wwPDB X-ray Structure Validation Summary Report (i)

Apr 21, 2024 – 08:54 pm BST

PDB ID	:	1E14
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 (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:

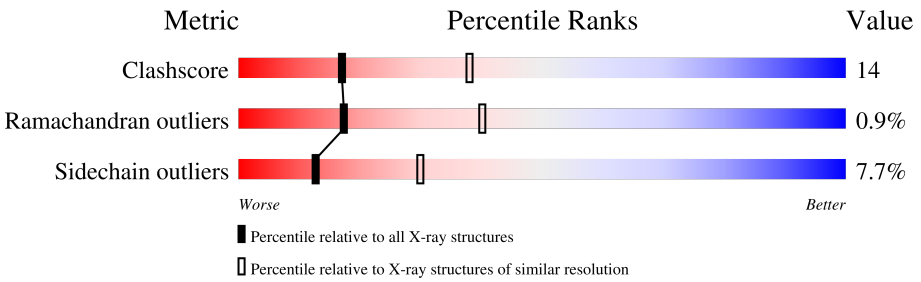
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.70 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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	H	260	57% 29% 5% • 7%
2	L	281	71% 25% ••
3	M	307	71% 21% 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 criteria:

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

2 Entry composition (i)

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
			Total	C	N	O	S			
1	H	241	1830	1169	315	337	9	0	0	1

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

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

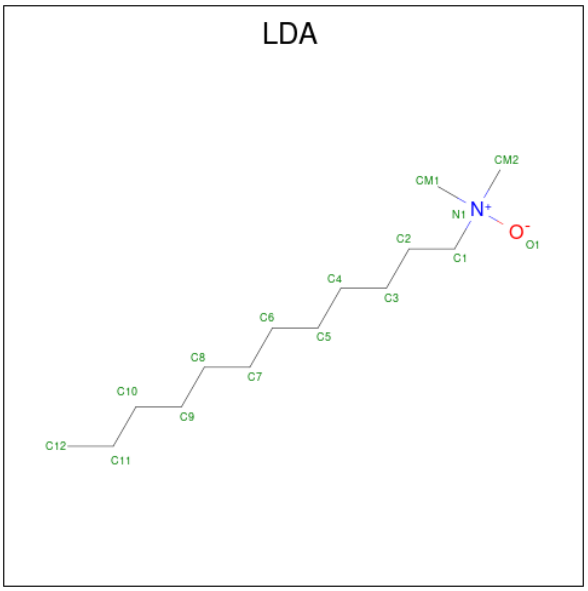
- Molecule 3 is a protein called Reaction center protein M chain.

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

There are 2 discrepancies between the modelled and reference sequences:

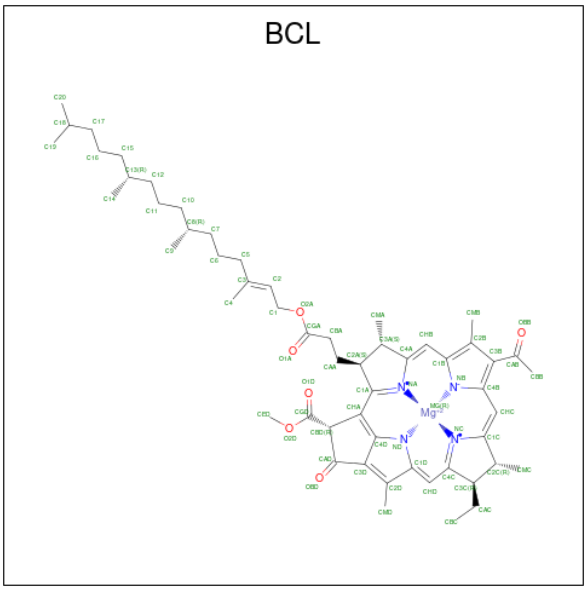
Chain	Residue	Modelled	Actual	Comment	Reference
M	197	ARG	PHE	conflict	UNP P0C0Y9
M	203	ASP	GLY	conflict	UNP P0C0Y9

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: 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	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 (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



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

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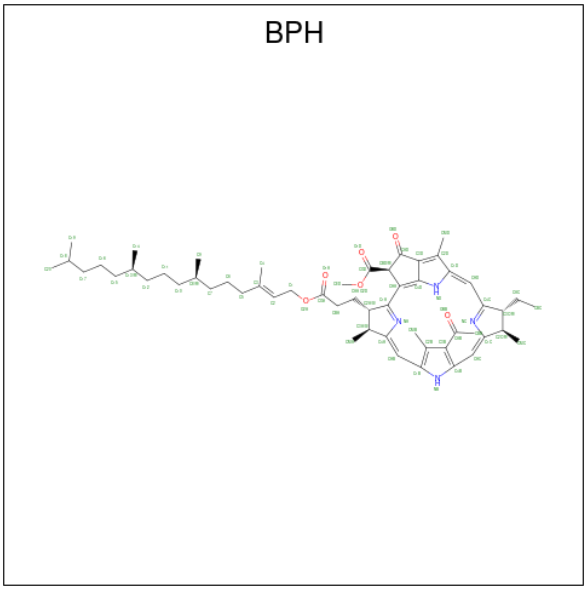
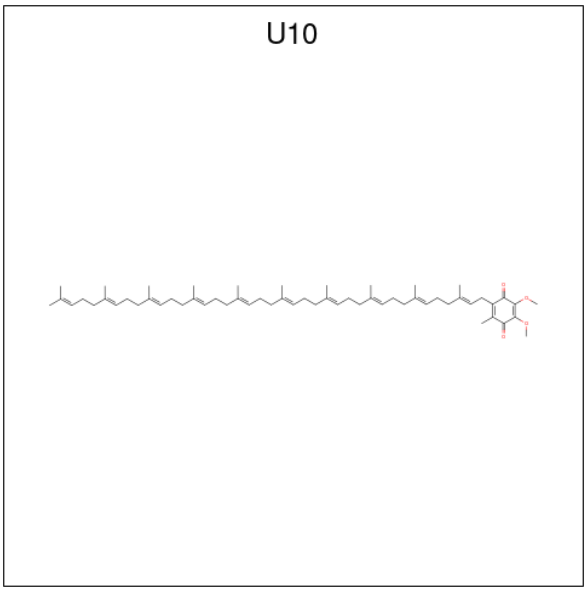
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
5	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	M	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	M	1	66	55	1	4	6	0	0

