wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 02:30 pm BST

PDB ID	:	1UMX
Title	:	PHOTOSYNTHETIC REACTION CENTER MUTANT WITH ARG M267 REPLACED WITH LEU (CHAIN M, R267L)
Authors	:	Fyfe, P.K.; Isaacs, N.W.; Cogdell, R.J.; Jones, M.R.
Deposited on	:	2003-09-02
Resolution	:	2.80 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:

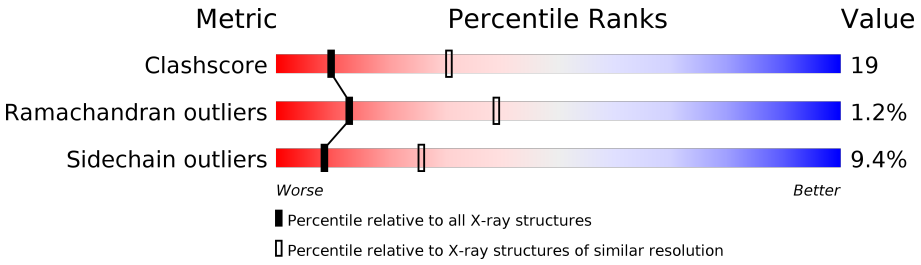
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 on 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% 30% 5% 7%
2	L	281	61% 32% 7%
3	M	307	67% 27% • •

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7007 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called REACTION CENTER PROTEIN H CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	241	Total	C	N	O	S	14	0	1
			1830	1169	315	337	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	10	0	0
			2232	1507	355	362	8			

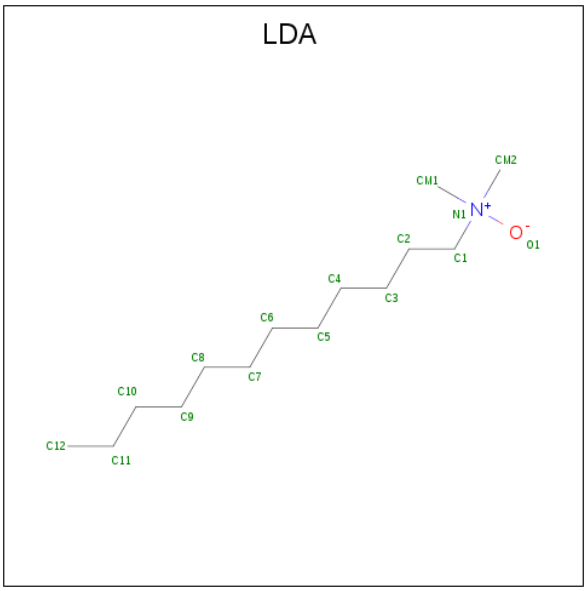
- Molecule 3 is a protein called REACTION CENTER PROTEIN M CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2406	1607	392	397	10			

There is a discrepancy between the modelled and reference sequences:

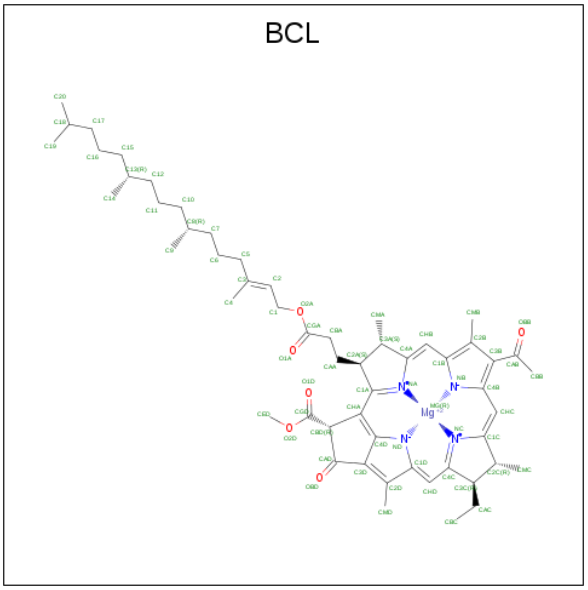
Chain	Residue	Modelled	Actual	Comment	Reference
M	267	LEU	ARG	engineered mutation	UNP P02953

