



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 10:39 AM UTC

PDB ID : 1EYS / pdb_00001eys
Title : CRYSTAL STRUCTURE OF PHOTOSYNTHETIC REACTION CENTER FROM A THERMOPHILIC BACTERIUM, THERMOCHROMATIUM TEPIDUM
Authors : Nogi, T.; Fathir, I.; Kobayashi, M.; Nozawa, T.; Miki, K.
Deposited on : 2000-05-08
Resolution : 2.20 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)
Xtrriage (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

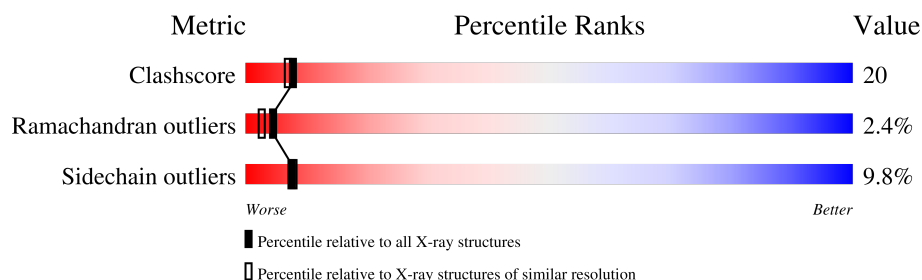
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	382	
2	L	280	
3	M	324	
4	H	259	

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	BPH	L	606	X	-	-	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 10044 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	310	Total	C	N	O	S	0	0	0
			2402	1514	421	451	16			

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	280	Total	C	N	O	S	0	0	0
			2233	1501	361	361	10			

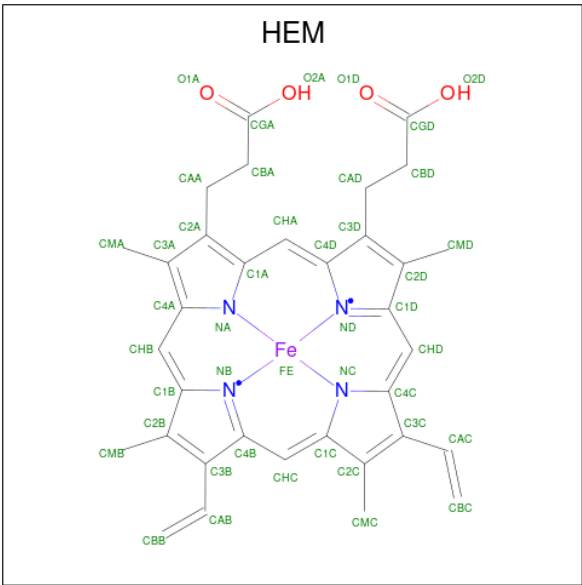
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	318	Total	C	N	O	S	0	0	0
			2537	1705	413	409	10			

- Molecule 4 is a protein called PHOTOSYNTHETIC REACTION CENTER.

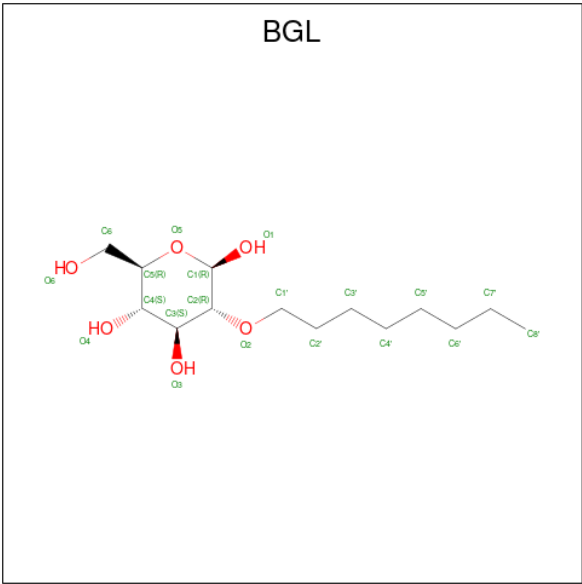
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	238	Total	C	N	O	S	0	0	0
			1837	1187	309	336	5			

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



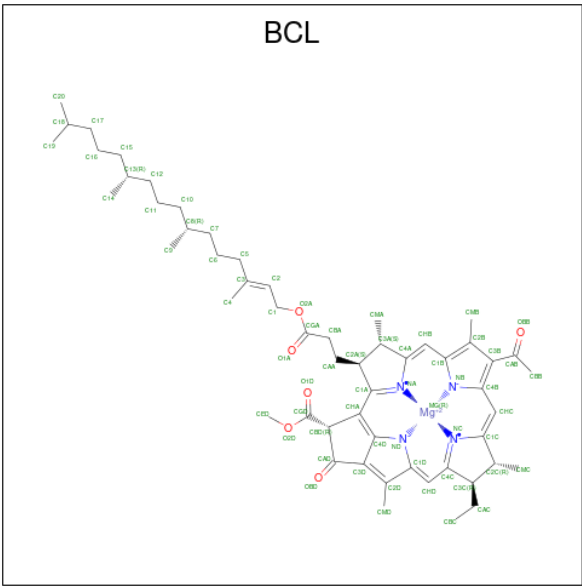
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is 2-O-octyl-beta-D-glucopyranose (CCD ID: BGL) (formula: $C_{14}H_{28}O_6$).



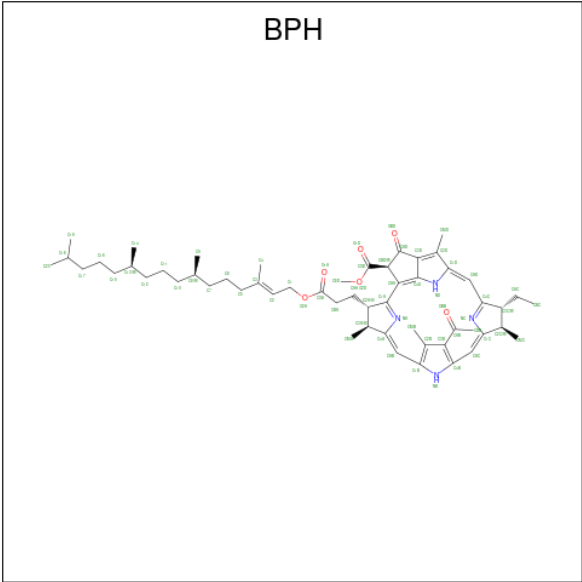
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			20	14	6		
6	L	1	Total	C	O	0	0
			20	14	6		
6	L	1	Total	C	O	0	0
			20	14	6		
6	M	1	Total	C	O	0	0
			20	14	6		
6	M	1	Total	C	O	0	0
			20	14	6		
6	M	1	Total	C	O	0	0
			20	14	6		

- Molecule 7 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



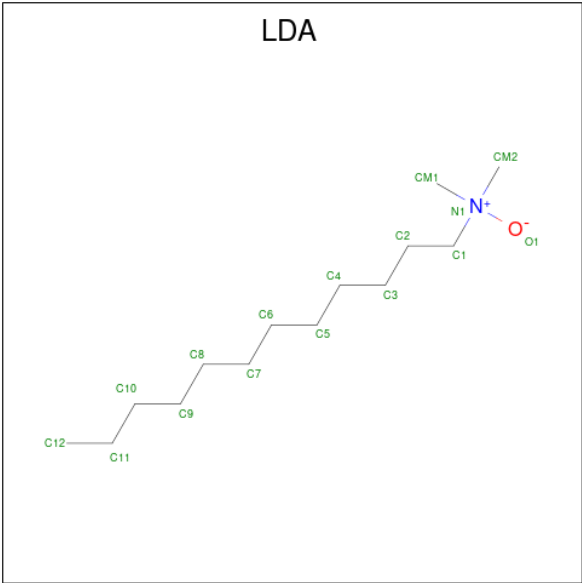
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 8 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



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

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).

