Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 10:58 pm GMT

PDB ID	:	5DIR
Title	:	membrane protein at 2.8 Angstroms
Authors	:	Vogeley, L.; El Arnaout, T.; Bailey, J.; Boland, C.; Caffrey, M.
Deposited on	:	2015-09-01
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

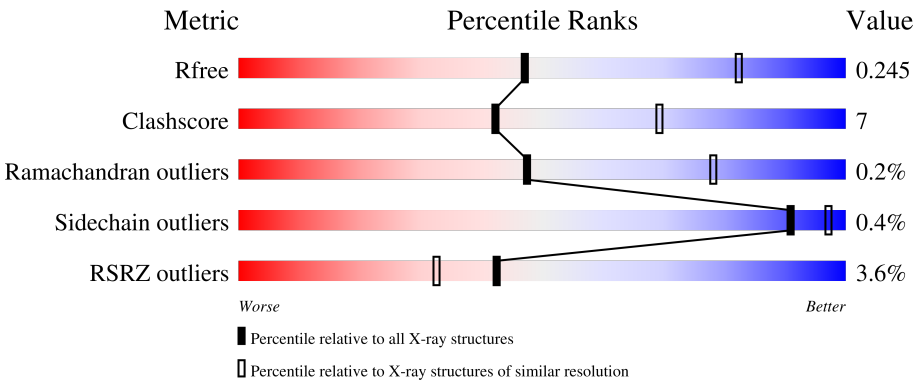
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	188	2%, 72%, 11%, 16%
1	B	188	4%, 65%, 14%, 21%
1	C	188	., 69%, 10%, 21%
1	D	188	5%, 70%, 9%, 21%
2	E	5	20%, 60%, 20%

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Mol	Chain	Length	Quality of chain
2	F	5	60% 40%
2	G	5	60% 40%
2	H	5	40% 40% 20%

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
3	OLC	B	202	-	-	-	X
3	OLC	C	204	-	-	-	X
3	OLC	D	202	-	-	-	X
3	OLC	D	203	-	-	-	X
3	OLC	D	205	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5653 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 Lipoprotein signal peptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	157	1261	848	202	207	4	0	0	0
			Total	C	N	O	S			
1	B	149	1198	806	194	195	3	0	0	0
			Total	C	N	O	S			
1	C	149	1197	807	191	195	4	0	0	0
			Total	C	N	O	S			
1	D	149	1197	807	191	195	4	0	0	0

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP Q9HVM5
A	-17	SER	-	expression tag	UNP Q9HVM5
A	-16	SER	-	expression tag	UNP Q9HVM5
A	-15	HIS	-	expression tag	UNP Q9HVM5
A	-14	HIS	-	expression tag	UNP Q9HVM5
A	-13	HIS	-	expression tag	UNP Q9HVM5
A	-12	HIS	-	expression tag	UNP Q9HVM5
A	-11	HIS	-	expression tag	UNP Q9HVM5
A	-10	HIS	-	expression tag	UNP Q9HVM5
A	-9	SER	-	expression tag	UNP Q9HVM5
A	-8	SER	-	expression tag	UNP Q9HVM5
A	-7	GLY	-	expression tag	UNP Q9HVM5
A	-6	LEU	-	expression tag	UNP Q9HVM5
A	-5	VAL	-	expression tag	UNP Q9HVM5
A	-4	PRO	-	expression tag	UNP Q9HVM5
A	-3	ARG	-	expression tag	UNP Q9HVM5
A	-2	GLY	-	expression tag	UNP Q9HVM5
A	-1	SER	-	expression tag	UNP Q9HVM5
A	0	HIS	-	expression tag	UNP Q9HVM5
B	-18	GLY	-	expression tag	UNP Q9HVM5
B	-17	SER	-	expression tag	UNP Q9HVM5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP Q9HVM5
B	-15	HIS	-	expression tag	UNP Q9HVM5
B	-14	HIS	-	expression tag	UNP Q9HVM5
B	-13	HIS	-	expression tag	UNP Q9HVM5
B	-12	HIS	-	expression tag	UNP Q9HVM5
B	-11	HIS	-	expression tag	UNP Q9HVM5
B	-10	HIS	-	expression tag	UNP Q9HVM5
B	-9	SER	-	expression tag	UNP Q9HVM5
B	-8	SER	-	expression tag	UNP Q9HVM5
B	-7	GLY	-	expression tag	UNP Q9HVM5
B	-6	LEU	-	expression tag	UNP Q9HVM5
B	-5	VAL	-	expression tag	UNP Q9HVM5
B	-4	PRO	-	expression tag	UNP Q9HVM5
B	-3	ARG	-	expression tag	UNP Q9HVM5
B	-2	GLY	-	expression tag	UNP Q9HVM5
B	-1	SER	-	expression tag	UNP Q9HVM5
B	0	HIS	-	expression tag	UNP Q9HVM5
C	-18	GLY	-	expression tag	UNP Q9HVM5
C	-17	SER	-	expression tag	UNP Q9HVM5
C	-16	SER	-	expression tag	UNP Q9HVM5
C	-15	HIS	-	expression tag	UNP Q9HVM5
C	-14	HIS	-	expression tag	UNP Q9HVM5
C	-13	HIS	-	expression tag	UNP Q9HVM5
C	-12	HIS	-	expression tag	UNP Q9HVM5
C	-11	HIS	-	expression tag	UNP Q9HVM5
C	-10	HIS	-	expression tag	UNP Q9HVM5
C	-9	SER	-	expression tag	UNP Q9HVM5
C	-8	SER	-	expression tag	UNP Q9HVM5
C	-7	GLY	-	expression tag	UNP Q9HVM5
C	-6	LEU	-	expression tag	UNP Q9HVM5
C	-5	VAL	-	expression tag	UNP Q9HVM5
C	-4	PRO	-	expression tag	UNP Q9HVM5
C	-3	ARG	-	expression tag	UNP Q9HVM5
C	-2	GLY	-	expression tag	UNP Q9HVM5
C	-1	SER	-	expression tag	UNP Q9HVM5
C	0	HIS	-	expression tag	UNP Q9HVM5
D	-18	GLY	-	expression tag	UNP Q9HVM5
D	-17	SER	-	expression tag	UNP Q9HVM5
D	-16	SER	-	expression tag	UNP Q9HVM5
D	-15	HIS	-	expression tag	UNP Q9HVM5
D	-14	HIS	-	expression tag	UNP Q9HVM5
D	-13	HIS	-	expression tag	UNP Q9HVM5

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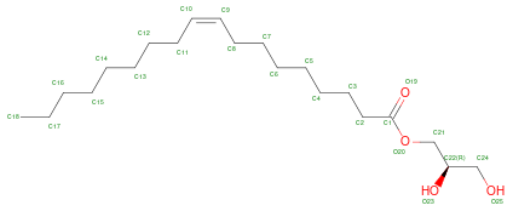
Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP Q9HVM5
D	-11	HIS	-	expression tag	UNP Q9HVM5
D	-10	HIS	-	expression tag	UNP Q9HVM5
D	-9	SER	-	expression tag	UNP Q9HVM5
D	-8	SER	-	expression tag	UNP Q9HVM5
D	-7	GLY	-	expression tag	UNP Q9HVM5
D	-6	LEU	-	expression tag	UNP Q9HVM5
D	-5	VAL	-	expression tag	UNP Q9HVM5
D	-4	PRO	-	expression tag	UNP Q9HVM5
D	-3	ARG	-	expression tag	UNP Q9HVM5
D	-2	GLY	-	expression tag	UNP Q9HVM5
D	-1	SER	-	expression tag	UNP Q9HVM5
D	0	HIS	-	expression tag	UNP Q9HVM5

- Molecule 2 is a protein called Globomycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	5	46	32	5	9	0	0	0
2	F	5	46	32	5	9	0	0	0
2	G	5	46	32	5	9	0	0	0
2	H	5	46	32	5	9	0	0	0

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

OLC



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	C	1	25	21	4	0	0
			Total	C	O		
3	C	1	25	21	4	0	0
			Total	C	O		
3	C	1	25	21	4	0	0
			Total	C	O		
3	D	1	25	21	4	0	0
			Total	C	O		
3	D	1	25	21	4	0	0
			Total	C	O		
3	D	1	25	21	4	0	0
			Total	C	O		
3	D	1	25	21	4	0	0
			Total	C	O		
3	D	1	25	21	4	0	0
			Total	C	O		
3	F	1	25	21	4	0	0
			Total	C	O		
3	F	1	25	21	4	0	0

- Molecule 4 is water.

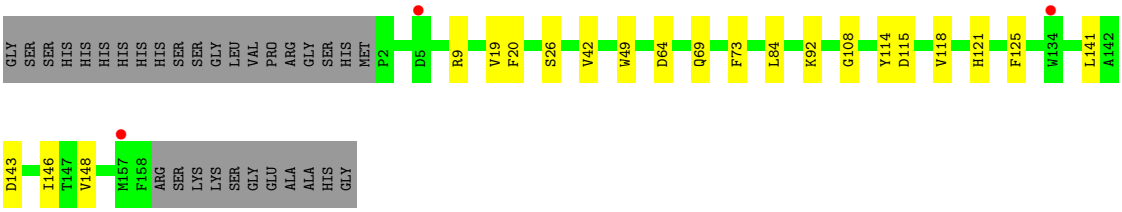
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	4	4	4	0	0
			Total	O		
4	B	2	2	2	0	0
			Total	O		
4	C	6	6	6	0	0
			Total	O		
4	D	4	4	4	0	0

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.

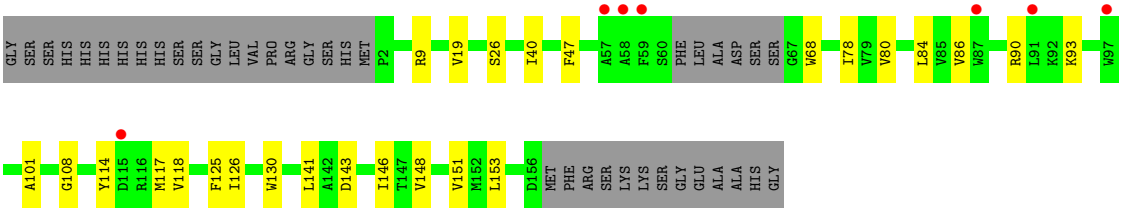
• Molecule 1: Lipoprotein signal peptidase

Chain A:



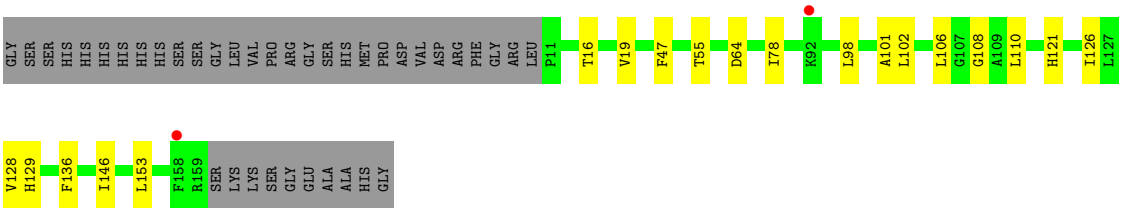
• Molecule 1: Lipoprotein signal peptidase

Chain B:



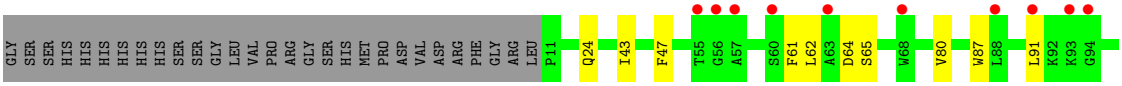
• Molecule 1: Lipoprotein signal peptidase

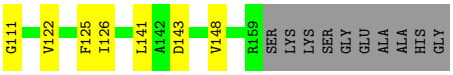
Chain C:



• Molecule 1: Lipoprotein signal peptidase

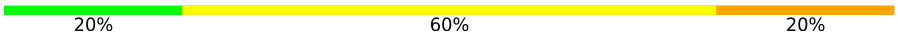
Chain D:





- Molecule 2: Globomycin

Chain E:



- Molecule 2: Globomycin

Chain F:

- Molecule 2: Globomycin

Chain G:

- Molecule 2: Globomycin

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	112.48Å 105.88Å 85.39Å 90.00° 96.92° 90.00°	Depositor
Resolution (Å)	44.90 – 2.80 44.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (44.90-2.80) 97.6 (44.90-2.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.81Å)	Xtriage
Refinement program	PHENIX dev_1894	Depositor
R, R_{free}	0.219 , 0.245 0.219 , 0.245	Depositor DCC
R_{free} test set	1207 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	66.5	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 62.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5653	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OLC, MLE, 5BV, IIL, ALO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.26	0/1300	0.46	0/1777
1	B	0.27	0/1234	0.49	0/1687
1	C	0.27	0/1234	0.49	0/1687
1	D	0.26	0/1234	0.48	0/1687
2	E	0.17	0/5	0.65	0/5
2	F	0.33	0/5	0.96	0/5
2	G	0.27	0/5	0.74	0/5
2	H	0.34	0/5	0.85	0/5
All	All	0.27	0/5022	0.48	0/6858

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 (i)

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	1261	0	1273	15	0
1	B	1198	0	1215	20	0
1	C	1197	0	1213	13	0
1	D	1197	0	1213	14	0
2	E	46	0	35	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	46	0	35	0	0
2	G	46	0	35	3	0
2	H	46	0	35	1	0
3	A	150	0	240	14	0
3	B	175	0	280	9	0
3	C	100	0	160	10	0
3	D	125	0	200	6	0
3	F	50	0	80	1	0
4	A	4	0	0	0	0
4	B	2	0	0	0	0
4	C	6	0	0	1	0
4	D	4	0	0	0	0
All	All	5653	0	6014	80	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 7.

