



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:03 PM EDT

PDB ID : 7B1K / pdb_00007b1k
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 types of validation reports are described at

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

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

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

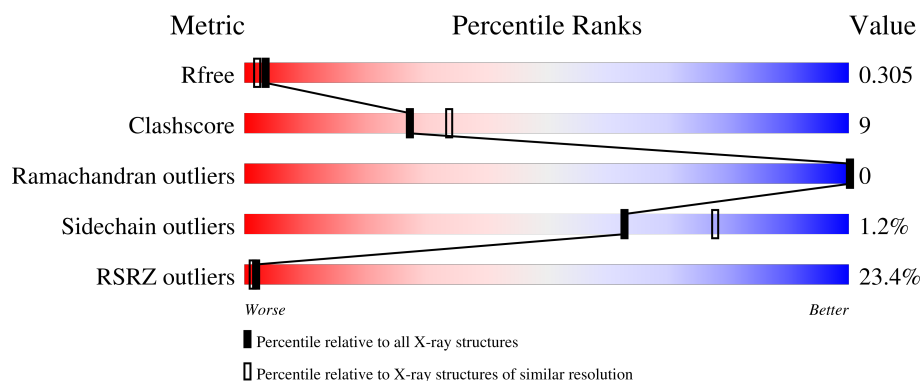
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 $\leq 5\%$. 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	225	23% 73% 16% 11%
1	B	225	19% 69% 20% 10%

2 Entry composition

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:

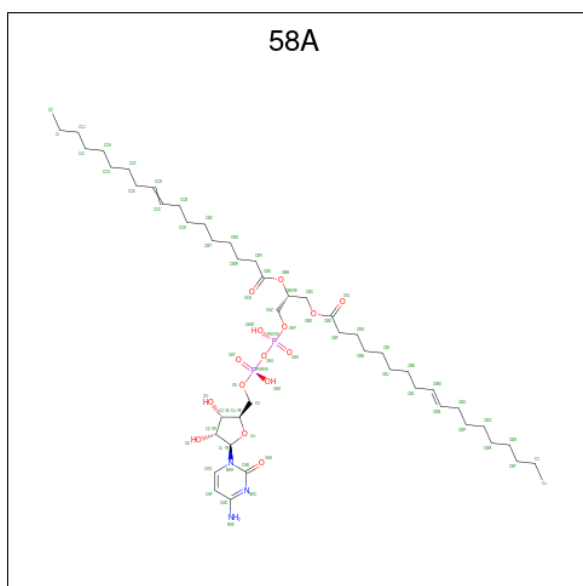
Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q58609
A	-20	GLY	-	expression tag	UNP Q58609
A	-19	SER	-	expression tag	UNP Q58609
A	-18	SER	-	expression tag	UNP Q58609
A	-17	HIS	-	expression tag	UNP Q58609
A	-16	HIS	-	expression tag	UNP Q58609
A	-15	HIS	-	expression 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

Continued on next page...

Continued from previous page...

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 (CCD ID: 58A) (formula: C₄₈H₈₅N₃O₁₅P₂).



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 (CCD ID: 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		

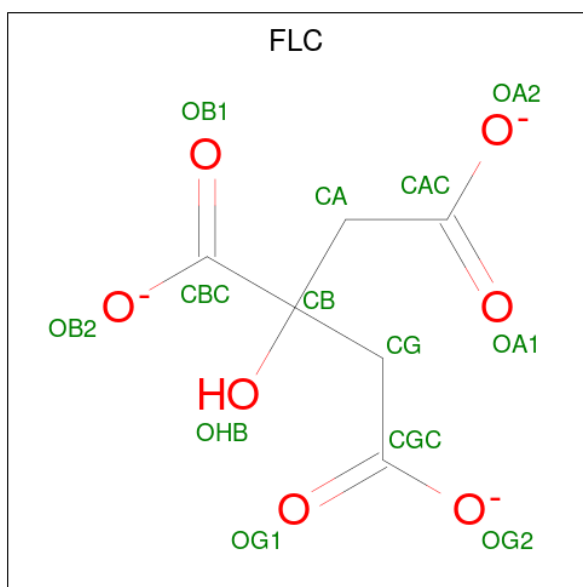
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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 (CCD ID: 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 (CCD ID: FLC) (formula: C₆H₅O₇).

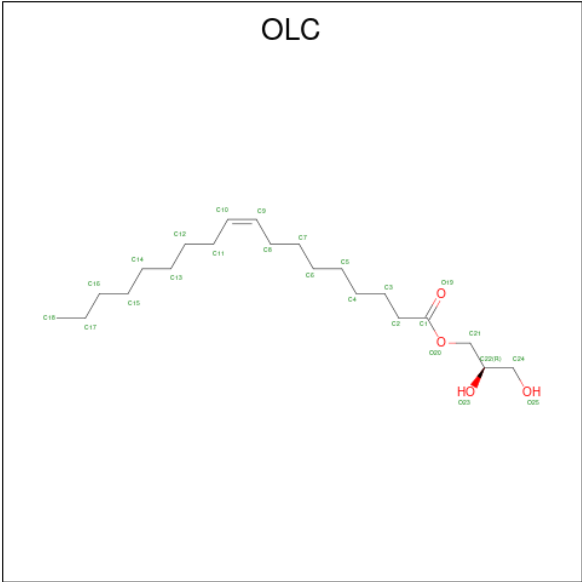


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	6	7		
6	B	1	Total	C	O	0	0
			13	6	7		
6	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 8 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: C₂₁H₄₀O₄).



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

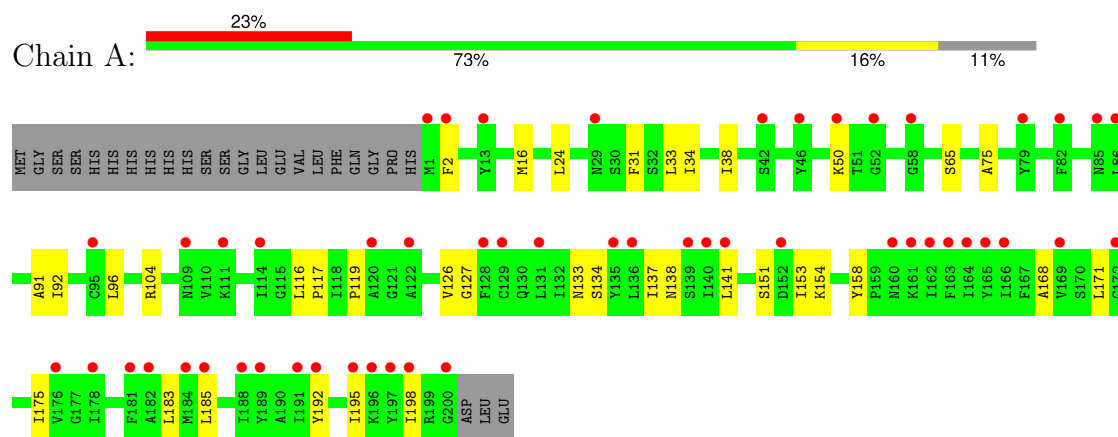
- Molecule 9 is water.

