



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:53 am BST

PDB ID : 6EIG  
Title : Crystal structure of N24Q/C128T mutant of Channelrhodopsin 2  
Authors : Kovalev, K.; Borshchevskiy, V.; Volkov, O.; Polovinkin, V.; Marin, E.; Balandin, T.; Astashkin, R.; Bamann, C.; Bueldt, G.; Willbold, D.; Popov, A.; Bamberg, E.; Gordeliy, V.  
Deposited on : 2017-09-19  
Resolution : 2.70 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 : 2.11  
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) : 2.11

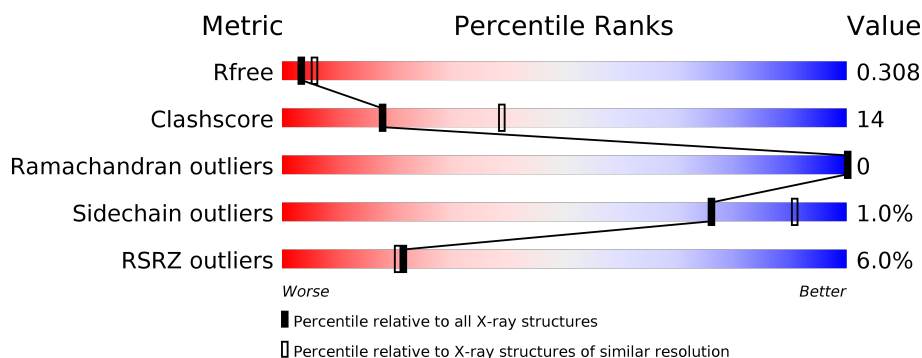
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	315	<div> <div>6%</div> <div> <div></div> <div>61%</div> <div>18%</div> <div>21%</div> </div> </div>
1	B	315	<div> <div>4%</div> <div> <div></div> <div>62%</div> <div>17%</div> <div>21%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4104 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.

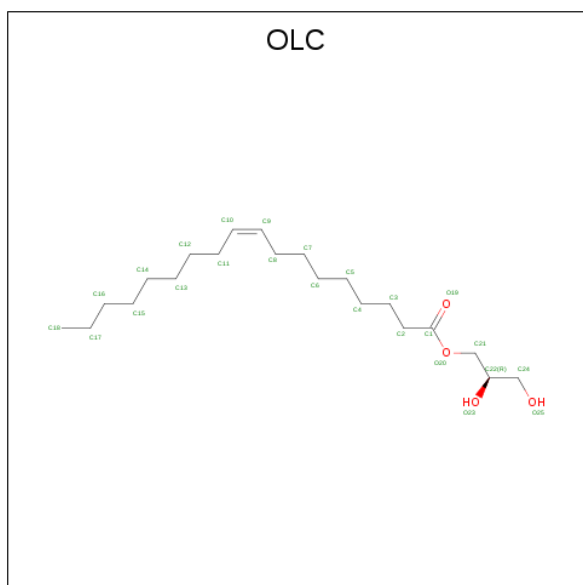
- Molecule 1 is a protein called Archaeal-type opsin 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1967	1310	312	330	15			
1	B	250	Total	C	N	O	S	0	0	0
			1971	1310	314	332	15			

There are 4 discrepancies between the modelled and reference sequences:

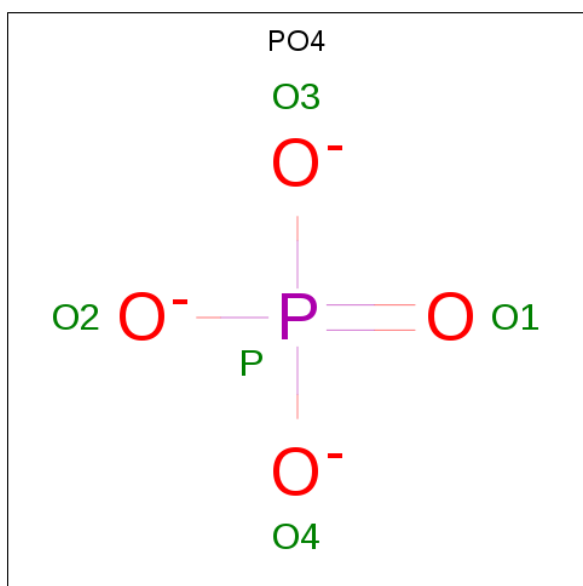
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLN	ASN	engineered mutation	UNP Q8RUT8
A	128	THR	CYS	engineered mutation	UNP Q8RUT8
B	24	GLN	ASN	engineered mutation	UNP Q8RUT8
B	128	THR	CYS	engineered mutation	UNP Q8RUT8

- Molecule 2 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



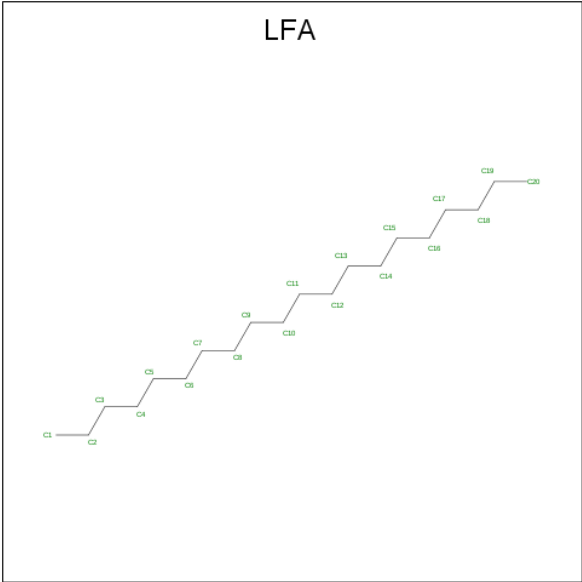
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 16 12 4	0	0
2	A	1	Total C O 17 14 3	0	0
2	A	1	Total C O 15 14 1	0	0
2	A	1	Total C 12 12	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C O 16 12 4	0	0
2	B	1	Total C O 19 15 4	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

- Molecule 4 is EICOSANE (three-letter code: LFA) (formula: C<sub>20</sub>H<sub>42</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	0
			15	15		
4	A	1	Total	C	0	0
			4	4		

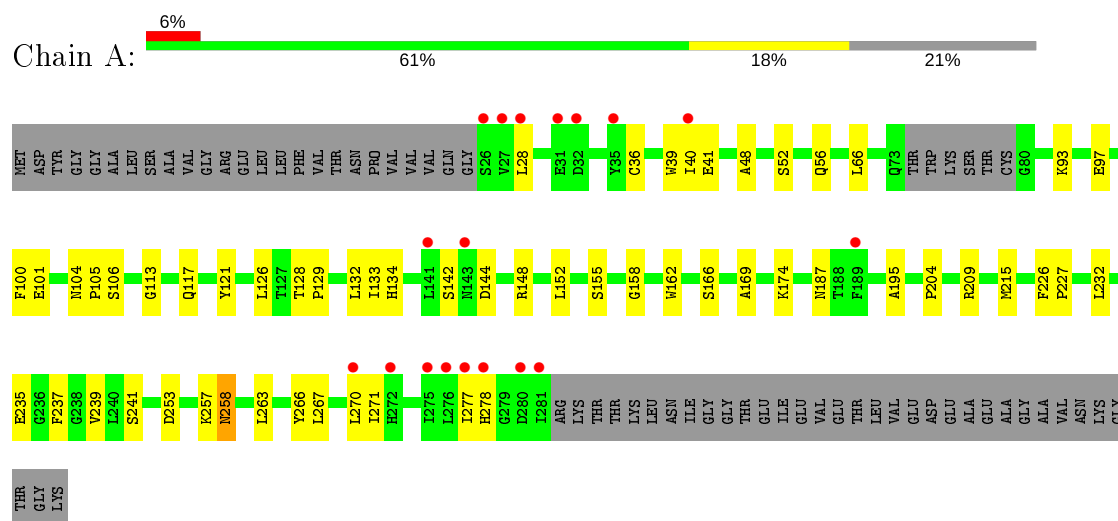
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	17	Total	O	0	0
			17	17		
5	B	16	Total	O	0	0
			16	16		

