wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2021 – 11:22 AM EDT

PDB ID	:	1FNP
Title	:	CRYSTAL STRUCTURE ANALYSIS OF THE MUTANT REACTION CENTER PRO L209-> PHE FROM THE PHOTOSYNTHETIC PURPLE BACTERIUM RHODOBACTER SPHAEROIDES
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Deposited on	:	2000-08-23
Resolution	:	2.60 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

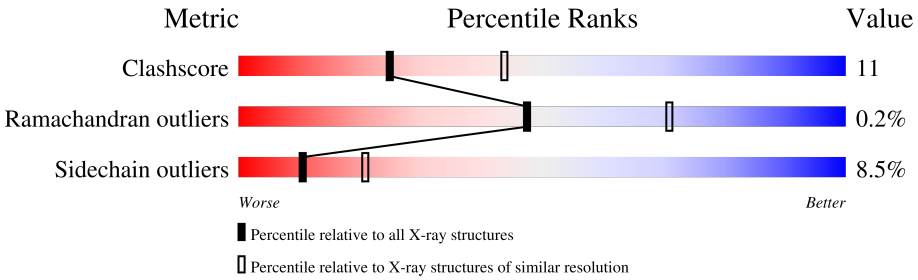
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	281	74% 24% •
2	M	307	73% 22% • •
3	H	260	76% 14% • 8%

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
4	BCL	L	304	X	-	-	-
4	BCL	M	801	X	-	-	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 7256 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 L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	0	0
			2236	1511	355	362	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	209	PHE	PRO	engineered mutation	UNP P02954

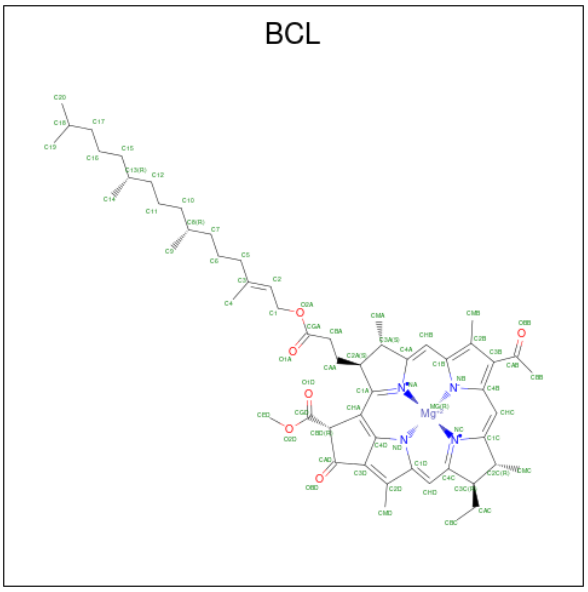
- Molecule 2 is a protein called REACTION CENTER PROTEIN M CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	301	Total	C	N	O	S	0	0	0
			2399	1600	393	396	10			

- Molecule 3 is a protein called REACTION CENTER PROTEIN H CHAIN.

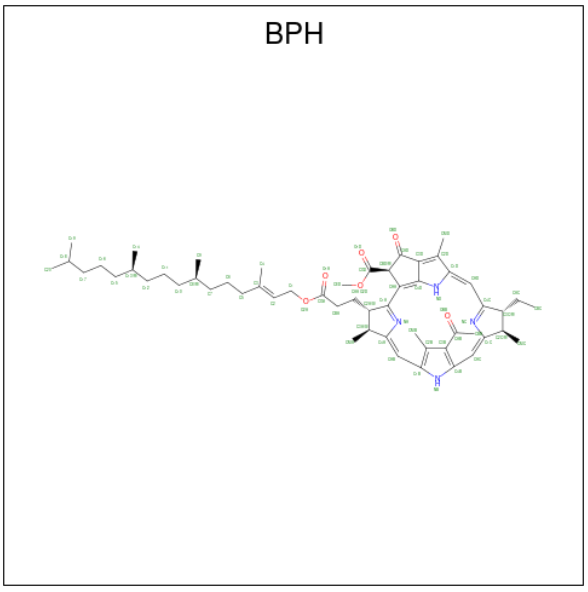
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



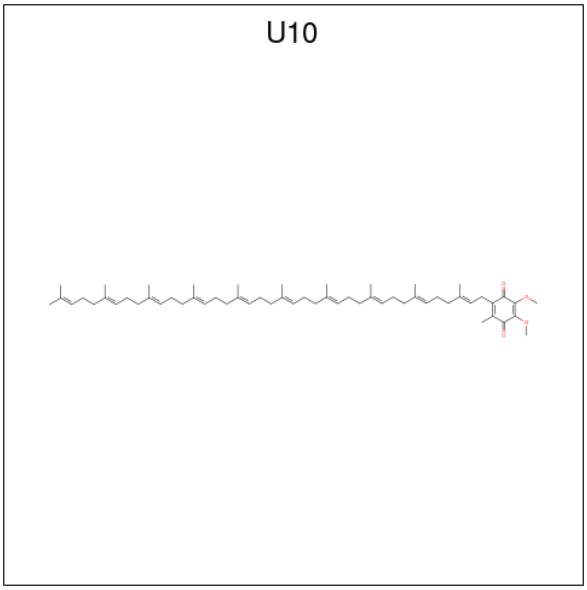
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