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

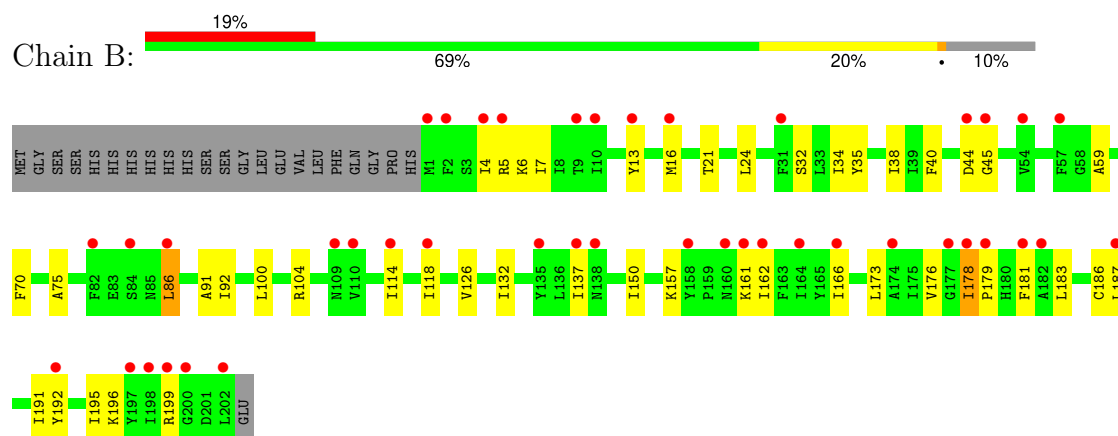
3 Residue-property plots [i](#)

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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	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 57.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	75.2 (57.00-2.20) 86.1 (57.00-2.20)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.17 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.19rc5_4047	Depositor
R, R_{free}	0.254 , 0.307 0.252 , 0.305	Depositor DCC
R_{free} test set	835 reflections (2.28%)	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)	0.34 , 66.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	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.*

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: NA, CL, CA, MG, 58A, OLC, FLC

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	0.10	0/1574	0.26	0/2138
1	B	0.10	0/1587	0.27	0/2156
All	All	0.10	0/3161	0.27	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	36	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

Continued on next page...

Continued from previous page...

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	65	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 (65) 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:13:TYR:HA	1:B:16:MET:HE3	1.91	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:TYR:HE2	2:A:301:58A:H36	1.78	0.48
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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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%)	168 (99%)	1 (1%)	78	89
1	B	170/191 (89%)	167 (98%)	3 (2%)	51	68
All	All	339/382 (89%)	335 (99%)	4 (1%)	63	78

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

Mol	Chain	Res	Type
1	A	65	SER
1	B	86	LEU
1	B	178	ILE
1	B	186	CYS

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	85	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
8	OLC	A	310	-	24,24,24	0.82	2 (8%)	25,25,25	0.98	1 (4%)
6	FLC	A	306	-	12,12,12	1.21	1 (8%)	17,17,17	1.21	1 (5%)
2	58A	A	301	3,7	65,65,69	2.83	22 (33%)	78,82,86	1.01	2 (2%)
8	OLC	A	309	-	24,24,24	0.81	2 (8%)	25,25,25	0.98	1 (4%)
8	OLC	B	308	-	24,24,24	0.82	2 (8%)	25,25,25	0.95	1 (4%)
8	OLC	A	311	-	24,24,24	0.82	2 (8%)	25,25,25	0.99	1 (4%)
6	FLC	B	306	-	12,12,12	1.07	0	17,17,17	1.58	4 (23%)
8	OLC	A	308	-	24,24,24	0.81	2 (8%)	25,25,25	0.98	1 (4%)
2	58A	B	301	3	65,65,69	2.86	22 (33%)	78,82,86	0.98	2 (2%)
8	OLC	B	309	-	24,24,24	0.80	2 (8%)	25,25,25	0.96	1 (4%)
6	FLC	B	307	-	12,12,12	1.11	0	17,17,17	1.17	2 (11%)

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
8	OLC	A	310	-	-	11/24/24/24	-
6	FLC	A	306	-	-	11/16/16/16	-
2	58A	A	301	3,7	-	21/61/77/81	0/2/2/2
8	OLC	A	309	-	-	9/24/24/24	-
8	OLC	B	308	-	-	12/24/24/24	-
8	OLC	A	311	-	-	15/24/24/24	-
6	FLC	B	306	-	-	12/16/16/16	-
8	OLC	A	308	-	-	15/24/24/24	-
2	58A	B	301	3	-	35/61/77/81	0/2/2/2
8	OLC	B	309	-	-	13/24/24/24	-
6	FLC	B	307	-	-	5/16/16/16	-

