



Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2021 – 04:08 pm BST

PDB ID : 7B0O
Title : In meso structure of the membrane integral lipoprotein intramolecular transacylase Lit from Bacillus cereus in space group P21
Authors : Huang, C.-Y.; Olatunji, S.; Olieric, V.; Caffrey, M.
Deposited on : 2020-11-20
Resolution : 2.33 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

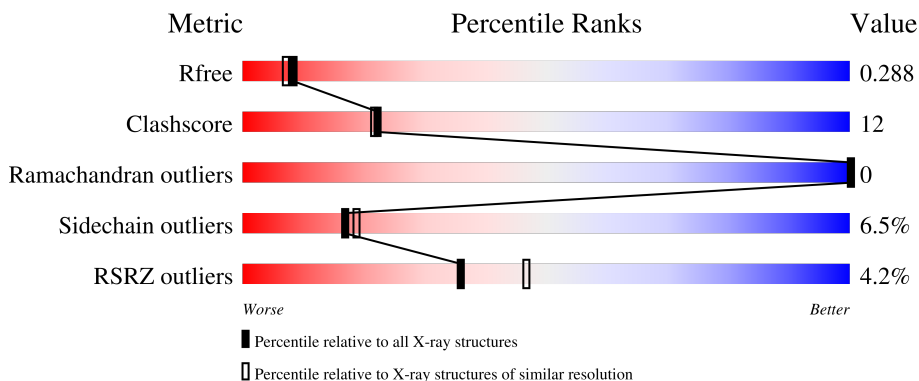
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	237	 4% 64% 26% • 9%
1	B	237	 3% 65% 22% • 11%

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
2	OLC	A	312	-	-	-	X

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 3911 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 Hypothetical Membrane Spanning Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	216	1771	1195	269	296	11	0	0	0
1	B	211	1723	1163	260	289	11	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

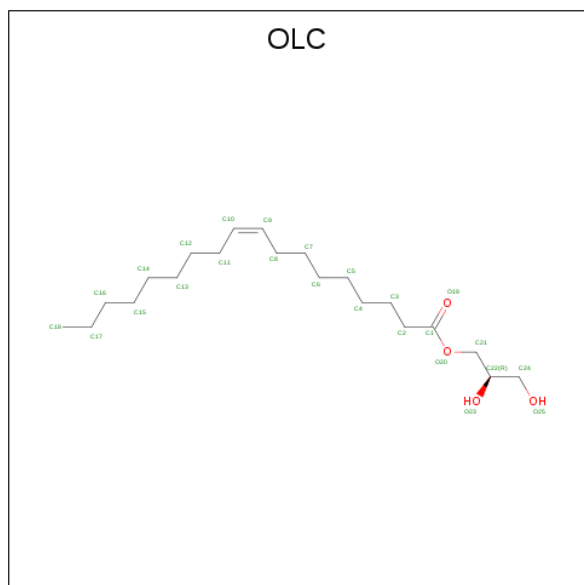
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q813T3
A	-18	HIS	-	expression tag	UNP Q813T3
A	-17	HIS	-	expression tag	UNP Q813T3
A	-16	HIS	-	expression tag	UNP Q813T3
A	-15	HIS	-	expression tag	UNP Q813T3
A	-14	HIS	-	expression tag	UNP Q813T3
A	-13	HIS	-	expression tag	UNP Q813T3
A	-12	SER	-	expression tag	UNP Q813T3
A	-11	SER	-	expression tag	UNP Q813T3
A	-10	GLY	-	expression tag	UNP Q813T3
A	-9	ARG	-	expression tag	UNP Q813T3
A	-8	GLU	-	expression tag	UNP Q813T3
A	-7	ASN	-	expression tag	UNP Q813T3
A	-6	LEU	-	expression tag	UNP Q813T3
A	-5	TYR	-	expression tag	UNP Q813T3
A	-4	PHE	-	expression tag	UNP Q813T3
A	-3	GLN	-	expression tag	UNP Q813T3
A	-2	GLY	-	expression tag	UNP Q813T3
A	-1	HIS	-	expression tag	UNP Q813T3
B	-18	MET	-	initiating methionine	UNP Q813T3
B	-17	HIS	-	expression tag	UNP Q813T3
B	-16	HIS	-	expression tag	UNP Q813T3
B	-15	HIS	-	expression tag	UNP Q813T3
B	-14	HIS	-	expression tag	UNP Q813T3
B	-13	HIS	-	expression tag	UNP Q813T3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP Q813T3
B	-11	SER	-	expression tag	UNP Q813T3
B	-10	SER	-	expression tag	UNP Q813T3
B	-9	GLY	-	expression tag	UNP Q813T3
B	-8	ARG	-	expression tag	UNP Q813T3
B	-7	GLU	-	expression tag	UNP Q813T3
B	-6	ASN	-	expression tag	UNP Q813T3
B	-5	LEU	-	expression tag	UNP Q813T3
B	-4	TYR	-	expression tag	UNP Q813T3
B	-3	PHE	-	expression tag	UNP Q813T3
B	-2	GLN	-	expression tag	UNP Q813T3
B	-1	GLY	-	expression tag	UNP Q813T3
B	0	HIS	-	expression tag	UNP Q813T3

- Molecule 2 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄) (labeled as "Ligand of Interest" by depositor).



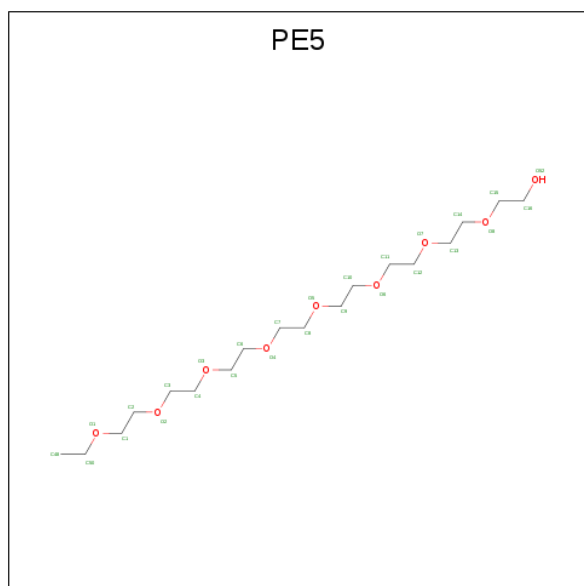
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			25	21	4		

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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	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
			25	21	4		
2	B	1	Total	C	O	0	0
			25	21	4		

- Molecule 3 is 3,6,9,12,15,18,21,24-OCTAOXAHEXACOSAN-1-OL (three-letter code: PE5) (formula: C₁₈H₃₈O₉).



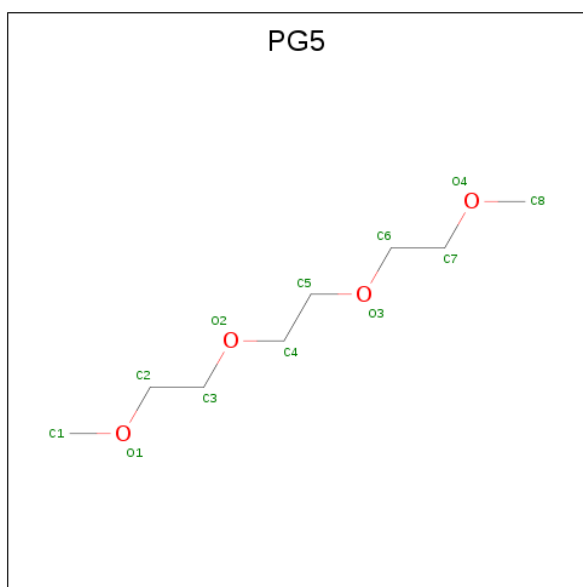
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is 1-METHOXY-2-[2-(2-METHOXY-ETHOXY)]-ETHANE (three-letter code: PG5) (formula: C₈H₁₈O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 11 7 4	0	0
5	B	1	Total C O 12 8 4	0	0

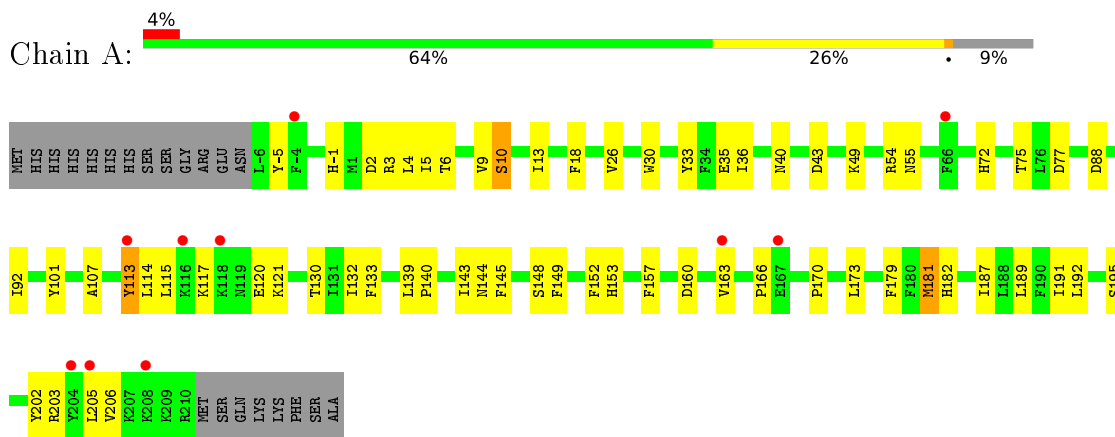
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	23	Total O 23 23	0	0
6	B	20	Total O 20 20	0	0

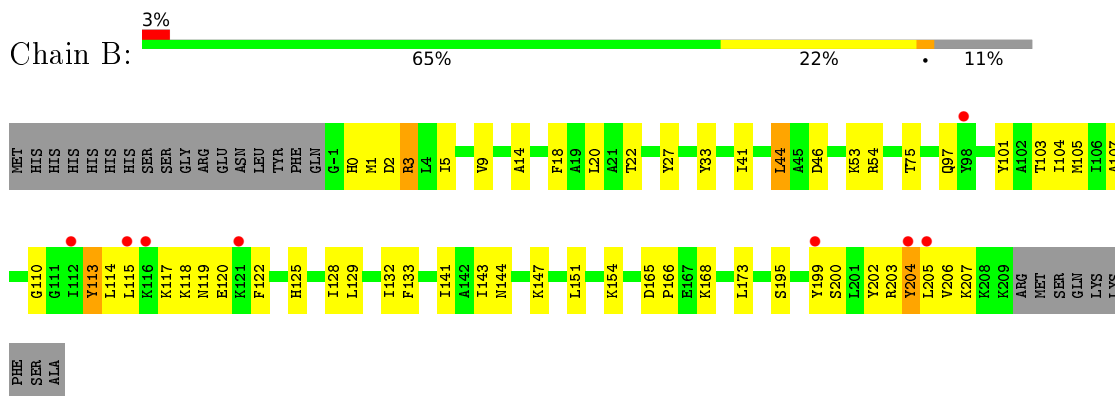
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Hypothetical Membrane Spanning Protein



