wwPDB X-ray Structure Validation Summary Report (i)

Aug 22, 2026 – 07:17 am BST

PDB ID	:	1E6D / pdb_00001e6d
Title	:	PHOTOSYNTHETIC REACTION CENTER MUTANT WITH TRP M115 REPLACED WITH PHE (CHAIN M, WM115F) PHE M197 REPLACED WITH ARG (CHAIN M, FM197R)
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Deposited on	:	2000-08-11
Resolution	:	2.30 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

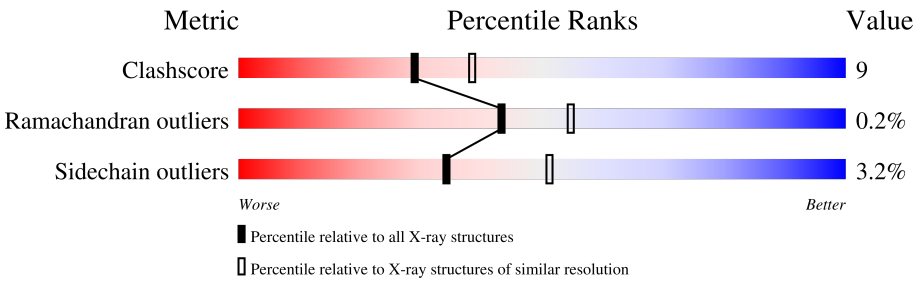
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	H	260	77% 13% • 8%
2	L	281	80% 17% •
3	M	307	77% 20% • •

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
10	PO4	M	1800	-	X	-	-
10	PO4	M	1801	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BCL	L	1304	X	-	-	-
5	BCL	M	1301	X	-	-	-
6	BPH	M	1401	X	-	-	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 7334 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 H SUBUNIT.

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

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

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

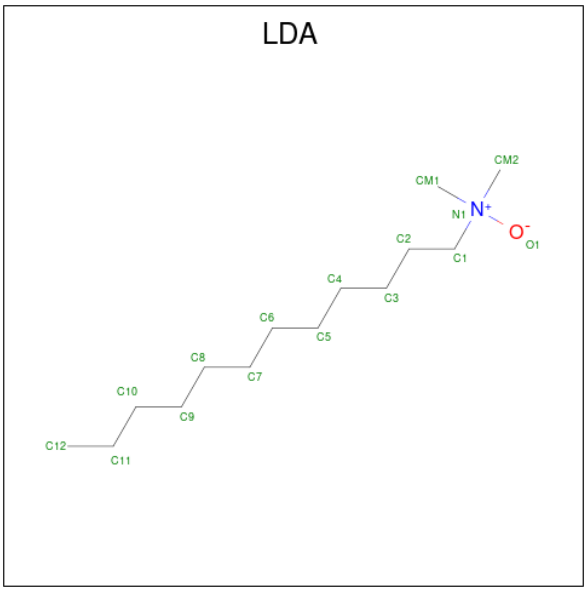
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER M SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	302	2405	1602	396	397	10	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	197	ARG	PHE	engineered mutation	UNP P02953
M	115	PHE	TRP	engineered mutation	UNP P02953

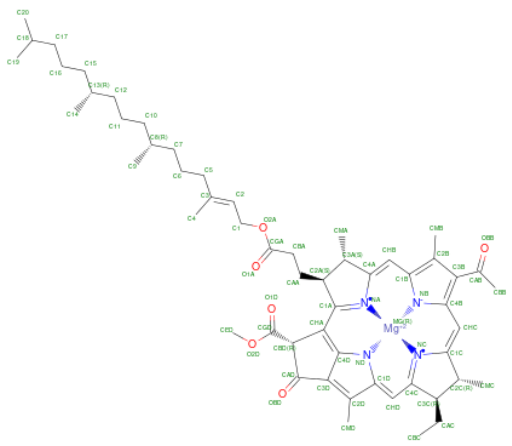
- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).



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

- Molecule 5 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).

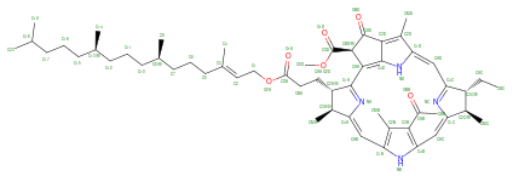
BCL



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

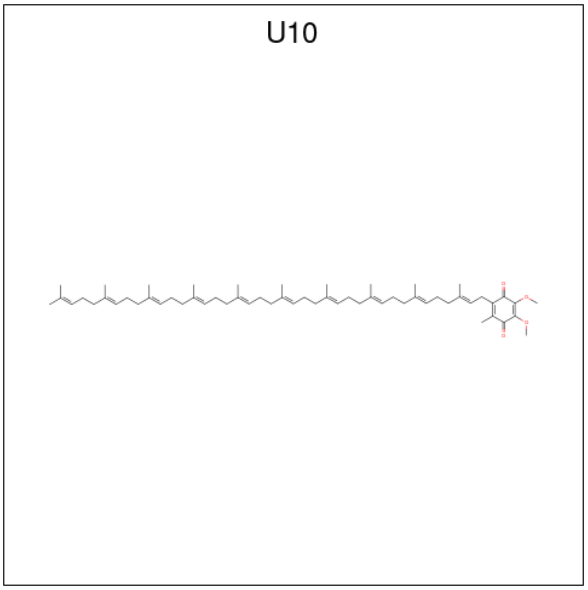
- Molecule 6 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).

