



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:45 AM UTC

PDB ID : 1DXR / pdb_00001dxr
Title : Photosynthetic reaction center from Rhodopseudomonas viridis - His L168 Phe mutant (terbutryn complex)
Authors : Lancaster, C.R.D.; Bibikova, M.; Sabatino, P.; Oesterhelt, D.; Michel, H.
Deposited on : 2000-01-15
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

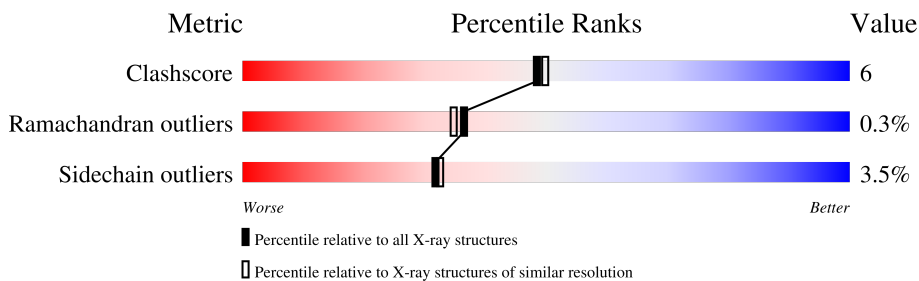
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	336	 88% 10% ..
2	H	258	 86% 12% .
3	L	273	 89% 10% .
4	M	323	 86% 12% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	BCB	L	400	X	-	-	-
8	BCB	L	401	X	-	-	-
8	BCB	M	400	X	-	-	-
8	BCB	M	401	X	-	-	-
9	BPB	M	402	X	-	-	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 10777 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	332	Total	C	N	O	S	39	4	0
			2636	1658	474	486	18			

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER H SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	258	Total	C	N	O	S	118	0	0
			2018	1292	344	380	2			

- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER L SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	273	Total	C	N	O	S	13	0	0
			2172	1462	348	355	7			

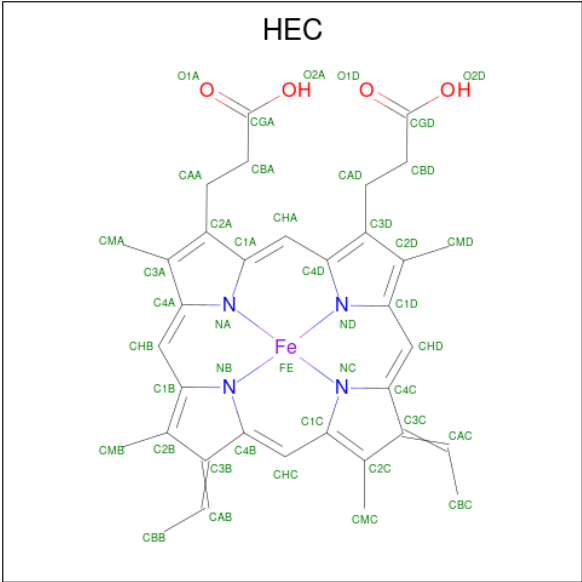
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	168	PHE	HIS	engineered mutation	UNP P06009

- Molecule 4 is a protein called PHOTOSYNTHETIC REACTION CENTER M SUBUNIT.

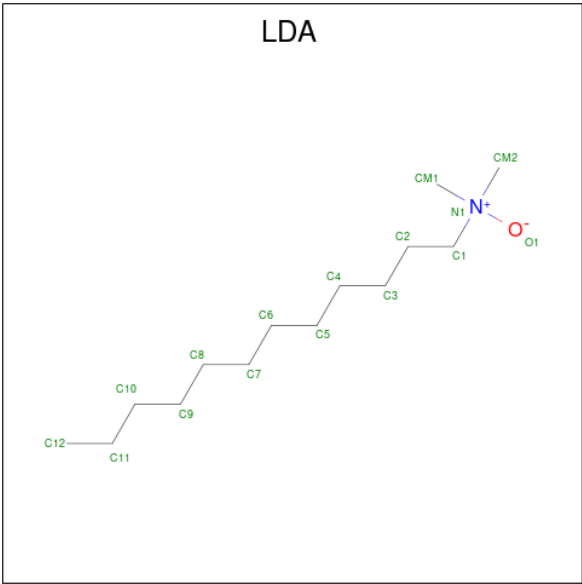
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	15	2	0
			2569	1710	421	425	13			

- Molecule 5 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



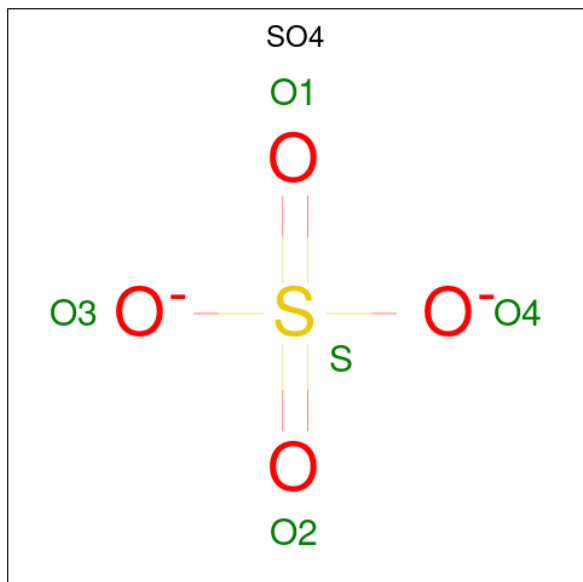
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



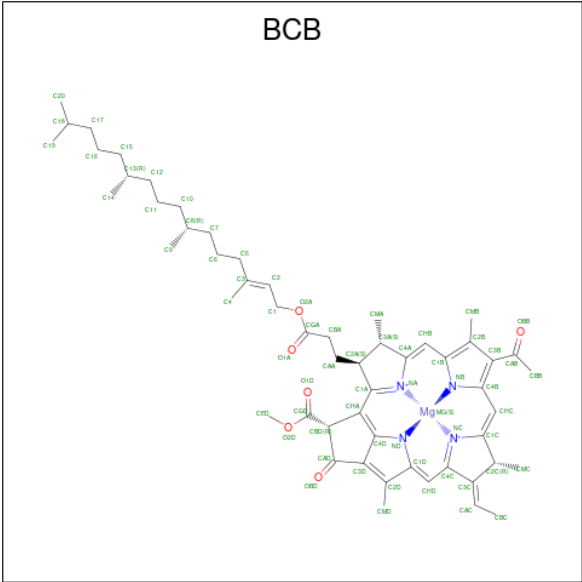
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	3	0
			16	14	1	1		
6	M	1	Total	C	N	O	4	0
			16	14	1	1		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