- Molecule 1: Hypothetical Membrane Spanning Protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.72Å 44.70Å 116.86Å 90.00° 92.38° 90.00°	Depositor
Resolution (Å)	43.32 – 2.33 67.67 – 2.33	Depositor EDS
% Data completeness (in resolution range)	64.3 (43.32-2.33) 64.4 (67.67-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.32Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.245 , 0.287 0.246 , 0.288	Depositor DCC
R_{free} test set	982 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtrriage
Anisotropy	0.041	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.093 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3911	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.70% 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, OLC, PG5, PE5

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	0/1820	0.41	0/2467
1	B	0.27	0/1770	0.42	0/2400
All	All	0.26	0/3590	0.41	0/4867

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	1771	0	1829	52	0
1	B	1723	0	1788	34	0
2	A	150	0	240	20	0
2	B	125	0	200	8	0
3	A	16	0	20	0	0
4	A	30	0	40	3	0
4	B	30	0	40	4	0
5	B	23	0	33	0	0
6	A	23	0	0	0	0
6	B	20	0	0	0	0
All	All	3911	0	4190	94	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 (94) 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:192:LEU:HD22	2:A:303:OLC:H10	1.57	0.85
1:A:9:VAL:HG22	1:A:107:ALA:HA	1.63	0.80
1:A:157:PHE:HA	4:A:311:GOL:H31	1.67	0.76
1:A:101:TYR:HE2	4:A:310:GOL:H32	1.54	0.70
2:A:304:OLC:H7A	2:A:304:OLC:H12	1.73	0.70
1:B:2:ASP:O	1:B:5:ILE:HG22	1.93	0.68
1:B:5:ILE:HG23	1:B:114:LEU:HD11	1.75	0.67
1:B:5:ILE:O	1:B:9:VAL:HG23	1.94	0.66
1:A:140:PRO:HA	1:A:144:ASN:HD21	1.60	0.66
1:A:101:TYR:HE1	2:A:304:OLC:H4	1.62	0.65
1:A:5:ILE:HD13	1:A:113:TYR:HE2	1.64	0.63
1:A:3:ARG:O	1:A:6:THR:HG22	1.99	0.62
1:B:203:ARG:HA	1:B:206:VAL:HG22	1.81	0.62
1:A:2:ASP:HB3	1:A:114:LEU:HD21	1.81	0.62
1:A:132:ILE:HD11	2:B:304:OLC:H12A	1.82	0.60
1:A:187:ILE:O	1:A:191:ILE:HG12	2.01	0.60
2:A:304:OLC:H17	2:A:304:OLC:H12A	1.83	0.59
1:A:140:PRO:HA	1:A:144:ASN:ND2	2.16	0.59
1:B:200:SER:O	1:B:204:TYR:HB2	2.03	0.58
1:B:147:LYS:HD3	1:B:151:LEU:HD23	1.86	0.57
1:A:133:PHE:HE1	2:A:301:OLC:H15	1.68	0.57
1:B:141:ILE:HD11	2:B:302:OLC:H16	1.86	0.57
1:B:113:TYR:HE2	1:B:117:LYS:HD2	1.70	0.57
1:B:75:THR:HB	4:B:310:GOL:H2	1.86	0.56
1:B:133:PHE:HB2	4:B:311:GOL:H31	1.88	0.56
1:A:5:ILE:O	1:A:9:VAL:HB	2.05	0.55
1:A:88:ASP:O	1:A:92:ILE:HG12	2.07	0.55
1:A:189:LEU:HD12	2:A:306:OLC:H9	1.89	0.55
1:B:97:GLN:HE21	2:B:303:OLC:H2	1.72	0.55
1:B:41:ILE:HA	1:B:44:LEU:HB2	1.88	0.54
1:A:101:TYR:CE1	2:A:304:OLC:H6A	2.43	0.54
1:A:144:ASN:OD1	1:A:148:SER:OG	2.26	0.54
1:A:55:ASN:HD21	1:A:75:THR:HB	1.71	0.53
1:B:103:THR:O	1:B:107:ALA:N	2.41	0.53
1:A:5:ILE:HD13	1:A:113:TYR:CE2	2.44	0.52
1:A:33:TYR:HA	1:A:36:ILE:HD12	1.91	0.52
1:A:115:LEU:HD11	1:A:205:LEU:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ALA:HB1	4:B:311:GOL:H2	1.92	0.52
1:B:128:ILE:O	1:B:132:ILE:HG12	2.09	0.52
1:B:22:THR:HG21	2:B:301:OLC:H4A	1.92	0.51
1:A:143:ILE:HG13	1:A:144:ASN:HD22	1.75	0.51
1:A:40:ASN:ND2	1:A:43:ASP:OD2	2.44	0.51
1:B:105:MET:HG2	2:B:303:OLC:H14A	1.92	0.51
1:A:133:PHE:CE1	2:A:301:OLC:H15	2.45	0.50
1:A:26:VAL:HG22	2:A:302:OLC:H9	1.92	0.50
1:A:145:PHE:CG	1:A:181:MET:HG3	2.47	0.50
1:A:149:PHE:CZ	1:A:153:HIS:HE1	2.30	0.50
1:B:202:TYR:O	1:B:206:VAL:HG13	2.11	0.49
1:A:-1:HIS:O	1:A:4:LEU:N	2.43	0.48
1:A:182:HIS:HE1	2:A:306:OLC:H24	1.78	0.48
1:A:182:HIS:CE1	2:A:306:OLC:H24	2.49	0.47
1:A:117:LYS:HA	1:A:117:LYS:HD3	1.62	0.47
1:A:77:ASP:O	1:A:170:PRO:HD2	2.15	0.47
1:A:143:ILE:CG1	1:A:144:ASN:HD22	2.27	0.46
1:A:166:PRO:HB3	1:A:173:LEU:HD21	1.96	0.46
1:A:36:ILE:HG21	1:A:49:LYS:HG3	1.96	0.46
1:A:130:THR:HG23	1:A:195:SER:HB2	1.96	0.46
1:B:101:TYR:HE1	2:B:303:OLC:H7A	1.80	0.46
1:A:35:GLU:HG2	1:A:179:PHE:HB2	1.98	0.46
2:A:306:OLC:H2A	2:A:306:OLC:H21A	1.53	0.46
1:A:2:ASP:O	1:A:114:LEU:HD11	2.16	0.46
1:A:18:PHE:HA	1:A:191:ILE:CD1	2.47	0.45
1:A:181:MET:HE1	2:A:306:OLC:H21	1.98	0.45
1:A:202:TYR:O	1:A:206:VAL:HG23	2.16	0.45
1:B:3:ARG:H	1:B:3:ARG:HG2	1.35	0.45
1:A:120:GLU:N	1:A:120:GLU:OE1	2.50	0.44
1:B:133:PHE:HB2	4:B:311:GOL:C3	2.48	0.44
1:B:166:PRO:HB3	1:B:173:LEU:HD21	2.00	0.44
1:A:179:PHE:CZ	2:A:302:OLC:H7	2.53	0.44
1:B:195:SER:O	1:B:199:TYR:N	2.45	0.44
1:B:165:ASP:OD2	1:B:168:LYS:HE3	2.17	0.43
1:A:101:TYR:CE2	4:A:310:GOL:H32	2.44	0.43
1:B:114:LEU:HB2	1:B:122:PHE:CE2	2.54	0.43
1:A:120:GLU:HG2	1:A:202:TYR:CE1	2.53	0.43
1:B:125:HIS:O	1:B:129:LEU:HD12	2.18	0.43
1:A:160:ASP:O	1:A:163:VAL:HG22	2.18	0.43
2:A:312:OLC:H18B	2:A:312:OLC:H15A	1.66	0.42
1:B:113:TYR:CE2	1:B:117:LYS:HD2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:PHE:HZ	2:A:301:OLC:H3	1.84	0.42
1:B:20:LEU:HD11	1:B:104:ILE:HD11	2.01	0.42
1:A:54:ARG:HA	1:A:54:ARG:HD3	1.87	0.42
2:B:307:OLC:H11A	2:B:307:OLC:H8A	1.78	0.42
1:A:139:LEU:O	1:A:143:ILE:HG12	2.20	0.41
1:B:27:TYR:CG	2:B:303:OLC:H22	2.55	0.41
1:B:33:TYR:CE2	1:B:53:LYS:HG2	2.54	0.41
1:B:114:LEU:HD23	1:B:114:LEU:HA	1.90	0.41
1:B:117:LYS:C	1:B:119:ASN:H	2.23	0.41
1:B:110:GLY:O	1:B:113:TYR:HB3	2.21	0.41
1:B:114:LEU:HB2	1:B:122:PHE:HE2	1.84	0.41
1:A:153:HIS:CE1	2:A:301:OLC:HO25	2.35	0.41
1:A:10:SER:HA	1:A:13:ILE:HD12	2.02	0.40
2:A:301:OLC:H6A	2:A:301:OLC:H3A	1.89	0.40
2:A:301:OLC:H18B	2:A:301:OLC:H15A	1.71	0.40
2:A:304:OLC:H12	2:A:304:OLC:H15	1.85	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	214/237 (90%)	214 (100%)	0	0	100	100
1	B	209/237 (88%)	202 (97%)	7 (3%)	0	100	100
All	All	423/474 (89%)	416 (98%)	7 (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	193/213 (91%)	185 (96%)	8 (4%)	30	38
1	B	189/213 (89%)	172 (91%)	17 (9%)	9	8
All	All	382/426 (90%)	357 (94%)	25 (6%)	17	19

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-5	TYR
1	A	10	SER
1	A	30	TRP
1	A	72	HIS
1	A	113	TYR
1	A	121	LYS
1	A	181	MET
1	A	203	ARG
1	B	0	HIS
1	B	1	MET
1	B	3	ARG
1	B	18	PHE
1	B	44	LEU
1	B	46	ASP
1	B	54	ARG
1	B	113	TYR
1	B	115	LEU
1	B	118	LYS
1	B	120	GLU
1	B	143	ILE
1	B	144	ASN
1	B	154	LYS
1	B	204	TYR
1	B	205	LEU
1	B	207	LYS

