.44
1:BE:159:ASN:ND2	8:BE:305:HOH:O	2.49	0.44
4:BL:97:GLU:OE2	4:BL:187:SER:OG	2.33	0.44
2:AT:27:LEU:HD23	2:AT:27:LEU:HA	1.89	0.44
1:BE:8:ALA:HB1	1:BE:23:GLU:HG3	1.98	0.44
1:BG:40:ALA:HB2	1:BG:146:ALA:HB1	1.99	0.44
2:AD:150:ARG:HD2	2:AD:150:ARG:HA	1.68	0.44
1:AG:40:ALA:HB2	1:AG:146:ALA:HB1	2.00	0.44
1:AG:75:ALA:HA	1:AG:80:GLY:HA3	2.00	0.44
2:AP:135:LYS:HE3	2:AP:161:ALA:HB1	1.99	0.44
2:AR:114:ARG:NH1	2:AR:172:ALA:O	2.51	0.44
2:BB:132:GLN:O	2:BB:136:GLU:HG2	2.18	0.44
4:BL:120:LEU:HD23	4:BL:129:ASP:HA	2.00	0.44
5:BM:67:ILE:HB	5:BM:71:ASP:HB2	2.00	0.44
1:AM:128:TRP:CD2	7:AM:201:CYC:HMC3	2.52	0.44
1:AY:32:ARG:NH2	1:AY:33:GLN:OE1	2.48	0.44
1:BG:114:GLY:O	1:BG:118:ILE:HG12	2.17	0.44
1:AA:118:ILE:HD13	7:AA:201:CYC:HMA3	2.00	0.43
2:AL:106:GLU:OE1	2:AL:110:LEU:HD12	2.18	0.43
1:AY:29:GLY:HA3	1:BG:25:GLN:O	2.18	0.43
2:BB:84:ARG:NH1	7:BB:201:CYC:O1A	2.51	0.43
2:BD:69:PRO:HA	2:BD:74:TYR:CG	2.53	0.43
4:BL:235:ALA:HA	4:BL:266:GLU:OE1	2.19	0.43
1:BA:27:ALA:HB2	2:BB:98:PHE:CZ	2.53	0.43
2:AX:43:ARG:NH1	2:AX:144:ASP:O	2.50	0.43
2:AX:60:PHE:HB3	2:AX:67:ILE:HD13	2.00	0.43
1:BI:128:TRP:CD2	7:BI:201:CYC:HMC3	2.54	0.43
6:BN:56:ASN:O	6:BN:60:ARG:HG3	2.18	0.43
1:AO:108:ASP:HA	1:AO:112:ILE:HB	2.01	0.43
7:AX:201:CYC:CGA	4:BL:115:ILE:HG12	2.48	0.43
1:BA:23:GLU:OE1	1:BA:23:GLU:N	2.52	0.43
1:AI:155:ASP:HA	1:AI:158:ILE:HB	2.01	0.43
2:AN:114:ARG:HB2	2:AN:170:ALA:O	2.18	0.43
2:AR:43:ARG:NH1	2:AR:144:ASP:O	2.40	0.43
1:BI:23:GLU:OE1	1:BI:23:GLU:N	2.52	0.43
1:BI:47:ASN:ND2	1:BI:50:SER:HG	2.17	0.43
2:BJ:2:PHE:H	2:BJ:103:SER:HG	1.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AO:23:GLU:HA	1:AO:26:ILE:HD12	2.01	0.43
1:AS:24:LEU:HD22	2:AT:38:ILE:HG23	2.00	0.43
1:AY:25:GLN:NE2	1:BG:102:GLY:O	2.39	0.43
1:AU:84:CYS:HA	7:AU:201:CYC:HAC1	1.84	0.43
1:BC:91:TYR:CZ	1:BC:111:LEU:HD21	2.54	0.43
2:AR:119:ALA:O	5:BM:192:ARG:NH2	2.52	0.43
1:AY:128:TRP:CD2	7:AY:201:CYC:HMC3	2.54	0.43
2:BH:127:VAL:HG22	7:BH:201:CYC:H3C	2.00	0.43
2:AF:69:PRO:HA	2:AF:74:TYR:CG	2.54	0.43
1:AQ:133:LEU:HB2	1:AQ:158:ILE:HD11	2.01	0.43
1:AU:117:GLU:OE1	1:AU:117:GLU:N	2.52	0.43
2:BJ:69:PRO:HA	2:BJ:74:TYR:CG	2.54	0.43
1:AC:25:GLN:NE2	1:AG:102:GLY:O	2.52	0.43
2:AD:15:ARG:HH22	2:AD:23:GLN:HE22	1.66	0.43
2:AJ:39:ASP:OD2	7:AJ:202:CYC:ND	2.42	0.43
2:AL:150:ARG:HD2	2:AL:150:ARG:HA	1.77	0.43
1:AU:118:ILE:HD13	7:AU:201:CYC:HMA3	2.00	0.43
7:AX:201:CYC:HB	7:AX:201:CYC:CMA	2.31	0.43
1:AY:19:LEU:O	8:AY:301:HOH:O	2.21	0.43
1:BG:65:TYR:O	1:BG:69:THR:HG22	2.19	0.43
2:BJ:106:GLU:OE2	2:BJ:166:ARG:HD3	2.18	0.43
2:AB:135:LYS:NZ	2:AB:165:ASP:OD1	2.46	0.42
1:AW:84:CYS:HA	7:AW:201:CYC:HAC1	1.90	0.42
1:AW:91:TYR:CZ	1:AW:111:LEU:HD21	2.54	0.42
2:BB:60:PHE:CE2	2:BB:79:MET:HE1	2.54	0.42
2:BH:15:ARG:NH2	2:BH:17:GLU:OE2	2.43	0.42
2:BH:106:GLU:OE2	2:BH:110:LEU:HD12	2.19	0.42
1:BI:155:ASP:O	1:BI:159:ASN:ND2	2.52	0.42
6:BN:55:MET:O	6:BN:59:MET:HG2	2.19	0.42
1:AM:159:ASN:ND2	8:AM:305:HOH:O	2.38	0.42
2:AP:86:MET:HE2	2:AP:134:MET:HE2	2.01	0.42
1:AS:140:HIS:HE1	1:AS:147:ARG:HG3	1.83	0.42
2:AV:76:SER:OG	1:AW:111:LEU:O	2.30	0.42
1:AW:75:ALA:HA	1:AW:80:GLY:HA3	2.02	0.42
1:BA:72:ASN:O	1:BA:79:ARG:NH2	2.48	0.42
5:BM:65:ARG:HA	5:BM:65:ARG:HD3	1.87	0.42
1:AA:140:HIS:CD2	1:AA:142:LEU:H	2.37	0.42
2:AJ:79:MET:HE3	7:AK:201:CYC:HBA1	2.00	0.42
1:AK:93:ARG:O	1:AK:96:THR:OG1	2.35	0.42
2:AL:27:LEU:HD23	2:AL:27:LEU:HA	1.91	0.42
2:AL:69:PRO:HA	2:AL:74:TYR:CG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AQ:84:CYS:HA	7:AQ:201:CYC:HAC1	1.90	0.42
1:AA:24:LEU:HD22	2:AB:38:ILE:HG23	2.01	0.42
1:AC:1:MET:HE2	2:AD:6:THR:HB	2.01	0.42
1:AI:122:PHE:CE2	7:AI:201:CYC:HAA1	2.55	0.42
1:AK:75:ALA:HA	1:AK:80:GLY:HA3	2.00	0.42
1:BG:79:ARG:NH2	7:BG:201:CYC:HAD1	2.34	0.42
1:AI:125:SER:HB3	1:AI:128:TRP:CE2	2.54	0.42
1:AM:8:ALA:HB1	1:AM:23:GLU:HG3	2.00	0.42
1:AM:84:CYS:HA	7:AM:201:CYC:HAC1	1.88	0.42
2:AZ:108:ARG:HG2	4:BL:228:GLY:HA3	2.01	0.42
2:BB:69:PRO:HA	2:BB:74:TYR:CD2	2.53	0.42
6:BN:13:THR:HG22	6:BN:16:ALA:H	1.85	0.42
1:AG:39:GLN:NE2	1:AG:39:GLN:N	2.67	0.42
2:AT:12:ALA:O	2:AT:16:GLY:N	2.51	0.42
1:BA:84:CYS:HA	7:BA:201:CYC:HAC1	1.93	0.42
1:BA:91:TYR:CD2	1:BA:133:LEU:HD21	2.55	0.42
2:BF:128:ALA:O	2:BF:132:GLN:HG2	2.20	0.42
1:BG:84:CYS:O	1:BG:88:ILE:HG12	2.19	0.42
5:BM:51:SER:HA	5:BM:54:ARG:HG3	2.01	0.42
5:BM:165:PHE:O	5:BM:168:SER:HB3	2.20	0.42
2:AD:115:GLU:HG2	6:BN:71:ASN:HA	2.01	0.42
2:AJ:60:PHE:HB3	2:AJ:67:ILE:HD13	2.00	0.42
2:AJ:91:ARG:O	2:AJ:94:THR:OG1	2.25	0.42
1:AK:23:GLU:HA	1:AK:26:ILE:HD12	2.02	0.42
2:BB:58:ALA:HB3	2:BB:133:LYS:HD3	2.02	0.42
2:BH:84:ARG:CZ	3:BK:127:ILE:HG12	2.50	0.42
1:AS:23:GLU:HA	1:AS:26:ILE:HD12	2.01	0.42
2:AX:89:ILE:HD13	2:AX:109:CYS:SG	2.59	0.42
2:BD:128:ALA:HB2	2:BD:172:ALA:HB2	2.01	0.42
7:BH:201:CYC:HMA1	7:BH:201:CYC:NB	2.34	0.42
1:BI:114:GLY:O	1:BI:118:ILE:HG12	2.20	0.42
2:AL:58:ALA:HB3	2:AL:133:LYS:HD3	2.00	0.42
2:AV:92:TYR:CG	2:AV:109:CYS:HB2	2.55	0.42
2:BB:66:LEU:HD11	2:BB:126:SER:HB3	2.02	0.42
2:BF:135:LYS:O	2:BF:139:LEU:HG	2.20	0.42
5:BM:152:ARG:HB3	5:BM:157:GLN:NE2	2.35	0.42
1:AC:114:GLY:O	1:AC:117:GLU:HG2	2.19	0.42
1:AQ:117:GLU:HA	1:AQ:120:ARG:HG2	2.02	0.42
1:BA:13:ASP:OD2	2:BB:108:ARG:NH1	2.42	0.42
5:BM:211:LEU:HD23	5:BM:211:LEU:HA	1.93	0.42
1:AA:108:ASP:HA	1:AA:112:ILE:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AH:43:ARG:NH1	2:AH:144:ASP:O	2.42	0.41
2:AN:114:ARG:HH11	5:BM:187:ARG:HH22	1.66	0.41
1:AY:99:LEU:HD23	1:AY:149:GLU:HG2	2.01	0.41
1:BG:108:ASP:HA	1:BG:112:ILE:HB	2.02	0.41
3:BK:146:GLU:OE2	3:BK:160:ARG:NH2	2.52	0.41
3:BK:173:PRO:HD2	3:BK:176:ILE:HD12	2.01	0.41
2:AX:119:ALA:HB2	4:BL:191:THR:HA	2.01	0.41
2:AD:127:VAL:HG22	7:AD:201:CYC:H3C	2.01	0.41
2:AN:114:ARG:NH2	2:AN:172:ALA:O	2.42	0.41
1:BE:125:SER:HB3	1:BE:128:TRP:CE2	2.54	0.41
2:BH:63:GLN:HB3	2:BH:65:GLN:HE22	1.85	0.41
2:BJ:64:PRO:O	2:BJ:68:GLN:HG2	2.20	0.41
1:AG:84:CYS:HA	7:AG:201:CYC:HAC1	1.91	0.41
1:AS:40:ALA:HB2	1:AS:146:ALA:HB1	2.03	0.41
1:AU:15:GLN:HG2	1:AU:17:ARG:HG2	2.01	0.41
2:AV:65:GLN:CD	2:BB:68:GLN:HG3	2.45	0.41
1:BE:1:MET:H1	1:BE:109:GLU:CD	2.27	0.41
2:AN:69:PRO:HA	2:AN:74:TYR:CG	2.55	0.41
2:AN:102:ALA:O	2:AN:106:GLU:HG2	2.21	0.41
2:AP:107:ASP:O	5:BM:212:ARG:HD2	2.20	0.41
2:AT:107:ASP:OD2	4:BL:196:ASN:ND2	2.53	0.41
1:AU:65:TYR:O	1:AU:69:THR:HG22	2.21	0.41
1:BE:113:ALA:O	2:BJ:76:SER:OG	2.35	0.41
1:AC:21:SER:O	1:AC:25:GLN:HG3	2.21	0.41
2:AD:60:PHE:CE2	2:AD:79:MET:HE1	2.56	0.41
1:AM:93:ARG:O	1:AM:96:THR:OG1	2.36	0.41
7:AW:201:CYC:HAC1	7:AW:201:CYC:HHD	1.93	0.41
2:AZ:166:ARG:HA	2:AZ:166:ARG:HD2	1.94	0.41
7:BB:202:CYC:HHD	7:BB:202:CYC:HAC1	1.89	0.41
1:AE:35:ASN:O	1:AE:39:GLN:HG3	2.21	0.41
2:AB:86:MET:HB3	2:AB:86:MET:HE3	1.85	0.41
2:AB:92:TYR:CG	2:AB:109:CYS:HB2	2.56	0.41
1:AS:149:GLU:HG2	1:AS:153:TYR:CE2	2.55	0.41
2:AV:85:ASP:OD1	4:BL:48:TYR:OH	2.33	0.41
1:BA:125:SER:HB3	1:BA:128:TRP:CE2	2.55	0.41
2:BB:43:ARG:HB3	2:BB:141:ILE:HG22	2.02	0.41
1:AA:2:LYS:HE2	1:AI:17:ARG:NH1	2.36	0.41
2:AD:162:GLY:O	2:AD:166:ARG:HG3	2.21	0.41
1:AI:62:LYS:HD3	1:AI:131:GLU:HG2	2.03	0.41
2:AL:166:ARG:HA	2:AL:166:ARG:HD2	1.90	0.41
2:AN:106:GLU:OE1	2:AN:166:ARG:NH1	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AO:201:CYC:CMD	7:AO:201:CYC:HC	2.34	0.41
2:AT:150:ARG:HD2	2:AT:150:ARG:HA	1.85	0.41
1:AW:38:LEU:HD23	1:AW:100:VAL:HG12	2.02	0.41
1:BE:93:ARG:O	1:BE:96:THR:OG1	2.28	0.41
1:AU:1:MET:HG2	1:AU:105:GLY:HA3	2.03	0.41
5:BM:117:HIS:HB3	5:BM:129:GLU:OE2	2.21	0.41
1:AA:2:LYS:HE2	1:AI:17:ARG:HH11	1.86	0.40
2:AN:27:LEU:HD23	2:AN:27:LEU:HA	1.88	0.40
1:AU:83:LYS:NZ	7:AU:201:CYC:O2A	2.45	0.40
2:AT:20:SER:OG	2:AT:23:GLN:HG3	2.22	0.40
1:BA:40:ALA:HB2	1:BA:146:ALA:HB1	2.03	0.40
1:BG:142:LEU:C	1:BG:147:ARG:HB2	2.46	0.40
2:BH:17:GLU:HB2	8:BH:326:HOH:O	2.21	0.40
2:BJ:84:ARG:HH22	7:BJ:201:CYC:CGA	2.34	0.40
2:AP:27:LEU:HD23	2:AP:27:LEU:HA	1.90	0.40
2:BB:136:GLU:HG2	2:BB:136:GLU:H	1.72	0.40
2:BB:172:ALA:OXT	4:BL:184:ARG:NH1	2.54	0.40
1:BE:65:TYR:O	1:BE:69:THR:HG22	2.21	0.40
1:BG:55:ALA:O	1:BG:59:VAL:HG23	2.22	0.40
3:BK:59:LYS:HE3	3:BK:59:LYS:HB3	1.95	0.40
5:BM:83:ARG:HH22	6:BN:10:TYR:HD2	1.69	0.40
1:AC:2:LYS:NZ	1:AC:7:GLU:OE1	2.51	0.40
1:AS:18:PHE:HB3	2:AT:45:THR:HG23	2.04	0.40
2:AX:65:GLN:HA	2:AX:68:GLN:HE21	1.85	0.40
4:BL:36:ILE:HG13	4:BL:62:LEU:HD23	2.04	0.40
1:AK:84:CYS:HA	7:AK:201:CYC:HAC1	1.96	0.40
2:AL:12:ALA:O	2:AL:16:GLY:N	2.53	0.40
1:AU:149:GLU:HG2	1:AU:153:TYR:CE2	2.56	0.40
4:BL:177:SER:C	4:BL:179:ARG:H	2.30	0.40
5:BM:203:TYR:HB3	5:BM:208:ALA:HB2	2.03	0.40

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	AA	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
1	AC	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
1	AE	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
1	AG	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
1	AI	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
1	AK	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
1	AM	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
1	AO	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
1	AQ	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
1	AS	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
1	AU	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
1	AW	160/162 (99%)	160 (100%)	0	0	100	100
1	AY	160/162 (99%)	160 (100%)	0	0	100	100
1	BA	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
1	BC	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
1	BE	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
1	BG	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
1	BI	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
2	AB	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
2	AD	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
2	AF	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
2	AH	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
2	AJ	170/172 (99%)	169 (99%)	1 (1%)	0	100	100
2	AL	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	21	18
2	AN	170/172 (99%)	169 (99%)	1 (1%)	0	100	100
2	AP	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
2	AR	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
2	AT	170/172 (99%)	169 (99%)	1 (1%)	0	100	100
2	AV	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
2	AX	170/172 (99%)	169 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AZ	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
2	BB	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
2	BD	170/172 (99%)	169 (99%)	1 (1%)	0	100	100
2	BF	170/172 (99%)	169 (99%)	1 (1%)	0	100	100
2	BH	170/172 (99%)	169 (99%)	1 (1%)	0	100	100
2	BJ	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
3	BK	192/249 (77%)	188 (98%)	4 (2%)	0	100	100
4	BL	287/291 (99%)	282 (98%)	5 (2%)	0	100	100
5	BM	260/273 (95%)	255 (98%)	5 (2%)	0	100	100
6	BN	73/83 (88%)	72 (99%)	1 (1%)	0	100	100
All	All	6752/6908 (98%)	6684 (99%)	67 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AL	75	THR

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	AA	126/126 (100%)	125 (99%)	1 (1%)	73	81
1	AC	126/126 (100%)	126 (100%)	0	100	100
1	AE	126/126 (100%)	125 (99%)	1 (1%)	73	81
1	AG	126/126 (100%)	125 (99%)	1 (1%)	73	81
1	AI	126/126 (100%)	126 (100%)	0	100	100
1	AK	126/126 (100%)	126 (100%)	0	100	100
1	AM	126/126 (100%)	123 (98%)	3 (2%)	43	49
1	AO	126/126 (100%)	125 (99%)	1 (1%)	73	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AQ	126/126 (100%)	126 (100%)	0	100	100
1	AS	126/126 (100%)	125 (99%)	1 (1%)	73	81
1	AU	126/126 (100%)	125 (99%)	1 (1%)	73	81
1	AW	126/126 (100%)	124 (98%)	2 (2%)	55	64
1	AY	126/126 (100%)	126 (100%)	0	100	100
1	BA	126/126 (100%)	125 (99%)	1 (1%)	73	81
1	BC	126/126 (100%)	125 (99%)	1 (1%)	73	81
1	BE	126/126 (100%)	125 (99%)	1 (1%)	73	81
1	BG	126/126 (100%)	124 (98%)	2 (2%)	55	64
1	BI	126/126 (100%)	124 (98%)	2 (2%)	55	64
2	AB	128/128 (100%)	126 (98%)	2 (2%)	55	64
2	AD	128/128 (100%)	128 (100%)	0	100	100
2	AF	128/128 (100%)	128 (100%)	0	100	100
2	AH	128/128 (100%)	126 (98%)	2 (2%)	55	64
2	AJ	128/128 (100%)	127 (99%)	1 (1%)	73	81
2	AL	128/128 (100%)	127 (99%)	1 (1%)	73	81
2	AN	128/128 (100%)	128 (100%)	0	100	100
2	AP	128/128 (100%)	128 (100%)	0	100	100
2	AR	128/128 (100%)	127 (99%)	1 (1%)	73	81
2	AT	128/128 (100%)	127 (99%)	1 (1%)	73	81
2	AV	128/128 (100%)	128 (100%)	0	100	100
2	AX	128/128 (100%)	127 (99%)	1 (1%)	73	81
2	AZ	128/128 (100%)	127 (99%)	1 (1%)	73	81
2	BB	128/128 (100%)	128 (100%)	0	100	100
2	BD	128/128 (100%)	126 (98%)	2 (2%)	55	64
2	BF	128/128 (100%)	128 (100%)	0	100	100
2	BH	128/128 (100%)	127 (99%)	1 (1%)	73	81
2	BJ	128/128 (100%)	128 (100%)	0	100	100
3	BK	175/221 (79%)	174 (99%)	1 (1%)	78	86
4	BL	244/246 (99%)	240 (98%)	4 (2%)	55	64
5	BM	225/230 (98%)	222 (99%)	3 (1%)	61	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	BN	64/71 (90%)	63 (98%)	1 (2%)	55 64
All	All	5280/5340 (99%)	5240 (99%)	40 (1%)	70 81

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	49	GLN
2	AB	39	ASP
2	AB	86	MET
1	AE	70	GLN
1	AG	39	GLN
2	AH	132	GLN
2	AH	139	LEU
2	AJ	8	VAL
2	AL	65	GLN
1	AM	1	MET
1	AM	39	GLN
1	AM	109	GLU
1	AO	120	ARG
2	AR	139	LEU
1	AS	137	LYS
2	AT	33	GLU
1	AU	15	GLN
1	AW	1	MET
1	AW	49	GLN
2	AX	106	GLU
2	AZ	84	ARG
1	BA	78	GLN
1	BC	120	ARG
2	BD	65	GLN
2	BD	150	ARG
1	BE	1	MET
1	BG	14	SER
1	BG	79	ARG
2	BH	150	ARG
1	BI	39	GLN
1	BI	42	LYS
3	BK	42	MET
4	BL	29	LEU
4	BL	47	ASP
4	BL	84	LYS
4	BL	273	GLN

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Mol	Chain	Res	Type
5	BM	96	ILE
5	BM	123	GLN
5	BM	238	ARG
6	BN	39	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	35	ASN
1	AA	57	GLN
1	AA	70	GLN
2	AB	68	GLN
1	AC	57	GLN
1	AE	57	GLN
1	AE	78	GLN
2	AF	23	GLN
2	AF	72	ASN
2	AF	111	ASN
1	AG	70	GLN
2	AH	63	GLN
1	AI	53	ASN
1	AI	70	GLN
1	AI	78	GLN
1	AK	57	GLN
1	AK	78	GLN
2	AL	47	ASN
2	AL	132	GLN
1	AM	49	GLN
1	AM	57	GLN
1	AM	78	GLN
1	AM	139	ASN
1	AO	15	GLN
1	AQ	78	GLN
1	AS	57	GLN
2	AT	42	ASN
2	AT	47	ASN
2	AT	132	GLN
1	AU	15	GLN
1	AU	47	ASN
2	AV	42	ASN
1	AW	15	GLN
1	AW	47	ASN

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Mol	Chain	Res	Type
1	AW	49	GLN
1	AY	57	GLN
1	AY	72	ASN
1	AY	139	ASN
2	AZ	65	GLN
2	BB	132	GLN
1	BC	68	GLN
2	BD	63	GLN
2	BD	72	ASN
1	BE	49	GLN
1	BG	49	GLN
1	BG	57	GLN
2	BH	42	ASN
2	BH	132	GLN
1	BI	15	GLN
1	BI	47	ASN
4	BL	64	ASN
5	BM	111	GLN
5	BM	252	ASN
5	BM	259	GLN
6	BN	14	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

54 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
7	CYC	AM	201	1	46,46,46	0.48	0	63,67,67	0.94	1 (1%)
7	CYC	BJ	201	2	46,46,46	0.42	0	63,67,67	1.15	4 (6%)
7	CYC	AI	201	1	46,46,46	0.53	0	63,67,67	0.98	2 (3%)
7	CYC	AK	201	1	46,46,46	0.47	0	63,67,67	1.00	2 (3%)
7	CYC	AD	202	2	46,46,46	0.41	0	63,67,67	0.74	2 (3%)
7	CYC	AJ	201	2	46,46,46	0.42	0	63,67,67	1.01	4 (6%)
7	CYC	BH	202	2	46,46,46	0.43	0	63,67,67	0.95	3 (4%)
7	CYC	AN	201	2	46,46,46	0.40	0	63,67,67	0.98	2 (3%)
7	CYC	BB	202	2	46,46,46	0.36	0	63,67,67	0.77	4 (6%)
7	CYC	BF	201	2	46,46,46	0.53	0	63,67,67	1.18	4 (6%)
7	CYC	AB	201	2	46,46,46	0.37	0	63,67,67	1.09	3 (4%)
7	CYC	BJ	202	2	46,46,46	0.40	0	63,67,67	0.86	3 (4%)
7	CYC	BI	201	1	46,46,46	0.51	0	63,67,67	0.97	1 (1%)
7	CYC	AU	201	1	46,46,46	0.56	0	63,67,67	0.94	2 (3%)
7	CYC	AX	201	2	46,46,46	0.57	0	63,67,67	1.12	3 (4%)
7	CYC	BG	201	1	46,46,46	0.45	0	63,67,67	1.03	2 (3%)
7	CYC	AW	201	1	46,46,46	0.47	0	63,67,67	0.88	2 (3%)
7	CYC	AN	202	2	46,46,46	0.40	0	63,67,67	0.87	4 (6%)
7	CYC	AR	201	2	46,46,46	0.43	0	63,67,67	0.91	2 (3%)
7	CYC	BA	201	1	46,46,46	0.54	1 (2%)	63,67,67	0.99	1 (1%)
7	CYC	BD	201	2	46,46,46	0.37	0	63,67,67	0.96	3 (4%)
7	CYC	AL	201	2	46,46,46	0.40	0	63,67,67	0.94	3 (4%)
7	CYC	AZ	202	2	46,46,46	0.43	0	63,67,67	0.80	2 (3%)
7	CYC	AB	202	2	46,46,46	0.33	0	63,67,67	0.88	3 (4%)
7	CYC	BB	201	2	46,46,46	0.51	0	63,67,67	1.22	3 (4%)
7	CYC	AX	202	2	46,46,46	0.41	0	63,67,67	0.95	3 (4%)
7	CYC	BD	202	2	46,46,46	0.39	0	63,67,67	0.86	3 (4%)
7	CYC	AA	201	1	46,46,46	0.43	0	63,67,67	0.90	1 (1%)
7	CYC	AS	201	1	46,46,46	0.51	0	63,67,67	0.81	1 (1%)
7	CYC	AT	201	2	46,46,46	0.56	0	63,67,67	1.12	4 (6%)
7	CYC	AR	202	2	46,46,46	0.47	0	63,67,67	0.92	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	CYC	AF	202	2	46,46,46	0.44	0	63,67,67	0.90	3 (4%)
7	CYC	AV	202	2	46,46,46	0.50	0	63,67,67	0.82	1 (1%)
7	CYC	AL	202	2	46,46,46	0.34	0	63,67,67	0.78	3 (4%)
7	CYC	AQ	201	1	46,46,46	0.49	0	63,67,67	0.95	2 (3%)
7	CYC	BE	201	1	46,46,46	0.46	0	63,67,67	0.93	2 (3%)
7	CYC	AE	201	1	46,46,46	0.47	0	63,67,67	0.78	1 (1%)
7	CYC	AH	202	2	46,46,46	0.41	0	63,67,67	0.75	3 (4%)
7	CYC	AV	201	2	46,46,46	0.47	0	63,67,67	0.98	2 (3%)
7	CYC	AZ	201	2	46,46,46	0.55	0	63,67,67	1.05	3 (4%)
7	CYC	AG	201	1	46,46,46	0.52	0	63,67,67	1.00	1 (1%)
7	CYC	AP	201	2	46,46,46	0.46	0	63,67,67	1.00	2 (3%)
7	CYC	BH	201	2	46,46,46	0.55	0	63,67,67	1.13	3 (4%)
7	CYC	AJ	202	2	46,46,46	0.39	0	63,67,67	0.86	4 (6%)
7	CYC	AP	202	2	46,46,46	0.47	0	63,67,67	0.83	3 (4%)
7	CYC	BC	201	1	46,46,46	0.47	0	63,67,67	0.94	2 (3%)
7	CYC	AF	201	2	46,46,46	0.34	0	63,67,67	0.94	2 (3%)
7	CYC	AT	202	2	46,46,46	0.48	0	63,67,67	1.01	3 (4%)
7	CYC	AC	201	1	46,46,46	0.47	0	63,67,67	0.86	2 (3%)
7	CYC	BF	202	2	46,46,46	0.39	0	63,67,67	0.82	4 (6%)
7	CYC	AD	201	2	46,46,46	0.37	0	63,67,67	0.92	3 (4%)
7	CYC	AY	201	1	46,46,46	0.49	0	63,67,67	0.93	2 (3%)
7	CYC	AH	201	2	46,46,46	0.42	0	63,67,67	0.97	3 (4%)
7	CYC	AO	201	1	46,46,46	0.56	0	63,67,67	0.95	1 (1%)

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
7	CYC	AM	201	1	-	10/26/74/74	0/4/4/4
7	CYC	BJ	201	2	-	6/26/74/74	0/4/4/4
7	CYC	AI	201	1	-	13/26/74/74	0/4/4/4
7	CYC	AK	201	1	-	12/26/74/74	0/4/4/4
7	CYC	AD	202	2	-	8/26/74/74	0/4/4/4
7	CYC	AJ	201	2	-	6/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CYC	BH	202	2	-	9/26/74/74	0/4/4/4
7	CYC	AN	201	2	-	5/26/74/74	0/4/4/4
7	CYC	BB	202	2	-	10/26/74/74	0/4/4/4
7	CYC	BF	201	2	-	8/26/74/74	0/4/4/4
7	CYC	AB	201	2	-	6/26/74/74	0/4/4/4
7	CYC	BJ	202	2	-	8/26/74/74	0/4/4/4
7	CYC	BI	201	1	-	11/26/74/74	0/4/4/4
7	CYC	AU	201	1	-	13/26/74/74	0/4/4/4
7	CYC	AX	201	2	-	9/26/74/74	0/4/4/4
7	CYC	BG	201	1	-	11/26/74/74	0/4/4/4
7	CYC	AW	201	1	-	11/26/74/74	0/4/4/4
7	CYC	AN	202	2	-	10/26/74/74	0/4/4/4
7	CYC	AR	201	2	-	9/26/74/74	0/4/4/4
7	CYC	BA	201	1	-	14/26/74/74	0/4/4/4
7	CYC	BD	201	2	-	7/26/74/74	0/4/4/4
7	CYC	AL	201	2	-	7/26/74/74	0/4/4/4
7	CYC	AZ	202	2	-	9/26/74/74	0/4/4/4
7	CYC	AB	202	2	-	8/26/74/74	0/4/4/4
7	CYC	BB	201	2	-	11/26/74/74	0/4/4/4
7	CYC	AX	202	2	-	9/26/74/74	0/4/4/4
7	CYC	BD	202	2	-	8/26/74/74	0/4/4/4
7	CYC	AA	201	1	-	13/26/74/74	0/4/4/4
7	CYC	AS	201	1	-	13/26/74/74	0/4/4/4
7	CYC	AT	201	2	-	7/26/74/74	0/4/4/4
7	CYC	AR	202	2	-	9/26/74/74	0/4/4/4
7	CYC	AF	202	2	-	10/26/74/74	0/4/4/4
7	CYC	AV	202	2	-	8/26/74/74	0/4/4/4
7	CYC	AL	202	2	-	9/26/74/74	0/4/4/4
7	CYC	AQ	201	1	-	12/26/74/74	0/4/4/4
7	CYC	BE	201	1	-	11/26/74/74	0/4/4/4
7	CYC	AE	201	1	-	13/26/74/74	0/4/4/4
7	CYC	AH	202	2	-	11/26/74/74	0/4/4/4
7	CYC	AV	201	2	-	10/26/74/74	0/4/4/4
7	CYC	AZ	201	2	-	8/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CYC	AG	201	1	-	11/26/74/74	0/4/4/4
7	CYC	AP	201	2	-	6/26/74/74	0/4/4/4
7	CYC	BH	201	2	-	6/26/74/74	0/4/4/4
7	CYC	AJ	202	2	-	9/26/74/74	0/4/4/4
7	CYC	AP	202	2	-	9/26/74/74	0/4/4/4
7	CYC	BC	201	1	-	12/26/74/74	0/4/4/4
7	CYC	AF	201	2	-	6/26/74/74	0/4/4/4
7	CYC	AT	202	2	-	7/26/74/74	0/4/4/4
7	CYC	AC	201	1	-	12/26/74/74	0/4/4/4
7	CYC	BF	202	2	-	10/26/74/74	0/4/4/4
7	CYC	AD	201	2	-	6/26/74/74	0/4/4/4
7	CYC	AY	201	1	-	11/26/74/74	0/4/4/4
7	CYC	AH	201	2	-	7/26/74/74	0/4/4/4
7	CYC	AO	201	1	-	11/26/74/74	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	BA	201	CYC	CHA-C1A	-2.16	1.34	1.38