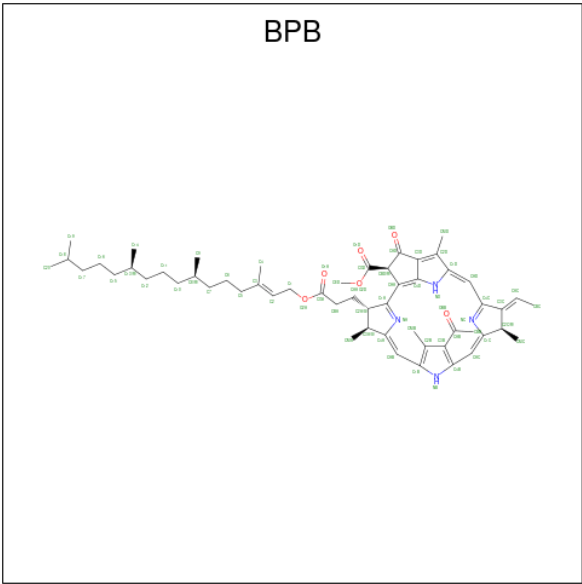
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	H	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is BACTERIOCHLOROPHYLL B (CCD ID: BCB) (formula: C₅₅H₇₂MgN₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
8	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
8	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
8	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 9 is BACTERIOPHEOPHYTIN B (CCD ID: BPB) (formula: C₅₅H₇₄N₄O₆).

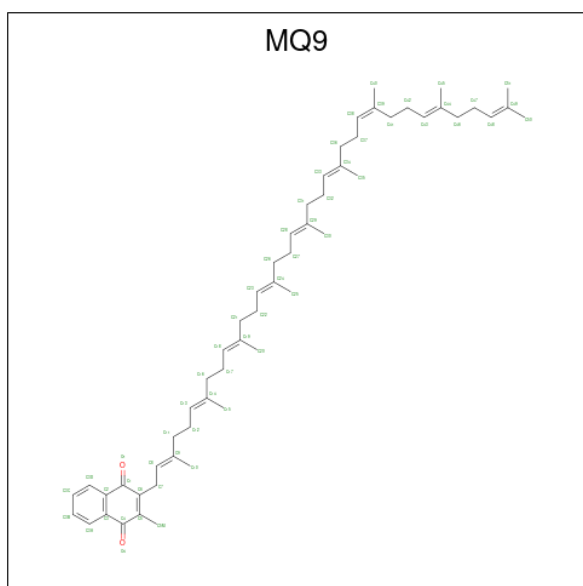


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	L	1	Total	C	N	O	0	0
			65	55	4	6		
9	M	1	Total	C	N	O	7	0
			65	55	4	6		

- Molecule 10 is FE (II) ION (CCD ID: FE2) (formula: Fe).

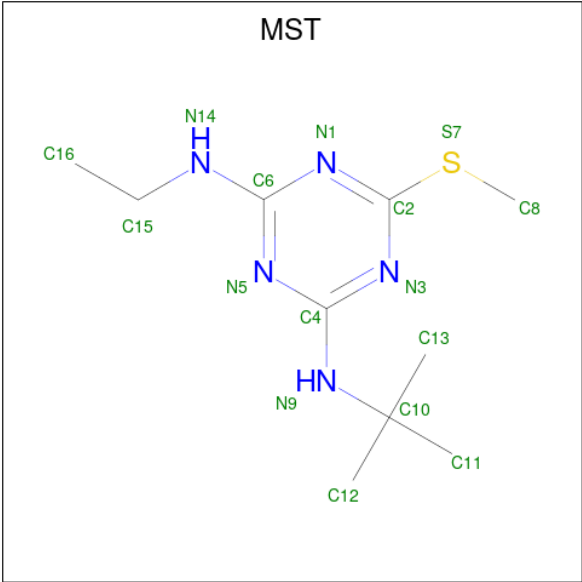
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	L	1	Total	Fe	0	0
			1	1		

- Molecule 11 is MENAQUINONE-9 (CCD ID: MQ9) (formula: C₅₆H₈₀O₂).



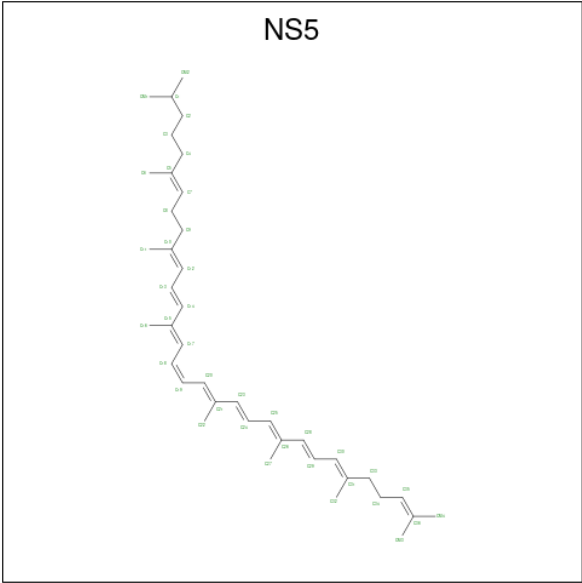
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	O	0	0
			58	56	2		

- Molecule 12 is 2-T-BUTYLAMINO-4-ETHYLAMINO-6-METHYLTHIO-S-TRIAZINE (CCD ID: MST) (formula: C₁₀H₁₉N₅S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	L	1	Total	C	N	S	0	0
			16	10	5	1		

- Molecule 13 is 15-cis-1,2-dihydroneurosporene (CCD ID: NS5) (formula: C₄₀H₆₀).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	M	1	Total	C	14	0
			40	40		

- Molecule 14 is water.

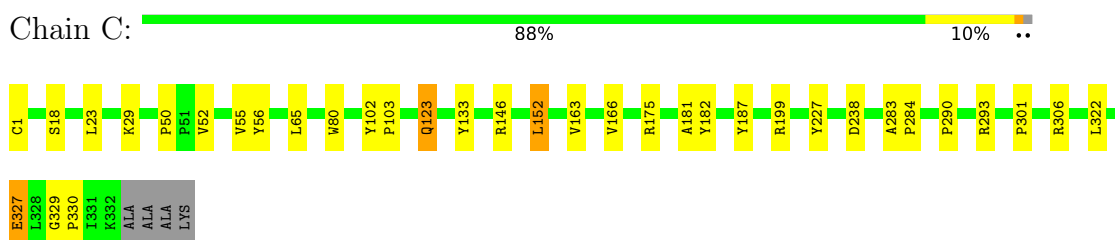
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	222	Total O 222 222	0	0
14	H	146	Total O 146 146	0	0
14	H	1	Total O 1 1	0	0
14	H	2	Total O 2 2	0	0
14	H	1	Total O 1 1	0	0
14	L	88	Total O 88 88	0	0
14	L	1	Total O 1 1	0	0
14	M	120	Total O 120 120	0	0
14	M	1	Total O 1 1	0	0
14	M	1	Total O 1 1	0	0
14	M	1	Total O 1 1	0	0
14	M	1	Total O 1 1	0	0

