Full wwPDB X-ray Structure Validation Report ⓘ

Feb 23, 2023 – 06:31 pm GMT

PDB ID	:	7POW
Title	:	Crystal structure of phosphatidyl serine synthase (PSS) in transition state.
Authors	:	Yildiz, O.; Centola, M.
Deposited on	:	2021-09-10
Resolution	:	2.51 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:

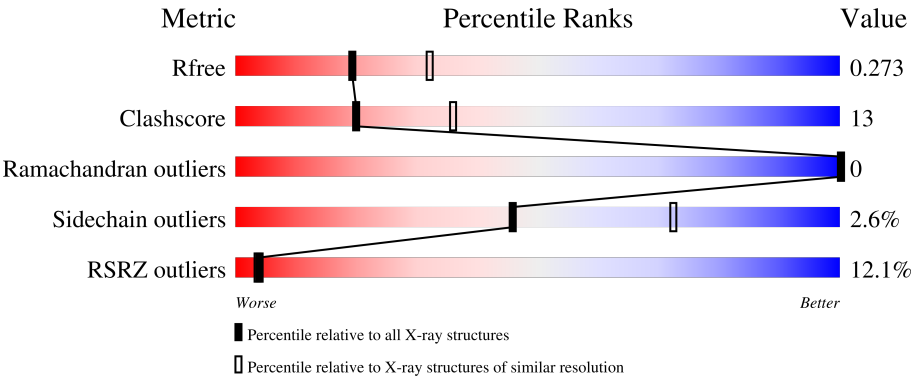
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	204	9% 75% 22%
1	B	204	14% 72% 27%

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
5	CL	A	307	-	-	X	-
6	OLC	A	312	-	-	-	X
6	OLC	B	309	-	-	-	X
8	SER	B	306	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 3613 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.

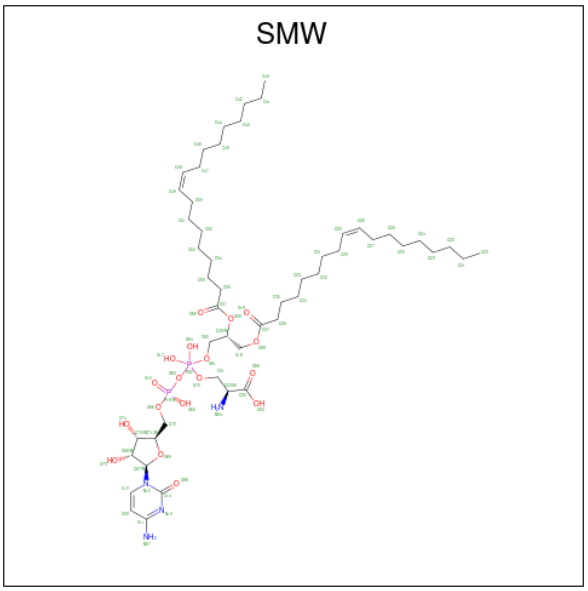
- Molecule 1 is a protein called CDP-diacylglycerol--serine O-phosphatidyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	Se	0	0	0
			1551	1043	235	264	5	4			
1	B	204	Total	C	N	O	S	Se	0	1	0
			1582	1065	240	268	5	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	expression tag	UNP Q58609
A	-1	PRO	-	expression tag	UNP Q58609
A	0	HIS	-	expression tag	UNP Q58609
B	-2	ALA	-	expression tag	UNP Q58609
B	-1	PRO	-	expression tag	UNP Q58609
B	0	HIS	-	expression tag	UNP Q58609

- Molecule 2 is (2S)-2-amino-3-[[[(2R,3S,4R,5R)-5-(4-amino-2-oxo-pyrimidin-1-yl)-3,4-dihydroxy-tetrahydrofuran-2-yl]methoxy-hydroxy-phosphoryl]oxy-[(2R)-2,3-bis[[(Z)-octadec-9-enoyl]oxy]propoxy]-dihydroxy-lambda^5-phosphanyl]oxy-propanoic acid (three-letter code: SMW) (formula: $C_{51}H_{92}N_4O_{18}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			75	51	4	18	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		

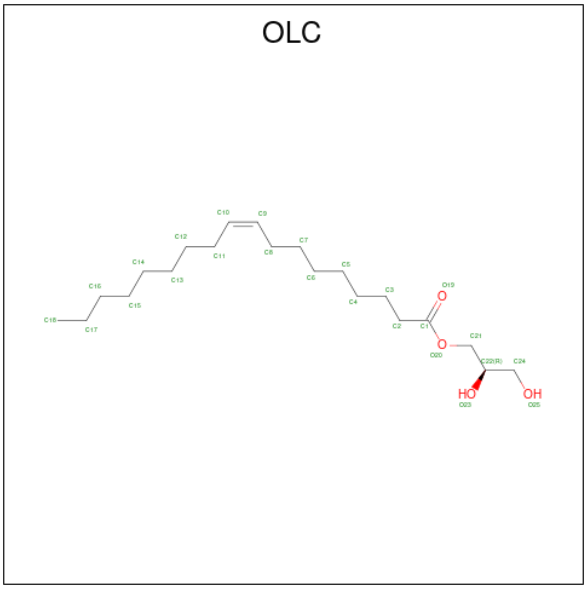
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

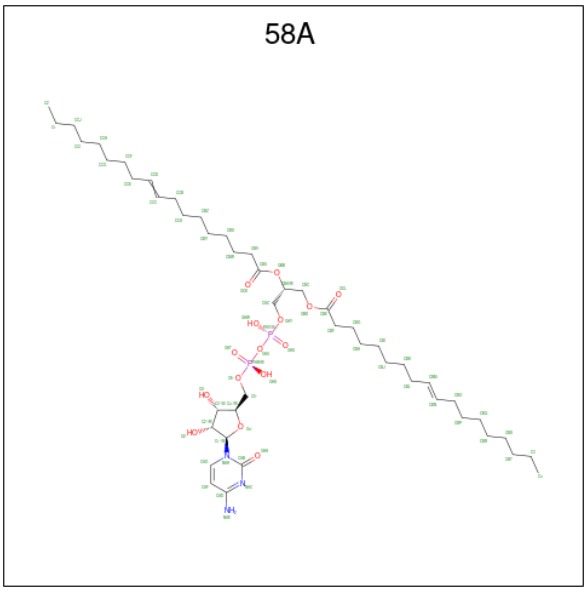
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Cl	0	0
			4	4		
5	B	2	Total	Cl	0	0
			2	2		

- Molecule 6 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



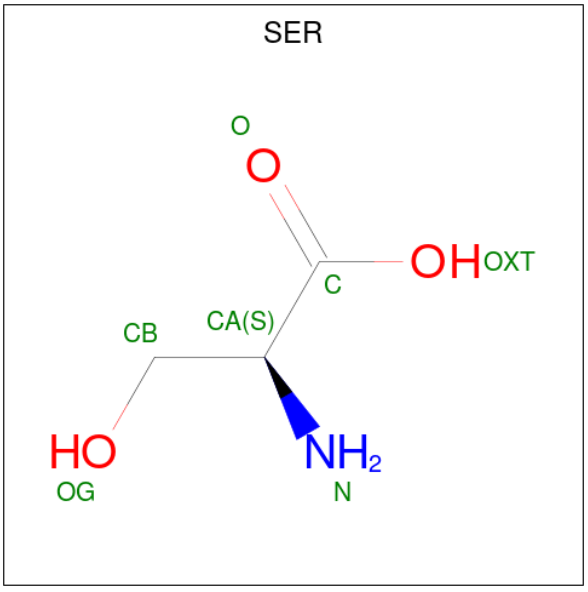
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 25 21 4	0	0
6	A	1	Total C O 25 21 4	0	0
6	A	1	Total C O 25 21 4	0	0
6	A	1	Total C O 25 21 4	0	0
6	A	1	Total C O 25 21 4	0	0
6	A	1	Total C O 25 21 4	0	0
6	B	1	Total C O 25 21 4	0	0
6	B	1	Total C O 25 21 4	0	0
6	B	1	Total C O 25 21 4	0	0
6	B	1	Total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

- Molecule 7 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: $C_{48}H_{85}N_3O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is SERINE (three-letter code: SER) (formula: $C_3H_7NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			7	3	1	3		

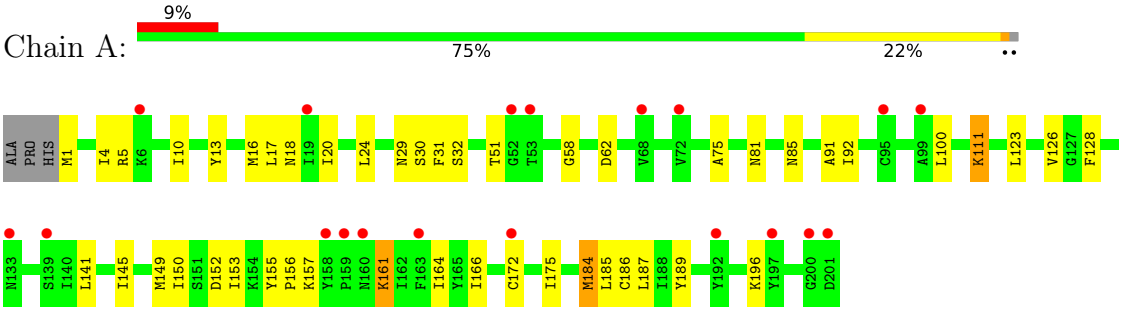
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	44	Total O 44 44	0	0
9	B	30	Total O 30 30	0	0

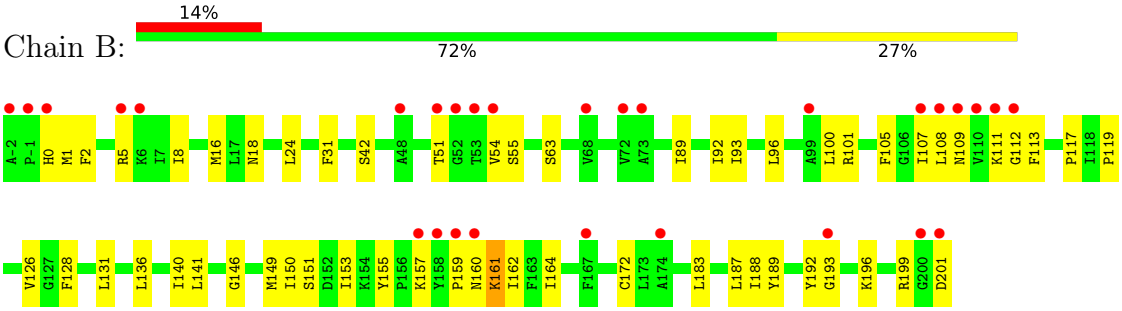
3 Residue-property plots (i)

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 (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	107.35Å 61.22Å 79.31Å 90.00° 118.72° 90.00°	Depositor
Resolution (Å)	38.04 – 2.51 38.04 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.5 (38.04-2.51) 99.9 (38.04-2.51)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.46 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.215 , 0.276 0.216 , 0.273	Depositor DCC
R_{free} test set	782 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 73.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l 0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	3613	wwPDB-VP
Average B, all atoms (Å^2)	31.0	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 24.51 % 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 3.7851e-03. 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: CA, CL, SMW, 58A, OLC, MG

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	0.42	0/1579	0.56	0/2140
1	B	0.39	0/1615	0.58	0/2189
All	All	0.41	0/3194	0.57	0/4329

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	1551	0	1655	41	0
1	B	1582	0	1683	51	0
2	A	75	0	0	2	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	4	0	0	4	0
5	B	2	0	0	1	0
6	A	150	0	240	15	0
6	B	100	0	160	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	64	0	69	6	0
8	B	7	0	4	1	0
9	A	44	0	0	1	0
9	B	30	0	0	1	0
All	All	3613	0	3811	92	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 13.