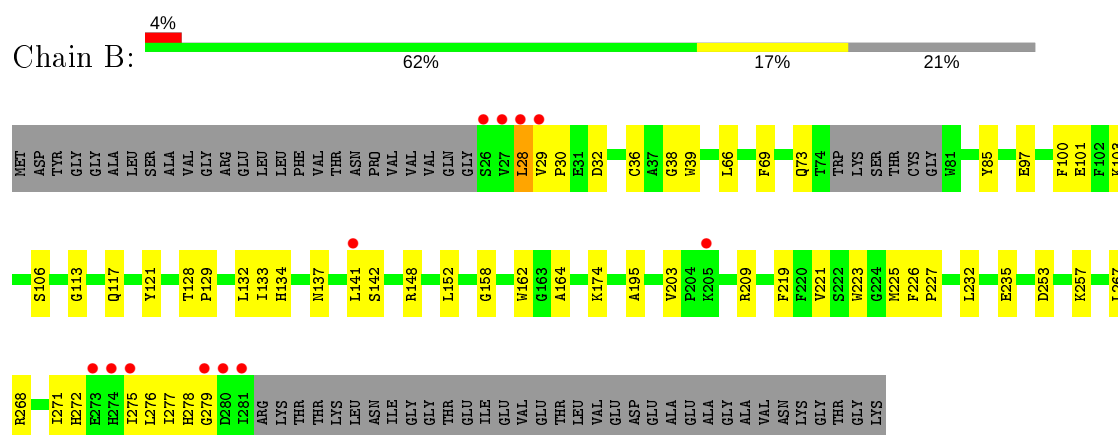
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Archaeal-type opsin 2



#### • Molecule 1: Archaeal-type opsin 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.51Å 134.06Å 78.47Å 90.00° 90.22° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 46.79 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.7 (20.00-2.70) 95.1 (46.79-2.70)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.265 , 0.297 0.273 , 0.308	Depositor DCC
$R_{free}$ test set	862 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.9	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 21.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.408 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4104	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.57% 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: PO4, OLC, LFA, 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	0.26	0/1996	0.35	0/2720
1	B	0.26	0/1999	0.35	0/2723
All	All	0.26	0/3995	0.35	0/5443

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	1967	0	1918	56	0
1	B	1971	0	1933	53	0
2	A	60	0	85	7	14
2	B	44	0	58	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	19	0	33	0	14
5	A	17	0	0	4	0
5	B	16	0	0	3	0
All	All	4104	0	4027	110	14

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 14.

All (110) 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:B:257:LYR:H9	1:B:257:LYR:H192	1.38	1.01
1:B:235:GLU:OE1	5:B:1201:HOH:O	1.79	1.00
1:A:257:LYR:H9	1:A:257:LYR:H192	1.40	0.98
1:B:257:LYR:H192	1:B:257:LYR:C9	2.06	0.84
1:A:257:LYR:C9	1:A:257:LYR:H192	2.07	0.84
1:B:174:LYS:HE2	1:B:235:GLU:O	1.78	0.83
1:B:36:CYS:SG	1:B:113:GLY:HA2	2.17	0.83
1:B:117:GLN:OE1	5:B:1201:HOH:O	1.99	0.80
1:A:128:THR:OG1	1:A:129:PRO:HD3	1.81	0.80
1:B:128:THR:OG1	1:B:129:PRO:HD3	1.83	0.78
1:A:253:ASP:O	1:A:257:LYR:HB3	1.86	0.74
1:A:166:SER:O	1:A:174:LYS:HE2	1.90	0.71
1:A:48:ALA:HB2	2:A:1102:OLC:H24	1.72	0.70
1:B:97:GLU:O	1:B:101:GLU:HB2	1.93	0.69
1:A:36:CYS:HB3	1:A:39:TRP:CD2	2.28	0.68
1:B:117:GLN:O	1:B:121:TYR:HD2	1.77	0.68
1:B:253:ASP:O	1:B:257:LYR:HB3	1.95	0.66
1:A:237:PHE:CE1	2:A:1101:OLC:H2A	2.31	0.65
1:A:257:LYR:H9	1:A:257:LYR:H183	1.78	0.64
1:B:36:CYS:HB3	1:B:39:TRP:CD2	2.33	0.64
1:A:36:CYS:SG	1:A:113:GLY:HA2	2.39	0.63
1:B:257:LYR:H9	1:B:257:LYR:H183	1.82	0.61
1:A:126:LEU:HD12	2:A:1103:OLC:H11	1.81	0.61
1:A:258:ASN:HD22	1:A:258:ASN:N	1.98	0.61
1:B:117:GLN:O	1:B:121:TYR:CD2	2.54	0.60
1:A:134:HIS:NE2	5:A:1203:HOH:O	2.32	0.60
1:B:272:HIS:O	1:B:276:LEU:HG	2.04	0.57
1:A:155:SER:HB3	1:A:187:ASN:HD22	1.69	0.57
1:B:277:ILE:CG2	1:B:278:HIS:CE1	2.88	0.56
1:A:277:ILE:HG22	1:A:278:HIS:CD2	2.40	0.56
1:A:257:LYR:C9	1:A:257:LYR:H183	2.35	0.56
1:A:52:SER:O	1:A:56:GLN:HG2	2.06	0.56
1:B:28:LEU:C	1:B:28:LEU:HD12	2.26	0.56
1:B:257:LYR:C19	1:B:257:LYR:H9	2.16	0.55
1:B:275:ILE:O	1:B:279:GLY:N	2.37	0.55
1:A:169:ALA:O	1:A:174:LYS:HE3	2.07	0.55
1:B:100:PHE:O	1:B:106:SER:HB3	2.08	0.54
1:A:237:PHE:CD1	2:A:1101:OLC:H2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:ILE:HG22	1:B:278:HIS:CE1	2.43	0.54
1:A:129:PRO:O	1:A:133:ILE:HG13	2.09	0.53
1:A:257:LYR:H9	1:A:257:LYR:C19	2.17	0.53
1:B:268:ARG:O	1:B:271:ILE:HG13	2.09	0.53
1:A:226:PHE:N	1:A:227:PRO:HD2	2.24	0.53
1:A:235:GLU:OE1	5:A:1201:HOH:O	2.19	0.52
1:B:257:LYR:C9	1:B:257:LYR:H183	2.38	0.52
1:B:226:PHE:N	1:B:227:PRO:HD2	2.23	0.52
1:A:134:HIS:O	1:A:134:HIS:HD2	1.92	0.52
1:A:117:GLN:O	1:A:121:TYR:HD2	1.93	0.52
1:B:271:ILE:HD12	1:B:272:HIS:N	2.26	0.51
1:A:40:ILE:HG22	1:A:40:ILE:O	2.11	0.51
1:A:241:SER:OG	2:A:1102:OLC:O25	2.26	0.50
1:A:277:ILE:CG2	1:A:278:HIS:CD2	2.94	0.50
1:B:32:ASP:OD1	1:B:32:ASP:N	2.45	0.50
1:A:257:LYR:C9	1:A:257:LYR:C19	2.78	0.50
1:B:36:CYS:HG	1:B:113:GLY:HA2	1.74	0.50
1:B:128:THR:N	1:B:129:PRO:CD	2.74	0.50
1:B:271:ILE:HD12	1:B:271:ILE:C	2.32	0.50
1:A:158:GLY:O	1:A:162:TRP:CD1	2.65	0.49
1:A:93:LYS:NZ	1:A:253:ASP:OD2	2.43	0.49
1:B:257:LYR:C19	1:B:257:LYR:C9	2.78	0.49
1:A:41:GLU:N	5:A:1208:HOH:O	2.46	0.48
2:A:1104:OLC:H9	1:B:232:LEU:HD21	1.94	0.48
1:A:117:GLN:O	1:A:121:TYR:CD2	2.66	0.48
1:A:100:PHE:O	1:A:106:SER:HB3	2.14	0.47
1:A:237:PHE:CD1	2:A:1101:OLC:C2	2.98	0.47
1:A:128:THR:N	1:A:129:PRO:CD	2.77	0.46
1:B:221:VAL:O	1:B:225:MET:HG2	2.15	0.46
1:B:203:VAL:HG23	1:B:209:ARG:HG2	1.98	0.46
1:A:134:HIS:CD2	5:A:1203:HOH:O	2.69	0.45
1:B:28:LEU:O	1:B:28:LEU:HG	2.16	0.45
1:A:36:CYS:HB3	1:A:39:TRP:CE2	2.51	0.45
1:A:267:LEU:O	1:A:271:ILE:HG12	2.17	0.45
1:B:69:PHE:O	1:B:73:GLN:HG2	2.17	0.45
1:B:36:CYS:SG	1:B:113:GLY:CA	2.99	0.45
1:A:128:THR:HG1	1:A:129:PRO:HD3	1.80	0.45
1:A:28:LEU:C	1:A:28:LEU:HD12	2.38	0.45
1:B:100:PHE:O	1:B:106:SER:CB	2.65	0.45
1:B:134:HIS:O	1:B:134:HIS:HD2	2.00	0.44
1:A:204:PRO:O	1:A:209:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:TYR:CD1	1:B:164:ALA:HB2	2.53	0.44
1:A:132:LEU:HD13	1:A:152:LEU:HG	2.00	0.44
1:A:148:ARG:NH1	1:A:195:ALA:HA	2.33	0.44
1:A:232:LEU:O	1:A:239:VAL:N	2.51	0.44
1:A:215:MET:HG2	1:A:263:LEU:HB3	1.99	0.43
2:B:1101:OLC:H11	2:B:1101:OLC:H8A	1.83	0.43
1:B:137:ASN:ND2	1:B:142:SER:O	2.35	0.43
1:A:97:GLU:O	1:A:101:GLU:HB2	2.18	0.43
1:A:134:HIS:CD2	1:A:134:HIS:O	2.72	0.43
1:B:132:LEU:HD13	1:B:152:LEU:HG	2.00	0.43
1:A:257:LYR:H10	1:A:257:LYR:H81	1.85	0.42
1:B:267:LEU:O	1:B:271:ILE:HG23	2.19	0.42
1:A:36:CYS:SG	1:A:113:GLY:CA	3.08	0.42
1:A:142:SER:HB2	1:A:144:ASP:OD1	2.19	0.42
1:B:257:LYR:H10	1:B:257:LYR:H81	1.85	0.42
1:B:219:PHE:O	1:B:223:TRP:HB2	2.20	0.42
1:B:85:TYR:OH	5:B:1202:HOH:O	2.16	0.41
1:B:134:HIS:CD2	1:B:134:HIS:O	2.73	0.41
1:B:38:GLY:HA3	1:B:113:GLY:O	2.20	0.41
1:B:235:GLU:CD	1:B:235:GLU:H	2.22	0.41
1:B:158:GLY:O	1:B:162:TRP:CD1	2.74	0.41
1:A:104:ASN:HA	1:A:105:PRO:HA	1.79	0.41
1:A:36:CYS:HB3	1:A:39:TRP:CE3	2.55	0.41
1:A:121:TYR:CD2	1:A:121:TYR:N	2.88	0.41
1:A:169:ALA:O	1:A:174:LYS:CE	2.68	0.41
1:A:266:TYR:CE2	1:A:270:LEU:HD11	2.56	0.41
1:B:148:ARG:NH1	1:B:195:ALA:HA	2.35	0.41
1:B:103:LYS:O	1:B:106:SER:HB3	2.21	0.41
1:B:129:PRO:O	1:B:133:ILE:HG13	2.21	0.40
1:B:141:LEU:HD21	1:B:271:ILE:HD13	2.03	0.40
1:B:29:VAL:HA	1:B:30:PRO:HD3	1.97	0.40

