wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 09:41 PM EDT

PDB ID	:	1AIG / pdb_00001aig
Title	:	PHOTOSYNTHETIC REACTION CENTER FROM RHODOBACTER SPHAEROIDES IN THE D+QB-CHARGE SEPARATED STATE
Authors	:	Stowell, M.H.B.; Mcphillips, T.M.; Soltis, S.M.; Rees, D.C.; Abresch, E.; Feher, G.
Deposited on	:	1997-04-17
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 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:

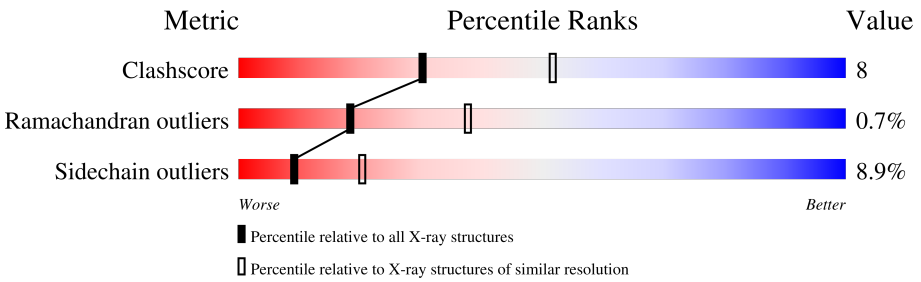
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.60 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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (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	66% 27% 7%
1	N	281	67% 27% 6% •
2	M	307	67% 26% • • •
2	O	307	66% 25% 6% •
3	H	260	63% 28% • • 5%
3	P	260	63% 28% • • 5%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BCL	M	309	X	-	-	-
4	BCL	M	310	X	-	-	-
4	BCL	N	282	X	-	-	-
4	BCL	O	309	X	-	-	-
5	BPH	L	284	X	-	-	-
5	BPH	L	285	X	-	-	-
5	BPH	N	285	X	-	-	-
5	BPH	O	310	X	-	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 14138 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 (L SUBUNIT).

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

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	299	2390	1597	391	392	10	0	0	0
2	O	299	2390	1597	391	392	10	0	0	0

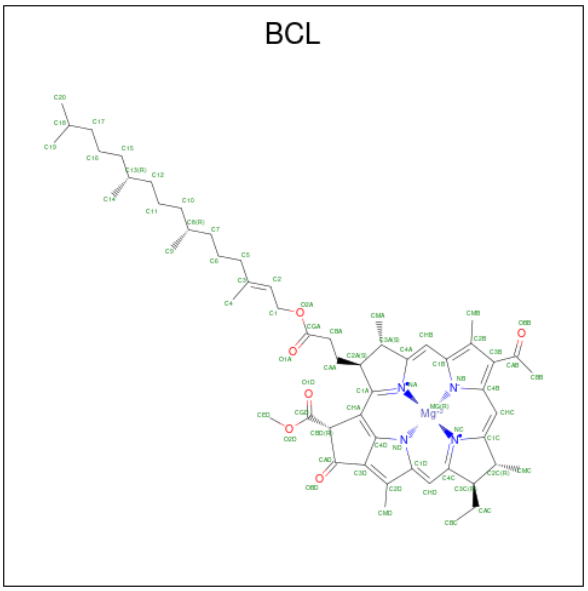
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	248	1883	1204	322	347	10	0	0	0
3	P	248	1883	1204	322	347	10	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	8	GLN	GLY	conflict	UNP P11846
P	8	GLN	GLY	conflict	UNP P11846

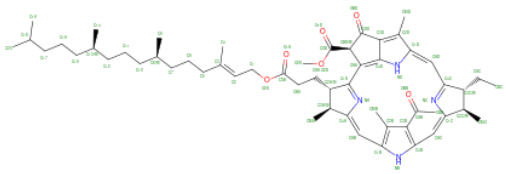
- Molecule 4 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



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

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

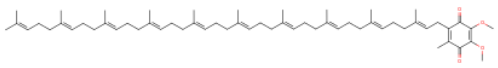
BPH



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	L	1	65	55	4	6	14	0
			Total	C	N	O		
5	L	1	65	55	4	6	0	0
			Total	C	N	O		
5	N	1	65	55	4	6	0	0
			Total	C	N	O		
5	O	1	65	55	4	6	0	0

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

U10



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	L	1	63	59	4	0	0
6	M	1	63	59	4	0	0
6	N	1	63	59	4	19	0
6	O	1	63	59	4	0	0

- Molecule 7 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
7	M	1	1	1	0	0
7	O	1	1	1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	L	19	19	19	0	0
8	M	21	21	21	0	0
8	H	13	13	13	0	0
8	N	13	13	13	0	0
8	O	15	15	15	0	0
8	P	5	5	5	0	0

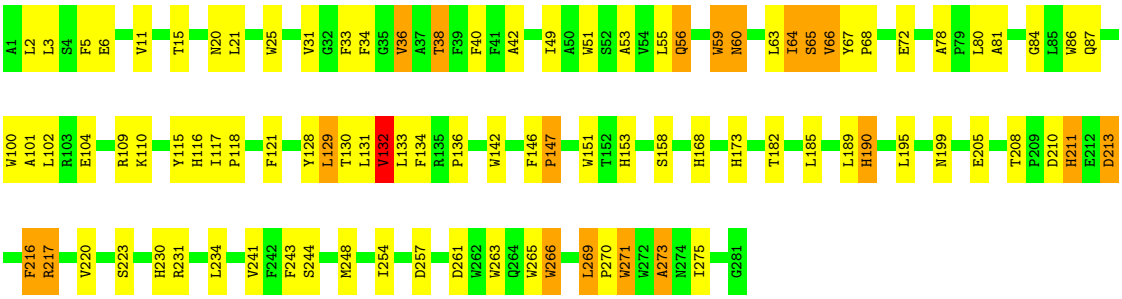
3 Residue-property plots (i)

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.

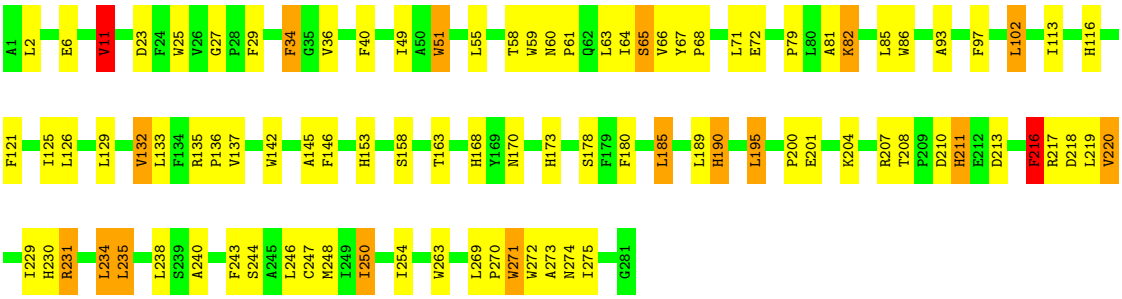
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER (L SUBUNIT)

Chain L:



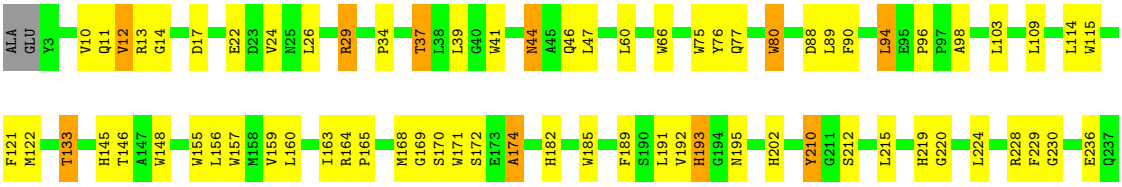
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER (L SUBUNIT)

Chain N:



• Molecule 2: PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT)

Chain M:



I238 T243 A244 R247 F251 W254 F258 N259 A260 T261 M262 E263 G264 I265 H266 R267 L275 T279 L286 S287 G288 D292 V296 W297 N300 H301 GLY MET ALA PRO LEU ASN

• Molecule 2: PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT)

Chain O: 66% 25% 6% •

ALA GLU Y3 F7 S8 Q9 V12 D17 E22 D23 V24 N25 L26 R29 T37 F42 Q46 L60 F61 S62 I72 W75 Y76 Q77 W80 N81 R87 D88 L89 L94 L114 F120 F121 M122 F123 V124 T133 Y134 L135 M142 H145

T146 A147 W148 A149 F150 L151 S152 A153 I154 W155 L156 W157 M158 V159 L160 R164 P165 M168 W171 S172 E173 H182 W185 T186 F189 S190 L191 V192 H193 G194 N195 L196 F197 Y198 N199 H202 G203 L204 S205 I206 H219 T222 V226 S227 R228 F229 E234 L235 E236

Q237 I238 A239 D240 A244 F251 M256 G257 F258 N259 A260 T261 M262 E263 G264 I265 H266 R267 W271 V274 L275 L278 I284 L285 L286 S287 G288 T289 V290 V291 W294 W297 H301 GLY MET ALA PRO LEU ASN

• Molecule 3: PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT)

Chain H: 63% 28% • • 5%

MET VAL GLY VAL THR ALA PHE GLN ASN PHE D11 L12 I17 W21 T33 E34 N35 M36 R37 P49 K60 P61 K62 T63 F64 I65 L66 P67 H68 G69 R70 L73 T74 V75 E79 D82 R83 P84 I85 A86 L87 F96 P97 H98 D103 D107 G108 V109

S113 D119 E122 L123 D124 G125 H126 G127 H128 N129 K130 F140 H141 V142 S143 A144 G145 K146 L151 R154 D157 W168 V169 D170 Q174 M175 A176 R177 F178 V181 E182 L183 S187 T188 R189 M193 Q194 M195 R202 V203 H204 L208 S209 S210 D211 L212

I216 I219 K220 S221 P222 T223 E224 V225 T226 L227 L228 E229 E230 D231 L241 M242 Y243 R248 K249 A254 M255 L256 A257 E258 TYR ALA

• Molecule 3: PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT)

Chain P: 63% 28% • • 5%

MET VAL GLY VAL THR ALA PHE GLN ASN PHE D11 L12 I17 W21 E34 R37 P41 N44 E45 D46 F56 P57 L58 P59 K60 P61 K62 T63 F64 I65 L66 P67 H68 G69 R70 L73 T74 V75 D82 L87 H98 D103 G108 V109 G110 P111 A112

D119 E122 L123 D124 G125 H126 G127 H128 N129 K130 I131 K132 K135 A138 H141 R154 D157 D166 I167 W168 V169 D170 I171 P172 E173 F178 L179 E180 L183 K184 D185 T188 R189 P192 M193 Q194 M195 V196 K197 V198 Q199 S200 V203 H204 V205 N206 A207

L208 L212 I216 I219 K220 S221 P222 T223 E224 V225 T226 L227 L228 E229 E230 D231 V237 L241 M242 Y243 R248 V251 V252 E258 TYR ALA

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	140.10Å 140.10Å 271.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60	Depositor
% Data completeness (in resolution range)	88.0 (30.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	X-PLOR 3.89	Depositor
R, R_{free}	0.215 , 0.299	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14138	wwPDB-VP
Average B, all atoms (Å^2)	56.0	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: BCL, BPH, U10, FE2

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	1.07	12/2320 (0.5%)	1.80	60/3175 (1.9%)
1	N	1.01	9/2320 (0.4%)	1.77	51/3175 (1.6%)
2	M	1.05	9/2482 (0.4%)	1.77	49/3389 (1.4%)
2	O	1.05	12/2482 (0.5%)	1.71	45/3389 (1.3%)
3	H	0.98	6/1931 (0.3%)	1.76	33/2627 (1.3%)
3	P	0.96	6/1931 (0.3%)	1.75	38/2627 (1.4%)
All	All	1.02	54/13466 (0.4%)	1.76	276/18382 (1.5%)

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	211	HIS	CD2-NE2	-7.82	1.29	1.37
2	O	145	HIS	CD2-NE2	-7.20	1.29	1.37
2	M	145	HIS	CD2-NE2	-7.07	1.30	1.37
3	H	128	HIS	CD2-NE2	-7.06	1.30	1.37
1	L	211	HIS	CD2-NE2	-6.98	1.30	1.37

The worst 5 of 276 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	75	VAL	N-CA-CB	-11.56	100.11	112.37
1	N	220	VAL	N-CA-CB	-9.88	100.58	112.33
3	H	124	ASP	CA-CB-CG	9.65	122.25	112.60
3	H	75	VAL	CB-CA-C	9.51	119.35	110.13
3	P	124	ASP	CA-CB-CG	8.91	121.51	112.60

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	L	2232	0	2187	38	0
1	N	2232	0	2187	39	0
2	M	2390	0	2304	37	0
2	O	2390	0	2304	47	0
3	H	1883	0	1895	31	0
3	P	1883	0	1895	33	0
4	L	132	0	148	7	0
4	M	132	0	148	11	0
4	N	198	0	222	16	0
4	O	66	0	74	7	0
5	L	130	0	152	11	0
5	N	65	0	76	7	0
5	O	65	0	76	4	0
6	L	63	0	90	4	0
6	M	63	0	90	1	0
6	N	63	0	90	6	0
6	O	63	0	90	3	0
7	M	1	0	0	0	0
7	O	1	0	0	0	0
8	H	13	0	0	3	0
8	L	19	0	0	4	0
8	M	21	0	0	0	0
8	N	13	0	0	0	0
8	O	15	0	0	1	0
8	P	5	0	0	0	0
All	All	14138	0	14028	235	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 8.