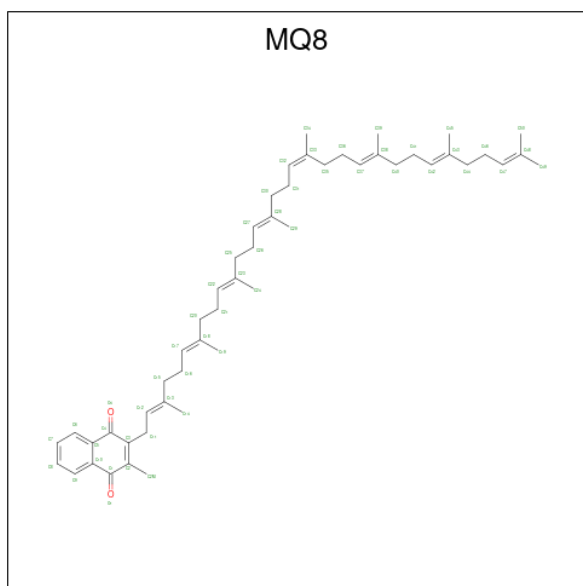


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	L	1	Total	C	N	O	0	0
			16	14	1	1		

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

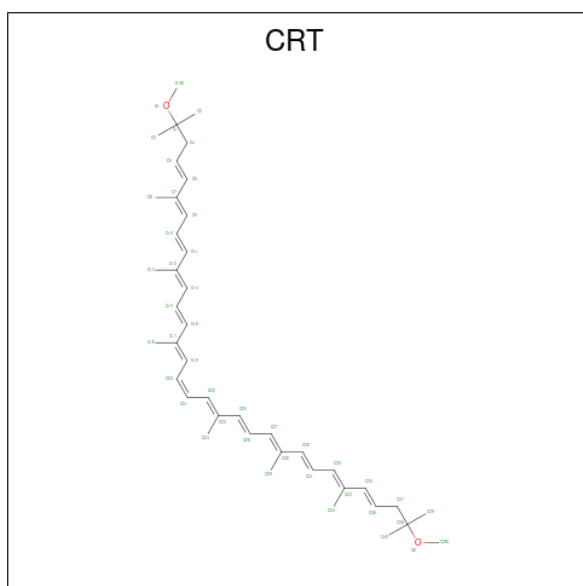
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	1	Total	Fe	0	0
			1	1		

- Molecule 11 is MENAQUINONE 8 (CCD ID: MQ8) (formula: $C_{51}H_{72}O_2$).



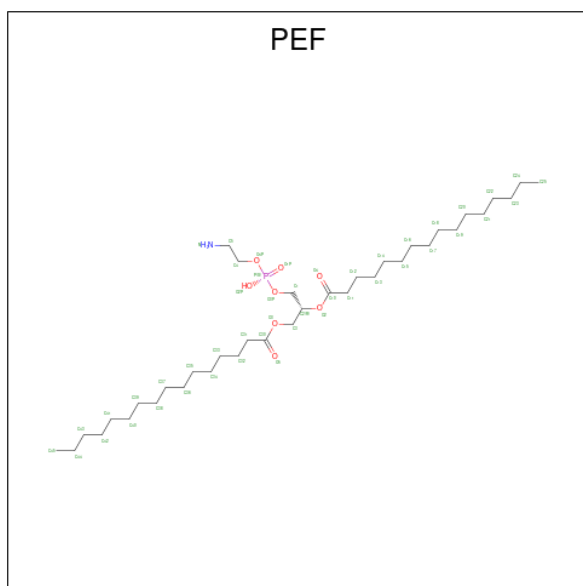
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	M	1	Total	C	O	0	0
			53	51	2		

- Molecule 12 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: $C_{42}H_{60}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			44	42	2		

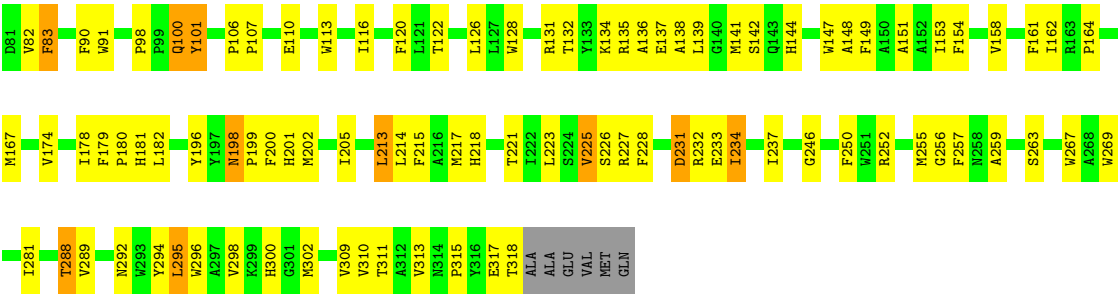
- Molecule 13 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: $C_{37}H_{74}NO_8P$).



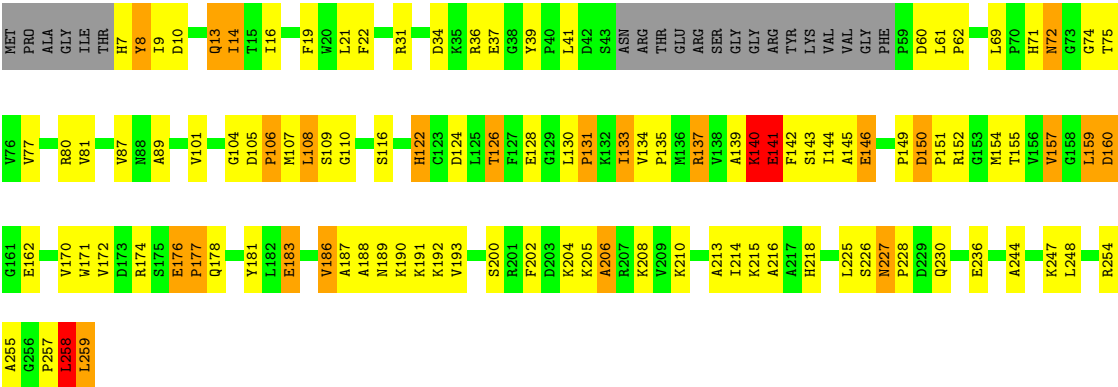
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	H	1	Total	C	N	O	P	0	0
			47	37	1	8	1		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	94	Total	O	0	0
			94	94		
14	L	37	Total	O	0	0
			37	37		
14	M	35	Total	O	0	0
			35	35		
14	H	22	Total	O	0	0
			22	22		



• Molecule 4: PHOTOSYNTHETIC REACTION CENTER



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	133.30Å 196.60Å 84.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.231 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10044	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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: MQ8, LDA, BCL, FE, BPH, PEF, BGL, CRT, HEM

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	0.69	0/2471	1.09	22/3374 (0.7%)
2	L	0.68	0/2320	0.99	14/3170 (0.4%)
3	M	0.67	0/2637	1.04	14/3610 (0.4%)
4	H	0.60	0/1890	1.12	14/2576 (0.5%)
All	All	0.66	0/9318	1.06	64/12730 (0.5%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	109	SER	N-CA-C	8.85	121.73	111.11
3	M	39	LEU	N-CA-C	-8.56	101.95	111.28
1	C	44	ASP	N-CA-C	-8.43	97.66	110.30
4	H	254	ARG	N-CA-C	-8.03	102.22	110.97
4	H	8	TYR	N-CA-C	-7.97	104.04	113.21

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	2402	0	2323	82	0
2	L	2233	0	2195	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	2537	0	2511	133	0
4	H	1837	0	1831	87	0
5	C	172	0	120	5	0
6	L	60	0	84	9	0
6	M	60	0	84	1	0
7	L	132	0	148	14	0
7	M	132	0	148	16	0
8	L	65	0	75	7	0
8	M	65	0	75	4	0
9	L	16	0	31	2	0
10	M	1	0	0	0	0
11	M	53	0	72	1	0
12	M	44	0	60	2	0
13	H	47	0	73	7	0
14	C	94	0	0	0	0
14	H	22	0	0	1	0
14	L	37	0	0	0	0
14	M	35	0	0	1	0
All	All	10044	0	9830	391	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 20.

