Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2023 – 03:59 AM EDT

PDB ID	:	1C3W
Title	:	BACTERIORHODOPSIN/LIPID COMPLEX AT 1.55 A RESOLUTION
Authors	:	Luecke, H.
Deposited on	:	1999-07-28
Resolution	:	1.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

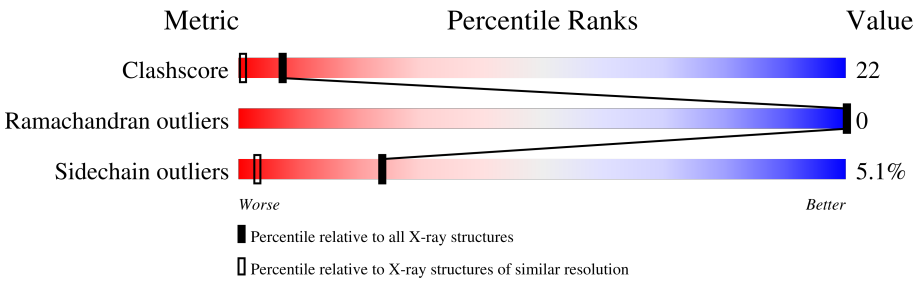
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 1.55 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	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)

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	A	222	67% 29% .

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
2	LI1	A	601	X	-	-	-
2	LI1	A	611	X	-	-	-
2	LI1	A	613	X	-	-	-
3	SQU	A	701	-	X	-	-

2 Entry composition (i)

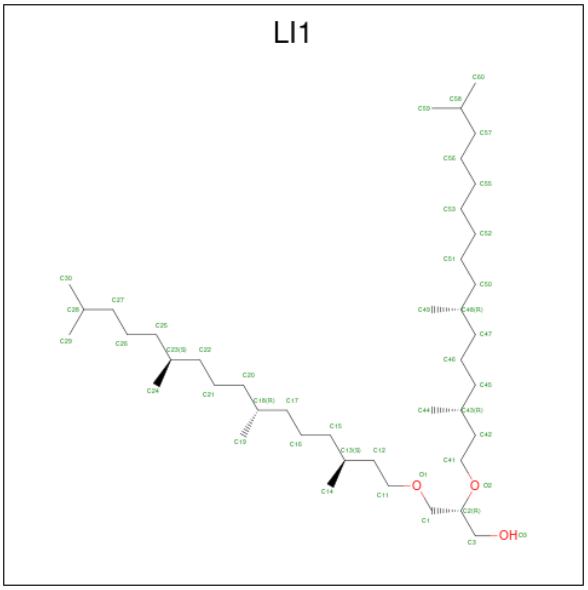
There are 5 unique types of molecules in this entry. The entry contains 2073 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BACTERIORHODOPSIN (GROUND STATE WILD TYPE "BR").

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	222	1720	1159	262	290	9	0	0	0

- Molecule 2 is 1-[2,6,10.14-TETRAMETHYL-HEXADECAN-16-YL]-2-[2,10,14-TRIMETHYLHEXADECAN-16-YL]GLYCEROL (three-letter code: LI1) (formula: $C_{42}H_{86}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	32	29	3	0	0
			Total	C	O		
2	A	1	41	38	3	0	0
			Total	C			
2	A	1	18	18		0	0
			Total	C			
2	A	1	16	16		0	0

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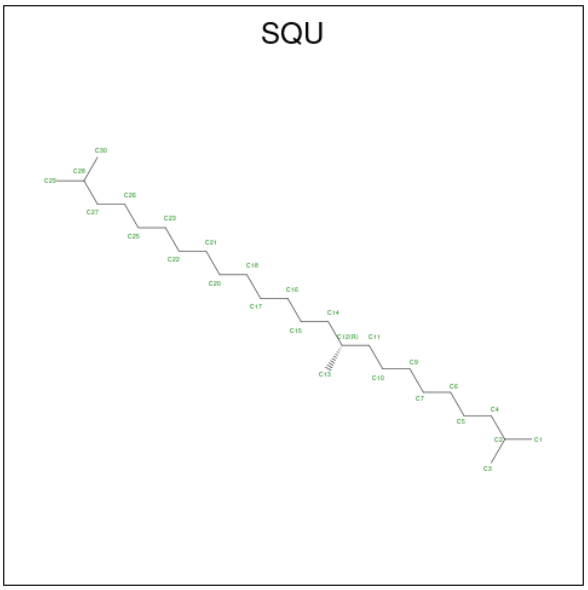
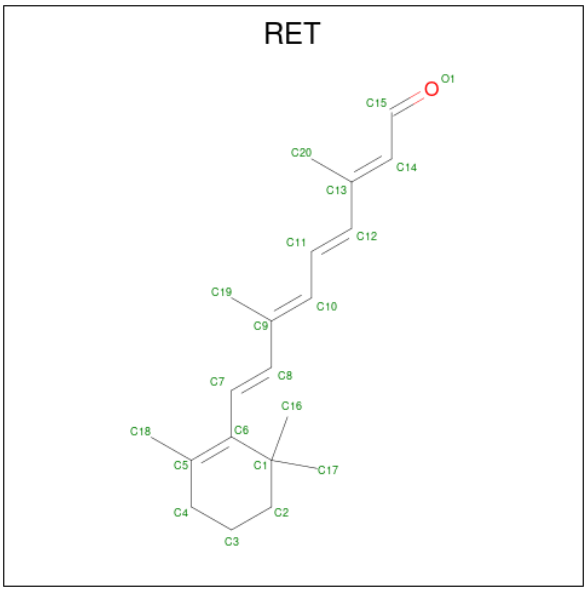
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 8 8	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C O 38 35 3	0	0
2	A	1	Total C 18 18	0	0
2	A	1	Total C 16 16	0	0
2	A	1	Total C O 40 37 3	0	0
2	A	1	Total C 17 17	0	0
2	A	1	Total C 18 18	0	0
2	A	1	Total C 13 13	0	0

- Molecule 3 is 2,10,23-TRIMETHYL-TETRACOSANE (three-letter code: SQU) (formula: $C_{27}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 27 27	0	0

- Molecule 4 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
4	A	1	20	20	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	23	23	23	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: BACTERIORHODOPSIN (GROUND STATE WILD TYPE "BR")

Chain A:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	60.63Å 60.63Å 108.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	12.00 – 1.55	Depositor
% Data completeness (in resolution range)	99.1 (12.00-1.55)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.158 , 0.225	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2073	wwPDB-VP
Average B, all atoms (Å^2)	30.0	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: LI1, RET, SQU

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	A	0.66	0/1767	1.58	20/2413 (0.8%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	7	ARG	NE-CZ-NH2	-14.17	113.22	120.30
1	A	7	ARG	NE-CZ-NH1	12.37	126.49	120.30
1	A	175	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	A	175	ARG	NE-CZ-NH2	-8.99	115.80	120.30
1	A	164	ARG	CD-NE-CZ	7.67	134.33	123.60
1	A	219	PHE	CB-CG-CD1	7.51	126.06	120.80
1	A	7	ARG	CD-NE-CZ	6.80	133.12	123.60
1	A	164	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	A	83	TYR	CB-CG-CD1	-6.49	117.11	121.00
1	A	57	TYR	CB-CG-CD1	-6.47	117.12	121.00
1	A	82	ARG	CD-NE-CZ	-6.38	114.67	123.60
1	A	83	TYR	CG-CD1-CE1	-6.20	116.34	121.30
1	A	185	TYR	CB-CG-CD2	-6.07	117.36	121.00
1	A	137	TRP	CZ3-CH2-CZ2	5.94	128.73	121.60
1	A	88	PHE	CB-CG-CD1	-5.42	117.00	120.80
1	A	219	PHE	C-N-CA	-5.38	111.01	122.30
1	A	135	PHE	CB-CG-CD1	-5.24	117.14	120.80
1	A	133	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	A	43	TYR	CB-CG-CD1	-5.21	117.88	121.00
1	A	175	ARG	CD-NE-CZ	5.18	130.85	123.60

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	A	1720	0	1776	63	0
2	A	283	0	457	63	0
3	A	27	0	53	6	0
4	A	20	0	27	2	0
5	A	23	0	0	1	0
All	All	2073	0	2313	98	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 22.

