



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:09 AM UTC

PDB ID : 6EDQ / pdb_00006edq
Title : Crystal Structure of the Light-Gated Anion Channelrhodopsin GtACR1
Authors : Li, H.; Huang, C.Y.; Wang, M.; Zheng, L.; Spudich, J.L.
Deposited on : 2018-08-10
Resolution : 2.90 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

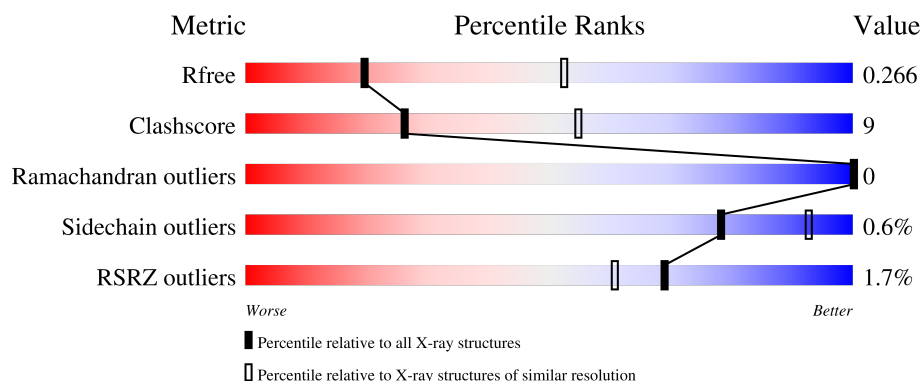
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	303	% 68% 19% • 12%
1	B	303	2% 71% 19% • 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4568 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.

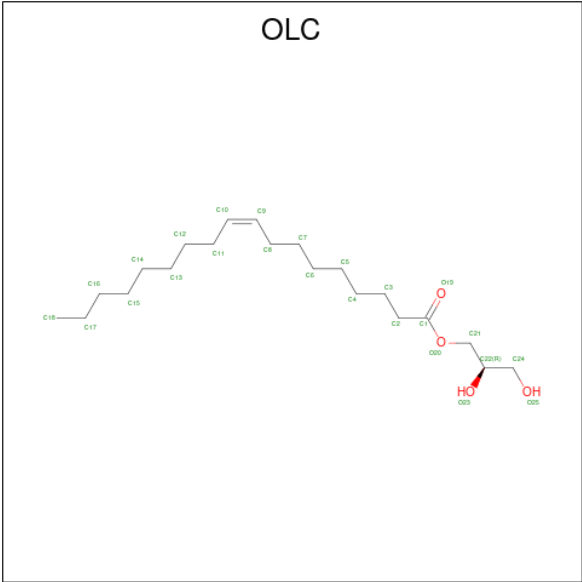
- Molecule 1 is a protein called Anion channelrhodopsin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2129	1414	329	363	23			
1	B	275	Total	C	N	O	S	0	0	0
			2198	1457	338	380	23			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	296	HIS	-	expression tag	UNP L1J207
A	297	HIS	-	expression tag	UNP L1J207
A	298	HIS	-	expression tag	UNP L1J207
A	299	HIS	-	expression tag	UNP L1J207
A	300	HIS	-	expression tag	UNP L1J207
A	301	HIS	-	expression tag	UNP L1J207
A	302	HIS	-	expression tag	UNP L1J207
A	303	HIS	-	expression tag	UNP L1J207
B	296	HIS	-	expression tag	UNP L1J207
B	297	HIS	-	expression tag	UNP L1J207
B	298	HIS	-	expression tag	UNP L1J207
B	299	HIS	-	expression tag	UNP L1J207
B	300	HIS	-	expression tag	UNP L1J207
B	301	HIS	-	expression tag	UNP L1J207
B	302	HIS	-	expression tag	UNP L1J207
B	303	HIS	-	expression tag	UNP L1J207

- Molecule 2 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			18	14	4		
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			25	21	4		
2	B	1	Total	C	O	0	0
			25	21	4		
2	B	1	Total	C	O	0	0
			25	21	4		
2	B	1	Total	C	O	0	0
			21	17	4		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

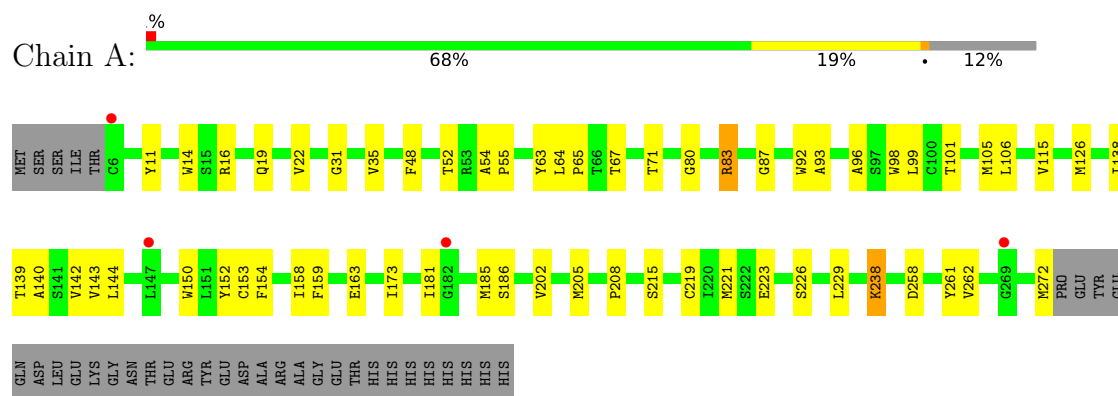
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		
4	B	9	Total	O	0	0
			9	9		