All (14) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1103:OLC:C3	4:A:1106:LFA:C6[2_555]	1.01	1.19
2:A:1103:OLC:C7	4:A:1106:LFA:C10[2_555]	1.04	1.16
2:A:1103:OLC:C5	4:A:1106:LFA:C7[2_555]	1.81	0.39
2:A:1103:OLC:C7	4:A:1106:LFA:C12[2_555]	1.81	0.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1103:OLC:C8	4:A:1106:LFA:C11[2_555]	1.85	0.35
2:A:1103:OLC:C8	4:A:1106:LFA:C12[2_555]	1.85	0.35
2:A:1103:OLC:C9	4:A:1106:LFA:C11[2_555]	1.91	0.29
2:A:1103:OLC:C10	4:A:1106:LFA:C12[2_555]	1.99	0.21
2:A:1103:OLC:C12	4:A:1106:LFA:C15[2_555]	2.12	0.08
2:A:1103:OLC:C10	4:A:1106:LFA:C13[2_555]	2.12	0.08
2:A:1103:OLC:C9	4:A:1106:LFA:C13[2_555]	2.13	0.07
2:A:1103:OLC:C4	4:A:1106:LFA:C6[2_555]	2.14	0.06
2:A:1103:OLC:C7	4:A:1106:LFA:C9[2_555]	2.14	0.06
2:A:1103:OLC:C8	4:A:1106:LFA:C10[2_555]	2.18	0.02

## 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	245/315 (78%)	239 (98%)	6 (2%)	0	100	100
1	B	245/315 (78%)	240 (98%)	5 (2%)	0	100	100
All	All	490/630 (78%)	479 (98%)	11 (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	196/258 (76%)	194 (99%)	2 (1%)	76	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	199/258 (77%)	197 (99%)	2 (1%)	76	91
All	All	395/516 (77%)	391 (99%)	4 (1%)	76	91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LEU
1	A	258	ASN
1	B	28	LEU
1	B	66	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	49	GLN
1	A	73	GLN
1	A	114	HIS
1	A	134	HIS
1	A	187	ASN
1	A	258	ASN
1	A	265	HIS
1	A	278	HIS
1	B	33	GLN
1	B	49	GLN
1	B	114	HIS
1	B	134	HIS

### 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	B	257	1	27,29,30	0.60	0	30,37,39	2.05	8 (26%)
1	LYR	A	257	1	27,29,30	0.62	0	30,37,39	2.05	8 (26%)

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	B	257	1	-	4/22/40/42	0/1/1/1
1	LYR	A	257	1	-	4/22/40/42	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	257	LYR	C13-C12-C11	-5.19	118.70	124.53
1	A	257	LYR	C13-C12-C11	-5.15	118.75	124.53
1	A	257	LYR	C1-NZ-CE	5.08	121.39	113.33
1	B	257	LYR	C1-NZ-CE	5.05	121.33	113.33
1	B	257	LYR	C6-C7-C80	-3.52	122.28	127.31
1	A	257	LYR	C6-C7-C80	-3.47	122.35	127.31
1	B	257	LYR	C10-C9-C80	-3.29	121.26	126.23
1	A	257	LYR	C10-C9-C80	-3.26	121.31	126.23
1	A	257	LYR	C1-C2-C3	-2.78	121.63	126.97
1	B	257	LYR	C1-C2-C3	-2.78	121.64	126.97
1	A	257	LYR	C9-C10-C11	-2.74	119.51	127.20
1	B	257	LYR	C9-C10-C11	-2.70	119.62	127.20
1	A	257	LYR	C13-C12-C14	2.52	118.45	113.62
1	B	257	LYR	C13-C12-C14	2.50	118.42	113.62
1	A	257	LYR	C15-C14-C12	-2.14	110.26	114.08
1	B	257	LYR	C15-C14-C12	-2.11	110.31	114.08

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	257	LYR	N-CA-CB-CG
1	B	257	LYR	C-CA-CB-CG
1	B	257	LYR	CD-CE-NZ-C1
1	A	257	LYR	N-CA-CB-CG
1	A	257	LYR	C-CA-CB-CG
1	A	257	LYR	CD-CE-NZ-C1
1	B	257	LYR	CE-CD-CG-CB
1	A	257	LYR	CE-CD-CG-CB

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	257	LYR	8	0
1	A	257	LYR	8	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