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



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

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

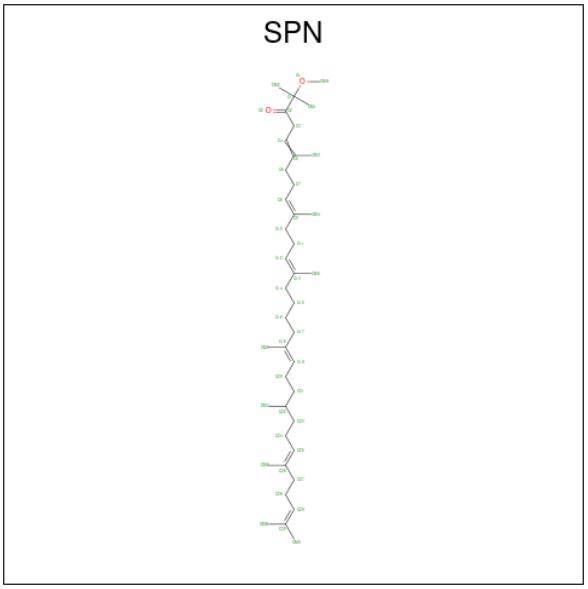


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	L	1	48	44	4	22	0
			Total	C	O		
7	M	1	48	44	4	0	0

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

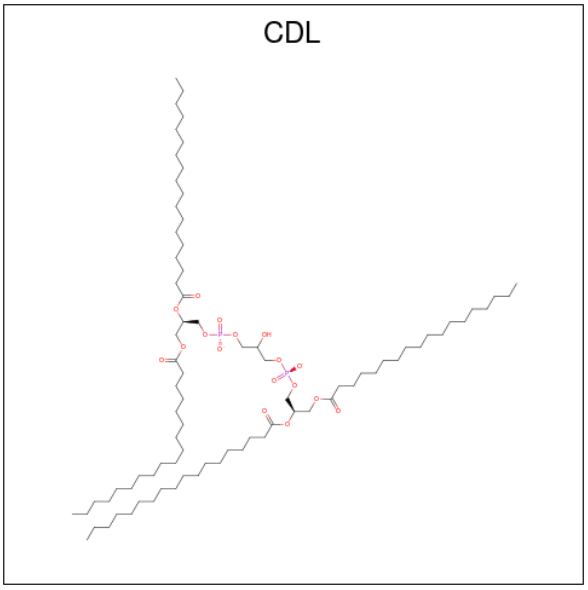
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
8	M	1	1	1	0	0

- Molecule 9 is SPEROIDENONE (three-letter code: 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 CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 11 is water.

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

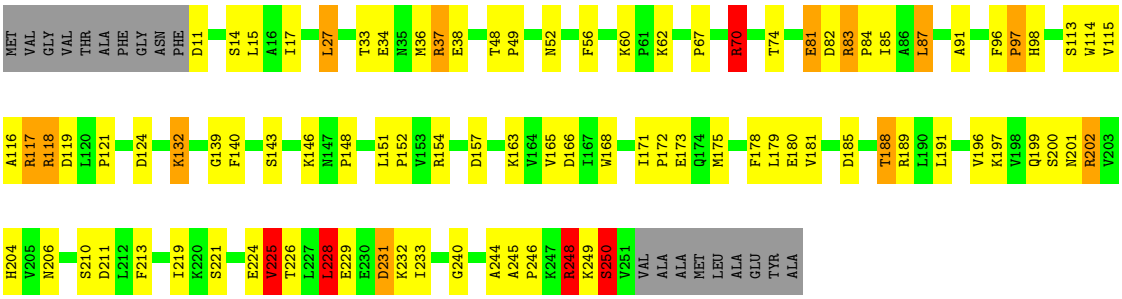
3 Residue-property plots (i)

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.

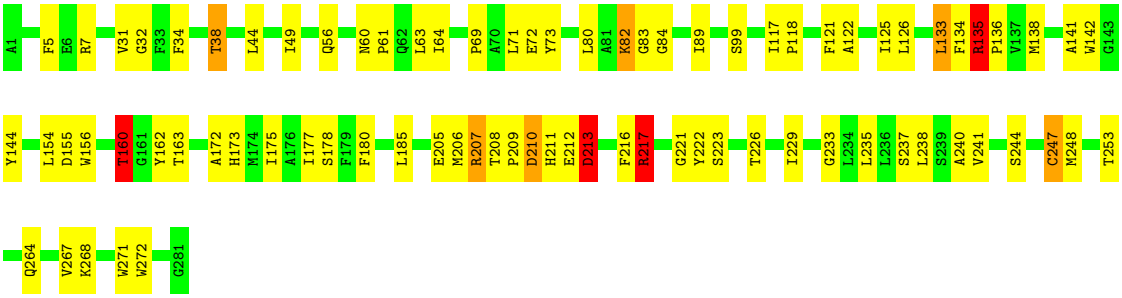
• Molecule 1: Reaction center protein H chain

Chain H: 57% 29% 5% • 7%



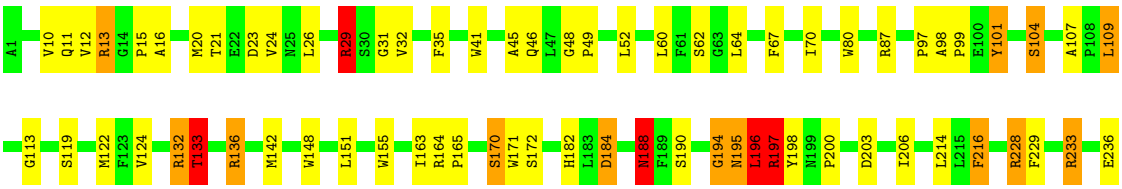
• Molecule 2: Reaction center protein L chain

Chain L: 71% 25% • •



• Molecule 3: Reaction center protein M chain

Chain M: 71% 21% 5% • •



A239
D240
R241
G242
T243
A244
A245
E246
R247
R253
N259
I270
L285
D292
N293
W294
Y295
H301
G302
M303
ALA
PRO
LEU
ASN

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	140.00Å 140.00Å 184.60Å 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, BPH, BCL, U10, SPN, CDL, FE

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	0.66	0/1878	1.75	30/2555 (1.2%)
2	L	0.63	0/2320	1.48	12/3175 (0.4%)
3	M	0.61	0/2504	1.56	36/3419 (1.1%)
All	All	0.63	0/6702	1.59	78/9149 (0.9%)

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

There are no bond length outliers.