BPH



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

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

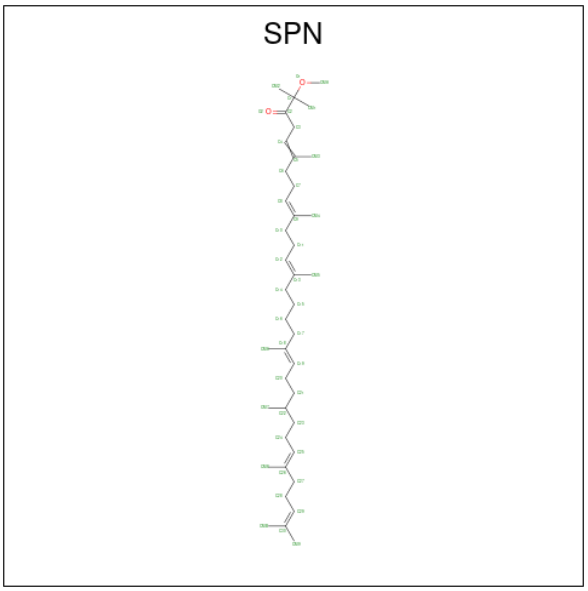


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	L	1	48	44	4	0	0
7	M	1	48	44	4	0	0

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

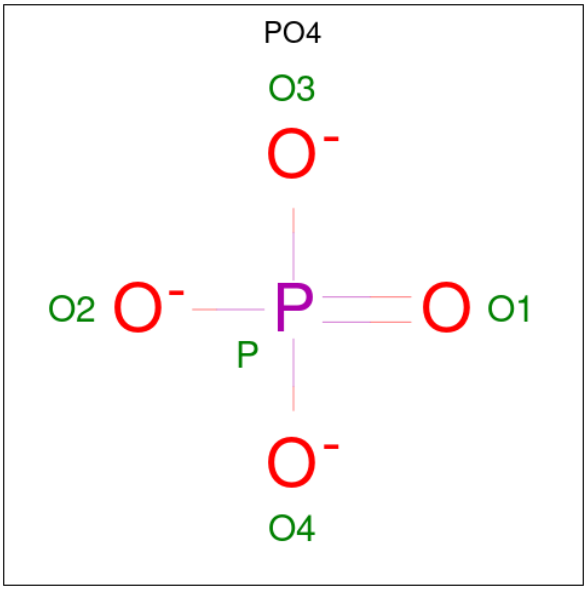
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
8	M	1	1	1	0	0

- Molecule 9 is SPEROIDENONE (CCD ID: SPN) (formula: $C_{41}H_{70}O_2$).



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

- Molecule 10 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	H	1	1	1	0	0
			Total	O		
11	H	94	94	94	0	0
			Total	O		
11	L	1	1	1	0	0
			Total	O		
11	L	1	1	1	0	0
			Total	O		
11	L	47	47	47	0	0
			Total	O		
11	M	2	2	2	0	0
			Total	O		
11	M	1	1	1	0	0
			Total	O		
11	M	65	65	65	0	0

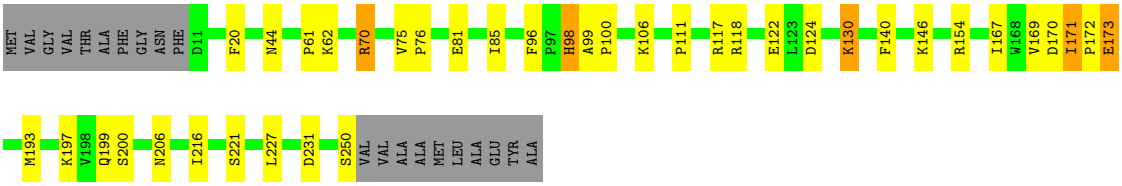
3 Residue-property plots (i)

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.

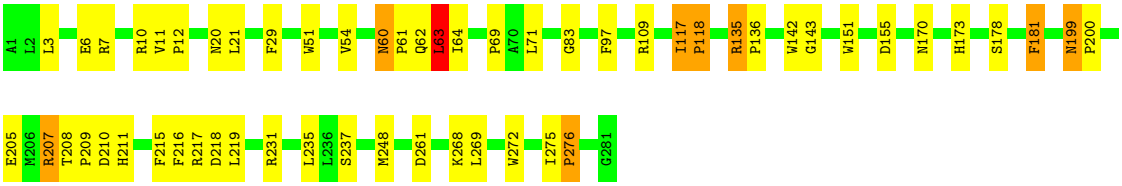
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER H SUBUNIT

Chain H:



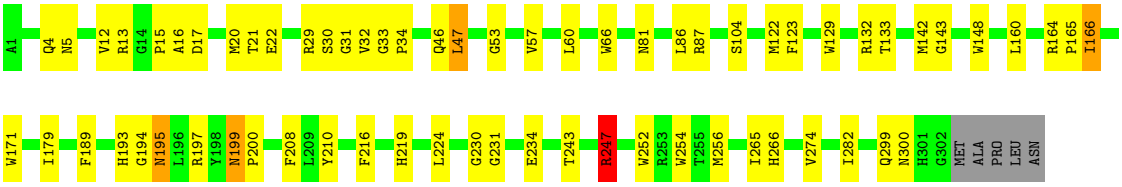
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER L SUBUNIT

Chain L:



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER M SUBUNIT

Chain M:



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	141.20Å 141.20Å 187.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.40 – 2.30	Depositor
% Data completeness (in resolution range)	94.5 (26.40-2.30)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.174 , 0.200	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7334	wwPDB-VP
Average B, all atoms (Å^2)	42.0	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: FE, U10, BCL, BPH, LDA, SPN, PO4