All (80) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:VAL:HG11	3:B:201:OLC:H13A	1.69	0.72
1:A:49:TRP:HE1	3:A:203:OLC:H4A	1.56	0.70
1:A:148:VAL:HG21	3:A:201:OLC:H12A	1.76	0.67
3:A:202:OLC:H18A	3:A:203:OLC:H15A	1.79	0.64
1:C:129:HIS:NE2	4:C:301:HOH:O	2.30	0.64
1:B:148:VAL:HG21	3:B:201:OLC:H11	1.82	0.61
1:B:78:ILE:HD11	1:B:117:MET:HE3	1.83	0.59
1:D:143:ASP:OD2	2:G:203:SER:OG	2.19	0.59
3:C:202:OLC:H18A	3:C:203:OLC:H18A	1.85	0.58
1:A:108:GLY:HA3	1:A:146:ILE:HG13	1.86	0.57
1:A:20:PHE:HE2	3:A:205:OLC:H17A	1.70	0.57
3:A:201:OLC:H17	3:A:204:OLC:H12A	1.88	0.56
1:C:19:VAL:HG22	3:F:301:OLC:H17A	1.88	0.56
1:C:110:LEU:HB3	3:C:202:OLC:H10	1.88	0.55
1:D:80:VAL:HG11	2:G:201:MLE:HD21	1.89	0.55
1:D:148:VAL:HG21	3:D:201:OLC:H11A	1.89	0.55
1:C:101:ALA:HB1	1:C:153:LEU:HD12	1.89	0.54
1:C:47:PHE:HE1	1:C:126:ILE:HG23	1.73	0.53
1:B:47:PHE:HE1	1:B:126:ILE:HG23	1.74	0.53
1:B:130:TRP:CD2	3:B:206:OLC:H3A	2.44	0.53
1:A:19:VAL:HG22	3:A:204:OLC:H16	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ASP:OD2	2:H:203:SER:OG	2.28	0.51
1:D:141:LEU:HD21	3:D:202:OLC:H12	1.93	0.50
1:C:16:THR:HG21	1:C:106:LEU:HD22	1.93	0.50
1:A:143:ASP:HB3	3:A:201:OLC:H21A	1.93	0.50
1:B:108:GLY:HA3	1:B:146:ILE:HG13	1.94	0.50
1:A:42:VAL:HG22	3:A:203:OLC:H2A	1.93	0.50
1:B:151:VAL:HG12	3:B:202:OLC:H7A	1.94	0.50
1:D:47:PHE:HE1	1:D:126:ILE:HG23	1.77	0.49
1:B:101:ALA:HB1	1:B:153:LEU:HD12	1.95	0.49
1:A:141:LEU:HD21	3:A:202:OLC:H14A	1.94	0.49
1:D:122:VAL:HG11	2:G:203:SER:HB3	1.93	0.49
1:B:26:SER:HB3	1:B:125:PHE:CZ	2.48	0.49
1:D:43:ILE:HD11	3:D:205:OLC:H15	1.95	0.48
1:C:55:THR:HG22	1:C:121:HIS:HB3	1.95	0.48
1:D:24:GLN:NE2	1:D:111:GLY:O	2.47	0.48
1:C:128:VAL:HG23	1:C:136:PHE:HB3	1.96	0.47
1:B:9:ARG:CZ	1:B:93:LYS:HG3	2.45	0.47
3:A:201:OLC:H11	3:A:201:OLC:H8A	1.66	0.46
1:B:148:VAL:O	1:B:151:VAL:HG22	2.15	0.46
1:A:26:SER:HB3	1:A:125:PHE:CZ	2.50	0.46
1:B:40:ILE:HD13	3:B:207:OLC:H21A	1.97	0.46
1:D:125:PHE:HZ	1:D:141:LEU:HD13	1.81	0.46
1:B:114:TYR:CE1	1:B:118:VAL:HG21	2.51	0.46
3:D:203:OLC:H8A	3:D:203:OLC:H11	1.43	0.45
3:D:202:OLC:H11	3:D:202:OLC:H8	1.43	0.45
1:C:108:GLY:HA3	1:C:146:ILE:HG13	1.99	0.45
3:A:202:OLC:H11A	3:A:202:OLC:H8	1.46	0.45
1:A:69:GLN:HB3	1:A:73:PHE:CE2	2.52	0.45
3:A:205:OLC:H11	3:A:205:OLC:H8	1.75	0.45
1:A:9:ARG:HH21	1:A:92:LYS:HA	1.81	0.45
3:C:203:OLC:H11A	3:C:203:OLC:H8	1.76	0.44
1:D:87:TRP:O	1:D:91:LEU:HD13	2.16	0.44
3:B:207:OLC:H8	3:B:207:OLC:H11A	1.39	0.44
3:C:202:OLC:H8	3:C:202:OLC:H11	1.49	0.44
1:A:114:TYR:CZ	1:A:118:VAL:HG21	2.52	0.44
3:C:201:OLC:H16	3:C:204:OLC:H17A	1.99	0.43
3:C:203:OLC:H12	3:C:203:OLC:H15	1.62	0.43
1:B:86:VAL:O	1:B:90:ARG:HG2	2.19	0.43
3:C:201:OLC:H11	3:C:201:OLC:H8	1.55	0.43
1:A:84:LEU:HD12	1:A:84:LEU:HA	1.86	0.43
3:A:204:OLC:H11	3:A:204:OLC:H8A	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:TRP:CH2	1:D:62:LEU:HD22	2.54	0.43
1:B:141:LEU:HD23	1:B:141:LEU:HA	1.84	0.42
1:B:19:VAL:HG22	3:B:204:OLC:H16	2.01	0.42
3:C:201:OLC:H14	3:C:204:OLC:H15A	2.01	0.42
1:B:68:TRP:NE1	1:D:65:SER:OG	2.52	0.42
1:D:64:ASP:OD1	1:D:64:ASP:N	2.52	0.42
3:B:203:OLC:H8	3:B:203:OLC:H11A	1.67	0.42
1:A:115:ASP:HB3	1:A:121:HIS:O	2.20	0.42
1:D:143:ASP:HB3	3:D:201:OLC:H21A	2.02	0.42
1:C:110:LEU:HD13	3:C:202:OLC:H10	2.02	0.41
3:A:201:OLC:H21	2:E:202:IIL:HD12	2.03	0.41
3:B:204:OLC:H9	3:B:204:OLC:H6	1.72	0.41
2:E:201:MLE:HG	2:E:205:5BV:C	2.49	0.41
1:C:78:ILE:HG12	3:C:203:OLC:H10	2.01	0.41
1:B:80:VAL:O	1:B:84:LEU:HD13	2.21	0.41
1:C:98:LEU:O	1:C:102:LEU:HD13	2.21	0.40
1:A:64:ASP:OD1	1:A:64:ASP:N	2.54	0.40
1:C:64:ASP:N	1:C:64:ASP:OD1	2.52	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	155/188 (82%)	153 (99%)	2 (1%)	0	100	100
1	B	145/188 (77%)	143 (99%)	2 (1%)	0	100	100
1	C	147/188 (78%)	140 (95%)	7 (5%)	0	100	100
1	D	147/188 (78%)	142 (97%)	4 (3%)	1 (1%)	22	53
2	E	1/5 (20%)	1 (100%)	0	0	100	100
2	F	1/5 (20%)	1 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	1/5 (20%)	1 (100%)	0	0	100	100
2	H	1/5 (20%)	1 (100%)	0	0	100	100
All	All	598/772 (78%)	582 (97%)	15 (2%)	1 (0%)	47	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	61	PHE

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	130/154 (84%)	130 (100%)	0	100	100
1	B	123/154 (80%)	123 (100%)	0	100	100
1	C	123/154 (80%)	123 (100%)	0	100	100
1	D	123/154 (80%)	123 (100%)	0	100	100
2	E	1/1 (100%)	1 (100%)	0	100	100
2	F	1/1 (100%)	1 (100%)	0	100	100
2	G	1/1 (100%)	0	1 (100%)	0	0
2	H	1/1 (100%)	0	1 (100%)	0	0
All	All	503/620 (81%)	501 (100%)	2 (0%)	91	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	203	SER
2	H	203	SER

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)

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	IIL	E	202	2	6,7,8	0.40	0	5,8,10	0.95	0
2	ALO	H	204	2	5,6,7	0.56	0	6,7,9	1.25	1 (16%)
2	IIL	G	202	2	6,7,8	0.40	0	5,8,10	1.05	0
2	IIL	H	202	2	6,7,8	0.38	0	5,8,10	0.94	0
2	MLE	G	201	2	7,8,9	0.54	0	6,9,11	1.04	1 (16%)
2	MLE	H	201	2	7,8,9	0.57	0	6,9,11	0.95	1 (16%)
2	ALO	G	204	2	5,6,7	0.52	0	6,7,9	0.91	0
2	ALO	F	204	2	5,6,7	0.48	0	6,7,9	1.09	1 (16%)
2	IIL	F	202	2	6,7,8	0.38	0	5,8,10	1.13	0
2	MLE	F	201	2	7,8,9	0.50	0	6,9,11	1.07	1 (16%)
2	MLE	E	201	2	7,8,9	0.52	0	6,9,11	1.14	1 (16%)
2	ALO	E	204	2	5,6,7	0.50	0	6,7,9	1.24	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IIL	E	202	2	-	3/7/8/10	-
2	ALO	H	204	2	-	1/5/6/8	-
2	IIL	G	202	2	-	2/7/8/10	-
2	IIL	H	202	2	-	4/7/8/10	-
2	MLE	G	201	2	-	0/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLE	H	201	2	-	1/5/8/10	-
2	ALO	G	204	2	-	1/5/6/8	-
2	ALO	F	204	2	-	1/5/6/8	-
2	IIL	F	202	2	-	4/7/8/10	-
2	MLE	F	201	2	-	1/5/8/10	-
2	MLE	E	201	2	-	1/5/8/10	-
2	ALO	E	204	2	-	0/5/6/8	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	204	ALO	CB-CA-C	-2.69	107.48	111.77
2	E	204	ALO	CB-CA-C	-2.59	107.63	111.77
2	E	201	MLE	O-C-CA	-2.41	118.47	124.78
2	F	201	MLE	O-C-CA	-2.40	118.49	124.78
2	F	204	ALO	CB-CA-C	-2.28	108.13	111.77
2	G	201	MLE	O-C-CA	-2.26	118.85	124.78
2	H	201	MLE	O-C-CA	-2.13	119.20	124.78