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	182	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 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$
4	GOL	A	310	-	5,5,5	1.03	0	5,5,5	0.86	0
2	OLC	A	304	-	24,24,24	0.69	1 (4%)	25,25,25	1.03	1 (4%)
4	GOL	B	312	-	5,5,5	0.92	0	5,5,5	0.98	0
4	GOL	A	308	-	5,5,5	0.91	0	5,5,5	0.98	0
2	OLC	B	302	-	24,24,24	0.69	1 (4%)	25,25,25	0.90	1 (4%)
3	PE5	A	305	-	15,15,26	0.54	0	14,14,25	0.24	0
4	GOL	B	306	-	5,5,5	0.90	0	5,5,5	1.00	0
2	OLC	A	303	-	24,24,24	0.67	1 (4%)	25,25,25	0.94	1 (4%)
2	OLC	A	302	-	24,24,24	0.68	1 (4%)	25,25,25	1.06	1 (4%)
4	GOL	B	305	-	5,5,5	0.93	0	5,5,5	1.00	0
4	GOL	B	310	-	5,5,5	0.96	0	5,5,5	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PG5	B	309	-	11,11,11	0.50	0	10,10,10	0.23	0
5	PG5	B	308	-	10,10,11	0.50	0	9,9,10	0.23	0
2	OLC	A	306	-	24,24,24	0.69	1 (4%)	25,25,25	0.92	1 (4%)
2	OLC	A	301	-	24,24,24	0.68	1 (4%)	25,25,25	0.96	1 (4%)
2	OLC	B	307	-	24,24,24	0.69	1 (4%)	25,25,25	0.97	1 (4%)
2	OLC	A	312	-	24,24,24	0.68	1 (4%)	25,25,25	1.01	1 (4%)
2	OLC	B	303	-	24,24,24	0.68	1 (4%)	25,25,25	0.87	1 (4%)
2	OLC	B	301	-	24,24,24	0.67	1 (4%)	25,25,25	1.00	1 (4%)
4	GOL	A	311	-	5,5,5	0.94	0	5,5,5	0.99	0
2	OLC	B	304	-	24,24,24	0.68	1 (4%)	25,25,25	0.93	1 (4%)
4	GOL	B	311	-	5,5,5	0.95	0	5,5,5	0.92	0
4	GOL	A	309	-	5,5,5	0.90	0	5,5,5	1.00	0
4	GOL	A	307	-	5,5,5	0.91	0	5,5,5	1.01	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
4	GOL	A	310	-	-	1/4/4/4	-
2	OLC	A	304	-	-	13/24/24/24	-
4	GOL	B	312	-	-	0/4/4/4	-
4	GOL	A	308	-	-	2/4/4/4	-
2	OLC	B	302	-	-	15/24/24/24	-
3	PE5	A	305	-	-	4/13/13/24	-
4	GOL	B	306	-	-	0/4/4/4	-
2	OLC	A	303	-	-	14/24/24/24	-
2	OLC	A	302	-	-	12/24/24/24	-
4	GOL	B	305	-	-	2/4/4/4	-
4	GOL	B	310	-	-	0/4/4/4	-
5	PG5	B	309	-	-	6/9/9/9	-
5	PG5	B	308	-	-	5/8/8/9	-
2	OLC	A	306	-	-	10/24/24/24	-
2	OLC	A	301	-	-	10/24/24/24	-
2	OLC	B	307	-	-	7/24/24/24	-
2	OLC	A	312	-	-	12/24/24/24	-
2	OLC	B	303	-	-	9/24/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	B	301	-	-	14/24/24/24	-
4	GOL	A	311	-	-	3/4/4/4	-
2	OLC	B	304	-	-	8/24/24/24	-
4	GOL	B	311	-	-	2/4/4/4	-
4	GOL	A	309	-	-	4/4/4/4	-
4	GOL	A	307	-	-	3/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	306	OLC	O20-C1	2.65	1.41	1.33
2	A	302	OLC	O20-C1	2.65	1.41	1.33
2	B	302	OLC	O20-C1	2.65	1.41	1.33
2	B	304	OLC	O20-C1	2.61	1.41	1.33
2	B	307	OLC	O20-C1	2.61	1.41	1.33
2	A	312	OLC	O20-C1	2.60	1.40	1.33
2	B	303	OLC	O20-C1	2.58	1.40	1.33
2	A	304	OLC	O20-C1	2.58	1.40	1.33
2	A	301	OLC	O20-C1	2.56	1.40	1.33
2	A	303	OLC	O20-C1	2.55	1.40	1.33
2	B	301	OLC	O20-C1	2.53	1.40	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	302	OLC	O20-C1-C2	2.82	120.76	111.91
2	A	312	OLC	O20-C1-C2	2.81	120.74	111.91
2	B	302	OLC	O20-C1-C2	2.69	120.34	111.91
2	A	301	OLC	O20-C1-C2	2.64	120.20	111.91
2	B	301	OLC	O20-C1-C2	2.64	120.20	111.91
2	A	306	OLC	O20-C1-C2	2.59	120.03	111.91
2	B	307	OLC	O20-C1-C2	2.58	120.00	111.91
2	B	304	OLC	O20-C1-C2	2.51	119.79	111.91
2	B	303	OLC	O20-C1-C2	2.49	119.71	111.91
2	A	304	OLC	O20-C1-C2	2.39	119.40	111.91
2	A	303	OLC	O20-C1-C2	2.37	119.36	111.91

There are no chirality outliers.

All (156) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	302	OLC	C21-C22-C24-O25
2	A	306	OLC	C2-C1-O20-C21
2	A	306	OLC	O19-C1-O20-C21
2	B	302	OLC	O20-C21-C22-C24
2	B	302	OLC	O20-C21-C22-O23
2	B	303	OLC	C21-C22-C24-O25
2	B	307	OLC	O20-C21-C22-C24
2	B	307	OLC	O20-C21-C22-O23
4	A	309	GOL	C1-C2-C3-O3
4	A	311	GOL	O1-C1-C2-C3
4	B	311	GOL	C1-C2-C3-O3
2	B	301	OLC	O19-C1-O20-C21
2	B	301	OLC	C2-C1-O20-C21
2	A	303	OLC	O19-C1-O20-C21
2	A	303	OLC	C2-C1-O20-C21
2	B	301	OLC	O20-C21-C22-O23
2	A	304	OLC	C12-C13-C14-C15
2	A	301	OLC	C3-C4-C5-C6
2	A	304	OLC	C2-C1-O20-C21
2	A	312	OLC	C2-C1-O20-C21
2	B	307	OLC	C1-C2-C3-C4
2	A	312	OLC	O19-C1-O20-C21
2	B	302	OLC	C2-C1-O20-C21
4	A	308	GOL	O1-C1-C2-O2
2	A	301	OLC	C1-C2-C3-C4
2	A	302	OLC	C1-C2-C3-C4
2	A	303	OLC	C1-C2-C3-C4
2	B	302	OLC	C1-C2-C3-C4
2	A	304	OLC	O19-C1-O20-C21
2	A	312	OLC	C1-C2-C3-C4
2	B	301	OLC	C1-C2-C3-C4
2	A	306	OLC	C10-C11-C12-C13
2	A	304	OLC	C13-C14-C15-C16
2	A	304	OLC	C3-C4-C5-C6
2	A	312	OLC	C11-C12-C13-C14
2	A	312	OLC	C4-C5-C6-C7
2	B	304	OLC	C11-C12-C13-C14
2	B	307	OLC	C11-C12-C13-C14
2	A	304	OLC	C2-C3-C4-C5
2	B	301	OLC	C13-C14-C15-C16
2	B	304	OLC	C2-C1-O20-C21
2	A	304	OLC	C14-C15-C16-C17
2	B	302	OLC	O19-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
2	A	312	OLC	C14-C15-C16-C17
2	B	302	OLC	C3-C4-C5-C6
2	B	302	OLC	C12-C13-C14-C15
4	A	307	GOL	O1-C1-C2-C3
4	A	307	GOL	C1-C2-C3-O3
4	A	308	GOL	O1-C1-C2-C3
4	A	309	GOL	O1-C1-C2-C3
4	A	310	GOL	C1-C2-C3-O3
4	A	311	GOL	C1-C2-C3-O3
2	A	302	OLC	C12-C13-C14-C15
3	A	305	PE5	O3-C5-C6-O4
2	A	303	OLC	C6-C7-C8-C9
2	B	304	OLC	C10-C11-C12-C13
2	A	303	OLC	C12-C13-C14-C15
2	A	312	OLC	C13-C14-C15-C16
2	B	303	OLC	C4-C5-C6-C7
2	B	301	OLC	C14-C15-C16-C17
2	A	302	OLC	O23-C22-C24-O25
2	B	303	OLC	O23-C22-C24-O25
4	A	311	GOL	O1-C1-C2-O2
2	A	304	OLC	C4-C5-C6-C7
2	B	302	OLC	C10-C11-C12-C13
2	A	303	OLC	C11-C12-C13-C14
2	A	301	OLC	C2-C3-C4-C5
2	B	302	OLC	C13-C14-C15-C16
2	B	304	OLC	O19-C1-O20-C21
2	A	312	OLC	C15-C16-C17-C18
2	B	301	OLC	C6-C7-C8-C9
2	B	303	OLC	C6-C7-C8-C9
2	A	301	OLC	C12-C13-C14-C15
5	B	309	PG5	O2-C4-C5-O3
2	B	304	OLC	C5-C6-C7-C8
2	A	303	OLC	C3-C4-C5-C6
2	B	307	OLC	C2-C3-C4-C5
2	B	302	OLC	C11-C12-C13-C14
2	B	302	OLC	C6-C7-C8-C9
2	B	304	OLC	C12-C13-C14-C15
2	A	303	OLC	C4-C5-C6-C7
2	A	306	OLC	C13-C14-C15-C16
5	B	309	PG5	C2-C3-O2-C4
4	A	309	GOL	O1-C1-C2-O2
4	A	309	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	B	311	GOL	O2-C2-C3-O3
2	B	307	OLC	C6-C7-C8-C9
5	B	309	PG5	O3-C6-C7-O4
2	A	303	OLC	C13-C14-C15-C16
3	A	305	PE5	O4-C7-C8-O5
2	A	306	OLC	C1-C2-C3-C4
2	A	303	OLC	O20-C21-C22-O23
2	A	304	OLC	C7-C8-C9-C10
2	A	304	OLC	C15-C16-C17-C18
2	B	302	OLC	C4-C5-C6-C7
2	A	306	OLC	C5-C6-C7-C8
2	A	312	OLC	C6-C7-C8-C9
2	A	301	OLC	C5-C6-C7-C8
2	B	301	OLC	C15-C16-C17-C18
2	A	302	OLC	C3-C4-C5-C6
5	B	308	PG5	C2-C3-O2-C4
4	B	305	GOL	O2-C2-C3-O3
2	A	312	OLC	C12-C13-C14-C15
2	B	301	OLC	O20-C21-C22-C24
2	A	301	OLC	C15-C16-C17-C18
2	A	301	OLC	C10-C11-C12-C13
2	B	307	OLC	C10-C11-C12-C13
2	A	302	OLC	C15-C16-C17-C18
2	A	304	OLC	C5-C6-C7-C8
2	B	301	OLC	C5-C6-C7-C8
3	A	305	PE5	C4-C3-O2-C2
2	A	303	OLC	C5-C6-C7-C8
4	A	307	GOL	O2-C2-C3-O3
5	B	308	PG5	C4-C5-O3-C6
2	A	301	OLC	C13-C14-C15-C16
2	A	303	OLC	C15-C16-C17-C18
2	A	303	OLC	C9-C10-C11-C12
2	B	301	OLC	C9-C10-C11-C12
2	A	303	OLC	C10-C11-C12-C13
5	B	309	PG5	O1-C2-C3-O2
5	B	308	PG5	C5-C4-O2-C3
2	A	304	OLC	C6-C7-C8-C9
2	B	303	OLC	C13-C14-C15-C16
2	A	301	OLC	C9-C10-C11-C12
2	A	302	OLC	C9-C10-C11-C12
2	A	306	OLC	C2-C3-C4-C5
2	B	303	OLC	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
3	A	305	PE5	O2-C3-C4-O3
2	B	302	OLC	C15-C16-C17-C18
5	B	309	PG5	C5-C4-O2-C3
2	A	302	OLC	O19-C1-O20-C21
2	A	306	OLC	C7-C8-C9-C10
2	B	301	OLC	C7-C8-C9-C10
2	A	304	OLC	C1-C2-C3-C4
2	A	302	OLC	C2-C1-O20-C21
5	B	308	PG5	C7-C6-O3-C5
2	A	302	OLC	C11-C12-C13-C14
2	B	302	OLC	C9-C10-C11-C12
2	A	301	OLC	C11-C12-C13-C14
2	A	312	OLC	C2-C3-C4-C5
2	A	302	OLC	O20-C1-C2-C3
2	B	304	OLC	C9-C10-C11-C12
5	B	309	PG5	C4-C5-O3-C6
2	B	304	OLC	C7-C8-C9-C10
2	B	301	OLC	C4-C5-C6-C7
2	B	301	OLC	C2-C3-C4-C5
2	B	302	OLC	C14-C15-C16-C17
2	A	302	OLC	O19-C1-C2-C3
4	B	305	GOL	C1-C2-C3-O3
2	B	303	OLC	O20-C1-C2-C3
2	A	306	OLC	C9-C10-C11-C12
2	B	303	OLC	C9-C10-C11-C12
5	B	308	PG5	O3-C6-C7-O4
2	B	303	OLC	O19-C1-C2-C3
2	A	306	OLC	C4-C5-C6-C7
2	A	312	OLC	C7-C8-C9-C10