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



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

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



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

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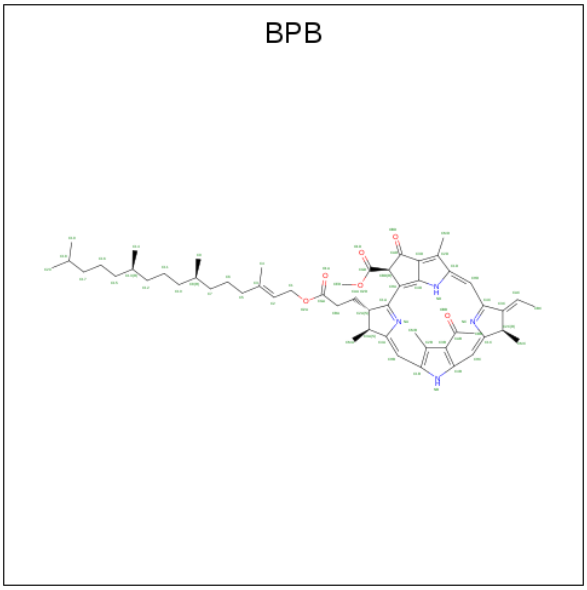
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 6 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: $C_{55}H_{74}N_4O_6$).

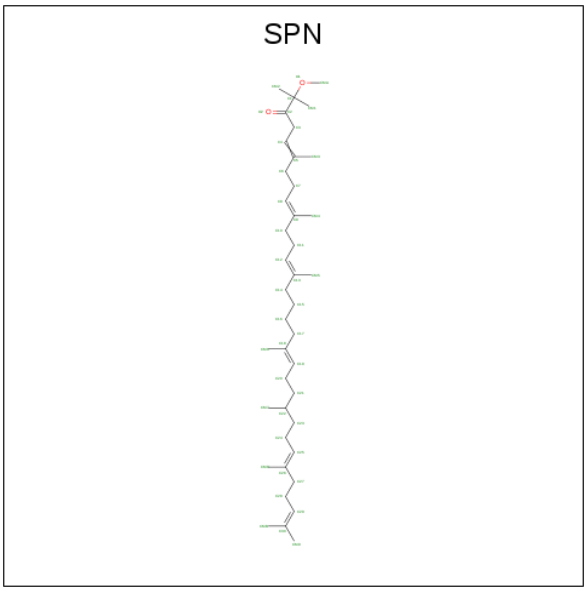


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			65	55	4	6		
6	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 7 is FE (III) ION (three-letter code: FE) (formula: Fe).

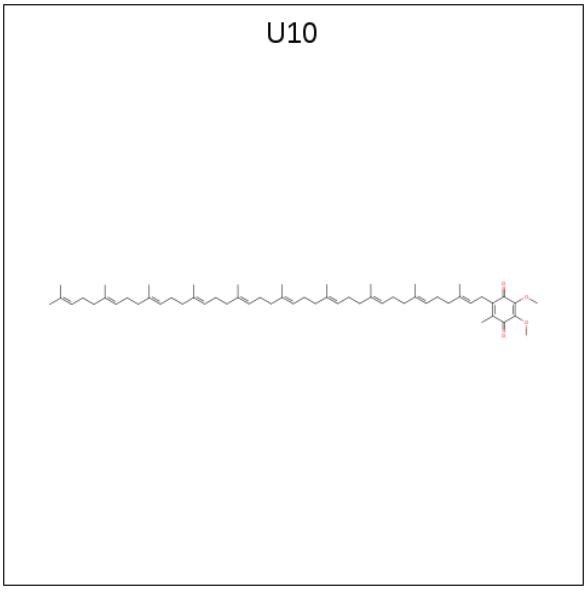
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total	Fe	0	0
			1	1		

- Molecule 8 is SPEROIDENONE (three-letter code: SPN) (formula: $C_{41}H_{70}O_2$).



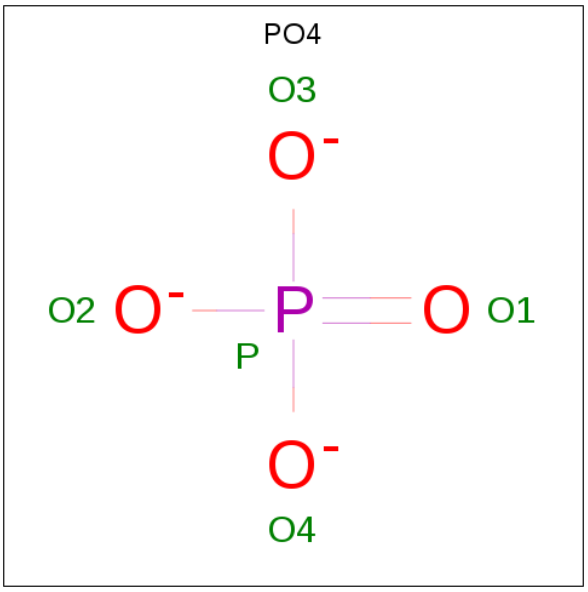
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			43	41	2		