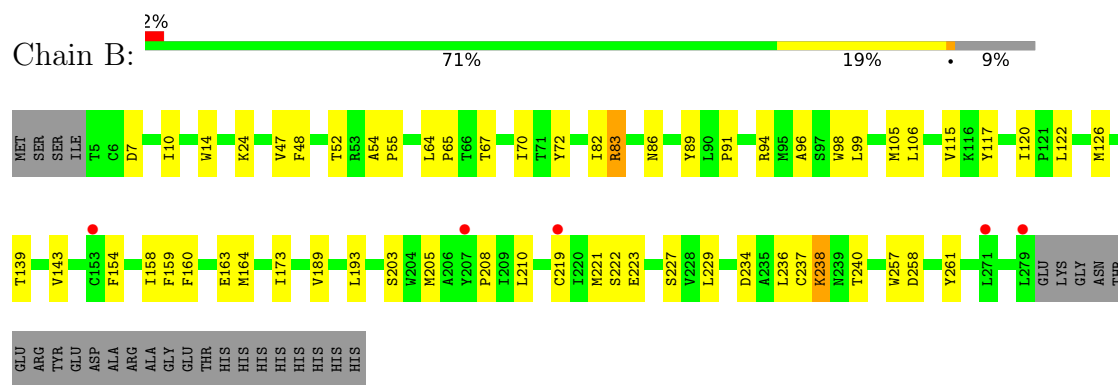
3 Residue-property plots

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 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	77.79Å 149.55Å 62.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.91 – 2.90 47.91 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.91-2.90) 99.8 (47.91-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.14_3211)	Depositor
R, R_{free}	0.230 , 0.267 0.232 , 0.266	Depositor DCC
R_{free} test set	838 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	65.7	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4568	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.43 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5276e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: LYR, GOL, OLC

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	0.22	0/2158	0.45	0/2941
1	B	0.22	0/2229	0.44	0/3039
All	All	0.22	0/4387	0.45	0/5980

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	2129	0	2164	44	0
1	B	2198	0	2222	39	0
2	A	118	0	183	15	0
2	B	71	0	109	2	0
3	A	12	0	16	0	0
3	B	18	0	24	0	0
4	A	13	0	0	0	0
4	B	9	0	0	0	0
All	All	4568	0	4718	87	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 9.