3 Residue-property plots

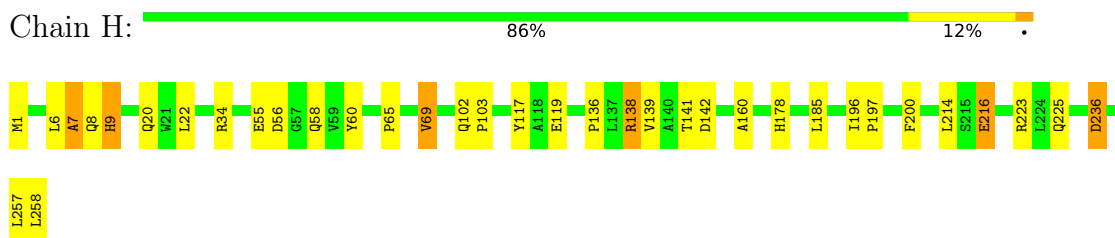
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

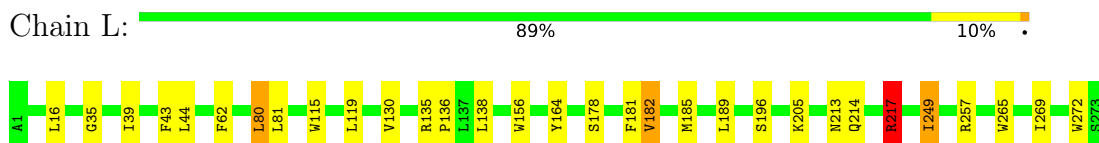
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT



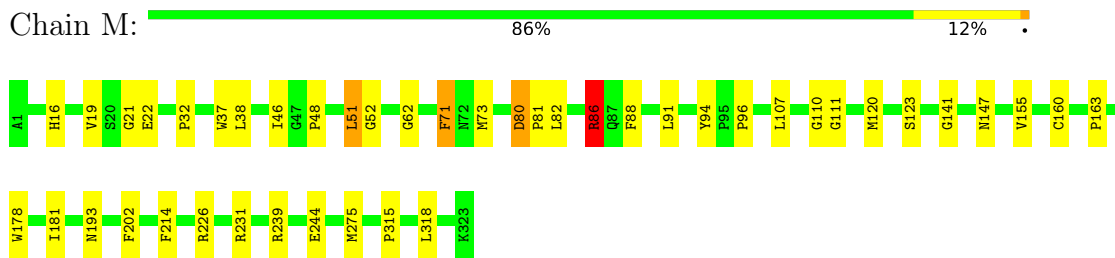
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER H SUBUNIT



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER L SUBUNIT



• Molecule 4: PHOTOSYNTHETIC REACTION CENTER M SUBUNIT



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	223.50 Å 223.50 Å 113.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00	Depositor
% Data completeness (in resolution range)	97.5 (10.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.194 , 0.218	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10777	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, MST, NS5, MQ9, LDA, SO4, FME, BCB, BPB, FE2

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	C	0.61	0/2703	0.81	0/3683
2	H	0.65	0/2055	0.79	0/2807
3	L	0.64	0/2260	0.80	1/3085 (0.0%)
4	M	0.61	0/2673	0.80	4/3655 (0.1%)
All	All	0.63	0/9691	0.80	5/13230 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	4
2	H	0	4
3	L	0	2
4	M	0	2
All	All	0	12

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	182	VAL	CB-CA-C	-5.32	104.96	112.14
4	M	80	ASP	CA-C-N	5.31	124.50	118.97
4	M	80	ASP	C-N-CA	5.31	124.50	118.97
4	M	94	TYR	CA-C-N	5.04	125.58	120.38
4	M	94	TYR	C-N-CA	5.04	125.58	120.38

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	187	TYR	Sidechain
1	C	199[A]	ARG	Sidechain
1	C	227	TYR	Sidechain
1	C	327	GLU	Mainchain
2	H	8	GLN	Peptide

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	C	2636	0	2599	20	0
2	H	2018	0	2020	21	0
3	L	2172	0	2100	34	0
4	M	2569	0	2464	30	0
5	C	172	0	120	2	0
6	H	32	0	62	3	0
6	L	16	0	31	4	0
6	M	48	0	93	2	0
7	H	5	0	0	0	0
7	M	15	0	0	1	0
8	L	132	0	144	4	0
8	M	132	0	144	12	0
9	L	65	0	74	2	0
9	M	65	0	74	7	0
10	L	1	0	0	0	0
11	L	58	0	80	1	0
12	L	16	0	19	0	0
13	M	40	0	60	2	0
14	C	222	0	0	0	0
14	H	150	0	0	0	0
14	L	89	0	0	2	0
14	M	124	0	0	2	0
All	All	10777	0	10084	109	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 6.

The worst 5 of 109 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)
9:M:402:BPB:HHC	9:M:402:BPB:HBBB	1.46	0.94
8:M:400:BCB:HBB2	8:M:400:BCB:HHC	1.50	0.91
3:L:62:PHE:HD2	6:L:1274:LDA:HM11	1.48	0.77
3:L:185:MET:SD	8:M:400:BCB:H41	2.29	0.73
2:H:65:PRO:HG3	6:H:1260:LDA:H72	1.70	0.72

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 X-ray entries followed by that with respect to entries of similar resolution.

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	C	334/336 (99%)	327 (98%)	7 (2%)	0	100	100
2	H	256/258 (99%)	245 (96%)	9 (4%)	2 (1%)	16	11
3	L	271/273 (99%)	265 (98%)	6 (2%)	0	100	100
4	M	323/323 (100%)	314 (97%)	8 (2%)	1 (0%)	36	35
All	All	1184/1190 (100%)	1151 (97%)	30 (2%)	3 (0%)	36	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	7	ALA
2	H	9	HIS
4	M	193	ASN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	C	284/282 (101%)	276 (97%)	8 (3%)	38	41
2	H	212/212 (100%)	201 (95%)	11 (5%)	21	18
3	L	218/218 (100%)	211 (97%)	7 (3%)	34	35
4	M	251/249 (101%)	242 (96%)	9 (4%)	31	31
All	All	965/961 (100%)	930 (96%)	35 (4%)	32	31

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	M	37	TRP
4	M	51	LEU
4	M	147	ASN
2	H	185	LEU
2	H	141	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
4	M	16	HIS
3	L	239	ASN
3	L	183	ASN
3	L	158	ASN
3	L	214	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
2	FME	H	1	2	8,9,10	0.59	0	8,9,11	2.15	2 (25%)

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
2	FME	H	1	2	-	2/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	H	1	FME	O1-CN-N	-4.36	114.05	125.32
2	H	1	FME	CA-N-CN	-3.35	117.68	122.82