- Molecule 9 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



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

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	H	6	Total O 6 6	0	0
11	L	6	Total O 6 6	0	0
11	M	4	Total O 4 4	0	0

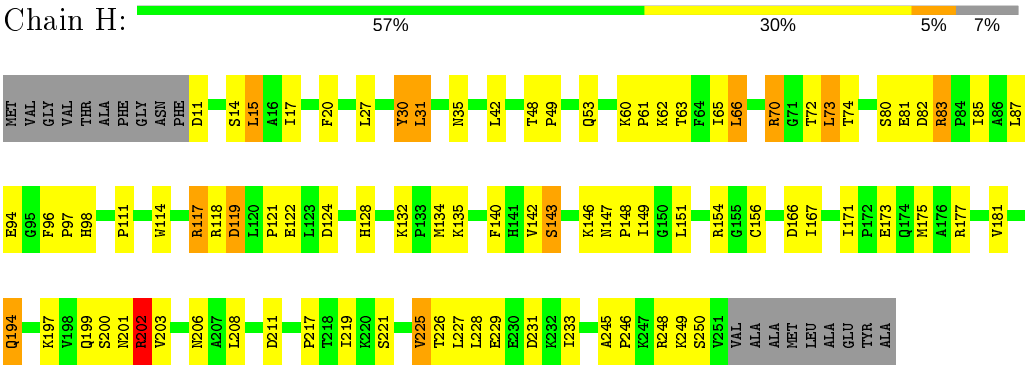
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

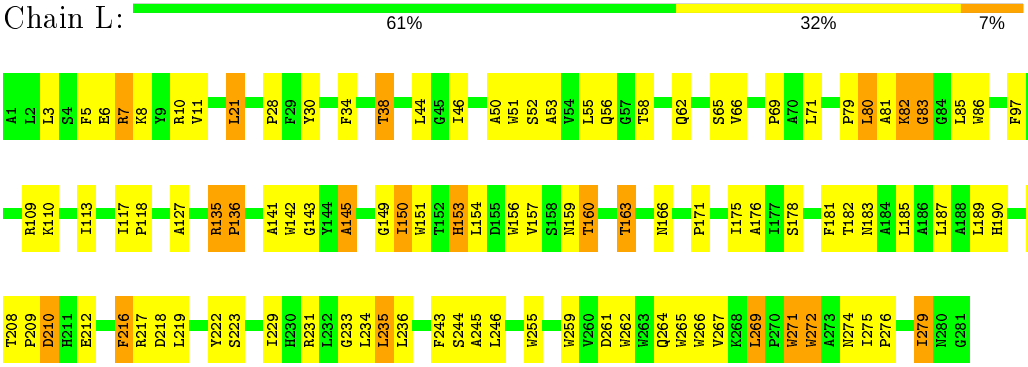
- Molecule 1: REACTION CENTER PROTEIN H CHAIN

Chain H:



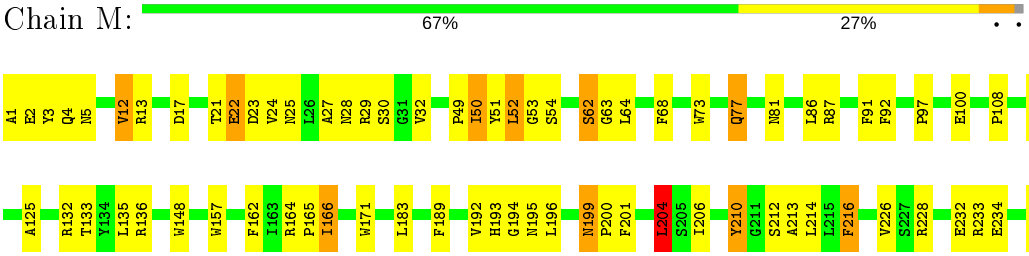
- Molecule 2: REACTION CENTER PROTEIN L CHAIN

Chain L:



- Molecule 3: REACTION CENTER PROTEIN M CHAIN

Chain M:




T243
E246
R247
R253
W254
T255
A260
T261
G264
I265
H266
L275
L278
T279
G280
W297
N300
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	141.64Å 141.64Å 187.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.00 – 2.80	Depositor
% Data completeness (in resolution range)	97.5 (29.00-2.80)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.224 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7007	wwPDB-VP
Average B, all atoms (Å^2)	44.0	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, LDA, BPB, PO4, FE, SPN, U10

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	1.09	0/1878	1.34	18/2555 (0.7%)
2	L	1.29	3/2320 (0.1%)	1.15	13/3175 (0.4%)
3	M	0.98	0/2498	1.09	8/3412 (0.2%)
All	All	1.13	3/6696 (0.0%)	1.18	39/9142 (0.4%)