11 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	1102	-	16,16,24	0.37	0	16,16,25	0.84	0
2	OLC	B	1102	-	15,15,24	1.16	1 (6%)	16,16,25	0.99	1 (6%)
3	PO4	B	1104	-	4,4,4	0.91	0	6,6,6	0.43	0
2	OLC	B	1101	-	8,8,24	0.27	0	7,7,25	0.49	0
4	LFA	A	1107	-	3,3,19	0.38	0	2,2,18	0.63	0
2	OLC	A	1104	-	11,11,24	0.28	0	9,10,25	0.57	0
2	OLC	A	1103	4	14,14,24	0.53	0	12,13,25	0.86	0
3	PO4	A	1105	-	4,4,4	0.92	0	6,6,6	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OLC	A	1101	-	15,15,24	1.16	1 (6%)	16,16,25	0.98	1 (6%)
2	OLC	B	1103	-	18,18,24	1.06	1 (5%)	18,19,25	0.96	1 (5%)
4	LFA	A	1106	2	14,14,19	0.26	0	13,13,18	0.58	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	1102	-	-	9/15/15/24	-
2	OLC	B	1102	-	-	7/15/15/24	-
2	OLC	B	1101	-	-	2/6/6/24	-
4	LFA	A	1107	-	-	1/1/1/17	-
2	OLC	A	1104	-	-	4/9/9/24	-
2	OLC	A	1103	4	-	5/12/12/24	-
2	OLC	A	1101	-	-	7/15/15/24	-
2	OLC	B	1103	-	-	8/18/18/24	-
4	LFA	A	1106	2	-	8/12/12/17	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	OLC	O20-C1	4.31	1.45	1.33
2	B	1102	OLC	O20-C1	4.30	1.45	1.33
2	B	1103	OLC	O20-C1	4.28	1.45	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1103	OLC	O20-C1-C2	2.67	120.29	111.91
2	B	1102	OLC	O20-C1-C2	2.66	120.27	111.91
2	A	1101	OLC	O20-C1-C2	2.62	120.12	111.91

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1102	OLC	C21-C22-C24-O25

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Mol	Chain	Res	Type	Atoms
4	A	1107	LFA	C10-C11-C12-C13
2	A	1103	OLC	C9-C10-C11-C12
2	B	1103	OLC	C9-C10-C11-C12
2	B	1102	OLC	C2-C1-O20-C21
2	B	1102	OLC	O19-C1-O20-C21
2	A	1101	OLC	C2-C1-O20-C21
2	A	1101	OLC	O20-C21-C22-O23
2	A	1101	OLC	O19-C1-O20-C21
2	B	1103	OLC	C1-C2-C3-C4
2	A	1102	OLC	O20-C1-C2-C3
2	A	1104	OLC	C10-C11-C12-C13
2	A	1101	OLC	C4-C5-C6-C7
2	B	1103	OLC	C4-C5-C6-C7
4	A	1106	LFA	C5-C6-C7-C8
4	A	1106	LFA	C3-C4-C5-C6
2	A	1102	OLC	C2-C3-C4-C5
2	A	1102	OLC	O23-C22-C24-O25
2	A	1103	OLC	C1-C2-C3-C4
2	B	1102	OLC	C4-C5-C6-C7
2	A	1103	OLC	C6-C7-C8-C9
4	A	1106	LFA	C7-C8-C9-C10
2	B	1102	OLC	C3-C4-C5-C6
2	B	1103	OLC	C3-C4-C5-C6
2	A	1104	OLC	C12-C13-C14-C15
2	A	1102	OLC	C6-C7-C8-C9
2	A	1102	OLC	C22-C21-O20-C1
2	B	1103	OLC	C2-C1-O20-C21
4	A	1106	LFA	C9-C10-C11-C12
2	B	1103	OLC	O23-C22-C24-O25
2	B	1103	OLC	O19-C1-O20-C21
4	A	1106	LFA	C11-C12-C13-C14
2	A	1102	OLC	C3-C4-C5-C6
2	A	1101	OLC	C2-C3-C4-C5
2	A	1101	OLC	C5-C6-C7-C8
4	A	1106	LFA	C11-C10-C9-C8
2	B	1102	OLC	O20-C21-C22-C24
2	A	1101	OLC	O20-C21-C22-C24
2	A	1104	OLC	C13-C14-C15-C16
4	A	1106	LFA	C10-C11-C12-C13
2	B	1101	OLC	C6-C7-C8-C9
2	B	1102	OLC	C6-C7-C8-C9
2	A	1103	OLC	C22-C21-O20-C1

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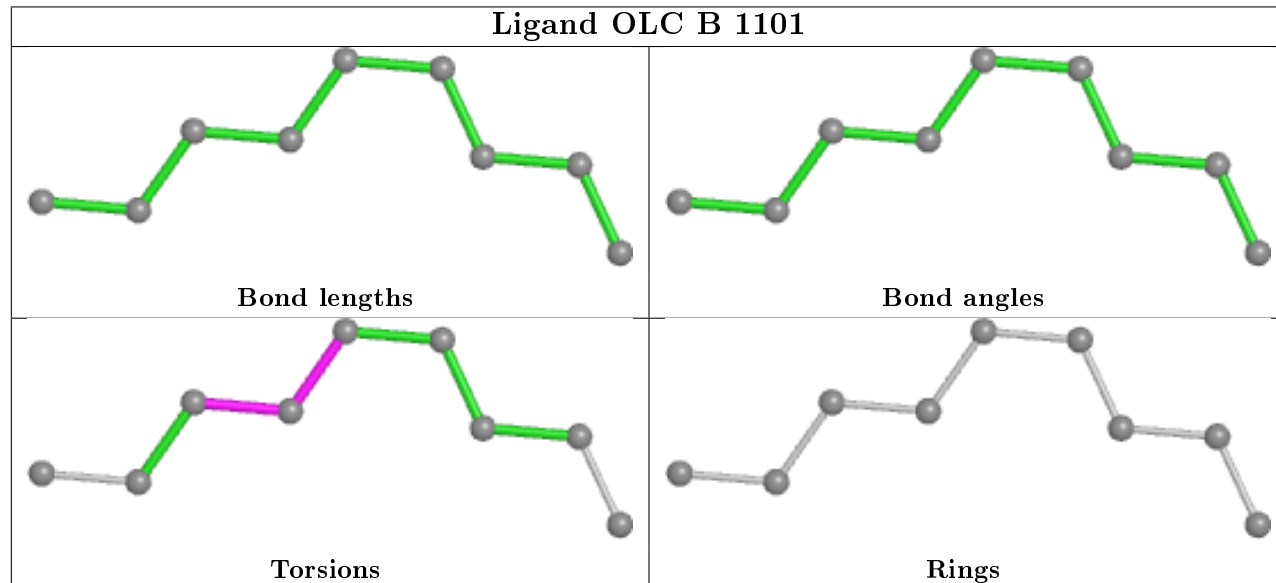
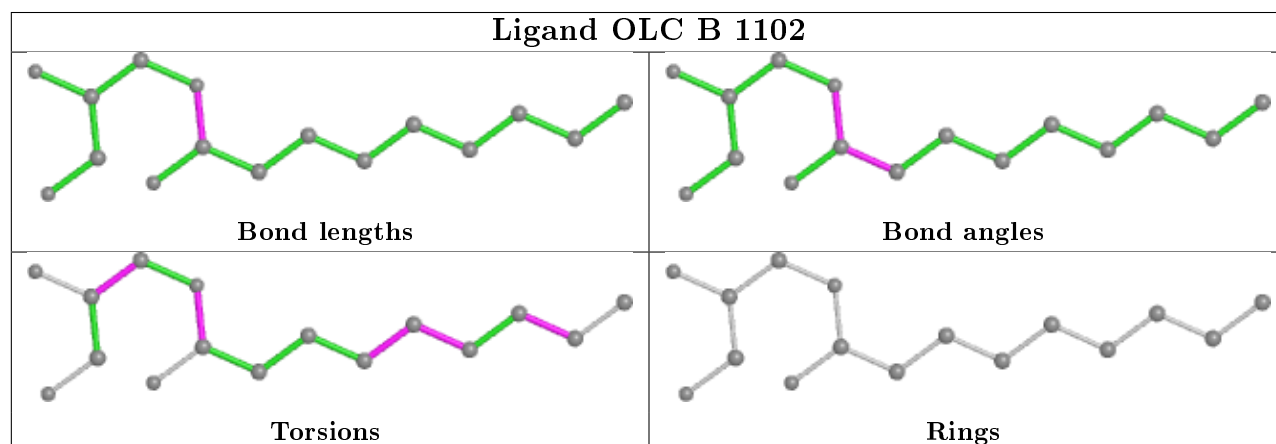
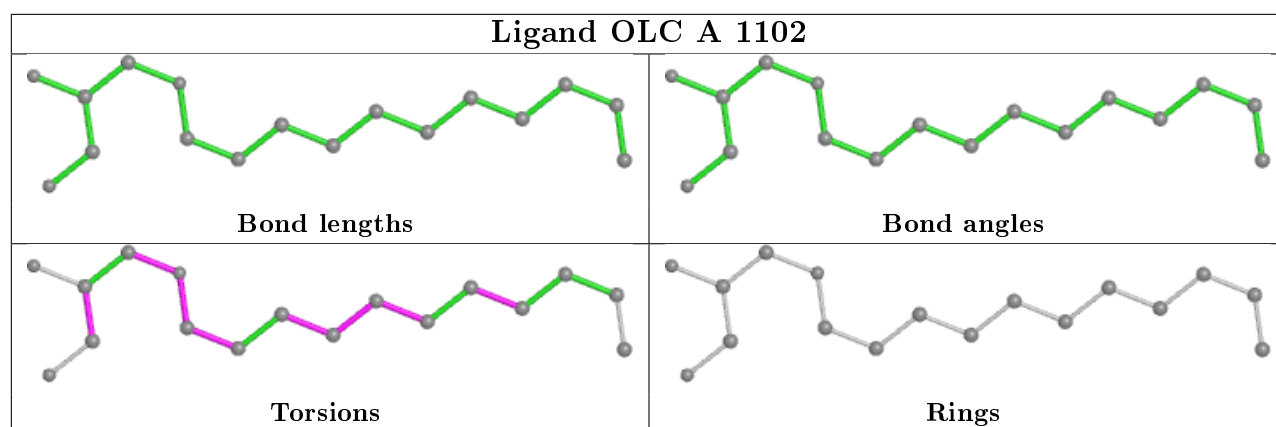
Mol	Chain	Res	Type	Atoms
2	B	1102	OLC	O20-C21-C22-O23
2	A	1104	OLC	C9-C10-C11-C12
4	A	1106	LFA	C4-C5-C6-C7
2	B	1103	OLC	C21-C22-C24-O25
2	A	1102	OLC	C2-C1-O20-C21
2	A	1103	OLC	O20-C1-C2-C3
2	A	1102	OLC	C4-C5-C6-C7
2	B	1101	OLC	C7-C8-C9-C10