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	0.93	0/1877	1.63	19/2553 (0.7%)
2	L	0.97	1/2320 (0.0%)	1.52	23/3175 (0.7%)
3	M	0.88	3/2495 (0.1%)	1.48	21/3404 (0.6%)
All	All	0.93	4/6692 (0.1%)	1.54	63/9132 (0.7%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	254	TRP	NE1-CE2	-5.23	1.31	1.37
2	L	29	PHE	N-CA	-5.16	1.39	1.46
3	M	252	TRP	NE1-CE2	-5.09	1.31	1.37
3	M	219	HIS	CE1-NE2	-5.00	1.27	1.32

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	70	ARG	CD-NE-CZ	18.28	149.99	124.40
2	L	237	SER	CA-CB-OG	-7.96	95.19	111.10
1	H	98	HIS	CA-CB-CG	-7.27	106.53	113.80
1	H	173	GLU	CB-CG-CD	6.96	124.43	112.60
1	H	96	PHE	CA-CB-CG	-6.92	106.88	113.80

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	H	1829	0	1836	18	0
2	L	2232	0	2187	38	0
3	M	2405	0	2324	47	0
4	H	32	0	62	0	0
4	M	80	0	155	11	0
5	L	132	0	148	5	0
5	M	132	0	148	12	0
6	L	65	0	75	6	0
6	M	65	0	76	10	0
7	L	48	0	63	8	0
7	M	48	0	63	3	0
8	M	1	0	0	0	0
9	M	43	0	69	2	0
10	M	10	0	0	3	0
11	H	95	0	0	1	0
11	L	49	0	0	8	0
11	M	68	0	0	1	0
All	All	7334	0	7206	125	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 9.

The worst 5 of 125 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:L:215:PHE:HB2	3:M:142:MET:HE1	1.38	1.06
3:M:243:THR:O	3:M:247:ARG:HG2	1.58	1.02
5:M:1303:BCL:H191	4:M:1706:LDA:H121	1.47	0.97
6:L:1402:BPH:HHC	6:L:1402:BPH:HBB3	1.51	0.93
4:M:1701:LDA:H91	4:M:1702:LDA:H121	1.54	0.88

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	238/260 (92%)	233 (98%)	5 (2%)	0	100	100
2	L	279/281 (99%)	271 (97%)	8 (3%)	0	100	100
3	M	300/307 (98%)	290 (97%)	8 (3%)	2 (1%)	18	23
All	All	817/848 (96%)	794 (97%)	21 (3%)	2 (0%)	43	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	30	SER
3	M	195	ASN

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	195/208 (94%)	190 (97%)	5 (3%)	40	59
2	L	220/220 (100%)	213 (97%)	7 (3%)	34	51
3	M	236/240 (98%)	227 (96%)	9 (4%)	29	44
All	All	651/668 (98%)	630 (97%)	21 (3%)	34	51

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	86	LEU
3	M	216	PHE
3	M	299	GLN
3	M	247	ARG
3	M	199	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
3	M	193	HIS
3	M	199	ASN
3	M	299	GLN
2	L	199	ASN
2	L	280	ASN

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 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	$\#\|Z\| > 2$
5	BCL	M	1301	3	69,74,74	1.47	9 (13%)	83,115,115	2.20	22 (26%)
4	LDA	M	1705	-	12,15,15	2.24	1 (8%)	14,17,17	0.70	0
5	BCL	M	1303	3	69,74,74	1.44	10 (14%)	83,115,115	2.32	19 (22%)
7	U10	L	1502	-	48,48,63	2.05	16 (33%)	58,61,79	1.67	10 (17%)
4	LDA	M	1701	-	12,15,15	2.26	1 (8%)	14,17,17	0.64	0
6	BPH	M	1401	-	59,70,70	1.99	14 (23%)	61,101,101	2.78	19 (31%)
4	LDA	H	1707	-	12,15,15	2.27	1 (8%)	14,17,17	0.75	0
9	SPN	M	1600	-	40,42,42	3.80	17 (42%)	50,52,52	2.40	19 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	BCL	L	1304	2	69,74,74	1.47	10 (14%)	83,115,115	2.33	20 (24%)
10	PO4	M	1801	-	4,4,4	2.21	1 (25%)	6,6,6	1.29	0
10	PO4	M	1800	-	4,4,4	3.26	2 (50%)	6,6,6	1.88	2 (33%)
7	U10	M	1501	-	48,48,63	1.89	15 (31%)	58,61,79	1.53	10 (17%)
4	LDA	M	1703	-	12,15,15	2.27	1 (8%)	14,17,17	0.67	0
6	BPH	L	1402	-	59,70,70	2.13	14 (23%)	61,101,101	2.58	19 (31%)
5	BCL	L	1302	2	69,74,74	1.46	9 (13%)	83,115,115	2.38	23 (27%)
4	LDA	M	1706	-	12,15,15	2.46	1 (8%)	14,17,17	0.86	0
4	LDA	M	1702	-	12,15,15	2.50	1 (8%)	14,17,17	0.64	0
4	LDA	H	1704	-	12,15,15	2.25	1 (8%)	14,17,17	0.43	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
5	BCL	M	1301	3	1/1/21/25	14/41/137/137	-
4	LDA	M	1705	-	-	7/13/13/13	-
5	BCL	M	1303	3	-	5/41/137/137	-
7	U10	L	1502	-	-	18/45/69/87	0/1/1/1
4	LDA	M	1701	-	-	2/13/13/13	-
6	BPH	M	1401	-	1/1/18/22	15/37/105/105	0/5/6/6
4	LDA	H	1707	-	-	4/13/13/13	-
9	SPN	M	1600	-	-	21/50/51/51	-
5	BCL	L	1304	2	1/1/21/25	6/41/137/137	-
7	U10	M	1501	-	-	8/45/69/87	0/1/1/1
4	LDA	M	1703	-	-	7/13/13/13	-
6	BPH	L	1402	-	-	5/37/105/105	0/5/6/6
5	BCL	L	1302	2	-	1/41/137/137	-
4	LDA	M	1706	-	-	9/13/13/13	-
4	LDA	M	1702	-	-	6/13/13/13	-
4	LDA	H	1704	-	-	8/13/13/13	-

