



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 12:01 AM UTC

PDB ID : 1E14 / pdb_00001e14
Title : PHOTOSYNTHETIC REACTION CENTER MUTANT WITH PHE M197 REPLACED WITH ARG (CHAIN M, FM197R) AND GLY M203 REPLACED WITH ASP (CHAIN M, GM203D)
Authors : Fyfe, P.K.; Ridge, J.P.; McAuley, K.E.; Cogdell, R.J.; Isaacs, N.W.; Jones, M.R.
Deposited on : 2000-04-18
Resolution : 2.70 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

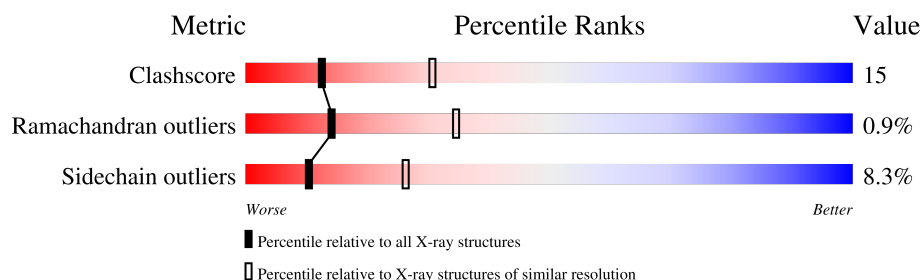
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	H	260	49% 30% 11% 7%
2	L	281	60% 32% 6%
3	M	307	62% 28% 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BCL	M	1301	X	-	-	-
6	BPH	L	401	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	SPN	M	600	-	X	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7250 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 Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	241	Total	C	N	O	S	0	0	1
			1830	1169	315	337	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

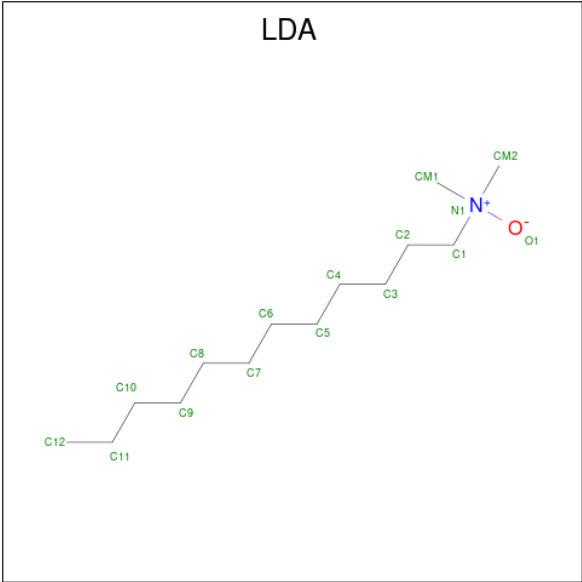
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2413	1606	398	399	10			

There are 2 discrepancies between the modelled and reference sequences:

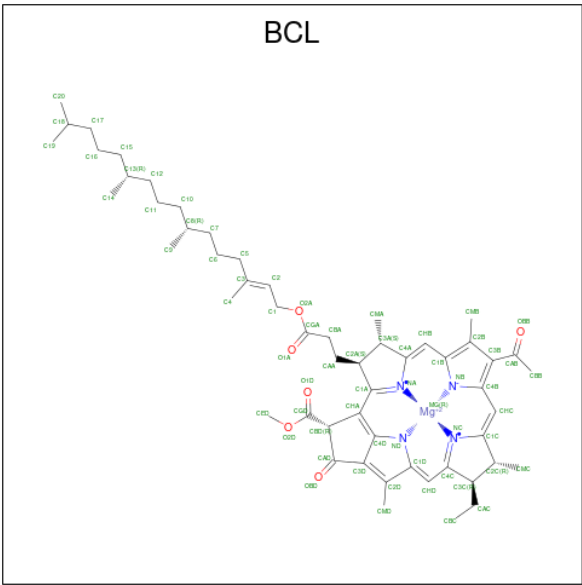
Chain	Residue	Modelled	Actual	Comment	Reference
M	197	ARG	PHE	conflict	UNP P0C0Y9
M	203	ASP	GLY	conflict	UNP P0C0Y9

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



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

- Molecule 5 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



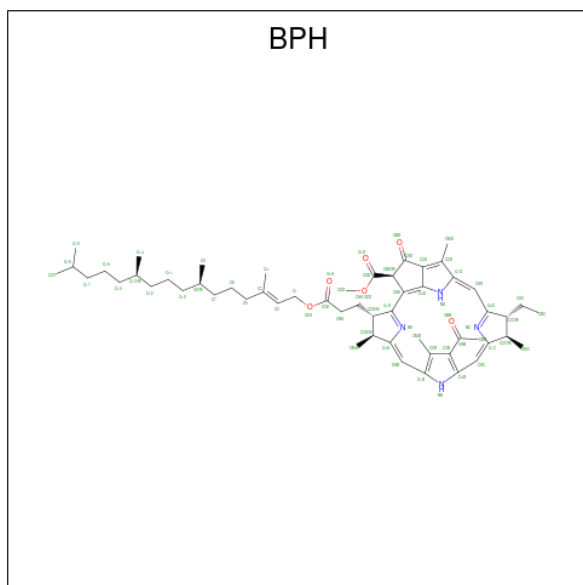
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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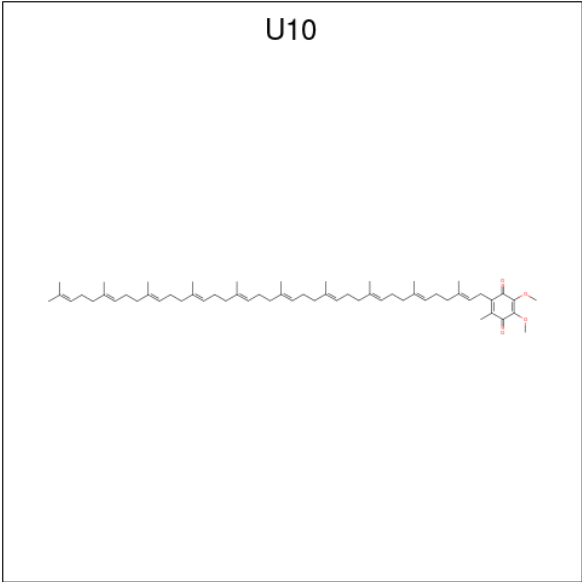
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 6 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



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

- Molecule 7 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).

