



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 07:55 pm BST

PDB ID : 1M0L
Title : BACTERIORHODOPSIN/LIPID COMPLEX AT 1.47 Å RESOLUTION
Authors : Lanyi, J.K.
Deposited on : 2002-06-13
Resolution : 1.47 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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

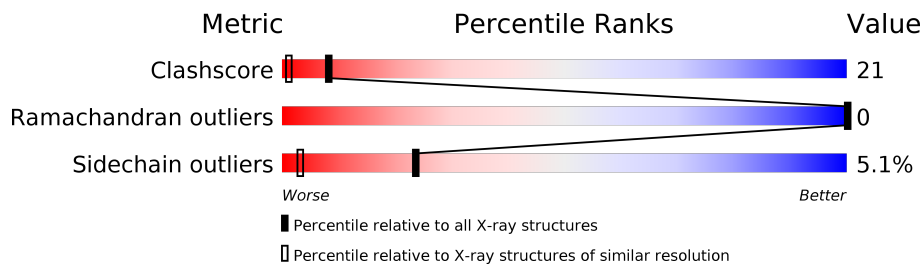
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.47 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	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	262	

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

2 Entry composition [i](#)

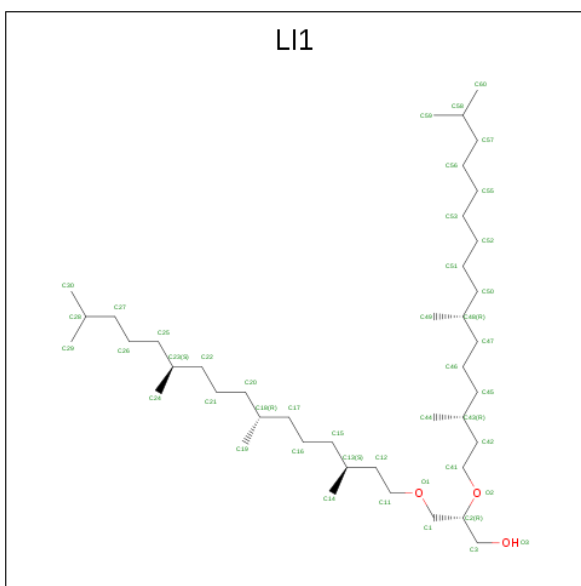
There are 5 unique types of molecules in this entry. The entry contains 2073 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

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: $C_{42}H_{86}O_3$).



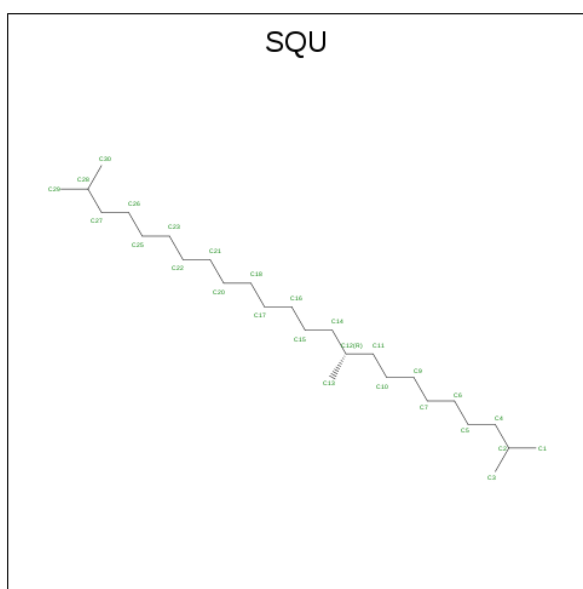
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C O	0	0
			32	29 3		
2	A	1	Total	C O	0	0
			41	38 3		
2	A	1	Total	C	0	0
			18	18		
2	A	1	Total	C	0	0
			16	16		
2	A	1	Total	C	0	0
			8	8		

Continued on next page...

Continued from previous page...

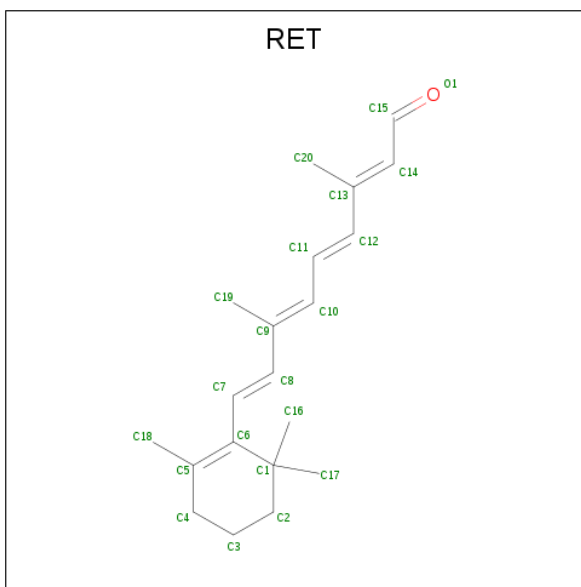
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 8 8	0	0
2	A	1	Total C O 38 35 3	0	0
2	A	1	Total C 18 18	0	0
2	A	1	Total C 16 16	0	0
2	A	1	Total C O 40 37 3	0	0
2	A	1	Total C 17 17	0	0
2	A	1	Total C 18 18	0	0
2	A	1	Total C 13 13	0	0

- 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.

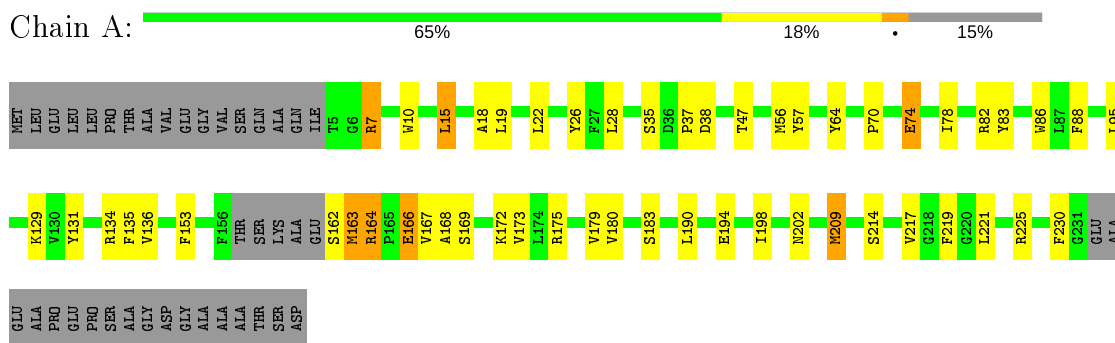
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	23	Total O 23 23	0	0

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: BACTERIORHODOPSIN



4 Data and refinement statistics

Xtrriage (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	60.94Å 60.94Å 110.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 1.47	Depositor
% Data completeness (in resolution range)	97.3 (25.00-1.47)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.149 , 0.179	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2073	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: SQU, RET, LI1

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	0.71	0/1767	1.50	17/2413 (0.7%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ARG	NE-CZ-NH1	12.14	126.37	120.30
1	A	7	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	A	175	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	A	83	TYR	CG-CD1-CE1	-6.58	116.03	121.30
1	A	57	TYR	CB-CG-CD1	-6.55	117.07	121.00
1	A	7	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	A	135	PHE	CB-CG-CD1	-6.04	116.57	120.80
1	A	209	MET	CA-CB-CG	-5.95	103.19	113.30
1	A	88	PHE	CB-CG-CD1	-5.92	116.66	120.80
1	A	86	TRP	CZ3-CH2-CZ2	-5.70	114.76	121.60
1	A	183	SER	O-C-N	-5.57	113.79	122.70
1	A	86	TRP	CH2-CZ2-CE2	5.34	122.74	117.40
1	A	57	TYR	CD1-CG-CD2	5.33	123.77	117.90
1	A	83	TYR	CZ-CE2-CD2	-5.15	115.17	119.80
1	A	134	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	219	PHE	CB-CG-CD1	5.08	124.36	120.80
1	A	82	ARG	NE-CZ-NH2	-5.05	117.77	120.30

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	48	0
2	A	283	0	456	67	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	2312	92	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 21.

