



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 03:49 PM BST

PDB ID : 4FPD  
Title : Deprotonation of D96 in bacteriorhodopsin opens the proton uptake pathway  
Authors : Wang, T.; Sessions, A.O.; Lunde, C.S.; Rouani, S.; Glaeser, R.M.; Facciotti, M.T.; Duan, Y.  
Deposited on : 2012-06-22  
Resolution : 2.65 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](mailto: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.

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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 : 2.13.1  
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) : 2.13.1

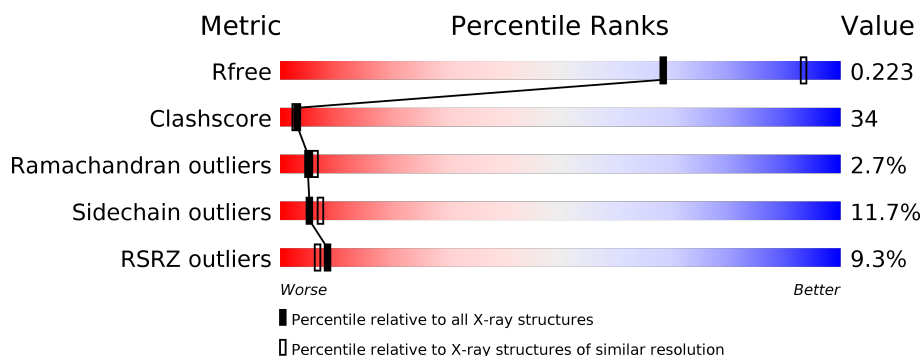
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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))
$R_{free}$	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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  $\geq 3$ , 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	262	<div> <div>8%</div> <div>48%</div> <div>31%</div> <div>6%</div> <div>14%</div> </div>

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
4	LI1	A	303	-	-	-	X
4	LI1	A	304	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	LI1	A	306	-	-	-	X
4	LI1	A	308	-	-	-	X
4	LI1	A	310	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 1899 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.

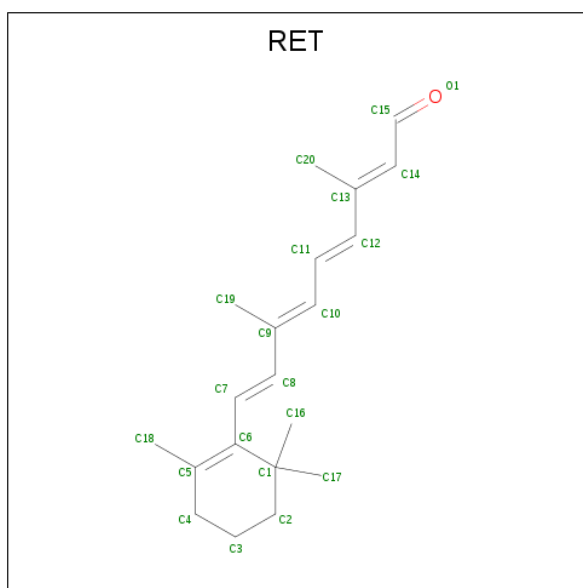
- Molecule 1 is a protein called Bacteriorhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	225	1729	1158	266	295	10	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	GLY	ASP	ENGINEERED MUTATION	UNP P02945
A	171	CYS	PHE	ENGINEERED MUTATION	UNP P02945
A	219	LEU	PHE	ENGINEERED MUTATION	UNP P02945

- Molecule 2 is RETINAL (three-letter code: RET) (formula:  $C_{20}H_{28}O$ ).

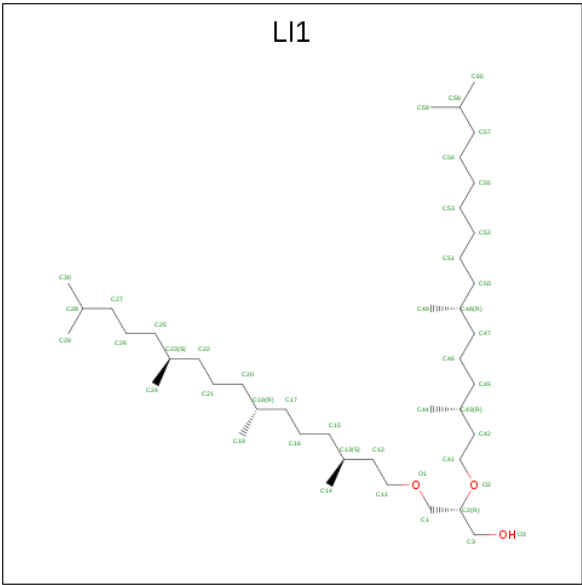


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	1
			40	40		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0

- Molecule 4 is 1-[2,6,10,14-TETRAMETHYL-HEXADECAN-16-YL]-2-[2,10,14-TRIMETHYLHEXADECAN-16-YL]GLYCEROL (three-letter code: LI1) (formula: C<sub>42</sub>H<sub>86</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 11 11	0	0
4	A	1	Total C 18 18	0	0
4	A	1	Total C 8 8	0	0
4	A	1	Total C 5 5	0	0
4	A	1	Total C O 29 26 3	0	0
4	A	1	Total C 3 3	0	0
4	A	1	Total C 14 14	0	0
4	A	1	Total C 10 10	0	0

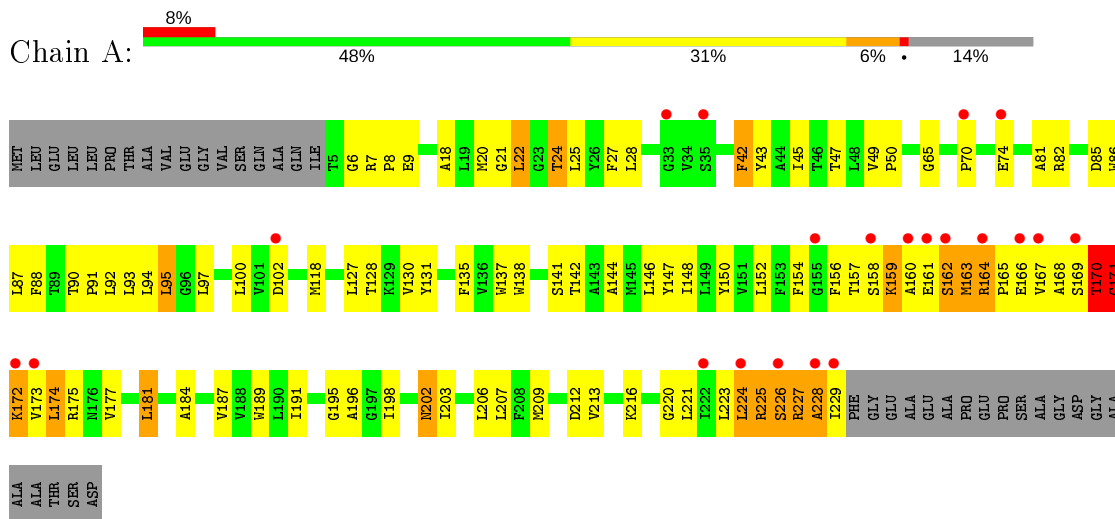
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	31	Total	O	0	0
			31	31		

### 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 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, $\alpha$ , $\beta$ , $\gamma$	60.93 Å 60.93 Å 107.70 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.95 – 2.65 47.39 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.95-2.65) 99.5 (47.39-2.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.65 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.223 , 0.240 0.230 , 0.223	Depositor DCC
$R_{free}$ test set	322 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.4	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 62.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.088 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	1899	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LI1, RET, CL

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	0.45	0/1774	0.64	0/2424

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	1729	0	1797	128	0
2	A	40	0	53	5	0
3	A	1	0	0	1	0
4	A	98	0	135	9	0
5	A	31	0	0	5	0
All	All	1899	0	1985	131	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 34.

