



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 05:14 PM EDT

PDB ID : 2I21
Title : Bacteriorhodopsin/lipid complex, T46V mutant
Authors : Lanyi, J.K.; Schobert, B.
Deposited on : 2006-08-15
Resolution : 1.84 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) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

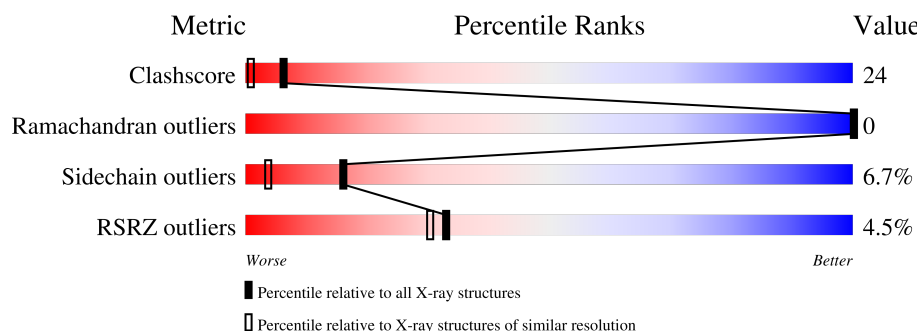
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	249	

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
3	LI1	A	601	X	-	-	-
3	LI1	A	611	X	-	-	-
3	LI1	A	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	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.

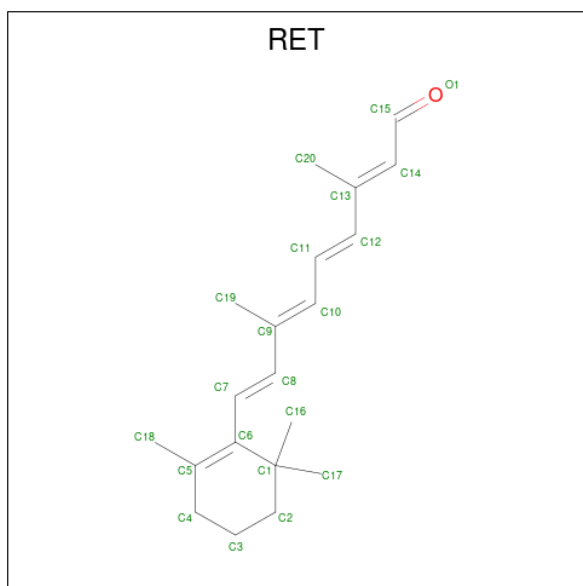
- Molecule 1 is a protein called Bacteriorhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	222	1720	1160	262	289	9	0	0	0

There is a discrepancy between the modelled and reference sequences:

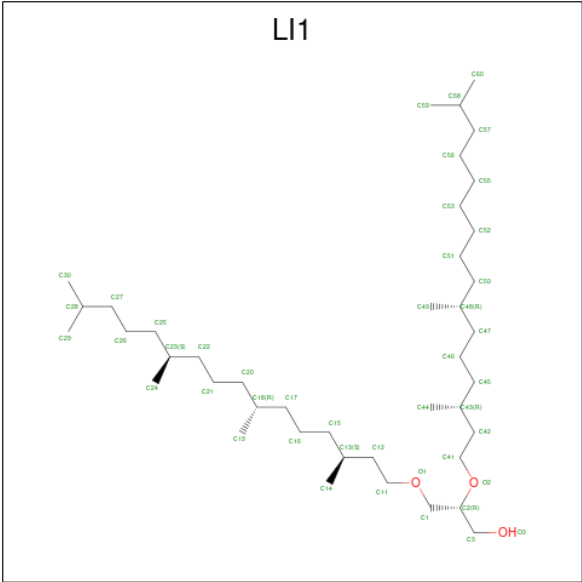
Chain	Residue	Modelled	Actual	Comment	Reference
A	46	VAL	THR	engineered mutation	UNP P02945

- Molecule 2 is RETINAL (three-letter code: RET) (formula: C₂₀H₂₈O).



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

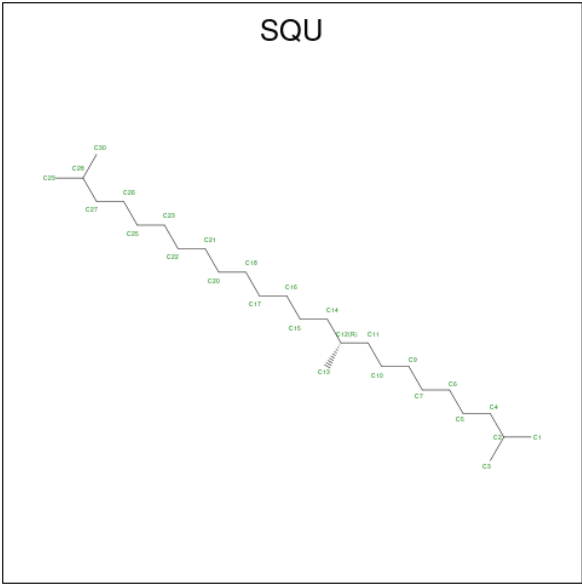
- Molecule 3 is 1-[2,6,10,14-TETRAMETHYL-HEXADECAN-16-YL]-2-[2,10,14-TRIMETHYLHEXADECAN-16-YL]GLYCEROL (three-letter code: LI1) (formula: C₄₂H₈₆O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 32 29 3	0	0
3	A	1	Total C O 41 38 3	0	0
3	A	1	Total C 18 18	0	0
3	A	1	Total C 16 16	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C O 38 35 3	0	0
3	A	1	Total C 18 18	0	0
3	A	1	Total C 16 16	0	0
3	A	1	Total C O 40 37 3	0	0
3	A	1	Total C 17 17	0	0
3	A	1	Total C 18 18	0	0
3	A	1	Total C 13 13	0	0

- Molecule 4 is 2,10,23-TRIMETHYL-TETRACOSANE (three-letter code: SQU) (formula:

C₂₇H₅₆).



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

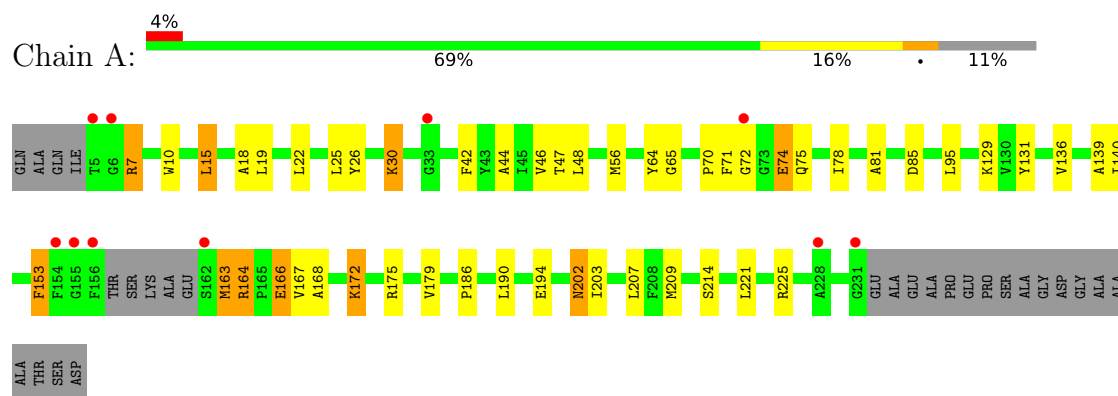
- Molecule 5 is water.

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: Bacteriorhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	61.07Å 61.07Å 110.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 1.84 24.49 – 1.84	Depositor EDS
% Data completeness (in resolution range)	95.5 (25.00-1.84) 86.2 (24.49-1.84)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 1.84Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.195 , 0.260 0.180 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 99.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.065 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2074	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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, SQU, RET

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	0.32	0/1767	0.91	2/2413 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	7	ARG	NE-CZ-NH2	-5.21	117.70	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	1778	64	0
2	A	20	0	27	3	0
3	A	283	0	452	72	0
4	A	27	0	53	4	0
5	A	24	0	0	1	0
All	All	2074	0	2310	106	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 24.