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	70	ARG	NE-CZ-NH2	-21.92	109.34	120.30
3	M	247	ARG	NE-CZ-NH1	17.87	129.24	120.30
2	L	135	ARG	NE-CZ-NH1	16.24	128.42	120.30
2	L	135	ARG	CD-NE-CZ	15.24	144.93	123.60
2	L	135	ARG	NE-CZ-NH2	-14.98	112.81	120.30

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 (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	1830	0	1836	61	0
2	L	2232	0	2187	59	0
3	M	2413	0	2326	58	0
4	H	16	0	31	0	0
4	M	32	0	62	5	0
5	L	132	0	148	15	0
5	M	132	0	148	10	0
6	L	65	0	76	10	0
6	M	65	0	76	3	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	200	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 14.

The worst 5 of 200 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:206:MET:HE1	3:M:239:ALA:HB2	1.51	0.89

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%)	19 43
2	L	279/281 (99%)	262 (94%)	17 (6%)	0	100 100
3	M	301/307 (98%)	275 (91%)	21 (7%)	5 (2%)	9 23
All	All	819/848 (97%)	761 (93%)	51 (6%)	7 (1%)	17 40

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%)	182 (93%)	13 (7%)	16	37
2	L	220/220 (100%)	199 (90%)	21 (10%)	8	20
3	M	237/241 (98%)	221 (93%)	16 (7%)	16	36
All	All	652/669 (98%)	602 (92%)	50 (8%)	13	30

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	223	SER
3	M	52	LEU
3	M	259	ASN
2	L	235	LEU
2	L	271	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
1	H	126	HIS
1	H	199	GLN
1	H	204	HIS
1	H	206	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
5	BCL	M	1303	3	64,74,74	1.57	10 (15%)	78,115,115	1.87	24 (30%)
10	CDL	M	800	-	80,80,99	0.50	0	86,92,111	0.90	3 (3%)
6	BPH	L	401	-	51,70,70	1.80	11 (21%)	52,101,101	3.41	12 (23%)
6	BPH	M	402	-	51,70,70	1.62	10 (19%)	52,101,101	3.17	18 (34%)
5	BCL	M	1301	3	64,74,74	1.55	8 (12%)	78,115,115	2.31	24 (30%)
7	U10	M	502	-	48,48,63	1.79	14 (29%)	58,61,79	1.51	13 (22%)
4	LDA	H	701	-	12,15,15	2.46	1 (8%)	14,17,17	0.79	1 (7%)
9	SPN	M	600	-	40,42,42	3.79	18 (45%)	50,52,52	2.93	19 (38%)
5	BCL	L	1304	2	64,74,74	1.56	9 (14%)	78,115,115	2.84	25 (32%)
4	LDA	M	702	-	12,15,15	2.45	1 (8%)	14,17,17	0.85	1 (7%)
7	U10	L	501	-	47,47,63	2.03	13 (27%)	54,58,79	2.66	21 (38%)
4	LDA	M	703	-	12,15,15	2.42	1 (8%)	14,17,17	0.81	1 (7%)
5	BCL	L	1302	2	64,74,74	1.58	10 (15%)	78,115,115	2.15	20 (25%)

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	1303	3	-	6/37/137/137	-
10	CDL	M	800	-	-	35/91/91/110	-
6	BPH	L	401	-	2/2/18/22	14/37/105/105	0/5/6/6
6	BPH	M	402	-	-	18/37/105/105	0/5/6/6
5	BCL	M	1301	3	1/1/21/25	17/37/137/137	-
7	U10	M	502	-	-	6/45/69/87	0/1/1/1
4	LDA	H	701	-	-	12/13/13/13	-
9	SPN	M	600	-	-	18/50/51/51	-
5	BCL	L	1304	2	-	9/37/137/137	-
4	LDA	M	702	-	-	12/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	U10	L	501	-	-	15/41/65/87	0/1/1/1
4	LDA	M	703	-	-	8/13/13/13	-
5	BCL	L	1302	2	-	9/37/137/137	-

The worst 5 of 106 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	600	SPN	C4-C5	8.89	1.54	1.33
9	M	600	SPN	C8-C9	8.50	1.53	1.33
4	H	701	LDA	O1-N1	-8.48	1.22	1.42
4	M	702	LDA	O1-N1	-8.47	1.22	1.42
4	M	703	LDA	O1-N1	-8.38	1.22	1.42

The worst 5 of 182 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	401	BPH	O2D-CGD-CBD	18.87	134.91	111.00
6	M	402	BPH	O2D-CGD-CBD	14.16	128.94	111.00
5	L	1304	BCL	O2D-CGD-CBD	11.19	131.15	111.27
7	L	501	U10	C37-C38-C39	10.29	152.45	127.66
5	L	1304	BCL	C1C-NC-C4C	9.36	110.92	106.71

All (3) chirality outliers are listed below:

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

5 of 179 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

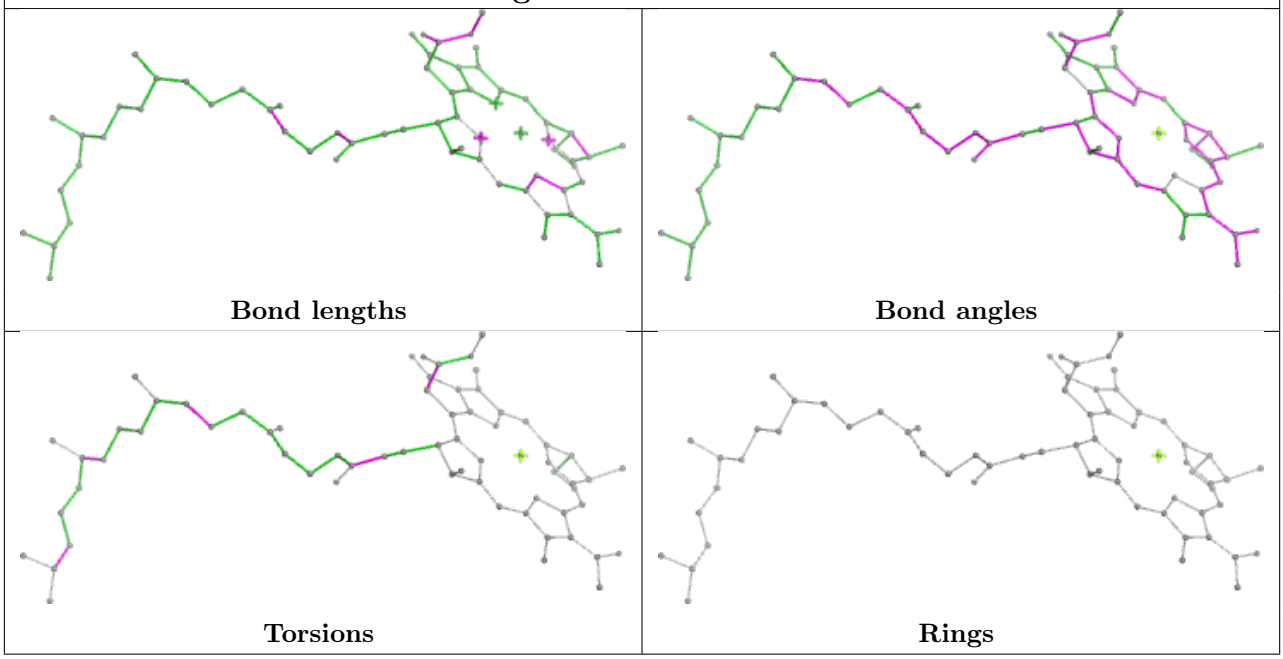
There are no ring outliers.

11 monomers are involved in 62 short contacts:

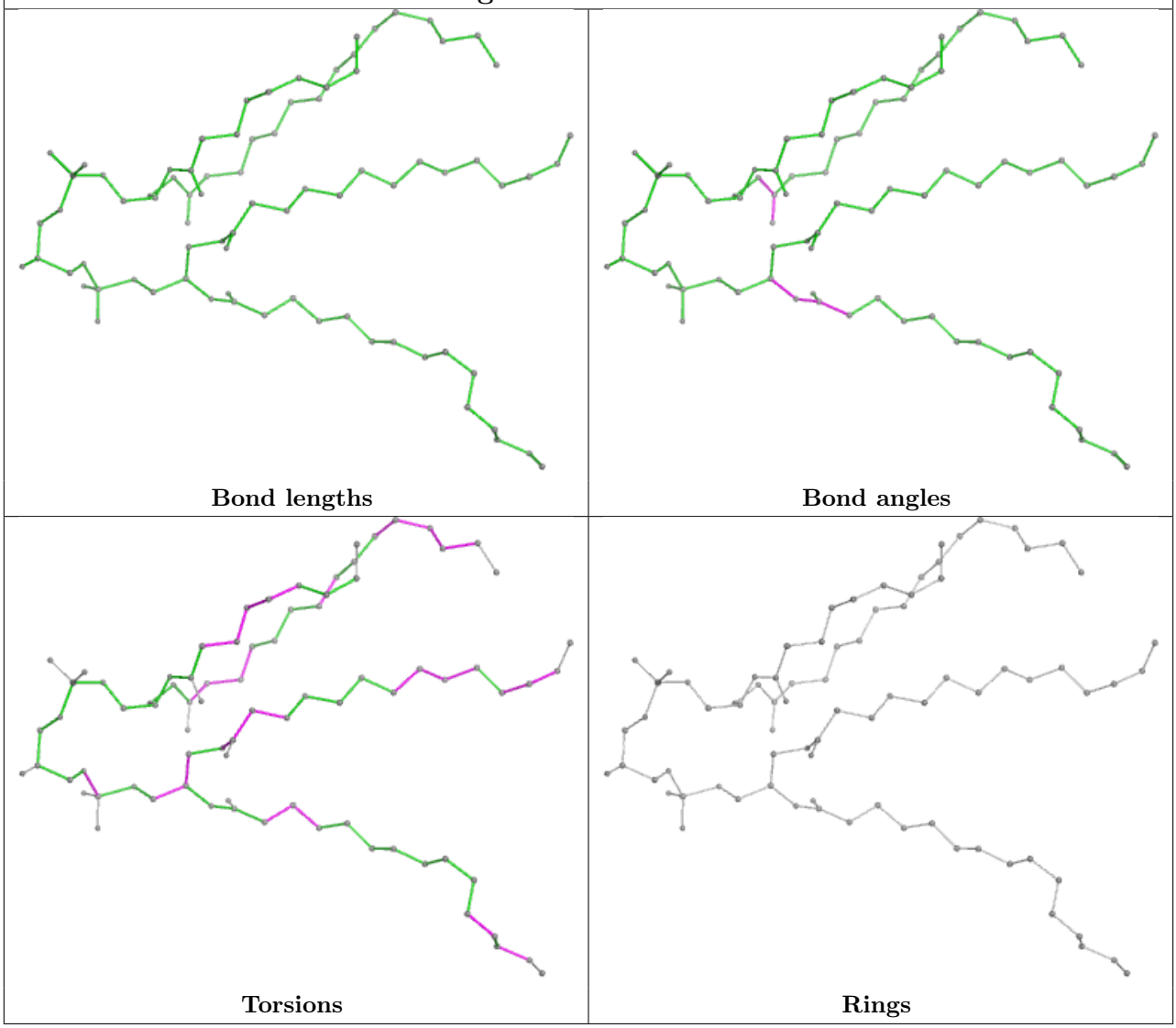
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	1303	BCL	6	0
10	M	800	CDL	16	0
6	L	401	BPH	10	0
6	M	402	BPH	3	0
5	M	1301	BCL	5	0
9	M	600	SPN	5	0
5	L	1304	BCL	8	0
4	M	702	LDA	3	0
7	L	501	U10	1	0
4	M	703	LDA	2	0
5	L	1302	BCL	9	0

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.