The worst 5 of 391 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)
3:M:69:ILE:HD13	3:M:116:ILE:HG23	1.36	1.06
4:H:7:HIS:HB3	4:H:9:ILE:HG12	1.40	1.00
4:H:151:PRO:HA	4:H:154:MET:SD	2.07	0.94
3:M:33:PRO:HG3	3:M:49:PRO:HD3	1.52	0.92
6:L:704:BGL:H1	3:M:302:MET:HE2	1.53	0.90

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	308/382 (81%)	268 (87%)	31 (10%)	9 (3%)	3	2
2	L	278/280 (99%)	249 (90%)	27 (10%)	2 (1%)	18	19
3	M	316/324 (98%)	279 (88%)	31 (10%)	6 (2%)	6	4
4	H	234/259 (90%)	191 (82%)	33 (14%)	10 (4%)	2	1
All	All	1136/1245 (91%)	987 (87%)	122 (11%)	27 (2%)	4	3

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2	GLU
1	C	4	PRO
4	H	140	LYS
4	H	142	PHE
4	H	146	GLU

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	259/300 (86%)	243 (94%)	16 (6%)	16	20
2	L	228/228 (100%)	211 (92%)	17 (8%)	12	14
3	M	254/258 (98%)	231 (91%)	23 (9%)	9	9
4	H	195/211 (92%)	159 (82%)	36 (18%)	1	1
All	All	936/997 (94%)	844 (90%)	92 (10%)	7	8

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	14	ILE
4	H	131	PRO
4	H	21	LEU

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Mol	Chain	Res	Type
4	H	106	PRO
4	H	141	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	219	HIS
3	M	143	GLN
4	H	218	HIS
3	M	100	GLN
3	M	144	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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	BPH	M	605	-	59,70,70	2.13	13 (22%)	59,101,101	2.43	19 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BCL	L	604	2	69,74,74	2.01	12 (17%)	79,115,115	2.20	22 (27%)
12	CRT	M	613	-	43,43,43	2.39	13 (30%)	48,54,54	2.61	5 (10%)
9	LDA	L	707	-	13,15,15	2.46	2 (15%)	14,17,17	0.64	0
6	BGL	L	703	-	20,20,20	0.93	1 (5%)	24,25,25	2.02	7 (29%)
6	BGL	M	702	-	20,20,20	1.09	1 (5%)	24,25,25	2.39	8 (33%)
13	PEF	H	708	-	46,46,46	2.19	7 (15%)	49,51,51	1.40	6 (12%)
11	MQ8	M	608	-	54,54,54	2.47	17 (31%)	67,69,69	2.79	20 (29%)
5	HEM	C	611	1	50,50,50	1.49	10 (20%)	67,82,82	0.92	1 (1%)
6	BGL	M	705	-	20,20,20	1.30	2 (10%)	24,25,25	2.01	6 (25%)
6	BGL	M	706	-	20,20,20	0.98	1 (5%)	24,25,25	2.04	6 (25%)
7	BCL	M	603	3	69,74,74	1.85	8 (11%)	79,115,115	2.09	21 (26%)
6	BGL	L	704	-	20,20,20	1.25	2 (10%)	24,25,25	2.39	9 (37%)
5	HEM	C	612	1	50,50,50	1.38	6 (12%)	67,82,82	0.64	0
6	BGL	L	701	-	20,20,20	1.28	2 (10%)	24,25,25	1.95	8 (33%)
5	HEM	C	610	1	50,50,50	1.78	10 (20%)	67,82,82	1.01	4 (5%)
7	BCL	M	601	3	69,74,74	2.02	9 (13%)	79,115,115	2.20	21 (26%)
7	BCL	L	602	2	69,74,74	1.89	10 (14%)	79,115,115	2.10	19 (24%)
8	BPH	L	606	-	59,70,70	2.02	12 (20%)	59,101,101	2.54	20 (33%)
5	HEM	C	609	1	50,50,50	1.72	11 (22%)	67,82,82	0.96	2 (2%)

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	BPH	M	605	-	-	11/37/105/105	0/5/6/6
7	BCL	L	604	2	-	8/41/137/137	-
12	CRT	M	613	-	-	5/51/51/51	-
9	LDA	L	707	-	-	4/13/13/13	-
6	BGL	L	703	-	-	6/11/31/31	0/1/1/1
6	BGL	M	702	-	-	7/11/31/31	0/1/1/1
13	PEF	H	708	-	-	34/50/50/50	-
11	MQ8	M	608	-	-	12/47/67/67	0/2/2/2
5	HEM	C	611	1	-	6/14/54/54	-
6	BGL	M	705	-	-	4/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BGL	M	706	-	-	5/11/31/31	0/1/1/1
7	BCL	M	603	3	-	8/41/137/137	-
6	BGL	L	704	-	-	5/11/31/31	0/1/1/1
5	HEM	C	612	1	-	6/14/54/54	-
6	BGL	L	701	-	-	7/11/31/31	0/1/1/1
5	HEM	C	610	1	-	8/14/54/54	-
7	BCL	M	601	3	-	21/41/137/137	-
7	BCL	L	602	2	-	10/41/137/137	-
8	BPH	L	606	-	1/1/18/22	15/37/105/105	0/5/6/6
5	HEM	C	609	1	-	4/14/54/54	-

The worst 5 of 149 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	601	BCL	C3C-C4C	-12.13	1.36	1.51
7	L	604	BCL	C3C-C4C	-12.06	1.36	1.51
7	M	603	BCL	C3C-C4C	-10.55	1.38	1.51
7	L	602	BCL	C3C-C4C	-10.39	1.38	1.51
11	M	608	MQ8	C34-C33	8.93	1.72	1.50

The worst 5 of 204 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	613	CRT	C37-C36-C35	-11.54	108.70	124.91
8	L	606	BPH	O2D-CGD-CBD	10.96	122.99	110.95
12	M	613	CRT	C4-C5-C6	-9.81	111.13	124.91
7	L	604	BCL	C4A-NA-C1A	8.88	110.73	106.68
7	M	601	BCL	C4A-NA-C1A	8.61	110.61	106.68

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	L	606	BPH	C8

5 of 186 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	610	HEM	C2C-C3C-CAC-CBC
5	C	611	HEM	C2B-C3B-CAB-CBB

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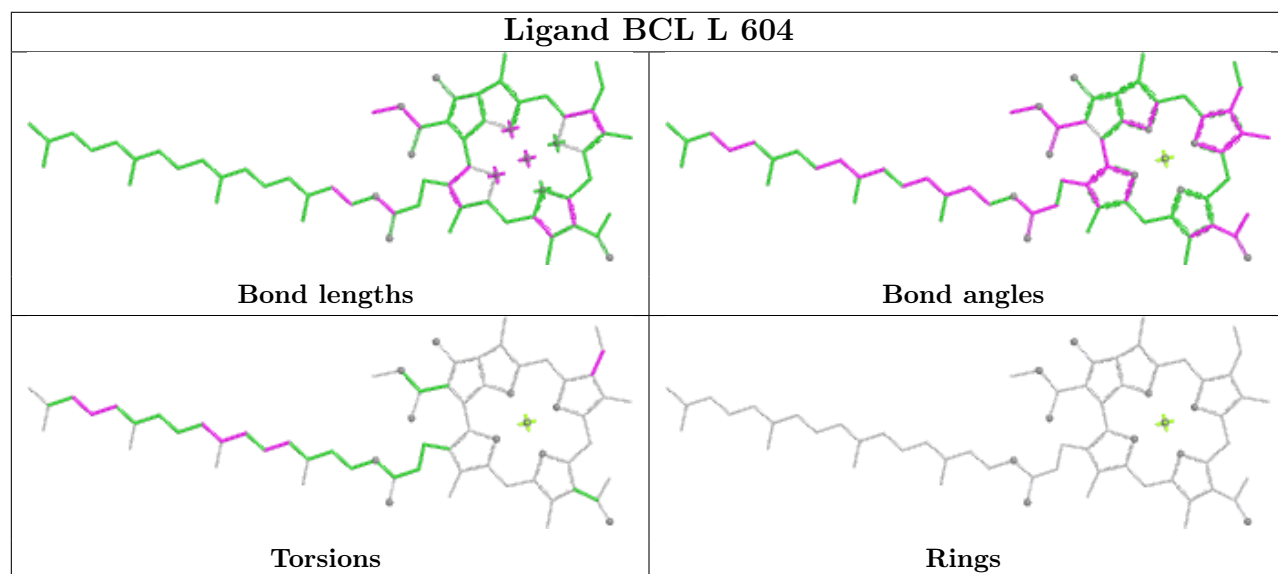
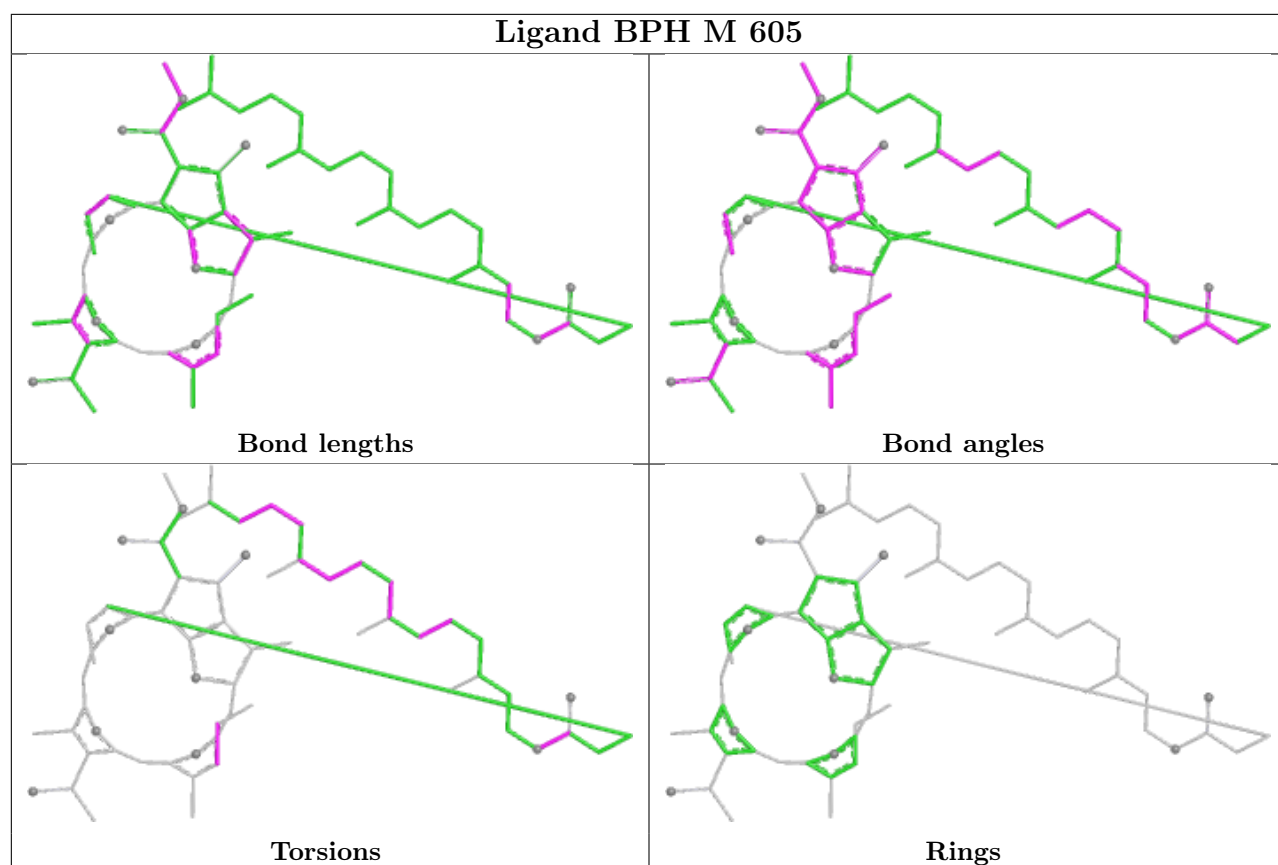
Mol	Chain	Res	Type	Atoms
5	C	611	HEM	C2C-C3C-CAC-CBC
5	C	611	HEM	C4C-C3C-CAC-CBC
5	C	612	HEM	C2C-C3C-CAC-CBC