All (106) 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)
3:A:603:LI1:C26	3:A:603:LI1:C25	1.74	1.64
3:A:610:LI1:C26	3:A:610:LI1:C25	1.74	1.62
3:A:611:LI1:C26	3:A:611:LI1:C25	1.74	1.57
3:A:611:LI1:C25	3:A:611:LI1:C27	2.51	0.88
1:A:19:LEU:HD21	4:A:701:SQU:H32	1.55	0.88
3:A:603:LI1:C25	3:A:603:LI1:C27	2.53	0.87
3:A:610:LI1:C25	3:A:610:LI1:C27	2.54	0.85
3:A:601:LI1:H303	3:A:608:LI1:H303	1.59	0.83
3:A:610:LI1:H593	3:A:610:LI1:H522	1.60	0.81
3:A:611:LI1:C26	3:A:611:LI1:C23	2.58	0.81
3:A:610:LI1:C26	3:A:610:LI1:C23	2.60	0.80
1:A:15:LEU:HB3	1:A:209:MET:HE2	1.64	0.80
1:A:136:VAL:HG22	3:A:602:LI1:H531	1.64	0.79
3:A:603:LI1:C26	3:A:603:LI1:C23	2.60	0.79
1:A:18:ALA:O	1:A:22:LEU:HD13	1.85	0.76
1:A:221:LEU:O	1:A:225:ARG:HG2	1.87	0.75
1:A:64:TYR:OH	3:A:607:LI1:H32	1.86	0.75
1:A:153:PHE:HE2	1:A:179:VAL:HG21	1.53	0.74
1:A:131:TYR:OH	3:A:602:LI1:H162	1.87	0.74
1:A:26:TYR:HD1	3:A:611:LI1:H152	1.52	0.72
1:A:172:LYS:HE2	3:A:610:LI1:O3	1.89	0.72
3:A:610:LI1:H122	3:A:610:LI1:H412	1.72	0.71
1:A:131:TYR:OH	3:A:602:LI1:H13	1.91	0.71
1:A:202:ASN:HD22	1:A:202:ASN:H	1.40	0.70
1:A:172:LYS:HD3	3:A:610:LI1:H32	1.75	0.68
1:A:78:ILE:HD12	1:A:194:GLU:HG3	1.76	0.68
1:A:70:PRO:HG2	1:A:129:LYS:HD3	1.75	0.67
1:A:42:PHE:O	1:A:46:VAL:HG13	1.95	0.67
1:A:139:ALA:HB2	3:A:602:LI1:H571	1.76	0.67
1:A:214:SER:OG	4:A:701:SQU:H132	1.96	0.65
1:A:179:VAL:HG12	3:A:610:LI1:H202	1.80	0.63
1:A:153:PHE:CE2	1:A:179:VAL:HG21	2.34	0.61
1:A:164:ARG:HG3	1:A:167:VAL:HG23	1.82	0.61
3:A:612:LI1:H143	5:A:512:HOH:O	2.00	0.61
1:A:131:TYR:CE2	3:A:602:LI1:H112	2.36	0.60
3:A:610:LI1:H593	3:A:610:LI1:C52	2.32	0.60
1:A:26:TYR:CE2	1:A:30:LYS:HD2	2.36	0.60
3:A:610:LI1:H122	3:A:610:LI1:C41	2.32	0.60
1:A:26:TYR:CE1	3:A:611:LI1:H121	2.38	0.59
3:A:602:LI1:H592	3:A:602:LI1:H522	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:601:LI1:O1	3:A:601:LI1:H152	2.02	0.59
1:A:190:LEU:CD2	3:A:603:LI1:H222	2.34	0.58
1:A:202:ASN:HD22	1:A:202:ASN:N	1.99	0.58
3:A:603:LI1:C25	3:A:603:LI1:H271	2.32	0.58
1:A:26:TYR:CD1	3:A:611:LI1:H152	2.38	0.57
1:A:153:PHE:HE1	3:A:610:LI1:H112	1.69	0.57
3:A:602:LI1:H152	3:A:603:LI1:H141	1.88	0.55
1:A:56:MET:HG3	1:A:85:ASP:HB2	1.88	0.54
3:A:602:LI1:H592	3:A:602:LI1:C52	2.37	0.54
1:A:26:TYR:CZ	1:A:30:LYS:HD2	2.43	0.54
3:A:602:LI1:H592	3:A:602:LI1:C51	2.38	0.53
1:A:19:LEU:CD2	4:A:701:SQU:H32	2.34	0.53
1:A:175:ARG:HH21	3:A:610:LI1:C1	2.23	0.52
3:A:602:LI1:H152	3:A:603:LI1:C14	2.40	0.51
1:A:140:ILE:HG13	3:A:601:LI1:H272	1.93	0.51
1:A:44:ALA:HA	3:A:612:LI1:H13	1.92	0.50
1:A:136:VAL:CG2	3:A:602:LI1:H531	2.37	0.50
1:A:164:ARG:HE	1:A:166:GLU:CD	2.15	0.50
1:A:175:ARG:HH21	3:A:610:LI1:H11	1.77	0.50
3:A:601:LI1:H172	3:A:601:LI1:H412	1.94	0.49
1:A:78:ILE:CD1	1:A:194:GLU:HG3	2.41	0.49
3:A:610:LI1:C25	3:A:610:LI1:H272	2.39	0.49
1:A:72:GLY:O	1:A:74:GLU:HG2	2.12	0.48
1:A:65:GLY:HA3	1:A:81:ALA:HB2	1.95	0.48
1:A:221:LEU:HD21	4:A:701:SQU:H271	1.96	0.47
3:A:601:LI1:H162	3:A:601:LI1:H193	1.33	0.47
3:A:601:LI1:H412	3:A:601:LI1:H12	1.60	0.47
1:A:140:ILE:CG1	3:A:601:LI1:H272	2.44	0.47
1:A:190:LEU:HD23	3:A:603:LI1:H222	1.95	0.47
3:A:602:LI1:H421	3:A:602:LI1:H12	1.97	0.47
3:A:601:LI1:H152	3:A:601:LI1:C1	2.45	0.47
3:A:610:LI1:H522	3:A:610:LI1:C59	2.36	0.47
1:A:47:THR:HG21	3:A:612:LI1:H141	1.97	0.46
3:A:608:LI1:H211	3:A:608:LI1:H172	1.78	0.46
1:A:190:LEU:HD11	3:A:602:LI1:H23	1.98	0.45
3:A:603:LI1:H271	3:A:603:LI1:H252	1.98	0.45
3:A:610:LI1:H593	3:A:610:LI1:H502	1.99	0.45
3:A:613:LI1:H211	3:A:613:LI1:H191	1.65	0.44
1:A:7:ARG:O	1:A:10:TRP:HD1	2.01	0.44
1:A:22:LEU:HD11	3:A:606:LI1:C22	2.46	0.44
1:A:166:GLU:H	1:A:166:GLU:HG3	1.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:610:LI1:H272	3:A:610:LI1:H251	1.98	0.44
1:A:56:MET:CE	3:A:607:LI1:H521	2.48	0.44
2:A:300:RET:H181	2:A:300:RET:H7	1.81	0.44
3:A:610:LI1:H593	3:A:610:LI1:C50	2.49	0.43
3:A:602:LI1:H202	3:A:602:LI1:H472	1.99	0.43
1:A:25:LEU:HB3	3:A:611:LI1:H191	2.01	0.43
1:A:190:LEU:HD21	3:A:603:LI1:H222	2.00	0.43
1:A:15:LEU:HD13	1:A:209:MET:HE1	2.01	0.42
1:A:25:LEU:HD13	3:A:611:LI1:H211	2.02	0.42
1:A:139:ALA:CB	3:A:602:LI1:H571	2.47	0.42
1:A:172:LYS:HD3	3:A:610:LI1:C3	2.47	0.42
1:A:70:PRO:O	1:A:71:PHE:HB3	2.20	0.41
1:A:15:LEU:HB3	1:A:209:MET:CE	2.42	0.41
3:A:607:LI1:H122	3:A:607:LI1:H2	2.01	0.41
1:A:25:LEU:HB3	3:A:611:LI1:C19	2.50	0.41
1:A:186:PRO:HB3	2:A:300:RET:H183	2.02	0.41
1:A:64:TYR:HH	3:A:607:LI1:H32	1.82	0.41
1:A:163:MET:CE	1:A:168:ALA:HB2	2.51	0.41
2:A:300:RET:H8	2:A:300:RET:H171	2.03	0.41
1:A:163:MET:HG3	1:A:167:VAL:HB	2.01	0.40
3:A:602:LI1:H202	3:A:602:LI1:C47	2.52	0.40
1:A:70:PRO:HA	1:A:74:GLU:O	2.21	0.40
3:A:611:LI1:C27	3:A:611:LI1:H251	2.44	0.40
1:A:203:ILE:O	1:A:207:LEU:HG	2.22	0.40
3:A:602:LI1:H592	3:A:602:LI1:C50	2.52	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	218/249 (88%)	216 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	178/195 (91%)	166 (93%)	12 (7%)	16 4

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	30	LYS
1	A	48	LEU
1	A	74	GLU
1	A	75	GLN
1	A	95	LEU
1	A	153	PHE
1	A	163	MET
1	A	164	ARG
1	A	166	GLU
1	A	172	LYS
1	A	202	ASN

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	176	ASN
1	A	202	ASN

5.3.3 RNA ⓘ

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	$\# Z > 2$
3	LI1	A	606	-	7,7,44	0.48	0	6,6,51	0.82	0
3	LI1	A	612	-	17,17,44	1.07	1 (5%)	18,18,51	1.14	1 (5%)
3	LI1	A	610	-	39,39,44	1.04	2 (5%)	41,41,51	1.11	2 (4%)
3	LI1	A	605	-	7,7,44	0.45	0	6,6,51	0.60	0
3	LI1	A	601	-	31,31,44	1.11	2 (6%)	33,33,51	1.27	4 (12%)
3	LI1	A	611	-	16,16,44	1.15	1 (6%)	18,18,51	2.22	4 (22%)
2	RET	A	300	1	20,20,21	0.97	1 (5%)	27,27,28	1.49	6 (22%)
3	LI1	A	604	-	15,15,44	1.11	1 (6%)	14,14,51	1.09	1 (7%)
3	LI1	A	613	-	12,12,44	0.45	0	12,12,51	0.98	1 (8%)
3	LI1	A	603	-	17,17,44	1.10	1 (5%)	18,18,51	1.15	1 (5%)
3	LI1	A	607	-	37,37,44	1.04	2 (5%)	37,38,51	1.08	3 (8%)
3	LI1	A	602	-	40,40,44	1.05	2 (5%)	43,45,51	3.24	9 (20%)
4	SQU	A	701	-	26,26,26	1.40	6 (23%)	28,28,28	1.86	10 (35%)
3	LI1	A	609	-	15,15,44	1.15	1 (6%)	14,14,51	1.17	2 (14%)
3	LI1	A	608	-	17,17,44	1.07	1 (5%)	18,18,51	1.28	3 (16%)

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
3	LI1	A	606	-	-	3/5/5/49	-
3	LI1	A	612	-	-	9/16/16/49	-
3	LI1	A	610	-	-	29/39/39/49	-
3	LI1	A	605	-	-	4/5/5/49	-
3	LI1	A	601	-	2/2/3/8	20/32/32/49	-
3	LI1	A	611	-	2/2/3/8	7/17/17/49	-
2	RET	A	300	1	-	2/13/30/31	0/1/1/1
3	LI1	A	613	-	1/1/1/8	4/11/11/49	-
3	LI1	A	604	-	-	7/13/13/49	-
3	LI1	A	603	-	-	9/16/16/49	-
4	SQU	A	701	-	1/1/3/3	16/25/25/25	-
3	LI1	A	602	-	-	19/44/44/49	-
3	LI1	A	607	-	-	21/38/38/49	-
3	LI1	A	609	-	-	8/13/13/49	-
3	LI1	A	608	-	-	10/16/16/49	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	611	LI1	C26-C25	4.16	1.74	1.51
3	A	610	LI1	C26-C25	4.14	1.74	1.51
3	A	603	LI1	C26-C25	4.12	1.74	1.51
3	A	602	LI1	C26-C25	4.10	1.74	1.51
3	A	609	LI1	C26-C25	4.07	1.74	1.51
3	A	607	LI1	C26-C25	4.06	1.74	1.51
3	A	612	LI1	C26-C25	4.04	1.74	1.51
3	A	608	LI1	C26-C25	4.00	1.74	1.51
3	A	604	LI1	C26-C25	3.95	1.73	1.51
3	A	601	LI1	C26-C25	3.88	1.73	1.51
4	A	701	SQU	C14-C12	-3.23	1.35	1.52
4	A	701	SQU	C23-C22	-3.17	1.33	1.51
3	A	602	LI1	O3-C3	3.09	1.55	1.42
3	A	601	LI1	O3-C3	3.04	1.55	1.42
3	A	610	LI1	O3-C3	2.95	1.54	1.42
3	A	607	LI1	O3-C3	2.92	1.54	1.42
4	A	701	SQU	C9-C7	-2.91	1.35	1.51
4	A	701	SQU	C18-C17	-2.90	1.35	1.51
4	A	701	SQU	C4-C2	-2.47	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	SQU	C27-C28	-2.20	1.36	1.51
2	A	300	RET	C2-C3	-2.12	1.47	1.52