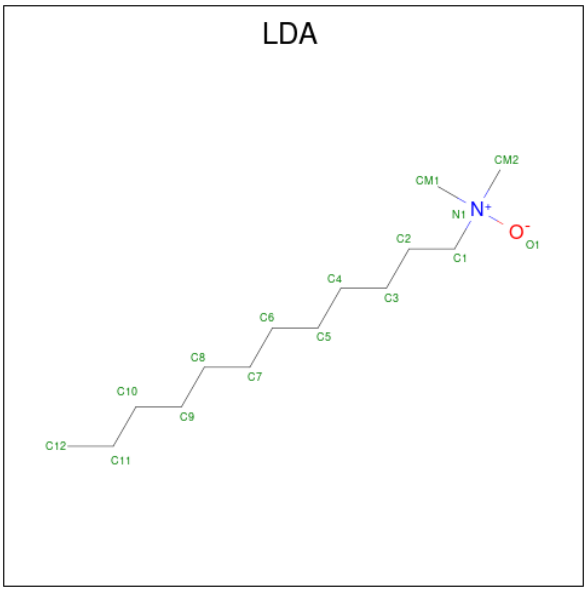
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 6 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



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

- Molecule 7 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).

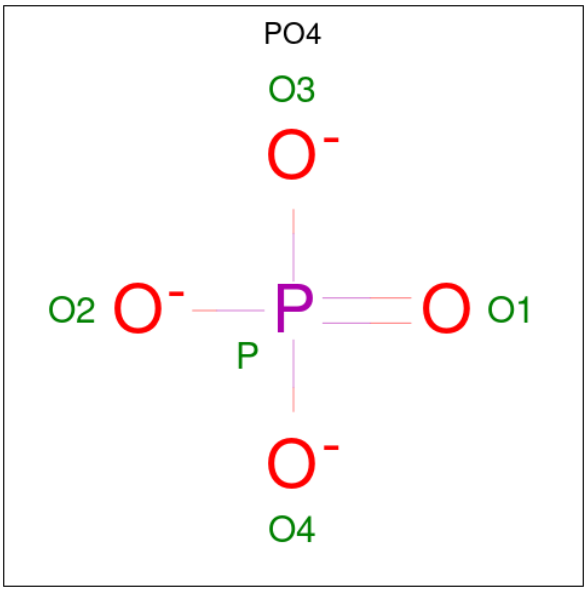


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	M	1	Total	C	N	O	0	0
			16	14	1	1		
7	H	1	Total	C	N	O	0	0
			16	14	1	1		
7	H	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

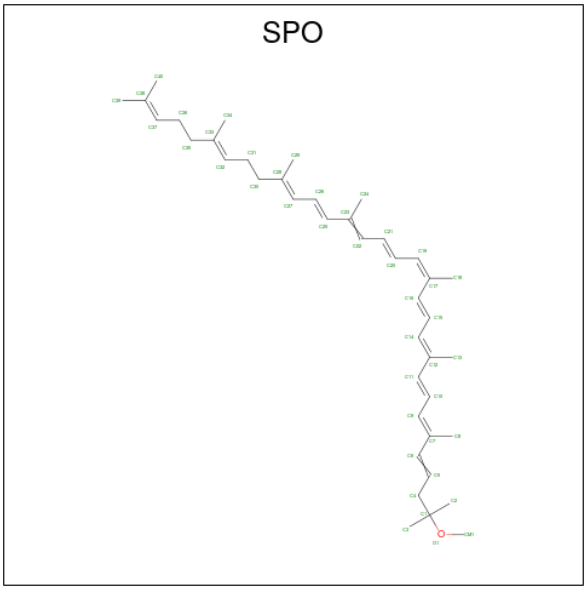
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total O P 5 4 1	0	0

- Molecule 10 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	M	1	Total C O 42 41 1	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	L	38	Total O 38 38	0	0
11	M	39	Total O 39 39	0	0
11	H	65	Total O 65 65	0	0

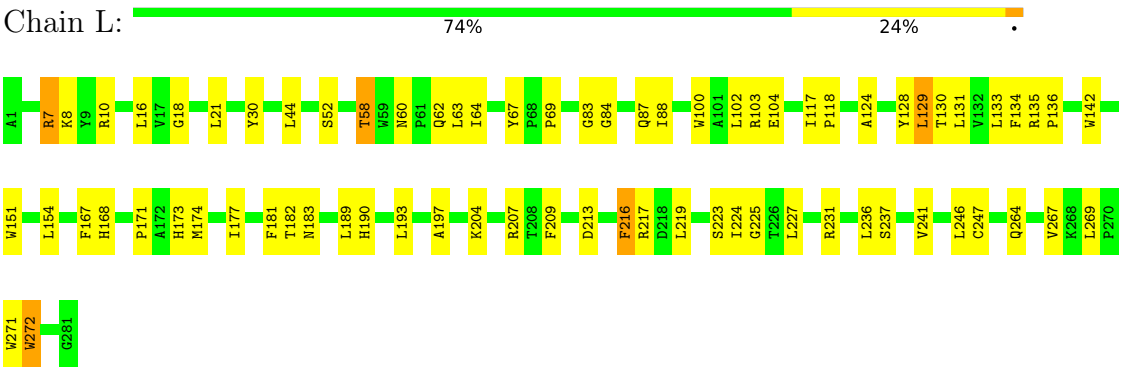
3 Residue-property plots (i)

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.