All (92) 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:611:LI1:C25	2:A:611:LI1:C26	1.74	1.62
2:A:610:LI1:C25	2:A:610:LI1:C26	1.74	1.61
2:A:609:LI1:C26	2:A:609:LI1:C25	1.74	1.56
1:A:217:VAL:HG11	3:A:701:SQU:H212	1.44	0.99
1:A:26:TYR:HD1	2:A:611:LI1:H152	1.38	0.88
2:A:611:LI1:C25	2:A:611:LI1:C27	2.53	0.86
2:A:610:LI1:C25	2:A:610:LI1:C27	2.53	0.86
2:A:609:LI1:C25	2:A:609:LI1:C27	2.54	0.85
2:A:611:LI1:C26	2:A:611:LI1:C23	2.58	0.82
2:A:609:LI1:C26	2:A:609:LI1:C23	2.57	0.81
2:A:610:LI1:C23	2:A:610:LI1:C26	2.60	0.80
1:A:221:LEU:O	1:A:225:ARG:HG2	1.85	0.77
1:A:214:SER:OG	3:A:701:SQU:H132	1.85	0.77
1:A:131:TYR:OH	2:A:602:LI1:H162	1.87	0.74
1:A:26:TYR:CE1	2:A:611:LI1:H121	2.24	0.72
1:A:136:VAL:HG22	2:A:602:LI1:H531	1.70	0.72
1:A:18:ALA:O	1:A:22:LEU:HD13	1.88	0.71
1:A:180:VAL:HG13	2:A:610:LI1:H591	1.73	0.69
1:A:198:ILE:HD11	2:A:603:LI1:H152	1.76	0.68
1:A:26:TYR:CD1	2:A:611:LI1:H152	2.27	0.68
1:A:131:TYR:OH	2:A:602:LI1:H13	1.95	0.67
1:A:153:PHE:HE1	2:A:610:LI1:H121	1.60	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:602:LI1:H412	2:A:602:LI1:H121	1.78	0.65
2:A:611:LI1:H262	2:A:611:LI1:H241	1.78	0.64
2:A:611:LI1:H262	2:A:611:LI1:C24	2.28	0.63
1:A:70:PRO:HG2	1:A:129:LYS:HD3	1.81	0.61
1:A:163:MET:HG3	1:A:168:ALA:HB2	1.82	0.61
2:A:601:LI1:H172	2:A:601:LI1:H11	1.82	0.60
1:A:26:TYR:CD1	2:A:611:LI1:H121	2.37	0.60
2:A:611:LI1:C26	2:A:611:LI1:C24	2.79	0.59
1:A:47:THR:HG21	2:A:612:LI1:H141	1.83	0.59
1:A:153:PHE:CE2	1:A:179:VAL:HG21	2.40	0.57
3:A:701:SQU:H182	3:A:701:SQU:H13	1.86	0.57
1:A:131:TYR:CE2	2:A:602:LI1:H112	2.39	0.57
2:A:610:LI1:C25	2:A:610:LI1:H272	2.33	0.57
1:A:136:VAL:HA	2:A:602:LI1:C55	2.35	0.56
2:A:601:LI1:H152	2:A:601:LI1:O1	2.05	0.55
1:A:56:MET:HE1	2:A:607:LI1:H501	1.87	0.55
2:A:602:LI1:C52	2:A:602:LI1:H592	2.38	0.54
1:A:190:LEU:CD2	2:A:603:LI1:H222	2.36	0.54
2:A:604:LI1:C28	2:A:610:LI1:H301	2.38	0.53
1:A:35:SER:O	1:A:37:PRO:HD3	2.08	0.53
1:A:19:LEU:HD21	3:A:701:SQU:H32	1.91	0.53
1:A:180:VAL:CG1	2:A:610:LI1:H591	2.37	0.53
1:A:47:THR:HG21	2:A:612:LI1:H162	1.93	0.51
2:A:610:LI1:H272	2:A:610:LI1:H251	1.91	0.51
1:A:70:PRO:HA	1:A:74:GLU:O	2.12	0.50
1:A:136:VAL:HG22	2:A:602:LI1:C53	2.41	0.49
1:A:198:ILE:HD11	2:A:603:LI1:C15	2.42	0.49
1:A:164:ARG:HG3	1:A:167:VAL:HG23	1.95	0.49
1:A:153:PHE:CE1	2:A:610:LI1:H121	2.46	0.49
1:A:131:TYR:CZ	2:A:602:LI1:H13	2.48	0.48
2:A:610:LI1:H501	2:A:610:LI1:H591	1.95	0.48
2:A:610:LI1:H122	2:A:610:LI1:H12	1.44	0.48
2:A:602:LI1:C59	2:A:602:LI1:H501	2.44	0.48
1:A:15:LEU:HD22	1:A:19:LEU:CD1	2.43	0.48
1:A:190:LEU:HD23	2:A:603:LI1:H222	1.96	0.47
1:A:166:GLU:H	1:A:166:GLU:HG3	1.39	0.47
1:A:131:TYR:CE2	2:A:602:LI1:H13	2.50	0.46
2:A:602:LI1:H411	2:A:602:LI1:H442	1.45	0.46
2:A:611:LI1:H252	2:A:611:LI1:H211	1.69	0.46
1:A:136:VAL:HA	2:A:602:LI1:H551	1.96	0.46
2:A:610:LI1:H593	2:A:610:LI1:C51	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LEU:HD21	2:A:603:LI1:H222	1.98	0.45
2:A:602:LI1:H592	2:A:602:LI1:H501	1.99	0.45
2:A:602:LI1:H592	2:A:602:LI1:H521	1.98	0.45
1:A:28:LEU:HD23	2:A:612:LI1:C14	2.46	0.44
1:A:70:PRO:CG	1:A:129:LYS:HD3	2.44	0.44
2:A:601:LI1:H302	2:A:608:LI1:H303	2.00	0.44
4:A:301:RET:H181	4:A:301:RET:H7	1.81	0.43
1:A:64:TYR:CZ	2:A:607:LI1:H32	2.54	0.43
2:A:608:LI1:H211	2:A:608:LI1:H172	1.91	0.43
1:A:164:ARG:NH2	1:A:230:PHE:O	2.48	0.42
2:A:603:LI1:H262	2:A:603:LI1:H303	1.85	0.42
2:A:613:LI1:H201	2:A:613:LI1:H162	1.33	0.42
1:A:15:LEU:HD13	1:A:209:MET:HE1	2.02	0.42
2:A:611:LI1:H193	2:A:611:LI1:H162	1.63	0.42
2:A:601:LI1:H301	2:A:608:LI1:H272	2.02	0.42
1:A:78:ILE:HD12	1:A:194:GLU:HG3	2.01	0.42
4:A:301:RET:H171	4:A:301:RET:H8	2.01	0.42
3:A:701:SQU:H133	3:A:701:SQU:H102	1.97	0.42
1:A:172:LYS:HD3	2:A:610:LI1:O3	2.21	0.41
2:A:601:LI1:H193	2:A:601:LI1:H162	1.42	0.41
1:A:7:ARG:O	1:A:10:TRP:HD1	2.03	0.41
1:A:164:ARG:HG2	1:A:164:ARG:H	1.50	0.41
2:A:610:LI1:H501	2:A:610:LI1:C59	2.51	0.41
2:A:602:LI1:H211	2:A:602:LI1:H243	1.70	0.41
2:A:610:LI1:H593	2:A:610:LI1:C52	2.51	0.41
1:A:169:SER:O	1:A:173:VAL:HG23	2.21	0.41
2:A:608:LI1:H262	2:A:608:LI1:H292	1.73	0.41
2:A:612:LI1:H143	5:A:512:HOH:O	2.21	0.40
3:A:701:SQU:C1	3:A:701:SQU:H182	2.51	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	218/262 (83%)	216 (99%)	2 (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	178/206 (86%)	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	95	LEU
1	A	162	SER
1	A	163	MET
1	A	164	ARG
1	A	166	GLU
1	A	202	ASN