All (92) 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:100:LEU:HD21	1:B:16:MSE:HE2	1.64	0.77
1:B:162:ILE:H	1:B:162:ILE:HD12	1.52	0.74
1:A:196:LYS:NZ	9:A:401:HOH:O	2.20	0.73
1:A:5:ARG:NH1	6:B:310:OLC:O25	2.23	0.72
6:A:312:OLC:H18A	6:B:307:OLC:H16A	1.72	0.72
1:B:188:ILE:HG22	7:B:301:58A:H43	1.73	0.71
1:A:62:ASP:HB3	2:A:301:SMW:O02	1.90	0.70
1:B:172:CYS:HB3	6:B:308:OLC:H14A	1.75	0.68
1:A:10:ILE:HD11	1:A:51:THR:HG21	1.77	0.66
1:B:63:SER:OG	8:B:306:SER:O	2.14	0.63
1:B:2:PHE:O	1:B:5:ARG:HG2	1.99	0.62
1:A:24:LEU:HD21	1:B:92:ILE:HD11	1.81	0.62
1:A:13:TYR:HB3	6:A:313:OLC:H13	1.82	0.62
1:A:30:SER:HB2	6:A:308:OLC:H21	1.81	0.61
1:A:1:MSE:HE1	1:B:153:ILE:HD11	1.83	0.61
1:B:8:ILE:HD13	1:B:16:MSE:HE1	1.83	0.60
1:A:172:CYS:HB3	6:A:308:OLC:H14	1.83	0.60
1:B:92:ILE:HG21	6:B:310:OLC:H12A	1.84	0.59
1:B:128:PHE:HZ	1:B:187:LEU:HD21	1.66	0.59
1:A:17:LEU:HD11	6:A:312:OLC:H15	1.85	0.58
1:B:51:THR:HA	6:B:309:OLC:H2A	1.86	0.57
1:B:101:ARG:NH2	5:B:305:CL:CL	2.75	0.56
1:B:51:THR:HG22	6:B:309:OLC:H6	1.88	0.56
1:A:166:ILE:HG22	1:A:185:LEU:HD11	1.88	0.55
1:A:29:ASN:HD21	1:A:81:ASN:HD21	1.55	0.55
1:B:155:TYR:HB3	1:B:189:TYR:OH	2.06	0.55
1:B:92:ILE:HD13	6:B:310:OLC:H14A	1.87	0.55
1:A:123:LEU:HD23	1:A:186:CYS:HB2	1.89	0.54
1:A:153:ILE:HD11	1:B:1:MSE:HE1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ILE:O	1:B:93:ILE:HG12	2.08	0.54
1:A:31:PHE:HD1	1:A:126:VAL:HG13	1.73	0.53
6:A:312:OLC:H16A	6:B:307:OLC:H18B	1.92	0.51
1:A:31:PHE:CD1	1:A:126:VAL:HG13	2.46	0.51
1:A:4:ILE:N	5:A:307:CL:CL	2.74	0.49
1:A:111:LYS:O	1:A:157:LYS:HD2	2.11	0.49
1:A:13:TYR:HE1	6:A:313:OLC:H21A	1.77	0.49
1:B:96:LEU:HD13	6:B:310:OLC:H6A	1.95	0.49
1:B:160:ASN:OD1	1:B:161:LYS:HD3	2.11	0.49
5:A:307:CL:CL	1:B:150:ILE:O	2.69	0.48
1:B:42:SER:HA	7:B:301:58A:H50	1.96	0.48
1:B:107:ILE:O	1:B:108:LEU:HD23	2.13	0.48
1:A:16:MSE:HE2	1:B:100:LEU:HD21	1.96	0.47
1:B:164:ILE:HG23	7:B:301:58A:H56	1.96	0.47
1:B:192:TYR:CE2	1:B:196:LYS:HE2	2.50	0.47
1:B:161:LYS:HD3	1:B:161:LYS:H	1.78	0.47
1:B:199:ARG:NH1	1:B:201:ASP:OD2	2.48	0.47
1:A:128:PHE:CG	1:A:141:LEU:HD13	2.50	0.47
6:A:309:OLC:H12	6:A:309:OLC:H15	1.60	0.47
1:A:175:ILE:HG21	6:A:308:OLC:H11A	1.98	0.45
1:B:128:PHE:CZ	1:B:187:LEU:HD21	2.49	0.45
1:A:156:PRO:HD2	1:A:189:TYR:CE1	2.51	0.45
1:A:155:TYR:HB3	1:A:189:TYR:OH	2.16	0.45
1:A:145:ILE:O	1:A:149:MSE:HG3	2.17	0.45
1:A:152:ASP:HB2	1:B:0:HIS:O	2.16	0.45
1:B:111:LYS:HB2	1:B:111:LYS:HE2	1.68	0.45
1:A:128:PHE:HZ	1:A:187:LEU:HD21	1.81	0.45
1:B:161:LYS:HB2	1:B:161:LYS:HE2	1.75	0.45
1:A:92:ILE:HD11	1:B:24:LEU:HD21	1.99	0.44
6:A:308:OLC:H3	6:B:307:OLC:H8A	1.99	0.44
1:B:92:ILE:CG2	6:B:310:OLC:H12A	2.48	0.44
6:A:312:OLC:H6A	6:A:313:OLC:H11A	1.98	0.44
1:A:161:LYS:HD2	1:A:161:LYS:H	1.84	0.43
1:B:159:PRO:HB2	1:B:164:ILE:HG13	1.99	0.43
1:B:117:PRO:HB2	1:B:119:PRO:HD2	2.01	0.43
1:A:4:ILE:HG22	5:A:307:CL:CL	2.56	0.43
1:B:151:SER:HB3	1:B:153:ILE:H	1.83	0.43
7:B:301:58A:H53	7:B:301:58A:H59	1.85	0.43
1:A:123:LEU:HD23	1:A:186:CYS:SG	2.59	0.42
1:B:55:SER:OG	9:B:401:HOH:O	2.21	0.42
1:B:112:GLY:HA2	1:B:157:LYS:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:PHE:CD2	1:A:141:LEU:HD13	2.54	0.42
1:A:184:MSE:HE2	1:A:184:MSE:HB3	1.96	0.42
1:B:113:PHE:HB2	1:B:155:TYR:O	2.19	0.42
1:B:136:LEU:O	1:B:140:ILE:HG13	2.20	0.42
1:A:75:ALA:HB1	1:A:91:ALA:HB1	2.01	0.42
6:A:310:OLC:H15A	6:A:310:OLC:H18A	1.80	0.42
1:B:54:VAL:HA	7:B:301:58A:OAA	2.20	0.42
1:A:58:GLY:HA3	2:A:301:SMW:N13	2.35	0.42
1:B:31:PHE:HD1	1:B:126:VAL:HB	1.85	0.41
1:B:131:LEU:HD12	1:B:183:LEU:CD2	2.50	0.41
1:A:20:ILE:O	1:A:24:LEU:HG	2.20	0.41
1:A:150:ILE:O	5:A:306:CL:CL	2.75	0.41
1:B:128:PHE:CG	1:B:141:LEU:HD13	2.55	0.41
1:B:105:PHE:O	1:B:109:ASN:HB3	2.21	0.41
1:A:51:THR:HG22	6:A:310:OLC:H5A	2.02	0.41
1:A:10:ILE:HD13	6:A:312:OLC:H4A	2.03	0.41
1:B:107:ILE:HG13	1:B:108:LEU:N	2.36	0.41
1:A:85:ASN:OD1	6:A:311:OLC:H21	2.20	0.41
1:B:189:TYR:HB2	7:B:301:58A:H41	2.03	0.40
1:B:151:SER:HB3	1:B:153:ILE:HG13	2.02	0.40
1:B:146:GLY:HA2	1:B:149:MSE:HE2	2.04	0.40
1:B:155:TYR:CE1	1:B:193:GLY:HA3	2.56	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	199/204 (98%)	195 (98%)	4 (2%)	0	100	100
1	B	203/204 (100%)	198 (98%)	5 (2%)	0	100	100
All	All	402/408 (98%)	393 (98%)	9 (2%)	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	170/168 (101%)	164 (96%)	6 (4%)	36 62
1	B	173/168 (103%)	171 (99%)	2 (1%)	71 88
All	All	343/336 (102%)	335 (98%)	8 (2%)	46 76

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	32	SER
1	A	111	LYS
1	A	161	LYS
1	A	164	ILE
1	A	184	MSE
1	B	18	ASN
1	B	161	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	81	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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 23 ligands modelled in this entry, 10 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
6	OLC	B	307	-	24,24,24	0.95	1 (4%)	25,25,25	0.93	1 (4%)
6	OLC	A	313	-	24,24,24	0.96	1 (4%)	25,25,25	0.81	1 (4%)
7	58A	B	301	3	63,65,69	2.62	19 (30%)	75,82,86	1.10	4 (5%)
6	OLC	A	311	-	24,24,24	0.91	1 (4%)	25,25,25	0.86	1 (4%)
8	SER	B	306	-	5,6,6	1.00	1 (20%)	5,7,7	1.86	2 (40%)
6	OLC	A	309	-	24,24,24	0.88	1 (4%)	25,25,25	0.86	1 (4%)
6	OLC	A	312	-	24,24,24	0.96	1 (4%)	25,25,25	0.81	1 (4%)
6	OLC	B	308	-	24,24,24	0.91	1 (4%)	25,25,25	0.83	2 (8%)
6	OLC	A	308	-	24,24,24	0.93	1 (4%)	25,25,25	0.91	1 (4%)
6	OLC	B	310	-	24,24,24	0.93	1 (4%)	25,25,25	0.82	1 (4%)
6	OLC	A	310	-	24,24,24	0.93	1 (4%)	25,25,25	0.93	1 (4%)
2	SMW	A	301	3	70,76,76	2.69	18 (25%)	84,98,98	1.40	6 (7%)
6	OLC	B	309	-	24,24,24	0.94	1 (4%)	25,25,25	0.75	1 (4%)

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
6	OLC	B	307	-	-	12/24/24/24	-
6	OLC	A	313	-	-	15/24/24/24	-
7	58A	B	301	3	-	23/61/77/81	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OLC	A	311	-	-	7/24/24/24	-
8	SER	B	306	-	-	4/6/6/6	-
6	OLC	A	309	-	-	6/24/24/24	-
6	OLC	A	312	-	-	11/24/24/24	-
6	OLC	B	308	-	-	9/24/24/24	-
6	OLC	A	308	-	-	15/24/24/24	-
6	OLC	B	310	-	-	10/24/24/24	-
6	OLC	A	310	-	-	6/24/24/24	-
2	SMW	A	301	3	-	39/66/94/94	0/2/2/2
6	OLC	B	309	-	-	12/24/24/24	-

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	301	58A	C3'-C2'	-10.76	1.23	1.53
2	A	301	SMW	C70-C71	-9.92	1.27	1.53
2	A	301	SMW	C68-C67	-7.83	1.28	1.53
2	A	301	SMW	C10-C09	6.54	1.50	1.35
7	B	301	58A	CAG-CAF	5.95	1.48	1.35
2	A	301	SMW	O69-C67	5.72	1.55	1.42
7	B	301	58A	CAB-NAC	5.52	1.47	1.36
2	A	301	SMW	C14-N13	5.45	1.47	1.36
2	A	301	SMW	C11-N07	5.06	1.45	1.33
7	B	301	58A	CAD-NAC	4.99	1.44	1.34
7	B	301	58A	CAD-NAE	4.89	1.45	1.33
7	B	301	58A	O4'-C1'	-4.72	1.30	1.42
2	A	301	SMW	C11-N13	4.62	1.43	1.34
6	A	312	OLC	O20-C1	4.48	1.46	1.33
6	A	313	OLC	O20-C1	4.43	1.46	1.33
2	A	301	SMW	O69-C71	4.42	1.54	1.45
6	B	307	OLC	O20-C1	4.41	1.46	1.33
6	A	310	OLC	O20-C1	4.39	1.46	1.33
6	B	310	OLC	O20-C1	4.36	1.46	1.33
6	B	309	OLC	O20-C1	4.32	1.46	1.33
7	B	301	58A	C5'-C4'	-4.30	1.38	1.51
2	A	301	SMW	C70-C68	4.29	1.65	1.53
6	A	311	OLC	O20-C1	4.28	1.45	1.33
6	A	308	OLC	O20-C1	4.27	1.45	1.33
2	A	301	SMW	C14-N12	4.20	1.49	1.40
7	B	301	58A	C2'-C1'	4.16	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	308	OLC	O20-C1	4.16	1.45	1.33
7	B	301	58A	CAB-NAH	4.16	1.49	1.40
6	A	309	OLC	O20-C1	4.07	1.45	1.33
2	A	301	SMW	O38-C37	3.92	1.44	1.33
7	B	301	58A	OBD-CBE	3.72	1.44	1.33
2	A	301	SMW	C10-N12	3.49	1.46	1.38
7	B	301	58A	OBB-CBU	3.32	1.43	1.34
7	B	301	58A	CAG-NAH	3.27	1.45	1.38
2	A	301	SMW	O59-C57	3.15	1.43	1.34
2	A	301	SMW	C09-C11	3.15	1.50	1.42
2	A	301	SMW	O08-C14	-3.02	1.18	1.23
7	B	301	58A	O3'-C3'	3.01	1.50	1.43
7	B	301	58A	OAA-CAB	-2.81	1.18	1.23
7	B	301	58A	O4'-C4'	2.77	1.51	1.45
7	B	301	58A	CAF-CAD	2.72	1.49	1.42
2	A	301	SMW	P62-O61	2.67	1.70	1.62
7	B	301	58A	C3'-C4'	2.49	1.59	1.53
2	A	301	SMW	O59-C39	-2.41	1.40	1.46
7	B	301	58A	CBF-CBE	2.30	1.57	1.50
7	B	301	58A	O2'-C2'	2.27	1.48	1.43
2	A	301	SMW	C36-C37	2.13	1.56	1.50
8	B	306	SER	OXT-C	-2.11	1.23	1.30

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	SMW	O75-C01-C03	5.95	113.34	108.00
2	A	301	SMW	O59-C57-C56	4.42	121.03	111.50
7	B	301	58A	OBB-CBU-CBV	4.28	120.72	111.50
2	A	301	SMW	C71-O69-C67	-3.27	102.25	109.47
2	A	301	SMW	O02-C05-O06	-3.01	117.26	124.09
7	B	301	58A	PAV-OAU-PAR	-2.98	122.60	132.83
8	B	306	SER	OXT-C-O	-2.91	117.49	124.09
2	A	301	SMW	P62-O75-C01	-2.87	116.22	125.88
6	B	307	OLC	O20-C1-C2	2.82	120.75	111.91
8	B	306	SER	OXT-C-CA	2.78	122.85	113.38
7	B	301	58A	OBD-CBE-CBF	2.73	120.47	111.91
6	A	313	OLC	O20-C1-C2	2.65	120.21	111.91
6	A	312	OLC	O20-C1-C2	2.61	120.11	111.91
6	A	308	OLC	O20-C1-C2	2.61	120.09	111.91
2	A	301	SMW	O38-C37-C36	2.55	119.92	111.91
6	B	308	OLC	O20-C1-C2	2.51	119.80	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	309	OLC	O20-C1-C2	2.40	119.45	111.91
6	B	310	OLC	O20-C1-C2	2.32	119.18	111.91
6	A	310	OLC	C3-C2-C1	-2.19	105.66	113.62
6	A	311	OLC	O20-C1-C2	2.12	118.56	111.91
6	B	309	OLC	O20-C1-C2	2.12	118.56	111.91
7	B	301	58A	C4'-O4'-C1'	-2.11	104.81	109.47
6	B	308	OLC	O20-C1-O19	-2.05	118.42	123.59

There are no chirality outliers.