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	202	IIL	C-CA-CB-CG2
2	E	202	IIL	C-CA-CB-CG1
2	F	204	ALO	O-C-CA-CB
2	H	204	ALO	O-C-CA-CB
2	E	201	MLE	N-CA-CB-CG
2	H	202	IIL	CA-CB-CG1-CD1
2	H	201	MLE	N-CA-CB-CG
2	H	202	IIL	CG2-CB-CG1-CD1
2	F	201	MLE	N-CA-CB-CG
2	G	202	IIL	CA-CB-CG1-CD1
2	F	202	IIL	CG2-CB-CG1-CD1
2	F	202	IIL	CA-CB-CG1-CD1
2	F	202	IIL	C-CA-CB-CG1
2	G	202	IIL	C-CA-CB-CG1
2	H	202	IIL	C-CA-CB-CG1
2	E	202	IIL	O-C-CA-CB
2	F	202	IIL	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	H	202	IIL	O-C-CA-CB
2	G	204	ALO	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	202	IIL	1	0
2	G	201	MLE	1	0
2	E	201	MLE	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	OLC	A	202	-	24,24,24	0.52	0	25,25,25	0.79	0
3	OLC	A	205	-	24,24,24	0.53	0	25,25,25	0.75	0
3	OLC	F	302	-	24,24,24	0.50	0	25,25,25	0.81	0
3	OLC	C	201	-	24,24,24	0.51	0	25,25,25	0.80	0
3	OLC	A	204	-	24,24,24	0.51	0	25,25,25	0.75	0
3	OLC	A	203	-	24,24,24	0.49	0	25,25,25	0.84	0
3	OLC	A	206	-	24,24,24	0.52	0	25,25,25	0.78	0
3	OLC	B	202	-	24,24,24	0.51	0	25,25,25	0.82	0
3	OLC	D	202	-	24,24,24	0.53	0	25,25,25	0.79	0
3	OLC	C	202	-	24,24,24	0.51	0	25,25,25	0.80	0
3	OLC	B	207	-	24,24,24	0.51	0	25,25,25	0.78	0
3	OLC	C	204	-	24,24,24	0.53	0	25,25,25	0.84	0
3	OLC	B	205	-	24,24,24	0.52	0	25,25,25	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	OLC	C	203	-	24,24,24	0.54	0	25,25,25	0.71	0
3	OLC	D	201	-	24,24,24	0.53	0	25,25,25	0.72	0
3	OLC	B	204	-	24,24,24	0.53	0	25,25,25	0.90	0
3	OLC	D	205	-	24,24,24	0.57	0	25,25,25	0.66	0
3	OLC	D	204	-	24,24,24	0.55	0	25,25,25	0.77	0
3	OLC	B	203	-	24,24,24	0.48	0	25,25,25	0.89	0
3	OLC	B	206	-	24,24,24	0.54	0	25,25,25	0.70	0
3	OLC	D	203	-	24,24,24	0.52	0	25,25,25	0.76	0
3	OLC	F	301	-	24,24,24	0.52	0	25,25,25	0.76	0
3	OLC	B	201	-	24,24,24	0.53	0	25,25,25	0.79	0
3	OLC	A	201	-	24,24,24	0.54	0	25,25,25	0.88	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OLC	A	202	-	-	15/24/24/24	-
3	OLC	A	205	-	-	10/24/24/24	-
3	OLC	F	302	-	-	14/24/24/24	-
3	OLC	C	201	-	-	13/24/24/24	-
3	OLC	A	204	-	-	17/24/24/24	-
3	OLC	A	203	-	-	17/24/24/24	-
3	OLC	A	206	-	-	13/24/24/24	-
3	OLC	B	202	-	-	9/24/24/24	-
3	OLC	D	202	-	-	8/24/24/24	-
3	OLC	C	202	-	-	15/24/24/24	-
3	OLC	B	207	-	-	12/24/24/24	-
3	OLC	C	204	-	-	8/24/24/24	-
3	OLC	B	205	-	-	16/24/24/24	-
3	OLC	C	203	-	-	12/24/24/24	-
3	OLC	D	201	-	-	14/24/24/24	-
3	OLC	B	204	-	-	9/24/24/24	-
3	OLC	D	205	-	-	11/24/24/24	-
3	OLC	D	204	-	-	12/24/24/24	-
3	OLC	B	203	-	-	14/24/24/24	-
3	OLC	B	206	-	-	14/24/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OLC	D	203	-	-	13/24/24/24	-
3	OLC	F	301	-	-	11/24/24/24	-
3	OLC	B	201	-	-	7/24/24/24	-
3	OLC	A	201	-	-	12/24/24/24	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (296) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	OLC	C21-C22-C24-O25
3	A	201	OLC	O20-C21-C22-O23
3	A	202	OLC	O20-C21-C22-C24
3	A	202	OLC	O20-C21-C22-O23
3	A	205	OLC	C6-C7-C8-C9
3	A	206	OLC	C21-C22-C24-O25
3	A	206	OLC	O23-C22-C24-O25
3	B	203	OLC	C21-C22-C24-O25
3	B	205	OLC	C21-C22-C24-O25
3	B	207	OLC	C21-C22-C24-O25
3	C	202	OLC	C21-C22-C24-O25
3	C	202	OLC	O20-C21-C22-C24
3	C	202	OLC	O20-C21-C22-O23
3	C	204	OLC	C21-C22-C24-O25
3	D	201	OLC	C21-C22-C24-O25
3	D	201	OLC	O20-C21-C22-C24
3	D	201	OLC	O20-C21-C22-O23
3	D	203	OLC	O20-C21-C22-C24
3	D	203	OLC	O20-C21-C22-O23
3	D	204	OLC	C21-C22-C24-O25
3	D	205	OLC	C21-C22-C24-O25
3	D	205	OLC	O20-C21-C22-C24
3	F	301	OLC	C21-C22-C24-O25
3	F	302	OLC	O20-C21-C22-C24
3	F	302	OLC	O20-C21-C22-O23
3	A	203	OLC	O19-C1-O20-C21
3	C	202	OLC	O19-C1-O20-C21
3	C	203	OLC	O19-C1-O20-C21
3	D	202	OLC	O19-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
3	C	203	OLC	C2-C1-O20-C21
3	D	202	OLC	C2-C1-O20-C21
3	A	202	OLC	C2-C1-O20-C21
3	A	203	OLC	C2-C1-O20-C21
3	C	202	OLC	C2-C1-O20-C21
3	C	204	OLC	C2-C1-O20-C21
3	A	202	OLC	O19-C1-O20-C21
3	C	204	OLC	O19-C1-O20-C21
3	A	205	OLC	O20-C21-C22-O23
3	B	205	OLC	O20-C21-C22-O23
3	D	205	OLC	O20-C21-C22-O23
3	B	202	OLC	C2-C1-O20-C21
3	B	202	OLC	O19-C1-O20-C21
3	A	204	OLC	C2-C1-O20-C21
3	B	205	OLC	C2-C1-O20-C21
3	B	206	OLC	C2-C1-O20-C21
3	C	201	OLC	C2-C1-O20-C21
3	A	203	OLC	O20-C21-C22-C24
3	A	204	OLC	O20-C21-C22-C24
3	A	205	OLC	O20-C21-C22-C24
3	A	204	OLC	O20-C21-C22-O23
3	C	201	OLC	O20-C21-C22-O23
3	A	201	OLC	C1-C2-C3-C4
3	D	205	OLC	C2-C1-O20-C21
3	A	203	OLC	C1-C2-C3-C4
3	B	206	OLC	C1-C2-C3-C4
3	A	204	OLC	O19-C1-O20-C21
3	F	301	OLC	O23-C22-C24-O25
3	A	202	OLC	C1-C2-C3-C4
3	C	202	OLC	C1-C2-C3-C4
3	D	202	OLC	C1-C2-C3-C4
3	C	204	OLC	C1-C2-C3-C4
3	B	205	OLC	O19-C1-O20-C21
3	B	206	OLC	O19-C1-O20-C21
3	C	201	OLC	O19-C1-O20-C21
3	B	207	OLC	C2-C1-O20-C21
3	D	205	OLC	O19-C1-O20-C21
3	A	203	OLC	O20-C21-C22-O23
3	B	201	OLC	O20-C21-C22-O23
3	C	204	OLC	O20-C21-C22-O23
3	F	302	OLC	C2-C1-O20-C21
3	A	204	OLC	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
3	B	207	OLC	C6-C7-C8-C9
3	B	207	OLC	C11-C12-C13-C14
3	B	206	OLC	C13-C14-C15-C16
3	B	206	OLC	C2-C3-C4-C5
3	C	203	OLC	C14-C15-C16-C17
3	A	205	OLC	C2-C1-O20-C21
3	A	201	OLC	O20-C21-C22-C24
3	B	201	OLC	O20-C21-C22-C24
3	C	201	OLC	O20-C21-C22-C24
3	A	203	OLC	C3-C4-C5-C6
3	B	205	OLC	C4-C5-C6-C7
3	C	203	OLC	C2-C3-C4-C5
3	A	206	OLC	C2-C3-C4-C5
3	C	201	OLC	C3-C4-C5-C6
3	A	202	OLC	C11-C12-C13-C14
3	A	202	OLC	C3-C4-C5-C6
3	D	204	OLC	C14-C15-C16-C17
3	F	302	OLC	C1-C2-C3-C4
3	A	204	OLC	C14-C15-C16-C17
3	C	202	OLC	C5-C6-C7-C8
3	D	203	OLC	C11-C12-C13-C14
3	D	203	OLC	C2-C3-C4-C5
3	A	202	OLC	C21-C22-C24-O25
3	A	204	OLC	C21-C22-C24-O25
3	C	201	OLC	C21-C22-C24-O25
3	A	202	OLC	C5-C6-C7-C8
3	A	203	OLC	C6-C7-C8-C9
3	A	206	OLC	C10-C11-C12-C13
3	F	302	OLC	C6-C7-C8-C9
3	A	203	OLC	C13-C14-C15-C16
3	B	206	OLC	C5-C6-C7-C8
3	B	207	OLC	C12-C13-C14-C15
3	C	202	OLC	C13-C14-C15-C16
3	C	204	OLC	C3-C4-C5-C6
3	D	201	OLC	C3-C4-C5-C6
3	A	205	OLC	C13-C14-C15-C16
3	D	201	OLC	C12-C13-C14-C15
3	F	301	OLC	C11-C12-C13-C14
3	A	206	OLC	C12-C13-C14-C15
3	B	206	OLC	C14-C15-C16-C17
3	F	302	OLC	C3-C4-C5-C6
3	B	207	OLC	O19-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
3	A	203	OLC	C11-C12-C13-C14
3	B	201	OLC	C12-C13-C14-C15
3	A	202	OLC	C4-C5-C6-C7
3	B	205	OLC	C5-C6-C7-C8
3	F	301	OLC	C13-C14-C15-C16
3	D	202	OLC	C14-C15-C16-C17
3	A	201	OLC	O23-C22-C24-O25
3	B	203	OLC	O23-C22-C24-O25
3	B	207	OLC	O23-C22-C24-O25
3	D	201	OLC	O23-C22-C24-O25
3	D	204	OLC	O23-C22-C24-O25
3	A	203	OLC	C12-C13-C14-C15
3	A	203	OLC	C10-C11-C12-C13
3	D	201	OLC	C6-C7-C8-C9
3	A	205	OLC	O19-C1-O20-C21
3	D	203	OLC	C12-C13-C14-C15
3	F	302	OLC	O19-C1-O20-C21
3	C	201	OLC	C1-C2-C3-C4
3	B	207	OLC	C1-C2-C3-C4
3	D	201	OLC	C1-C2-C3-C4
3	B	203	OLC	C6-C7-C8-C9
3	C	202	OLC	C10-C11-C12-C13
3	C	203	OLC	C10-C11-C12-C13
3	D	202	OLC	C10-C11-C12-C13
3	F	302	OLC	C10-C11-C12-C13
3	F	301	OLC	C2-C1-O20-C21
3	D	201	OLC	C2-C3-C4-C5
3	B	203	OLC	C12-C13-C14-C15
3	B	204	OLC	C2-C3-C4-C5
3	D	203	OLC	C3-C4-C5-C6
3	B	204	OLC	C1-C2-C3-C4
3	A	203	OLC	C2-C3-C4-C5
3	F	302	OLC	C5-C6-C7-C8
3	A	206	OLC	C3-C4-C5-C6
3	A	205	OLC	C14-C15-C16-C17
3	A	206	OLC	C5-C6-C7-C8
3	C	203	OLC	C4-C5-C6-C7
3	B	206	OLC	C6-C7-C8-C9
3	D	203	OLC	C5-C6-C7-C8
3	C	201	OLC	C5-C6-C7-C8
3	B	203	OLC	C2-C1-O20-C21
3	B	204	OLC	C2-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
3	A	206	OLC	C1-C2-C3-C4
3	C	202	OLC	C3-C4-C5-C6
3	D	203	OLC	C6-C7-C8-C9
3	B	201	OLC	C13-C14-C15-C16
3	F	301	OLC	C12-C13-C14-C15
3	F	301	OLC	O19-C1-O20-C21
3	F	301	OLC	C15-C16-C17-C18
3	B	205	OLC	O23-C22-C24-O25
3	C	201	OLC	O23-C22-C24-O25
3	C	204	OLC	O23-C22-C24-O25
3	D	205	OLC	O23-C22-C24-O25
3	B	203	OLC	C4-C5-C6-C7
3	A	201	OLC	C10-C11-C12-C13
3	C	201	OLC	C10-C11-C12-C13
3	D	204	OLC	C6-C7-C8-C9
3	D	205	OLC	C6-C7-C8-C9
3	B	207	OLC	C15-C16-C17-C18
3	D	201	OLC	C4-C5-C6-C7
3	A	206	OLC	C15-C16-C17-C18
3	B	205	OLC	C14-C15-C16-C17
3	A	202	OLC	C13-C14-C15-C16
3	B	203	OLC	O19-C1-O20-C21
3	B	206	OLC	C12-C13-C14-C15
3	B	204	OLC	C5-C6-C7-C8
3	B	204	OLC	O19-C1-O20-C21
3	D	201	OLC	C14-C15-C16-C17
3	F	302	OLC	C21-C22-C24-O25
3	C	204	OLC	C4-C5-C6-C7
3	A	201	OLC	C3-C4-C5-C6
3	D	203	OLC	C4-C5-C6-C7
3	A	203	OLC	C4-C5-C6-C7
3	D	203	OLC	C1-C2-C3-C4
3	D	204	OLC	C11-C12-C13-C14
3	A	204	OLC	C6-C7-C8-C9
3	A	201	OLC	C11-C12-C13-C14
3	B	205	OLC	C15-C16-C17-C18
3	A	201	OLC	C14-C15-C16-C17
3	F	301	OLC	C14-C15-C16-C17
3	A	204	OLC	C11-C12-C13-C14
3	B	202	OLC	O20-C21-C22-C24
3	D	204	OLC	O20-C21-C22-C24
3	D	203	OLC	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
3	D	204	OLC	O20-C21-C22-O23
3	B	203	OLC	C2-C3-C4-C5
3	B	207	OLC	C2-C3-C4-C5
3	A	202	OLC	O23-C22-C24-O25
3	C	202	OLC	O23-C22-C24-O25
3	A	202	OLC	C14-C15-C16-C17
3	C	201	OLC	C15-C16-C17-C18
3	A	203	OLC	C5-C6-C7-C8
3	D	203	OLC	C14-C15-C16-C17
3	C	203	OLC	C12-C13-C14-C15
3	D	205	OLC	C12-C13-C14-C15
3	A	202	OLC	C15-C16-C17-C18
3	A	204	OLC	C2-C3-C4-C5
3	B	202	OLC	C13-C14-C15-C16
3	B	205	OLC	C11-C12-C13-C14
3	B	207	OLC	C13-C14-C15-C16
3	B	205	OLC	O20-C21-C22-C24
3	A	204	OLC	C1-C2-C3-C4
3	D	201	OLC	C5-C6-C7-C8
3	C	203	OLC	C5-C6-C7-C8
3	A	204	OLC	O23-C22-C24-O25
3	B	202	OLC	O23-C22-C24-O25
3	D	202	OLC	C4-C5-C6-C7
3	B	202	OLC	O20-C21-C22-O23
3	B	205	OLC	C1-C2-C3-C4
3	B	206	OLC	O20-C21-C22-C24
3	B	203	OLC	C5-C6-C7-C8
3	D	201	OLC	C11-C12-C13-C14
3	A	204	OLC	C13-C14-C15-C16
3	A	202	OLC	C6-C7-C8-C9
3	A	205	OLC	O23-C22-C24-O25
3	C	203	OLC	C6-C7-C8-C9
3	D	203	OLC	C13-C14-C15-C16
3	B	205	OLC	C3-C4-C5-C6
3	B	203	OLC	C13-C14-C15-C16
3	A	204	OLC	C5-C6-C7-C8
3	B	205	OLC	C13-C14-C15-C16
3	A	206	OLC	C11-C12-C13-C14
3	B	202	OLC	C11-C12-C13-C14
3	B	204	OLC	C7-C8-C9-C10
3	D	205	OLC	C10-C11-C12-C13
3	A	206	OLC	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
3	D	201	OLC	C9-C10-C11-C12
3	F	301	OLC	C10-C11-C12-C13
3	D	204	OLC	C2-C1-O20-C21
3	C	202	OLC	C14-C15-C16-C17
3	B	201	OLC	C5-C6-C7-C8
3	F	301	OLC	C9-C10-C11-C12
3	A	201	OLC	C4-C5-C6-C7
3	D	205	OLC	C14-C15-C16-C17
3	C	202	OLC	C6-C7-C8-C9
3	D	204	OLC	C9-C10-C11-C12
3	C	202	OLC	C2-C3-C4-C5
3	B	206	OLC	C11-C12-C13-C14
3	C	203	OLC	C1-C2-C3-C4
3	D	204	OLC	O19-C1-O20-C21
3	C	203	OLC	C11-C12-C13-C14
3	B	204	OLC	C6-C7-C8-C9
3	B	202	OLC	C21-C22-C24-O25
3	C	202	OLC	C11-C12-C13-C14
3	B	201	OLC	C10-C11-C12-C13
3	D	204	OLC	C7-C8-C9-C10
3	A	203	OLC	C7-C8-C9-C10
3	A	204	OLC	C9-C10-C11-C12
3	C	203	OLC	C9-C10-C11-C12
3	B	207	OLC	C3-C4-C5-C6
3	D	202	OLC	O20-C21-C22-C24
3	B	201	OLC	C9-C10-C11-C12
3	D	205	OLC	C7-C8-C9-C10
3	A	205	OLC	C9-C10-C11-C12
3	B	203	OLC	C9-C10-C11-C12
3	D	202	OLC	C6-C7-C8-C9
3	A	203	OLC	O20-C1-C2-C3
3	B	203	OLC	C7-C8-C9-C10
3	B	205	OLC	C9-C10-C11-C12
3	F	302	OLC	C7-C8-C9-C10
3	A	204	OLC	C3-C4-C5-C6
3	F	302	OLC	C11-C12-C13-C14
3	A	205	OLC	C3-C4-C5-C6
3	F	302	OLC	C4-C5-C6-C7
3	B	204	OLC	C4-C5-C6-C7
3	F	302	OLC	O23-C22-C24-O25
3	B	206	OLC	O20-C1-C2-C3
3	B	202	OLC	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
3	D	204	OLC	C12-C13-C14-C15
3	A	201	OLC	C2-C1-O20-C21
3	A	201	OLC	O19-C1-O20-C21
3	B	206	OLC	C7-C8-C9-C10
3	A	206	OLC	C2-C1-O20-C21
3	B	204	OLC	C11-C12-C13-C14
3	C	201	OLC	C13-C14-C15-C16
3	C	201	OLC	C12-C13-C14-C15
3	A	203	OLC	O19-C1-C2-C3
3	A	206	OLC	O19-C1-O20-C21
3	B	203	OLC	O20-C1-C2-C3
3	B	206	OLC	O19-C1-C2-C3
3	A	204	OLC	O20-C1-C2-C3
3	B	205	OLC	C6-C7-C8-C9
3	B	203	OLC	O19-C1-C2-C3

