Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2023 – 11:53 PM EDT

PDB ID	:	1F50
Title	:	BACTERIORHODOPSIN-BR STATE OF THE E204Q MUTANT AT 1.7 ANGSTROM RESOLUTION
Authors	:	Luecke, H.; Schobert, B.; Cartailler, J.P.; Richter, H.T.; Rosengarth, A.; Needleman, R.; Lanyi, J.K.
Deposited on	:	2000-06-10
Resolution	:	1.70 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:

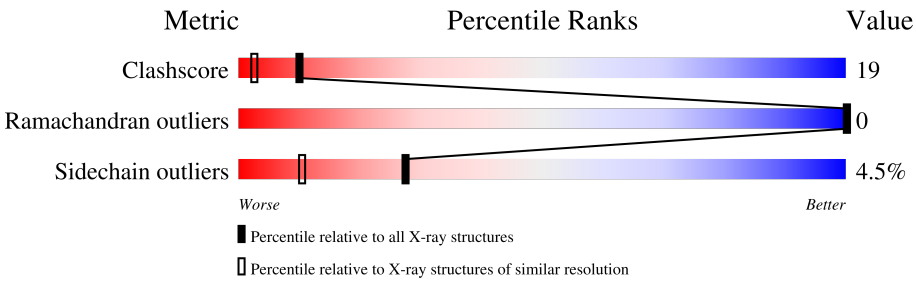
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.70 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	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)

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	A	227	70% 25% • •

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	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2074 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.

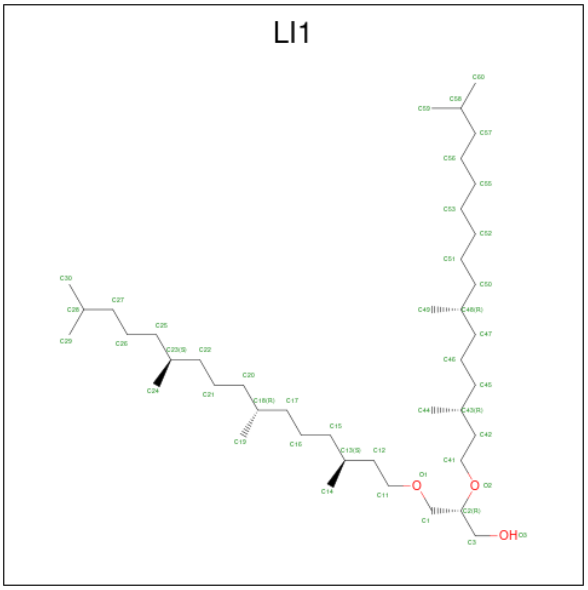
- Molecule 1 is a protein called BACTERIORHODOPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	222	1720	1159	263	289	9	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	204	GLN	GLU	engineered mutation	UNP P02945

- 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

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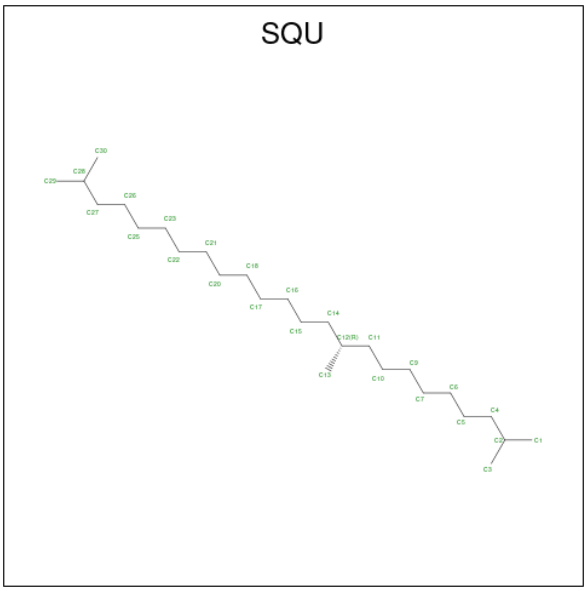
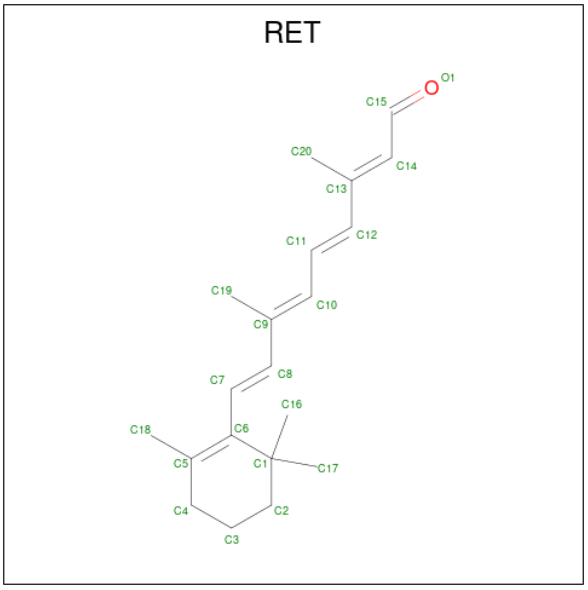
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 18 18	0	0
2	A	1	Total C 16 16	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C O 38 35 3	0	0
2	A	1	Total C 18 18	0	0
2	A	1	Total C 16 16	0	0
2	A	1	Total C O 40 37 3	0	0
2	A	1	Total C 17 17	0	0
2	A	1	Total C 18 18	0	0
2	A	1	Total C 13 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
4	A	1	Total C 20 20	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	24	Total O 24 24	0	0

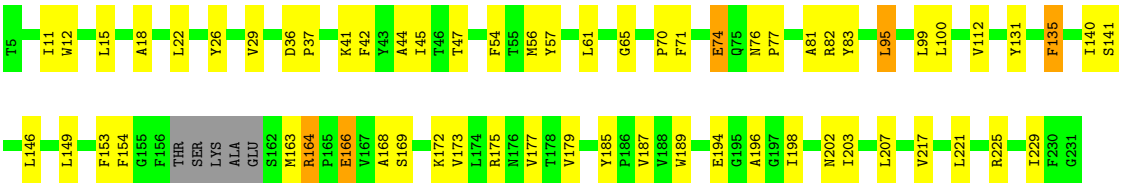
3 Residue-property plots (i)

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

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 – 1.70	Depositor
% Data completeness (in resolution range)	95.1 (12.00-1.70)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.132 , 0.191	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2074	wwPDB-VP
Average B, all atoms (Å^2)	29.0	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	0.49	0/1767	1.25	8/2413 (0.3%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	82	ARG	NE-CZ-NH1	-7.66	116.47	120.30
1	A	83	TYR	CB-CG-CD1	-7.16	116.71	121.00
1	A	175	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	A	82	ARG	NE-CZ-NH2	6.39	123.50	120.30
1	A	175	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	185	TYR	CB-CG-CD2	-5.59	117.64	121.00
1	A	57	TYR	CA-CB-CG	-5.50	102.94	113.40
1	A	135	PHE	CB-CG-CD1	-5.10	117.23	120.80

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	1778	58	0
2	A	283	0	457	51	0
3	A	27	0	53	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	20	0	27	4	0
5	A	24	0	0	1	0
All	All	2074	0	2315	83	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.