There are no ring outliers.

15 monomers are involved in 35 short contacts:

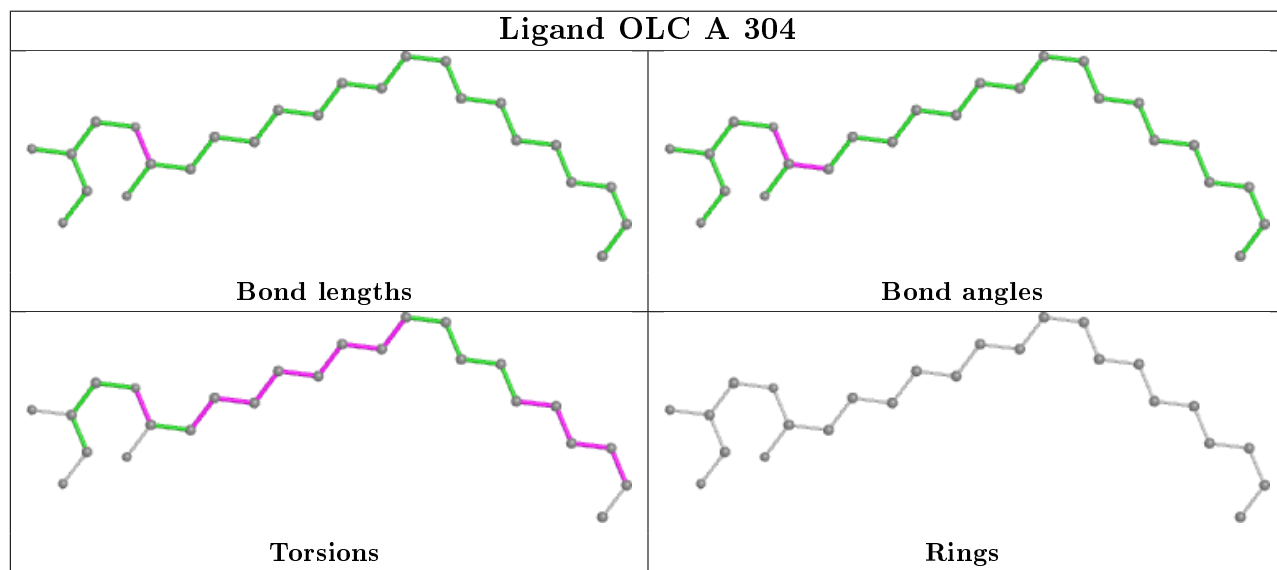
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	310	GOL	2	0
2	A	304	OLC	5	0
2	B	302	OLC	1	0
2	A	303	OLC	1	0
2	A	302	OLC	2	0
4	B	310	GOL	1	0
2	A	306	OLC	5	0
2	A	301	OLC	6	0

