



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 12:56 PM EDT

PDB ID : 1C8S
Title : BACTERIORHODOPSIN D96N LATE M STATE INTERMEDIATE
Authors : Luecke, H.
Deposited on : 1999-07-29
Resolution : 2.00 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)
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) : 2.23.2

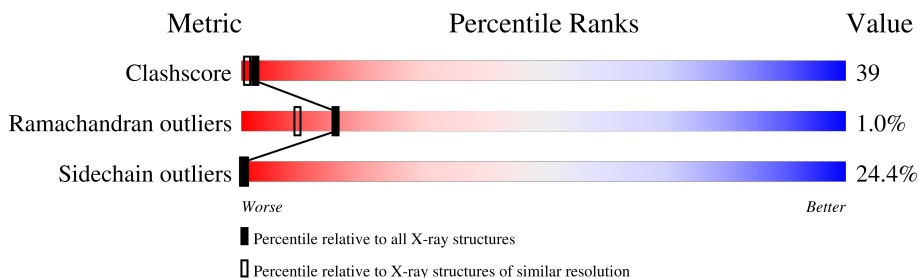
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	196	

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	613	X	-	-	-
3	SQU	A	701	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 1821 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.

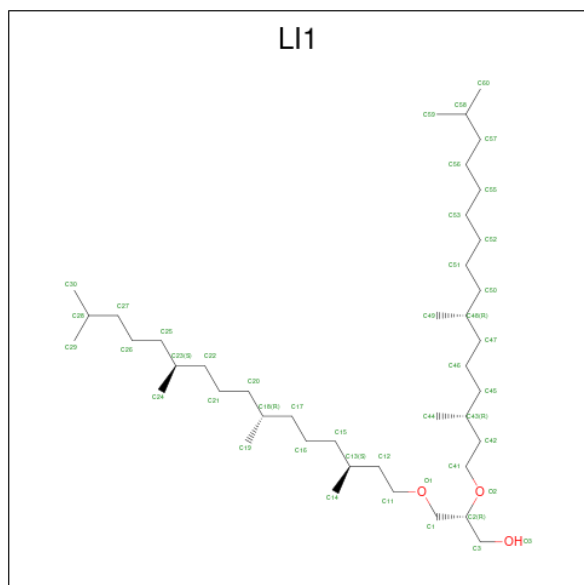
- Molecule 1 is a protein called BACTERIORHODOPSIN ("M" STATE INTERMEDIATE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	0	0
			1510	1021	224	257	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	ASN	ASP	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: C₄₂H₈₆O₃).



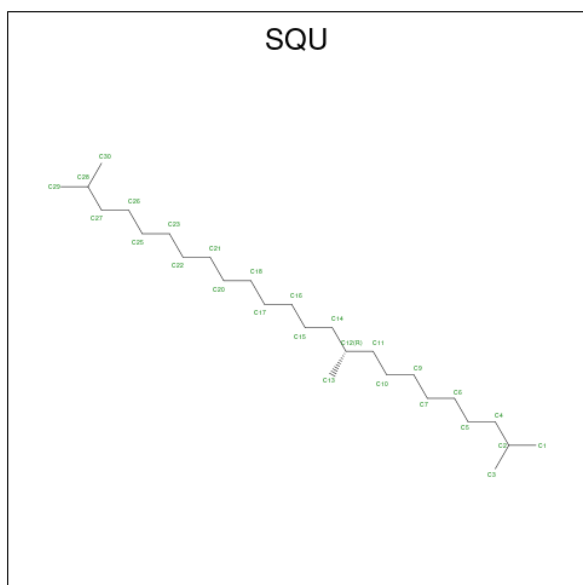
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			32	29	3		
2	A	1	Total	C	O	0	0
			41	38	3		

Continued on next page...

Continued from previous page...

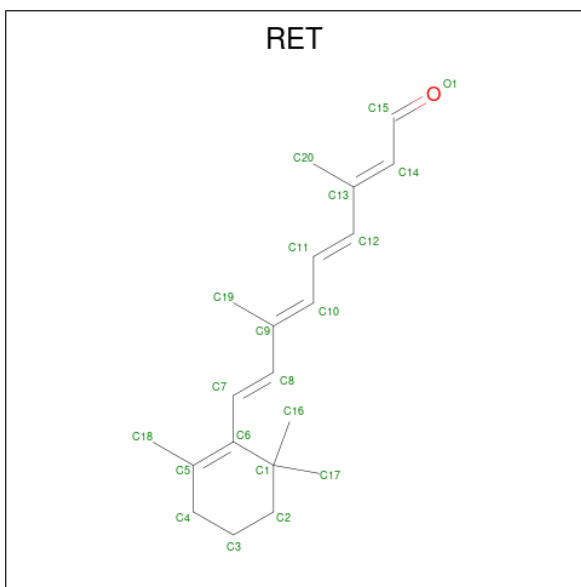
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 18 18	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C O 38 35 3	0	0
2	A	1	Total C 18 18	0	0
2	A	1	Total C 16 16	0	0
2	A	1	Total C O 40 37 3	0	0
2	A	1	Total C 18 18	0	0
2	A	1	Total C 13 13	0	0

- 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	14	Total O 14 14	0	0

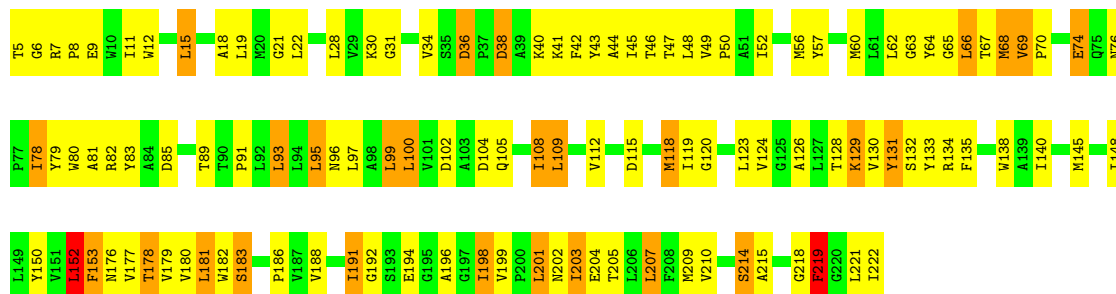
3 Residue-property plots

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 ("M" STATE INTERMEDIATE)

Chain A: 



4 Data and refinement statistics

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 – 2.00	Depositor
% Data completeness (in resolution range)	95.0 (12.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.173 , 0.219	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1821	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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	0.38	0/1552	1.07	3/2126 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	PHE	CB-CG-CD1	6.05	125.03	120.80
1	A	150	TYR	CB-CG-CD1	5.52	124.31	121.00
1	A	219	PHE	CA-CB-CG	5.30	126.62	113.90

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	1510	0	1555	117	0
2	A	250	0	404	60	0
3	A	27	0	53	3	0
4	A	20	0	27	1	0
5	A	14	0	0	5	0
All	All	1821	0	2039	149	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 39.