All (87) 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:215:SER:HA	1:A:219:CYS:HB3	1.76	0.67
1:B:117:TYR:HB2	1:B:122:LEU:HD11	1.77	0.66
1:B:7:ASP:HB3	1:B:10:ILE:HG12	1.78	0.66
1:B:54:ALA:HB3	1:B:55:PRO:HD3	1.78	0.66
1:A:153:CYS:SG	2:A:403:OLC:H4A	2.36	0.66
1:A:208:PRO:HB2	2:A:405:OLC:H15A	1.78	0.64
1:B:210:LEU:HD21	1:B:229:LEU:HB3	1.78	0.64
1:A:221:MET:HE1	1:A:229:LEU:HD12	1.80	0.64
1:A:238:LYR:H182	1:A:238:LYR:H9	1.80	0.63
1:A:202:VAL:HA	2:A:402:OLC:H5	1.81	0.62
1:A:54:ALA:HB3	1:A:55:PRO:HD3	1.83	0.60
1:A:106:LEU:HD11	1:A:163:GLU:OE1	2.00	0.60
1:A:150:TRP:NE1	2:A:405:OLC:O23	2.36	0.59
1:A:154:PHE:CZ	1:A:158:ILE:HD11	2.38	0.59
1:B:159:PHE:O	1:B:163:GLU:HG2	2.04	0.58
2:A:402:OLC:H10	2:A:404:OLC:H14A	1.86	0.58
1:A:258:ASP:HB3	1:A:261:TYR:HB3	1.86	0.57
1:A:205:MET:HE3	2:A:402:OLC:H5A	1.86	0.56
1:A:153:CYS:SG	2:A:403:OLC:H6	2.47	0.56
1:A:142:VAL:HG21	1:B:82:ILE:HD13	1.88	0.55
1:A:181:ILE:O	1:A:186:SER:OG	2.22	0.54
1:B:210:LEU:HD23	1:B:221:MET:HE1	1.90	0.53
1:B:106:LEU:HD11	1:B:163:GLU:OE2	2.08	0.53
1:B:208:PRO:HG3	1:B:238:LYR:H132	1.89	0.53
1:B:24:LYS:HB3	1:B:222:SER:HA	1.90	0.53
1:A:150:TRP:CZ3	2:A:403:OLC:H4	2.44	0.53
1:B:154:PHE:CZ	1:B:158:ILE:HD11	2.44	0.52
1:B:203:SER:HB2	1:B:237:CYS:HB3	1.91	0.52
1:B:64:LEU:HB2	1:B:65:PRO:HD3	1.92	0.52
1:B:238:LYR:H192	1:B:238:LYR:H9	1.92	0.51
1:B:189:VAL:O	1:B:193:LEU:HD13	2.10	0.51
2:A:403:OLC:H24A	2:A:405:OLC:H2A	1.92	0.51
1:A:63:TYR:HD1	2:A:401:OLC:H13	1.76	0.51
1:B:203:SER:CB	1:B:237:CYS:HB3	2.41	0.51
1:A:96:ALA:HA	1:A:99:LEU:HD12	1.93	0.50
1:A:101:THR:O	1:A:105:MET:HG3	2.12	0.50
1:A:105:MET:SD	1:A:238:LYR:H11	2.51	0.50
1:A:159:PHE:O	1:A:163:GLU:HG2	2.11	0.50
1:A:11:TYR:O	1:A:16:ARG:NH2	2.44	0.50
1:A:115:VAL:HG12	1:A:173:ILE:HD12	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:TRP:HB2	1:A:144:LEU:HD13	1.94	0.49
1:A:63:TYR:CD1	2:A:401:OLC:H13	2.47	0.49
1:B:83:ARG:HG3	1:B:89:TYR:CE1	2.47	0.49
1:A:106:LEU:HD13	1:A:126:MET:HG2	1.94	0.48
1:B:67:THR:HG22	2:B:401:OLC:H6	1.95	0.48
1:B:223:GLU:O	1:B:227:SER:OG	2.24	0.48
1:B:139:THR:O	1:B:143:VAL:HG23	2.13	0.48
1:B:72:TYR:OH	1:B:234:ASP:OD2	2.20	0.47
1:B:205:MET:O	1:B:208:PRO:HD2	2.14	0.47
1:B:91:PRO:HG2	1:B:94:ARG:HH22	1.78	0.47
1:A:258:ASP:O	1:A:262:VAL:HG23	2.14	0.47
1:B:236:LEU:O	1:B:240:THR:HB	2.14	0.47
2:A:402:OLC:H13	2:A:404:OLC:H16A	1.98	0.46
1:A:80:GLY:HA3	1:A:93:ALA:HB2	1.98	0.46
1:B:48:PHE:O	1:B:52:THR:HG23	2.16	0.46
1:B:193:LEU:HD11	1:B:257:TRP:CZ3	2.51	0.46
1:B:258:ASP:HB3	1:B:261:TYR:HB3	1.98	0.45
1:A:67:THR:O	1:A:71:THR:HG23	2.17	0.45
1:B:117:TYR:O	1:B:120:ILE:HG12	2.16	0.45
1:B:106:LEU:HD13	1:B:126:MET:HG2	1.99	0.44
1:A:48:PHE:O	1:A:52:THR:HG23	2.17	0.44
1:A:140:ALA:HB2	1:A:152:TYR:HB2	1.99	0.44
1:B:91:PRO:HG2	1:B:94:ARG:NH2	2.33	0.44
1:A:83:ARG:NH1	1:A:87:GLY:O	2.50	0.44
1:B:47:VAL:HG23	1:B:65:PRO:HB2	1.99	0.44
1:A:19:GLN:O	1:A:22:VAL:HG12	2.18	0.43
1:A:202:VAL:HG21	2:A:404:OLC:H9	1.99	0.43
1:B:70:ILE:HD12	2:B:401:OLC:H6A	1.99	0.43
2:A:403:OLC:H21	2:A:405:OLC:H2A	2.01	0.43
1:B:238:LYR:H10	1:B:238:LYR:H81	1.91	0.43
1:A:98:TRP:CD1	1:A:238:LYR:HC2	2.55	0.42
1:A:64:LEU:HB2	1:A:65:PRO:HD3	2.01	0.42
1:A:223:GLU:HA	1:A:226:SER:HB3	2.01	0.42
1:A:238:LYR:H182	1:A:238:LYR:C9	2.48	0.42
1:B:98:TRP:CD1	1:B:238:LYR:HC2	2.55	0.42
1:B:105:MET:SD	1:B:238:LYR:H11	2.60	0.42
1:A:92:TRP:HZ3	1:A:138:ILE:HD13	1.85	0.42
1:B:115:VAL:HG22	1:B:173:ILE:HD12	2.01	0.42
1:A:31:GLY:O	1:A:35:VAL:HG23	2.19	0.41
1:A:185:MET:HG2	1:A:262:VAL:HG13	2.02	0.41
1:B:160:PHE:O	1:B:164:MET:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:403:OLC:H6A	2:A:405:OLC:H13A	2.02	0.41
1:B:96:ALA:HA	1:B:99:LEU:HD12	2.03	0.41
1:A:101:THR:HG21	1:A:238:LYR:HE3	2.03	0.41
1:A:139:THR:O	1:A:143:VAL:HG23	2.21	0.41
1:A:272:MET:HE3	1:A:272:MET:HB2	1.95	0.40
1:B:14:TRP:HB3	1:B:86:ASN:O	2.21	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	264/303 (87%)	257 (97%)	7 (3%)	0	100	100
1	B	272/303 (90%)	266 (98%)	6 (2%)	0	100	100
All	All	536/606 (88%)	523 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	231/263 (88%)	230 (100%)	1 (0%)	84	94
1	B	239/263 (91%)	237 (99%)	2 (1%)	73	90

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	470/526 (89%)	467 (99%)	3 (1%)	78	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ARG
1	B	83	ARG
1	B	219	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	HIS
1	B	18	ASN
1	B	176	HIS
1	B	239	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	4.01	10 (37%)	30,37,39	2.25	12 (40%)
1	LYR	B	238	1	27,29,30	4.08	10 (37%)	30,37,39	2.11	12 (40%)

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	-	6/22/40/42	0/1/1/1
1	LYR	B	238	1	-	6/22/40/42	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	238	LYR	C12-C11	15.66	1.60	1.34
1	A	238	LYR	C12-C11	15.12	1.59	1.34
1	B	238	LYR	C16-C15	-6.87	1.36	1.52
1	A	238	LYR	C16-C15	-6.68	1.36	1.52
1	A	238	LYR	C17-C11	-5.99	1.46	1.53
1	B	238	LYR	C17-C11	-5.12	1.47	1.53
1	A	238	LYR	C16-C17	4.82	1.65	1.54
1	B	238	LYR	C16-C17	4.67	1.64	1.54
1	B	238	LYR	C5-C3	4.07	1.54	1.46
1	A	238	LYR	C6-C7	4.04	1.55	1.43
1	A	238	LYR	C15-C14	4.03	1.65	1.52
1	B	238	LYR	C15-C14	4.03	1.65	1.52
1	B	238	LYR	C14-C12	-3.97	1.43	1.51
1	A	238	LYR	C5-C3	3.89	1.54	1.46
1	B	238	LYR	C6-C7	3.87	1.55	1.43
1	A	238	LYR	C14-C12	-3.74	1.44	1.51
1	B	238	LYR	C9-C80	3.66	1.53	1.46
1	A	238	LYR	C9-C80	3.55	1.53	1.46
1	B	238	LYR	C10-C11	3.49	1.57	1.45
1	A	238	LYR	C10-C11	3.41	1.56	1.45