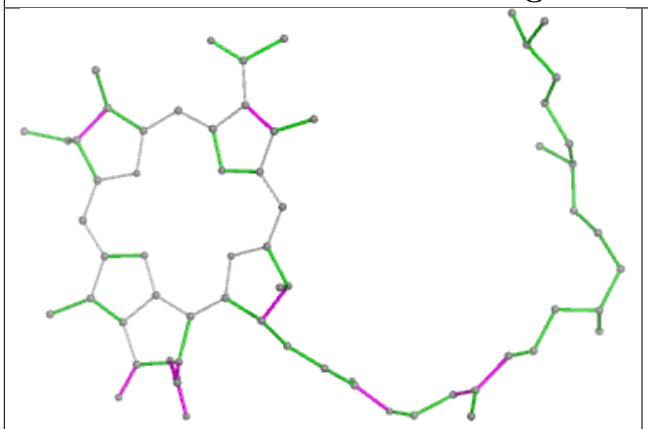
Ligand BCL M 1303



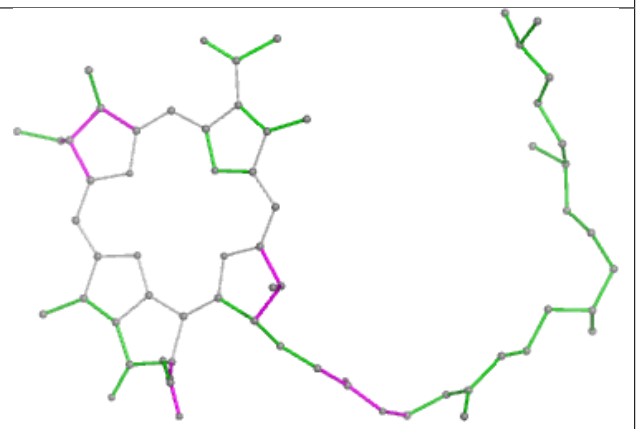
Ligand CDL M 800



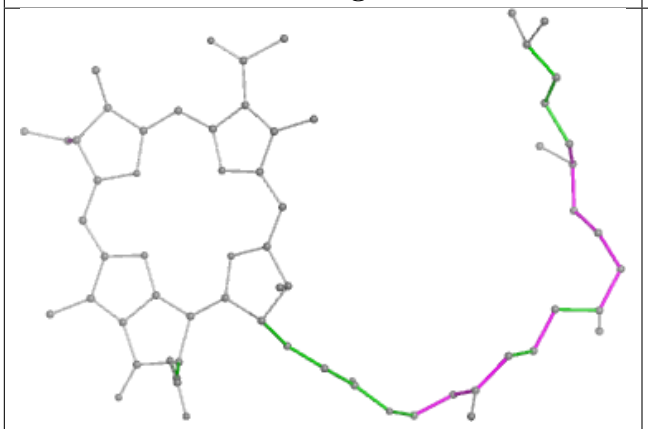
Ligand BPH L 401



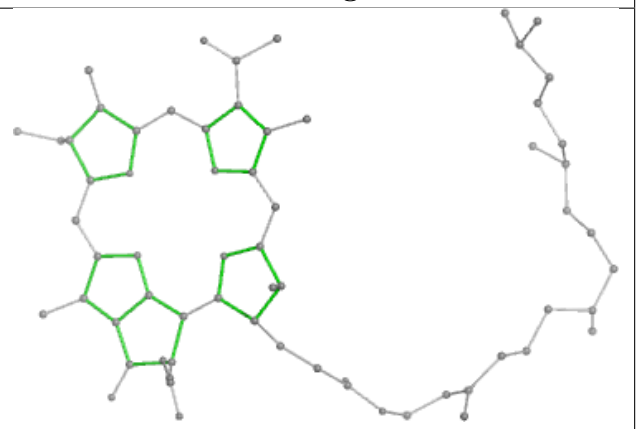
Bond lengths



Bond angles