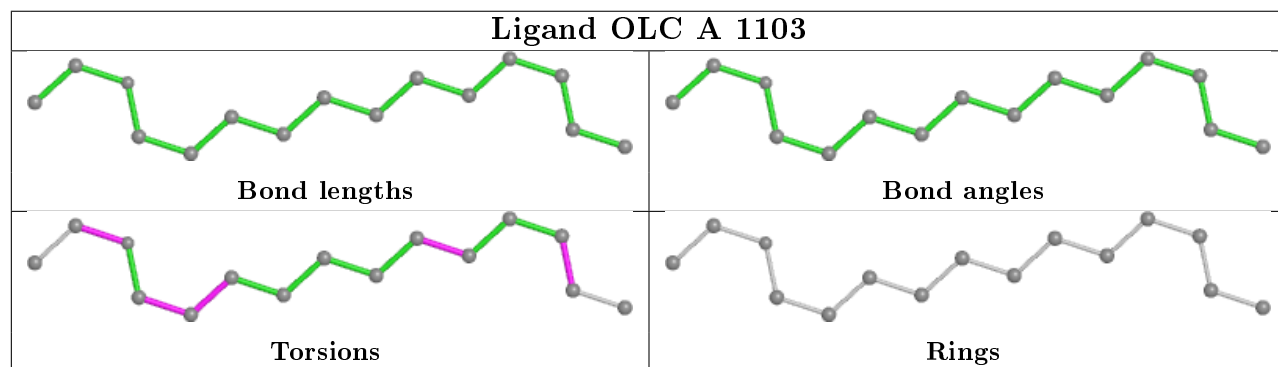
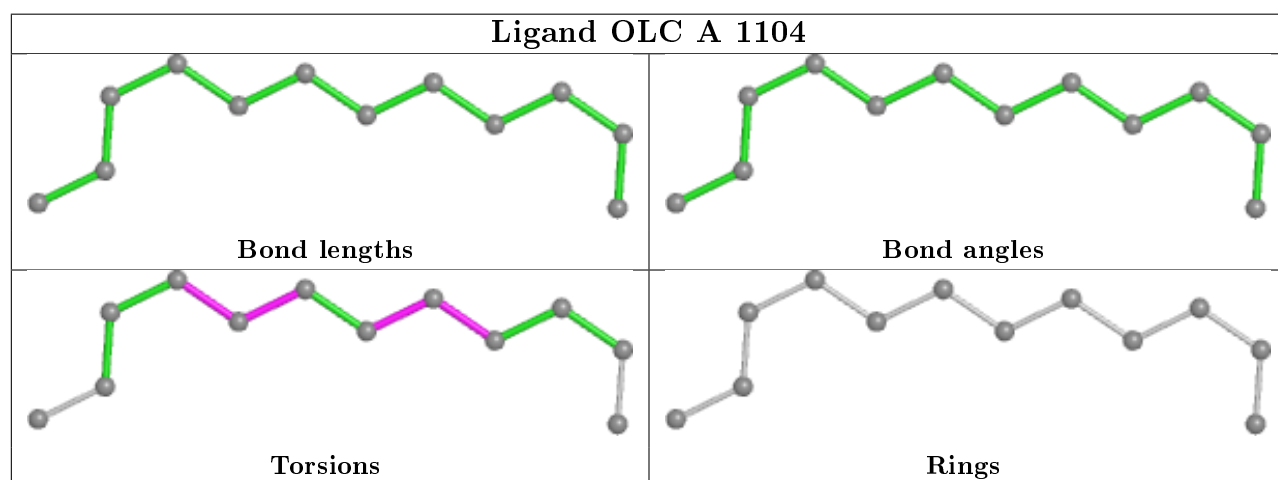
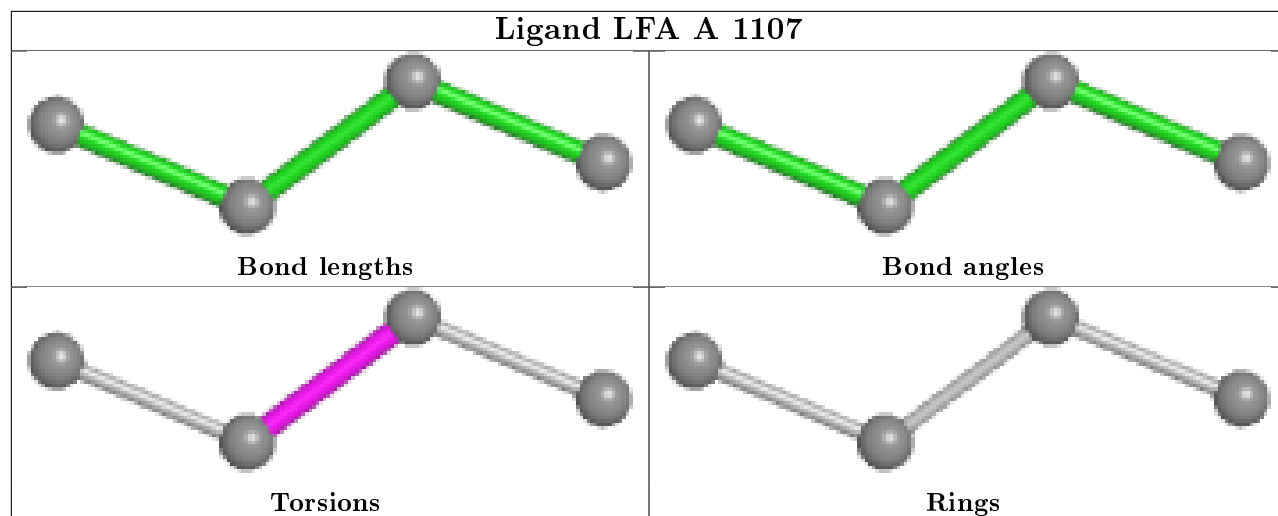
There are no ring outliers.

