Full wwPDB X-ray Structure Validation Report ⓘ

Dec 1, 2021 – 12:09 pm GMT

PDB ID	:	7B1K
Title	:	Crystal structure of phosphatidyl serine synthase (PSS) in the closed conformation with bound citrate.
Authors	:	Yildiz, O.; Centola, M.
Deposited on	:	2020-11-25
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

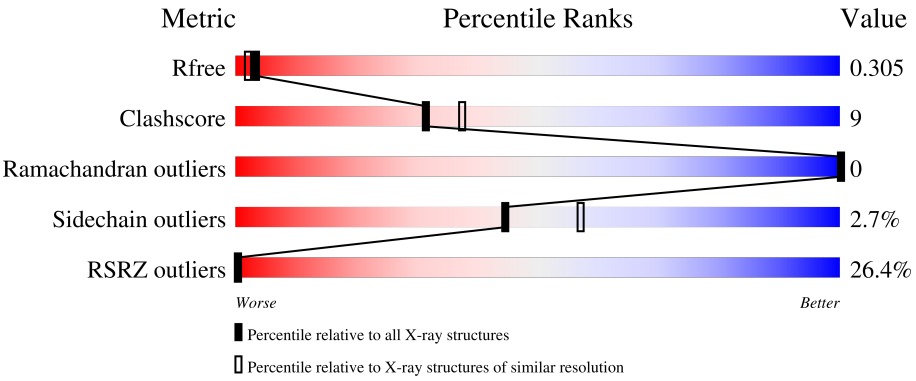
MolProbity	:	4.02b-467
Mogul	:	1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	225	24% 72% 17% 11%
1	B	225	23% 69% 20% · 10%

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
6	FLC	B	307	-	-	-	X
7	NA	A	307	-	-	-	X
7	NA	B	310	-	-	-	X
8	OLC	A	309	-	-	-	X
8	OLC	A	310	-	-	-	X
8	OLC	A	311	-	-	-	X
8	OLC	B	308	-	-	-	X
8	OLC	B	309	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 3455 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 CDP-diacylglycerol--serine O-phosphatidyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	0	0
			1543	1039	234	261	9			
1	B	202	Total	C	N	O	S	0	0	0
			1556	1046	236	265	9			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q58609
A	-20	GLY	-	expression tag	UNP Q58609
A	-19	SER	-	expression tag	UNP Q58609
A	-18	SER	-	expression tag	UNP Q58609
A	-17	HIS	-	expression tag	UNP Q58609
A	-16	HIS	-	expression tag	UNP Q58609
A	-15	HIS	-	expression tag	UNP Q58609
A	-14	HIS	-	expression tag	UNP Q58609
A	-13	HIS	-	expression tag	UNP Q58609
A	-12	HIS	-	expression tag	UNP Q58609
A	-11	SER	-	expression tag	UNP Q58609
A	-10	SER	-	expression tag	UNP Q58609
A	-9	GLY	-	expression tag	UNP Q58609
A	-8	LEU	-	expression tag	UNP Q58609
A	-7	GLU	-	expression tag	UNP Q58609
A	-6	VAL	-	expression tag	UNP Q58609
A	-5	LEU	-	expression tag	UNP Q58609
A	-4	PHE	-	expression tag	UNP Q58609
A	-3	GLN	-	expression tag	UNP Q58609
A	-2	GLY	-	expression tag	UNP Q58609
A	-1	PRO	-	expression tag	UNP Q58609
A	0	HIS	-	expression tag	UNP Q58609
A	202	LEU	-	expression tag	UNP Q58609
A	203	GLU	-	expression tag	UNP Q58609
B	-21	MET	-	initiating methionine	UNP Q58609

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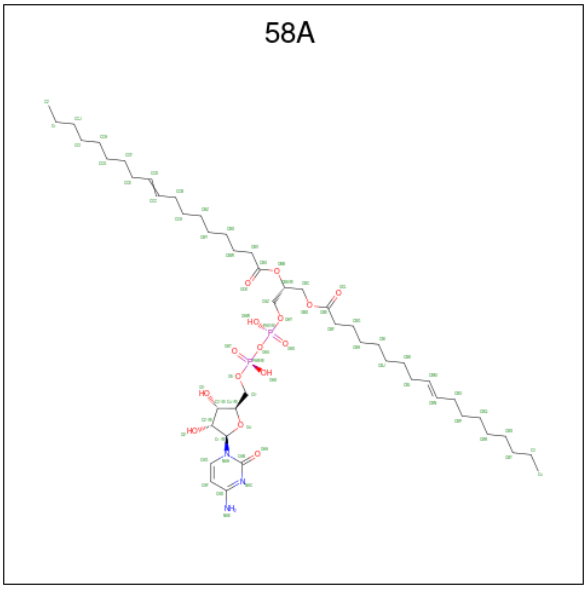
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	GLY	-	expression tag	UNP Q58609
B	-19	SER	-	expression tag	UNP Q58609
B	-18	SER	-	expression tag	UNP Q58609
B	-17	HIS	-	expression tag	UNP Q58609
B	-16	HIS	-	expression tag	UNP Q58609
B	-15	HIS	-	expression tag	UNP Q58609
B	-14	HIS	-	expression tag	UNP Q58609
B	-13	HIS	-	expression tag	UNP Q58609
B	-12	HIS	-	expression tag	UNP Q58609
B	-11	SER	-	expression tag	UNP Q58609
B	-10	SER	-	expression tag	UNP Q58609
B	-9	GLY	-	expression tag	UNP Q58609
B	-8	LEU	-	expression tag	UNP Q58609
B	-7	GLU	-	expression tag	UNP Q58609
B	-6	VAL	-	expression tag	UNP Q58609
B	-5	LEU	-	expression tag	UNP Q58609
B	-4	PHE	-	expression tag	UNP Q58609
B	-3	GLN	-	expression tag	UNP Q58609
B	-2	GLY	-	expression tag	UNP Q58609
B	-1	PRO	-	expression tag	UNP Q58609
B	0	HIS	-	expression tag	UNP Q58609
B	202	LEU	-	expression tag	UNP Q58609
B	203	GLU	-	expression tag	UNP Q58609