The worst 5 of 124 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1600	SPN	C8-C9	9.65	1.56	1.33
9	M	1600	SPN	C4-C5	8.95	1.54	1.33
4	M	1702	LDA	O1-N1	-8.62	1.22	1.42
9	M	1600	SPN	C12-C13	8.45	1.53	1.33
4	M	1706	LDA	O1-N1	-8.42	1.22	1.42

The worst 5 of 163 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	1401	BPH	O2D-CGD-CBD	15.11	130.15	111.00
6	L	1402	BPH	O2D-CGD-CBD	12.34	126.63	111.00
5	L	1302	BCL	C4A-NA-C1A	10.95	111.63	106.71
5	M	1303	BCL	C1C-NC-C4C	10.45	111.40	106.71
5	L	1302	BCL	C1C-NC-C4C	9.09	110.79	106.71

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	1304	BCL	C13
5	M	1301	BCL	C13
6	M	1401	BPH	C8

5 of 136 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	1703	LDA	C2-C1-N1-O1
4	M	1703	LDA	C2-C1-N1-CM1
4	M	1705	LDA	N1-C1-C2-C3
4	M	1706	LDA	C2-C1-N1-O1
4	M	1706	LDA	C2-C1-N1-CM1

There are no ring outliers.

15 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	1301	BCL	10	0
5	M	1303	BCL	3	0
7	L	1502	U10	8	0
4	M	1701	LDA	2	0
6	M	1401	BPH	10	0
9	M	1600	SPN	2	0
5	L	1304	BCL	1	0

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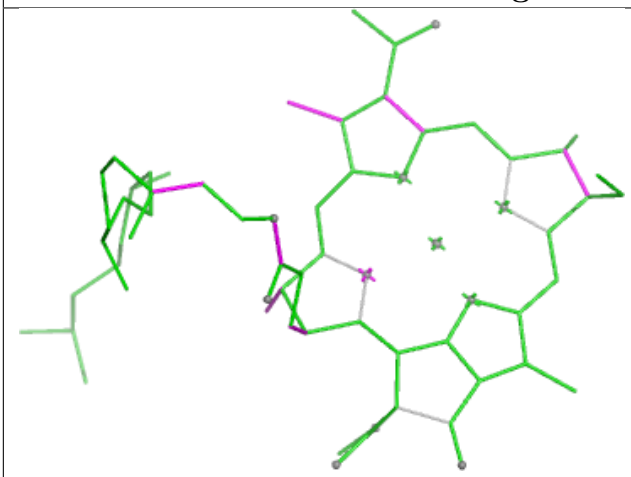
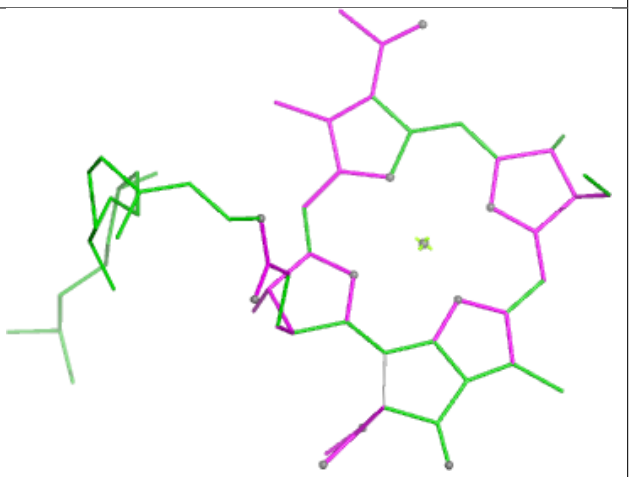
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	M	1801	PO4	2	0
10	M	1800	PO4	1	0
7	M	1501	U10	3	0
4	M	1703	LDA	5	0
6	L	1402	BPH	6	0
5	L	1302	BCL	4	0
4	M	1706	LDA	4	0
4	M	1702	LDA	2	0

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.