All (149) 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:180:VAL:HG22	2:A:610:LI1:H211	1.49	0.92
1:A:181:LEU:HD21	1:A:215:ALA:HB2	1.61	0.83
1:A:21:GLY:HA2	2:A:612:LI1:H291	1.59	0.82
2:A:602:LI1:H171	2:A:602:LI1:H451	1.60	0.82
1:A:78:ILE:HD13	1:A:194:GLU:HG2	1.63	0.80
1:A:96:ASN:HA	1:A:99:LEU:HD12	1.63	0.80
1:A:36:ASP:O	1:A:40:LYS:HG3	1.83	0.78
2:A:602:LI1:H592	2:A:608:LI1:H303	1.67	0.74
1:A:96:ASN:O	1:A:100:LEU:HD22	1.89	0.72
1:A:203:ILE:O	1:A:207:LEU:HG	1.89	0.72
1:A:9:GLU:OE1	1:A:201:LEU:HD21	1.90	0.71
2:A:610:LI1:H461	2:A:610:LI1:H151	1.72	0.70
1:A:28:LEU:HD21	2:A:612:LI1:H162	1.73	0.69
1:A:69:VAL:HG23	1:A:78:ILE:HG13	1.75	0.69
1:A:180:VAL:HG11	2:A:610:LI1:H552	1.75	0.68
1:A:56:MET:HG3	1:A:85:ASP:HB2	1.75	0.67
1:A:188:VAL:HG13	1:A:207:LEU:HD12	1.78	0.65
1:A:31:GLY:HA3	5:A:512:HOH:O	1.95	0.65
2:A:602:LI1:H443	2:A:602:LI1:H121	1.79	0.64
1:A:69:VAL:HG12	1:A:129:LYS:HD3	1.81	0.63
1:A:97:LEU:HD21	1:A:219:PHE:CZ	2.33	0.63
1:A:218:GLY:O	1:A:222:ILE:HD13	1.99	0.62
1:A:135:PHE:CD1	2:A:602:LI1:H212	2.34	0.62
1:A:97:LEU:HD21	1:A:219:PHE:HZ	1.65	0.61
1:A:44:ALA:HA	2:A:612:LI1:H143	1.81	0.61
1:A:47:THR:HB	2:A:612:LI1:H142	1.83	0.61
1:A:131:TYR:HE2	2:A:602:LI1:H112	1.67	0.60
1:A:68:MET:HA	1:A:76:ASN:O	2.03	0.59
1:A:34:VAL:HG12	1:A:40:LYS:HG2	1.85	0.59
1:A:78:ILE:HD12	1:A:126:ALA:O	2.02	0.58
2:A:601:LI1:C30	2:A:608:LI1:H252	2.33	0.58
1:A:178:THR:HG1	1:A:182:TRP:HE1	1.51	0.58
2:A:603:LI1:H201	2:A:603:LI1:H151	1.85	0.58
1:A:180:VAL:HA	2:A:610:LI1:C23	2.33	0.58
1:A:221:LEU:HD11	3:A:701:SQU:H292	1.85	0.57
1:A:214:SER:HB3	3:A:701:SQU:H132	1.87	0.57
2:A:601:LI1:H293	2:A:601:LI1:H251	1.86	0.56
2:A:601:LI1:H301	2:A:608:LI1:H252	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:PHE:CZ	1:A:99:LEU:HB2	2.40	0.56
1:A:152:LEU:O	1:A:153:PHE:HB2	2.05	0.56
1:A:96:ASN:HA	1:A:99:LEU:CD1	2.36	0.56
1:A:18:ALA:HA	2:A:606:LI1:H211	1.89	0.55
1:A:95:LEU:O	1:A:99:LEU:HG	2.06	0.55
1:A:201:LEU:HD23	5:A:415:HOH:O	2.06	0.55
1:A:45:ILE:HD11	1:A:95:LEU:HD22	1.88	0.54
1:A:31:GLY:O	1:A:34:VAL:HG23	2.07	0.54
1:A:63:GLY:O	1:A:66:LEU:HD22	2.07	0.54
1:A:179:VAL:HG11	2:A:610:LI1:H171	1.88	0.54
1:A:181:LEU:HD21	1:A:215:ALA:CB	2.35	0.54
1:A:221:LEU:CD1	3:A:701:SQU:H292	2.37	0.53
1:A:45:ILE:HD13	1:A:95:LEU:HB3	1.91	0.53
1:A:48:LEU:O	1:A:52:ILE:HG13	2.09	0.53
1:A:135:PHE:HA	1:A:138:TRP:HB3	1.91	0.53
2:A:602:LI1:H572	2:A:608:LI1:H303	1.91	0.52
1:A:118:MET:HE2	1:A:145:MET:HA	1.92	0.52
2:A:602:LI1:H451	2:A:602:LI1:C17	2.34	0.52
1:A:60:MET:HB3	1:A:79:TYR:CD1	2.45	0.51
1:A:148:ILE:O	1:A:152:LEU:HB2	2.10	0.51
1:A:18:ALA:HA	2:A:606:LI1:H202	1.91	0.51
1:A:78:ILE:CD1	1:A:194:GLU:HG2	2.37	0.51
1:A:138:TRP:CZ3	2:A:602:LI1:H251	2.45	0.51
1:A:179:VAL:CG1	2:A:610:LI1:H202	2.41	0.51
2:A:610:LI1:O1	2:A:610:LI1:H411	2.08	0.51
1:A:34:VAL:HG21	1:A:43:TYR:CD2	2.46	0.50
1:A:145:MET:CE	1:A:186:PRO:HG3	2.41	0.50
1:A:56:MET:HE3	2:A:607:LI1:H511	1.94	0.50
1:A:201:LEU:HD23	1:A:202:ASN:N	2.26	0.50
1:A:97:LEU:HA	1:A:100:LEU:CD2	2.42	0.49
1:A:93:LEU:HD22	4:A:301:RET:H201	1.94	0.49
1:A:176:ASN:OD1	2:A:610:LI1:H162	2.12	0.49
1:A:31:GLY:HA3	5:A:513:HOH:O	2.12	0.49
1:A:210:VAL:O	1:A:214:SER:OG	2.29	0.49
1:A:41:LYS:HE3	1:A:99:LEU:CD2	2.43	0.48
1:A:97:LEU:HA	1:A:100:LEU:HD23	1.95	0.48
1:A:67:THR:HG22	1:A:80:TRP:HD1	1.78	0.48
