



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2021 – 04:06 PM EDT

PDB ID : 7L1E
Title : The Crystal Structure of Bromide-Bound GtACR1
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Deposited on : 2020-12-14
Resolution : 3.20 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 : 2.18
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) : 2.18

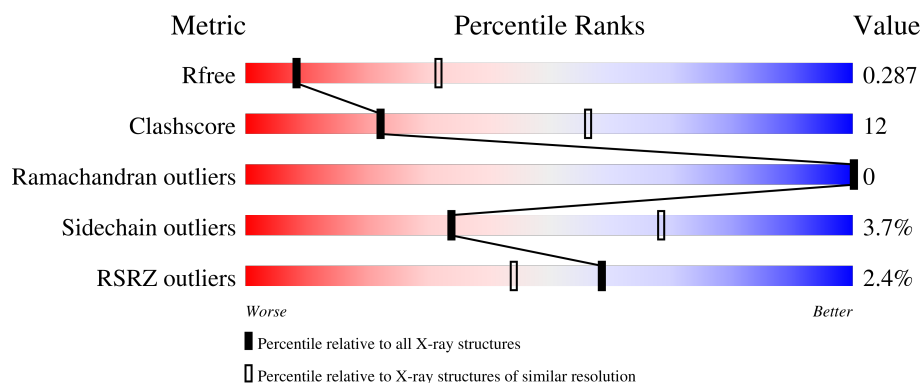
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	269	<div> <div>3%</div> <div>70%</div> <div>27%</div> <div>..</div> </div>
1	B	269	<div> <div>2%</div> <div>71%</div> <div>28%</div> <div>.</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
3	OLC	A	303	-	-	-	X
4	GOL	B	306	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4438 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.

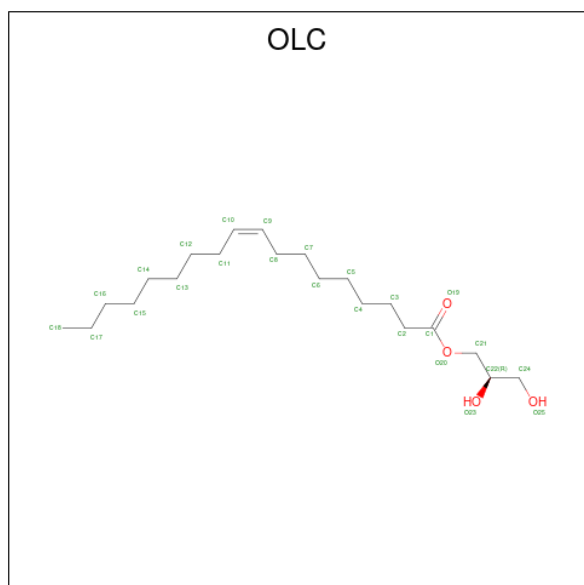
- Molecule 1 is a protein called Anion channelrhodopsin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2113	1403	327	361	22			
1	B	269	Total	C	N	O	S	0	0	0
			2144	1424	331	366	23			

- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br) (labeled as "Ligand of Interest" by depositor).

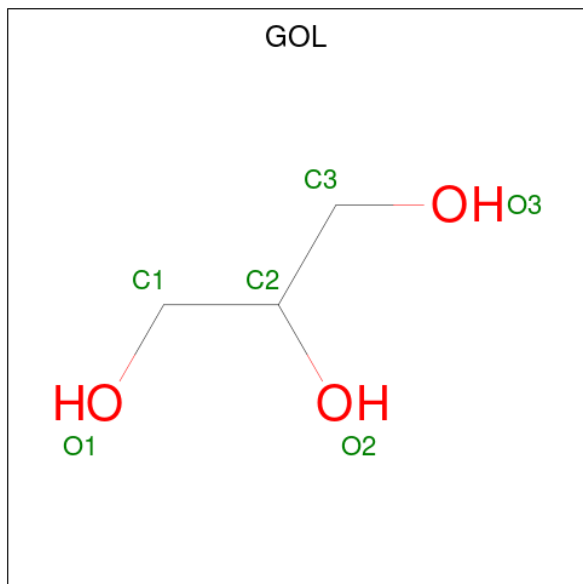
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Br	0	0
			1	1		
2	B	1	Total	Br	0	0
			1	1		

- Molecule 3 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			25	21	4		
3	A	1	Total	C	O	0	0
			25	21	4		
3	B	1	Total	C	O	0	0
			25	21	4		
3	B	1	Total	C	O	0	0
			25	21	4		
3	B	1	Total	C	O	0	0
			25	21	4		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

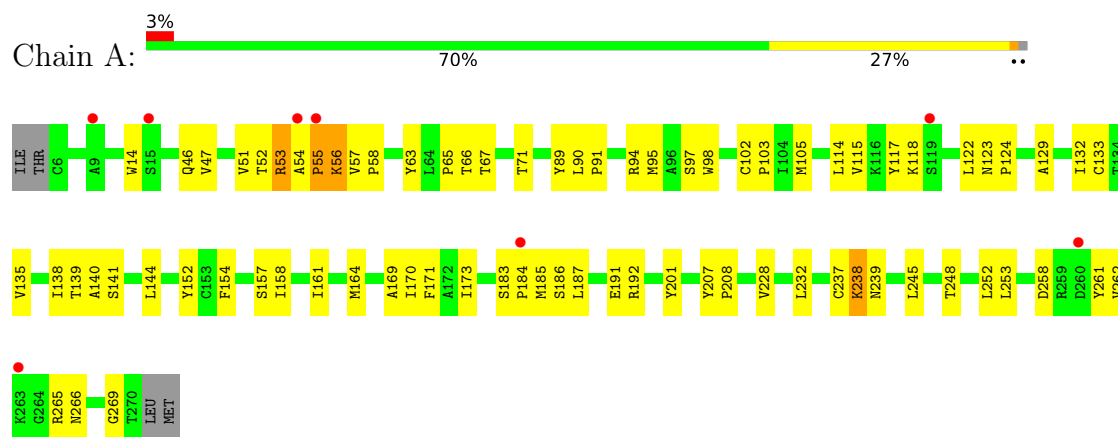
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	O	0	0
			9	9		
5	B	8	Total	O	0	0
			8	8		