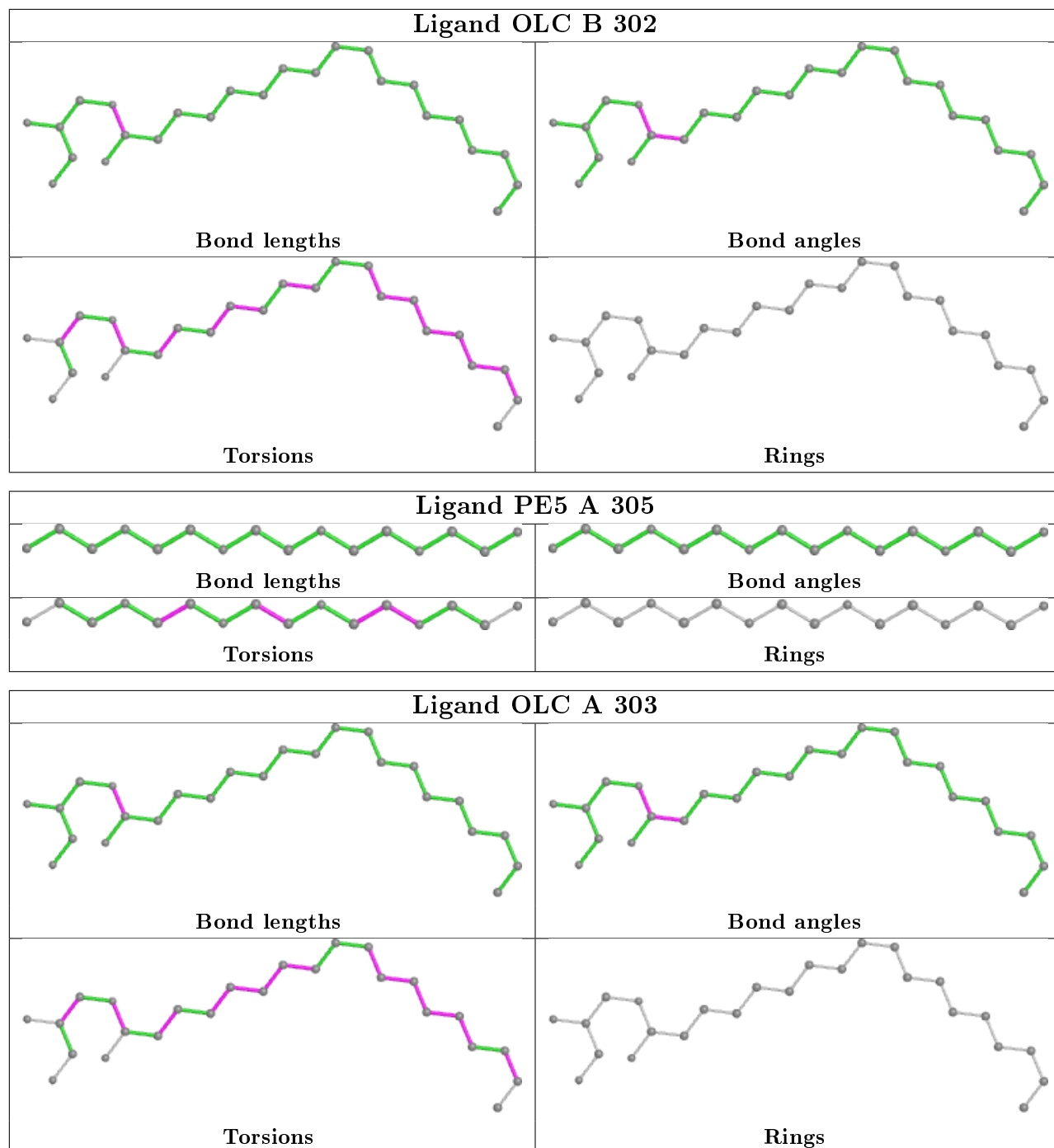
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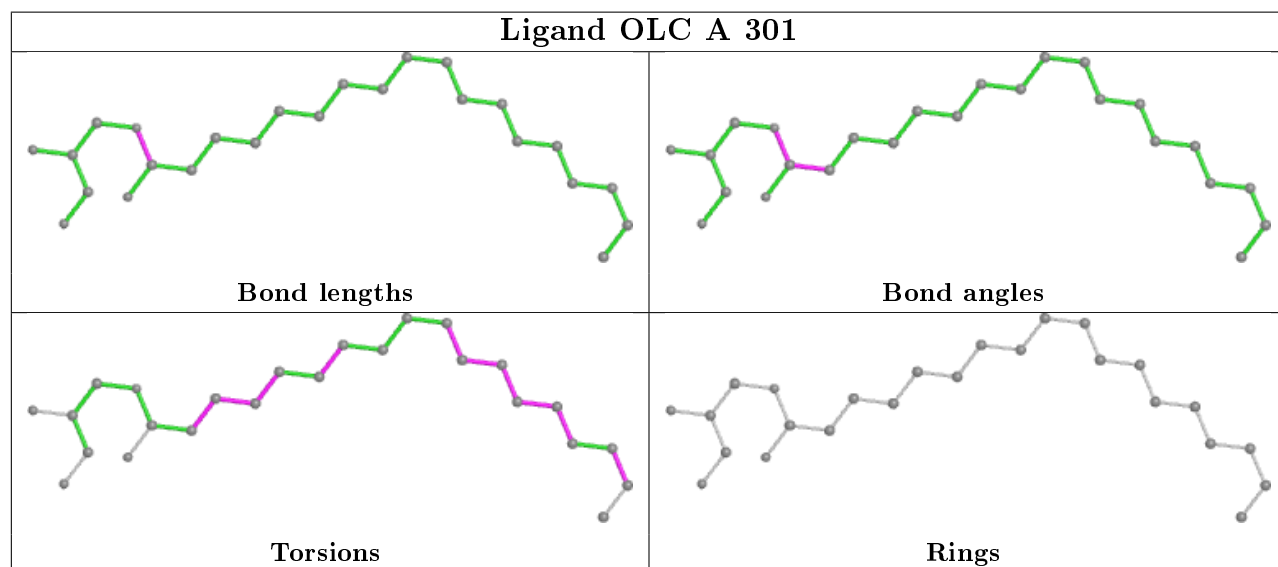
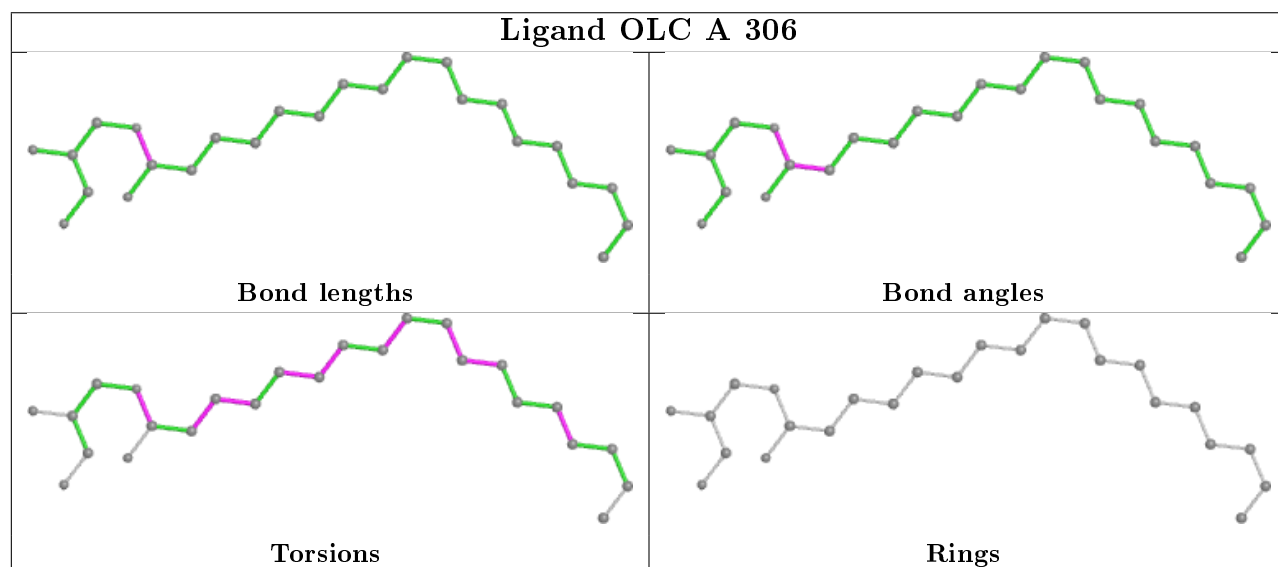
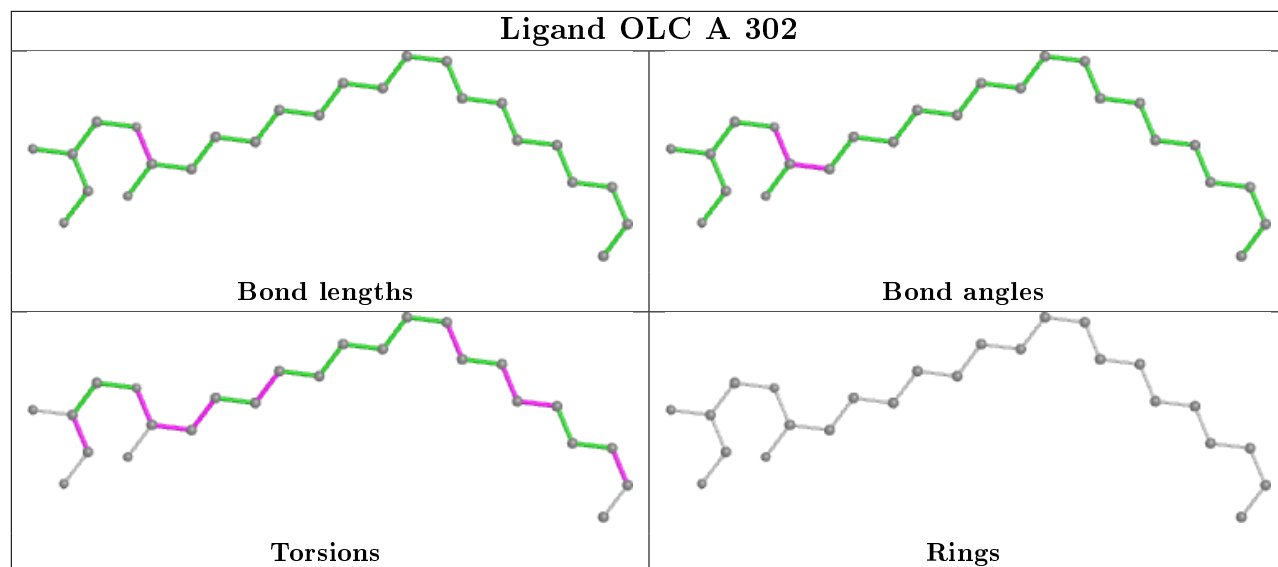
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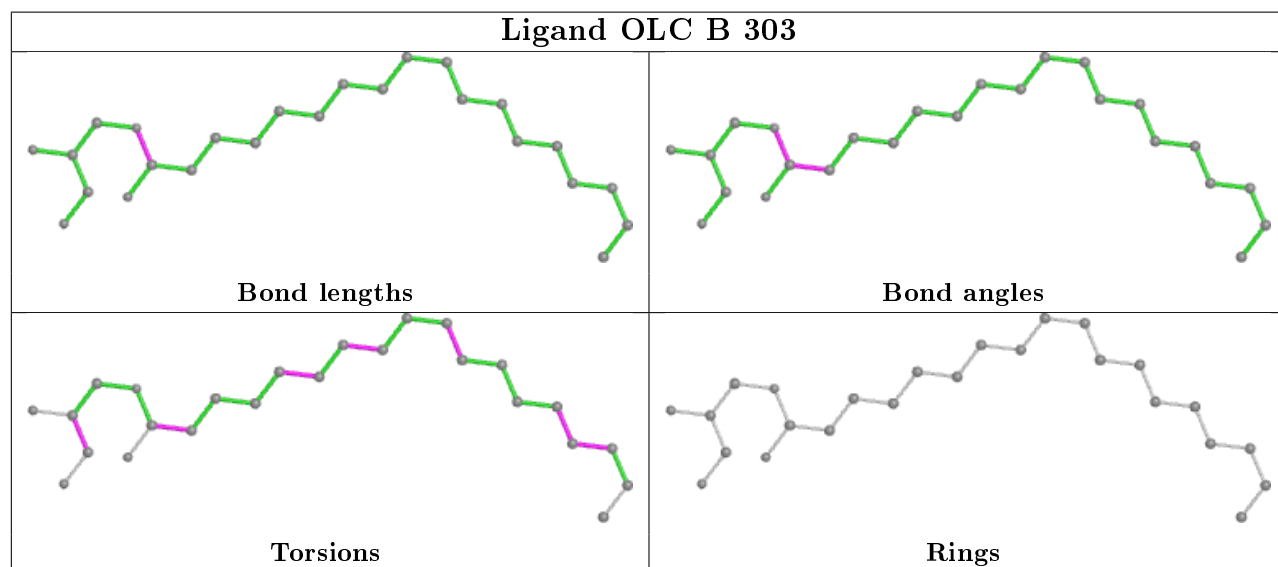
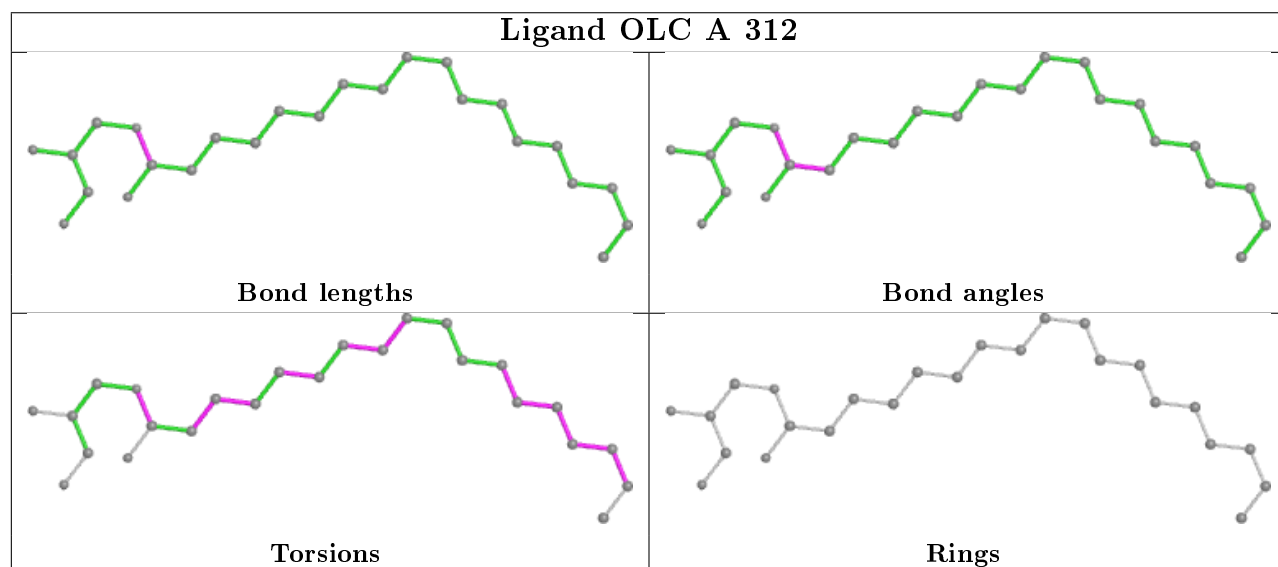
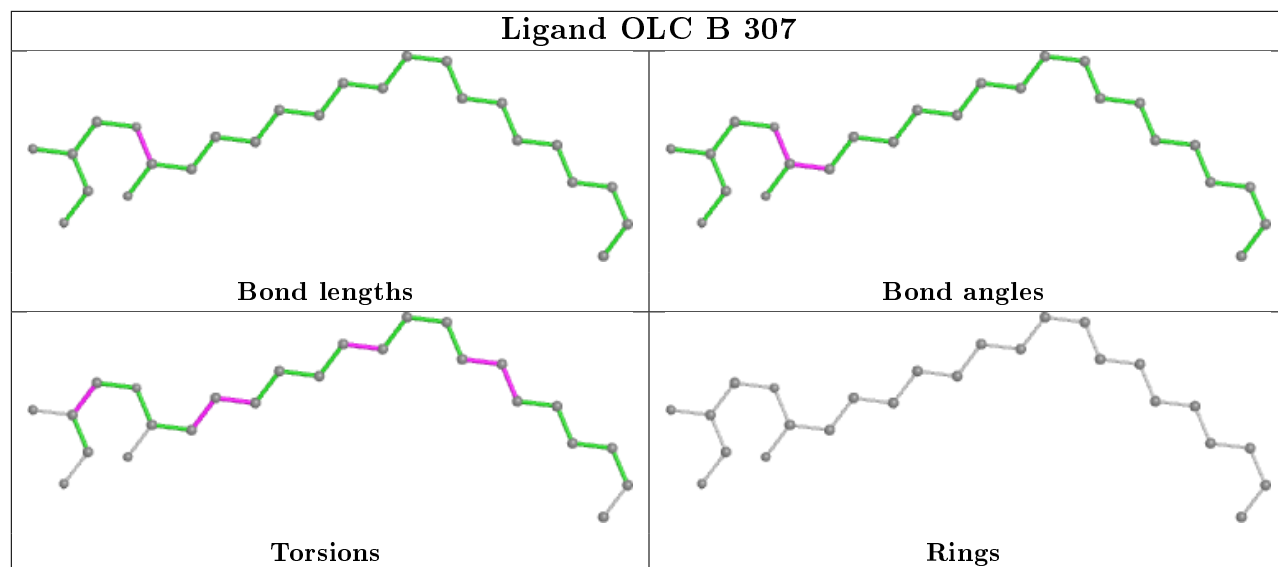
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	307	OLC	1	0
2	A	312	OLC	1	0
2	B	303	OLC	4	0
2	B	301	OLC	1	0
4	A	311	GOL	1	0
2	B	304	OLC	1	0
4	B	311	GOL	3	0