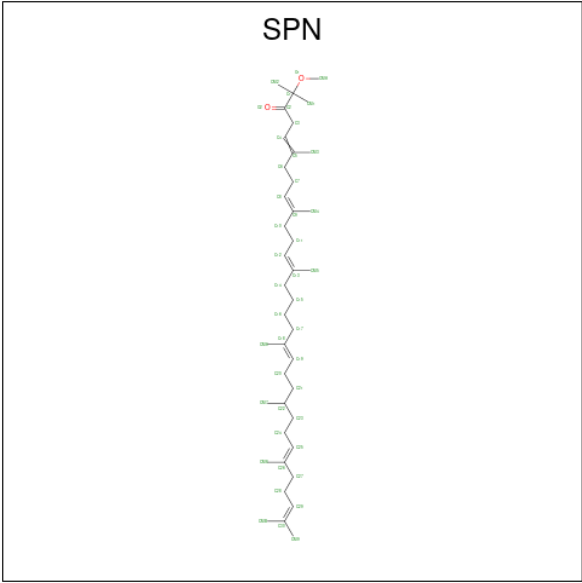


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	22	0
			48	44	4		
7	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 8 is FE (III) ION (CCD ID: FE) (formula: Fe).

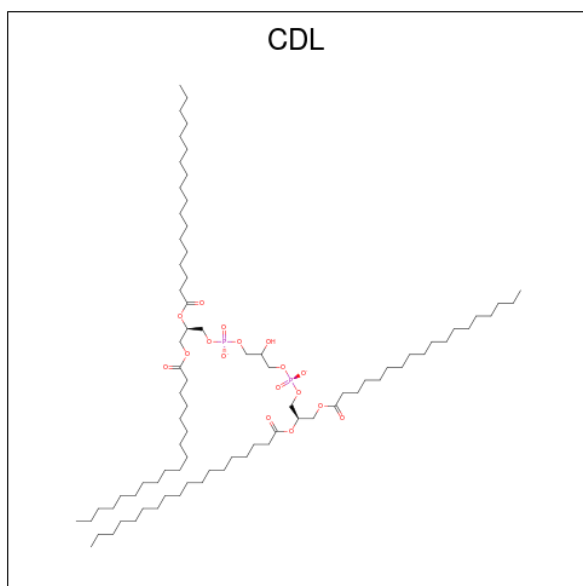
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- Molecule 9 is SPEROIDENONE (CCD ID: SPN) (formula: C₄₁H₇₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			43	41	2		

- Molecule 10 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 11 is water.

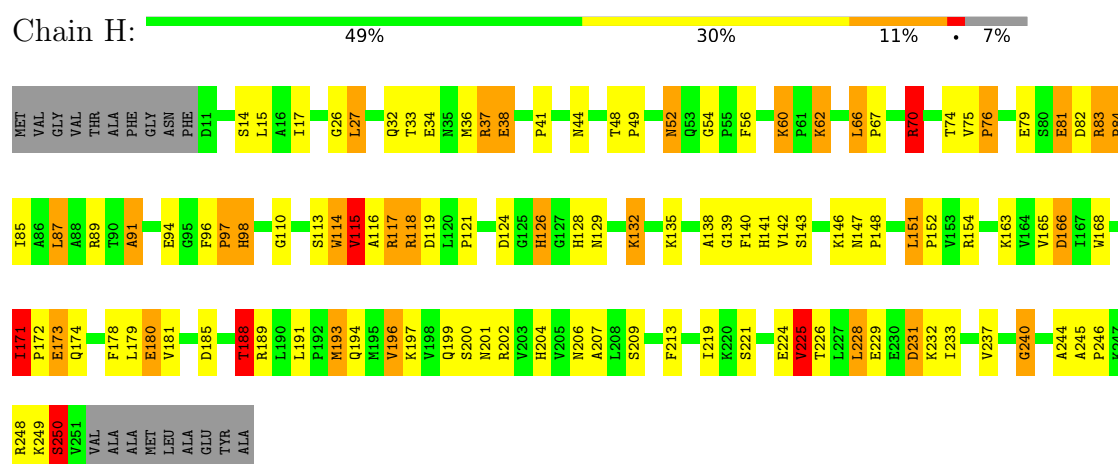
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	42	Total	O	0	0
			42	42		
11	L	28	Total	O	0	0
			28	28		
11	M	42	Total	O	0	0
			42	42		

