



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 20, 2021 – 04:21 am BST

PDB ID : 6ZHW
Title : Ultrafast Structural Response to Charge Redistribution Within a Photosynthetic Reaction Centre - 1 ps structure
Authors : Baath, P.; Dods, R.; Branden, G.; Neutze, R.
Deposited on : 2020-06-23
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

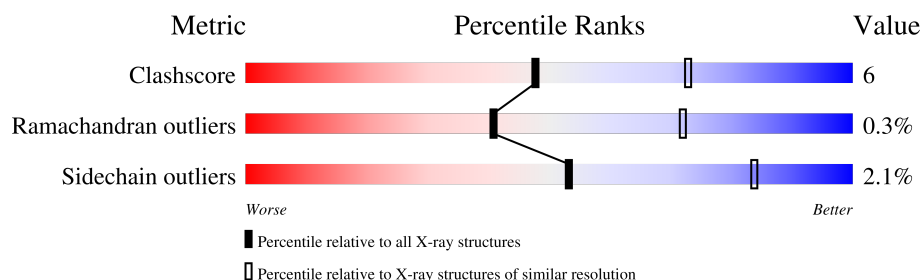
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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	
2	H	258	
3	L	273	
4	M	323	

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
7	SO4	M	407	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 11472 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	0	0	0
			2602	1640	466	478	18			

- Molecule 2 is a protein called Reaction center protein H chain.

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

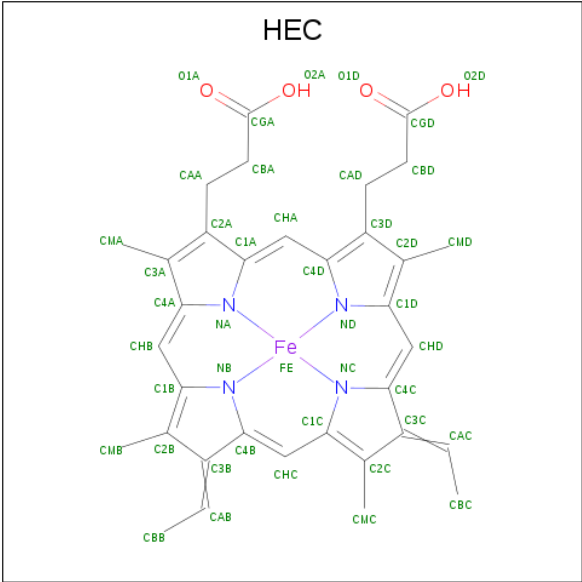
- Molecule 3 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	273	Total	C	N	O	S	0	41	0
			2508	1678	409	413	8			

- Molecule 4 is a protein called Reaction center protein M chain.

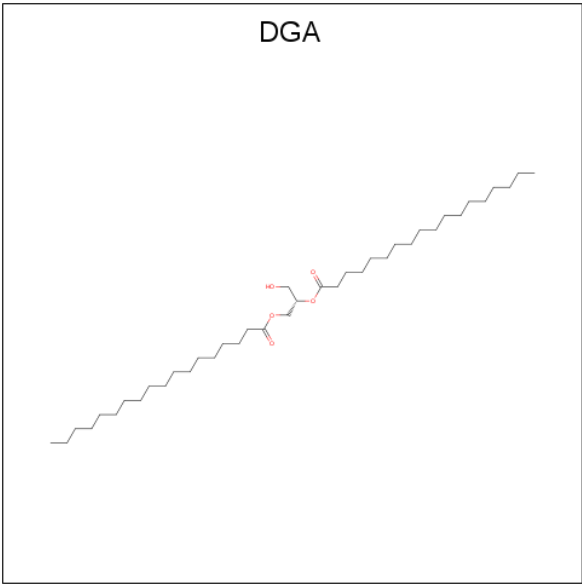
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	51	0
			2977	1983	491	490	13			

- Molecule 5 is HEME C (three-letter code: 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 DIACYL GLYCEROL (three-letter code: DGA) (formula: C₃₉H₇₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			37	33	4		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



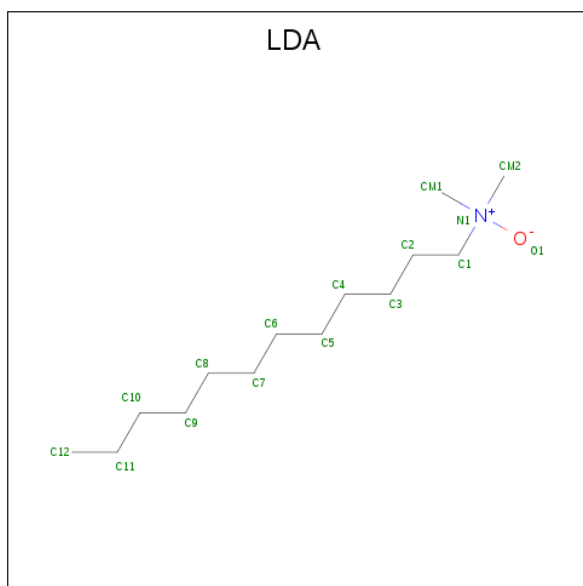
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total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

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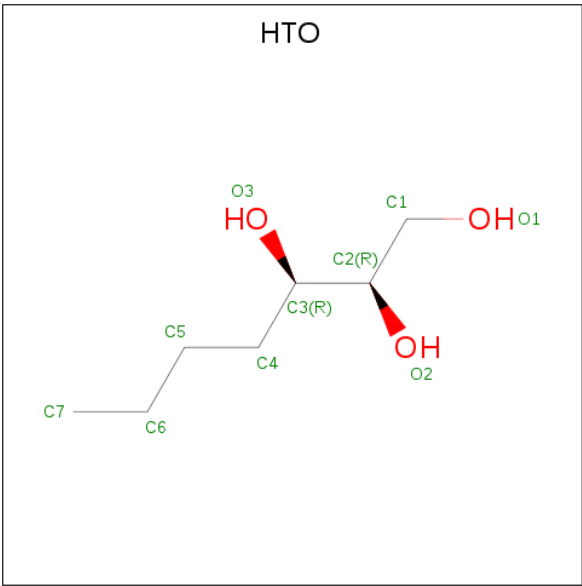
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



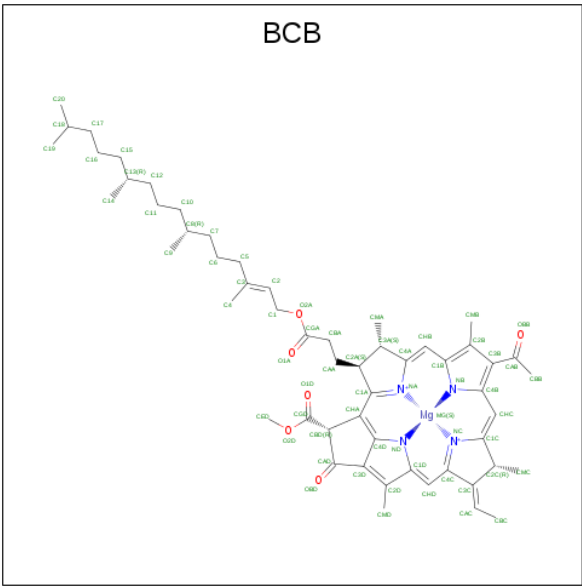
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	L	1	Total	C	N	O	0	0
			16	14	1	1		
8	L	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 9 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C₇H₁₆O₃).