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	58A	C3'-C2'	-10.81	1.24	1.53
2	A	301	58A	C3'-C2'	-10.76	1.24	1.53
2	B	301	58A	CAB-NAC	6.39	1.49	1.36
2	A	301	58A	CAG-CAF	6.38	1.49	1.35
2	A	301	58A	CAB-NAC	6.38	1.49	1.36
2	B	301	58A	CAG-CAF	6.38	1.49	1.35
2	B	301	58A	PAR-OAU	5.95	1.65	1.59
2	B	301	58A	CAD-NAC	5.71	1.45	1.34
2	A	301	58A	PAR-OAU	5.69	1.65	1.59
2	A	301	58A	CAD-NAC	5.67	1.45	1.34
2	B	301	58A	PAV-OAU	5.32	1.65	1.59
2	A	301	58A	CAD-NAE	5.27	1.46	1.33
2	B	301	58A	CAD-NAE	5.25	1.46	1.33
2	A	301	58A	PAV-OAU	5.11	1.65	1.59
2	B	301	58A	CAB-NAH	4.80	1.50	1.40
2	A	301	58A	CAB-NAH	4.78	1.50	1.40
2	A	301	58A	O4'-C1'	-4.68	1.31	1.42
2	B	301	58A	O4'-C1'	-4.61	1.31	1.42
2	B	301	58A	C2'-C1'	4.28	1.66	1.53
2	A	301	58A	C2'-C1'	4.27	1.66	1.53
2	A	301	58A	C5'-C4'	-4.21	1.38	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	58A	C5'-C4'	-4.17	1.39	1.51
2	B	301	58A	OBD-CBE	3.76	1.44	1.33
2	A	301	58A	OBD-CBE	3.63	1.43	1.33
2	B	301	58A	OBB-CBU	3.43	1.44	1.34
2	A	301	58A	CAG-NAH	3.35	1.46	1.38
2	B	301	58A	CAG-NAH	3.35	1.46	1.38
2	A	301	58A	OBB-CBU	3.33	1.43	1.34
2	A	301	58A	O3'-C3'	3.29	1.51	1.43
2	B	301	58A	O3'-C3'	3.27	1.51	1.43
2	A	301	58A	C3'-C4'	2.99	1.60	1.53
2	B	301	58A	C3'-C4'	2.95	1.60	1.53
2	A	301	58A	O4'-C4'	2.93	1.51	1.45
2	B	301	58A	O4'-C4'	2.93	1.51	1.45
2	B	301	58A	OAA-CAB	-2.62	1.18	1.23
2	A	301	58A	OAA-CAB	-2.56	1.18	1.23
2	B	301	58A	CAF-CAD	2.53	1.48	1.42
2	A	301	58A	CAF-CAD	2.53	1.48	1.42
8	A	311	OLC	O20-C1	2.46	1.40	1.33
8	B	308	OLC	O20-C1	2.43	1.40	1.33
8	A	308	OLC	O20-C1	2.39	1.40	1.33
8	A	309	OLC	O20-C1	2.38	1.40	1.33
8	A	310	OLC	O20-C1	2.37	1.40	1.33
8	B	309	OLC	O20-C1	2.33	1.40	1.33
2	A	301	58A	OBB-CBA	-2.30	1.41	1.46
6	A	306	FLC	CB-CBC	-2.27	1.51	1.53
2	B	301	58A	CBF-CBE	2.23	1.57	1.50
8	B	309	OLC	O20-C21	-2.23	1.40	1.45
8	A	310	OLC	O20-C21	-2.18	1.40	1.45
8	A	309	OLC	O20-C21	-2.18	1.40	1.45
8	A	308	OLC	O20-C21	-2.17	1.40	1.45
2	B	301	58A	OBB-CBA	-2.14	1.41	1.46
8	A	311	OLC	O20-C21	-2.13	1.40	1.45
8	B	308	OLC	O20-C21	-2.12	1.40	1.45
2	A	301	58A	O2'-C2'	2.11	1.48	1.43
2	B	301	58A	O2'-C2'	2.10	1.48	1.43
2	A	301	58A	CBF-CBE	2.09	1.56	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	58A	OBB-CBU-CBV	4.06	120.27	111.48
2	A	301	58A	OBB-CBU-CBV	3.79	119.67	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	306	FLC	OB2-CBC-CB	3.67	120.18	113.14
6	B	307	FLC	OB2-CBC-CB	3.12	119.13	113.14
8	A	311	OLC	O20-C1-C2	2.92	120.73	111.83
8	A	310	OLC	O20-C1-C2	2.84	120.50	111.83
8	B	308	OLC	O20-C1-C2	2.74	120.19	111.83
6	A	306	FLC	OB2-CBC-CB	2.70	118.32	113.14
2	B	301	58A	OBD-CBE-CBF	2.67	119.99	111.83
8	A	309	OLC	O20-C1-C2	2.66	119.94	111.83
8	A	308	OLC	O20-C1-C2	2.65	119.91	111.83
8	B	309	OLC	O20-C1-C2	2.58	119.72	111.83
2	A	301	58A	OBD-CBE-CBF	2.56	119.65	111.83
6	B	306	FLC	OB1-CBC-CB	-2.26	117.70	122.09
6	B	306	FLC	OG2-CGC-CG	2.22	121.38	114.35
6	B	307	FLC	OB1-CBC-CB	-2.05	118.12	122.09
6	B	306	FLC	OG1-CGC-CG	-2.04	117.18	122.95

There are no chirality outliers.