There are no ring outliers.

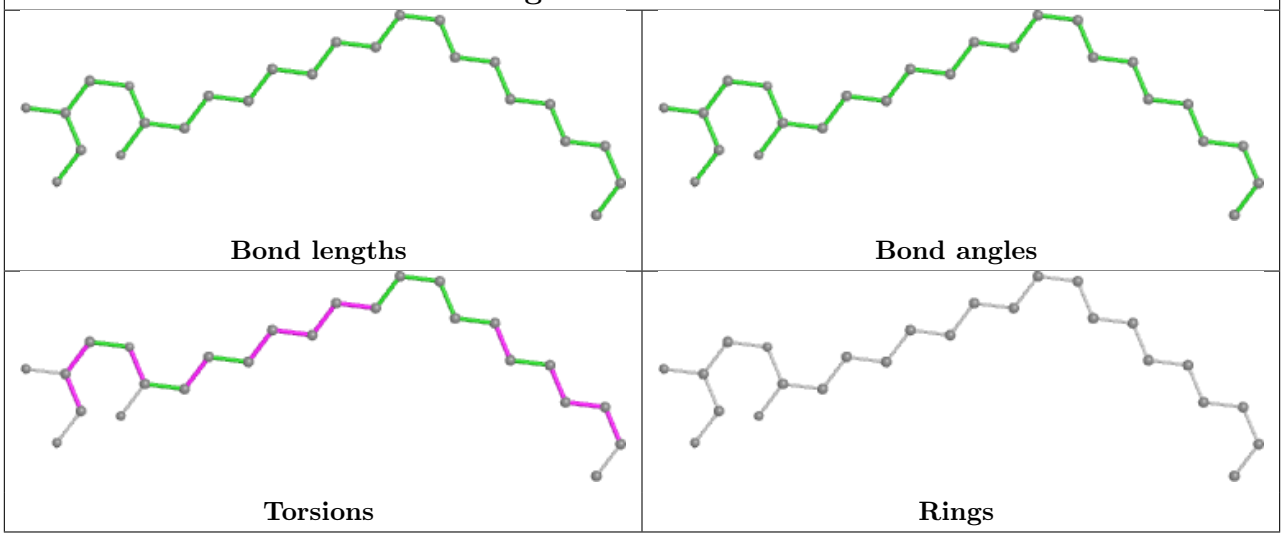
20 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	202	OLC	3	0
3	A	205	OLC	2	0
3	C	201	OLC	3	0
3	A	204	OLC	3	0
3	A	203	OLC	3	0
3	B	202	OLC	1	0
3	D	202	OLC	2	0
3	C	202	OLC	4	0
3	B	207	OLC	2	0
3	C	204	OLC	2	0
3	C	203	OLC	4	0
3	D	201	OLC	2	0
3	B	204	OLC	2	0
3	D	205	OLC	1	0
3	B	203	OLC	1	0
3	B	206	OLC	1	0
3	D	203	OLC	1	0
3	F	301	OLC	1	0
3	B	201	OLC	2	0
3	A	201	OLC	5	0

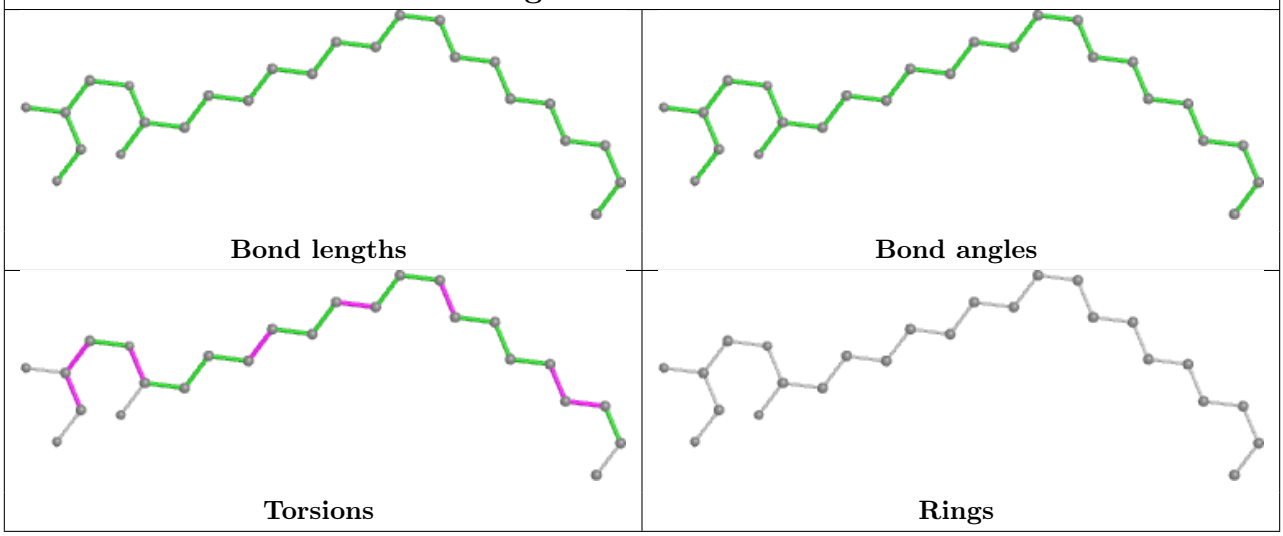
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