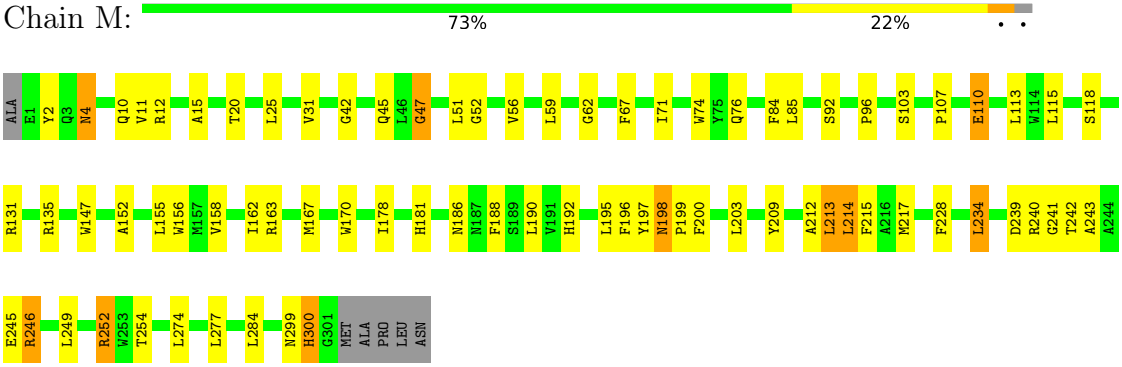
• Molecule 1: REACTION CENTER PROTEIN L CHAIN

Chain L:



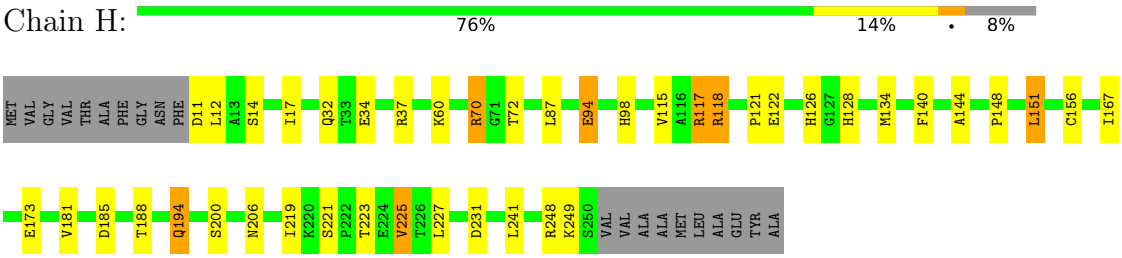
• Molecule 2: REACTION CENTER PROTEIN M CHAIN

Chain M:



• Molecule 3: REACTION CENTER PROTEIN H CHAIN

Chain H:



4 Data and refinement statistics (i)

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	141.75Å 141.75Å 187.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.60	Depositor
% Data completeness (in resolution range)	92.2 (50.00-2.60)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.3	Depositor
R, R_{free}	0.216 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7256	wwPDB-VP
Average B, all atoms (Å^2)	60.0	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: BCL, BPH, PO4, U10, SPO, 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	L	0.44	0/2324	0.48	0/3179
2	M	0.43	0/2491	0.49	1/3400 (0.0%)
3	H	0.42	0/1877	0.53	0/2553
All	All	0.43	0/6692	0.50	1/9132 (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	L	0	1
2	M	0	3
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	213	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	10	ARG	Sidechain
2	M	197	TYR	Sidechain
2	M	252	ARG	Sidechain
2	M	47	GLY	Peptide

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	L	2236	0	2189	53	0
2	M	2399	0	2306	59	0
3	H	1829	0	1836	34	0
4	L	132	0	148	12	0
4	M	132	0	148	12	0
5	L	65	0	76	8	0
5	M	65	0	76	11	0
6	L	48	0	63	8	0
6	M	48	0	63	2	0
7	H	32	0	62	2	0
7	L	16	0	31	0	0
7	M	64	0	124	1	0
8	M	1	0	0	0	0
9	M	5	0	0	1	0
10	M	42	0	60	1	0
11	H	65	0	0	4	0
11	L	38	0	0	6	0
11	M	39	0	0	0	0
All	All	7256	0	7182	154	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 11.

The worst 5 of 154 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)
4:L:304:BCL:HHC	4:L:304:BCL:HBB2	1.42	1.02
5:L:402:BPH:HHC	5:L:402:BPH:HBB3	1.48	0.95
4:M:801:BCL:HBB2	4:M:801:BCL:HHC	1.49	0.92
2:M:152:ALA:HB2	5:M:401:BPH:HAC1	1.54	0.90
3:H:194:GLN:HE21	3:H:194:GLN:H	1.21	0.85

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	L	279/281 (99%)	269 (96%)	10 (4%)	0	100 100
2	M	299/307 (97%)	283 (95%)	14 (5%)	2 (1%)	22 43
3	H	238/260 (92%)	229 (96%)	9 (4%)	0	100 100
All	All	816/848 (96%)	781 (96%)	33 (4%)	2 (0%)	47 71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	4	ASN
2	M	300	HIS

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	L	220/220 (100%)	203 (92%)	17 (8%)	13 25
2	M	235/240 (98%)	213 (91%)	22 (9%)	8 17
3	H	195/208 (94%)	179 (92%)	16 (8%)	11 22
All	All	650/668 (97%)	595 (92%)	55 (8%)	10 21

