

wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2020 – 07:11 am BST

PDB ID : 1E14

Title : PHOTOSYNTHETIC REACTION CENTER MUTANT WITH PHE M197

REPLACED WITH ARG (CHAIN M, FM197R) AND GLY M203 RE-

PLACED WITH ASP (CHAIN M, GM203D)

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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 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)

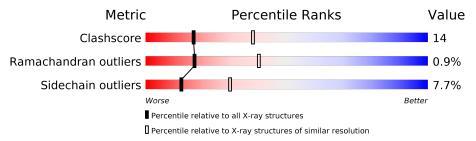
Validation Pipeline (wwPDB-VP) : 2.11

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 2.70 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	Similar resolution
Metric	$(\# { m Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$
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 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 cl	hain	
1	Н	260	57%	29%	5% • 7%
2	L	281	71%	25%	
3	М	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:

	\mathbf{Mol}	Type	Chain	${ m Res}$	Chirality	$\mathbf{Geometry}$	Clashes	Electron density
Ī	5	BCL	M	1301	X	-	=	-
	6	ВРН	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		\mathbf{At}	oms			ZeroOcc	AltConf	Trace
1	Н	241	Total 1830	C 1169	N 315	O 337	S 9	0	0	1

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

\mathbf{Mol}	Chain	Residues		\mathbf{At}	oms			ZeroOcc	AltConf	Trace	
2	L	281	Total 2232	C 1507	N 355	O 362	S 8	0	0	0	

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

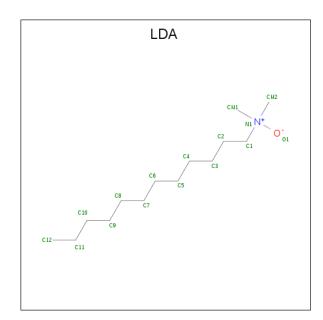
Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
3	М	303	Total 2413	C 1606	N 398	O 399	S 10	0	0	1

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

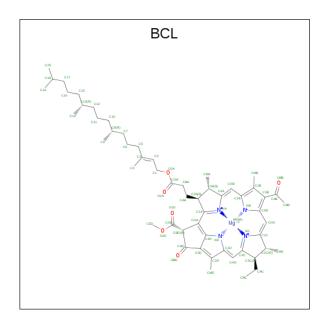
• Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
1	Н	1	Total C N O	0	0	
4	11	1	16 14 1 1	U	0	
4	М	1	Total C N O	0	0	
4	1V1	1	16 14 1 1	0	0	
4	М	1	Total C N O	0	0	
4	1V1	1	16 14 1 1	0	U	

 $\bullet \ \ \mathrm{Molecule} \ 5 \ \mathrm{is} \ \mathrm{BACTERIOCHLOROPHYLL} \ \mathrm{A} \ (\mathrm{three-letter} \ \mathrm{code} \colon \ \mathrm{BCL}) \ (\mathrm{formula} \colon \ \mathrm{C}_{55} \mathrm{H}_{74} \mathrm{MgN}_4 \mathrm{O}_6).$



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf
5	Т	1	Total	С	Mg	Ν	О	0	0
5	L	1	66	55	1	4	6	U	0

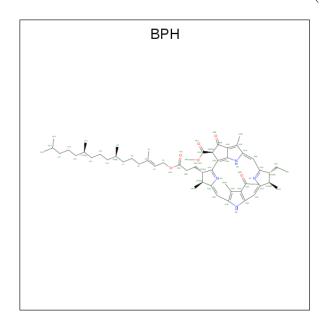
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Mol	Chain	Residues		$\mathbf{A}\mathbf{t}$	$\overline{\mathrm{oms}}$			ZeroOcc	AltConf	
5	T.	1	Total	С	Mg	N	О	0	0	
	L	1	66	55	1	4	6	U		
5	M	1	Total	С	Mg	Ν	Ο	0	0	
0	101	1	66	55	1	4	6	0	0	
5	M	1	Total	С	Mg	N	О	0	0	
3	1V1	1	66	55	1	4	6	U		