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	1	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	202	LYS	CD-CE	30.62	2.27	1.51
2	L	202	LYS	CG-CD	-24.89	0.67	1.52
2	L	5	PHE	CD2-CE2	5.88	1.51	1.39

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	202	LYS	CB-CG-CD	-17.59	65.86	111.60
1	H	31	LEU	N-CA-C	-15.57	68.97	111.00
2	L	202	LYS	CD-CE-NZ	11.23	137.54	111.70
3	M	17	ASP	CB-CG-OD2	10.95	128.16	118.30
1	H	65	ILE	C-N-CA	9.02	144.24	121.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	H	66	LEU	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	30	TYR	Mainchain,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	H	1830	0	1836	64	0
2	L	2232	0	2187	92	0
3	M	2406	0	2319	98	0
4	H	16	0	31	4	0
4	M	16	0	31	5	0
5	L	132	0	148	11	0
5	M	132	0	148	28	0
6	L	65	0	74	5	0
6	M	65	0	74	11	0
7	M	1	0	0	0	0
8	M	43	0	69	8	0
9	M	48	0	63	2	0
10	M	5	0	0	0	0
11	H	6	0	0	1	0
11	L	6	0	0	1	0
11	M	4	0	0	0	0
All	All	7007	0	6980	268	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 19.

The worst 5 of 268 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)
5:M:1303:BCL:H51	6:M:1307:BPB:HMBB	1.25	1.12
3:M:50:ILE:HD13	3:M:51:TYR:N	1.67	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:1251:LDA:H121	4:M:1305:LDA:H91	1.14	1.07
3:M:50:ILE:HD13	3:M:51:TYR:H	1.16	1.07
2:L:272:TRP:HA	2:L:275:ILE:HD12	1.36	1.05

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%)	221 (92%)	14 (6%)	4 (2%)	9 29
2	L	279/281 (99%)	251 (90%)	26 (9%)	2 (1%)	22 53
3	M	301/307 (98%)	267 (89%)	30 (10%)	4 (1%)	12 36
All	All	819/848 (97%)	739 (90%)	70 (8%)	10 (1%)	13 39

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	250	SER
2	L	145	ALA
3	M	22	GLU
3	M	301	HIS
2	L	80	LEU

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%)	172 (88%)	23 (12%)	5 16
2	L	220/220 (100%)	198 (90%)	22 (10%)	7 22
3	M	236/240 (98%)	220 (93%)	16 (7%)	16 42
All	All	651/668 (98%)	590 (91%)	61 (9%)	8 26

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	46	ILE
2	L	163	THR
3	M	199	ASN
2	L	58	THR
2	L	136	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
3	M	4	GLN
3	M	11	GLN
3	M	193	HIS
2	L	280	ASN
3	M	77	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	LDA	M	1305	-	12,15,15	2.84	1 (8%)	14,17,17	1.70	3 (21%)
8	SPN	M	1308	-	40,42,42	3.76	15 (37%)	50,52,52	2.14	17 (34%)
5	BCL	M	1304	3	58,74,74	1.46	5 (8%)	69,115,115	1.86	16 (23%)
6	BPB	L	1284	-	64,70,70	1.57	7 (10%)	64,101,101	1.87	18 (28%)
6	BPB	M	1307	-	64,70,70	1.26	4 (6%)	64,101,101	2.26	20 (31%)
5	BCL	L	1283	2	58,74,74	1.39	6 (10%)	69,115,115	2.21	22 (31%)
4	LDA	H	1251	-	12,15,15	2.39	1 (8%)	14,17,17	3.26	3 (21%)
10	PO4	M	1310	-	4,4,4	0.79	0	6,6,6	0.80	0
5	BCL	L	1282	2	58,74,74	1.37	5 (8%)	69,115,115	1.71	19 (27%)
5	BCL	M	1303	3	58,74,74	1.33	5 (8%)	69,115,115	2.05	20 (28%)
9	U10	M	1309	-	48,48,63	1.63	3 (6%)	58,61,79	1.88	15 (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
4	LDA	M	1305	-	-	8/13/13/13	-
8	SPN	M	1308	-	-	20/50/51/51	-
5	BCL	M	1304	3	-	9/37/137/137	-
6	BPB	L	1284	-	-	11/47/105/105	0/5/6/6
6	BPB	M	1307	-	-	21/47/105/105	0/5/6/6
5	BCL	L	1283	2	-	7/37/137/137	-
4	LDA	H	1251	-	-	2/13/13/13	-
5	BCL	L	1282	2	-	8/37/137/137	-
5	BCL	M	1303	3	-	12/37/137/137	-
9	U10	M	1309	-	-	8/45/69/87	0/1/1/1