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	AB	201	CYC	C1D-CHD-C4C	6.81	139.39	127.76
7	BF	201	CYC	C1B-CHB-C4A	6.06	142.92	128.06
7	BA	201	CYC	C1D-CHD-C4C	5.97	137.96	127.76
7	BG	201	CYC	C1D-CHD-C4C	5.92	137.86	127.76
7	AM	201	CYC	C1D-CHD-C4C	5.82	137.70	127.76
7	AK	201	CYC	C1D-CHD-C4C	5.74	137.57	127.76
7	AG	201	CYC	C1D-CHD-C4C	5.74	137.56	127.76
7	AV	201	CYC	C1D-CHD-C4C	5.73	137.55	127.76
7	AT	201	CYC	C1D-CHD-C4C	5.72	137.53	127.76
7	BD	201	CYC	C1D-CHD-C4C	5.71	137.51	127.76
7	BC	201	CYC	C1D-CHD-C4C	5.68	137.46	127.76
7	AI	201	CYC	C1D-CHD-C4C	5.67	137.45	127.76
7	BI	201	CYC	C1D-CHD-C4C	5.63	137.38	127.76
7	BE	201	CYC	C1D-CHD-C4C	5.63	137.37	127.76
7	BB	201	CYC	C1D-CHD-C4C	5.63	137.37	127.76
7	AN	201	CYC	C1D-CHD-C4C	5.62	137.37	127.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	AL	201	CYC	C1D-CHD-C4C	5.62	137.35	127.76
7	BB	201	CYC	C1B-CHB-C4A	5.60	141.79	128.06
7	AP	201	CYC	C1D-CHD-C4C	5.59	137.30	127.76
7	AQ	201	CYC	C1D-CHD-C4C	5.51	137.17	127.76
7	AH	201	CYC	C1D-CHD-C4C	5.47	137.10	127.76
7	AF	201	CYC	C1D-CHD-C4C	5.45	137.07	127.76
7	AR	201	CYC	C1D-CHD-C4C	5.37	136.93	127.76
7	AU	201	CYC	C1D-CHD-C4C	5.35	136.90	127.76
7	AY	201	CYC	C1D-CHD-C4C	5.33	136.87	127.76
7	BJ	201	CYC	C1D-CHD-C4C	5.28	136.78	127.76
7	AA	201	CYC	C1D-CHD-C4C	5.13	136.52	127.76
7	BH	201	CYC	C1B-CHB-C4A	5.12	140.62	128.06
7	AJ	201	CYC	C1D-CHD-C4C	5.06	136.41	127.76
7	AX	201	CYC	C1B-CHB-C4A	5.05	140.46	128.06
7	AT	202	CYC	C1B-CHB-C4A	4.93	140.15	128.06
7	BH	201	CYC	C1D-CHD-C4C	4.92	136.17	127.76
7	AZ	201	CYC	C1D-CHD-C4C	4.84	136.03	127.76
7	AC	201	CYC	C1D-CHD-C4C	4.83	136.01	127.76
7	AD	201	CYC	C1D-CHD-C4C	4.77	135.91	127.76
7	AO	201	CYC	C1D-CHD-C4C	4.72	135.82	127.76
7	AE	201	CYC	C1D-CHD-C4C	4.58	135.59	127.76
7	BJ	201	CYC	C1B-CHB-C4A	4.53	139.19	128.06
7	AW	201	CYC	C1D-CHD-C4C	4.37	135.23	127.76
7	AS	201	CYC	C1D-CHD-C4C	4.27	135.05	127.76
7	AX	202	CYC	C1B-CHB-C4A	4.23	138.44	128.06
7	BF	201	CYC	C1D-CHD-C4C	3.99	134.57	127.76
7	BD	202	CYC	C1B-CHB-C4A	3.97	137.79	128.06
7	AX	201	CYC	C1D-CHD-C4C	3.94	134.49	127.76
7	BH	202	CYC	C1B-CHB-C4A	3.90	137.62	128.06
7	AV	202	CYC	C1B-CHB-C4A	3.90	137.62	128.06
7	AF	202	CYC	C1B-CHB-C4A	3.84	137.47	128.06
7	AF	202	CYC	C1D-CHD-C4C	3.80	134.24	127.76
7	BJ	202	CYC	C1B-CHB-C4A	3.79	137.36	128.06
7	AB	202	CYC	C1B-CHB-C4A	3.74	137.25	128.06
7	AR	202	CYC	C1B-CHB-C4A	3.74	137.24	128.06
7	BH	202	CYC	C1D-CHD-C4C	3.64	133.97	127.76
7	BF	202	CYC	C1B-CHB-C4A	3.53	136.71	128.06
7	AR	202	CYC	C1D-CHD-C4C	3.48	133.71	127.76
7	AP	202	CYC	C1B-CHB-C4A	3.45	136.53	128.06
7	AJ	202	CYC	C1B-CHB-C4A	3.39	136.39	128.06
7	AX	202	CYC	C1D-CHD-C4C	3.35	133.48	127.76
7	AN	202	CYC	C1B-CHB-C4A	3.32	136.19	128.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	AT	201	CYC	C2C-C3C-C4C	3.31	106.29	101.34
7	AB	202	CYC	C1D-CHD-C4C	3.26	133.33	127.76
7	AL	202	CYC	C1B-CHB-C4A	3.18	135.86	128.06
7	AN	201	CYC	C2C-C3C-C4C	3.14	106.05	101.34
7	AZ	201	CYC	C2C-C3C-C4C	3.11	106.00	101.34
7	AD	202	CYC	C1B-CHB-C4A	3.08	135.62	128.06
7	AT	202	CYC	C1D-CHD-C4C	3.04	132.95	127.76
7	AH	202	CYC	C1B-CHB-C4A	2.96	135.32	128.06
7	BD	202	CYC	C1D-CHD-C4C	2.92	132.75	127.76
7	BJ	202	CYC	C1D-CHD-C4C	2.92	132.75	127.76
7	BB	202	CYC	C1B-CHB-C4A	2.89	135.15	128.06
7	AJ	202	CYC	C1D-CHD-C4C	2.85	132.63	127.76
7	BJ	201	CYC	C4D-CHA-C1A	2.85	134.44	128.22
7	AZ	201	CYC	C1B-CHB-C4A	2.84	135.02	128.06
7	AB	201	CYC	C2C-C3C-C4C	2.80	105.53	101.34
7	AJ	201	CYC	C2C-C3C-C4C	2.76	105.48	101.34
7	BH	201	CYC	C2C-C3C-C4C	2.74	105.44	101.34
7	AP	201	CYC	C2C-C3C-C4C	2.74	105.44	101.34
7	AF	201	CYC	C2C-C3C-C4C	2.74	105.44	101.34
7	AZ	202	CYC	C1D-CHD-C4C	2.73	132.43	127.76
7	AL	202	CYC	C1D-CHD-C4C	2.73	132.42	127.76
7	AZ	202	CYC	C1B-CHB-C4A	2.70	134.68	128.06
7	AD	201	CYC	C2C-C3C-C4C	2.69	105.37	101.34
7	AX	201	CYC	C2C-C3C-C4C	2.68	105.35	101.34
7	AF	202	CYC	C2C-C3C-C4C	2.60	105.23	101.34
7	AN	202	CYC	C1D-CHD-C4C	2.59	132.19	127.76
7	BJ	201	CYC	C2C-C3C-C4C	2.58	105.20	101.34
7	AD	201	CYC	C4D-CHA-C1A	2.57	133.83	128.22
7	BF	202	CYC	C1D-CHD-C4C	2.56	132.13	127.76
7	BD	201	CYC	C2C-C3C-C4C	2.56	105.17	101.34
7	AV	201	CYC	C2C-C3C-C4C	2.54	105.15	101.34
7	AL	201	CYC	C2C-C3C-C4C	2.54	105.14	101.34
7	AX	202	CYC	C2C-C3C-C4C	2.53	105.13	101.34
7	AW	201	CYC	C1C-NC-C4C	-2.52	110.25	113.41
7	AR	202	CYC	C2C-C3C-C4C	2.52	105.11	101.34
7	AJ	201	CYC	C4D-CHA-C1A	2.49	133.66	128.22
7	BB	202	CYC	CAC-C3C-C4C	-2.47	106.34	112.67
7	AL	202	CYC	C2C-C3C-C4C	2.46	105.03	101.34
7	AP	202	CYC	C1D-CHD-C4C	2.44	131.93	127.76
7	AD	202	CYC	C2C-C3C-C4C	2.44	104.99	101.34
7	AB	201	CYC	C4D-CHA-C1A	2.43	133.53	128.22
7	BD	202	CYC	C2C-C3C-C4C	2.42	104.96	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	BF	201	CYC	C4D-CHA-C1A	2.39	133.43	128.22
7	AB	202	CYC	C2C-C3C-C4C	2.37	104.89	101.34
7	BF	202	CYC	C2C-C3C-C4C	2.36	104.88	101.34
7	AN	202	CYC	C4D-CHA-C1A	2.35	133.36	128.22
7	BG	201	CYC	C4D-CHA-C1A	2.35	133.35	128.22
7	AT	201	CYC	C4D-CHA-C1A	2.30	133.25	128.22
7	AR	201	CYC	C2C-C3C-C4C	2.29	104.77	101.34
7	AH	201	CYC	C2C-C3C-C4C	2.28	104.75	101.34
7	AP	202	CYC	C2C-C3C-C4C	2.28	104.75	101.34
7	BF	201	CYC	C2C-C3C-C4C	2.27	104.74	101.34
7	AJ	201	CYC	CAA-C2A-C1A	2.27	129.00	125.02
7	AK	201	CYC	C4D-CHA-C1A	2.25	133.14	128.22
7	AN	202	CYC	C2C-C3C-C4C	2.24	104.70	101.34
7	AI	201	CYC	C4D-CHA-C1A	2.24	133.12	128.22
7	AT	201	CYC	C1B-CHB-C4A	2.22	133.50	128.06
7	BH	202	CYC	C2C-C3C-C4C	2.20	104.64	101.34
7	AC	201	CYC	C1B-CHB-C4A	2.19	133.44	128.06
7	AJ	202	CYC	C2C-C3C-C4C	2.18	104.61	101.34
7	BE	201	CYC	C4D-CHA-C1A	2.18	132.98	128.22
7	AU	201	CYC	C4D-CHA-C1A	2.18	132.98	128.22
7	AH	201	CYC	C4D-CHA-C1A	2.14	132.91	128.22
7	BC	201	CYC	C4D-CHA-C1A	2.14	132.90	128.22
7	BB	201	CYC	C2C-C3C-C4C	2.12	104.51	101.34
7	AT	202	CYC	C4D-CHA-C1A	2.11	132.83	128.22
7	AQ	201	CYC	C4D-CHA-C1A	2.09	132.80	128.22
7	AL	201	CYC	C4D-CHA-C1A	2.09	132.78	128.22
7	BF	202	CYC	C4D-CHA-C1A	2.08	132.77	128.22
7	AY	201	CYC	C4D-CHA-C1A	2.06	132.71	128.22
7	BB	202	CYC	C2C-C3C-C4C	2.05	104.41	101.34
7	AH	202	CYC	C4D-CHA-C1A	2.04	132.67	128.22
7	BD	201	CYC	C4D-CHA-C1A	2.04	132.67	128.22
7	AJ	202	CYC	C4D-CHA-C1A	2.04	132.67	128.22
7	BJ	202	CYC	C2C-C3C-C4C	2.03	104.38	101.34
7	AH	202	CYC	C1D-CHD-C4C	2.00	131.19	127.76
7	BB	202	CYC	C4D-CHA-C1A	2.00	132.59	128.22

There are no chirality outliers.

All (505) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	AA	201	CYC	NA-C4A-CHB-C1B
7	AA	201	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
7	AA	201	CYC	C4C-C3C-CAC-CBC
7	AA	201	CYC	NC-C4C-CHD-C1D
7	AB	201	CYC	NA-C4A-CHB-C1B
7	AB	201	CYC	C3A-C4A-CHB-C1B
7	AB	202	CYC	NA-C4A-CHB-C1B
7	AB	202	CYC	C3A-C4A-CHB-C1B
7	AB	202	CYC	NC-C4C-CHD-C1D
7	AC	201	CYC	NA-C4A-CHB-C1B
7	AC	201	CYC	C3A-C4A-CHB-C1B
7	AC	201	CYC	C2C-C3C-CAC-CBC
7	AC	201	CYC	C4C-C3C-CAC-CBC
7	AC	201	CYC	NC-C4C-CHD-C1D
7	AD	201	CYC	NA-C4A-CHB-C1B
7	AD	201	CYC	C3A-C4A-CHB-C1B
7	AD	202	CYC	NA-C4A-CHB-C1B
7	AD	202	CYC	C3A-C4A-CHB-C1B
7	AE	201	CYC	NA-C4A-CHB-C1B
7	AE	201	CYC	C3A-C4A-CHB-C1B
7	AE	201	CYC	C2C-C3C-CAC-CBC
7	AE	201	CYC	C4C-C3C-CAC-CBC
7	AE	201	CYC	NC-C4C-CHD-C1D
7	AF	201	CYC	NA-C4A-CHB-C1B
7	AF	201	CYC	C3A-C4A-CHB-C1B
7	AF	202	CYC	NA-C4A-CHB-C1B
7	AF	202	CYC	C3A-C4A-CHB-C1B
7	AG	201	CYC	NA-C4A-CHB-C1B
7	AG	201	CYC	C3A-C4A-CHB-C1B
7	AG	201	CYC	C4C-C3C-CAC-CBC
7	AG	201	CYC	NC-C4C-CHD-C1D
7	AG	201	CYC	C3C-C4C-CHD-C1D
7	AH	201	CYC	NA-C4A-CHB-C1B
7	AH	201	CYC	C3A-C4A-CHB-C1B
7	AH	202	CYC	NA-C4A-CHB-C1B
7	AH	202	CYC	C3A-C4A-CHB-C1B
7	AI	201	CYC	NA-C4A-CHB-C1B
7	AI	201	CYC	C3A-C4A-CHB-C1B
7	AI	201	CYC	C4C-C3C-CAC-CBC
7	AI	201	CYC	NC-C4C-CHD-C1D
7	AI	201	CYC	C3C-C4C-CHD-C1D
7	AJ	201	CYC	NA-C4A-CHB-C1B
7	AJ	201	CYC	C3A-C4A-CHB-C1B
7	AJ	202	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
7	AJ	202	CYC	C3A-C4A-CHB-C1B
7	AK	201	CYC	NA-C4A-CHB-C1B
7	AK	201	CYC	C3A-C4A-CHB-C1B
7	AK	201	CYC	C4C-C3C-CAC-CBC
7	AK	201	CYC	NC-C4C-CHD-C1D
7	AK	201	CYC	C3C-C4C-CHD-C1D
7	AL	201	CYC	NA-C4A-CHB-C1B
7	AL	201	CYC	C3A-C4A-CHB-C1B
7	AL	202	CYC	NA-C4A-CHB-C1B
7	AL	202	CYC	C3A-C4A-CHB-C1B
7	AM	201	CYC	NA-C4A-CHB-C1B
7	AM	201	CYC	C3A-C4A-CHB-C1B
7	AM	201	CYC	C2C-C3C-CAC-CBC
7	AM	201	CYC	C4C-C3C-CAC-CBC
7	AM	201	CYC	NC-C4C-CHD-C1D
7	AN	201	CYC	NA-C4A-CHB-C1B
7	AN	201	CYC	C3A-C4A-CHB-C1B
7	AN	202	CYC	NA-C4A-CHB-C1B
7	AN	202	CYC	C3A-C4A-CHB-C1B
7	AO	201	CYC	NA-C4A-CHB-C1B
7	AO	201	CYC	C3A-C4A-CHB-C1B
7	AO	201	CYC	C4C-C3C-CAC-CBC
7	AO	201	CYC	NC-C4C-CHD-C1D
7	AO	201	CYC	C3C-C4C-CHD-C1D
7	AP	201	CYC	NA-C4A-CHB-C1B
7	AP	201	CYC	C3A-C4A-CHB-C1B
7	AP	202	CYC	NA-C4A-CHB-C1B
7	AP	202	CYC	C3A-C4A-CHB-C1B
7	AQ	201	CYC	NA-C4A-CHB-C1B
7	AQ	201	CYC	C3A-C4A-CHB-C1B
7	AQ	201	CYC	C4C-C3C-CAC-CBC
7	AQ	201	CYC	NC-C4C-CHD-C1D
7	AQ	201	CYC	C3C-C4C-CHD-C1D
7	AR	201	CYC	NA-C4A-CHB-C1B
7	AR	201	CYC	C3A-C4A-CHB-C1B
7	AR	202	CYC	NA-C4A-CHB-C1B
7	AR	202	CYC	C3A-C4A-CHB-C1B
7	AS	201	CYC	NA-C4A-CHB-C1B
7	AS	201	CYC	C3A-C4A-CHB-C1B
7	AS	201	CYC	C4C-C3C-CAC-CBC
7	AS	201	CYC	NC-C4C-CHD-C1D
7	AS	201	CYC	C3C-C4C-CHD-C1D

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Mol	Chain	Res	Type	Atoms
7	AT	201	CYC	NA-C4A-CHB-C1B
7	AT	201	CYC	C3A-C4A-CHB-C1B
7	AU	201	CYC	NA-C4A-CHB-C1B
7	AU	201	CYC	C3A-C4A-CHB-C1B
7	AU	201	CYC	C4C-C3C-CAC-CBC
7	AU	201	CYC	NC-C4C-CHD-C1D
7	AV	201	CYC	NA-C4A-CHB-C1B
7	AV	201	CYC	C3A-C4A-CHB-C1B
7	AV	202	CYC	NA-C4A-CHB-C1B
7	AV	202	CYC	C3A-C4A-CHB-C1B
7	AW	201	CYC	NA-C4A-CHB-C1B
7	AW	201	CYC	C3A-C4A-CHB-C1B
7	AW	201	CYC	C2C-C3C-CAC-CBC
7	AW	201	CYC	C4C-C3C-CAC-CBC
7	AX	202	CYC	NA-C4A-CHB-C1B
7	AX	202	CYC	C3A-C4A-CHB-C1B
7	AY	201	CYC	NA-C4A-CHB-C1B
7	AY	201	CYC	C3A-C4A-CHB-C1B
7	AY	201	CYC	C4C-C3C-CAC-CBC
7	AY	201	CYC	NC-C4C-CHD-C1D
7	AY	201	CYC	C3C-C4C-CHD-C1D
7	AZ	201	CYC	NA-C4A-CHB-C1B
7	AZ	201	CYC	C3A-C4A-CHB-C1B
7	AZ	202	CYC	NA-C4A-CHB-C1B
7	AZ	202	CYC	C3A-C4A-CHB-C1B
7	BA	201	CYC	NA-C4A-CHB-C1B
7	BA	201	CYC	C3A-C4A-CHB-C1B
7	BA	201	CYC	C4C-C3C-CAC-CBC
7	BA	201	CYC	NC-C4C-CHD-C1D
7	BA	201	CYC	C3C-C4C-CHD-C1D
7	BB	202	CYC	NA-C4A-CHB-C1B
7	BB	202	CYC	C3A-C4A-CHB-C1B
7	BC	201	CYC	NA-C4A-CHB-C1B
7	BC	201	CYC	C3A-C4A-CHB-C1B
7	BC	201	CYC	C4C-C3C-CAC-CBC
7	BC	201	CYC	NC-C4C-CHD-C1D
7	BC	201	CYC	C3C-C4C-CHD-C1D
7	BD	201	CYC	NA-C4A-CHB-C1B
7	BD	201	CYC	C3A-C4A-CHB-C1B
7	BD	202	CYC	NA-C4A-CHB-C1B
7	BD	202	CYC	C3A-C4A-CHB-C1B
7	BE	201	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
7	BE	201	CYC	C3A-C4A-CHB-C1B
7	BE	201	CYC	C4C-C3C-CAC-CBC
7	BE	201	CYC	NC-C4C-CHD-C1D
7	BE	201	CYC	C3C-C4C-CHD-C1D
7	BF	201	CYC	C3A-C4A-CHB-C1B
7	BF	202	CYC	NA-C4A-CHB-C1B
7	BF	202	CYC	C3A-C4A-CHB-C1B
7	BF	202	CYC	C2C-C3C-CAC-CBC
7	BF	202	CYC	C4C-C3C-CAC-CBC
7	BG	201	CYC	NA-C4A-CHB-C1B
7	BG	201	CYC	C3A-C4A-CHB-C1B
7	BG	201	CYC	C4C-C3C-CAC-CBC
7	BG	201	CYC	NC-C4C-CHD-C1D
7	BG	201	CYC	C3C-C4C-CHD-C1D
7	BH	202	CYC	NA-C4A-CHB-C1B
7	BH	202	CYC	C3A-C4A-CHB-C1B
7	BI	201	CYC	NA-C4A-CHB-C1B
7	BI	201	CYC	C3A-C4A-CHB-C1B
7	BI	201	CYC	C4C-C3C-CAC-CBC
7	BI	201	CYC	NC-C4C-CHD-C1D
7	BI	201	CYC	C3C-C4C-CHD-C1D
7	BJ	201	CYC	NA-C4A-CHB-C1B
7	BJ	201	CYC	C3A-C4A-CHB-C1B
7	BJ	202	CYC	NA-C4A-CHB-C1B
7	BJ	202	CYC	C3A-C4A-CHB-C1B
7	AX	201	CYC	C2B-C3B-CAB-CBB
7	BF	201	CYC	C2B-C3B-CAB-CBB
7	AT	201	CYC	C2B-C3B-CAB-CBB
7	BG	201	CYC	C2B-C3B-CAB-CBB
7	AC	201	CYC	C2B-C3B-CAB-CBB
7	AE	201	CYC	C2B-C3B-CAB-CBB
7	BC	201	CYC	C2B-C3B-CAB-CBB
7	AQ	201	CYC	C2B-C3B-CAB-CBB
7	BE	201	CYC	C2B-C3B-CAB-CBB
7	AY	201	CYC	C2B-C3B-CAB-CBB
7	AM	201	CYC	C2B-C3B-CAB-CBB
7	AA	201	CYC	C2B-C3B-CAB-CBB
7	AG	201	CYC	C2B-C3B-CAB-CBB
7	AO	201	CYC	C2B-C3B-CAB-CBB
7	AR	201	CYC	C2B-C3B-CAB-CBB
7	AS	201	CYC	C2B-C3B-CAB-CBB
7	AW	201	CYC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
7	BA	201	CYC	C2B-C3B-CAB-CBB
7	BI	201	CYC	C2B-C3B-CAB-CBB
7	AI	201	CYC	C2B-C3B-CAB-CBB
7	AA	201	CYC	ND-C1D-CHD-C4C
7	AB	201	CYC	ND-C1D-CHD-C4C
7	AB	202	CYC	ND-C1D-CHD-C4C
7	AD	201	CYC	ND-C1D-CHD-C4C
7	AG	201	CYC	ND-C1D-CHD-C4C
7	AH	201	CYC	ND-C1D-CHD-C4C
7	AJ	201	CYC	ND-C1D-CHD-C4C
7	AK	201	CYC	ND-C1D-CHD-C4C
7	AN	201	CYC	ND-C1D-CHD-C4C
7	AO	201	CYC	ND-C1D-CHD-C4C
7	AP	201	CYC	ND-C1D-CHD-C4C
7	AT	201	CYC	ND-C1D-CHD-C4C
7	AX	201	CYC	ND-C1D-CHD-C4C
7	AX	202	CYC	ND-C1D-CHD-C4C
7	AY	201	CYC	ND-C1D-CHD-C4C
7	AZ	201	CYC	ND-C1D-CHD-C4C
7	BA	201	CYC	ND-C1D-CHD-C4C
7	BB	201	CYC	ND-C1D-CHD-C4C
7	BD	201	CYC	ND-C1D-CHD-C4C
7	BF	201	CYC	ND-C1D-CHD-C4C
7	BH	201	CYC	ND-C1D-CHD-C4C
7	BH	202	CYC	ND-C1D-CHD-C4C
7	BI	201	CYC	ND-C1D-CHD-C4C
7	BJ	201	CYC	ND-C1D-CHD-C4C
7	BJ	202	CYC	ND-C1D-CHD-C4C
7	AA	201	CYC	C2D-C1D-CHD-C4C
7	AB	202	CYC	C2D-C1D-CHD-C4C
7	AD	201	CYC	C2D-C1D-CHD-C4C
7	AD	202	CYC	C2D-C1D-CHD-C4C
7	AE	201	CYC	C2D-C1D-CHD-C4C
7	AF	201	CYC	C2D-C1D-CHD-C4C
7	AF	202	CYC	C2D-C1D-CHD-C4C
7	AG	201	CYC	C2D-C1D-CHD-C4C
7	AH	201	CYC	C2D-C1D-CHD-C4C
7	AH	202	CYC	C2D-C1D-CHD-C4C
7	AI	201	CYC	C2D-C1D-CHD-C4C
7	AJ	201	CYC	C2D-C1D-CHD-C4C
7	AJ	202	CYC	C2D-C1D-CHD-C4C
7	AK	201	CYC	C2D-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
7	AL	201	CYC	C2D-C1D-CHD-C4C
7	AL	202	CYC	C2D-C1D-CHD-C4C
7	AM	201	CYC	C2D-C1D-CHD-C4C
7	AN	201	CYC	C2D-C1D-CHD-C4C
7	AN	202	CYC	C2D-C1D-CHD-C4C
7	AO	201	CYC	C2D-C1D-CHD-C4C
7	AP	201	CYC	C2D-C1D-CHD-C4C
7	AQ	201	CYC	C2D-C1D-CHD-C4C
7	AR	201	CYC	C2D-C1D-CHD-C4C
7	AR	202	CYC	C2D-C1D-CHD-C4C
7	AT	202	CYC	C2D-C1D-CHD-C4C
7	AU	201	CYC	C2D-C1D-CHD-C4C
7	AV	202	CYC	C2D-C1D-CHD-C4C
7	AX	201	CYC	C2D-C1D-CHD-C4C
7	AX	202	CYC	C2D-C1D-CHD-C4C
7	AY	201	CYC	C2D-C1D-CHD-C4C
7	AZ	202	CYC	C2D-C1D-CHD-C4C
7	BA	201	CYC	C2D-C1D-CHD-C4C
7	BC	201	CYC	C2D-C1D-CHD-C4C
7	BD	201	CYC	C2D-C1D-CHD-C4C
7	BD	202	CYC	C2D-C1D-CHD-C4C
7	BE	201	CYC	C2D-C1D-CHD-C4C
7	BF	201	CYC	C2D-C1D-CHD-C4C
7	BF	202	CYC	C2D-C1D-CHD-C4C
7	BG	201	CYC	C2D-C1D-CHD-C4C
7	BH	202	CYC	C2D-C1D-CHD-C4C
7	BI	201	CYC	C2D-C1D-CHD-C4C
7	BJ	201	CYC	C2D-C1D-CHD-C4C
7	BJ	202	CYC	C2D-C1D-CHD-C4C
7	AU	201	CYC	C2B-C3B-CAB-CBB
7	BB	201	CYC	C2B-C3B-CAB-CBB
7	AC	201	CYC	ND-C1D-CHD-C4C
7	AD	202	CYC	ND-C1D-CHD-C4C
7	AE	201	CYC	ND-C1D-CHD-C4C
7	AF	201	CYC	ND-C1D-CHD-C4C
7	AF	202	CYC	ND-C1D-CHD-C4C
7	AH	202	CYC	ND-C1D-CHD-C4C
7	AI	201	CYC	ND-C1D-CHD-C4C
7	AJ	202	CYC	ND-C1D-CHD-C4C
7	AL	201	CYC	ND-C1D-CHD-C4C
7	AL	202	CYC	ND-C1D-CHD-C4C
7	AM	201	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
7	AN	202	CYC	ND-C1D-CHD-C4C
7	AP	202	CYC	ND-C1D-CHD-C4C
7	AQ	201	CYC	ND-C1D-CHD-C4C
7	AR	201	CYC	ND-C1D-CHD-C4C
7	AR	202	CYC	ND-C1D-CHD-C4C
7	AS	201	CYC	ND-C1D-CHD-C4C
7	AT	202	CYC	ND-C1D-CHD-C4C
7	AU	201	CYC	ND-C1D-CHD-C4C
7	AV	201	CYC	ND-C1D-CHD-C4C
7	AV	202	CYC	ND-C1D-CHD-C4C
7	AW	201	CYC	ND-C1D-CHD-C4C
7	AZ	202	CYC	ND-C1D-CHD-C4C
7	BB	202	CYC	ND-C1D-CHD-C4C
7	BC	201	CYC	ND-C1D-CHD-C4C
7	BD	202	CYC	ND-C1D-CHD-C4C
7	BE	201	CYC	ND-C1D-CHD-C4C
7	BF	202	CYC	ND-C1D-CHD-C4C
7	BG	201	CYC	ND-C1D-CHD-C4C
7	AB	201	CYC	C2D-C1D-CHD-C4C
7	AC	201	CYC	C2D-C1D-CHD-C4C
7	AP	202	CYC	C2D-C1D-CHD-C4C
7	AS	201	CYC	C2D-C1D-CHD-C4C
7	AT	201	CYC	C2D-C1D-CHD-C4C
7	AV	201	CYC	C2D-C1D-CHD-C4C
7	AW	201	CYC	C2D-C1D-CHD-C4C
7	AZ	201	CYC	C2D-C1D-CHD-C4C
7	BB	201	CYC	C2D-C1D-CHD-C4C
7	BB	202	CYC	C2D-C1D-CHD-C4C
7	BH	201	CYC	C2D-C1D-CHD-C4C
7	AK	201	CYC	C2B-C3B-CAB-CBB
7	AT	202	CYC	NA-C4A-CHB-C1B
7	AX	201	CYC	NA-C4A-CHB-C1B
7	BB	201	CYC	NA-C4A-CHB-C1B
7	BF	201	CYC	NA-C4A-CHB-C1B
7	BH	201	CYC	NA-C4A-CHB-C1B
7	AT	202	CYC	C3A-C4A-CHB-C1B
7	AX	201	CYC	C3A-C4A-CHB-C1B
7	BB	201	CYC	C3A-C4A-CHB-C1B
7	BH	201	CYC	C3A-C4A-CHB-C1B
7	AL	201	CYC	C2B-C3B-CAB-CBB
7	AV	201	CYC	C2A-CAA-CBA-CGA
7	AJ	201	CYC	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
7	AL	202	CYC	C2B-C3B-CAB-CBB
7	BB	201	CYC	C2B-C1B-CHB-C4A
7	AA	201	CYC	C2C-C3C-CAC-CBC
7	AG	201	CYC	C2C-C3C-CAC-CBC
7	AI	201	CYC	C2C-C3C-CAC-CBC
7	AK	201	CYC	C2C-C3C-CAC-CBC
7	AQ	201	CYC	C2C-C3C-CAC-CBC
7	AS	201	CYC	C2C-C3C-CAC-CBC
7	AU	201	CYC	C2C-C3C-CAC-CBC
7	BC	201	CYC	C2C-C3C-CAC-CBC
7	BB	201	CYC	NB-C1B-CHB-C4A
7	AJ	201	CYC	C3A-C2A-CAA-CBA
7	BA	201	CYC	C2A-CAA-CBA-CGA
7	AF	202	CYC	C4C-C3C-CAC-CBC
7	AH	202	CYC	C4C-C3C-CAC-CBC
7	AJ	202	CYC	C4C-C3C-CAC-CBC
7	AN	202	CYC	C4C-C3C-CAC-CBC
7	AP	202	CYC	C4C-C3C-CAC-CBC
7	AR	202	CYC	C4C-C3C-CAC-CBC
7	AX	202	CYC	C4C-C3C-CAC-CBC
7	AZ	202	CYC	C4C-C3C-CAC-CBC
7	BB	202	CYC	C4C-C3C-CAC-CBC
7	AV	201	CYC	C2B-C3B-CAB-CBB
7	AN	202	CYC	C2C-C3C-CAC-CBC
7	AO	201	CYC	C2C-C3C-CAC-CBC
7	AY	201	CYC	C2C-C3C-CAC-CBC
7	BA	201	CYC	C2C-C3C-CAC-CBC
7	BE	201	CYC	C2C-C3C-CAC-CBC
7	BG	201	CYC	C2C-C3C-CAC-CBC
7	BI	201	CYC	C2C-C3C-CAC-CBC
7	AU	201	CYC	C3C-C4C-CHD-C1D
7	AH	202	CYC	C2A-C1A-CHA-C4D
7	AZ	201	CYC	C2A-CAA-CBA-CGA
7	BJ	201	CYC	C4B-C3B-CAB-CBB
7	AF	202	CYC	CAA-CBA-CGA-O2A
7	AZ	201	CYC	CAA-CBA-CGA-O2A
7	AP	202	CYC	CAD-CBD-CGD-O2D
7	AY	201	CYC	CAA-CBA-CGA-O1A
7	AP	202	CYC	CAD-CBD-CGD-O1D
7	AT	202	CYC	CAA-CBA-CGA-O2A
7	AZ	201	CYC	CAA-CBA-CGA-O1A
7	BI	201	CYC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
7	BG	201	CYC	CAA-CBA-CGA-O1A
7	BB	201	CYC	C2A-CAA-CBA-CGA
7	BF	201	CYC	C3D-CAD-CBD-CGD
7	AD	202	CYC	CAA-CBA-CGA-O1A
7	AE	201	CYC	CAA-CBA-CGA-O1A
7	AF	202	CYC	CAD-CBD-CGD-O1D
7	AF	202	CYC	CAD-CBD-CGD-O2D
7	AG	201	CYC	CAA-CBA-CGA-O1A
7	AT	202	CYC	CAA-CBA-CGA-O1A
7	AV	202	CYC	CAA-CBA-CGA-O1A
7	BJ	202	CYC	CAA-CBA-CGA-O1A
7	AA	201	CYC	CAA-CBA-CGA-O2A
7	AF	202	CYC	CAA-CBA-CGA-O1A
7	AM	201	CYC	CAA-CBA-CGA-O2A
7	AE	201	CYC	CAA-CBA-CGA-O2A
7	AG	201	CYC	CAA-CBA-CGA-O2A
7	AN	202	CYC	CAA-CBA-CGA-O2A
7	AV	202	CYC	CAA-CBA-CGA-O2A
7	BF	201	CYC	CAD-CBD-CGD-O1D
7	AI	201	CYC	CAA-CBA-CGA-O2A
7	AK	201	CYC	CAA-CBA-CGA-O2A
7	AP	201	CYC	CAA-CBA-CGA-O1A
7	AP	202	CYC	CAA-CBA-CGA-O1A
7	AQ	201	CYC	CAA-CBA-CGA-O1A
7	AR	201	CYC	CAA-CBA-CGA-O2A
7	AI	201	CYC	CAA-CBA-CGA-O1A
7	BH	202	CYC	CAA-CBA-CGA-O1A
7	BH	202	CYC	CAA-CBA-CGA-O2A
7	AC	201	CYC	CAA-CBA-CGA-O2A
7	AL	201	CYC	CAA-CBA-CGA-O1A
7	AL	201	CYC	CAA-CBA-CGA-O2A
7	AN	202	CYC	CAA-CBA-CGA-O1A
7	AP	201	CYC	CAA-CBA-CGA-O2A
7	AW	201	CYC	CAA-CBA-CGA-O1A
7	BA	201	CYC	CAA-CBA-CGA-O1A
7	BB	201	CYC	CAA-CBA-CGA-O1A
7	AC	201	CYC	CAA-CBA-CGA-O1A
7	AJ	202	CYC	CAA-CBA-CGA-O1A
7	AP	202	CYC	CAA-CBA-CGA-O2A
7	AU	201	CYC	CAA-CBA-CGA-O1A
7	AX	201	CYC	CAD-CBD-CGD-O1D
7	BG	201	CYC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
7	BJ	202	CYC	CAA-CBA-CGA-O2A
7	AO	201	CYC	CAA-CBA-CGA-O2A
7	AR	201	CYC	CAD-CBD-CGD-O1D
7	AR	201	CYC	CAD-CBD-CGD-O2D
7	AU	201	CYC	CAA-CBA-CGA-O2A
7	AX	201	CYC	CAA-CBA-CGA-O1A
7	AF	202	CYC	C2C-C3C-CAC-CBC
7	AZ	202	CYC	C2C-C3C-CAC-CBC
7	BB	202	CYC	C2C-C3C-CAC-CBC
7	AD	202	CYC	CAA-CBA-CGA-O2A
7	AF	201	CYC	CAA-CBA-CGA-O1A
7	AY	201	CYC	CAA-CBA-CGA-O2A
7	BA	201	CYC	CAA-CBA-CGA-O2A
7	BC	201	CYC	CAA-CBA-CGA-O2A
7	BF	201	CYC	CAD-CBD-CGD-O2D
7	AB	202	CYC	CAA-CBA-CGA-O2A
7	AJ	202	CYC	CAA-CBA-CGA-O2A
7	BD	202	CYC	CAA-CBA-CGA-O2A
7	BE	201	CYC	CAA-CBA-CGA-O2A
7	AH	202	CYC	CAA-CBA-CGA-O2A
7	AN	201	CYC	C3A-C2A-CAA-CBA
7	AO	201	CYC	CAA-CBA-CGA-O1A
7	AZ	202	CYC	CAA-CBA-CGA-O2A
7	BE	201	CYC	CAA-CBA-CGA-O1A
7	AH	202	CYC	NA-C1A-CHA-C4D
7	BC	201	CYC	CAA-CBA-CGA-O1A
7	AF	201	CYC	CAA-CBA-CGA-O2A
7	AQ	201	CYC	CAA-CBA-CGA-O2A
7	AR	201	CYC	CAA-CBA-CGA-O1A
7	BI	201	CYC	CAA-CBA-CGA-O1A
7	AW	201	CYC	CAD-CBD-CGD-O2D
7	AX	201	CYC	CAD-CBD-CGD-O2D
7	BB	201	CYC	CAA-CBA-CGA-O2A
7	AH	202	CYC	CAD-CBD-CGD-O2D
7	AM	201	CYC	CAA-CBA-CGA-O1A
7	BB	202	CYC	CAA-CBA-CGA-O2A
7	AT	202	CYC	C4C-C3C-CAC-CBC
7	BH	202	CYC	C4C-C3C-CAC-CBC
7	AA	201	CYC	CAA-CBA-CGA-O1A
7	AD	202	CYC	CAD-CBD-CGD-O2D
7	AK	201	CYC	CAA-CBA-CGA-O1A
7	AW	201	CYC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
7	AB	202	CYC	CAA-CBA-CGA-O1A
7	AB	201	CYC	CAA-CBA-CGA-O1A
7	AD	201	CYC	CAD-CBD-CGD-O1D
7	AR	202	CYC	CAD-CBD-CGD-O2D
7	AE	201	CYC	CAD-CBD-CGD-O2D
7	AX	201	CYC	CAA-CBA-CGA-O2A
7	BB	202	CYC	CAD-CBD-CGD-O2D
7	BD	201	CYC	CAA-CBA-CGA-O2A
7	AX	202	CYC	CAA-CBA-CGA-O2A
7	BB	202	CYC	CAA-CBA-CGA-O1A
7	AA	201	CYC	CAD-CBD-CGD-O2D
7	AH	202	CYC	CAA-CBA-CGA-O1A
7	AS	201	CYC	CAA-CBA-CGA-O1A
7	AS	201	CYC	CAA-CBA-CGA-O2A
7	AX	202	CYC	CAD-CBD-CGD-O2D
7	BJ	202	CYC	CAD-CBD-CGD-O2D
7	AV	202	CYC	CAD-CBD-CGD-O2D
7	AZ	202	CYC	CAA-CBA-CGA-O1A
7	BD	202	CYC	CAA-CBA-CGA-O1A
7	BB	202	CYC	CAD-CBD-CGD-O1D
7	BF	202	CYC	CAD-CBD-CGD-O2D
7	AV	201	CYC	CAA-CBA-CGA-O2A
7	BD	201	CYC	CAA-CBA-CGA-O1A
7	BF	202	CYC	CAA-CBA-CGA-O2A
7	AX	202	CYC	CAA-CBA-CGA-O1A
7	AN	202	CYC	CAD-CBD-CGD-O2D
7	BA	201	CYC	CAD-CBD-CGD-O1D
7	BD	202	CYC	CAD-CBD-CGD-O2D
7	BH	201	CYC	CAD-CBD-CGD-O2D
7	AD	202	CYC	CAD-CBD-CGD-O1D
7	AH	202	CYC	CAD-CBD-CGD-O1D
7	AX	202	CYC	CAD-CBD-CGD-O1D
7	BF	202	CYC	CAA-CBA-CGA-O1A
7	BJ	202	CYC	CAD-CBD-CGD-O1D
7	AL	202	CYC	CAD-CBD-CGD-O2D
7	BD	201	CYC	CAD-CBD-CGD-O2D
7	BF	202	CYC	CAD-CBD-CGD-O1D
7	AR	202	CYC	CAA-CBA-CGA-O2A
7	AR	202	CYC	CAD-CBD-CGD-O1D
7	AN	202	CYC	CAD-CBD-CGD-O1D
7	AR	202	CYC	CAA-CBA-CGA-O1A
7	AV	201	CYC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
7	AW	201	CYC	CAD-CBD-CGD-O1D
7	BA	201	CYC	CAD-CBD-CGD-O2D
7	AL	202	CYC	CAA-CBA-CGA-O2A
7	AV	201	CYC	CAD-CBD-CGD-O1D
7	AD	201	CYC	CAD-CBD-CGD-O2D
7	AL	202	CYC	CAA-CBA-CGA-O1A
7	AV	202	CYC	CAD-CBD-CGD-O1D
7	BD	202	CYC	CAD-CBD-CGD-O1D
7	AB	201	CYC	CAA-CBA-CGA-O2A
7	AL	202	CYC	CAD-CBD-CGD-O1D
7	AE	201	CYC	CAD-CBD-CGD-O1D
7	BH	201	CYC	CAD-CBD-CGD-O1D
7	AZ	202	CYC	C2A-CAA-CBA-CGA
7	BH	202	CYC	CAD-CBD-CGD-O2D
7	AC	201	CYC	CAD-CBD-CGD-O2D
7	BJ	201	CYC	CAD-CBD-CGD-O2D
7	AJ	202	CYC	CAD-CBD-CGD-O2D
7	AH	201	CYC	CAA-CBA-CGA-O1A
7	AA	201	CYC	CAD-CBD-CGD-O1D
7	AJ	202	CYC	CAD-CBD-CGD-O1D
7	AH	201	CYC	CAD-CBD-CGD-O2D
7	AU	201	CYC	CAD-CBD-CGD-O2D
7	BH	202	CYC	CAD-CBD-CGD-O1D
7	AV	201	CYC	CAA-CBA-CGA-O1A
7	AI	201	CYC	CAD-CBD-CGD-O2D
7	AZ	201	CYC	CAD-CBD-CGD-O2D
7	AS	201	CYC	CAD-CBD-CGD-O2D
7	AA	201	CYC	C3C-C4C-CHD-C1D
7	AB	202	CYC	C3C-C4C-CHD-C1D
7	AE	201	CYC	C3C-C4C-CHD-C1D
7	AC	201	CYC	CAD-CBD-CGD-O1D
7	AK	201	CYC	CAD-CBD-CGD-O2D
7	AQ	201	CYC	CAD-CBD-CGD-O2D
7	AT	201	CYC	CAD-CBD-CGD-O1D
7	AT	201	CYC	CAD-CBD-CGD-O2D
7	AH	201	CYC	CAA-CBA-CGA-O2A
7	BB	201	CYC	CAD-CBD-CGD-O2D
7	BC	201	CYC	CAD-CBD-CGD-O2D
7	AI	201	CYC	CAD-CBD-CGD-O1D
7	AS	201	CYC	CAD-CBD-CGD-O1D
7	AU	201	CYC	CAD-CBD-CGD-O1D

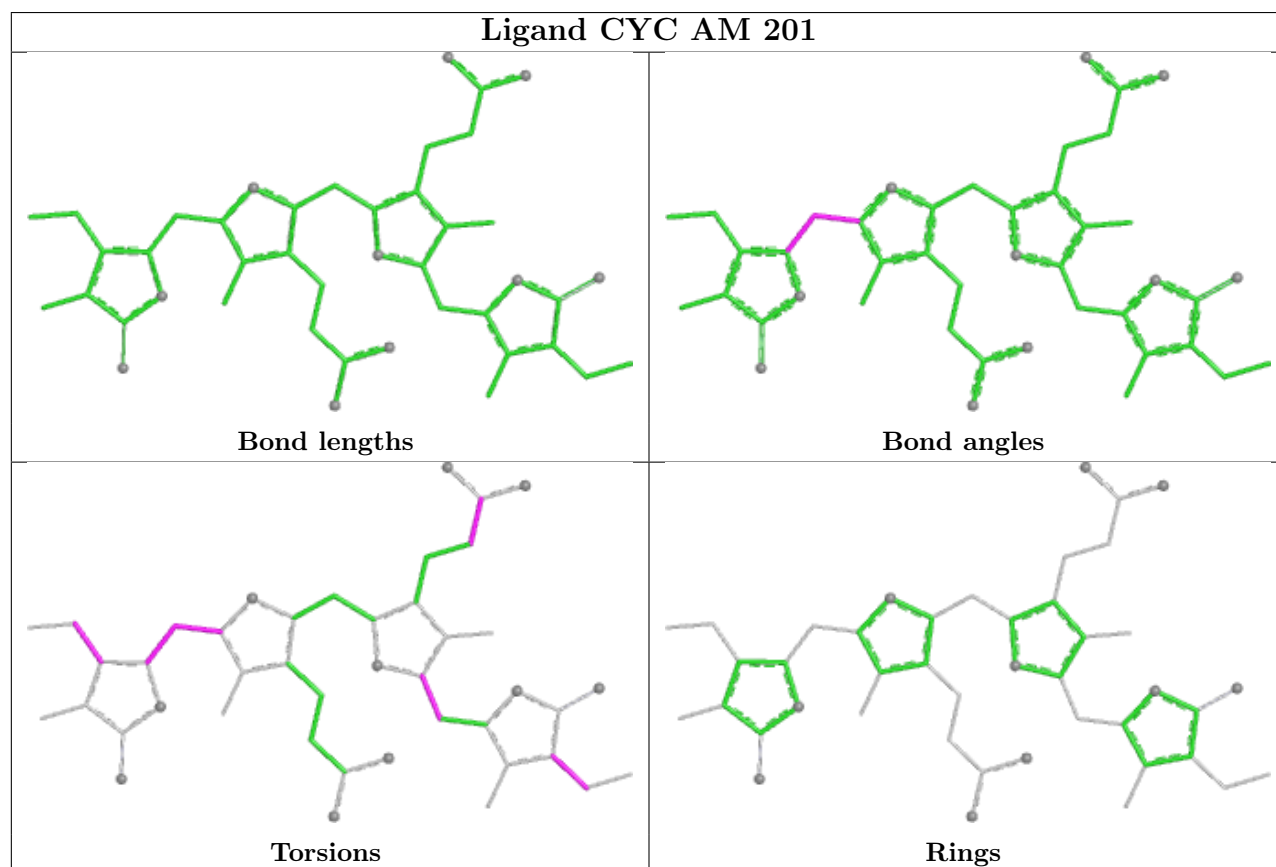
There are no ring outliers.