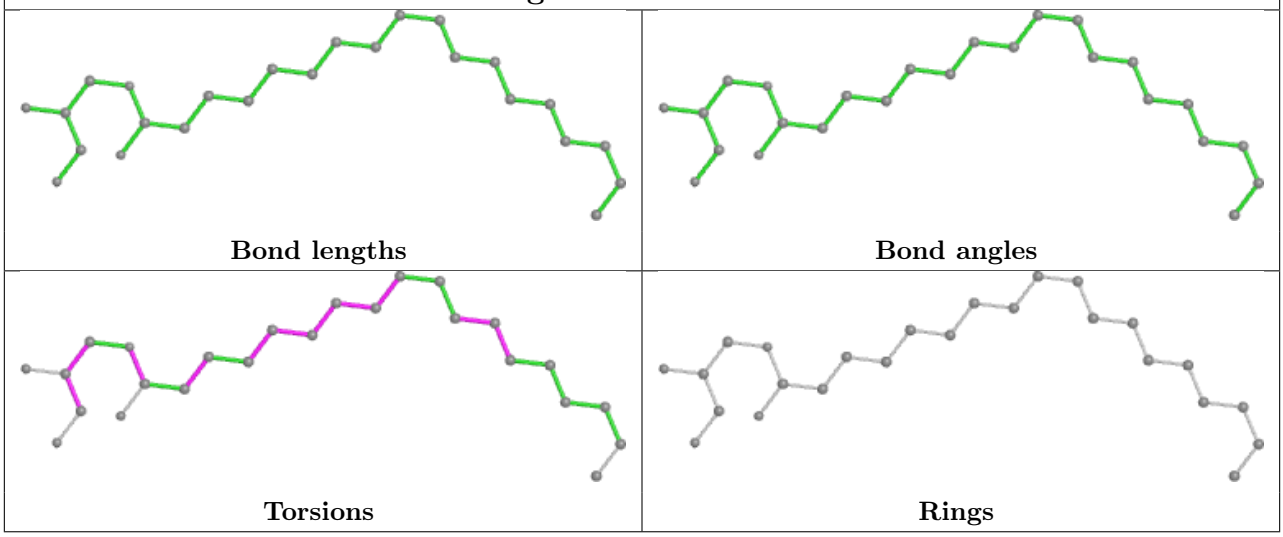
Ligand OLC A 202



Ligand OLC A 205



Ligand OLC F 302



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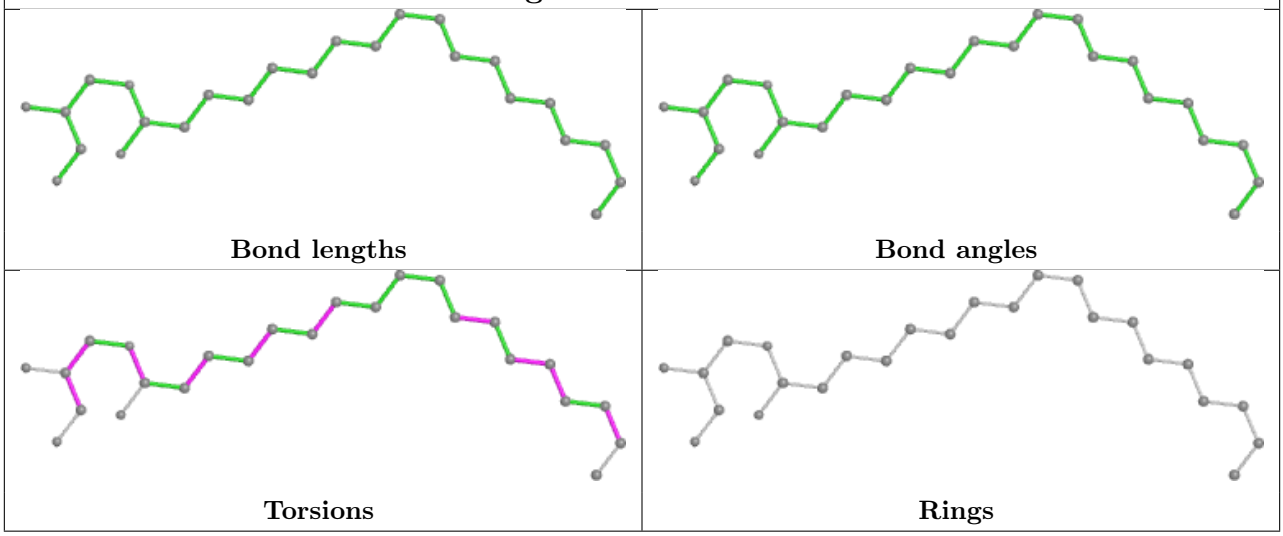

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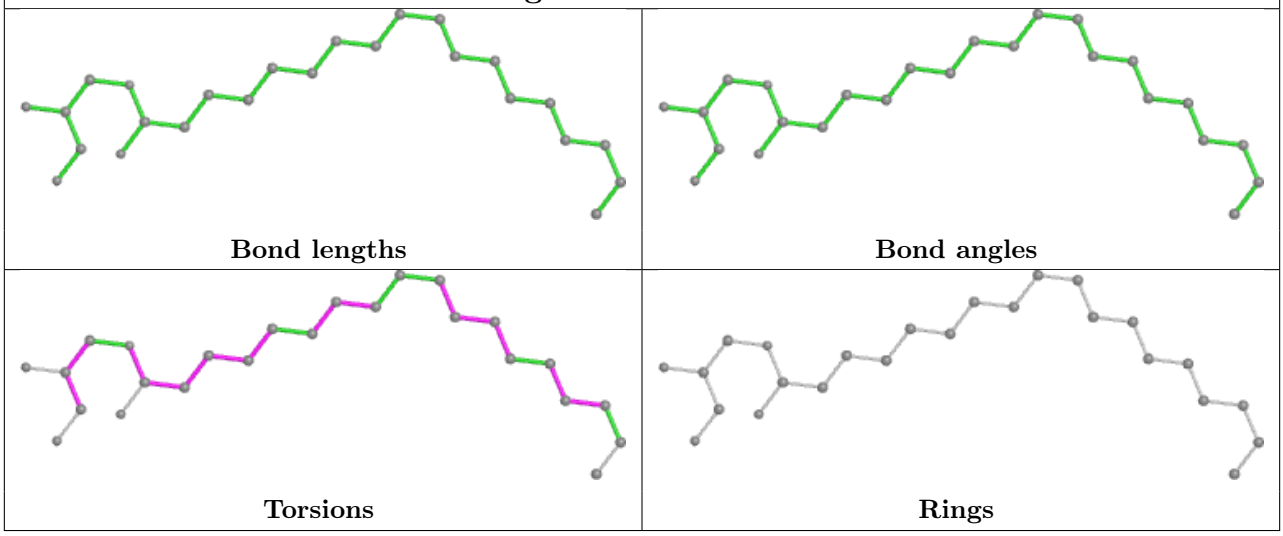

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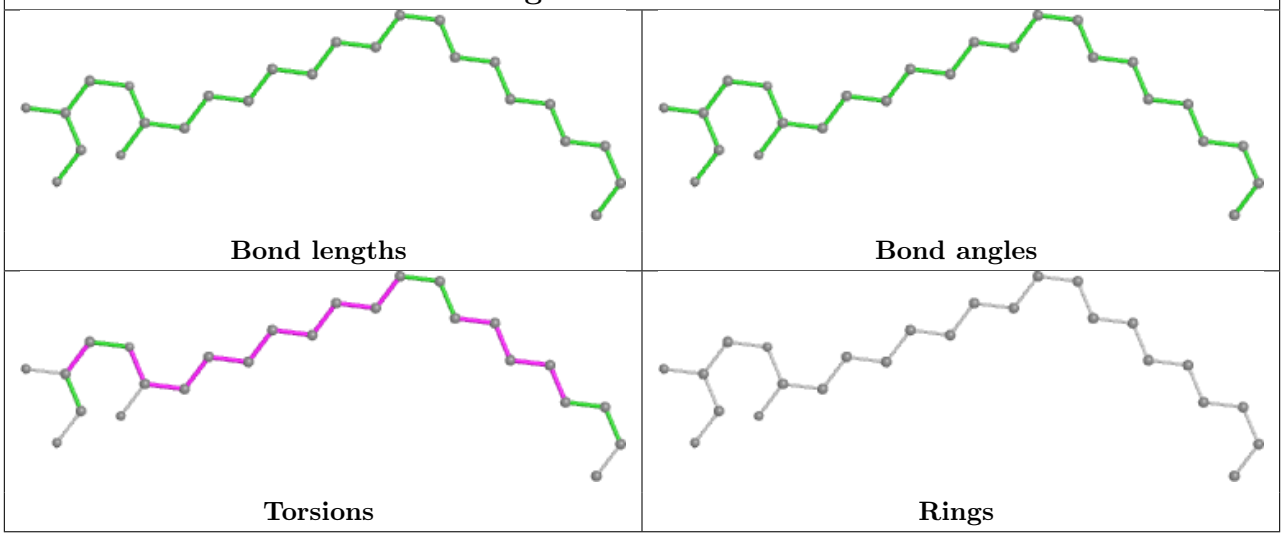

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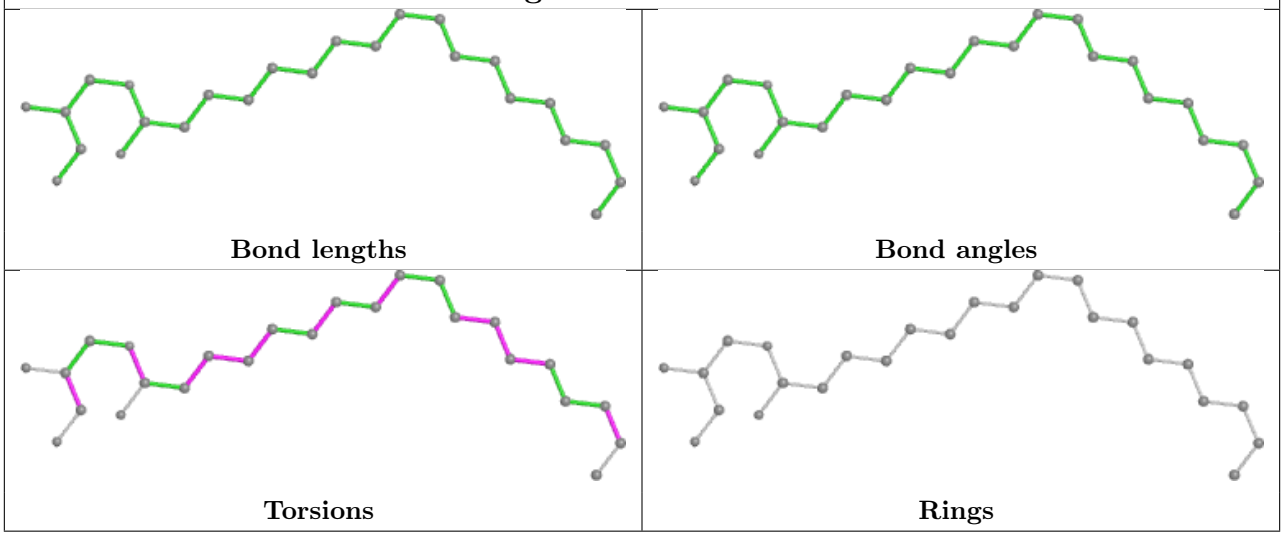