The worst 5 of 235 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:O:122:MET:HE3	2:O:157:TRP:HE1	1.37	0.89
2:M:275:LEU:O	2:M:279:THR:HB	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:122:MET:HE3	2:M:157:TRP:HE1	1.52	0.75
4:N:282:BCL:HBB3	4:O:309:BCL:H41	1.71	0.72
4:N:284:BCL:HED2	2:O:203:GLY:HA3	1.72	0.70

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%)	261 (94%)	14 (5%)	4 (1%)	9	19
1	N	279/281 (99%)	261 (94%)	15 (5%)	3 (1%)	11	25
2	M	297/307 (97%)	284 (96%)	11 (4%)	2 (1%)	18	38
2	O	297/307 (97%)	284 (96%)	11 (4%)	2 (1%)	18	38
3	H	246/260 (95%)	238 (97%)	8 (3%)	0	100	100
3	P	246/260 (95%)	238 (97%)	7 (3%)	1 (0%)	30	51
All	All	1644/1696 (97%)	1566 (95%)	66 (4%)	12 (1%)	18	38

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	270	PRO
2	M	259	ASN
2	O	259	ASN
1	L	271	TRP
2	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	L	220/220 (100%)	205 (93%)	15 (7%)	14	32
1	N	220/220 (100%)	200 (91%)	20 (9%)	9	19
2	M	235/240 (98%)	217 (92%)	18 (8%)	12	27
2	O	235/240 (98%)	215 (92%)	20 (8%)	10	22
3	H	200/209 (96%)	178 (89%)	22 (11%)	6	13
3	P	200/209 (96%)	178 (89%)	22 (11%)	6	13
All	All	1310/1338 (98%)	1193 (91%)	117 (9%)	9	20

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	64	ILE
3	P	223	THR
1	N	234	LEU
3	P	220	LYS
3	P	66	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
3	H	204	HIS
1	N	199	ASN
3	P	52	ASN
1	N	159	ASN
1	N	211	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 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	282	1	69,74,74	1.19	7 (10%)	79,115,115	1.71	20 (25%)
4	BCL	N	283	1	69,74,74	1.14	5 (7%)	79,115,115	1.98	22 (27%)
6	U10	M	311	-	63,63,63	1.74	14 (22%)	78,79,79	1.29	7 (8%)
6	U10	N	286	-	63,63,63	1.73	16 (25%)	78,79,79	1.59	9 (11%)
6	U10	O	311	-	63,63,63	1.61	14 (22%)	78,79,79	1.19	11 (14%)
4	BCL	M	310	2	69,74,74	1.10	5 (7%)	79,115,115	1.97	20 (25%)
4	BCL	N	284	1	69,74,74	1.20	9 (13%)	79,115,115	2.12	24 (30%)
4	BCL	L	283	1	69,74,74	1.15	6 (8%)	79,115,115	1.99	25 (31%)
5	BPH	L	285	-	59,70,70	1.61	7 (11%)	59,101,101	2.39	21 (35%)
4	BCL	O	309	2	69,74,74	1.10	7 (10%)	79,115,115	1.76	17 (21%)
5	BPH	N	285	-	59,70,70	1.44	6 (10%)	59,101,101	2.82	19 (32%)
4	BCL	M	309	2	69,74,74	1.22	8 (11%)	79,115,115	2.18	24 (30%)
5	BPH	O	310	-	59,70,70	1.39	7 (11%)	59,101,101	2.86	20 (33%)
4	BCL	N	282	2	69,74,74	1.28	8 (11%)	79,115,115	1.85	19 (24%)
5	BPH	L	284	-	59,70,70	1.72	9 (15%)	59,101,101	2.45	20 (33%)
6	U10	L	286	-	63,63,63	1.74	16 (25%)	78,79,79	1.32	8 (10%)

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	282	1	-	3/41/137/137	-
4	BCL	N	283	1	-	11/41/137/137	-
6	U10	M	311	-	-	15/63/87/87	0/1/1/1
6	U10	N	286	-	-	19/63/87/87	0/1/1/1
6	U10	O	311	-	-	13/63/87/87	0/1/1/1
4	BCL	M	310	2	2/2/21/25	3/41/137/137	-
4	BCL	N	284	1	-	5/41/137/137	-
5	BPH	L	285	-	1/1/18/22	10/37/105/105	0/5/6/6
5	BPH	N	285	-	1/1/18/22	9/37/105/105	0/5/6/6
4	BCL	O	309	2	1/1/21/25	4/41/137/137	-
4	BCL	L	283	1	-	6/41/137/137	-
4	BCL	M	309	2	2/2/21/25	11/41/137/137	-
5	BPH	O	310	-	1/1/18/22	10/37/105/105	0/5/6/6
4	BCL	N	282	2	2/2/21/25	6/41/137/137	-
5	BPH	L	284	-	2/2/18/22	9/37/105/105	0/5/6/6
6	U10	L	286	-	-	13/63/87/87	0/1/1/1

The worst 5 of 144 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	285	BPH	C3A-C2A	-7.85	1.47	1.54
5	L	284	BPH	C2C-C3C	-6.89	1.48	1.54
5	L	284	BPH	C3A-C2A	-5.74	1.49	1.54
5	N	285	BPH	C3D-CAD	-5.04	1.38	1.47
5	O	310	BPH	C3D-CAD	-5.00	1.38	1.47

The worst 5 of 286 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	N	285	BPH	O2D-CGD-CBD	9.79	121.70	110.95
5	O	310	BPH	O2D-CGD-CBD	9.55	121.44	110.95
5	O	310	BPH	C4D-CHA-CBD	-9.44	103.93	108.45
4	M	309	BCL	C1C-NC-C4C	8.00	110.33	106.68
5	N	285	BPH	C4D-CHA-CBD	-7.92	104.66	108.45

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	M	309	BCL	C13
4	M	309	BCL	C8
4	M	310	BCL	C13
4	M	310	BCL	C8
4	N	282	BCL	C13

5 of 147 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	283	BCL	CBD-CGD-O2D-CED
4	N	283	BCL	CBD-CGD-O2D-CED
4	N	284	BCL	CBD-CGD-O2D-CED
5	N	285	BPH	C4C-C3C-CAC-CBC
5	O	310	BPH	C4C-C3C-CAC-CBC

There are no ring outliers.

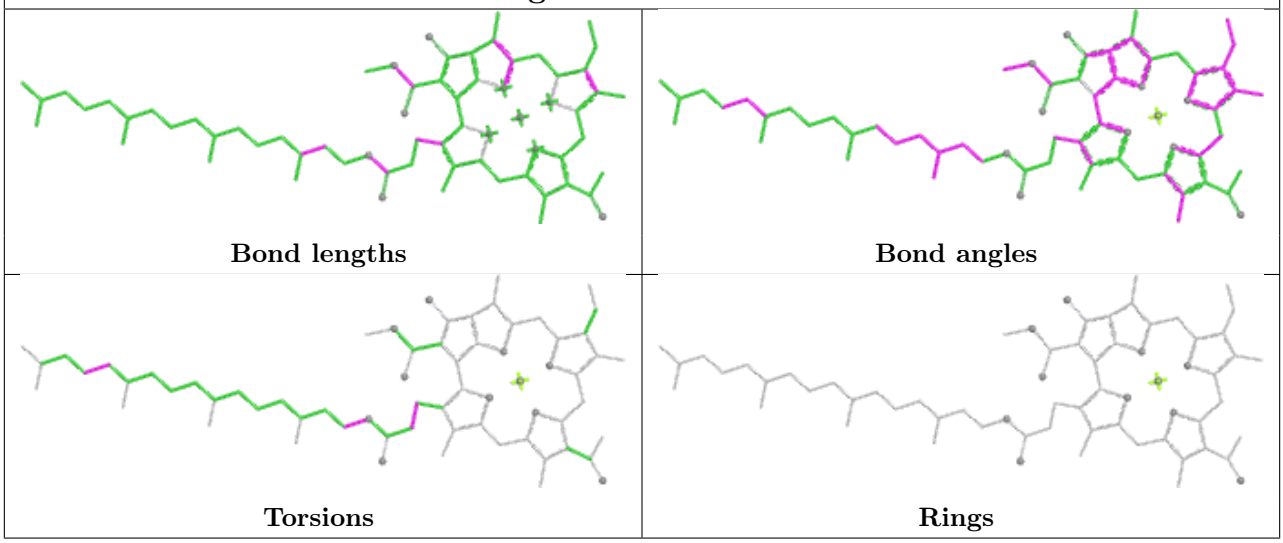
16 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	282	BCL	6	0
4	N	283	BCL	5	0
6	M	311	U10	1	0
6	N	286	U10	6	0
6	O	311	U10	3	0
4	M	310	BCL	4	0
4	N	284	BCL	5	0
4	L	283	BCL	4	0
5	L	285	BPH	9	0
4	O	309	BCL	7	0
5	N	285	BPH	7	0
4	M	309	BCL	7	0
5	O	310	BPH	4	0
4	N	282	BCL	8	0
5	L	284	BPH	2	0
6	L	286	U10	4	0