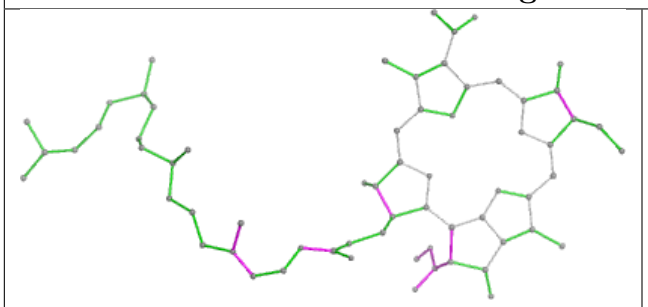


Torsions

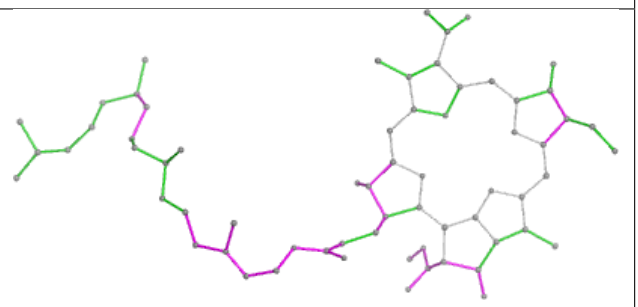


Rings

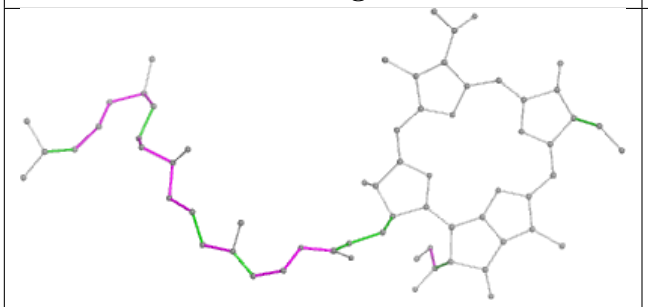
Ligand BPH M 402



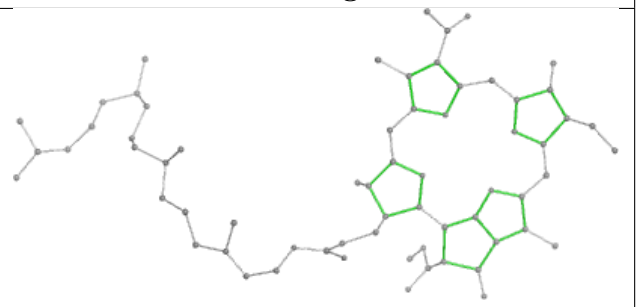
Bond lengths



Bond angles

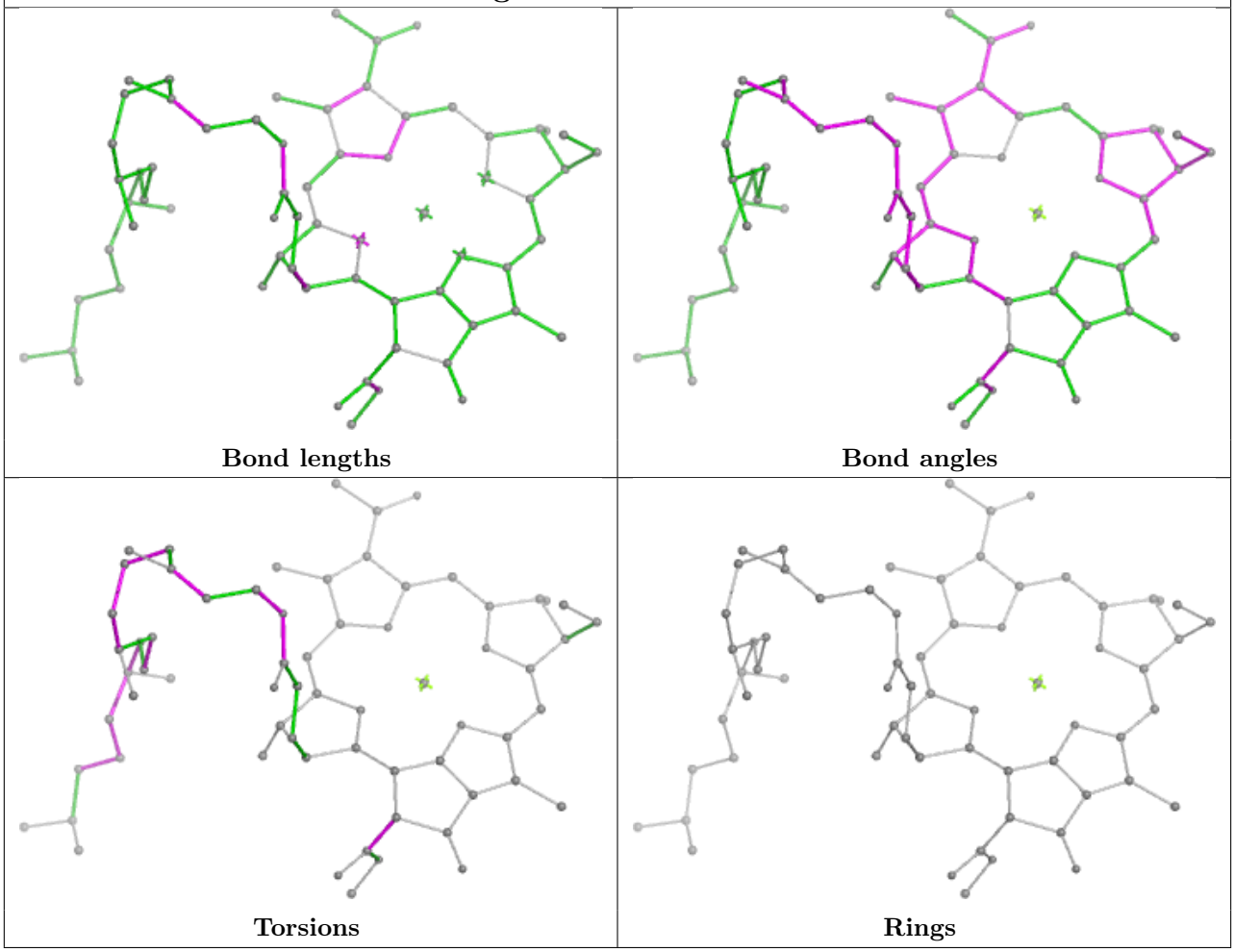