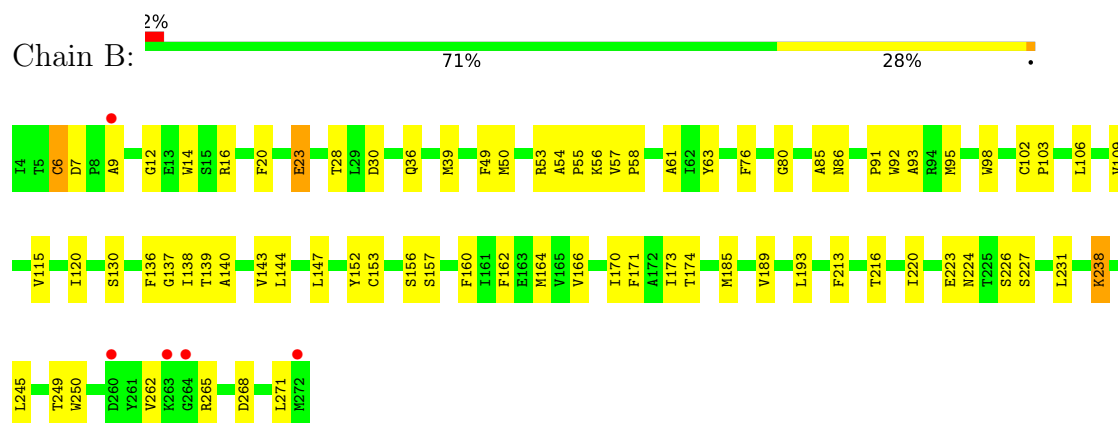
3 Residue-property plots

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: Anion channelrhodopsin-1



• Molecule 1: Anion channelrhodopsin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.66Å 77.64Å 73.63Å 90.00° 95.59° 90.00°	Depositor
Resolution (Å)	44.94 – 3.20 48.14 – 3.20	Depositor EDS
% Data completeness (in resolution range)	93.8 (44.94-3.20) 81.2 (48.14-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.53 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660)	Depositor
R, R_{free}	0.241 , 0.286 0.241 , 0.287	Depositor DCC
R_{free} test set	553 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	4438	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.21% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BR, OLC, LYR

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	0.25	0/2142	0.45	0/2920
1	B	0.25	0/2173	0.43	0/2962
All	All	0.25	0/4315	0.44	0/5882

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	2113	0	2144	51	0
1	B	2144	0	2182	51	0
2	A	1	0	0	1	0
2	B	1	0	0	1	0
3	A	50	0	80	7	0
3	B	100	0	160	4	0
4	A	6	0	8	0	0
4	B	6	0	8	1	0
5	A	9	0	0	3	0
5	B	8	0	0	0	0
All	All	4438	0	4582	105	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 12.

All (105) 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:58:PRO:HD2	2:A:301:BR:BR	2.26	0.90
3:A:302:OLC:H16	3:B:303:OLC:H13	1.72	0.72
1:A:55:PRO:HD2	1:A:56:LYS:HD2	1.71	0.72
1:B:238:LYR:H192	1:B:238:LYR:H9	1.70	0.71
1:B:58:PRO:HD2	2:B:301:BR:BR	2.47	0.69
1:A:52:THR:HB	1:A:53:ARG:HH21	1.58	0.69
1:B:147:LEU:HD12	4:B:306:GOL:H11	1.75	0.69
1:A:185:MET:HG2	1:A:262:VAL:HG13	1.76	0.68
1:B:115:VAL:HG12	1:B:173:ILE:HD12	1.79	0.64
1:A:185:MET:HE2	1:A:265:ARG:HB3	1.79	0.64
1:B:265:ARG:HD3	1:B:271:LEU:HG	1.80	0.63
1:A:238:LYR:H182	1:A:238:LYR:H9	1.81	0.63
1:A:98:TRP:CD1	1:A:238:LYR:HC2	2.35	0.62
1:B:174:THR:HG22	1:B:193:LEU:HD21	1.82	0.61
1:A:140:ALA:HB2	1:A:152:TYR:HB2	1.82	0.61
5:A:403:HOH:O	1:B:6:CYS:HB3	2.00	0.60
1:B:223:GLU:HA	1:B:226:SER:HB2	1.83	0.60
1:A:54:ALA:HB3	1:A:55:PRO:HD3	1.83	0.59
1:B:50:MET:HB3	1:B:57:VAL:HG21	1.85	0.59
1:A:14:TRP:HB2	1:A:144:LEU:HD13	1.85	0.58
1:A:115:VAL:HG12	1:A:173:ILE:HD12	1.84	0.58
1:B:12:GLY:N	1:B:85:ALA:O	2.37	0.58
1:A:115:VAL:HG22	1:A:123:ASN:HD21	1.68	0.58
1:B:14:TRP:HB3	1:B:86:ASN:O	2.04	0.57
1:A:157:SER:O	1:A:161:ILE:HG12	2.05	0.56
1:B:56:LYS:HB3	1:B:250:TRP:CE3	2.41	0.56
1:B:120:ILE:HG13	1:B:120:ILE:O	2.05	0.56
1:B:98:TRP:CD1	1:B:238:LYR:HC2	2.40	0.55
5:A:403:HOH:O	1:B:6:CYS:CB	2.54	0.55
3:A:302:OLC:H11A	3:B:303:OLC:H9	1.89	0.54
1:B:9:ALA:H	1:B:16:ARG:NH1	2.05	0.54
1:B:80:GLY:HA3	1:B:93:ALA:HB2	1.90	0.54
1:B:92:TRP:HZ3	1:B:138:ILE:HD13	1.74	0.53
1:A:164:MET:O	1:A:201:TYR:OH	2.27	0.53
1:A:102:CYS:HB2	1:A:103:PRO:HD3	1.91	0.52
1:A:123:ASN:HD22	1:A:170:ILE:HD11	1.74	0.52
1:A:135:VAL:O	1:A:139:THR:OG1	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ASP:HB3	1:A:261:TYR:HB3	1.93	0.51
1:B:140:ALA:HB2	1:B:152:TYR:HB2	1.92	0.51
1:A:258:ASP:O	1:A:262:VAL:HG23	2.12	0.50
1:B:56:LYS:HD2	1:B:250:TRP:CZ3	2.46	0.50
1:A:105:MET:HE1	1:A:237:CYS:HB2	1.93	0.50
1:B:137:GLY:HA3	1:B:238:LYR:H182	1.93	0.49
1:A:94:ARG:NH1	5:A:401:HOH:O	2.45	0.49
1:A:183:SER:HB3	1:A:186:SER:HB2	1.94	0.49
1:B:185:MET:O	1:B:189:VAL:HG23	2.12	0.49
1:A:123:ASN:ND2	1:A:170:ILE:HD11	2.28	0.49
1:A:185:MET:HE1	1:A:265:ARG:HD2	1.94	0.49
1:A:114:LEU:HD23	1:A:123:ASN:OD1	2.12	0.49
1:A:63:TYR:HA	3:A:302:OLC:H17	1.96	0.48
1:B:185:MET:HG2	1:B:262:VAL:HG12	1.95	0.48
1:B:49:PHE:CE2	1:B:53:ARG:HD2	2.50	0.47
1:A:265:ARG:HG2	1:A:269:GLY:O	2.14	0.47
1:B:36:GLN:NE2	1:B:227:SER:HB3	2.30	0.47
1:A:228:VAL:O	1:A:232:LEU:N	2.35	0.47
1:B:57:VAL:HG23	1:B:61:ALA:HB3	1.96	0.47
1:B:54:ALA:HB1	1:B:55:PRO:HD2	1.96	0.46
1:B:49:PHE:O	1:B:53:ARG:HG2	2.14	0.46
3:A:302:OLC:H14A	3:B:303:OLC:H10	1.97	0.46
1:A:53:ARG:O	1:A:57:VAL:HG22	2.15	0.46
1:B:14:TRP:HB2	1:B:144:LEU:CD2	2.46	0.46
1:A:66:THR:HG21	3:A:302:OLC:H15A	1.98	0.46
1:A:154:PHE:CZ	1:A:158:ILE:HD11	2.51	0.46
1:A:192:ARG:NH1	1:A:252:LEU:HD12	2.31	0.46
1:A:47:VAL:O	1:A:51:VAL:HG23	2.16	0.46
1:B:213:PHE:CG	1:B:220:ILE:HD11	2.51	0.46
1:B:9:ALA:H	1:B:16:ARG:HH12	1.63	0.45
1:A:169:ALA:O	1:A:173:ILE:HG13	2.17	0.45
1:A:117:TYR:HB2	1:A:122:LEU:HD11	1.98	0.45
1:A:207:TYR:HB2	1:A:208:PRO:HD3	1.98	0.45
1:B:28:THR:HG1	1:B:224:ASN:HD21	1.63	0.45
1:B:91:PRO:HD2	1:B:95:MET:HE2	1.98	0.45
1:B:271:LEU:H	1:B:271:LEU:HD12	1.80	0.45
1:A:46:GLN:OE1	1:A:239:ASN:ND2	2.41	0.44
1:B:162:PHE:O	1:B:166:VAL:HG23	2.17	0.44
1:B:245:LEU:O	1:B:249:THR:OG1	2.28	0.44
1:B:238:LYR:H41	1:B:238:LYR:H6	1.55	0.44
1:B:106:LEU:HD12	1:B:130:SER:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:CYS:O	1:B:157:SER:OG	2.29	0.44
1:B:160:PHE:O	1:B:164:MET:HG2	2.18	0.44
1:A:187:LEU:O	1:A:191:GLU:HG2	2.18	0.43
1:B:102:CYS:HB2	1:B:103:PRO:HD3	2.00	0.43
1:A:123:ASN:HB2	1:A:124:PRO:HD3	2.00	0.43
1:A:67:THR:O	1:A:71:THR:HG23	2.19	0.43
1:B:23:GLU:H	1:B:23:GLU:HG3	1.66	0.43
1:B:39:MET:HB2	1:B:231:LEU:HD21	2.01	0.43
1:A:47:VAL:HG22	1:A:65:PRO:HB2	2.01	0.43
1:B:56:LYS:HB3	1:B:250:TRP:CD2	2.53	0.42
1:B:63:TYR:CD1	3:B:302:OLC:H14A	2.54	0.42
1:A:71:THR:HG21	1:A:97:SER:HB3	2.02	0.42
1:A:63:TYR:CD1	3:A:302:OLC:H14	2.55	0.41
1:B:36:GLN:HE22	1:B:227:SER:HB3	1.85	0.41
1:B:227:SER:O	1:B:231:LEU:HB2	2.20	0.41
1:A:90:LEU:HD13	1:A:141:SER:HB2	2.00	0.41
1:A:95:MET:HB3	1:A:138:ILE:HD11	2.01	0.41
1:A:129:ALA:HA	1:A:132:ILE:HD12	2.03	0.41
1:A:63:TYR:CE1	3:A:302:OLC:H12A	2.56	0.41
1:A:91:PRO:O	1:A:95:MET:HG3	2.21	0.41
1:B:109:VAL:HG12	1:B:170:ILE:HG21	2.02	0.41
1:A:248:THR:O	1:A:253:LEU:HD12	2.21	0.40
1:A:184:PRO:HB2	1:A:266:ASN:HA	2.04	0.40
1:A:185:MET:CE	1:A:265:ARG:HD2	2.51	0.40
1:B:136:PHE:HB2	1:B:156:SER:HB2	2.04	0.40
1:B:50:MET:O	1:B:57:VAL:HG11	2.22	0.40
1:B:139:THR:O	1:B:143:VAL:HG23	2.21	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	262/269 (97%)	254 (97%)	8 (3%)	0	100	100
1	B	266/269 (99%)	252 (95%)	14 (5%)	0	100	100
All	All	528/538 (98%)	506 (96%)	22 (4%)	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	229/233 (98%)	221 (96%)	8 (4%)	36	69
1	B	233/233 (100%)	224 (96%)	9 (4%)	32	67
All	All	462/466 (99%)	445 (96%)	17 (4%)	34	68