- Molecule 2 is 5'-O-[(R)-{[(S)-{(2R)-2,3-bis[(9E)-octadec-9-enoyloxy]propoxy}(hydroxy)phosphoryl]oxy}(hydroxy)phosphoryl]cytidine (three-letter code: 58A) (formula: $C_{48}H_{85}N_3O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			64	44	3	15	2		
2	B	1	Total	C	N	O	P	0	0
			64	44	3	15	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

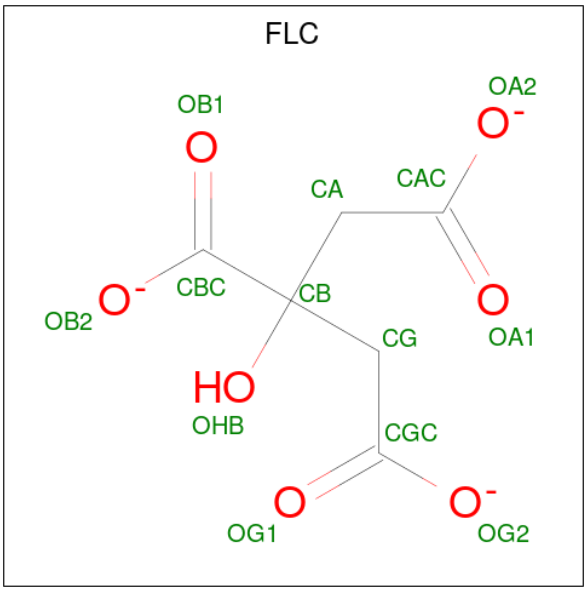
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Cl	0	0
			2	2		
5	B	2	Total	Cl	0	0
			2	2		

- Molecule 6 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).

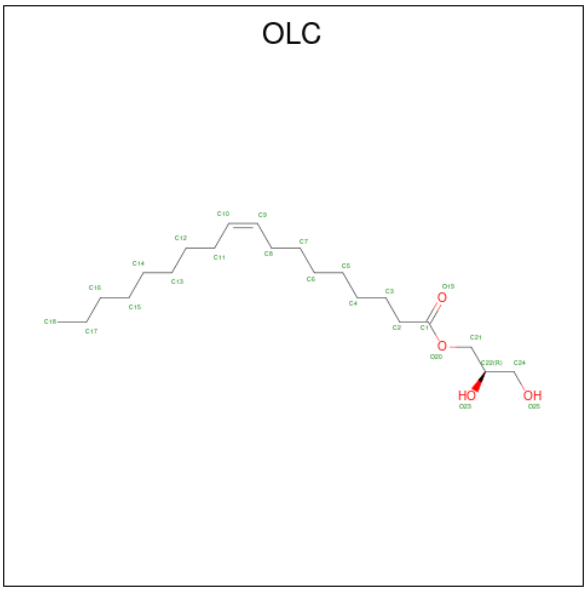


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 13 6 7	0	0
6	B	1	Total C O 13 6 7	0	0
6	B	1	Total C O 13 6 7	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Na 1 1	0	0
7	B	1	Total Na 1 1	0	0

- Molecule 8 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



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

- Molecule 9 is water.

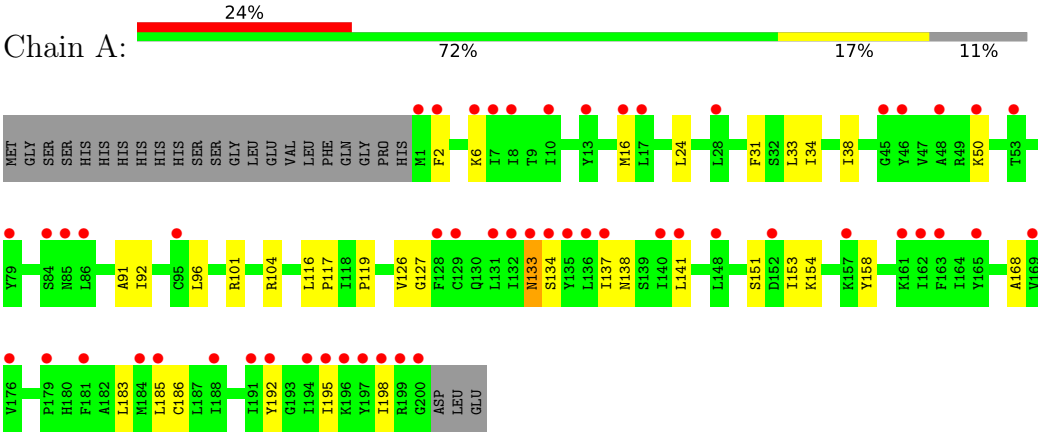
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	16	Total O 16 16	0	0
9	B	13	Total O 13 13	0	0

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.

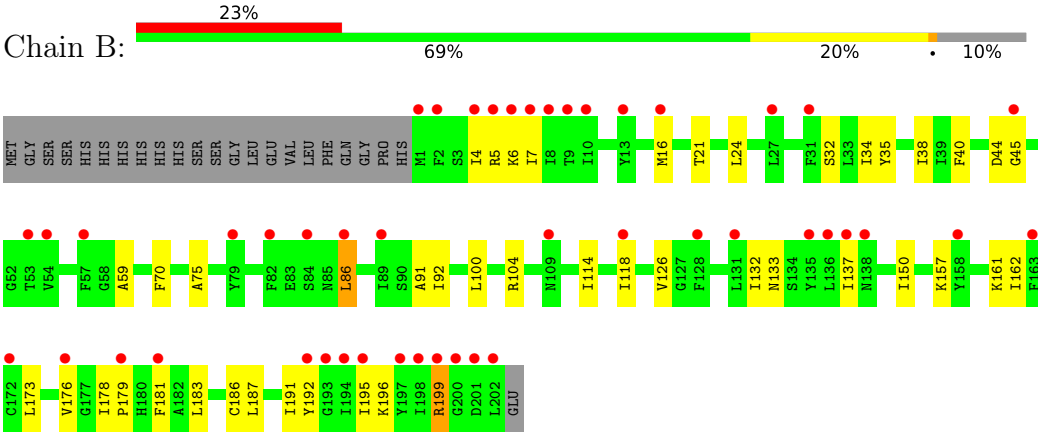
• Molecule 1: CDP-diacylglycerol--serine O-phosphatidyltransferase