All (98) 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)
1:A:140:ILE:HG13	2:A:601:LI1:H272	1.52	0.92
1:A:44:ALA:HA	2:A:612:LI1:H13	1.53	0.89
2:A:602:LI1:H451	2:A:602:LI1:H172	1.55	0.86
1:A:139:ALA:HB1	2:A:608:LI1:H301	1.58	0.83
1:A:26:TYR:HD1	2:A:611:LI1:H152	1.44	0.81
1:A:221:LEU:HD13	3:A:701:SQU:H292	1.64	0.78
1:A:131:TYR:OH	2:A:602:LI1:H162	1.86	0.76
1:A:78:ILE:HD12	1:A:194:GLU:HG3	1.70	0.74
1:A:18:ALA:O	1:A:22:LEU:HD13	1.87	0.74
1:A:70:PRO:HG2	1:A:129:LYS:HD3	1.69	0.74
1:A:221:LEU:O	1:A:225:ARG:HG2	1.90	0.71
1:A:180:VAL:HG22	2:A:610:LI1:H211	1.72	0.71
1:A:187:VAL:HG21	2:A:610:LI1:H293	1.72	0.71
1:A:217:VAL:HG11	3:A:701:SQU:H212	1.77	0.66
1:A:221:LEU:HD11	3:A:701:SQU:H271	1.76	0.65
2:A:610:LI1:H593	2:A:610:LI1:H303	1.80	0.64
2:A:602:LI1:H161	2:A:603:LI1:H141	1.79	0.64
2:A:603:LI1:H293	2:A:609:LI1:H301	1.79	0.63
1:A:154:PHE:HZ	2:A:609:LI1:H152	1.64	0.62
1:A:18:ALA:HA	2:A:606:LI1:H202	1.81	0.62
2:A:610:LI1:H122	2:A:610:LI1:H411	1.82	0.62
1:A:131:TYR:CE2	2:A:602:LI1:H112	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:VAL:HG21	2:A:610:LI1:H512	1.83	0.60
1:A:149:LEU:HD22	1:A:179:VAL:HG22	1.82	0.60
2:A:610:LI1:H303	2:A:610:LI1:C59	2.32	0.59
1:A:153:PHE:CE2	1:A:179:VAL:HG21	2.36	0.59
1:A:26:TYR:CD1	2:A:611:LI1:H152	2.33	0.58
1:A:54:PHE:CD2	2:A:612:LI1:H292	2.39	0.58
1:A:45:ILE:HD11	1:A:95:LEU:HD13	1.85	0.58
2:A:610:LI1:H152	2:A:610:LI1:H461	1.86	0.57
1:A:198:ILE:HD11	2:A:603:LI1:H152	1.87	0.57
1:A:35:SER:O	1:A:37:PRO:HD3	2.06	0.56
1:A:64:TYR:OH	2:A:607:LI1:H31	2.06	0.56
1:A:19:LEU:HD21	3:A:701:SQU:H32	1.87	0.55
2:A:602:LI1:H443	2:A:602:LI1:C15	2.36	0.55
1:A:70:PRO:CG	1:A:129:LYS:HD3	2.36	0.55
1:A:19:LEU:CD2	3:A:701:SQU:H32	2.38	0.54
1:A:26:TYR:CE1	2:A:611:LI1:H121	2.43	0.53
1:A:70:PRO:HA	1:A:74:GLU:O	2.08	0.53
2:A:601:LI1:H303	2:A:608:LI1:H303	1.90	0.53
2:A:602:LI1:H172	2:A:602:LI1:H443	1.91	0.52
2:A:602:LI1:H451	2:A:602:LI1:C17	2.36	0.52
1:A:139:ALA:HB1	2:A:608:LI1:C30	2.34	0.52
1:A:214:SER:OG	3:A:701:SQU:H132	2.10	0.51
2:A:612:LI1:H143	5:A:512:HOH:O	2.09	0.51
1:A:164:ARG:HE	1:A:166:GLU:CD	2.15	0.49
1:A:131:TYR:OH	2:A:602:LI1:H13	2.13	0.49
2:A:602:LI1:H172	2:A:602:LI1:C44	2.43	0.49
1:A:169:SER:O	1:A:173:VAL:HG23	2.13	0.48
1:A:44:ALA:HA	2:A:612:LI1:C13	2.36	0.48
1:A:140:ILE:CG1	2:A:601:LI1:H272	2.34	0.47
1:A:180:VAL:CG1	2:A:610:LI1:H551	2.44	0.47
2:A:601:LI1:C30	2:A:608:LI1:H303	2.43	0.47
2:A:601:LI1:C30	2:A:608:LI1:H272	2.45	0.47
1:A:56:MET:HG3	1:A:85:ASP:HB2	1.96	0.47
2:A:603:LI1:H293	2:A:609:LI1:C28	2.45	0.47
1:A:88:PHE:HD1	2:A:613:LI1:H191	1.81	0.46
2:A:602:LI1:H443	2:A:602:LI1:H151	1.98	0.46
1:A:166:GLU:H	1:A:166:GLU:HG3	1.21	0.46
2:A:611:LI1:H222	2:A:611:LI1:H191	1.98	0.46
2:A:611:LI1:H193	2:A:611:LI1:H162	1.50	0.45
2:A:603:LI1:C29	2:A:609:LI1:H301	2.47	0.45
1:A:154:PHE:CZ	2:A:609:LI1:H152	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ARG:HG3	1:A:167:VAL:CG2	2.46	0.45
2:A:613:LI1:H202	2:A:613:LI1:H162	1.58	0.45
2:A:610:LI1:H411	2:A:610:LI1:H12	1.69	0.45
2:A:610:LI1:H122	2:A:610:LI1:H12	1.62	0.45
1:A:30:LYS:HE3	1:A:225:ARG:HD3	1.99	0.45
1:A:184:ALA:O	1:A:188:VAL:HG23	2.17	0.45
2:A:608:LI1:H292	2:A:608:LI1:H262	1.85	0.44
4:A:301:RET:H181	4:A:301:RET:H7	1.78	0.44
2:A:607:LI1:H122	2:A:607:LI1:H12	1.72	0.44
2:A:602:LI1:H243	2:A:602:LI1:H211	1.67	0.44
2:A:601:LI1:H303	2:A:608:LI1:H272	1.99	0.44
1:A:29:VAL:O	1:A:32:MET:HB2	2.18	0.43
1:A:163:MET:HG3	1:A:168:ALA:HB2	2.00	0.43
1:A:164:ARG:H	1:A:164:ARG:HG2	1.49	0.43
1:A:7:ARG:O	1:A:10:TRP:HD1	2.02	0.43
1:A:25:LEU:HD13	2:A:611:LI1:H221	2.00	0.43
1:A:190:LEU:CD2	2:A:603:LI1:H222	2.49	0.42
2:A:601:LI1:H193	2:A:601:LI1:H162	1.42	0.42
1:A:164:ARG:NH2	1:A:230:PHE:O	2.50	0.42
1:A:131:TYR:CE2	2:A:602:LI1:H13	2.55	0.42
1:A:54:PHE:CG	2:A:612:LI1:H292	2.53	0.42
2:A:611:LI1:H242	2:A:611:LI1:H262	1.51	0.42
1:A:203:ILE:O	1:A:207:LEU:HG	2.20	0.42
1:A:11:ILE:HG23	1:A:12:TRP:N	2.35	0.42
2:A:603:LI1:H293	2:A:609:LI1:C30	2.45	0.42
2:A:613:LI1:H191	2:A:613:LI1:H211	1.84	0.41
1:A:15:LEU:HB3	1:A:209:MET:HE2	2.01	0.41
1:A:190:LEU:HD23	2:A:603:LI1:H222	2.01	0.41
4:A:301:RET:H8	4:A:301:RET:H171	2.01	0.41
1:A:56:MET:HE1	2:A:607:LI1:H501	2.02	0.41
1:A:98:ALA:HB1	1:A:108:ILE:HG12	2.02	0.41
1:A:43:TYR:CE1	1:A:224:LEU:HD13	2.55	0.41
2:A:602:LI1:H2	2:A:602:LI1:H121	2.01	0.41
2:A:602:LI1:H592	2:A:608:LI1:H302	2.02	0.41
1:A:26:TYR:HE1	2:A:611:LI1:H121	1.85	0.40