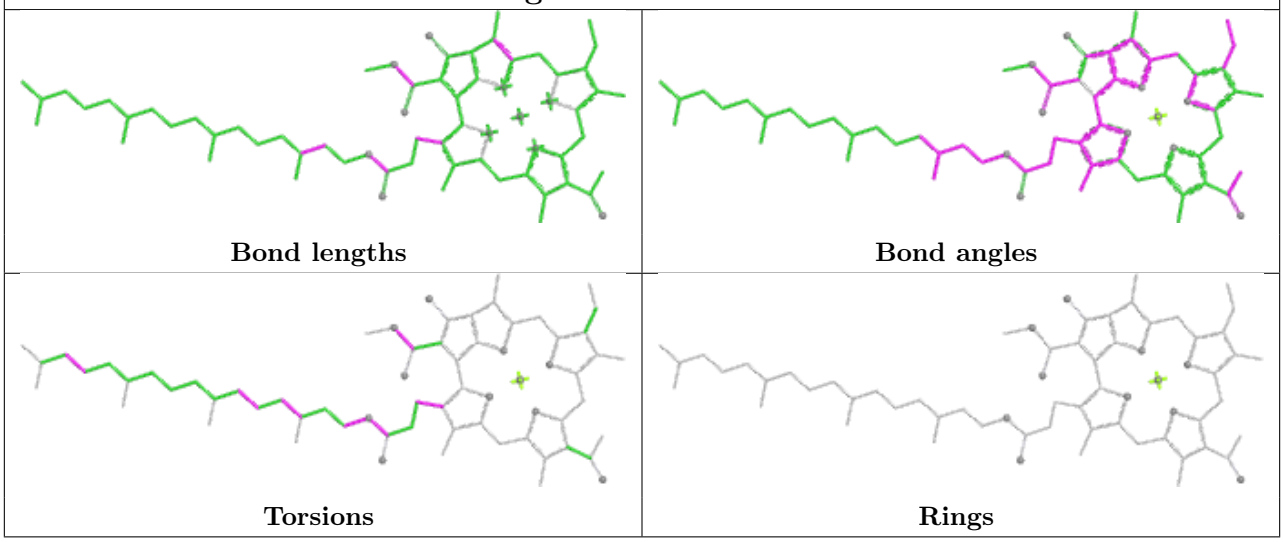
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