Chain A:



• Molecule 1: CDP-diacylglycerol--serine O-phosphatidyltransferase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.31Å 70.76Å 95.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.00 – 2.20 56.86 – 2.20	Depositor EDS
% Data completeness (in resolution range)	75.2 (57.00-2.20) 86.1 (56.86-2.20)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.17 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.19rc5_4047	Depositor
R, R_{free}	0.254 , 0.307 0.251 , 0.305	Depositor DCC
R_{free} test set	835 reflections (3.93%)	wwPDB-VP
Wilson B-factor (Å^2)	29.8	Xtriage
Anisotropy	0.789	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3455	wwPDB-VP
Average B, all atoms (Å^2)	52.0	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 61.00 % 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 1.3985e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FLC, MG, NA, OLC, 58A, CA, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.25	0/1574	0.42	0/2138
1	B	0.25	0/1587	0.42	0/2156
All	All	0.25	0/3161	0.42	0/4294

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	1543	0	1647	25	0
1	B	1556	0	1657	35	0
2	A	64	0	69	7	0
2	B	64	0	69	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	1	0
6	A	13	0	5	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	26	0	10	2	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	100	0	160	2	0
8	B	50	0	80	2	0
9	A	16	0	0	1	0
9	B	13	0	0	1	0
All	All	3455	0	3697	64	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 (64) 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:96:LEU:HD11	1:B:16:MET:HG2	1.72	0.72
1:B:132:ILE:HD11	8:B:308:OLC:H9	1.74	0.70
1:B:166:ILE:HG21	2:B:301:58A:H77	1.78	0.64
1:A:31:PHE:HD2	1:A:126:VAL:HG13	1.65	0.61
1:B:157:LYS:NZ	6:B:306:FLC:OG2	2.35	0.60
1:B:187:LEU:O	1:B:191:ILE:HG13	2.02	0.59
6:A:306:FLC:OG2	6:A:306:FLC:OHB	2.22	0.58
1:A:151:SER:OG	1:A:153:ILE:HG13	2.05	0.56
1:B:70:PHE:HB2	1:B:118:ILE:HG12	1.89	0.55
2:A:301:58A:H65	2:A:301:58A:H24	1.89	0.53
1:B:196:LYS:HA	1:B:199:ARG:HG2	1.90	0.53
1:B:75:ALA:HB1	1:B:91:ALA:HB1	1.90	0.53
1:A:24:LEU:HD13	1:B:92:ILE:HD11	1.91	0.52
1:A:24:LEU:HB3	1:A:33:LEU:HD13	1.90	0.52
1:B:191:ILE:O	1:B:195:ILE:HG12	2.09	0.52
1:A:104:ARG:NH2	1:A:151:SER:O	2.43	0.52
1:B:44:ASP:OD1	1:B:45:GLY:N	2.43	0.51
1:A:154:LYS:NZ	9:A:404:HOH:O	2.43	0.51
1:A:158:TYR:HB2	2:A:301:58A:H30	1.92	0.50
2:A:301:58A:H4	2:A:301:58A:H11	1.94	0.50
2:B:301:58A:H29	2:B:301:58A:H65	1.93	0.50
1:B:104:ARG:NH1	9:B:401:HOH:O	2.40	0.49
1:B:5:ARG:HE	1:B:6:LYS:HE2	1.77	0.49
1:B:173:LEU:HD13	1:B:181:PHE:HD2	1.78	0.49
1:A:133:ASN:O	1:A:133:ASN:ND2	2.46	0.48
1:A:192:TYR:HE2	2:A:301:58A:H36	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:VAL:HG23	1:B:178:ILE:HD12	1.95	0.48
1:B:118:ILE:HG22	5:B:304:CL:CL	2.50	0.47
1:B:157:LYS:HZ2	6:B:306:FLC:CGC	2.26	0.47
1:A:127:GLY:HA3	1:A:183:LEU:HD13	1.94	0.47
1:A:175:ILE:HG22	8:A:308:OLC:H11A	1.96	0.47
1:B:4:ILE:HD12	1:B:7:ILE:HD11	1.96	0.47
1:A:134:SER:HB3	1:A:137:ILE:HB	1.96	0.47
1:B:86:LEU:HD12	1:B:86:LEU:HA	1.72	0.46
1:B:21:THR:HG21	1:B:40:PHE:HE2	1.80	0.46
2:A:301:58A:H44	2:A:301:58A:H38	1.60	0.46
1:B:173:LEU:HD13	1:B:181:PHE:CD2	2.51	0.46
1:A:34:ILE:O	1:A:38:ILE:HG13	2.16	0.45
1:A:185:LEU:HD23	2:A:301:58A:H70	1.97	0.45
1:A:168:ALA:HA	1:A:171:LEU:HD12	1.97	0.45
1:A:195:ILE:HA	1:A:198:ILE:HG12	1.99	0.45
1:A:75:ALA:HB1	1:A:91:ALA:HB1	1.99	0.45
2:A:301:58A:H65	2:A:301:58A:H60	1.67	0.45
1:A:92:ILE:HD11	1:B:24:LEU:HD21	2.00	0.44
1:B:34:ILE:HG21	1:B:126:VAL:HG21	2.00	0.44
1:A:50:LYS:HD3	1:A:50:LYS:HA	1.68	0.43
1:B:32:SER:HA	1:B:35:TYR:HD2	1.82	0.43
1:B:59:ALA:HB2	2:B:301:58A:H6	2.01	0.42
2:B:301:58A:H77	2:B:301:58A:H72	1.32	0.42
2:B:301:58A:H25	2:B:301:58A:H18	1.78	0.42
1:B:161:LYS:HB2	1:B:161:LYS:HE3	1.87	0.42
1:B:162:ILE:H	1:B:162:ILE:HD12	1.84	0.42
1:A:138:ASN:HA	1:A:141:LEU:HD12	2.01	0.42
1:B:104:ARG:NH2	1:B:114:ILE:O	2.52	0.42
8:A:309:OLC:H4	8:A:309:OLC:H7A	1.78	0.41
1:B:137:ILE:HG23	8:B:309:OLC:H15	2.01	0.41
1:A:116:LEU:HD12	1:A:117:PRO:HD2	2.03	0.41
1:B:34:ILE:O	1:B:38:ILE:HG13	2.20	0.41
1:B:187:LEU:HD23	1:B:187:LEU:HA	1.82	0.41
1:A:2:PHE:HE1	1:B:150:ILE:HG13	1.85	0.41
1:A:117:PRO:HB2	1:A:119:PRO:HD2	2.02	0.41
1:A:16:MET:SD	1:B:100:LEU:HD21	2.61	0.41
1:B:192:TYR:CZ	2:B:301:58A:H45	2.57	0.40
1:B:179:PRO:O	1:B:183:LEU:HB2	2.22	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	198/225 (88%)	189 (96%)	9 (4%)	0	100	100
1	B	200/225 (89%)	195 (98%)	5 (2%)	0	100	100
All	All	398/450 (88%)	384 (96%)	14 (4%)	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	169/191 (88%)	164 (97%)	5 (3%)	41	53
1	B	170/191 (89%)	166 (98%)	4 (2%)	49	62
All	All	339/382 (89%)	330 (97%)	9 (3%)	44	57