All (169) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	SMW	O75-C01-C03-C05
2	A	301	SMW	O75-C01-C03-N04
2	A	301	SMW	C56-C57-O59-C39
2	A	301	SMW	O69-C71-C72-O66
2	A	301	SMW	C72-O66-P16-O15
2	A	301	SMW	C72-O66-P16-O63
2	A	301	SMW	C72-O66-P16-O65
6	A	312	OLC	O20-C21-C22-C24
6	B	307	OLC	O20-C21-C22-C24
6	B	308	OLC	C21-C22-C24-O25
6	B	309	OLC	O20-C21-C22-C24
6	B	310	OLC	O20-C21-C22-O23
7	B	301	58A	C5'-O5'-PAR-OAT
7	B	301	58A	C5'-O5'-PAR-OAU
7	B	301	58A	CAZ-OAY-PAV-OAX
8	B	306	SER	O-C-CA-CB
8	B	306	SER	OXT-C-CA-CB
8	B	306	SER	N-CA-CB-OG
8	B	306	SER	C-CA-CB-OG
2	A	301	SMW	O19-C37-O38-C18
6	B	308	OLC	O19-C1-O20-C21
2	A	301	SMW	C36-C37-O38-C18
6	B	308	OLC	C2-C1-O20-C21
2	A	301	SMW	O58-C57-O59-C39
6	B	307	OLC	C2-C1-O20-C21
6	A	312	OLC	O20-C21-C22-O23
2	A	301	SMW	C21-C22-C23-C24
7	B	301	58A	CBZ-CCA-CCB-CCC
2	A	301	SMW	C70-C71-C72-O66
6	B	307	OLC	O19-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
7	B	301	58A	CBV-CBU-OBB-CBA
6	A	311	OLC	C2-C1-O20-C21
6	B	310	OLC	O20-C21-C22-C24
2	A	301	SMW	O59-C39-C60-O61
6	B	307	OLC	O20-C21-C22-O23
6	B	309	OLC	O20-C21-C22-O23
6	A	311	OLC	O19-C1-O20-C21
6	A	309	OLC	C1-C2-C3-C4
6	A	312	OLC	C1-C2-C3-C4
6	A	313	OLC	C1-C2-C3-C4
6	B	308	OLC	O23-C22-C24-O25
6	B	307	OLC	C1-C2-C3-C4
7	B	301	58A	CBE-CBF-CBG-CBH
7	B	301	58A	OCK-CBU-OBB-CBA
2	A	301	SMW	C54-C55-C56-C57
6	B	309	OLC	C2-C1-O20-C21
2	A	301	SMW	C41-C42-C43-C44
6	A	308	OLC	C5-C6-C7-C8
7	B	301	58A	CCF-CCG-CCH-CCI
6	A	308	OLC	C2-C3-C4-C5
7	B	301	58A	CBO-CBP-CBQ-CBR
6	A	310	OLC	C5-C6-C7-C8
6	A	308	OLC	C12-C13-C14-C15
6	A	308	OLC	C1-C2-C3-C4
2	A	301	SMW	C51-C52-C53-C54
6	A	312	OLC	C21-C22-C24-O25
6	A	313	OLC	C21-C22-C24-O25
6	B	307	OLC	C21-C22-C24-O25
6	B	309	OLC	C21-C22-C24-O25
6	A	312	OLC	C4-C5-C6-C7
6	B	308	OLC	C14-C15-C16-C17
2	A	301	SMW	C45-C46-C47-C48
2	A	301	SMW	C32-C33-C34-C35
6	A	310	OLC	C14-C15-C16-C17
7	B	301	58A	CBW-CBX-CBY-CBZ
2	A	301	SMW	C22-C23-C24-C25
6	B	309	OLC	O19-C1-O20-C21
6	A	313	OLC	C4-C5-C6-C7
6	A	312	OLC	C5-C6-C7-C8
6	B	309	OLC	O23-C22-C24-O25
6	B	307	OLC	C13-C14-C15-C16
6	B	308	OLC	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
6	B	309	OLC	C3-C4-C5-C6
6	B	310	OLC	C5-C6-C7-C8
6	A	308	OLC	C13-C14-C15-C16
2	A	301	SMW	C50-C51-C52-C53
6	A	308	OLC	C11-C12-C13-C14
6	B	309	OLC	C4-C5-C6-C7
6	A	313	OLC	C10-C11-C12-C13
6	B	310	OLC	C10-C11-C12-C13
6	A	313	OLC	C2-C1-O20-C21
7	B	301	58A	CBI-CBJ-CBK-CBL
6	A	313	OLC	O20-C21-C22-C24
6	B	307	OLC	C11-C12-C13-C14
6	A	308	OLC	C10-C11-C12-C13
6	A	311	OLC	C3-C4-C5-C6
6	A	311	OLC	C1-C2-C3-C4
2	A	301	SMW	C18-C39-C60-O61
6	A	313	OLC	C2-C3-C4-C5
2	A	301	SMW	C25-C26-C27-C28
6	A	310	OLC	C13-C14-C15-C16
6	B	308	OLC	C15-C16-C17-C18
6	B	308	OLC	C2-C3-C4-C5
6	A	313	OLC	O23-C22-C24-O25
6	A	309	OLC	C12-C13-C14-C15
6	A	312	OLC	C10-C11-C12-C13
7	B	301	58A	CCD-CCE-CCF-CCG
6	B	309	OLC	C2-C3-C4-C5
2	A	301	SMW	C20-C21-C22-C23
2	A	301	SMW	C18-C39-O59-C57
2	A	301	SMW	C23-C24-C25-C26
6	A	313	OLC	O19-C1-O20-C21
6	A	308	OLC	C2-C1-O20-C21
6	A	309	OLC	C2-C1-O20-C21
6	A	308	OLC	C3-C4-C5-C6
7	B	301	58A	CBJ-CBK-CBL-CBM
6	A	310	OLC	C4-C5-C6-C7
2	A	301	SMW	O38-C18-C39-C60
7	B	301	58A	CAZ-CBA-CBC-OBD
6	A	312	OLC	C13-C14-C15-C16
6	A	308	OLC	C14-C15-C16-C17
6	A	313	OLC	O20-C21-C22-O23
7	B	301	58A	CBP-CBQ-CBR-CBS
2	A	301	SMW	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
6	A	308	OLC	C4-C5-C6-C7
2	A	301	SMW	C42-C43-C44-C45
6	A	310	OLC	C15-C16-C17-C18
7	B	301	58A	PAR-OAU-PAV-OAY
7	B	301	58A	CBU-CBV-CBW-CBX
6	A	308	OLC	O19-C1-O20-C21
6	A	309	OLC	O19-C1-O20-C21
6	A	312	OLC	O23-C22-C24-O25
6	A	311	OLC	C4-C5-C6-C7
7	B	301	58A	C3'-C4'-C5'-O5'
6	A	311	OLC	C12-C13-C14-C15
2	A	301	SMW	C30-C31-C32-C33
2	A	301	SMW	C49-C50-C51-C52
6	B	309	OLC	C12-C13-C14-C15
2	A	301	SMW	C03-C01-O75-P62
2	A	301	SMW	O38-C18-C39-O59
6	B	307	OLC	C2-C3-C4-C5
2	A	301	SMW	C46-C47-C48-C49
6	A	312	OLC	C7-C8-C9-C10
6	B	310	OLC	C2-C3-C4-C5
6	B	309	OLC	C13-C14-C15-C16
2	A	301	SMW	P62-O63-P16-O65
6	B	310	OLC	C15-C16-C17-C18
2	A	301	SMW	C48-C49-C50-C51
6	A	310	OLC	C9-C10-C11-C12
6	B	307	OLC	C15-C16-C17-C18
6	A	312	OLC	C11-C12-C13-C14
6	A	308	OLC	C6-C7-C8-C9
6	A	309	OLC	C9-C10-C11-C12
2	A	301	SMW	P62-O63-P16-O66
6	A	313	OLC	C5-C6-C7-C8
7	B	301	58A	OBB-CBA-CBC-OBD
2	A	301	SMW	P62-O63-P16-O15
6	A	311	OLC	C7-C8-C9-C10
6	A	313	OLC	C7-C8-C9-C10
6	A	308	OLC	C9-C10-C11-C12
6	A	309	OLC	C2-C3-C4-C5
6	A	313	OLC	C9-C10-C11-C12
7	B	301	58A	CBN-CBO-CBP-CBQ
7	B	301	58A	CBV-CBW-CBX-CBY
6	B	310	OLC	C4-C5-C6-C7
7	B	301	58A	CCA-CCB-CCC-CCD

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Mol	Chain	Res	Type	Atoms
6	B	307	OLC	C7-C8-C9-C10
6	B	308	OLC	C5-C6-C7-C8
6	A	308	OLC	O20-C21-C22-C24
6	A	313	OLC	C13-C14-C15-C16
7	B	301	58A	CBK-CBL-CBM-CBN
6	B	310	OLC	C7-C8-C9-C10
6	B	310	OLC	C2-C1-O20-C21
6	B	307	OLC	C5-C6-C7-C8
2	A	301	SMW	C39-C60-O61-P62
6	A	313	OLC	C3-C4-C5-C6
6	B	310	OLC	O20-C1-C2-C3
6	B	309	OLC	C7-C8-C9-C10
2	A	301	SMW	C35-C36-C37-O38

There are no ring outliers.

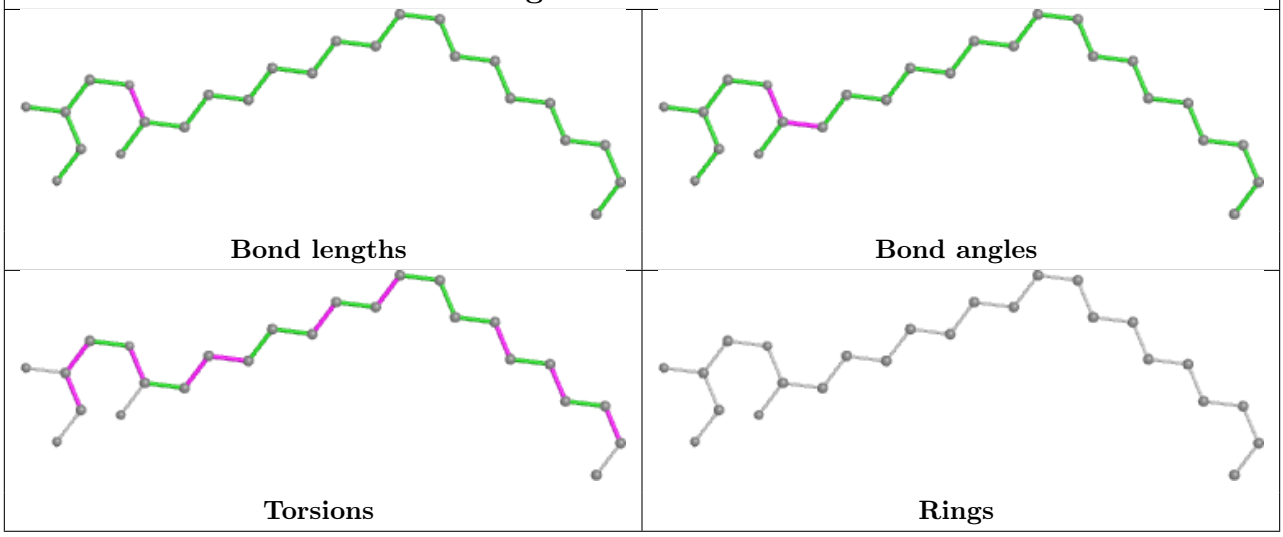
13 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	307	OLC	3	0
6	A	313	OLC	3	0
7	B	301	58A	6	0
6	A	311	OLC	1	0
8	B	306	SER	1	0
6	A	309	OLC	1	0
6	A	312	OLC	5	0
6	B	308	OLC	1	0
6	A	308	OLC	4	0
6	B	310	OLC	5	0
6	A	310	OLC	2	0
2	A	301	SMW	2	0
6	B	309	OLC	2	0