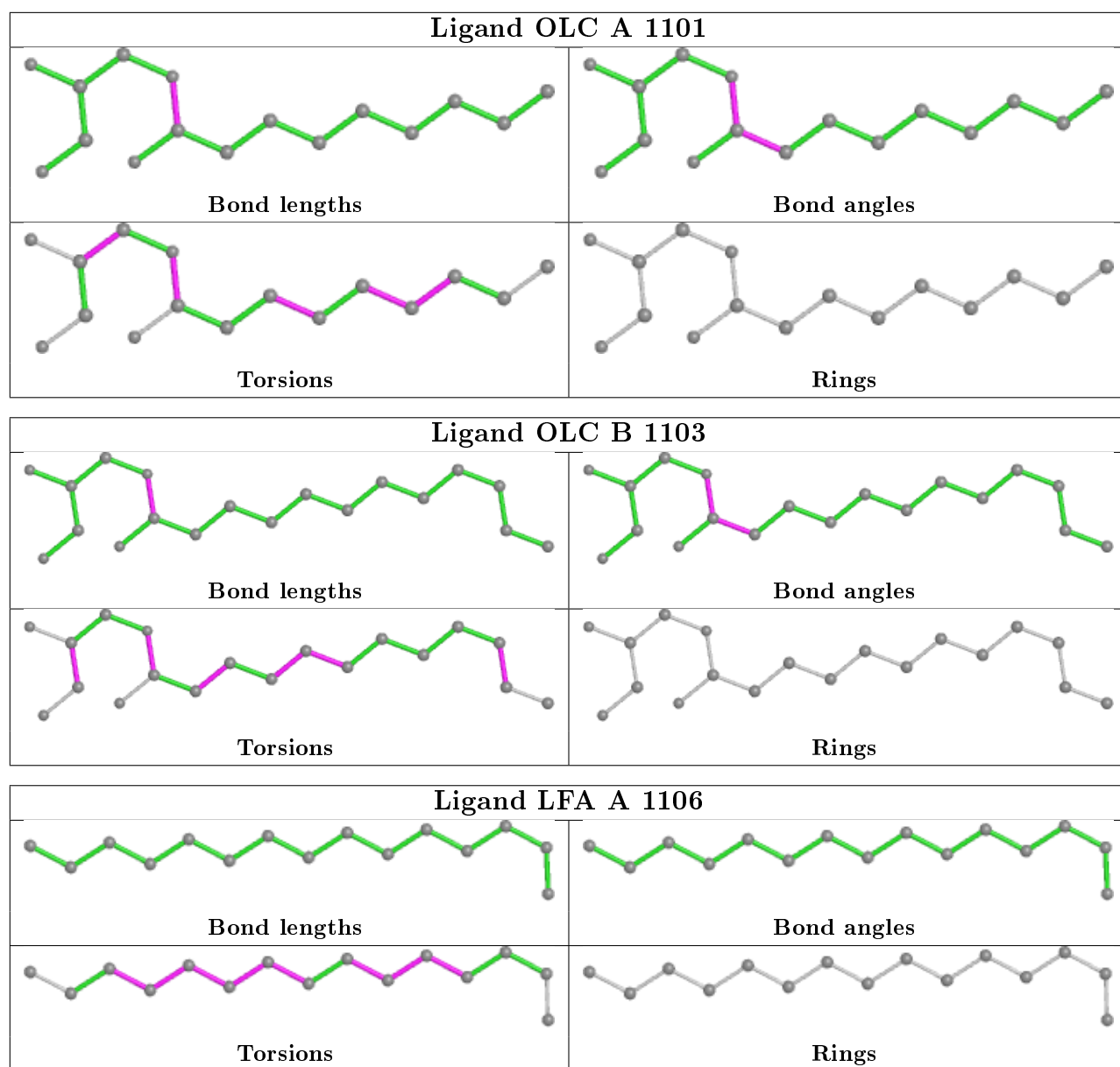
6 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1102	OLC	2	0
2	B	1101	OLC	1	0
2	A	1104	OLC	1	0
2	A	1103	OLC	1	14
2	A	1101	OLC	3	0
4	A	1106	LFA	0	14

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	249/315 (79%)	0.10	18 (7%) 15 13	32, 62, 90, 126	0
1	B	249/315 (79%)	0.05	12 (4%) 30 28	33, 63, 100, 122	0
All	All	498/630 (79%)	0.07	30 (6%) 21 20	32, 63, 95, 126	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	280	ASP	10.8
1	B	281	ILE	6.9
1	A	281	ILE	6.2
1	A	280	ASP	5.9
1	A	141	LEU	5.3
1	A	275	ILE	5.0
1	A	26	SER	4.6
1	B	26	SER	4.4
1	B	28	LEU	4.2
1	B	279	GLY	4.1
1	A	27	VAL	4.1
1	A	28	LEU	4.0
1	A	40	ILE	4.0
1	B	29	VAL	4.0
1	A	276	LEU	3.5
1	B	275	ILE	3.5
1	B	27	VAL	2.9
1	A	270	LEU	2.8
1	A	143	ASN	2.7
1	B	205	LYS	2.6
1	A	277	ILE	2.6
1	A	272	HIS	2.5
1	A	278	HIS	2.4
1	B	274	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	273	GLU	2.4
1	B	141	LEU	2.3
1	A	32	ASP	2.2
1	A	35	TYR	2.2
1	A	31	GLU	2.1
1	A	189	PHE	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, 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
1	LYR	A	257	29/30	0.92	0.21	52,67,78,85	0
1	LYR	B	257	29/30	0.94	0.19	56,64,76,76	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 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.