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	A	218/222 (98%)	217 (100%)	1 (0%)	0	100 100

There are no Ramachandran outliers to report.

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	A	178/178 (100%)	169 (95%)	9 (5%)	24 3

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	38	ASP
1	A	74	GLU
1	A	75	GLN
1	A	95	LEU
1	A	100	LEU
1	A	164	ARG
1	A	166	GLU
1	A	202	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	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)

15 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	LI1	A	609	-	15,15,44	0.54	0	14,14,51	1.02	0
2	LI1	A	608	-	17,17,44	0.51	0	18,18,51	1.17	1 (5%)
2	LI1	A	602	-	40,40,44	0.73	1 (2%)	43,45,51	1.27	2 (4%)
2	LI1	A	613	-	12,12,44	0.52	0	12,12,51	1.38	3 (25%)
4	RET	A	301	1	20,20,21	1.32	3 (15%)	27,27,28	2.13	11 (40%)
2	LI1	A	603	-	17,17,44	0.48	0	18,18,51	0.83	0
2	LI1	A	607	-	37,37,44	0.74	1 (2%)	37,38,51	1.04	0
2	LI1	A	611	-	16,16,44	0.52	0	18,18,51	1.46	3 (16%)
2	LI1	A	610	-	39,39,44	0.80	1 (2%)	41,41,51	1.01	1 (2%)
2	LI1	A	612	-	17,17,44	0.52	0	18,18,51	1.14	1 (5%)
2	LI1	A	605	-	7,7,44	0.51	0	6,6,51	0.80	0
2	LI1	A	601	-	31,31,44	0.82	1 (3%)	33,33,51	1.16	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SQU	A	701	-	26,26,26	1.41	6 (23%)	28,28,28	1.89	10 (35%)
2	LI1	A	606	-	7,7,44	0.52	0	6,6,51	0.89	0
2	LI1	A	604	-	15,15,44	0.51	0	14,14,51	1.00	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LI1	A	609	-	-	5/13/13/49	-
2	LI1	A	608	-	-	7/16/16/49	-
2	LI1	A	602	-	-	18/44/44/49	-
2	LI1	A	613	-	1/1/1/8	5/11/11/49	-
4	RET	A	301	1	-	2/13/30/31	0/1/1/1
2	LI1	A	603	-	-	6/16/16/49	-
2	LI1	A	607	-	-	19/38/38/49	-
2	LI1	A	611	-	1/1/3/8	13/17/17/49	-
2	LI1	A	610	-	-	24/39/39/49	-
2	LI1	A	612	-	-	10/16/16/49	-
2	LI1	A	605	-	-	4/5/5/49	-
2	LI1	A	601	-	2/2/3/8	17/32/32/49	-
3	SQU	A	701	-	-	16/25/25/25	-
2	LI1	A	606	-	-	3/5/5/49	-
2	LI1	A	604	-	-	8/13/13/49	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	SQU	C14-C12	-3.35	1.35	1.52
4	A	301	RET	C14-C13	3.10	1.36	1.33
3	A	701	SQU	C23-C22	-3.08	1.34	1.51
2	A	610	LI1	O3-C3	3.00	1.55	1.42
3	A	701	SQU	C18-C17	-2.93	1.35	1.51
3	A	701	SQU	C9-C7	-2.89	1.35	1.51
2	A	601	LI1	O3-C3	2.84	1.54	1.42
2	A	602	LI1	O3-C3	2.70	1.53	1.42
4	A	301	RET	C17-C1	2.58	1.58	1.53
2	A	607	LI1	O3-C3	2.58	1.53	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	SQU	C4-C2	-2.41	1.35	1.51
3	A	701	SQU	C27-C28	-2.28	1.36	1.51
4	A	301	RET	C2-C3	-2.18	1.47	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	701	SQU	C15-C14-C12	5.08	132.33	115.92
4	A	301	RET	C11-C10-C9	-4.75	120.53	127.31
4	A	301	RET	C18-C5-C6	4.11	129.14	124.53
4	A	301	RET	C8-C9-C10	-3.60	113.42	118.94
4	A	301	RET	C10-C11-C12	-3.49	112.31	123.22
2	A	611	LI1	C16-C17-C18	-3.42	104.86	115.92
2	A	610	LI1	O3-C3-C2	-3.13	103.49	111.78
4	A	301	RET	C7-C6-C5	-3.02	114.16	121.46
3	A	701	SQU	C10-C9-C7	2.96	129.44	114.42
2	A	602	LI1	C21-C22-C23	-2.90	106.54	115.92
2	A	601	LI1	C16-C17-C18	-2.83	106.79	115.92
3	A	701	SQU	C5-C4-C2	2.78	129.09	115.98
2	A	601	LI1	O3-C3-C2	-2.68	104.68	111.78
3	A	701	SQU	C25-C23-C22	2.67	127.98	114.42
2	A	608	LI1	C21-C20-C18	-2.61	107.49	115.92
2	A	613	LI1	C16-C17-C18	-2.60	107.50	115.92
3	A	701	SQU	C23-C22-C21	2.59	127.59	114.42
4	A	301	RET	C19-C9-C8	2.56	122.11	118.08
2	A	612	LI1	C17-C16-C15	-2.51	104.75	113.62
2	A	602	LI1	C51-C50-C48	-2.48	107.90	115.92
3	A	701	SQU	C18-C17-C16	2.47	126.96	114.42
2	A	611	LI1	C21-C20-C18	-2.45	108.01	115.92
3	A	701	SQU	C14-C12-C11	2.42	124.84	112.13
4	A	301	RET	C17-C1-C6	2.41	114.20	110.30
3	A	701	SQU	C26-C27-C28	2.38	127.19	115.98
4	A	301	RET	C1-C6-C7	2.38	122.50	115.78
3	A	701	SQU	C9-C7-C6	2.35	126.36	114.42
3	A	701	SQU	C20-C18-C17	2.34	126.32	114.42
2	A	613	LI1	C21-C20-C18	-2.25	108.66	115.92
2	A	611	LI1	C21-C22-C23	-2.22	108.75	115.92
2	A	601	LI1	C21-C20-C18	-2.22	108.75	115.92
4	A	301	RET	C4-C5-C6	-2.10	119.68	122.73
4	A	301	RET	C20-C13-C12	2.09	121.37	118.08
4	A	301	RET	C2-C1-C6	2.04	113.62	110.48
2	A	613	LI1	C22-C21-C20	-2.03	106.44	113.62