All (131) 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:228:ALA:O	1:A:229:ILE:CG1	1.95	1.15
1:A:172:LYS:HD3	1:A:175:ARG:NH2	1.65	1.10
1:A:228:ALA:O	1:A:229:ILE:HG13	1.59	1.02
1:A:224:LEU:O	1:A:227:ARG:HD3	1.64	0.98
1:A:225:ARG:O	1:A:227:ARG:N	1.94	0.98
1:A:227:ARG:HH11	1:A:227:ARG:CG	1.78	0.96
1:A:212:ASP:O	1:A:216:LYS:HG3	1.67	0.94
1:A:20:MET:O	1:A:24:THR:HG22	1.69	0.93
1:A:227:ARG:O	1:A:229:ILE:N	2.02	0.92
1:A:167:VAL:CG2	1:A:229:ILE:HG12	1.98	0.92
1:A:42:PHE:HD1	1:A:224:LEU:HD23	1.34	0.91
1:A:170:THR:C	1:A:172:LYS:H	1.72	0.90
1:A:228:ALA:O	1:A:229:ILE:CD1	2.20	0.90
1:A:227:ARG:HH11	1:A:227:ARG:CB	1.83	0.89
1:A:227:ARG:HH11	1:A:227:ARG:HB3	1.36	0.88
1:A:152:LEU:HD22	5:A:430:HOH:O	1.75	0.85
1:A:227:ARG:HH11	1:A:227:ARG:HG3	1.40	0.84
1:A:228:ALA:O	1:A:229:ILE:HD12	1.78	0.83
1:A:170:THR:C	1:A:172:LYS:N	2.32	0.81
1:A:43:TYR:CE1	1:A:224:LEU:HD11	2.15	0.80
1:A:154:PHE:HA	1:A:157:THR:HG22	1.63	0.80
1:A:167:VAL:HG23	1:A:229:ILE:HG12	1.64	0.79
1:A:227:ARG:NH1	1:A:227:ARG:HG3	1.95	0.78
1:A:42:PHE:CD1	1:A:224:LEU:HD23	2.18	0.77
1:A:228:ALA:O	1:A:229:ILE:CB	2.33	0.76
1:A:43:TYR:CZ	1:A:224:LEU:HD11	2.21	0.75
1:A:172:LYS:CD	1:A:175:ARG:NH2	2.50	0.73
1:A:227:ARG:HB3	1:A:227:ARG:NH1	2.04	0.73
1:A:156:PHE:CE2	1:A:174:LEU:HD13	2.24	0.73
1:A:227:ARG:O	1:A:228:ALA:C	2.24	0.72
1:A:172:LYS:HD3	1:A:175:ARG:HH22	1.50	0.71
1:A:163:MET:HE2	1:A:167:VAL:O	1.91	0.71
1:A:82:ARG:HD3	5:A:404:HOH:O	1.92	0.70
1:A:137:TRP:NE1	3:A:302:CL:CL	2.56	0.69
1:A:224:LEU:O	1:A:227:ARG:CD	2.39	0.68
1:A:170:THR:O	1:A:173:VAL:N	2.26	0.68
1:A:42:PHE:HD1	1:A:224:LEU:CD2	2.04	0.68
1:A:202:ASN:H	1:A:202:ASN:HD22	1.41	0.68
1:A:160:ALA:O	1:A:168:ALA:HB1	1.94	0.67
1:A:173:VAL:O	1:A:177:VAL:HG23	1.93	0.67
1:A:156:PHE:CB	1:A:175:ARG:HB2	2.27	0.65
1:A:156:PHE:HE2	1:A:174:LEU:HD13	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:THR:O	1:A:172:LYS:N	2.32	0.62
1:A:141:SER:HB3	2:A:301[A]:RET:H41	1.81	0.62
1:A:18:ALA:O	1:A:22:LEU:HD13	2.00	0.62
1:A:160:ALA:O	1:A:163:MET:HG3	2.00	0.62
1:A:170:THR:HG22	1:A:171:CYS:N	2.13	0.61
1:A:163:MET:HG3	1:A:168:ALA:HA	1.82	0.61
1:A:177:VAL:O	1:A:181:LEU:HB2	2.01	0.61
1:A:163:MET:HB2	1:A:167:VAL:HG13	1.83	0.60
1:A:49:VAL:HB	1:A:50:PRO:HD3	1.82	0.60
1:A:156:PHE:CG	1:A:175:ARG:HB2	2.38	0.59
1:A:65:GLY:HA3	1:A:81:ALA:HB2	1.86	0.58
1:A:220:GLY:HA3	5:A:415:HOH:O	2.05	0.57
1:A:90:THR:N	1:A:91:PRO:HD2	2.19	0.57
1:A:43:TYR:CZ	1:A:224:LEU:CD1	2.87	0.57
1:A:142:THR:O	1:A:146:LEU:HG	2.04	0.56
1:A:91:PRO:HB2	4:A:310:LI1:H212	1.87	0.56
1:A:92:LEU:HG	4:A:310:LI1:H243	1.87	0.56
2:A:301[A]:RET:H171	2:A:301[A]:RET:H8	1.87	0.55
1:A:170:THR:CG2	1:A:171:CYS:N	2.69	0.55
1:A:172:LYS:HZ2	1:A:175:ARG:NH1	2.04	0.55
1:A:93:LEU:O	1:A:97:LEU:HG	2.07	0.54
1:A:202:ASN:N	1:A:202:ASN:HD22	2.04	0.54
1:A:135:PHE:CZ	1:A:195:GLY:O	2.60	0.54
1:A:172:LYS:NZ	1:A:175:ARG:CZ	2.71	0.53
1:A:209:MET:O	1:A:213:VAL:HG12	2.08	0.53
1:A:196:ALA:HB1	1:A:198:ILE:HD13	1.90	0.53
1:A:160:ALA:O	1:A:168:ALA:CB	2.57	0.53
1:A:196:ALA:CB	1:A:198:ILE:HD13	2.38	0.53
1:A:187:VAL:O	1:A:191:ILE:HG12	2.10	0.52
1:A:224:LEU:O	1:A:227:ARG:HG2	2.09	0.52
1:A:163:MET:CE	1:A:167:VAL:O	2.57	0.52
1:A:118:MET:SD	2:A:301[A]:RET:H192	2.50	0.52
1:A:135:PHE:CE2	4:A:304:LI1:H121	2.44	0.52
1:A:82:ARG:NH2	5:A:402:HOH:O	2.35	0.52
1:A:156:PHE:HB3	1:A:175:ARG:HB2	1.91	0.52
1:A:90:THR:N	1:A:91:PRO:CD	2.73	0.51
1:A:173:VAL:HG12	1:A:173:VAL:O	2.10	0.51
1:A:164:ARG:O	1:A:168:ALA:CB	2.59	0.50
1:A:184:ALA:O	1:A:187:VAL:HG13	2.12	0.50
1:A:203:ILE:O	1:A:207:LEU:HG	2.10	0.50
1:A:6:GLY:O	1:A:7:ARG:C	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LEU:HD23	4:A:309:LI1:H561	1.94	0.49
1:A:174:LEU:C	1:A:174:LEU:CD2	2.82	0.49
1:A:90:THR:OG1	1:A:91:PRO:HD3	2.13	0.48
1:A:94:LEU:CD2	1:A:152:LEU:HD11	2.44	0.48
1:A:227:ARG:HD2	1:A:227:ARG:HA	1.47	0.47
1:A:135:PHE:HZ	1:A:195:GLY:O	1.97	0.47
1:A:154:PHE:O	1:A:158:SER:HB3	2.15	0.47
1:A:172:LYS:HZ3	1:A:175:ARG:CZ	2.28	0.47
1:A:88:PHE:CD1	4:A:307:LI1:H571	2.50	0.46
1:A:224:LEU:O	1:A:227:ARG:CG	2.63	0.46
1:A:131:TYR:OH	4:A:304:LI1:C11	2.63	0.46
1:A:174:LEU:HD21	1:A:223:LEU:HD21	1.98	0.46
1:A:70:PRO:HA	1:A:74:GLU:O	2.15	0.46
1:A:167:VAL:CG2	1:A:229:ILE:CG1	2.84	0.45
1:A:225:ARG:HB3	1:A:226:SER:H	1.38	0.45
1:A:184:ALA:O	1:A:187:VAL:CG1	2.65	0.45
1:A:160:ALA:HA	1:A:171:CYS:SG	2.57	0.44
1:A:161:GLU:OE2	1:A:161:GLU:HA	2.17	0.44
1:A:25:LEU:HB2	4:A:308:LI1:H161	2.00	0.44
1:A:147:TYR:O	1:A:150:TYR:HB3	2.17	0.44
1:A:224:LEU:HD23	1:A:224:LEU:HA	1.80	0.44
1:A:21:GLY:O	1:A:25:LEU:HG	2.18	0.43
1:A:86:TRP:CD1	2:A:301[A]:RET:H14	2.53	0.43
1:A:82:ARG:O	1:A:85:ASP:HB3	2.18	0.43
4:A:304:LI1:H193	4:A:304:LI1:H161	1.77	0.43
1:A:223:LEU:O	1:A:224:LEU:C	2.55	0.43
1:A:161:GLU:O	1:A:162:SER:CB	2.66	0.43
1:A:128:THR:HG22	1:A:130:VAL:H	1.84	0.43
1:A:167:VAL:HG21	1:A:229:ILE:HG12	1.93	0.43
1:A:144:ALA:O	1:A:148:ILE:HG13	2.19	0.42
1:A:138:TRP:CD1	1:A:189:TRP:CE3	3.08	0.42
1:A:49:VAL:HB	1:A:50:PRO:CD	2.49	0.42
1:A:160:ALA:O	1:A:163:MET:CG	2.67	0.42
1:A:159:LYS:C	1:A:161:GLU:N	2.72	0.42
1:A:221:LEU:O	1:A:225:ARG:HB2	2.19	0.42
1:A:165:PRO:O	1:A:169:SER:HB2	2.20	0.42
1:A:88:PHE:C	1:A:91:PRO:HD2	2.39	0.41
1:A:43:TYR:CE1	1:A:224:LEU:CD1	2.97	0.41
1:A:45:ILE:HD11	1:A:95:LEU:HD12	2.02	0.41
1:A:161:GLU:O	1:A:162:SER:HB2	2.20	0.41
1:A:172:LYS:HE2	1:A:172:LYS:HB2	1.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:VAL:HG12	1:A:216:LYS:HB3	2.02	0.41
1:A:87:LEU:HD12	5:A:416:HOH:O	2.21	0.41
1:A:164:ARG:HG2	1:A:164:ARG:H	1.49	0.41
2:A:301[B]:RET:H161	2:A:301[B]:RET:H8	2.02	0.40
1:A:27:PHE:HB3	1:A:47:THR:OG1	2.20	0.40
1:A:170:THR:HG22	1:A:171:CYS:H	1.81	0.40
1:A:127:LEU:HD11	4:A:307:LI1:H122	2.04	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	223/262 (85%)	204 (92%)	13 (6%)	6 (3%)	<b>5</b> <b>6</b>