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ARG
1	A	55	PRO
1	A	56	LYS
1	A	89	TYR
1	A	118	LYS
1	A	133	CYS
1	A	171	PHE
1	A	245	LEU
1	B	6	CYS
1	B	7	ASP
1	B	20	PHE
1	B	23	GLU
1	B	30	ASP
1	B	76	PHE
1	B	171	PHE
1	B	216	THR
1	B	268	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	LYR	A	238	1	27,29,30	0.69	0	30,37,39	1.42	3 (10%)
1	LYR	B	238	1	27,29,30	0.78	0	30,37,39	2.14	11 (36%)

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
1	LYR	A	238	1	-	4/22/40/42	0/1/1/1
1	LYR	B	238	1	-	5/22/40/42	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	238	LYR	C19-C17-C11	5.62	119.41	110.30
1	B	238	LYR	C13-C12-C11	-4.86	119.07	124.53
1	A	238	LYR	C18-C17-C11	4.68	117.89	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	LYR	C15-C14-C12	-3.22	108.33	114.08
1	B	238	LYR	C4-C3-C5	-3.14	113.13	118.08
1	B	238	LYR	C1-C2-C3	-2.71	121.76	126.97
1	B	238	LYR	C15-C16-C17	2.63	123.99	114.60
1	B	238	LYR	C14-C12-C11	2.38	126.19	122.73
1	B	238	LYR	C18-C17-C11	2.26	113.96	110.30
1	B	238	LYR	C17-C11-C10	2.25	122.14	115.78
1	B	238	LYR	C15-C14-C12	2.11	117.84	114.08
1	A	238	LYR	C9-C80-C7	-2.07	115.77	118.94
1	B	238	LYR	C18-C17-C16	-2.06	100.67	108.91
1	B	238	LYR	C8-C80-C9	-2.03	114.89	118.08

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	238	LYR	C-CA-CB-CG
1	B	238	LYR	C-CA-CB-CG
1	A	238	LYR	CG-CD-CE-NZ
1	B	238	LYR	CG-CD-CE-NZ
1	A	238	LYR	CA-CB-CG-CD
1	A	238	LYR	NZ-C1-C2-C3
1	B	238	LYR	NZ-C1-C2-C3
1	B	238	LYR	CA-CB-CG-CD
1	B	238	LYR	CD-CE-NZ-C1