1:A:47:THR:O	1:A:50:PRO:HD2	2.14	0.48
1:A:191:ILE:HB	1:A:198:ILE:HB	1.95	0.48
1:A:6:GLY:O	1:A:8:PRO:HD3	2.14	0.48
1:A:69:VAL:CG2	1:A:78:ILE:HG13	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LEU:HD12	1:A:109:LEU:O	2.15	0.47
1:A:140:ILE:HG13	2:A:601:LI1:H272	1.96	0.47
2:A:602:LI1:H603	2:A:602:LI1:H562	1.61	0.47
2:A:602:LI1:C59	2:A:608:LI1:H303	2.42	0.47
1:A:47:THR:HG21	2:A:612:LI1:H122	1.97	0.47
1:A:131:TYR:CE2	2:A:602:LI1:H112	2.47	0.47
2:A:612:LI1:H212	2:A:612:LI1:H172	1.61	0.47
1:A:115:ASP:O	1:A:119:ILE:HD12	2.14	0.47
1:A:105:GLN:HA	1:A:108:ILE:HB	1.96	0.47
1:A:135:PHE:CE1	2:A:602:LI1:H212	2.49	0.47
1:A:179:VAL:HG11	2:A:610:LI1:H202	1.95	0.47
1:A:179:VAL:O	1:A:183:SER:OG	2.30	0.46
1:A:196:ALA:O	2:A:602:LI1:H141	2.15	0.46
2:A:607:LI1:H112	2:A:607:LI1:H152	1.30	0.46
2:A:608:LI1:H261	2:A:608:LI1:H292	1.43	0.46
2:A:602:LI1:H12	2:A:602:LI1:H412	1.75	0.46
1:A:57:TYR:OH	1:A:209:MET:HA	2.16	0.46
2:A:601:LI1:H112	2:A:601:LI1:H152	1.38	0.46
2:A:602:LI1:H121	2:A:602:LI1:H162	1.53	0.46
1:A:21:GLY:HA2	2:A:612:LI1:C29	2.37	0.46
1:A:152:LEU:HD22	1:A:178:THR:HG21	1.98	0.46
1:A:42:PHE:HZ	1:A:100:LEU:HD13	1.81	0.45
1:A:49:VAL:HB	1:A:50:PRO:HD3	1.99	0.45
1:A:56:MET:HG3	1:A:85:ASP:CB	2.44	0.45
2:A:613:LI1:H191	2:A:613:LI1:H212	1.68	0.45
2:A:602:LI1:H443	2:A:602:LI1:H411	1.56	0.45
1:A:9:GLU:HA	1:A:12:TRP:CD1	2.52	0.45
1:A:128:THR:HG23	5:A:412:HOH:O	2.16	0.44
2:A:602:LI1:H121	2:A:602:LI1:H411	1.99	0.44
1:A:188:VAL:O	1:A:192:GLY:N	2.49	0.44
1:A:191:ILE:HG13	1:A:199:VAL:HG13	1.99	0.44
1:A:119:ILE:HD12	1:A:119:ILE:H	1.83	0.43
1:A:176:ASN:CG	2:A:610:LI1:H162	2.39	0.43
1:A:56:MET:CE	2:A:607:LI1:H511	2.48	0.43
1:A:78:ILE:HD11	1:A:134:ARG:HH22	1.83	0.43
1:A:83:TYR:OH	1:A:194:GLU:OE1	2.36	0.43
1:A:130:VAL:HG11	1:A:133:TYR:CE2	2.53	0.43
1:A:178:THR:HG23	1:A:182:TRP:CD1	2.54	0.43
1:A:70:PRO:HA	1:A:74:GLU:O	2.18	0.43
2:A:602:LI1:H443	2:A:602:LI1:C12	2.46	0.43
1:A:49:VAL:HG13	1:A:89:THR:HB	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:PRO:HB3	1:A:112:VAL:HG13	2.00	0.43
1:A:131:TYR:HD1	1:A:134:ARG:HD3	1.84	0.43
2:A:603:LI1:H162	2:A:603:LI1:H142	1.76	0.42
1:A:15:LEU:O	1:A:19:LEU:HG	2.19	0.42
1:A:7:ARG:HA	1:A:8:PRO:HD2	1.85	0.42
1:A:64:TYR:OH	2:A:607:LI1:H411	2.19	0.42
1:A:129:LYS:H	1:A:129:LYS:HG2	1.63	0.42
1:A:192:GLY:HA3	1:A:204:GLU:OE2	2.19	0.42
1:A:176:ASN:ND2	2:A:610:LI1:O1	2.50	0.42
1:A:82:ARG:HH12	1:A:205:THR:HG23	1.85	0.42
1:A:60:MET:HG2	1:A:81:ALA:HB3	2.02	0.42
1:A:120:GLY:O	1:A:124:VAL:HG23	2.19	0.42
2:A:602:LI1:C55	2:A:602:LI1:H261	2.50	0.42
2:A:602:LI1:H443	2:A:602:LI1:H162	2.01	0.41
2:A:601:LI1:H302	2:A:608:LI1:H252	2.03	0.41
1:A:82:ARG:HB2	5:A:405:HOH:O	2.20	0.41
2:A:601:LI1:H11	2:A:601:LI1:H411	1.51	0.41
2:A:602:LI1:H491	2:A:602:LI1:H511	1.86	0.41
2:A:607:LI1:H422	2:A:607:LI1:O3	2.21	0.41
1:A:70:PRO:HD2	1:A:129:LYS:HD2	2.02	0.41
1:A:56:MET:CG	1:A:85:ASP:HB2	2.48	0.41
2:A:601:LI1:H221	2:A:601:LI1:H18	1.52	0.41
2:A:610:LI1:H151	2:A:610:LI1:C46	2.47	0.41
1:A:65:GLY:HA3	1:A:81:ALA:HB2	2.03	0.41
1:A:62:LEU:HD23	1:A:62:LEU:HA	1.74	0.40
1:A:178:THR:OG1	1:A:182:TRP:NE1	2.50	0.40
1:A:196:ALA:HA	2:A:602:LI1:H152	2.02	0.40
1:A:130:VAL:HB	1:A:133:TYR:CD2	2.56	0.40
1:A:38:ASP:OD1	1:A:38:ASP:N	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	192/196 (98%)	179 (93%)	11 (6%)	2 (1%)	15 9