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	LI1	C49-C48-C50	13.05	158.54	111.29
3	A	602	LI1	C49-C48-C47	-10.31	73.94	111.29
3	A	602	LI1	C24-C23-C25	-9.97	75.20	111.29
3	A	611	LI1	C24-C23-C25	7.29	137.70	111.29
4	A	701	SQU	C15-C14-C12	4.16	129.37	115.92
3	A	610	LI1	C25-C26-C27	-3.55	101.06	113.62
3	A	612	LI1	C25-C26-C27	-3.54	101.10	113.62
3	A	603	LI1	C25-C26-C27	-3.53	101.13	113.62
3	A	608	LI1	C25-C26-C27	-3.52	101.16	113.62
3	A	602	LI1	O3-C3-C2	-3.30	103.04	111.78
3	A	601	LI1	O3-C3-C2	-3.23	103.22	111.78
3	A	602	LI1	C21-C22-C23	-3.15	105.72	115.92
4	A	701	SQU	C23-C22-C21	3.15	130.43	114.42
4	A	701	SQU	C10-C9-C7	3.15	130.41	114.42
3	A	601	LI1	C25-C26-C27	-3.14	102.53	113.62
4	A	701	SQU	C5-C4-C2	3.10	130.59	115.98
3	A	602	LI1	C51-C50-C48	-3.09	105.92	115.92
4	A	701	SQU	C25-C23-C22	3.02	129.74	114.42
3	A	611	LI1	C27-C26-C25	-2.88	99.39	113.29
3	A	602	LI1	C26-C25-C23	-2.87	102.11	115.86
3	A	610	LI1	O3-C3-C2	-2.84	104.25	111.78
3	A	609	LI1	C27-C26-C25	-2.80	100.20	114.42
3	A	611	LI1	C26-C25-C23	-2.68	103.00	115.86
3	A	601	LI1	C16-C17-C18	-2.68	107.25	115.92
2	A	300	RET	C20-C13-C12	2.62	122.21	118.08
3	A	611	LI1	C21-C20-C18	-2.59	107.54	115.92
2	A	300	RET	C18-C5-C6	2.53	127.36	124.53
3	A	607	LI1	C46-C45-C43	-2.52	107.77	115.92
3	A	604	LI1	C27-C26-C25	-2.49	101.76	114.42
3	A	607	LI1	O3-C3-C2	-2.48	105.21	111.78
3	A	602	LI1	C27-C26-C25	-2.47	101.38	113.29
2	A	300	RET	C18-C5-C4	-2.46	108.89	113.62
3	A	601	LI1	C21-C20-C18	-2.42	108.10	115.92
4	A	701	SQU	C9-C7-C6	2.38	126.52	114.42
3	A	608	LI1	C21-C20-C18	-2.37	108.27	115.92
4	A	701	SQU	C18-C17-C16	2.35	126.37	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	SQU	C20-C18-C17	2.32	126.22	114.42
3	A	609	LI1	C26-C25-C23	-2.30	102.75	114.42
3	A	613	LI1	C21-C20-C18	-2.24	108.68	115.92
4	A	701	SQU	C14-C12-C11	2.21	123.73	112.13
2	A	300	RET	C17-C1-C6	2.05	113.63	110.30
3	A	608	LI1	C26-C25-C23	-2.05	104.01	114.42
2	A	300	RET	C7-C6-C5	-2.05	116.49	121.46
3	A	607	LI1	C26-C25-C23	-2.05	104.03	114.42
4	A	701	SQU	C1-C2-C4	2.03	124.11	111.54
3	A	602	LI1	C46-C47-C48	-2.02	109.40	115.92
2	A	300	RET	C1-C6-C7	2.00	121.45	115.78

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	601	LI1	C2
3	A	601	LI1	C18
3	A	611	LI1	C23
3	A	611	LI1	C13
3	A	613	LI1	C18
4	A	701	SQU	C12

All (168) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	RET	C12-C13-C14-C15
2	A	300	RET	C20-C13-C14-C15
3	A	601	LI1	C1-C2-O2-C41
3	A	602	LI1	C11-C12-C13-C14
3	A	607	LI1	C42-C41-O2-C2
3	A	610	LI1	O2-C2-C3-O3
3	A	610	LI1	C12-C11-O1-C1
4	A	701	SQU	C20-C21-C22-C23
3	A	610	LI1	C47-C48-C50-C51
3	A	610	LI1	C52-C53-C55-C56
3	A	610	LI1	C55-C56-C57-C58
3	A	601	LI1	C16-C17-C18-C19
3	A	602	LI1	C46-C47-C48-C49
3	A	607	LI1	C44-C43-C45-C46
3	A	611	LI1	C24-C23-C25-C26
3	A	612	LI1	C14-C13-C15-C16
4	A	701	SQU	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
3	A	604	LI1	C20-C21-C22-C23
3	A	603	LI1	C25-C26-C27-C28
4	A	701	SQU	C11-C12-C14-C15
3	A	607	LI1	O1-C11-C12-C13
3	A	601	LI1	O2-C41-C42-C43
3	A	611	LI1	C23-C25-C26-C27
3	A	611	LI1	C20-C21-C22-C23
3	A	607	LI1	C12-C11-O1-C1
3	A	601	LI1	C15-C16-C17-C18
3	A	603	LI1	C18-C20-C21-C22
3	A	610	LI1	C16-C17-C18-C20
3	A	610	LI1	C56-C57-C58-C60
3	A	604	LI1	C25-C26-C27-C28
3	A	610	LI1	C46-C47-C48-C50
4	A	701	SQU	C6-C7-C9-C10
4	A	701	SQU	C14-C15-C16-C17
3	A	604	LI1	C21-C22-C23-C25
3	A	610	LI1	C53-C55-C56-C57
4	A	701	SQU	C16-C17-C18-C20
3	A	608	LI1	C26-C27-C28-C30
3	A	605	LI1	C15-C16-C17-C18
3	A	603	LI1	C22-C23-C25-C26
4	A	701	SQU	C23-C25-C26-C27
3	A	607	LI1	C12-C13-C15-C16
3	A	610	LI1	C20-C21-C22-C23
3	A	601	LI1	C12-C13-C15-C16
3	A	609	LI1	C13-C15-C16-C17
3	A	609	LI1	C20-C21-C22-C23
3	A	607	LI1	C23-C25-C26-C27
3	A	610	LI1	C26-C27-C28-C29
3	A	610	LI1	C26-C27-C28-C30
3	A	602	LI1	C15-C16-C17-C18
3	A	605	LI1	C16-C17-C18-C20
3	A	608	LI1	C12-C13-C15-C16
4	A	701	SQU	C11-C10-C9-C7
3	A	608	LI1	C20-C21-C22-C23
4	A	701	SQU	C3-C2-C4-C5
3	A	609	LI1	C16-C17-C18-C20
3	A	607	LI1	C20-C21-C22-C23
3	A	601	LI1	C43-C45-C46-C47
3	A	604	LI1	C23-C25-C26-C27
3	A	610	LI1	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
3	A	610	LI1	C21-C22-C23-C25
3	A	604	LI1	C17-C18-C20-C21
3	A	613	LI1	C16-C17-C18-C20
3	A	610	LI1	C25-C26-C27-C28
4	A	701	SQU	C26-C27-C28-C29
3	A	610	LI1	O2-C41-C42-C43
3	A	610	LI1	C23-C25-C26-C27
3	A	601	LI1	C45-C46-C47-C48
4	A	701	SQU	C17-C18-C20-C21
3	A	606	LI1	C15-C16-C17-C18
3	A	607	LI1	C52-C53-C55-C56
3	A	602	LI1	C53-C55-C56-C57
3	A	612	LI1	C15-C16-C17-C18
3	A	612	LI1	C23-C25-C26-C27
3	A	602	LI1	C44-C43-C45-C46
3	A	610	LI1	C17-C18-C20-C21
3	A	612	LI1	C16-C17-C18-C20
3	A	609	LI1	C18-C20-C21-C22
3	A	605	LI1	C17-C18-C20-C21
3	A	609	LI1	C21-C22-C23-C25
4	A	701	SQU	C26-C27-C28-C30
3	A	610	LI1	C50-C51-C52-C53
3	A	610	LI1	C41-C42-C43-C45
3	A	601	LI1	C20-C21-C22-C23
3	A	607	LI1	C21-C22-C23-C25
3	A	609	LI1	C26-C27-C28-C30
3	A	607	LI1	O2-C41-C42-C43
3	A	613	LI1	C21-C22-C23-C24
3	A	610	LI1	C42-C43-C45-C46
3	A	610	LI1	C12-C13-C15-C16
3	A	601	LI1	C16-C17-C18-C20
3	A	601	LI1	C17-C18-C20-C21
3	A	602	LI1	C42-C43-C45-C46
3	A	603	LI1	C12-C13-C15-C16
3	A	611	LI1	C12-C13-C15-C16
3	A	611	LI1	C14-C13-C15-C16
3	A	609	LI1	C23-C25-C26-C27
4	A	701	SQU	C22-C23-C25-C26
3	A	602	LI1	C48-C50-C51-C52
3	A	602	LI1	C13-C15-C16-C17
3	A	607	LI1	C51-C52-C53-C55
3	A	612	LI1	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
3	A	606	LI1	C18-C20-C21-C22
3	A	602	LI1	C55-C56-C57-C58
3	A	603	LI1	C21-C22-C23-C25
3	A	607	LI1	C17-C18-C20-C21
3	A	602	LI1	C2-C1-O1-C11
3	A	610	LI1	C1-C2-C3-O3
3	A	608	LI1	C11-C12-C13-C15
3	A	603	LI1	C23-C25-C26-C27
3	A	601	LI1	C21-C22-C23-C25
3	A	607	LI1	C45-C46-C47-C48
3	A	608	LI1	C26-C27-C28-C29
3	A	608	LI1	C22-C23-C25-C26
3	A	607	LI1	C53-C55-C56-C57
3	A	610	LI1	C56-C57-C58-C59
3	A	602	LI1	C52-C53-C55-C56
3	A	607	LI1	C42-C43-C45-C46
3	A	609	LI1	C25-C26-C27-C28
3	A	604	LI1	C16-C17-C18-C20
3	A	602	LI1	C11-C12-C13-C15
3	A	608	LI1	C21-C22-C23-C25
3	A	603	LI1	C14-C13-C15-C16
4	A	701	SQU	C21-C22-C23-C25
3	A	607	LI1	C16-C17-C18-C20
3	A	607	LI1	C48-C50-C51-C52
3	A	603	LI1	C16-C17-C18-C20
3	A	607	LI1	C47-C48-C50-C51
3	A	601	LI1	C11-C12-C13-C15
3	A	608	LI1	C16-C17-C18-C20
3	A	612	LI1	C12-C13-C15-C16
3	A	601	LI1	O1-C11-C12-C13
3	A	610	LI1	C43-C45-C46-C47
3	A	601	LI1	C42-C43-C45-C46
3	A	602	LI1	C41-C42-C43-C44
3	A	601	LI1	C19-C18-C20-C21
3	A	612	LI1	C22-C23-C25-C26
3	A	604	LI1	C11-C12-C13-C15
3	A	601	LI1	C12-C11-O1-C1
3	A	606	LI1	C13-C15-C16-C17
3	A	607	LI1	C18-C20-C21-C22
3	A	612	LI1	C11-C12-C13-C15
3	A	601	LI1	C2-C1-O1-C11
3	A	607	LI1	C2-C1-O1-C11