3 Residue-property plots

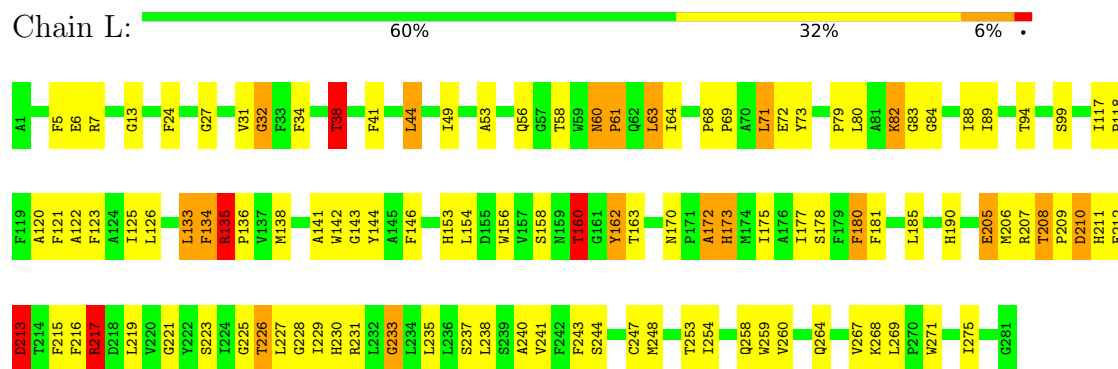
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

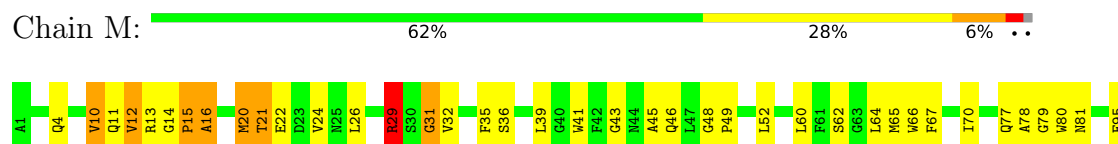
• Molecule 1: Reaction center protein H chain

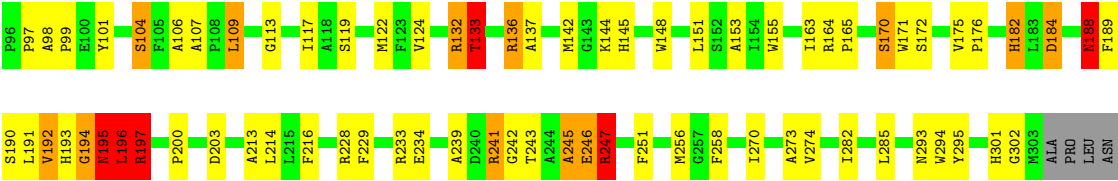


• Molecule 2: Reaction center protein L chain



• Molecule 3: Reaction center protein M chain





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.00 Å 140.00 Å 184.60 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	92.6 (30.00-2.70)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.226 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7250	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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: CDL, U10, BPH, BCL, SPN, FE, LDA

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	H	0.86	0/1878	2.10	77/2555 (3.0%)
2	L	0.81	1/2320 (0.0%)	1.93	73/3175 (2.3%)
3	M	0.77	0/2504	1.90	63/3419 (1.8%)
All	All	0.81	1/6702 (0.0%)	1.97	213/9149 (2.3%)

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	H	0	7
2	L	0	5
3	M	0	2
All	All	0	14

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	32	GLY	N-CA	6.85	1.52	1.45

The worst 5 of 213 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	188	ASN	OD1-CG-ND2	16.29	138.89	122.60
2	L	135	ARG	CD-NE-CZ	14.67	144.93	124.40
3	M	188	ASN	CA-CB-CG	-11.39	101.21	112.60
1	H	70	ARG	NE-CZ-NH2	-10.96	109.34	119.20
1	H	83	ARG	CD-NE-CZ	10.49	139.08	124.40

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	113	SER	Mainchain
1	H	114	TRP	Mainchain
1	H	115	VAL	Mainchain
1	H	87	LEU	Mainchain
1	H	91	ALA	Mainchain

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	H	1830	0	1836	68	0
2	L	2232	0	2187	66	0
3	M	2413	0	2326	67	0
4	H	16	0	31	0	0
4	M	32	0	62	5	0
5	L	132	0	148	11	0
5	M	132	0	148	9	0
6	L	65	0	76	12	0
6	M	65	0	76	5	0
7	L	48	0	58	1	0
7	M	48	0	63	0	0
8	M	1	0	0	0	0
9	M	43	0	69	5	0
10	M	81	0	106	16	0
11	H	42	0	0	3	0
11	L	28	0	0	1	0
11	M	42	0	0	1	0
All	All	7250	0	7186	218	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 15.

The worst 5 of 218 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)
10:M:800:CDL:CA6	10:M:800:CDL:HB4	1.62	1.28
10:M:800:CDL:HB4	10:M:800:CDL:HA61	1.10	1.10
10:M:800:CDL:HA61	10:M:800:CDL:CB4	1.83	1.08
1:H:27:LEU:HD23	10:M:800:CDL:H132	1.51	0.92
1:H:81:GLU:HG3	1:H:85:ILE:HD11	1.57	0.86

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	H	239/260 (92%)	224 (94%)	13 (5%)	2 (1%)	16	37
2	L	279/281 (99%)	262 (94%)	17 (6%)	0	100	100
3	M	301/307 (98%)	275 (91%)	21 (7%)	5 (2%)	7	19
All	All	819/848 (97%)	761 (93%)	51 (6%)	7 (1%)	14	35

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	250	SER
1	H	116	ALA
3	M	195	ASN
3	M	301	HIS
3	M	80	TRP

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	H	195/208 (94%)	178 (91%)	17 (9%)	9	24
2	L	220/220 (100%)	203 (92%)	17 (8%)	12	30
3	M	237/241 (98%)	217 (92%)	20 (8%)	10	26
All	All	652/669 (98%)	598 (92%)	54 (8%)	10	26

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	210	ASP
3	M	10	VAL
3	M	192	VAL
2	L	217	ARG
2	L	237	SER