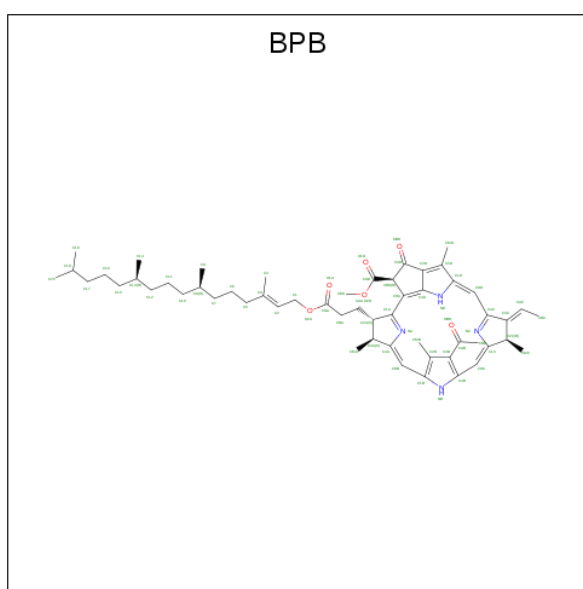
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	H	1	Total	C	O	0	0
			10	7	3		
9	H	1	Total	C	O	0	0
			10	7	3		
9	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 10 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: C₅₅H₇₂MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	L	1	Total	C	Mg	N	O	0	1
			132	110	2	8	12		
10	L	1	Total	C	Mg	N	O	0	1
			132	110	2	8	12		
10	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
10	M	1	Total	C	Mg	N	O	0	1
			132	110	2	8	12		

- Molecule 11 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: $C_{55}H_{74}N_4O_6$) (labeled as "Ligand of Interest" by depositor).

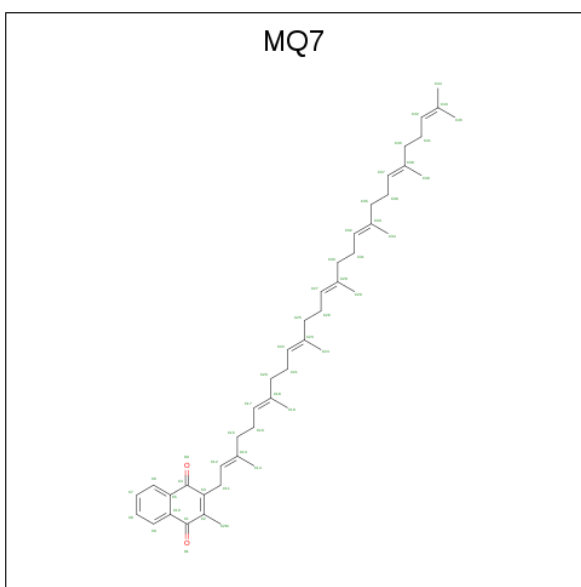


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	L	1	Total	C	N	O	0	1
			130	110	8	12		
11	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 12 is FE (III) ION (three-letter code: FE) (formula: Fe).

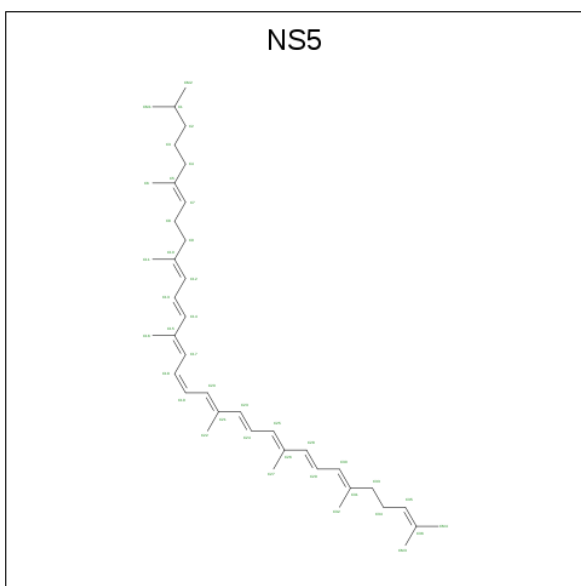
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	M	1	Total	Fe	0	1
			2	2		

- Molecule 13 is MENAQUINONE-7 (three-letter code: MQ7) (formula: $C_{46}H_{64}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	M	1	Total	C	O	0	1
			96	92	4		

- Molecule 14 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: C₄₀H₆₀).



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

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	C	56	Total 56	O 56	0	0
15	H	26	Total 26	O 26	0	0
15	L	25	Total 25	O 25	0	0
15	M	39	Total 39	O 39	0	0

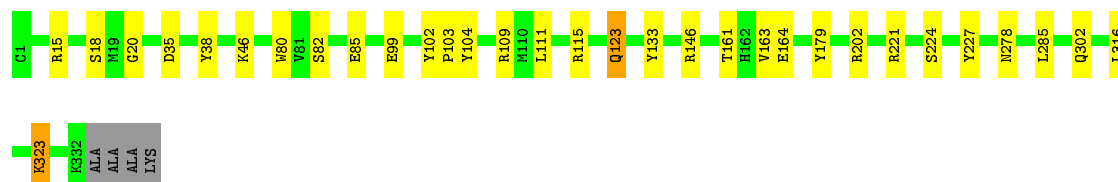
3 Residue-property plots [i](#)

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. 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.

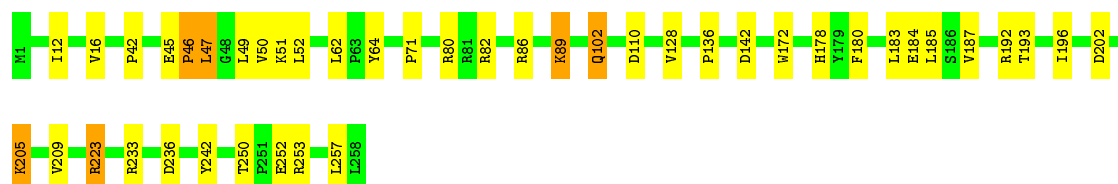
- Molecule 1: Photosynthetic reaction center cytochrome c subunit

Chain C: 




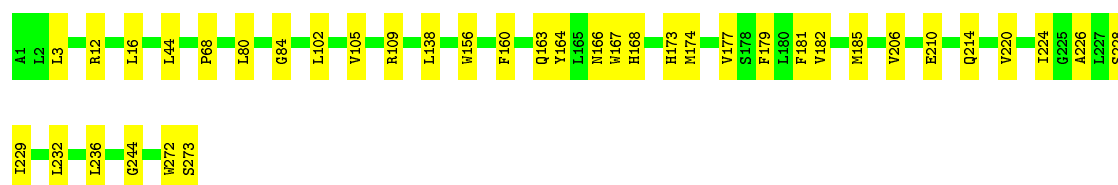
- Molecule 2: Reaction center protein H chain

Chain H: 



- Molecule 3: Reaction center protein L chain

Chain L: 



- Molecule 4: Reaction center protein M chain

Chain M: 





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	226.50Å 226.50Å 113.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.55 – 2.80	Depositor
% Data completeness (in resolution range)	98.7 (35.55-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.8.0158, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.170 , 0.193	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11472	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, NS5, SO4, BCB, DGA, MQ7, BPB, FME, HEC, HTO, FE

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	0.42	0/2669	0.57	0/3637
2	H	0.43	0/2055	0.60	0/2807
3	L	0.43	0/2612	0.56	0/3568
4	M	0.45	0/3101	0.55	0/4242
All	All	0.43	0/10437	0.57	0/14254

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2602	0	2578	25	0
2	H	2018	0	2020	37	0
3	L	2508	0	2390	42	0
4	M	2977	0	2832	24	0
5	C	172	0	120	4	0
6	C	37	0	58	0	0
7	C	15	0	0	0	0
7	H	25	0	0	0	0
7	M	35	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	48	0	93	5	0
8	L	32	0	62	2	0
8	M	32	0	62	0	0
9	H	20	0	32	0	0
9	L	10	0	16	0	0
10	L	330	0	360	18	0
10	M	132	0	144	6	0
11	L	195	0	222	14	0
12	M	2	0	0	0	0
13	M	96	0	128	1	0
14	M	40	0	60	2	0
15	C	56	0	0	0	0
15	H	26	0	0	1	0
15	L	25	0	0	0	0
15	M	39	0	0	0	0
All	All	11472	0	11177	137	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 137 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:H:205:LYS:HD3	2:H:205:LYS:H	1.46	0.80
1:C:161:THR:HG21	3:L:273:SER:O	1.83	0.79
4:M:160:CYS:O	4:M:164:THR:HG23	1.82	0.78
2:H:184:GLU:OE2	2:H:193:THR:HG21	1.82	0.77
11:L:305:BPB:HHC	11:L:305:BPB:HBBB	1.67	0.77