Torsions

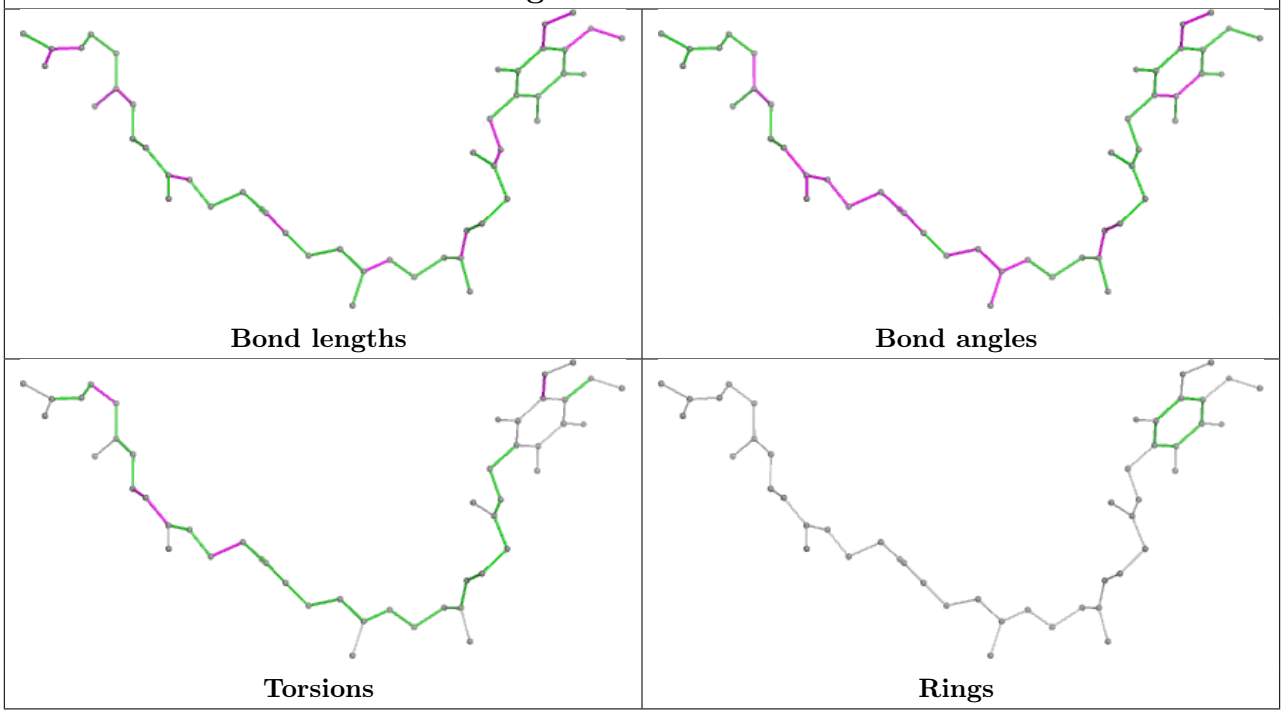


Rings

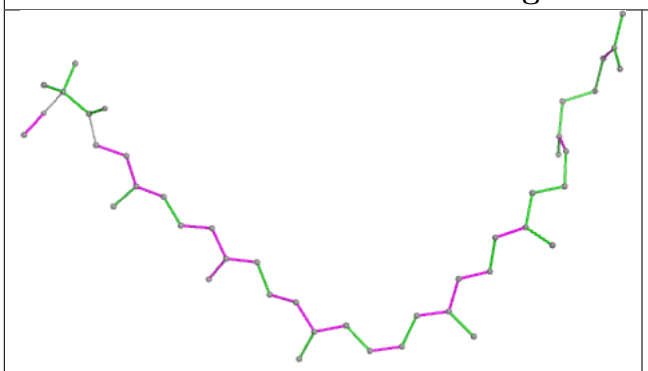
Ligand BCL M 1301



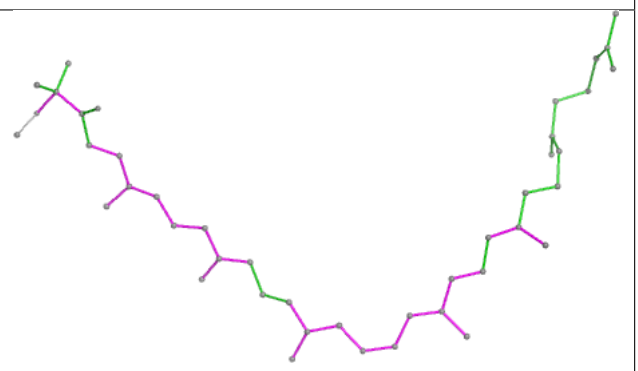
Ligand U10 M 502



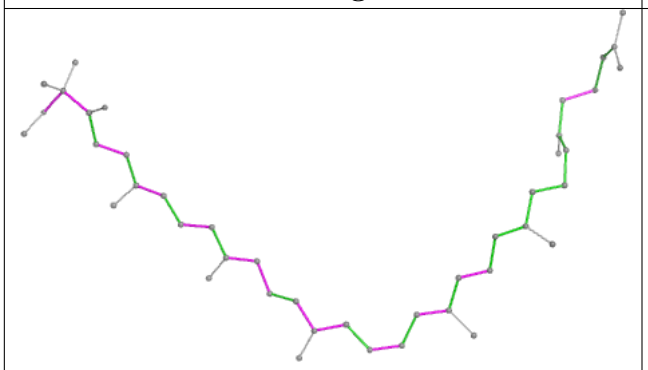
Ligand SPN M 600



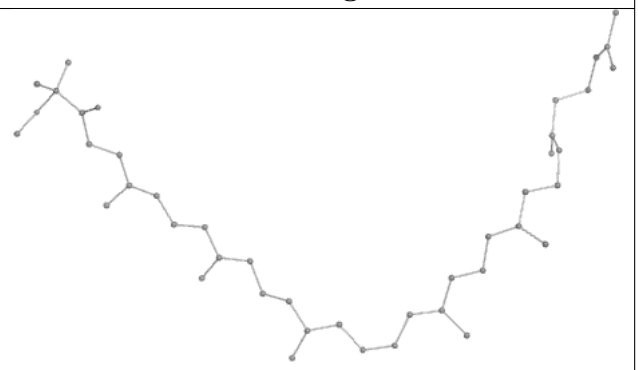