All (159) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	58A	CBV-CBU-OB2-CBA
2	A	301	58A	CBJ-CBK-CBL-CBM
2	B	301	58A	C5'-O5'-PAR-OAT
2	B	301	58A	CAZ-OAY-PAV-OAU
2	B	301	58A	CAZ-OAY-PAV-OAW
2	B	301	58A	CBV-CBU-OB2-CBA
6	A	306	FLC	CG-CB-CBC-OB2
6	A	306	FLC	CBC-CB-CG-CGC
6	A	306	FLC	OHB-CB-CG-CGC
6	B	306	FLC	CAC-CA-CB-CBC
6	B	306	FLC	CAC-CA-CB-CG
6	B	306	FLC	CAC-CA-CB-OHB
6	B	306	FLC	CG-CB-CBC-OB2
6	B	306	FLC	OHB-CB-CBC-OB1
6	B	306	FLC	OHB-CB-CBC-OB2
6	B	307	FLC	CG-CB-CBC-OB1
6	B	307	FLC	CG-CB-CBC-OB2
6	B	307	FLC	OHB-CB-CBC-OB1
6	B	307	FLC	OHB-CB-CBC-OB2
8	A	309	OLC	C21-C22-C24-O25
8	A	311	OLC	O20-C21-C22-O23
8	A	311	OLC	C2-C1-O20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	A	311	OLC	O19-C1-O20-C21
8	B	308	OLC	O20-C21-C22-C24
8	B	308	OLC	O20-C21-C22-O23
8	B	309	OLC	O20-C21-C22-C24
8	B	309	OLC	O20-C21-C22-O23
2	A	301	58A	OCK-CBU-OBB-CBA
2	B	301	58A	OCK-CBU-OBB-CBA
2	B	301	58A	O4'-C4'-C5'-O5'
2	B	301	58A	C3'-C4'-C5'-O5'
2	B	301	58A	CBP-CBQ-CBR-CBS
2	B	301	58A	CCF-CCG-CCH-CCI
6	A	306	FLC	CA-CB-CG-CGC
8	A	308	OLC	O20-C21-C22-O23
2	B	301	58A	CBF-CBE-OBD-CBC
8	A	310	OLC	C2-C1-O20-C21
2	B	301	58A	CBE-CBF-CBG-CBH
2	B	301	58A	OCL-CBE-OBD-CBC
8	A	308	OLC	C2-C1-O20-C21
2	A	301	58A	CCF-CCG-CCH-CCI
8	A	308	OLC	O20-C21-C22-C24
8	A	311	OLC	O20-C21-C22-C24
8	A	311	OLC	C1-C2-C3-C4
8	A	310	OLC	O19-C1-O20-C21
8	A	308	OLC	C21-C22-C24-O25
8	B	308	OLC	C21-C22-C24-O25
2	A	301	58A	CBP-CBQ-CBR-CBS
2	B	301	58A	CBO-CBP-CBQ-CBR
8	B	309	OLC	C13-C14-C15-C16
8	A	309	OLC	C12-C13-C14-C15
8	A	308	OLC	O19-C1-O20-C21
2	B	301	58A	CBI-CBJ-CBK-CBL
8	A	311	OLC	C4-C5-C6-C7
8	B	309	OLC	C2-C3-C4-C5
8	B	308	OLC	C11-C12-C13-C14
8	B	309	OLC	C10-C11-C12-C13
2	A	301	58A	CCE-CCF-CCG-CCH
8	A	309	OLC	C11-C12-C13-C14
2	A	301	58A	CBH-CBI-CBJ-CBK
8	A	311	OLC	C3-C4-C5-C6
2	A	301	58A	CBO-CBP-CBQ-CBR
8	A	308	OLC	C13-C14-C15-C16
8	A	311	OLC	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	B	306	FLC	CB-CG-CGC-OG2
2	B	301	58A	CBH-CBI-CBJ-CBK
8	B	309	OLC	C5-C6-C7-C8
2	A	301	58A	CBX-CBY-CBZ-CCA
8	A	310	OLC	C4-C5-C6-C7
2	B	301	58A	CBZ-CCA-CCB-CCC
2	A	301	58A	CBF-CBG-CBH-CBI
8	A	311	OLC	C5-C6-C7-C8
8	A	308	OLC	C11-C12-C13-C14
6	B	306	FLC	CB-CG-CGC-OG1
8	A	308	OLC	O23-C22-C24-O25
8	A	309	OLC	O23-C22-C24-O25
2	A	301	58A	CBN-CBO-CBP-CBQ
8	A	310	OLC	C10-C11-C12-C13
2	B	301	58A	OAY-CAZ-CBA-CBC
2	A	301	58A	CBF-CBE-OBD-CBC
8	A	308	OLC	C10-C11-C12-C13
8	A	309	OLC	C6-C7-C8-C9
2	B	301	58A	CBG-CBH-CBI-CBJ
8	A	311	OLC	C14-C15-C16-C17
2	A	301	58A	CBY-CBZ-CCA-CCB
8	B	308	OLC	C10-C11-C12-C13
8	B	308	OLC	C6-C7-C8-C9
8	A	311	OLC	C15-C16-C17-C18
8	B	309	OLC	C15-C16-C17-C18
8	A	310	OLC	C5-C6-C7-C8
8	A	308	OLC	C4-C5-C6-C7
8	B	308	OLC	C13-C14-C15-C16
2	B	301	58A	PAR-OAU-PAV-OAX
6	A	306	FLC	OHB-CB-CBC-OB2
6	A	306	FLC	CA-CB-CBC-OB2
6	A	306	FLC	CG-CB-CBC-OB1
6	B	306	FLC	CG-CB-CBC-OB1
2	B	301	58A	CBQ-CBR-CBS-CBT
8	B	308	OLC	C15-C16-C17-C18
2	A	301	58A	CBV-CBW-CBX-CBY
8	B	308	OLC	O23-C22-C24-O25
8	B	308	OLC	C12-C13-C14-C15
2	A	301	58A	OCL-CBE-OBD-CBC
2	B	301	58A	CAZ-CBA-CBC-OB1
8	A	310	OLC	C12-C13-C14-C15
8	B	309	OLC	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	A	309	OLC	C2-C1-O20-C21
2	B	301	58A	CBN-CBO-CBP-CBQ
8	B	308	OLC	C2-C3-C4-C5
8	A	309	OLC	O19-C1-O20-C21
6	A	306	FLC	CA-CB-CBC-OB1
2	A	301	58A	CCA-CCB-CCC-CCD
2	B	301	58A	OAY-CAZ-CBA-OB
2	B	301	58A	OB-CBA-CBC-OB
2	A	301	58A	CBW-CBX-CBY-CBZ
8	B	309	OLC	C7-C8-C9-C10
8	A	311	OLC	C11-C12-C13-C14
2	B	301	58A	C5'-O5'-PAR-OAS
2	B	301	58A	C5'-O5'-PAR-OAU
2	B	301	58A	CAZ-OAY-PAV-OAX
2	B	301	58A	CBC-CBA-OB-CBU
8	A	311	OLC	C12-C13-C14-C15
8	A	310	OLC	C11-C12-C13-C14
6	B	307	FLC	CAC-CA-CB-OHB
2	A	301	58A	PAR-OAU-PAV-OAW
8	A	308	OLC	C12-C13-C14-C15
6	A	306	FLC	OHB-CB-CBC-OB1
6	B	306	FLC	CA-CB-CBC-OB1
6	B	306	FLC	CA-CB-CBC-OB2
2	B	301	58A	CCA-CCB-CCC-CCD
2	B	301	58A	CBF-CBG-CBH-CBI
8	B	309	OLC	C11-C12-C13-C14
2	B	301	58A	PAR-OAU-PAV-OAW
8	A	308	OLC	C5-C6-C7-C8
8	A	309	OLC	C7-C8-C9-C10
8	A	310	OLC	C7-C8-C9-C10
2	B	301	58A	CCE-CCF-CCG-CCH
8	A	308	OLC	C9-C10-C11-C12
6	B	306	FLC	OHB-CB-CG-CGC
8	A	311	OLC	C6-C7-C8-C9
8	B	309	OLC	C9-C10-C11-C12
2	A	301	58A	CBK-CBL-CBM-CBN
8	A	310	OLC	C9-C10-C11-C12
8	A	309	OLC	O20-C21-C22-O23
8	A	310	OLC	O20-C21-C22-O23
8	B	308	OLC	C7-C8-C9-C10
8	A	311	OLC	C9-C10-C11-C12
2	B	301	58A	OB-CBE-CBF-CBG

Continued on next page...

Continued from previous page...