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	65	SER
1	A	101	ARG
1	A	133	ASN
1	A	186	CYS
1	B	86	LEU
1	B	133	ASN
1	B	186	CYS

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Mol	Chain	Res	Type
1	B	199	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 21 ligands modelled in this entry, 10 are monoatomic - leaving 11 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

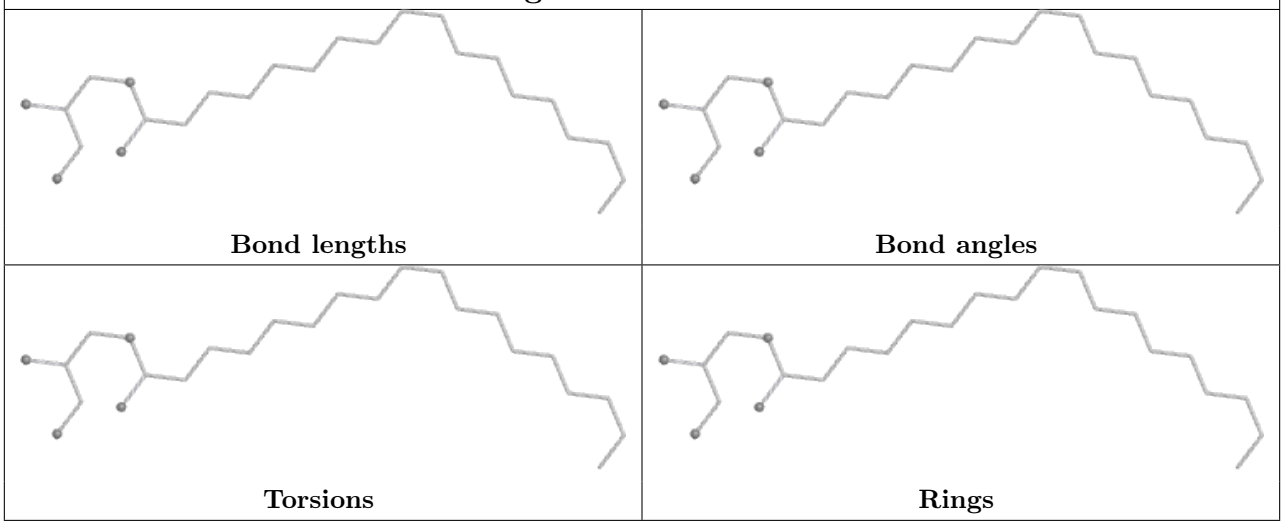
There are no ring outliers.

No monomer is involved in short contacts.

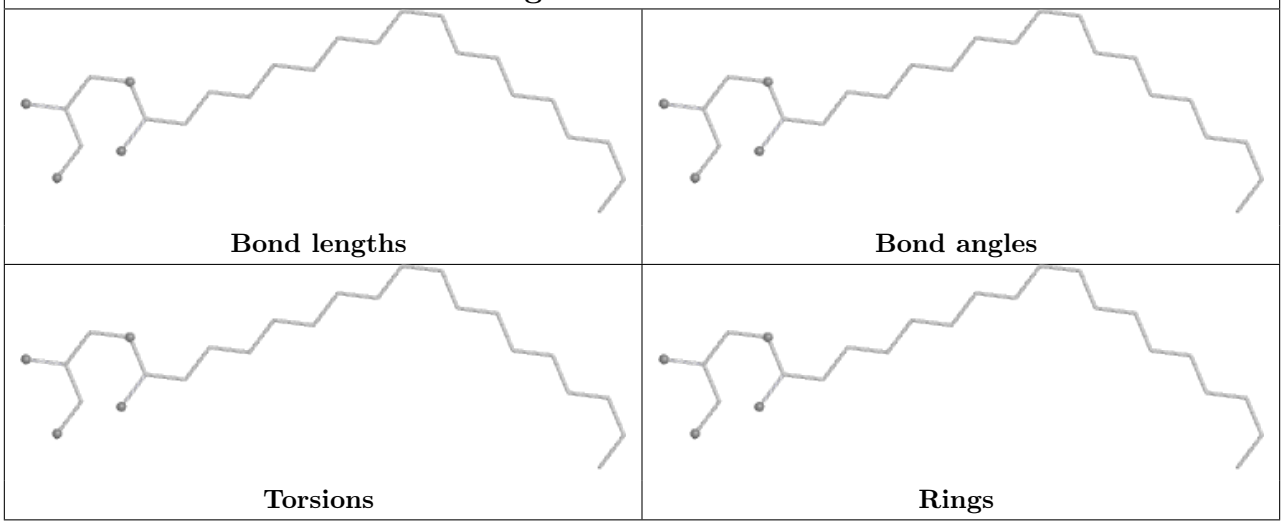
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