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	SER
1	A	225	ARG
1	A	226	SER
1	A	228	ALA
1	A	171	CYS
1	A	170	THR

### 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	180/205 (88%)	159 (88%)	21 (12%)	5 7

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PRO
1	A	9	GLU
1	A	22	LEU
1	A	24	THR
1	A	42	PHE
1	A	95	LEU
1	A	100	LEU
1	A	102	ASP
1	A	159	LYS
1	A	163	MET
1	A	164	ARG
1	A	166	GLU
1	A	170	THR
1	A	171	CYS
1	A	172	LYS
1	A	174	LEU
1	A	181	LEU
1	A	202	ASN
1	A	206	LEU
1	A	224	LEU
1	A	227	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
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](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

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
4	LI1	A	303	-	9,9,44	1.50	2 (22%)	7,7,51	1.48	1 (14%)
4	LI1	A	304	-	16,16,44	1.43	4 (25%)	16,16,51	2.35	6 (37%)
2	RET	A	301[A]	1	20,20,21	3.19	7 (35%)	27,27,28	1.70	4 (14%)
4	LI1	A	306	-	4,4,44	0.95	0	3,3,51	1.21	0
4	LI1	A	310	-	9,9,44	1.66	2 (22%)	9,9,51	3.85	4 (44%)
2	RET	A	301[B]	-	20,20,21	3.97	8 (40%)	27,27,28	3.99	14 (51%)
4	LI1	A	305	-	6,6,44	1.27	1 (16%)	4,4,51	0.97	0
4	LI1	A	309	-	13,13,44	1.08	2 (15%)	13,13,51	1.13	1 (7%)
4	LI1	A	307	-	27,27,44	1.82	5 (18%)	26,26,51	2.83	7 (26%)
4	LI1	A	308	-	2,2,44	0.56	0	0,1,51	0.00	-

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
4	LI1	A	303	-	-	2/5/5/49	-
4	LI1	A	304	-	1/1/2/8	3/13/13/49	-
2	RET	A	301[A]	1	-	0/13/30/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LI1	A	306	-	-	2/2/2/49	-
4	LI1	A	310	-	-	3/8/8/49	-
2	RET	A	301[B]	-	-	0/13/30/31	0/1/1/1
4	LI1	A	305	-	-	1/2/2/49	-
4	LI1	A	309	-	-	4/11/11/49	-
4	LI1	A	307	-	-	6/25/25/49	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301[B]	RET	C14-C13	12.68	1.43	1.33
2	A	301[A]	RET	C14-C13	9.70	1.41	1.33
2	A	301[B]	RET	C20-C13	-7.71	1.34	1.50
2	A	301[A]	RET	C11-C12	-6.75	1.17	1.34
2	A	301[B]	RET	C8-C7	6.25	1.52	1.33
4	A	307	LI1	C3-C2	-4.94	1.38	1.51
2	A	301[A]	RET	C11-C10	4.67	1.57	1.43
2	A	301[B]	RET	C12-C13	4.58	1.55	1.45
4	A	307	LI1	O2-C2	4.45	1.56	1.43
4	A	307	LI1	O1-C1	-4.38	1.31	1.42
4	A	303	LI1	C19-C18	-3.44	1.21	1.49
2	A	301[A]	RET	C5-C6	3.38	1.40	1.34
2	A	301[A]	RET	C1-C6	3.21	1.58	1.53
4	A	310	LI1	C22-C23	3.20	1.69	1.52
4	A	310	LI1	C25-C23	-2.93	1.37	1.52
4	A	307	LI1	C46-C45	-2.87	1.35	1.51
4	A	305	LI1	C52-C51	2.86	1.73	1.49
2	A	301[B]	RET	C2-C3	-2.84	1.45	1.52
4	A	309	LI1	C48-C47	2.79	1.67	1.51
4	A	304	LI1	C46-C45	2.76	1.64	1.52
4	A	303	LI1	C22-C21	-2.72	1.32	1.51
2	A	301[B]	RET	C1-C6	2.64	1.57	1.53
4	A	304	LI1	C19-C18	2.55	1.60	1.52
4	A	307	LI1	O1-C11	-2.50	1.31	1.42
2	A	301[A]	RET	C20-C13	-2.49	1.45	1.50
4	A	304	LI1	C20-C18	2.45	1.69	1.51
2	A	301[A]	RET	C2-C3	-2.23	1.47	1.52
4	A	309	LI1	C45-C46	-2.22	1.31	1.49
2	A	301[B]	RET	C15-C14	-2.14	1.41	1.49
2	A	301[B]	RET	C17-C1	2.09	1.57	1.53
4	A	304	LI1	C45-C43	2.04	1.65	1.51



All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301[B]	RET	C20-C13-C12	13.76	139.75	118.08
4	A	307	LI1	C1-C2-C3	-10.00	88.39	111.80
4	A	310	LI1	C27-C26-C25	8.42	143.43	113.62
2	A	301[B]	RET	C20-C13-C14	-7.68	101.03	123.71
2	A	301[B]	RET	C8-C9-C10	-6.70	108.67	118.94
4	A	310	LI1	C24-C23-C22	-6.69	87.07	111.29
2	A	301[A]	RET	C11-C10-C9	5.34	134.94	127.31
4	A	307	LI1	C41-O2-C2	-5.09	103.70	115.40
2	A	301[B]	RET	C7-C8-C9	-4.91	118.81	126.23
4	A	307	LI1	O2-C41-C42	4.71	126.09	109.56
4	A	304	LI1	C44-C43-C42	-4.65	89.06	110.51
2	A	301[B]	RET	C11-C10-C9	-4.58	120.77	127.31
2	A	301[B]	RET	C19-C9-C8	4.36	124.94	118.08
2	A	301[A]	RET	C20-C13-C12	4.20	124.70	118.08
4	A	304	LI1	C16-C17-C18	-4.03	102.89	115.92
4	A	304	LI1	C46-C45-C43	-4.02	97.04	115.98
2	A	301[B]	RET	C18-C5-C6	3.93	128.94	124.53
4	A	307	LI1	C45-C43-C42	-3.87	94.78	114.42
2	A	301[B]	RET	C15-C14-C13	3.84	149.84	127.65
4	A	307	LI1	O2-C2-C1	3.84	121.16	109.06
4	A	304	LI1	C19-C18-C17	-3.59	98.28	111.29
4	A	307	LI1	O1-C1-C2	-3.05	102.26	109.44
4	A	304	LI1	C47-C46-C45	-3.01	102.99	113.62
4	A	303	LI1	C18-C20-C21	-2.87	88.66	115.30
4	A	309	LI1	C50-C48-C47	-2.55	101.48	114.42
4	A	304	LI1	C19-C18-C20	-2.53	94.63	111.56
4	A	310	LI1	C21-C22-C23	2.51	127.90	115.86
4	A	310	LI1	C24-C23-C25	2.48	120.27	111.29
2	A	301[B]	RET	C18-C5-C4	-2.47	108.87	113.62
2	A	301[B]	RET	C19-C9-C10	2.47	126.38	122.92
2	A	301[B]	RET	C1-C6-C7	2.29	122.25	115.78
2	A	301[B]	RET	C17-C1-C6	2.18	113.84	110.30
2	A	301[B]	RET	C17-C1-C2	-2.06	100.66	108.91
2	A	301[A]	RET	C1-C6-C7	2.05	121.59	115.78
4	A	307	LI1	C16-C15-C13	-2.03	104.12	114.42
2	A	301[B]	RET	C11-C12-C13	-2.01	120.76	126.42
2	A	301[A]	RET	C17-C1-C6	2.01	113.56	110.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	304	LI1	C18

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	305	LI1	C48-C50-C51-C52
4	A	310	LI1	C24-C23-C25-C26
4	A	309	LI1	C53-C55-C56-C57
4	A	309	LI1	C56-C57-C58-C59
4	A	310	LI1	C25-C26-C27-C28
4	A	309	LI1	C51-C52-C53-C55
4	A	307	LI1	C42-C43-C45-C46
4	A	307	LI1	O2-C41-C42-C43
4	A	307	LI1	O1-C11-C12-C13
4	A	307	LI1	O1-C1-C2-C3
4	A	306	LI1	C50-C51-C52-C53
4	A	307	LI1	O1-C1-C2-O2
4	A	306	LI1	C51-C52-C53-C55
4	A	309	LI1	C56-C57-C58-C60
4	A	307	LI1	C11-C12-C13-C15
4	A	310	LI1	C22-C23-C25-C26
4	A	304	LI1	C17-C18-C20-C21
4	A	303	LI1	C20-C21-C22-C23
4	A	303	LI1	C18-C20-C21-C22
4	A	304	LI1	C46-C47-C48-C49
4	A	304	LI1	C44-C43-C45-C46