All (83) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:602:LI1:H451	2:A:602:LI1:H172	1.67	0.75
1:A:18:ALA:O	1:A:22:LEU:HD13	1.86	0.73
1:A:131:TYR:OH	2:A:602:LI1:H162	1.88	0.73
1:A:26:TYR:HD1	2:A:611:LI1:H152	1.55	0.72
1:A:41:LYS:HD2	1:A:99:LEU:HD13	1.72	0.71
2:A:601:LI1:H462	2:A:601:LI1:H222	1.72	0.70
1:A:47:THR:HG21	2:A:612:LI1:H141	1.73	0.69
1:A:44:ALA:HA	2:A:612:LI1:H13	1.75	0.69
2:A:602:LI1:H161	2:A:603:LI1:H141	1.73	0.68
1:A:169:SER:O	1:A:173:VAL:HG23	1.94	0.67
1:A:221:LEU:HD11	3:A:701:SQU:H272	1.77	0.66
3:A:701:SQU:H202	3:A:701:SQU:H261	1.76	0.66
1:A:187:VAL:HG21	2:A:610:LI1:H293	1.77	0.65
2:A:602:LI1:H12	2:A:602:LI1:H422	1.77	0.65
1:A:131:TYR:OH	2:A:602:LI1:H13	1.96	0.64
1:A:146:LEU:HD12	2:A:608:LI1:H262	1.80	0.64
1:A:70:PRO:HA	1:A:74:GLU:O	1.97	0.64
1:A:153:PHE:CE2	1:A:179:VAL:HG21	2.32	0.63
1:A:26:TYR:CE1	2:A:611:LI1:H121	2.34	0.62
1:A:141:SER:HB3	4:A:301:RET:H41	1.80	0.62
1:A:61:LEU:HD21	2:A:606:LI1:H152	1.81	0.61
3:A:701:SQU:H172	3:A:701:SQU:H111	1.84	0.60
2:A:601:LI1:H222	2:A:601:LI1:H471	1.84	0.60
2:A:602:LI1:H152	2:A:603:LI1:H141	1.83	0.60
1:A:198:ILE:HG22	2:A:604:LI1:H162	1.85	0.59
1:A:112:VAL:HG21	2:A:613:LI1:H121	1.84	0.58
1:A:131:TYR:CZ	2:A:602:LI1:H13	2.39	0.57
1:A:65:GLY:HA3	1:A:81:ALA:HB2	1.86	0.57
1:A:217:VAL:HG11	3:A:701:SQU:H212	1.87	0.57
1:A:44:ALA:HA	2:A:612:LI1:C13	2.36	0.55
1:A:153:PHE:HZ	2:A:610:LI1:H162	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:PHE:HB2	2:A:602:LI1:H522	1.88	0.55
2:A:612:LI1:H143	5:A:512:HOH:O	2.06	0.54
2:A:601:LI1:H222	2:A:601:LI1:C46	2.38	0.54
1:A:54:PHE:CD2	2:A:612:LI1:H28	2.43	0.54
1:A:26:TYR:CD1	2:A:611:LI1:H152	2.40	0.52
2:A:602:LI1:H451	2:A:602:LI1:C17	2.40	0.51
2:A:602:LI1:C16	2:A:603:LI1:H141	2.41	0.51
1:A:154:PHE:HZ	2:A:609:LI1:H161	1.76	0.50
4:A:301:RET:H8	4:A:301:RET:H171	1.94	0.50
1:A:173:VAL:O	1:A:177:VAL:HG23	2.11	0.50
1:A:140:ILE:CG1	2:A:601:LI1:H272	2.41	0.50
1:A:54:PHE:CE2	2:A:612:LI1:H28	2.46	0.50
1:A:187:VAL:HG21	2:A:610:LI1:C29	2.40	0.50
1:A:141:SER:CB	4:A:301:RET:H41	2.41	0.49
1:A:149:LEU:HD22	1:A:179:VAL:HG22	1.95	0.48
1:A:56:MET:HE1	2:A:607:LI1:H501	1.96	0.48
1:A:131:TYR:CE2	2:A:602:LI1:H13	2.48	0.48
1:A:135:PHE:CB	2:A:602:LI1:H522	2.43	0.48
1:A:153:PHE:CE1	2:A:610:LI1:H121	2.48	0.48
2:A:610:LI1:H122	2:A:610:LI1:H12	1.45	0.47
1:A:203:ILE:O	1:A:207:LEU:HG	2.15	0.47
1:A:163:MET:HE3	1:A:168:ALA:HA	1.97	0.47
1:A:189:TRP:CD1	4:A:301:RET:H22	2.50	0.47
2:A:601:LI1:H303	2:A:608:LI1:H28	1.97	0.46
2:A:607:LI1:H552	2:A:607:LI1:H511	1.49	0.46
1:A:168:ALA:O	1:A:172:LYS:HG3	2.17	0.45
2:A:601:LI1:H222	2:A:601:LI1:C47	2.44	0.45
1:A:187:VAL:HG22	2:A:603:LI1:H28	1.97	0.45
3:A:701:SQU:H172	3:A:701:SQU:C11	2.46	0.45
2:A:602:LI1:H262	2:A:602:LI1:H241	1.55	0.44
1:A:76:ASN:HA	1:A:77:PRO:HD2	1.84	0.44
2:A:605:LI1:H172	2:A:605:LI1:H212	1.79	0.44
1:A:45:ILE:HD11	1:A:95:LEU:HD13	2.00	0.44
1:A:47:THR:CG2	2:A:612:LI1:H141	2.46	0.44
1:A:217:VAL:HG11	3:A:701:SQU:C21	2.47	0.44
1:A:42:PHE:CD2	1:A:229:ILE:HB	2.53	0.43
2:A:602:LI1:C15	2:A:603:LI1:H141	2.45	0.43
1:A:74:GLU:H	1:A:74:GLU:HG2	1.63	0.43
1:A:70:PRO:O	1:A:71:PHE:HB3	2.17	0.43
1:A:140:ILE:HG12	2:A:601:LI1:H272	2.01	0.43
1:A:198:ILE:HD11	2:A:603:LI1:H151	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ASP:HA	1:A:37:PRO:HD2	1.88	0.43
2:A:602:LI1:H12	2:A:602:LI1:H121	1.67	0.43
1:A:131:TYR:OH	1:A:196:ALA:HA	2.20	0.42
2:A:607:LI1:H443	2:A:607:LI1:H462	1.54	0.42
1:A:100:LEU:HD12	1:A:100:LEU:HA	1.92	0.42
2:A:613:LI1:H202	2:A:613:LI1:H162	1.64	0.41
1:A:164:ARG:H	1:A:164:ARG:HG2	1.52	0.41
2:A:611:LI1:H161	2:A:611:LI1:H193	1.49	0.41
1:A:29:VAL:HG21	2:A:611:LI1:C19	2.52	0.40
1:A:11:ILE:HG23	1:A:12:TRP:N	2.37	0.40
1:A:166:GLU:H	1:A:166:GLU:HG3	1.55	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	218/227 (96%)	215 (99%)	3 (1%)	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	178/182 (98%)	170 (96%)	8 (4%)	27 10