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	238	LYR	2	0
1	B	238	LYR	4	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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
3	OLC	B	302	-	24,24,24	0.68	1 (4%)	25,25,25	0.94	1 (4%)
3	OLC	A	302	-	24,24,24	0.68	1 (4%)	25,25,25	0.89	1 (4%)
4	GOL	A	304	-	5,5,5	0.90	0	5,5,5	1.00	0
3	OLC	B	304	-	24,24,24	0.68	1 (4%)	25,25,25	0.85	1 (4%)
3	OLC	B	305	-	24,24,24	0.68	1 (4%)	25,25,25	0.93	1 (4%)
3	OLC	B	303	-	24,24,24	0.67	1 (4%)	25,25,25	0.99	1 (4%)
3	OLC	A	303	-	24,24,24	0.68	1 (4%)	25,25,25	0.94	1 (4%)
4	GOL	B	306	-	5,5,5	0.91	0	5,5,5	1.00	0

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	OLC	B	302	-	-	8/24/24/24	-
3	OLC	A	302	-	-	11/24/24/24	-
4	GOL	A	304	-	-	0/4/4/4	-
3	OLC	B	304	-	-	12/24/24/24	-
3	OLC	B	305	-	-	13/24/24/24	-
3	OLC	B	303	-	-	9/24/24/24	-
3	OLC	A	303	-	-	12/24/24/24	-
4	GOL	B	306	-	-	0/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	305	OLC	O20-C1	2.64	1.41	1.33
3	B	302	OLC	O20-C1	2.64	1.41	1.33
3	B	304	OLC	O20-C1	2.63	1.41	1.33
3	A	303	OLC	O20-C1	2.61	1.41	1.33
3	B	303	OLC	O20-C1	2.60	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	OLC	O20-C1	2.60	1.40	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	305	OLC	O20-C1-C2	2.67	120.30	111.91
3	B	302	OLC	O20-C1-C2	2.62	120.14	111.91
3	B	303	OLC	O20-C1-C2	2.60	120.07	111.91
3	A	302	OLC	O20-C1-C2	2.55	119.91	111.91
3	A	303	OLC	O20-C1-C2	2.52	119.80	111.91
3	B	304	OLC	O20-C1-C2	2.35	119.29	111.91

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	OLC	O20-C21-C22-C24
3	B	304	OLC	C21-C22-C24-O25
3	B	305	OLC	O19-C1-O20-C21
3	A	303	OLC	C2-C1-O20-C21
3	B	305	OLC	C2-C1-O20-C21
3	A	303	OLC	O19-C1-O20-C21
3	A	302	OLC	O20-C21-C22-O23
3	B	304	OLC	O20-C21-C22-O23
3	A	302	OLC	C14-C15-C16-C17
3	A	302	OLC	C1-C2-C3-C4
3	A	303	OLC	C4-C5-C6-C7
3	B	303	OLC	C11-C12-C13-C14
3	B	303	OLC	C4-C5-C6-C7
3	B	305	OLC	C21-C22-C24-O25
3	A	303	OLC	C6-C7-C8-C9
3	B	302	OLC	C10-C11-C12-C13
3	A	302	OLC	C3-C4-C5-C6
3	A	303	OLC	C3-C4-C5-C6
3	B	303	OLC	C14-C15-C16-C17
3	B	303	OLC	C1-C2-C3-C4
3	B	304	OLC	O23-C22-C24-O25
3	B	302	OLC	C14-C15-C16-C17
3	B	305	OLC	C6-C7-C8-C9
3	B	302	OLC	C4-C5-C6-C7
3	B	305	OLC	C13-C14-C15-C16
3	A	303	OLC	C10-C11-C12-C13

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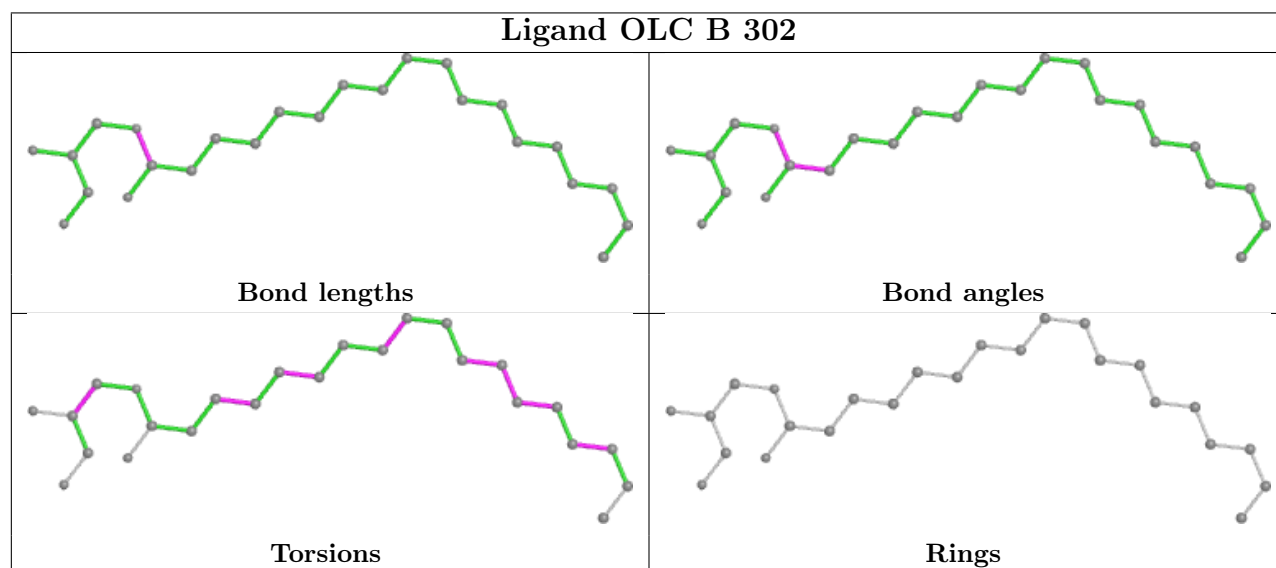
Mol	Chain	Res	Type	Atoms
3	B	303	OLC	C10-C11-C12-C13
3	B	303	OLC	C13-C14-C15-C16
3	A	303	OLC	C5-C6-C7-C8
3	B	305	OLC	C2-C3-C4-C5
3	B	302	OLC	C2-C3-C4-C5
3	B	305	OLC	O23-C22-C24-O25
3	B	304	OLC	C1-C2-C3-C4
3	A	303	OLC	C15-C16-C17-C18
3	A	303	OLC	C2-C3-C4-C5
3	B	302	OLC	C11-C12-C13-C14
3	A	303	OLC	C12-C13-C14-C15
3	B	303	OLC	O20-C21-C22-O23
3	B	305	OLC	C14-C15-C16-C17
3	A	302	OLC	C4-C5-C6-C7
3	A	302	OLC	C2-C3-C4-C5
3	B	305	OLC	C10-C11-C12-C13
3	B	304	OLC	O20-C21-C22-C24
3	B	305	OLC	C4-C5-C6-C7
3	B	302	OLC	C12-C13-C14-C15
3	B	305	OLC	C11-C12-C13-C14
3	B	302	OLC	C7-C8-C9-C10
3	B	304	OLC	C9-C10-C11-C12
3	B	303	OLC	C9-C10-C11-C12
3	A	302	OLC	C10-C11-C12-C13
3	B	304	OLC	C3-C4-C5-C6
3	A	303	OLC	C9-C10-C11-C12
3	B	305	OLC	C1-C2-C3-C4
3	B	304	OLC	C11-C12-C13-C14
3	B	303	OLC	C7-C8-C9-C10
3	B	304	OLC	C7-C8-C9-C10
3	B	305	OLC	C9-C10-C11-C12
3	A	302	OLC	C9-C10-C11-C12
3	B	304	OLC	C10-C11-C12-C13
3	A	302	OLC	C7-C8-C9-C10
3	A	302	OLC	C5-C6-C7-C8
3	A	303	OLC	C7-C8-C9-C10
3	B	304	OLC	C2-C3-C4-C5
3	B	304	OLC	C6-C7-C8-C9
3	B	302	OLC	O20-C21-C22-O23