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	LYR	C13-C12-C11	-5.42	118.57	124.48
1	A	238	LYR	C1-NZ-CE	-4.54	103.65	112.85
1	B	238	LYR	C1-NZ-CE	-4.27	104.19	112.85
1	A	238	LYR	C6-C7-C80	-4.04	121.62	127.28
1	B	238	LYR	C13-C12-C11	-3.84	120.29	124.48
1	B	238	LYR	C6-C7-C80	-3.76	122.00	127.28
1	B	238	LYR	C10-C9-C80	-3.45	121.13	126.23
1	A	238	LYR	C17-C11-C10	3.29	124.58	115.65
1	B	238	LYR	C17-C11-C10	3.20	124.33	115.65
1	A	238	LYR	C13-C12-C14	2.94	119.87	113.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	LYR	C16-C17-C11	2.81	114.52	110.44
1	A	238	LYR	C8-C80-C9	2.81	122.37	118.09
1	B	238	LYR	C7-C6-C5	-2.80	115.10	123.20
1	B	238	LYR	C16-C17-C11	2.74	114.42	110.44
1	A	238	LYR	C10-C11-C12	-2.66	115.42	121.56
1	B	238	LYR	C13-C12-C14	2.55	119.03	113.60
1	A	238	LYR	C7-C6-C5	-2.50	115.97	123.20
1	B	238	LYR	C10-C11-C12	-2.48	115.83	121.56
1	A	238	LYR	C17-C11-C12	-2.13	119.72	122.64
1	B	238	LYR	CD-CG-CB	-2.13	105.60	113.62
1	B	238	LYR	C8-C80-C9	2.07	121.25	118.09
1	B	238	LYR	C17-C11-C12	-2.05	119.84	122.64
1	A	238	LYR	C6-C5-C3	-2.05	120.75	126.36
1	A	238	LYR	C4-C3-C5	2.00	121.15	118.09

There are no chirality outliers.

All (12) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	238	LYR	5	0
1	B	238	LYR	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	OLC	A	405	-	24,24,24	0.73	1 (4%)	25,25,25	0.86	1 (4%)
2	OLC	A	404	-	24,24,24	0.69	1 (4%)	25,25,25	0.98	1 (4%)
2	OLC	B	402	-	24,24,24	0.70	1 (4%)	25,25,25	0.98	1 (4%)
3	GOL	A	407	-	5,5,5	0.33	0	5,5,5	0.23	0
2	OLC	A	402	-	24,24,24	0.74	1 (4%)	25,25,25	0.89	1 (4%)
3	GOL	A	406	-	5,5,5	0.36	0	5,5,5	0.34	0
2	OLC	A	401	-	24,24,24	0.76	1 (4%)	25,25,25	0.96	1 (4%)
2	OLC	B	401	-	24,24,24	0.75	1 (4%)	25,25,25	0.87	1 (4%)
3	GOL	B	405	-	5,5,5	0.36	0	5,5,5	0.18	0
2	OLC	B	403	-	20,20,24	0.80	1 (5%)	21,21,25	0.99	1 (4%)
3	GOL	B	404	-	5,5,5	0.31	0	5,5,5	0.31	0
2	OLC	A	403	-	17,17,24	0.84	1 (5%)	18,18,25	1.20	1 (5%)
3	GOL	B	406	-	5,5,5	0.34	0	5,5,5	0.31	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
2	OLC	A	405	-	-	7/24/24/24	-
2	OLC	A	404	-	-	10/24/24/24	-
2	OLC	B	402	-	-	9/24/24/24	-
3	GOL	A	407	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	A	402	-	-	12/24/24/24	-
3	GOL	A	406	-	-	2/4/4/4	-
2	OLC	A	401	-	-	7/24/24/24	-
2	OLC	B	401	-	-	9/24/24/24	-
3	GOL	B	405	-	-	1/4/4/4	-
2	OLC	B	403	-	-	7/20/20/24	-
3	GOL	B	404	-	-	0/4/4/4	-
2	OLC	A	403	-	-	7/17/17/24	-
3	GOL	B	406	-	-	0/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	OLC	O20-C1	3.23	1.42	1.33
2	B	401	OLC	O20-C1	3.14	1.42	1.33
2	B	403	OLC	O20-C1	3.09	1.42	1.33
2	A	405	OLC	O20-C1	2.94	1.41	1.33
2	A	402	OLC	O20-C1	2.87	1.41	1.33
2	A	403	OLC	O20-C1	2.81	1.41	1.33
2	B	402	OLC	O20-C1	2.79	1.41	1.33
2	A	404	OLC	O20-C1	2.72	1.41	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	OLC	O20-C1-C2	3.37	122.11	111.83
2	A	402	OLC	O20-C1-C2	3.08	121.22	111.83
2	B	402	OLC	O20-C1-C2	3.06	121.18	111.83
2	A	403	OLC	O20-C1-C2	3.06	121.16	111.83
2	B	403	OLC	O20-C1-C2	3.00	120.98	111.83
2	A	405	OLC	O20-C1-C2	2.90	120.66	111.83
2	A	404	OLC	O20-C1-C2	2.84	120.48	111.83
2	B	401	OLC	O20-C1-C2	2.60	119.77	111.83