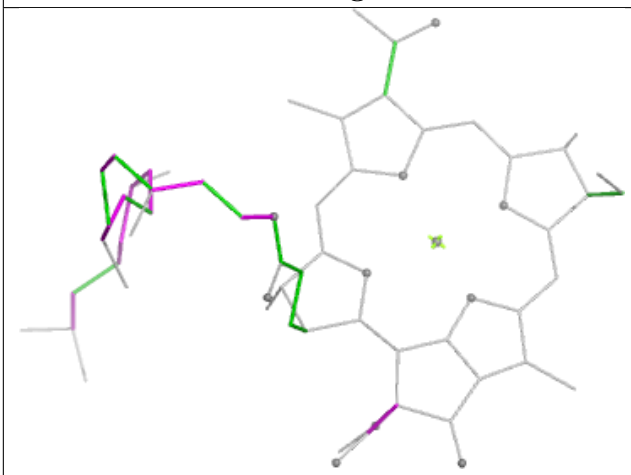
Ligand BCL M 1301



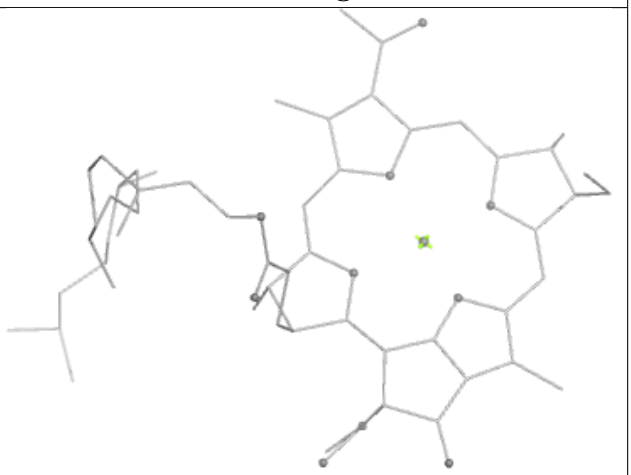
Bond lengths



Bond angles

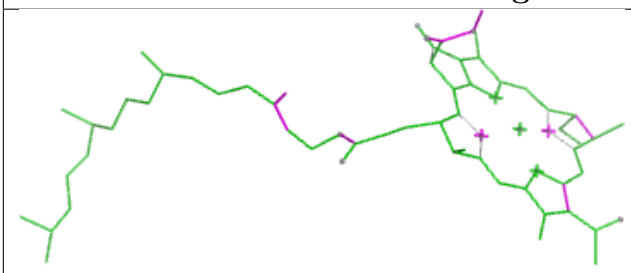


Torsions

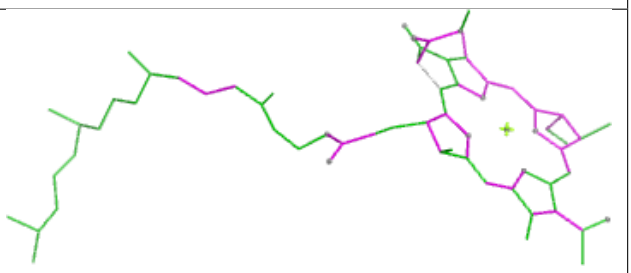


Rings

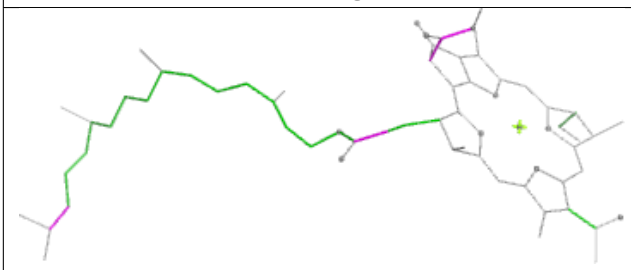
Ligand BCL M 1303



Bond lengths



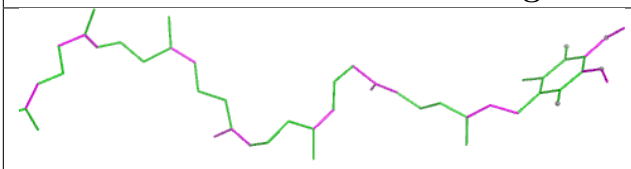
Bond angles



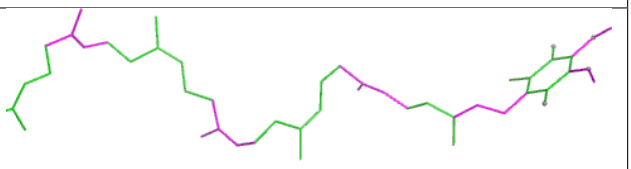
Torsions

Rings

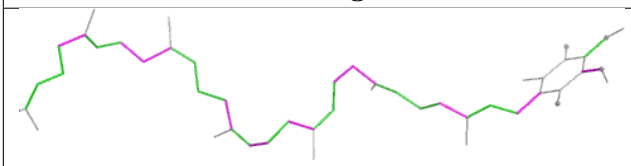
Ligand U10 L 1502



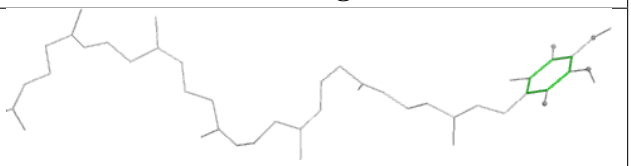
Bond lengths



Bond angles

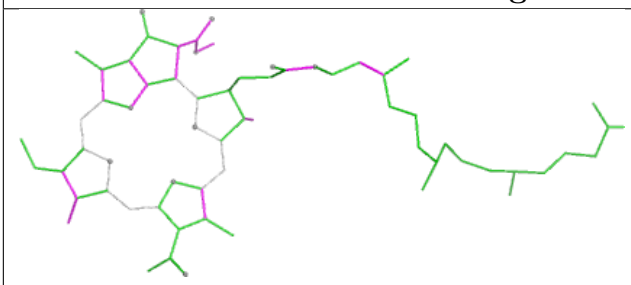


Torsions



Rings

Ligand BPH M 1401



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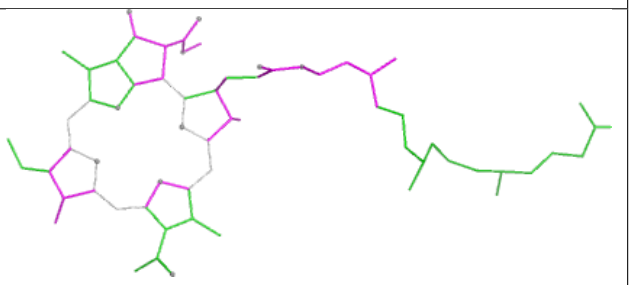
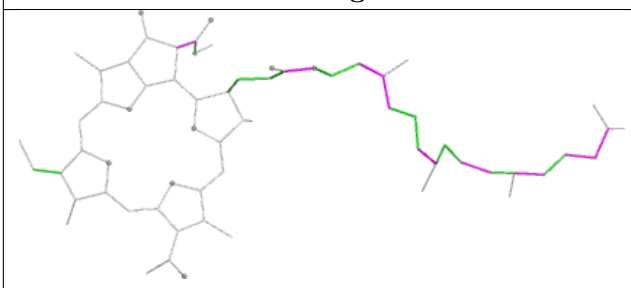
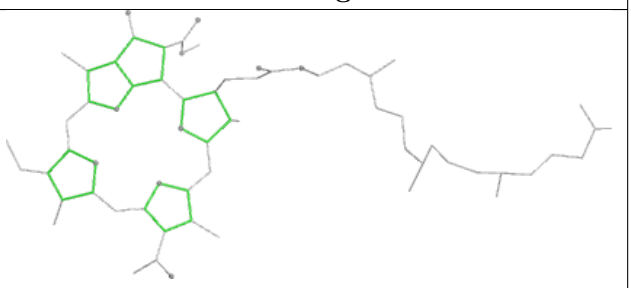