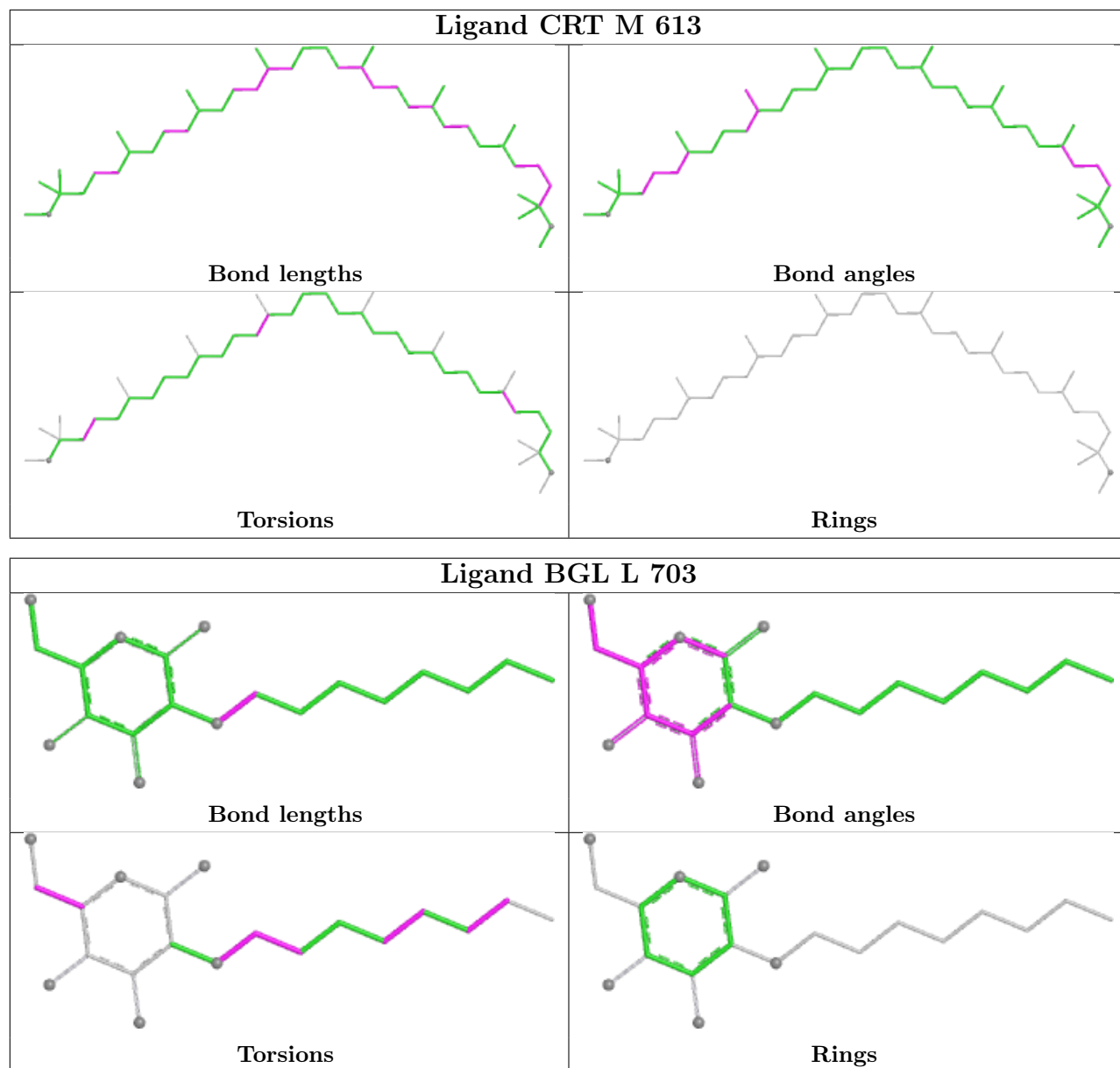
There are no ring outliers.