Some 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 carbohydrates 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	602	-	40,40,44	1.03	2 (5%)	43,45,51	2.23	8 (18%)
2	LI1	A	605	-	7,7,44	0.47	0	6,6,51	0.53	0
2	LI1	A	611	-	16,16,44	1.14	1 (6%)	18,18,51	1.61	5 (27%)
2	LI1	A	607	-	37,37,44	1.00	2 (5%)	37,38,51	1.08	2 (5%)
2	LI1	A	612	-	17,17,44	1.11	1 (5%)	18,18,51	1.29	2 (11%)
2	LI1	A	603	-	17,17,44	1.09	1 (5%)	18,18,51	1.18	2 (11%)
2	LI1	A	604	-	15,15,44	1.13	1 (6%)	14,14,51	1.07	1 (7%)
2	LI1	A	610	-	39,39,44	1.07	2 (5%)	41,41,51	1.13	2 (4%)
4	RET	A	301	1	20,20,21	1.29	3 (15%)	27,27,28	1.97	11 (40%)
2	LI1	A	601	-	31,31,44	1.11	2 (6%)	33,33,51	1.23	3 (9%)
2	LI1	A	613	-	12,12,44	0.47	0	12,12,51	1.05	1 (8%)
3	SQU	A	701	-	26,26,26	1.41	6 (23%)	28,28,28	1.75	7 (25%)
2	LI1	A	608	-	17,17,44	1.06	1 (5%)	18,18,51	1.29	2 (11%)
2	LI1	A	606	-	7,7,44	0.47	0	6,6,51	0.69	0
2	LI1	A	609	-	15,15,44	1.15	1 (6%)	14,14,51	1.19	2 (14%)

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	602	-	1/1/6/8	26/44/44/49	-
2	LI1	A	605	-	-	4/5/5/49	-
2	LI1	A	611	-	1/1/3/8	13/17/17/49	-
2	LI1	A	607	-	-	23/38/38/49	-
2	LI1	A	612	-	-	8/16/16/49	-
2	LI1	A	603	-	-	10/16/16/49	-
2	LI1	A	604	-	-	7/13/13/49	-
2	LI1	A	610	-	-	28/39/39/49	-
4	RET	A	301	1	-	2/13/30/31	0/1/1/1
2	LI1	A	601	-	2/2/3/8	19/32/32/49	-
2	LI1	A	613	-	1/1/1/8	8/11/11/49	-
3	SQU	A	701	-	1/1/3/3	17/25/25/25	-
2	LI1	A	608	-	-	11/16/16/49	-
2	LI1	A	606	-	-	3/5/5/49	-
2	LI1	A	609	-	-	8/13/13/49	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	610	LI1	C26-C25	4.11	1.74	1.51
2	A	611	LI1	C26-C25	4.11	1.74	1.51
2	A	609	LI1	C26-C25	4.08	1.74	1.51
2	A	612	LI1	C26-C25	4.03	1.74	1.51
2	A	604	LI1	C26-C25	4.01	1.74	1.51
2	A	603	LI1	C26-C25	4.01	1.74	1.51
2	A	608	LI1	C26-C25	4.00	1.74	1.51
2	A	602	LI1	C26-C25	3.99	1.73	1.51
2	A	601	LI1	C26-C25	3.97	1.73	1.51
2	A	607	LI1	C26-C25	3.92	1.73	1.51
2	A	610	LI1	O3-C3	3.31	1.56	1.42
3	A	701	SQU	C14-C12	-3.18	1.35	1.52
2	A	601	LI1	O3-C3	3.12	1.55	1.42
4	A	301	RET	C14-C13	3.08	1.36	1.33
4	A	301	RET	C2-C3	-3.04	1.45	1.52
3	A	701	SQU	C23-C22	-3.03	1.34	1.51
3	A	701	SQU	C18-C17	-2.93	1.35	1.51
3	A	701	SQU	C9-C7	-2.92	1.35	1.51
2	A	602	LI1	O3-C3	2.89	1.54	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	607	LI1	O3-C3	2.89	1.54	1.42
3	A	701	SQU	C4-C2	-2.38	1.35	1.51
4	A	301	RET	C17-C1	2.31	1.58	1.53
3	A	701	SQU	C27-C28	-2.14	1.37	1.51

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	602	LI1	C49-C48-C47	-10.08	74.78	111.29
2	A	602	LI1	C49-C48-C50	5.58	131.50	111.29
4	A	301	RET	C11-C10-C9	-5.53	119.41	127.31
3	A	701	SQU	C15-C14-C12	4.37	130.04	115.92
4	A	301	RET	C8-C9-C10	-3.67	113.31	118.94
2	A	608	LI1	C25-C26-C27	-3.67	100.64	113.62
2	A	601	LI1	C25-C26-C27	-3.58	100.95	113.62
2	A	603	LI1	C25-C26-C27	-3.57	101.00	113.62
2	A	610	LI1	C25-C26-C27	-3.52	101.17	113.62
2	A	612	LI1	C25-C26-C27	-3.39	101.64	113.62
2	A	602	LI1	C51-C50-C48	-3.30	105.25	115.92
3	A	701	SQU	C10-C9-C7	3.29	131.13	114.42
2	A	602	LI1	C24-C23-C25	-3.29	99.39	111.29
2	A	611	LI1	C16-C17-C18	-3.11	105.87	115.92
2	A	602	LI1	O3-C3-C2	-2.99	103.86	111.78
3	A	701	SQU	C5-C4-C2	2.97	129.97	115.98
2	A	611	LI1	C24-C23-C25	2.97	122.03	111.29
2	A	607	LI1	O2-C41-C42	2.86	114.78	108.77
4	A	301	RET	C10-C11-C12	-2.82	114.43	123.22
2	A	610	LI1	O3-C3-C2	-2.76	104.46	111.78
2	A	601	LI1	O3-C3-C2	-2.71	104.59	111.78
3	A	701	SQU	C25-C23-C22	2.70	128.13	114.42
2	A	601	LI1	C16-C17-C18	-2.69	107.24	115.92
2	A	611	LI1	C27-C26-C25	-2.61	100.68	113.29
2	A	602	LI1	C21-C22-C23	-2.59	107.55	115.92
2	A	609	LI1	C27-C26-C25	-2.56	101.43	114.42
2	A	611	LI1	C26-C25-C23	-2.53	103.74	115.86
4	A	301	RET	C20-C13-C12	2.52	122.05	118.08
2	A	602	LI1	C26-C25-C23	-2.49	103.92	115.86
3	A	701	SQU	C18-C17-C16	2.48	127.03	114.42
2	A	604	LI1	C27-C26-C25	-2.44	102.05	114.42
2	A	611	LI1	C21-C20-C18	-2.41	108.11	115.92
3	A	701	SQU	C9-C7-C6	2.41	126.67	114.42
2	A	608	LI1	C21-C20-C18	-2.39	108.19	115.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	SQU	C20-C18-C17	2.38	126.51	114.42
2	A	602	LI1	C27-C26-C25	-2.38	101.81	113.29
2	A	613	LI1	C21-C20-C18	-2.32	108.43	115.92
4	A	301	RET	C1-C6-C7	2.28	122.22	115.78
4	A	301	RET	C18-C5-C4	-2.26	109.27	113.62
2	A	603	LI1	C26-C25-C23	-2.24	103.04	114.42
2	A	609	LI1	C26-C25-C23	-2.19	103.31	114.42
4	A	301	RET	C12-C13-C14	-2.14	112.02	118.80
4	A	301	RET	C18-C5-C6	2.13	126.92	124.53
4	A	301	RET	C19-C9-C8	2.12	121.41	118.08
2	A	612	LI1	C16-C15-C13	-2.09	109.15	115.92
4	A	301	RET	C2-C1-C6	2.06	113.66	110.48
4	A	301	RET	C17-C1-C2	-2.05	100.71	108.91
2	A	607	LI1	C26-C25-C23	-2.04	104.09	114.42