40 monomers are involved in 91 short contacts:

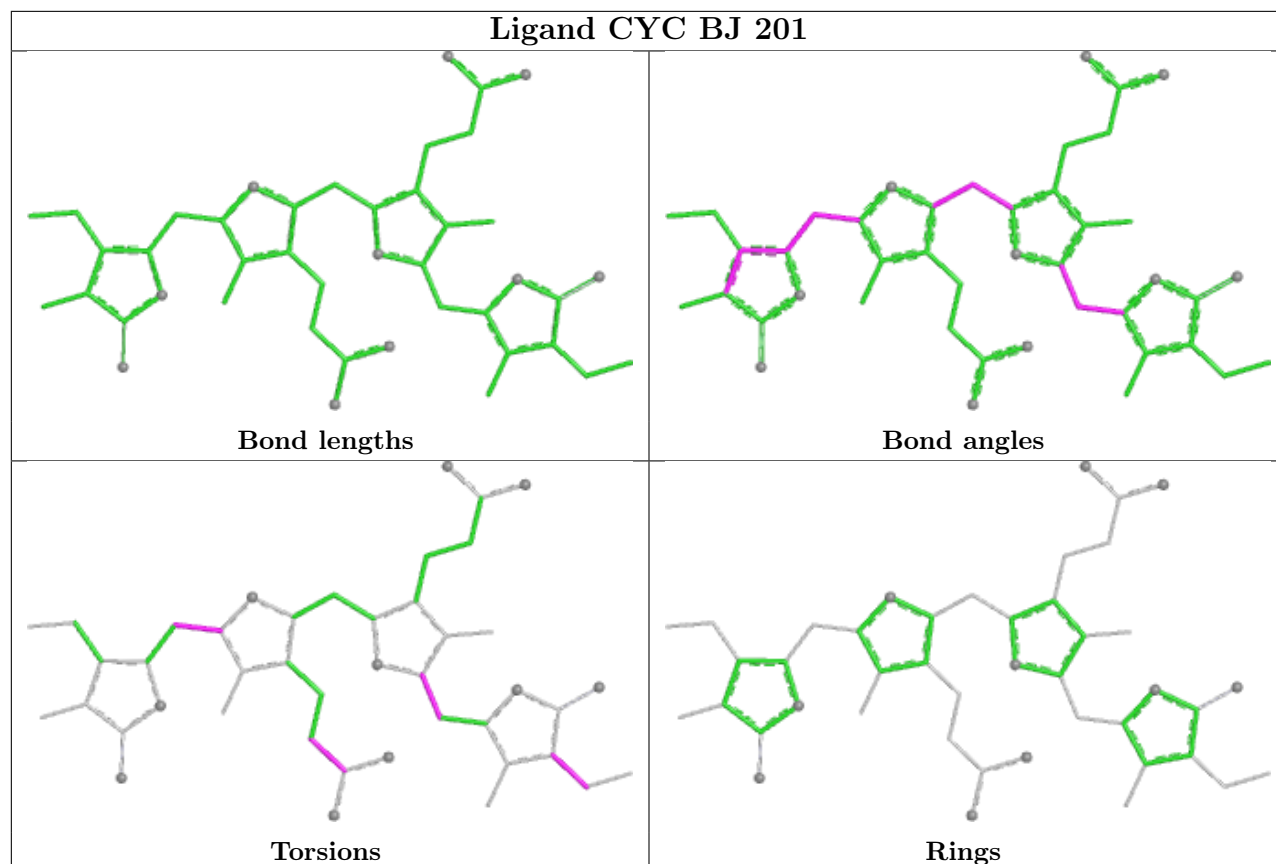
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	AM	201	CYC	4	0
7	BJ	201	CYC	3	0
7	AI	201	CYC	2	0
7	AK	201	CYC	4	0
7	AD	202	CYC	2	0
7	AJ	201	CYC	3	0
7	BH	202	CYC	1	0
7	AN	201	CYC	1	0
7	BB	202	CYC	1	0
7	BF	201	CYC	3	0
7	AB	201	CYC	2	0
7	BI	201	CYC	2	0
7	AU	201	CYC	6	0
7	AX	201	CYC	5	0
7	BG	201	CYC	3	0
7	AW	201	CYC	3	0
7	BA	201	CYC	3	0
7	BD	201	CYC	2	0
7	BB	201	CYC	2	0
7	AA	201	CYC	2	0
7	AS	201	CYC	2	0
7	AT	201	CYC	1	0
7	AR	202	CYC	1	0
7	AL	202	CYC	1	0
7	AQ	201	CYC	2	0
7	BE	201	CYC	2	0
7	AE	201	CYC	2	0
7	AH	202	CYC	1	0
7	AV	201	CYC	2	0
7	AZ	201	CYC	2	0
7	AG	201	CYC	3	0
7	AP	201	CYC	1	0
7	BH	201	CYC	4	0
7	AJ	202	CYC	1	0
7	BC	201	CYC	1	0
7	AF	201	CYC	1	0
7	BF	202	CYC	1	0
7	AD	201	CYC	3	0
7	AY	201	CYC	2	0
7	AO	201	CYC	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

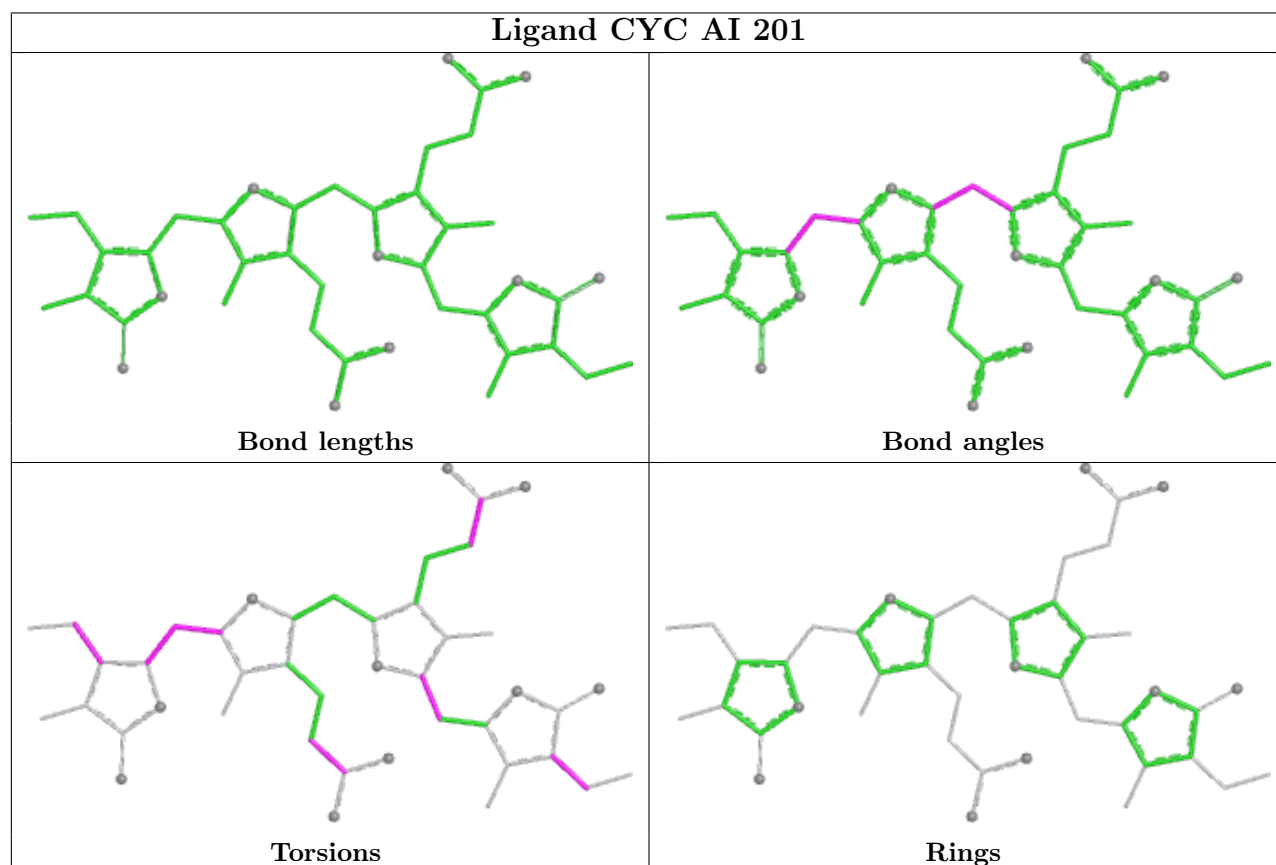
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