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	406	GOL	C1-C2-C3-O3
3	A	406	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	407	GOL	C1-C2-C3-O3
2	A	404	OLC	O19-C1-O20-C21
2	A	404	OLC	C2-C1-O20-C21
2	A	405	OLC	C2-C1-O20-C21
2	A	405	OLC	O19-C1-O20-C21
2	A	402	OLC	O20-C21-C22-C24
2	A	402	OLC	O20-C21-C22-O23
2	B	402	OLC	C2-C1-O20-C21
2	A	405	OLC	C2-C3-C4-C5
2	B	402	OLC	C12-C13-C14-C15
2	A	404	OLC	C2-C3-C4-C5
3	A	407	GOL	O2-C2-C3-O3
2	A	404	OLC	C12-C13-C14-C15
2	B	401	OLC	C13-C14-C15-C16
2	B	403	OLC	C2-C1-O20-C21
2	A	405	OLC	O20-C21-C22-O23
2	A	402	OLC	C13-C14-C15-C16
2	B	402	OLC	O19-C1-O20-C21
2	A	402	OLC	C11-C12-C13-C14
2	B	402	OLC	C6-C7-C8-C9
2	B	401	OLC	C2-C3-C4-C5
2	A	401	OLC	C4-C5-C6-C7
2	B	403	OLC	O19-C1-O20-C21
2	A	404	OLC	C1-C2-C3-C4
2	A	405	OLC	C10-C11-C12-C13
2	B	402	OLC	C10-C11-C12-C13
2	A	402	OLC	C14-C15-C16-C17
2	B	403	OLC	C3-C4-C5-C6
2	B	401	OLC	C6-C7-C8-C9
2	A	403	OLC	C5-C6-C7-C8
2	B	402	OLC	C14-C15-C16-C17
2	B	403	OLC	C2-C3-C4-C5
2	A	402	OLC	C6-C7-C8-C9
2	A	404	OLC	C10-C11-C12-C13
2	A	402	OLC	C2-C1-O20-C21
2	B	403	OLC	C5-C6-C7-C8
2	B	401	OLC	C5-C6-C7-C8
2	B	402	OLC	C15-C16-C17-C18
2	A	402	OLC	O19-C1-O20-C21
2	A	404	OLC	C15-C16-C17-C18
2	B	401	OLC	C11-C12-C13-C14
2	A	403	OLC	O23-C22-C24-O25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	405	GOL	O2-C2-C3-O3
2	A	403	OLC	C2-C1-O20-C21
2	A	403	OLC	C4-C5-C6-C7
2	A	402	OLC	C15-C16-C17-C18
2	A	403	OLC	C3-C4-C5-C6
2	A	403	OLC	O19-C1-O20-C21
2	A	401	OLC	C10-C11-C12-C13
2	A	402	OLC	C12-C13-C14-C15
2	A	402	OLC	C9-C10-C11-C12
2	A	404	OLC	C9-C10-C11-C12
2	A	404	OLC	C3-C4-C5-C6
2	A	401	OLC	C2-C3-C4-C5
2	B	401	OLC	C3-C4-C5-C6
2	A	401	OLC	O19-C1-O20-C21
2	A	401	OLC	C2-C1-O20-C21
2	B	402	OLC	C2-C3-C4-C5
2	B	403	OLC	C7-C8-C9-C10
2	A	405	OLC	C14-C15-C16-C17
2	B	401	OLC	C7-C8-C9-C10
2	A	404	OLC	C5-C6-C7-C8
2	A	401	OLC	C9-C10-C11-C12
2	A	403	OLC	C7-C8-C9-C10
2	B	401	OLC	C12-C13-C14-C15
2	A	405	OLC	C9-C10-C11-C12
2	B	402	OLC	C9-C10-C11-C12
2	A	401	OLC	C7-C8-C9-C10
2	B	403	OLC	C9-C10-C11-C12
2	A	402	OLC	C10-C11-C12-C13
2	B	401	OLC	C10-C11-C12-C13

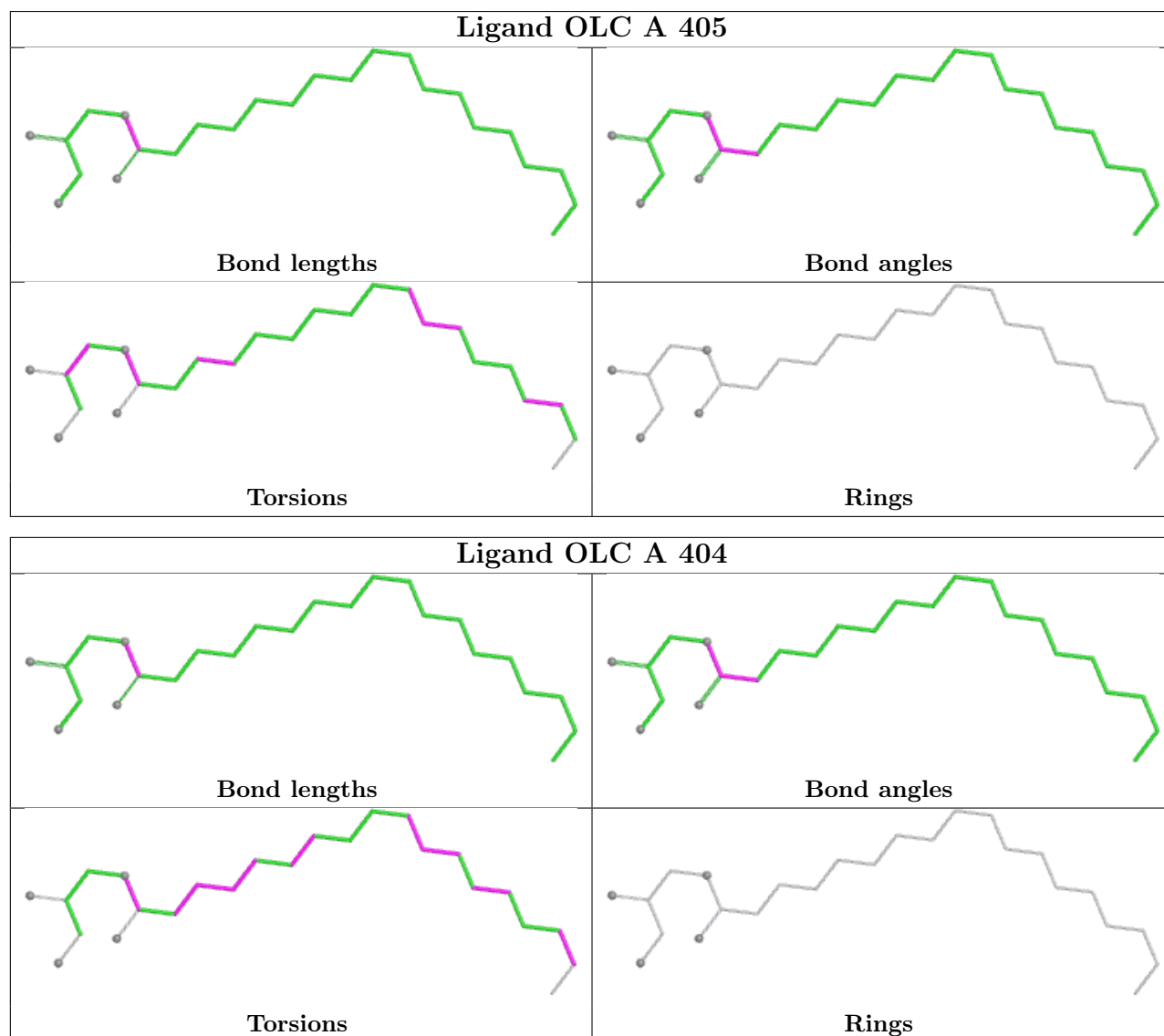
There are no ring outliers.