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	198	ASN

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Mol	Chain	Res	Type
2	M	249	LEU
3	H	249	LYS
3	H	200	SER
2	M	203	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	76	GLN
2	M	192	HIS
3	H	206	ASN
3	H	128	HIS
3	H	194	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 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	BCL	L	304	1	58,74,74	1.57	7 (12%)	69,115,115	2.11	12 (17%)
4	BCL	M	802	2	58,74,74	1.54	8 (13%)	69,115,115	2.03	12 (17%)
7	LDA	M	703	-	12,15,15	2.40	1 (8%)	14,17,17	0.58	0
4	BCL	L	302	1	58,74,74	1.49	9 (15%)	69,115,115	2.04	12 (17%)
6	U10	M	501	-	48,48,63	2.13	16 (33%)	58,61,79	1.05	4 (6%)
9	PO4	M	800	-	4,4,4	1.97	2 (50%)	6,6,6	0.92	0
5	BPH	M	401	-	64,70,70	1.18	5 (7%)	76,101,101	1.66	15 (19%)
7	LDA	M	701	-	12,15,15	2.49	1 (8%)	14,17,17	0.45	0
10	SPO	M	600	-	40,41,41	3.28	23 (57%)	47,50,50	1.97	12 (25%)
7	LDA	L	705	-	12,15,15	2.40	1 (8%)	14,17,17	0.50	0
7	LDA	M	707	-	12,15,15	2.21	1 (8%)	14,17,17	0.51	0
6	U10	L	502	-	48,48,63	1.92	14 (29%)	58,61,79	1.29	4 (6%)
7	LDA	H	706	-	12,15,15	2.25	1 (8%)	14,17,17	0.53	0
5	BPH	L	402	-	64,70,70	1.12	4 (6%)	76,101,101	1.62	11 (14%)
4	BCL	M	801	2	58,74,74	1.49	7 (12%)	69,115,115	2.08	12 (17%)
7	LDA	M	704	-	12,15,15	2.33	1 (8%)	14,17,17	0.52	0
7	LDA	H	702	-	12,15,15	2.40	1 (8%)	14,17,17	0.53	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
4	BCL	L	304	1	1/1/21/25	7/37/137/137	-
4	BCL	M	802	2	-	10/37/137/137	-
7	LDA	M	703	-	-	6/13/13/13	-
4	BCL	L	302	1	-	7/37/137/137	-
6	U10	M	501	-	-	8/45/69/87	0/1/1/1
5	BPH	M	401	-	-	17/54/105/105	0/5/6/6
7	LDA	M	701	-	-	1/13/13/13	-
10	SPO	M	600	-	-	17/47/47/47	-
7	LDA	L	705	-	-	0/13/13/13	-
7	LDA	M	707	-	-	1/13/13/13	-
6	U10	L	502	-	-	17/45/69/87	0/1/1/1
7	LDA	H	706	-	-	2/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BPH	L	402	-	-	12/54/105/105	0/5/6/6
4	BCL	M	801	2	1/1/21/25	12/37/137/137	-
7	LDA	M	704	-	-	2/13/13/13	-
7	LDA	H	702	-	-	5/13/13/13	-

The worst 5 of 102 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	600	SPO	C6-C5	8.83	1.55	1.32
7	M	701	LDA	O1-N1	-8.53	1.22	1.42
7	M	703	LDA	O1-N1	-8.30	1.22	1.42
7	H	702	LDA	O1-N1	-8.29	1.22	1.42
7	L	705	LDA	O1-N1	-8.25	1.22	1.42

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	304	BCL	C4A-NA-C1A	8.18	110.38	106.71
4	M	801	BCL	C4A-NA-C1A	8.07	110.33	106.71
4	L	304	BCL	O2D-CGD-CBD	7.95	125.40	111.27
4	M	802	BCL	C4A-NA-C1A	7.88	110.25	106.71
4	L	302	BCL	C4A-NA-C1A	7.75	110.19	106.71

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	L	304	BCL	C13
4	M	801	BCL	C8

5 of 124 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	302	BCL	CBD-CGD-O2D-CED
4	L	302	BCL	O1D-CGD-O2D-CED
4	M	801	BCL	C4C-C3C-CAC-CBC
5	L	402	BPH	C4C-C3C-CAC-CBC
5	L	402	BPH	C2C-C3C-CAC-CBC

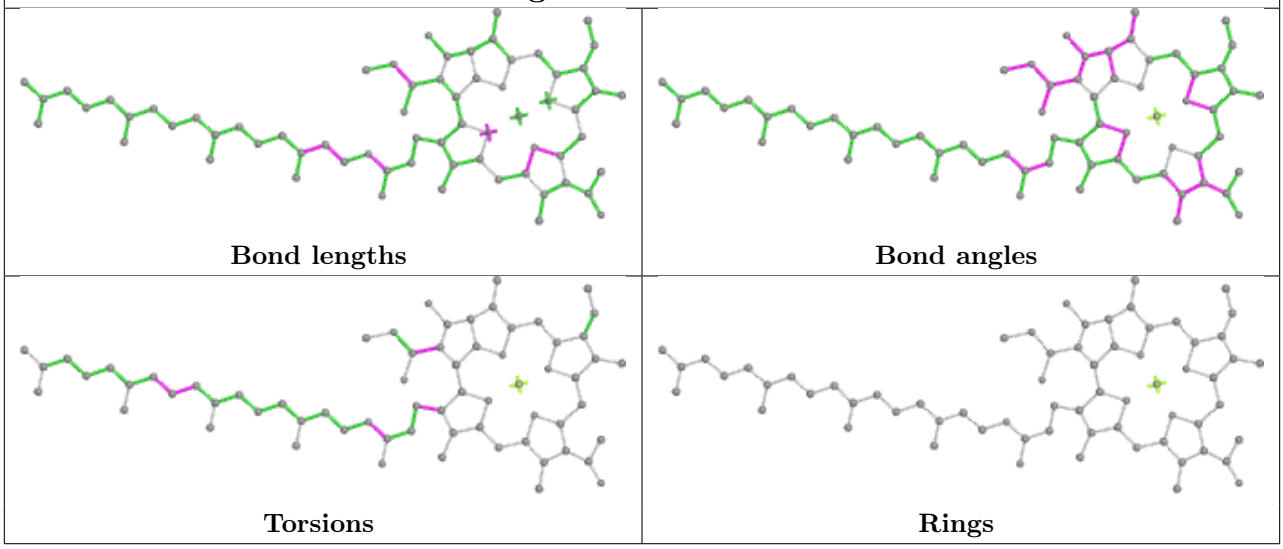
There are no ring outliers.