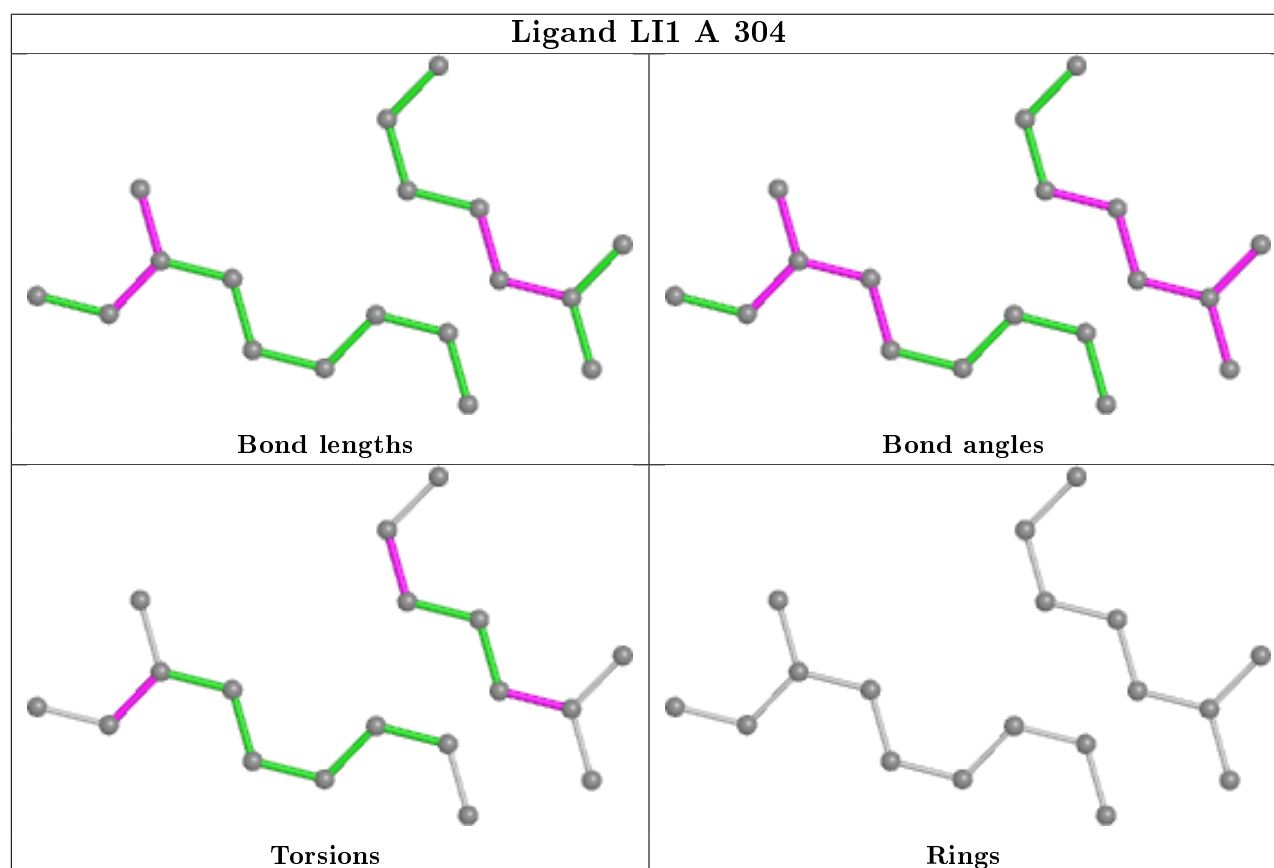
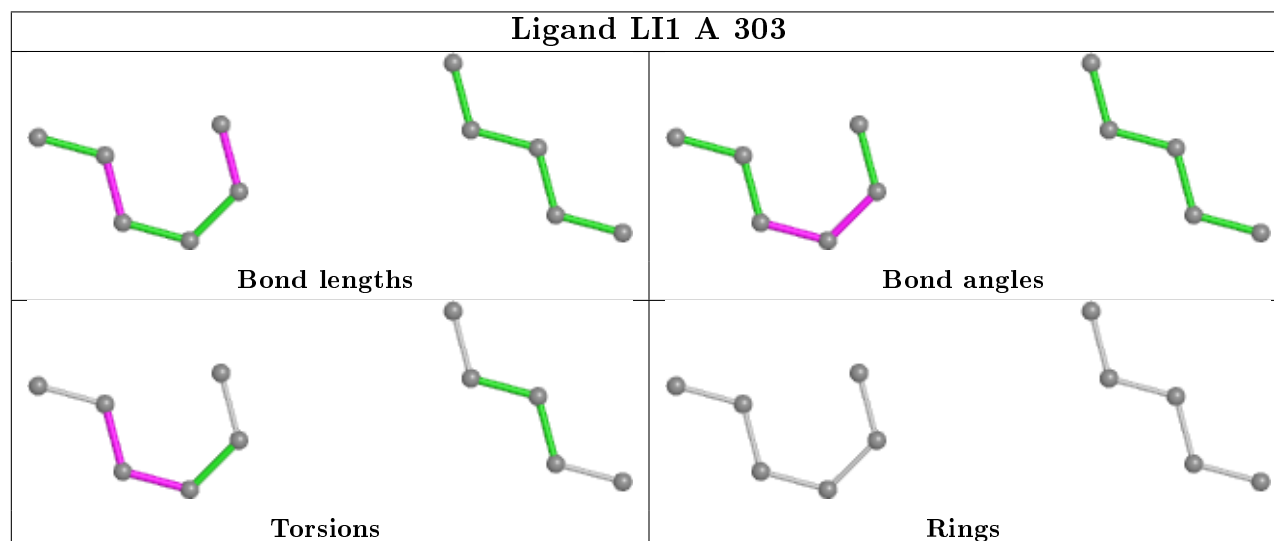
There are no ring outliers.