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601	LI1	C18
2	A	601	LI1	C2
2	A	611	LI1	C13
2	A	613	LI1	C18

All (157) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	LI1	C42-C41-O2-C2
2	A	602	LI1	C41-C42-C43-C44
2	A	602	LI1	C11-C12-C13-C14
2	A	607	LI1	C1-C2-C3-O3
2	A	607	LI1	O2-C2-C3-O3
2	A	607	LI1	C42-C41-O2-C2
2	A	607	LI1	C41-C42-C43-C44
2	A	610	LI1	C42-C41-O2-C2
2	A	611	LI1	C16-C17-C18-C19
2	A	613	LI1	C16-C17-C18-C20
3	A	701	SQU	C11-C12-C14-C15
2	A	607	LI1	C12-C11-O1-C1
2	A	610	LI1	C12-C11-O1-C1
3	A	701	SQU	C20-C21-C22-C23
2	A	604	LI1	C20-C21-C22-C23
2	A	602	LI1	C24-C23-C25-C26
2	A	611	LI1	C24-C23-C25-C26
2	A	612	LI1	C14-C13-C15-C16
3	A	701	SQU	C10-C11-C12-C13
2	A	601	LI1	C15-C16-C17-C18
2	A	601	LI1	C11-C12-C13-C15
2	A	610	LI1	C25-C26-C27-C28
2	A	601	LI1	O1-C11-C12-C13
2	A	611	LI1	C21-C22-C23-C25
2	A	603	LI1	C25-C26-C27-C28
2	A	611	LI1	C20-C21-C22-C23
2	A	610	LI1	C55-C56-C57-C58
2	A	607	LI1	C45-C46-C47-C48
3	A	701	SQU	C3-C2-C4-C5
2	A	601	LI1	C12-C13-C15-C16
2	A	603	LI1	C18-C20-C21-C22
2	A	607	LI1	C47-C48-C50-C51
2	A	610	LI1	C51-C52-C53-C55
3	A	701	SQU	C23-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
3	A	701	SQU	C17-C18-C20-C21
2	A	603	LI1	C23-C25-C26-C27
2	A	601	LI1	C45-C46-C47-C48
2	A	605	LI1	C17-C18-C20-C21
2	A	608	LI1	C23-C25-C26-C27
2	A	610	LI1	C56-C57-C58-C59
2	A	608	LI1	C22-C23-C25-C26
2	A	610	LI1	C23-C25-C26-C27
3	A	701	SQU	C4-C5-C6-C7
2	A	611	LI1	C21-C22-C23-C24
2	A	610	LI1	C16-C17-C18-C20
2	A	610	LI1	C22-C23-C25-C26
2	A	610	LI1	C12-C13-C15-C16
2	A	607	LI1	C23-C25-C26-C27
2	A	609	LI1	C20-C21-C22-C23
2	A	610	LI1	C17-C18-C20-C21
2	A	610	LI1	C21-C22-C23-C25
3	A	701	SQU	C14-C15-C16-C17
2	A	607	LI1	C52-C53-C55-C56
2	A	608	LI1	C21-C22-C23-C25
2	A	610	LI1	C47-C48-C50-C51
2	A	610	LI1	C20-C21-C22-C23
2	A	604	LI1	C22-C23-C25-C26
2	A	604	LI1	C21-C22-C23-C25
2	A	608	LI1	C20-C21-C22-C23
2	A	610	LI1	C56-C57-C58-C60
2	A	607	LI1	C51-C52-C53-C55
2	A	609	LI1	C16-C17-C18-C20
3	A	701	SQU	C22-C23-C25-C26
3	A	701	SQU	C25-C26-C27-C28
2	A	604	LI1	C25-C26-C27-C28
2	A	607	LI1	O1-C11-C12-C13
2	A	607	LI1	C18-C20-C21-C22
2	A	609	LI1	C13-C15-C16-C17
2	A	608	LI1	C12-C13-C15-C16
2	A	609	LI1	C12-C13-C15-C16
2	A	610	LI1	C18-C20-C21-C22
3	A	701	SQU	C16-C17-C18-C20
2	A	601	LI1	C41-C42-C43-C45
2	A	605	LI1	C15-C16-C17-C18
2	A	602	LI1	O2-C41-C42-C43
2	A	602	LI1	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
2	A	610	LI1	C42-C43-C45-C46
2	A	601	LI1	C26-C27-C28-C29
2	A	603	LI1	C11-C12-C13-C15
2	A	612	LI1	C18-C20-C21-C22
2	A	612	LI1	C22-C23-C25-C26
2	A	602	LI1	C55-C56-C57-C58
2	A	612	LI1	C23-C25-C26-C27
2	A	601	LI1	C26-C27-C28-C30
3	A	701	SQU	C26-C27-C28-C30
2	A	610	LI1	C41-C42-C43-C45
2	A	607	LI1	C12-C13-C15-C16
2	A	610	LI1	C45-C46-C47-C48
2	A	605	LI1	C16-C17-C18-C20
2	A	610	LI1	C43-C45-C46-C47
2	A	605	LI1	C18-C20-C21-C22
3	A	701	SQU	C6-C7-C9-C10
2	A	610	LI1	C15-C16-C17-C18
2	A	602	LI1	C13-C15-C16-C17
2	A	603	LI1	C22-C23-C25-C26
2	A	611	LI1	C16-C17-C18-C20
2	A	612	LI1	C12-C13-C15-C16
2	A	601	LI1	C21-C22-C23-C25
2	A	602	LI1	C44-C43-C45-C46
2	A	607	LI1	C44-C43-C45-C46
2	A	611	LI1	C14-C13-C15-C16
2	A	613	LI1	C16-C17-C18-C19
4	A	301	RET	C12-C13-C14-C15
2	A	613	LI1	C12-C13-C15-C16
2	A	608	LI1	C11-C12-C13-C15
2	A	603	LI1	C11-C12-C13-C14
2	A	602	LI1	C41-C42-C43-C45
2	A	611	LI1	C23-C25-C26-C27
2	A	606	LI1	C15-C16-C17-C18
2	A	612	LI1	C26-C27-C28-C30
2	A	601	LI1	C46-C47-C48-C50
2	A	601	LI1	C16-C17-C18-C19
2	A	604	LI1	C17-C18-C20-C21
2	A	602	LI1	C42-C43-C45-C46
2	A	602	LI1	C46-C47-C48-C50
2	A	611	LI1	C12-C13-C15-C16
2	A	601	LI1	C13-C15-C16-C17
2	A	602	LI1	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
2	A	607	LI1	C20-C21-C22-C23
2	A	610	LI1	C46-C47-C48-C50
2	A	607	LI1	C48-C50-C51-C52
2	A	611	LI1	C18-C20-C21-C22
3	A	701	SQU	C18-C20-C21-C22
2	A	606	LI1	C13-C15-C16-C17
2	A	604	LI1	C16-C17-C18-C20
2	A	607	LI1	C41-C42-C43-C45
2	A	610	LI1	C13-C15-C16-C17
2	A	601	LI1	C12-C11-O1-C1
2	A	607	LI1	C2-C1-O1-C11
2	A	608	LI1	C13-C15-C16-C17
2	A	601	LI1	O1-C1-C2-O2
2	A	612	LI1	C11-C12-C13-C14
2	A	601	LI1	O1-C1-C2-C3
2	A	611	LI1	C22-C23-C25-C26
2	A	602	LI1	C46-C47-C48-C49
2	A	612	LI1	C20-C21-C22-C23
2	A	601	LI1	C2-C1-O1-C11
3	A	701	SQU	C26-C27-C28-C29
2	A	604	LI1	C11-C12-C13-C15
3	A	701	SQU	C12-C14-C15-C16
2	A	613	LI1	C11-C12-C13-C15
2	A	601	LI1	C22-C23-C25-C26
4	A	301	RET	C20-C13-C14-C15
2	A	612	LI1	C26-C27-C28-C29
2	A	609	LI1	C18-C20-C21-C22
2	A	606	LI1	C16-C17-C18-C20
2	A	602	LI1	C2-C1-O1-C11
2	A	602	LI1	C56-C57-C58-C60
2	A	612	LI1	C11-C12-C13-C15
2	A	611	LI1	C19-C18-C20-C21
2	A	604	LI1	C26-C27-C28-C29
2	A	613	LI1	C21-C22-C23-C24
2	A	610	LI1	C50-C51-C52-C53
2	A	607	LI1	C42-C43-C45-C46
2	A	602	LI1	O1-C11-C12-C13
2	A	602	LI1	C43-C45-C46-C47
2	A	611	LI1	C17-C18-C20-C21