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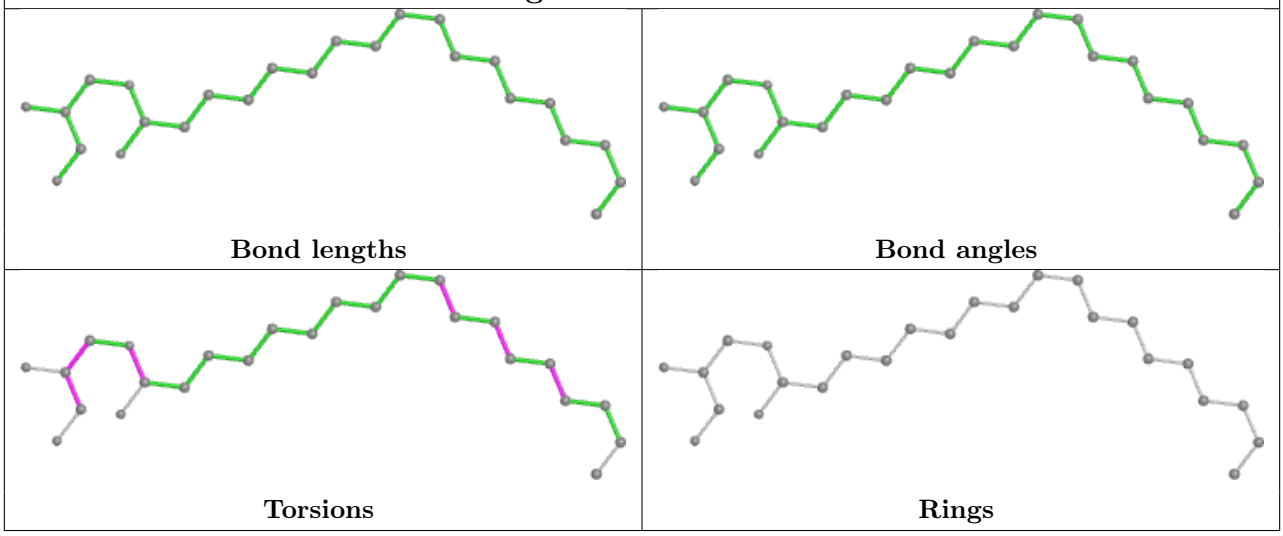
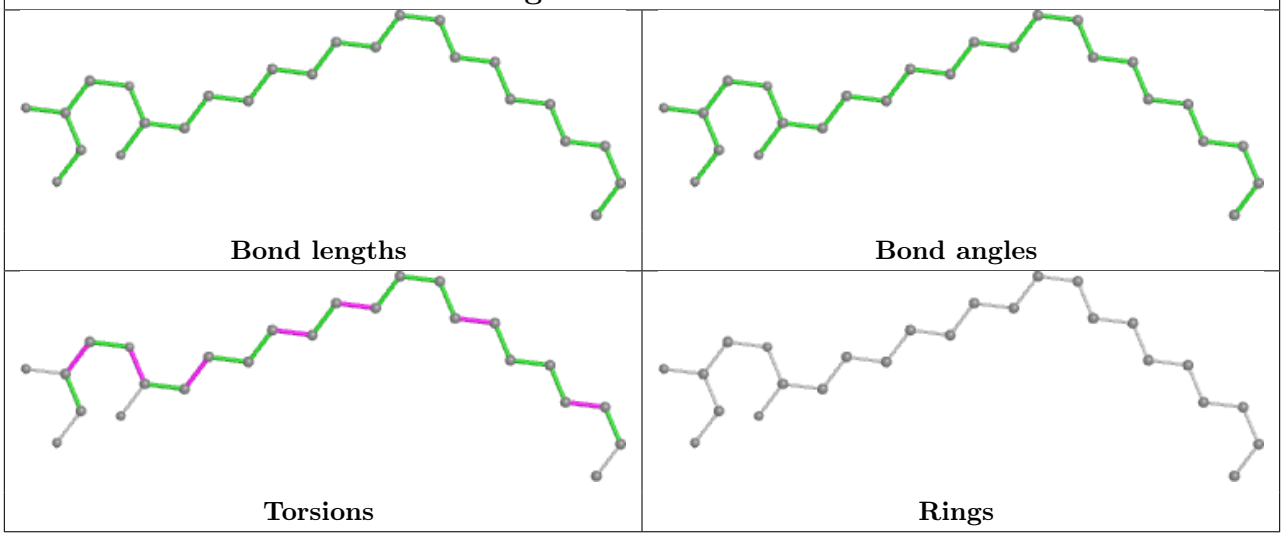


Ligand OLC D 202



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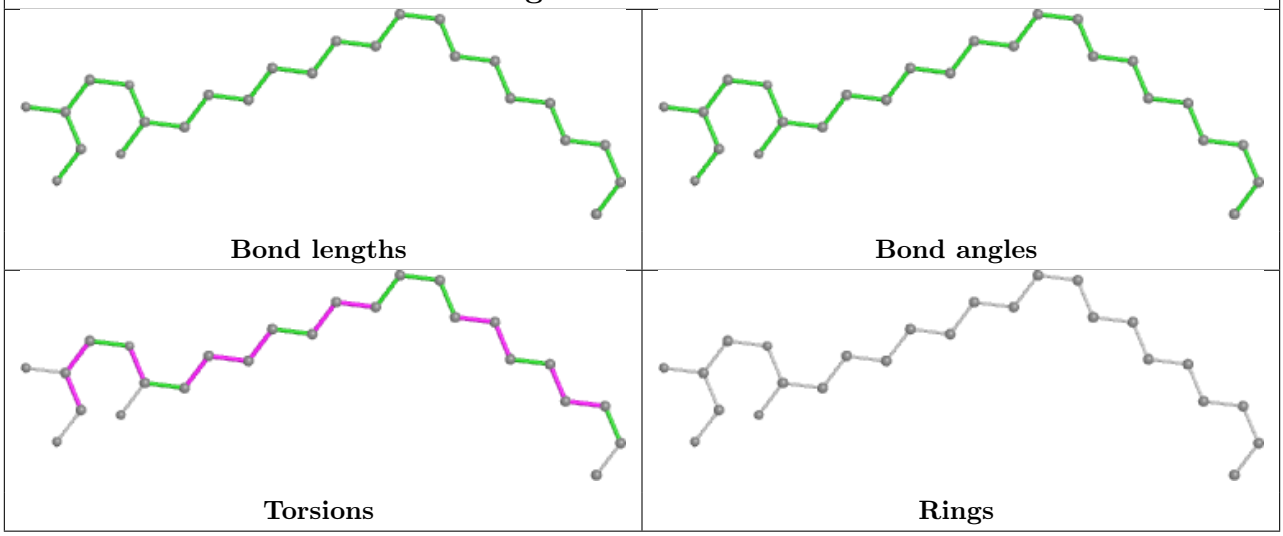

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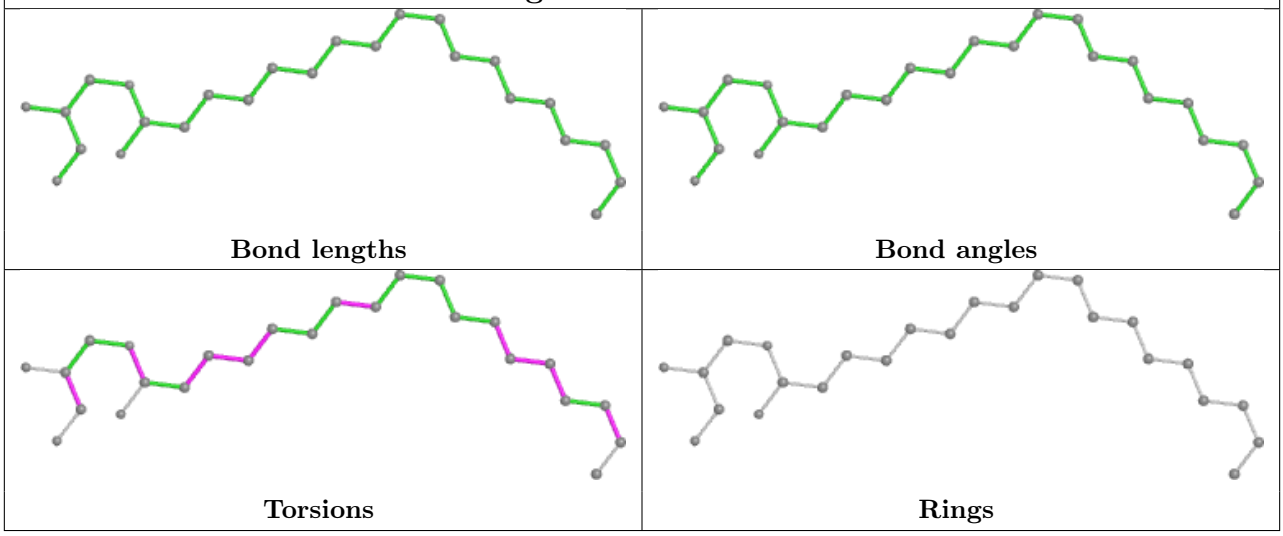

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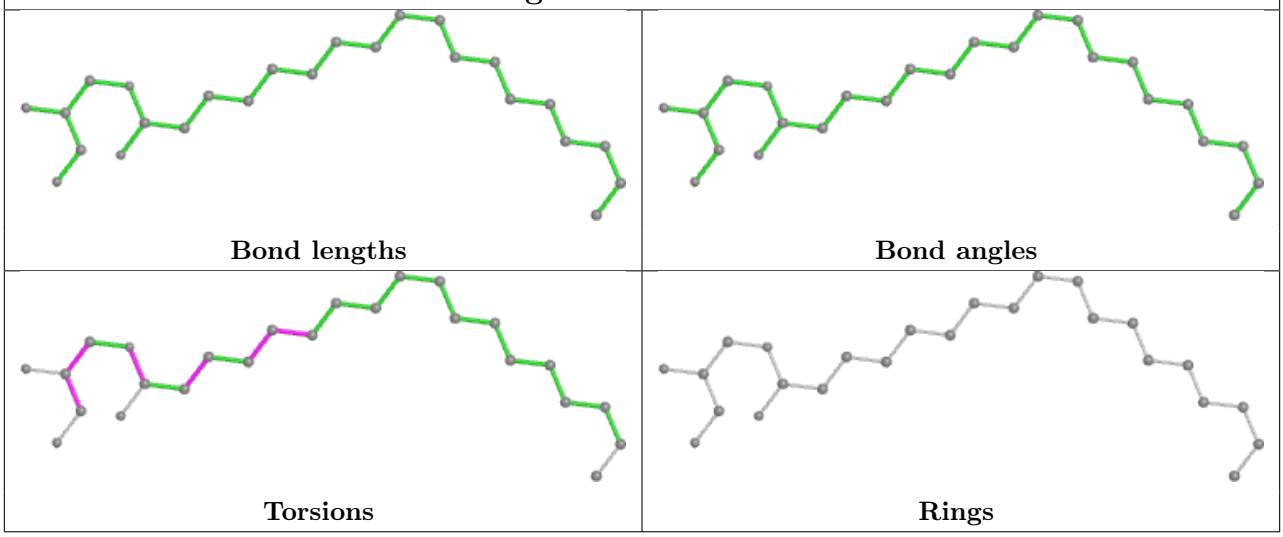