12 monomers are involved in 55 short contacts:

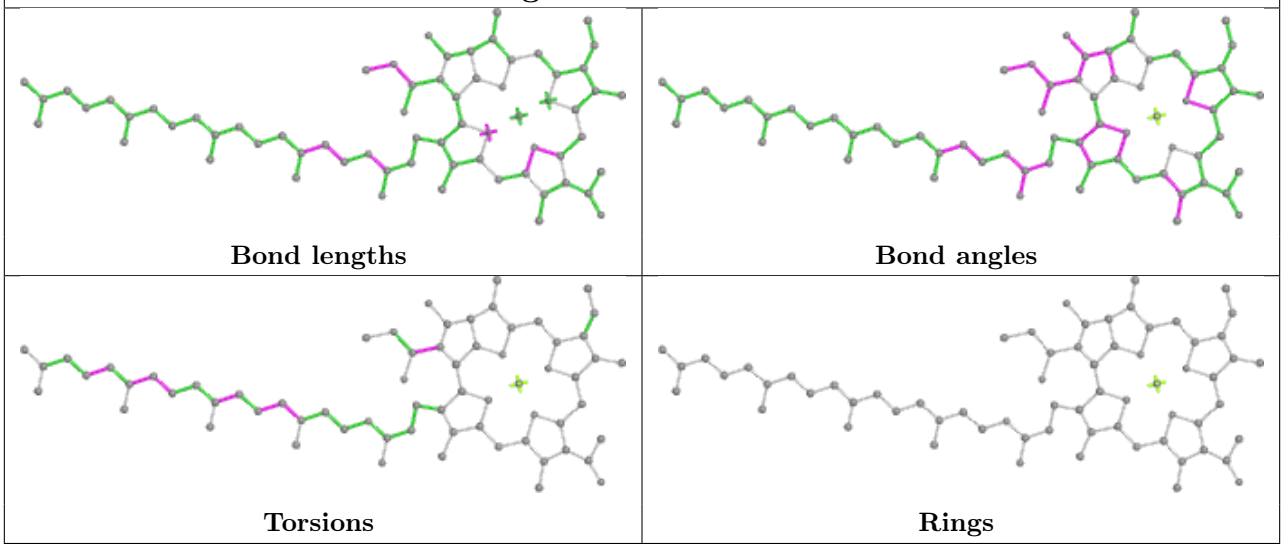
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	304	BCL	5	0
4	M	802	BCL	8	0
4	L	302	BCL	8	0
6	M	501	U10	2	0
9	M	800	PO4	1	0
5	M	401	BPH	11	0
10	M	600	SPO	1	0
6	L	502	U10	8	0
5	L	402	BPH	8	0
4	M	801	BCL	6	0
7	M	704	LDA	1	0
7	H	702	LDA	2	0

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 then 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.