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

Mol	Chain	Res	Type
3	M	299	GLN
3	M	4	GLN
1	H	206	ASN
1	H	204	HIS
2	L	87	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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$
4	LDA	M	703	-	13,15,15	2.78	2 (15%)	14,17,17	0.80	1 (7%)
4	LDA	H	701	-	13,15,15	2.67	2 (15%)	14,17,17	0.79	1 (7%)
7	U10	L	501	-	47,47,63	2.05	14 (29%)	56,58,79	2.66	19 (33%)
7	U10	M	502	-	48,48,63	1.83	17 (35%)	60,61,79	1.49	11 (18%)
6	BPH	M	402	-	59,70,70	1.97	15 (25%)	59,101,101	3.30	21 (35%)
9	SPN	M	600	-	42,42,42	4.02	20 (47%)	50,52,52	2.88	19 (38%)
5	BCL	L	1302	2	69,74,74	1.49	8 (11%)	79,115,115	2.07	20 (25%)
6	BPH	L	401	-	59,70,70	2.00	15 (25%)	59,101,101	3.67	16 (27%)
5	BCL	M	1301	3	69,74,74	1.39	7 (10%)	79,115,115	2.14	24 (30%)
5	BCL	L	1304	2	69,74,74	1.36	7 (10%)	79,115,115	2.70	24 (30%)
10	CDL	M	800	-	80,80,99	0.50	0	86,92,111	0.91	3 (3%)
4	LDA	M	702	-	13,15,15	2.71	2 (15%)	14,17,17	0.84	1 (7%)
5	BCL	M	1303	3	69,74,74	1.36	7 (10%)	79,115,115	1.75	19 (24%)

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
4	LDA	M	703	-	-	8/13/13/13	-
4	LDA	H	701	-	-	12/13/13/13	-
7	U10	L	501	-	-	15/41/65/87	0/1/1/1
7	U10	M	502	-	-	6/45/69/87	0/1/1/1
6	BPH	M	402	-	-	18/37/105/105	0/5/6/6
9	SPN	M	600	-	-	19/50/51/51	-
5	BCL	L	1302	2	-	8/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BPH	L	401	-	2/2/18/22	14/37/105/105	0/5/6/6
5	BCL	M	1301	3	1/1/21/25	16/41/137/137	-
5	BCL	L	1304	2	-	9/41/137/137	-
10	CDL	M	800	-	-	35/91/91/110	-
4	LDA	M	702	-	-	12/13/13/13	-
5	BCL	M	1303	3	-	4/41/137/137	-

The worst 5 of 116 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	600	SPN	C4-C5	9.23	1.54	1.33
9	M	600	SPN	C8-C9	8.82	1.53	1.33
9	M	600	SPN	C3-C2	8.76	1.60	1.52
9	M	600	SPN	C19-C18	8.61	1.52	1.33
9	M	600	SPN	C12-C13	8.38	1.52	1.33

The worst 5 of 179 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	401	BPH	O2D-CGD-CBD	21.81	134.91	110.95
6	M	402	BPH	O2D-CGD-CBD	16.37	128.94	110.95
5	L	1304	BCL	O2D-CGD-CBD	11.39	131.15	111.23
7	L	501	U10	C37-C38-C39	10.84	152.45	127.62
5	L	1304	BCL	C1C-NC-C4C	9.28	110.92	106.68

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	1301	BCL	C13
6	L	401	BPH	C8
6	L	401	BPH	C13

5 of 176 torsion outliers are listed below:

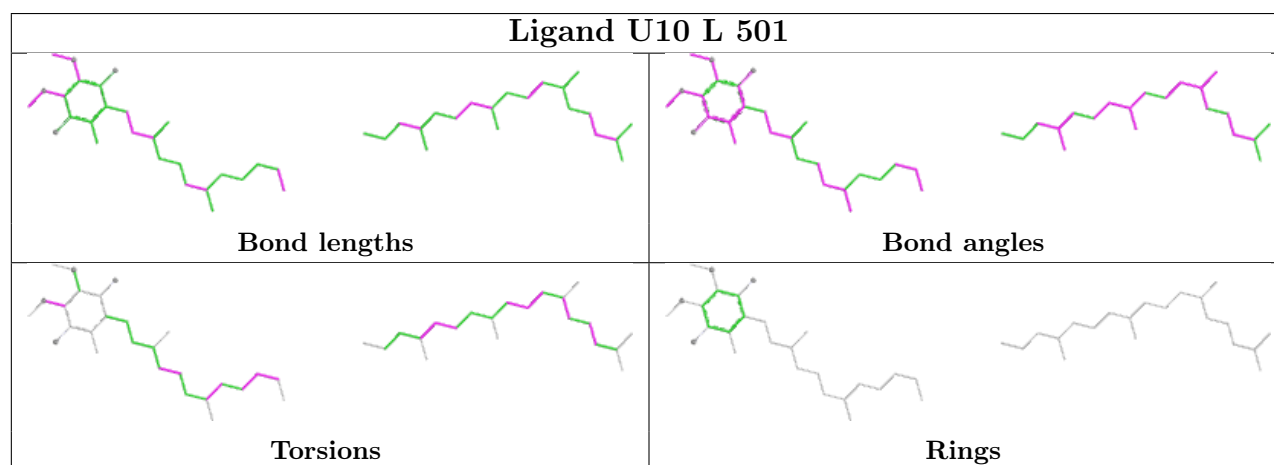
Mol	Chain	Res	Type	Atoms
4	H	701	LDA	C2-C1-N1-O1
4	H	701	LDA	C2-C1-N1-CM2
4	H	701	LDA	N1-C1-C2-C3
4	M	702	LDA	C2-C1-N1-O1
4	M	702	LDA	C2-C1-N1-CM1