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	1305	LDA	O1-N1	-9.68	1.19	1.42
8	M	1308	SPN	C3-C4	-9.44	1.37	1.50
8	M	1308	SPN	C10-C9	-8.23	1.34	1.51
4	H	1251	LDA	O1-N1	-8.16	1.23	1.42
8	M	1308	SPN	C17-C18	-7.74	1.35	1.51

The worst 5 of 153 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	1307	BPB	C1-C2-C3	-8.34	111.62	126.04
4	H	1251	LDA	CM2-N1-C1	-7.97	93.50	110.23
4	H	1251	LDA	CM1-N1-C1	-7.59	94.28	110.23
6	M	1307	BPB	CBC-CAC-C3C	-6.67	107.21	126.72
5	L	1283	BCL	CHD-C4C-NC	6.27	132.04	125.08

There are no chirality outliers.

5 of 106 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	1305	LDA	C2-C1-N1-CM1
4	M	1305	LDA	N1-C1-C2-C3
8	M	1308	SPN	C20-C21-C22-CM7
5	M	1304	BCL	C2C-C3C-CAC-CBC
5	M	1304	BCL	C4C-C3C-CAC-CBC

There are no ring outliers.

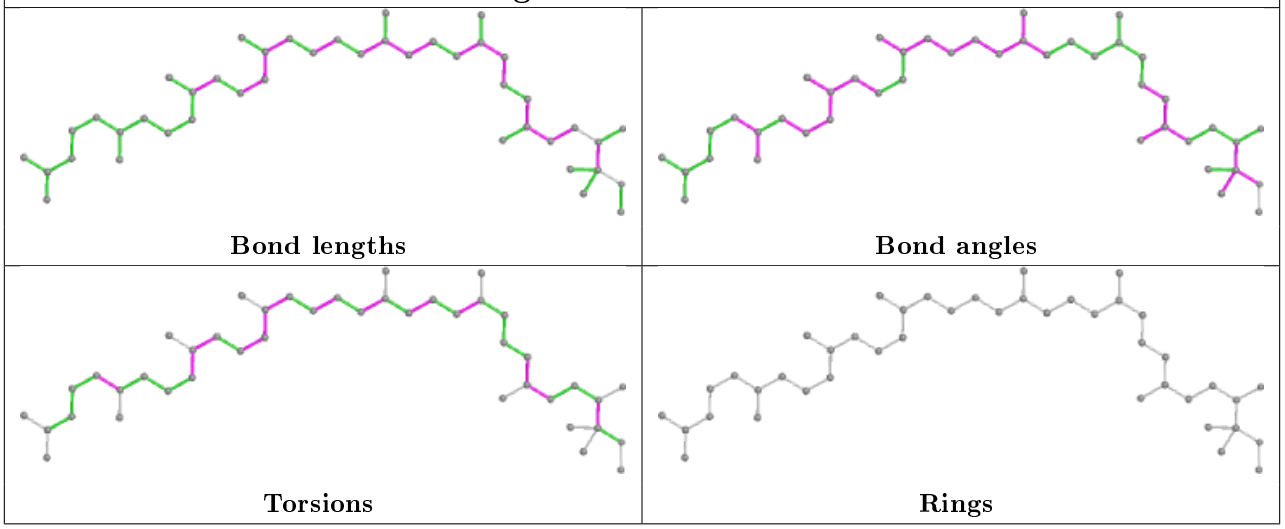
10 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	1305	LDA	5	0
8	M	1308	SPN	8	0
5	M	1304	BCL	15	0
6	L	1284	BPB	5	0
6	M	1307	BPB	11	0
5	L	1283	BCL	4	0
4	H	1251	LDA	4	0
5	L	1282	BCL	7	0
5	M	1303	BCL	18	0
9	M	1309	U10	2	0