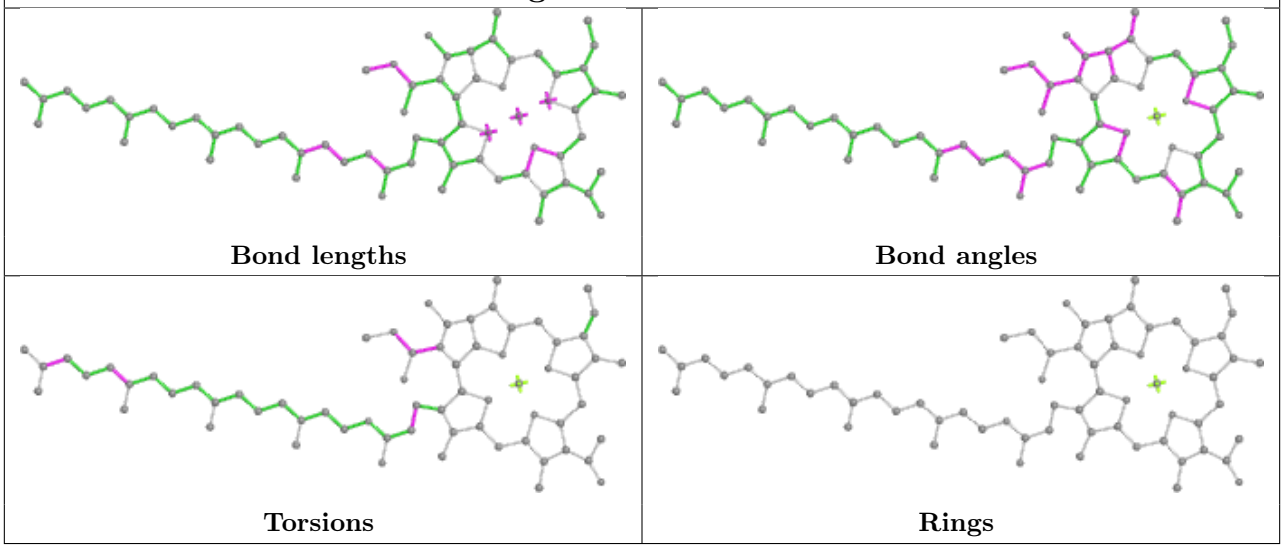
Ligand BCL L 304



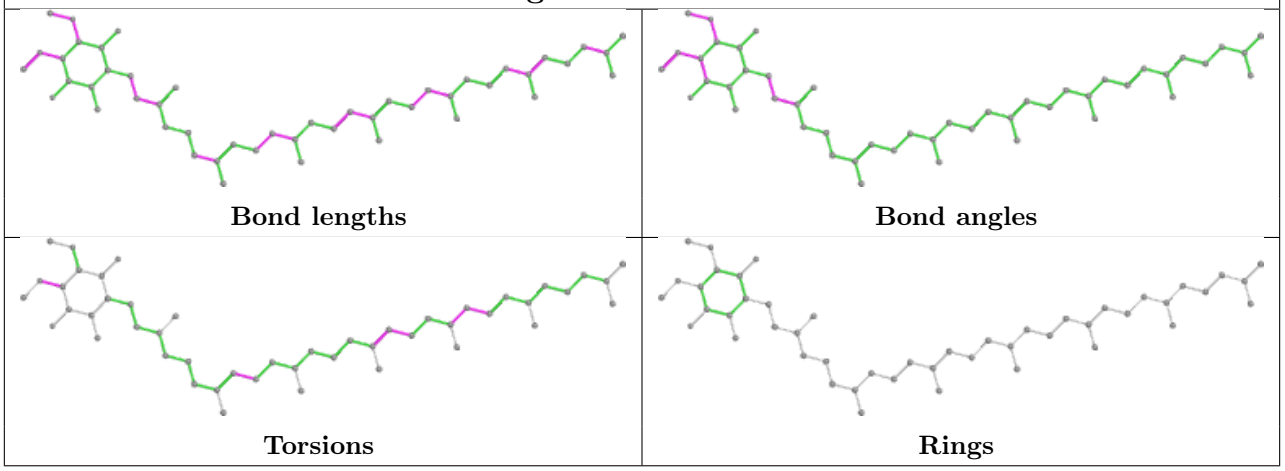
Ligand BCL M 802



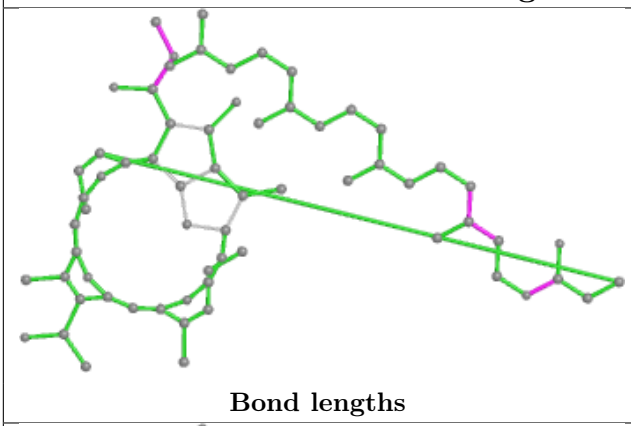
Ligand BCL L 302



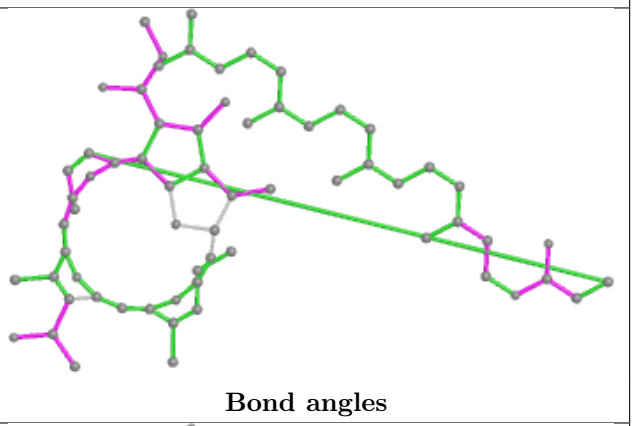
Ligand U10 M 501



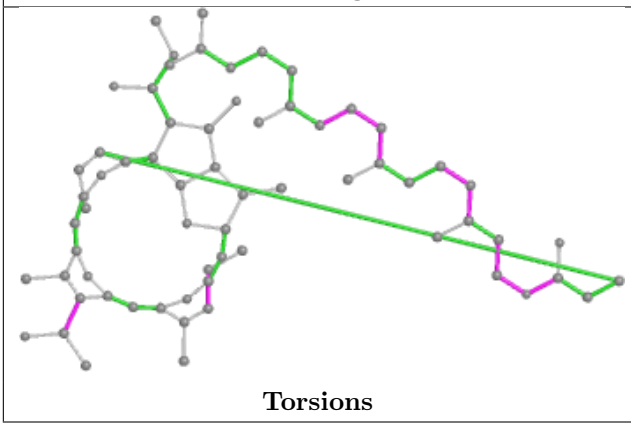
Ligand BPH M 401



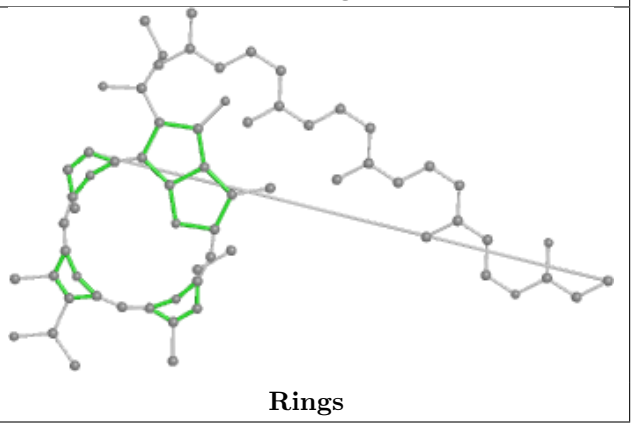