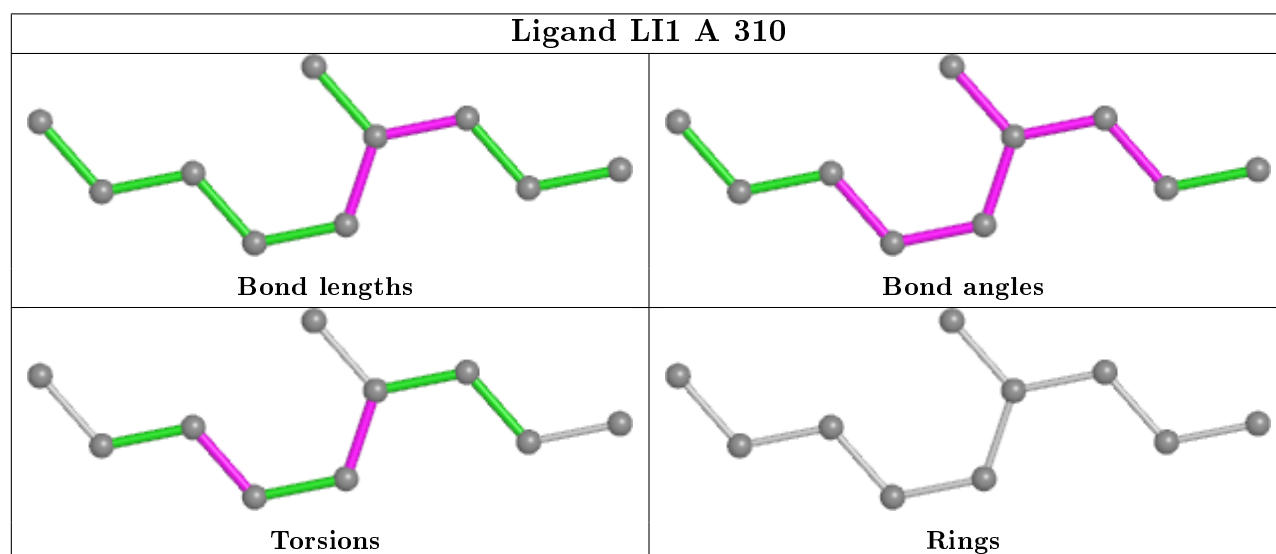
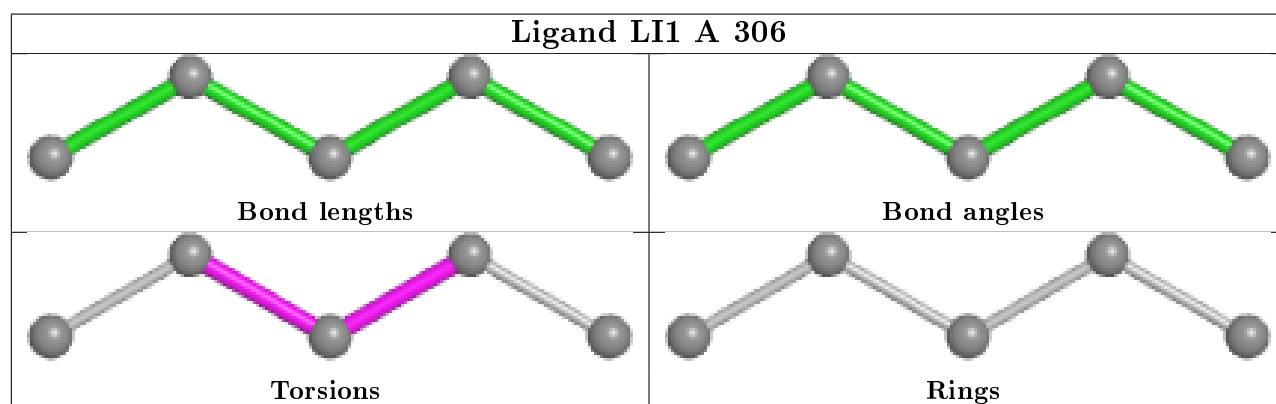
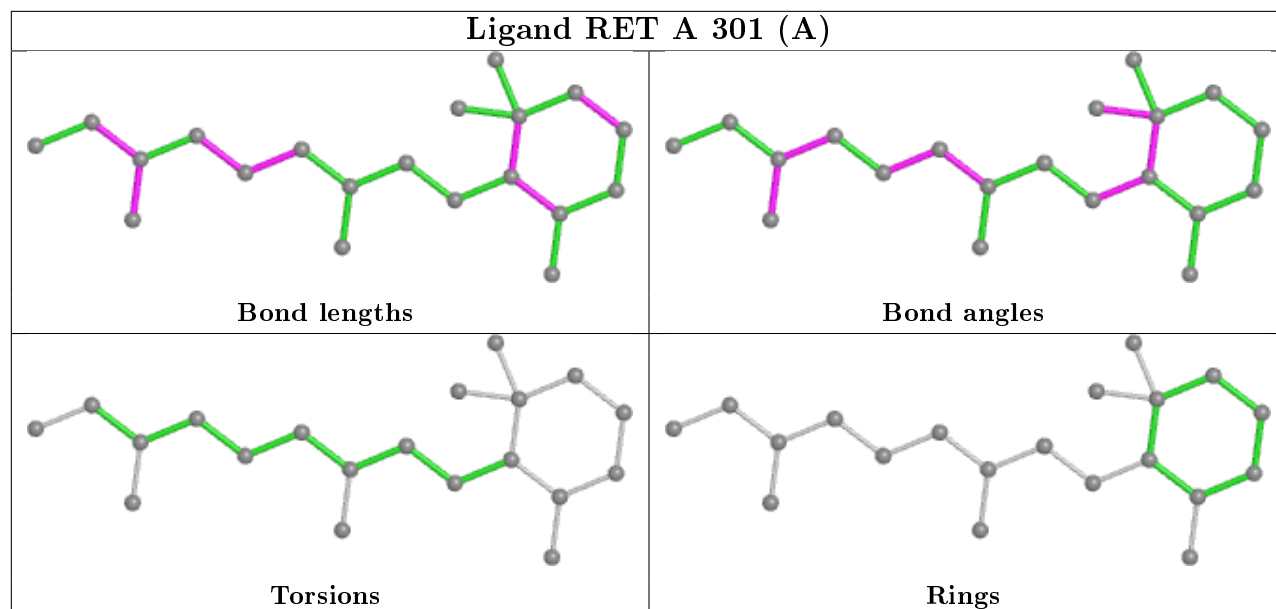
7 monomers are involved in 14 short contacts:

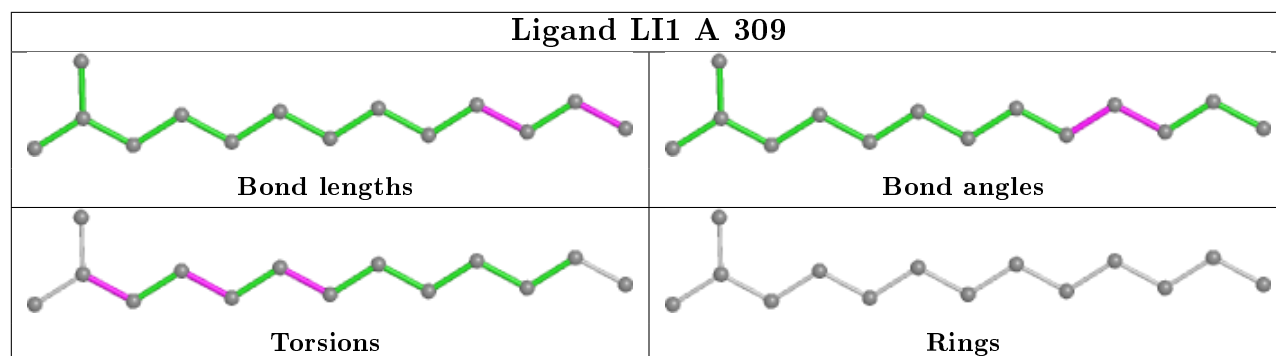
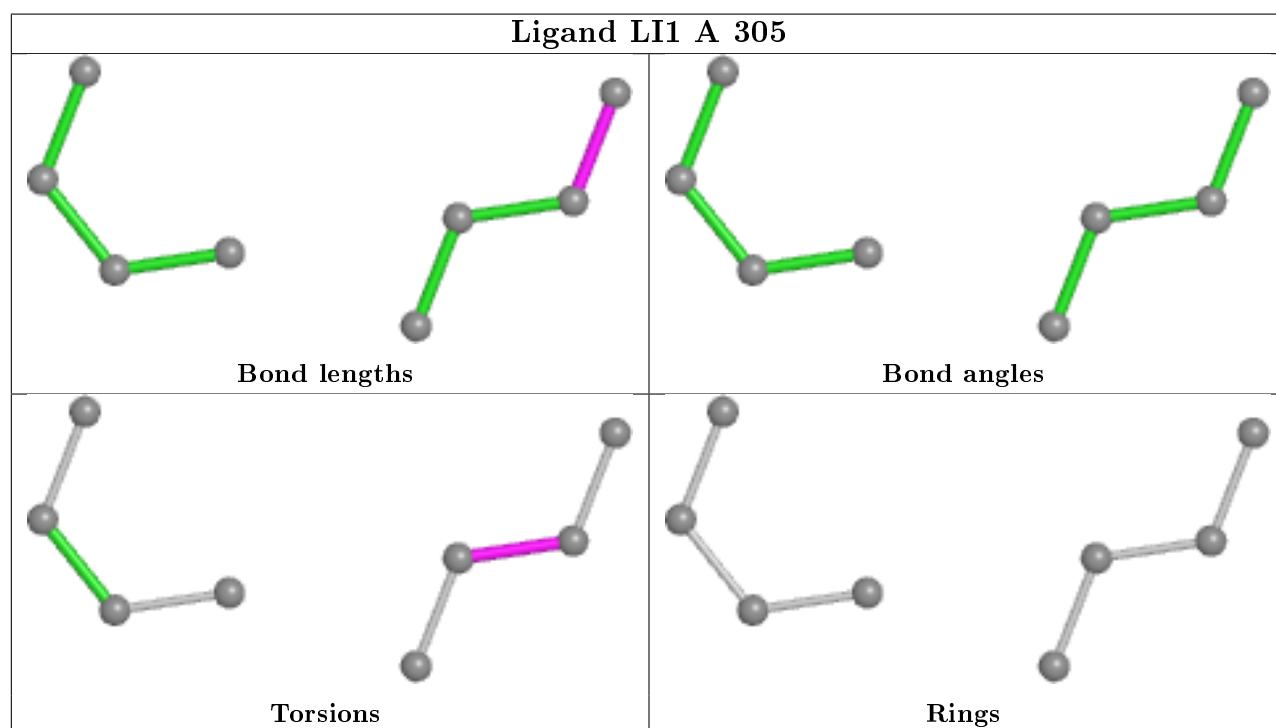
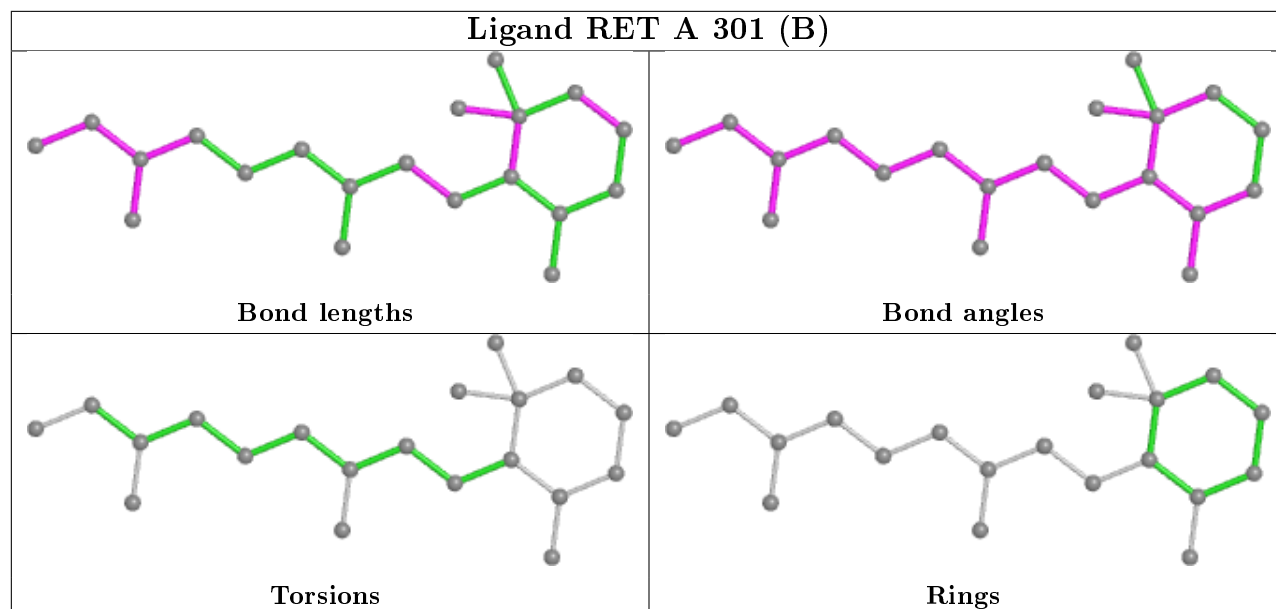
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	304	LI1	3	0
2	A	301[A]	RET	4	0
4	A	310	LI1	2	0
2	A	301[B]	RET	1	0
4	A	309	LI1	1	0
4	A	307	LI1	2	0
4	A	308	LI1	1	0