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	330/336 (98%)	320 (97%)	10 (3%)	0	100	100
2	H	256/258 (99%)	248 (97%)	5 (2%)	3 (1%)	13	39
3	L	312/273 (114%)	296 (95%)	16 (5%)	0	100	100
4	M	372/323 (115%)	356 (96%)	15 (4%)	1 (0%)	41	72
All	All	1270/1190 (107%)	1220 (96%)	46 (4%)	4 (0%)	41	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	M	177	ILE
2	H	46	PRO
2	H	47	LEU
2	H	50	VAL

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 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	281/282 (100%)	277 (99%)	4 (1%)	67	90
2	H	212/212 (100%)	202 (95%)	10 (5%)	26	59
3	L	253/218 (116%)	250 (99%)	3 (1%)	71	92
4	M	288/249 (116%)	282 (98%)	6 (2%)	53	84
All	All	1034/961 (108%)	1011 (98%)	23 (2%)	53	83

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	160[A]	PHE
4	M	27	ASP
3	L	272	TRP
4	M	194[A]	PHE
2	H	89	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	C	120	ASN
1	C	123	GLN
1	C	302	GLN
1	C	310	GLN
2	H	102	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	0.98	0	7,9,11	1.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	H	1	2	-	1/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	FME	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 2 are monoatomic - leaving 43 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	LDA	H	701	-	12,15,15	0.36	0	14,17,17	0.76	0
7	SO4	M	406	-	4,4,4	0.16	0	6,6,6	0.17	0
10	BCB	L	301[A]	-	60,74,74	2.81	19 (31%)	48,115,115	2.30	16 (33%)
14	NS5	M	404	-	39,39,39	1.39	2 (5%)	44,46,46	2.04	14 (31%)
6	DGA	C	405	1	36,36,43	1.18	3 (8%)	38,38,45	1.17	3 (7%)
7	SO4	C	406	-	4,4,4	0.25	0	6,6,6	0.39	0
7	SO4	M	409	-	4,4,4	0.15	0	6,6,6	0.18	0
10	BCB	L	302[B]	-	60,74,74	2.77	20 (33%)	48,115,115	2.19	16 (33%)
8	LDA	L	307	-	12,15,15	0.39	0	14,17,17	0.64	0
7	SO4	M	407	-	4,4,4	0.14	0	6,6,6	0.25	0
9	HTO	H	709	-	9,9,9	0.85	0	10,10,10	0.59	0
10	BCB	L	302[A]	-	60,74,74	2.75	19 (31%)	48,115,115	2.34	17 (35%)
7	SO4	C	408	-	4,4,4	0.16	0	6,6,6	0.11	0
5	HEC	C	403	1	26,50,50	1.53	4 (15%)	18,82,82	1.93	8 (44%)
7	SO4	H	705	-	4,4,4	0.27	0	6,6,6	0.36	0
11	BPB	L	303[B]	-	64,70,70	2.09	15 (23%)	64,101,101	2.06	16 (25%)
7	SO4	H	703	-	4,4,4	0.22	0	6,6,6	0.12	0
7	SO4	H	702	-	4,4,4	0.23	0	6,6,6	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	HEC	C	404	1	26,50,50	1.58	3 (11%)	18,82,82	1.95	7 (38%)
13	MQ7	M	402[B]	-	49,49,49	1.51	2 (4%)	60,63,63	1.42	12 (20%)
7	SO4	H	706	-	4,4,4	0.18	0	6,6,6	0.09	0
7	SO4	M	408	-	4,4,4	0.30	0	6,6,6	0.27	0
9	HTO	H	710	-	9,9,9	0.85	0	10,10,10	1.04	1 (10%)
8	LDA	M	412	-	12,15,15	0.42	0	14,17,17	0.55	0
5	HEC	C	401	1	26,50,50	1.64	4 (15%)	18,82,82	2.71	6 (33%)
11	BPB	L	303[A]	-	64,70,70	2.11	16 (25%)	64,101,101	1.97	17 (26%)
9	HTO	L	308	-	9,9,9	0.72	0	10,10,10	1.20	1 (10%)
5	HEC	C	402	1	26,50,50	1.51	3 (11%)	18,82,82	2.22	8 (44%)
10	BCB	L	304	-	60,74,74	2.70	20 (33%)	48,115,115	2.30	14 (29%)
13	MQ7	M	402[A]	-	49,49,49	1.53	2 (4%)	60,63,63	1.57	14 (23%)
7	SO4	H	704	-	4,4,4	0.12	0	6,6,6	0.16	0
11	BPB	L	305	-	64,70,70	2.18	16 (25%)	64,101,101	1.89	14 (21%)
10	BCB	M	403[B]	-	60,74,74	2.73	21 (35%)	48,115,115	2.40	19 (39%)
7	SO4	C	407	-	4,4,4	0.16	0	6,6,6	0.14	0
8	LDA	H	707	-	12,15,15	0.36	0	14,17,17	0.82	0
7	SO4	M	405	-	4,4,4	0.11	0	6,6,6	0.26	0
8	LDA	H	708	-	12,15,15	0.27	0	14,17,17	0.84	0
7	SO4	M	410	-	4,4,4	0.28	0	6,6,6	0.33	0
8	LDA	M	413	-	12,15,15	0.48	0	14,17,17	0.52	0
10	BCB	L	301[B]	-	60,74,74	2.79	22 (36%)	48,115,115	2.25	14 (29%)
8	LDA	L	306	-	12,15,15	0.39	0	14,17,17	0.70	0
10	BCB	M	403[A]	-	60,74,74	2.81	21 (35%)	48,115,115	2.32	16 (33%)
7	SO4	M	411	-	4,4,4	0.25	0	6,6,6	0.21	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	LDA	H	701	-	-	3/13/13/13	-
10	BCB	L	301[A]	-	-	12/41/177/177	-
14	NS5	M	404	-	-	10/43/43/43	-
6	DGA	C	405	1	-	15/37/37/45	-
10	BCB	L	302[B]	-	-	8/41/177/177	-
8	LDA	L	307	-	-	10/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HTO	H	709	-	-	4/10/10/10	-
10	BCB	L	302[A]	-	-	10/41/177/177	-
5	HEC	C	403	1	-	0/6/54/54	-
11	BPB	L	303[B]	-	-	13/47/105/105	0/5/6/6
5	HEC	C	404	1	-	0/6/54/54	-
13	MQ7	M	402[B]	-	-	1/41/61/61	0/2/2/2
9	HTO	H	710	-	-	0/10/10/10	-
8	LDA	M	412	-	-	4/13/13/13	-
5	HEC	C	401	1	-	0/6/54/54	-
11	BPB	L	303[A]	-	-	6/47/105/105	0/5/6/6
9	HTO	L	308	-	-	4/10/10/10	-
5	HEC	C	402	1	-	1/6/54/54	-
10	BCB	L	304	-	-	15/41/177/177	-
13	MQ7	M	402[A]	-	-	0/41/61/61	0/2/2/2
11	BPB	L	305	-	-	8/47/105/105	0/5/6/6
10	BCB	M	403[B]	-	-	17/41/177/177	-
8	LDA	H	707	-	-	6/13/13/13	-
8	LDA	H	708	-	-	7/13/13/13	-
8	LDA	M	413	-	-	4/13/13/13	-
10	BCB	L	301[B]	-	-	16/41/177/177	-
8	LDA	L	306	-	-	5/13/13/13	-
10	BCB	M	403[A]	-	-	14/41/177/177	-

The worst 5 of 212 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	402[A]	MQ7	C3-C2	8.62	1.51	1.35
10	M	403[A]	BCB	CHB-C4A	-8.46	1.33	1.52
10	L	301[B]	BCB	CHB-C4A	-8.44	1.33	1.52
10	L	301[A]	BCB	CHB-C4A	-8.39	1.33	1.52
10	L	302[B]	BCB	CHB-C4A	-8.29	1.33	1.52

The worst 5 of 233 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	301[B]	BCB	CMB-C2B-C3B	8.15	134.52	114.29
10	M	403[A]	BCB	CMB-C2B-C3B	7.81	133.68	114.29
10	L	301[A]	BCB	CMB-C2B-C3B	7.73	133.50	114.29
10	M	403[B]	BCB	CMB-C2B-C3B	7.52	132.96	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	302[A]	BCB	CMB-C2B-C3B	7.30	132.42	114.29

There are no chirality outliers.