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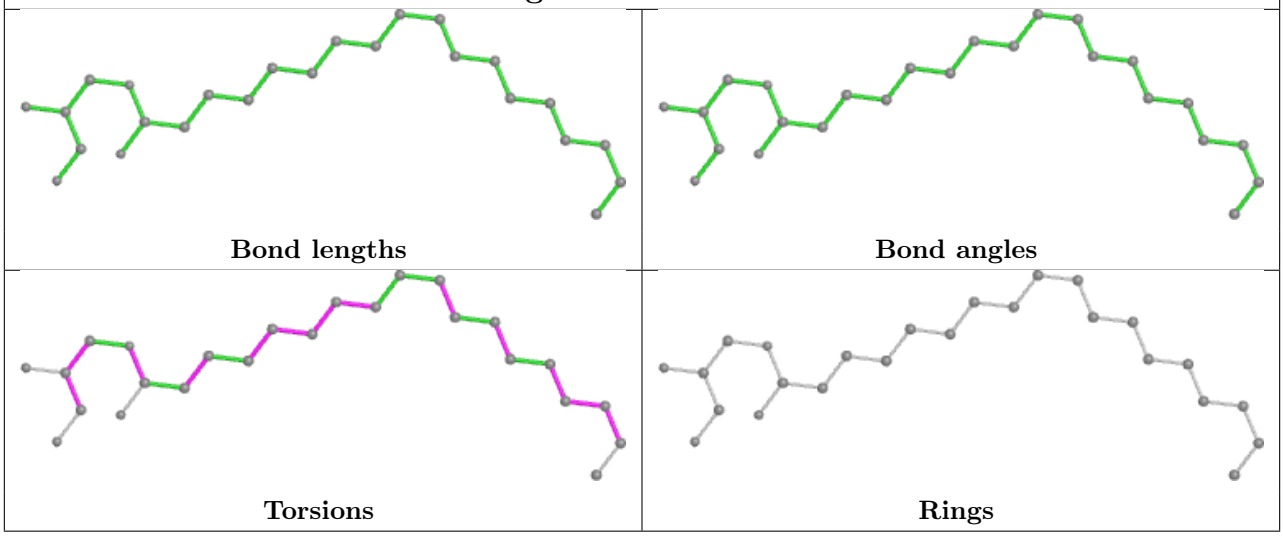

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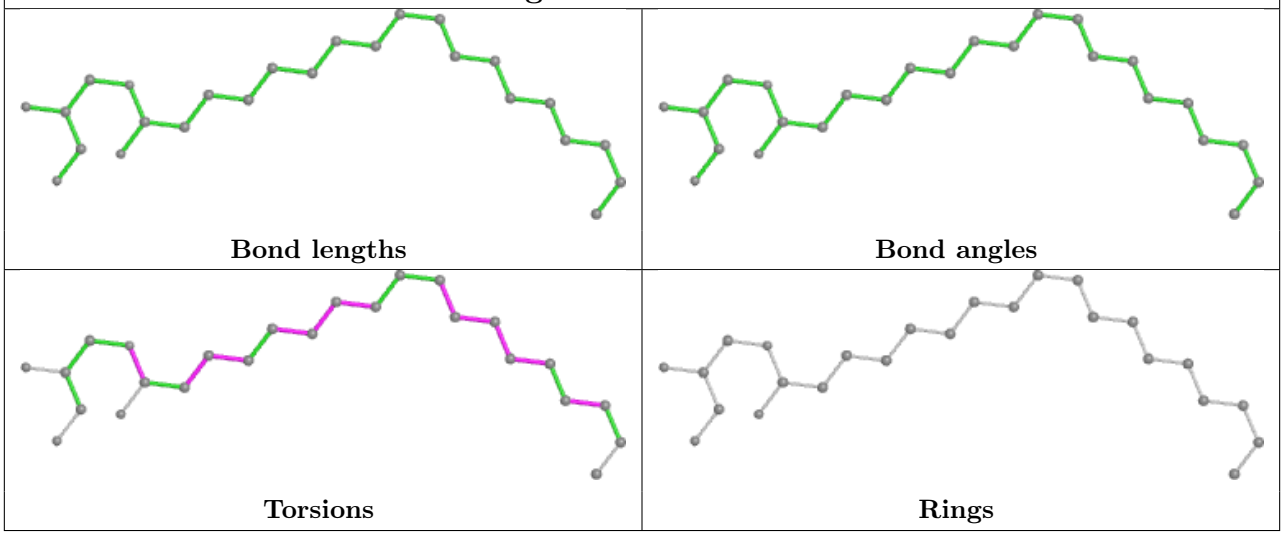

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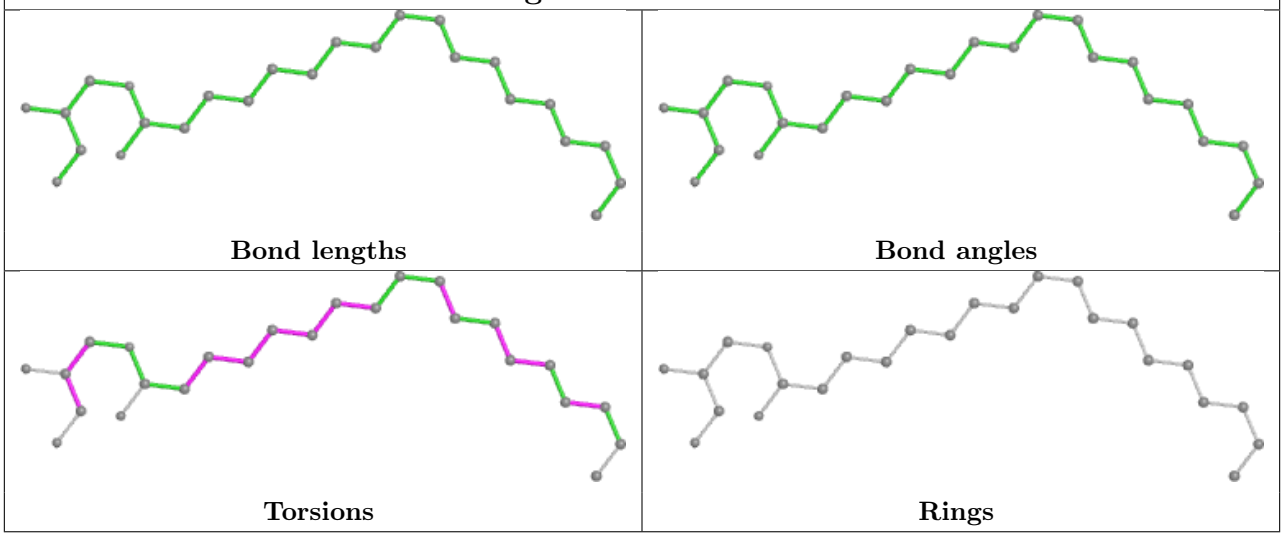

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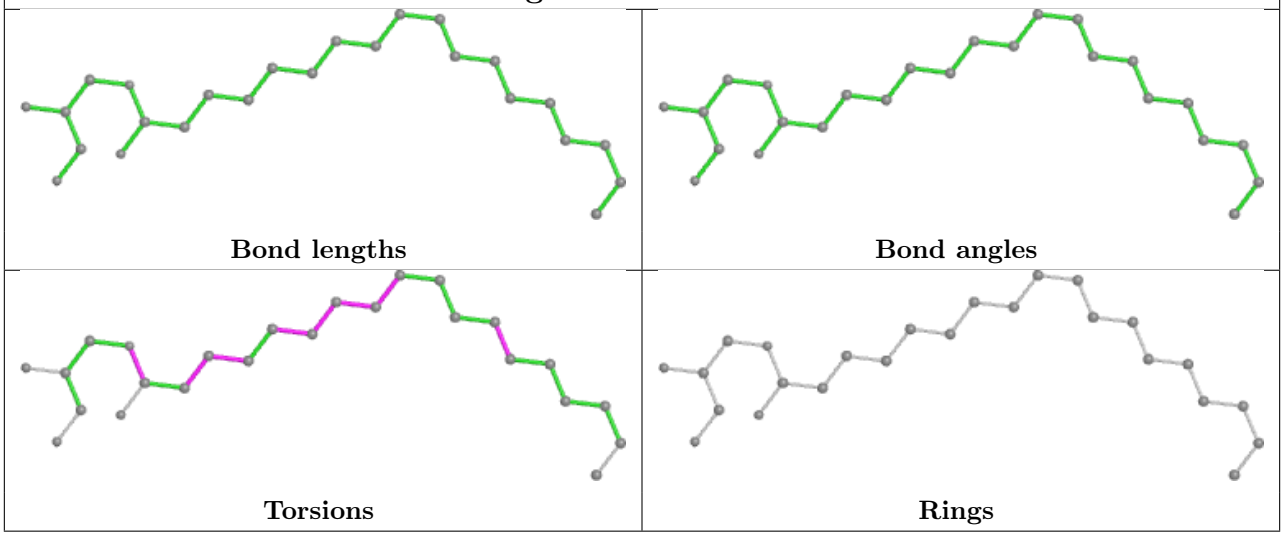

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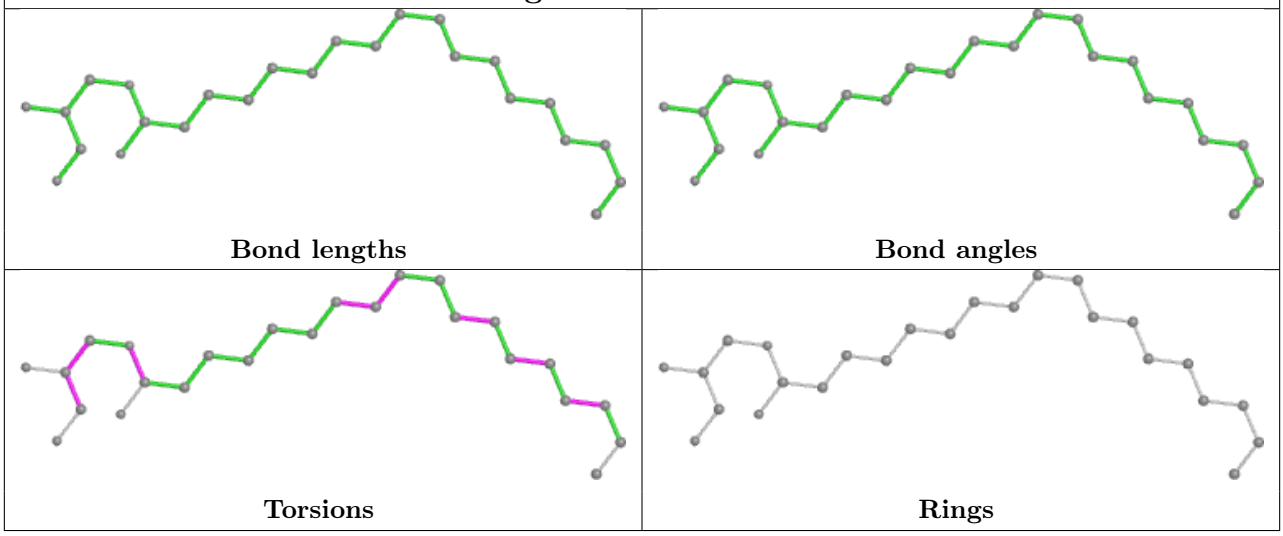
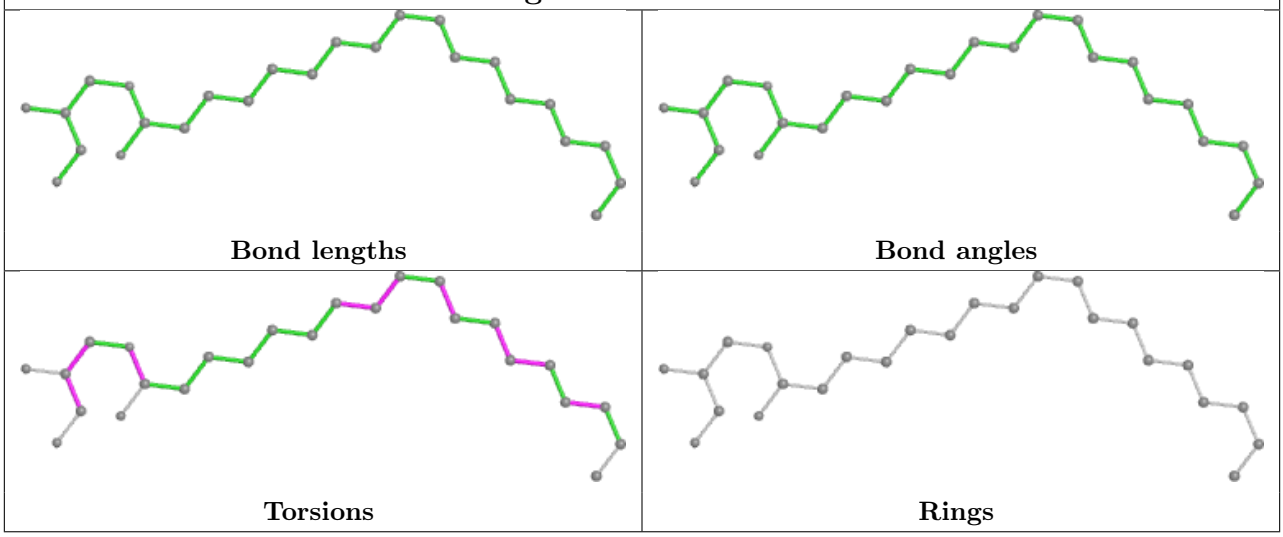
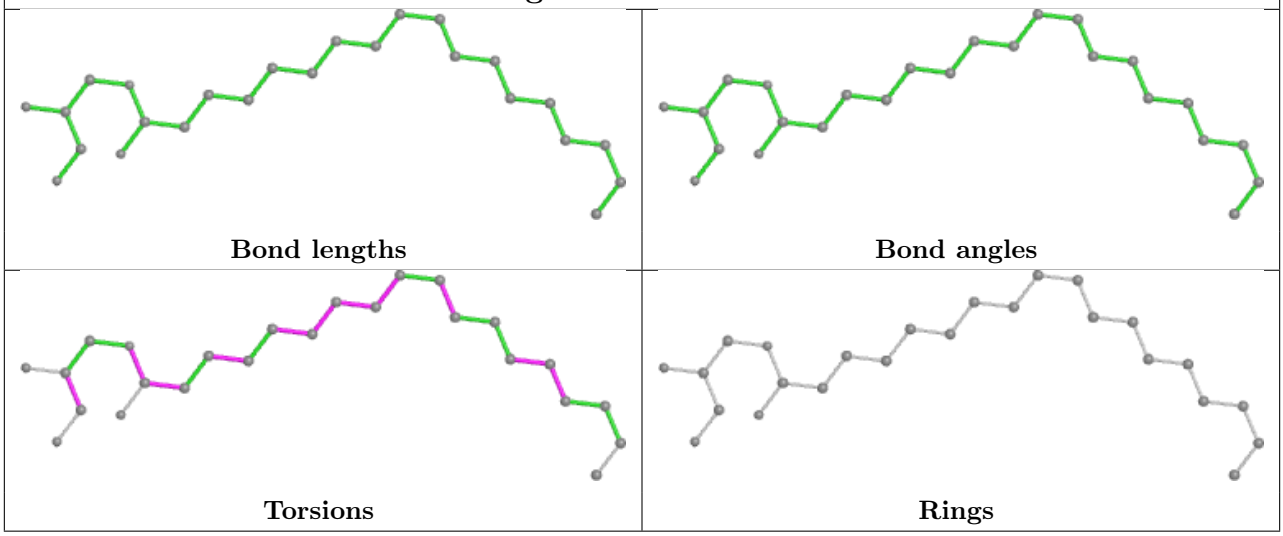