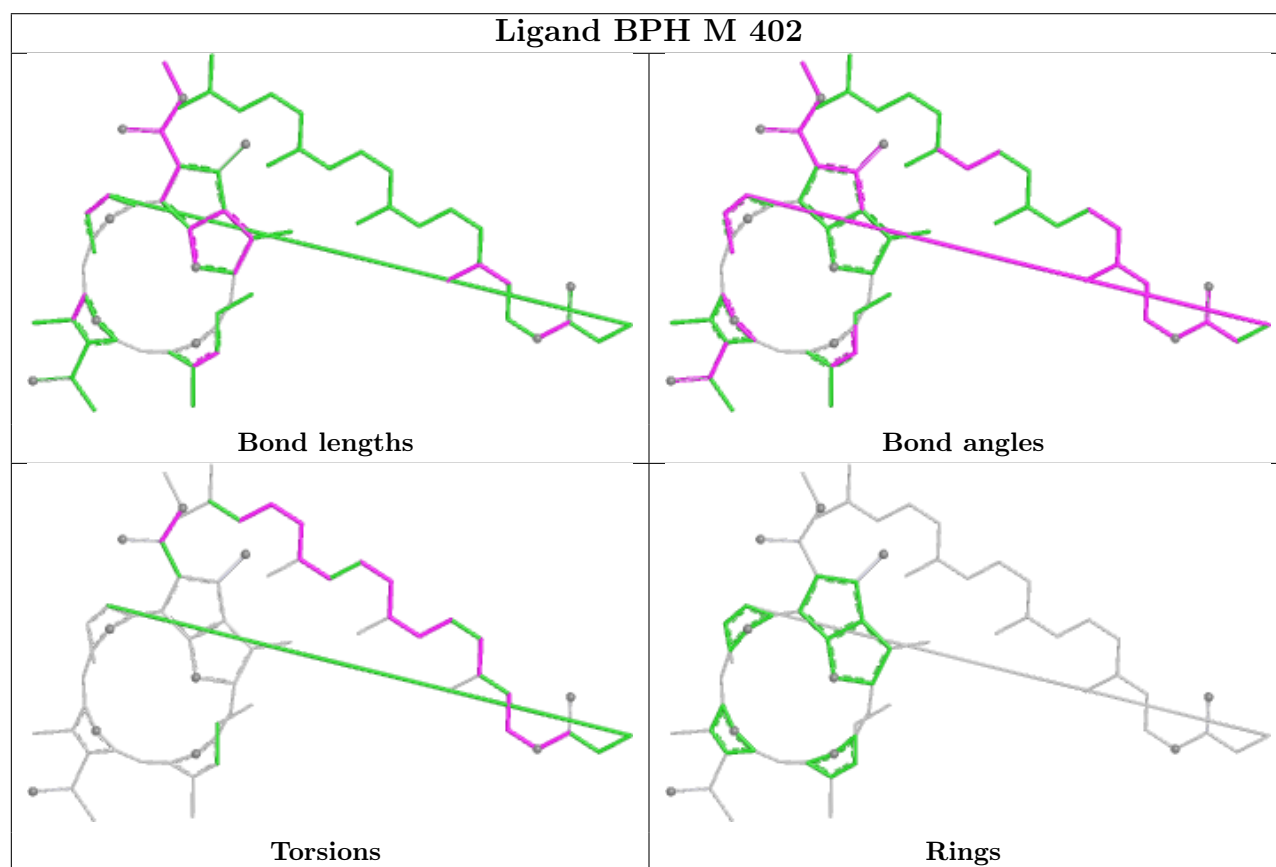
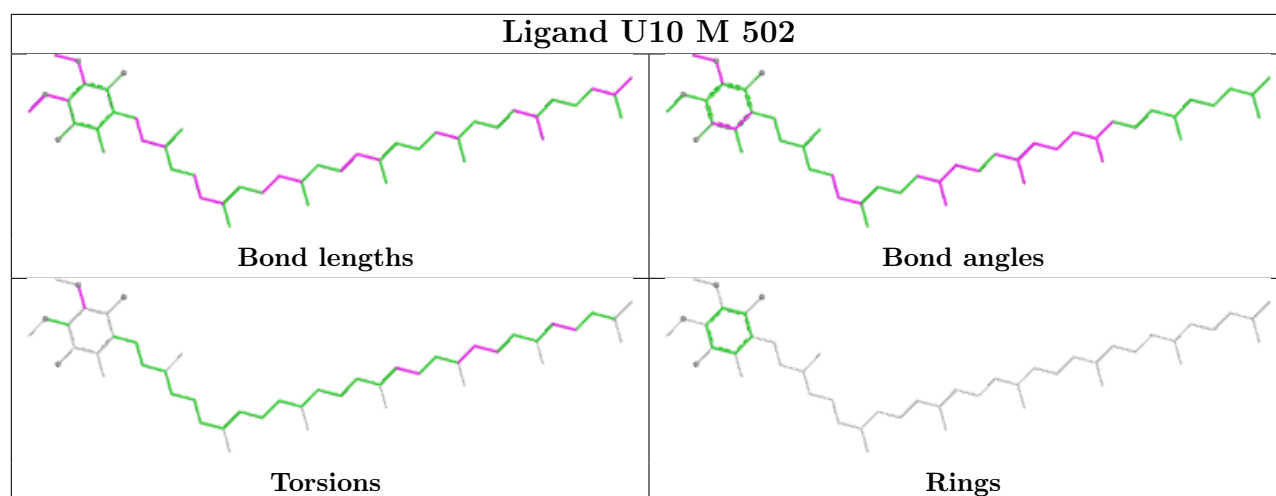
There are no ring outliers.