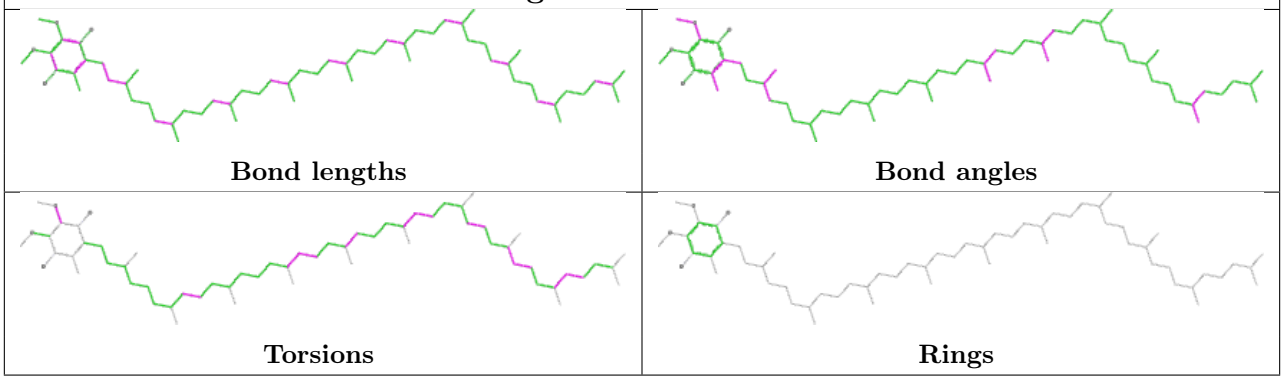
Ligand BCL L 282



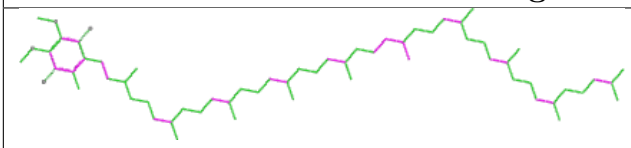
Ligand BCL N 283



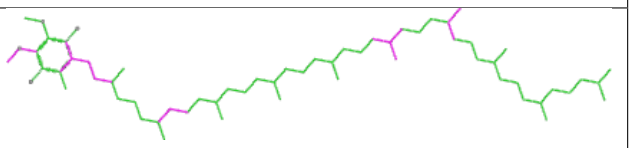
Ligand U10 M 311



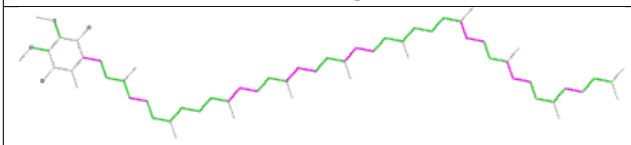
Ligand U10 N 286



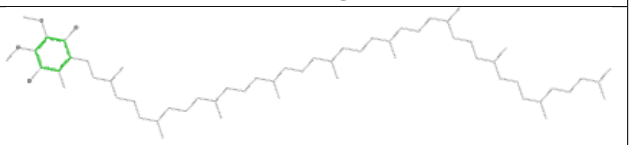
Bond lengths



Bond angles

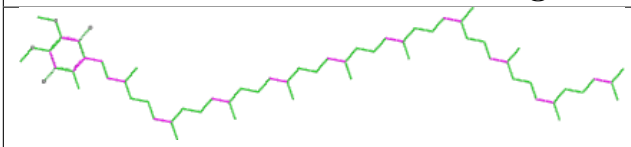


Torsions

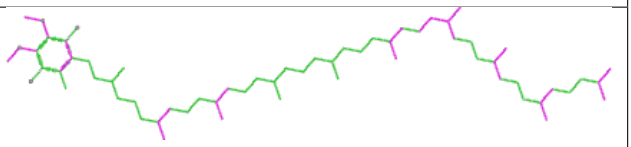


Rings

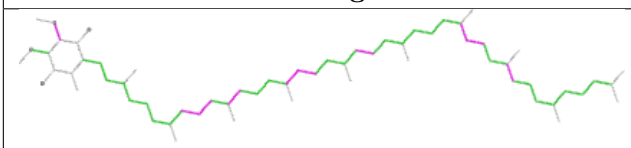
Ligand U10 O 311



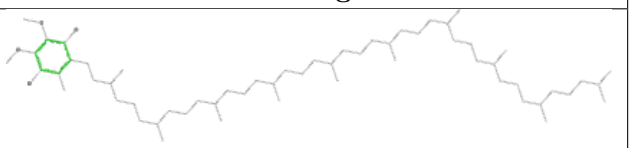
Bond lengths



Bond angles

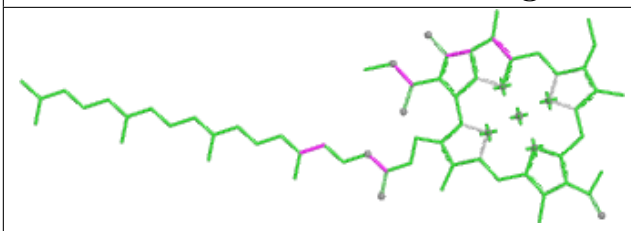


Torsions