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	ASP
1	A	152	LEU

5.3.2 Protein sidechains ⓘ

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	156/156 (100%)	118 (76%)	38 (24%)	0 0

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	11	ILE
1	A	15	LEU
1	A	22	LEU
1	A	30	LYS
1	A	36	ASP
1	A	38	ASP
1	A	46	THR
1	A	66	LEU
1	A	68	MET
1	A	69	VAL
1	A	74	GLU
1	A	78	ILE
1	A	93	LEU
1	A	95	LEU
1	A	99	LEU
1	A	100	LEU
1	A	104	ASP
1	A	108	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	109	LEU
1	A	118	MET
1	A	123	LEU
1	A	129	LYS
1	A	131	TYR
1	A	132	SER
1	A	152	LEU
1	A	153	PHE
1	A	177	VAL
1	A	178	THR
1	A	181	LEU
1	A	183	SER
1	A	191	ILE
1	A	198	ILE
1	A	201	LEU
1	A	203	ILE
1	A	207	LEU
1	A	214	SER
1	A	219	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

13 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	606	-	7,7,44	0.49	0	6,6,51	0.87	0
2	LI1	A	605	-	7,7,44	0.50	0	6,6,51	0.82	0
2	LI1	A	607	-	37,37,44	0.80	1 (2%)	37,38,51	1.05	1 (2%)
2	LI1	A	603	-	17,17,44	0.51	0	18,18,51	1.16	1 (5%)
3	SQU	A	701	-	26,26,26	1.40	6 (23%)	28,28,28	1.78	10 (35%)
2	LI1	A	612	-	17,17,44	0.47	0	18,18,51	1.02	1 (5%)
2	LI1	A	602	-	40,40,44	0.75	1 (2%)	43,45,51	1.14	3 (6%)
2	LI1	A	608	-	17,17,44	0.50	0	18,18,51	1.21	2 (11%)
2	LI1	A	609	-	15,15,44	0.50	0	14,14,51	0.94	0
4	RET	A	301	1	20,20,21	0.74	0	27,27,28	1.36	3 (11%)
2	LI1	A	613	-	12,12,44	0.51	0	12,12,51	1.39	2 (16%)
2	LI1	A	610	-	39,39,44	0.79	1 (2%)	41,41,51	1.02	1 (2%)
2	LI1	A	601	-	31,31,44	0.82	1 (3%)	33,33,51	1.13	3 (9%)

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	606	-	-	4/5/5/49	-
2	LI1	A	605	-	-	4/5/5/49	-
2	LI1	A	607	-	-	18/38/38/49	-
2	LI1	A	603	-	-	10/16/16/49	-
3	SQU	A	701	-	1/1/3/3	14/25/25/25	-
2	LI1	A	612	-	-	8/16/16/49	-
2	LI1	A	602	-	-	21/44/44/49	-
2	LI1	A	608	-	-	7/16/16/49	-
2	LI1	A	609	-	-	11/13/13/49	-
4	RET	A	301	1	-	0/13/30/31	0/1/1/1
2	LI1	A	613	-	1/1/1/8	5/11/11/49	-
2	LI1	A	610	-	-	30/39/39/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LI1	A	601	-	2/2/3/8	17/32/32/49	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	SQU	C14-C12	-3.33	1.35	1.52
3	A	701	SQU	C9-C7	-2.94	1.35	1.51
3	A	701	SQU	C23-C22	-2.92	1.35	1.51
2	A	607	LI1	O3-C3	2.91	1.54	1.42
3	A	701	SQU	C18-C17	-2.88	1.35	1.51
2	A	602	LI1	O3-C3	2.86	1.54	1.42
2	A	610	LI1	O3-C3	2.79	1.54	1.42
2	A	601	LI1	O3-C3	2.78	1.54	1.42
3	A	701	SQU	C4-C2	-2.40	1.35	1.51
3	A	701	SQU	C27-C28	-2.39	1.35	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	SQU	C15-C14-C12	4.41	130.16	115.92
4	A	301	RET	C11-C12-C13	-3.66	116.12	126.42
2	A	613	LI1	C16-C17-C18	-2.96	106.36	115.92
2	A	602	LI1	O3-C3-C2	-2.85	104.22	111.78
2	A	607	LI1	O3-C3-C2	-2.83	104.29	111.78
3	A	701	SQU	C10-C9-C7	2.78	128.54	114.42
2	A	601	LI1	O3-C3-C2	-2.71	104.60	111.78
3	A	701	SQU	C18-C17-C16	2.71	128.17	114.42
2	A	613	LI1	C21-C20-C18	-2.67	107.28	115.92
3	A	701	SQU	C5-C4-C2	2.58	128.13	115.98
2	A	601	LI1	C21-C20-C18	-2.56	107.65	115.92
3	A	701	SQU	C14-C12-C11	2.52	125.37	112.13
2	A	610	LI1	O3-C3-C2	-2.52	105.11	111.78
2	A	608	LI1	C21-C20-C18	-2.41	108.12	115.92
2	A	603	LI1	C16-C15-C13	-2.34	108.37	115.92
4	A	301	RET	C20-C13-C12	2.30	121.70	118.08
2	A	602	LI1	C21-C22-C23	-2.30	108.50	115.92
4	A	301	RET	C1-C6-C5	-2.29	119.39	122.61
2	A	612	LI1	C16-C15-C13	-2.28	108.54	115.92
3	A	701	SQU	C26-C27-C28	2.27	126.70	115.98
3	A	701	SQU	C23-C22-C21	2.21	125.65	114.42
2	A	608	LI1	C16-C17-C18	-2.21	108.79	115.92
2	A	602	LI1	C16-C15-C13	-2.19	108.83	115.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	LI1	C16-C17-C18	-2.17	108.89	115.92
3	A	701	SQU	C30-C28-C27	2.08	124.41	111.54
3	A	701	SQU	C9-C7-C6	2.05	124.83	114.42
3	A	701	SQU	C1-C2-C4	2.02	124.01	111.54

All (4) chirality outliers are listed below:

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

All (149) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	612	LI1	C20-C21-C22-C23
2	A	603	LI1	C21-C22-C23-C25
2	A	610	LI1	C48-C50-C51-C52
2	A	602	LI1	C56-C57-C58-C59
2	A	612	LI1	C26-C27-C28-C30
2	A	610	LI1	C47-C48-C50-C51
2	A	610	LI1	C53-C55-C56-C57
2	A	610	LI1	C16-C17-C18-C20
2	A	607	LI1	C20-C21-C22-C23
3	A	701	SQU	C16-C17-C18-C20
2	A	602	LI1	C51-C52-C53-C55
2	A	610	LI1	C21-C22-C23-C25
3	A	701	SQU	C15-C16-C17-C18
3	A	701	SQU	C22-C23-C25-C26
2	A	605	LI1	C15-C16-C17-C18
2	A	609	LI1	C20-C21-C22-C23
2	A	610	LI1	C26-C27-C28-C30
2	A	607	LI1	C44-C43-C45-C46
2	A	610	LI1	C42-C43-C45-C46
2	A	610	LI1	C45-C46-C47-C48
3	A	701	SQU	C14-C15-C16-C17
2	A	601	LI1	C12-C13-C15-C16
2	A	608	LI1	C21-C22-C23-C25
2	A	601	LI1	C23-C25-C26-C27
2	A	605	LI1	C17-C18-C20-C21
2	A	610	LI1	O2-C41-C42-C43
2	A	603	LI1	C18-C20-C21-C22
2	A	610	LI1	C51-C52-C53-C55
2	A	608	LI1	C26-C27-C28-C30
2	A	610	LI1	C26-C27-C28-C29
2	A	601	LI1	C13-C15-C16-C17
2	A	606	LI1	C16-C17-C18-C20
2	A	609	LI1	C17-C18-C20-C21
2	A	610	LI1	C23-C25-C26-C27
2	A	608	LI1	C20-C21-C22-C23
2	A	610	LI1	C50-C51-C52-C53
2	A	610	LI1	C11-C12-C13-C15
2	A	601	LI1	C20-C21-C22-C23
3	A	701	SQU	C5-C6-C7-C9
2	A	613	LI1	C11-C12-C13-C15
3	A	701	SQU	C1-C2-C4-C5
2	A	603	LI1	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	608	LI1	C25-C26-C27-C28
2	A	602	LI1	C56-C57-C58-C60
2	A	602	LI1	C44-C43-C45-C46
2	A	602	LI1	C21-C22-C23-C24
2	A	613	LI1	C19-C18-C20-C21
2	A	610	LI1	C20-C21-C22-C23
2	A	601	LI1	C26-C27-C28-C29
2	A	610	LI1	C56-C57-C58-C60
2	A	607	LI1	C52-C53-C55-C56
2	A	610	LI1	C41-C42-C43-C45
2	A	601	LI1	C45-C46-C47-C48
2	A	610	LI1	C56-C57-C58-C59
2	A	612	LI1	C26-C27-C28-C29
2	A	602	LI1	C16-C17-C18-C20
3	A	701	SQU	C6-C7-C9-C10
2	A	601	LI1	O1-C1-C2-C3
2	A	613	LI1	C21-C22-C23-C24
2	A	610	LI1	C52-C53-C55-C56
2	A	612	LI1	C23-C25-C26-C27
2	A	605	LI1	C18-C20-C21-C22
2	A	601	LI1	C43-C45-C46-C47
2	A	601	LI1	C46-C47-C48-C50
2	A	608	LI1	C13-C15-C16-C17
3	A	701	SQU	C2-C4-C5-C6
2	A	609	LI1	C25-C26-C27-C28
2	A	612	LI1	C21-C22-C23-C25
2	A	603	LI1	C15-C16-C17-C18
3	A	701	SQU	C4-C5-C6-C7
2	A	602	LI1	C42-C43-C45-C46
2	A	602	LI1	C21-C22-C23-C25
3	A	701	SQU	C10-C11-C12-C14
2	A	606	LI1	C13-C15-C16-C17
2	A	609	LI1	C21-C22-C23-C25
2	A	606	LI1	C18-C20-C21-C22
2	A	612	LI1	C22-C23-C25-C26
2	A	609	LI1	C23-C25-C26-C27
2	A	603	LI1	C20-C21-C22-C23
2	A	601	LI1	C18-C20-C21-C22
3	A	701	SQU	C25-C26-C27-C28
2	A	602	LI1	O2-C41-C42-C43
2	A	603	LI1	C11-C12-C13-C14
2	A	601	LI1	C26-C27-C28-C30