Bond angles

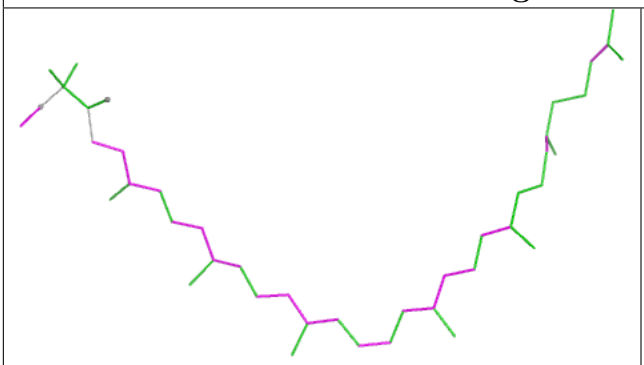


Torsions

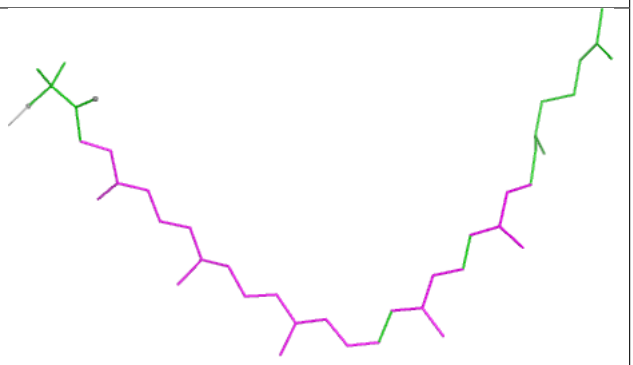


Rings

Ligand SPN M 1600



Bond lengths



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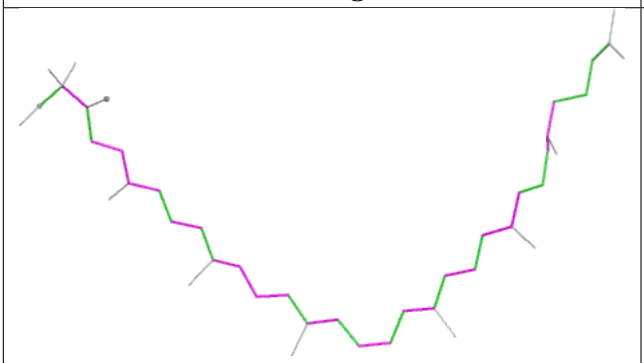
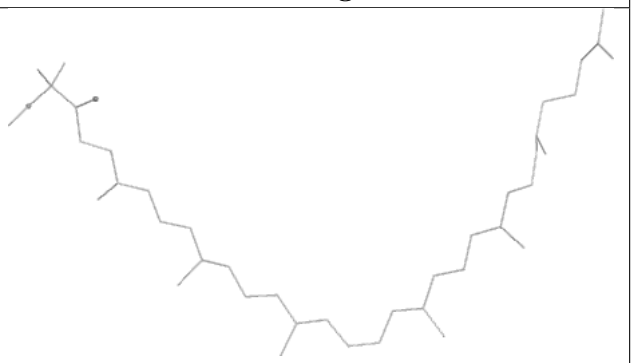
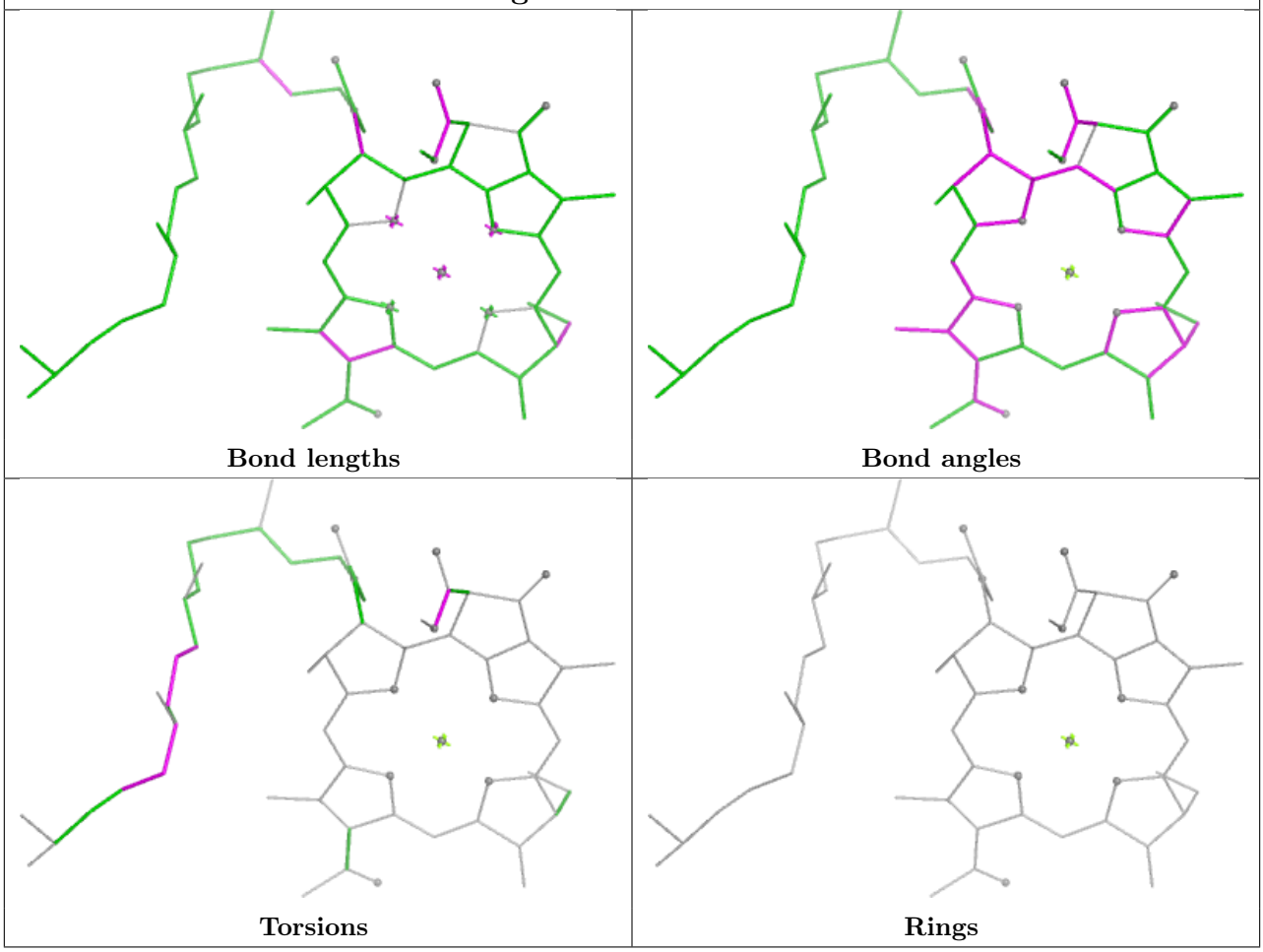