5 of 193 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	405	DGA	OG1-CG1-CG2-OG2
6	C	405	DGA	OG1-CG1-CG2-CG3
8	H	707	LDA	C2-C1-N1-O1
8	H	707	LDA	C2-C1-N1-CM1
8	H	707	LDA	C2-C1-N1-CM2

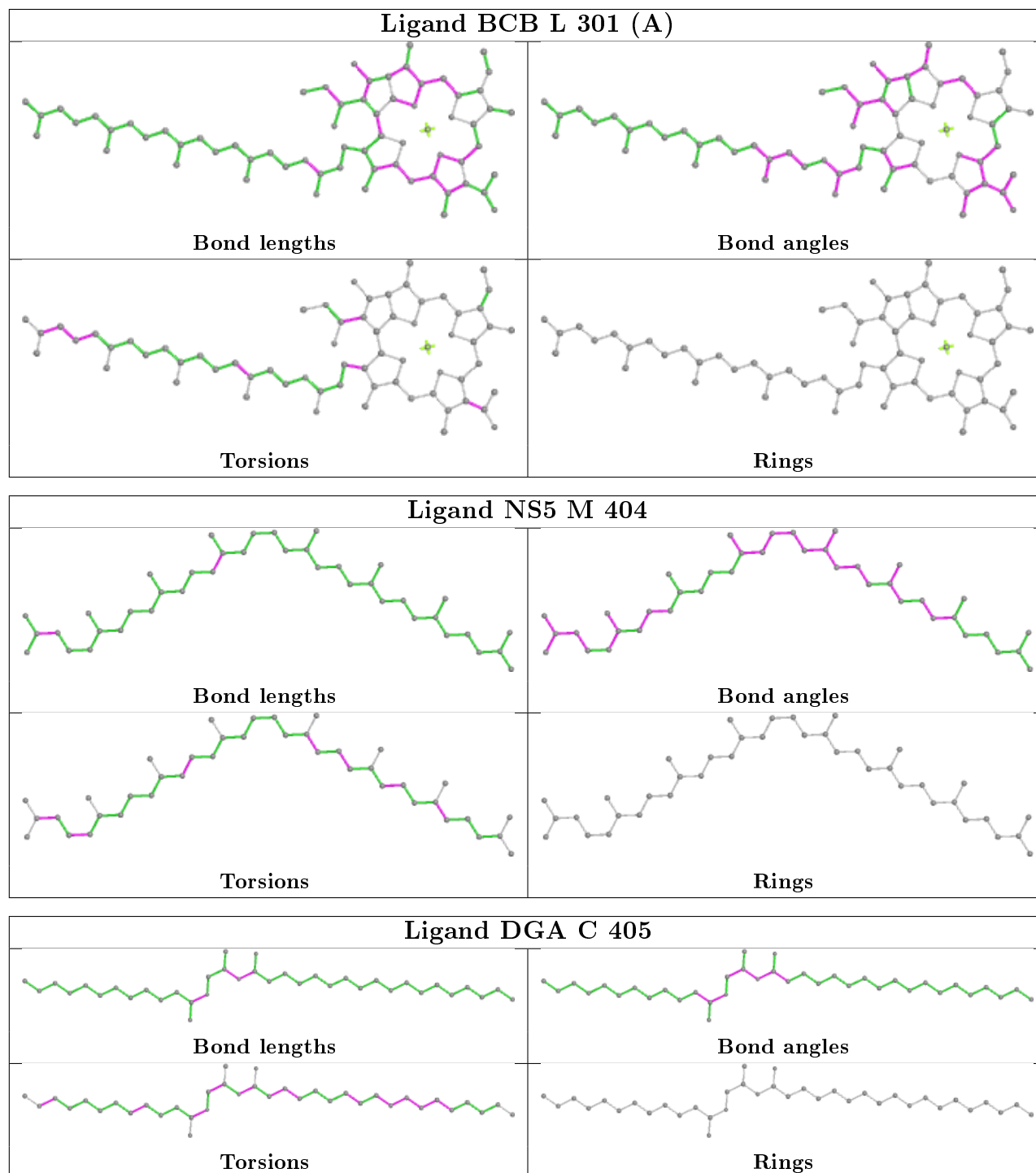
There are no ring outliers.

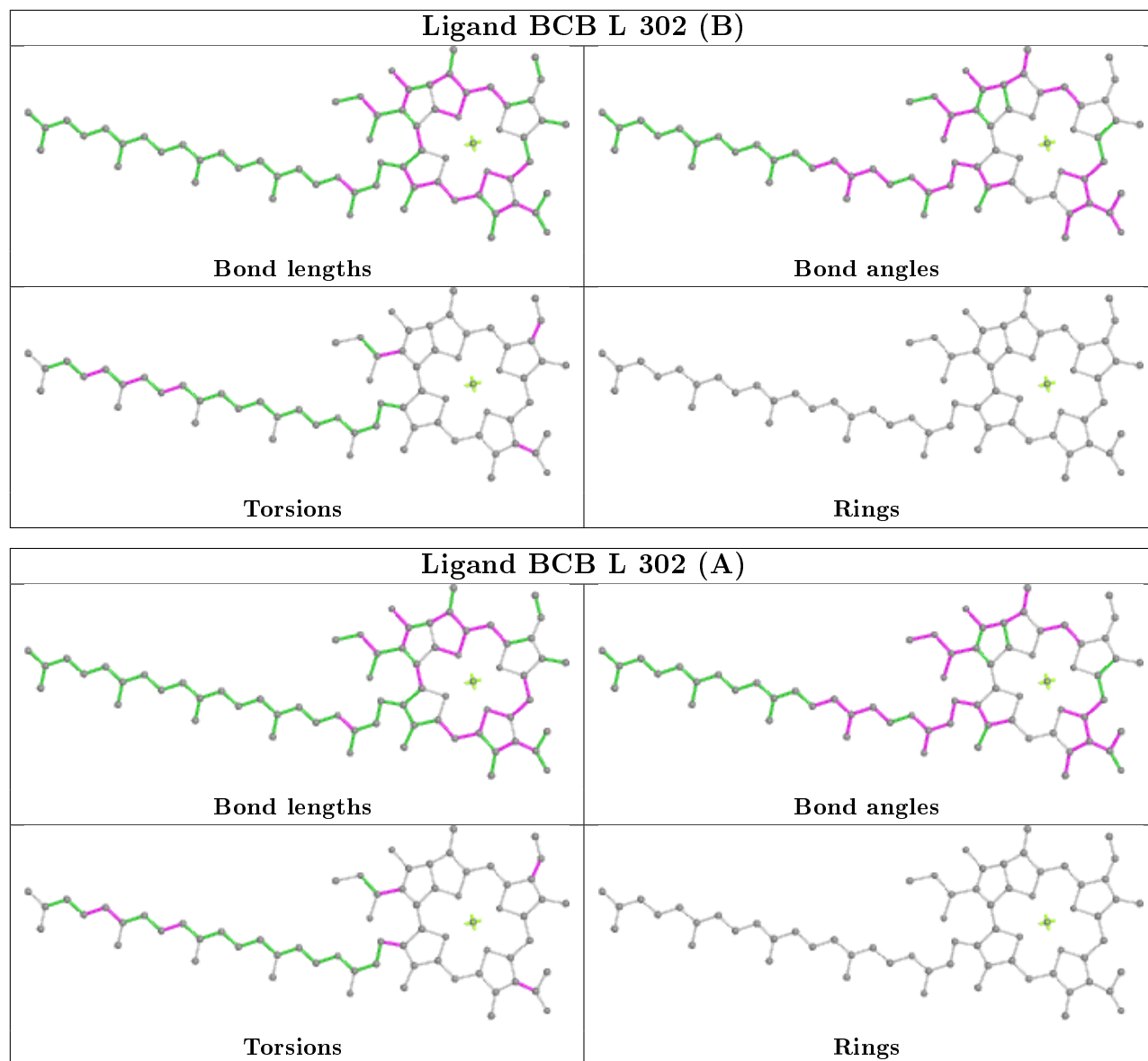
20 monomers are involved in 49 short contacts:

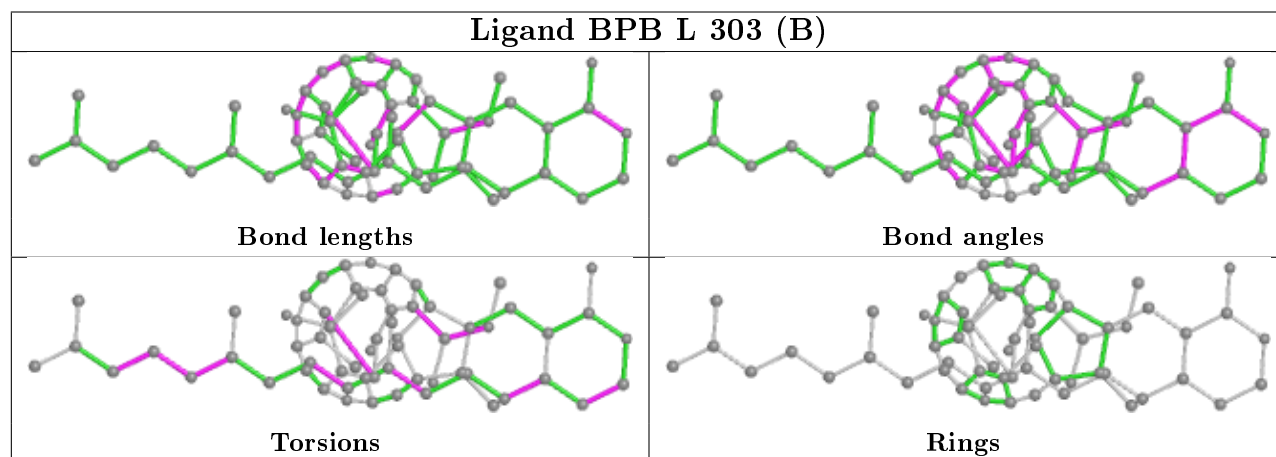
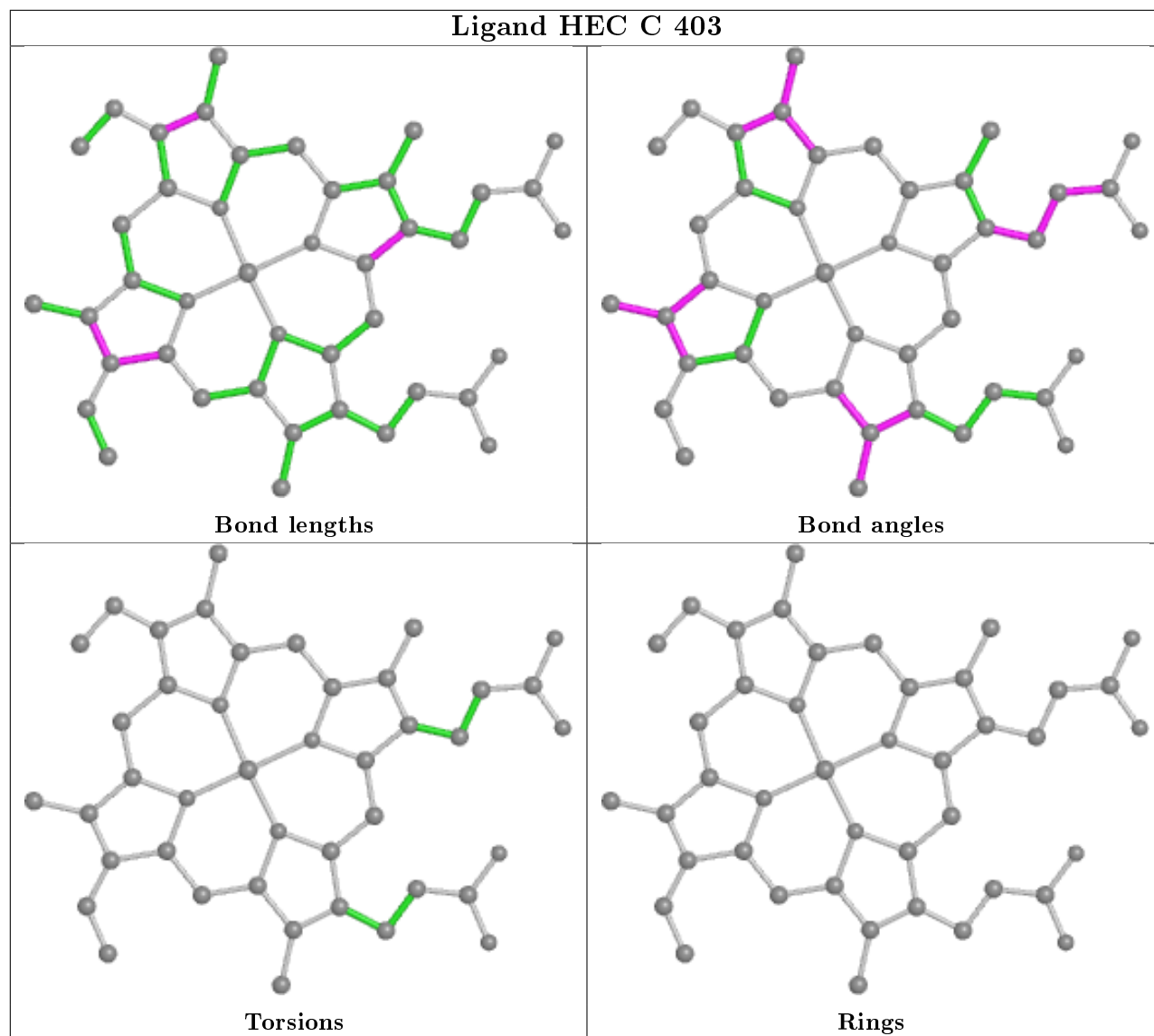
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	H	701	LDA	1	0
10	L	301[A]	BCB	4	0
14	M	404	NS5	2	0
10	L	302[B]	BCB	4	0
7	M	407	SO4	2	0
5	C	403	HEC	2	0
11	L	303[B]	BPB	5	0
5	C	404	HEC	1	0
5	C	401	HEC	1	0
11	L	303[A]	BPB	3	0
5	C	402	HEC	1	0
10	L	304	BCB	8	0
13	M	402[A]	MQ7	1	0
11	L	305	BPB	6	0
10	M	403[B]	BCB	5	0
8	H	707	LDA	1	0
8	H	708	LDA	3	0
10	L	301[B]	BCB	2	0
8	L	306	LDA	2	0
10	M	403[A]	BCB	1	0