Continued on next page...

Continued from previous page...

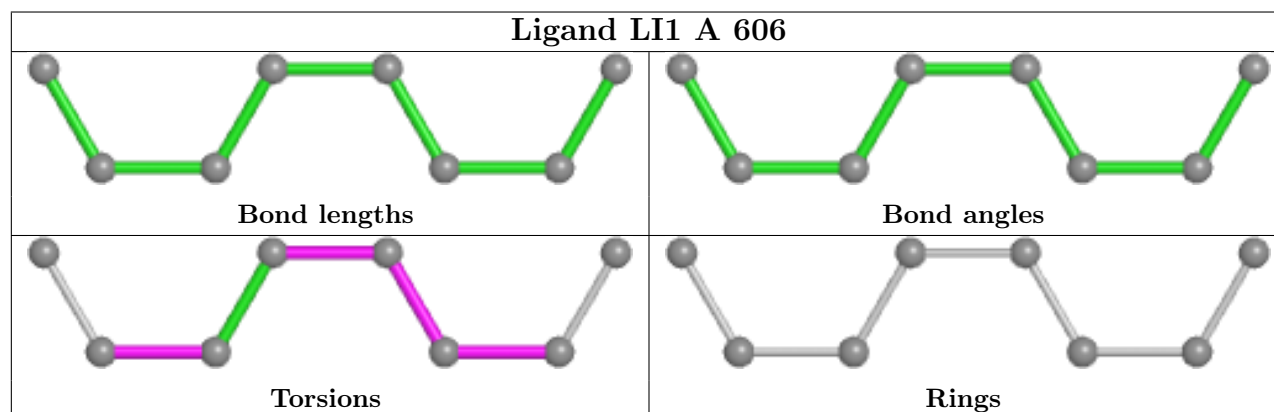
Mol	Chain	Res	Type	Atoms
2	A	607	LI1	O1-C1-C2-C3
2	A	607	LI1	C47-C48-C50-C51
2	A	610	LI1	C17-C18-C20-C21
2	A	602	LI1	C53-C55-C56-C57
2	A	608	LI1	C26-C27-C28-C29
2	A	607	LI1	O1-C1-C2-O2
2	A	607	LI1	C50-C51-C52-C53
2	A	606	LI1	C15-C16-C17-C18
2	A	609	LI1	C26-C27-C28-C30
2	A	610	LI1	C55-C56-C57-C58
3	A	701	SQU	C26-C27-C28-C29
2	A	609	LI1	C13-C15-C16-C17
2	A	601	LI1	C22-C23-C25-C26
2	A	602	LI1	C12-C11-O1-C1
2	A	602	LI1	C41-C42-C43-C45
2	A	609	LI1	C12-C13-C15-C16
2	A	610	LI1	C25-C26-C27-C28
3	A	701	SQU	C20-C21-C22-C23
2	A	607	LI1	C22-C23-C25-C26
2	A	603	LI1	C16-C17-C18-C20
2	A	602	LI1	C18-C20-C21-C22
2	A	609	LI1	C11-C12-C13-C15
2	A	613	LI1	C18-C20-C21-C22
2	A	601	LI1	C1-C2-O2-C41
2	A	601	LI1	O1-C1-C2-O2
2	A	603	LI1	C22-C23-C25-C26
2	A	607	LI1	C55-C56-C57-C58
2	A	610	LI1	C18-C20-C21-C22
2	A	602	LI1	C1-C2-C3-O3
2	A	607	LI1	C1-C2-C3-O3
2	A	613	LI1	C13-C15-C16-C17
2	A	608	LI1	C11-C12-C13-C15
2	A	609	LI1	C18-C20-C21-C22
2	A	607	LI1	C12-C11-O1-C1
2	A	609	LI1	C22-C23-C25-C26
2	A	605	LI1	C16-C17-C18-C20
2	A	607	LI1	C42-C43-C45-C46
2	A	607	LI1	C48-C50-C51-C52
2	A	607	LI1	C53-C55-C56-C57