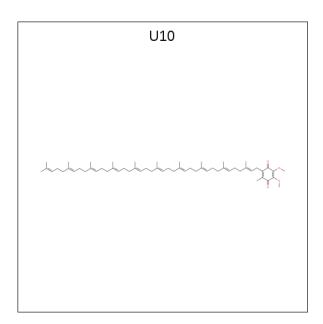
 $\bullet \ \ Molecule\ 6 \ is\ BACTERIOPHEOPHYTIN\ A\ (three-letter\ code:\ BPH)\ (formula:\ C_{55}H_{76}N_4O_6).$



I	Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
	6	L	1	Total C N O 65 55 4 6	0	0
	6	M	1	Total C N O 65 55 4 6	0	0

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



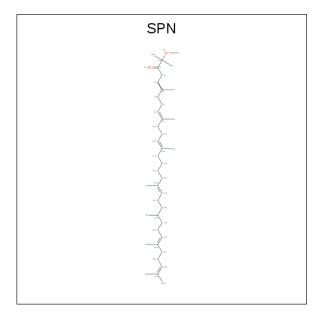


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C O 48 44 4	22	0
7	M	1	Total C O 48 44 4	0	0

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

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

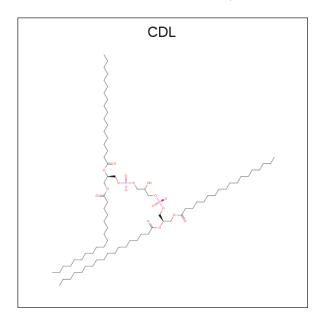
 \bullet Molecule 9 is SPEROIDENONE (three-letter code: SPN) (formula: $\mathrm{C_{41}H_{70}O_2}).$





Mol	Chain	Residues	${f Atoms}$		ZeroOcc	AltConf	
9	М	1	Total 43	C 41	O 2	0	0

 \bullet Molecule 10 is CARDIOLIPIN (three-letter code: CDL) (formula: $\mathrm{C_{81}H_{156}O_{17}P_2}).$



\mathbf{N}	Iol	Chain	Residues	Atoms		ZeroOcc	AltConf		
_	10	М	1	Total	С	О	Р	0	0
-	LU	1V1	1	81	62	17	2	0	0

• Molecule 11 is water.

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

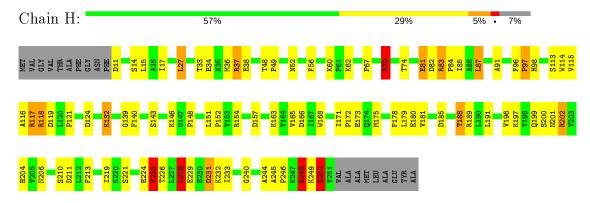


3 Residue-property plots (i)

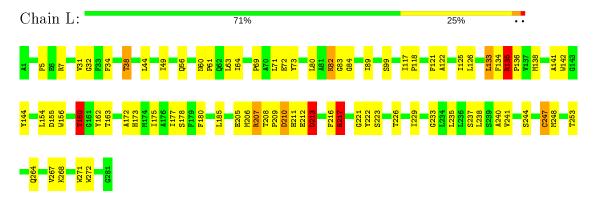
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

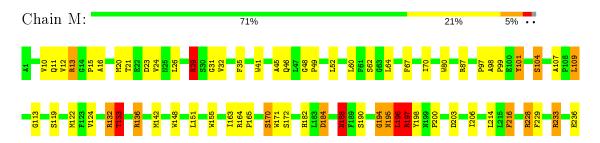
• Molecule 1: Reaction center protein H chain



• Molecule 2: Reaction center protein L chain



• Molecule 3: Reaction center protein M chain









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	140.00Å 140.00Å 184.60Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 - 2.70	Depositor
% Data completeness	92.6 (30.00-2.70)	Depositor
(in resolution range)	32.0 (30.00 2.10)	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: BCL, LDA, CDL, BPH, 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	\mathbf{B}_{0}	ond angles
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z > 5
1	Н	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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Н	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	${f Res}$	Type	${f Atoms}$	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
1	Н	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	Н	113	SER	Mainchain
1	Н	114	TRP	Mainchain
1	Н	115	VAL	Mainchain
1	Н	87	LEU	Mainchain
1	Н	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	Н	1830	0	1836	61	0
2	L	2232	0	2187	59	0
3	M	2413	0	2326	58	0
4	Н	16	0	31	0	0
4	Μ	32	0	62	5	0
5	L	132	0	148	15	0
5	Μ	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	Μ	48	0	63	0	0
8	Μ	1	0	0	0	0
9	Μ	43	0	69	5	0
10	Μ	81	0	106	16	0
11	Н	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	$egin{array}{ll} ext{Interatomic} \ ext{distance } (ext{Å}) \end{array}$	Clash overlap (Å)
10:M:800:CDL:CA6	10:M:800:CDL:HB4	1.62	1.28
10:M:800:CDL:HA61	10:M:800:CDL:HB4	1.10	1.10