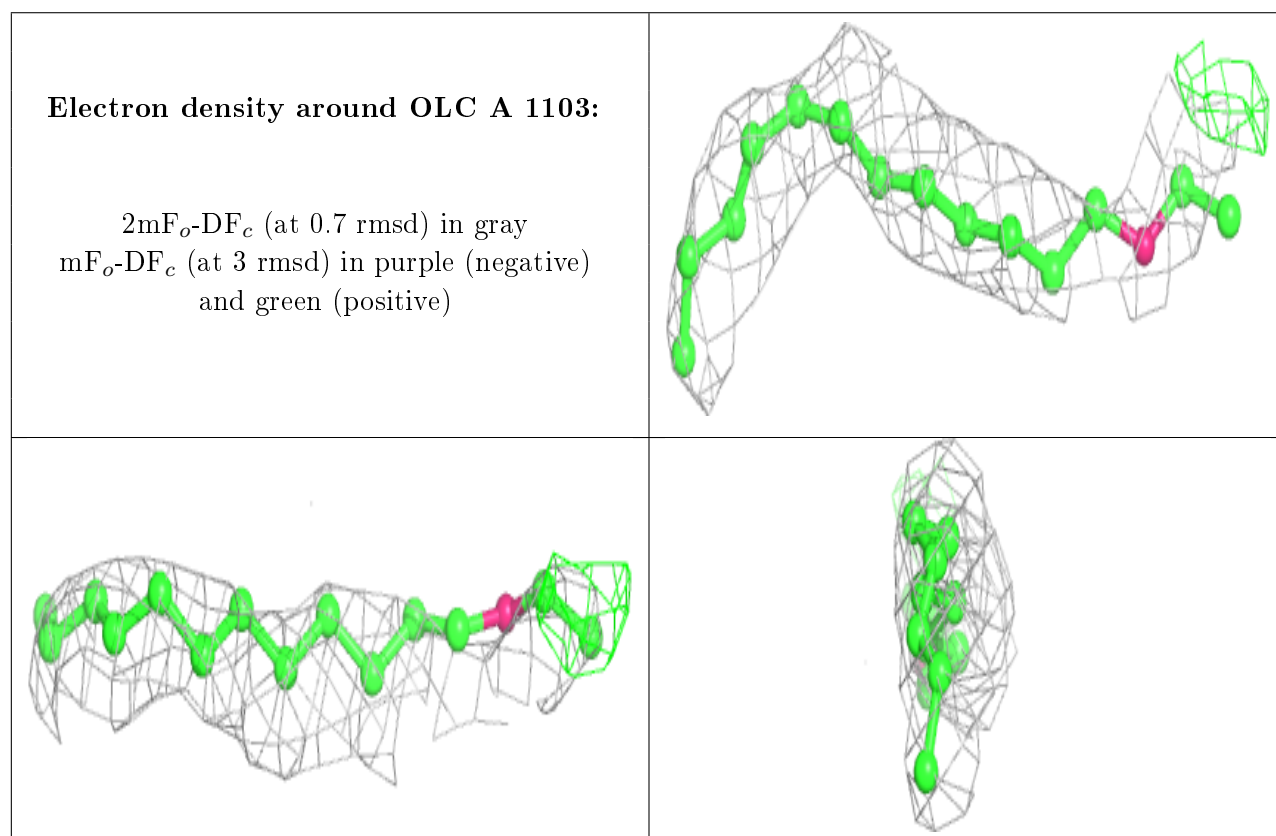
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	OLC	A	1103	15/25	0.82	0.38	93,112,162,170	0
2	OLC	A	1104	12/25	0.84	0.68	69,74,92,94	0
2	OLC	A	1101	16/25	0.88	0.22	57,83,119,131	0
4	LFA	A	1106	15/20	0.89	0.53	166,222,263,270	0
2	OLC	A	1102	17/25	0.91	0.29	69,77,89,91	0
2	OLC	B	1102	16/25	0.91	0.28	65,89,96,101	0
2	OLC	B	1103	19/25	0.92	0.27	59,70,104,115	0
3	PO4	A	1105	5/5	0.93	0.12	94,102,107,119	0
2	OLC	B	1101	9/25	0.93	0.23	37,57,63,65	0
3	PO4	B	1104	5/5	0.94	0.11	102,102,114,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	LFA	A	1107	4/20	0.97	0.15	28,28,29,31	0

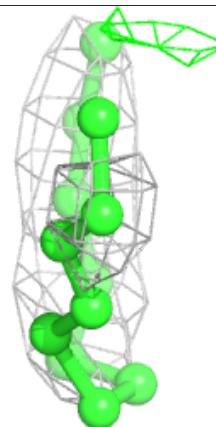
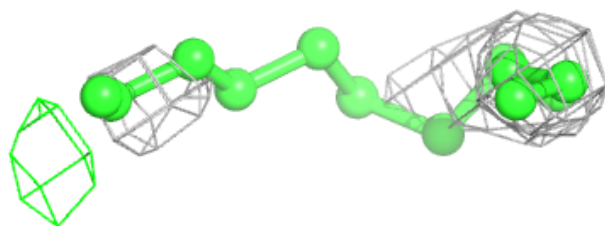
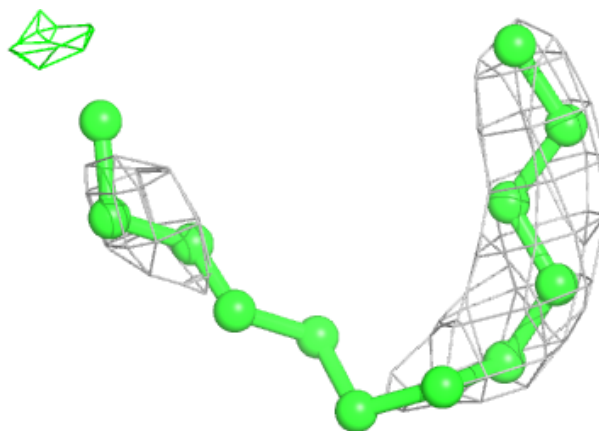
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



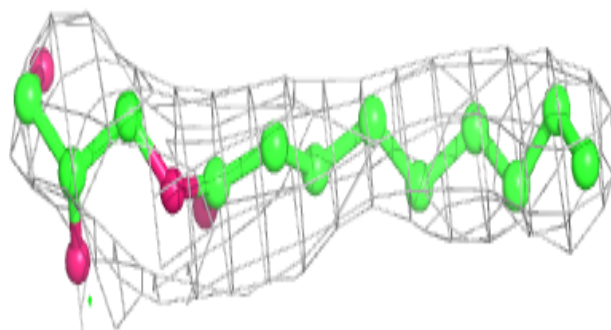
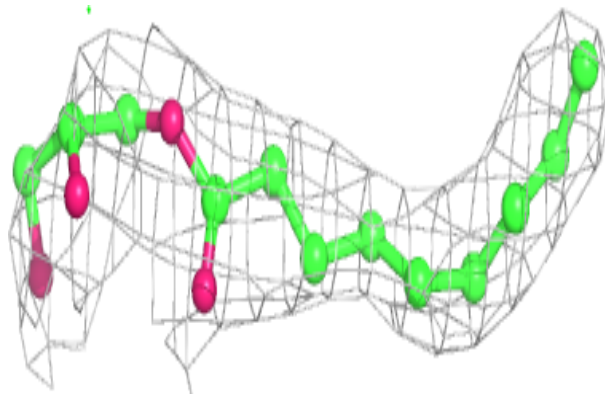


**Electron density around OLC A 1104:**

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

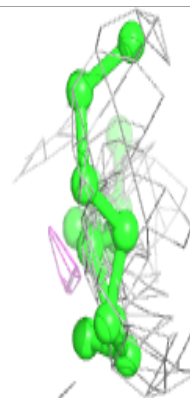
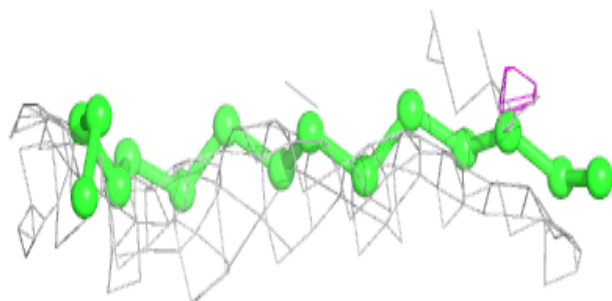
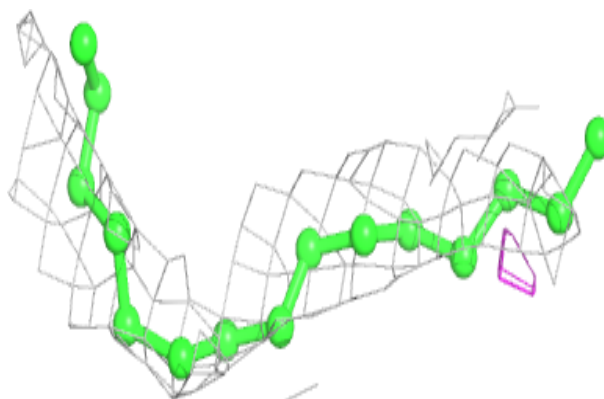
**Electron density around OLC A 1101:**