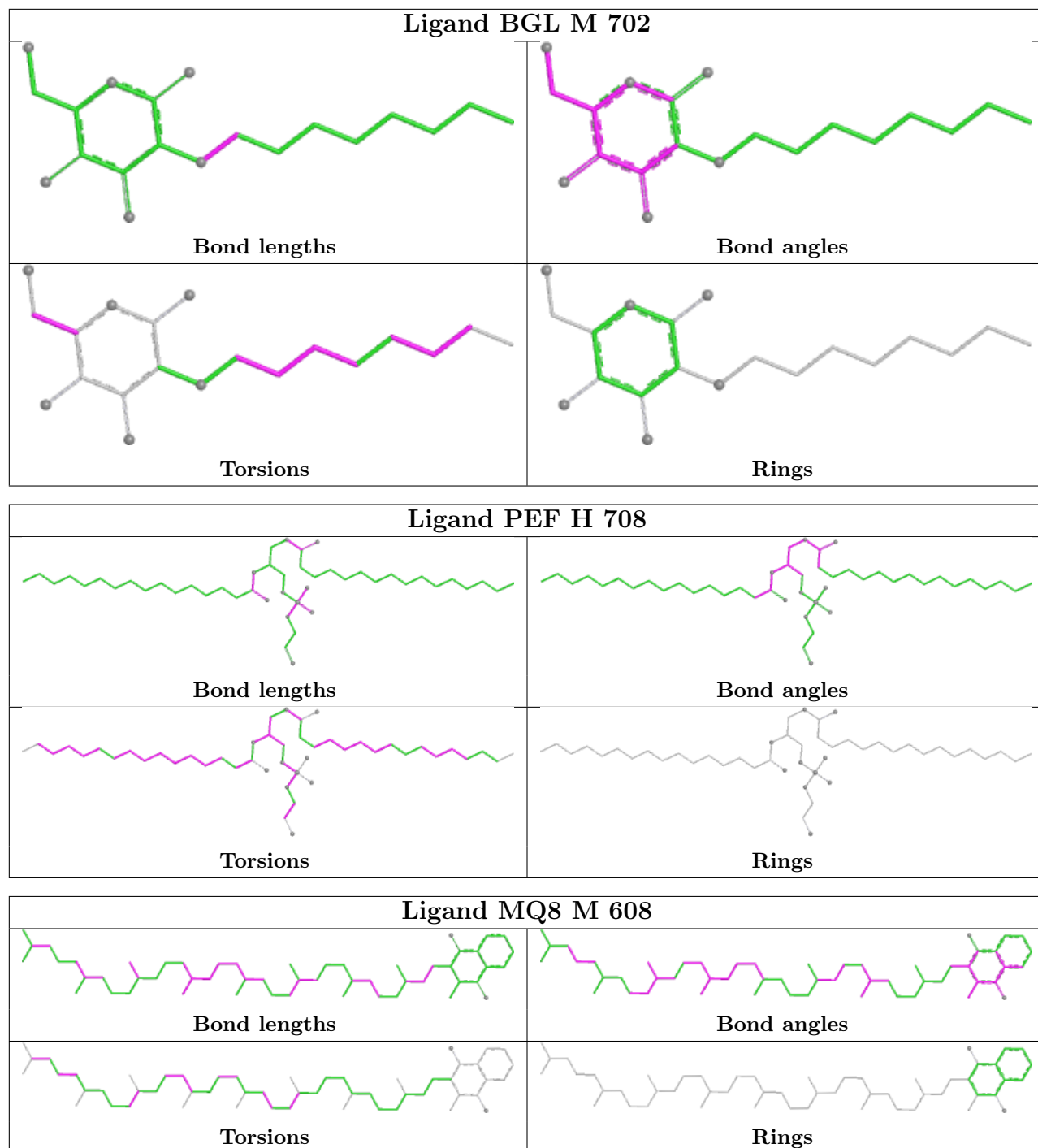
17 monomers are involved in 65 short contacts:

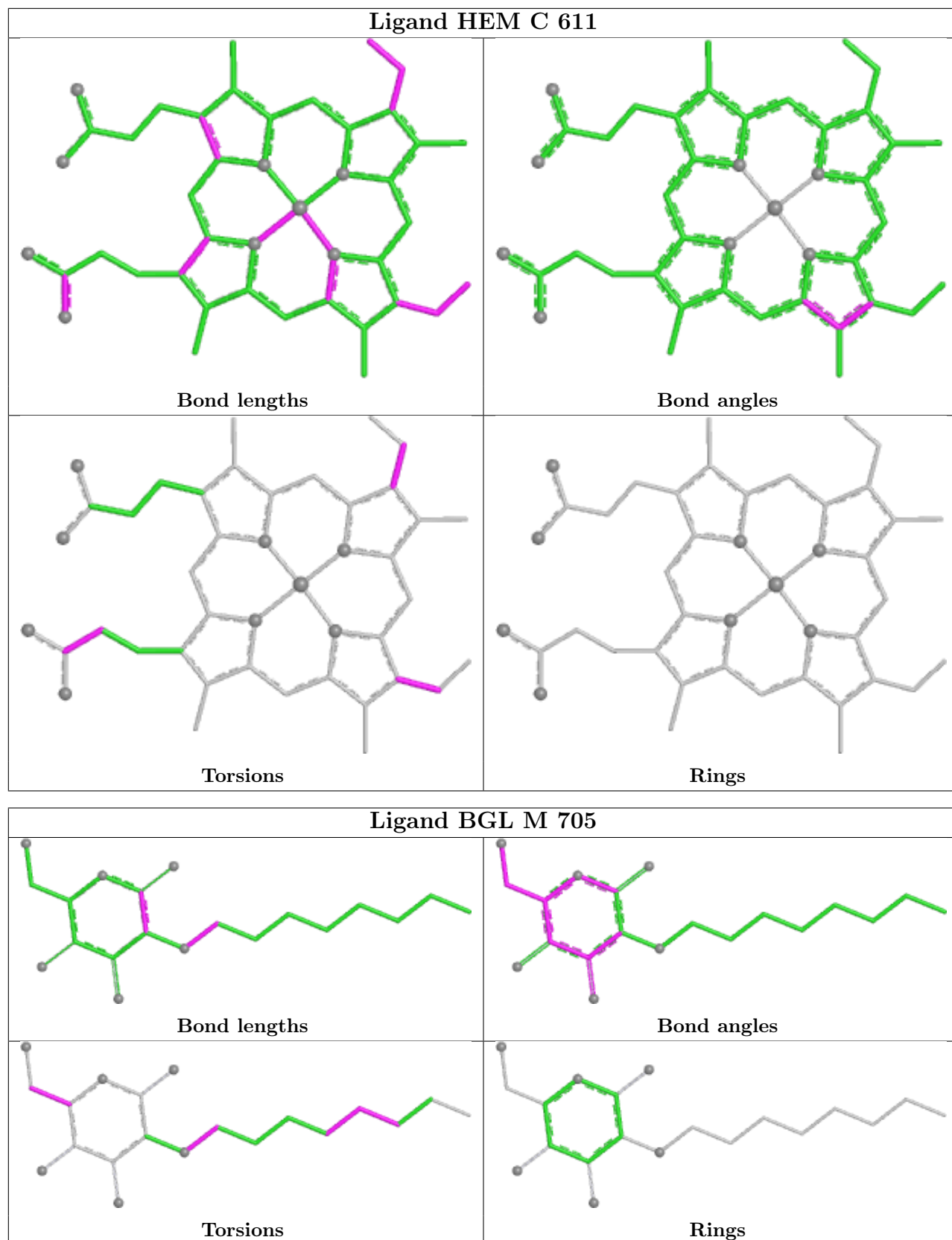
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	605	BPH	4	0
7	L	604	BCL	10	0
12	M	613	CRT	2	0
9	L	707	LDA	2	0
6	L	703	BGL	4	0
6	M	702	BGL	1	0
13	H	708	PEF	7	0
11	M	608	MQ8	1	0
7	M	603	BCL	6	0
6	L	704	BGL	2	0
5	C	612	HEM	2	0
6	L	701	BGL	3	0
5	C	610	HEM	2	0
7	M	601	BCL	10	0
7	L	602	BCL	7	0
8	L	606	BPH	7	0
5	C	609	HEM	1	0