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	602	LI1	C48
2	A	611	LI1	C13
2	A	601	LI1	C2
2	A	601	LI1	C18
2	A	613	LI1	C18
3	A	701	SQU	C12

All (187) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	611	LI1	C11-C12-C13-C15
2	A	607	LI1	C42-C41-O2-C2
2	A	612	LI1	C14-C13-C15-C16
2	A	610	LI1	C1-C2-C3-O3
2	A	610	LI1	O2-C2-C3-O3
4	A	301	RET	C20-C13-C14-C15
2	A	610	LI1	C12-C11-O1-C1
3	A	701	SQU	C20-C21-C22-C23
2	A	602	LI1	O2-C41-C42-C43
2	A	603	LI1	C25-C26-C27-C28
2	A	602	LI1	C49-C48-C50-C51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	611	LI1	C16-C17-C18-C19
2	A	611	LI1	C24-C23-C25-C26
2	A	607	LI1	C44-C43-C45-C46
2	A	601	LI1	C16-C17-C18-C19
3	A	701	SQU	C10-C11-C12-C13
2	A	607	LI1	O1-C11-C12-C13
2	A	602	LI1	C45-C46-C47-C48
2	A	613	LI1	C16-C17-C18-C20
3	A	701	SQU	C11-C12-C14-C15
2	A	603	LI1	C13-C15-C16-C17
2	A	610	LI1	C25-C26-C27-C28
2	A	611	LI1	C18-C20-C21-C22
2	A	601	LI1	C25-C26-C27-C28
2	A	610	LI1	O2-C41-C42-C43
2	A	602	LI1	C55-C56-C57-C58
2	A	608	LI1	C15-C16-C17-C18
2	A	610	LI1	C16-C17-C18-C20
3	A	701	SQU	C11-C10-C9-C7
2	A	606	LI1	C15-C16-C17-C18
3	A	701	SQU	C16-C17-C18-C20
2	A	609	LI1	C13-C15-C16-C17
2	A	610	LI1	C20-C21-C22-C23
3	A	701	SQU	C22-C23-C25-C26
2	A	612	LI1	C18-C20-C21-C22
2	A	604	LI1	C20-C21-C22-C23
3	A	701	SQU	C3-C2-C4-C5
2	A	610	LI1	C52-C53-C55-C56
2	A	607	LI1	C23-C25-C26-C27
2	A	610	LI1	C12-C13-C15-C16
2	A	602	LI1	C52-C53-C55-C56
2	A	610	LI1	C23-C25-C26-C27
3	A	701	SQU	C14-C15-C16-C17
3	A	701	SQU	C23-C25-C26-C27
2	A	602	LI1	C42-C41-O2-C2
2	A	607	LI1	C53-C55-C56-C57
2	A	604	LI1	C25-C26-C27-C28
2	A	610	LI1	C51-C52-C53-C55
2	A	607	LI1	C20-C21-C22-C23
2	A	612	LI1	C23-C25-C26-C27
2	A	611	LI1	C20-C21-C22-C23
2	A	602	LI1	C50-C51-C52-C53
2	A	608	LI1	C20-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	604	LI1	C16-C17-C18-C20
2	A	610	LI1	O1-C11-C12-C13
2	A	607	LI1	C52-C53-C55-C56
2	A	601	LI1	C12-C13-C15-C16
2	A	605	LI1	C16-C17-C18-C20
2	A	602	LI1	C56-C57-C58-C60
2	A	608	LI1	C26-C27-C28-C30
2	A	610	LI1	C41-C42-C43-C45
2	A	601	LI1	C46-C47-C48-C50
2	A	611	LI1	C11-C12-C13-C14
2	A	604	LI1	C21-C22-C23-C25
2	A	601	LI1	C21-C22-C23-C25
2	A	610	LI1	C22-C23-C25-C26
2	A	601	LI1	C45-C46-C47-C48
2	A	610	LI1	C47-C48-C50-C51
2	A	612	LI1	C15-C16-C17-C18
2	A	610	LI1	C15-C16-C17-C18
3	A	701	SQU	C18-C20-C21-C22
3	A	701	SQU	C9-C10-C11-C12
2	A	602	LI1	C15-C16-C17-C18
2	A	607	LI1	C15-C16-C17-C18
3	A	701	SQU	C4-C5-C6-C7
2	A	607	LI1	C22-C23-C25-C26
2	A	602	LI1	C56-C57-C58-C59
3	A	701	SQU	C26-C27-C28-C29
3	A	701	SQU	C25-C26-C27-C28
2	A	607	LI1	C55-C56-C57-C58
2	A	601	LI1	O1-C1-C2-C3
2	A	610	LI1	C48-C50-C51-C52
2	A	608	LI1	C25-C26-C27-C28
2	A	613	LI1	C11-C12-C13-C15
2	A	613	LI1	C21-C22-C23-C24
2	A	606	LI1	C13-C15-C16-C17
2	A	603	LI1	C23-C25-C26-C27
2	A	608	LI1	C23-C25-C26-C27
2	A	604	LI1	C17-C18-C20-C21
2	A	613	LI1	C12-C13-C15-C16
2	A	607	LI1	C47-C48-C50-C51
2	A	609	LI1	C23-C25-C26-C27
2	A	609	LI1	C26-C27-C28-C30
2	A	603	LI1	C20-C21-C22-C23
2	A	602	LI1	C12-C11-O1-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	611	LI1	C12-C13-C15-C16
2	A	612	LI1	C12-C13-C15-C16
2	A	602	LI1	C44-C43-C45-C46
2	A	602	LI1	C46-C47-C48-C49
2	A	601	LI1	C19-C18-C20-C21
2	A	613	LI1	C16-C17-C18-C19
2	A	601	LI1	C15-C16-C17-C18
2	A	601	LI1	C41-C42-C43-C45
2	A	602	LI1	C53-C55-C56-C57
4	A	301	RET	C12-C13-C14-C15
2	A	608	LI1	C21-C22-C23-C25
2	A	612	LI1	C21-C22-C23-C25
2	A	602	LI1	C13-C15-C16-C17
2	A	611	LI1	C23-C25-C26-C27
2	A	602	LI1	C11-C12-C13-C15
2	A	607	LI1	O1-C1-C2-C3
2	A	610	LI1	C53-C55-C56-C57
3	A	701	SQU	C6-C7-C9-C10
2	A	608	LI1	C26-C27-C28-C29
2	A	613	LI1	C15-C16-C17-C18
2	A	603	LI1	C21-C22-C23-C25
2	A	607	LI1	O1-C1-C2-O2
2	A	602	LI1	C1-C2-C3-O3
2	A	608	LI1	C22-C23-C25-C26
2	A	607	LI1	C18-C20-C21-C22
2	A	610	LI1	C50-C51-C52-C53
2	A	605	LI1	C18-C20-C21-C22
2	A	607	LI1	C45-C46-C47-C48
2	A	605	LI1	C13-C15-C16-C17
2	A	609	LI1	C21-C22-C23-C25
2	A	602	LI1	C42-C43-C45-C46
2	A	611	LI1	C22-C23-C25-C26
2	A	601	LI1	C17-C18-C20-C21
2	A	613	LI1	C17-C18-C20-C21
2	A	601	LI1	O2-C2-C3-O3
2	A	612	LI1	C17-C18-C20-C21
2	A	607	LI1	C12-C11-O1-C1
2	A	610	LI1	O1-C1-C2-C3
3	A	701	SQU	C5-C6-C7-C9
2	A	610	LI1	O1-C1-C2-O2
2	A	608	LI1	C16-C17-C18-C19
2	A	604	LI1	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	602	LI1	O1-C11-C12-C13
3	A	701	SQU	C26-C27-C28-C30
2	A	607	LI1	C12-C13-C15-C16
2	A	610	LI1	C17-C18-C20-C21
2	A	610	LI1	C56-C57-C58-C59
2	A	608	LI1	C12-C13-C15-C16
2	A	611	LI1	C16-C17-C18-C20
2	A	607	LI1	C42-C43-C45-C46
2	A	603	LI1	C12-C13-C15-C16
2	A	608	LI1	C16-C17-C18-C20
2	A	609	LI1	C20-C21-C22-C23
2	A	602	LI1	C2-C1-O1-C11
2	A	601	LI1	O1-C1-C2-O2
2	A	609	LI1	C12-C13-C15-C16
2	A	611	LI1	C14-C13-C15-C16
2	A	611	LI1	C21-C22-C23-C24
2	A	603	LI1	C14-C13-C15-C16
2	A	613	LI1	C19-C18-C20-C21
2	A	610	LI1	C2-C1-O1-C11
2	A	612	LI1	C22-C23-C25-C26
2	A	601	LI1	C12-C11-O1-C1
2	A	609	LI1	C16-C17-C18-C20
2	A	607	LI1	C48-C50-C51-C52
2	A	601	LI1	C26-C27-C28-C30
2	A	607	LI1	C46-C47-C48-C50
2	A	611	LI1	C21-C22-C23-C25
2	A	601	LI1	C16-C17-C18-C20
2	A	601	LI1	C2-C1-O1-C11
2	A	609	LI1	C11-C12-C13-C15
2	A	606	LI1	C16-C17-C18-C20
2	A	601	LI1	C26-C27-C28-C29
2	A	601	LI1	C20-C21-C22-C23
2	A	603	LI1	C18-C20-C21-C22
2	A	610	LI1	C26-C27-C28-C29
2	A	603	LI1	C11-C12-C13-C14
2	A	602	LI1	C12-C13-C15-C16
2	A	603	LI1	C15-C16-C17-C18
2	A	607	LI1	O2-C41-C42-C43
2	A	604	LI1	C22-C23-C25-C26
2	A	602	LI1	C41-C42-C43-C45
2	A	610	LI1	C45-C46-C47-C48
2	A	610	LI1	C46-C47-C48-C50