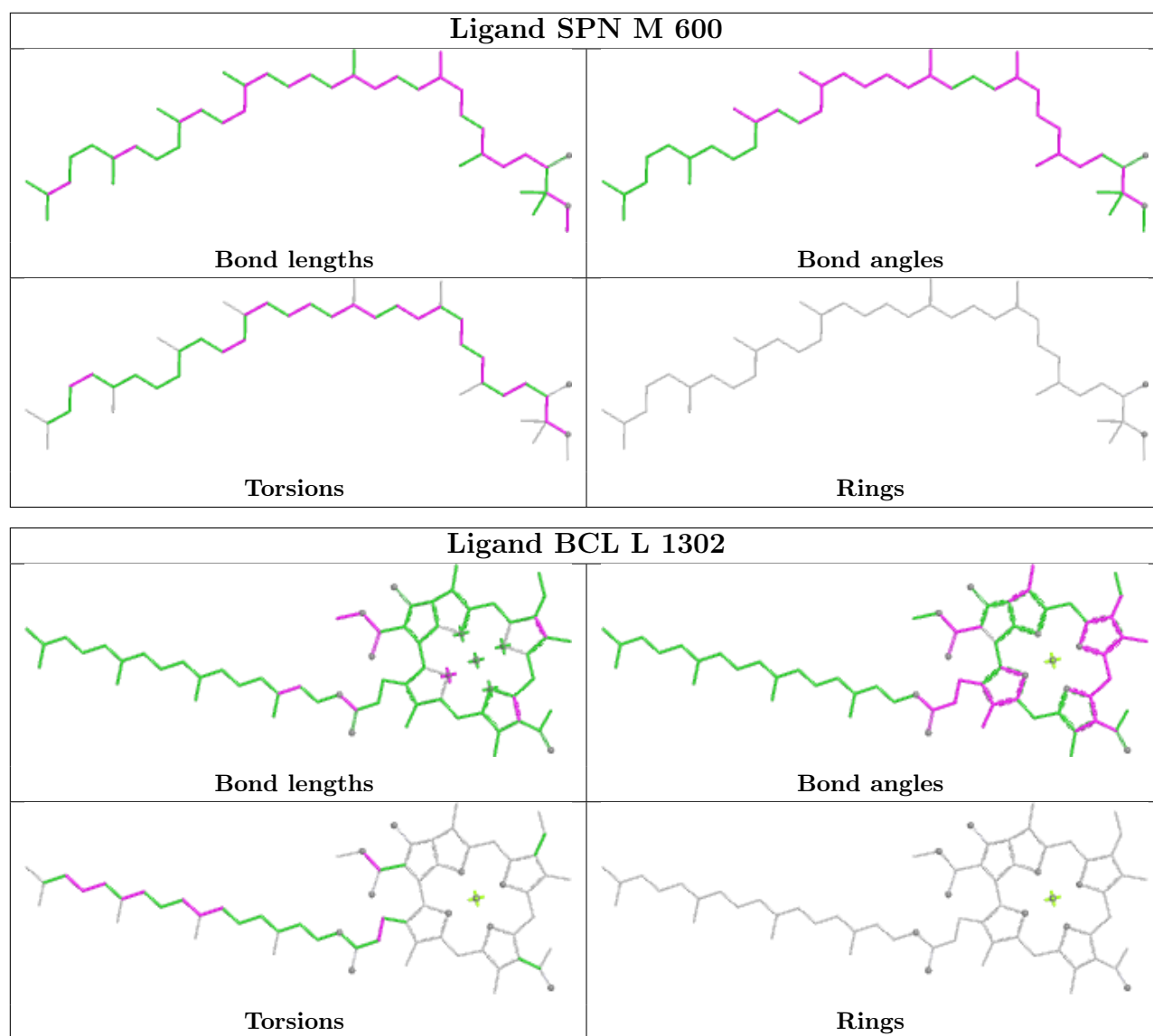
11 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	703	LDA	2	0
7	L	501	U10	1	0
6	M	402	BPH	5	0
9	M	600	SPN	5	0
5	L	1302	BCL	7	0
6	L	401	BPH	12	0
5	M	1301	BCL	5	0
5	L	1304	BCL	6	0
10	M	800	CDL	16	0
4	M	702	LDA	3	0
5	M	1303	BCL	5	0

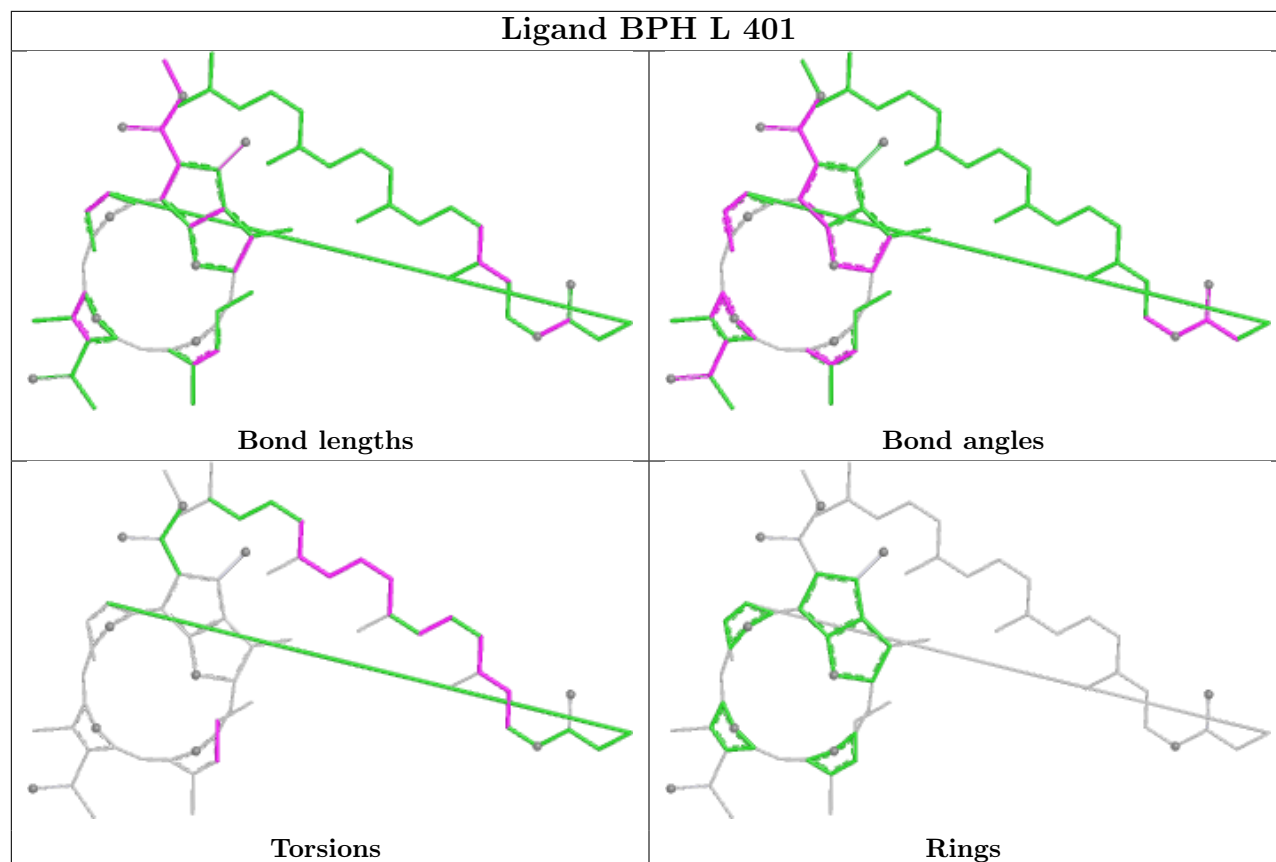
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