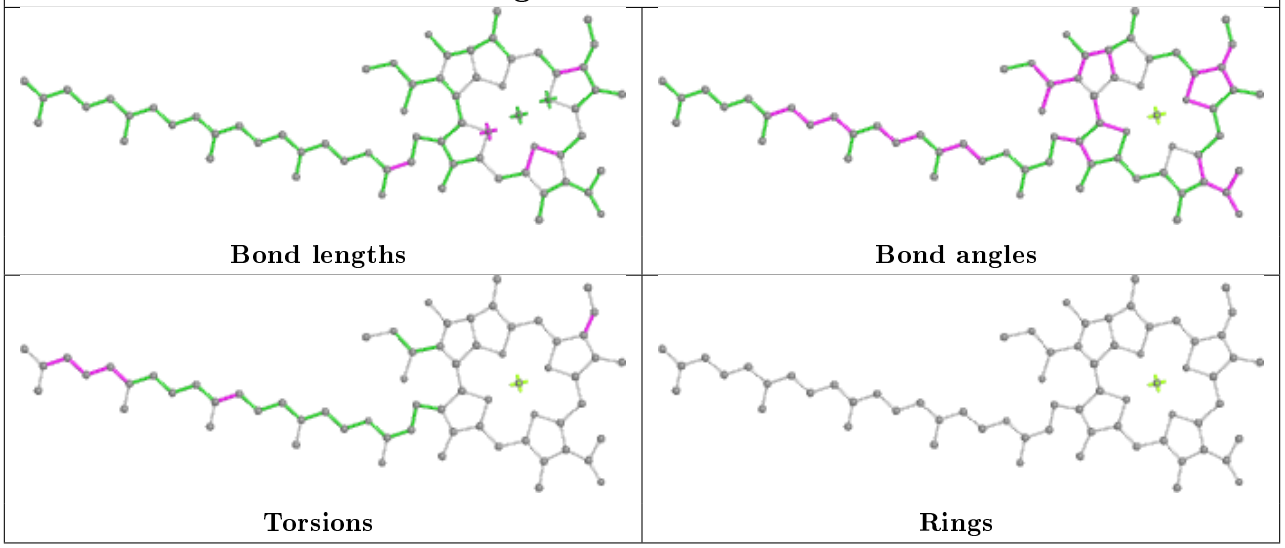
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