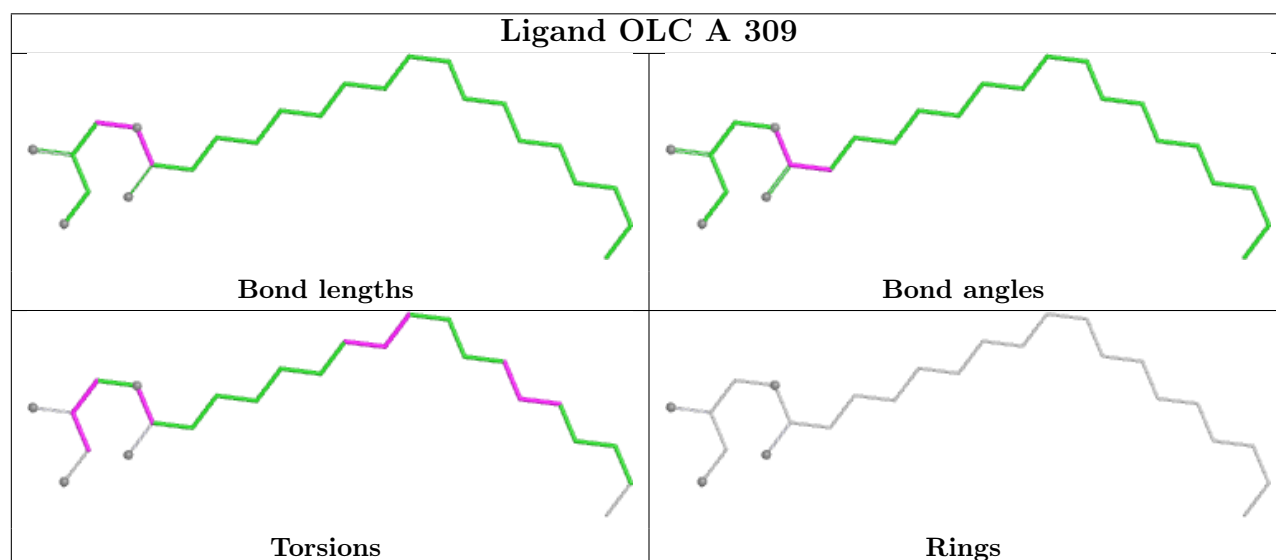
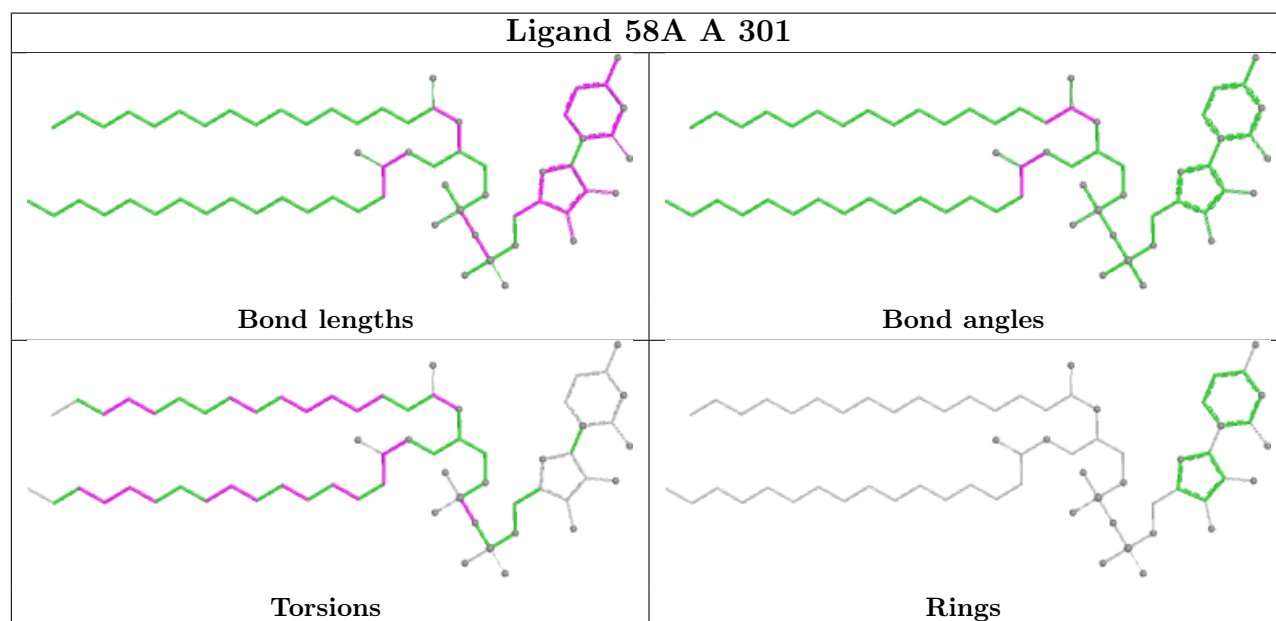
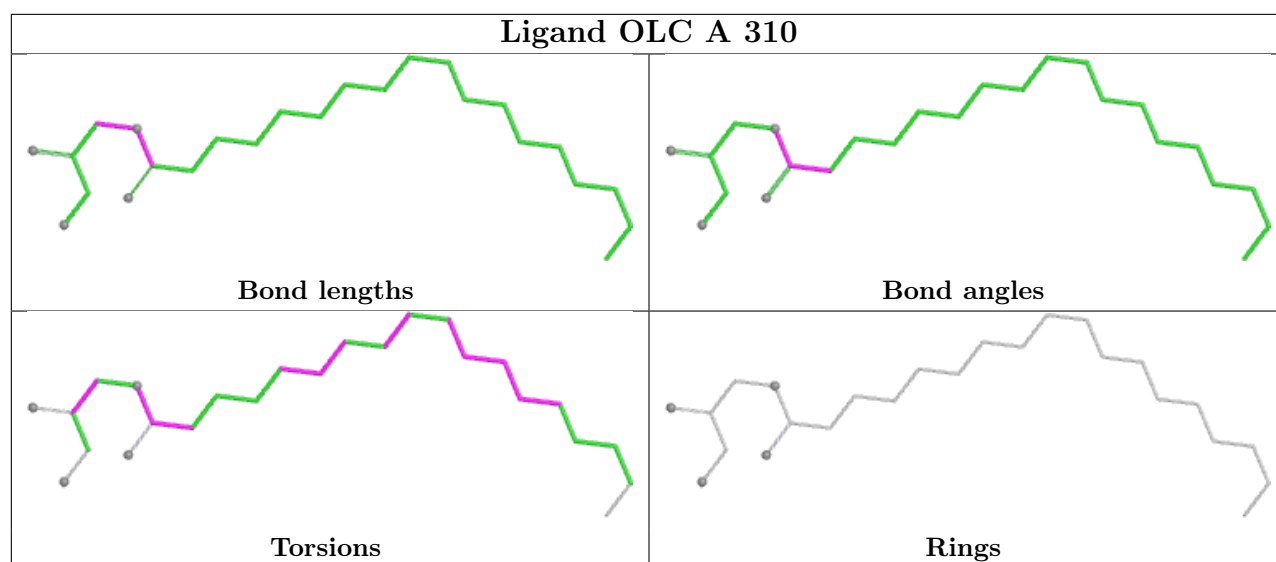
Mol	Chain	Res	Type	Atoms
6	A	306	FLC	CB-CG-CGC-OG1
8	B	309	OLC	O20-C1-C2-C3
8	A	308	OLC	C2-C3-C4-C5
8	A	308	OLC	C7-C8-C9-C10
8	B	309	OLC	O19-C1-C2-C3
2	A	301	58A	OBD-CBE-CBF-CBG
6	A	306	FLC	CB-CG-CGC-OG2
2	B	301	58A	OCL-CBE-CBF-CBG
2	B	301	58A	CCC-CCD-CCE-CCF
2	A	301	58A	PAR-OAU-PAV-OAX
8	A	310	OLC	O20-C1-C2-C3