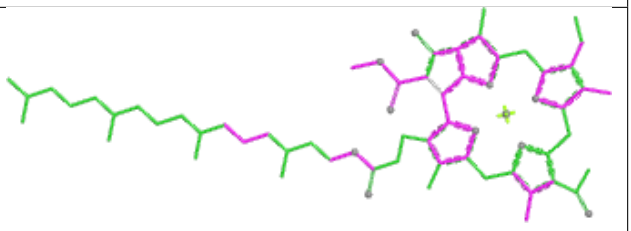


Rings

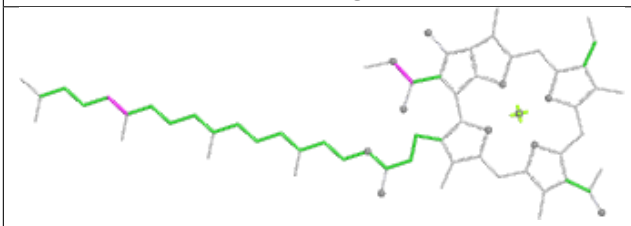
Ligand BCL M 310



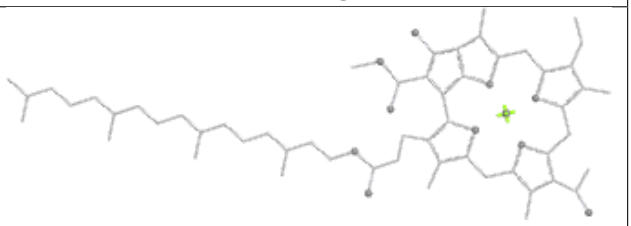
Bond lengths



Bond angles

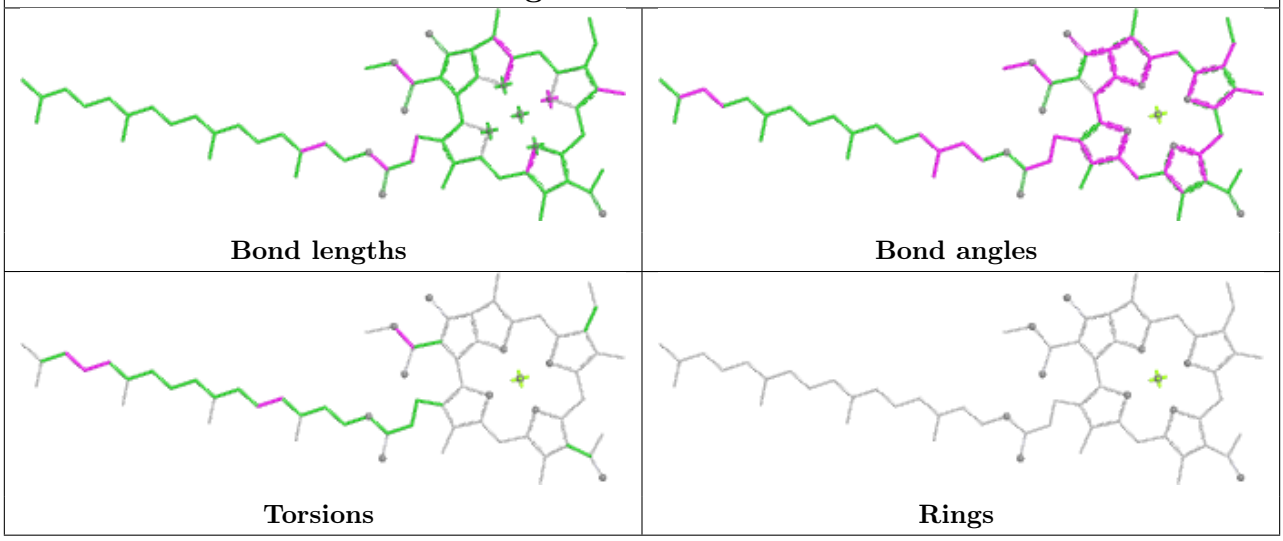


Torsions

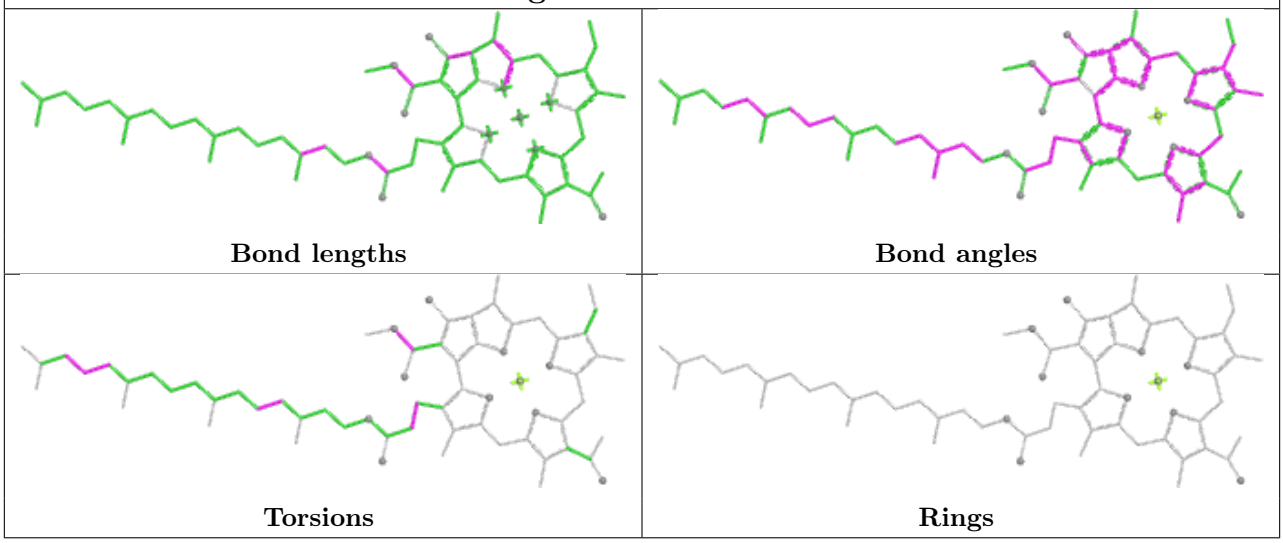


Rings

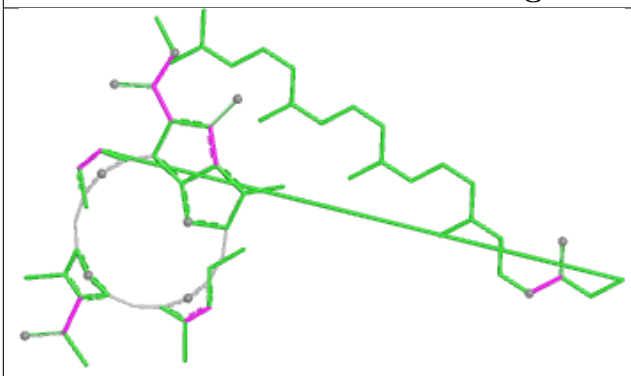
Ligand BCL N 284



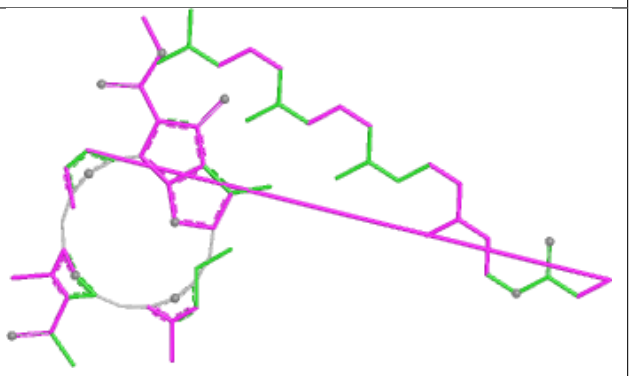
Ligand BCL L 283



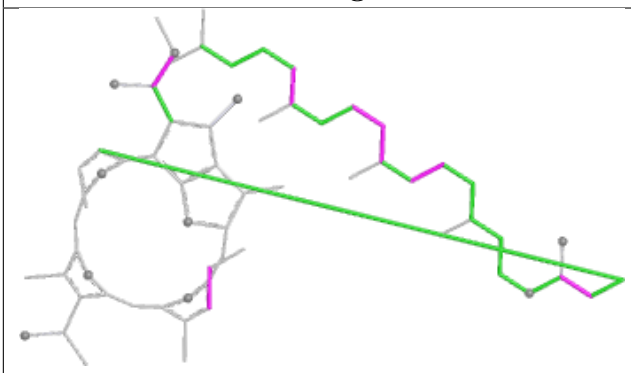
Ligand BPH L 285



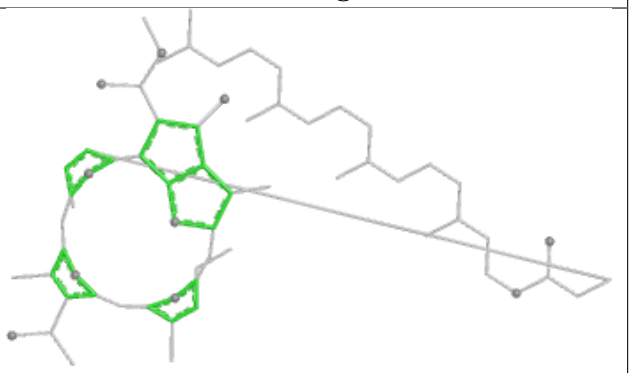
Bond lengths



Bond angles

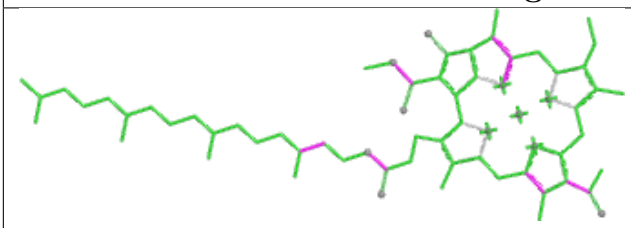


Torsions

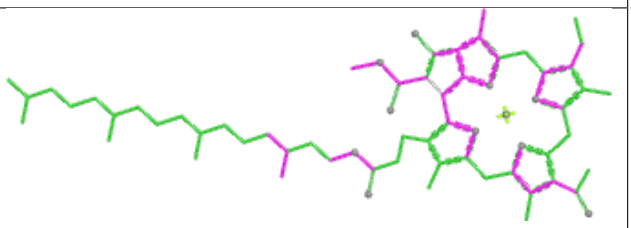