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	74	GLU
1	A	95	LEU
1	A	164	ARG
1	A	166	GLU
1	A	194	GLU
1	A	202	ASN
1	A	225	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
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	605	-	7,7,44	0.50	0	6,6,51	0.65	0
2	LI1	A	609	-	15,15,44	0.53	0	14,14,51	1.09	0
2	LI1	A	604	-	15,15,44	0.52	0	14,14,51	1.16	0
2	LI1	A	603	-	17,17,44	0.51	0	18,18,51	0.99	0
2	LI1	A	607	-	37,37,44	0.76	1 (2%)	37,38,51	1.03	1 (2%)
2	LI1	A	613	-	12,12,44	0.49	0	12,12,51	1.31	1 (8%)
2	LI1	A	611	-	16,16,44	0.49	0	18,18,51	1.36	4 (22%)
2	LI1	A	602	-	40,40,44	0.79	1 (2%)	43,45,51	1.21	2 (4%)
2	LI1	A	612	-	17,17,44	0.50	0	18,18,51	1.08	1 (5%)
4	RET	A	301	1	20,20,21	1.65	3 (15%)	27,27,28	1.74	7 (25%)
2	LI1	A	610	-	39,39,44	0.79	1 (2%)	41,41,51	0.97	1 (2%)
2	LI1	A	608	-	17,17,44	0.48	0	18,18,51	1.19	1 (5%)
3	SQU	A	701	-	26,26,26	1.39	6 (23%)	28,28,28	1.76	9 (32%)
2	LI1	A	606	-	7,7,44	0.49	0	6,6,51	0.85	0
2	LI1	A	601	-	31,31,44	0.78	1 (3%)	33,33,51	1.13	2 (6%)

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	605	-	-	2/5/5/49	-
2	LI1	A	609	-	-	11/13/13/49	-
2	LI1	A	604	-	-	8/13/13/49	-
2	LI1	A	603	-	-	11/16/16/49	-
2	LI1	A	607	-	-	20/38/38/49	-
2	LI1	A	613	-	1/1/1/8	6/11/11/49	-
2	LI1	A	611	-	1/1/3/8	11/17/17/49	-
2	LI1	A	602	-	-	25/44/44/49	-
2	LI1	A	612	-	-	10/16/16/49	-
4	RET	A	301	1	-	2/13/30/31	0/1/1/1
3	SQU	A	701	-	1/1/3/3	17/25/25/25	-
2	LI1	A	608	-	-	7/16/16/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LI1	A	610	-	-	25/39/39/49	-
2	LI1	A	606	-	-	2/5/5/49	-
2	LI1	A	601	-	2/2/3/8	23/32/32/49	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	RET	C15-C14	-5.76	1.27	1.49
3	A	701	SQU	C14-C12	-3.24	1.35	1.52
3	A	701	SQU	C9-C7	-2.97	1.34	1.51
2	A	602	LI1	O3-C3	2.96	1.54	1.42
3	A	701	SQU	C23-C22	-2.89	1.35	1.51
3	A	701	SQU	C18-C17	-2.88	1.35	1.51
2	A	610	LI1	O3-C3	2.86	1.54	1.42
2	A	607	LI1	O3-C3	2.82	1.54	1.42
2	A	601	LI1	O3-C3	2.71	1.53	1.42
4	A	301	RET	C2-C3	-2.67	1.46	1.52
3	A	701	SQU	C4-C2	-2.44	1.34	1.51
3	A	701	SQU	C27-C28	-2.39	1.35	1.51
4	A	301	RET	C14-C13	2.18	1.35	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	301	RET	C11-C10-C9	-3.88	121.78	127.31
4	A	301	RET	C8-C9-C10	-3.88	112.99	118.94
3	A	701	SQU	C15-C14-C12	3.81	128.25	115.92
2	A	602	LI1	O3-C3-C2	-3.50	102.50	111.78
2	A	613	LI1	C16-C17-C18	-3.14	105.78	115.92
2	A	611	LI1	C16-C17-C18	-3.09	105.92	115.92
4	A	301	RET	C18-C5-C6	3.07	127.97	124.53
2	A	601	LI1	C16-C17-C18	-3.06	106.03	115.92
3	A	701	SQU	C5-C4-C2	3.01	130.18	115.98
3	A	701	SQU	C10-C9-C7	2.99	129.59	114.42
3	A	701	SQU	C18-C17-C16	2.73	128.26	114.42
2	A	608	LI1	C21-C20-C18	-2.62	107.45	115.92
2	A	612	LI1	C16-C15-C13	-2.58	107.58	115.92
3	A	701	SQU	C9-C7-C6	2.55	127.38	114.42
4	A	301	RET	C19-C9-C10	2.55	126.50	122.92
4	A	301	RET	C16-C1-C2	-2.45	99.09	108.91
2	A	611	LI1	C21-C20-C18	-2.39	108.18	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	607	LI1	C46-C45-C43	-2.31	108.45	115.92
3	A	701	SQU	C14-C12-C11	2.22	123.82	112.13
2	A	611	LI1	C16-C15-C13	-2.21	108.79	115.92
2	A	602	LI1	C46-C45-C43	-2.15	108.97	115.92
2	A	610	LI1	O3-C3-C2	-2.13	106.13	111.78
2	A	601	LI1	O3-C3-C2	-2.10	106.21	111.78
4	A	301	RET	C10-C11-C12	-2.10	116.67	123.22
4	A	301	RET	C18-C5-C4	-2.10	109.59	113.62
3	A	701	SQU	C26-C27-C28	2.05	125.63	115.98
3	A	701	SQU	C30-C28-C27	2.04	124.12	111.54
2	A	611	LI1	C21-C22-C23	-2.02	109.40	115.92
3	A	701	SQU	C23-C22-C21	2.01	124.61	114.42

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601	LI1	C2
2	A	601	LI1	C18
2	A	611	LI1	C13
2	A	613	LI1	C18
3	A	701	SQU	C12