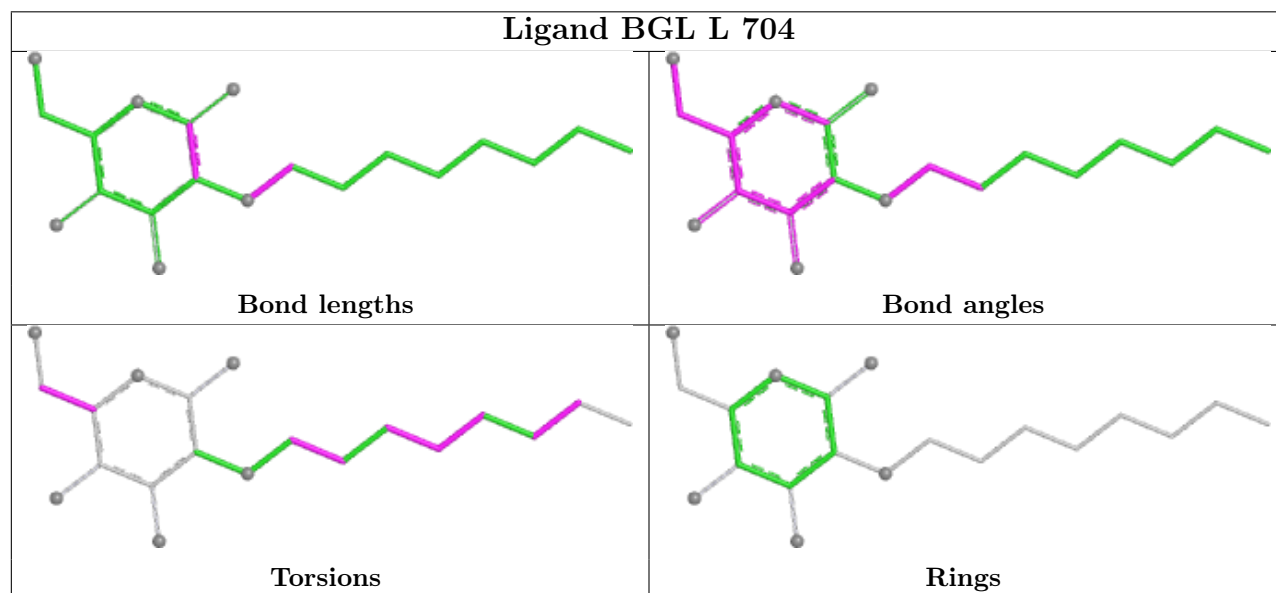
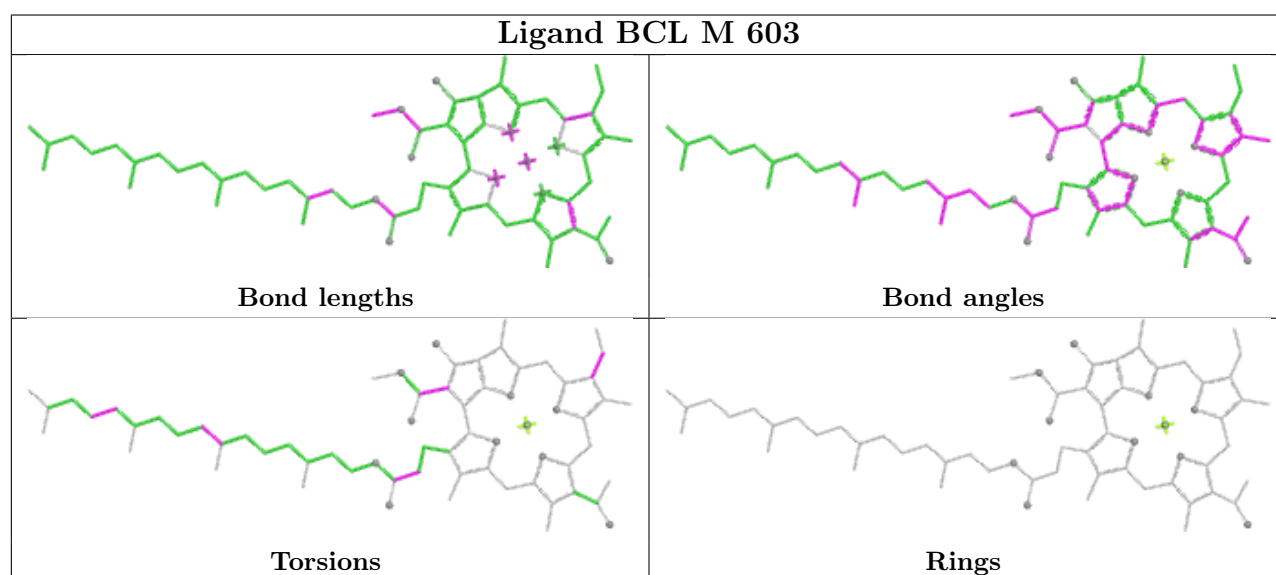
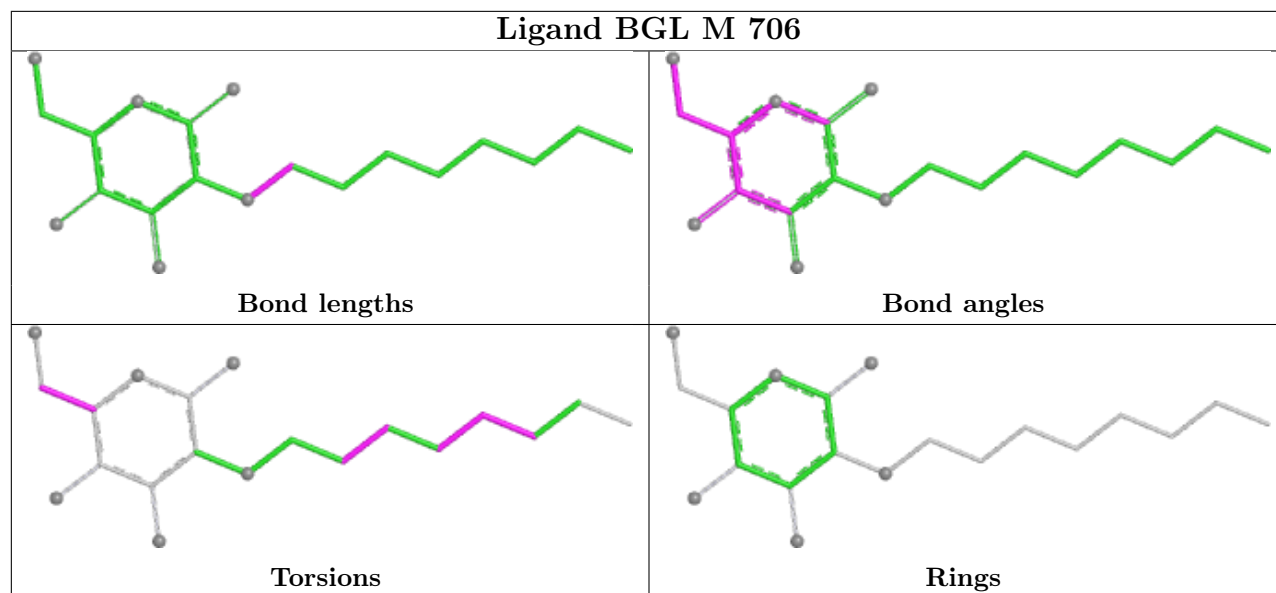
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