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	FME	O1-CN-N-CA
2	H	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
8	BCB	L	400	8,3	60,74,74	1.67	13 (21%)	59,115,115	2.54	21 (35%)
13	NS5	M	600	-	39,39,39	0.76	1 (2%)	46,46,46	1.12	4 (8%)
6	LDA	M	1326	-	13,15,15	2.58	2 (15%)	14,17,17	0.56	0
6	LDA	M	1325	-	13,15,15	2.33	2 (15%)	14,17,17	0.61	0
8	BCB	L	401	3	60,74,74	1.70	10 (16%)	59,115,115	2.88	14 (23%)
6	LDA	M	1324	-	13,15,15	1.77	1 (7%)	14,17,17	0.57	0
5	HEC	C	404	1	46,50,50	1.58	2 (4%)	58,82,82	1.45	3 (5%)
6	LDA	H	1259	-	13,15,15	2.36	2 (15%)	14,17,17	0.59	0
8	BCB	M	401	8,4	60,74,74	1.59	11 (18%)	59,115,115	3.00	17 (28%)
7	SO4	M	1329	-	4,4,4	1.21	0	6,6,6	0.79	0
7	SO4	M	1327	-	4,4,4	1.05	0	6,6,6	0.42	0
9	BPB	M	402	-	57,70,70	1.60	10 (17%)	55,101,101	2.56	15 (27%)
6	LDA	H	1260	-	13,15,15	2.71	2 (15%)	14,17,17	0.49	0
5	HEC	C	401	1	46,50,50	1.42	2 (4%)	58,82,82	1.66	5 (8%)
6	LDA	L	1274	-	13,15,15	2.07	1 (7%)	14,17,17	0.45	0
11	MQ9	L	501	-	59,59,59	1.71	20 (33%)	73,75,75	1.41	12 (16%)
7	SO4	H	1261	-	4,4,4	0.49	0	6,6,6	0.36	0
7	SO4	M	1328	-	4,4,4	0.88	0	6,6,6	0.50	0
5	HEC	C	403	1	46,50,50	1.61	3 (6%)	58,82,82	1.52	2 (3%)
8	BCB	M	400	4	60,74,74	1.69	9 (15%)	59,115,115	2.94	15 (25%)
9	BPB	L	402	-	57,70,70	1.60	7 (12%)	55,101,101	2.64	15 (27%)
5	HEC	C	402	1	46,50,50	1.41	2 (4%)	58,82,82	1.64	3 (5%)
12	MST	L	502	-	16,16,16	1.26	1 (6%)	22,22,22	1.03	2 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCB	L	400	8,3	3/3/21/26	6/37/137/137	-
13	NS5	M	600	-	-	12/43/43/43	-
6	LDA	M	1326	-	-	2/13/13/13	-
6	LDA	M	1325	-	-	3/13/13/13	-
8	BCB	L	401	3	2/2/21/26	3/37/137/137	-
6	LDA	M	1324	-	-	3/13/13/13	-
5	HEC	C	404	1	-	6/14/54/54	-
6	LDA	H	1259	-	-	5/13/13/13	-
8	BCB	M	401	8,4	3/3/21/26	6/37/137/137	-
9	BPB	M	402	-	1/1/18/23	1/37/105/105	0/5/6/6
6	LDA	H	1260	-	-	4/13/13/13	-
5	HEC	C	401	1	-	6/14/54/54	-
6	LDA	L	1274	-	-	3/13/13/13	-
11	MQ9	L	501	-	-	4/53/73/73	0/2/2/2
5	HEC	C	403	1	-	4/14/54/54	-
8	BCB	M	400	4	2/2/21/26	4/37/137/137	-
9	BPB	L	402	-	-	2/37/105/105	0/5/6/6
5	HEC	C	402	1	-	8/14/54/54	-
12	MST	L	502	-	-	0/10/10/10	0/1/1/1

The worst 5 of 101 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	1260	LDA	O1-N1	-7.74	1.23	1.42
6	M	1326	LDA	O1-N1	-7.56	1.23	1.42
6	M	1325	LDA	O1-N1	-7.43	1.24	1.42
6	L	1274	LDA	O1-N1	-7.27	1.24	1.42
6	H	1259	LDA	O1-N1	-7.20	1.24	1.42

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	402	BPB	O2D-CGD-CBD	13.09	125.33	110.95
8	L	401	BCB	O2D-CGD-CBD	12.90	125.12	110.95
8	M	401	BCB	O2D-CGD-CBD	12.88	125.10	110.95
9	L	402	BPB	O2D-CGD-CBD	11.98	124.11	110.95
8	M	400	BCB	O2D-CGD-CBD	11.86	123.98	110.95

5 of 11 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	L	400	BCB	NA
8	L	400	BCB	ND
8	L	400	BCB	NC
8	L	401	BCB	NA
8	L	401	BCB	NC

5 of 82 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	401	HEC	C2B-C3B-CAB-CBB
5	C	401	HEC	C4B-C3B-CAB-CBB
5	C	401	HEC	C2C-C3C-CAC-CBC
5	C	401	HEC	C4C-C3C-CAC-CBC
5	C	402	HEC	C2B-C3B-CAB-CBB

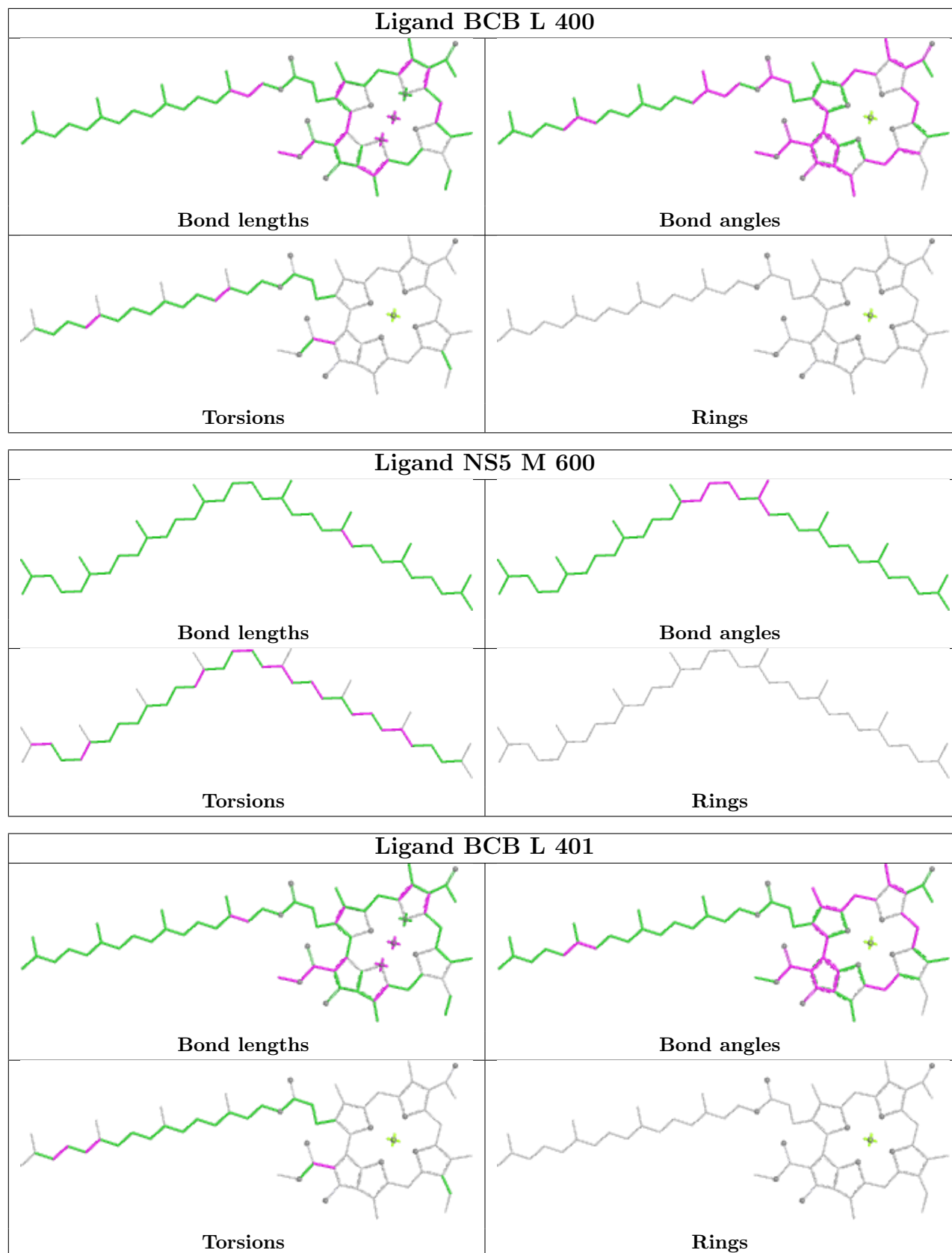
There are no ring outliers.