All (180) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	LI1	C1-C2-C3-O3
2	A	601	LI1	O2-C2-C3-O3
2	A	601	LI1	C42-C41-O2-C2
2	A	602	LI1	O2-C2-C3-O3
2	A	602	LI1	C41-C42-C43-C44
2	A	602	LI1	C11-C12-C13-C14
2	A	607	LI1	C42-C41-O2-C2
2	A	607	LI1	C41-C42-C43-C44
2	A	607	LI1	C44-C43-C45-C46
2	A	610	LI1	C1-C2-C3-O3
2	A	610	LI1	O2-C2-C3-O3
2	A	612	LI1	C14-C13-C15-C16
3	A	701	SQU	C11-C12-C14-C15
4	A	301	RET	C20-C13-C14-C15
2	A	607	LI1	C12-C11-O1-C1
2	A	610	LI1	C12-C11-O1-C1
3	A	701	SQU	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
3	A	701	SQU	C4-C5-C6-C7
2	A	601	LI1	C11-C12-C13-C15
2	A	602	LI1	C12-C11-O1-C1
2	A	603	LI1	C18-C20-C21-C22
3	A	701	SQU	C22-C23-C25-C26
2	A	605	LI1	C17-C18-C20-C21
2	A	601	LI1	C16-C17-C18-C19
2	A	602	LI1	C24-C23-C25-C26
2	A	611	LI1	C16-C17-C18-C19
3	A	701	SQU	C10-C11-C12-C13
2	A	602	LI1	C55-C56-C57-C58
2	A	610	LI1	C20-C21-C22-C23
2	A	607	LI1	C43-C45-C46-C47
2	A	608	LI1	C15-C16-C17-C18
2	A	607	LI1	O1-C11-C12-C13
2	A	601	LI1	C18-C20-C21-C22
2	A	610	LI1	O2-C41-C42-C43
2	A	603	LI1	C13-C15-C16-C17
3	A	701	SQU	C2-C4-C5-C6
2	A	613	LI1	C16-C17-C18-C20
2	A	603	LI1	C25-C26-C27-C28
2	A	611	LI1	C18-C20-C21-C22
2	A	610	LI1	O1-C11-C12-C13
2	A	601	LI1	C26-C27-C28-C29
2	A	602	LI1	O1-C11-C12-C13
2	A	604	LI1	C15-C16-C17-C18
3	A	701	SQU	C20-C21-C22-C23
3	A	701	SQU	C3-C2-C4-C5
2	A	601	LI1	C13-C15-C16-C17
2	A	604	LI1	C18-C20-C21-C22
2	A	607	LI1	C12-C13-C15-C16
2	A	610	LI1	C42-C43-C45-C46
2	A	602	LI1	C51-C52-C53-C55
2	A	612	LI1	C21-C22-C23-C25
2	A	601	LI1	C12-C13-C15-C16
2	A	610	LI1	C12-C13-C15-C16
3	A	701	SQU	C17-C18-C20-C21
2	A	609	LI1	C20-C21-C22-C23
2	A	610	LI1	C23-C25-C26-C27
2	A	601	LI1	C19-C18-C20-C21
2	A	602	LI1	C49-C48-C50-C51
2	A	608	LI1	C21-C22-C23-C25

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Mol	Chain	Res	Type	Atoms
2	A	608	LI1	C23-C25-C26-C27
2	A	610	LI1	C47-C48-C50-C51
2	A	610	LI1	C51-C52-C53-C55
3	A	701	SQU	C15-C16-C17-C18
3	A	701	SQU	C23-C25-C26-C27
2	A	612	LI1	C18-C20-C21-C22
2	A	601	LI1	C21-C22-C23-C25
2	A	604	LI1	C25-C26-C27-C28
2	A	608	LI1	C22-C23-C25-C26
2	A	607	LI1	C53-C55-C56-C57
2	A	613	LI1	C12-C13-C15-C16
2	A	603	LI1	C20-C21-C22-C23
2	A	609	LI1	C15-C16-C17-C18
2	A	601	LI1	C43-C45-C46-C47
2	A	602	LI1	C50-C51-C52-C53
2	A	607	LI1	C55-C56-C57-C58
2	A	609	LI1	C16-C17-C18-C20
3	A	701	SQU	C26-C27-C28-C30
2	A	602	LI1	C13-C15-C16-C17
2	A	610	LI1	C46-C47-C48-C50
2	A	601	LI1	C26-C27-C28-C30
2	A	610	LI1	C50-C51-C52-C53
2	A	609	LI1	C12-C13-C15-C16
2	A	601	LI1	C16-C17-C18-C20
2	A	601	LI1	C17-C18-C20-C21
2	A	611	LI1	C16-C17-C18-C20
2	A	610	LI1	C15-C16-C17-C18
2	A	609	LI1	C13-C15-C16-C17
2	A	608	LI1	C20-C21-C22-C23
2	A	610	LI1	C17-C18-C20-C21
2	A	601	LI1	C22-C23-C25-C26
2	A	604	LI1	C16-C17-C18-C20
2	A	607	LI1	C17-C18-C20-C21
2	A	612	LI1	C15-C16-C17-C18
2	A	601	LI1	C45-C46-C47-C48
2	A	603	LI1	C16-C17-C18-C20
3	A	701	SQU	C18-C20-C21-C22
2	A	602	LI1	C2-C1-O1-C11
2	A	602	LI1	C43-C45-C46-C47
2	A	604	LI1	C12-C13-C15-C16
2	A	613	LI1	C13-C15-C16-C17
2	A	609	LI1	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
2	A	606	LI1	C13-C15-C16-C17
2	A	601	LI1	C46-C47-C48-C50
2	A	607	LI1	C20-C21-C22-C23
2	A	607	LI1	C42-C43-C45-C46
2	A	612	LI1	C12-C13-C15-C16
2	A	613	LI1	C16-C17-C18-C19
2	A	610	LI1	C56-C57-C58-C60
4	A	301	RET	C12-C13-C14-C15
2	A	602	LI1	C23-C25-C26-C27
2	A	601	LI1	C25-C26-C27-C28
2	A	609	LI1	C22-C23-C25-C26
2	A	602	LI1	C41-C42-C43-C45
2	A	607	LI1	C41-C42-C43-C45
2	A	610	LI1	C56-C57-C58-C59
2	A	610	LI1	O1-C1-C2-C3
2	A	610	LI1	C2-C1-O1-C11
2	A	610	LI1	C45-C46-C47-C48
2	A	601	LI1	C41-C42-C43-C45
2	A	613	LI1	C21-C22-C23-C24
2	A	611	LI1	C20-C21-C22-C23
2	A	607	LI1	C46-C47-C48-C50
2	A	610	LI1	C13-C15-C16-C17
2	A	602	LI1	C46-C47-C48-C49
2	A	607	LI1	C16-C17-C18-C20
2	A	610	LI1	C41-C42-C43-C45
2	A	611	LI1	C11-C12-C13-C14
2	A	602	LI1	C46-C47-C48-C50
2	A	603	LI1	C12-C13-C15-C16
2	A	606	LI1	C18-C20-C21-C22
3	A	701	SQU	C12-C14-C15-C16
2	A	607	LI1	C18-C20-C21-C22
2	A	604	LI1	C11-C12-C13-C15
2	A	602	LI1	C11-C12-C13-C15
2	A	610	LI1	C21-C22-C23-C25
2	A	610	LI1	O1-C1-C2-O2
2	A	602	LI1	C15-C16-C17-C18
2	A	608	LI1	C12-C13-C15-C16
2	A	604	LI1	C23-C25-C26-C27
2	A	608	LI1	C11-C12-C13-C15
2	A	607	LI1	C52-C53-C55-C56
2	A	612	LI1	C23-C25-C26-C27
3	A	701	SQU	C11-C10-C9-C7