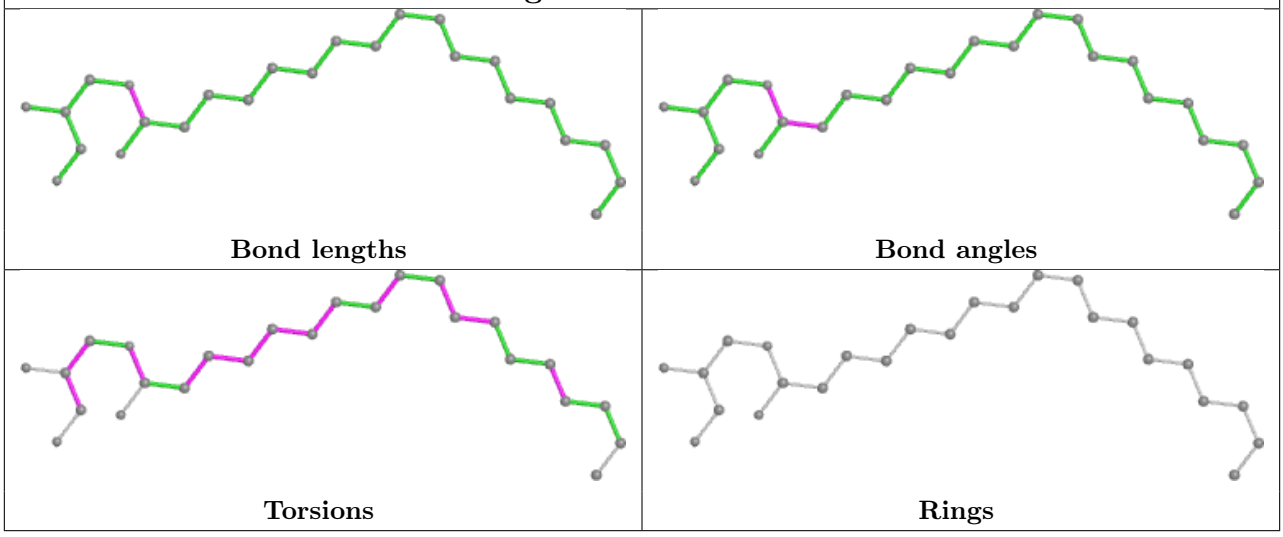
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