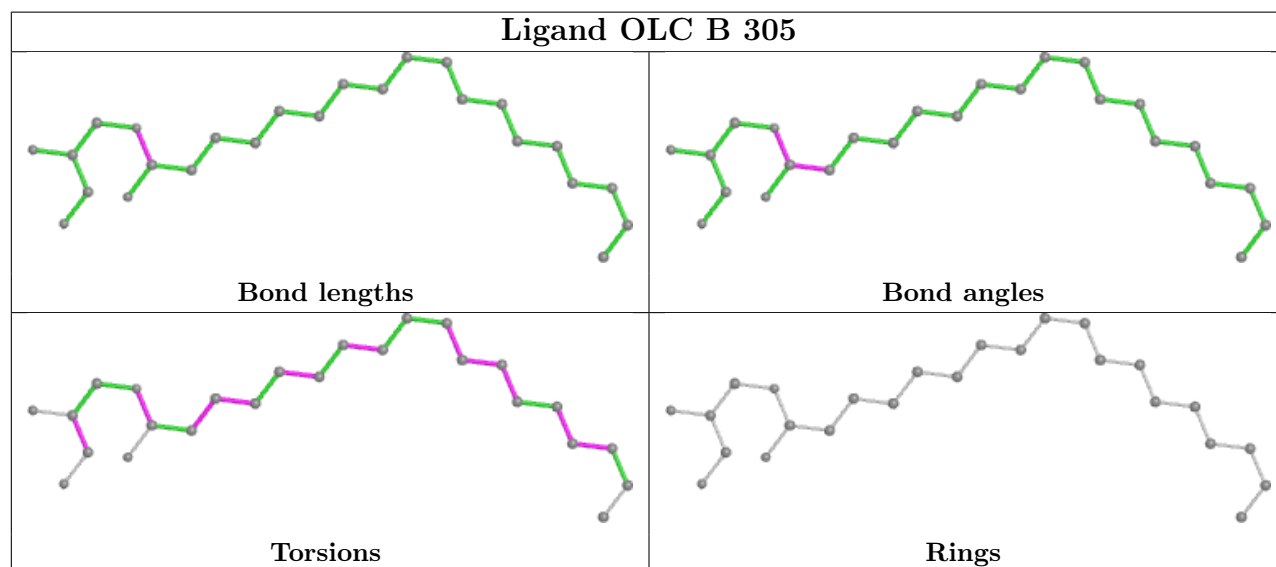
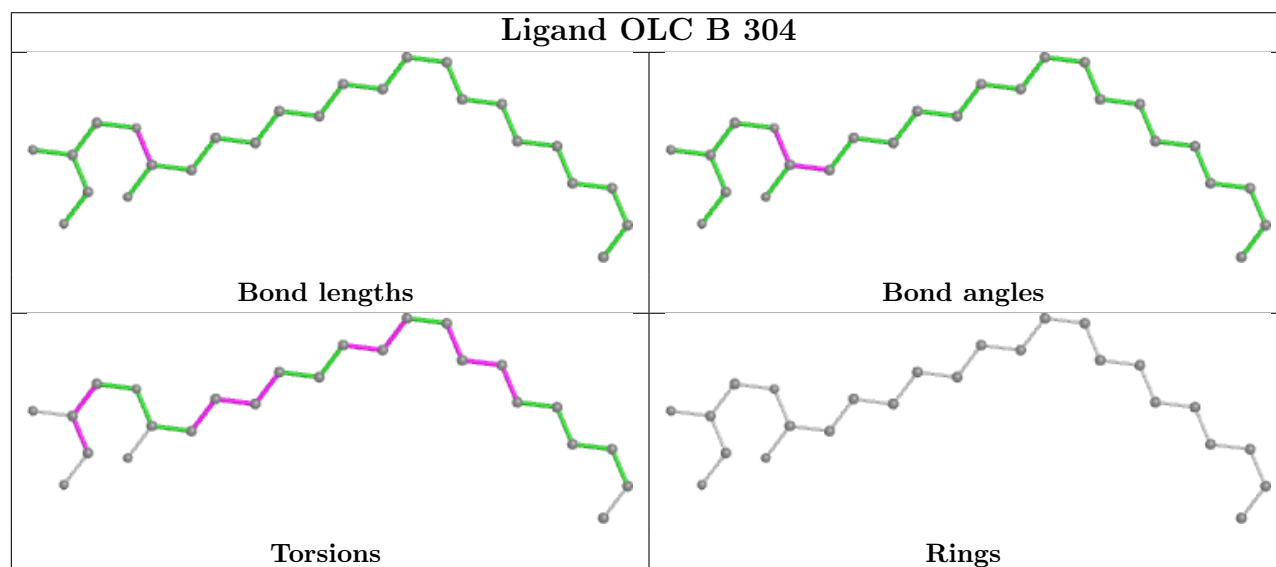
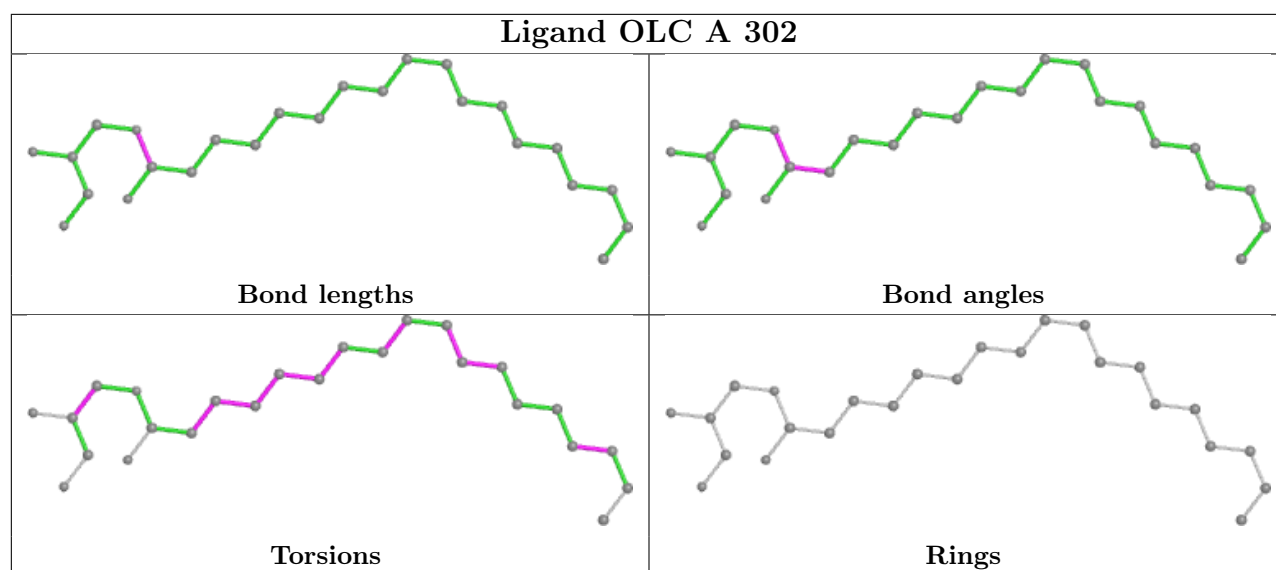
There are no ring outliers.