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Mol	Chain	Res	Type	Atoms
2	A	602	LI1	C42-C43-C45-C46
2	A	602	LI1	C22-C23-C25-C26
2	A	604	LI1	C21-C22-C23-C25
2	A	611	LI1	C23-C25-C26-C27
2	A	601	LI1	O2-C41-C42-C43
2	A	609	LI1	C26-C27-C28-C30
3	A	701	SQU	C5-C6-C7-C9
2	A	612	LI1	C20-C21-C22-C23
2	A	603	LI1	C22-C23-C25-C26
2	A	611	LI1	C17-C18-C20-C21
2	A	602	LI1	C44-C43-C45-C46
2	A	612	LI1	C16-C17-C18-C20
2	A	611	LI1	C11-C12-C13-C15
2	A	611	LI1	C15-C16-C17-C18
2	A	613	LI1	C11-C12-C13-C15
2	A	603	LI1	C21-C22-C23-C25
2	A	607	LI1	C51-C52-C53-C55
3	A	701	SQU	C21-C22-C23-C25
2	A	609	LI1	C25-C26-C27-C28
2	A	609	LI1	C18-C20-C21-C22
2	A	607	LI1	C2-C1-O1-C11
2	A	602	LI1	C1-C2-C3-O3
2	A	612	LI1	C26-C27-C28-C30
2	A	602	LI1	C42-C41-O2-C2
2	A	612	LI1	C11-C12-C13-C14
2	A	602	LI1	C47-C48-C50-C51
2	A	609	LI1	C17-C18-C20-C21
2	A	607	LI1	C11-C12-C13-C15
2	A	603	LI1	C23-C25-C26-C27
2	A	605	LI1	C13-C15-C16-C17
2	A	601	LI1	O1-C1-C2-O2
2	A	611	LI1	C12-C13-C15-C16
2	A	603	LI1	C14-C13-C15-C16
2	A	611	LI1	C14-C13-C15-C16
2	A	610	LI1	C43-C45-C46-C47
2	A	603	LI1	C11-C12-C13-C14
2	A	601	LI1	O1-C1-C2-C3

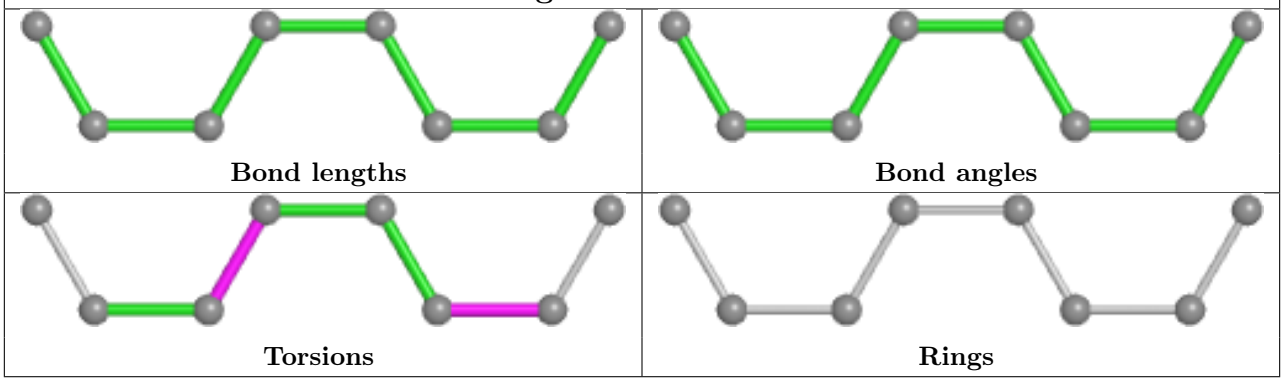
There are no ring outliers.

15 monomers are involved in 61 short contacts:

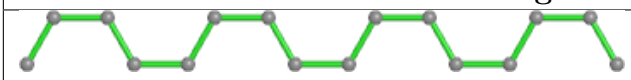
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	605	LI1	1	0
2	A	609	LI1	1	0
2	A	604	LI1	1	0
2	A	603	LI1	6	0
2	A	607	LI1	3	0
2	A	613	LI1	2	0
2	A	611	LI1	5	0
2	A	602	LI1	15	0
2	A	612	LI1	7	0
4	A	301	RET	4	0
2	A	610	LI1	5	0
2	A	608	LI1	2	0
3	A	701	SQU	6	0
2	A	606	LI1	1	0
2	A	601	LI1	7	0

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.