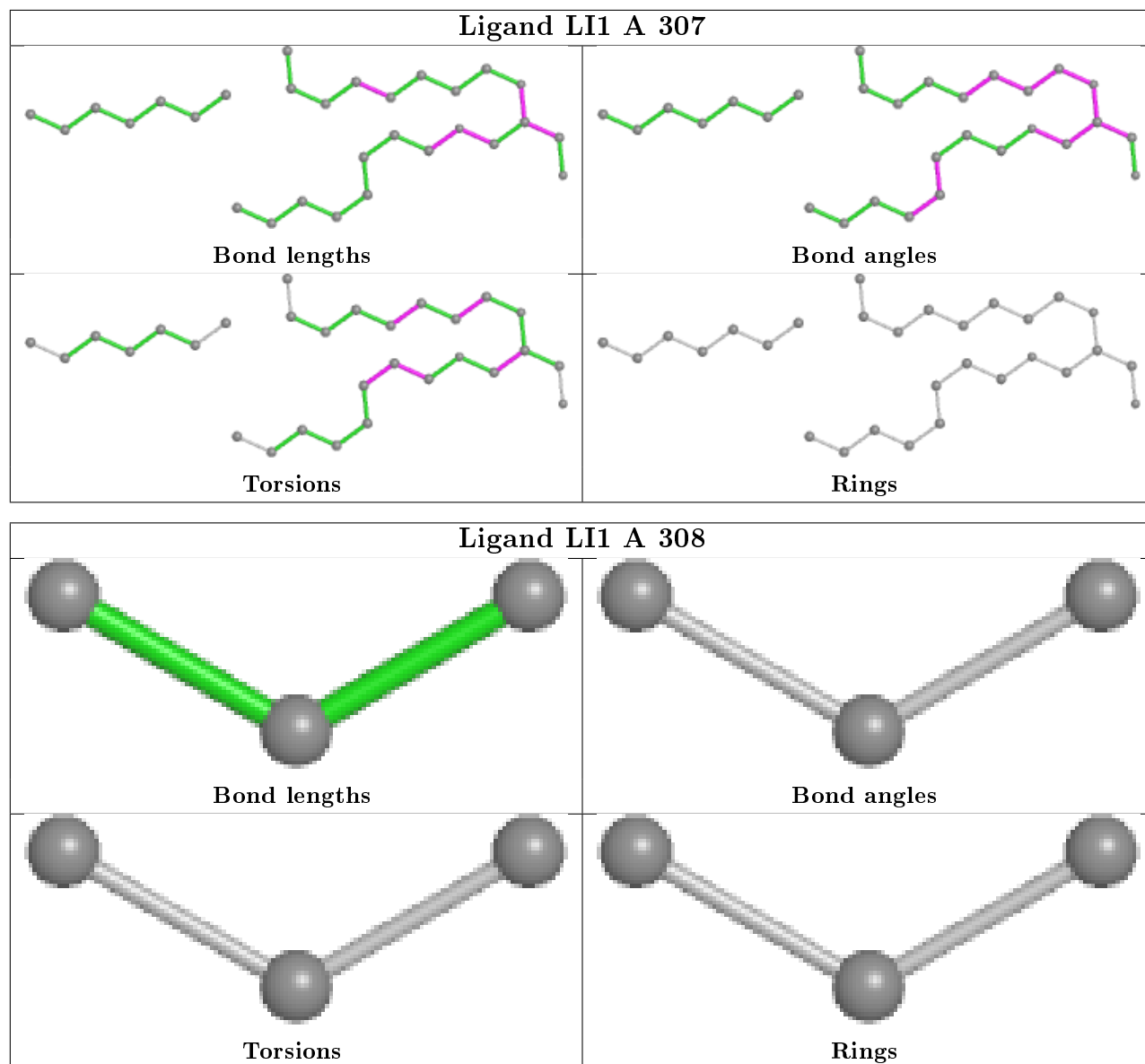
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	225/262 (85%)	0.18	21 (9%) <b>8</b> <b>7</b>	16, 29, 83, 93	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	74	GLU	4.9
1	A	160	ALA	4.6
1	A	228	ALA	4.1
1	A	35	SER	4.0
1	A	229	ILE	3.7
1	A	161	GLU	3.5
1	A	169	SER	3.5
1	A	167	VAL	2.7
1	A	226	SER	2.7
1	A	222	ILE	2.6
1	A	224	LEU	2.6
1	A	162	SER	2.5
1	A	166	GLU	2.4
1	A	33	GLY	2.4
1	A	158	SER	2.3
1	A	164	ARG	2.3
1	A	173	VAL	2.2
1	A	70	PRO	2.2
1	A	172	LYS	2.1
1	A	155	GLY	2.1
1	A	102	ASP	2.1

### 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 ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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.

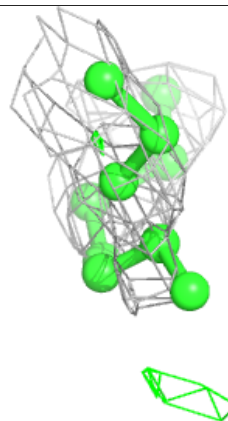
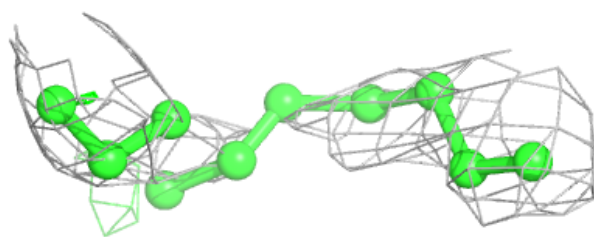
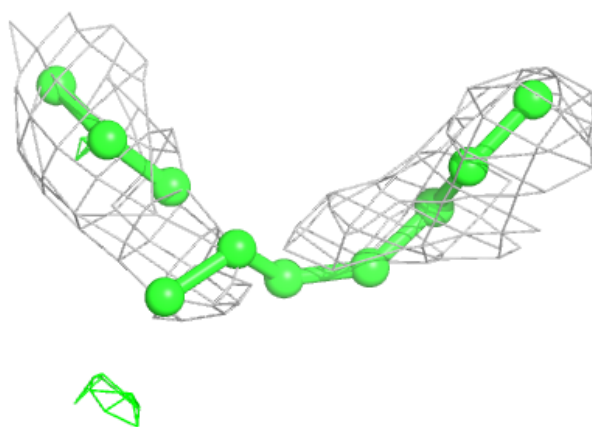
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	LI1	A	310	10/45	0.39	0.49	75,76,76,76	0
4	LI1	A	303	11/45	0.54	0.43	50,54,64,65	0
4	LI1	A	308	3/45	0.63	0.61	73,73,75,75	0
4	LI1	A	306	5/45	0.65	0.48	54,54,55,55	0
4	LI1	A	307	29/45	0.70	0.30	37,54,63,66	0
4	LI1	A	309	14/45	0.81	0.28	45,48,53,53	0
4	LI1	A	304	18/45	0.81	0.29	37,47,53,53	0
4	LI1	A	305	8/45	0.81	0.36	53,54,58,59	0
2	RET	A	301[A]	20/21	0.93	0.19	19,20,27,29	20
2	RET	A	301[B]	20/21	0.93	0.19	7,9,15,17	20
3	CL	A	302	1/1	0.99	0.20	38,38,38,38	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.