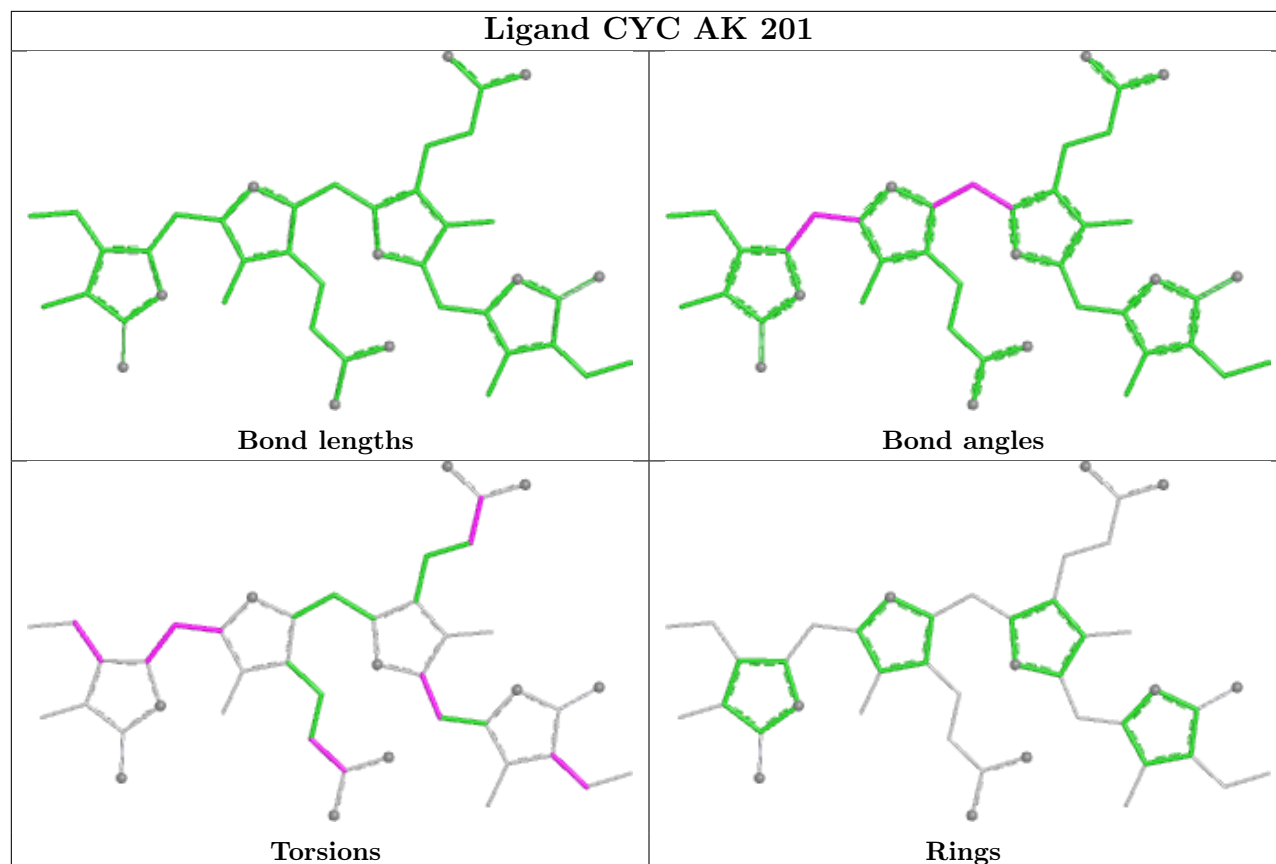
Ligand CYC BJ 201



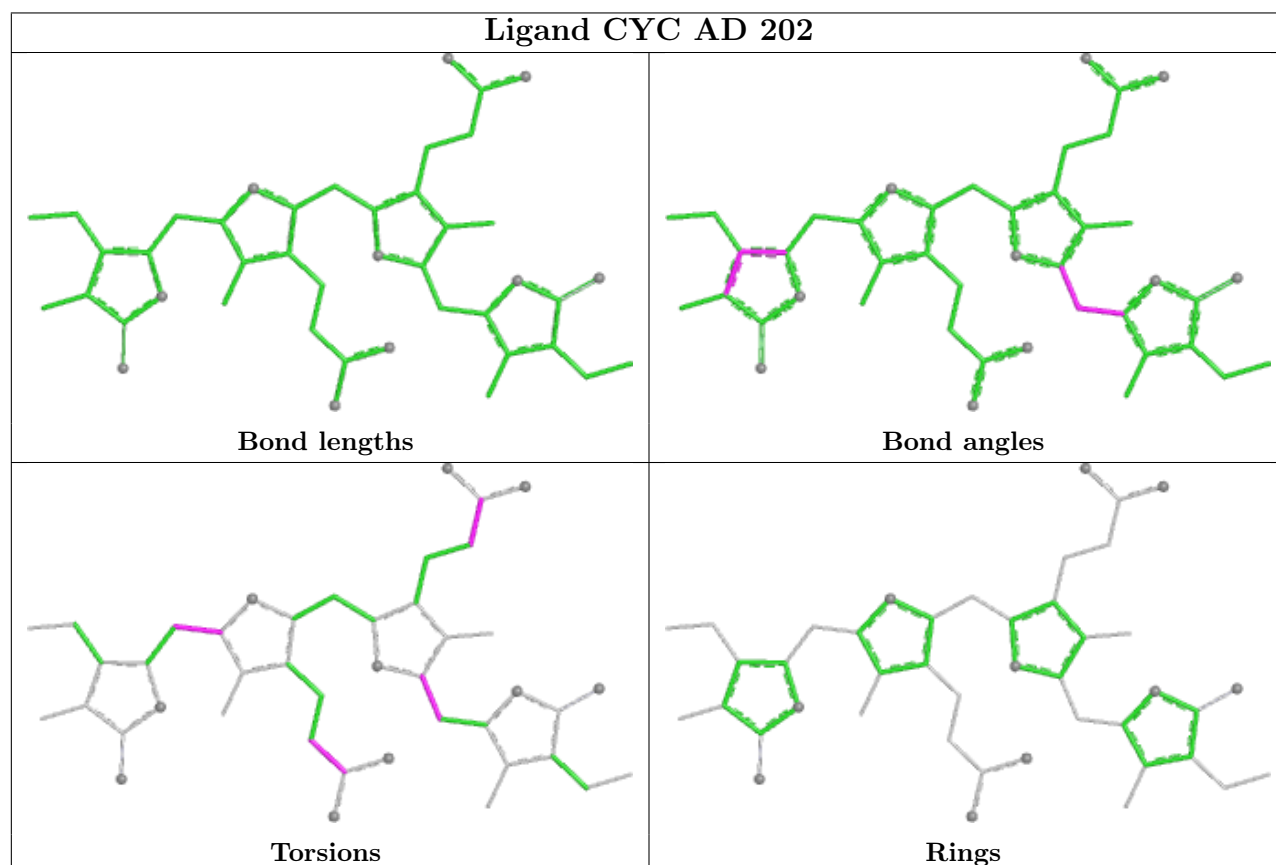
Ligand CYC AI 201



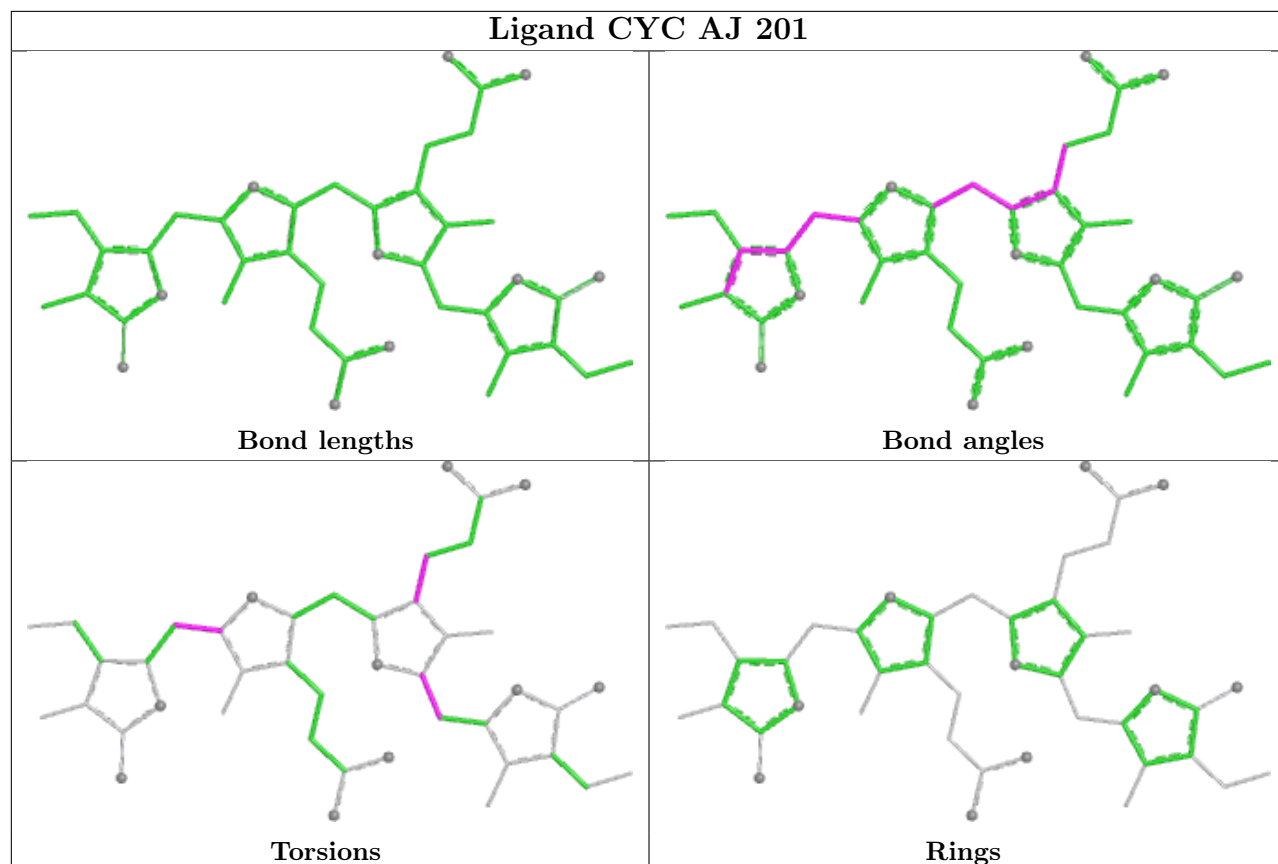
Ligand CYC AK 201



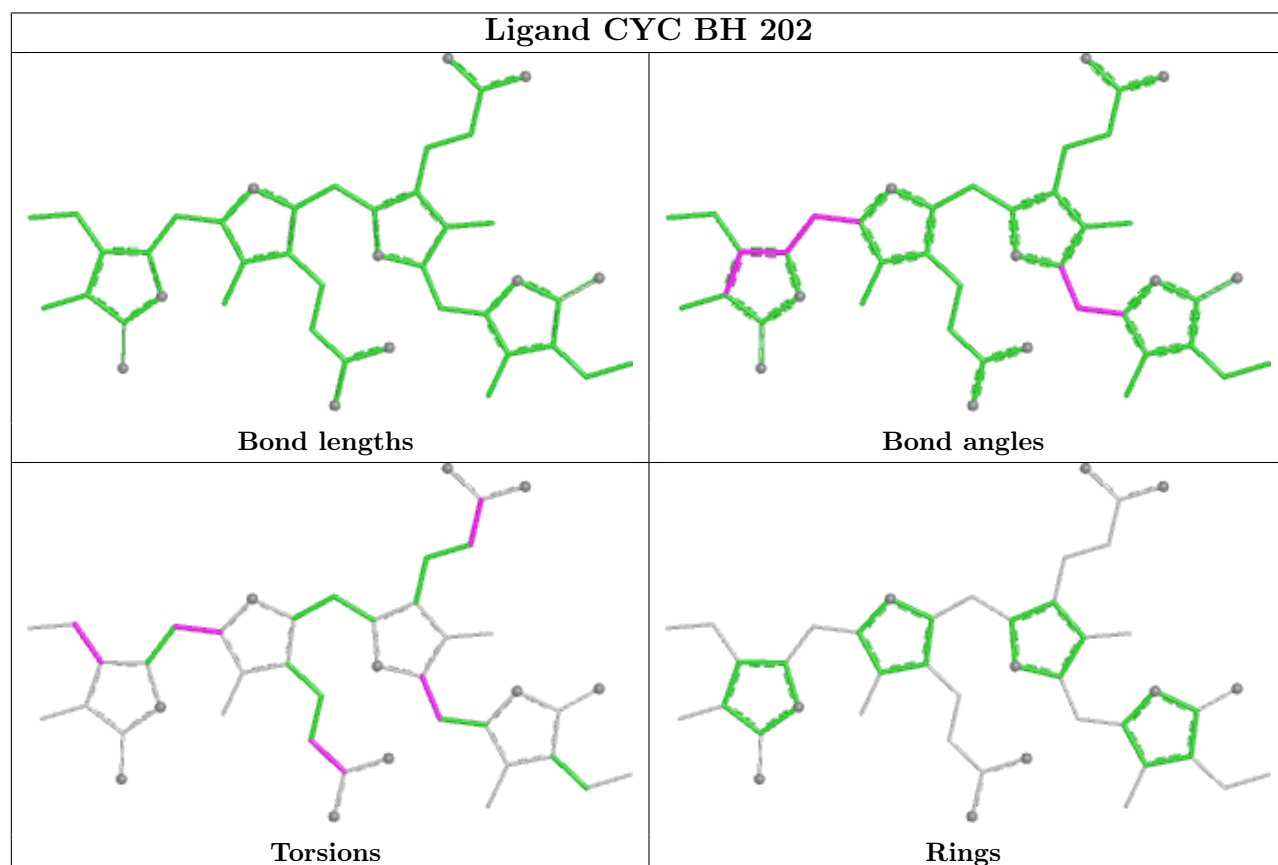
Ligand CYC AD 202



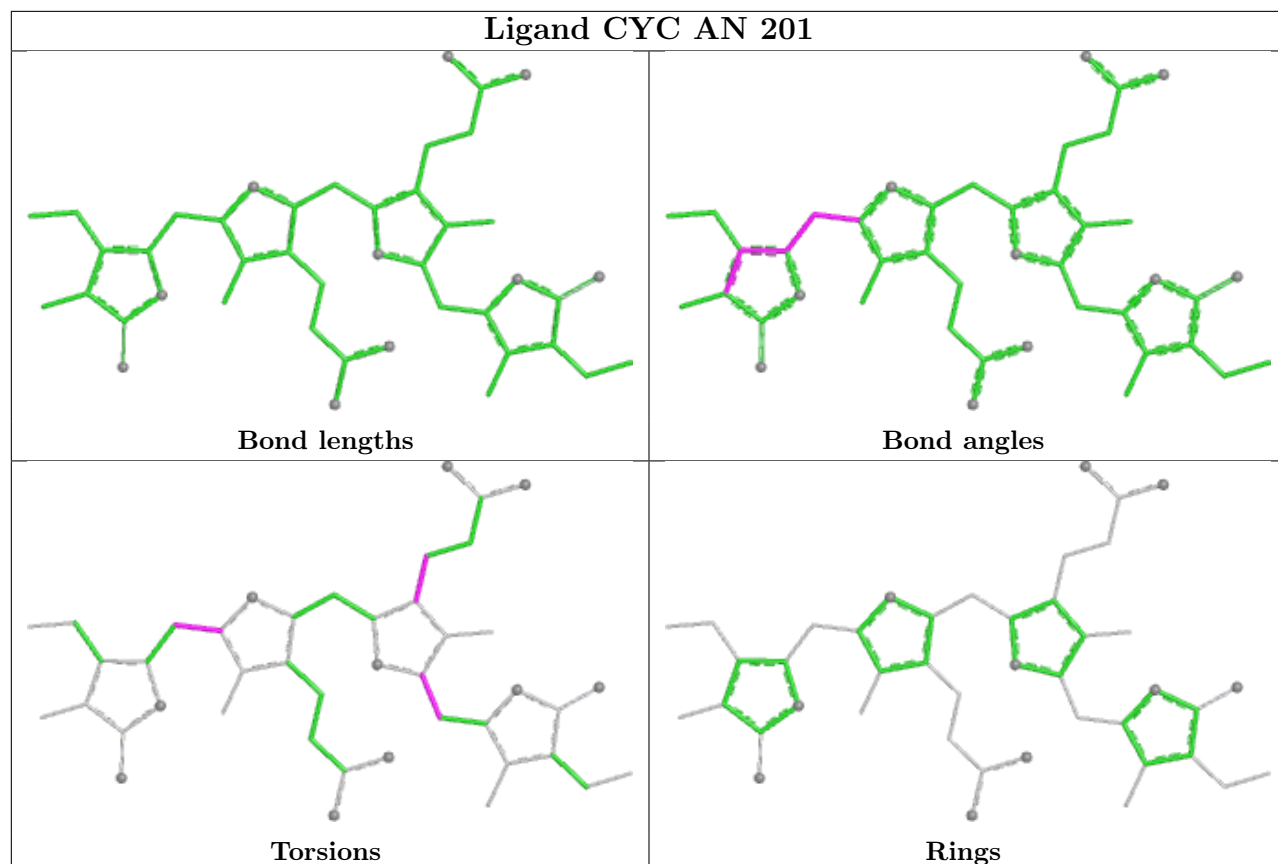
Ligand CYC AJ 201



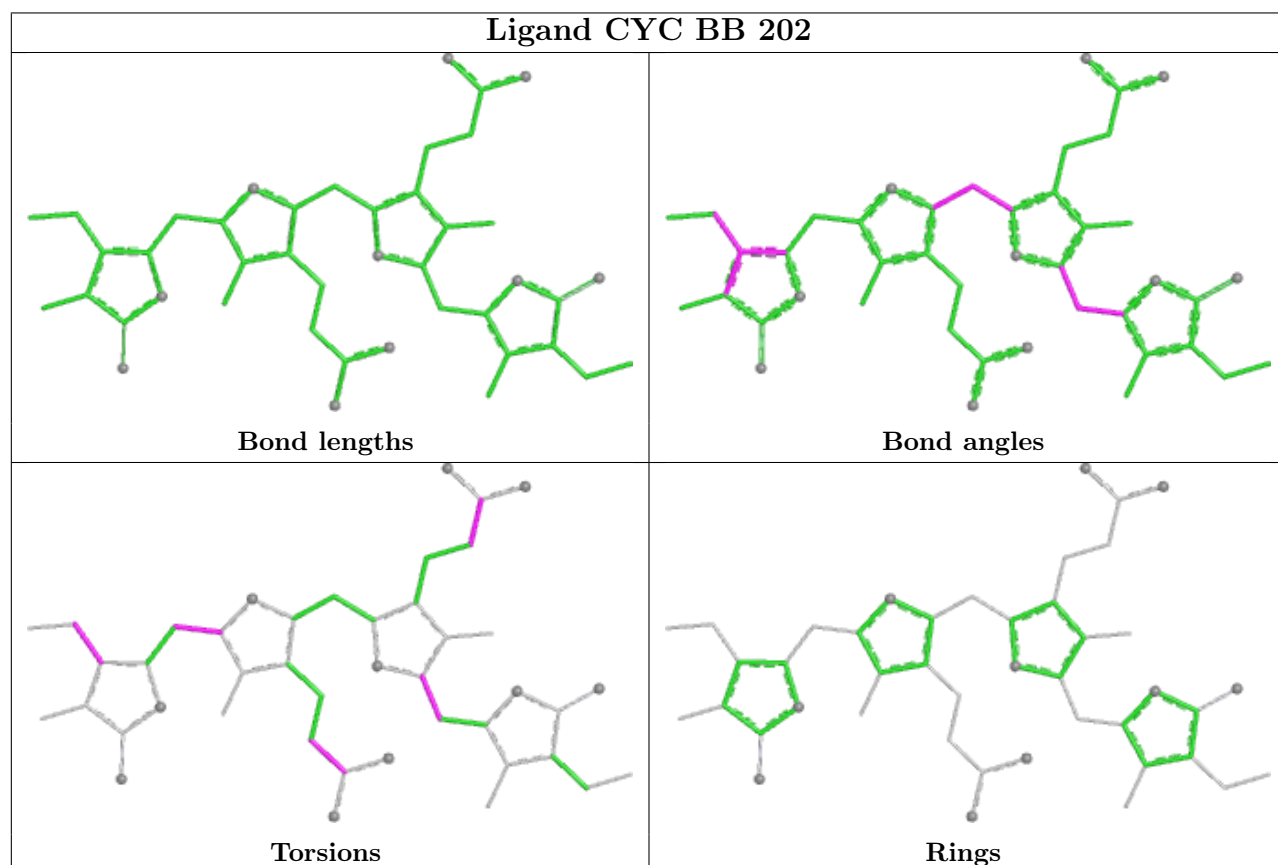
Ligand CYC BH 202



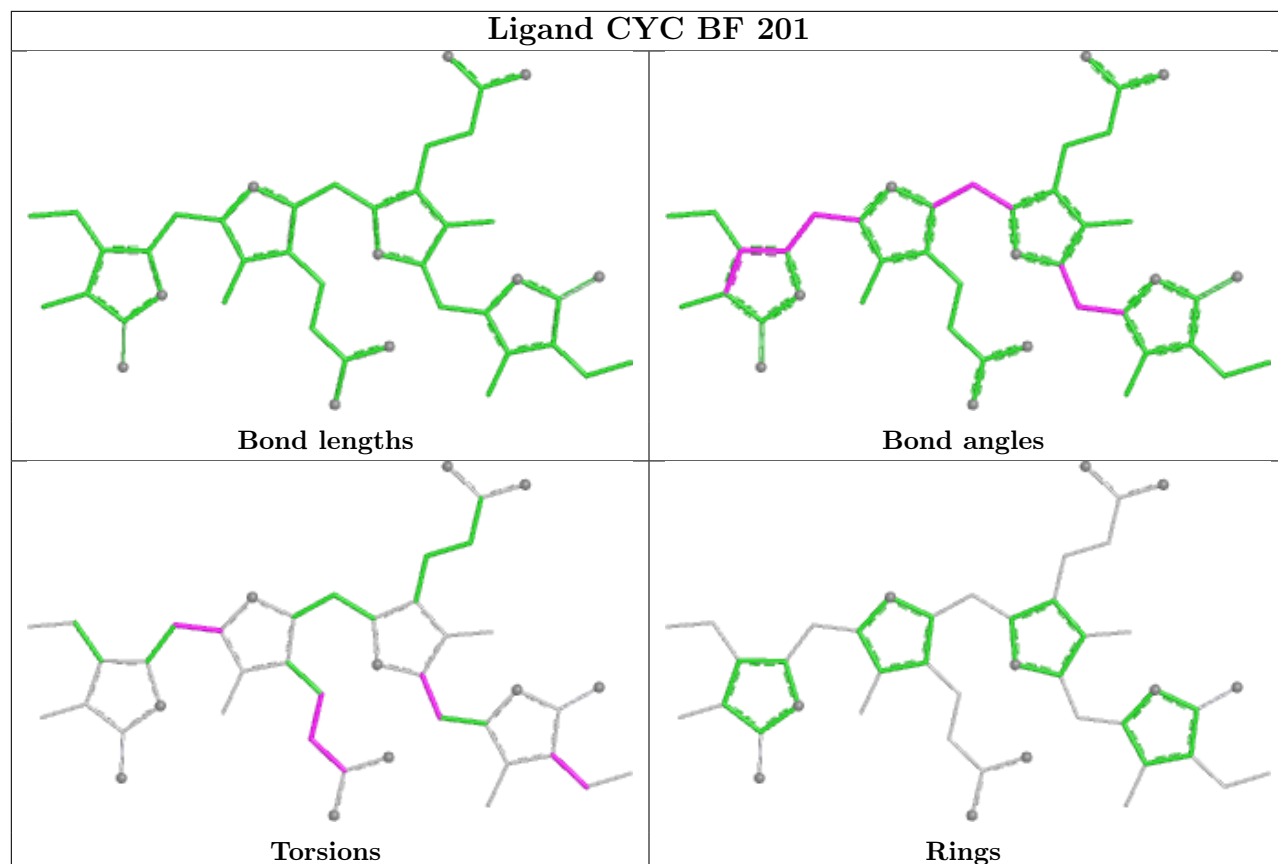
Ligand CYC AN 201



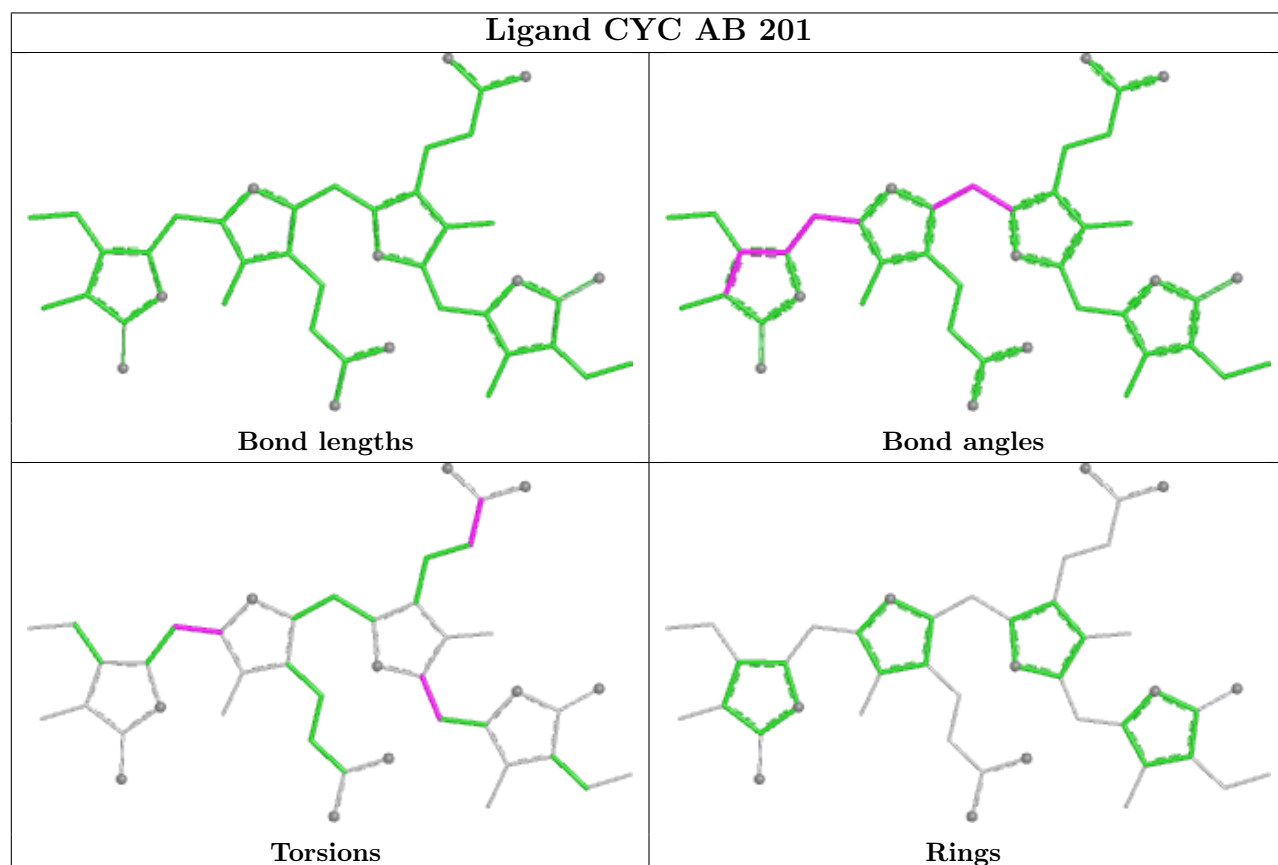
Ligand CYC BB 202

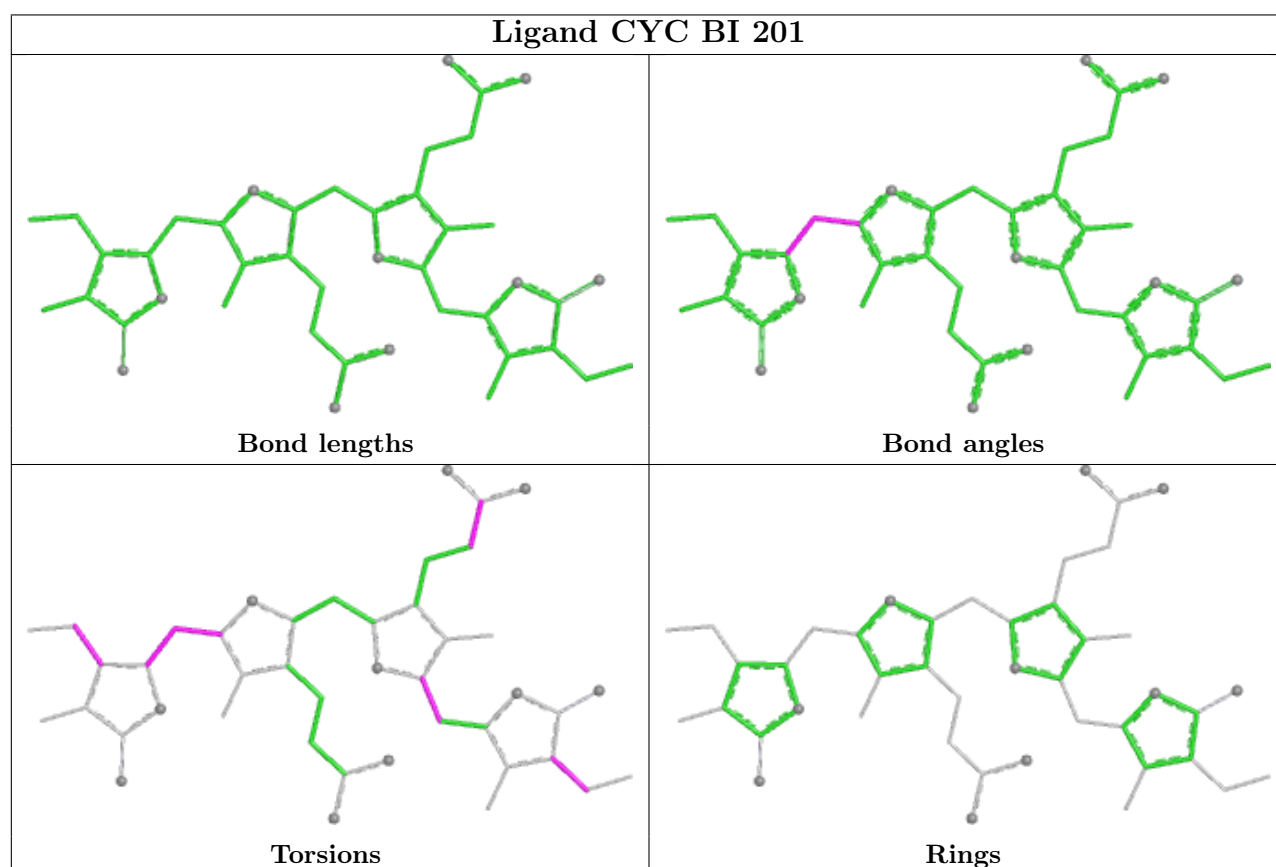
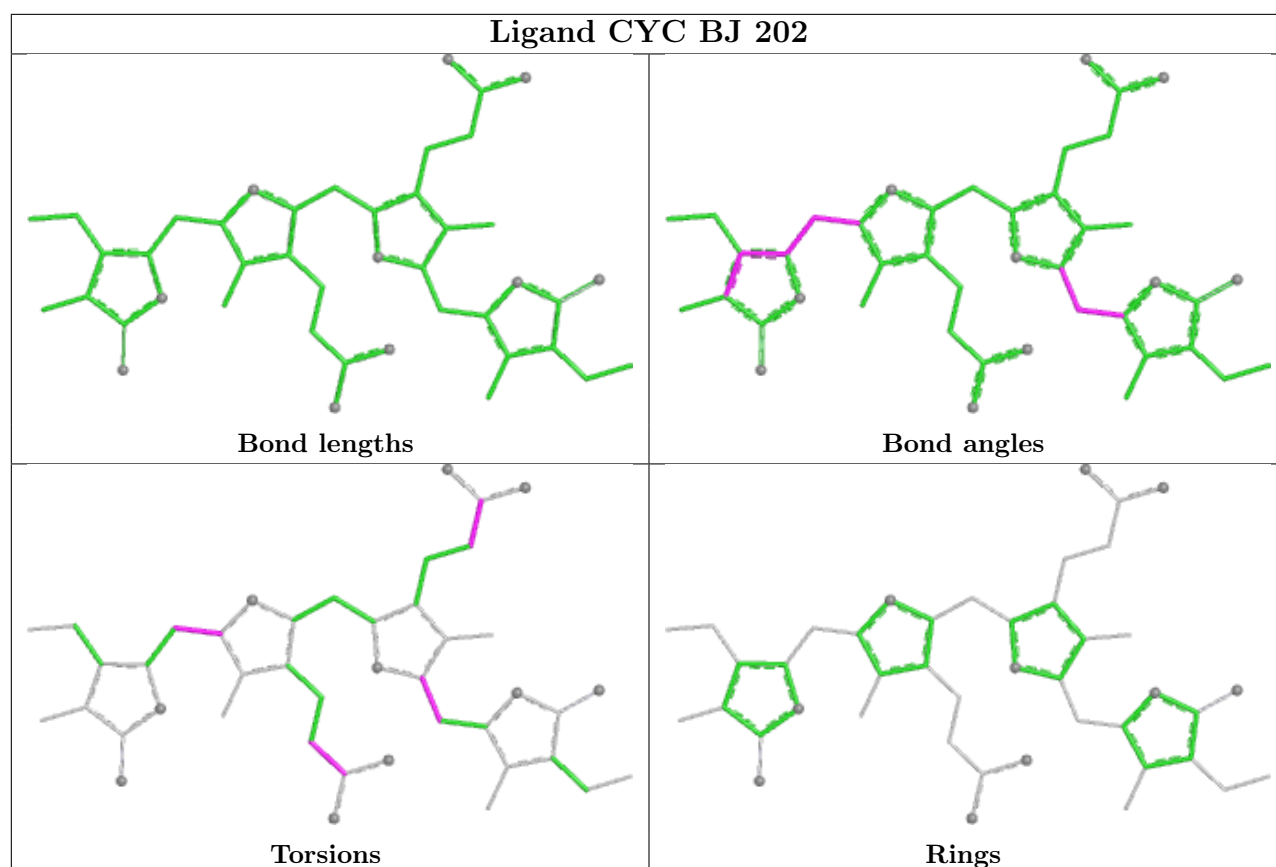


Ligand CYC BF 201

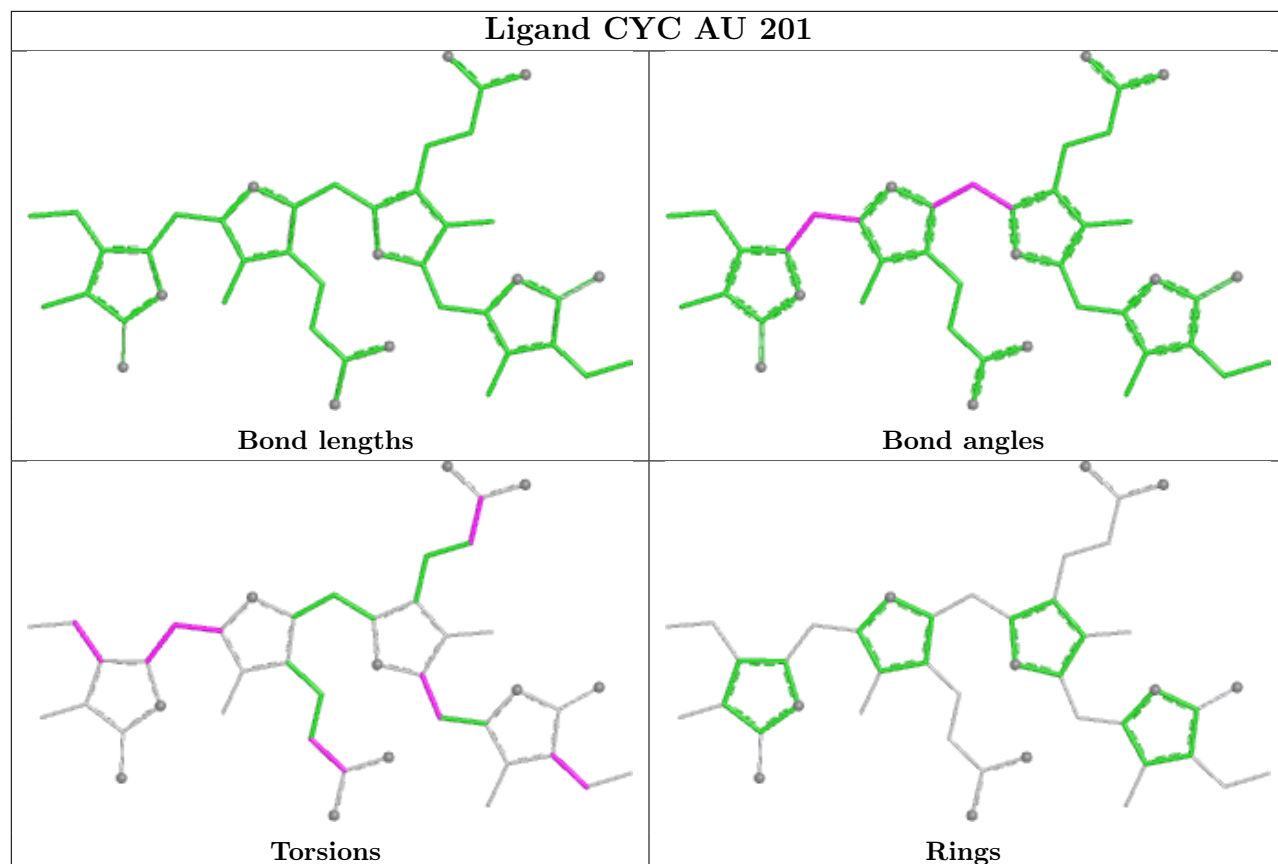


Ligand CYC AB 201

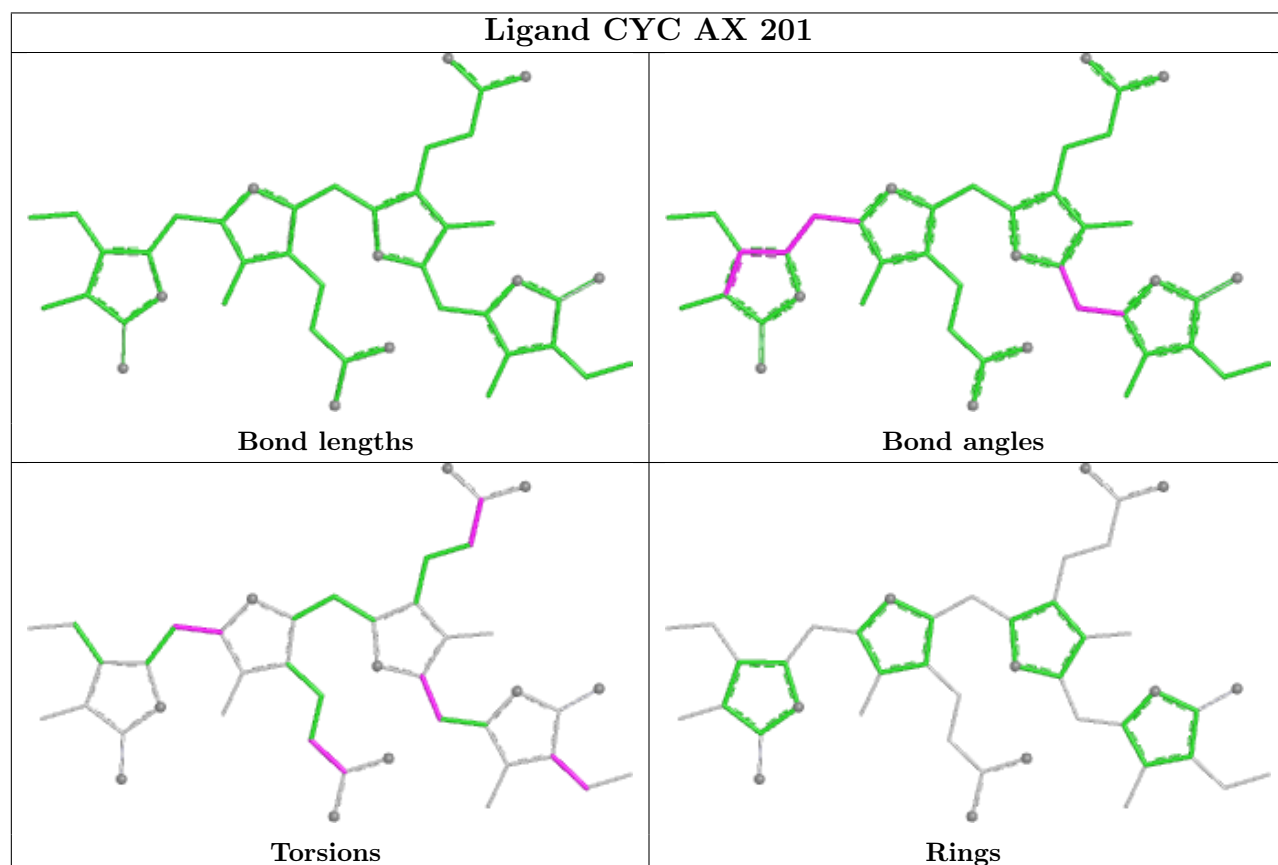




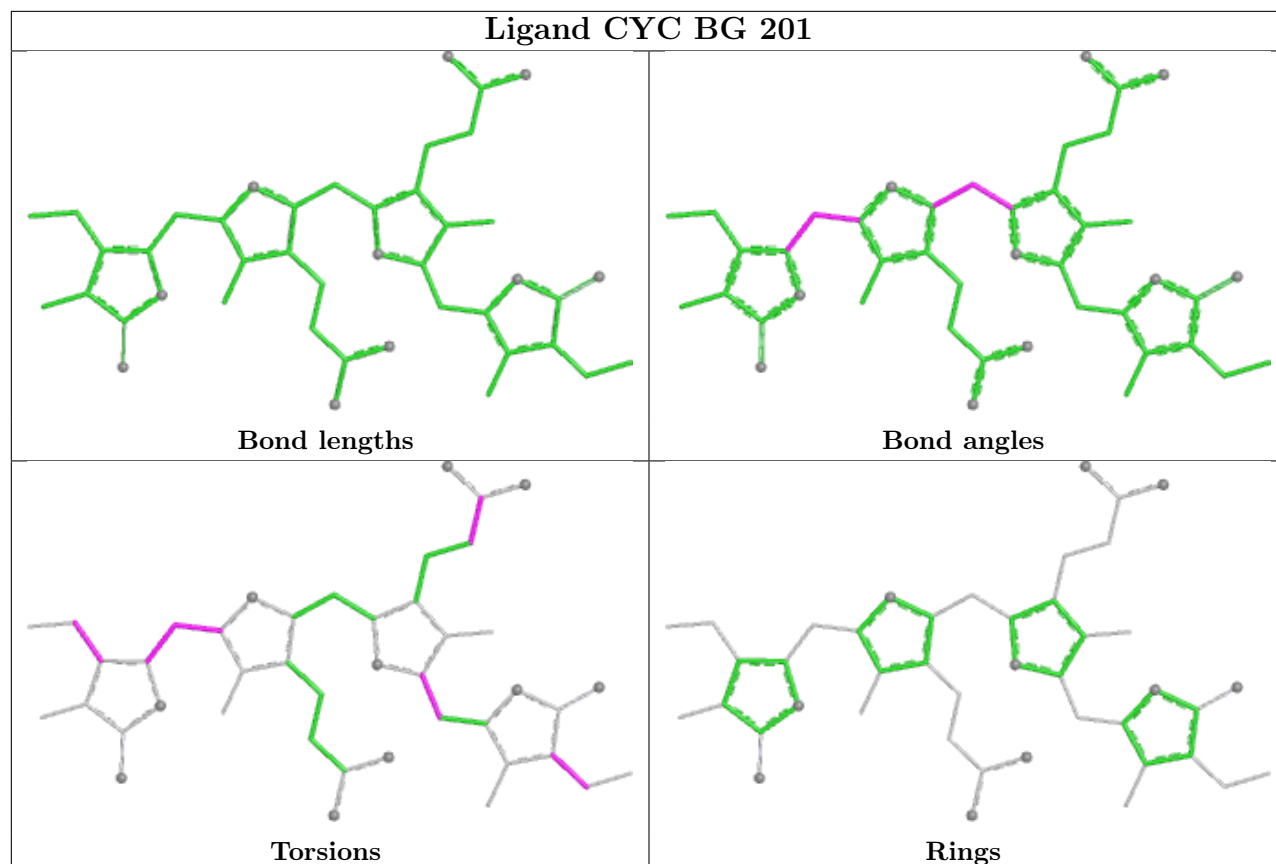
Ligand CYC AU 201



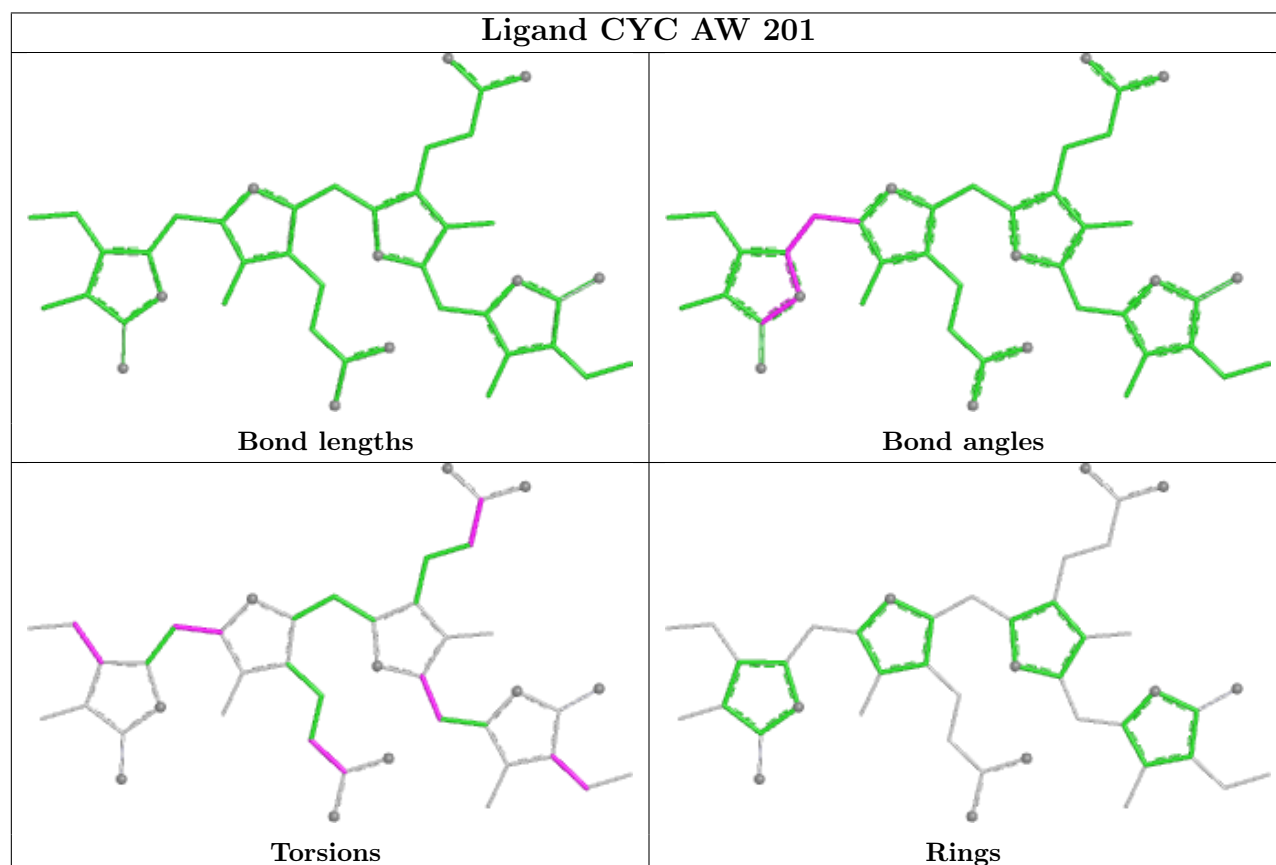
Ligand CYC AX 201

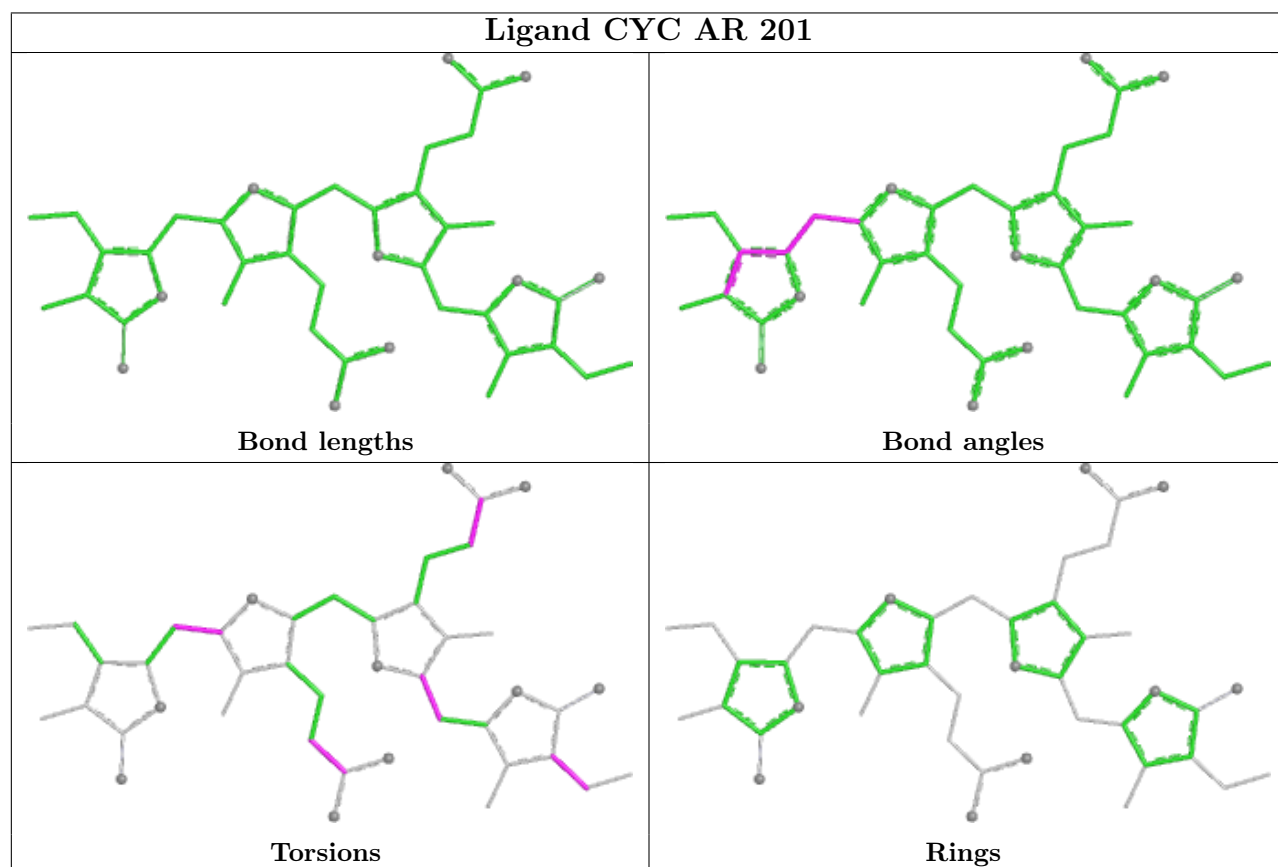
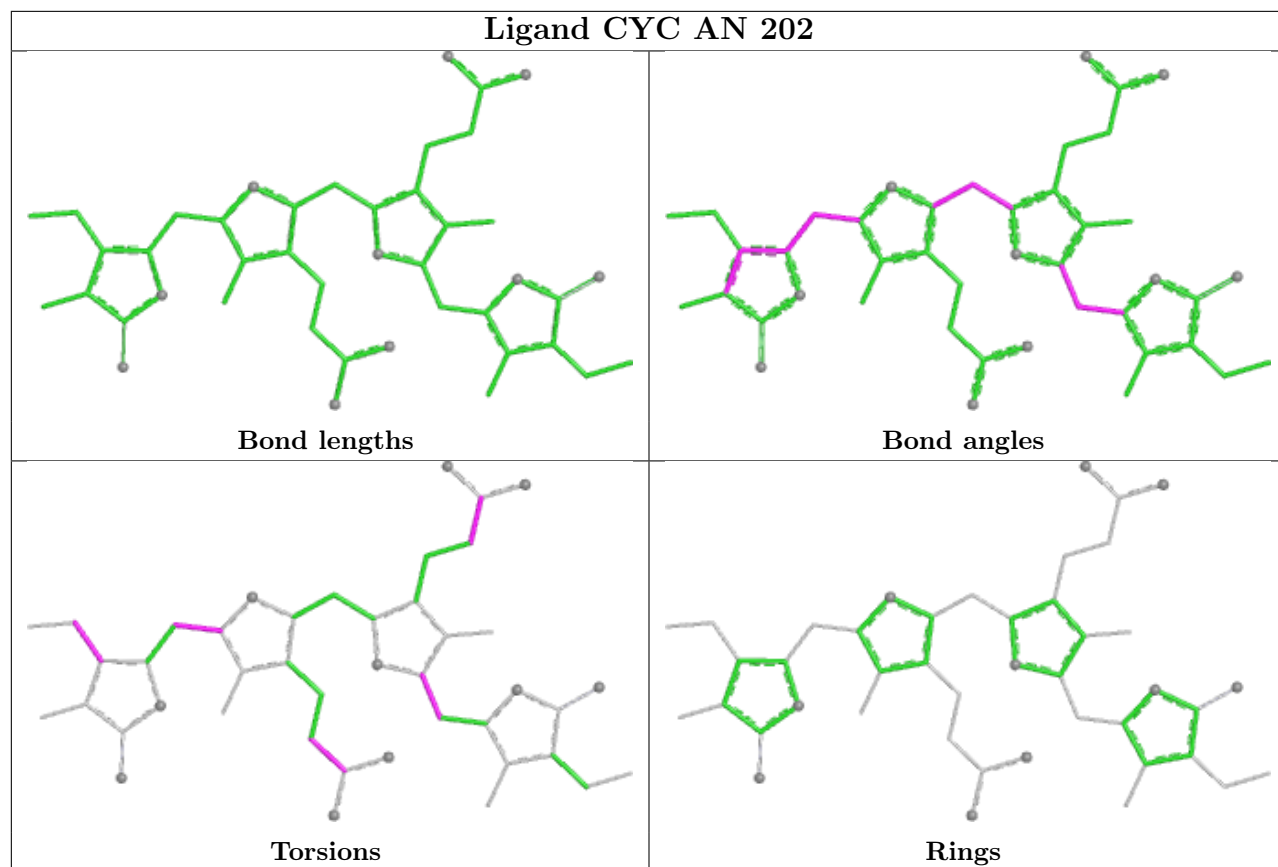