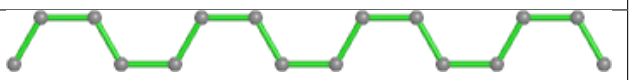
Ligand LI1 A 605



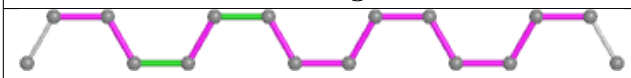
Ligand LI1 A 609



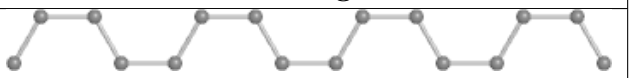
Bond lengths



Bond angles

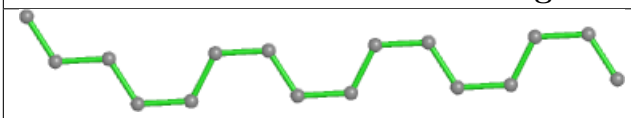


Torsions

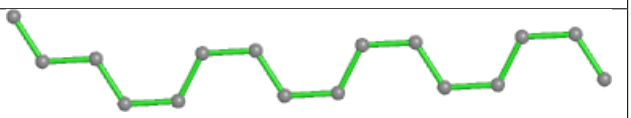


Rings

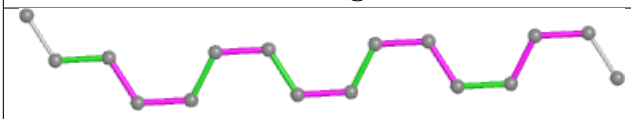
Ligand LI1 A 604



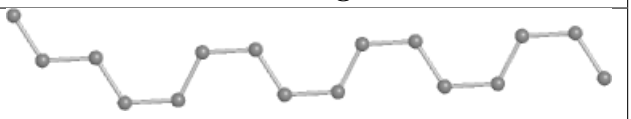
Bond lengths



Bond angles

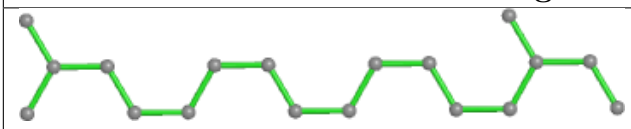


Torsions

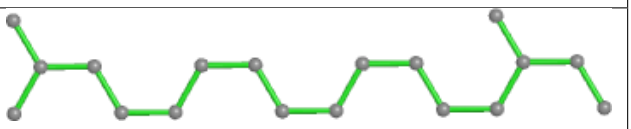


Rings

Ligand LI1 A 603



Bond lengths

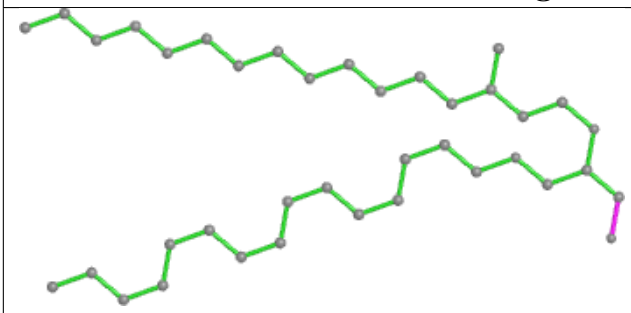


Bond angles

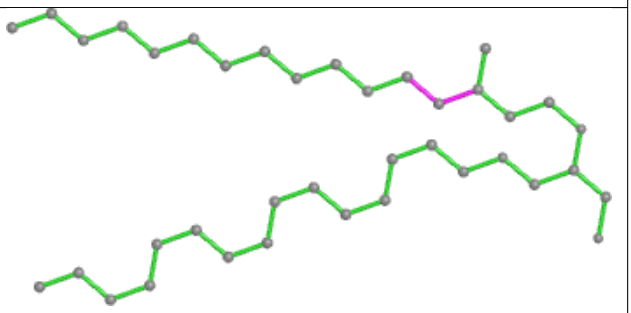
Torsions

Rings

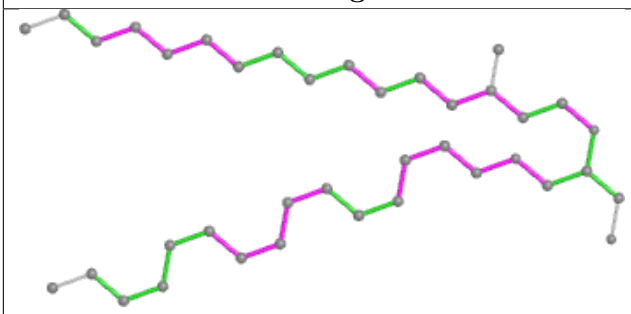
Ligand LI1 A 607



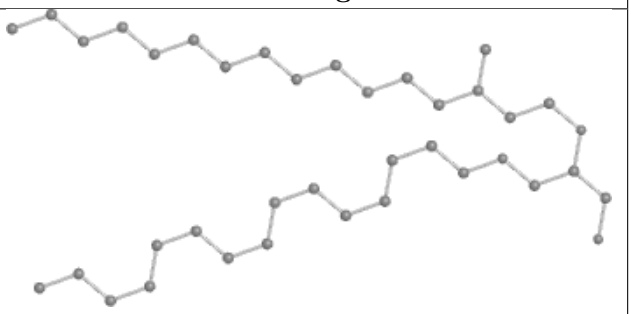
Bond lengths



Bond angles

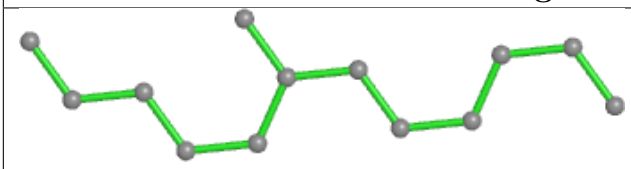


Torsions



Rings

Ligand LI1 A 613



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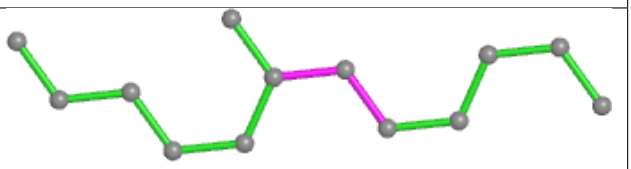
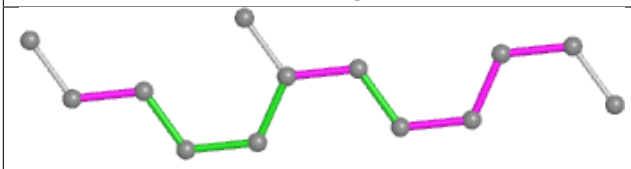


Bond angles



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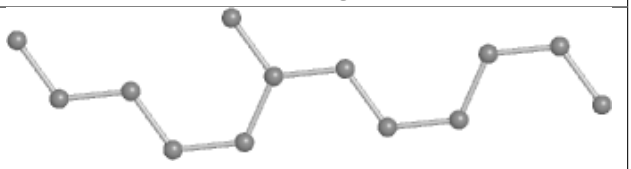
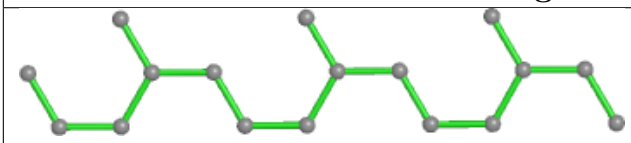
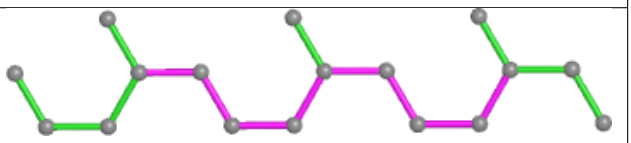


Rings

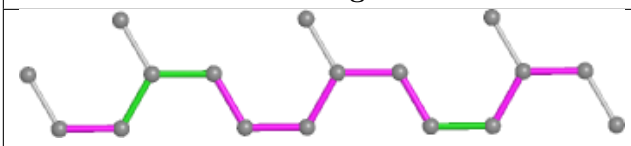
Ligand LI1 A 611



Bond lengths



Bond angles



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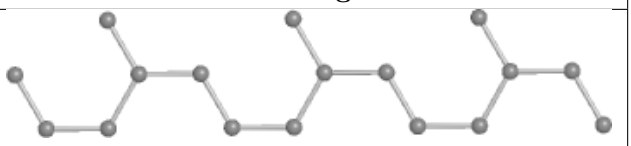
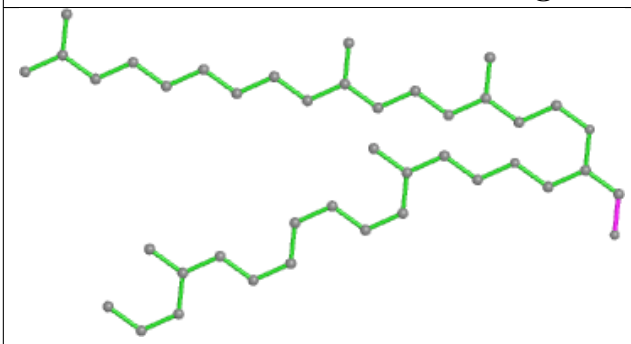


Rings

Ligand LI1 A 602



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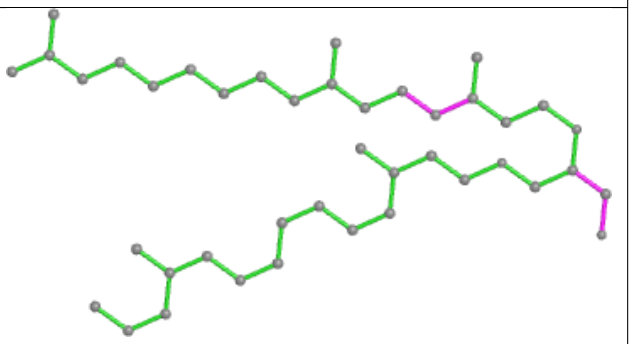
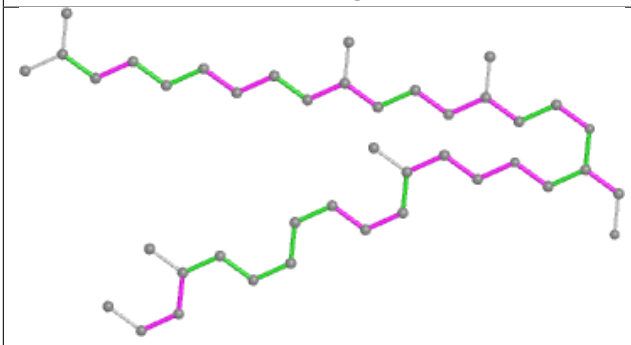
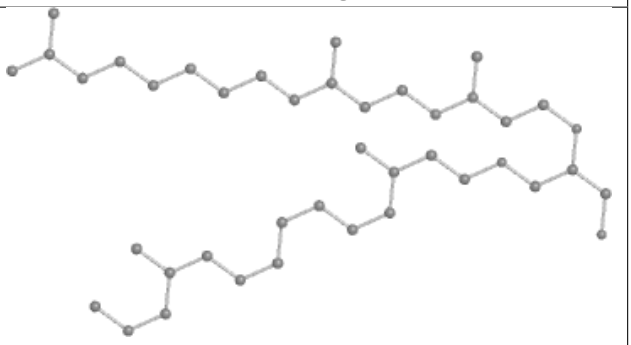