14 monomers are involved in 39 short contacts:

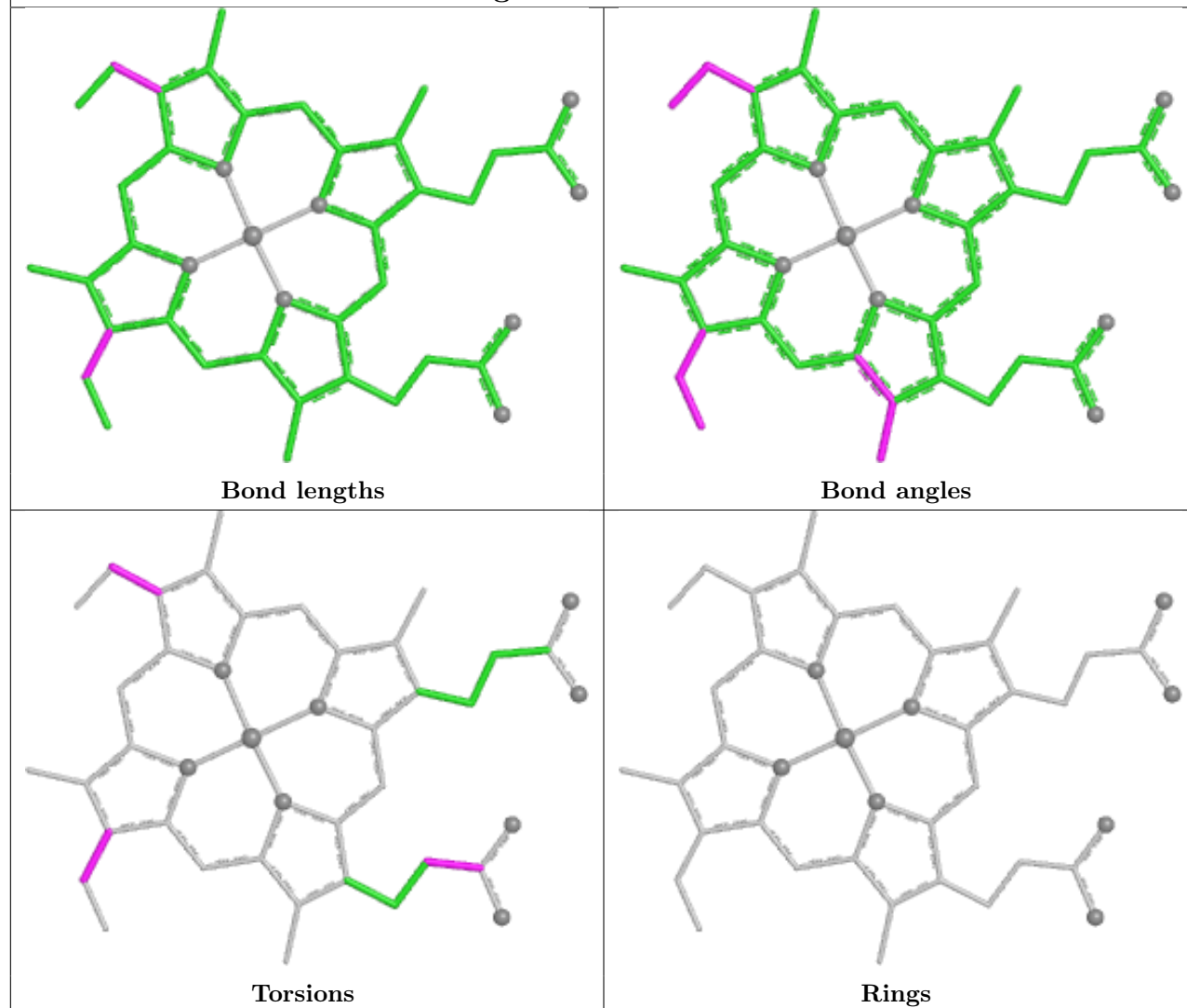
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	400	BCB	2	0
13	M	600	NS5	2	0
6	M	1326	LDA	1	0
8	L	401	BCB	3	0
6	M	1324	LDA	1	0
8	M	401	BCB	5	0
7	M	1329	SO4	1	0
9	M	402	BPB	7	0
6	H	1260	LDA	3	0
6	L	1274	LDA	4	0
11	L	501	MQ9	1	0
8	M	400	BCB	8	0
9	L	402	BPB	2	0
5	C	402	HEC	2	0