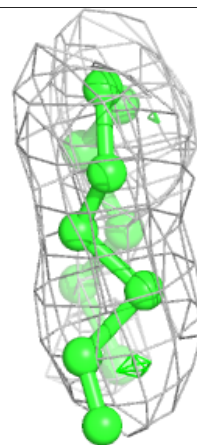
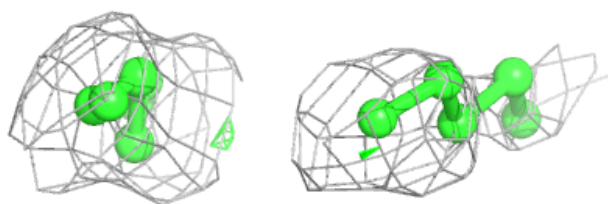
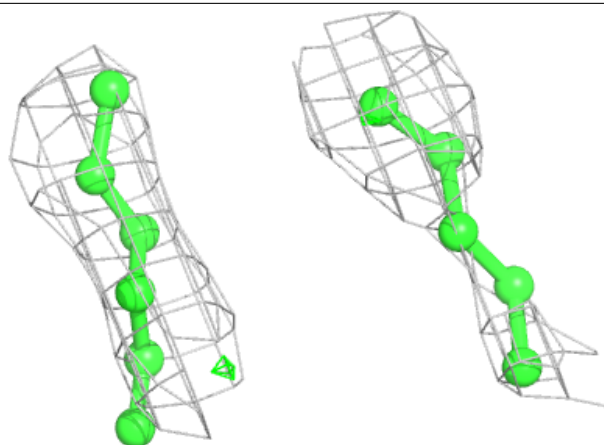
**Electron density around LI1 A 310:**

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



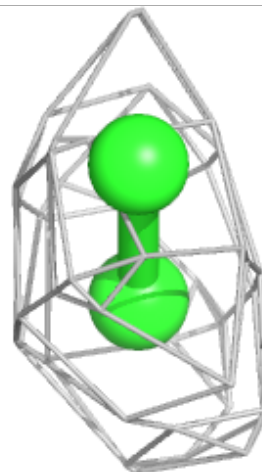
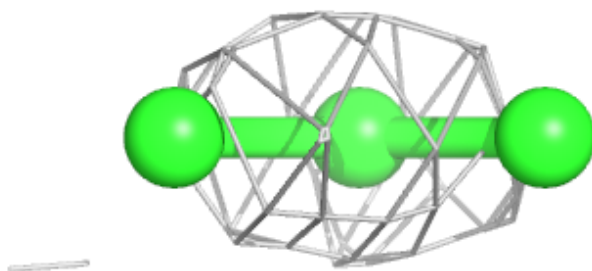
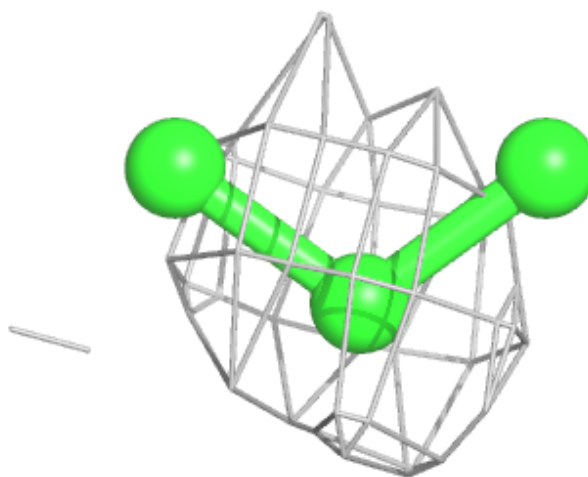
**Electron density around LI1 A 303:**

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



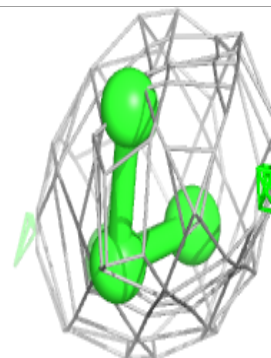
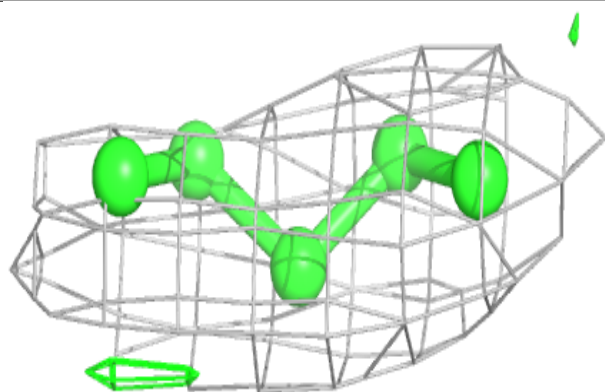
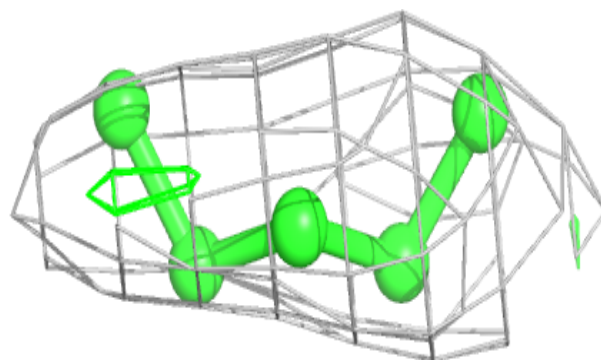
**Electron density around LI1 A 308:**

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

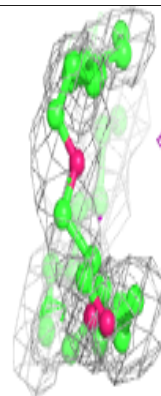
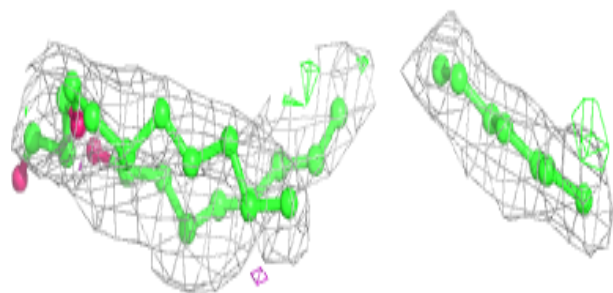
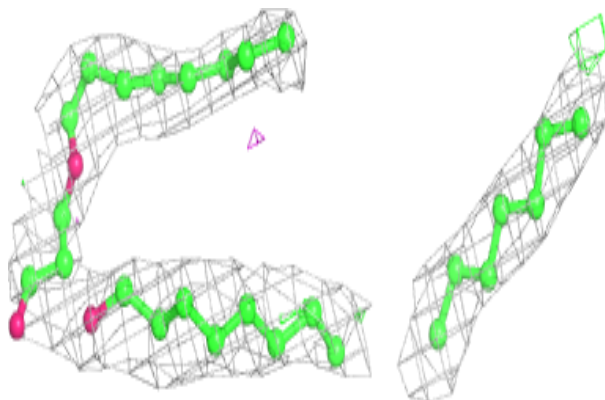


**Electron density around LI1 A 306:**

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

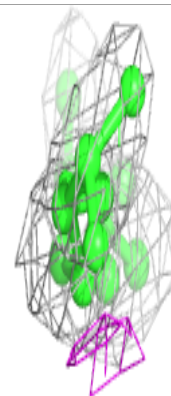
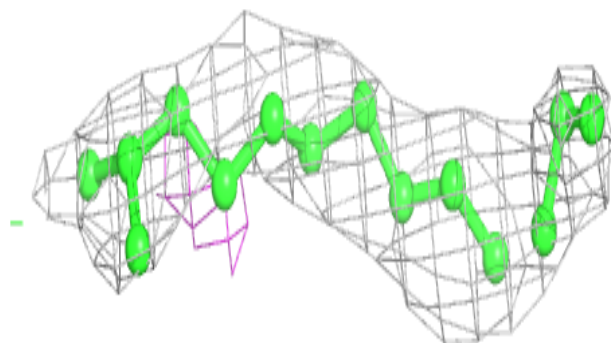
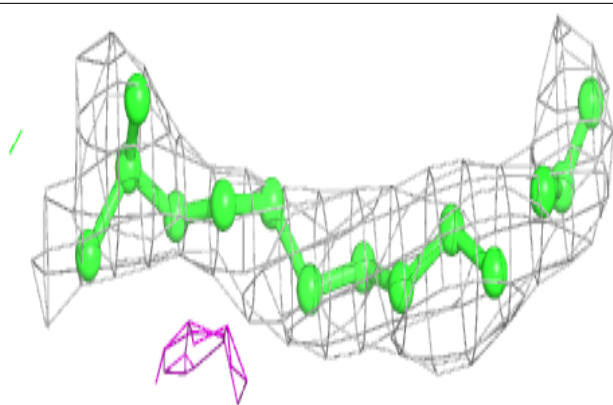
**Electron density around LI1 A 307:**