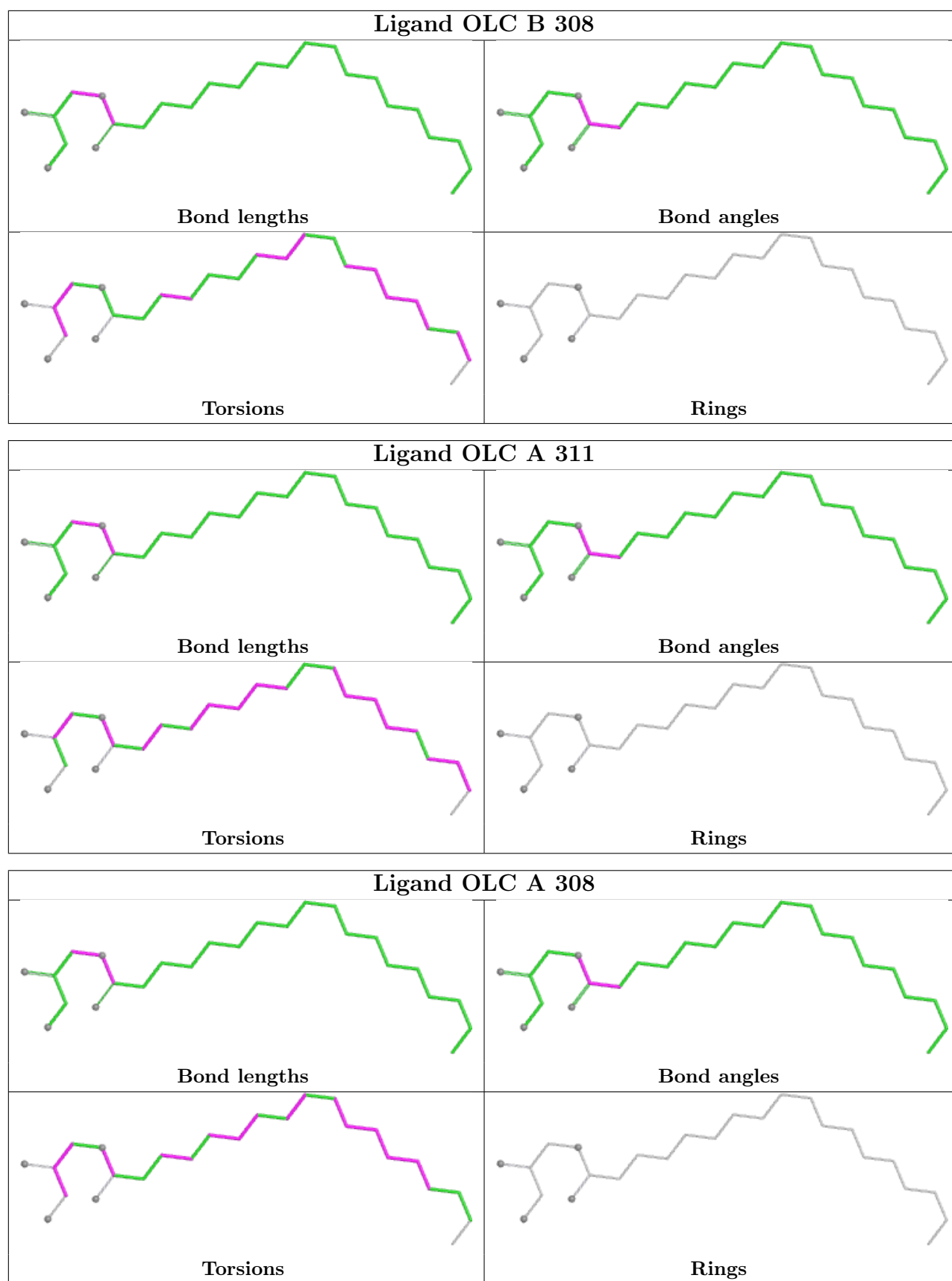
There are no ring outliers.

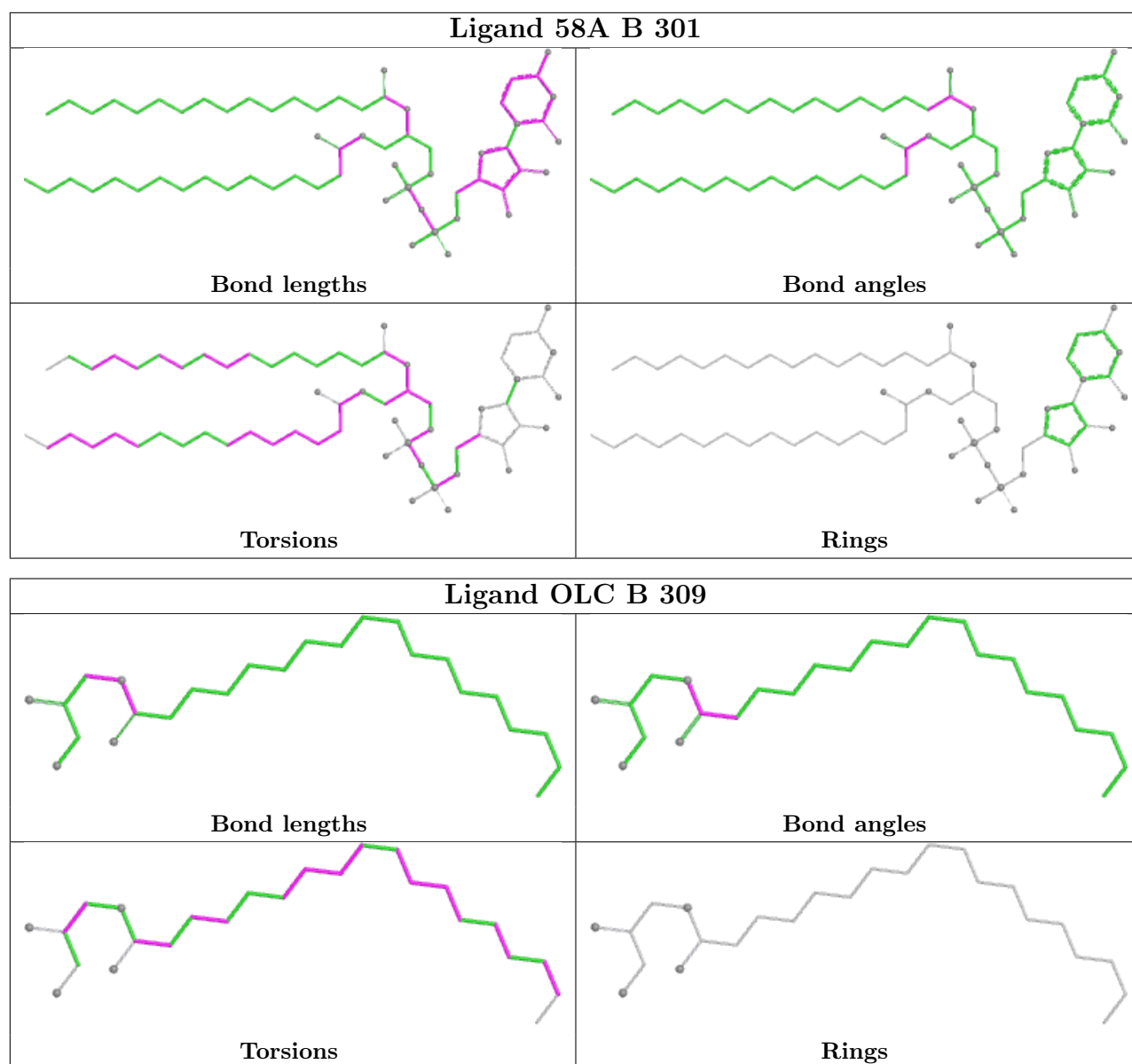
8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	306	FLC	1	0
2	A	301	58A	7	0
8	A	309	OLC	1	0
8	B	308	OLC	1	0
6	B	306	FLC	2	0
8	A	308	OLC	1	0
2	B	301	58A	6	0
8	B	309	OLC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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, 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	200/225 (88%)	1.62	52 (26%) 1 1	27, 45, 72, 106	0
1	B	202/225 (89%)	1.40	42 (20%) 2 2	28, 46, 69, 131	0
All	All	402/450 (89%)	1.51	94 (23%) 2 1	27, 46, 72, 131	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	198	ILE	5.6
1	B	86	LEU	5.3
1	A	200	GLY	4.9
1	A	165	TYR	4.5
1	B	202	LEU	4.3
1	B	2	PHE	4.0
1	B	109	ASN	3.9
1	A	13	TYR	3.8
1	A	1	MET	3.7
1	A	160	ASN	3.6
1	A	196	LYS	3.5
1	B	10	ILE	3.5
1	B	166	ILE	3.5
1	A	197	TYR	3.4
1	B	181	PHE	3.4
1	B	13	TYR	3.3
1	B	158	TYR	3.3
1	A	162	ILE	3.2
1	A	176	VAL	3.2
1	A	163	PHE	3.2
1	B	110	VAL	3.1
1	A	192	TYR	3.1
1	A	136	LEU	3.1
1	B	162	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	141	LEU	3.0
1	B	178	ILE	3.0
1	A	86	LEU	3.0
1	A	135	TYR	2.9
1	B	135	TYR	2.9
1	A	161	LYS	2.8
1	A	52	GLY	2.8
1	A	188	ILE	2.7
1	A	189	TYR	2.7
1	B	198	ILE	2.7
1	A	42	SER	2.6
1	B	187	LEU	2.6
1	A	46	TYR	2.6
1	A	111	LYS	2.5
1	A	164	ILE	2.5
1	A	166	ILE	2.5
1	A	50	LYS	2.5
1	A	58	GLY	2.5
1	A	181	PHE	2.5
1	A	114	ILE	2.5
1	A	95	CYS	2.5
1	A	169	VAL	2.5
1	A	79	TYR	2.5
1	B	138	ASN	2.5
1	A	140	ILE	2.4
1	A	195	ILE	2.4
1	A	182	ALA	2.4
1	B	174	ALA	2.4
1	B	31	PHE	2.4
1	B	57	PHE	2.4
1	B	182	ALA	2.4
1	A	184	MET	2.4
1	B	1	MET	2.4
1	A	109	ASN	2.4
1	B	4	ILE	2.3
1	B	199	ARG	2.3
1	A	128	PHE	2.3
1	B	179	PRO	2.3
1	B	197	TYR	2.3
1	A	85	ASN	2.3
1	A	185	LEU	2.2
1	A	172	CYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	200	GLY	2.2
1	B	160	ASN	2.2
1	A	120	ALA	2.2
1	B	164	ILE	2.2
1	A	152	ASP	2.2
1	B	16	MET	2.2
1	A	129	CYS	2.2
1	B	9	THR	2.2
1	A	178	ILE	2.1
1	B	114	ILE	2.1
1	B	54	VAL	2.1
1	B	84	SER	2.1
1	A	131	LEU	2.1
1	B	44	ASP	2.1
1	A	2	PHE	2.1
1	B	82	PHE	2.1
1	A	191	ILE	2.1
1	B	137	ILE	2.1
1	B	192	TYR	2.1
1	B	45	GLY	2.1
1	B	177	GLY	2.1
1	B	161	LYS	2.0
1	A	122	ALA	2.0
1	A	29	ASN	2.0
1	B	5	ARG	2.0
1	A	82	PHE	2.0
1	A	139	SER	2.0
1	B	118	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