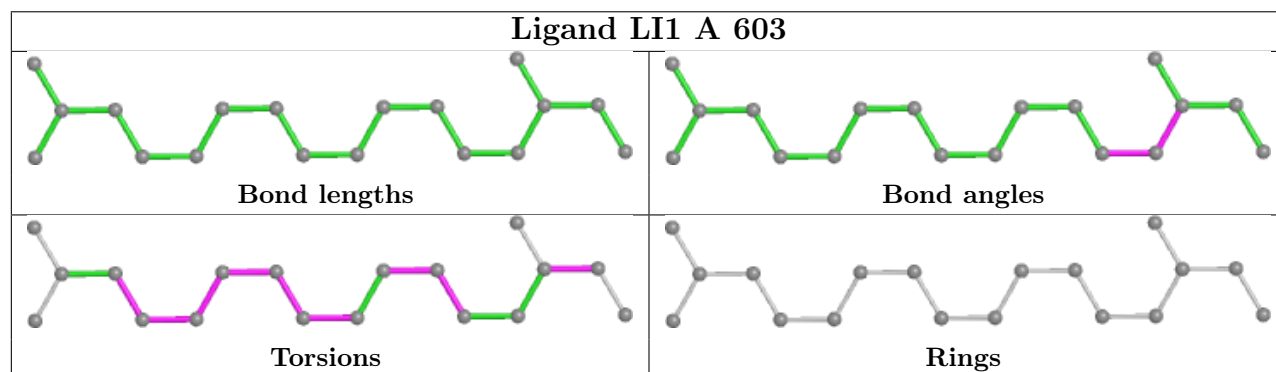
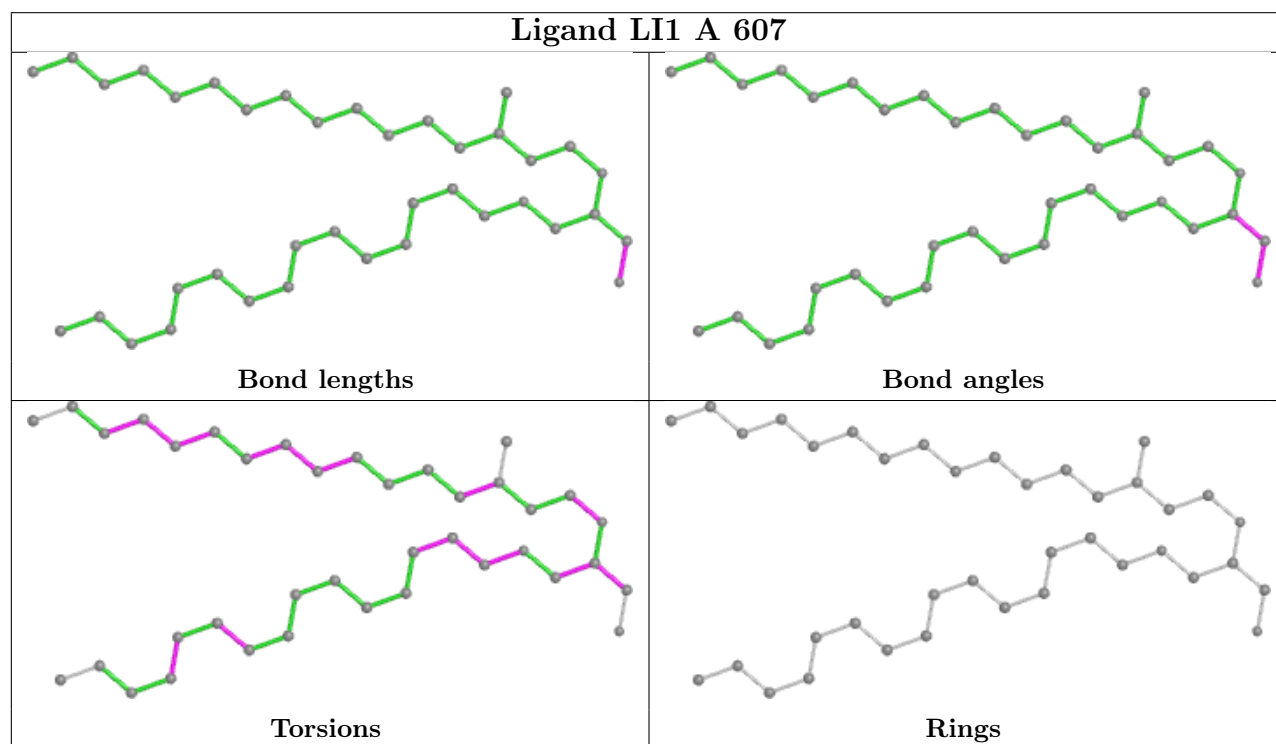
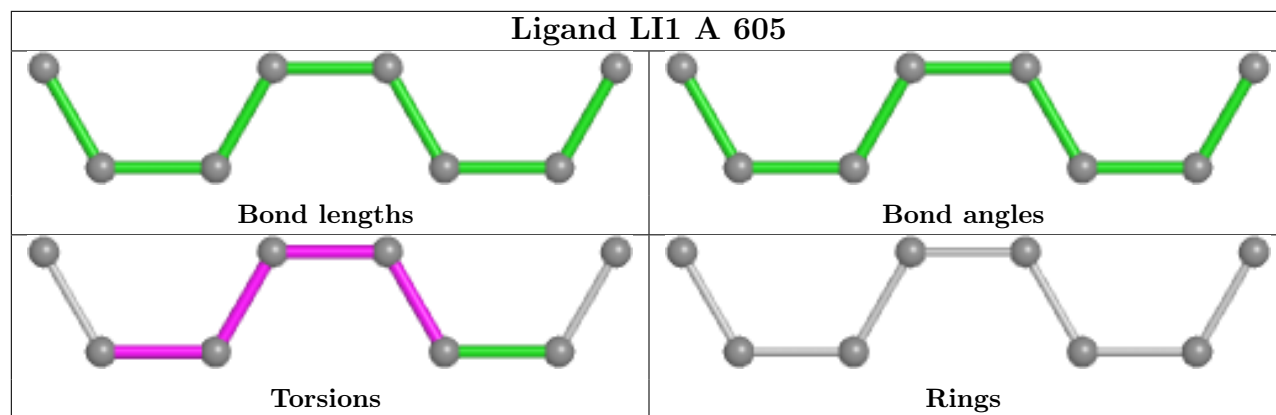
There are no ring outliers.