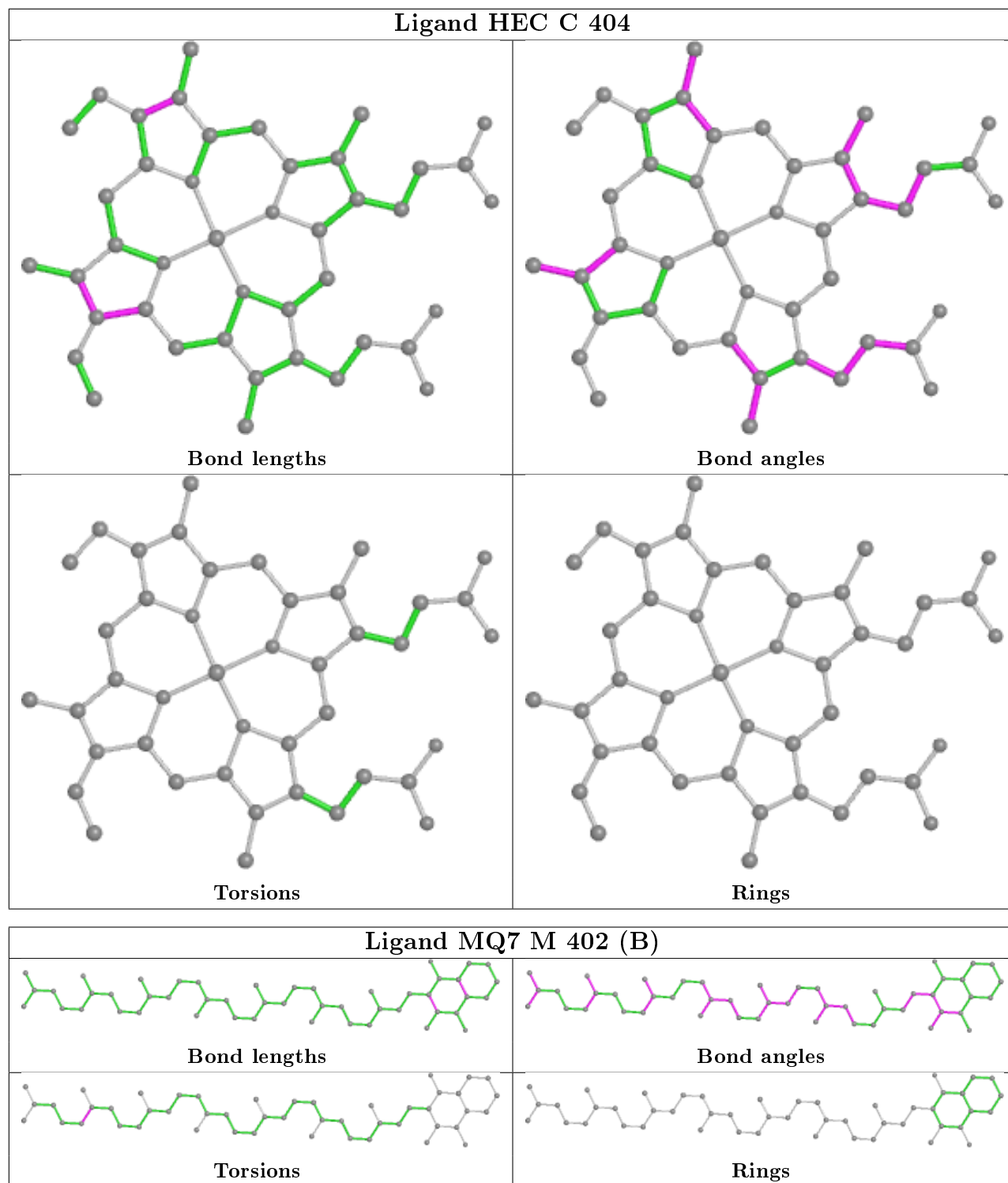
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

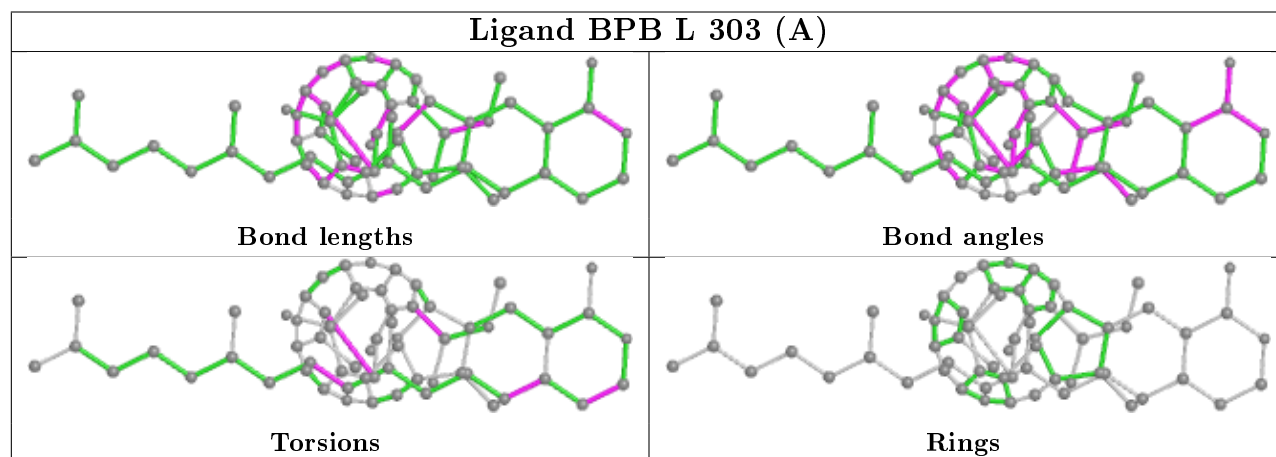
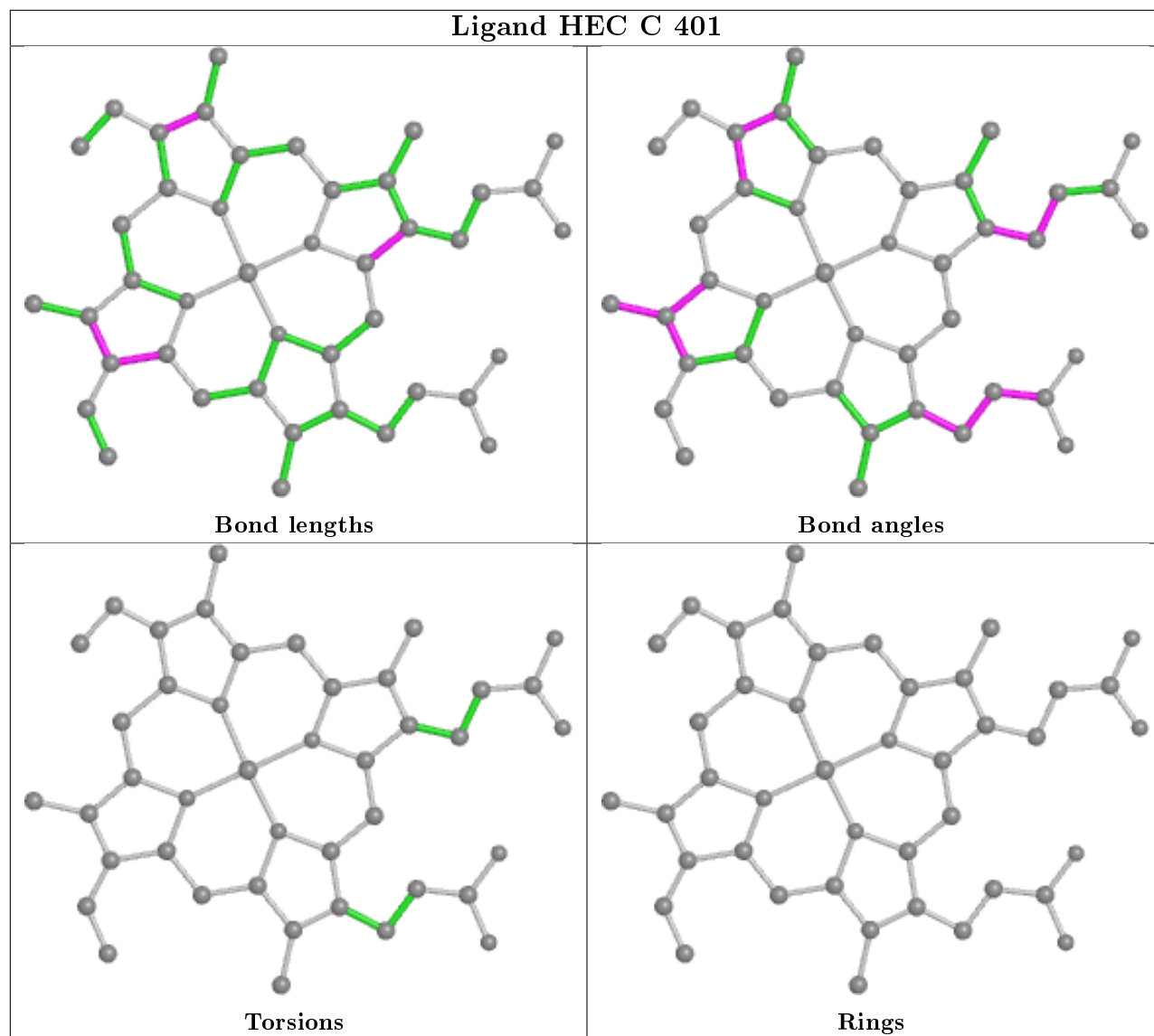
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