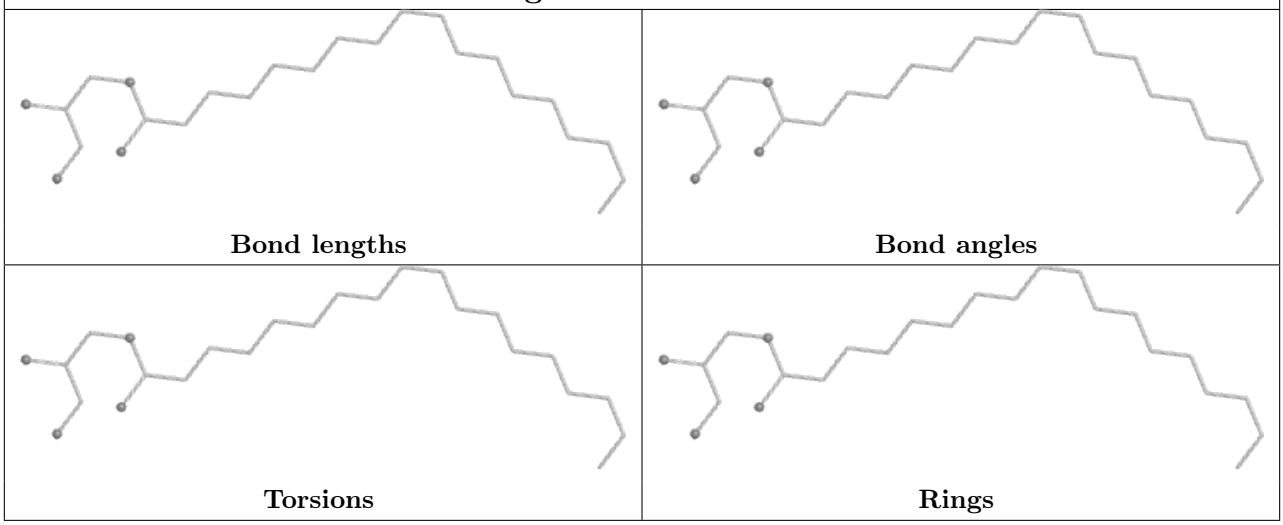
Ligand OLC A 309

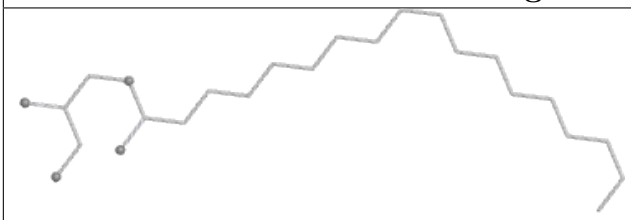
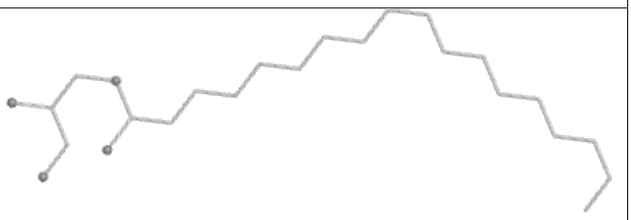
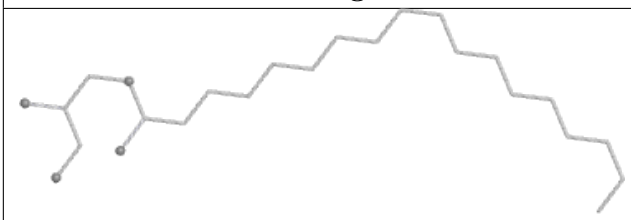
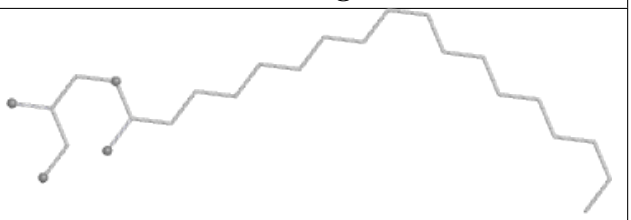


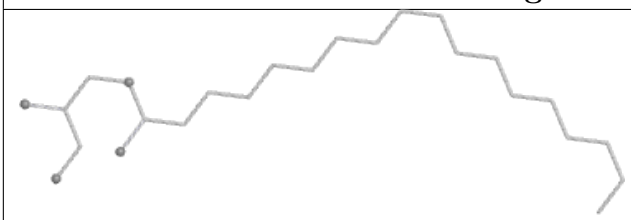
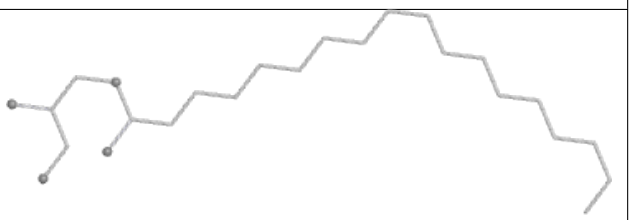
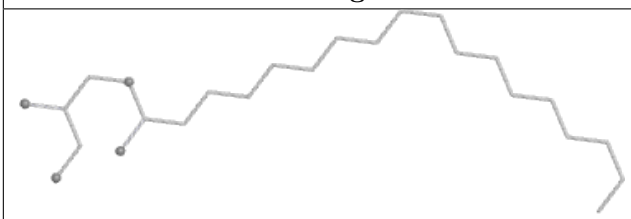
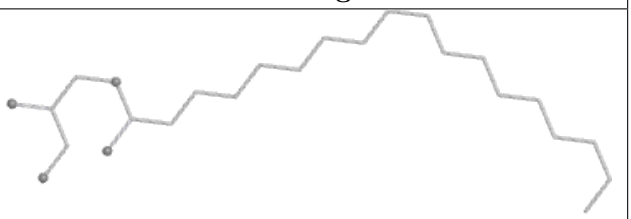
Ligand OLC A 310



Ligand OLC A 311



Ligand OLC B 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand OLC B 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