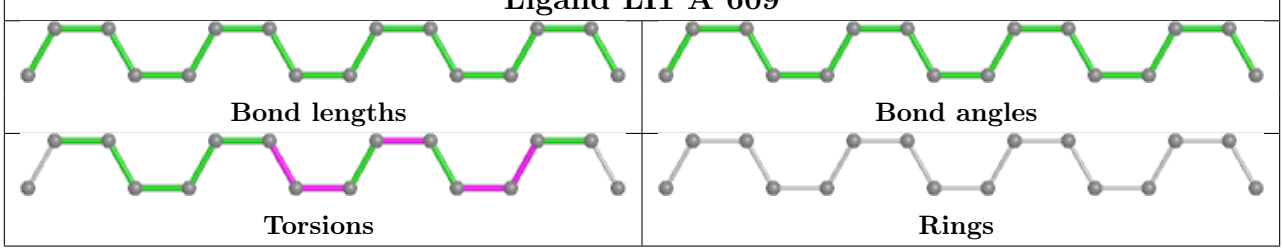
There are no ring outliers.

13 monomers are involved in 71 short contacts:

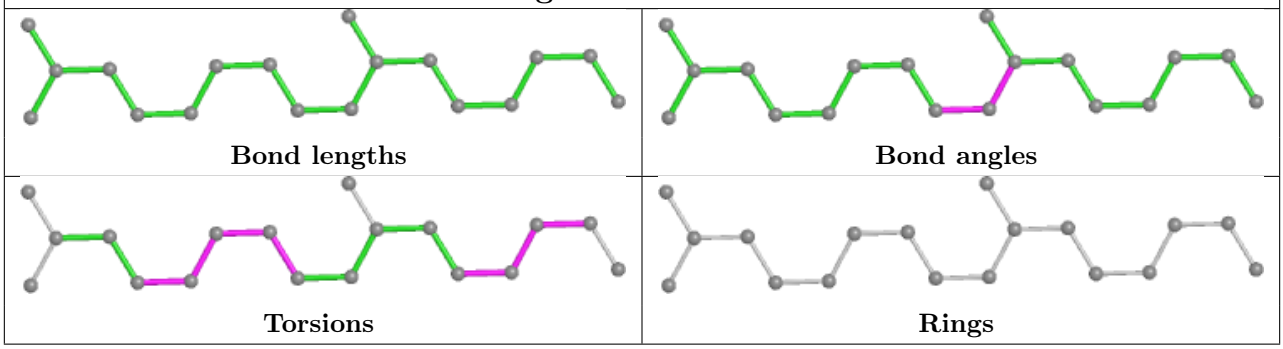
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	609	LI1	6	0
2	A	608	LI1	8	0
2	A	602	LI1	14	0
2	A	613	LI1	3	0
4	A	301	RET	2	0
2	A	603	LI1	8	0
2	A	607	LI1	3	0
2	A	611	LI1	8	0
2	A	610	LI1	10	0
2	A	612	LI1	5	0
2	A	601	LI1	7	0
3	A	701	SQU	6	0
2	A	606	LI1	1	0

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.