Bond lengths



Bond angles

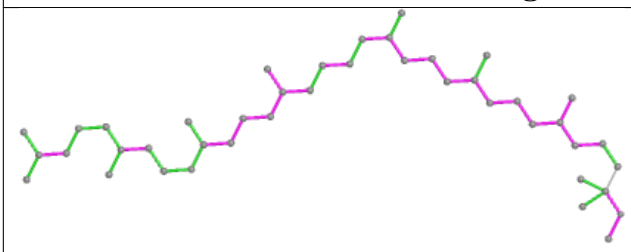


Torsions

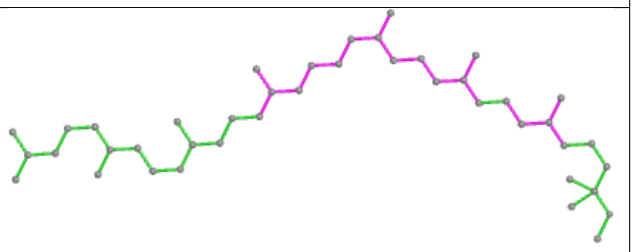


Rings

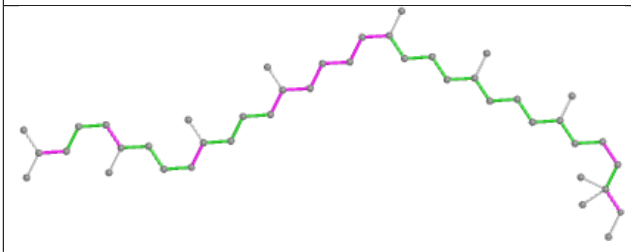
Ligand SPO M 600



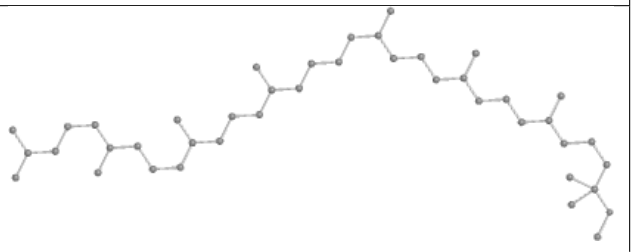
Bond lengths



Bond angles

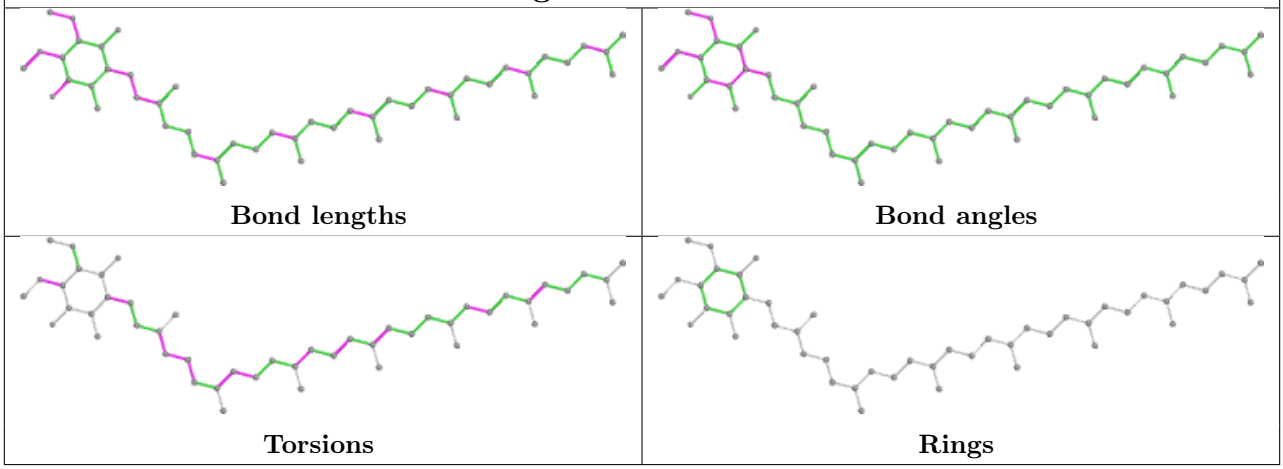


Torsions

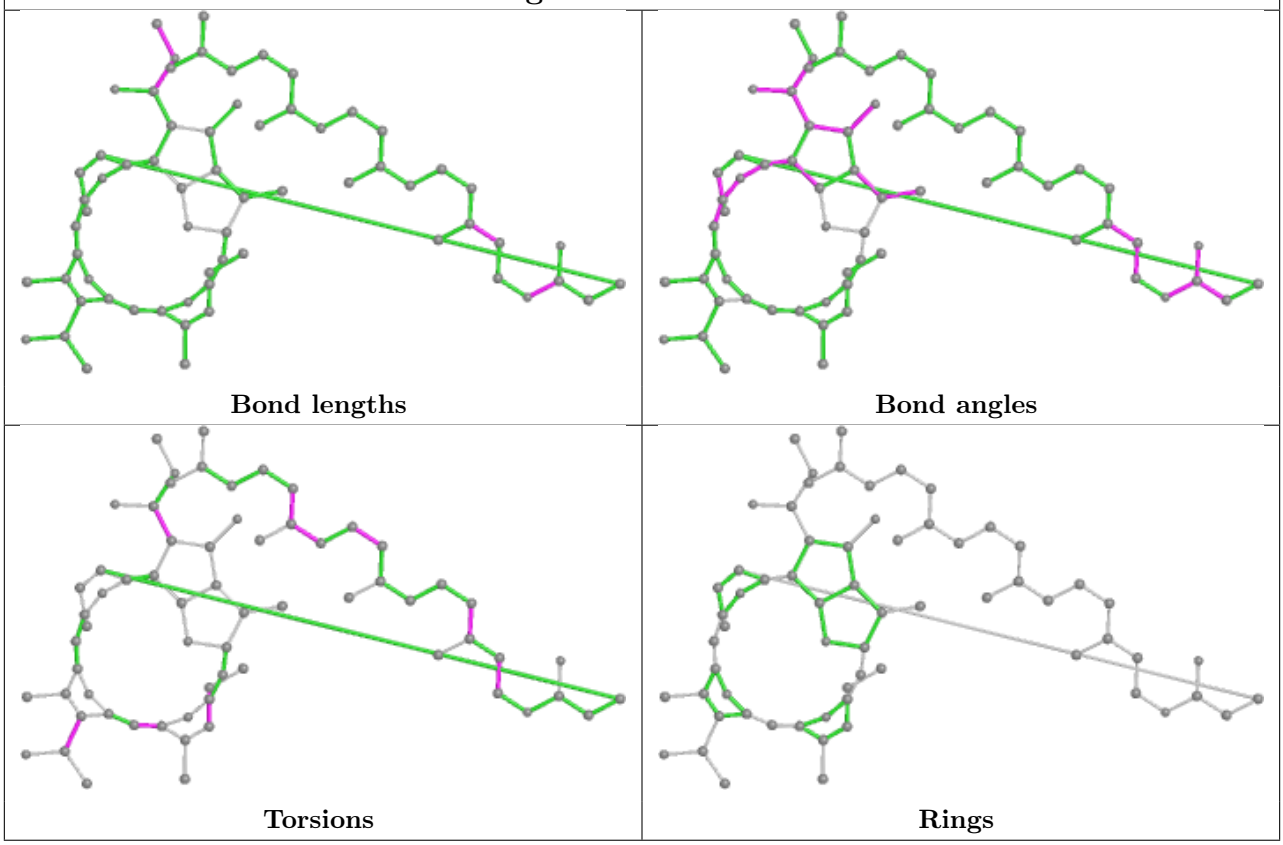