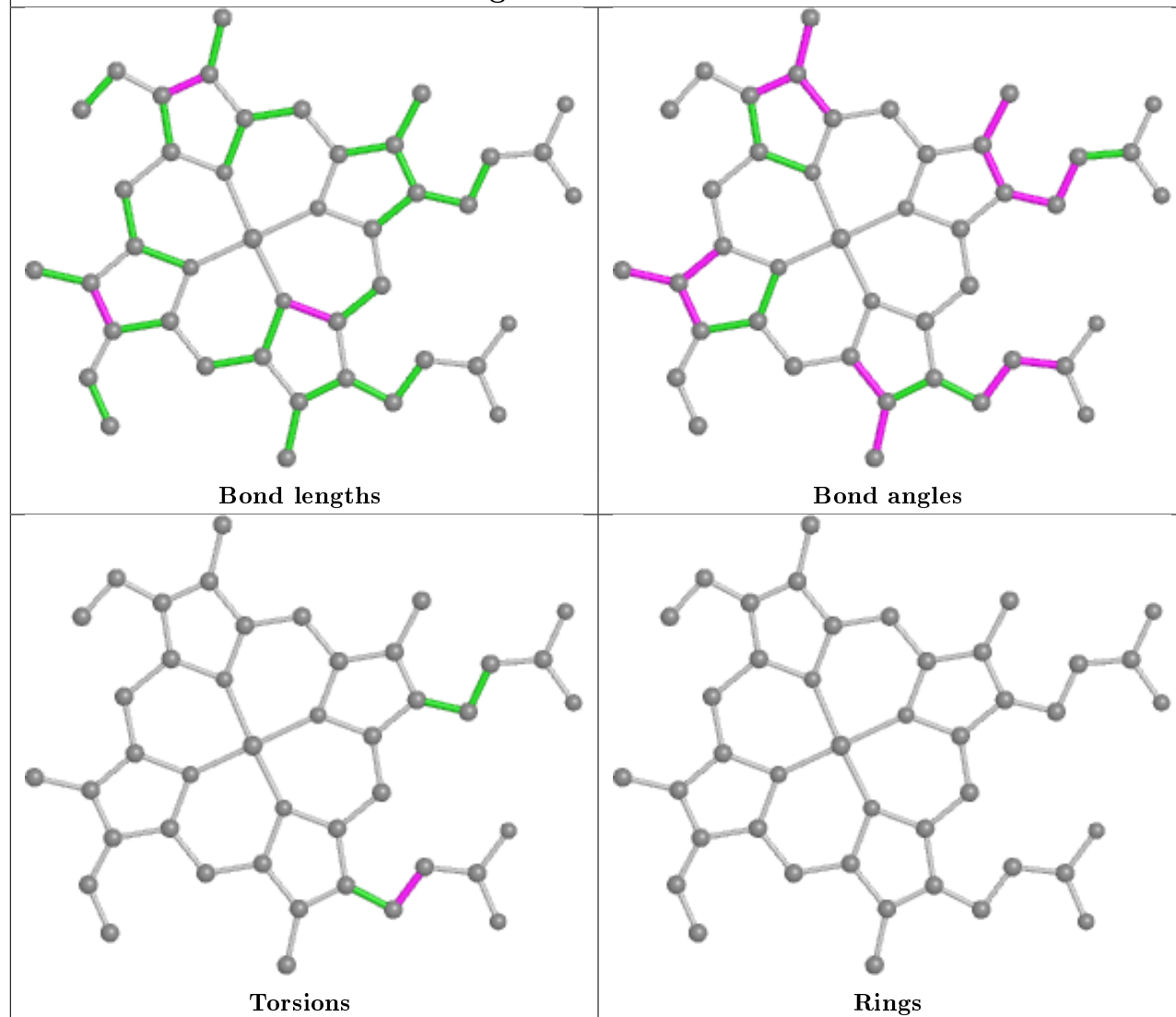




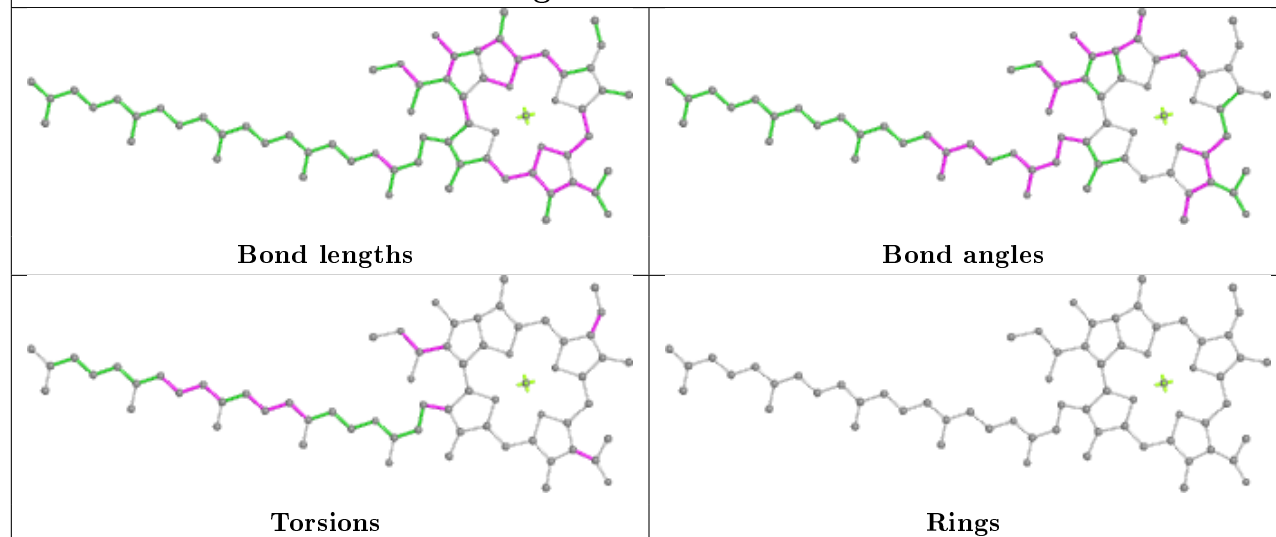


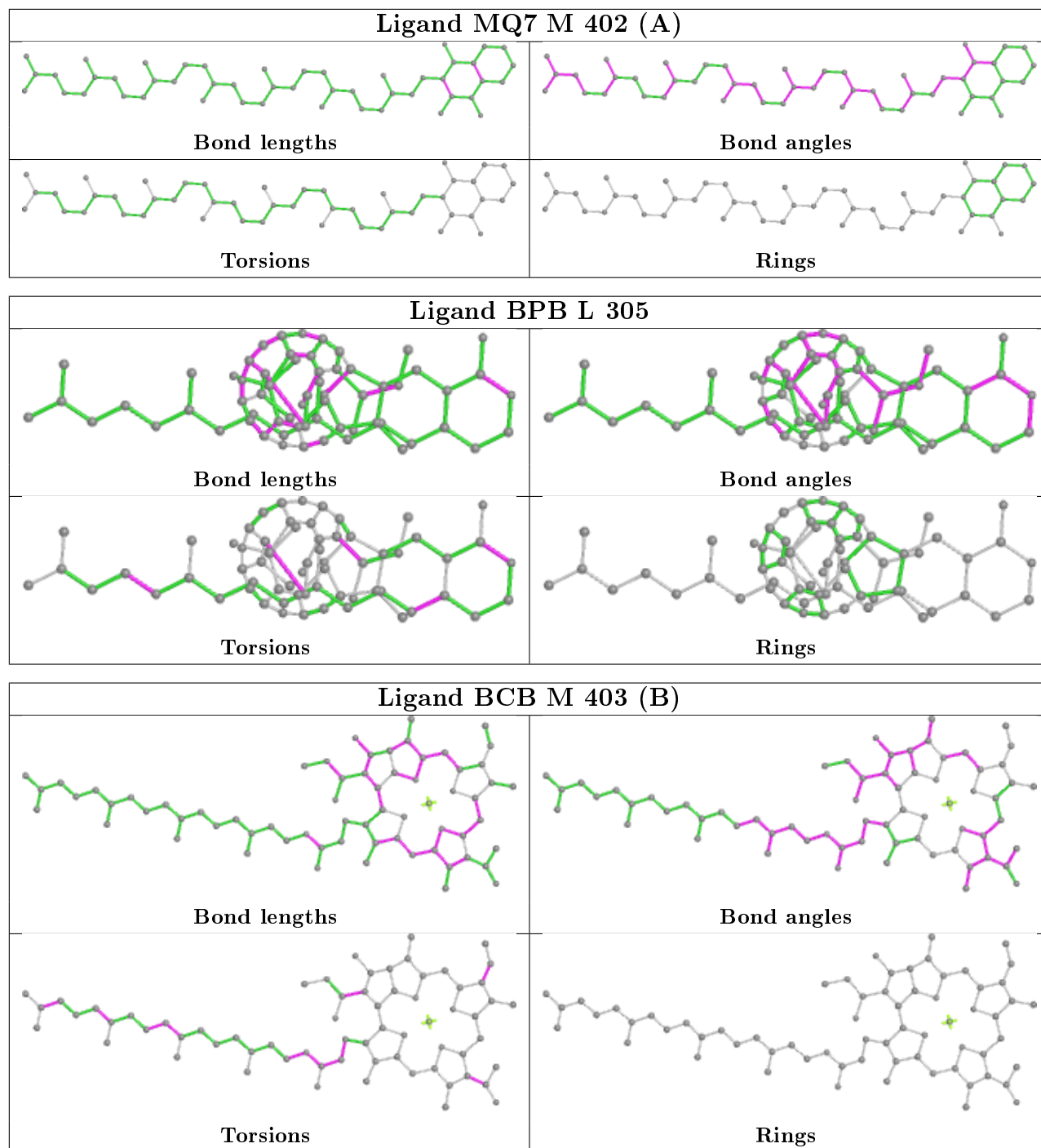


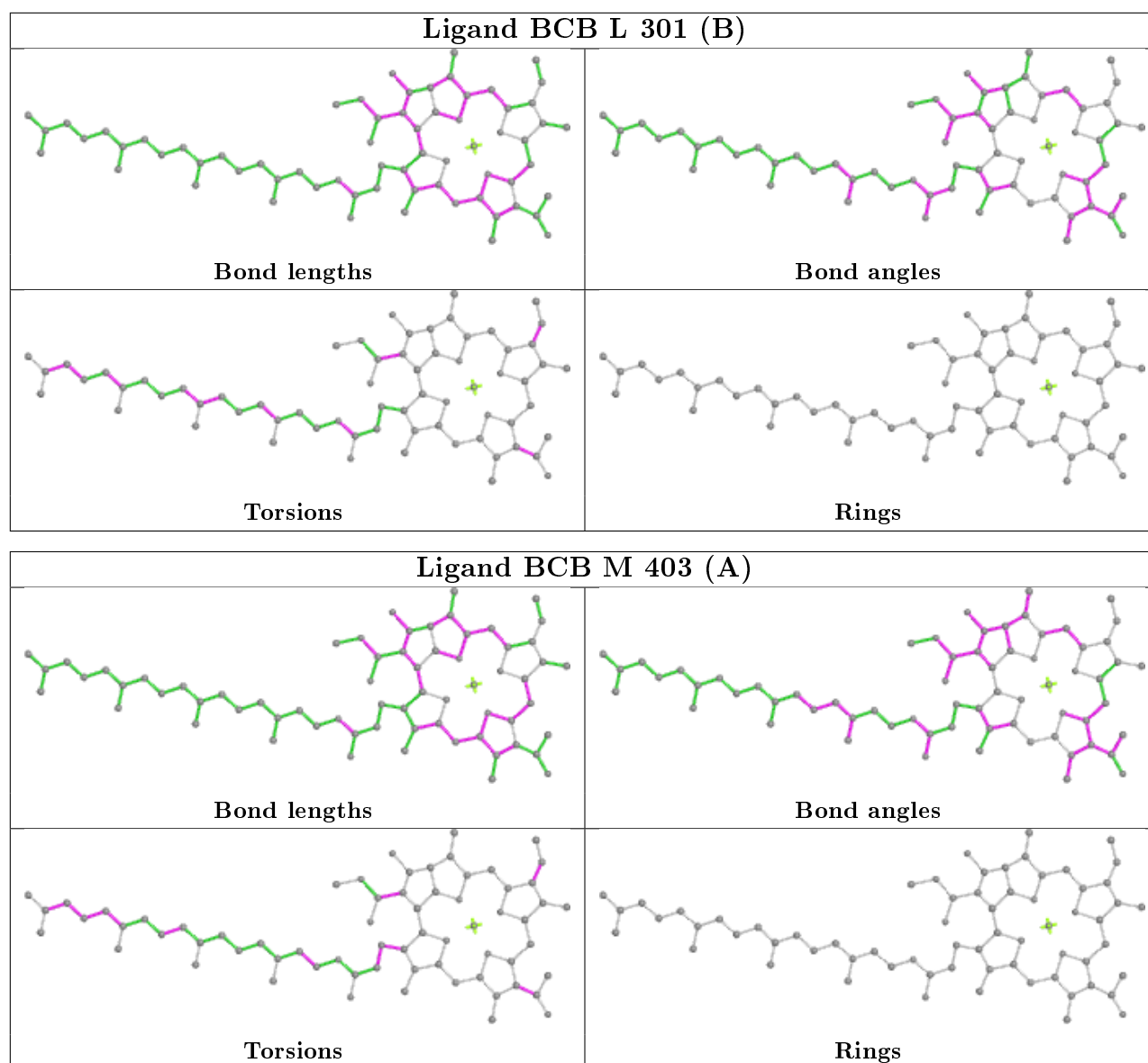
Ligand HEC C 402



Ligand BCB L 304







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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.