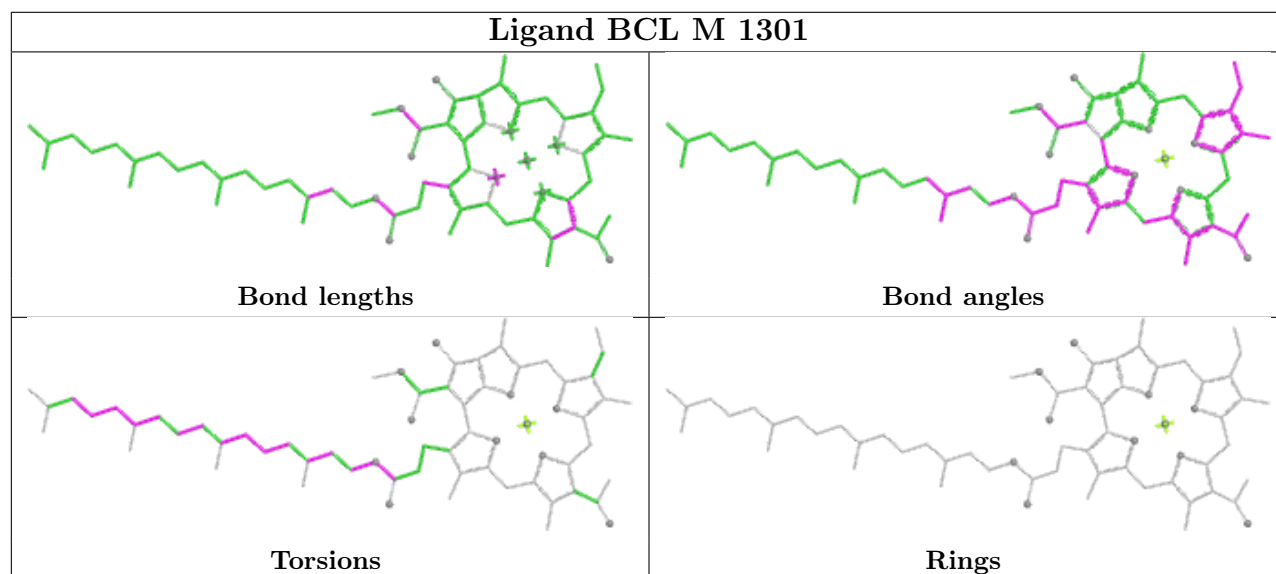


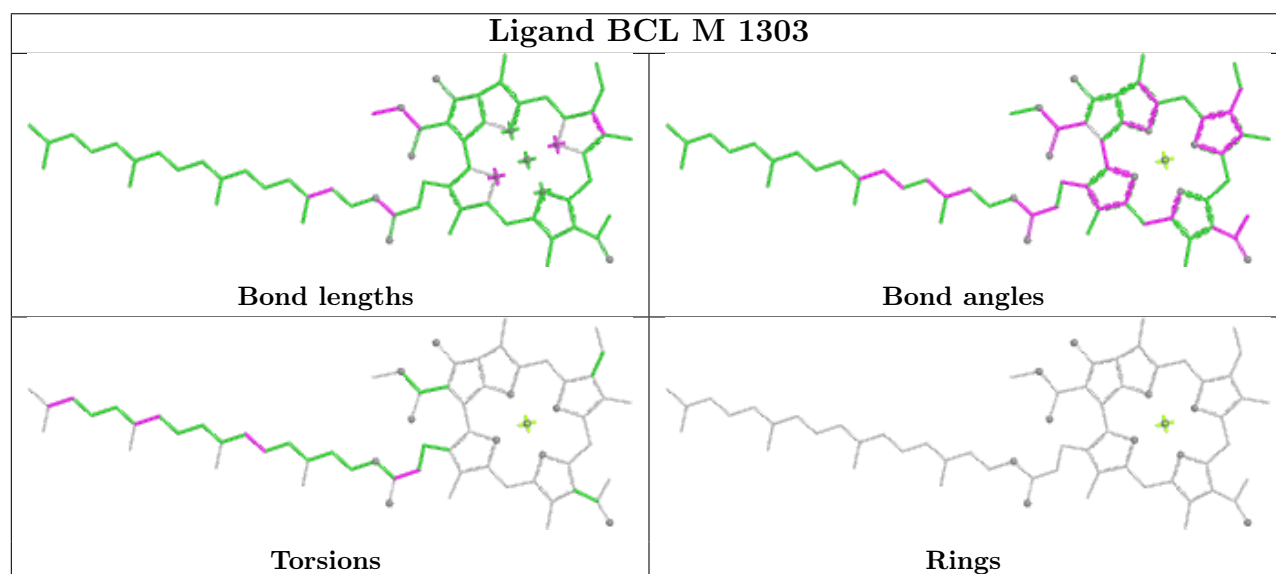
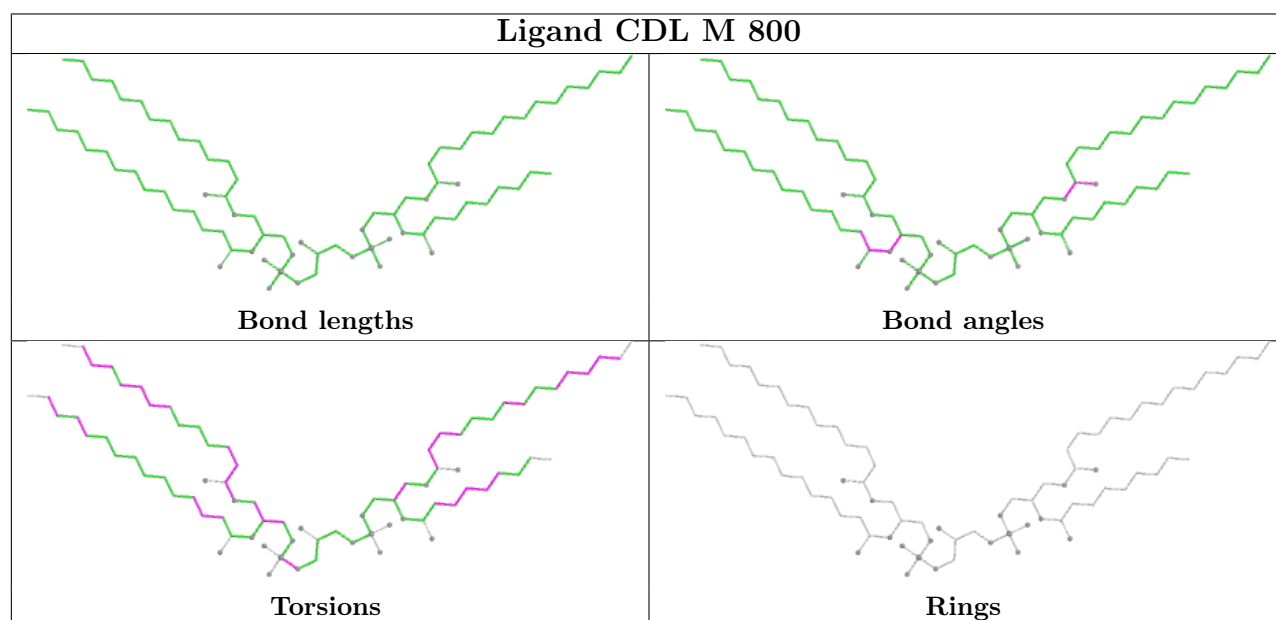