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

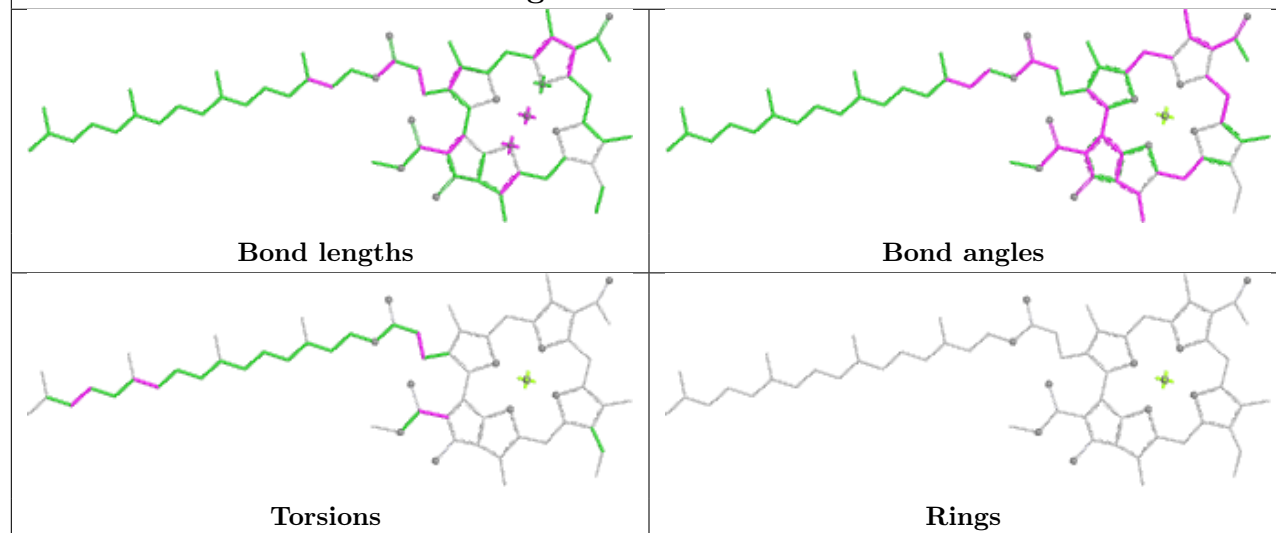
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

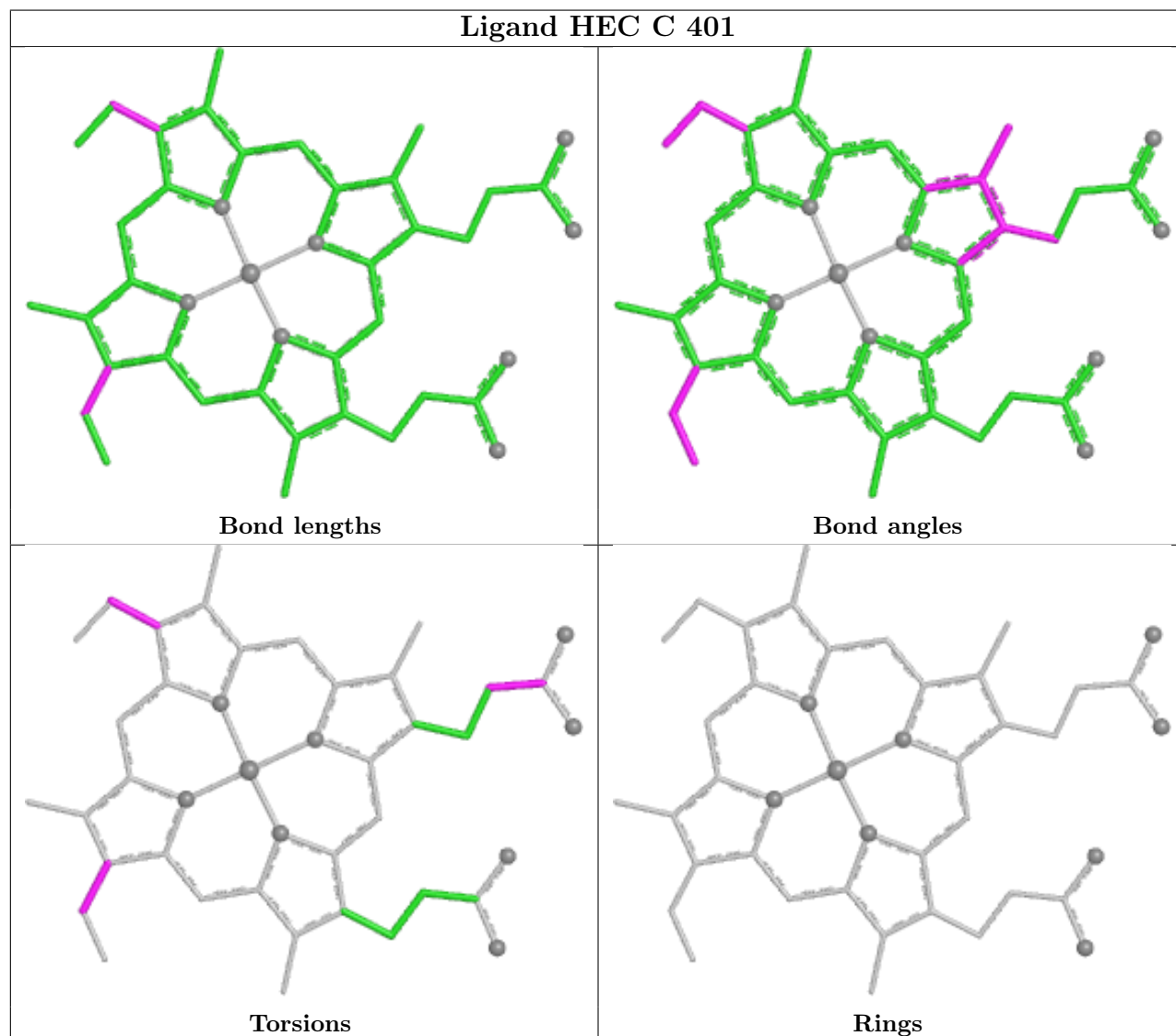
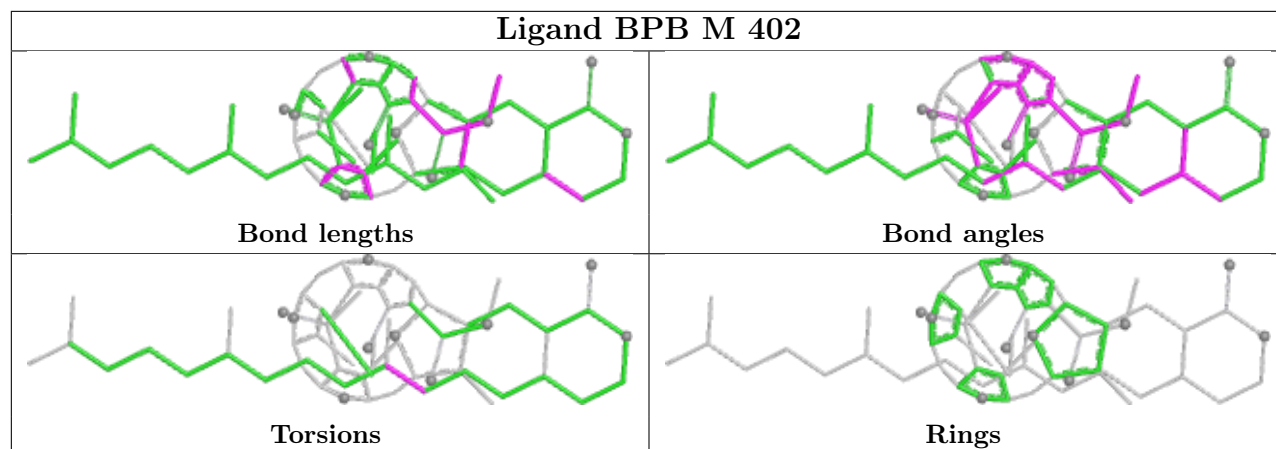