Torsions

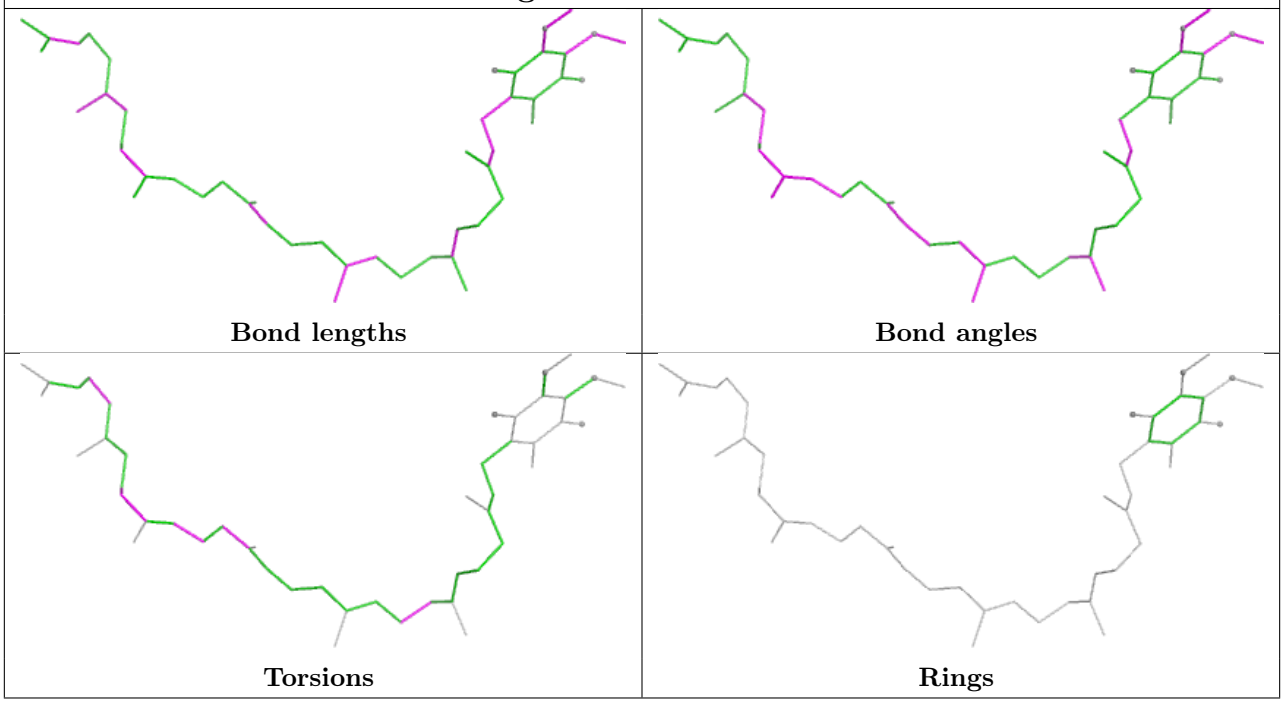


Rings

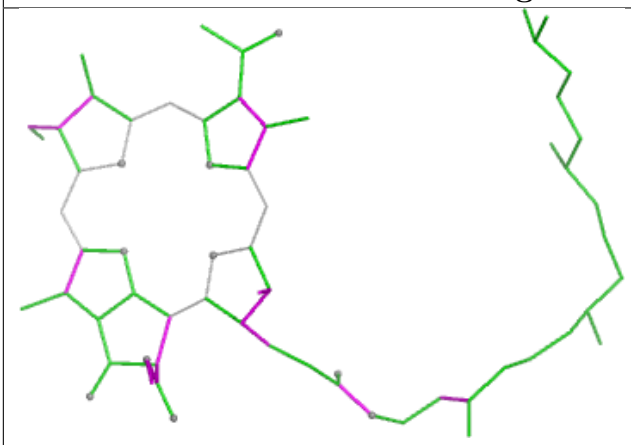
Ligand BCL L 1304



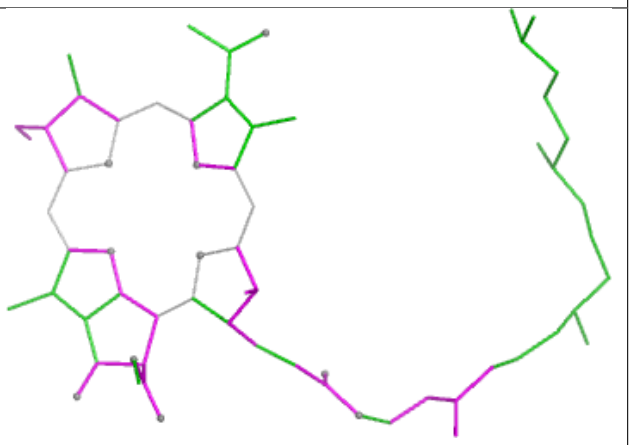
Ligand U10 M 1501



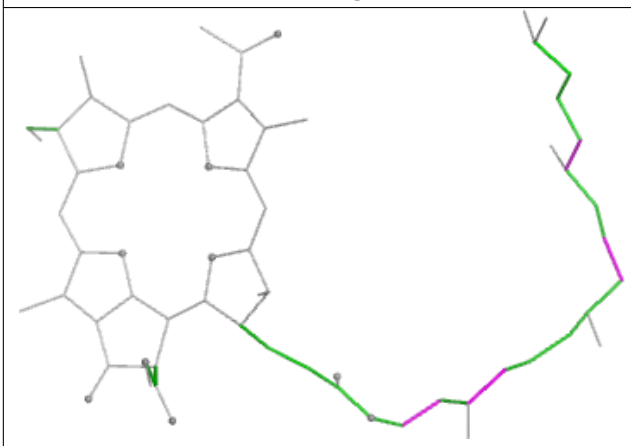
Ligand BPH L 1402



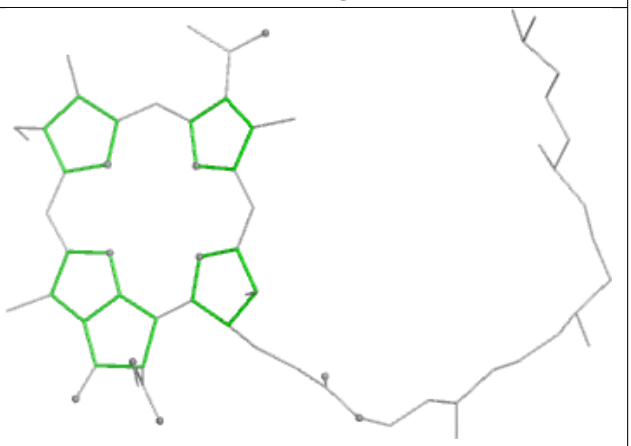
Bond lengths



Bond angles

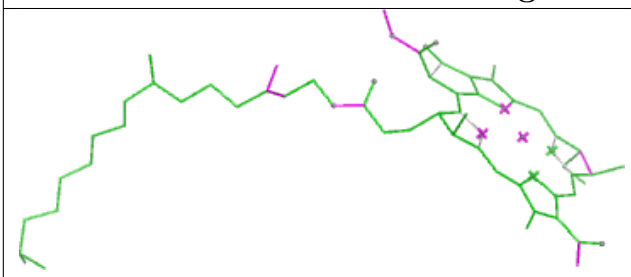


Torsions