Ligand CYC BG 201

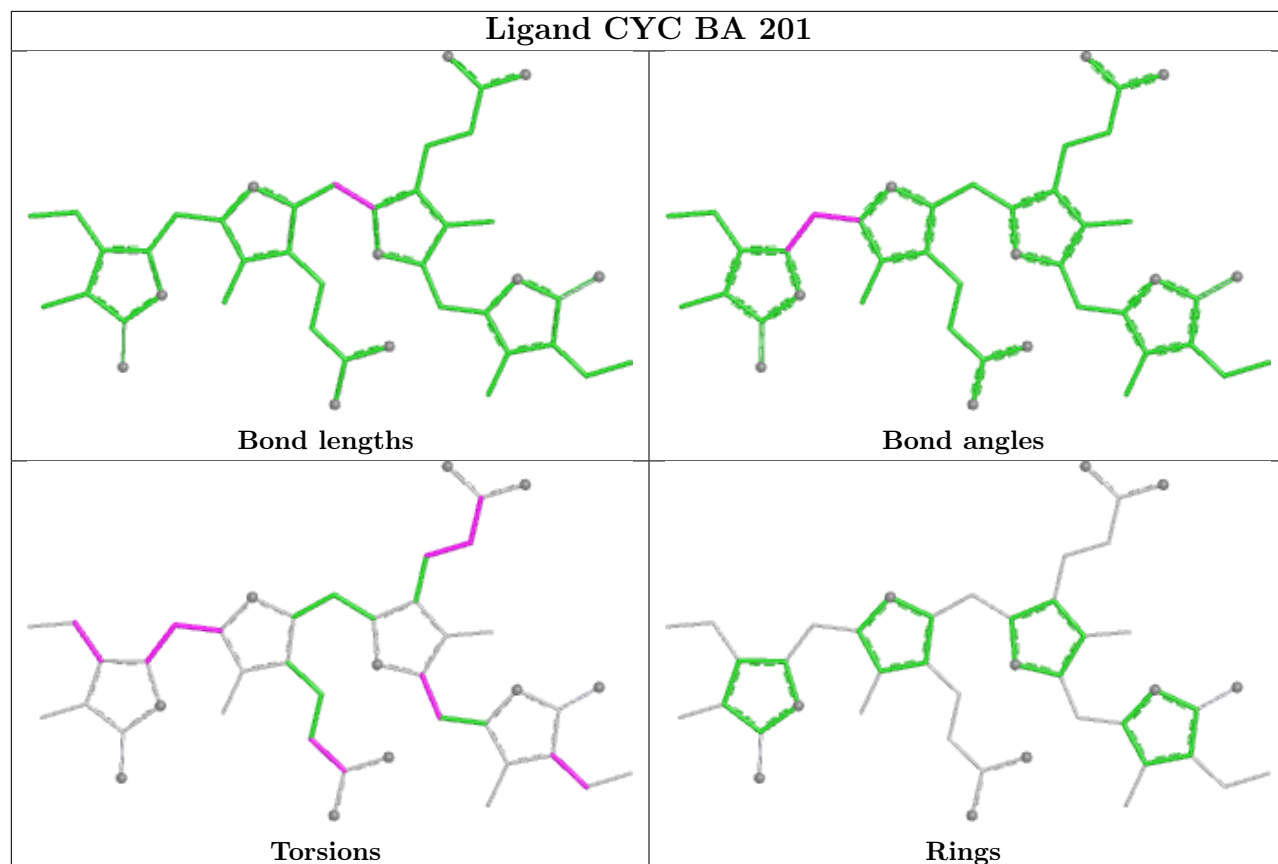


Ligand CYC AW 201

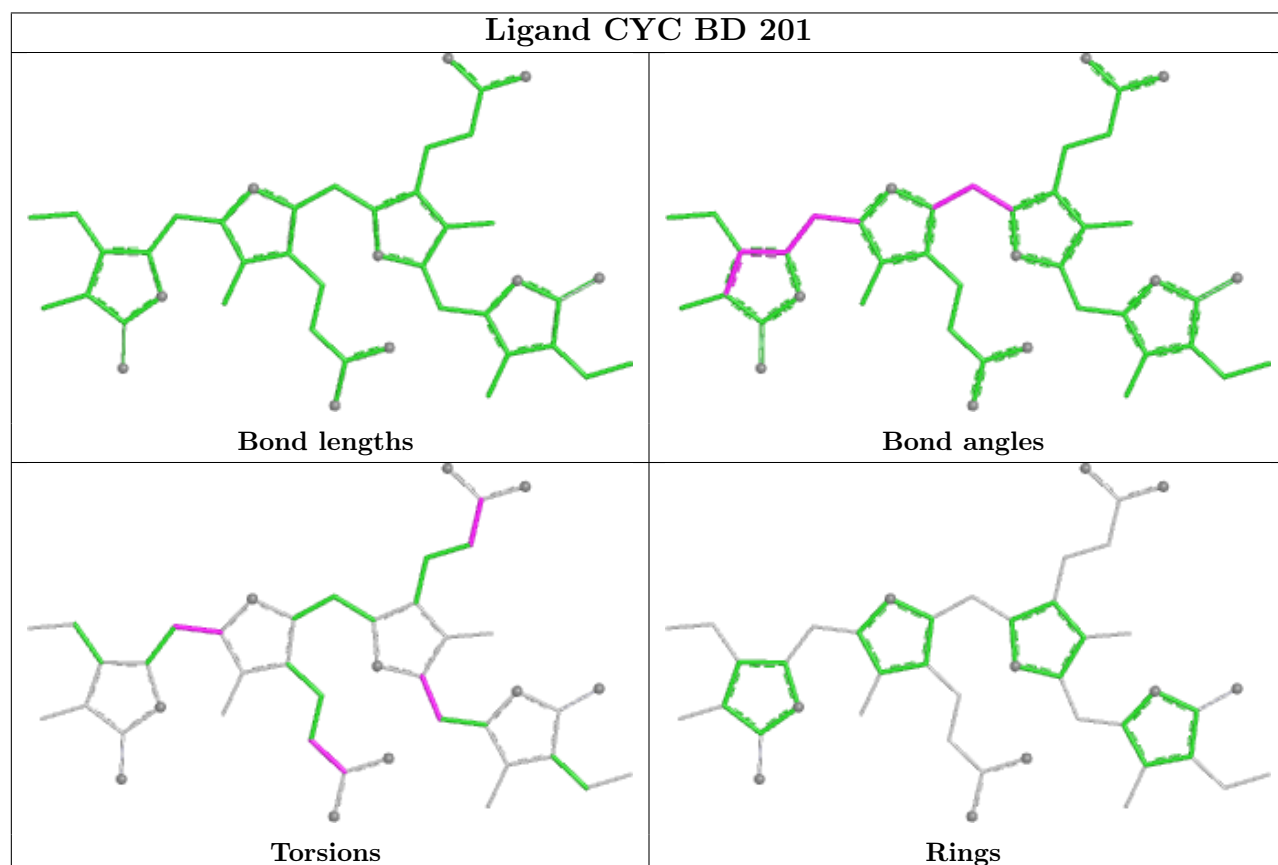




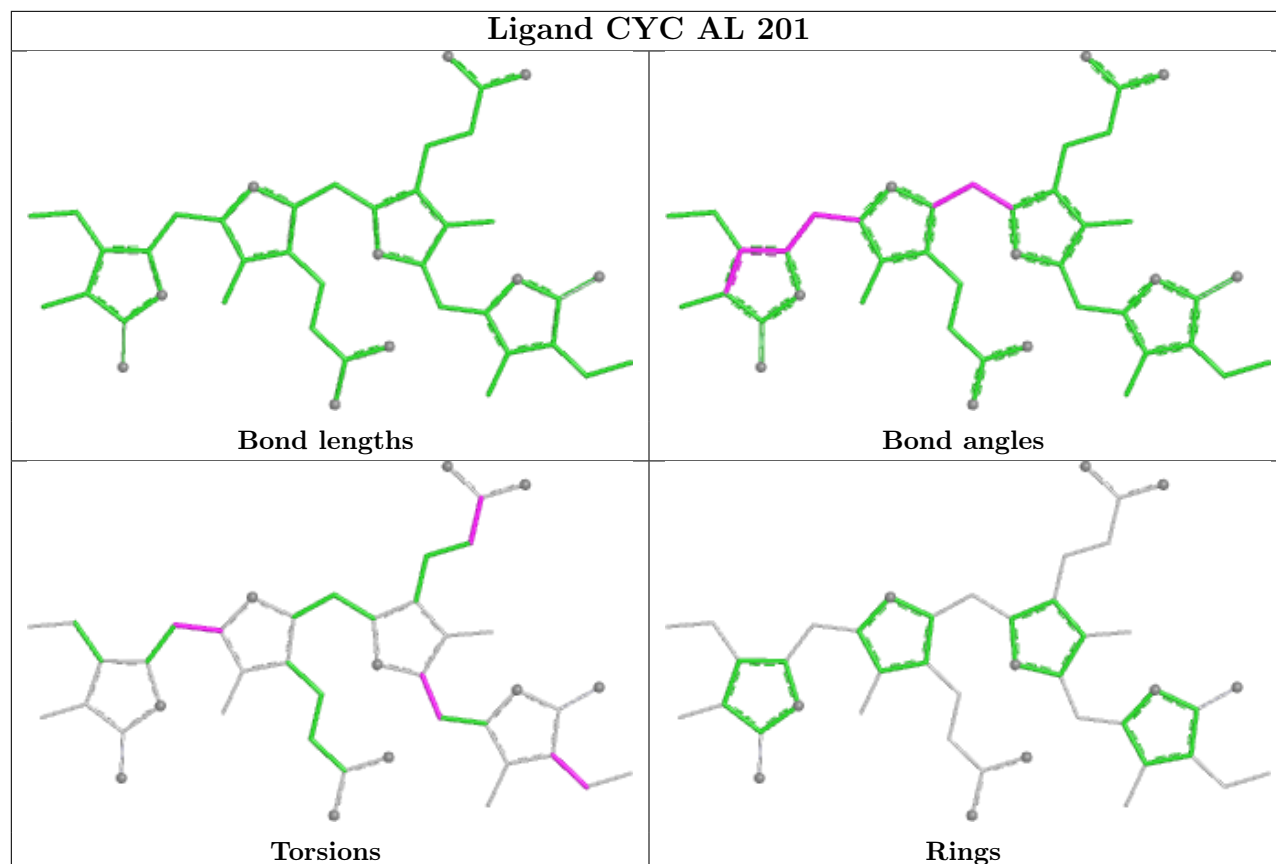
Ligand CYC BA 201



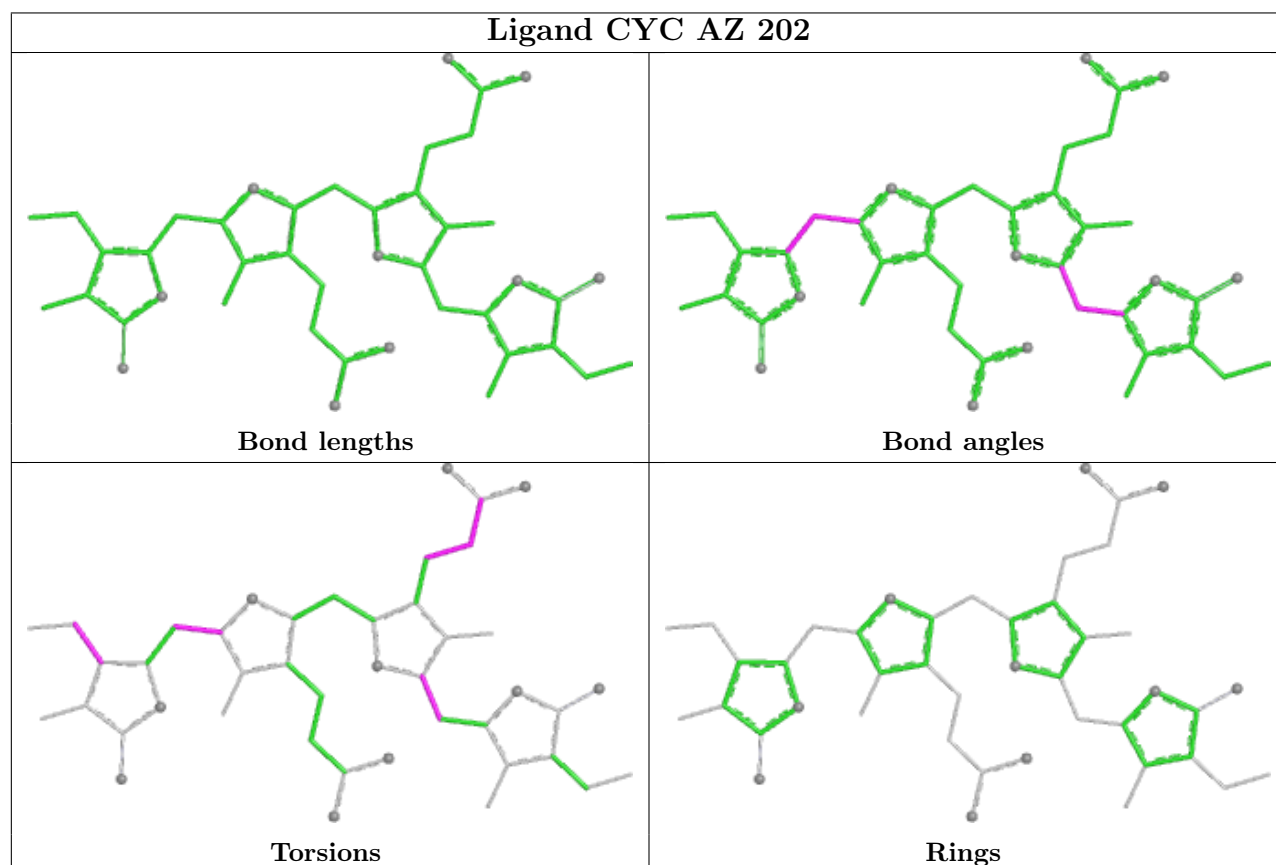
Ligand CYC BD 201



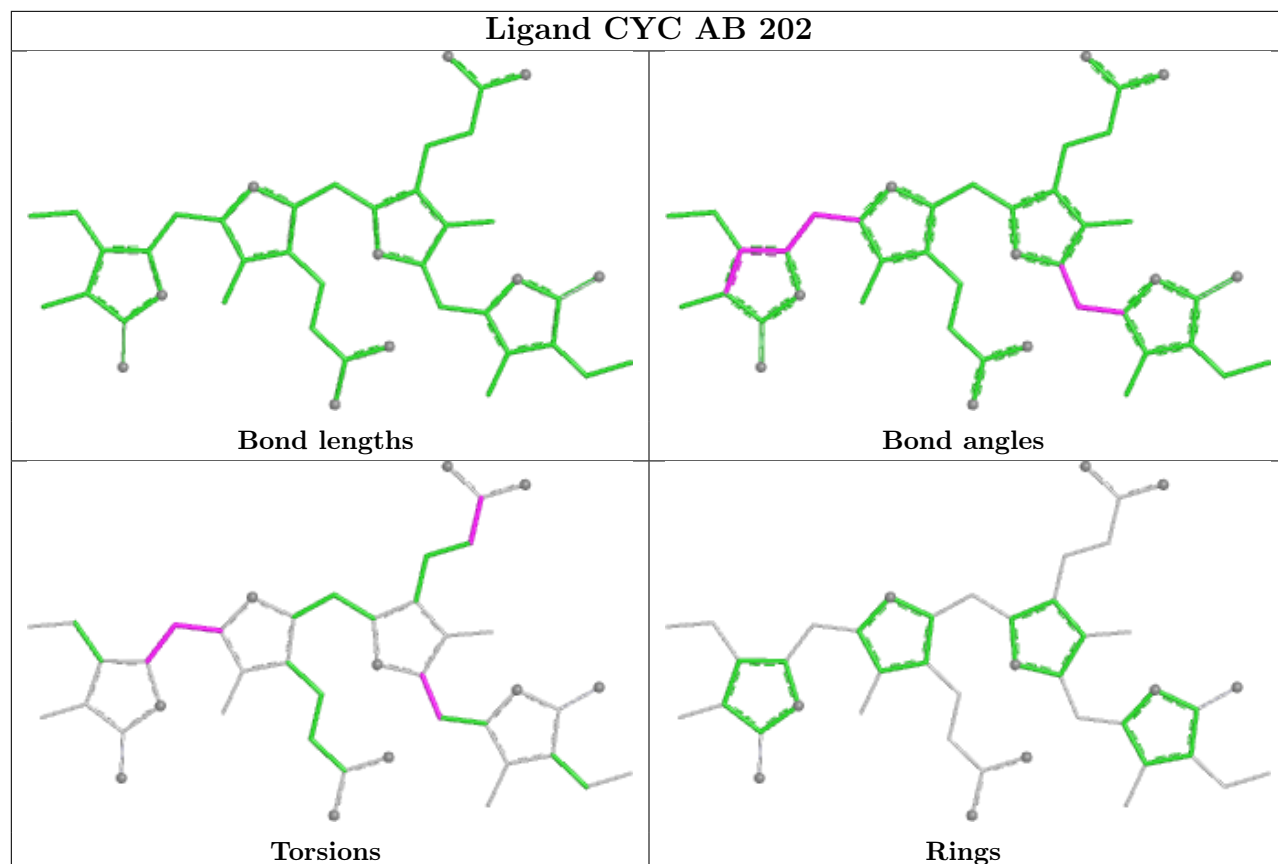
Ligand CYC AL 201



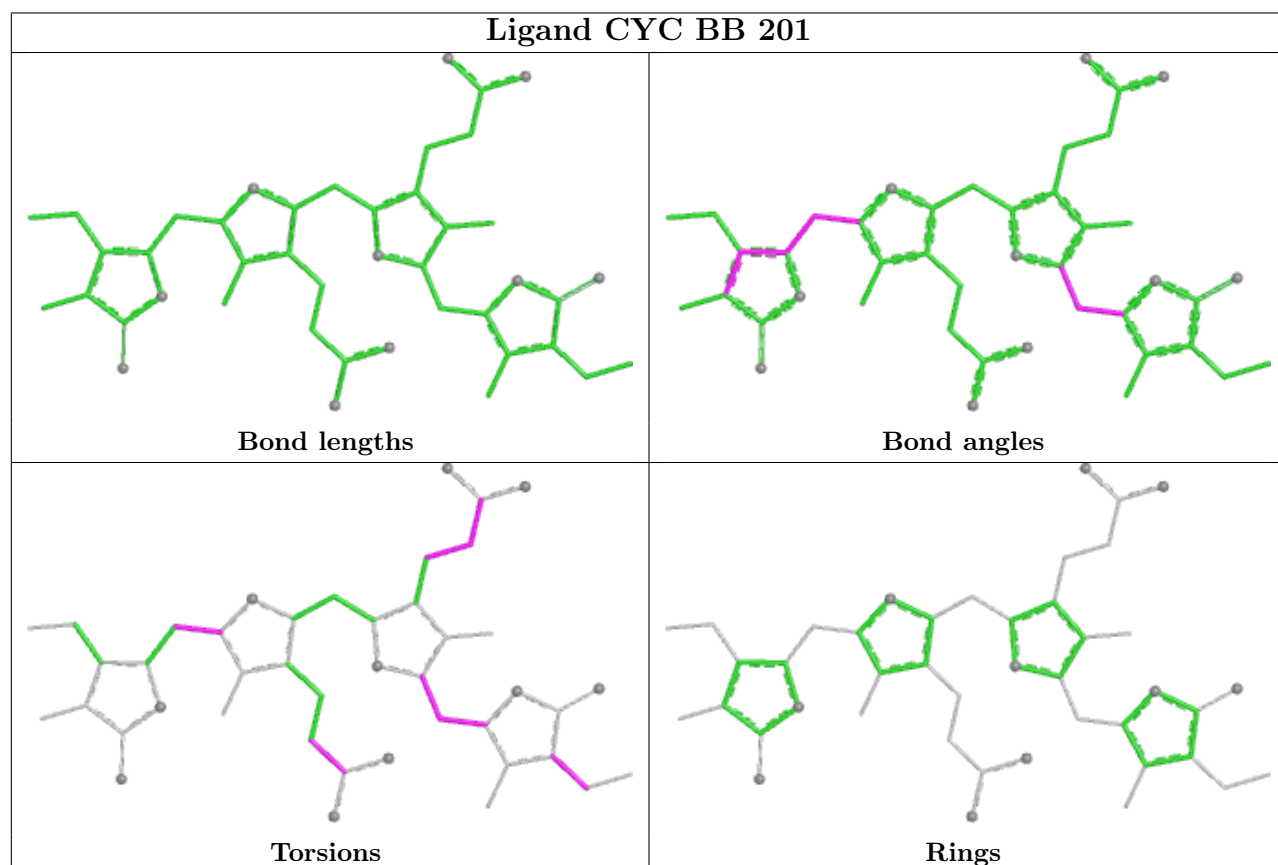
Ligand CYC AZ 202



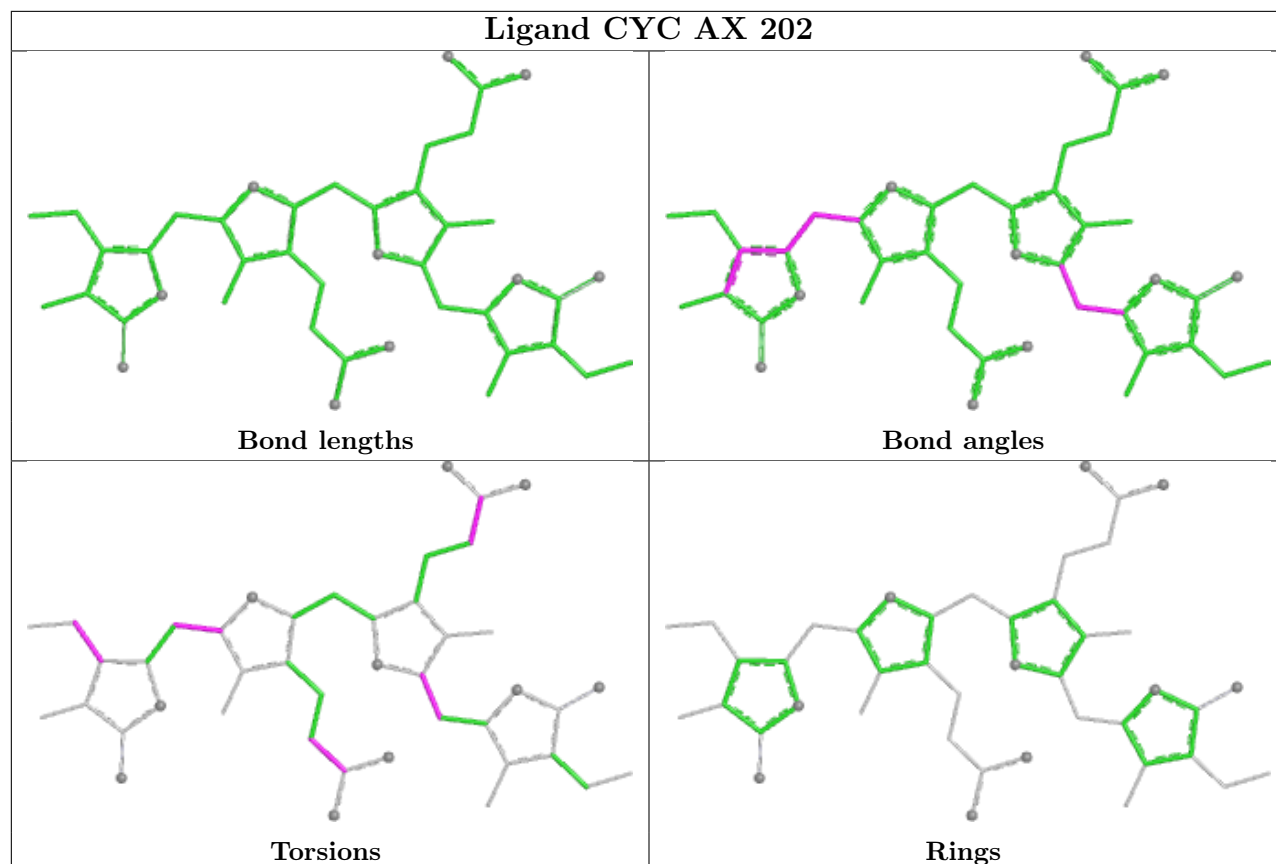
Ligand CYC AB 202



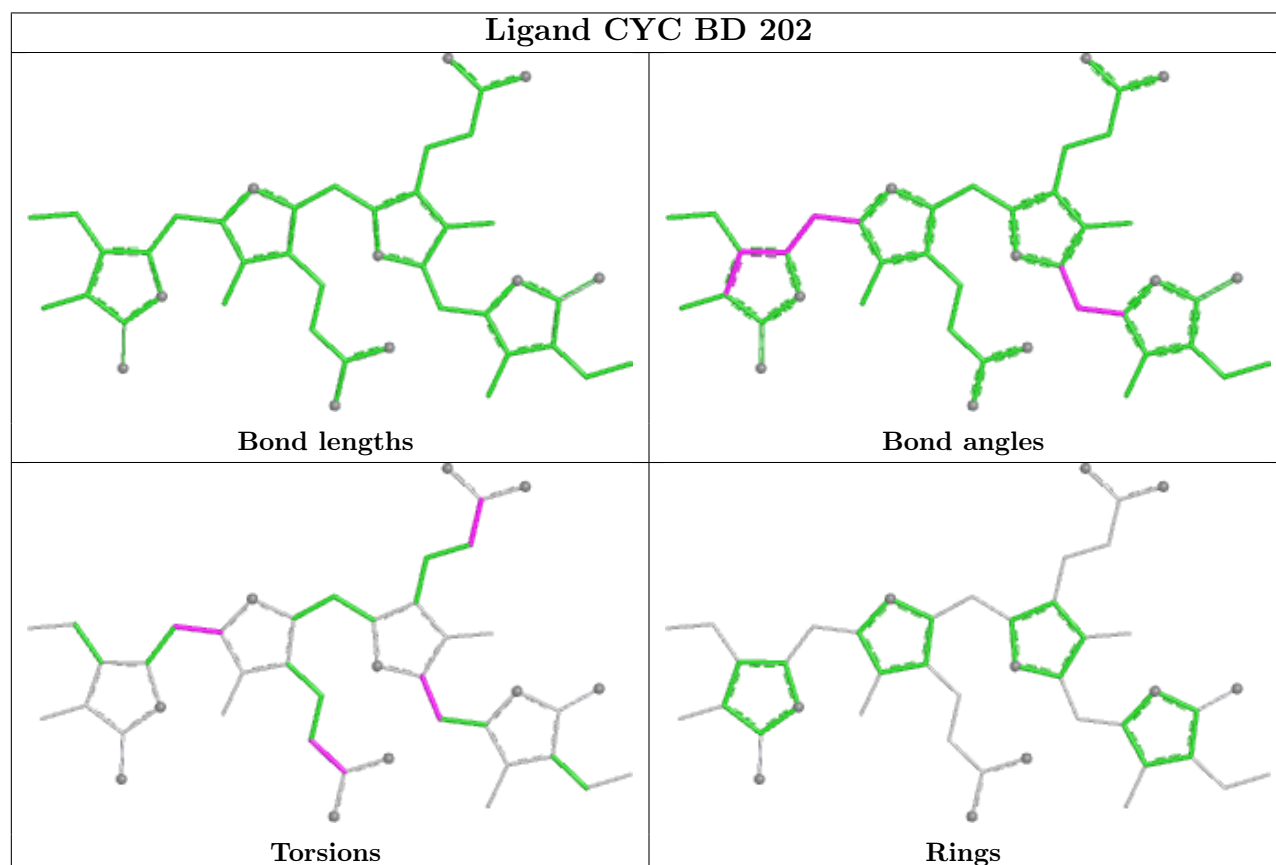
Ligand CYC BB 201



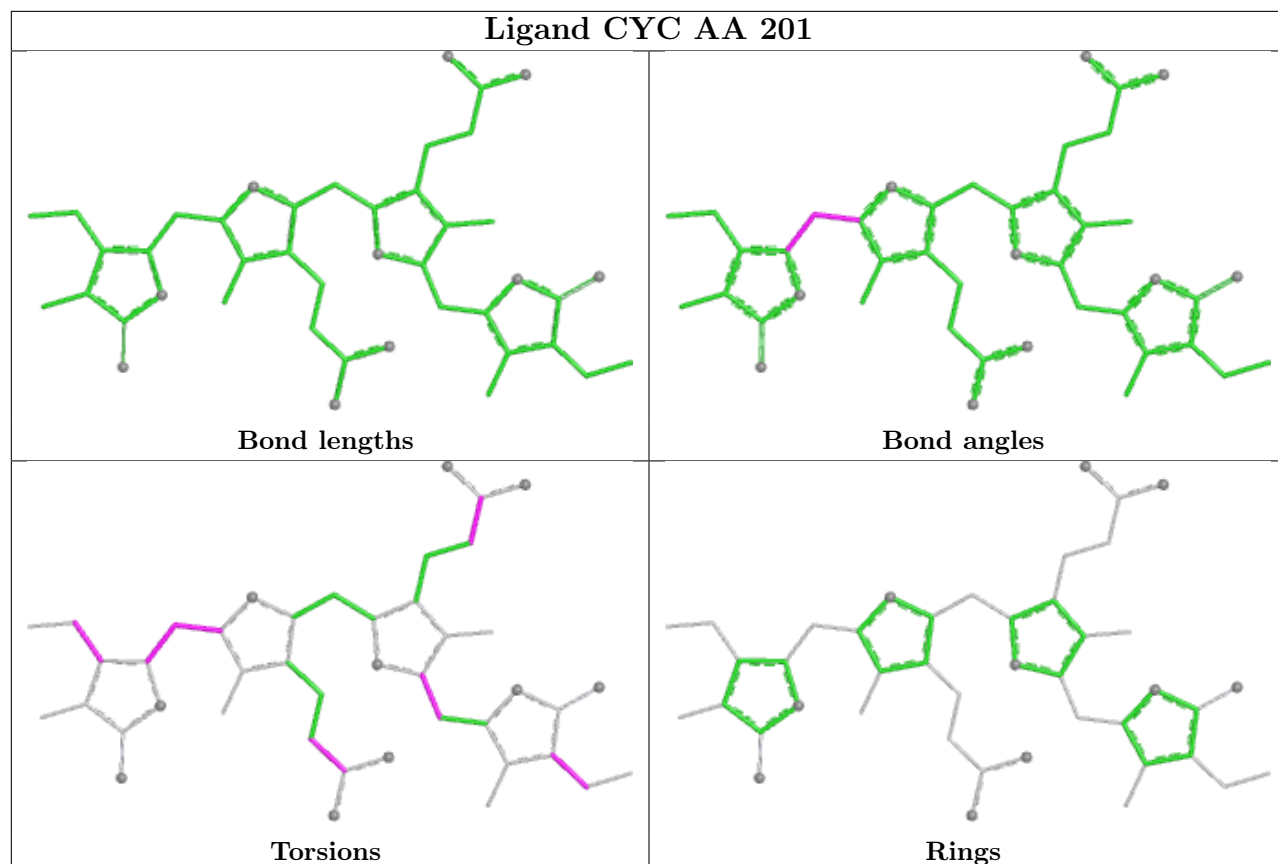
Ligand CYC AX 202



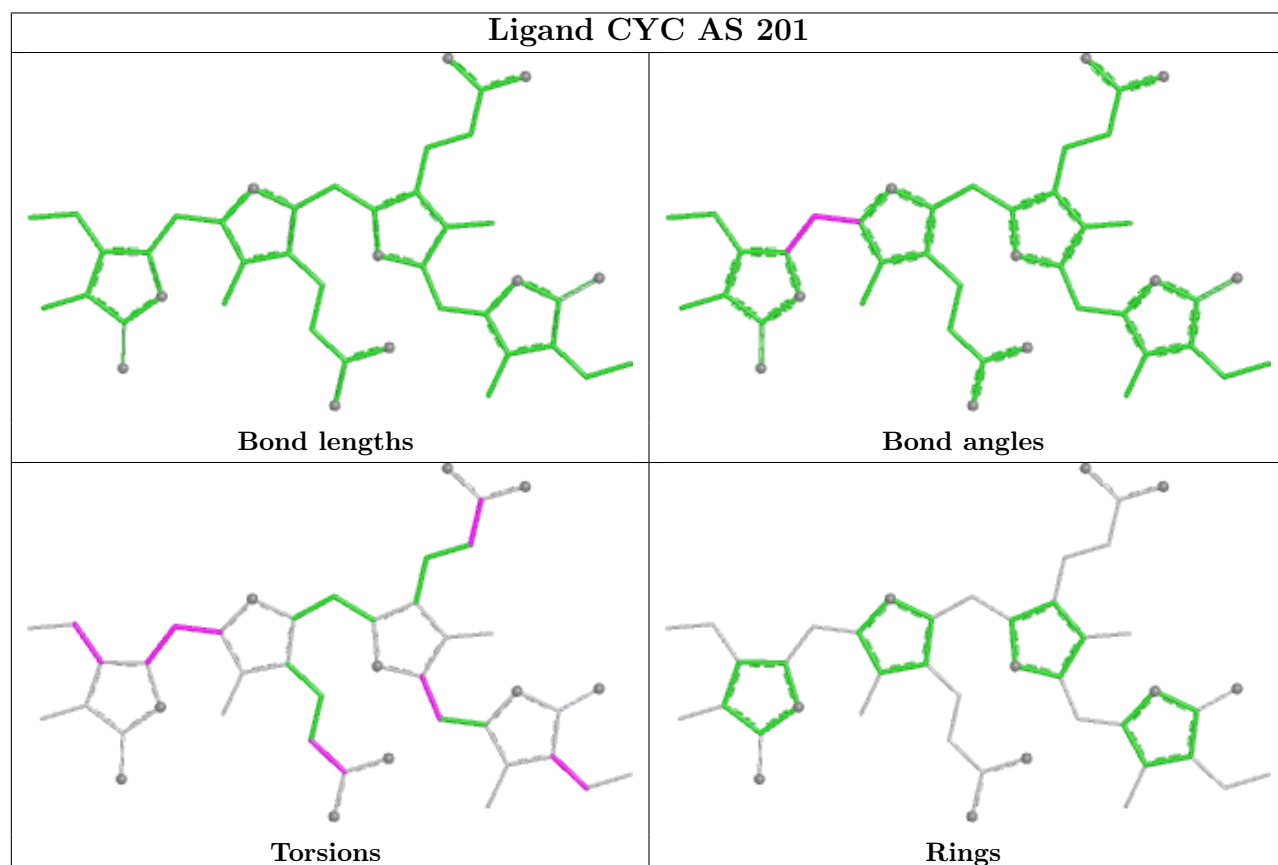
Ligand CYC BD 202



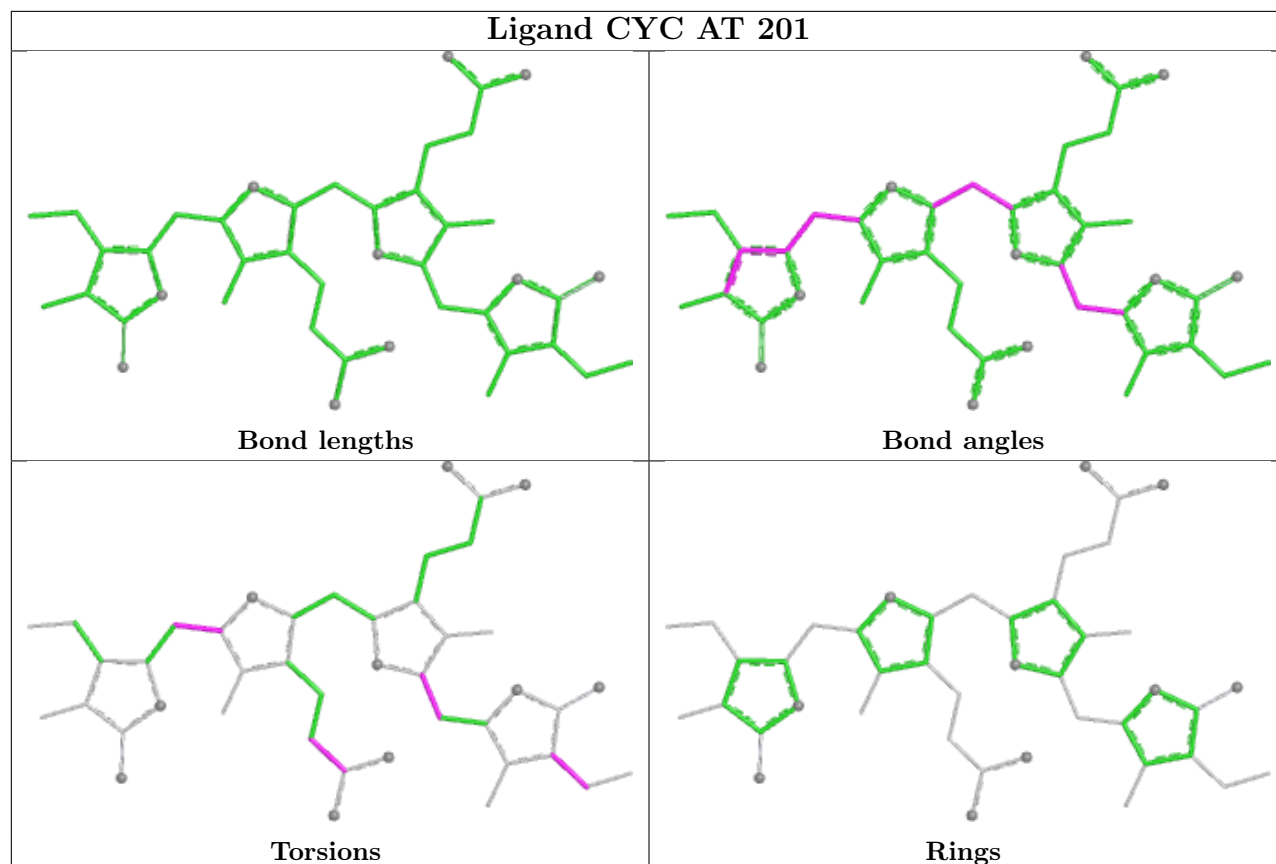
Ligand CYC AA 201



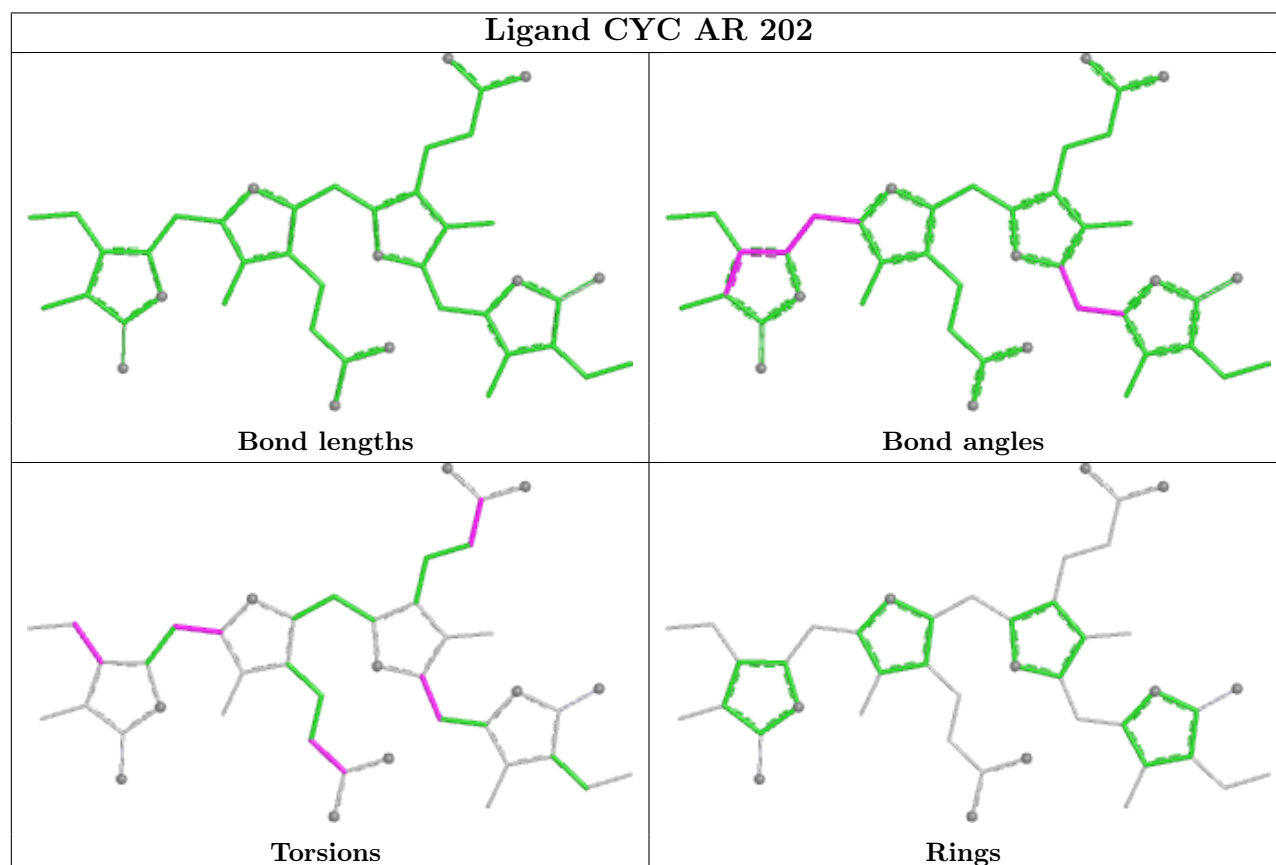
Ligand CYC AS 201

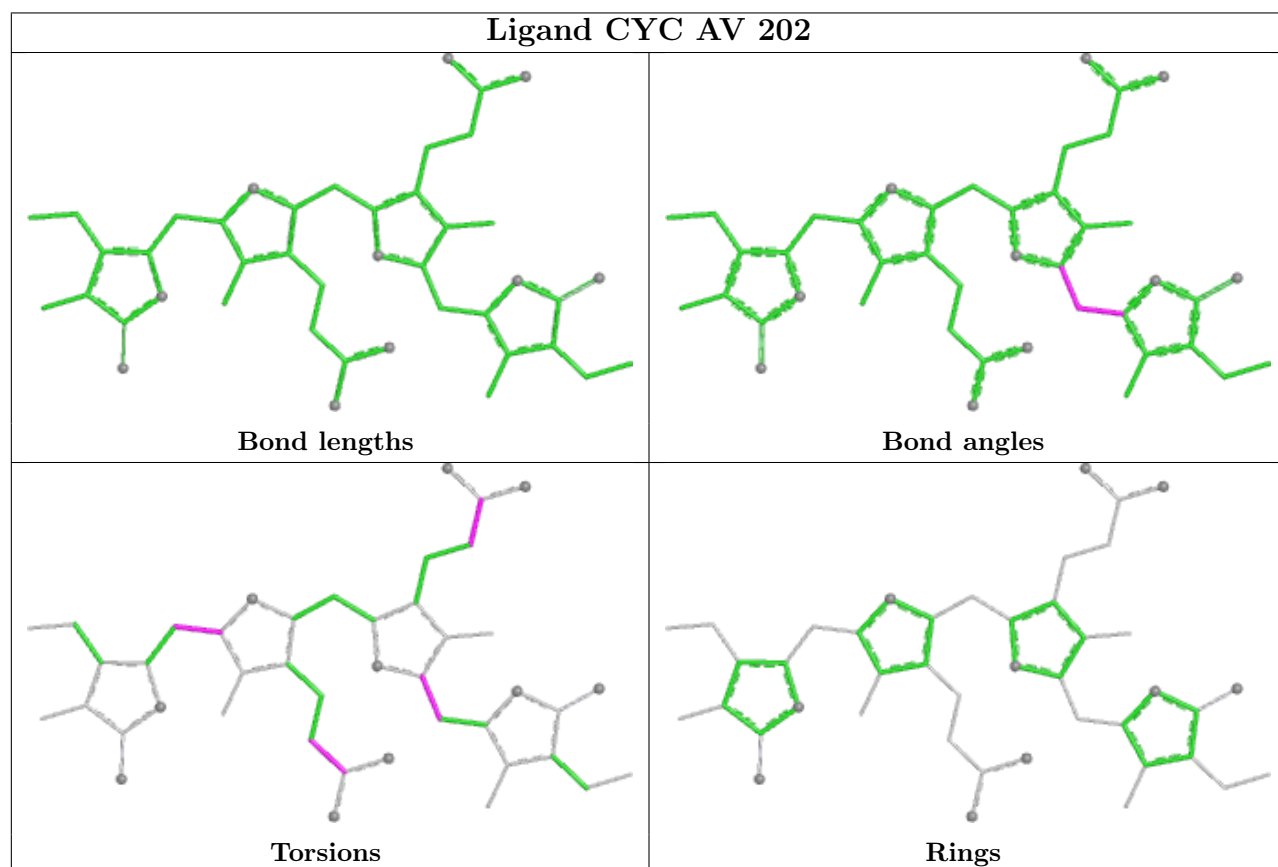
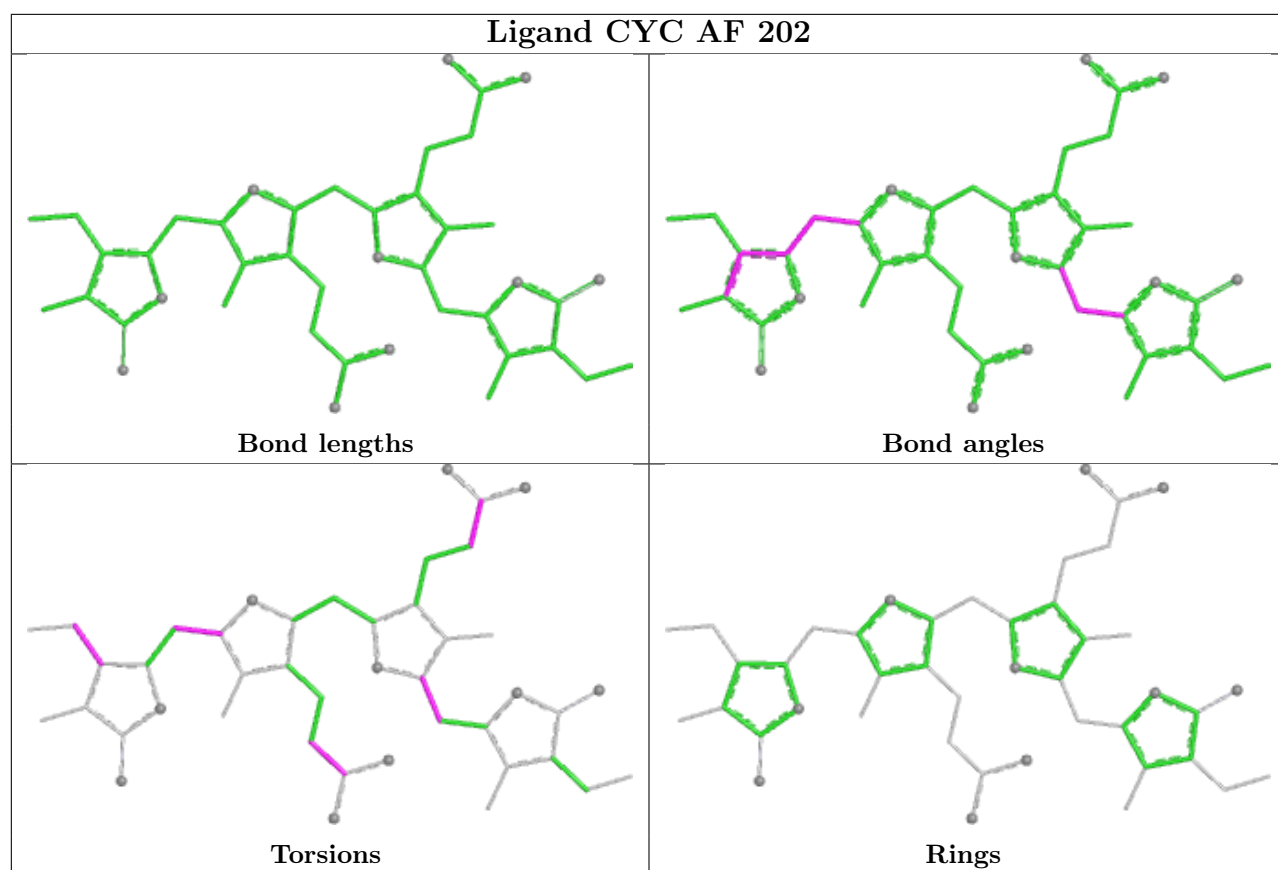