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^{th} 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	200/225 (88%)	1.58	55 (27%)	0	0	27, 45, 72, 106	0
1	B	202/225 (89%)	1.50	51 (25%)	0	0	28, 46, 69, 131	0
All	All	402/450 (89%)	1.54	106 (26%)	0	0	27, 46, 72, 131	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	198	ILE	11.1
1	A	1	MET	9.1
1	B	13	TYR	7.9
1	B	201	ASP	6.3
1	B	86	LEU	5.8
1	B	10	ILE	5.5
1	A	13	TYR	5.4
1	B	4	ILE	5.3
1	B	197	TYR	5.0
1	B	2	PHE	5.0
1	A	136	LEU	4.9
1	B	200	GLY	4.8
1	B	1	MET	4.6
1	B	50	LYS	4.5
1	B	8	ILE	4.3
1	A	165	TYR	4.1
1	B	202	LEU	4.0
1	A	141	LEU	4.0
1	A	135	TYR	3.9
1	A	195	ILE	3.9
1	B	9	THR	3.8
1	A	86	LEU	3.8
1	B	181	PHE	3.8
1	A	197	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	199	ARG	3.7
1	B	31	PHE	3.6
1	B	179	PRO	3.4
1	A	7	ILE	3.4
1	A	85	ASN	3.4
1	B	109	ASN	3.3
1	B	194	ILE	3.3
1	A	134	SER	3.3
1	B	195	ILE	3.2
1	B	198	ILE	3.2
1	A	128	PHE	3.2
1	A	50	LYS	3.2
1	A	199	ARG	3.2
1	A	184	MET	3.2
1	A	163	PHE	3.2
1	A	161	LYS	3.0
1	B	84	SER	3.0
1	B	57	PHE	3.0
1	B	82	PHE	3.0
1	B	138	ASN	2.9
1	A	176	VAL	2.9
1	A	132	ILE	2.8
1	B	118	ILE	2.8
1	B	193	GLY	2.8
1	A	188	ILE	2.8
1	B	54	VAL	2.8
1	B	16	MET	2.8
1	B	51	THR	2.8
1	A	192	TYR	2.8
1	A	152	ASP	2.7
1	A	10	ILE	2.7
1	A	140	ILE	2.7
1	B	136	LEU	2.7
1	B	5	ARG	2.7
1	A	181	PHE	2.7
1	B	137	ILE	2.7
1	B	89	ILE	2.6
1	A	8	ILE	2.6
1	A	2	PHE	2.6
1	B	131	LEU	2.6
1	B	7	ILE	2.5
1	A	175	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	169	VAL	2.5
1	A	196	LYS	2.5
1	A	46	TYR	2.5
1	B	192	TYR	2.5
1	A	28	LEU	2.5
1	A	6	LYS	2.4
1	A	162	ILE	2.4
1	B	27	LEU	2.4
1	B	79	TYR	2.4
1	A	185	LEU	2.4
1	B	53	THR	2.4
1	B	163	PHE	2.4
1	B	135	TYR	2.4
1	A	79	TYR	2.3
1	B	6	LYS	2.3
1	A	137	ILE	2.3
1	A	194	ILE	2.3
1	A	45	GLY	2.3
1	A	157	LYS	2.3
1	A	48	ALA	2.3
1	A	16	MET	2.2
1	A	129	CYS	2.2
1	A	191	ILE	2.2
1	B	158	TYR	2.2
1	A	95	CYS	2.2
1	B	48	ALA	2.2
1	A	53	THR	2.1
1	B	176	VAL	2.1
1	B	166	ILE	2.1
1	A	84	SER	2.1
1	A	148	LEU	2.1
1	B	128	PHE	2.1
1	B	45	GLY	2.1
1	A	133	ASN	2.1
1	B	172	CYS	2.1
1	A	131	LEU	2.0
1	A	179	PRO	2.0
1	A	17	LEU	2.0
1	B	165	TYR	2.0
1	A	200	GLY	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)

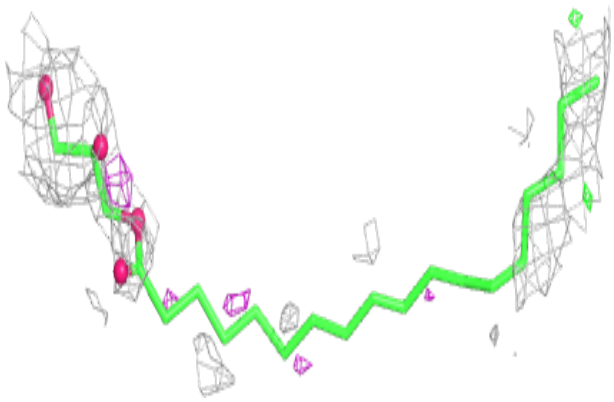
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

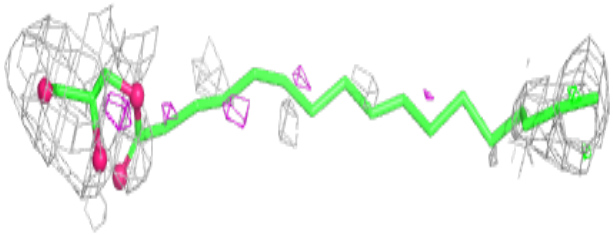
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NA	B	310	1/1	-0.25	0.44	57,57,57,57	0
8	OLC	A	310	25/25	0.18	0.64	59,72,91,95	0
8	OLC	A	311	25/25	0.21	0.63	46,89,110,114	0
6	FLC	B	306	13/13	0.27	0.34	126,129,141,142	0
5	CL	B	304	1/1	0.30	0.22	47,47,47,47	0
8	OLC	A	309	25/25	0.35	0.72	59,84,102,115	0
8	OLC	B	308	25/25	0.39	0.95	46,79,97,100	0
8	OLC	B	309	25/25	0.41	0.70	65,84,118,134	0
8	OLC	A	308	25/25	0.44	0.32	49,61,86,90	0
7	NA	A	307	1/1	0.46	0.45	49,49,49,49	0
6	FLC	B	307	13/13	0.46	0.45	87,102,122,126	0
3	CA	A	302	1/1	0.49	0.15	47,47,47,47	0
3	CA	B	302	1/1	0.53	0.10	55,55,55,55	0
6	FLC	A	306	13/13	0.55	0.29	100,108,113,113	0
5	CL	A	304	1/1	0.65	0.14	39,39,39,39	0
5	CL	A	305	1/1	0.72	0.18	46,46,46,46	0
4	MG	B	303	1/1	0.73	0.19	50,50,50,50	0
4	MG	A	303	1/1	0.74	0.09	49,49,49,49	0
2	58A	B	301	64/68	0.78	0.24	35,62,84,95	0
2	58A	A	301	64/68	0.79	0.23	28,54,74,87	0
5	CL	B	305	1/1	0.88	0.08	54,54,54,54	0