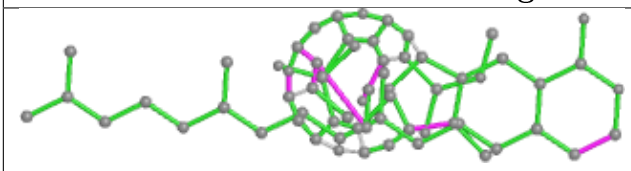
Ligand SPN M 1308



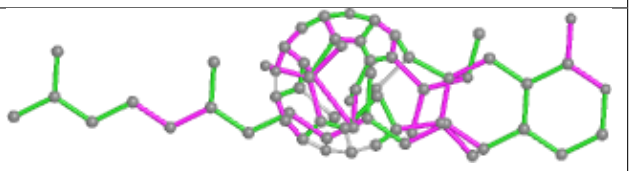
Ligand BCL M 1304



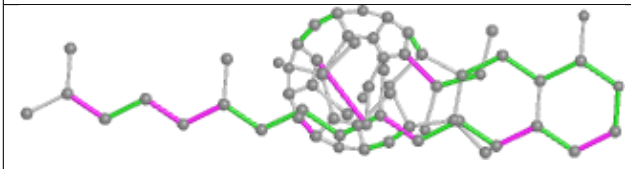
Ligand BPB L 1284



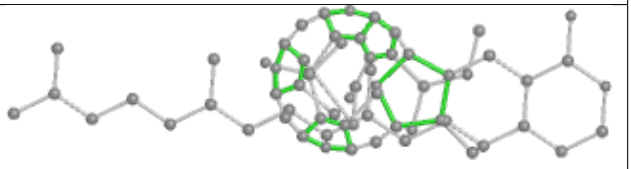
Bond lengths



Bond angles

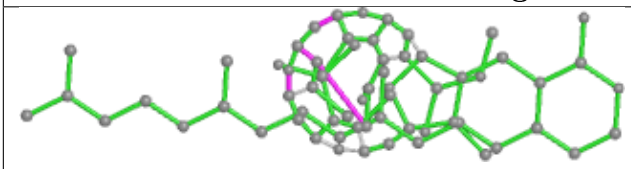


Torsions

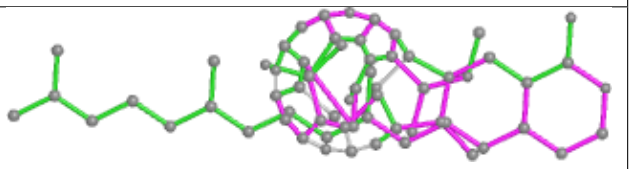


Rings

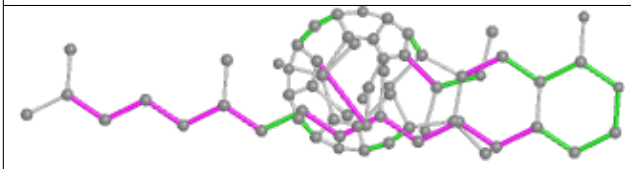
Ligand BPB M 1307



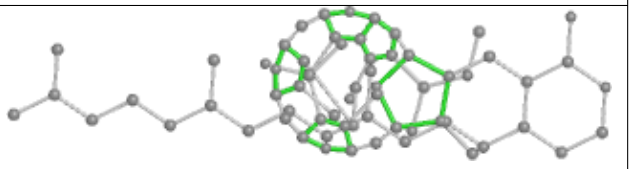
Bond lengths



Bond angles