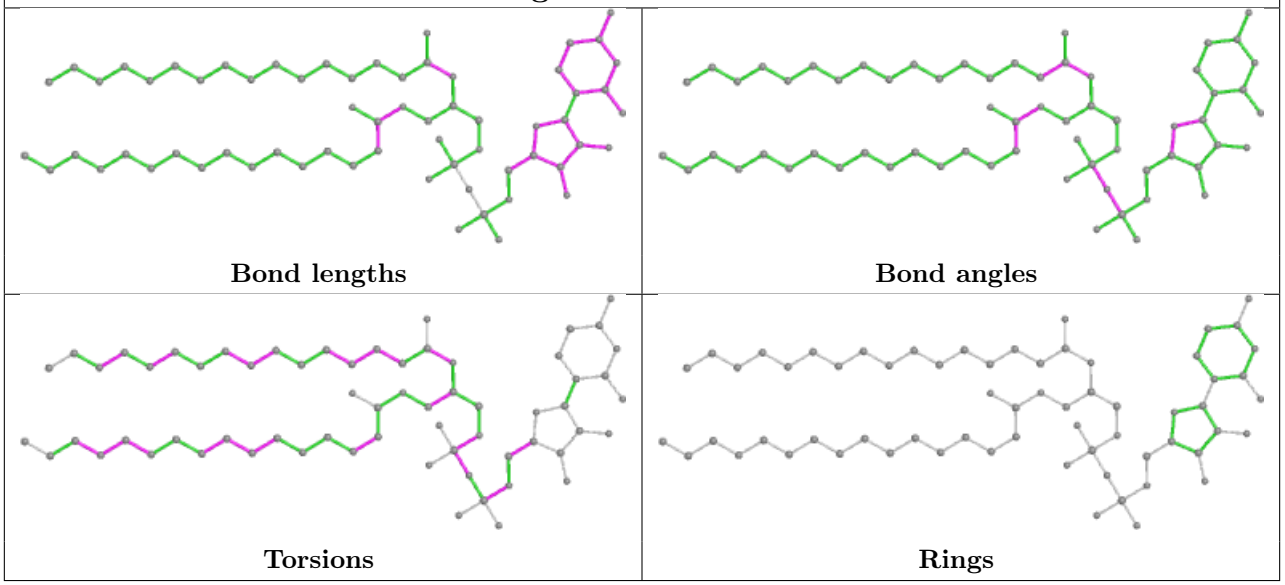
Ligand OLC B 307



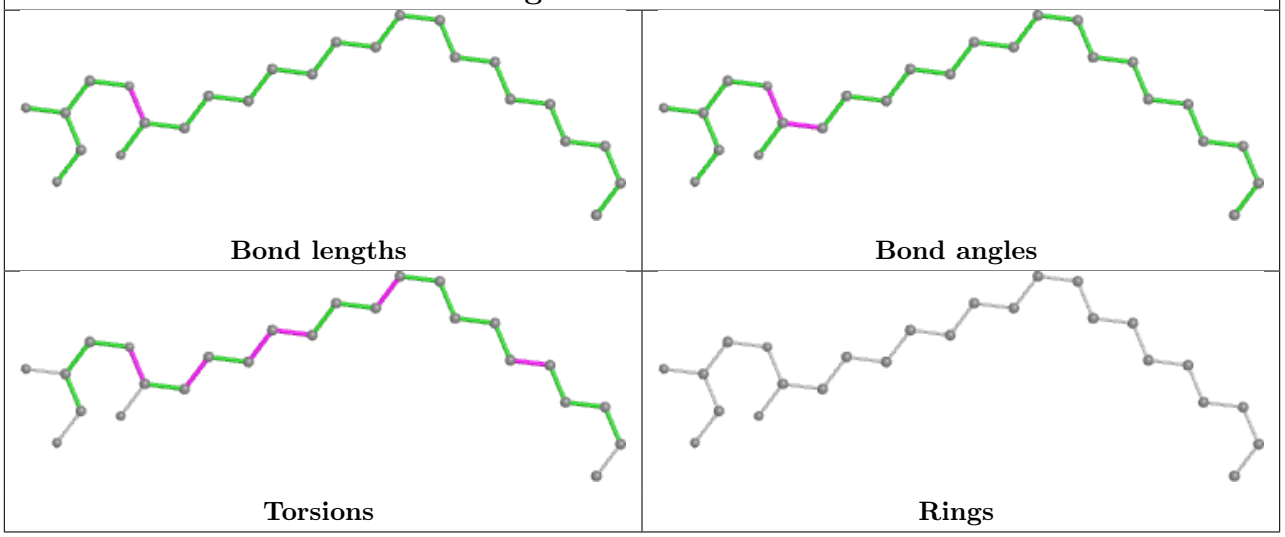
Ligand OLC A 313



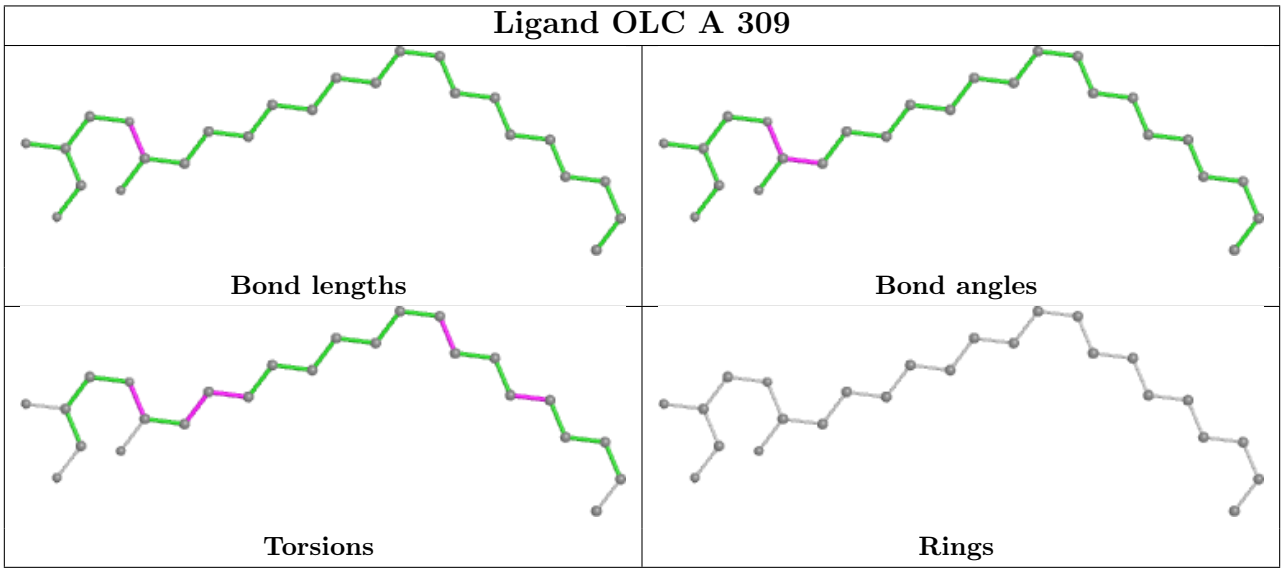
Ligand 58A B 301



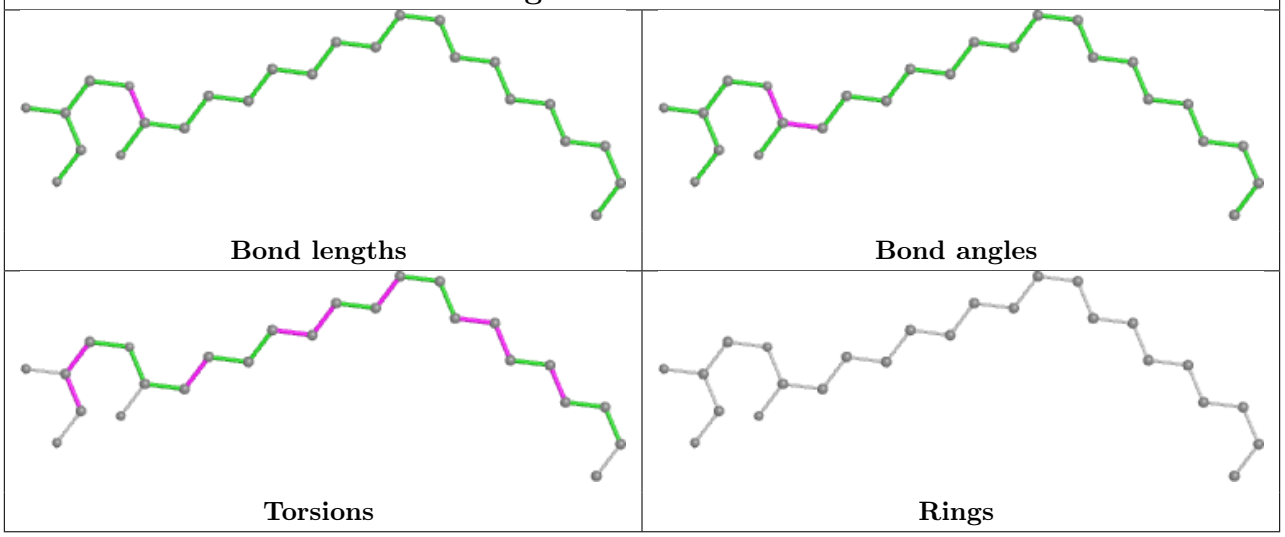
Ligand OLC A 311



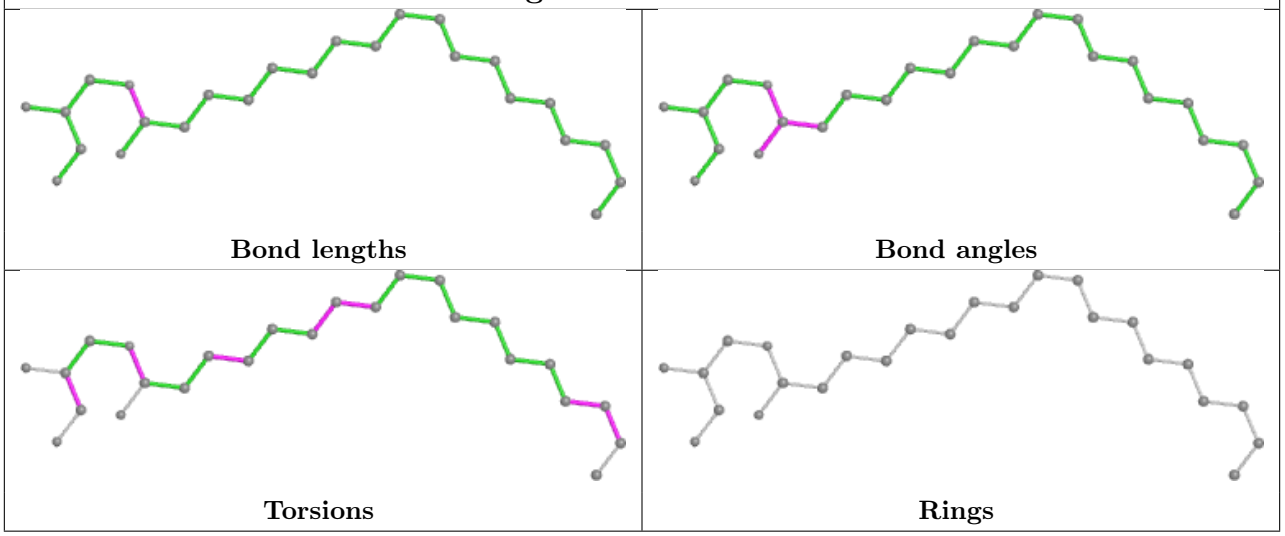
Ligand OLC A 309



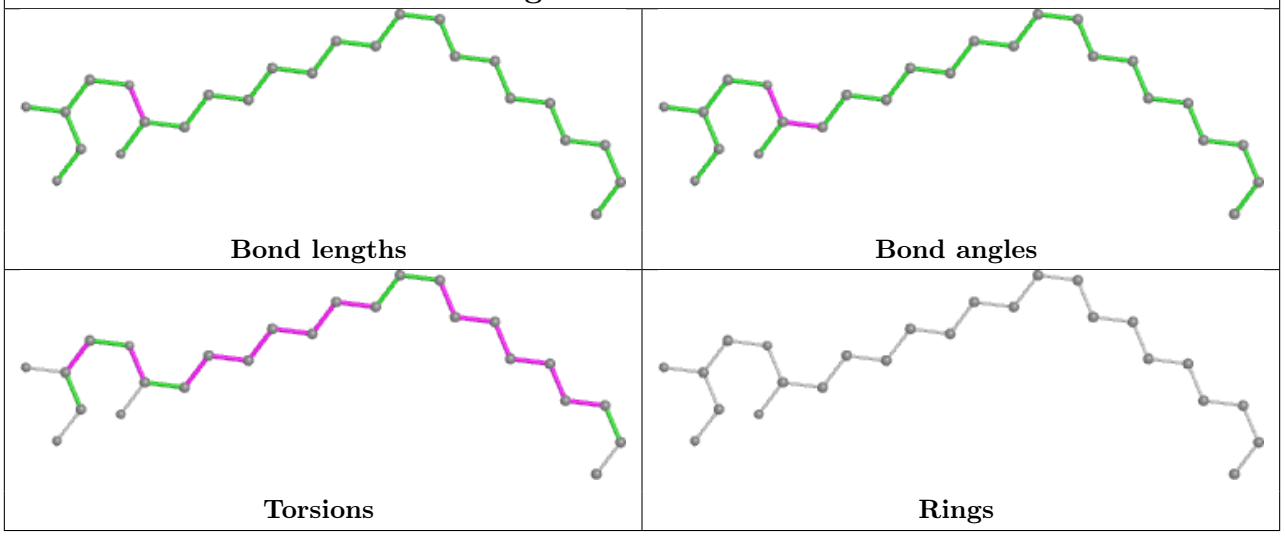
Ligand OLC A 312



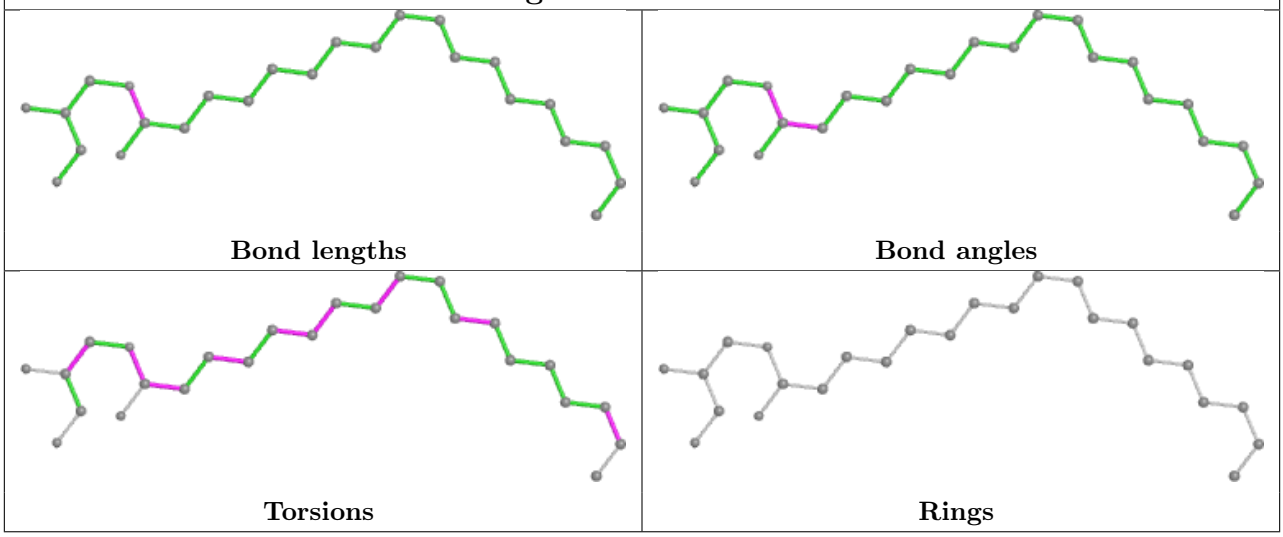
Ligand OLC B 308



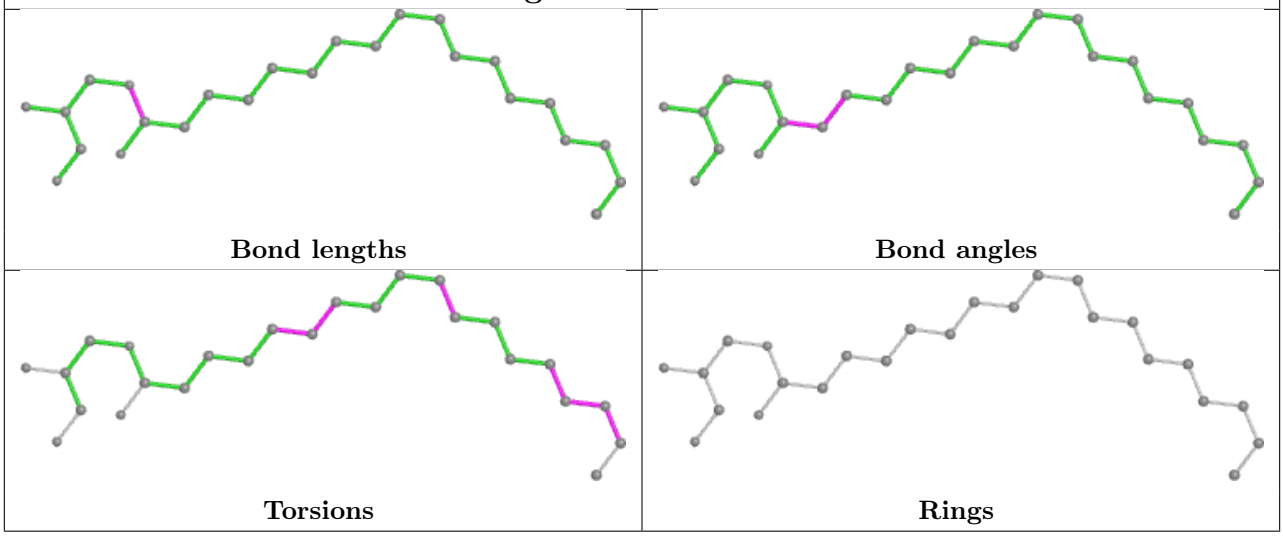
Ligand OLC A 308



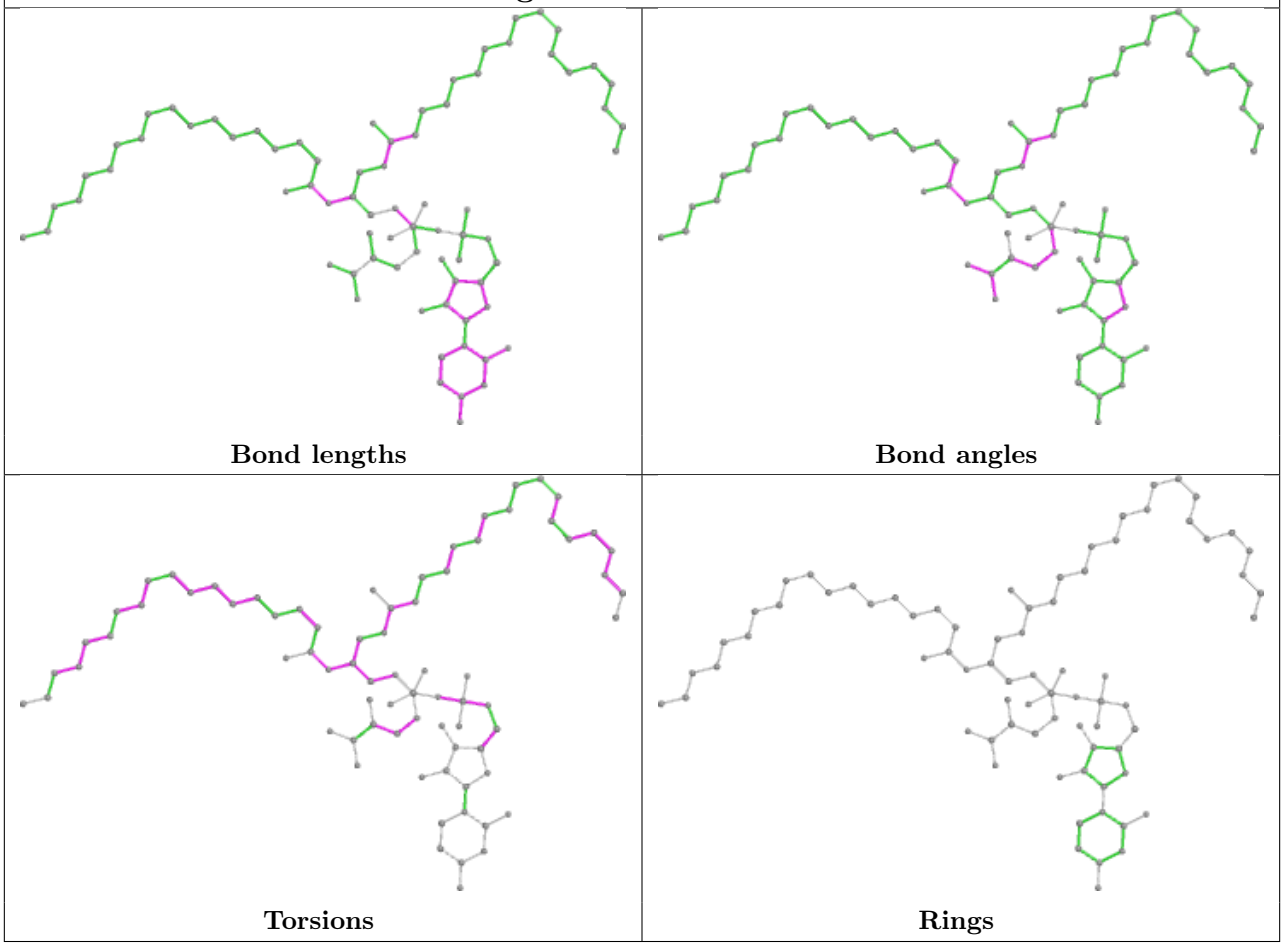
Ligand OLC B 310



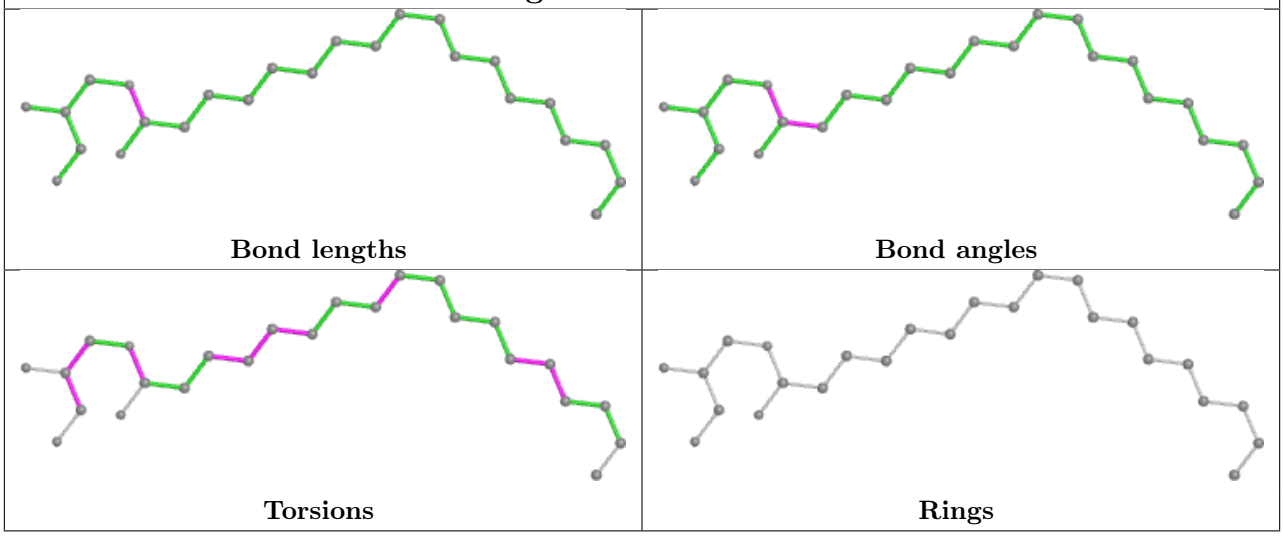
Ligand OLC A 310



Ligand SMW A 301



Ligand OLC B 309



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	197/204 (96%)	0.68	19 (9%)	8	7	15, 24, 50, 104	0
1	B	200/204 (98%)	0.92	29 (14%)	2	2	16, 25, 71, 118	0
All	All	397/408 (97%)	0.80	48 (12%)	4	4	15, 24, 57, 118	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	PRO	9.7
1	B	158	TYR	8.6
1	B	0	HIS	7.7
1	B	109	ASN	7.2
1	B	110	VAL	6.9
1	A	200	GLY	6.6
1	A	158	TYR	6.2
1	B	159	PRO	6.2
1	B	-1	PRO	5.8
1	B	52	GLY	5.6
1	B	201	ASP	5.5
1	A	201	ASP	5.3
1	B	200	GLY	5.3
1	B	111	LYS	4.9
1	A	192	TYR	4.0
1	B	-2	ALA	4.0
1	B	108	LEU	3.6
1	B	112	GLY	3.5
1	A	53	THR	3.5
1	A	6	LYS	3.2
1	B	157	LYS	3.1
1	B	53	THR	3.0
1	B	5	ARG	2.8
1	B	6	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	68	VAL	2.7
1	B	51	THR	2.7
1	B	160	ASN	2.6
1	B	99	ALA	2.5
1	B	48	ALA	2.5
1	A	160	ASN	2.5
1	B	193	GLY	2.5
1	A	133	ASN	2.4
1	B	167	PHE	2.4
1	B	174	ALA	2.4
1	B	68	VAL	2.3
1	A	52	GLY	2.3
1	A	197	TYR	2.3
1	B	72	VAL	2.3
1	A	139	SER	2.2
1	B	107	ILE	2.2
1	A	72	VAL	2.2
1	A	95	CYS	2.1
1	B	73	ALA	2.1
1	A	99	ALA	2.1
1	A	19	ILE	2.1
1	A	172	CYS	2.1
1	B	54	VAL	2.0
1	A	163	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)