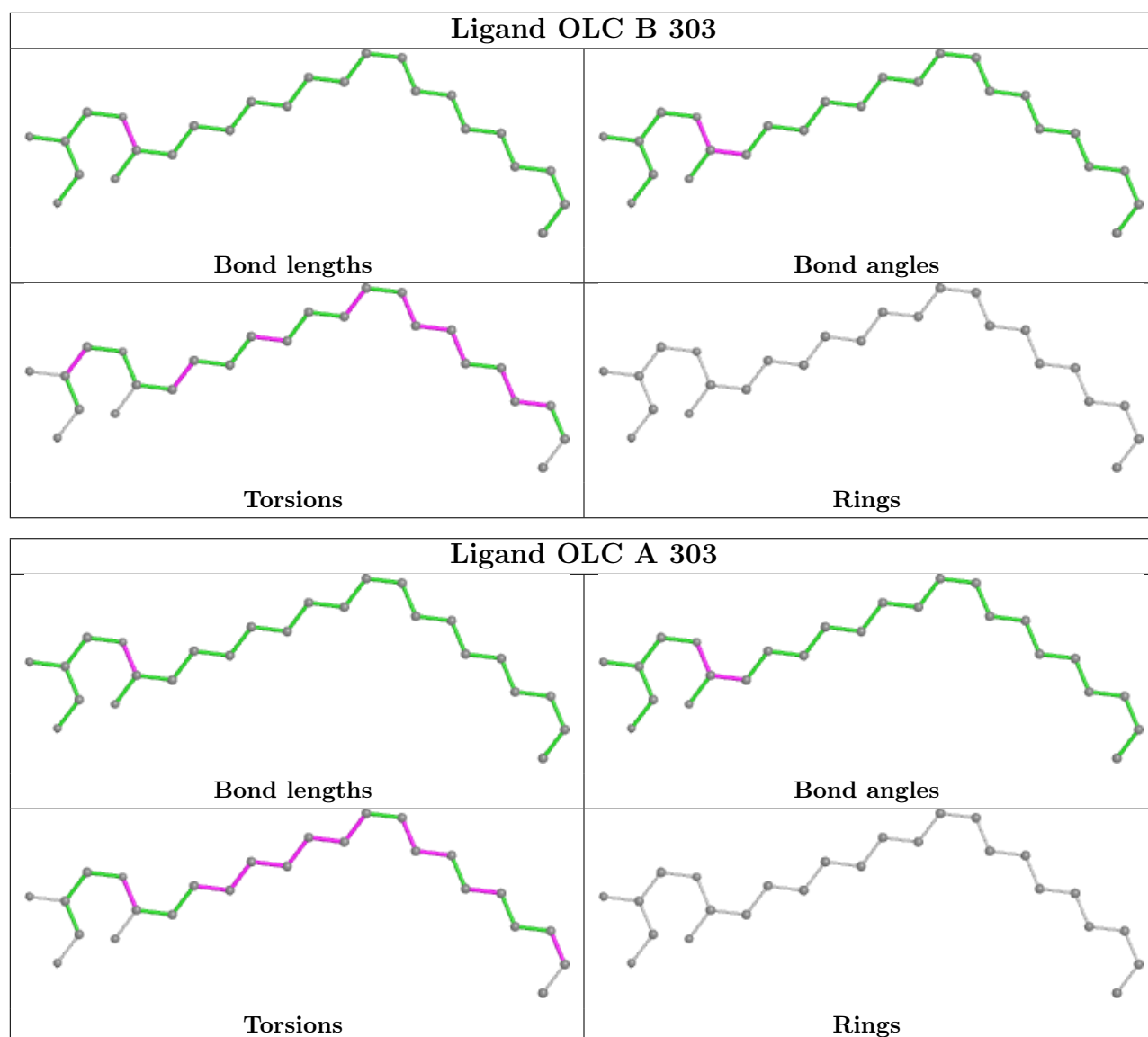
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	OLC	1	0
3	A	302	OLC	7	0
3	B	303	OLC	3	0
4	B	306	GOL	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, 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	264/269 (98%)	-0.00	8 (3%)	50 34	22, 50, 84, 103	0
1	B	268/269 (99%)	-0.01	5 (1%)	66 53	23, 46, 84, 104	0
All	All	532/538 (98%)	-0.01	13 (2%)	59 44	22, 49, 85, 104	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	264	GLY	4.3
1	A	260	ASP	2.7
1	A	9	ALA	2.7
1	A	184	PRO	2.6
1	B	260	ASP	2.5
1	A	119	SER	2.5
1	B	9	ALA	2.4
1	A	54	ALA	2.4
1	A	15	SER	2.3
1	B	272	MET	2.1
1	B	263	LYS	2.0
1	A	55	PRO	2.0
1	A	263	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q < 0.9
1	LYR	A	238	29/30	0.87	0.31	25,40,47,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	LYR	B	238	29/30	0.90	0.25	23,38,48,52	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