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Atom-1	Atom-2	$egin{array}{c} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{array}$	$egin{array}{c} ext{Clash} \ ext{overlap } (ext{Å}) \end{array}$
10:M:800:CDL:CB4	10:M:800:CDL:HA61	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	Perce	entiles
1	Н	$239/260 \ (92\%)$	224 (94%)	13 (5%)	2 (1%)	19	43
2	L	279/281 (99%)	262 (94%)	17 (6%)	0	100	100
3	М	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	Н	250	SER
1	Н	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	Н	195/208~(94%)	182 (93%)	13 (7%)	16	37	
2	L	220/220 (100%)	199 (90%)	21 (10%)	8	20	
3	М	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	185	LEU
2	L	217	ARG
3	M	197	ARG
2	L	205	GLU
2	L	210	ASP

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

Mol	Chain	Res	Type
1	Н	98	HIS
1	Н	126	HIS
1	Н	199	GLN
1	Н	204	HIS
1	Н	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 carbohydrates 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).

Mal	T	Chain	Dog	Link	В	ond leng	$_{ m gths}$	Во	ond angl	es
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LDA	M	703	-	12,15,15	2.42	1 (8%)	14,17,17	0.81	1 (7%)
4	LDA	M	702	-	12,15,15	2.45	1 (8%)	14,17,17	0.85	1 (7%)
5	BCL	M	1303	3	58,74,74	1.64	11 (18%)	69,115,115	1.97	23 (33%)
5	BCL	L	1304	2	58,74,74	1.60	7 (12%)	69,115,115	2.96	23 (33%)
10	CDL	M	800	-	80,80,99	0.50	0	86,92,111	0.90	3 (3%)
9	SPN	M	600	-	40,42,42	3.79	18 (45%)	50,52,52	2.93	19 (38%)
7	U10	M	502	-	48,48,63	1.79	14 (29%)	58,61,79	1.51	13 (22%)
5	BCL	M	1301	3	58,74,74	1.61	8 (13%)	69,115,115	2.48	27 (39%)
6	BPH	M	402	-	64,70,70	1.22	7 (10%)	76,101,101	2.58	25 (32%)
4	LDA	Н	701	-	12,15,15	2.46	1 (8%)	14,17,17	0.79	1 (7%)
7	U10	L	501	-	47,47,63	2.03	13 (27%)	54,58,79	2.66	21 (38%)
5	BCL	L	1302	2	58,74,74	1.66	10 (17%)	69,115,115	2.36	22 (31%)
6	ВРН	L	401	-	64,70,70	1.40	7 (10%)	76,101,101	2.46	21 (27%)

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	$\mathbf{Chirals}$	Torsions	Rings
4	LDA	M	703	-	-	8/13/13/13	-
4	LDA	M	702	-	-	12/13/13/13	-
5	BCL	M	1303	3	-	6/37/137/137	-
5	BCL	L	1304	2	-	9/37/137/137	-
10	CDL	M	800	-	-	35/91/91/110	_
9	SPN	M	600	-	-	18/50/51/51	_
7	U10	M	502	-	-	6/45/69/87	0/1/1/1
5	BCL	M	1301	3	1/1/21/25	17/37/137/137	_
6	BPH	M	402	-	-	22/54/105/105	0/5/6/6
4	LDA	Н	701	-	-	12/13/13/13	_

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Mol	Type	Chain	${f Res}$	Link	${ m Chirals}$	Torsions	Rings
7	U10	L	501	-	-	15/41/65/87	0/1/1/1
5	BCL	L	1302	2	-	9/37/137/137	-
6	BPH	L	401	-	2/2/18/22	15/54/105/105	0/5/6/6