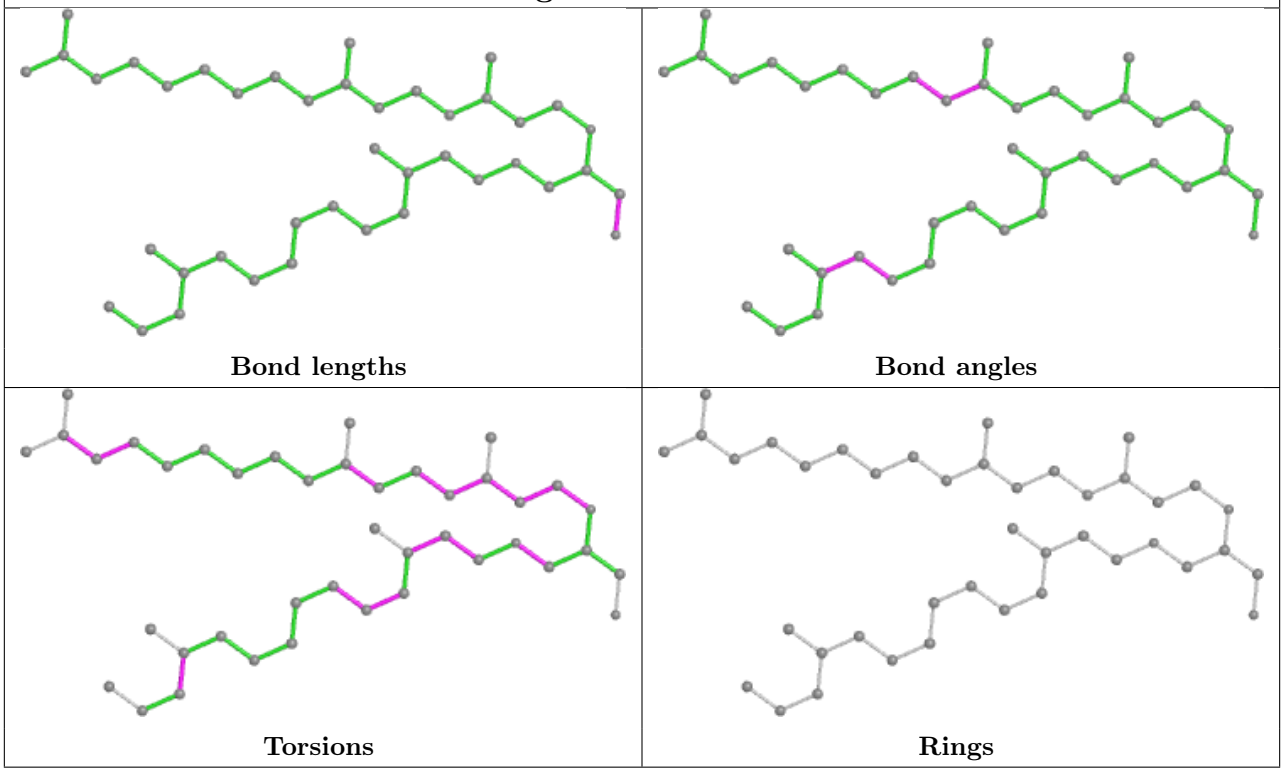
Ligand LI1 A 609



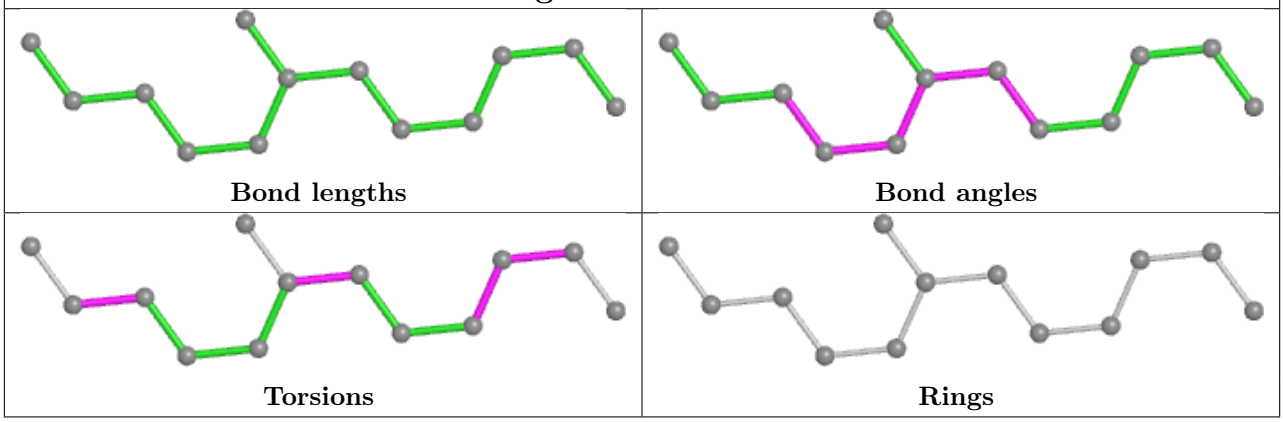
Ligand LI1 A 608



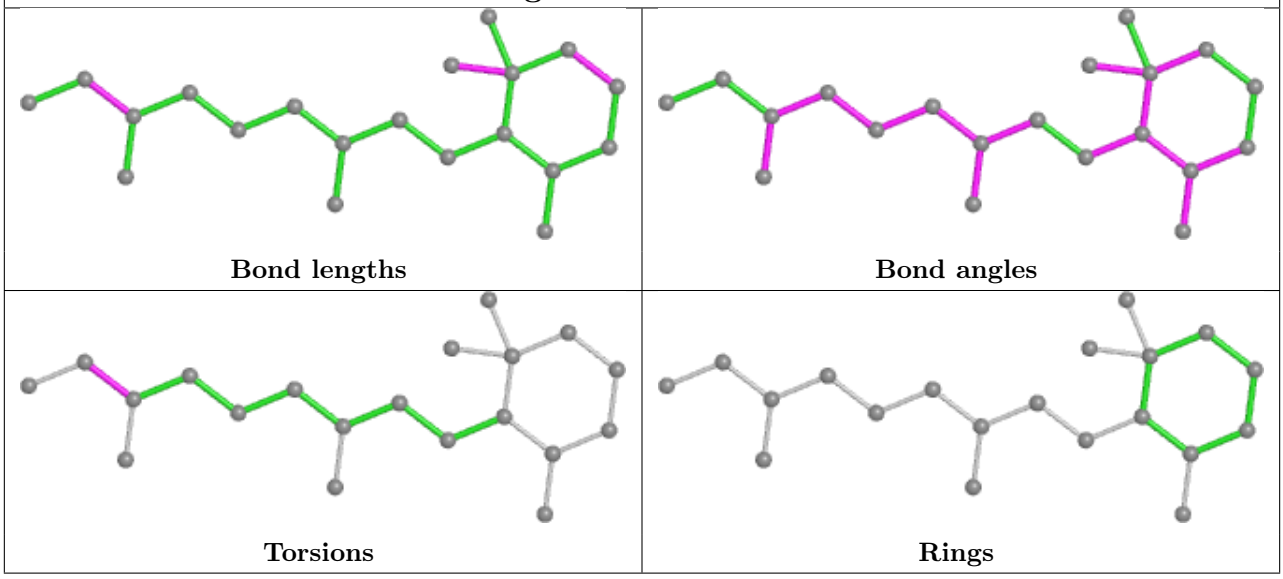
Ligand LI1 A 602



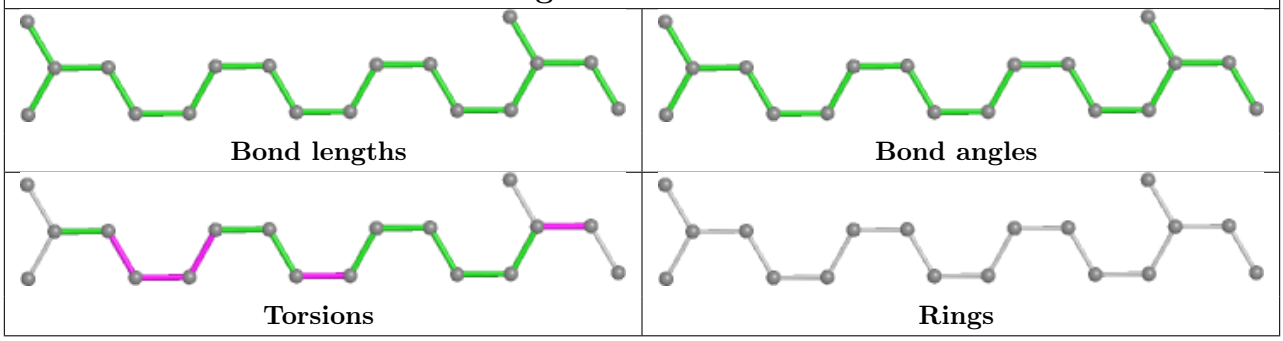
Ligand LI1 A 613



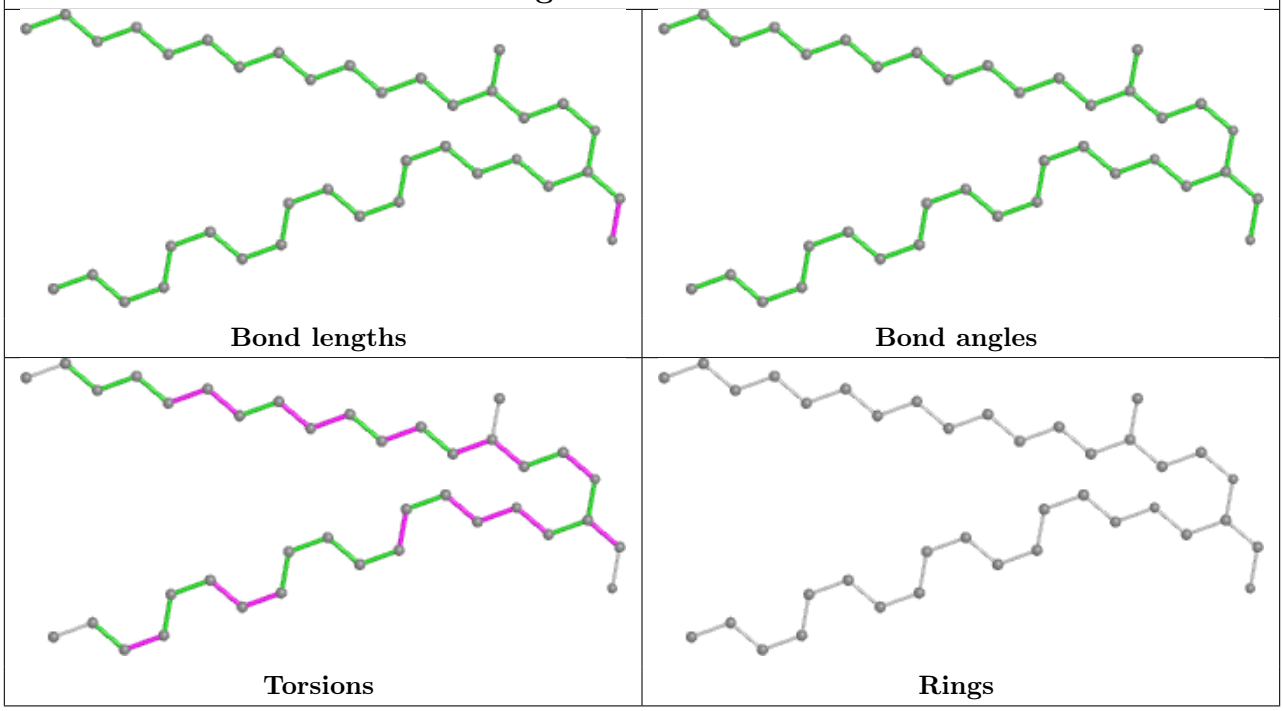
Ligand RET A 301



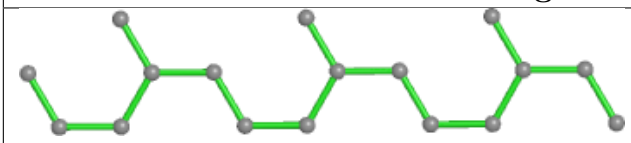
Ligand LI1 A 603



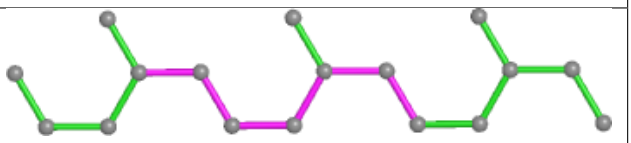
Ligand LI1 A 607



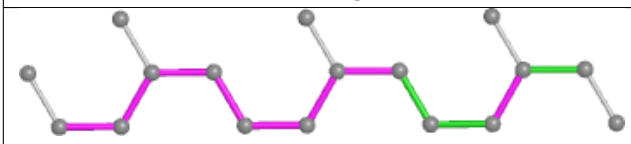
Ligand LI1 A 611



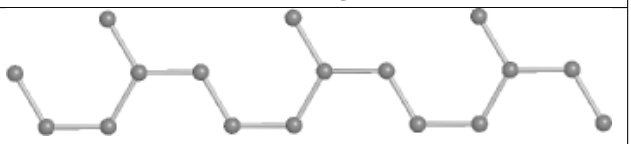
Bond lengths



Bond angles

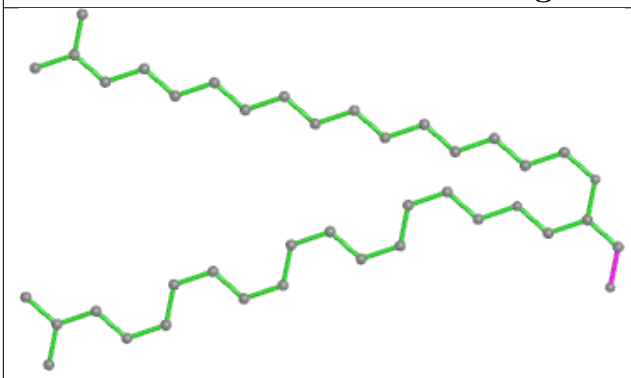


Torsions

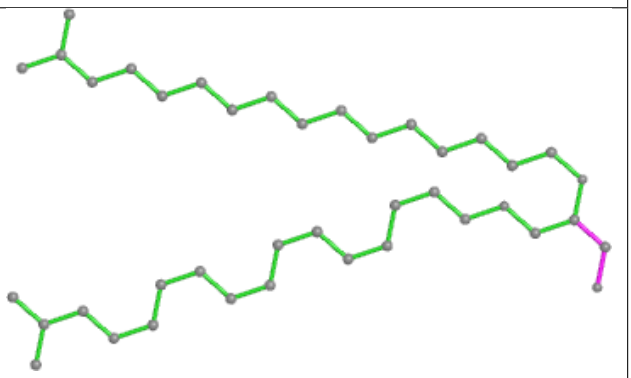