Continued on next page...

Continued from previous page...

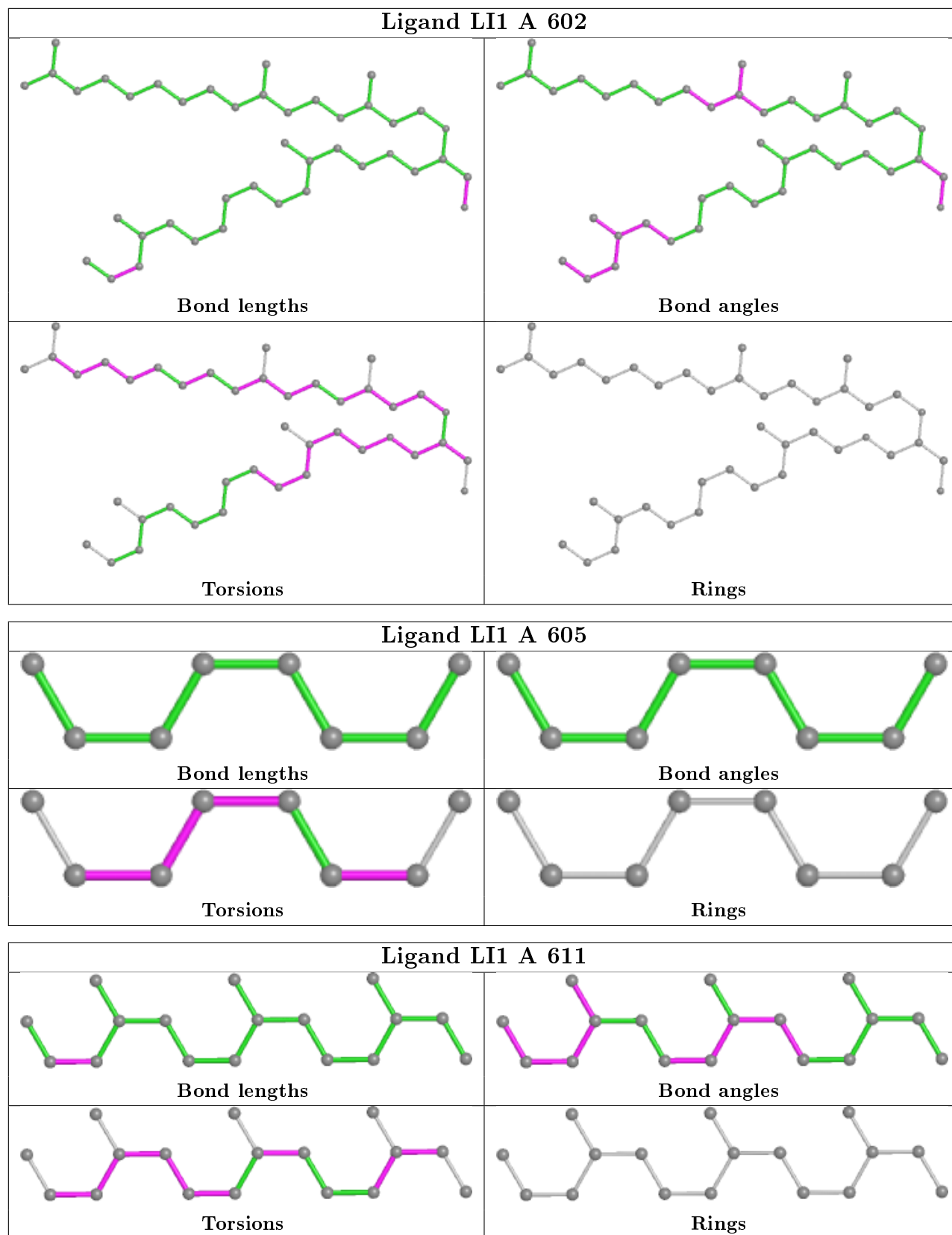
Mol	Chain	Res	Type	Atoms
2	A	602	LI1	O1-C1-C2-C3
2	A	605	LI1	C17-C18-C20-C21
2	A	610	LI1	C21-C22-C23-C25
2	A	607	LI1	C13-C15-C16-C17
2	A	607	LI1	C41-C42-C43-C45