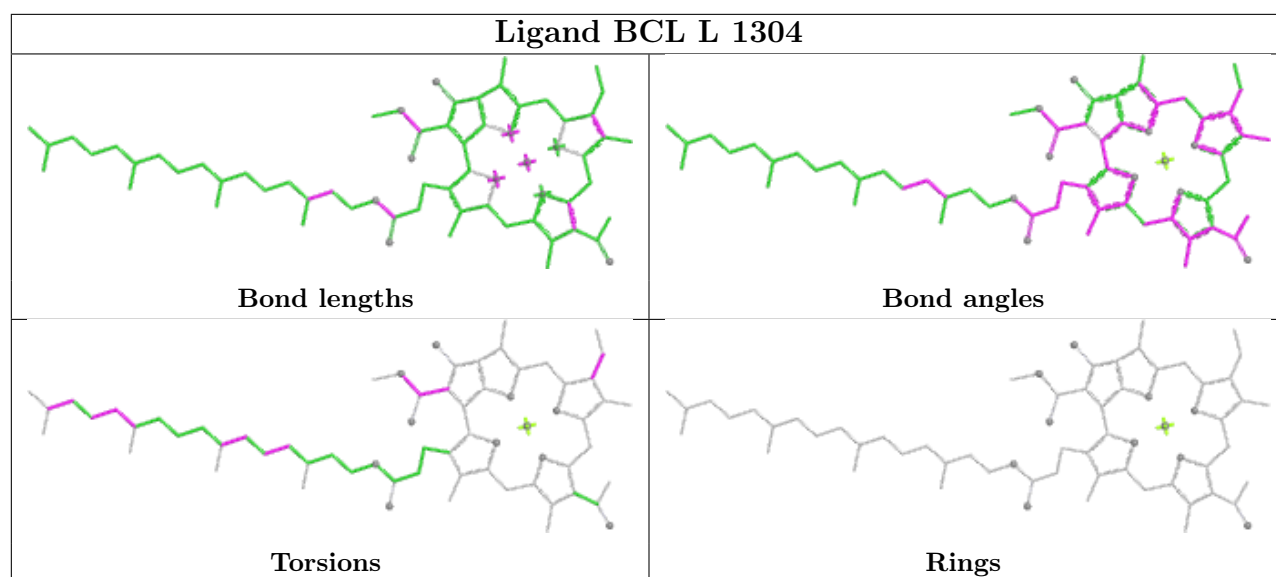


Ligand BPH L 401



Ligand BCL M 1301





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.