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



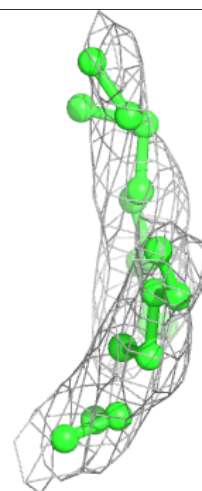
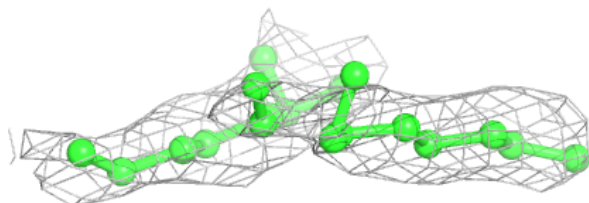
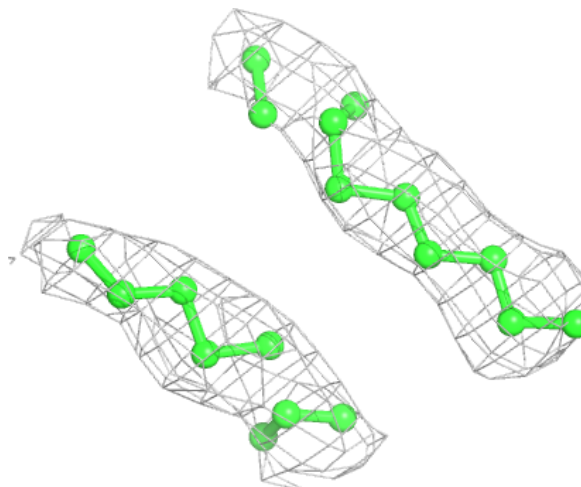
**Electron density around LI1 A 309:**

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



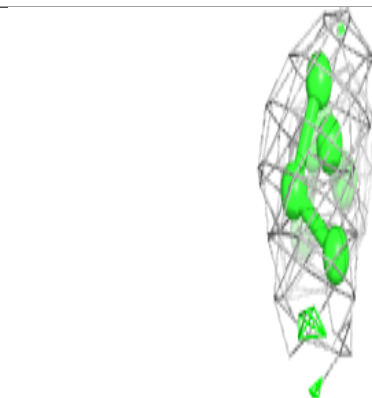
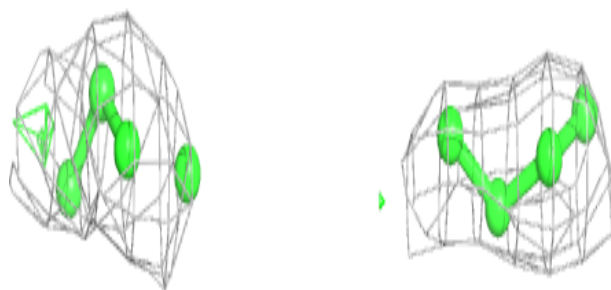
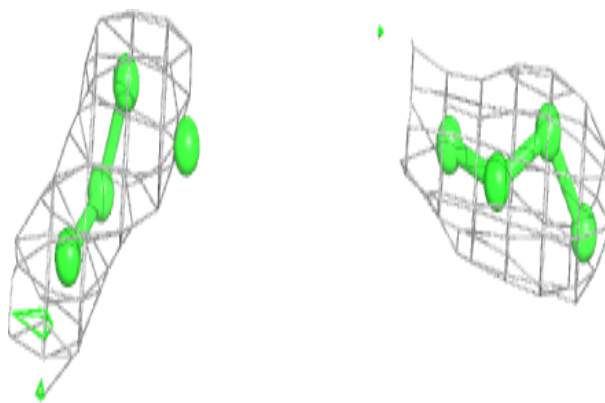
**Electron density around LI1 A 304:**

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

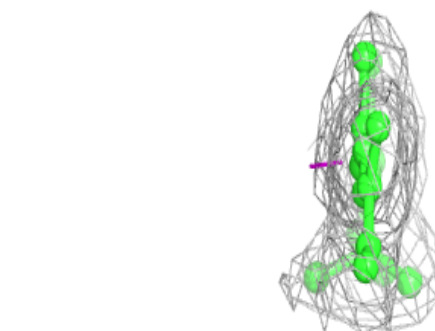
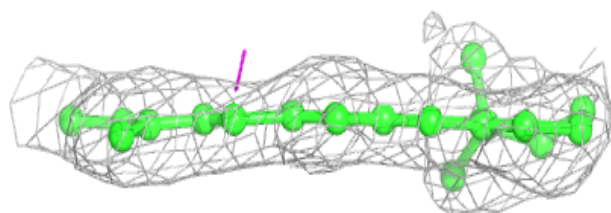
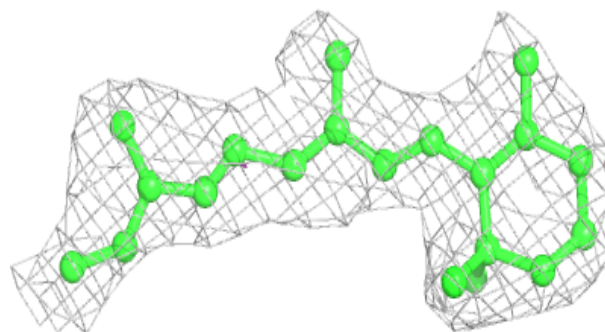


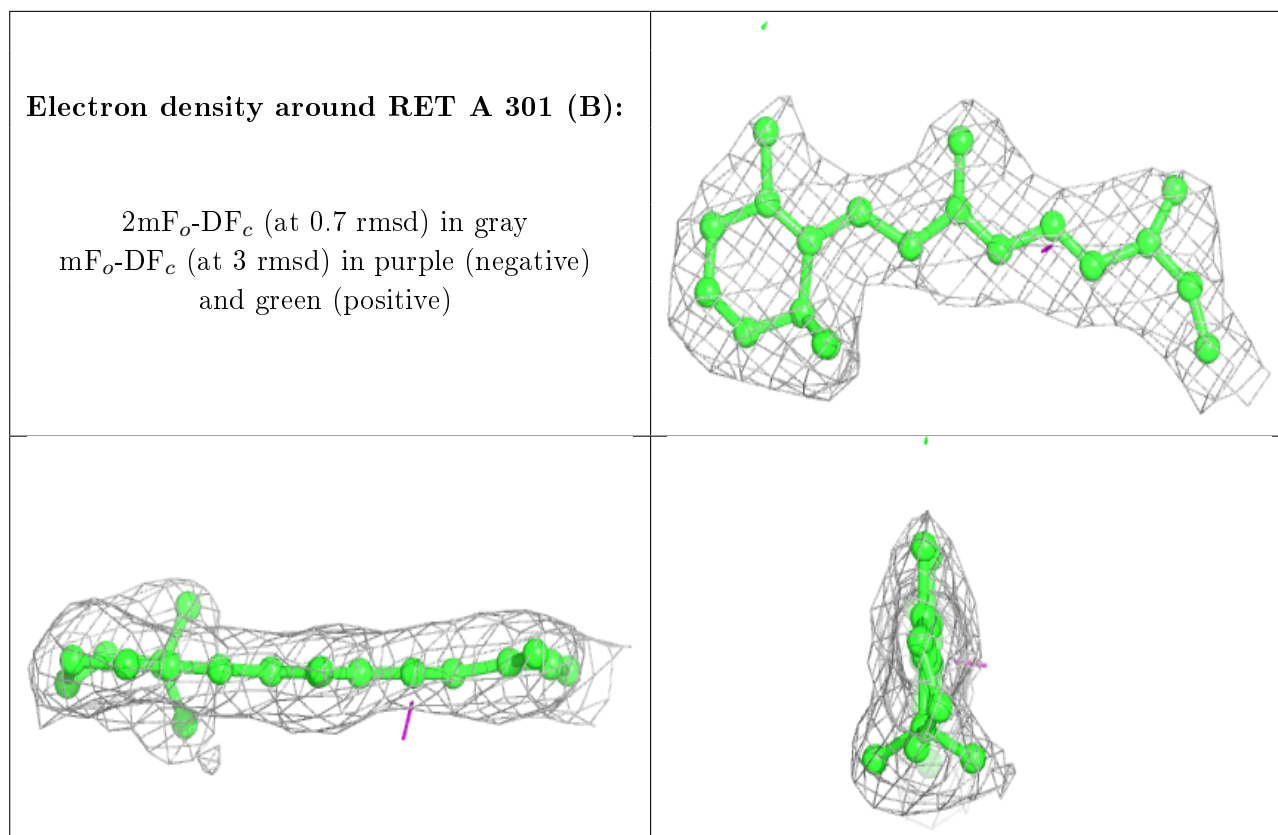
**Electron density around LI1 A 305:**

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

**Electron density around RET A 301 (A):**

$2mF_o-DF_c$  (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.