The worst 5 of 98 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(A)
9	Μ	600	SPN	C4-C5	8.89	1.54	1.33
9	M	600	SPN	C8-C9	8.50	1.53	1.33
4	Н	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 200 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
6	L	401	ВРН	O2D-CGD-CBD	13.31	134.91	111.27
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
6	M	402	ВРН	O2D-CGD-CBD	9.94	128.94	111.27
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	ВРН	C8
6	L	401	BPH	C13

5 of 184 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	703	LDA	C2-C1-N1-O1
4	M	703	LDA	C2-C1-N1-CM1
4	M	703	LDA	C2-C1-N1-CM2
4	M	702	LDA	C2-C1-N1-O1
4	M	702	LDA	C2-C1-N1-CM1

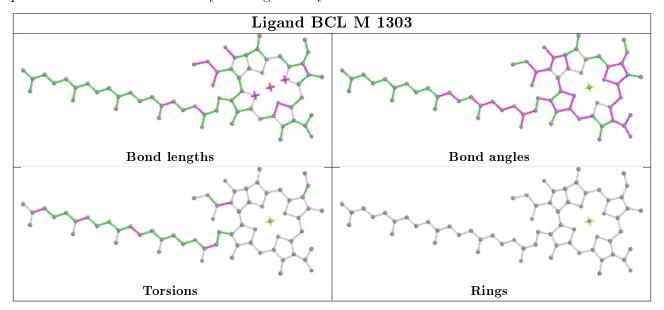
There are no ring outliers.

11 monomers are involved in 62 short contacts:

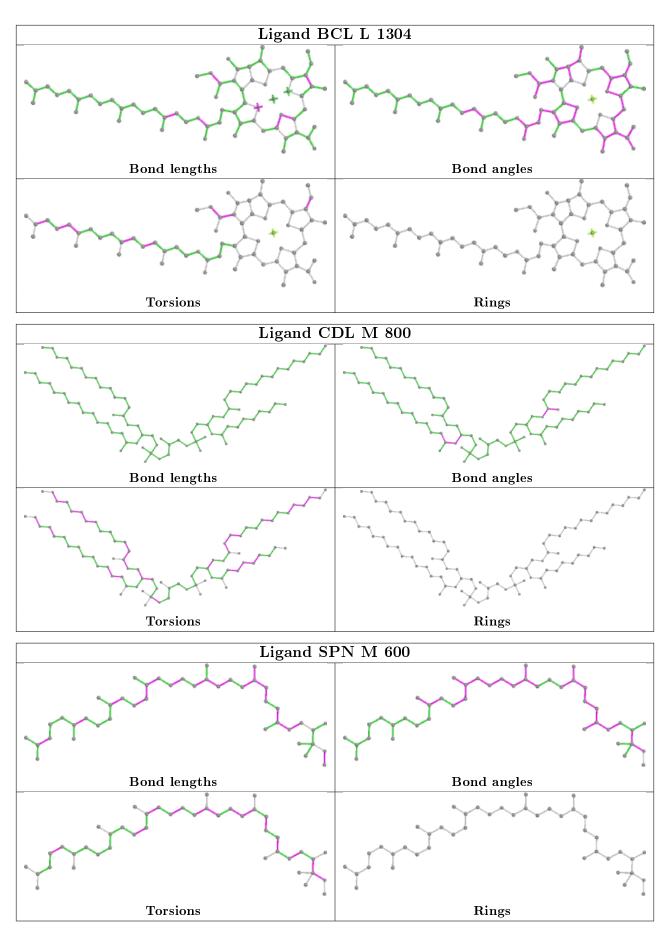


Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	703	LDA	2	0
4	M	702	LDA	3	0
5	M	1303	BCL	6	0
5	L	1304	BCL	8	0
10	M	800	CDL	16	0
9	M	600	SPN	5	0
5	M	1301	BCL	5	0
6	M	402	ВРН	3	0
7	L	501	U10	1	0
5	L	1302	BCL	9	0
6	L	401	BPH	10	0

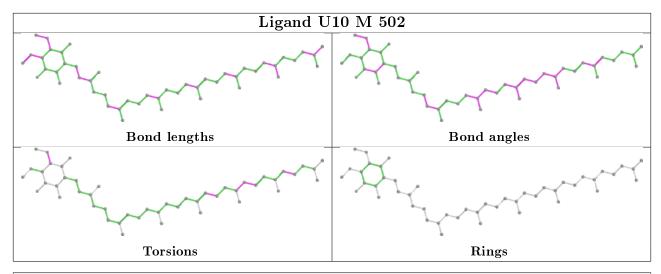
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