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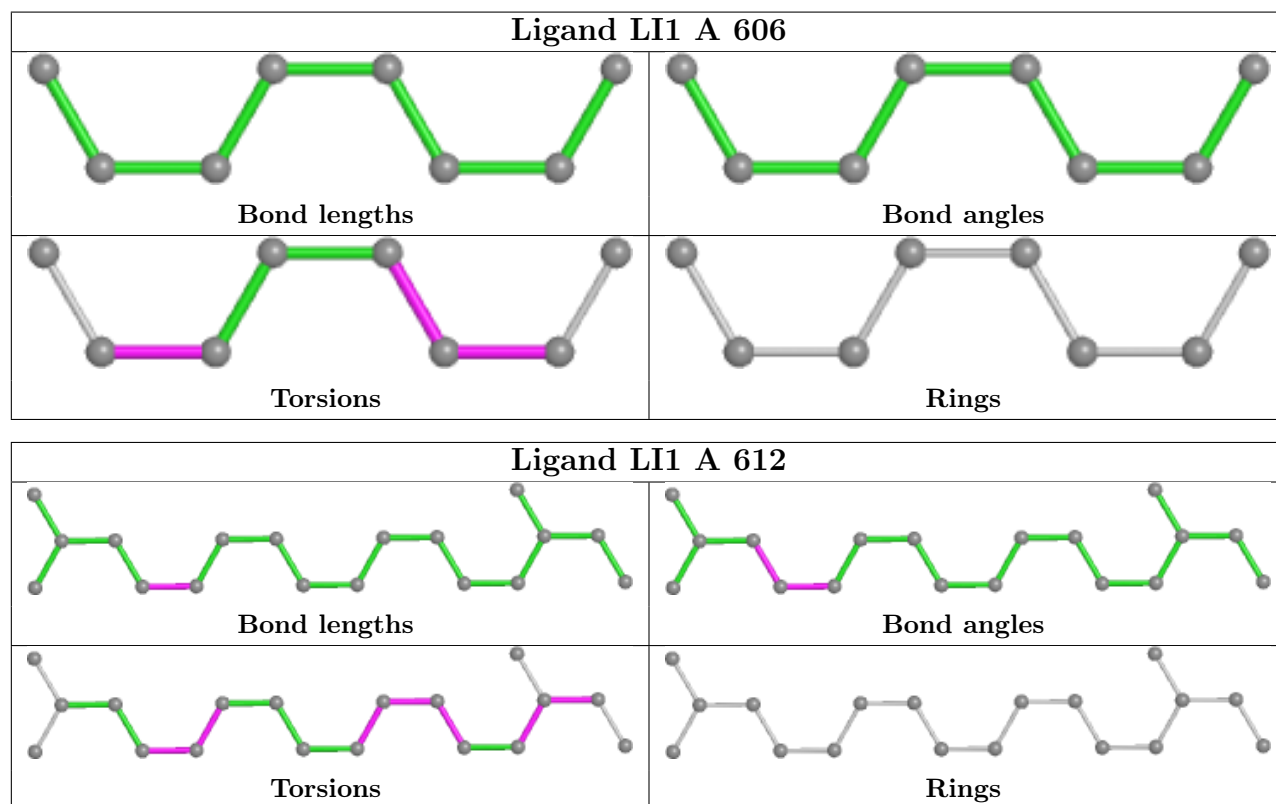
Mol	Chain	Res	Type	Atoms
3	A	610	LI1	O1-C1-C2-O2
3	A	612	LI1	C17-C18-C20-C21
3	A	608	LI1	C16-C17-C18-C19
3	A	611	LI1	C16-C17-C18-C19
3	A	610	LI1	C51-C52-C53-C55
4	A	701	SQU	C4-C5-C6-C7
3	A	611	LI1	C21-C22-C23-C25
3	A	613	LI1	C11-C12-C13-C15
3	A	601	LI1	C22-C23-C25-C26
3	A	602	LI1	C42-C41-O2-C2
3	A	613	LI1	C15-C16-C17-C18
3	A	601	LI1	C46-C47-C48-C50
3	A	608	LI1	C17-C18-C20-C21
3	A	602	LI1	O2-C2-C3-O3
3	A	602	LI1	C49-C48-C50-C51
3	A	602	LI1	C14-C13-C15-C16
3	A	601	LI1	C18-C20-C21-C22
3	A	603	LI1	C11-C12-C13-C14
3	A	610	LI1	O1-C1-C2-C3
3	A	605	LI1	C18-C20-C21-C22
3	A	602	LI1	C21-C22-C23-C24
4	A	701	SQU	C13-C12-C14-C15
3	A	610	LI1	C18-C20-C21-C22
3	A	607	LI1	C41-C42-C43-C45
3	A	602	LI1	C43-C45-C46-C47

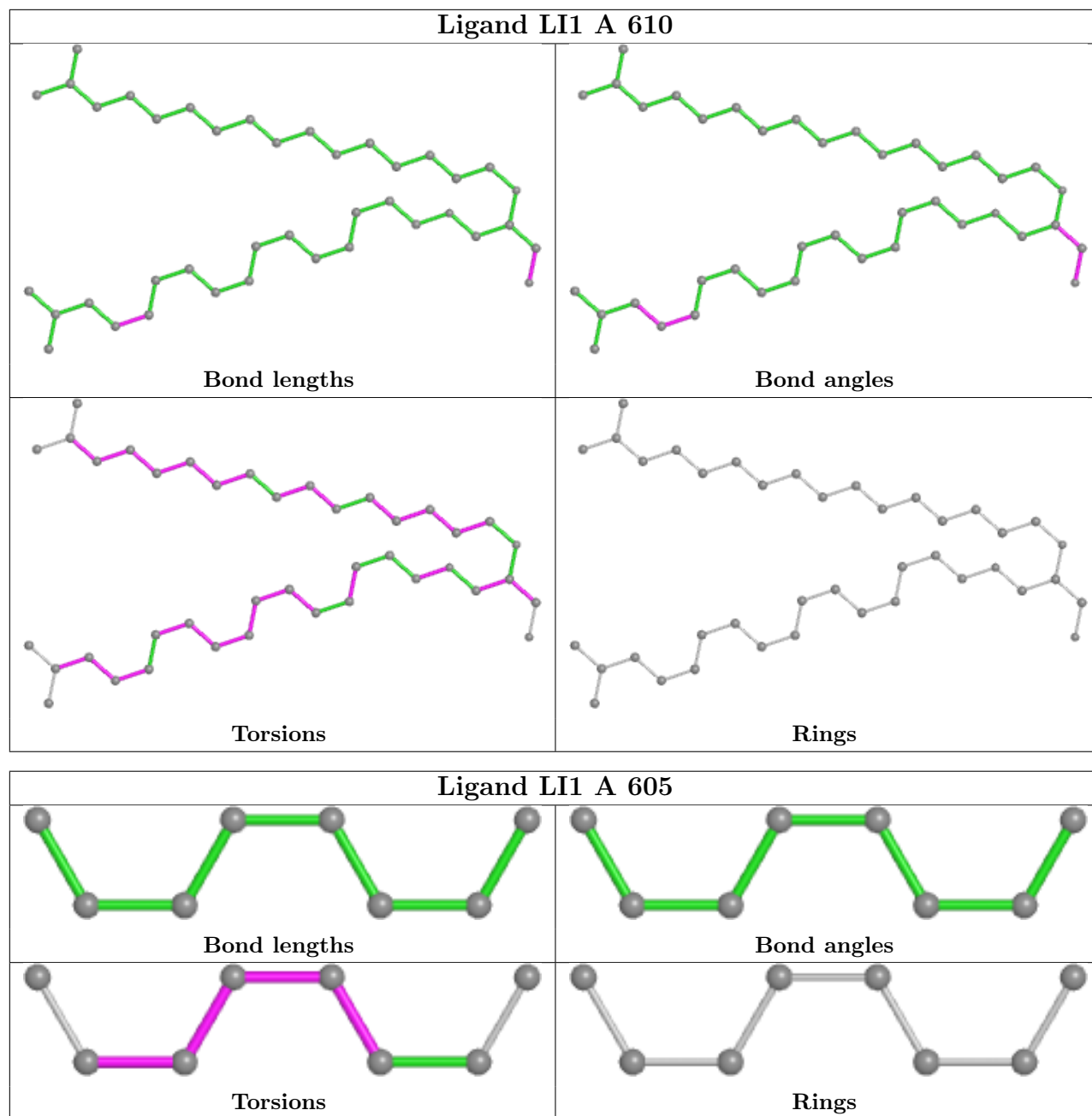
There are no ring outliers.

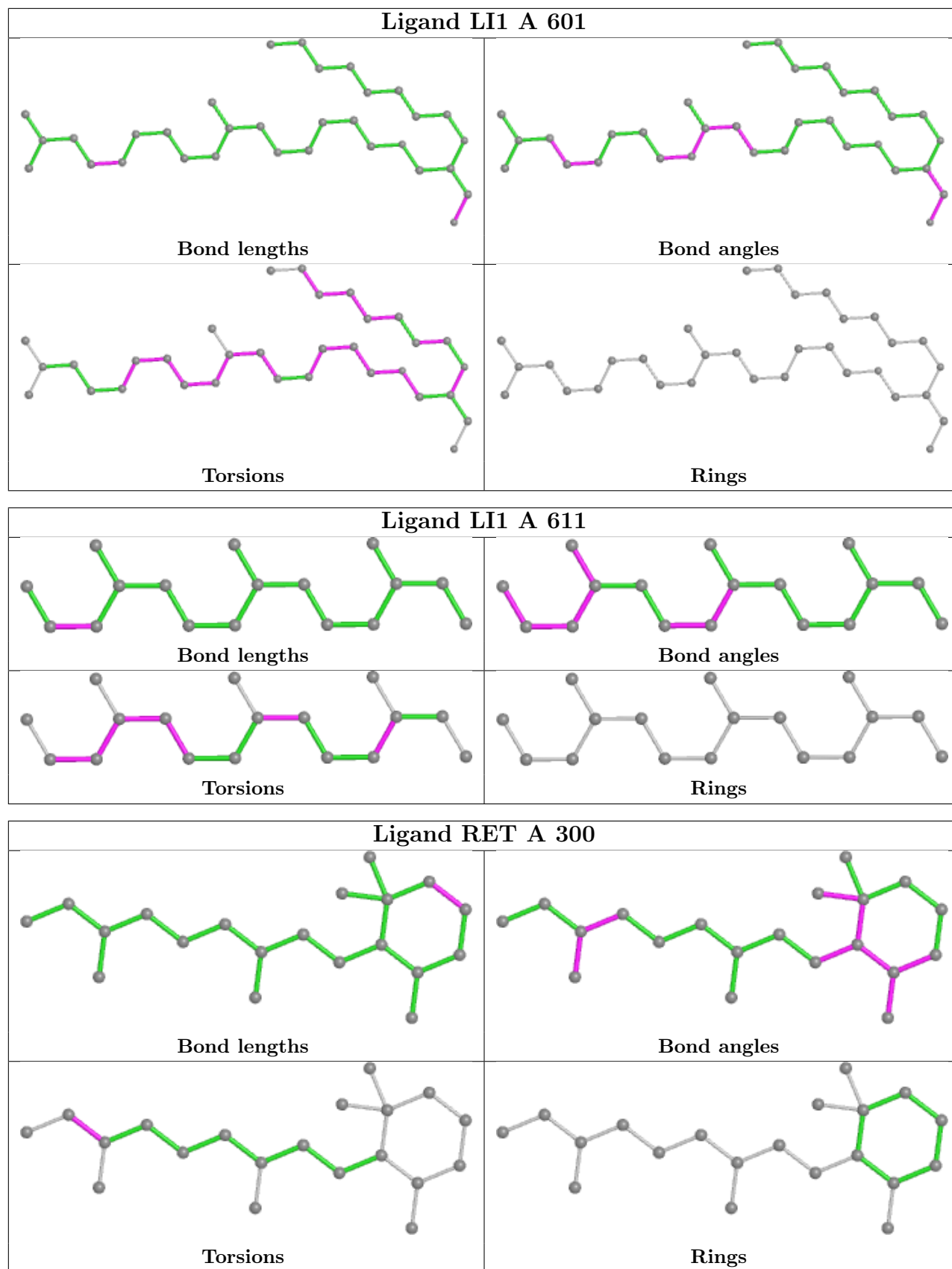
12 monomers are involved in 79 short contacts:

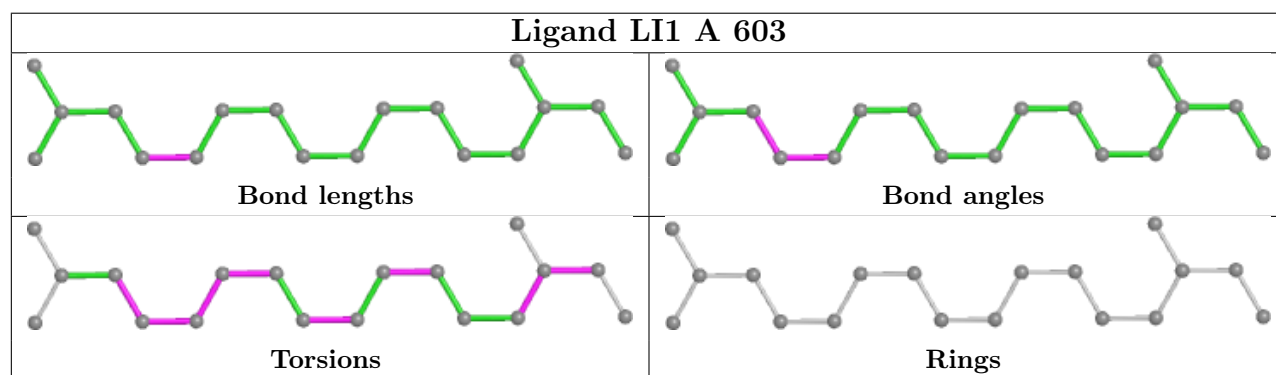
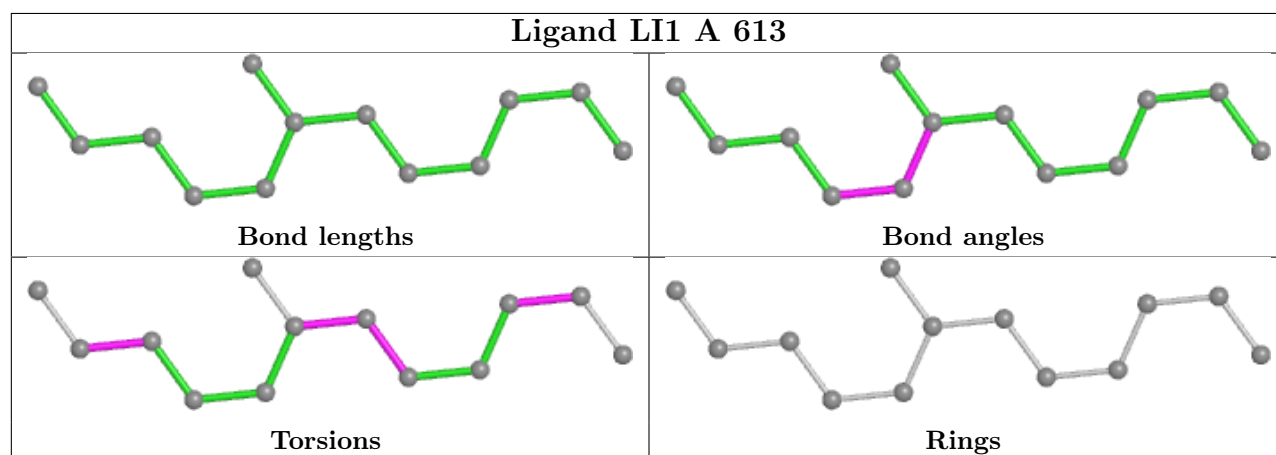
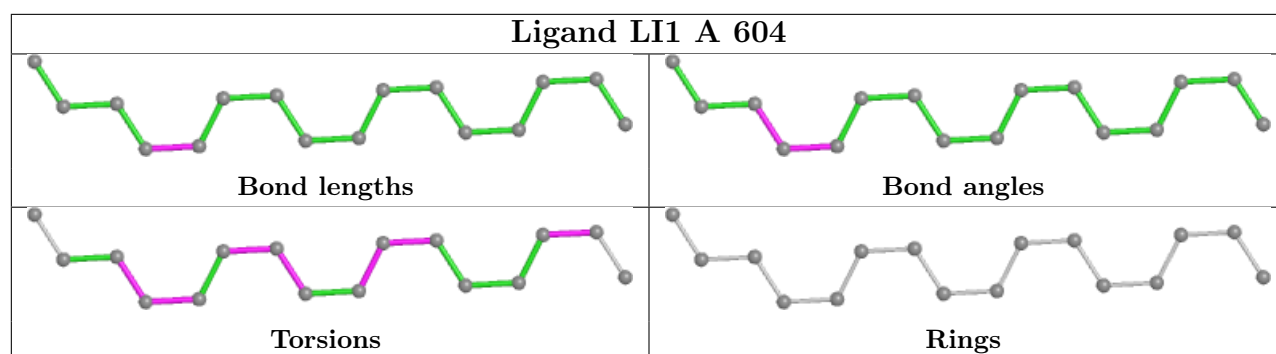
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	606	LI1	1	0
3	A	612	LI1	3	0
3	A	610	LI1	19	0
3	A	601	LI1	8	0
3	A	611	LI1	10	0
2	A	300	RET	3	0
3	A	613	LI1	1	0
3	A	603	LI1	10	0
3	A	607	LI1	4	0
3	A	602	LI1	17	0
4	A	701	SQU	4	0
3	A	608	LI1	2	0

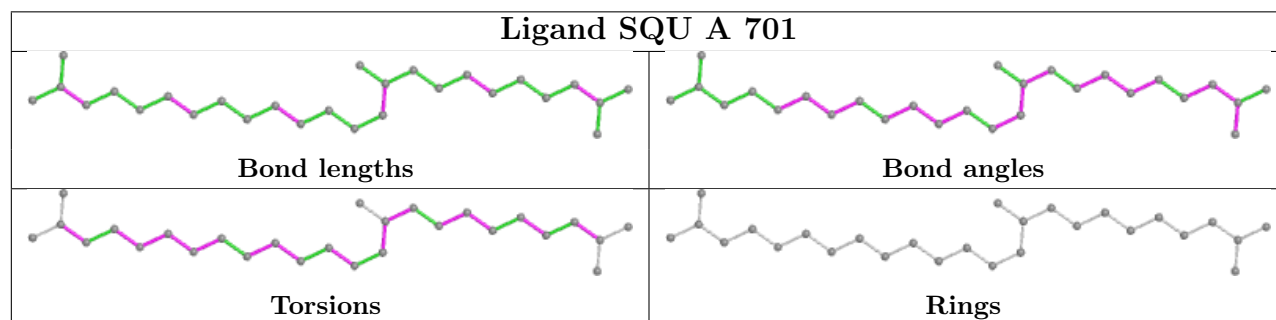
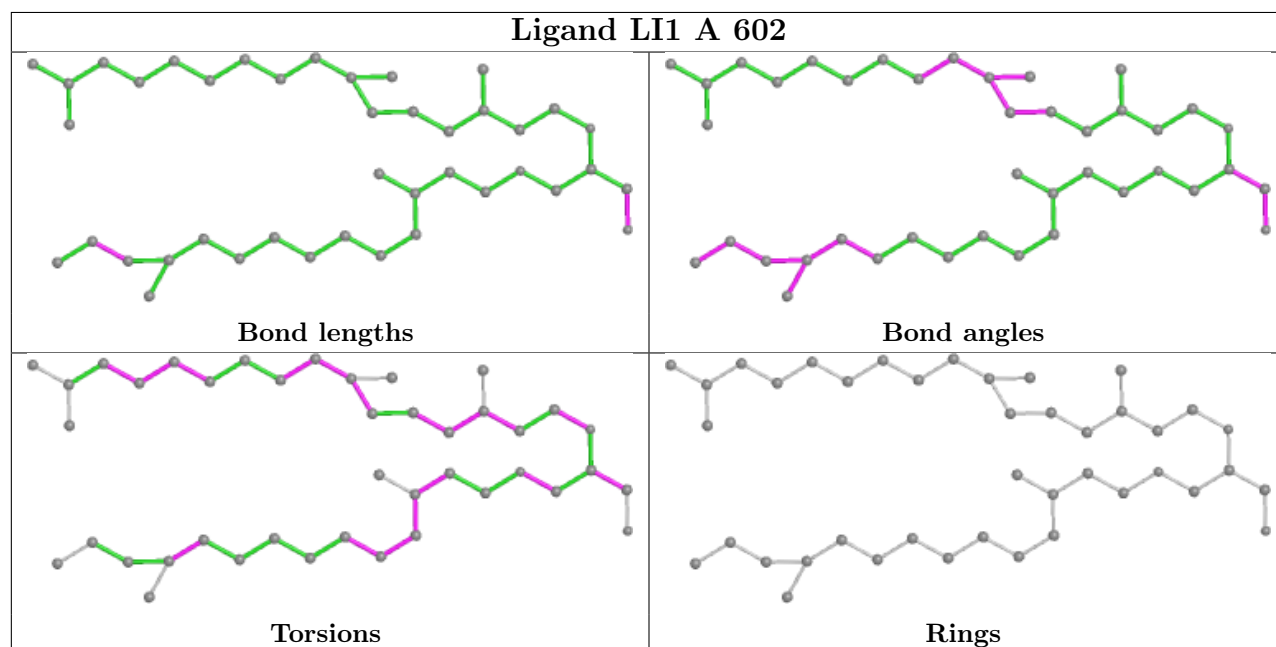
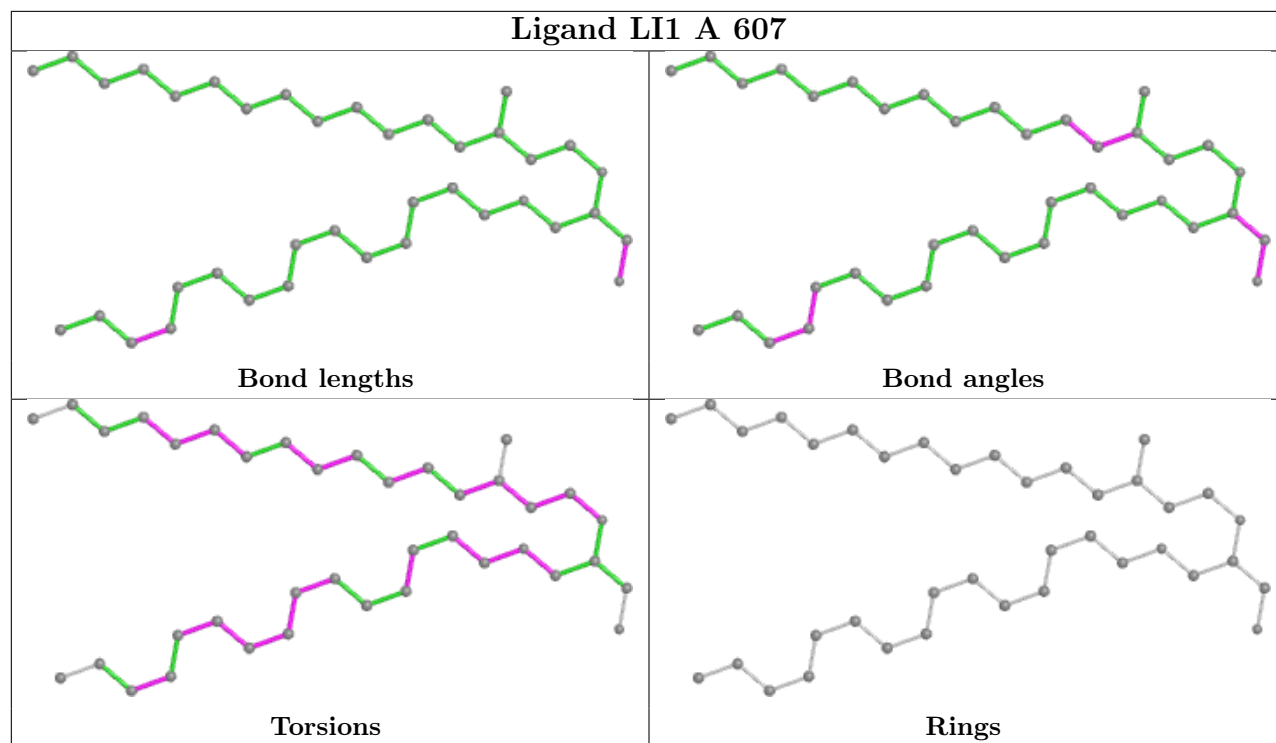
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