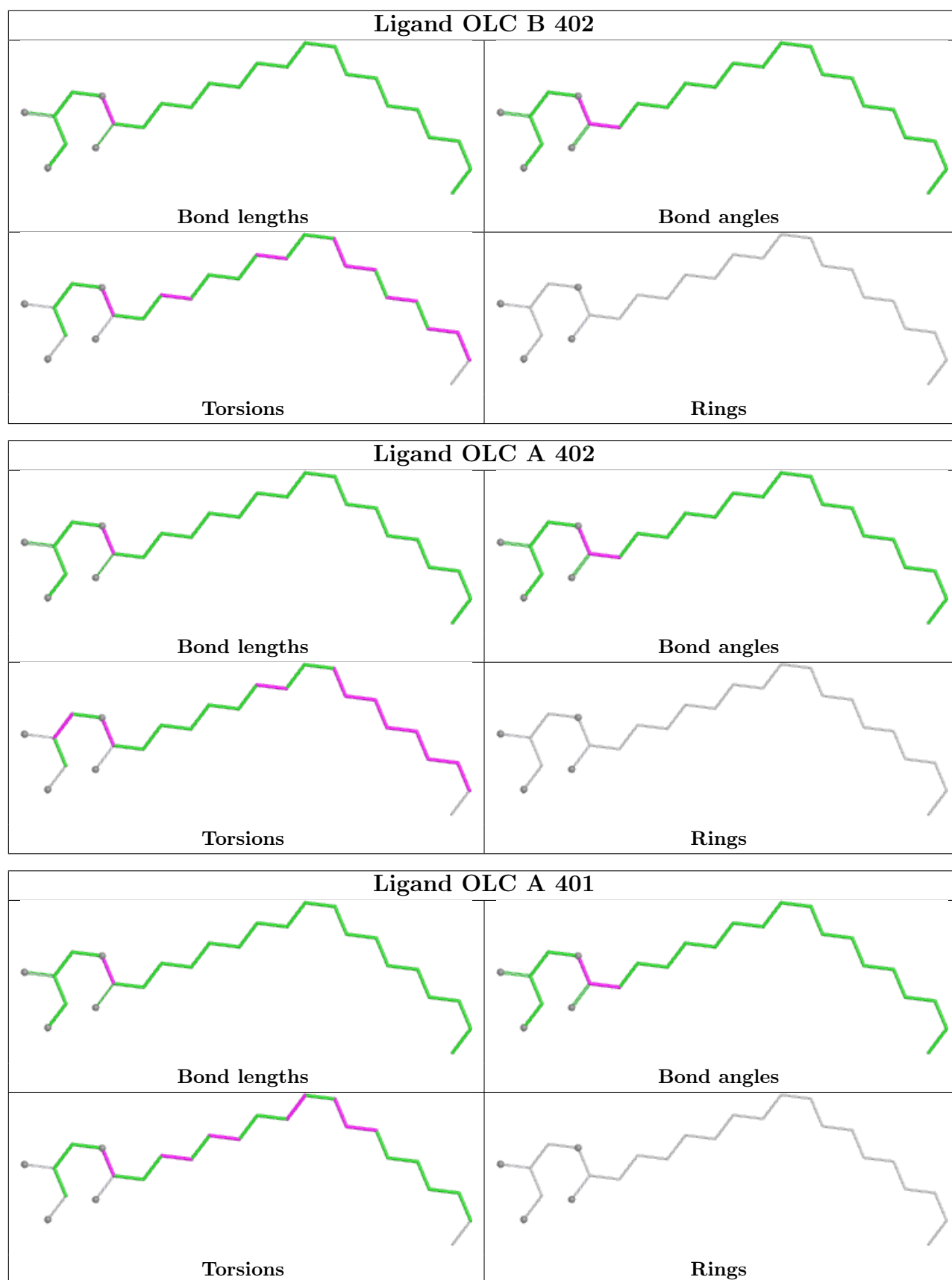
6 monomers are involved in 17 short contacts:

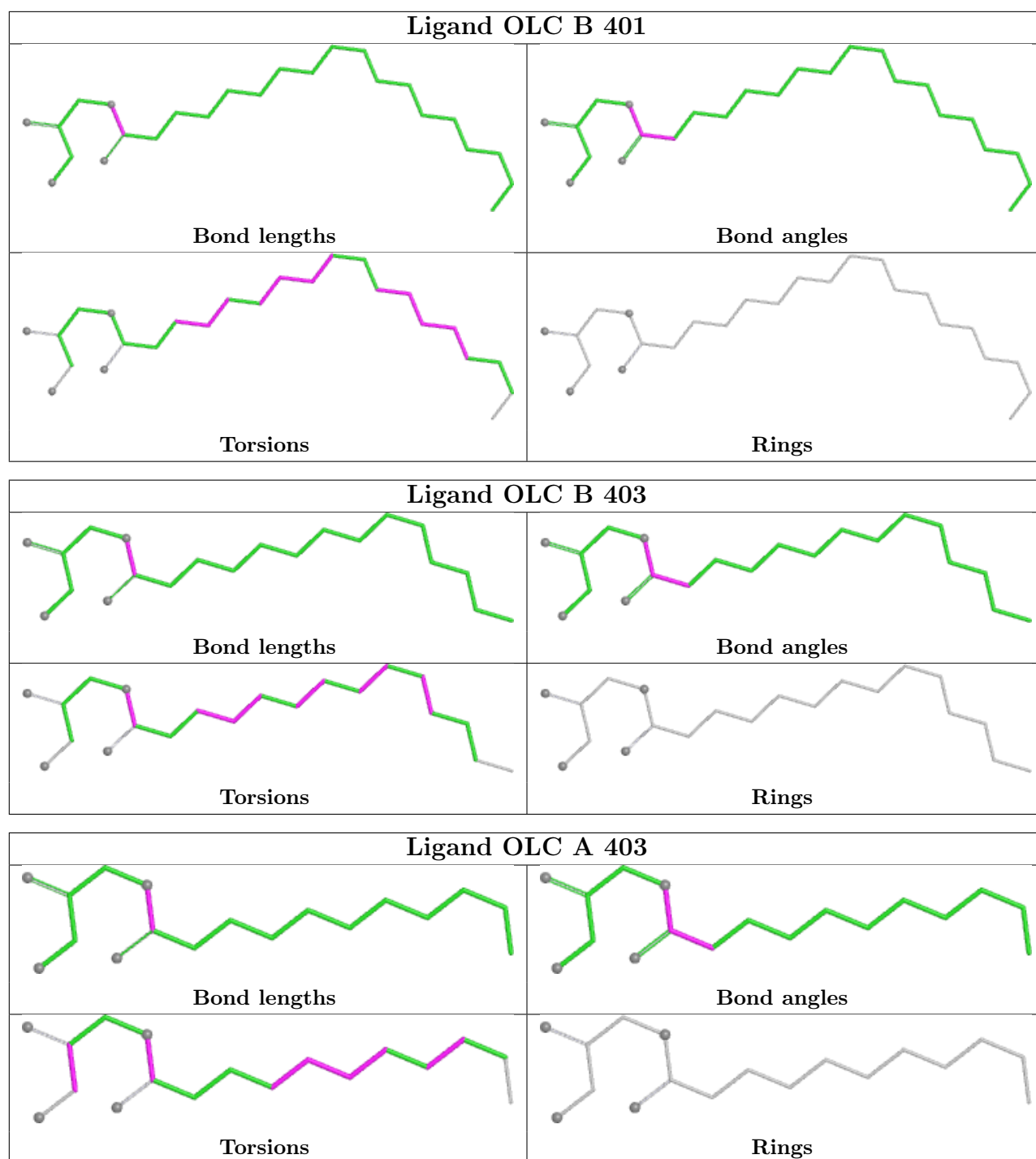
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	405	OLC	5	0
2	A	404	OLC	3	0
2	A	402	OLC	4	0
2	A	401	OLC	2	0
2	B	401	OLC	2	0
2	A	403	OLC	6	0

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	266/303 (87%)	0.01	4 (1%) 72 64	41, 59, 100, 154	0
1	B	274/303 (90%)	0.06	5 (1%) 67 59	42, 58, 94, 124	0
All	All	540/606 (89%)	0.03	9 (1%) 69 61	41, 59, 99, 154	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	CYS	5.0
1	B	279	LEU	3.5
1	A	182	GLY	2.7
1	A	269	GLY	2.5
1	A	147	LEU	2.2
1	B	219	CYS	2.1
1	B	271	LEU	2.0
1	B	153	CYS	2.0
1	B	207	TYR	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	0.93	0.11	40,44,54,57	0
1	LYR	B	238	29/30	0.94	0.16	52,57,64,66	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

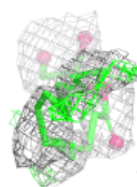
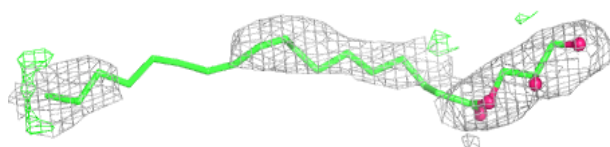
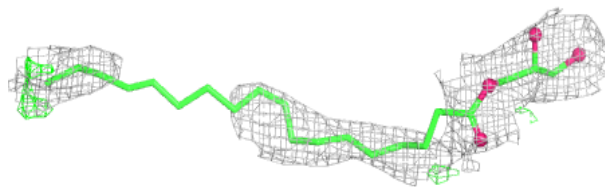
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	406	6/6	0.71	0.20	92,96,100,108	0
2	OLC	A	404	25/25	0.72	0.19	92,100,108,108	0
2	OLC	A	405	25/25	0.78	0.22	71,82,101,108	0
2	OLC	A	401	25/25	0.78	0.24	61,67,81,83	0
3	GOL	B	404	6/6	0.78	0.29	67,71,73,77	0
2	OLC	A	402	25/25	0.80	0.20	69,75,89,89	0
2	OLC	B	402	25/25	0.83	0.20	73,83,89,92	0
2	OLC	A	403	18/25	0.85	0.17	74,85,89,89	0
2	OLC	B	401	25/25	0.88	0.17	47,64,84,85	0
2	OLC	B	403	21/25	0.88	0.17	61,73,89,94	0
3	GOL	A	407	6/6	0.89	0.14	66,70,72,78	0
3	GOL	B	406	6/6	0.89	0.16	78,79,80,86	0
3	GOL	B	405	6/6	0.90	0.13	54,57,64,74	0