Bond angles

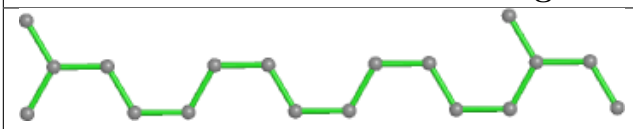


Torsions



Rings

Ligand LI1 A 612



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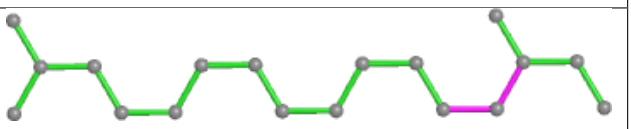
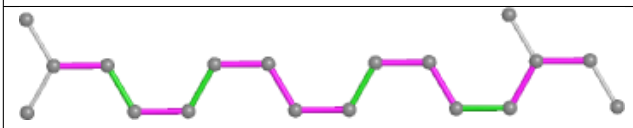


Bond angles



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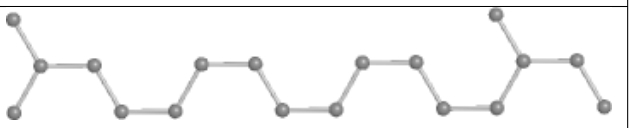
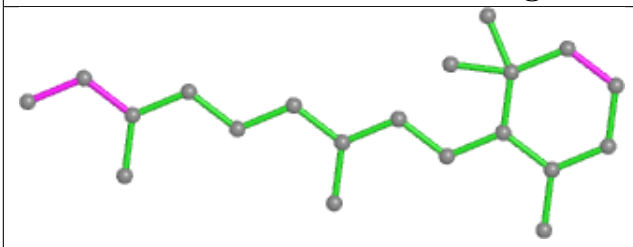


Rings

Ligand RET A 301



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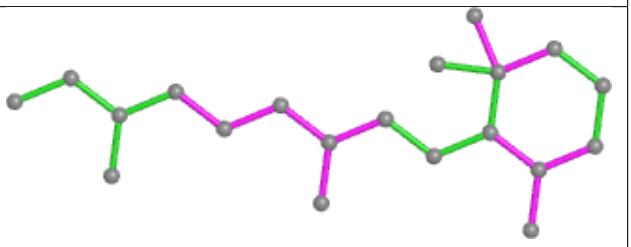
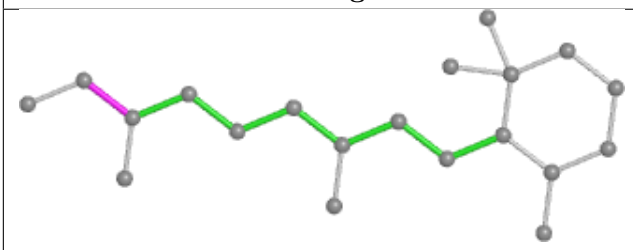


Bond angles



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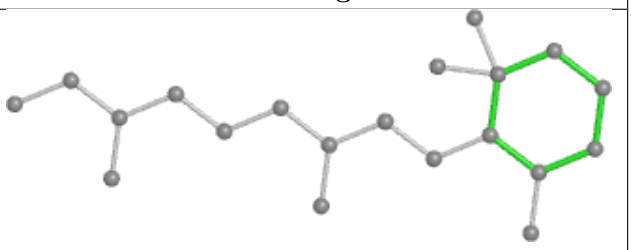
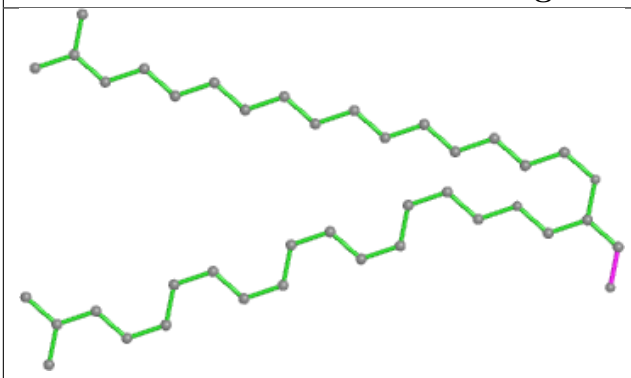
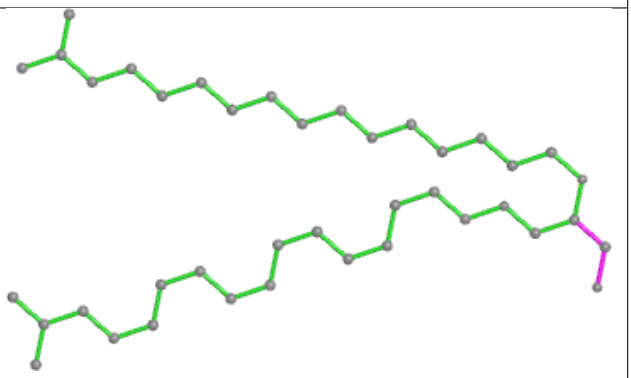


Rings

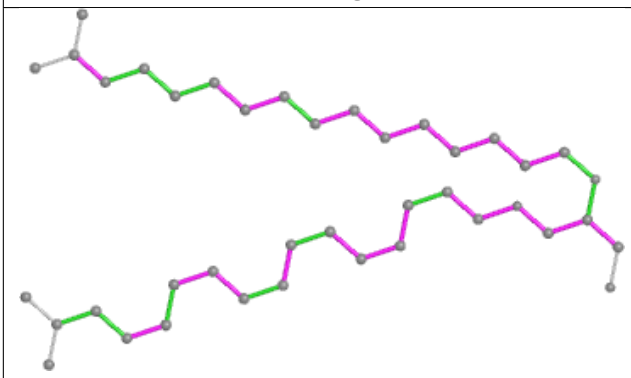
Ligand LI1 A 610



Bond lengths



Bond angles



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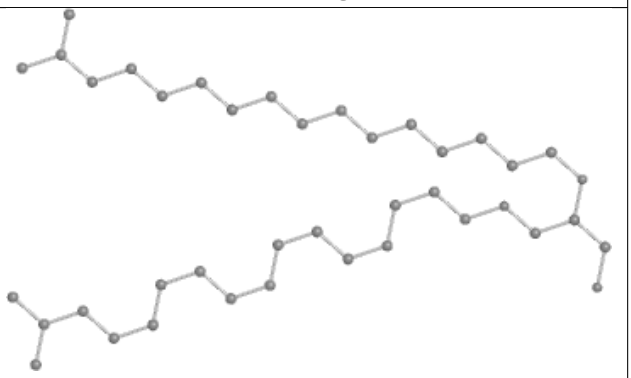
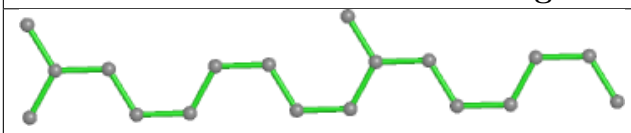