Ligand HEC C 404

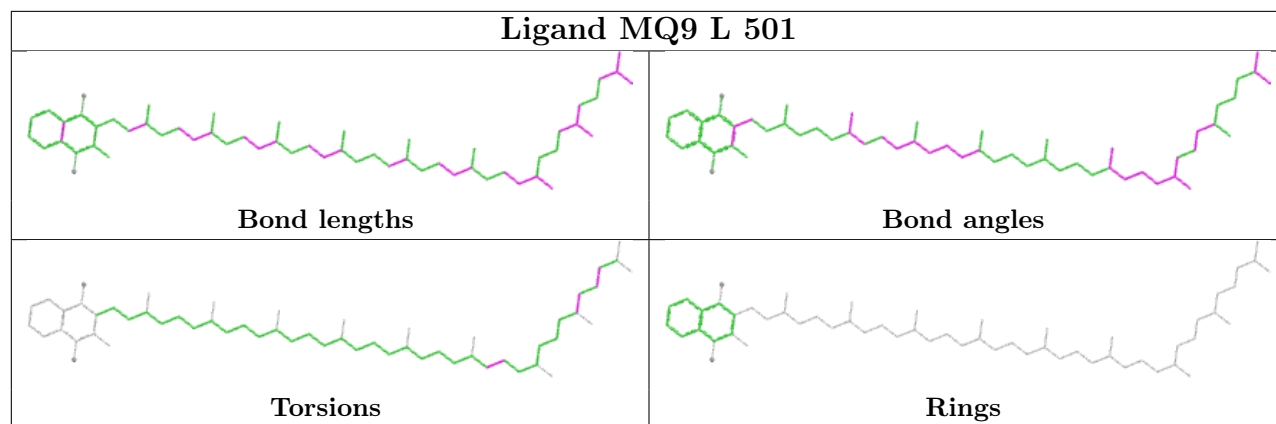


Ligand BCB M 401

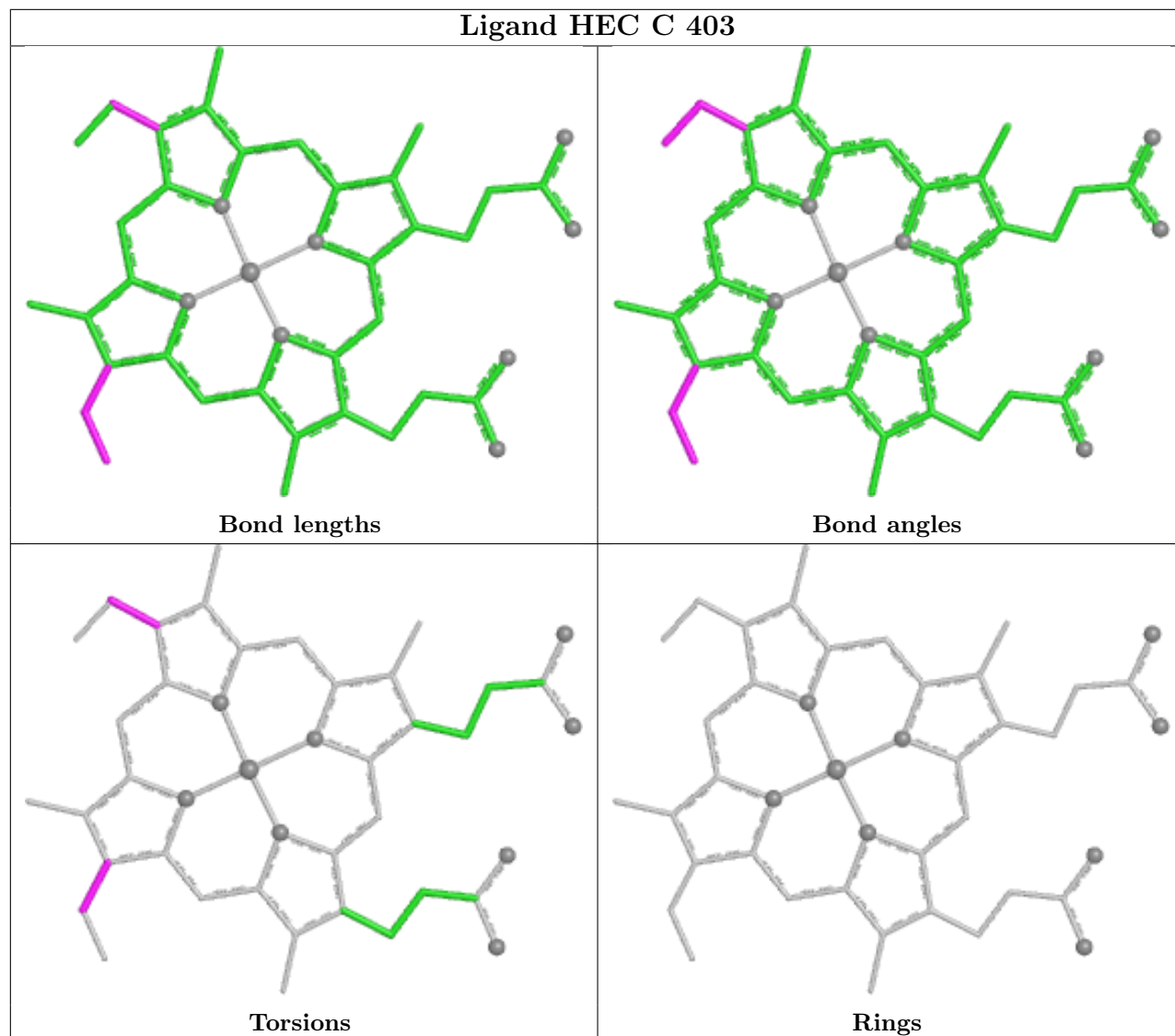


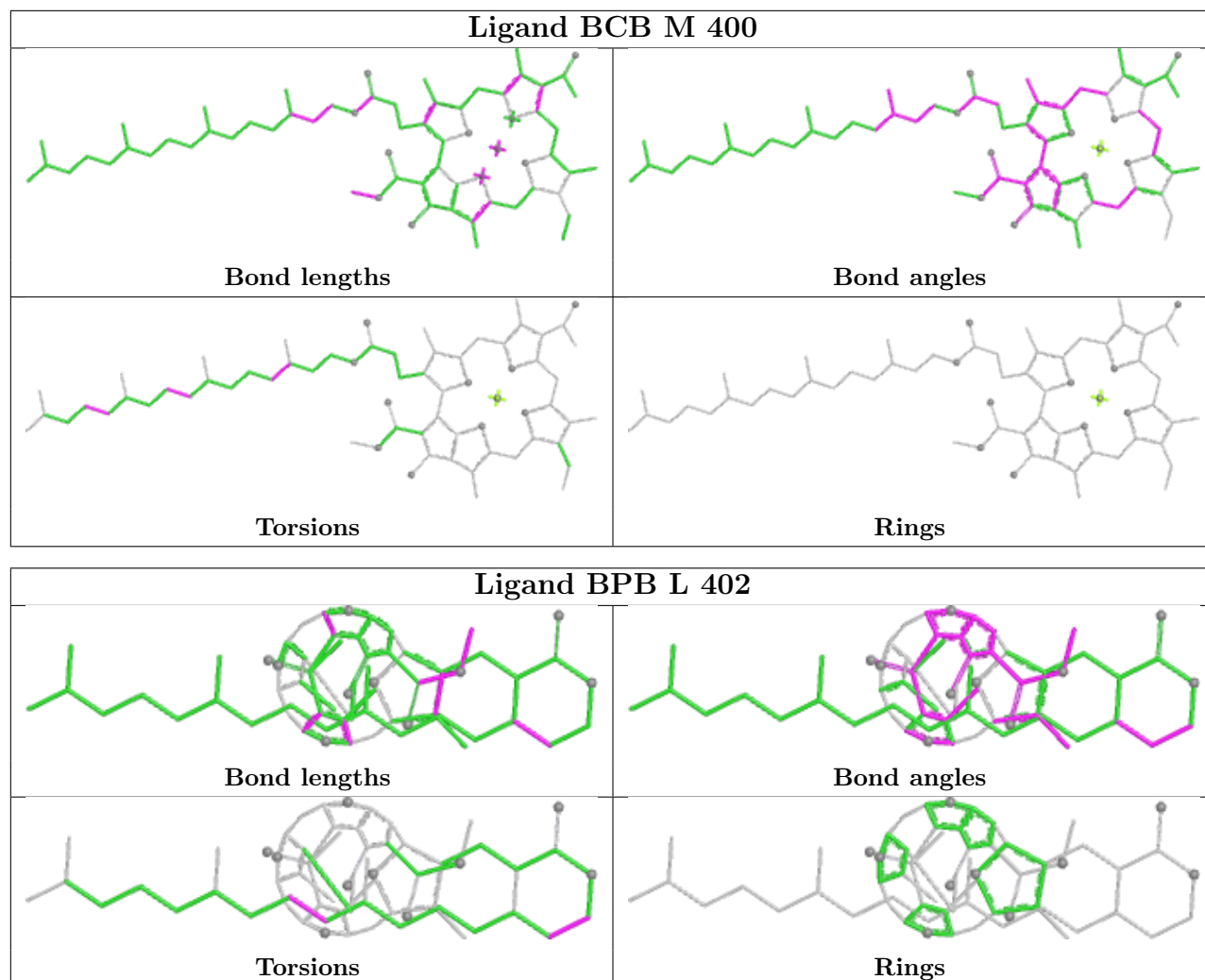