Rings

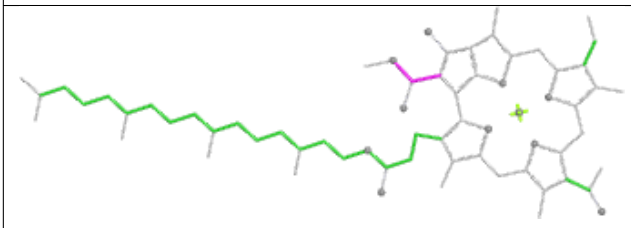
Ligand BCL O 309



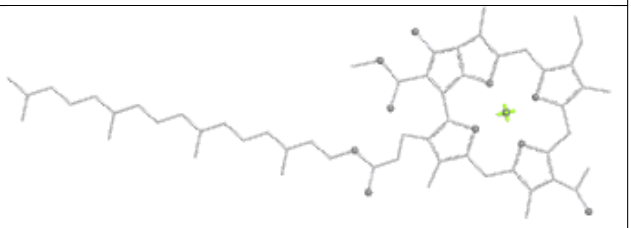
Bond lengths



Bond angles

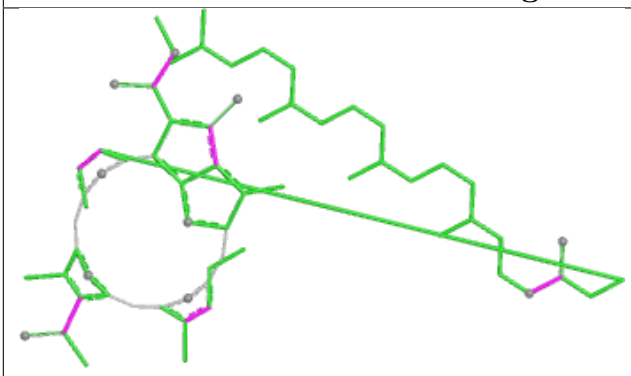


Torsions



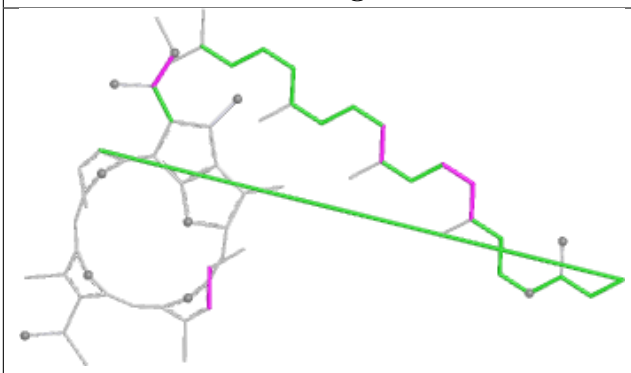
Rings

Ligand BPH N 285

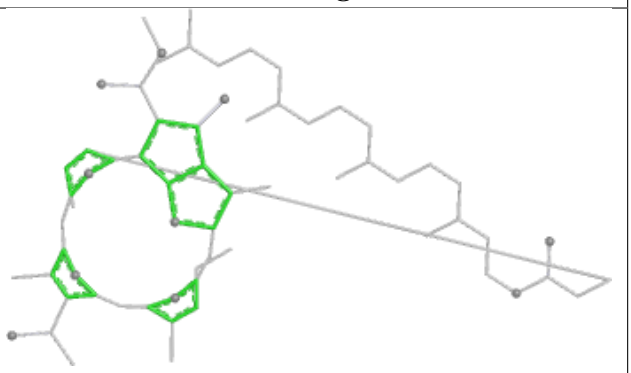


Bond lengths

Bond angles

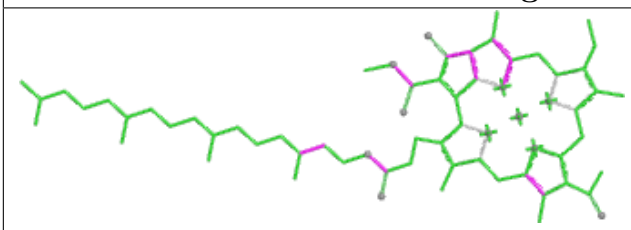


Torsions

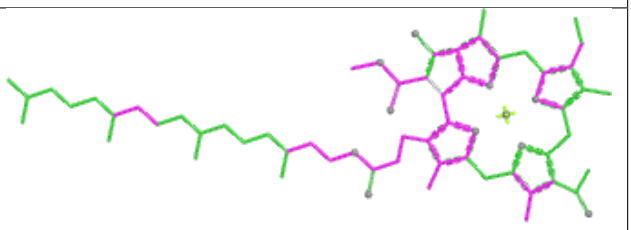


Rings

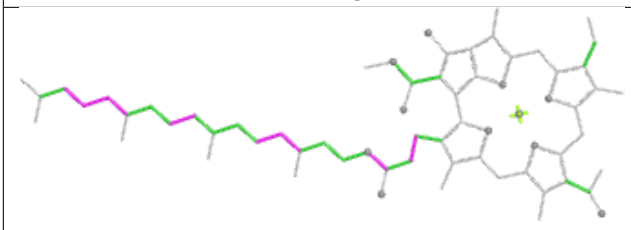
Ligand BCL M 309



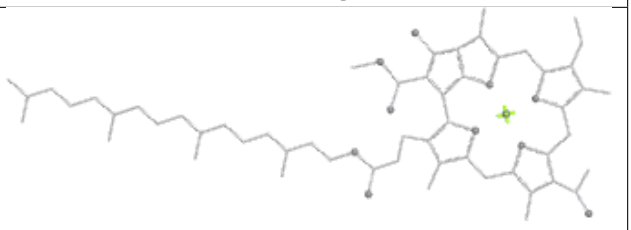
Bond lengths



Bond angles

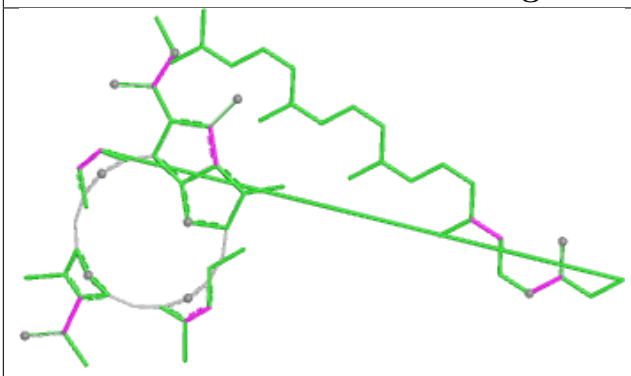


Torsions