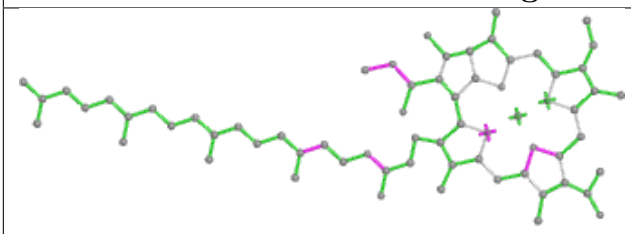
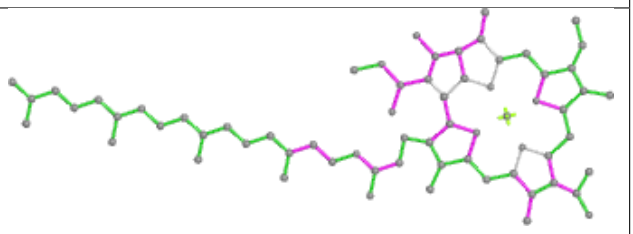
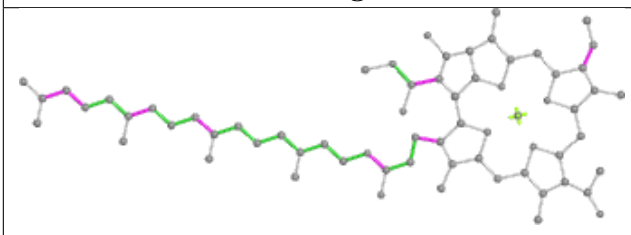
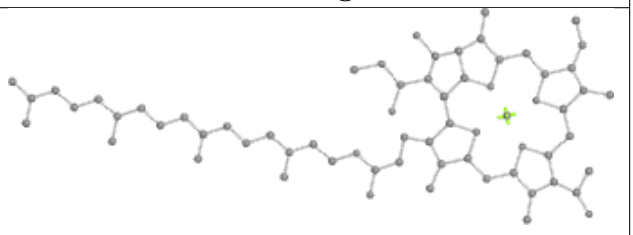
Rings

Ligand U10 L 502



Ligand BPH L 402



Ligand BCL M 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

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.