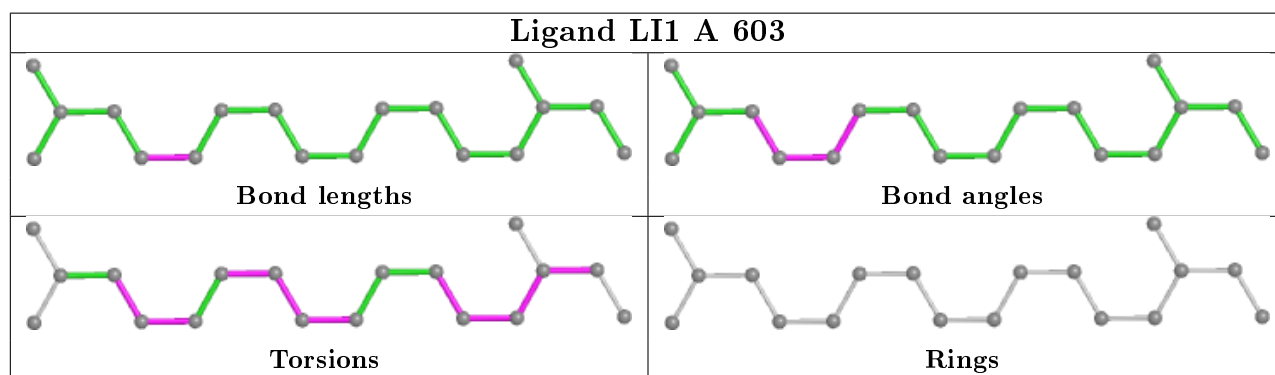
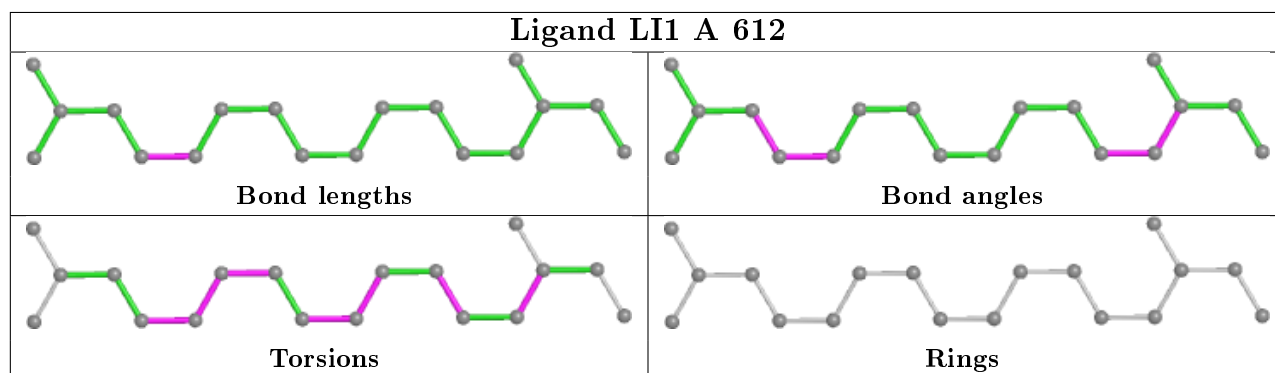
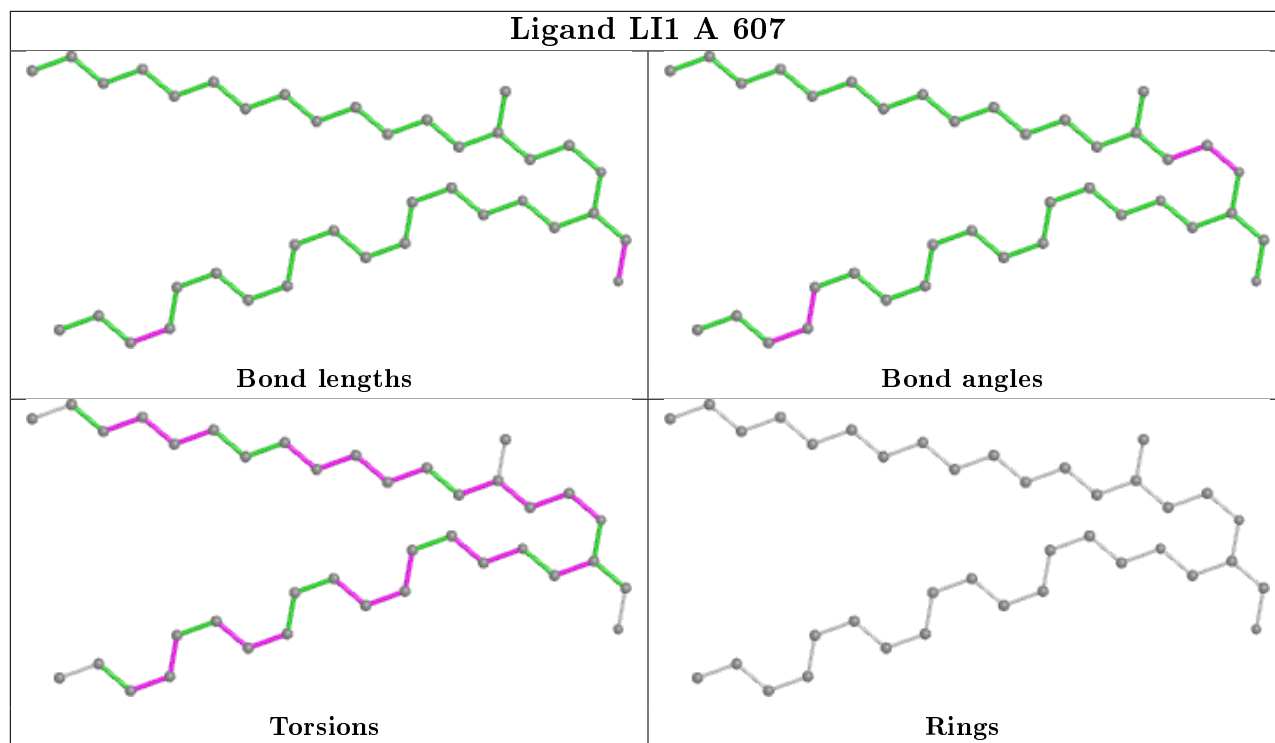
There are no ring outliers.