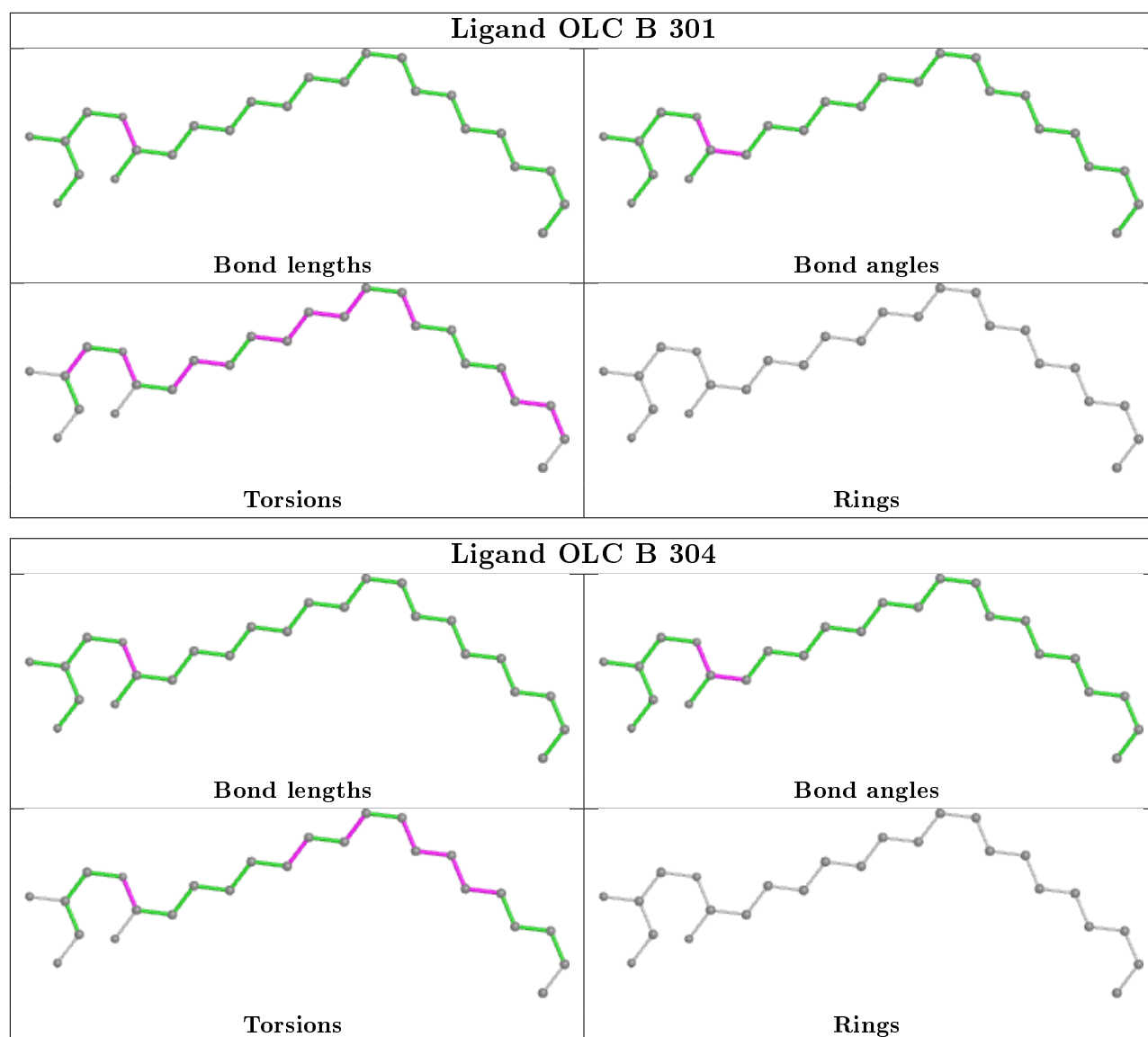
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	216/237 (91%)	0.03	10 (4%) 32 43	20, 43, 94, 115	0
1	B	211/237 (89%)	0.08	8 (3%) 40 51	23, 49, 95, 131	0
All	All	427/474 (90%)	0.06	18 (4%) 36 47	20, 47, 94, 131	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	204	TYR	4.2
1	A	118	LYS	4.0
1	A	205	LEU	3.9
1	A	204	TYR	3.5
1	B	98	TYR	3.5
1	A	66	PHE	3.4
1	B	112	ILE	3.1
1	A	208	LYS	2.8
1	A	163	VAL	2.7
1	B	121	LYS	2.6
1	A	116	LYS	2.5
1	B	205	LEU	2.4
1	B	115	LEU	2.3
1	B	199	TYR	2.3
1	A	167	GLU	2.3
1	B	116	LYS	2.3
1	A	113	TYR	2.1
1	A	-4	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

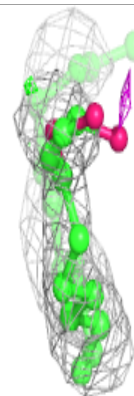
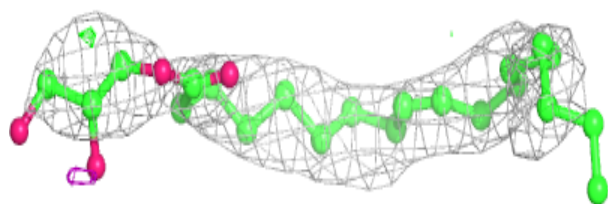
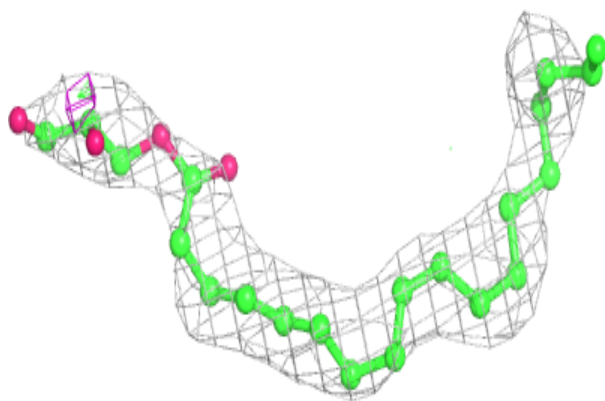
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	310	6/6	0.62	0.28	85,92,93,96	0
4	GOL	B	310	6/6	0.68	0.31	73,86,98,104	0
2	OLC	A	306	25/25	0.77	0.29	57,77,98,102	0
2	OLC	A	312	25/25	0.78	0.40	55,72,91,92	0
4	GOL	B	305	6/6	0.79	0.19	70,74,76,81	0
2	OLC	B	307	25/25	0.79	0.27	48,68,79,86	0
2	OLC	A	303	25/25	0.83	0.27	44,69,85,87	0
2	OLC	B	304	25/25	0.83	0.32	37,70,83,89	0
4	GOL	B	312	6/6	0.83	0.23	76,84,85,95	0
4	GOL	B	306	6/6	0.84	0.14	59,68,73,81	0
2	OLC	B	301	25/25	0.84	0.39	38,74,86,90	0
3	PE5	A	305	16/27	0.84	0.19	43,59,66,70	0
2	OLC	A	304	25/25	0.85	0.35	50,73,87,90	0
5	PG5	B	309	12/12	0.85	0.18	61,74,85,87	0
2	OLC	B	303	25/25	0.86	0.30	55,69,89,91	0
4	GOL	A	311	6/6	0.88	0.17	45,57,78,105	0
4	GOL	A	309	6/6	0.88	0.30	56,73,83,83	0
2	OLC	B	302	25/25	0.89	0.20	38,56,71,91	0
4	GOL	B	311	6/6	0.90	0.28	73,74,77,92	0
2	OLC	A	301	25/25	0.90	0.22	42,58,76,81	0
4	GOL	A	307	6/6	0.90	0.12	45,57,71,79	0
4	GOL	A	308	6/6	0.93	0.21	19,43,60,73	0
5	PG5	B	308	11/12	0.93	0.32	60,72,82,83	0
2	OLC	A	302	25/25	0.93	0.15	20,44,70,75	0