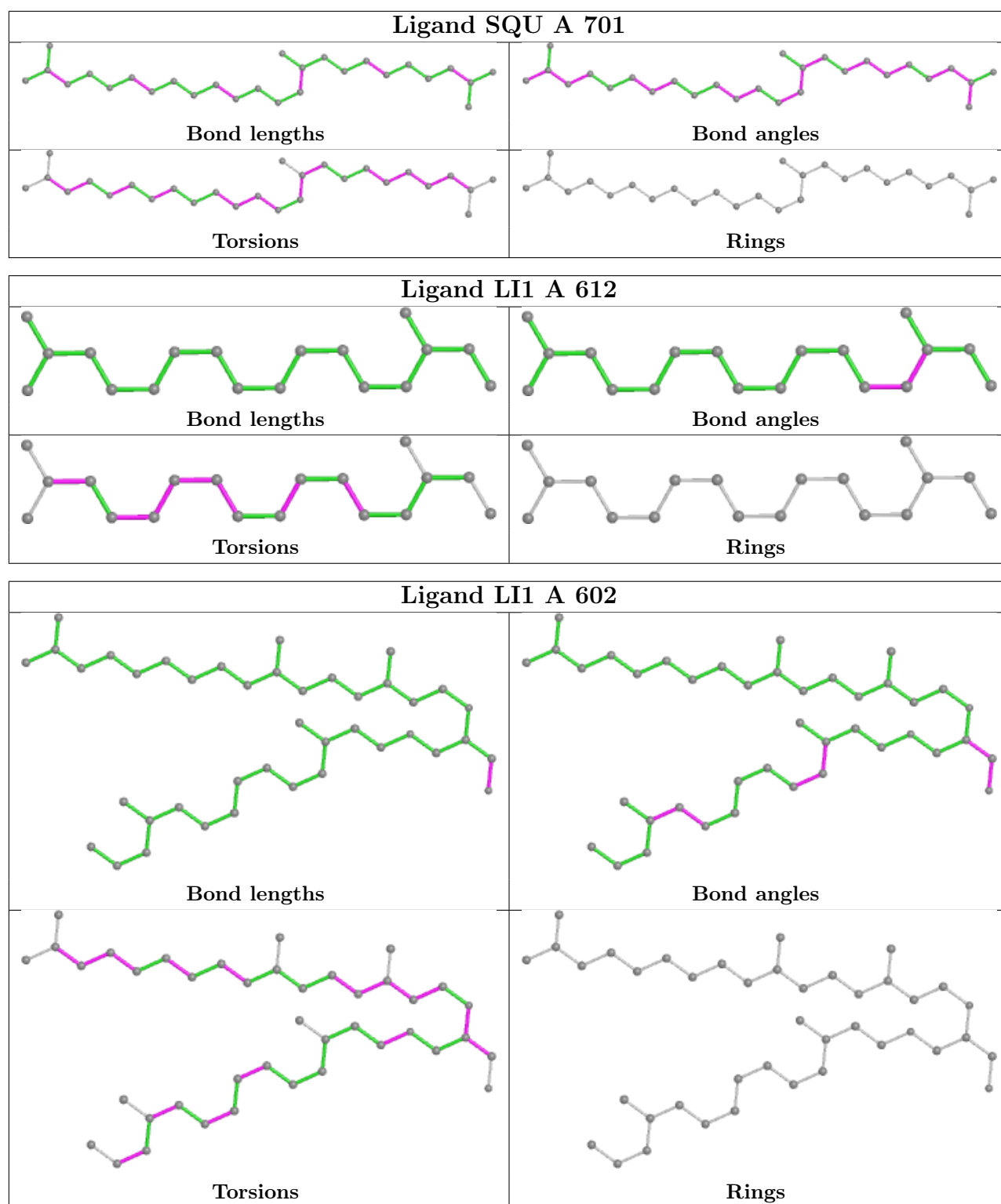
11 monomers are involved in 64 short contacts:

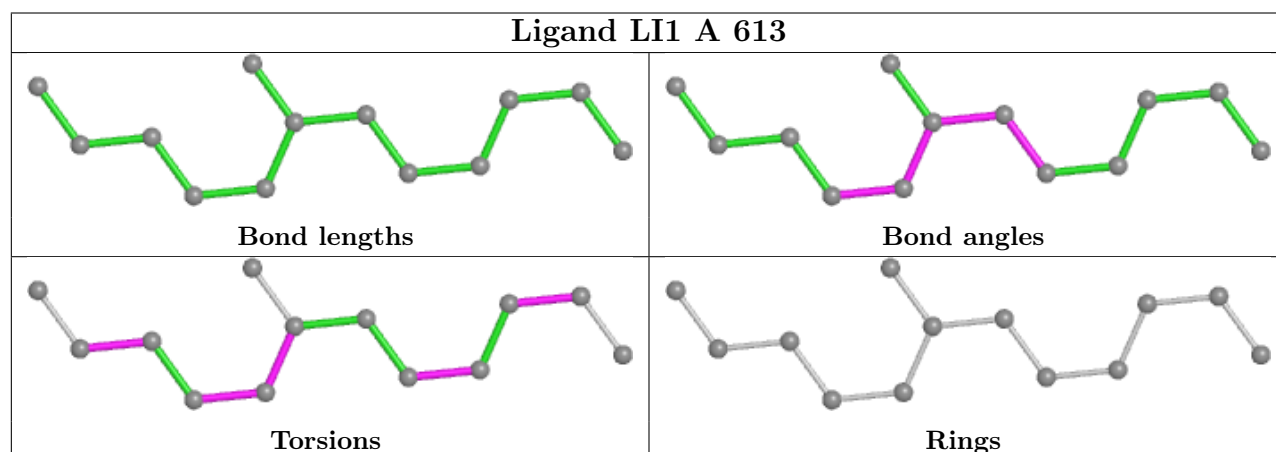
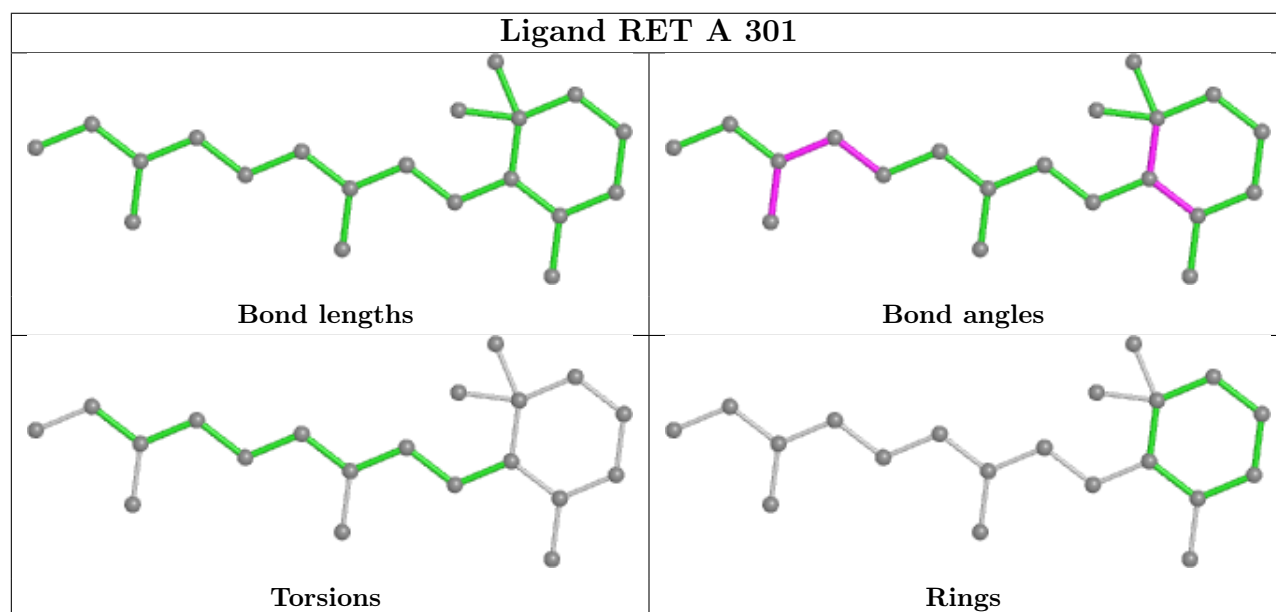
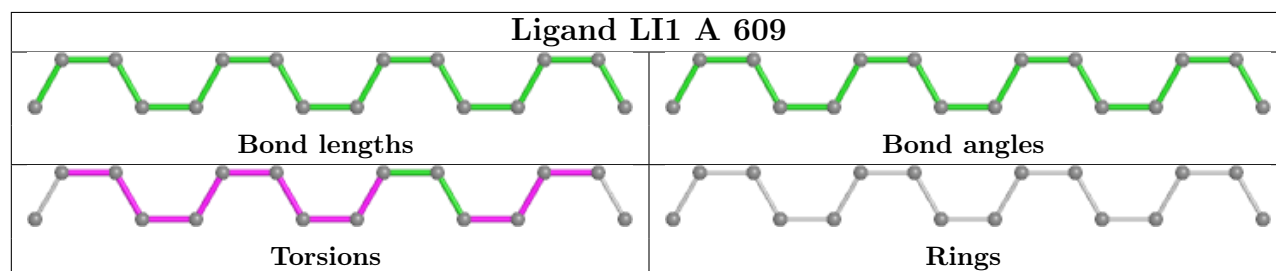
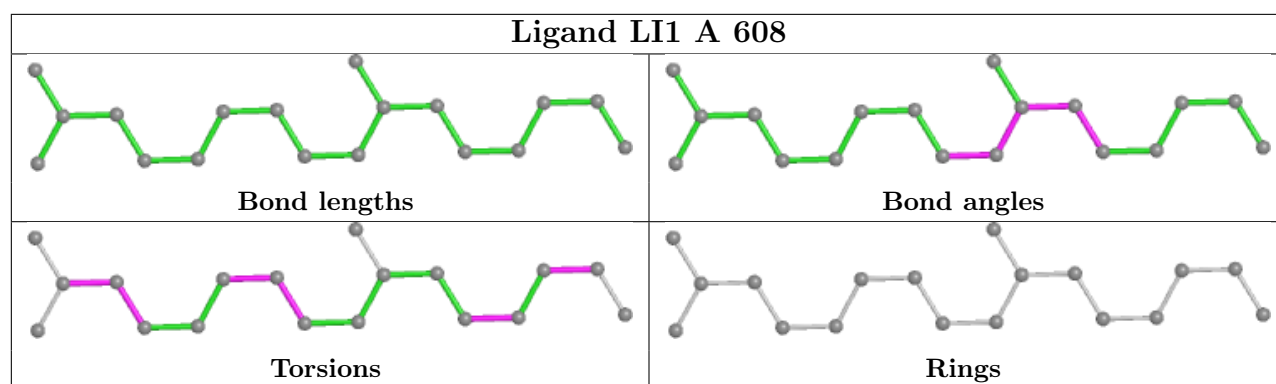
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	606	LI1	2	0
2	A	607	LI1	5	0
2	A	603	LI1	2	0
3	A	701	SQU	3	0
2	A	612	LI1	7	0
2	A	602	LI1	22	0
2	A	608	LI1	7	0
4	A	301	RET	1	0
2	A	613	LI1	1	0
2	A	610	LI1	12	0
2	A	601	LI1	8	0