Ligand CYC AT 201

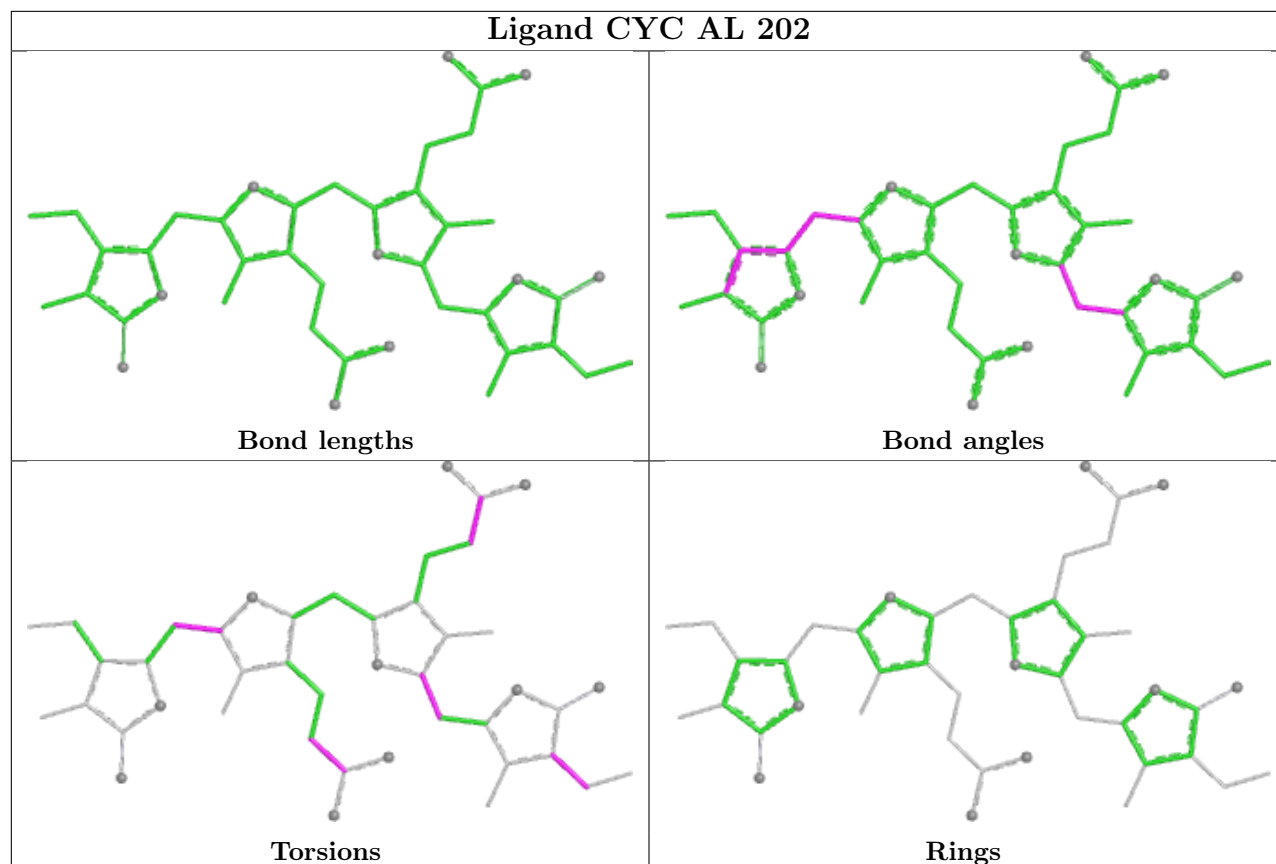


Ligand CYC AR 202

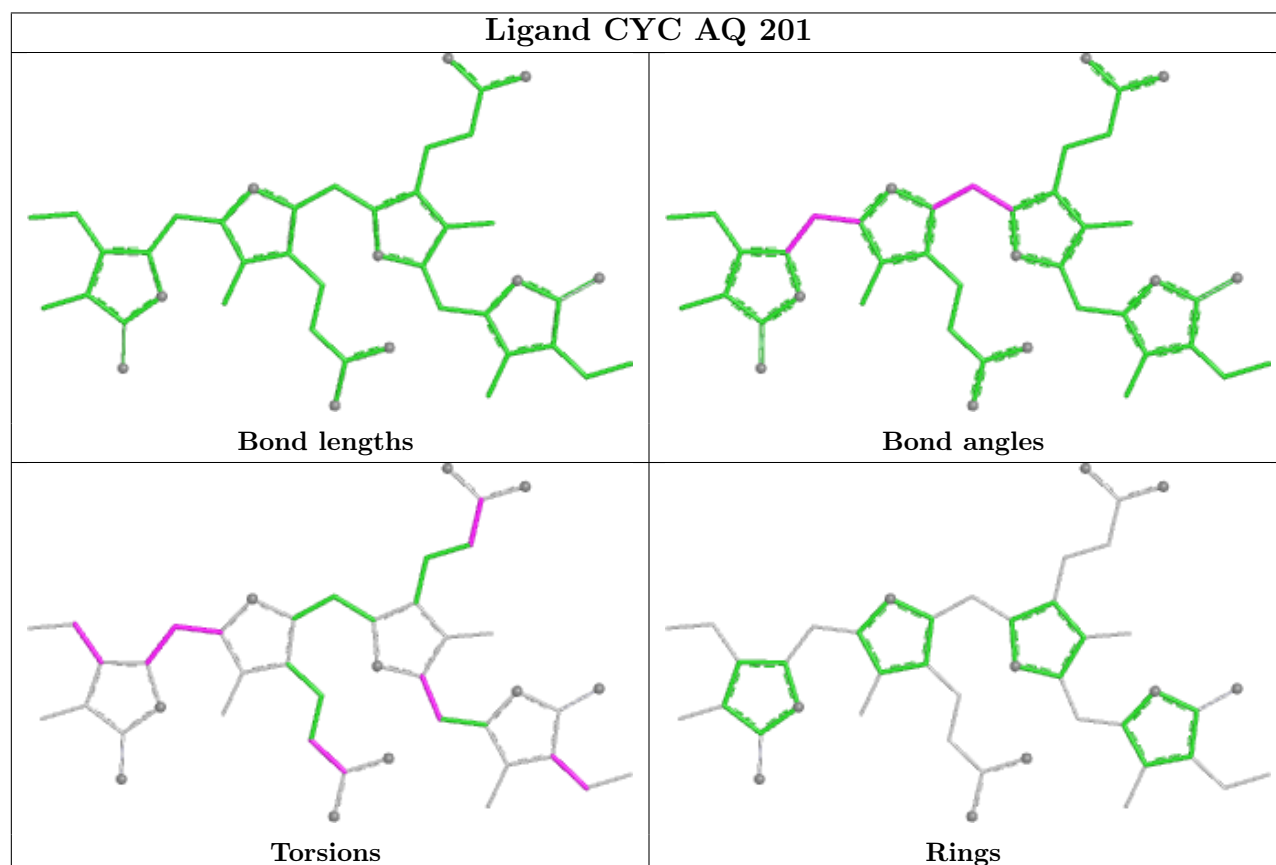




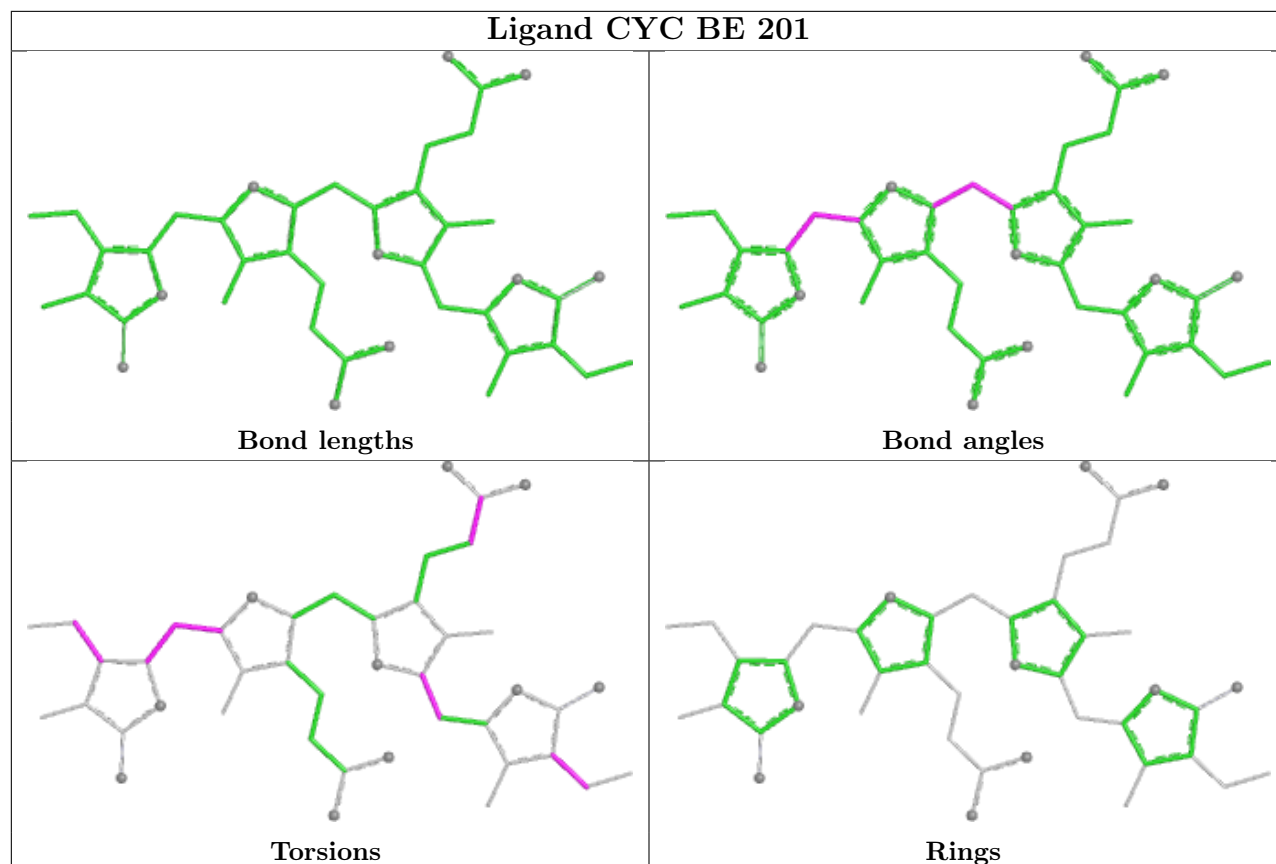
Ligand CYC AL 202



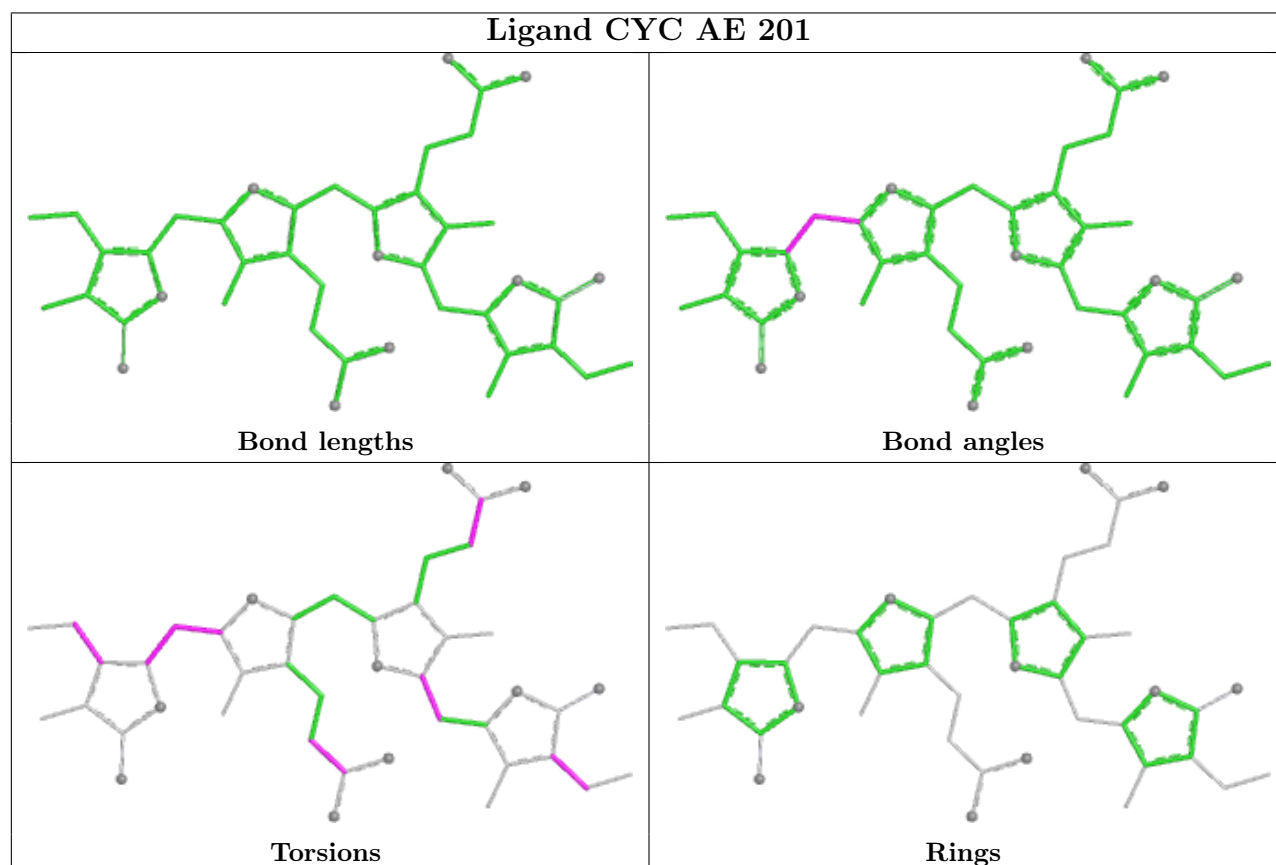
Ligand CYC AQ 201



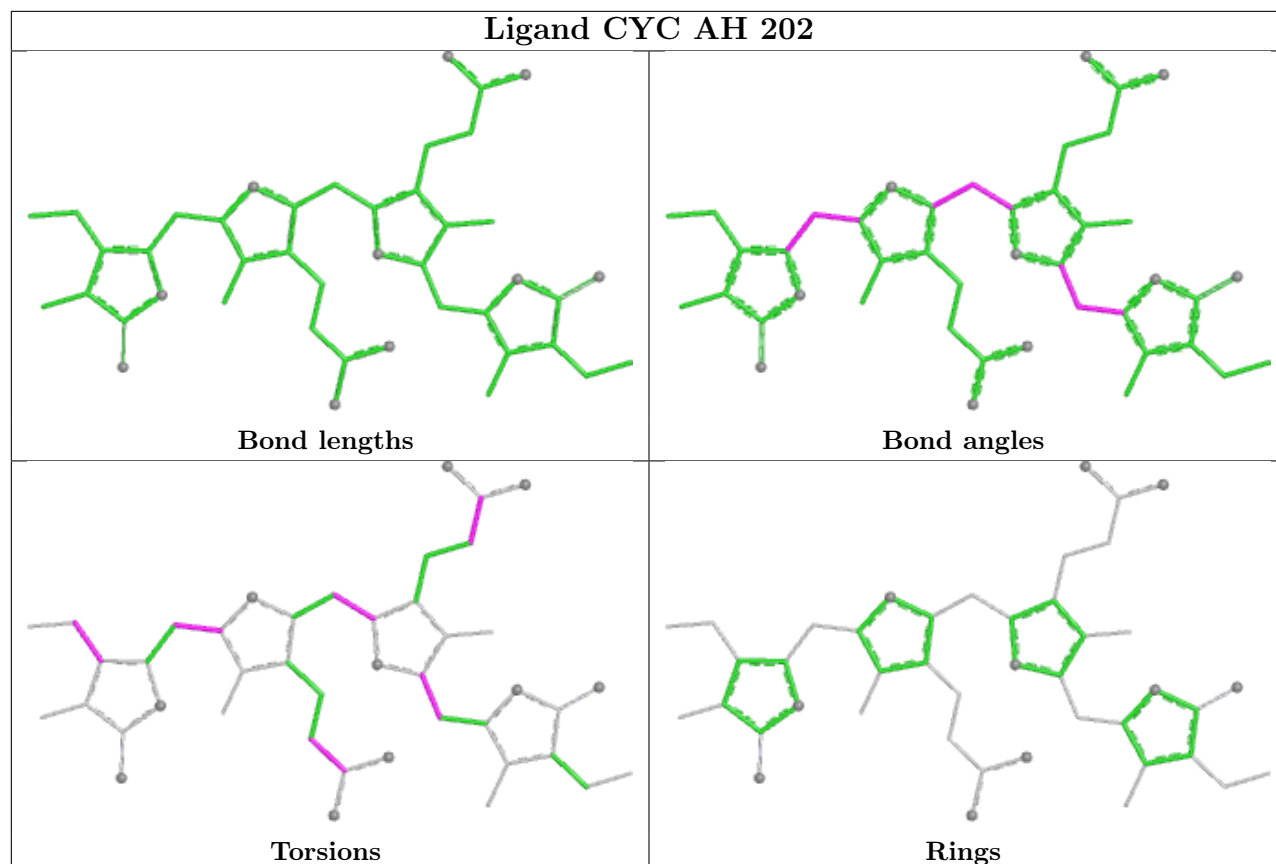
Ligand CYC BE 201



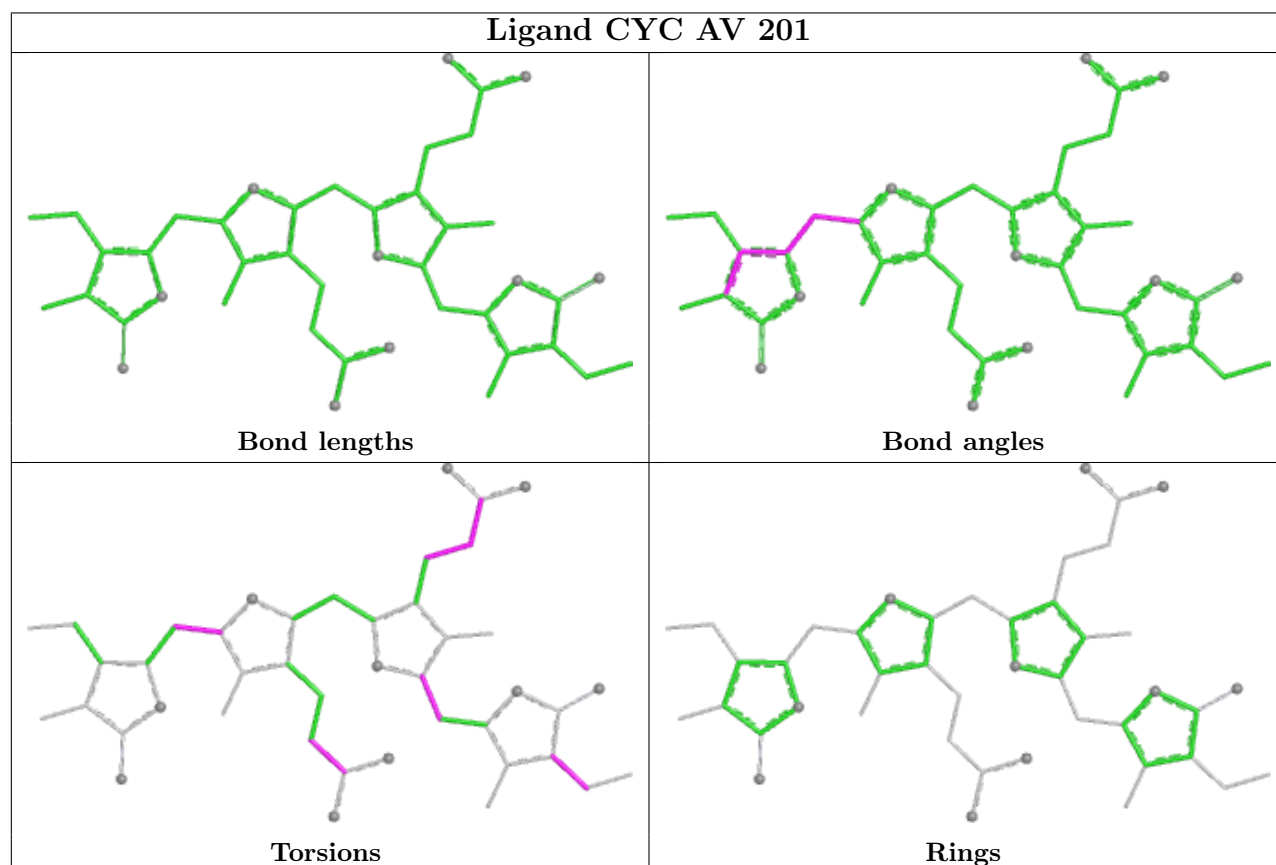
Ligand CYC AE 201



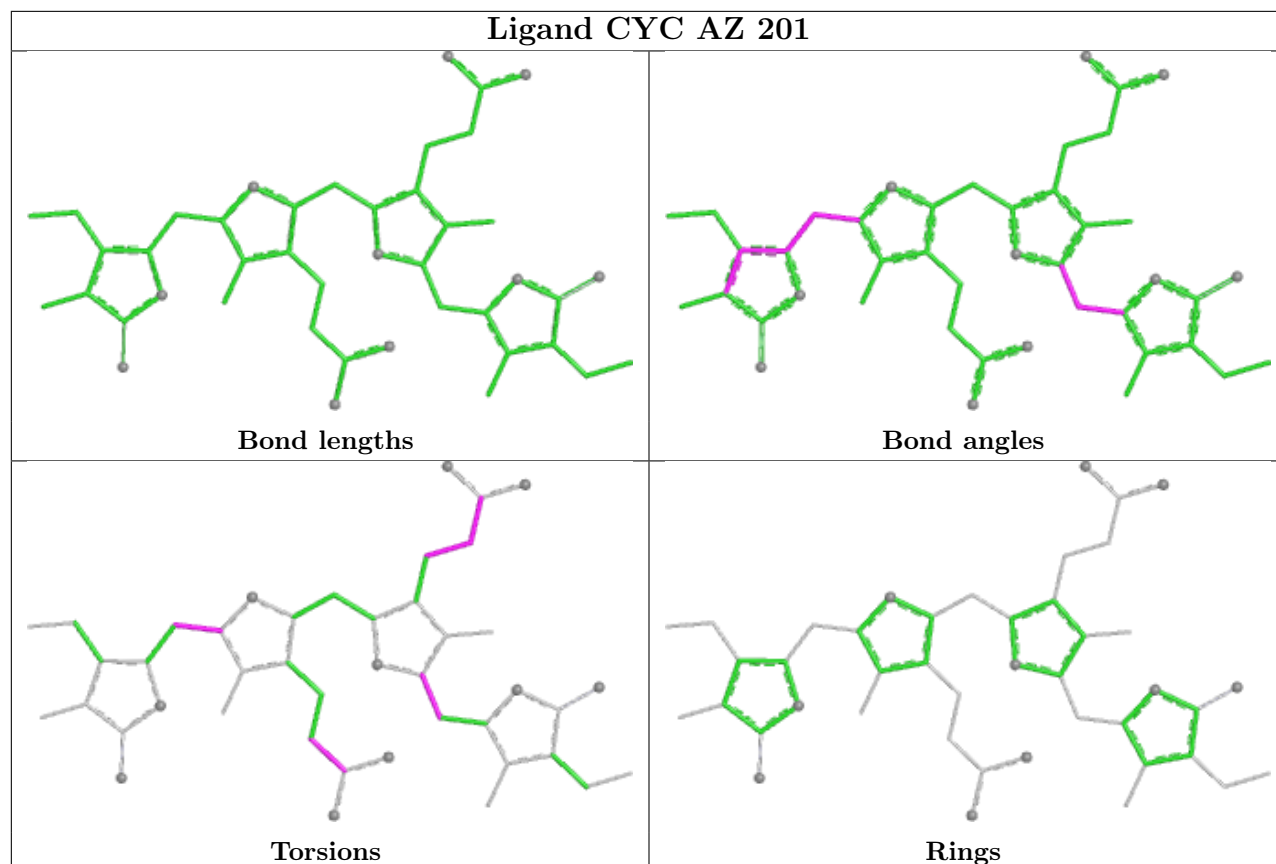
Ligand CYC AH 202



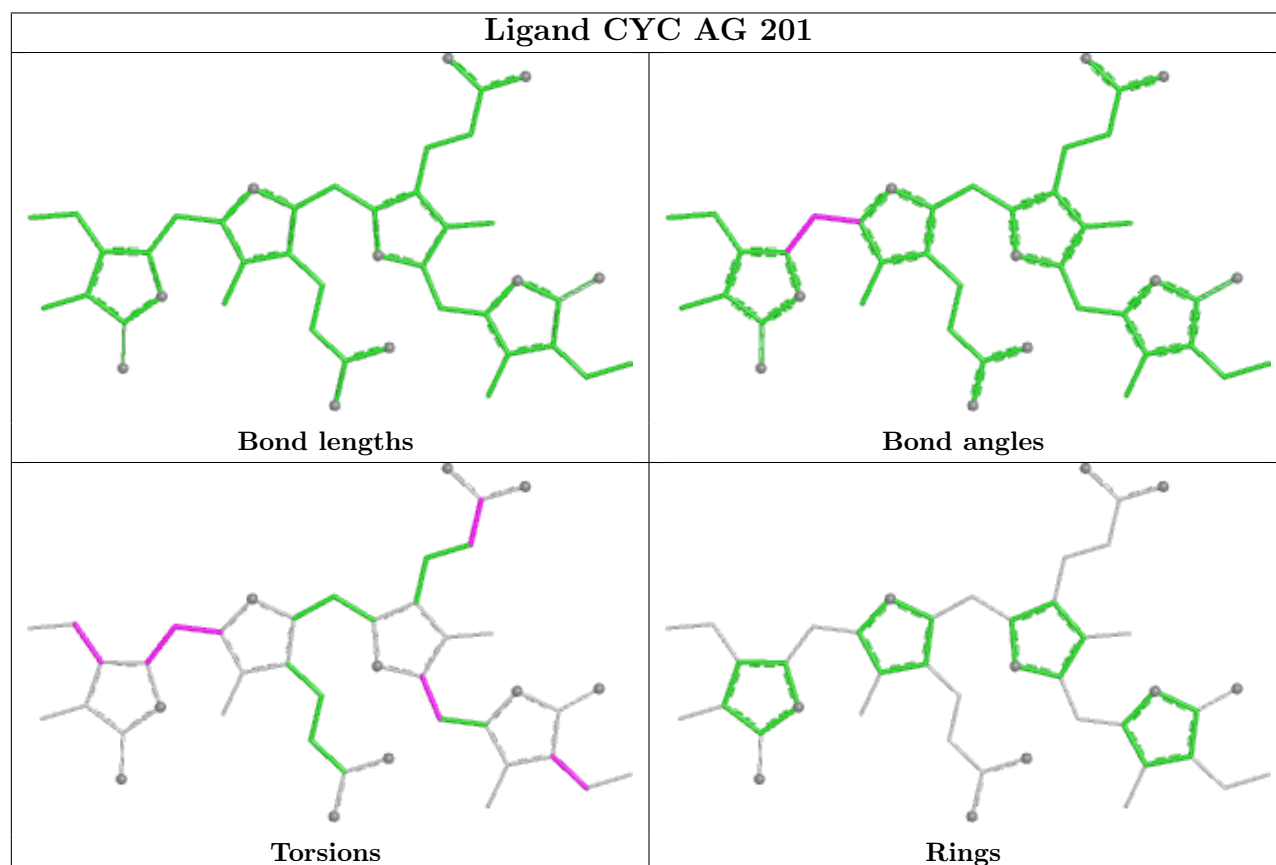
Ligand CYC AV 201



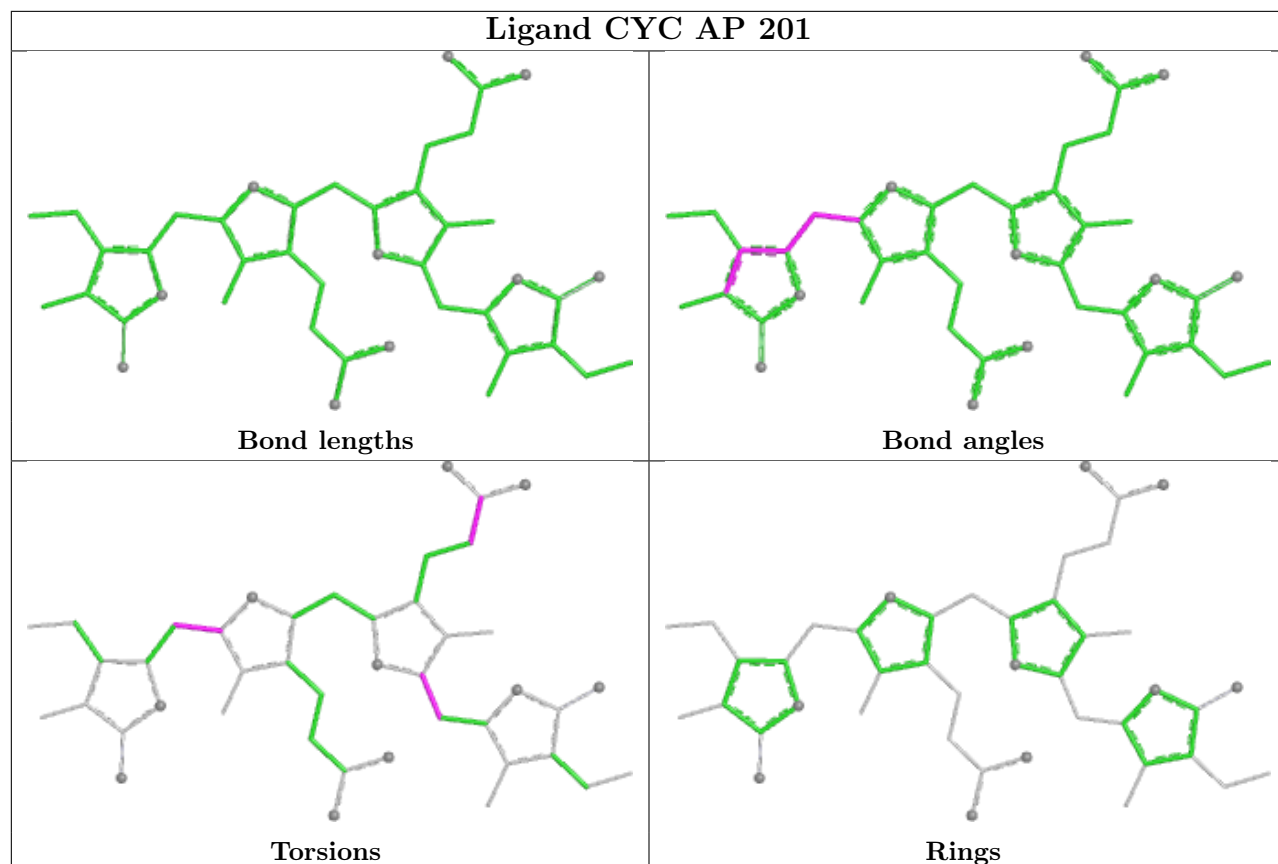
Ligand CYC AZ 201



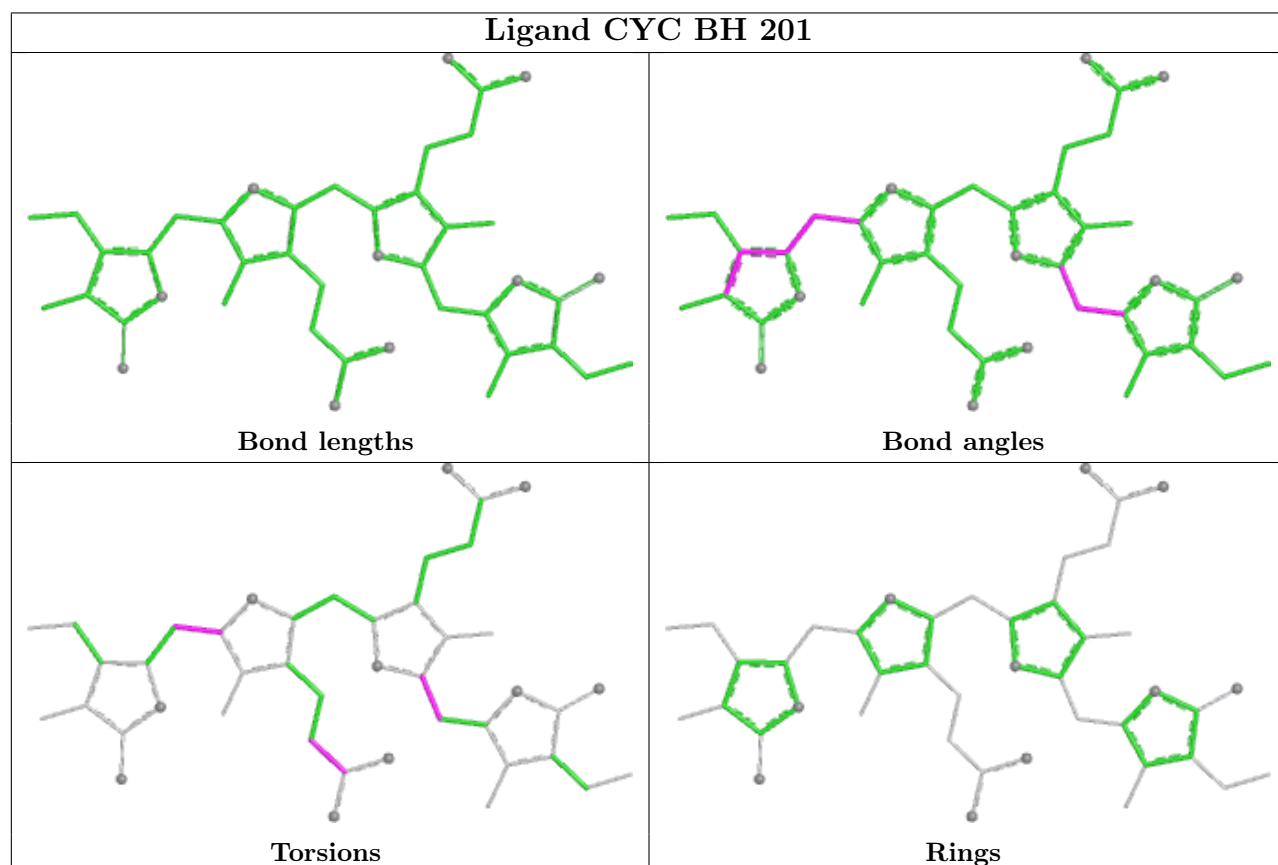
Ligand CYC AG 201



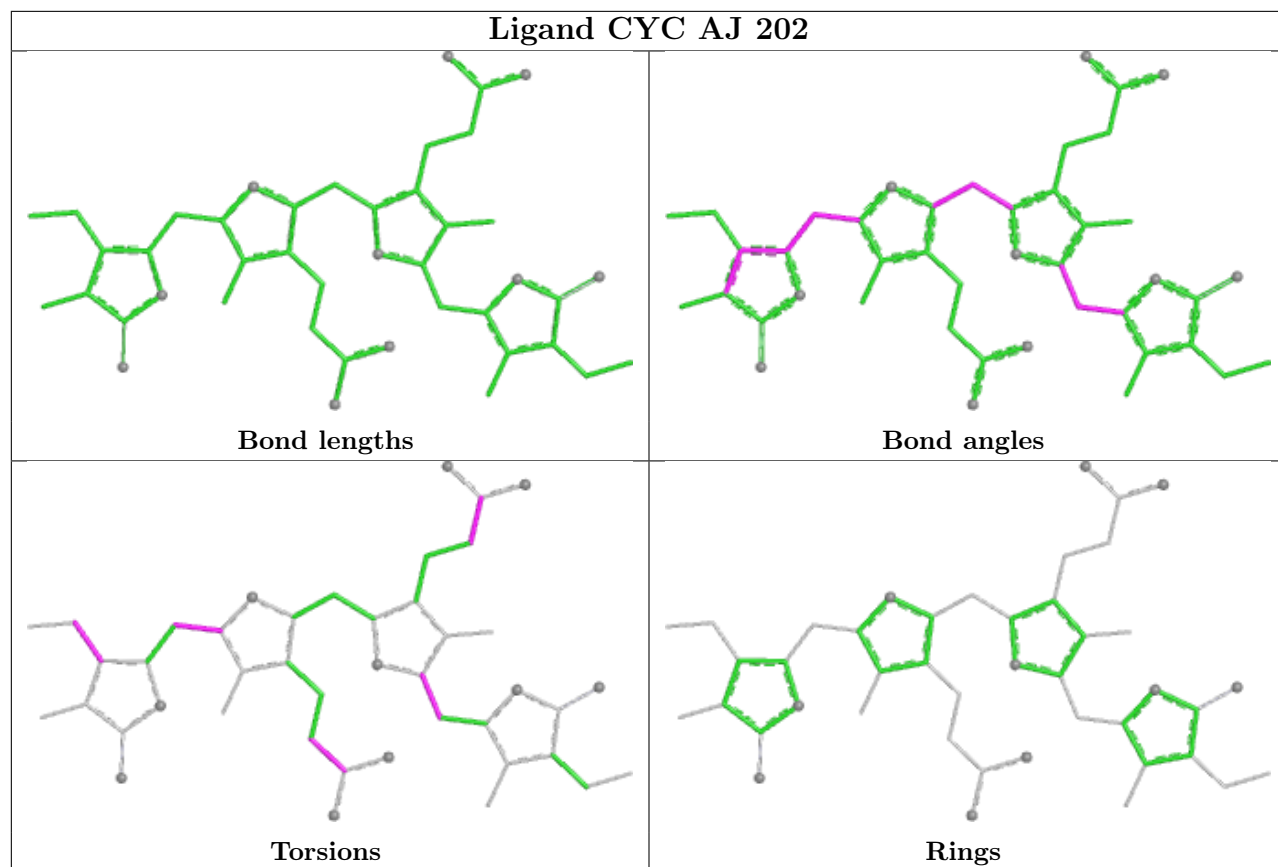
Ligand CYC AP 201



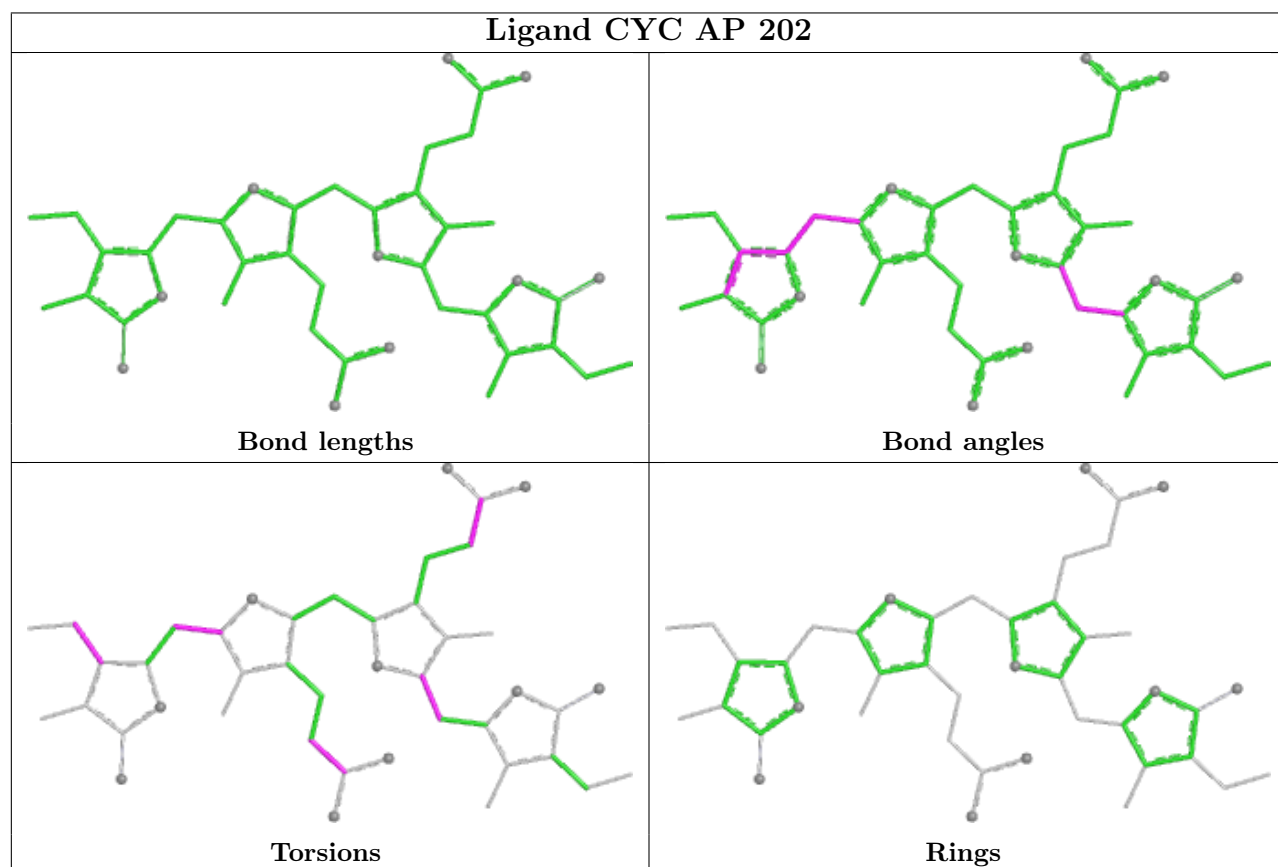
Ligand CYC BH 201