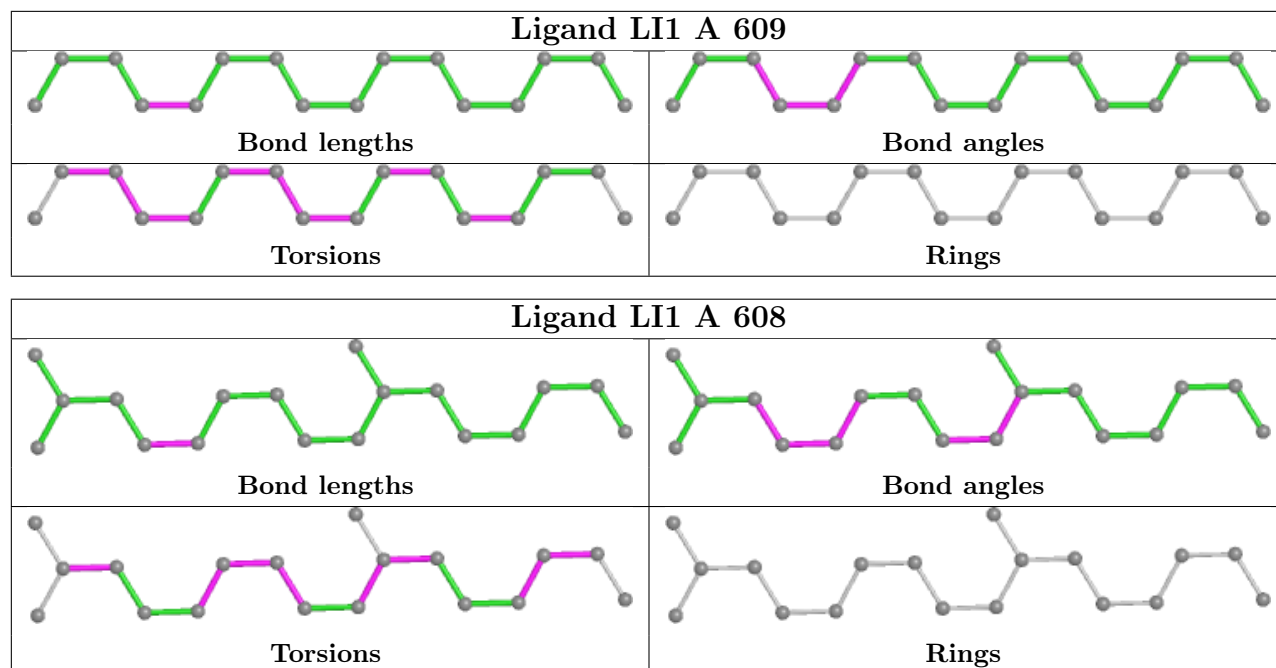












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	222/249 (89%)	-0.18	10 (4%) 33 30	18, 26, 57, 128	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	GLY	4.1
1	A	162	SER	3.9
1	A	156	PHE	3.8
1	A	5	THR	3.6
1	A	6	GLY	3.4
1	A	154	PHE	3.1
1	A	33	GLY	3.0
1	A	228	ALA	2.8
1	A	72	GLY	2.7
1	A	231	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

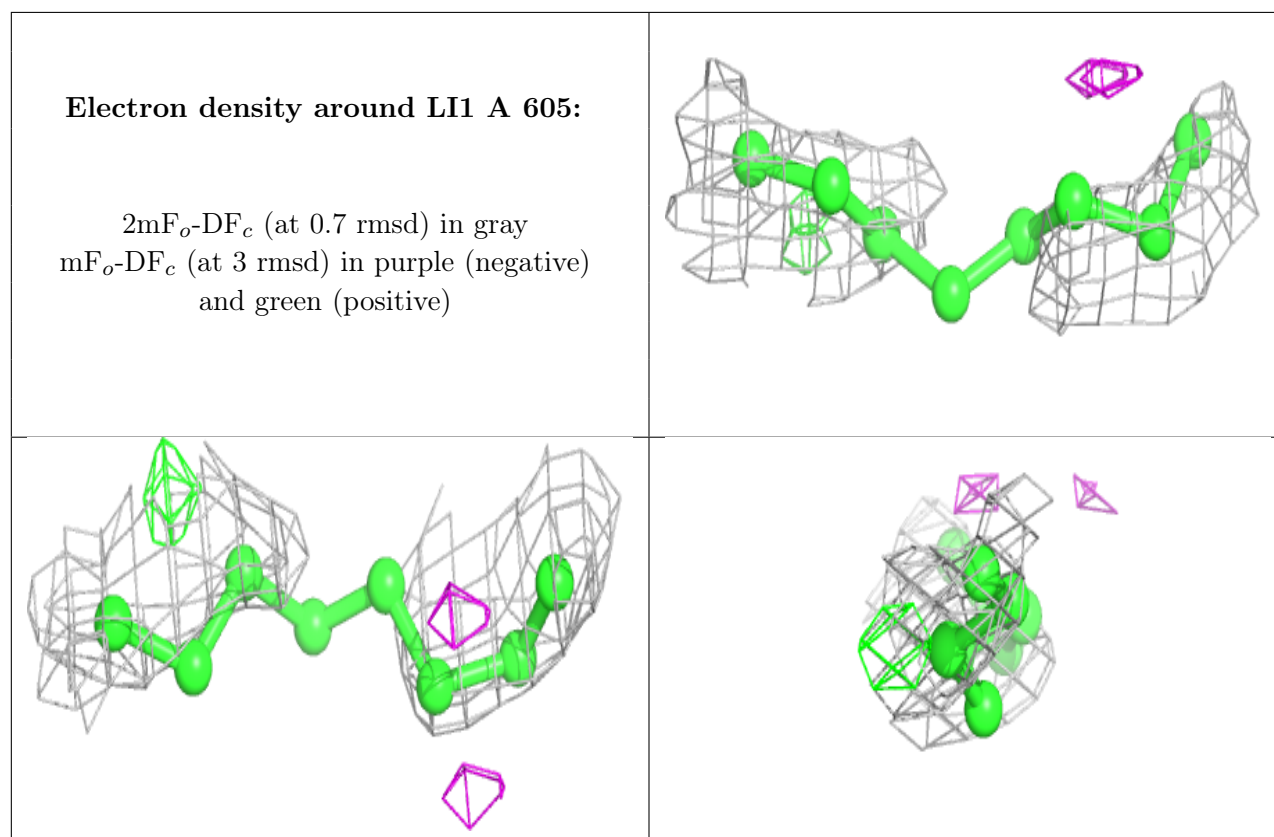
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

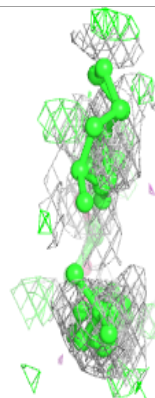
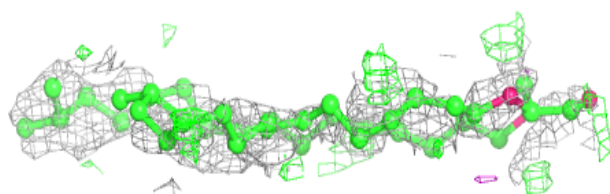
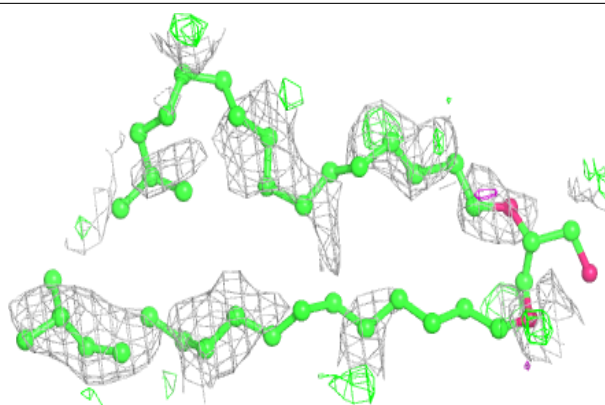
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	LI1	A	605	8/45	0.20	0.35	67,79,86,88	0
3	LI1	A	610	40/45	0.52	0.35	63,108,131,135	0
3	LI1	A	604	16/45	0.63	0.22	52,78,105,106	0
3	LI1	A	609	16/45	0.65	0.33	53,69,84,85	0
3	LI1	A	611	17/45	0.69	0.38	104,114,144,152	0
4	SQU	A	701	27/27	0.69	0.26	55,62,96,105	0
3	LI1	A	603	18/45	0.71	0.22	44,54,78,80	0
3	LI1	A	602	41/45	0.73	0.22	30,73,91,92	0
3	LI1	A	601	32/45	0.76	0.21	37,64,89,97	0
3	LI1	A	607	38/45	0.76	0.15	34,55,84,102	0
3	LI1	A	608	18/45	0.79	0.20	35,65,82,84	0
3	LI1	A	612	18/45	0.84	0.22	27,44,55,77	0
3	LI1	A	606	8/45	0.85	0.15	38,42,59,63	0
3	LI1	A	613	13/45	0.86	0.15	39,52,71,73	0
2	RET	A	300	20/21	0.95	0.10	16,20,25,27	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