Rings

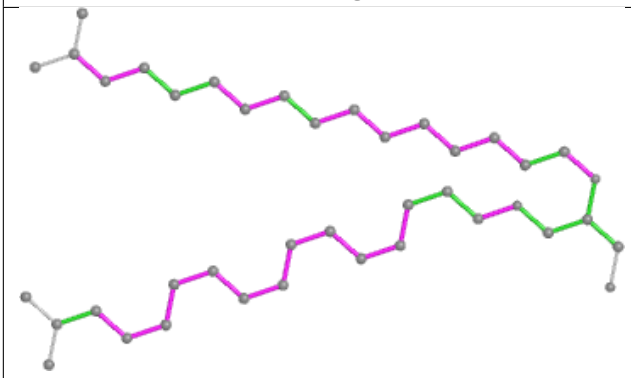
Ligand LI1 A 610



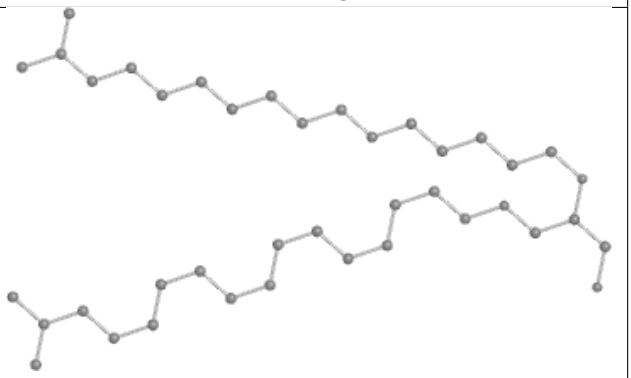
Bond lengths



Bond angles

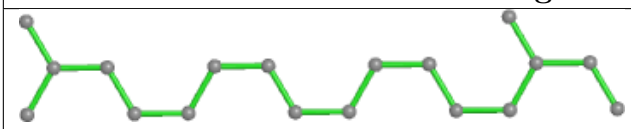


Torsions

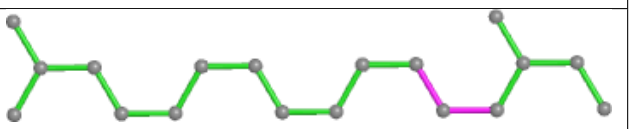


Rings

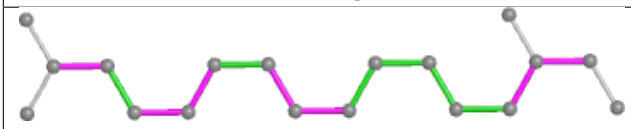
Ligand LI1 A 612



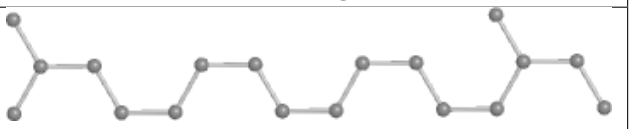
Bond lengths



Bond angles

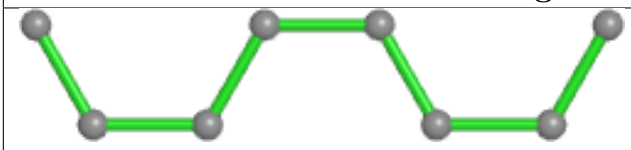


Torsions

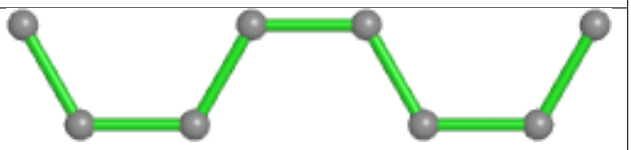


Rings

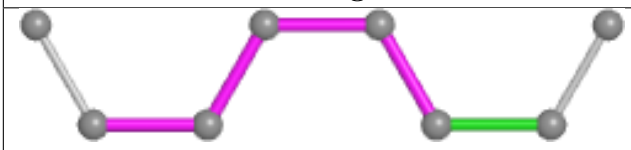
Ligand LI1 A 605



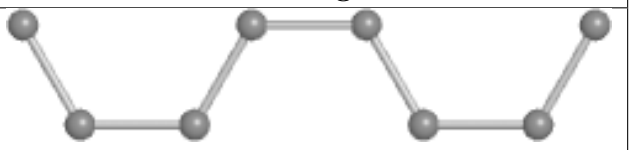
Bond lengths



Bond angles

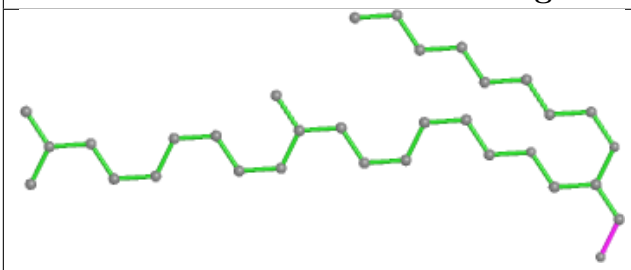


Torsions