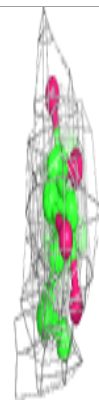
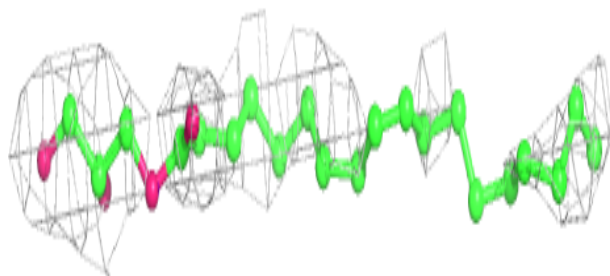
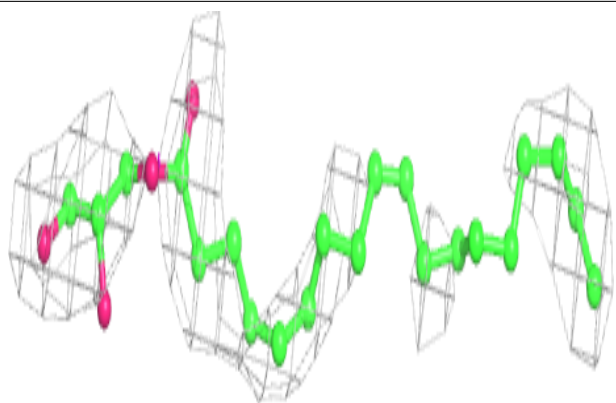
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	B	306	6/6	0.61	0.44	41,44,56,58	0
3	OLC	A	303	25/25	0.65	0.45	25,59,79,83	0
2	BR	B	301	1/1	0.69	0.14	71,71,71,71	1
3	OLC	B	305	25/25	0.74	0.37	40,53,68,71	0
2	BR	A	301	1/1	0.76	0.20	71,71,71,71	1
3	OLC	B	303	25/25	0.81	0.62	28,50,70,87	0
3	OLC	A	302	25/25	0.82	0.47	28,45,53,54	0
4	GOL	A	304	6/6	0.83	0.55	34,37,44,55	0
3	OLC	B	304	25/25	0.83	0.29	32,41,61,63	0
3	OLC	B	302	25/25	0.85	0.44	26,41,59,62	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.

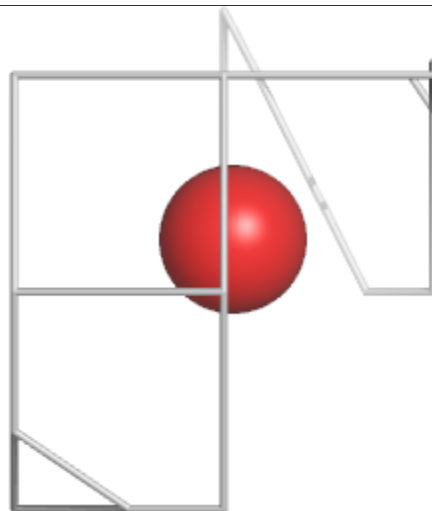
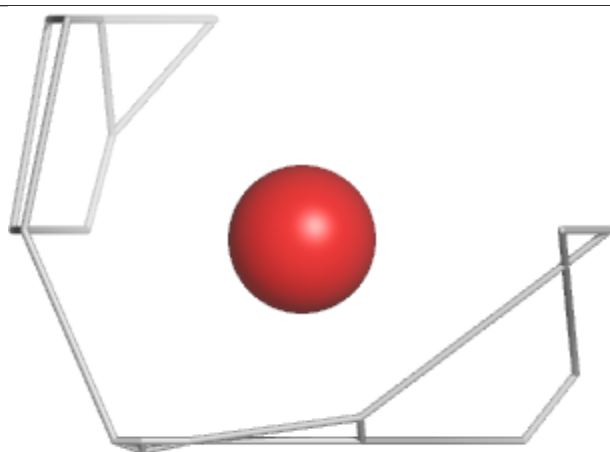
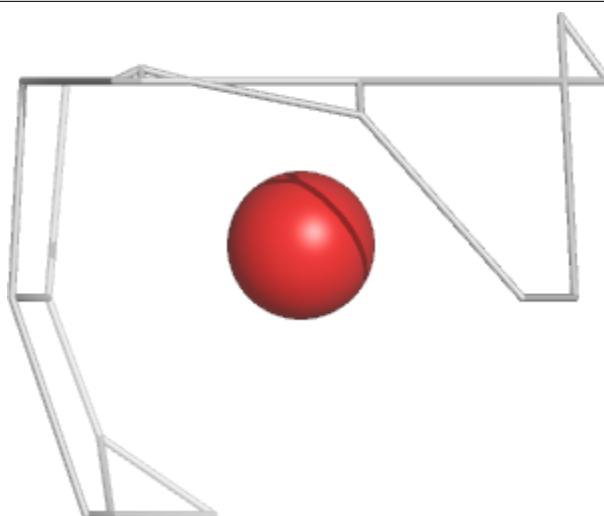
Electron density around OLC A 303:

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



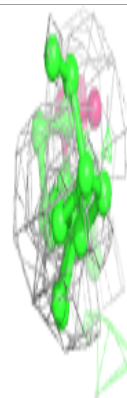
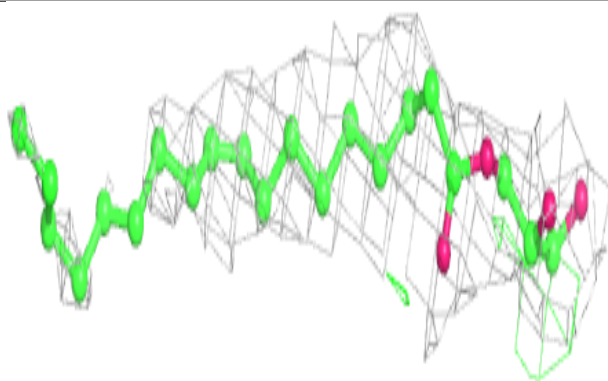
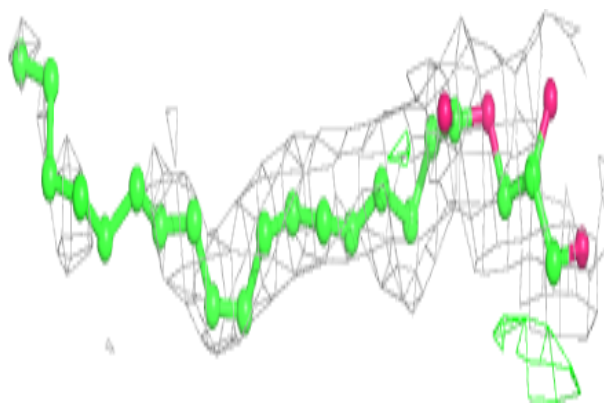
Electron density around BR B 301:

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



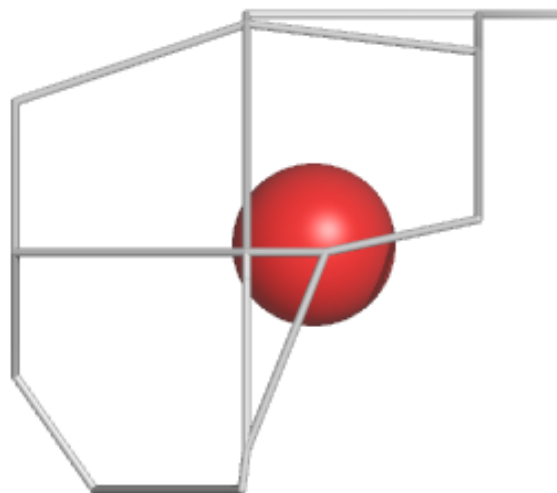
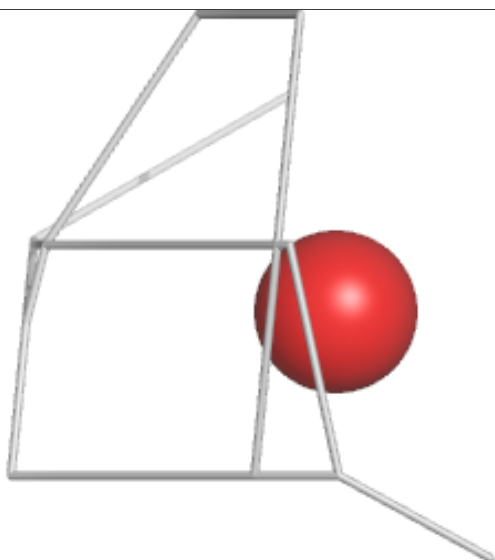
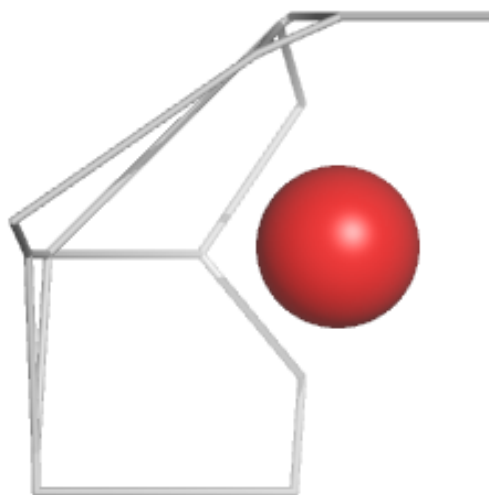
Electron density around OLC B 305:

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



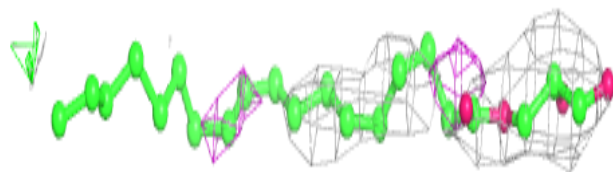
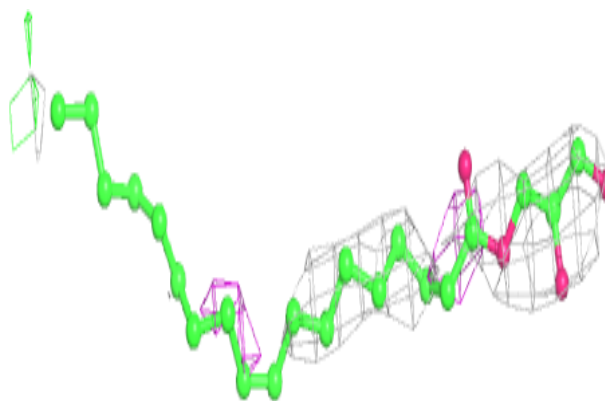
Electron density around BR A 301:

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

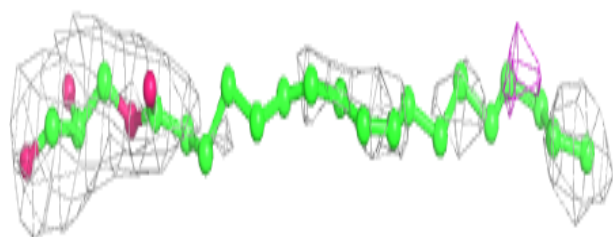
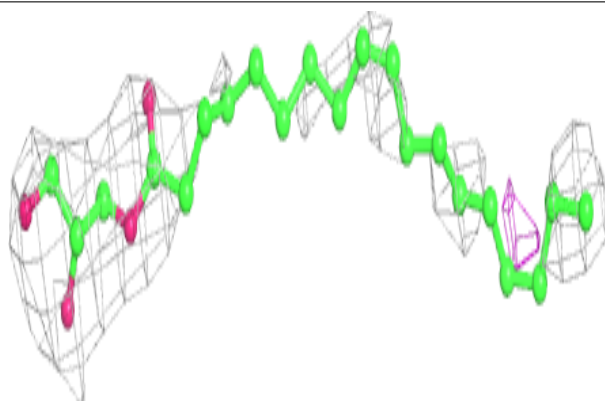


Electron density around OLC B 303:

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

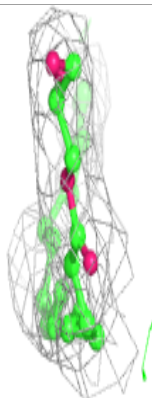
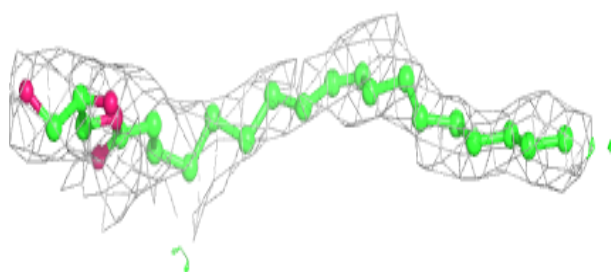
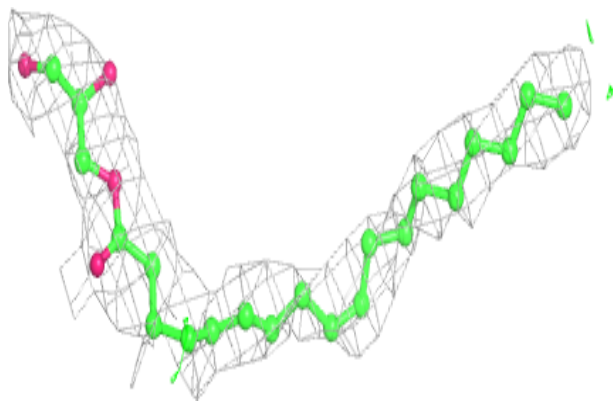
**Electron density around OLC A 302:**

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and green (positive)

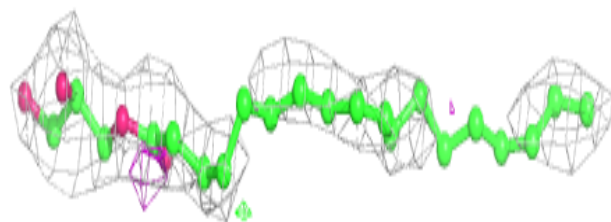
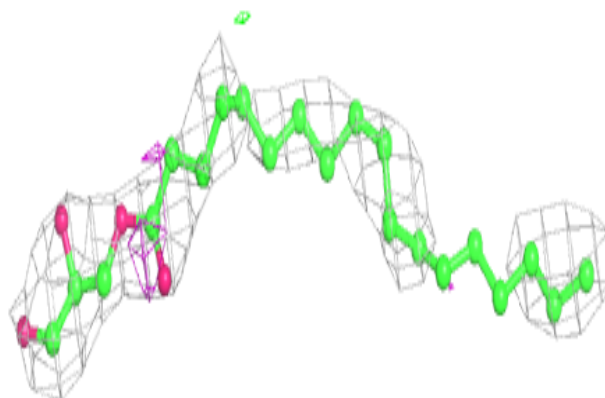


Electron density around OLC B 304:

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

**Electron density around OLC B 302:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.