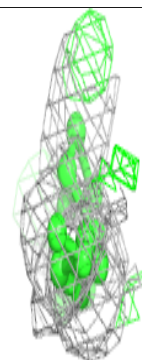
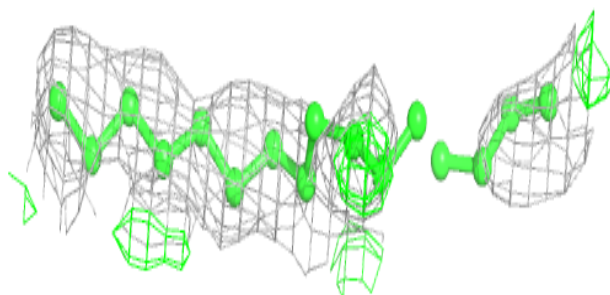
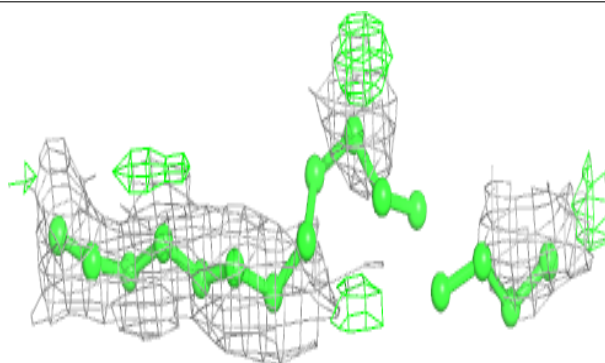


Electron density around LI1 A 610:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

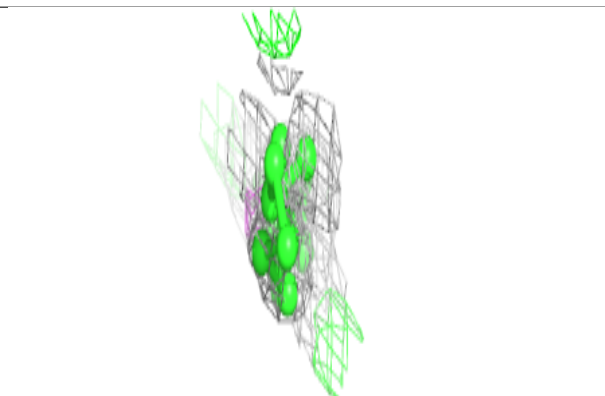
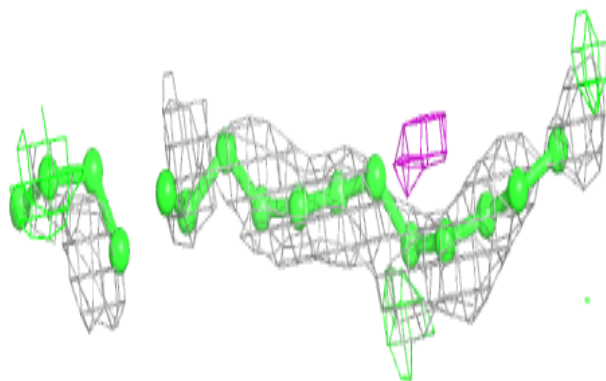
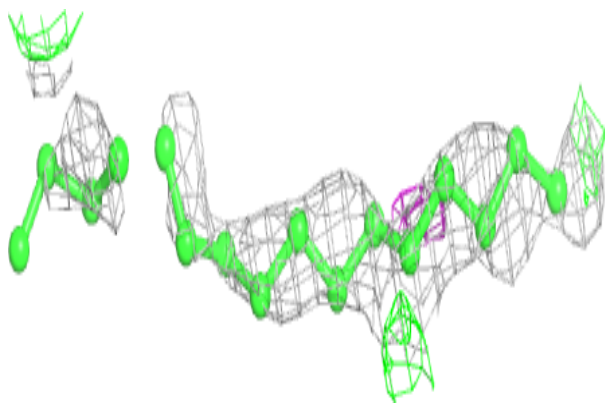
**Electron density around LI1 A 604:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

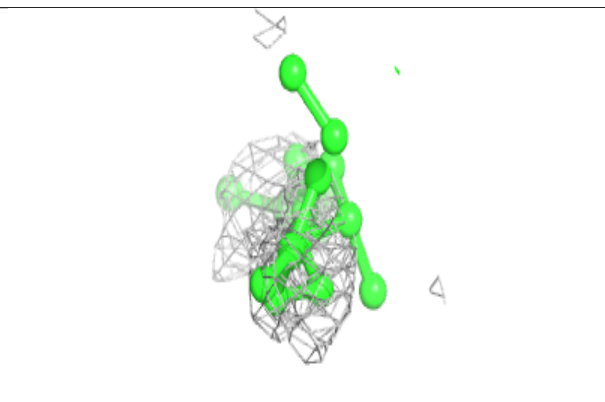
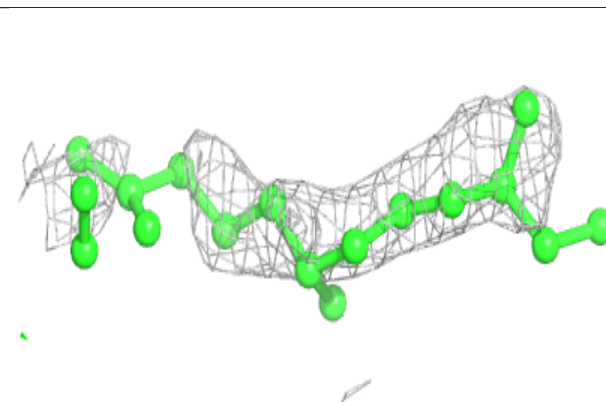
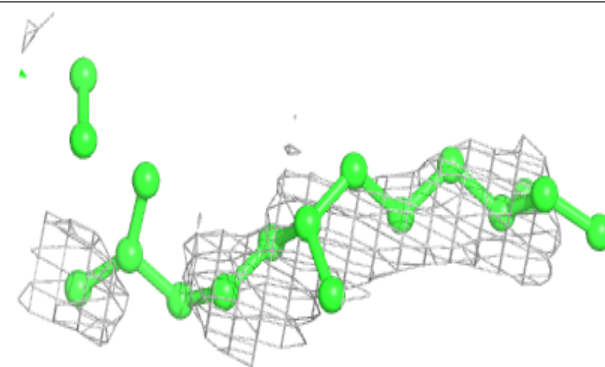


Electron density around LI1 A 609:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

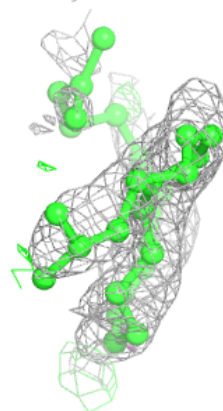
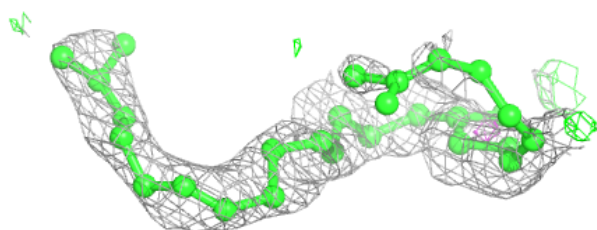
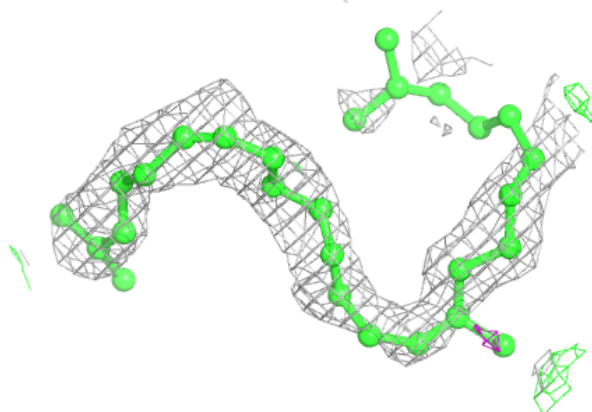
**Electron density around LI1 A 611:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

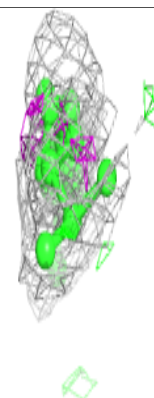
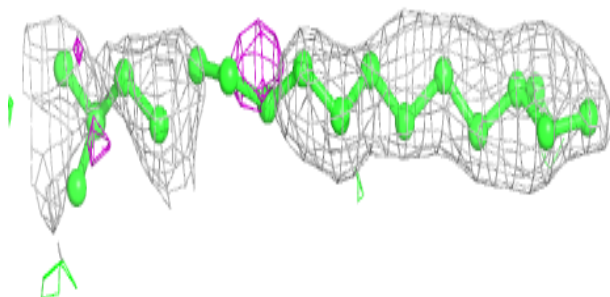
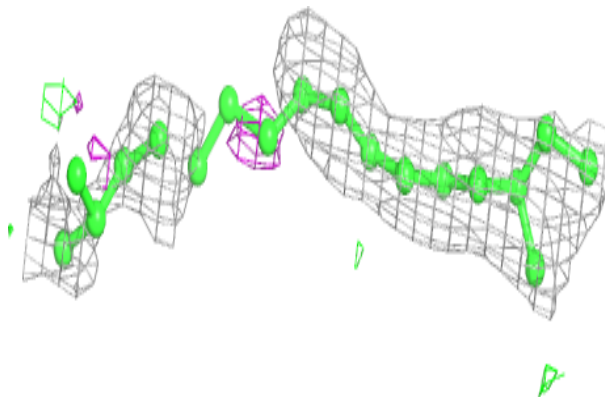


Electron density around SQU A 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

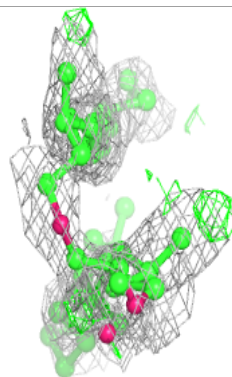
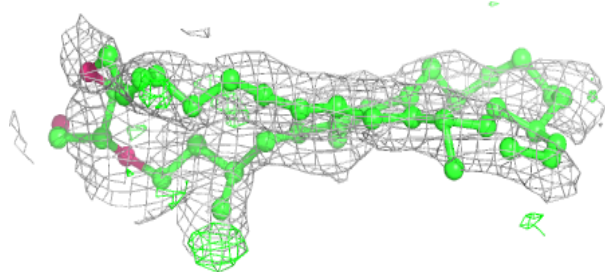
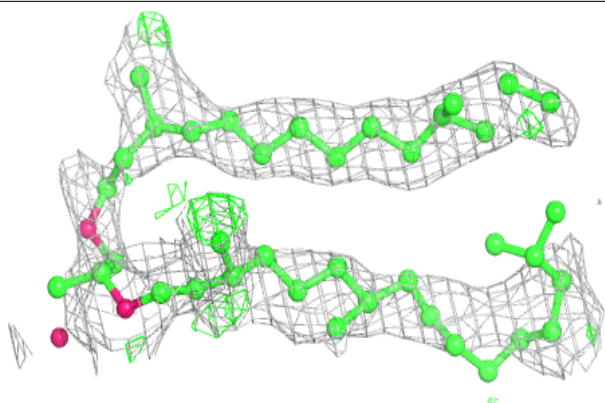
**Electron density around LI1 A 603:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