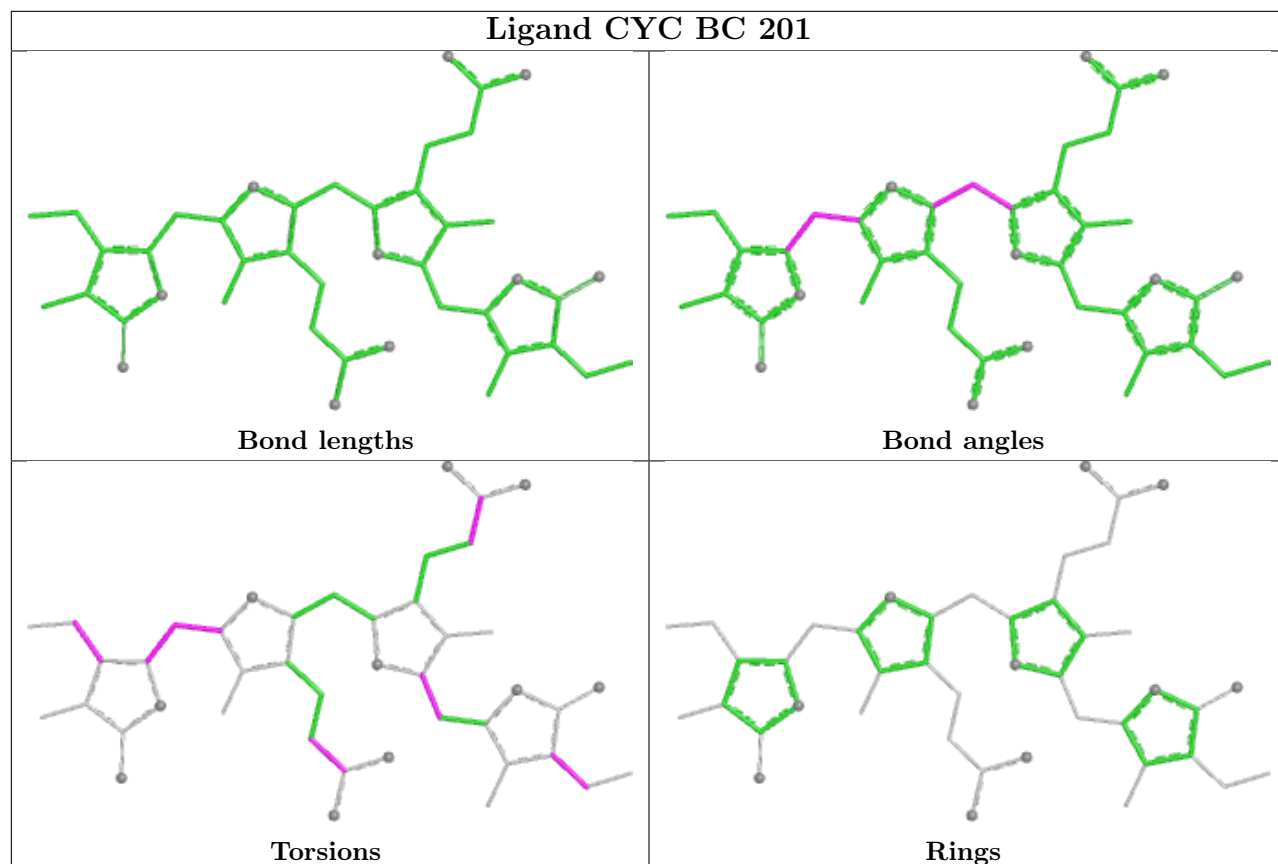
Ligand CYC AJ 202



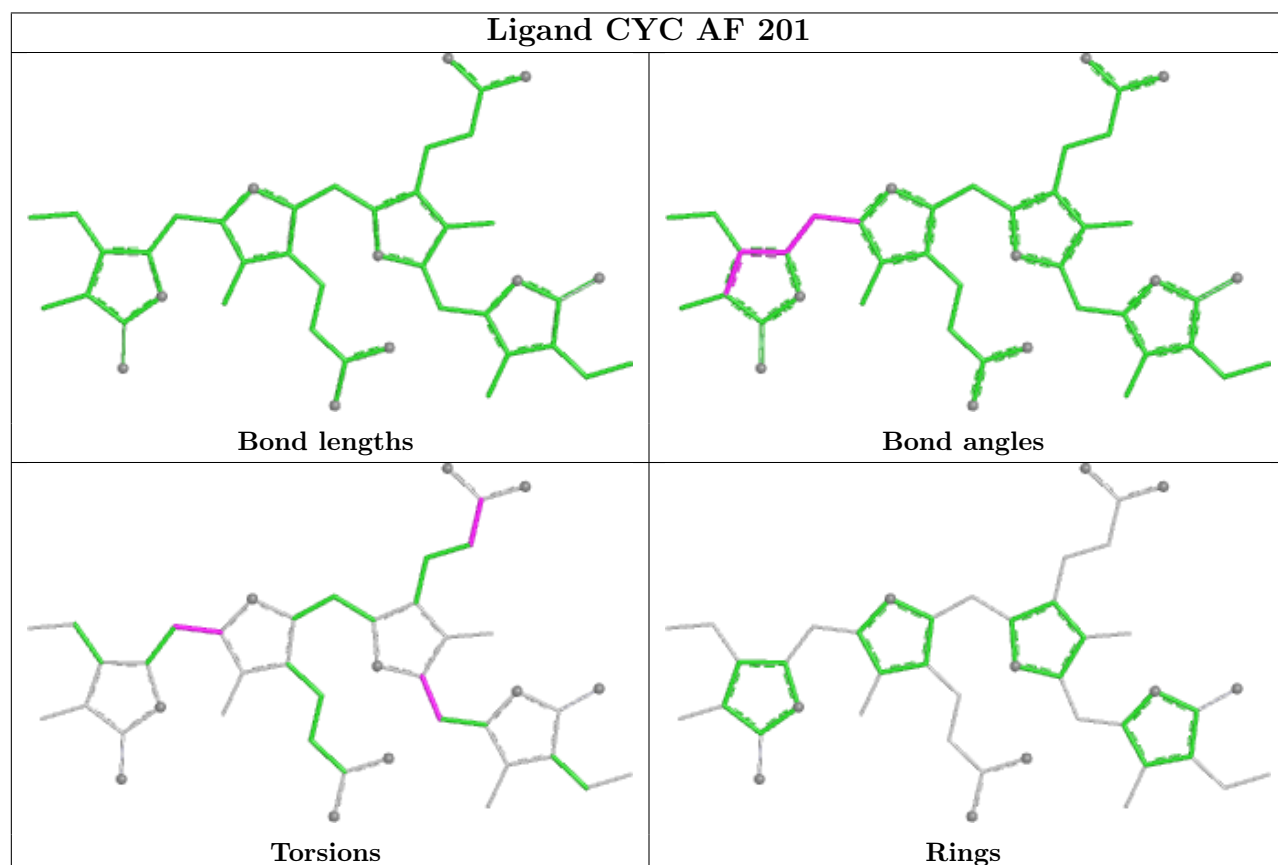
Ligand CYC AP 202



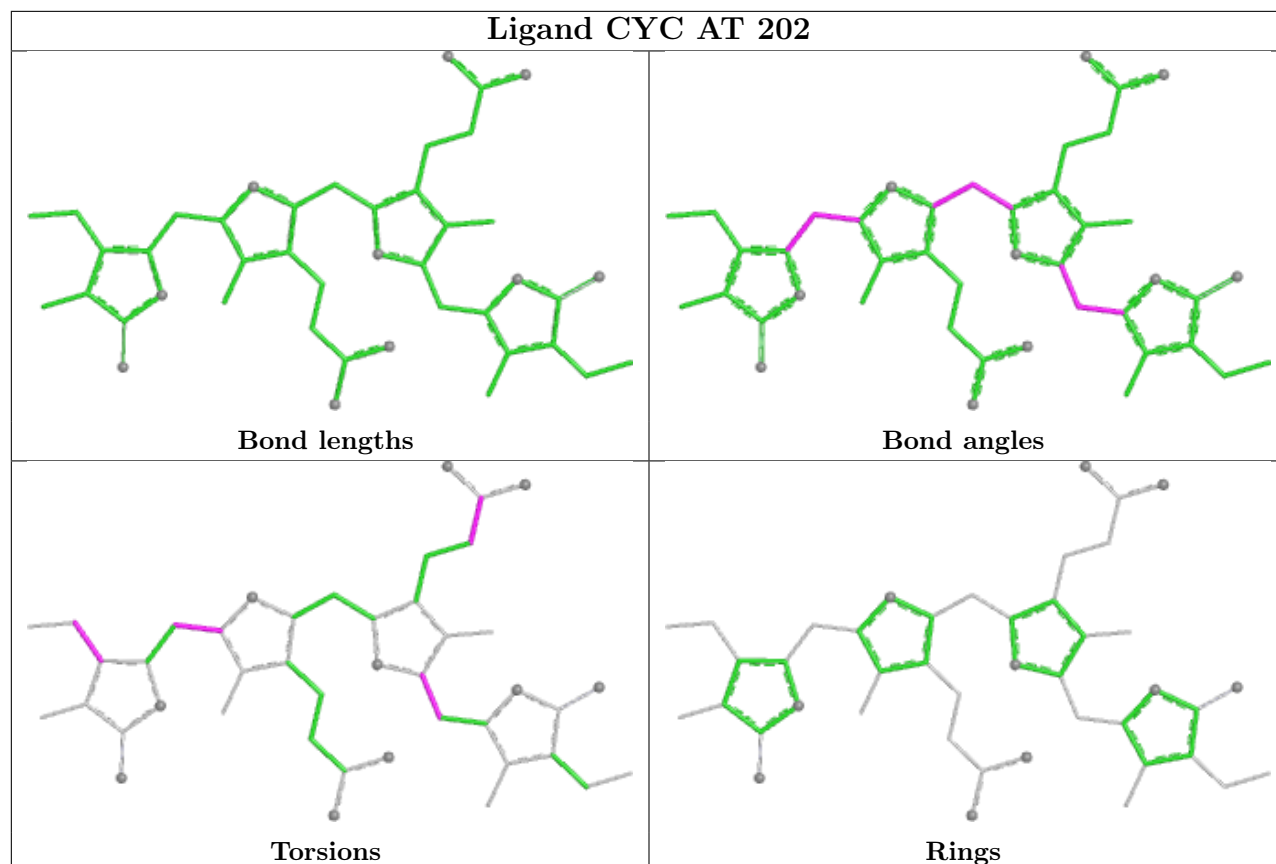
Ligand CYC BC 201



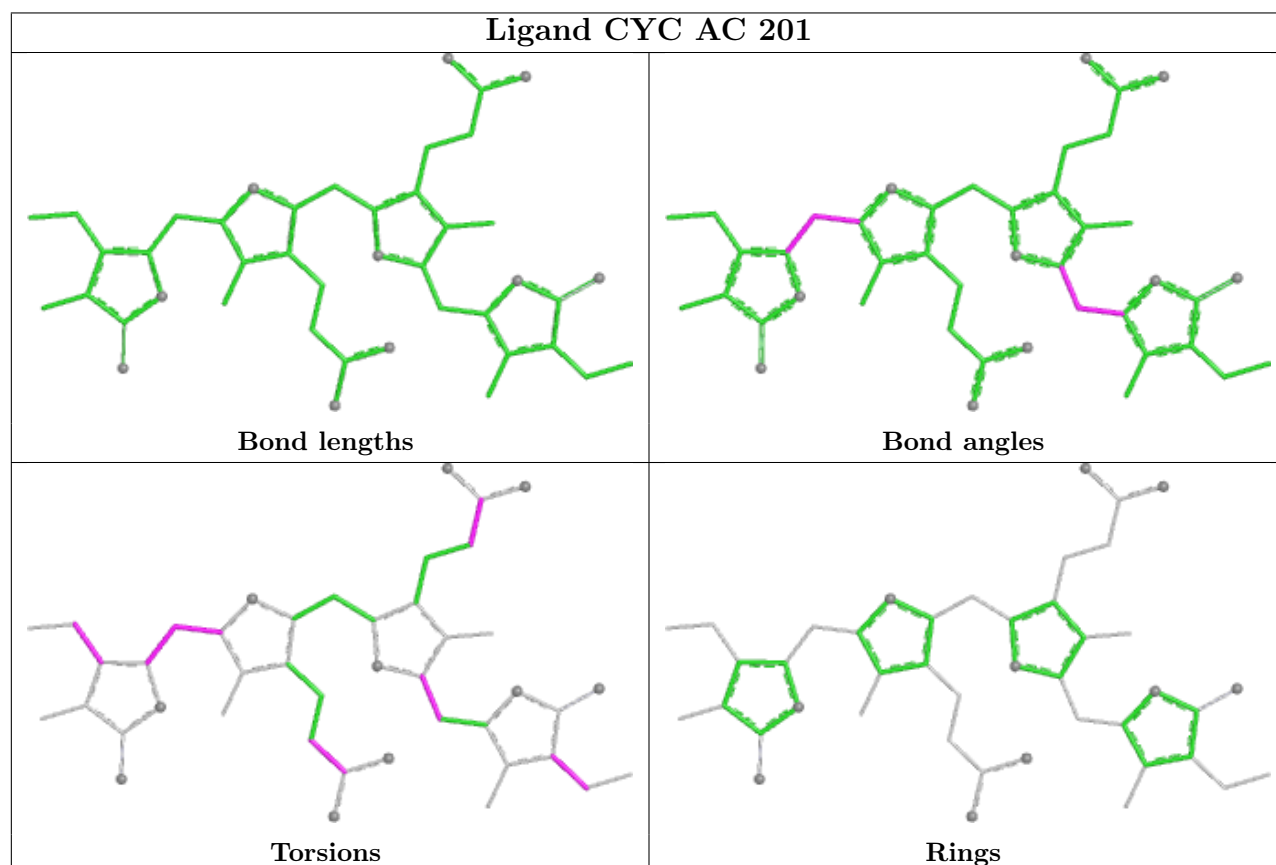
Ligand CYC AF 201



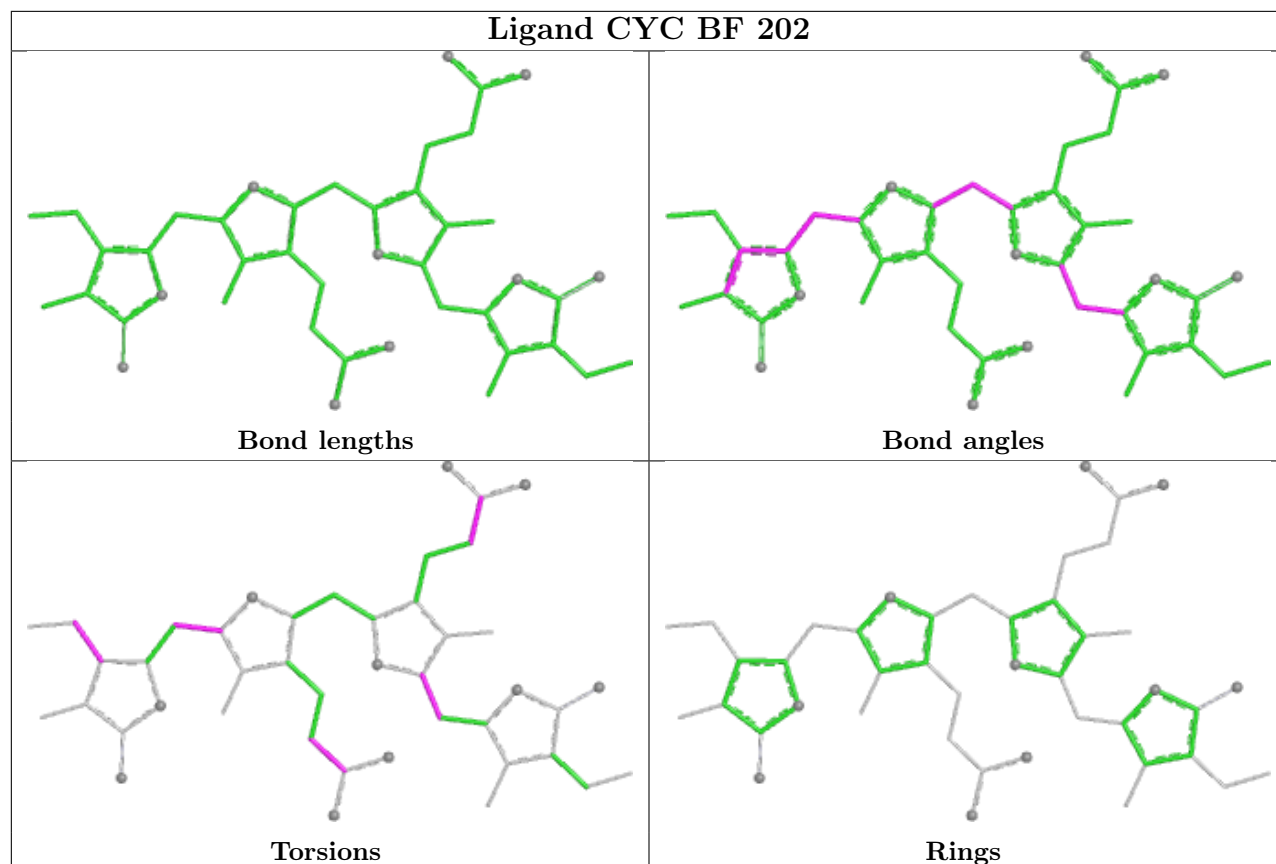
Ligand CYC AT 202



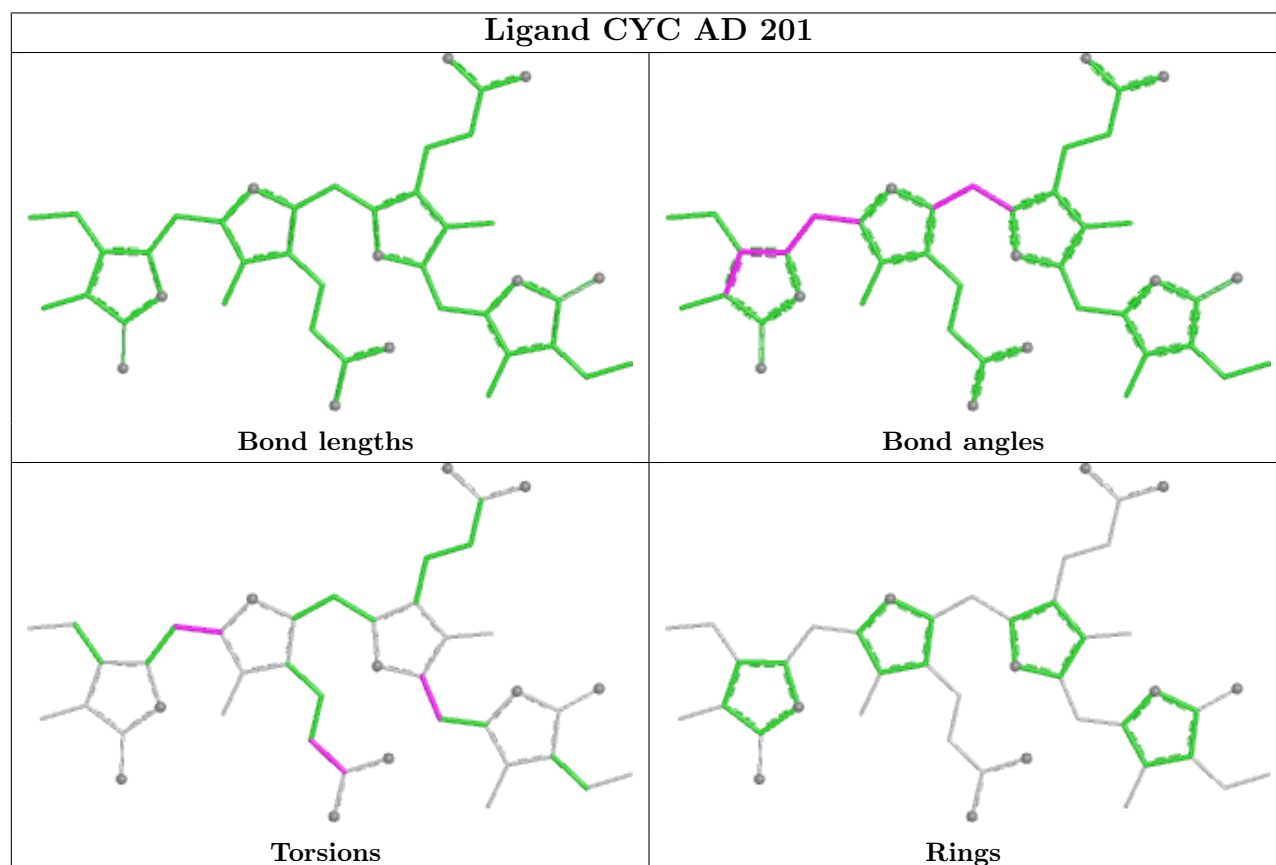
Ligand CYC AC 201

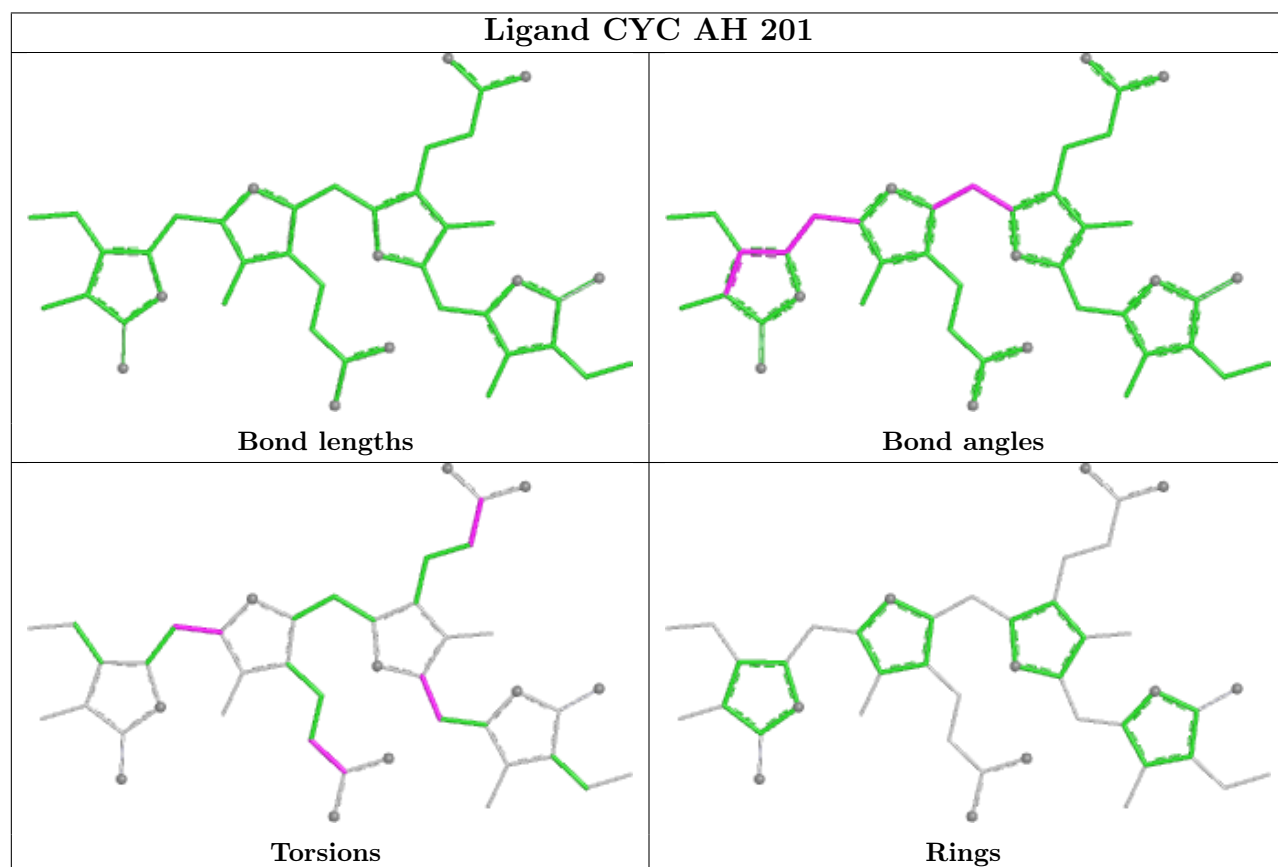
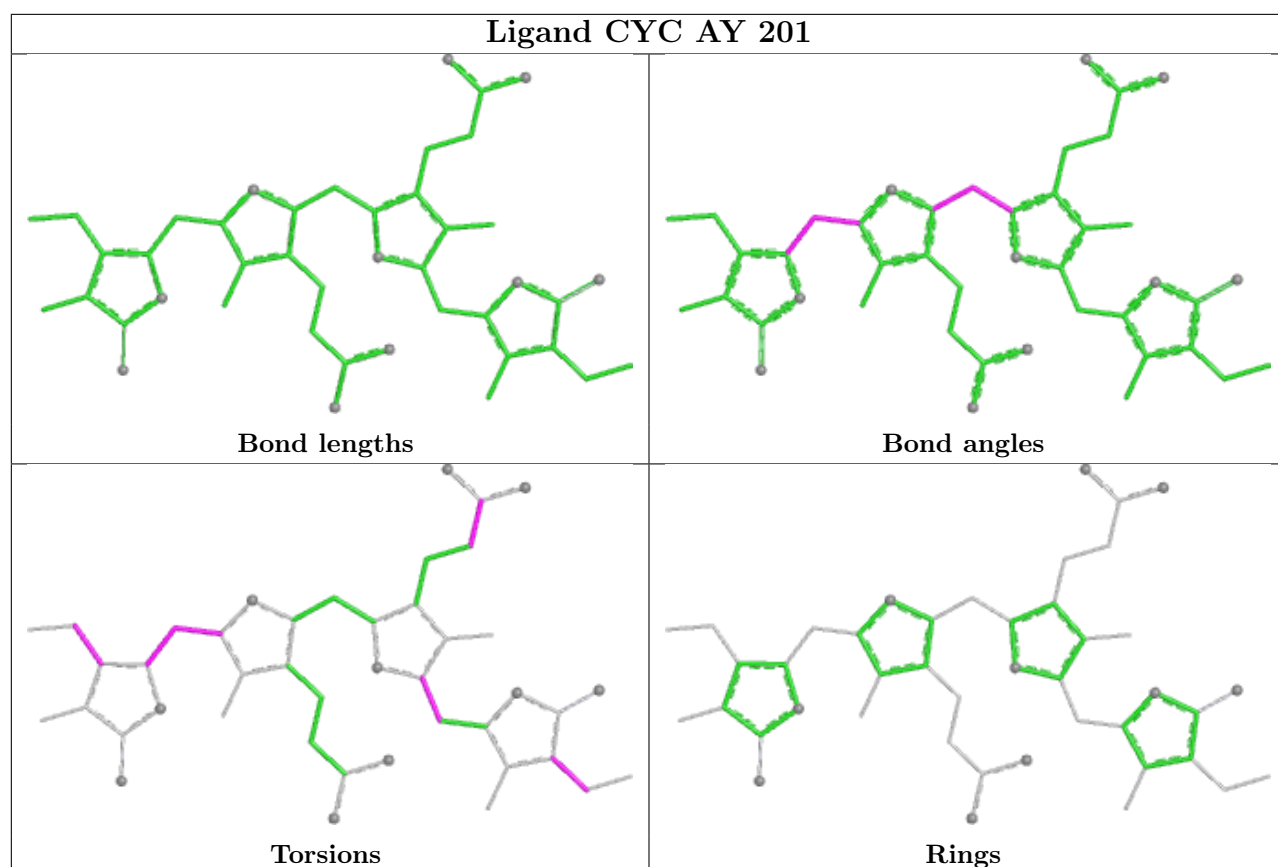


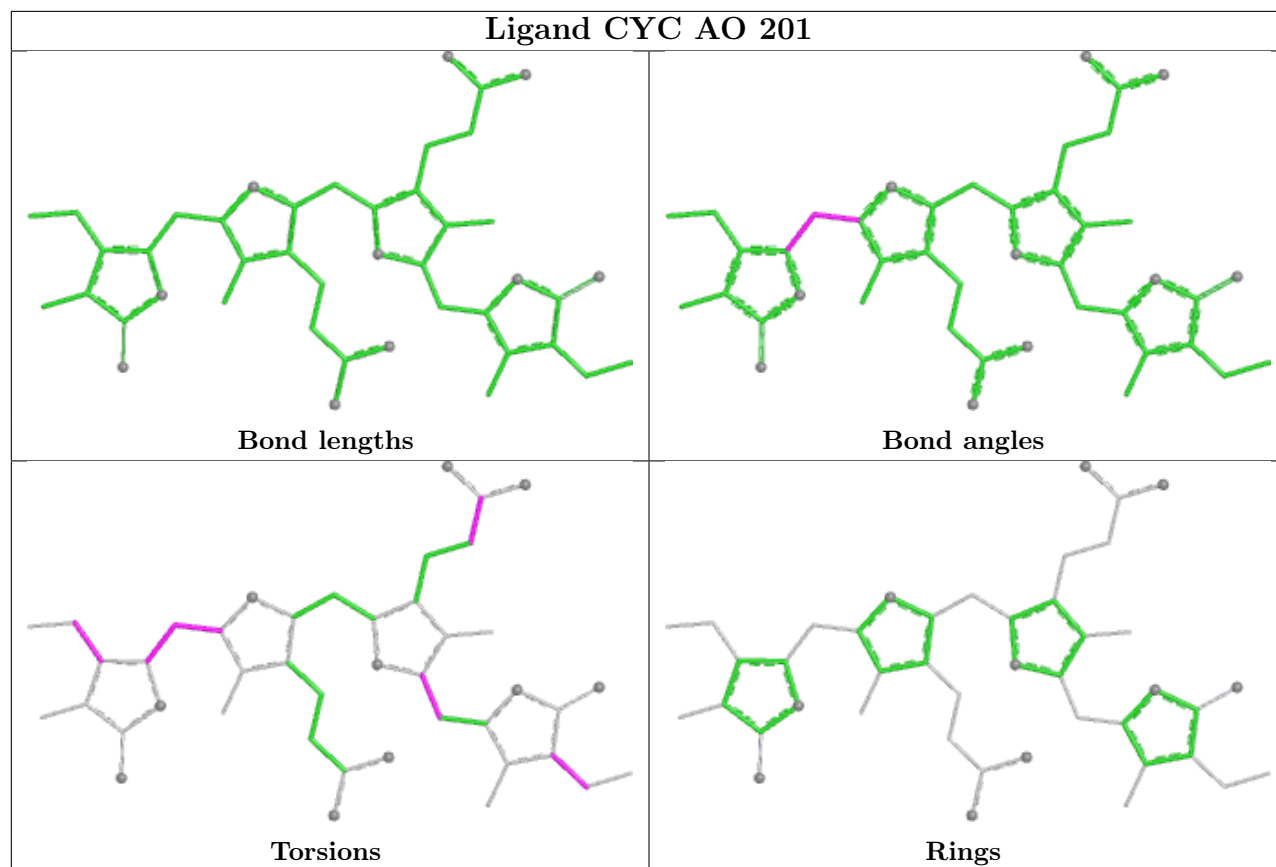
Ligand CYC BF 202



Ligand CYC AD 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.

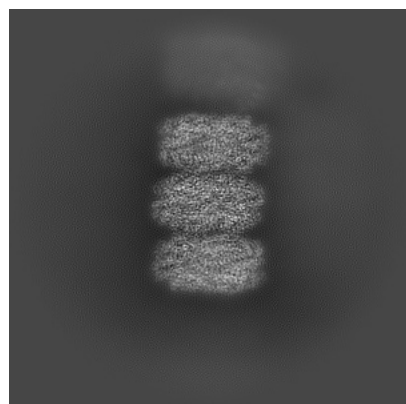
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25031. These allow visual inspection of the internal detail of the map and identification of artifacts.