Rings

Ligand BCL L 1302



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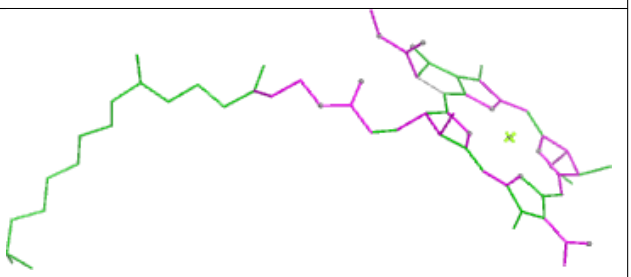

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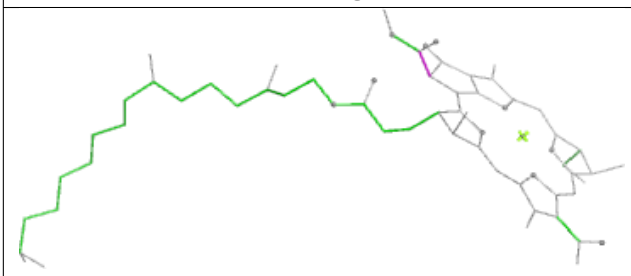

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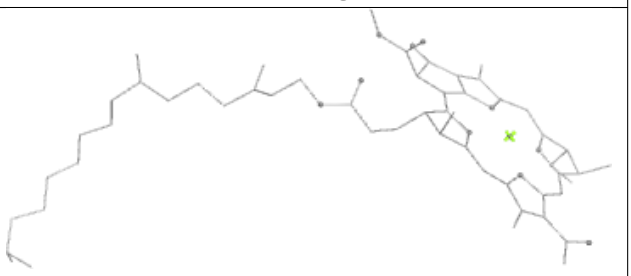

Rings

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.