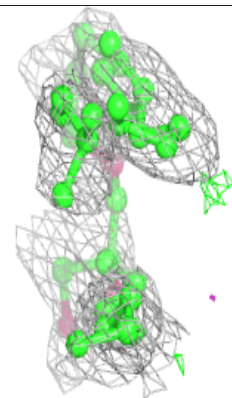
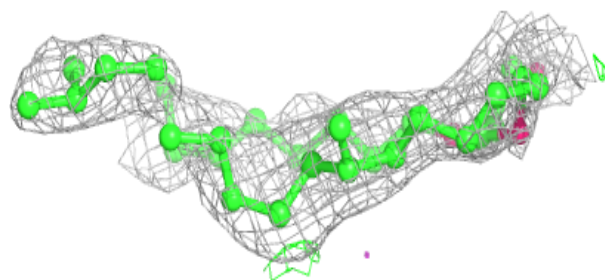
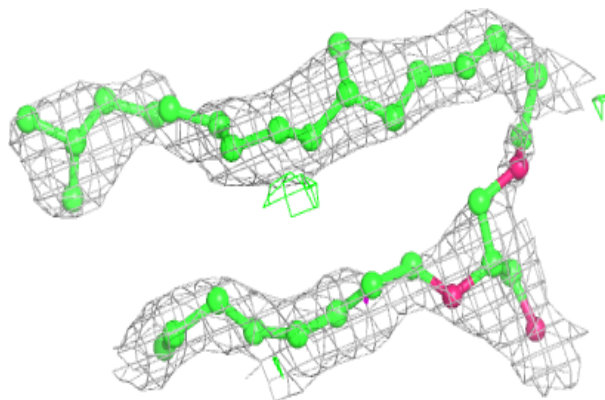


Electron density around LI1 A 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

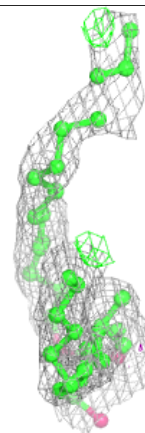
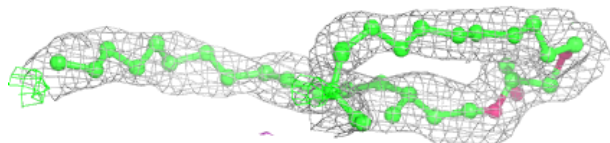
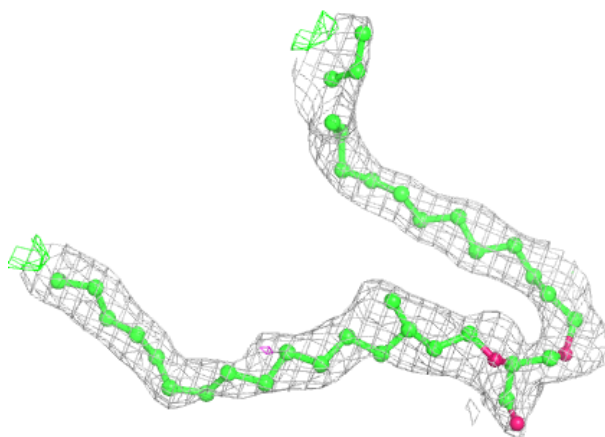
**Electron density around LI1 A 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

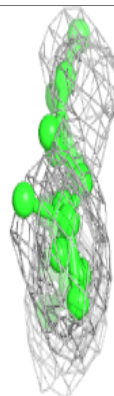
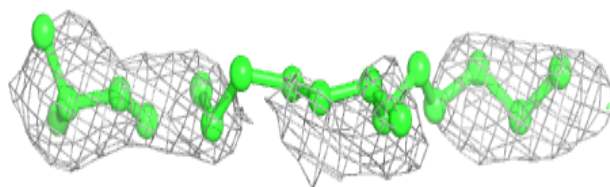
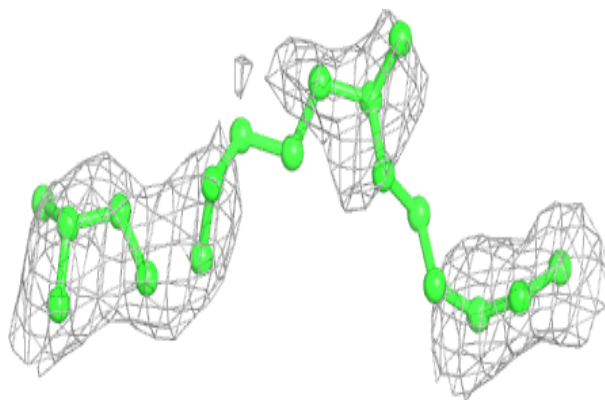


Electron density around LI1 A 607:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

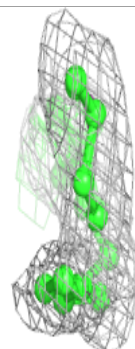
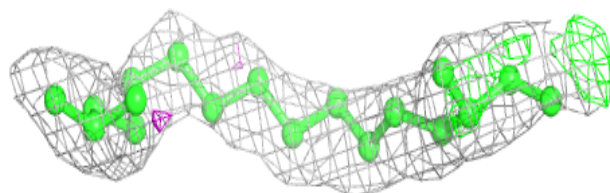
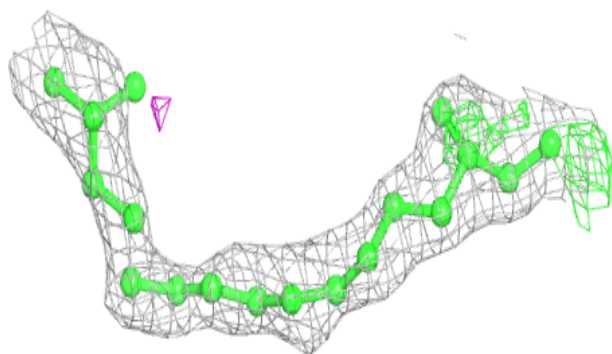
**Electron density around LI1 A 608:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

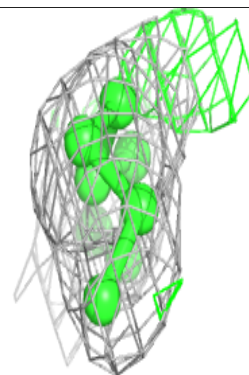
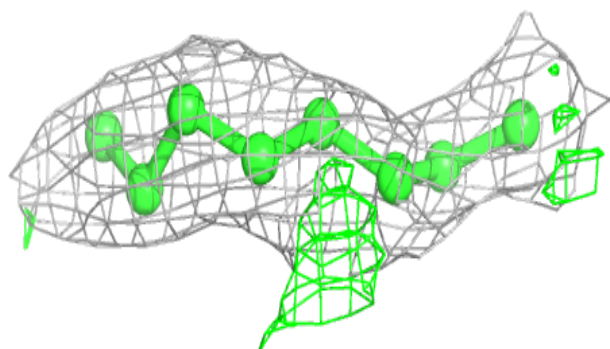
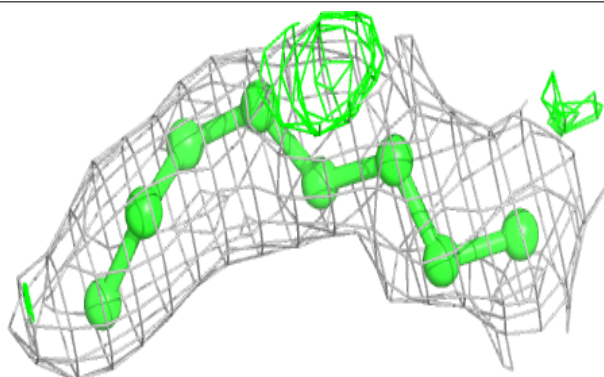


Electron density around LI1 A 612:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

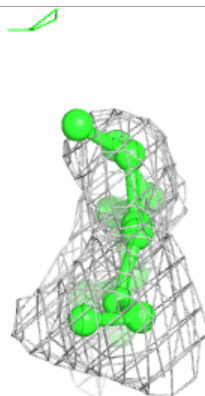
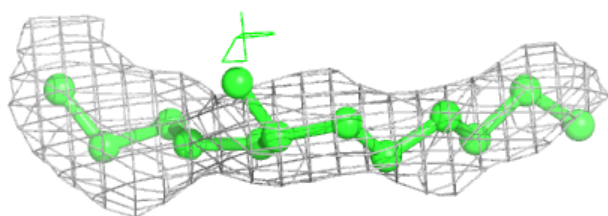
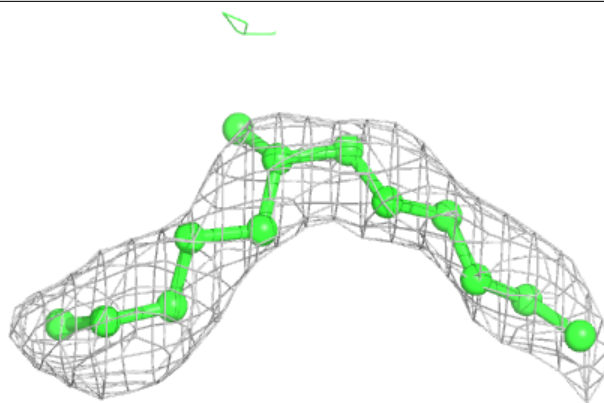
**Electron density around LI1 A 606:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

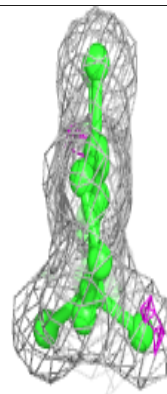
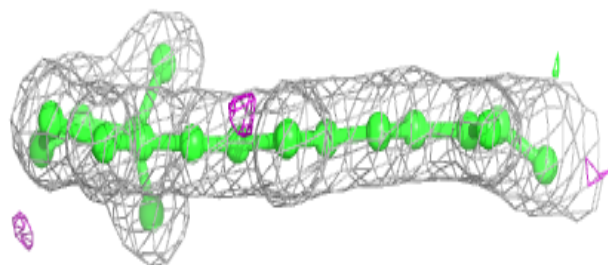
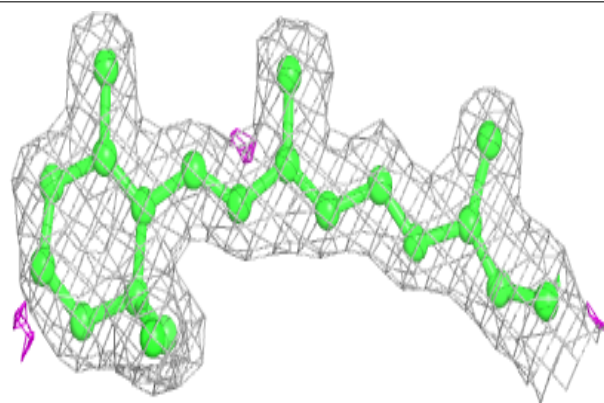


Electron density around LI1 A 613:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around RET A 300:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.