Bond lengths



Bond angles

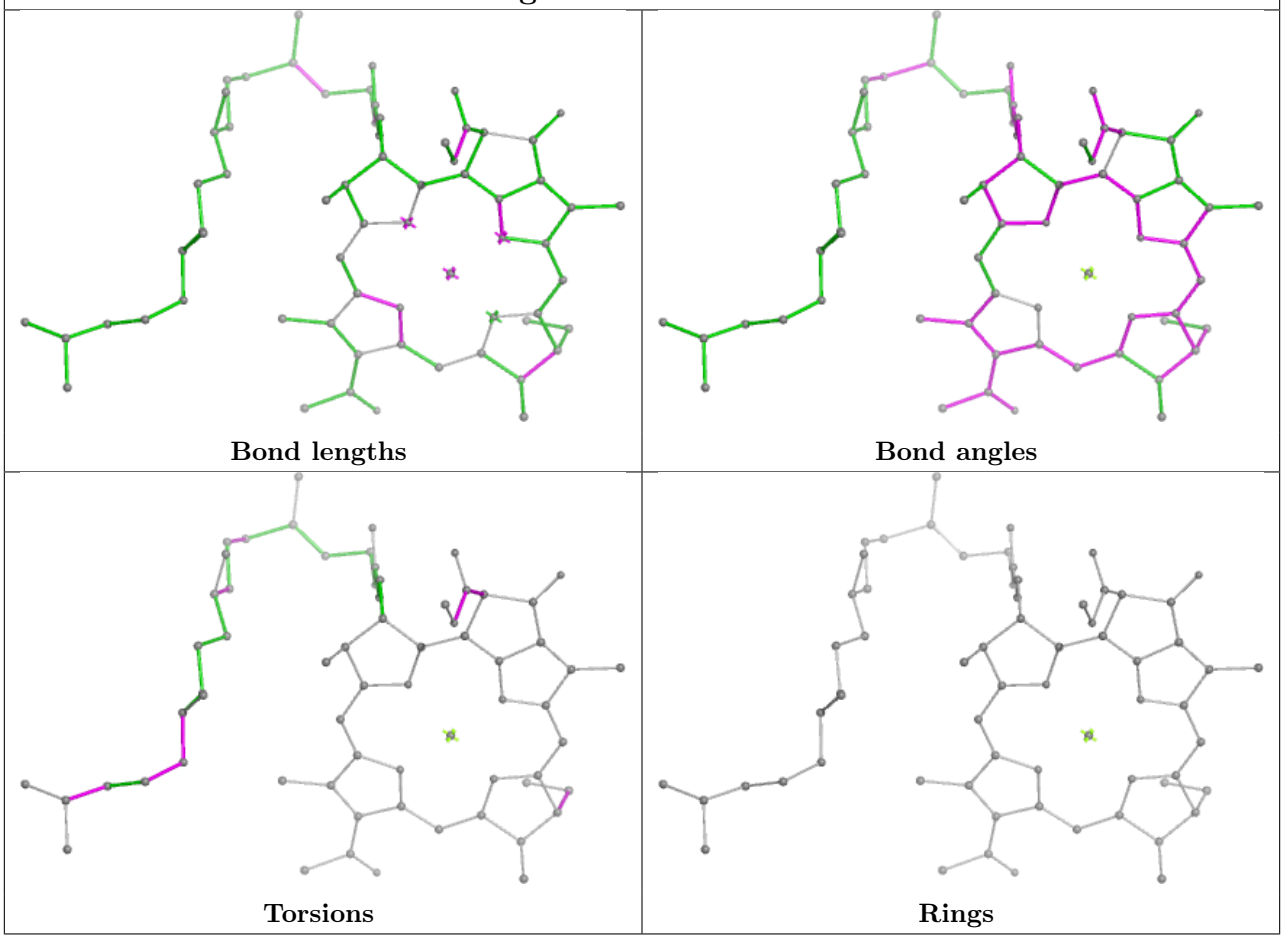


Torsions



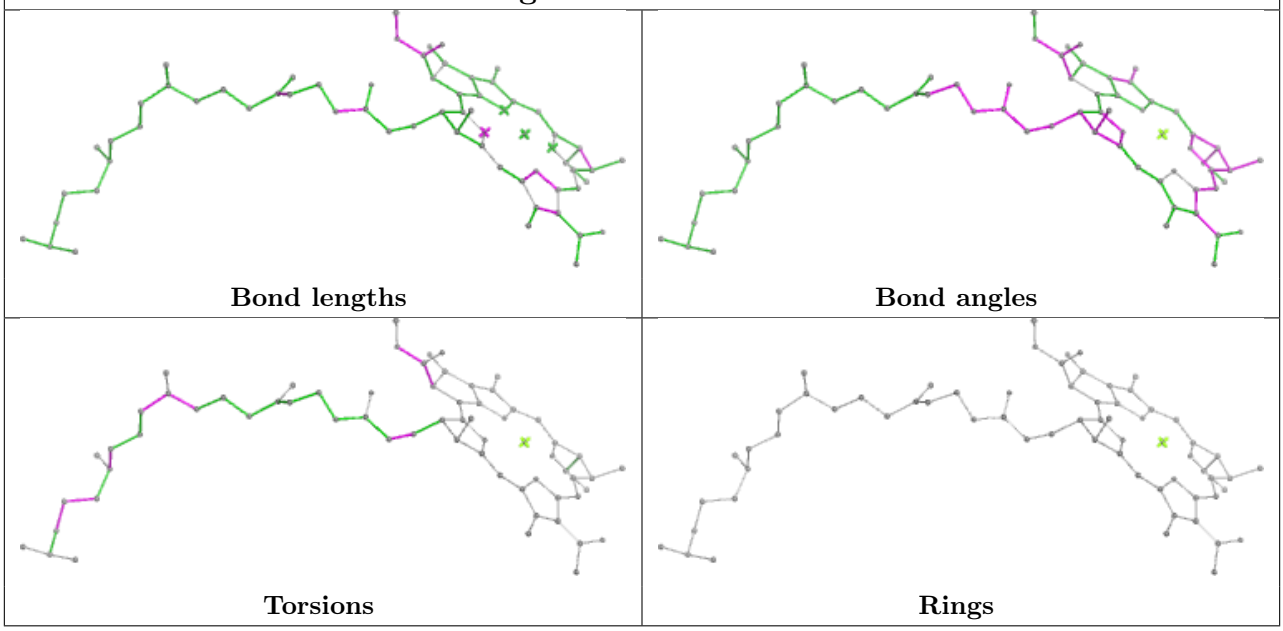
Rings

Ligand BCL L 1304



Ligand U10 L 501

Ligand BCL L 1302



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.