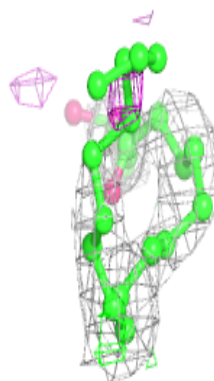
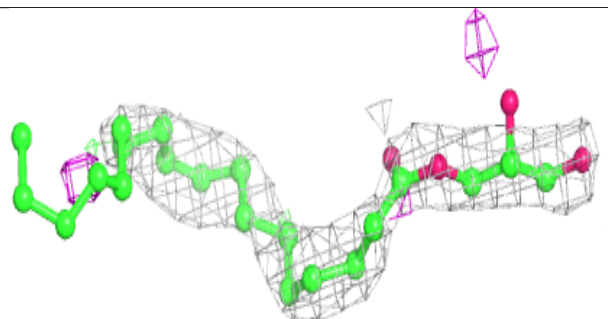
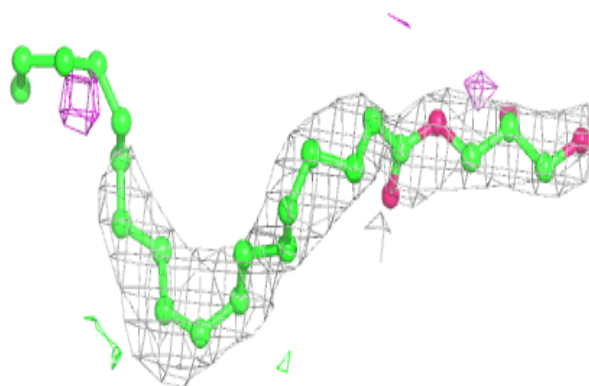
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 306:

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

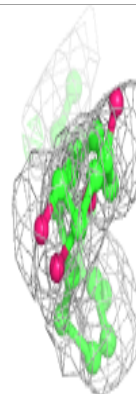
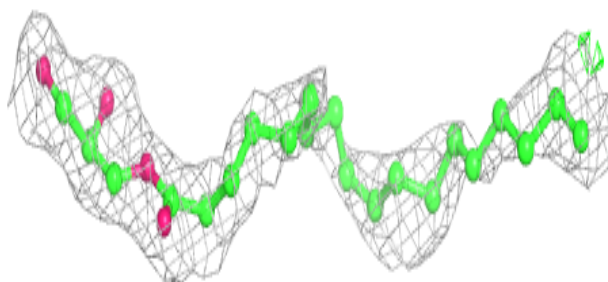
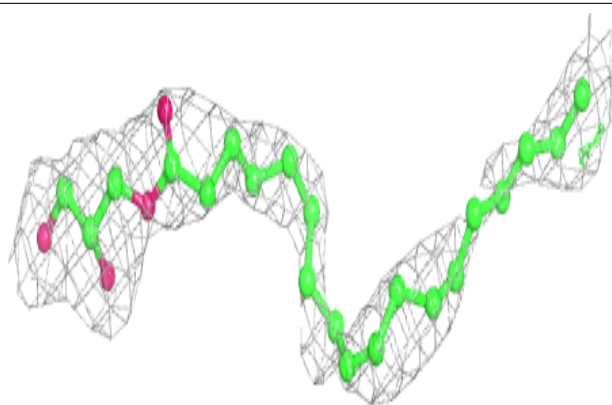
**Electron density around OLC A 312:**

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

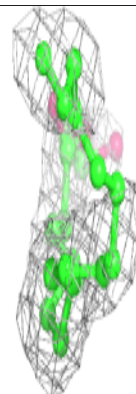
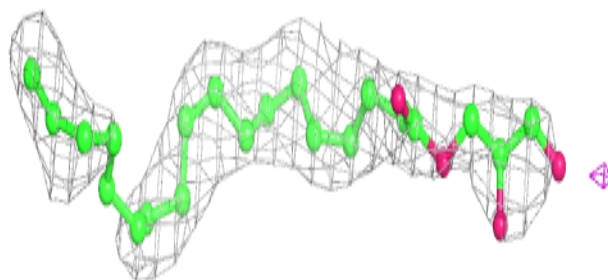
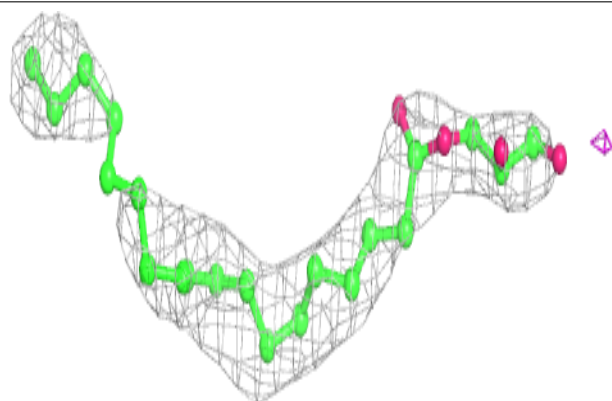


Electron density around OLC B 307:

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

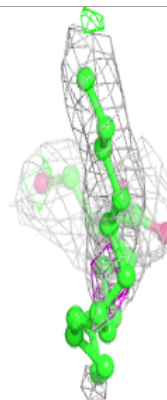
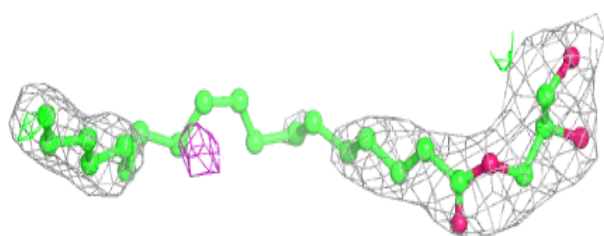
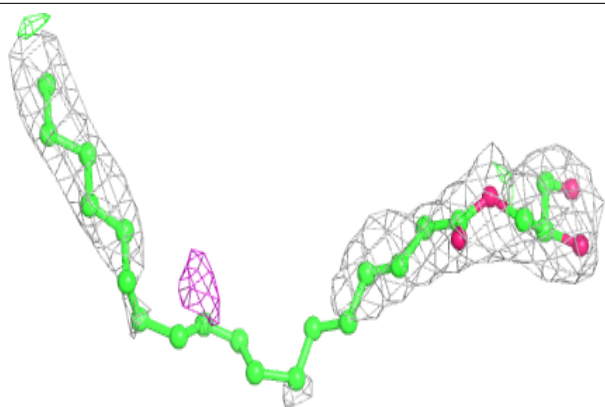
**Electron density around OLC A 303:**

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

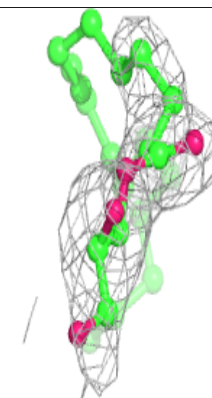
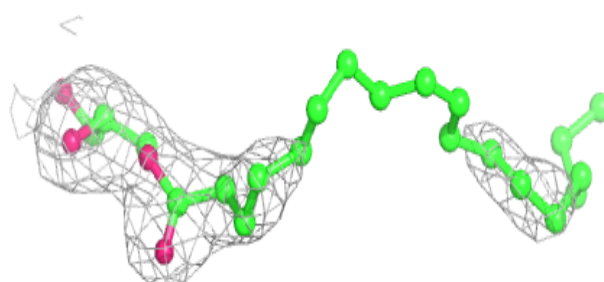
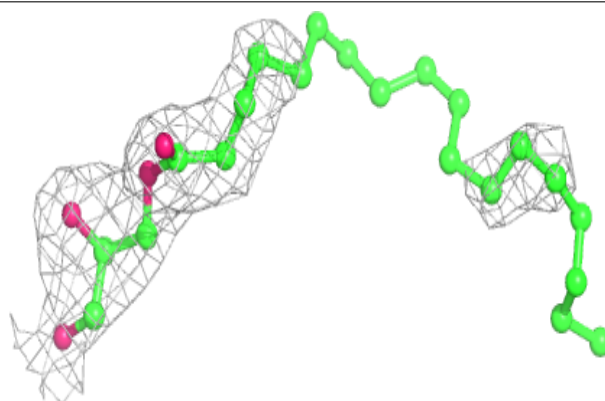


Electron density around OLC B 304:

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

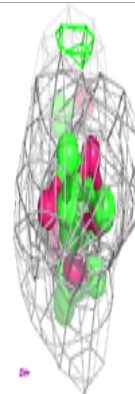
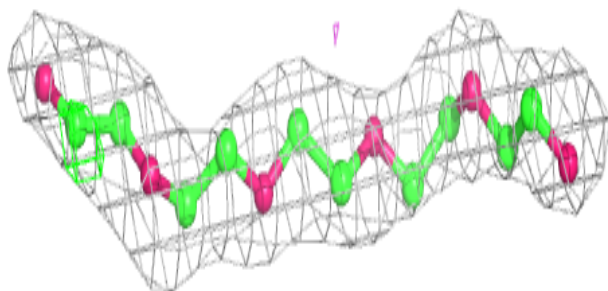
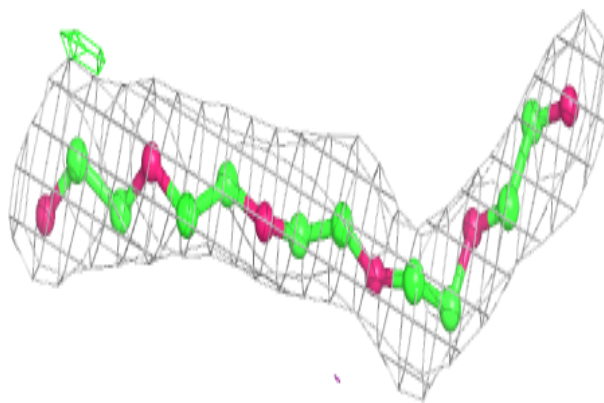
**Electron density around OLC B 301:**

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

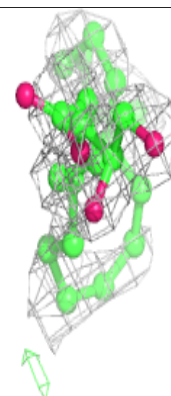
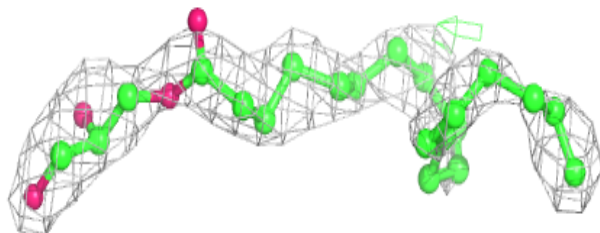
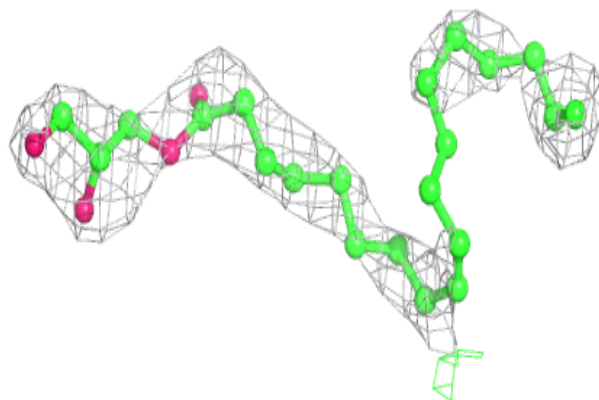


Electron density around PE5 A 305:

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

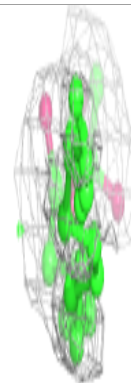
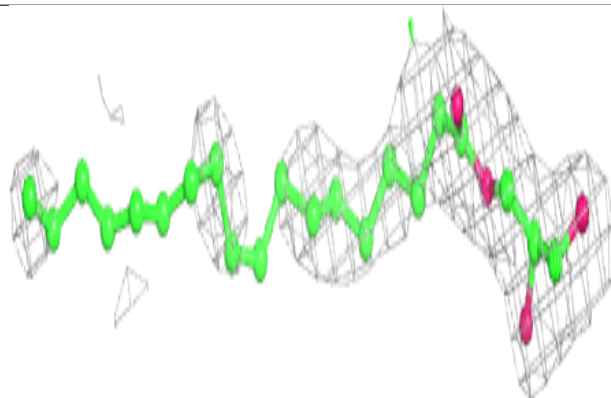
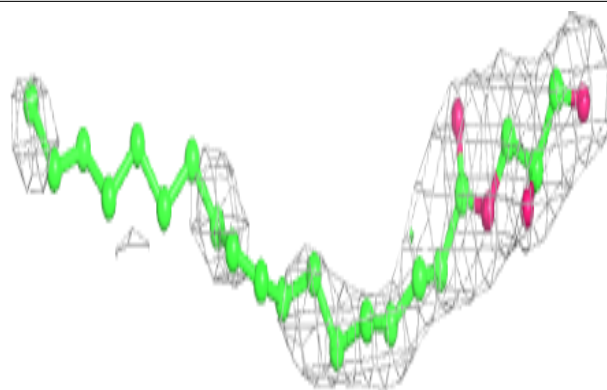
**Electron density around OLC A 304:**

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

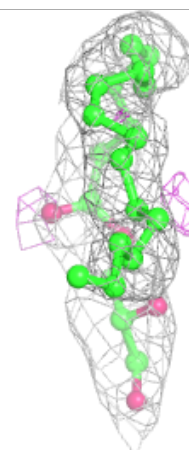
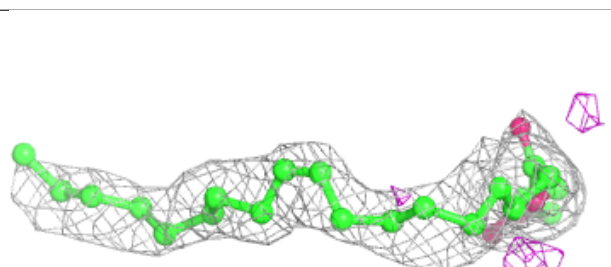
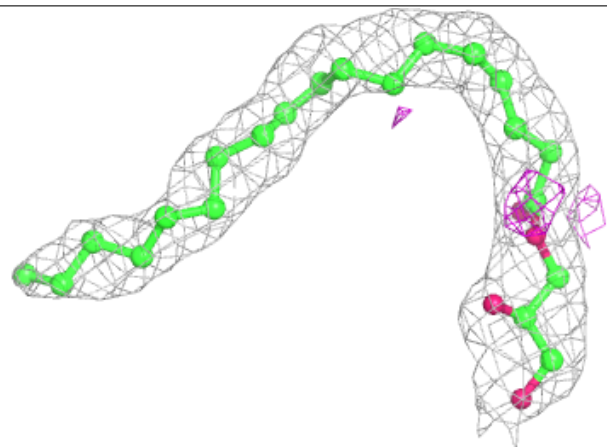


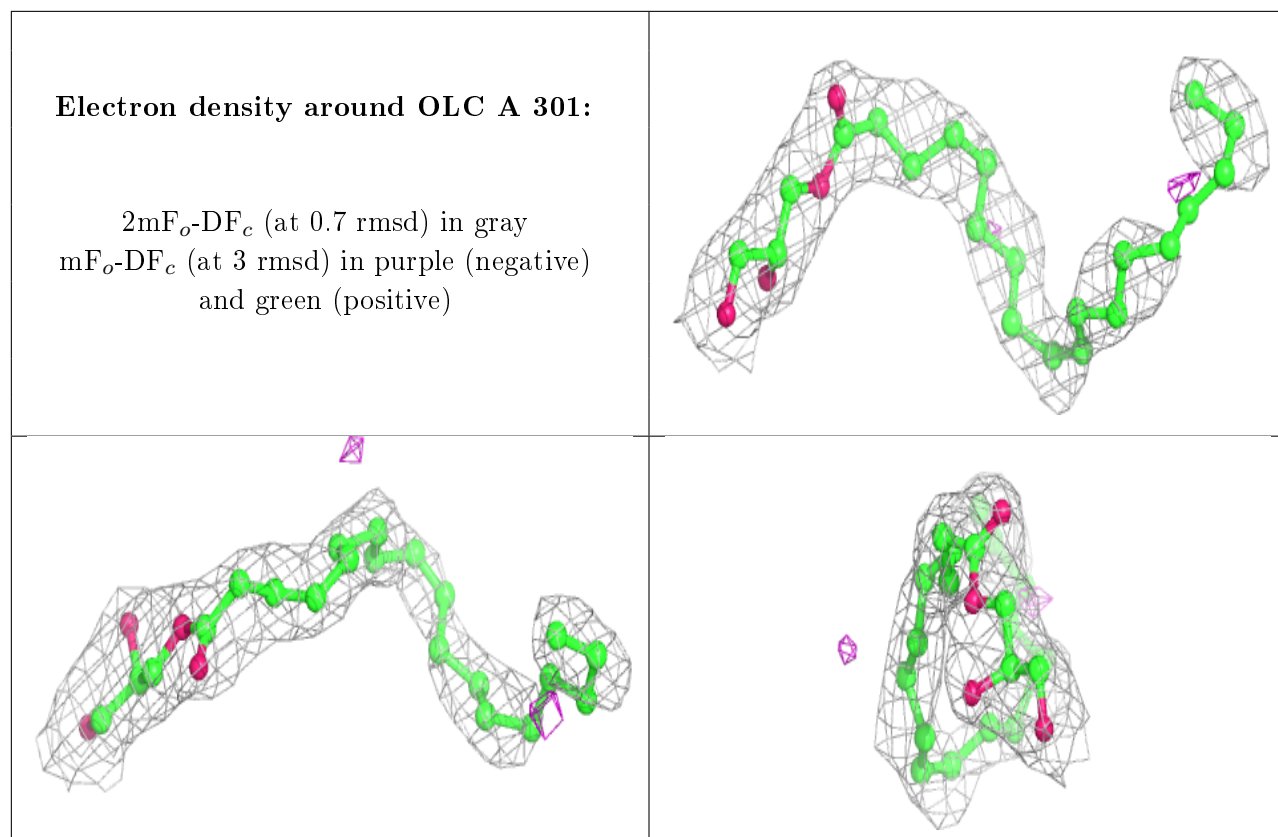
Electron density around OLC B 303:

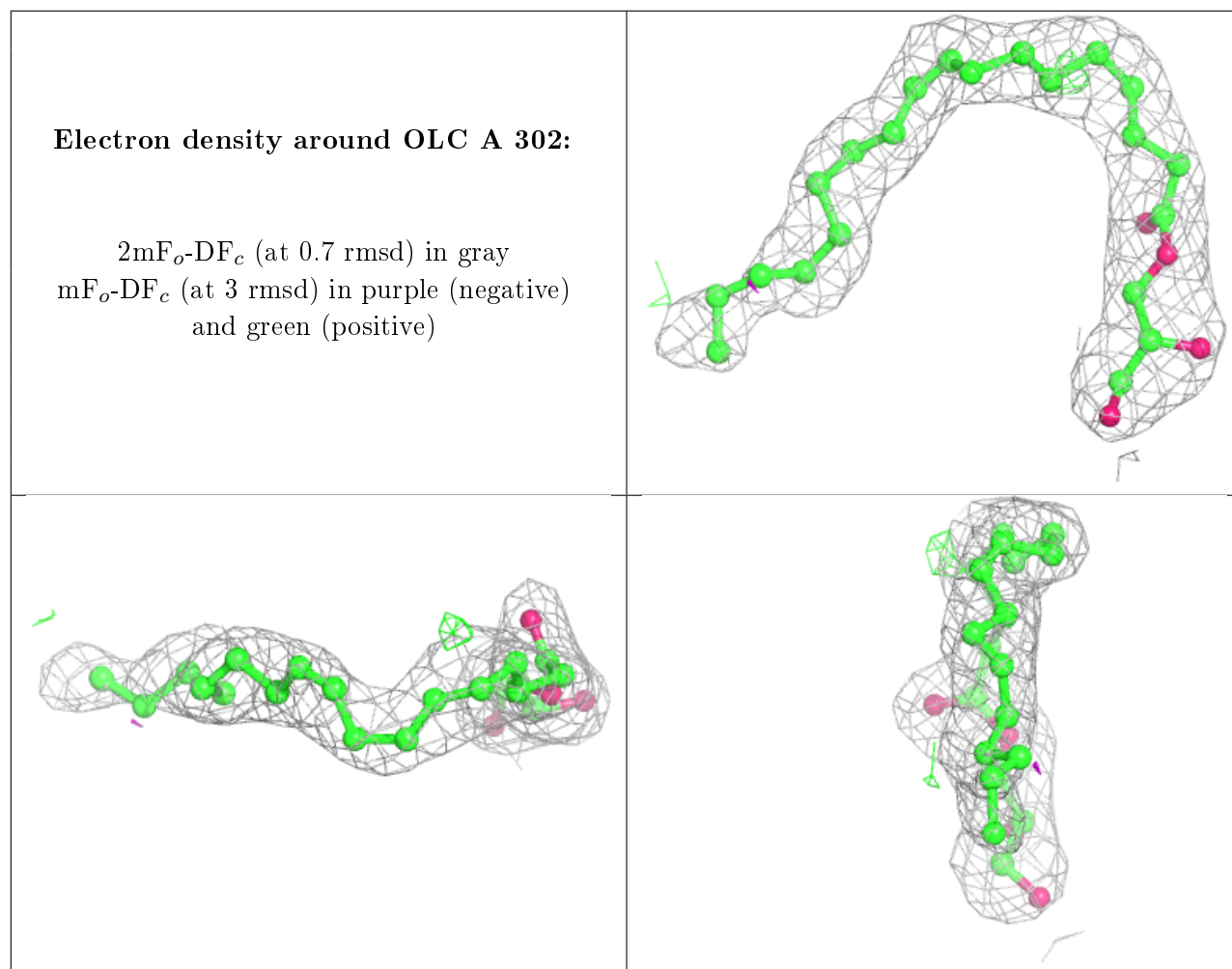
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around OLC 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 [i](#)

There are no such residues in this entry.