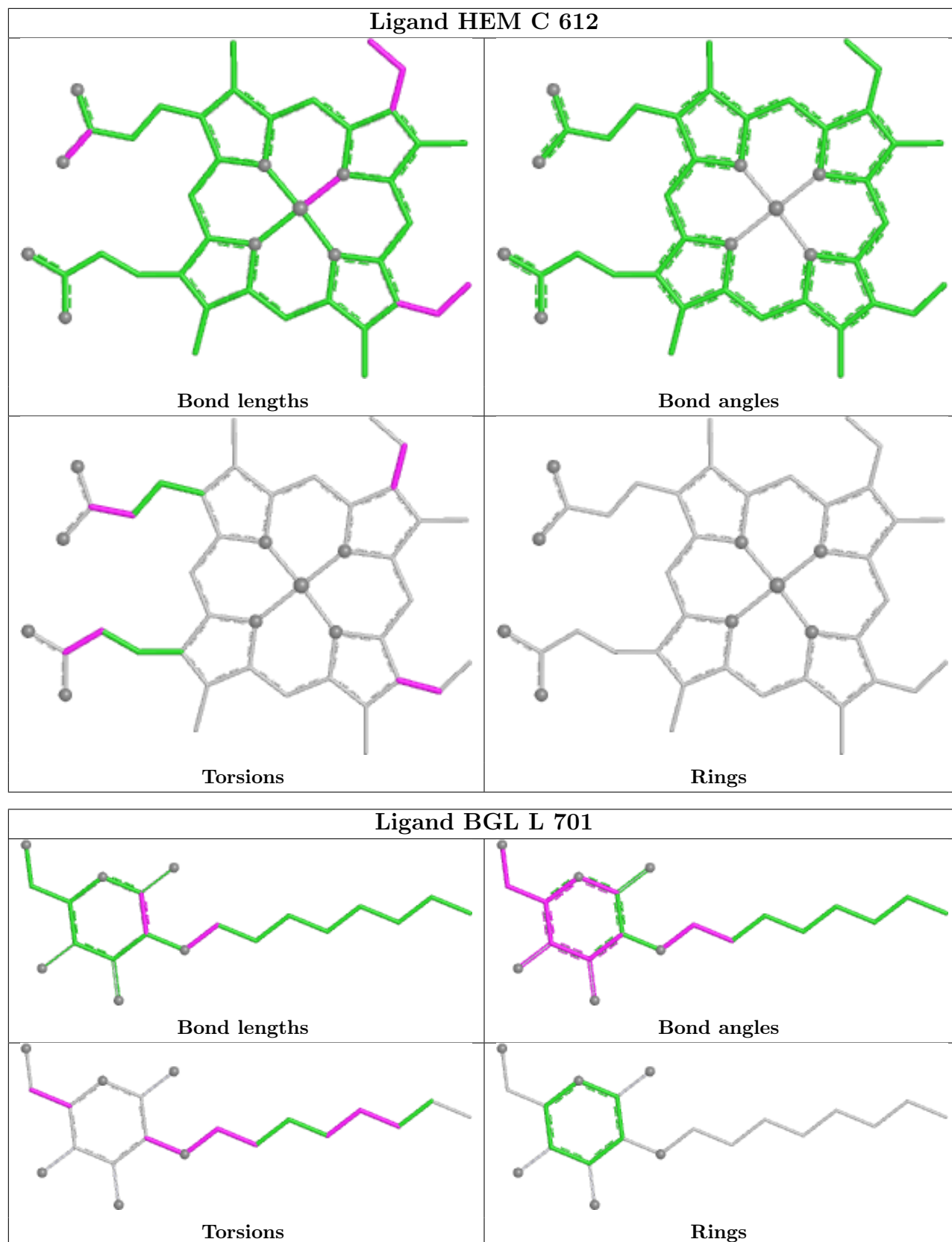


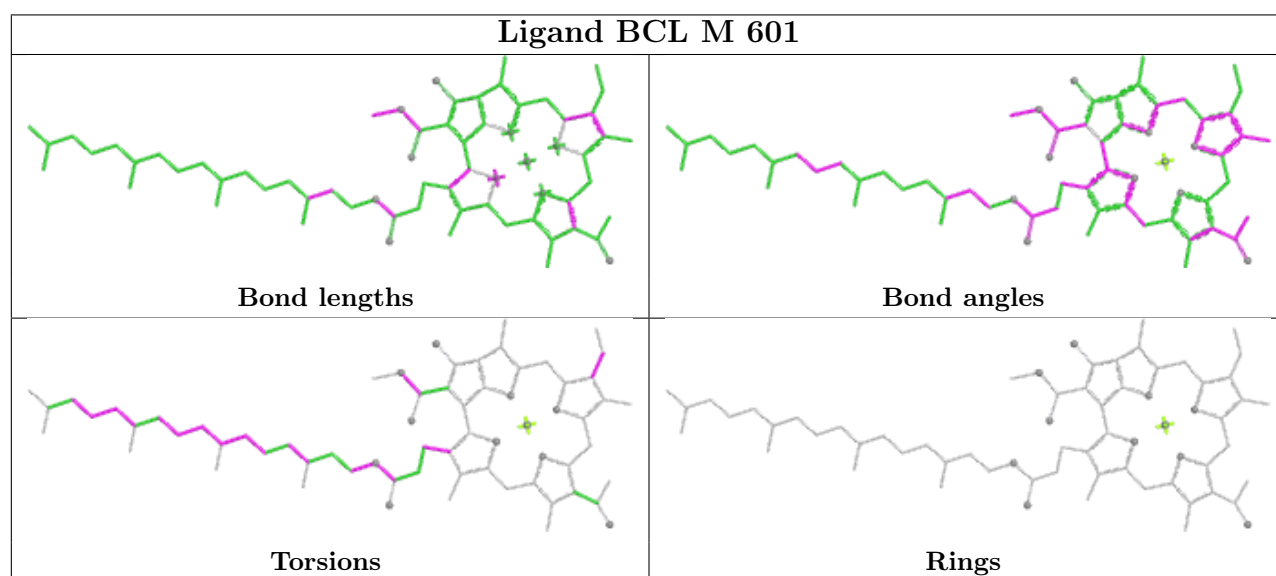
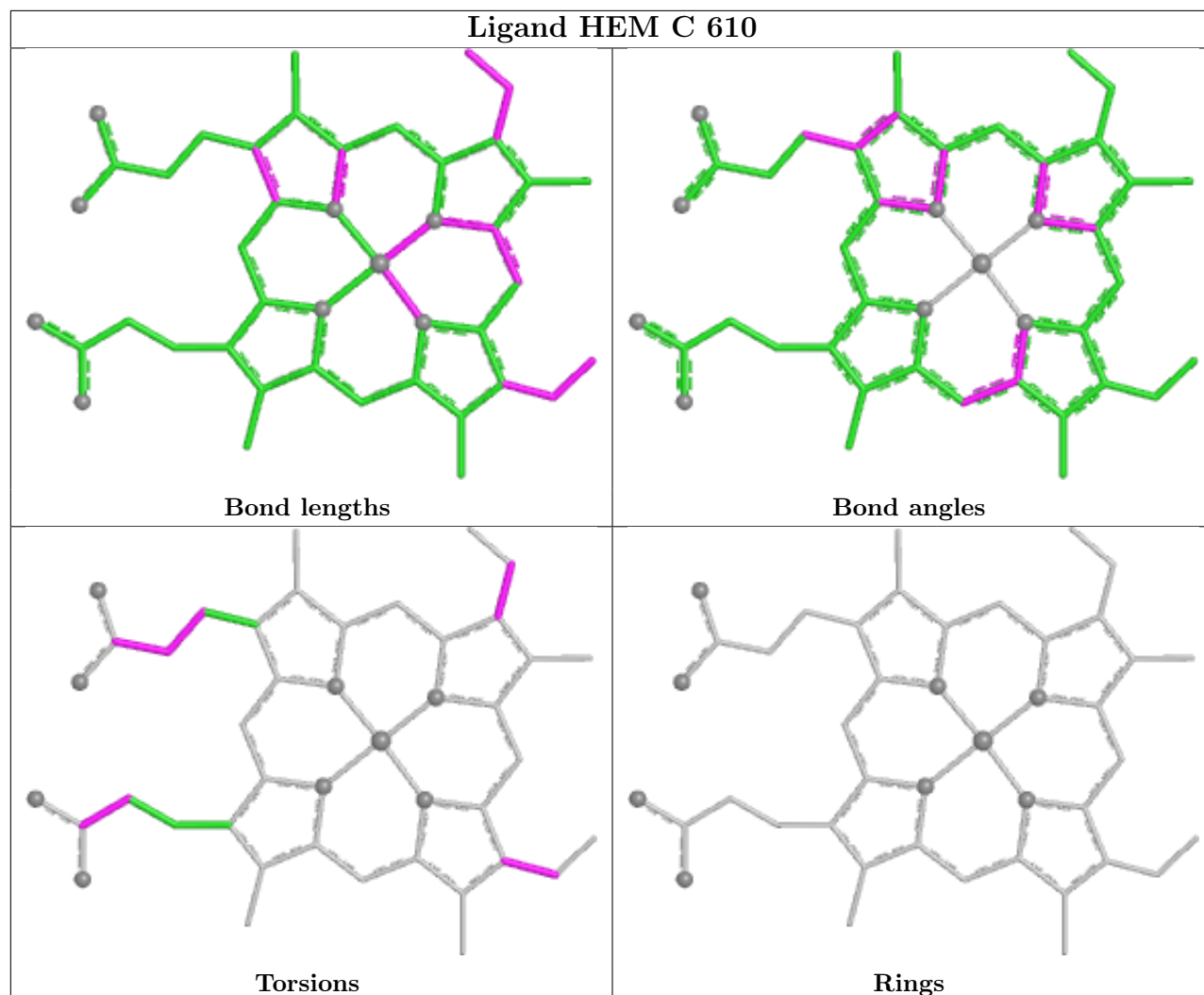