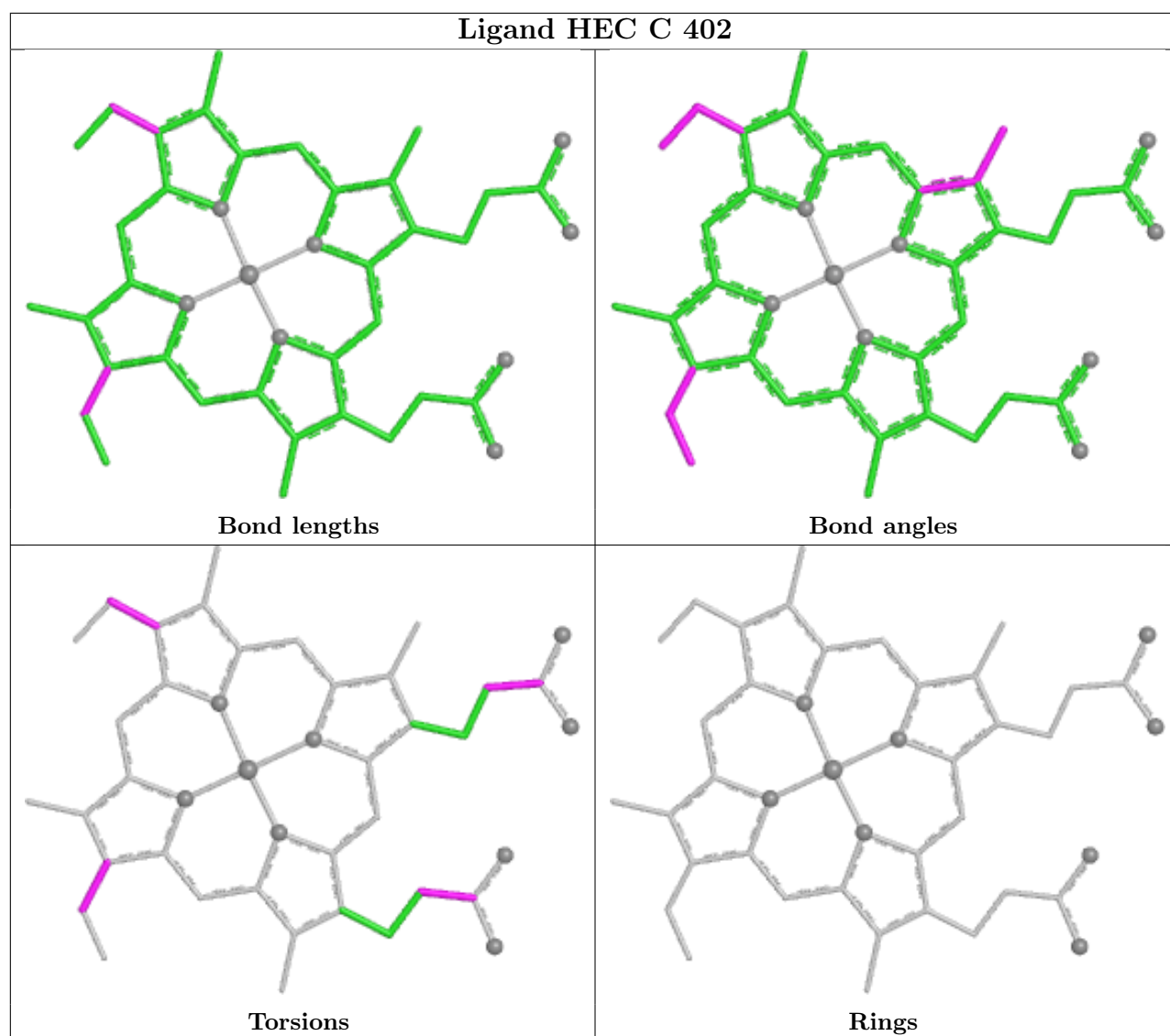
Ligand MQ9 L 501



Ligand HEC C 403







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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.