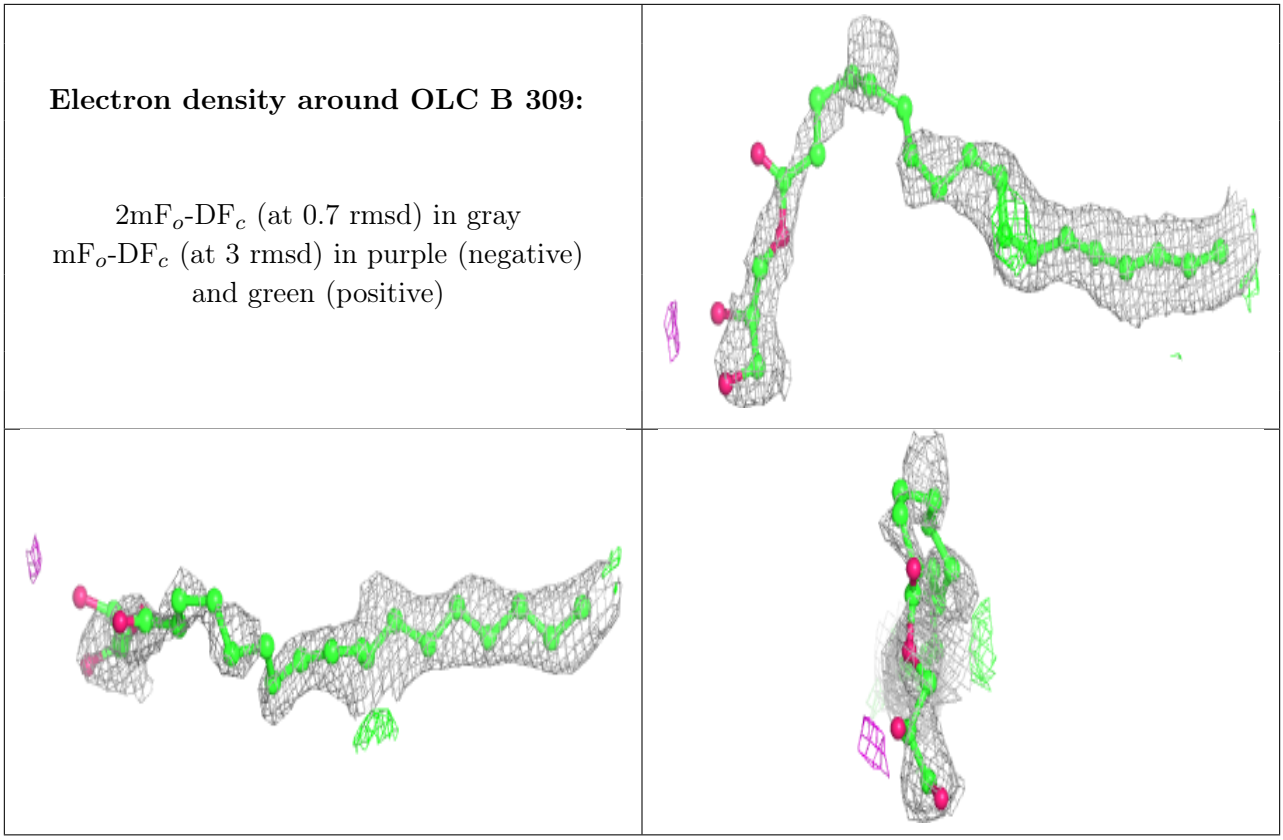
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	OLC	B	309	25/25	0.43	0.41	37,51,72,79	0
6	OLC	A	313	25/25	0.44	0.34	34,57,70,74	0
6	OLC	A	310	25/25	0.56	0.39	37,50,70,84	0
6	OLC	A	312	25/25	0.56	0.41	38,49,65,77	0
6	OLC	B	310	25/25	0.65	0.39	45,60,73,76	0
6	OLC	A	311	25/25	0.67	0.31	38,50,65,71	0
8	SER	B	306	7/7	0.70	0.43	58,60,68,70	0
6	OLC	B	307	25/25	0.75	0.24	33,46,61,68	0
6	OLC	A	309	25/25	0.75	0.25	42,53,64,71	0
6	OLC	B	308	25/25	0.78	0.24	19,33,47,50	0
4	MG	A	303	1/1	0.79	0.19	26,26,26,26	0
6	OLC	A	308	25/25	0.79	0.24	18,34,44,51	0
2	SMW	A	301	75/75	0.82	0.25	21,36,47,53	0
7	58A	B	301	64/68	0.86	0.23	17,34,50,63	0
5	CL	A	306	1/1	0.89	0.19	38,38,38,38	0
5	CL	A	307	1/1	0.91	0.32	41,41,41,41	0
4	MG	B	303	1/1	0.94	0.18	28,28,28,28	0
5	CL	B	305	1/1	0.94	0.07	35,35,35,35	0
5	CL	A	304	1/1	0.96	0.25	29,29,29,29	0
5	CL	A	305	1/1	0.97	0.09	32,32,32,32	0
3	CA	B	302	1/1	0.98	0.05	30,30,30,30	0
3	CA	A	302	1/1	0.98	0.05	28,28,28,28	0
5	CL	B	304	1/1	0.99	0.12	33,33,33,33	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.

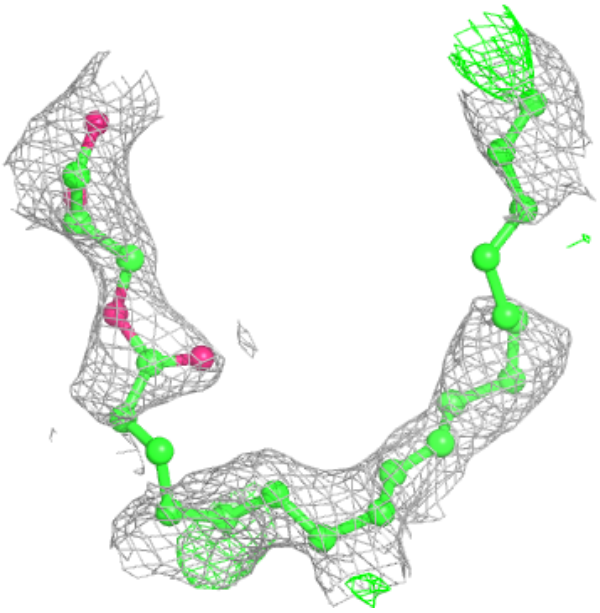
Electron density around OLC B 309:

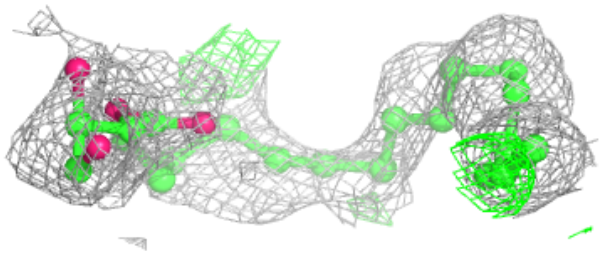
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

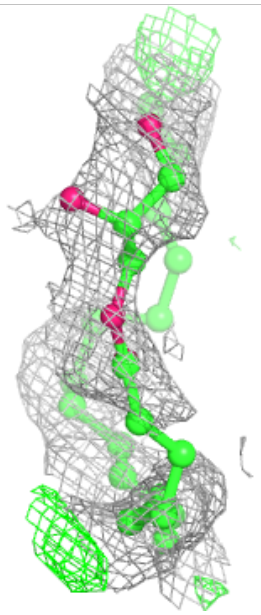


Electron density around OLC A 313:

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

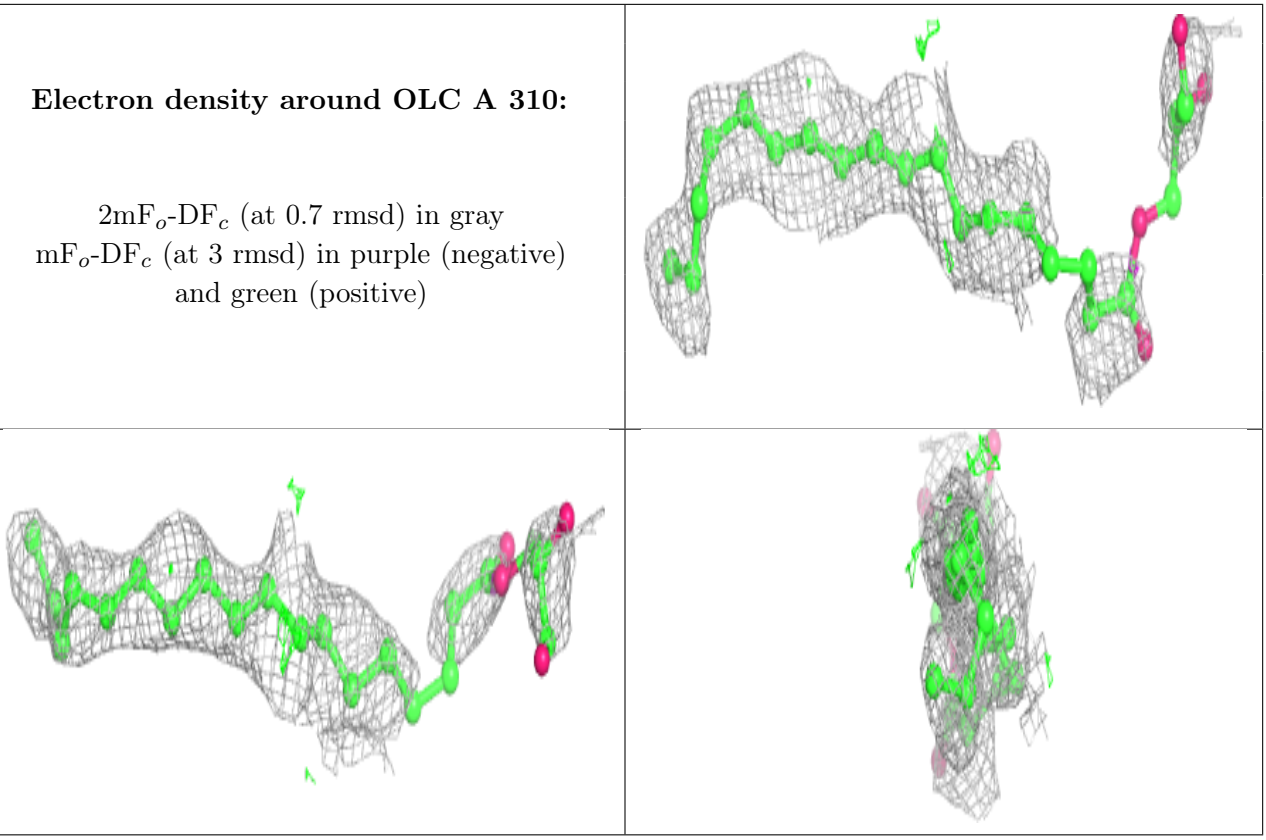






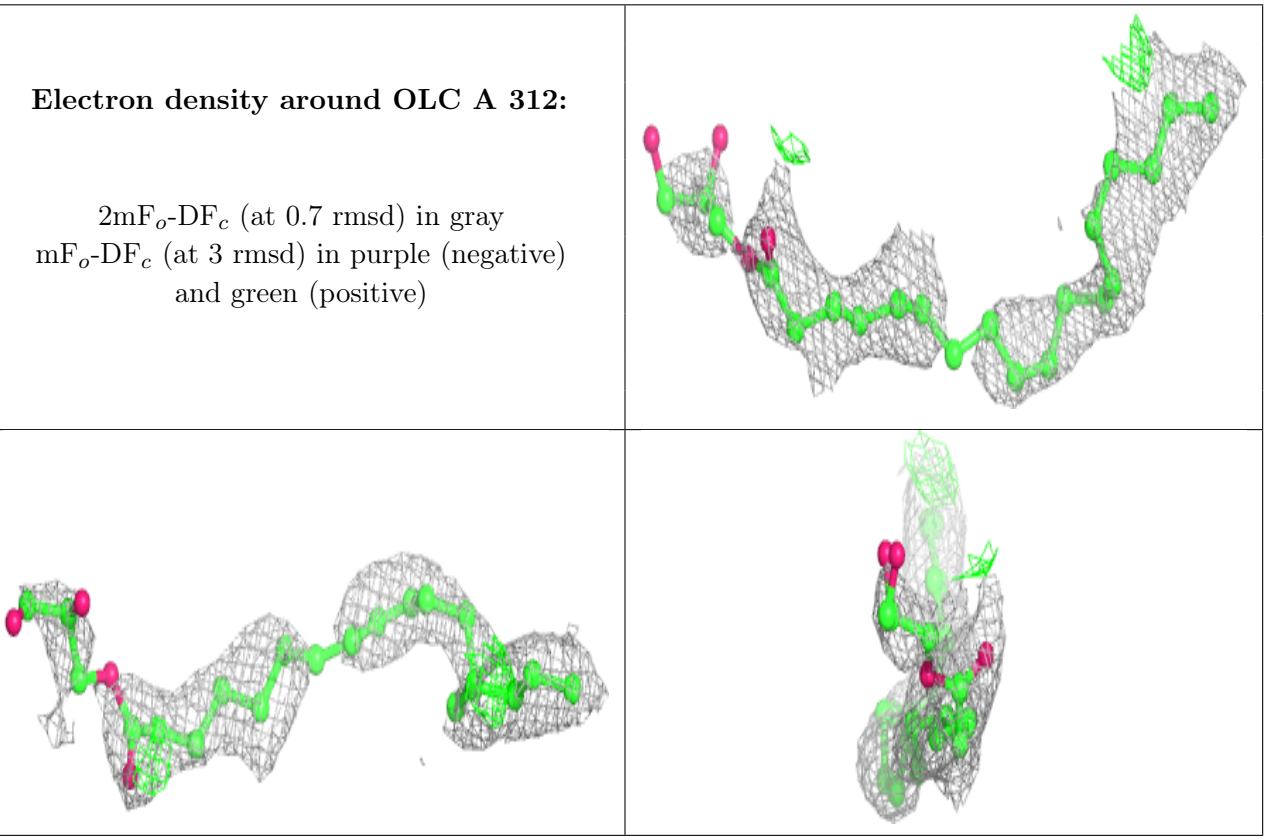
Electron density around OLC A 310:

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



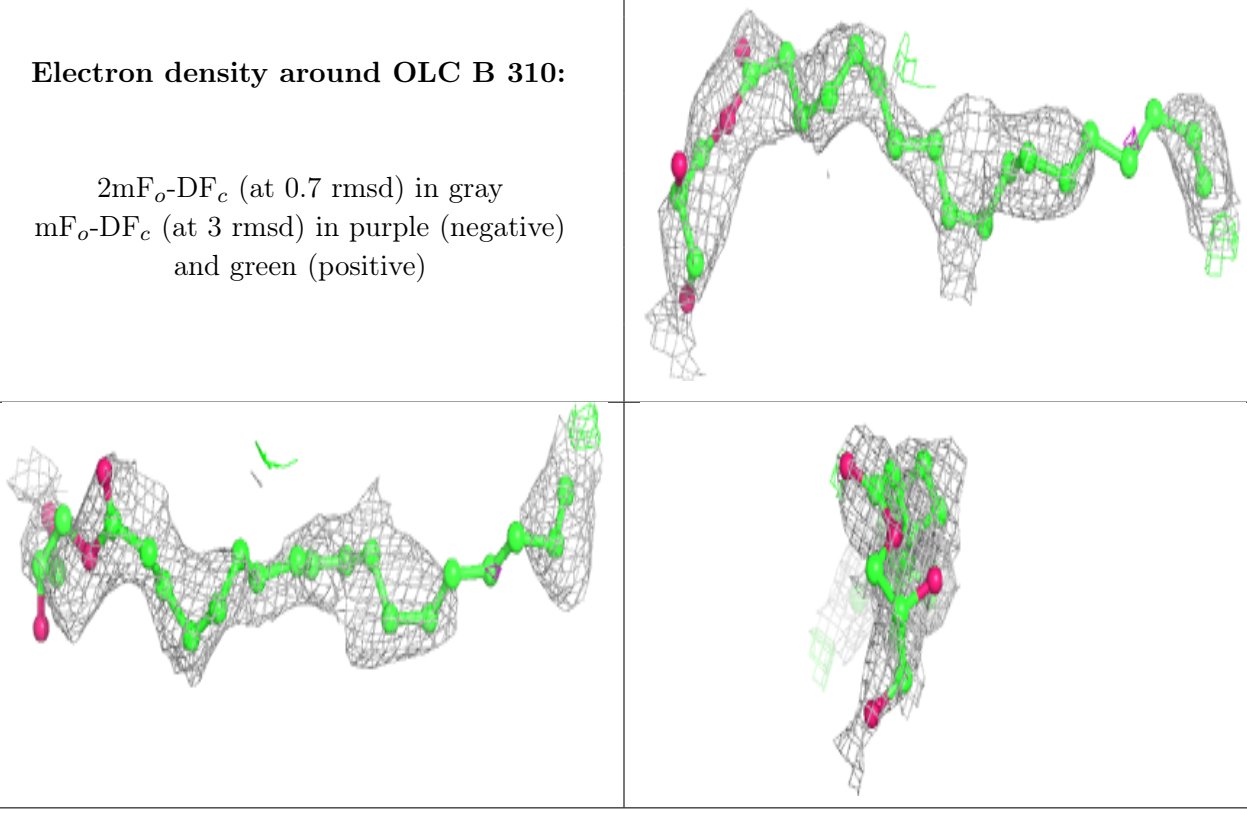
Electron density around OLC A 312:

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



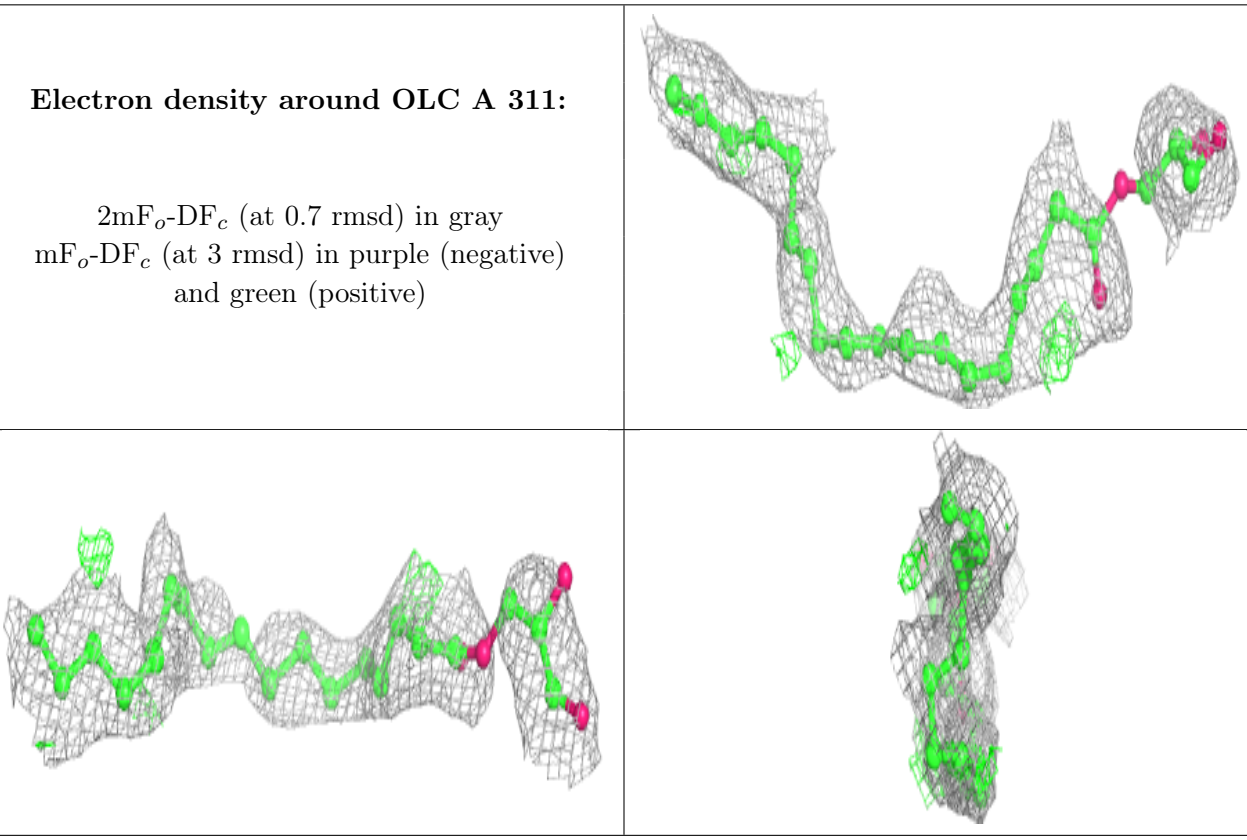
Electron density around OLC B 310:

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



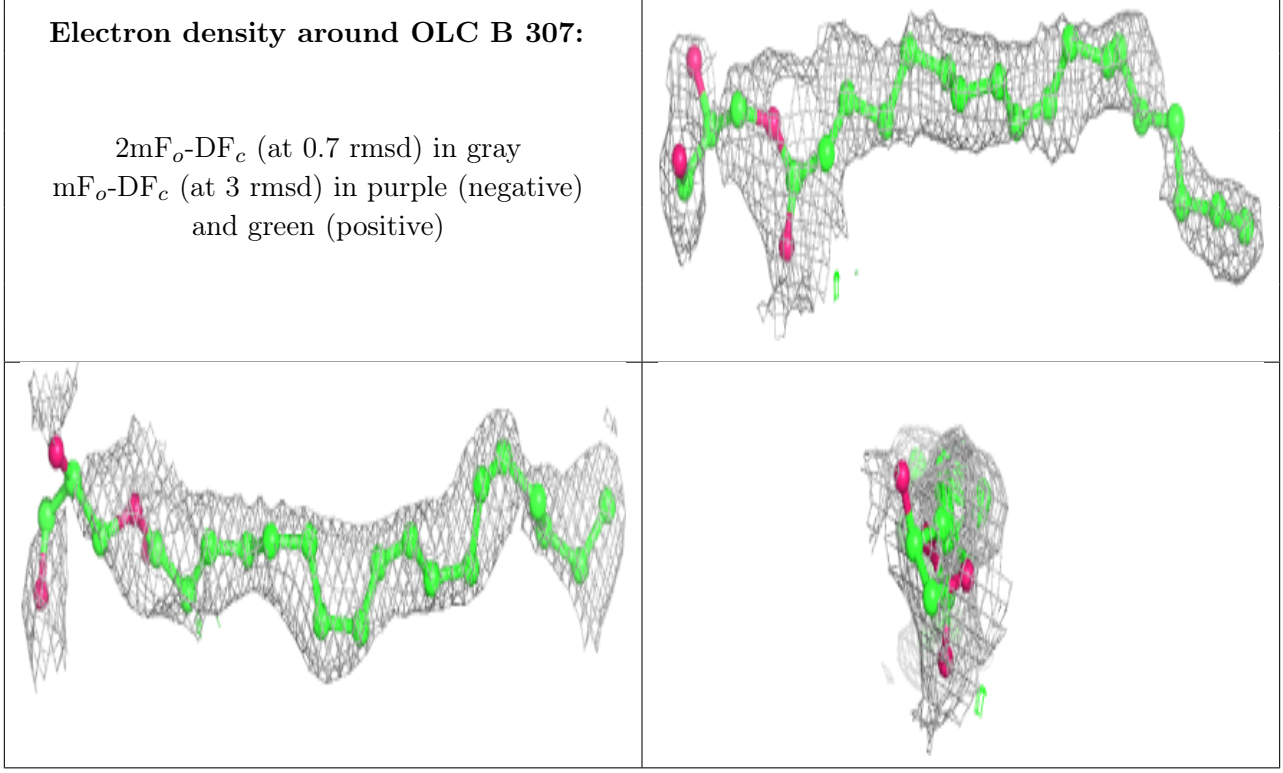
Electron density around OLC A 311:

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



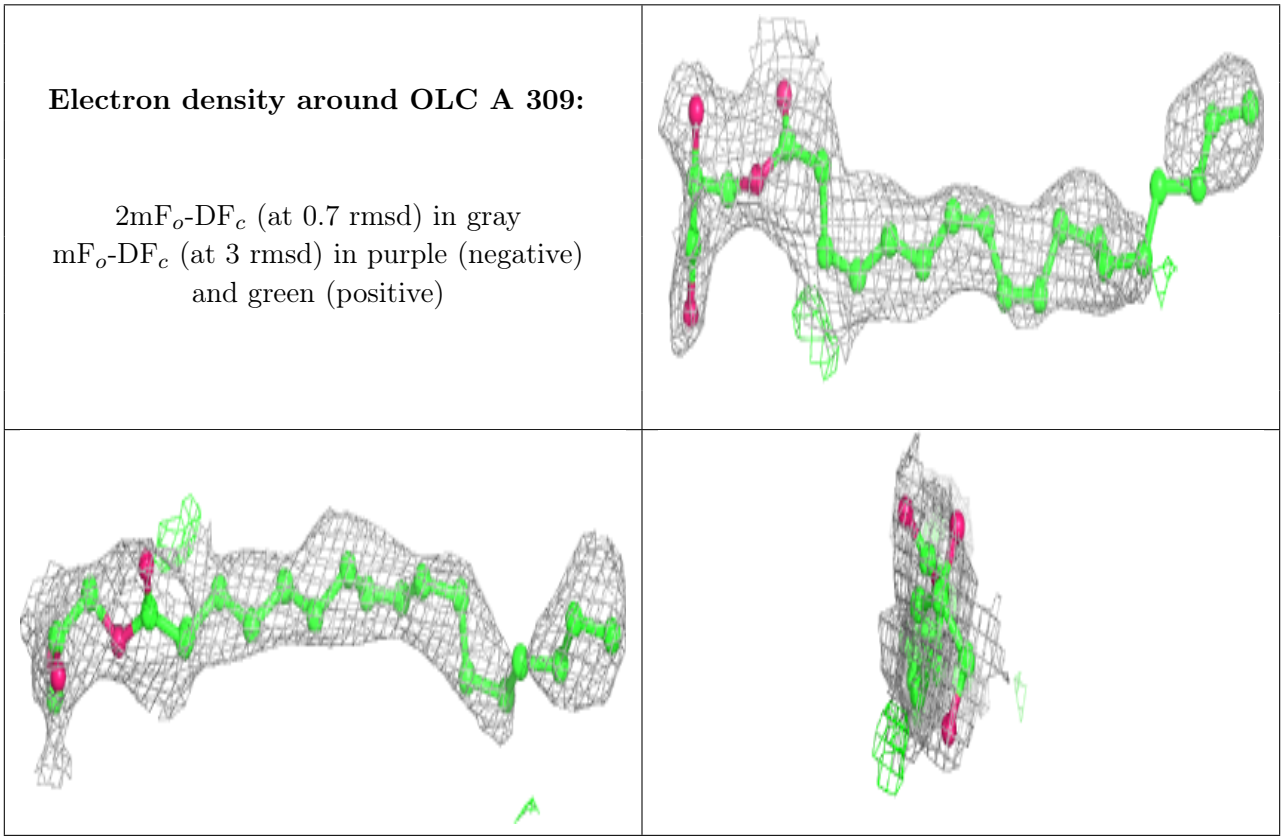
Electron density around OLC B 307:

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



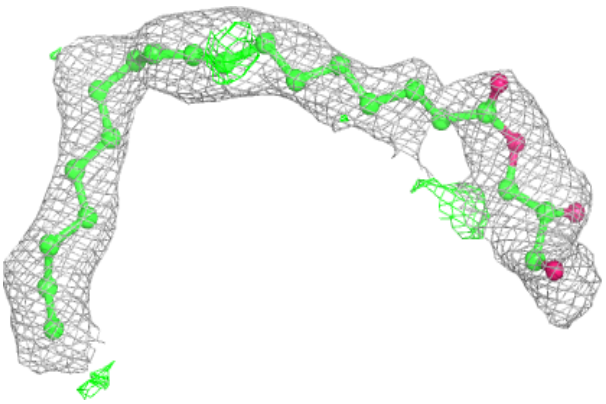
Electron density around OLC A 309:

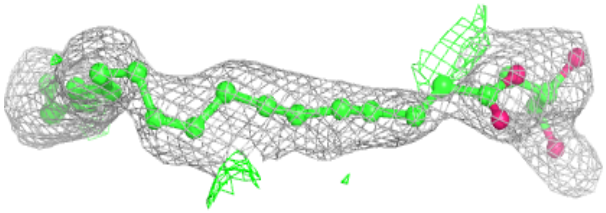
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

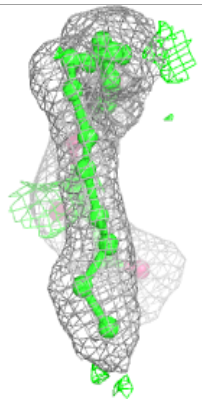


Electron density around OLC B 308:

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

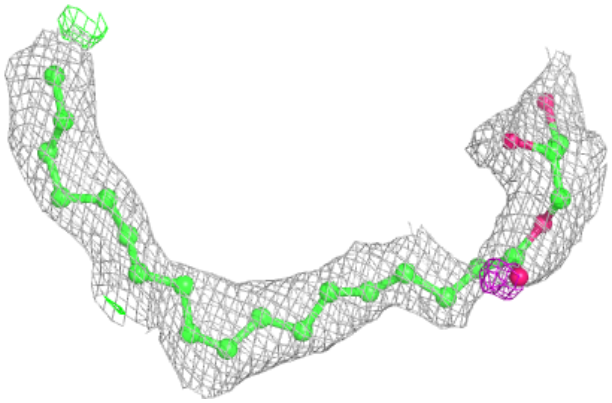


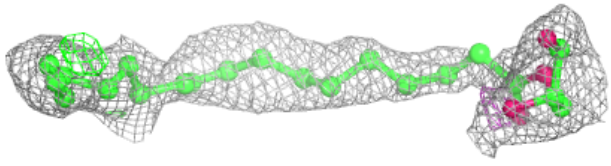


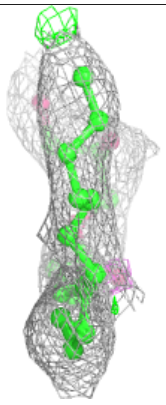


Electron density around OLC A 308:

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

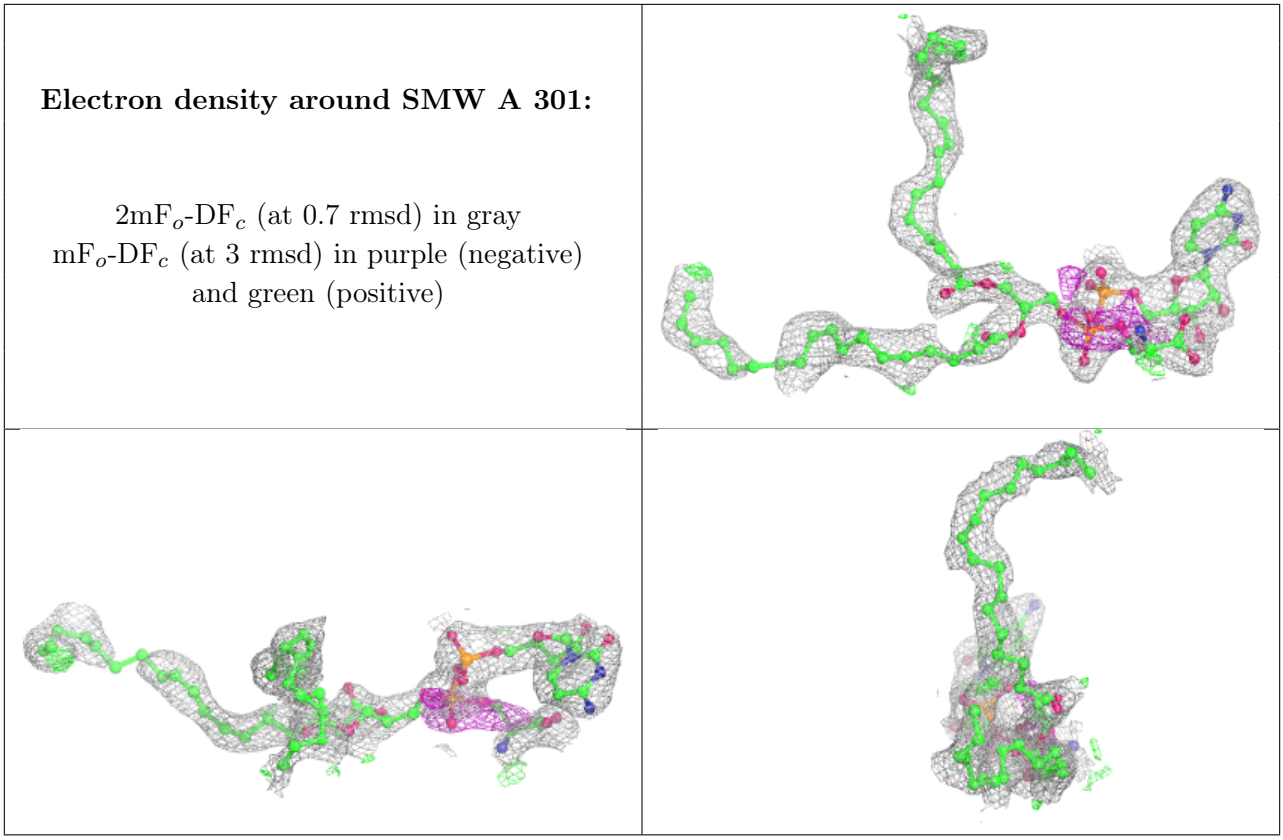






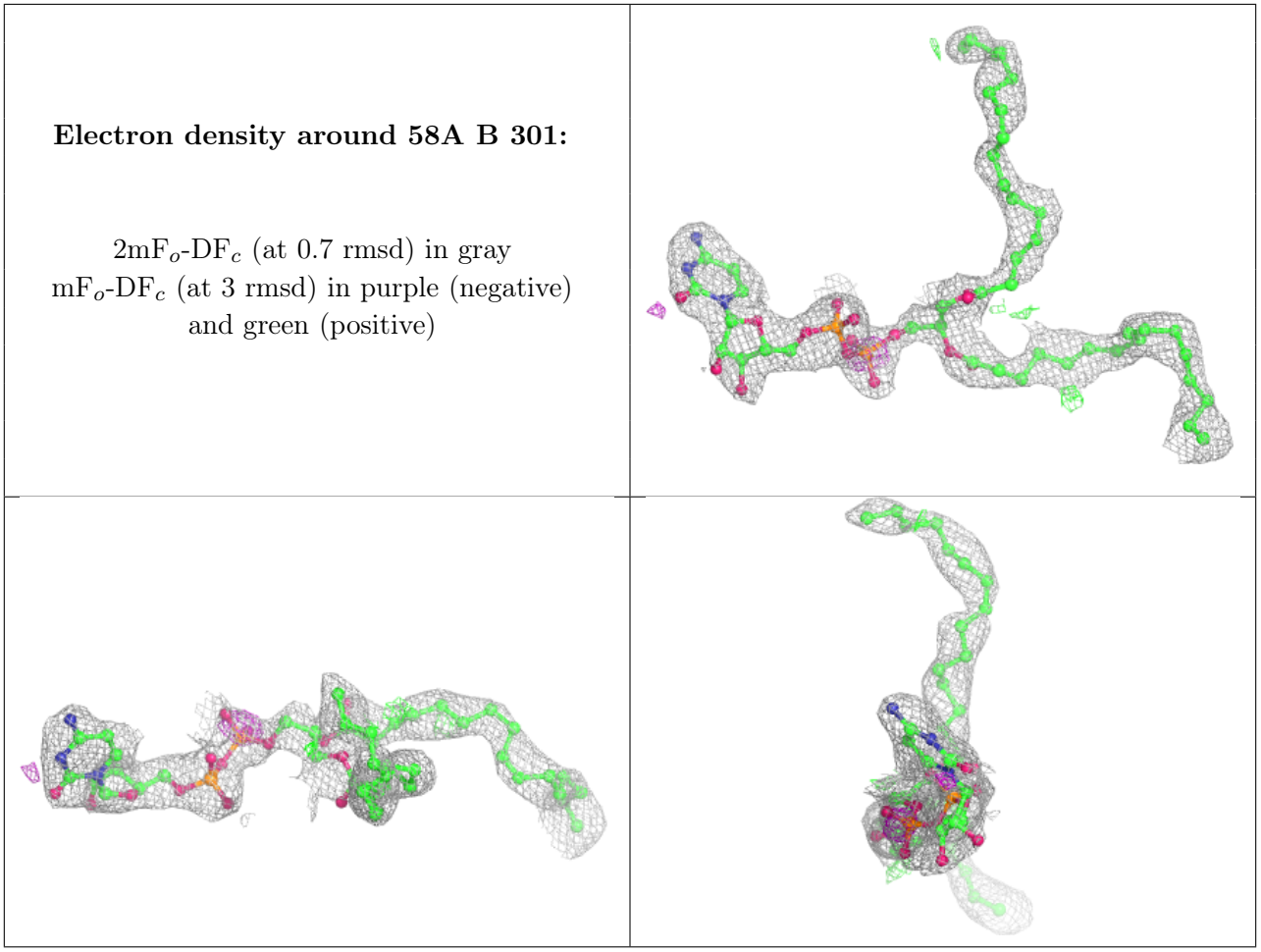
Electron density around SMW A 301:

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



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)



6.5 Other polymers

There are no such residues in this entry.