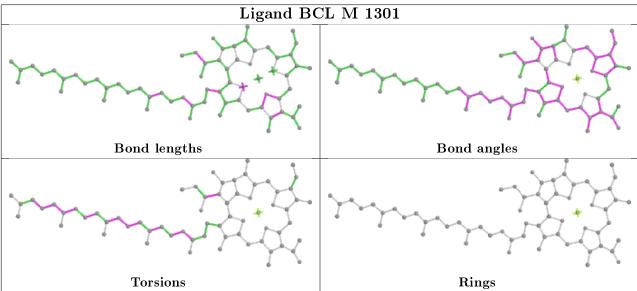




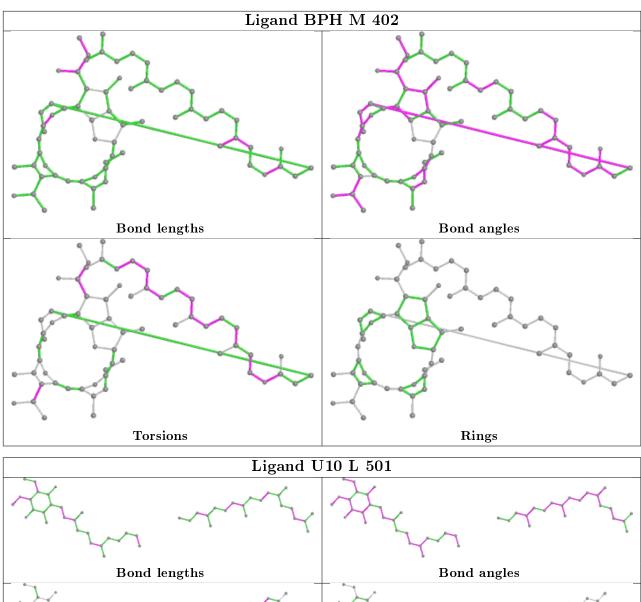


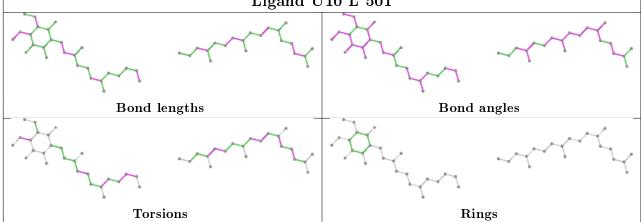




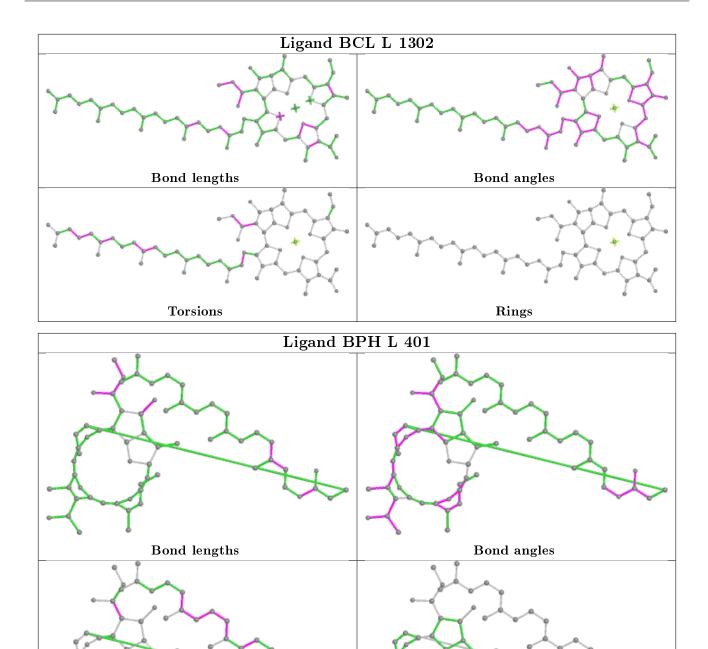


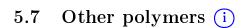












There are no such residues in this entry.

Torsions



Rings

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.