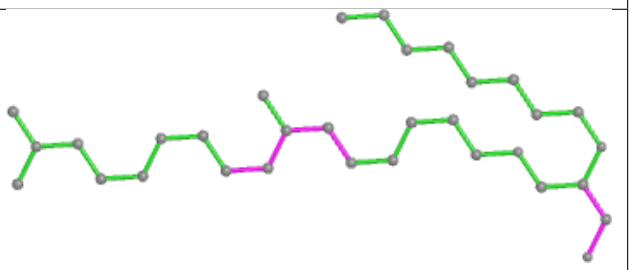


Rings

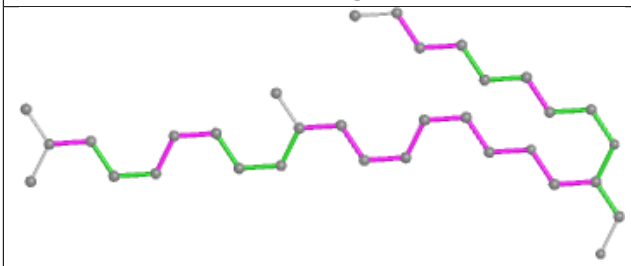
Ligand LI1 A 601



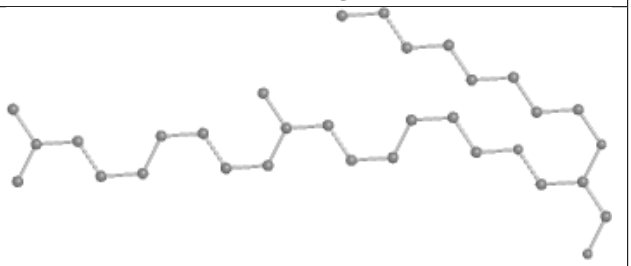
Bond lengths



Bond angles

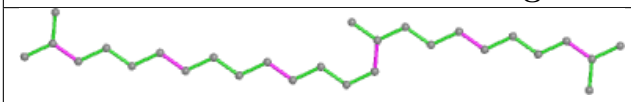


Torsions

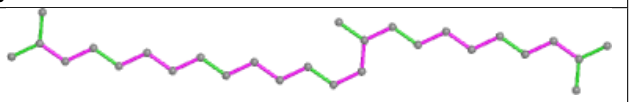


Rings

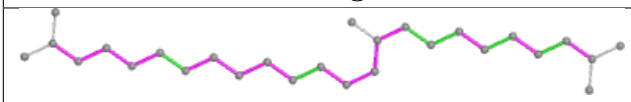
Ligand SQU A 701



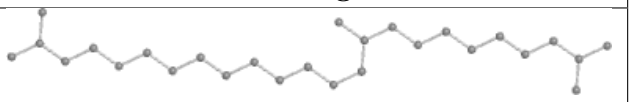
Bond lengths



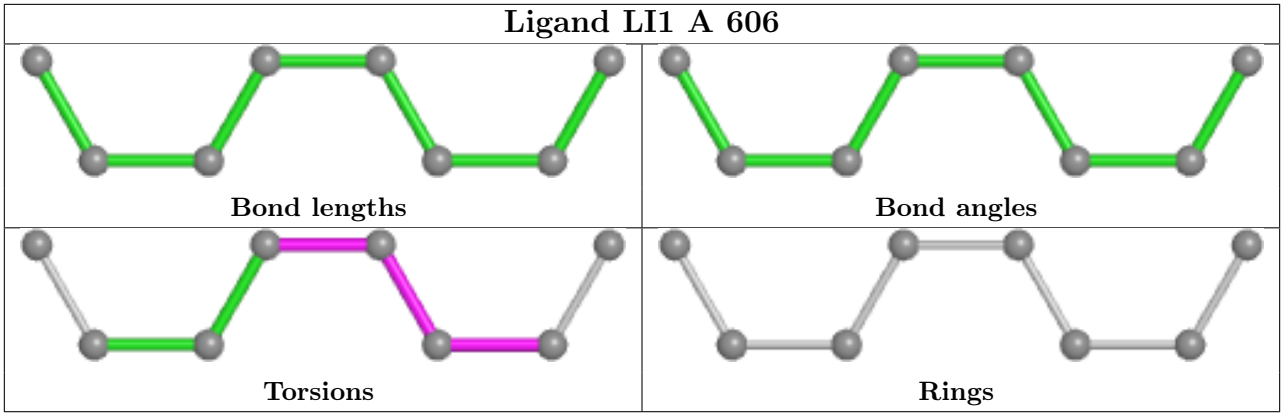
Bond angles

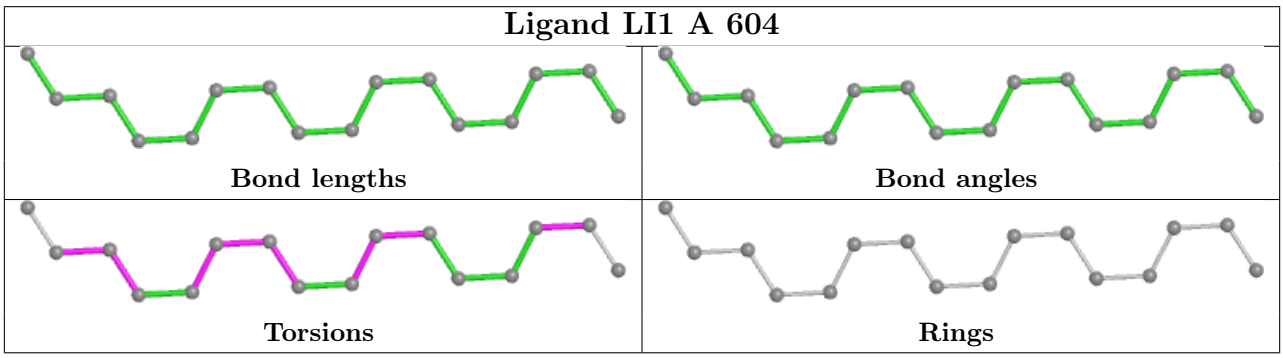


Torsions



Rings





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	156:PHE	C	162:SER	N	8.73

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.