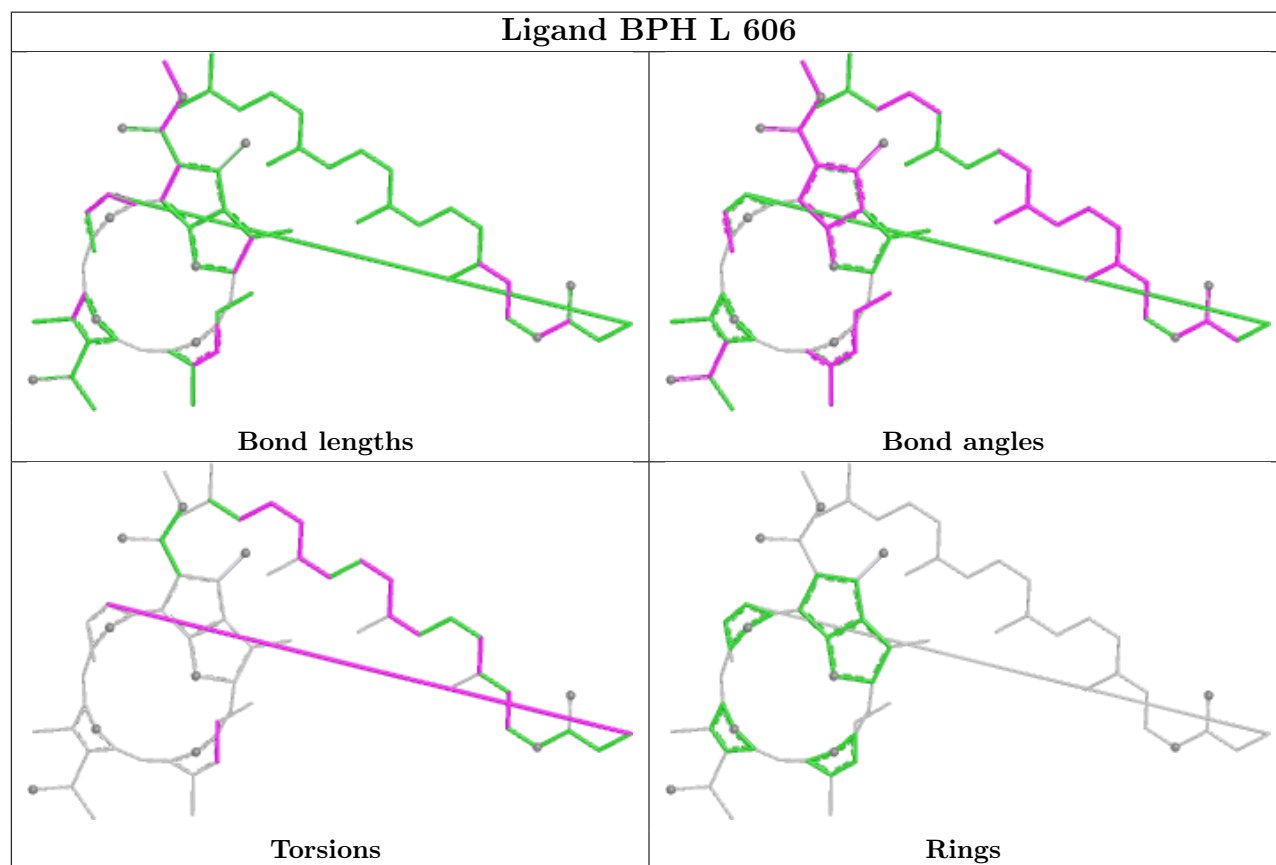
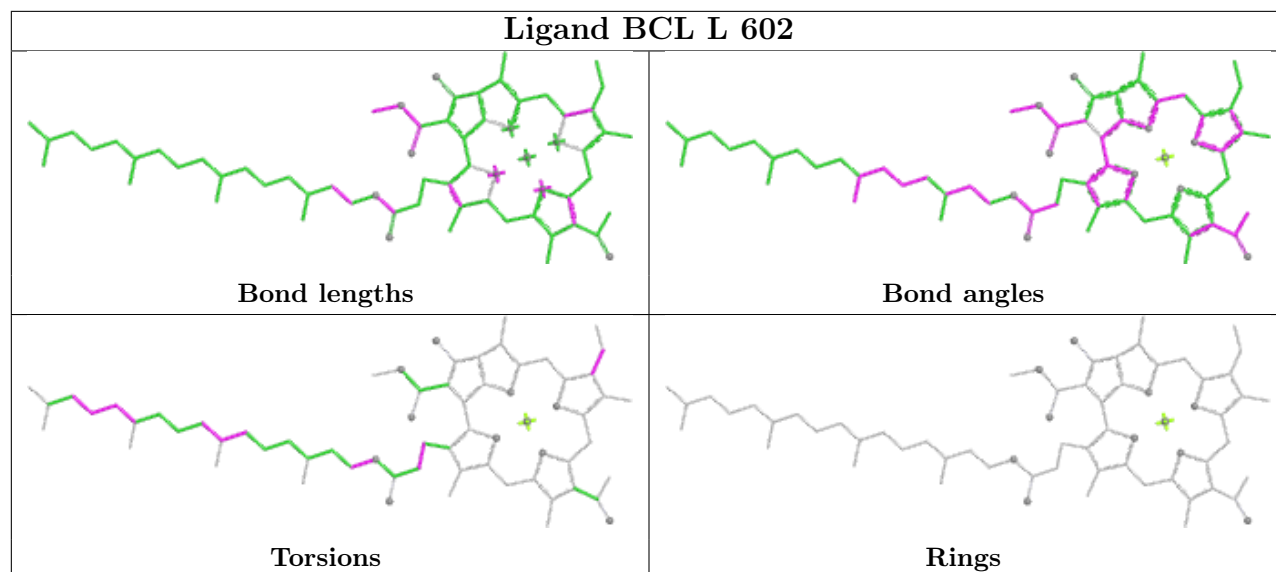


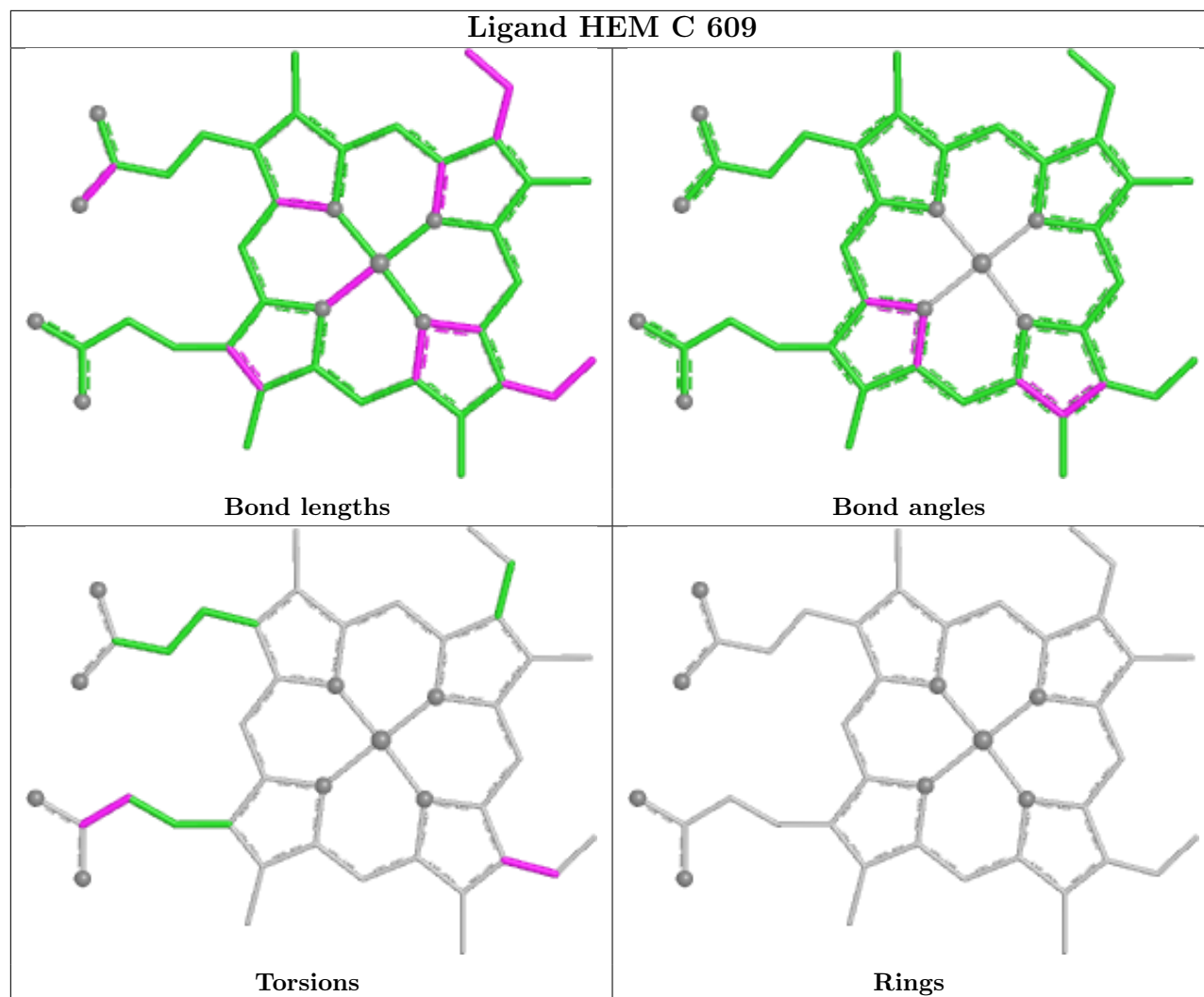












5.7 Other polymers [i](#)

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.