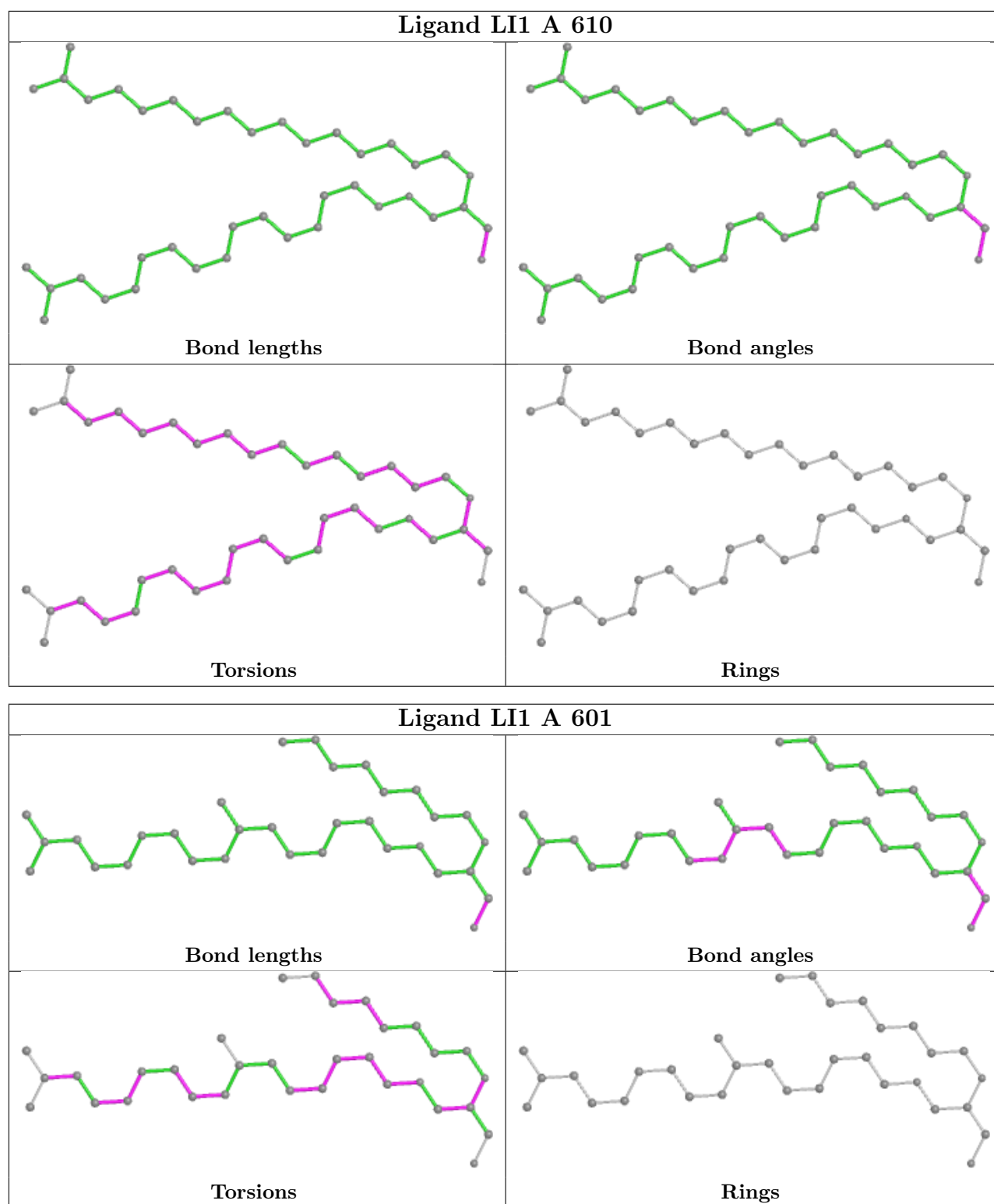
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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	153:PHE	C	176:ASN	N	9.48

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.