Rings

Ligand LI1 A 608



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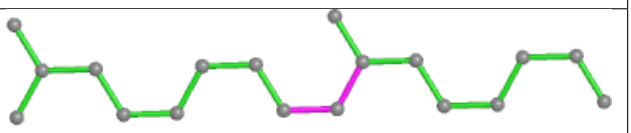
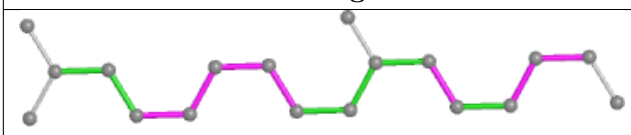
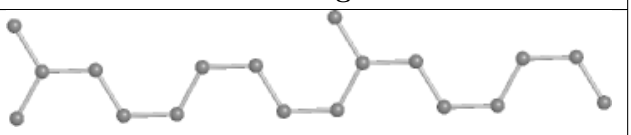


Bond angles

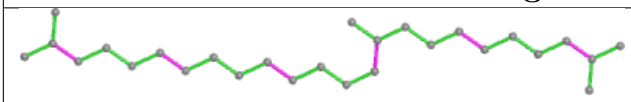


Torsions

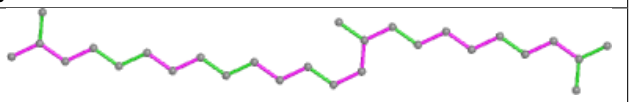


Rings

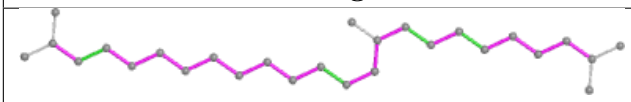
Ligand SQU A 701



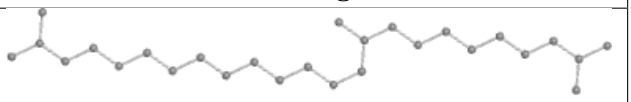
Bond lengths



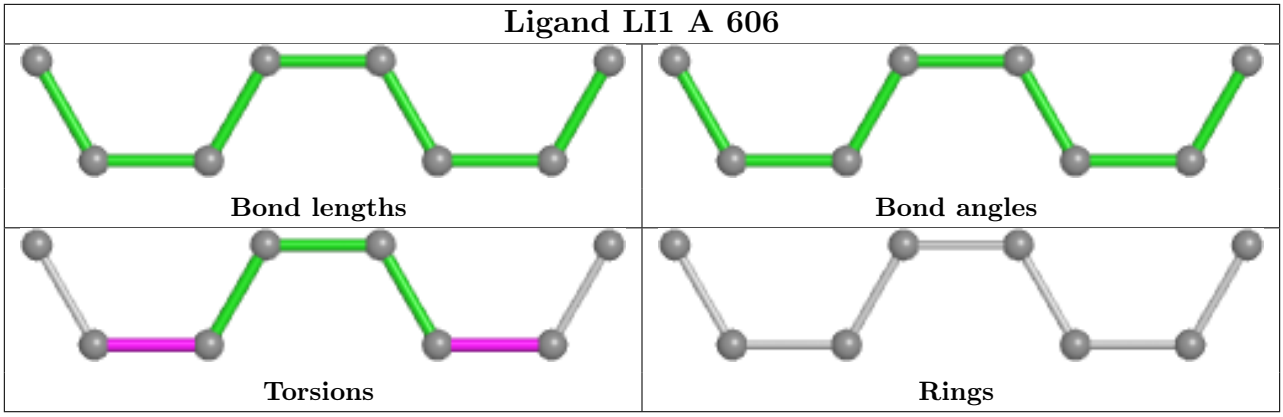
Bond angles

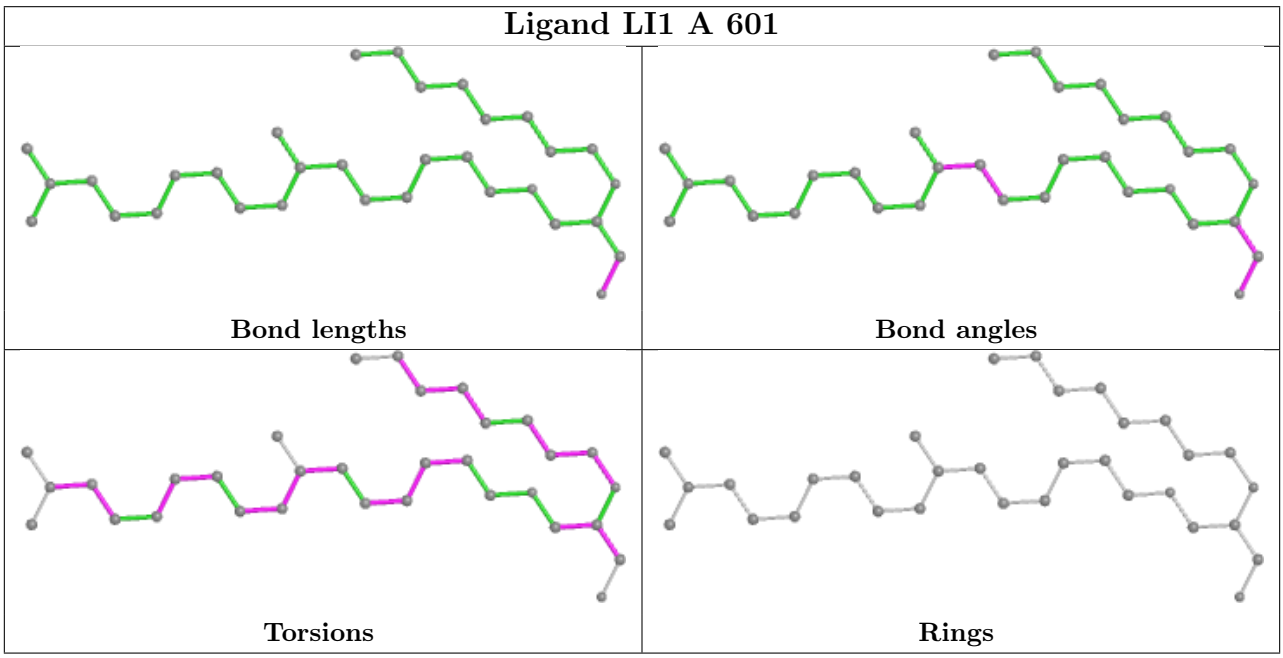


Torsions



Rings





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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.