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

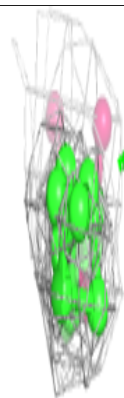
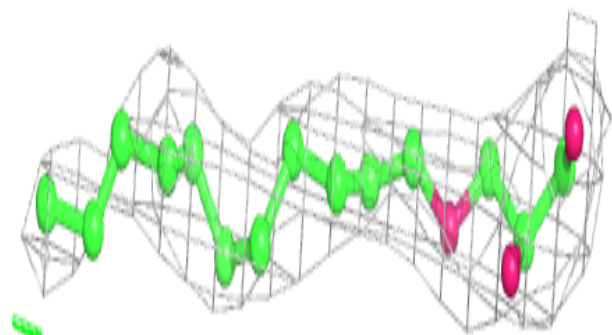
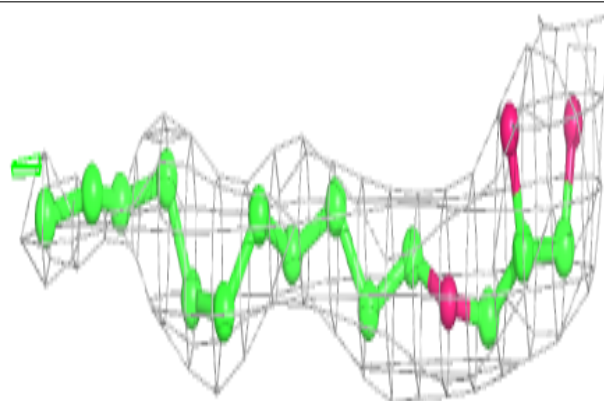


**Electron density around LFA A 1106:**

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

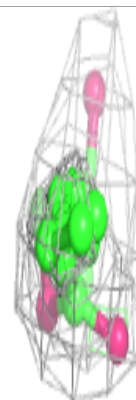
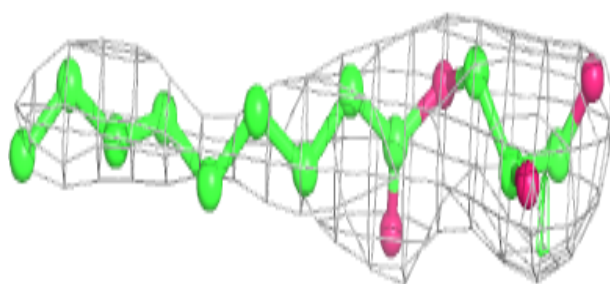
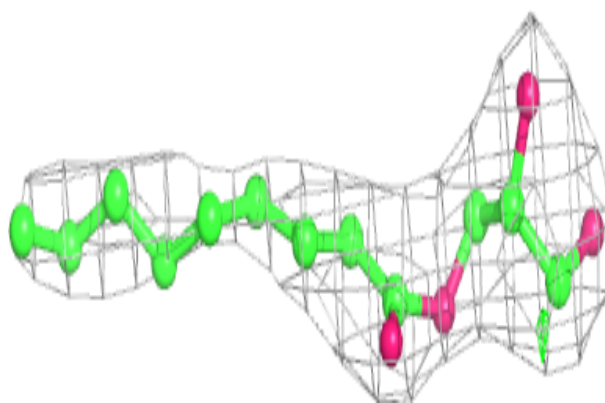
**Electron density around OLC A 1102:**

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

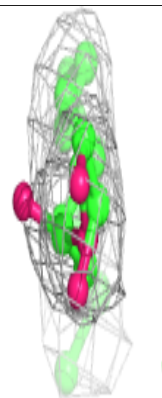
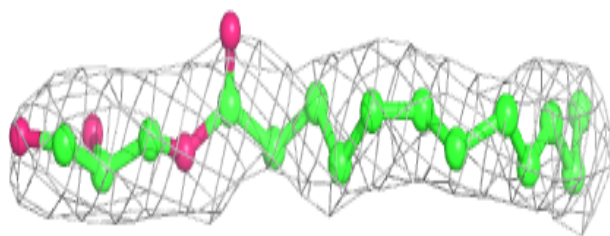
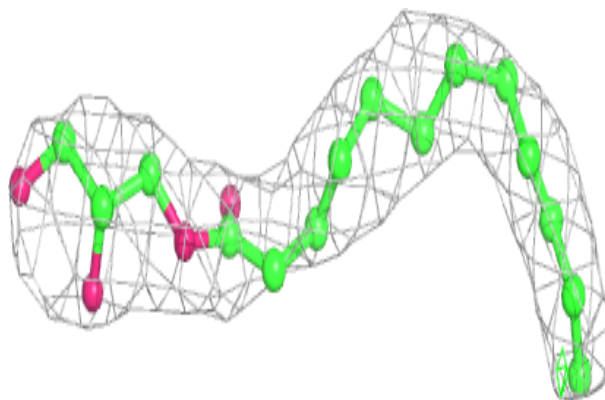


**Electron density around OLC B 1102:**

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

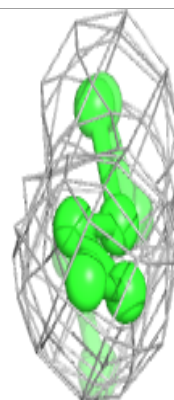
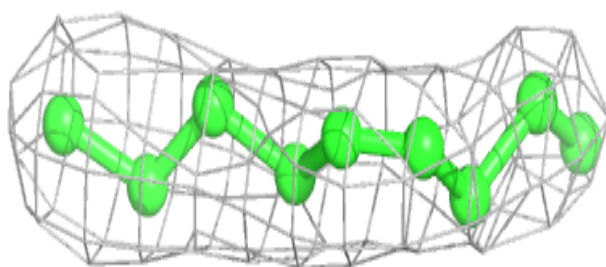
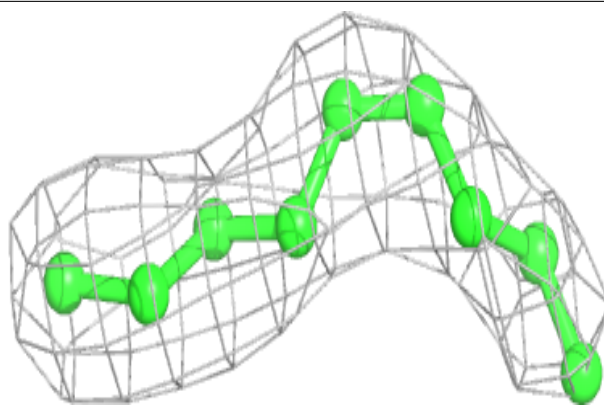
**Electron density around OLC B 1103:**

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

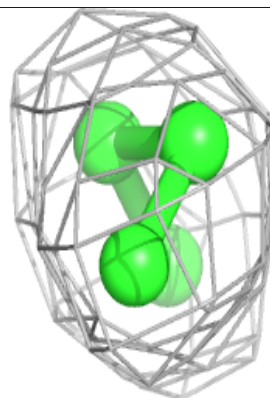
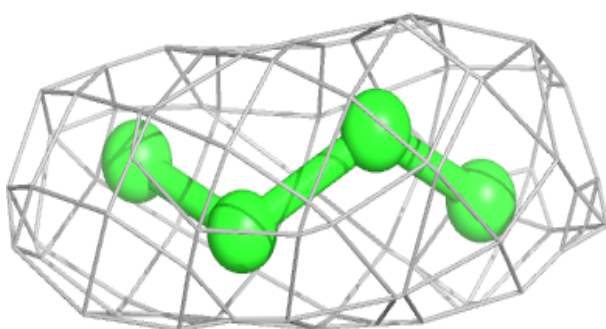
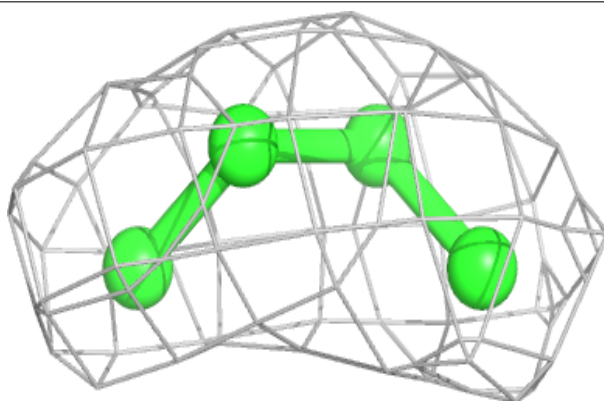


**Electron density around OLC B 1101:**

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

**Electron density around LFA A 1107:**

$2mF_o-DF_c$  (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.