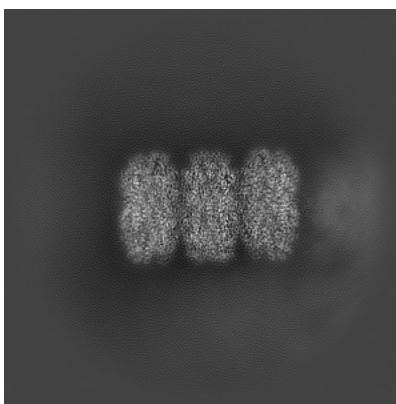
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

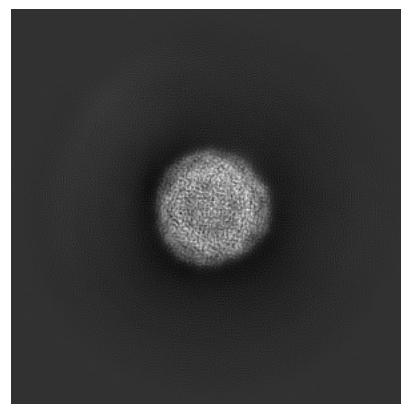
6.1.1 Primary map



X

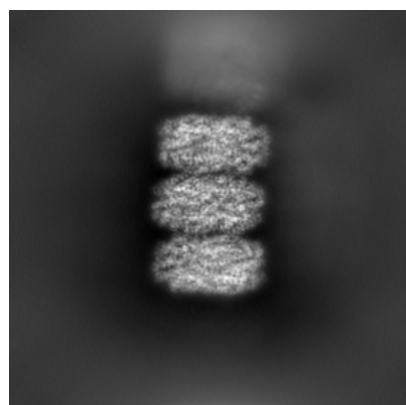


Y

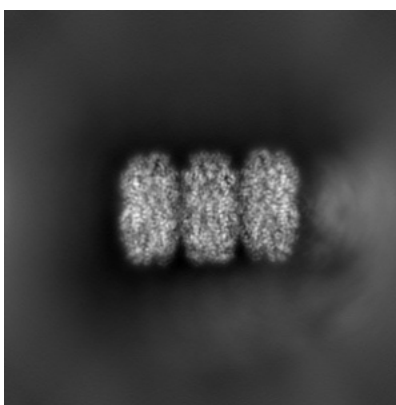


Z

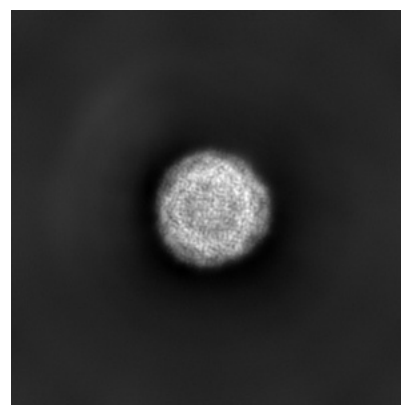
6.1.2 Raw map



X



Y

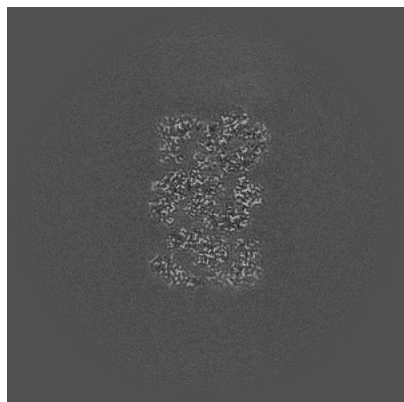


Z

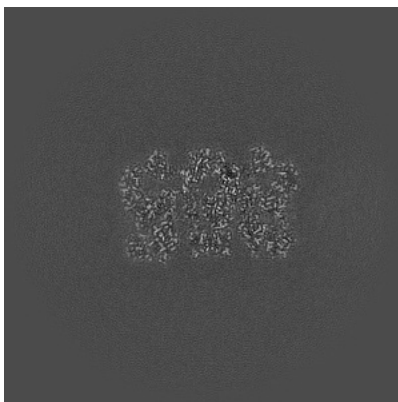
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

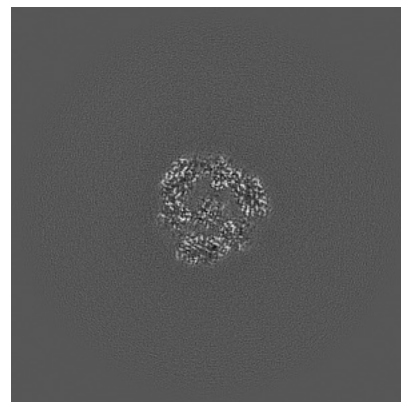
6.2.1 Primary map



X Index: 180

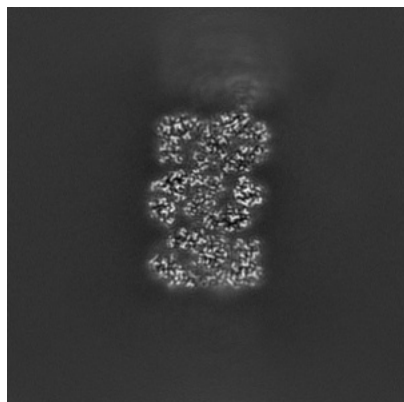


Y Index: 180

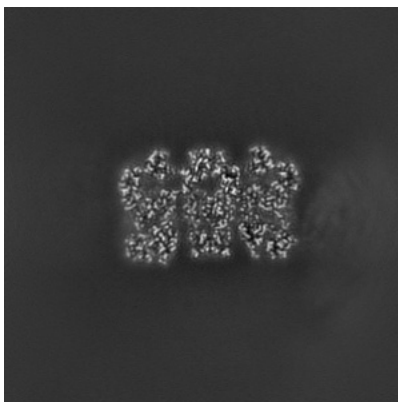


Z Index: 180

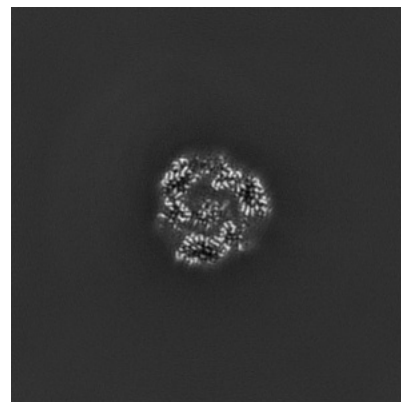
6.2.2 Raw map



X Index: 180



Y Index: 180

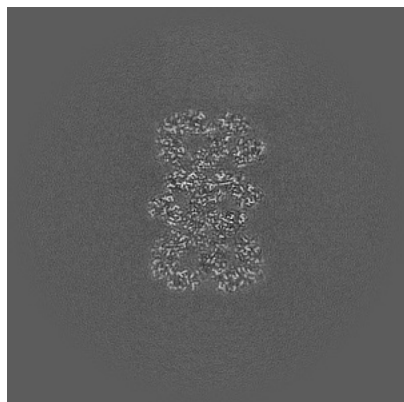


Z Index: 180

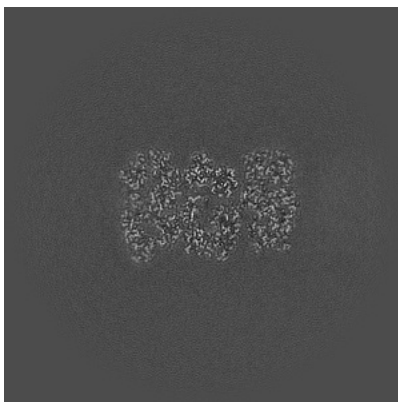
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

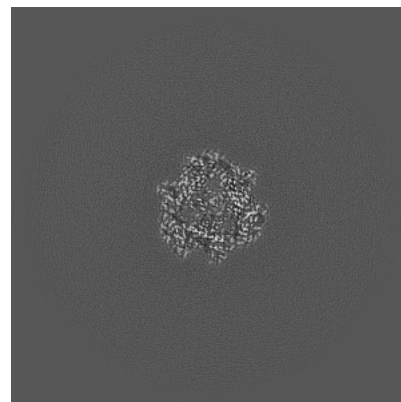
6.3.1 Primary map



X Index: 171

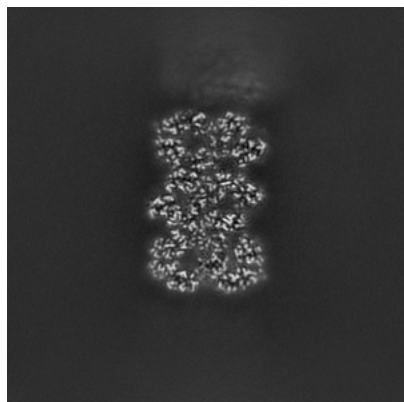


Y Index: 194

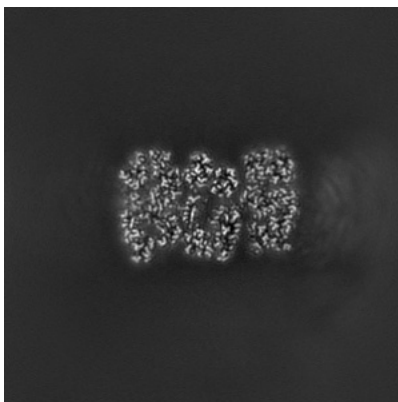


Z Index: 197

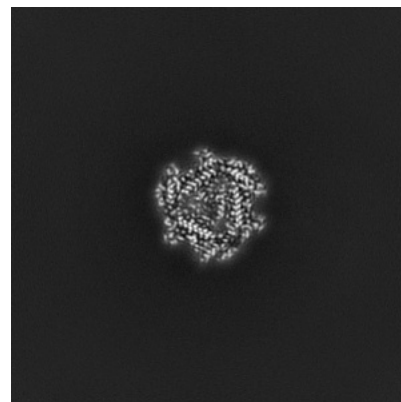
6.3.2 Raw map



X Index: 170



Y Index: 194

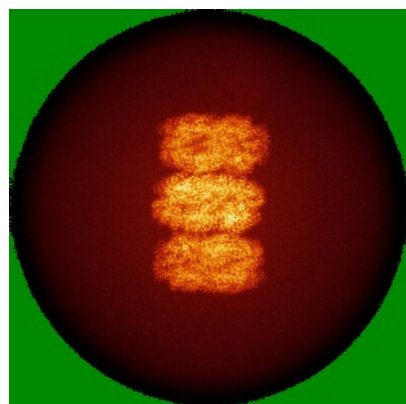


Z Index: 119

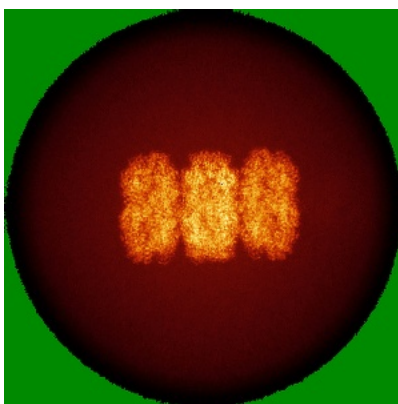
The images above show the largest variance slices of the map in three orthogonal directions.

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

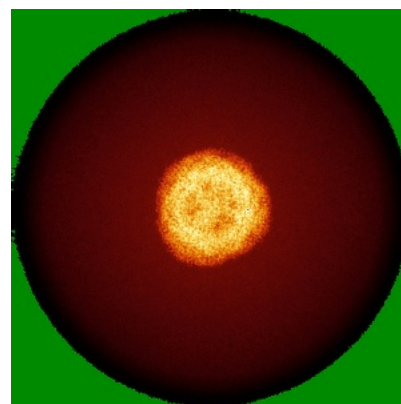
6.4.1 Primary map



X

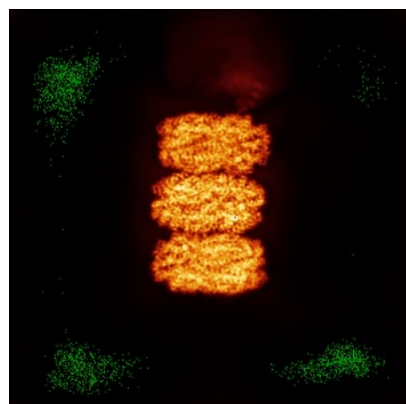


Y

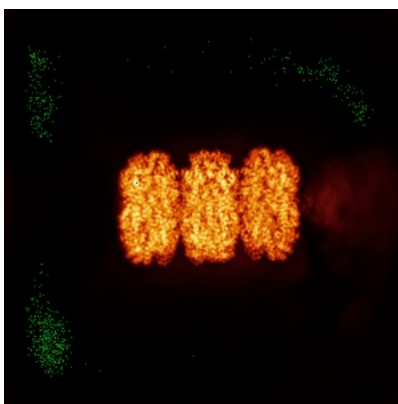


Z

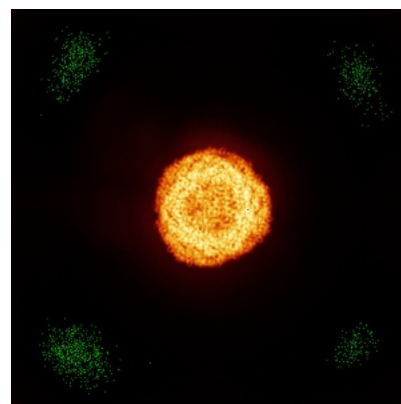
6.4.2 Raw map



X



Y

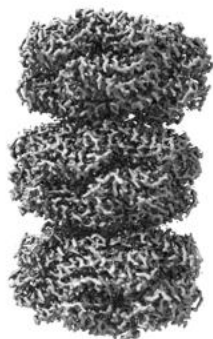


Z

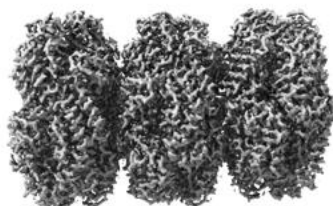
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

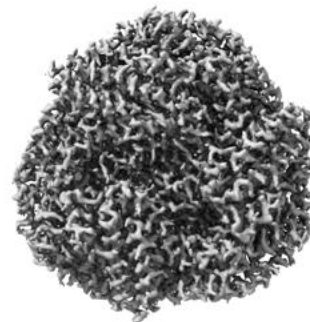
6.5.1 Primary map



X



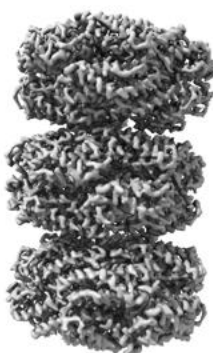
Y



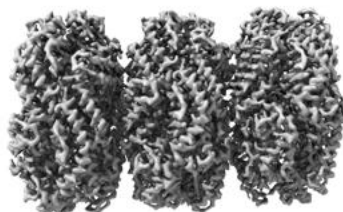
Z

The images above show the 3D surface view of the map at the recommended contour level 1.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

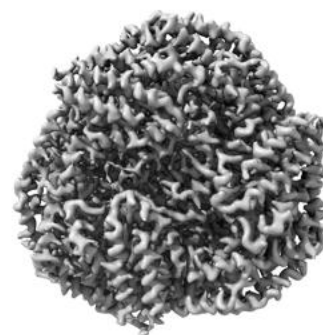
6.5.2 Raw map



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.

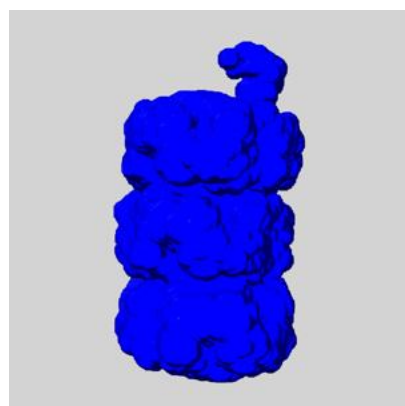
6.6 Mask visualisation [i](#)

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

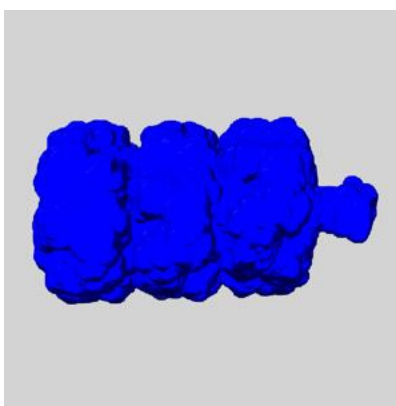
A mask typically either:

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

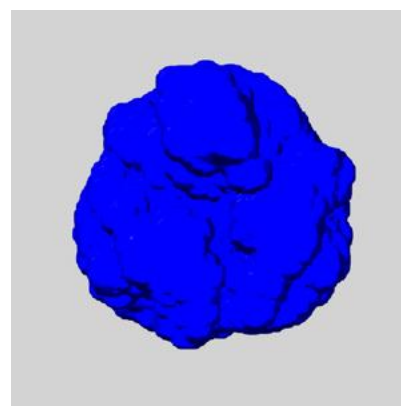
6.6.1 emd_25031_msk_1.map [i](#)



X



Y

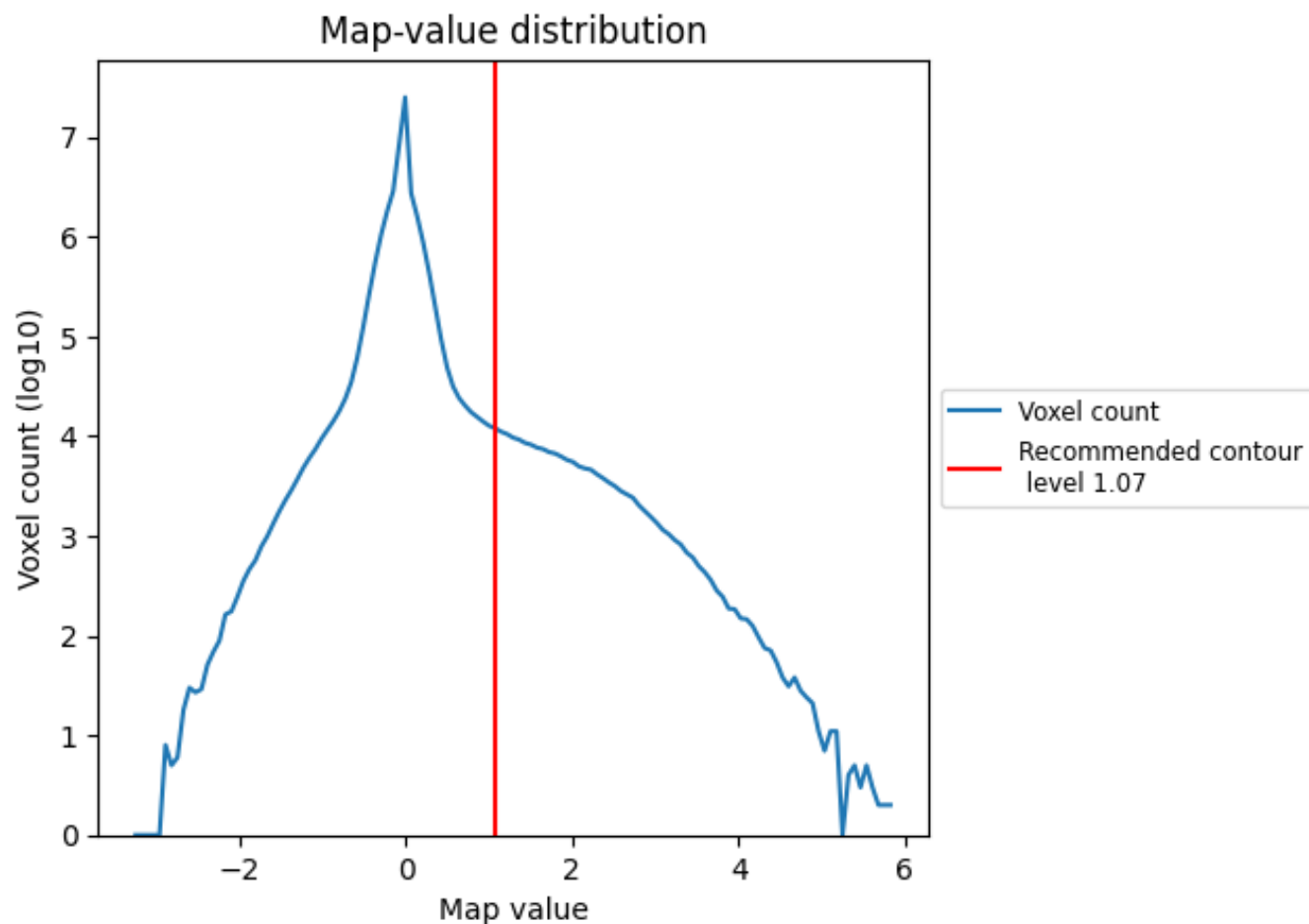


Z

7 Map analysis [i](#)

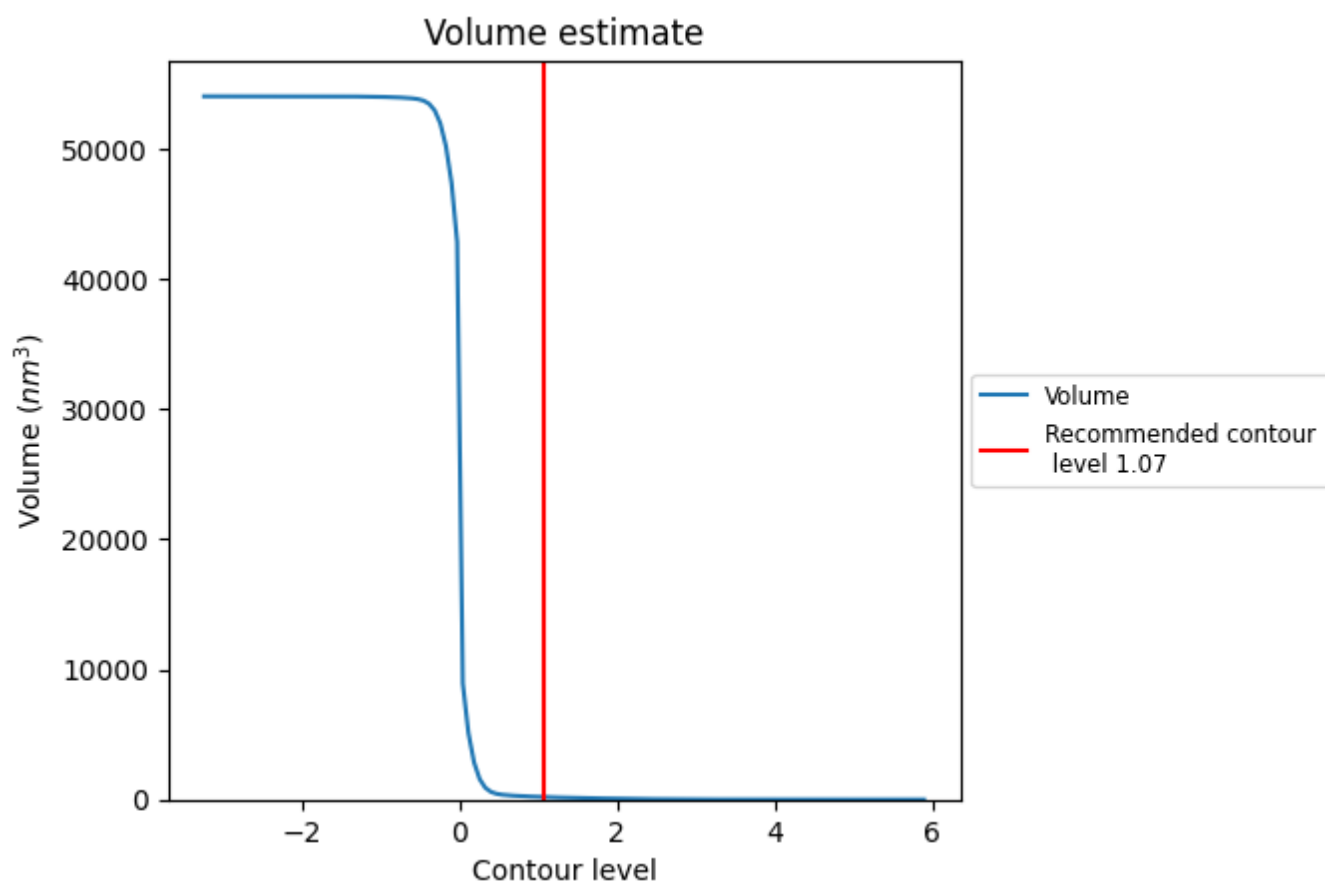
This section contains the results of statistical analysis of the map.

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.

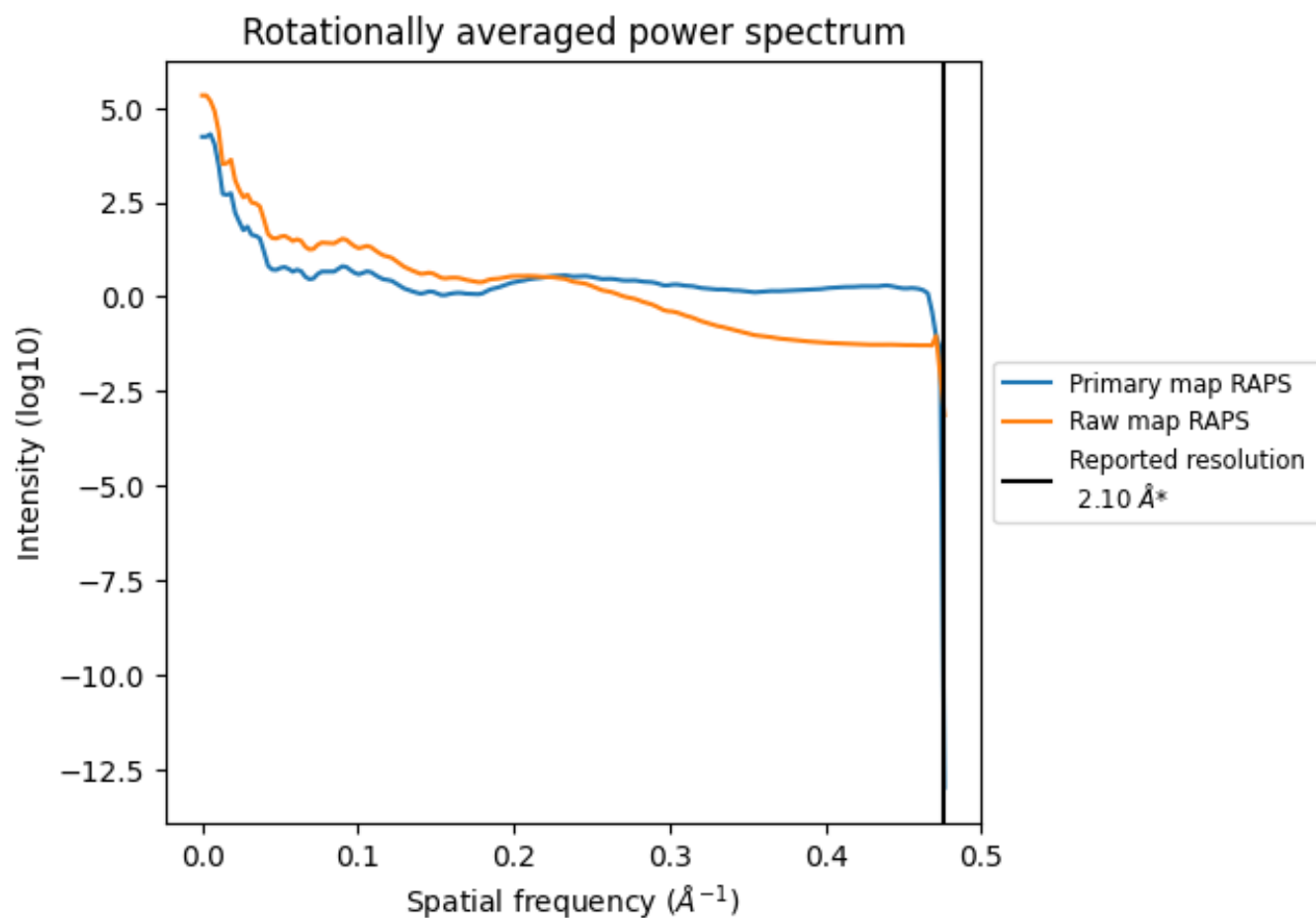
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 195 nm³; this corresponds to an approximate mass of 176 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 ⓘ

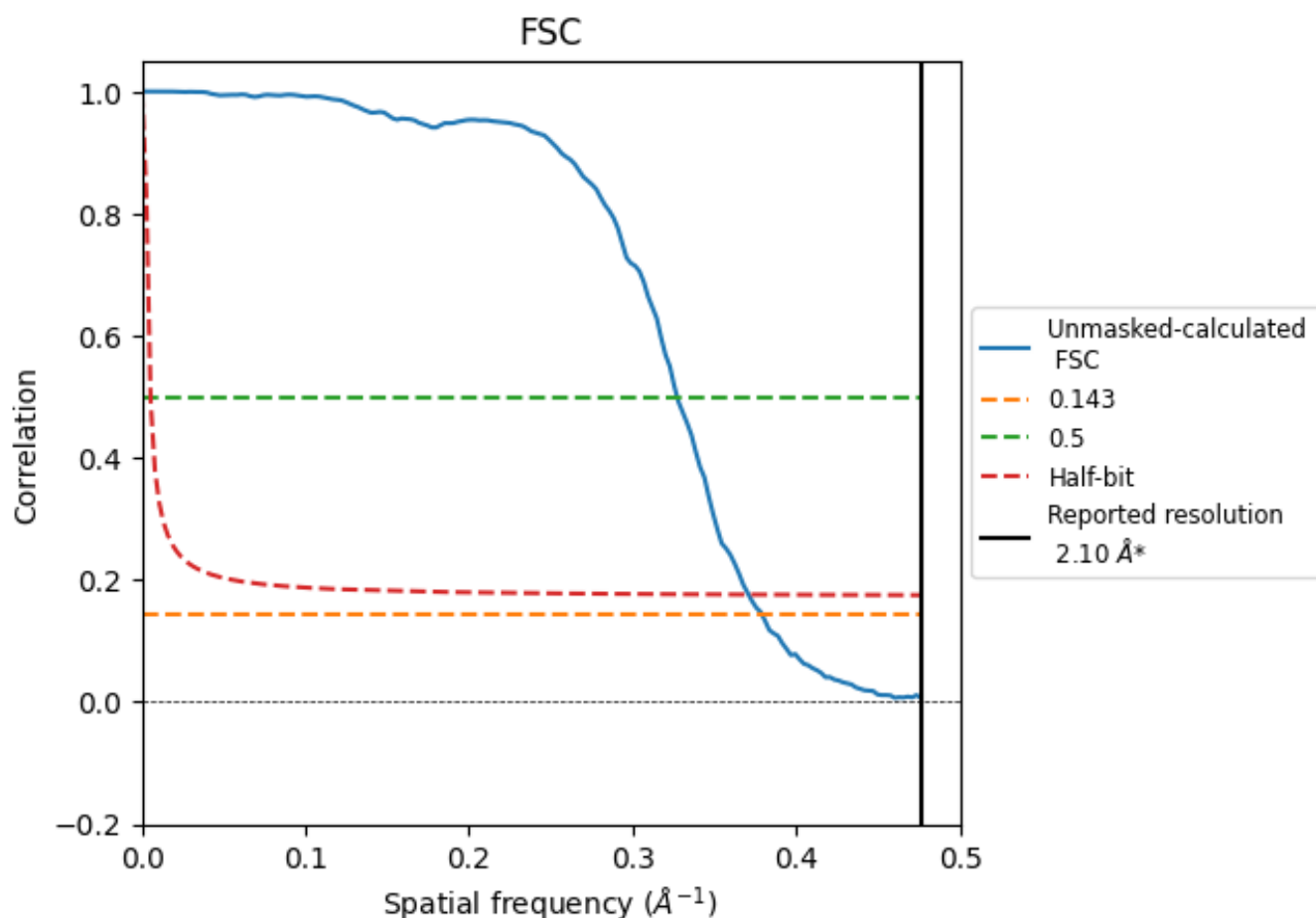


*Reported resolution corresponds to spatial frequency of 0.476 Å⁻¹

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 0.476 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

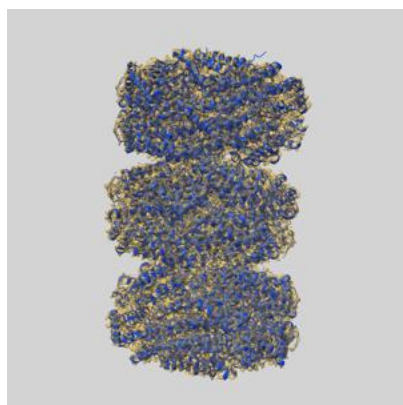
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.64	3.06	2.70

*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 2.64 differs from the reported value 2.1 by more than 10 %

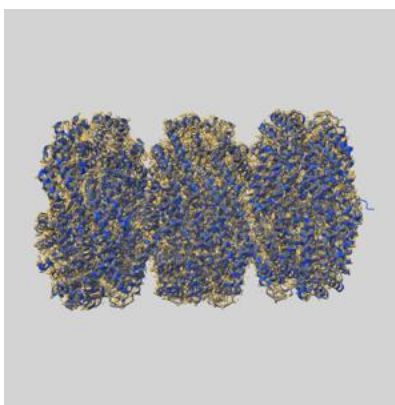
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25031 and PDB model 7SCA. Per-residue inclusion information can be found in section 3 on page 13.

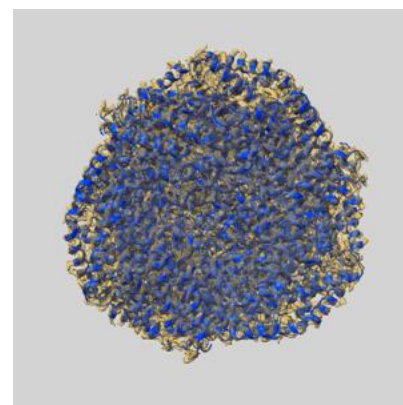
9.1 Map-model overlay [i](#)



X



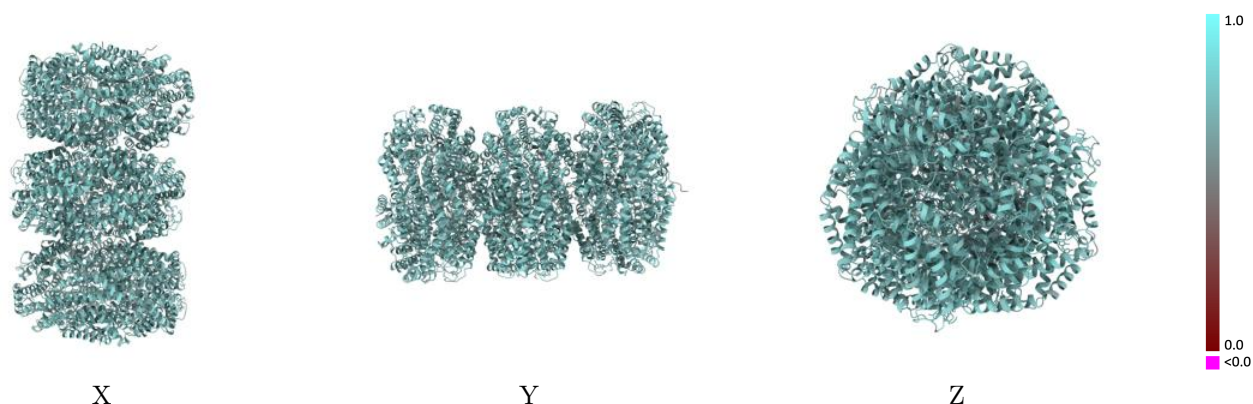
Y



Z

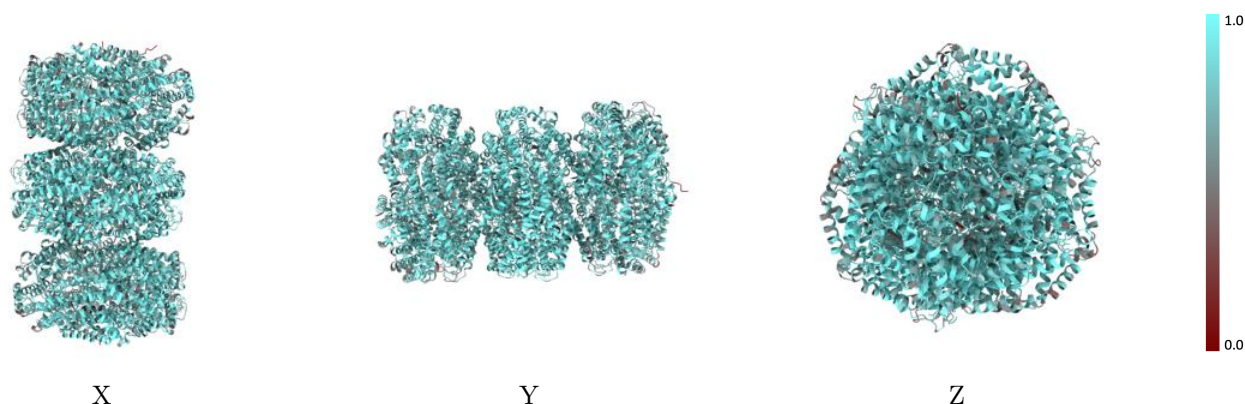
The images above show the 3D surface view of the map at the recommended contour level 1.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



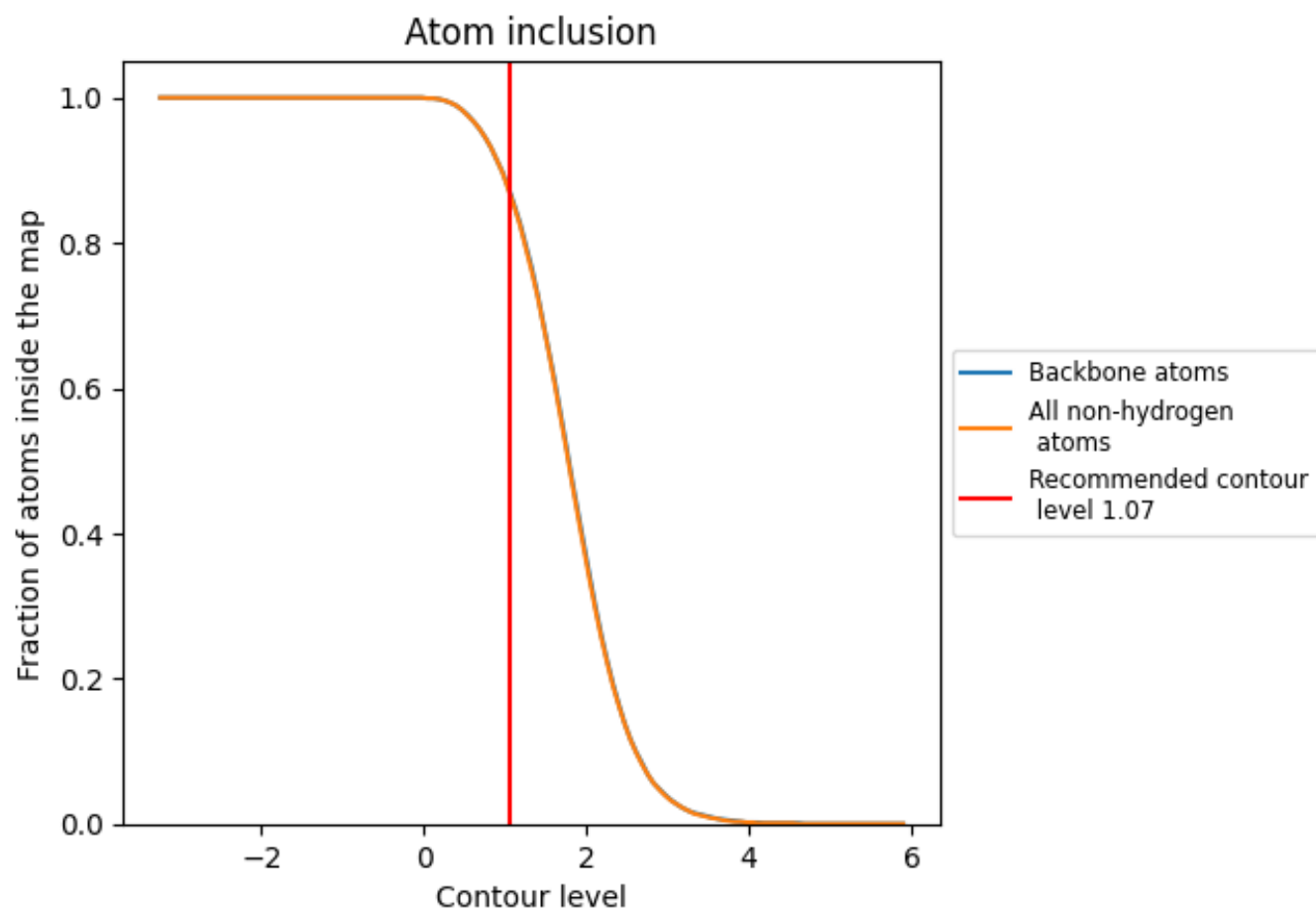
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 86% 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 (1.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8650	 0.7120
AA	 0.8400	 0.7030
AB	 0.8480	 0.7060
AC	 0.8450	 0.7030
AD	 0.8410	 0.6970
AE	 0.8420	 0.6910
AF	 0.8200	 0.6930
AG	 0.8760	 0.7050
AH	 0.8780	 0.7170
AI	 0.8680	 0.7100
AJ	 0.8820	 0.7210
AK	 0.8720	 0.7010
AL	 0.8840	 0.7140
AM	 0.9310	 0.7250
AN	 0.9350	 0.7320
AO	 0.9270	 0.7330
AP	 0.9120	 0.7250
AQ	 0.8910	 0.7090
AR	 0.8910	 0.7170
AS	 0.9280	 0.7250
AT	 0.9350	 0.7360
AU	 0.9280	 0.7310
AV	 0.9160	 0.7290
AW	 0.9200	 0.7240
AX	 0.9070	 0.7260
AY	 0.8600	 0.7060
AZ	 0.8790	 0.7170
BA	 0.8440	 0.6990
BB	 0.8510	 0.7160
BC	 0.8440	 0.7060
BD	 0.8550	 0.7140
BE	 0.8280	 0.7010
BF	 0.8160	 0.6970
BG	 0.8430	 0.6930
BH	 0.8230	 0.7000



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Chain	Atom inclusion	Q-score
BI	 0.8290	 0.7060
BJ	 0.8410	 0.7120
BK	 0.8400	 0.7110
BL	 0.8900	 0.7280
BM	 0.8520	 0.7150
BN	 0.6530	 0.6640