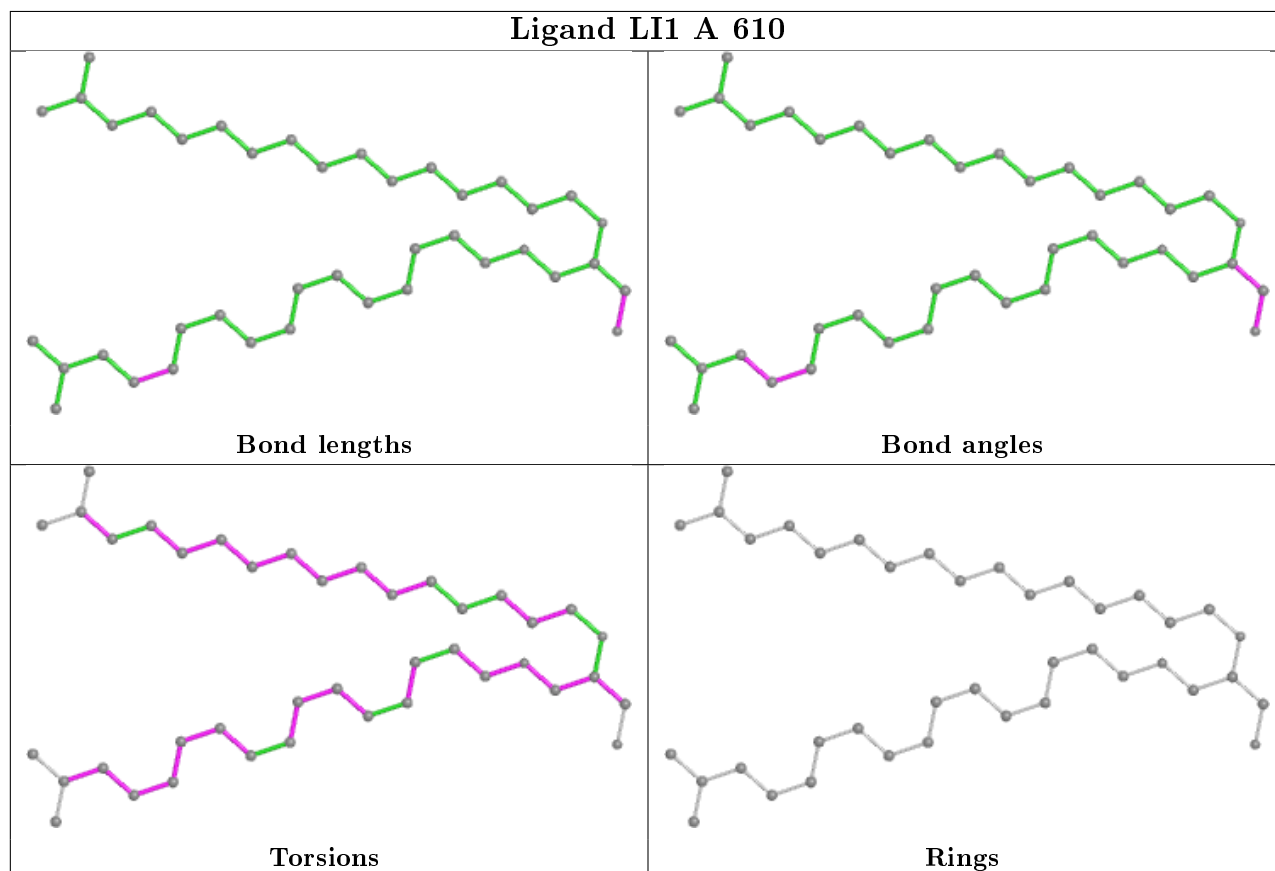
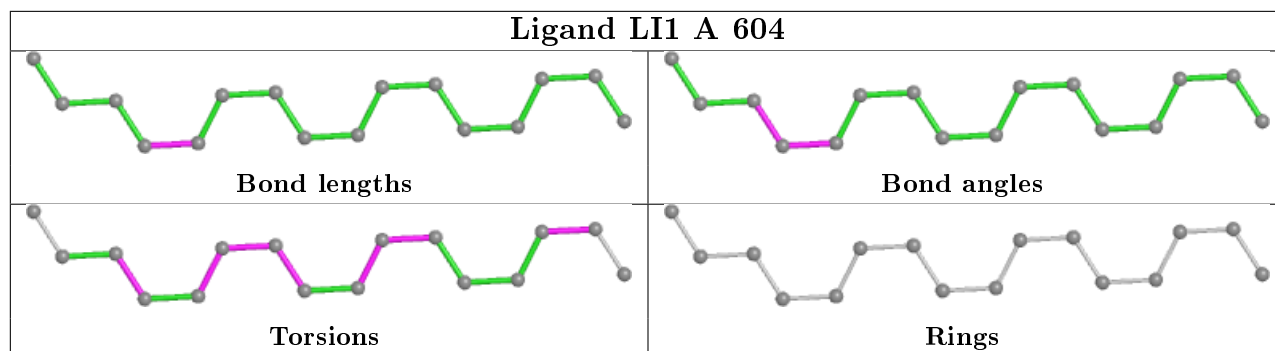
13 monomers are involved in 75 short contacts:

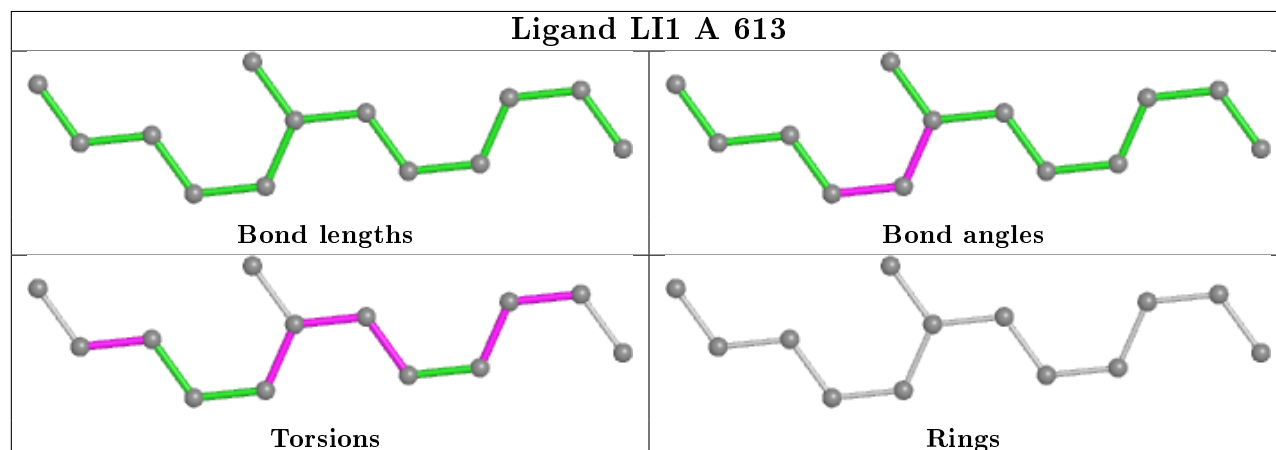
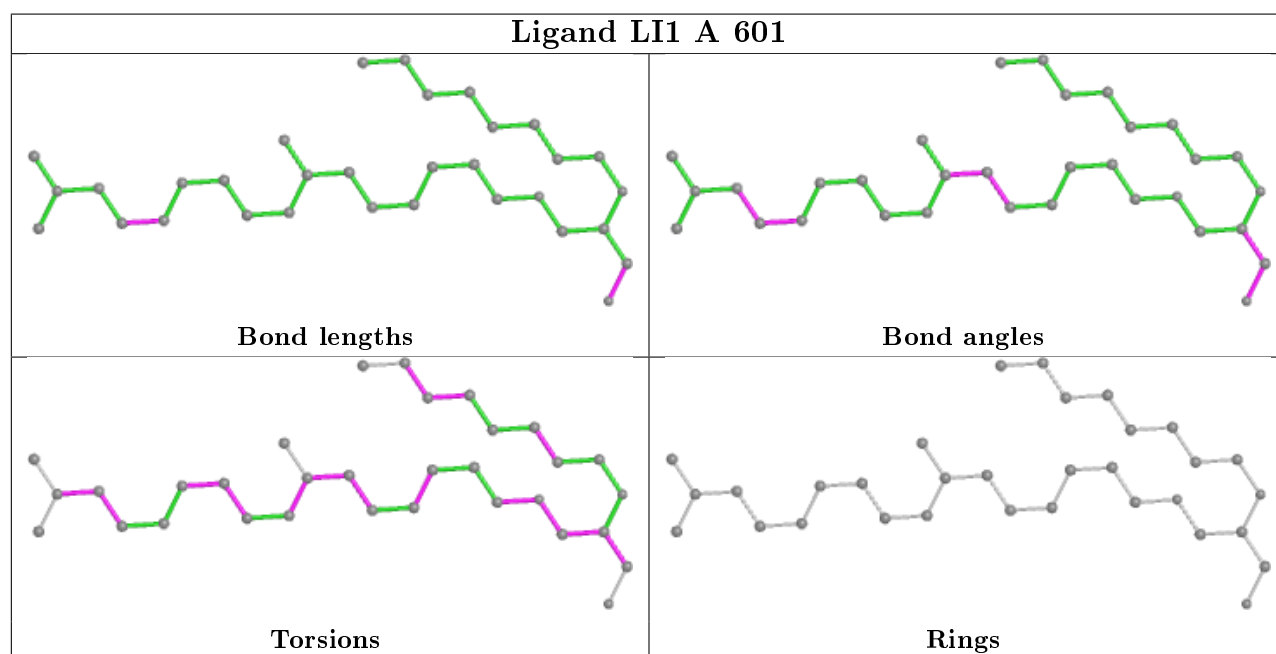
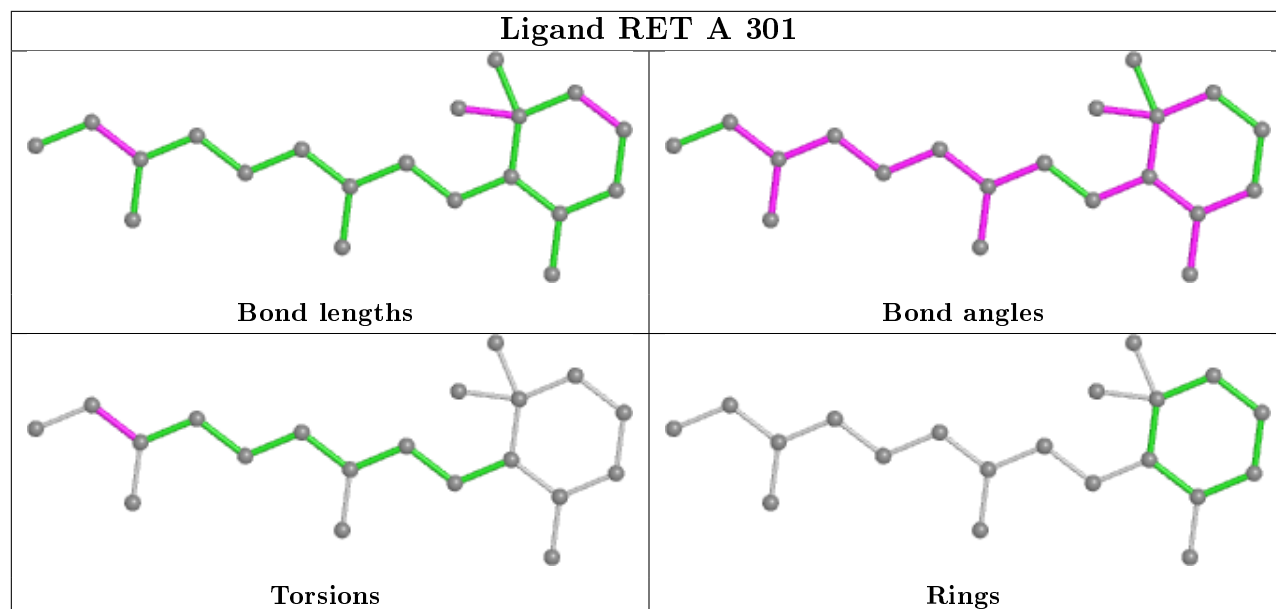
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	LI1	16	0
2	A	611	LI1	12	0
2	A	607	LI1	2	0
2	A	612	LI1	4	0
2	A	603	LI1	6	0
2	A	604	LI1	1	0
2	A	610	LI1	16	0
4	A	301	RET	2	0
2	A	601	LI1	5	0
2	A	613	LI1	1	0
3	A	701	SQU	6	0
2	A	608	LI1	4	0
2	A	609	LI1	3	0