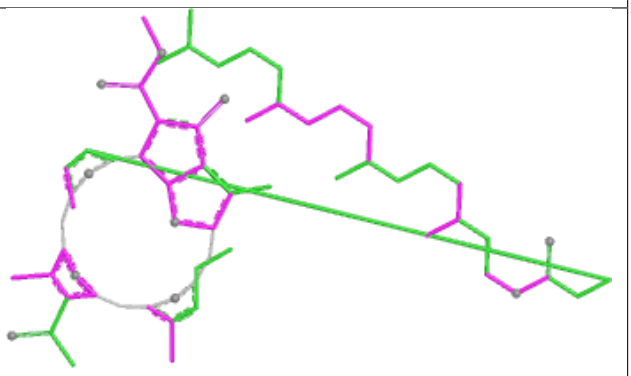


Rings

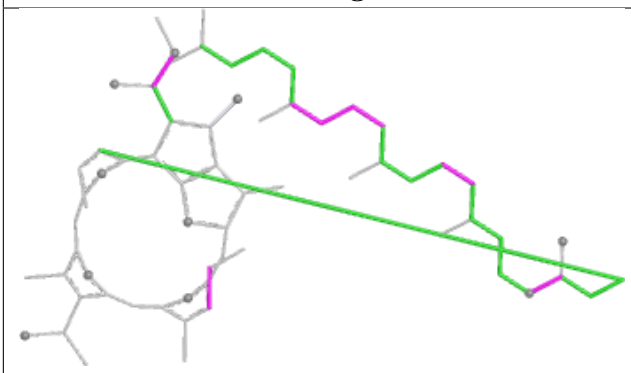
Ligand BPH O 310



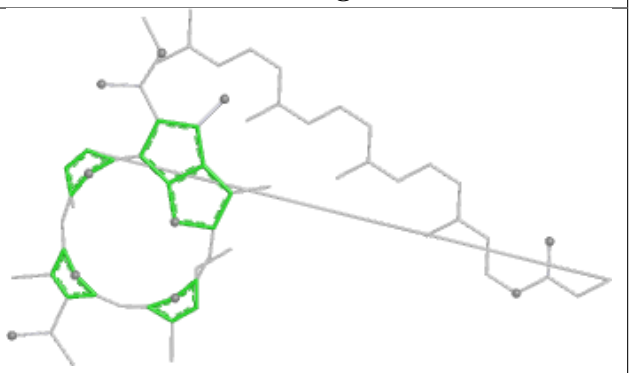
Bond lengths



Bond angles

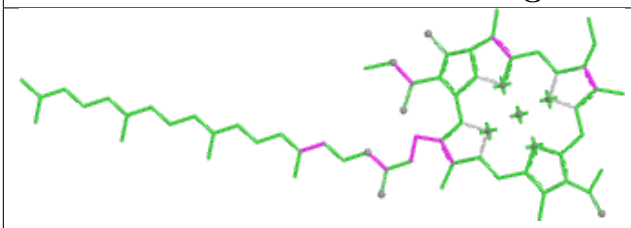


Torsions

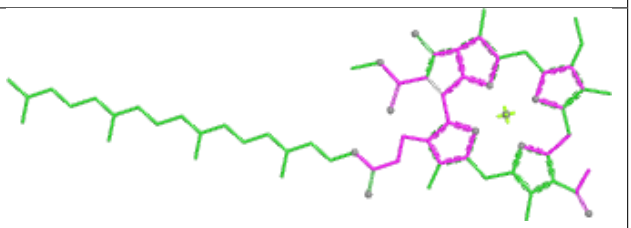


Rings

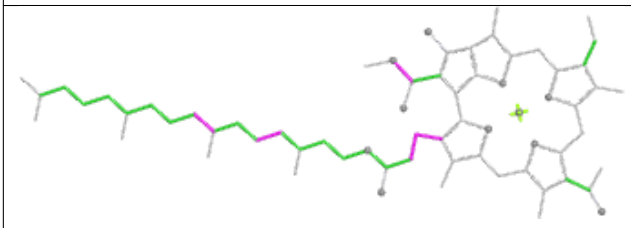
Ligand BCL N 282



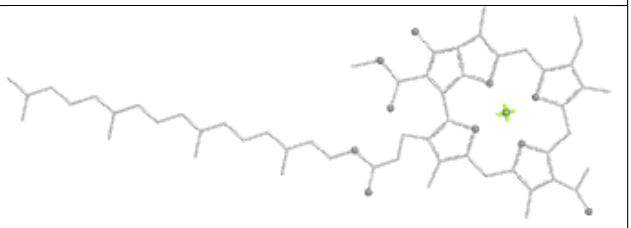
Bond lengths



Bond angles

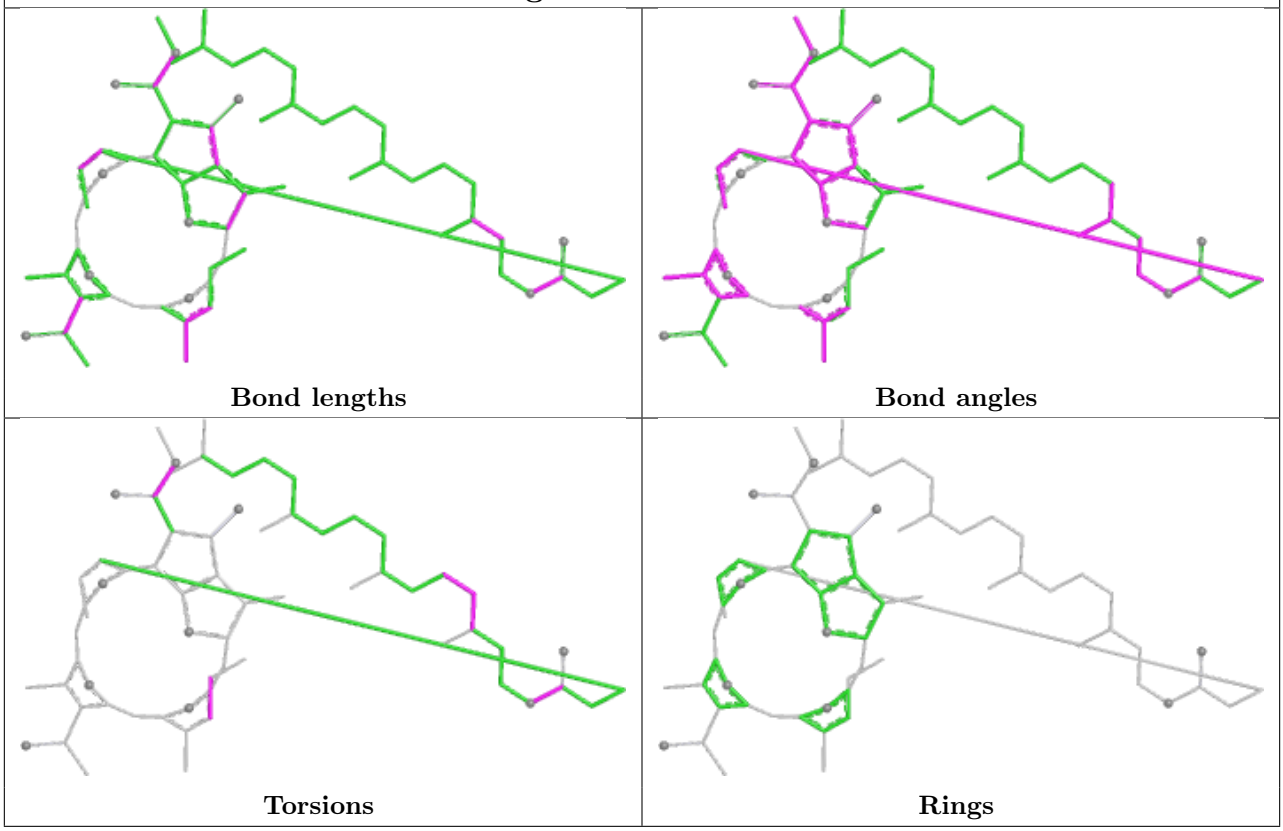


Torsions

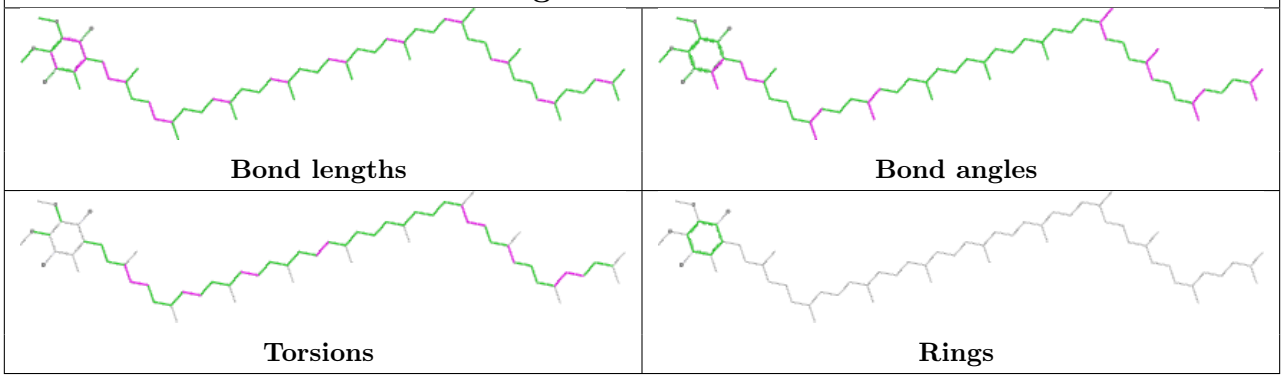


Rings

Ligand BPH L 284



Ligand U10 L 286



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.