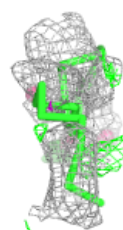
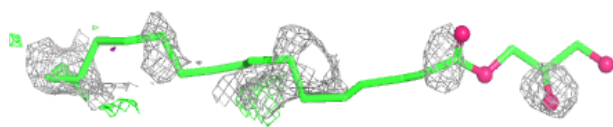
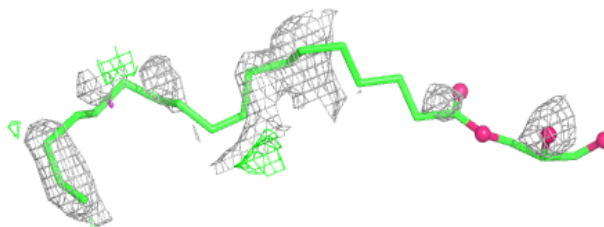
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NA	B	310	1/1	0.38	0.23	57,57,57,57	0
8	OLC	A	309	25/25	0.44	0.23	59,84,102,115	0
6	FLC	B	306	13/13	0.45	0.17	126,129,141,142	0
8	OLC	A	311	25/25	0.45	0.24	46,89,110,114	0
8	OLC	B	308	25/25	0.53	0.23	46,79,97,100	0
8	OLC	A	310	25/25	0.55	0.24	59,72,91,95	0
6	FLC	B	307	13/13	0.58	0.14	87,102,122,126	0
8	OLC	A	308	25/25	0.60	0.20	49,61,86,90	0
6	FLC	A	306	13/13	0.61	0.16	100,108,113,113	0
8	OLC	B	309	25/25	0.66	0.25	65,84,118,134	0
2	58A	B	301	64/68	0.77	0.18	35,62,84,95	0
3	CA	A	302	1/1	0.79	0.13	47,47,47,47	0
5	CL	B	304	1/1	0.79	0.17	47,47,47,47	0
2	58A	A	301	64/68	0.80	0.17	28,54,74,87	0
5	CL	A	304	1/1	0.81	0.13	39,39,39,39	0
7	NA	A	307	1/1	0.82	0.16	49,49,49,49	0
4	MG	B	303	1/1	0.84	0.09	50,50,50,50	0
3	CA	B	302	1/1	0.87	0.10	55,55,55,55	0
4	MG	A	303	1/1	0.88	0.07	49,49,49,49	0
5	CL	A	305	1/1	0.88	0.16	46,46,46,46	0
5	CL	B	305	1/1	0.93	0.13	54,54,54,54	0

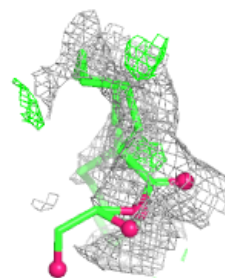
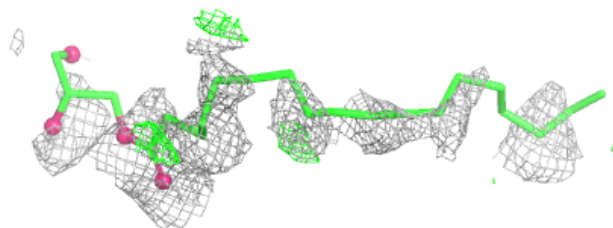
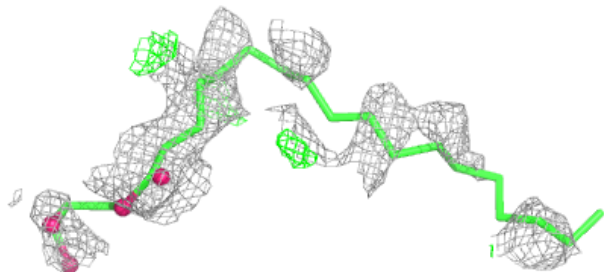
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 309:

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

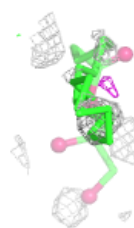
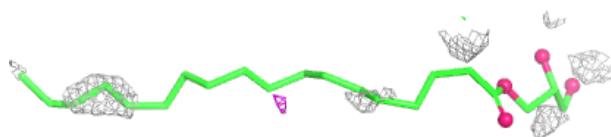
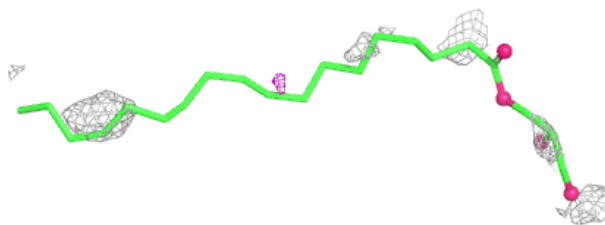
**Electron density around OLC A 311:**

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

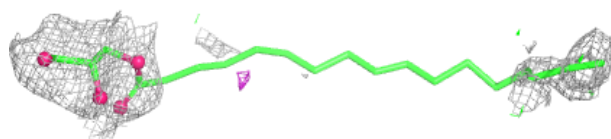


Electron density around OLC B 308:

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

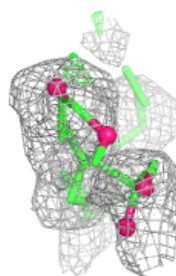
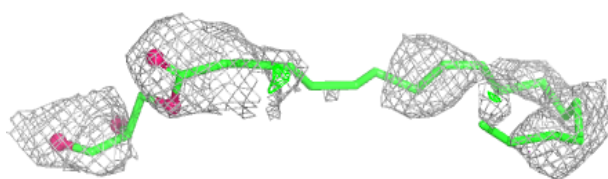
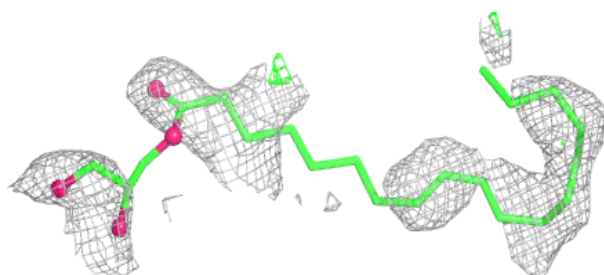
**Electron density around OLC A 310:**

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

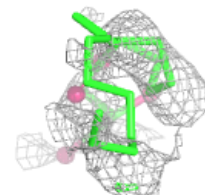
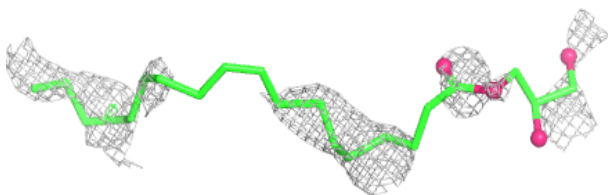
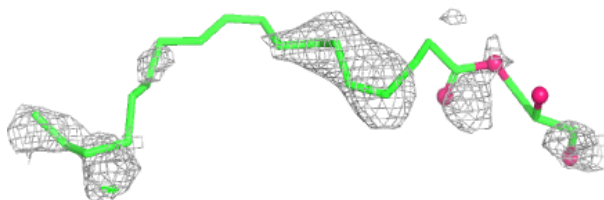


Electron density around OLC A 308:

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

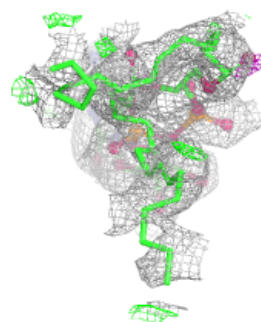
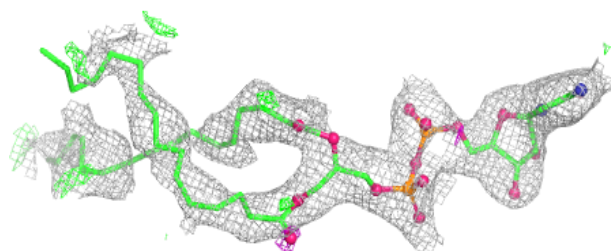
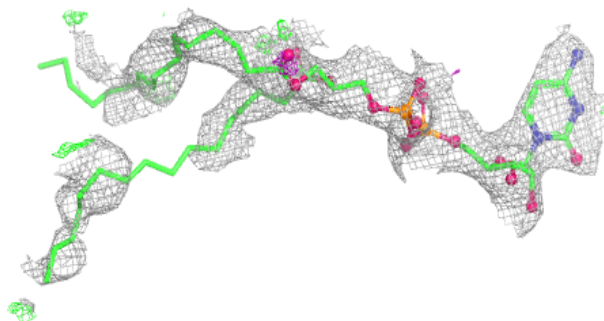
**Electron density around OLC B 309:**

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

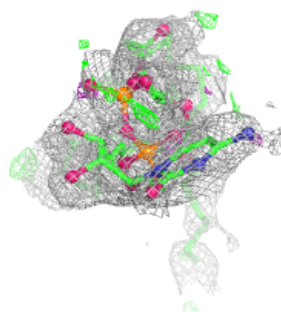
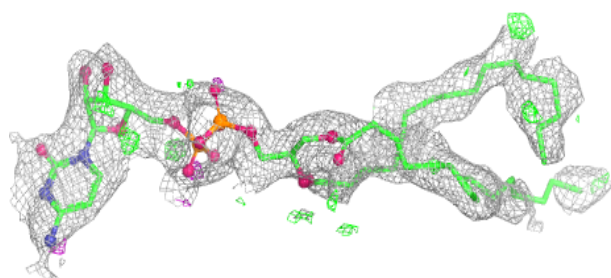
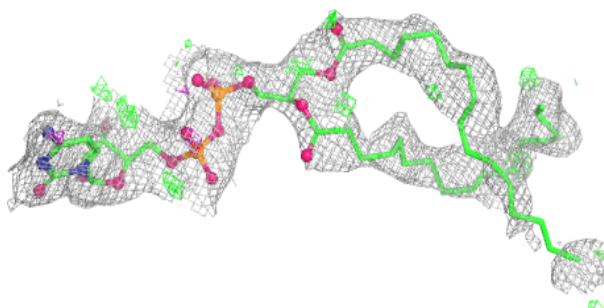


Electron density around 58A B 301:

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

**Electron density around 58A A 301:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.