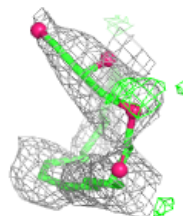
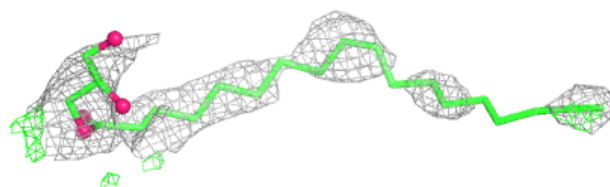
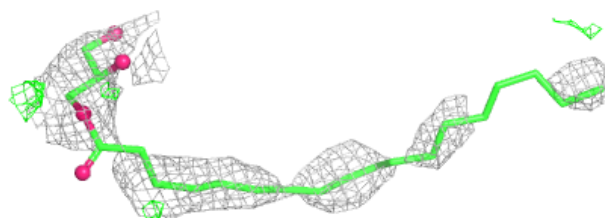
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 404:

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

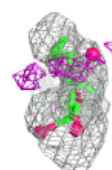
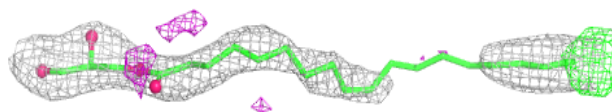
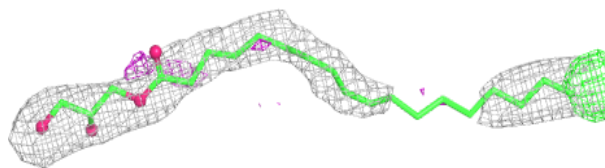
**Electron density around OLC A 405:**

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

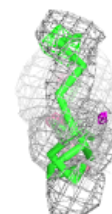
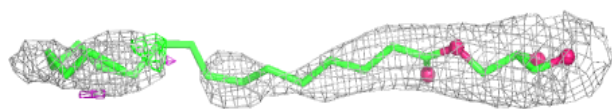
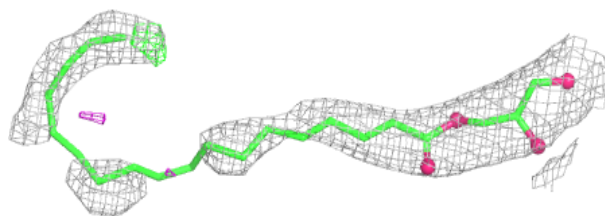


Electron density around OLC A 401:

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

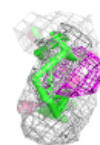
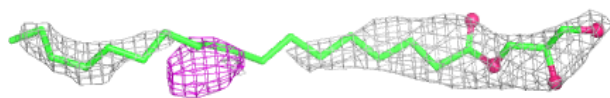
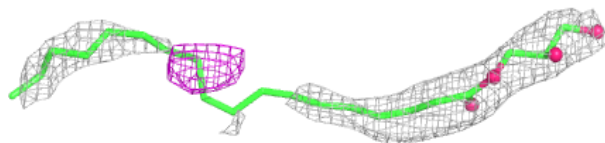
**Electron density around OLC A 402:**

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

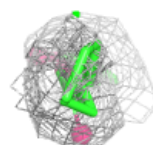
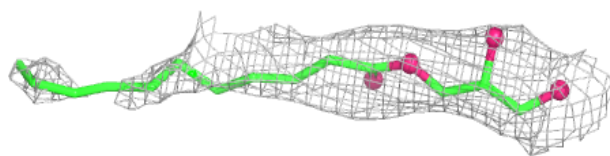
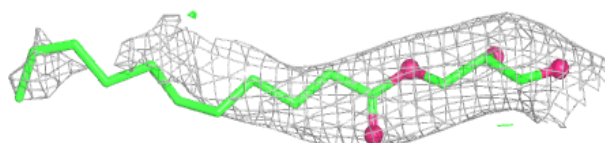


Electron density around OLC B 402:

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

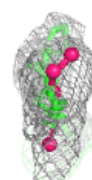
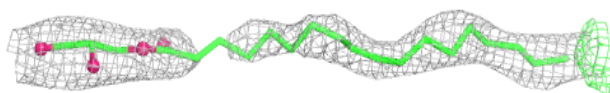
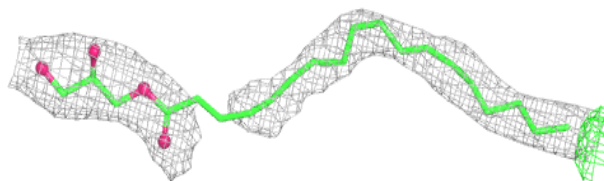
**Electron density around OLC A 403:**

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

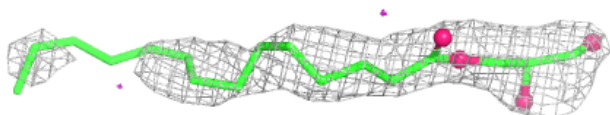
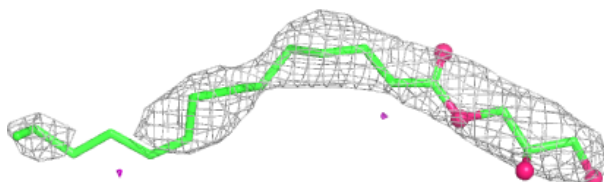


Electron density around OLC B 401:

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

**Electron density around OLC B 403:**

$2mF_o-DF_c$ (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.