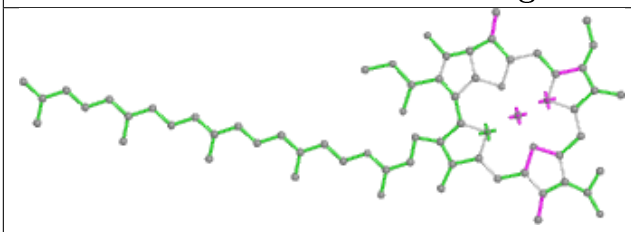


Torsions

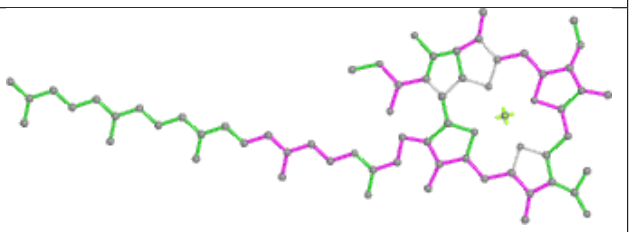


Rings

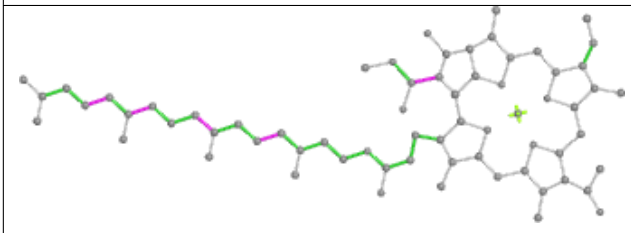
Ligand BCL L 1283



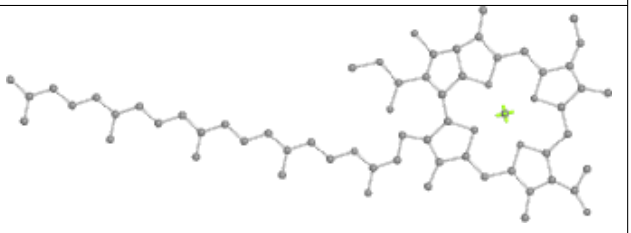
Bond lengths



Bond angles

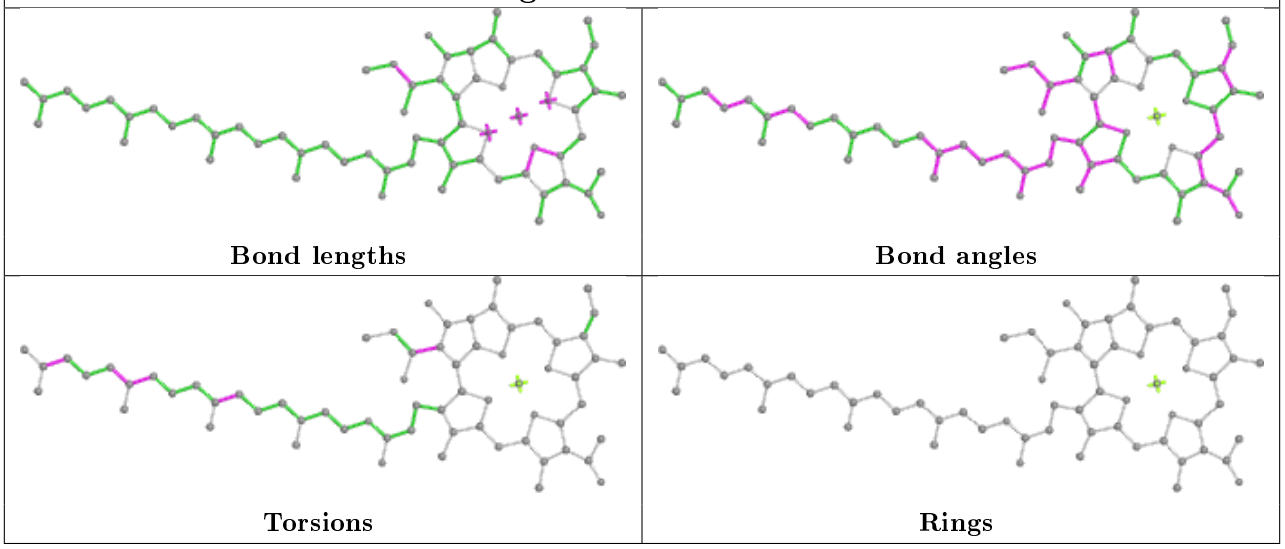


Torsions

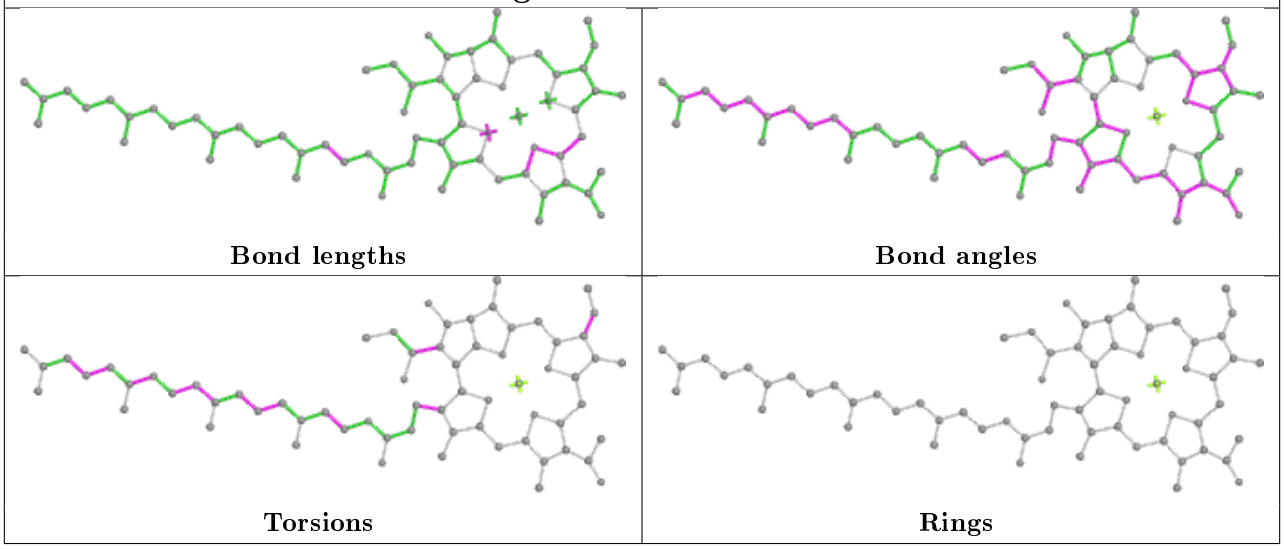


Rings

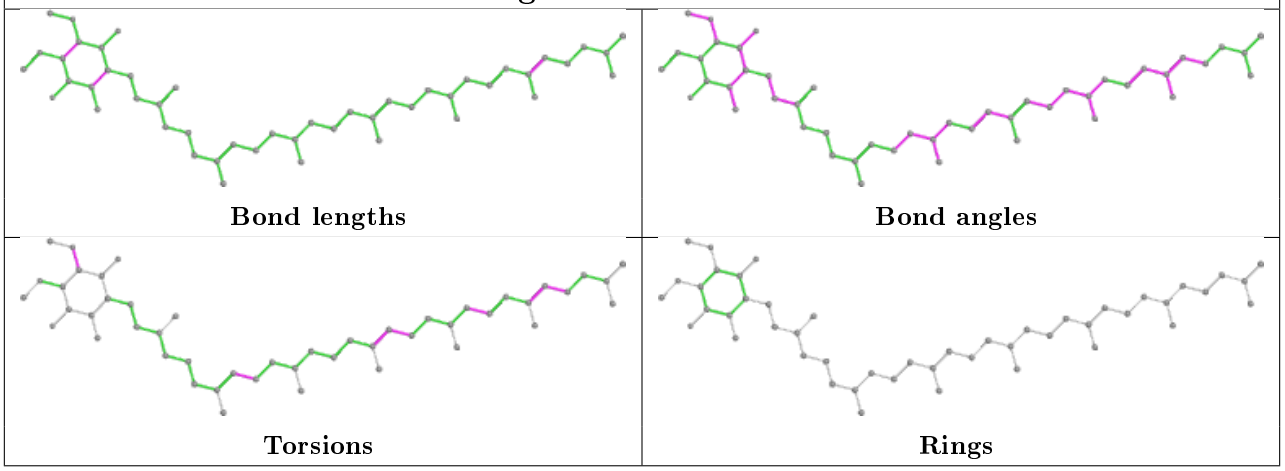
Ligand BCL L 1282



Ligand BCL M 1303



Ligand U10 M 1309



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.