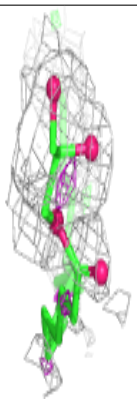
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 310:

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

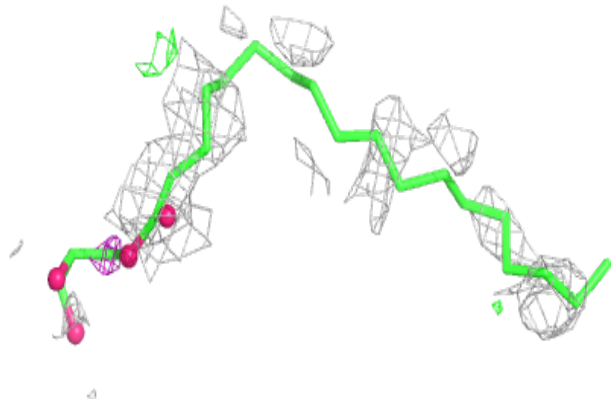


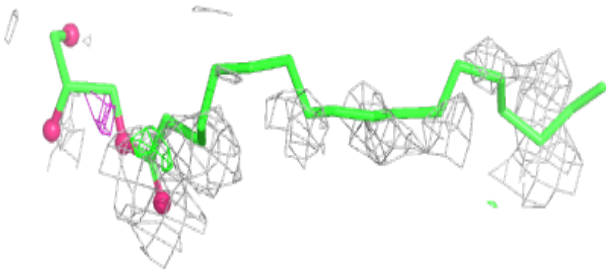




Electron density around OLC A 311:

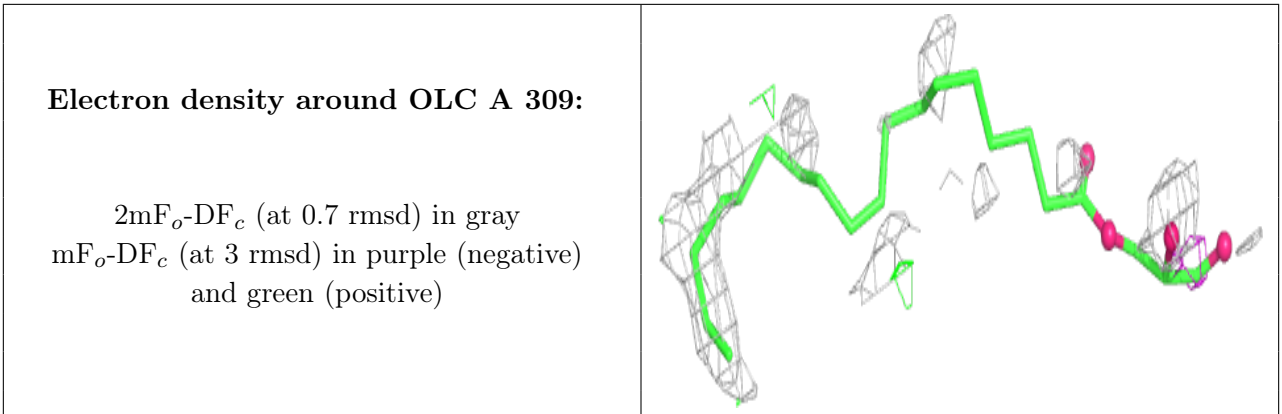
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

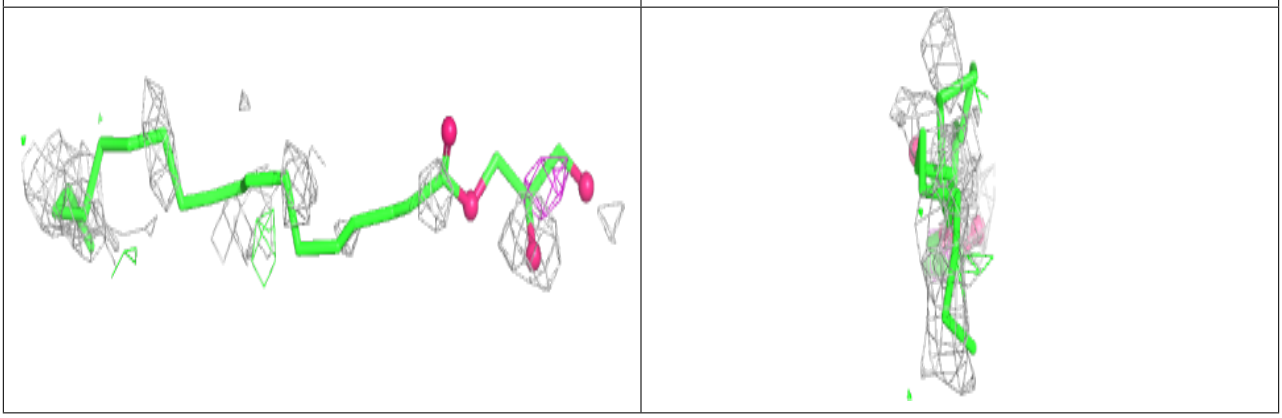




Electron density around OLC A 309:

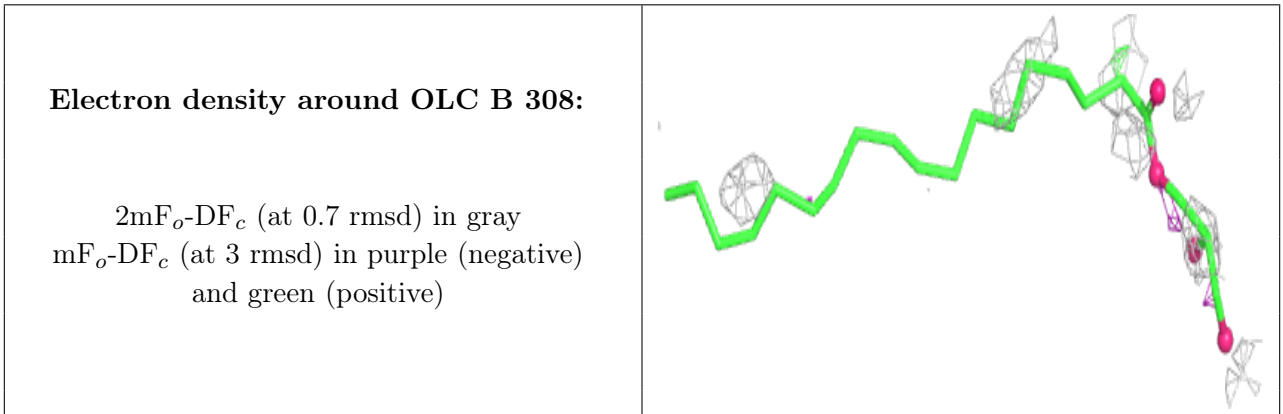
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

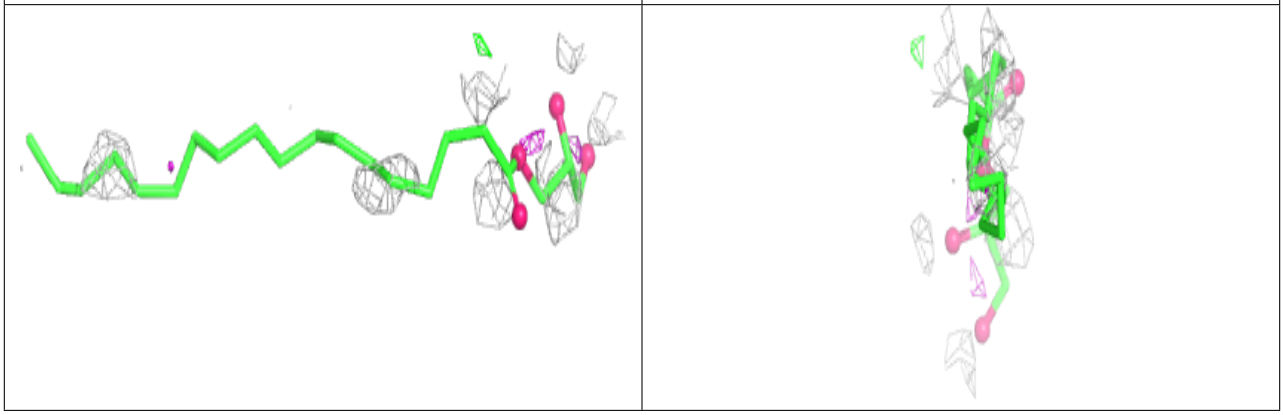




Electron density around OLC B 308:

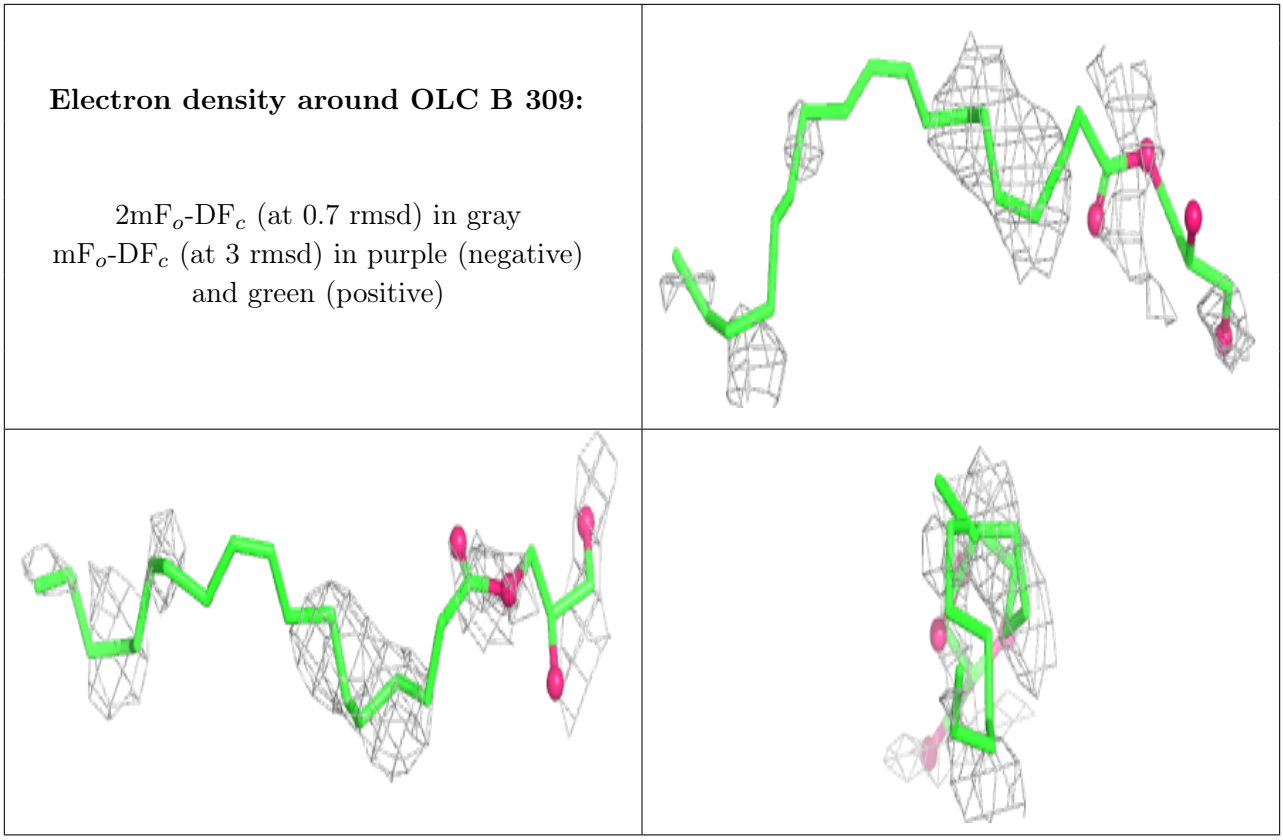
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around OLC B 309:

$2mF_o$-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.