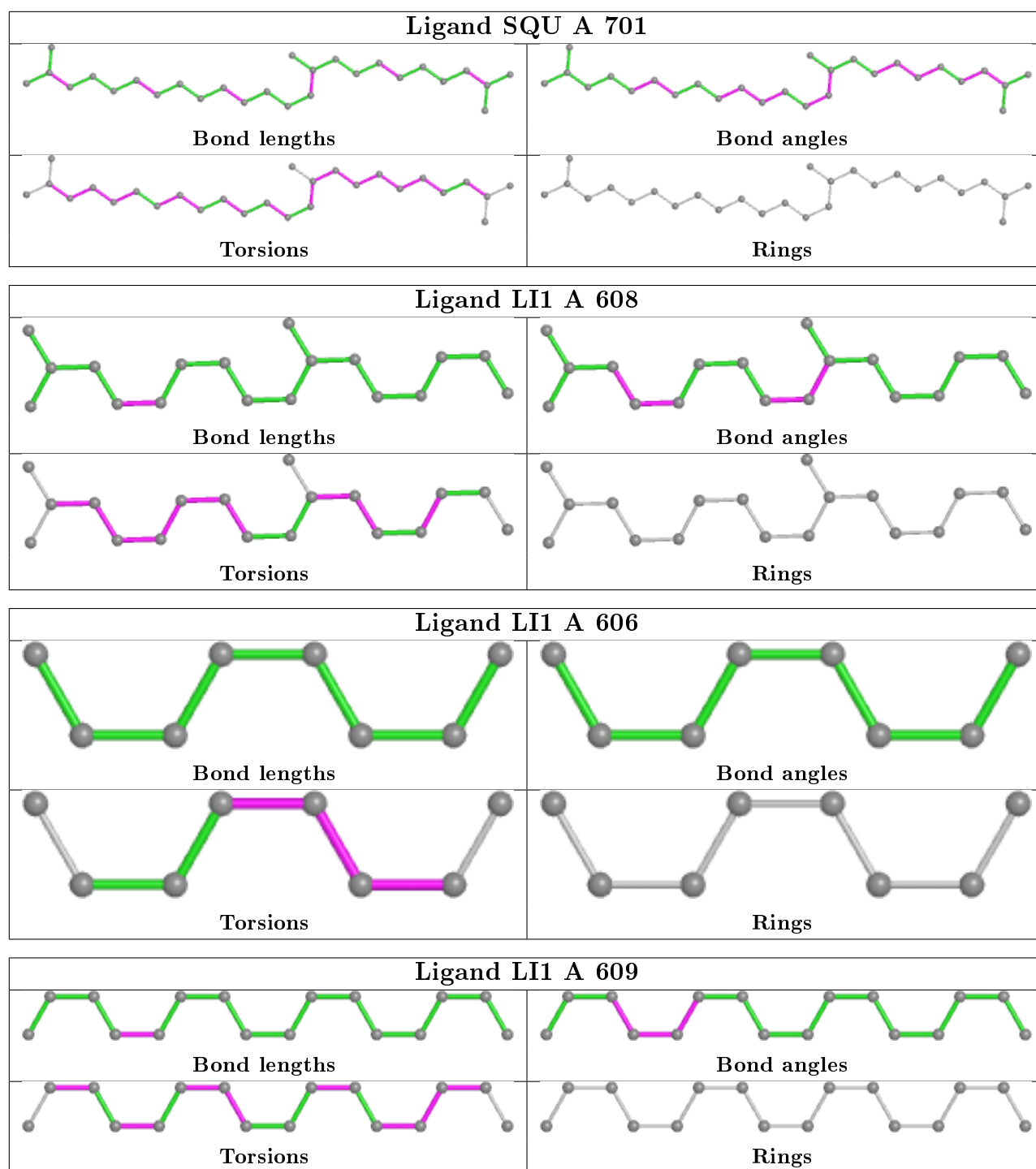
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.