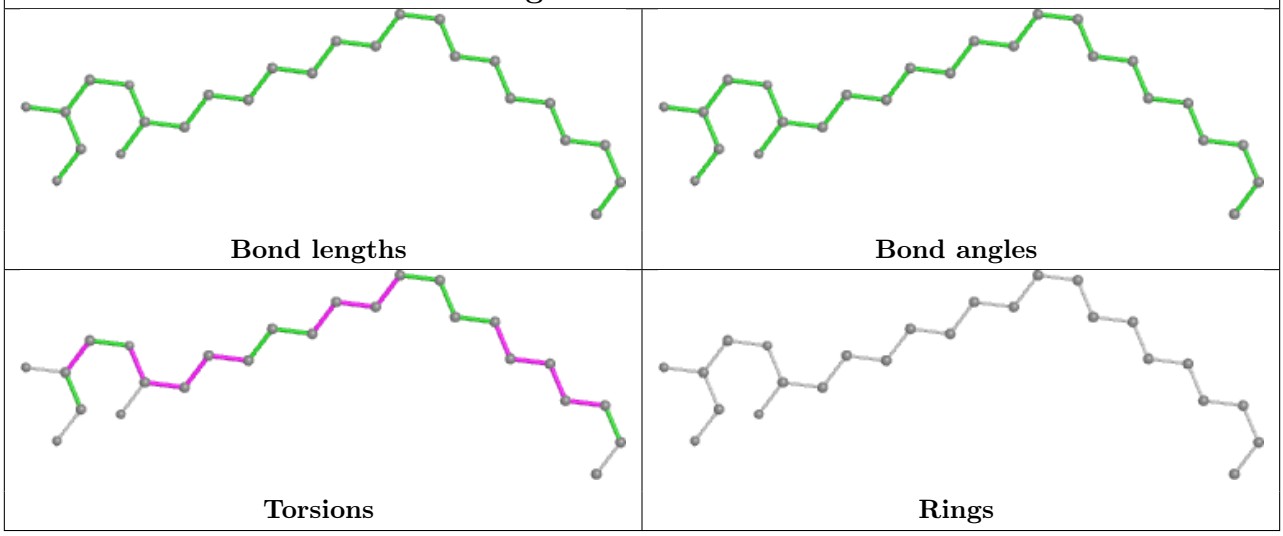
Ligand OLC D 204



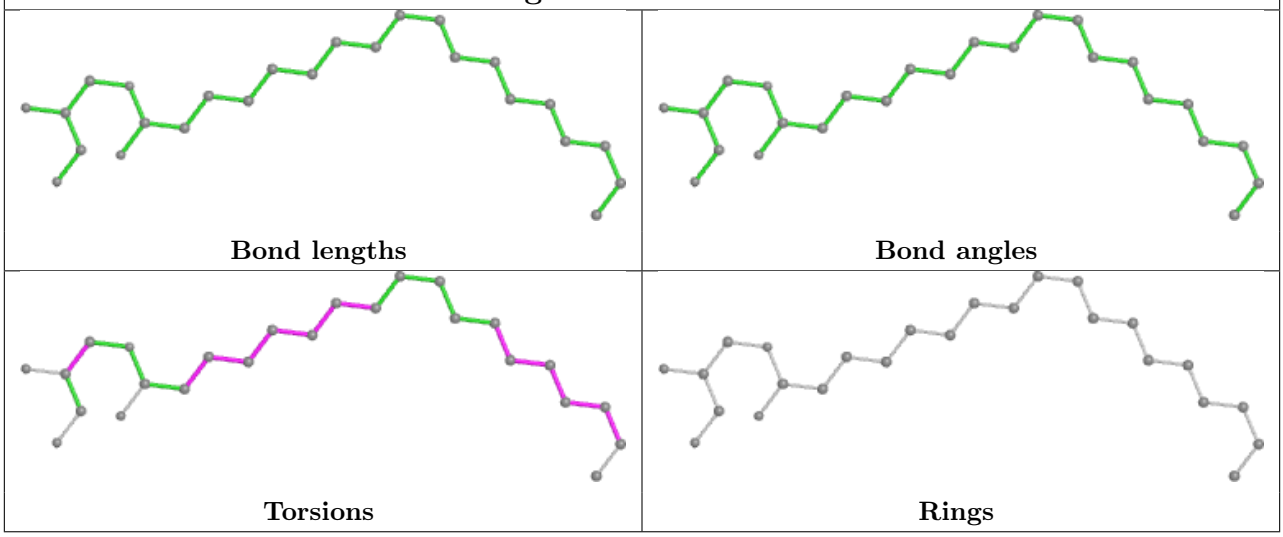
Ligand OLC B 203



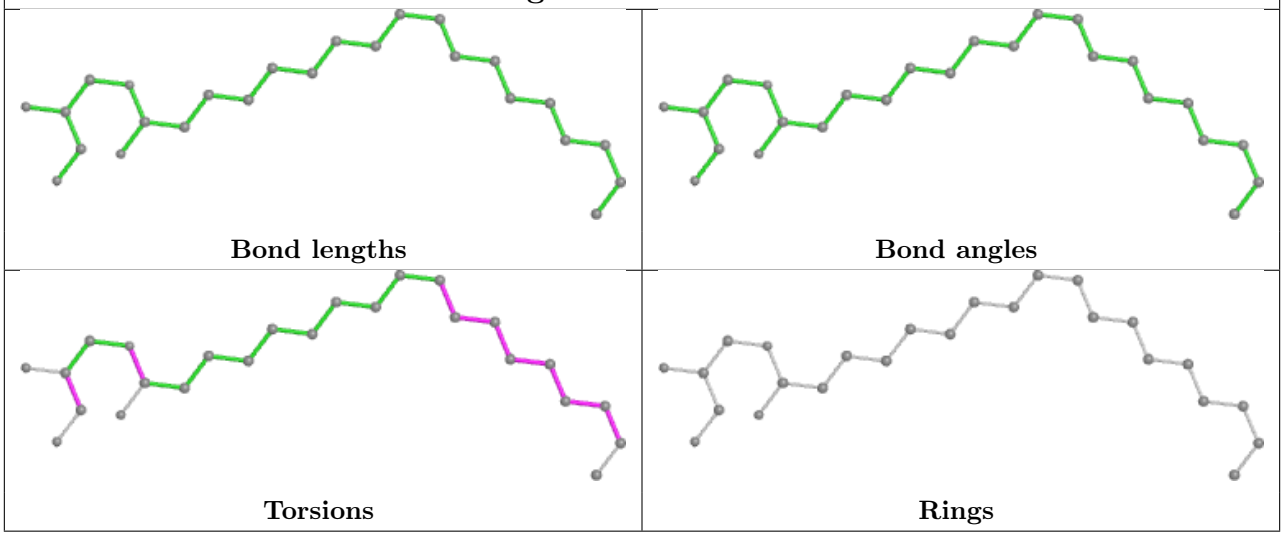
Ligand OLC B 206



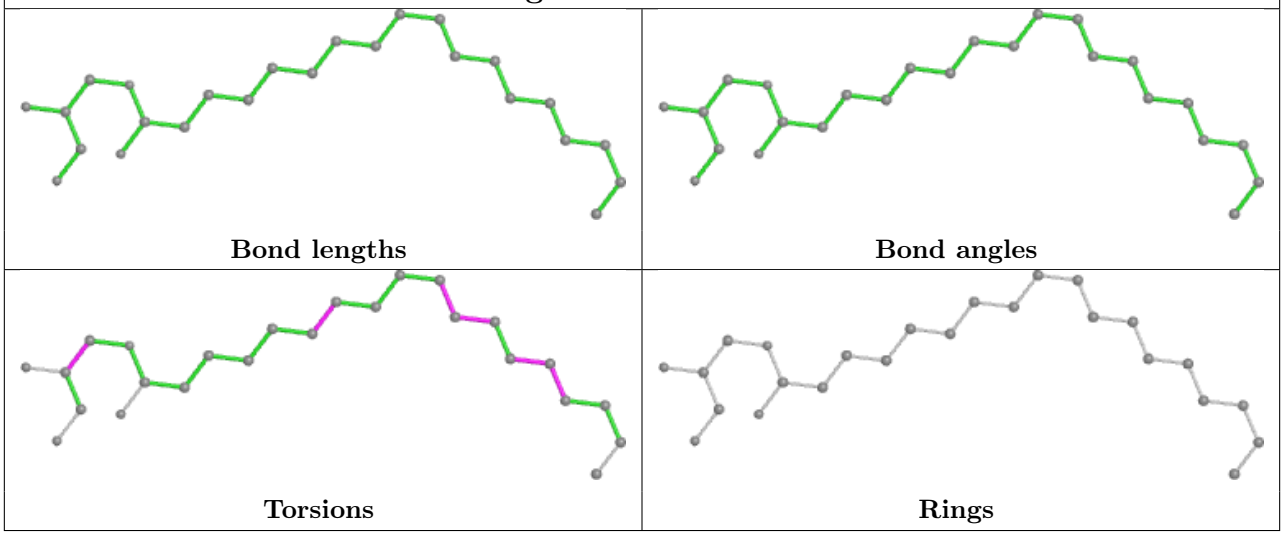
Ligand OLC D 203



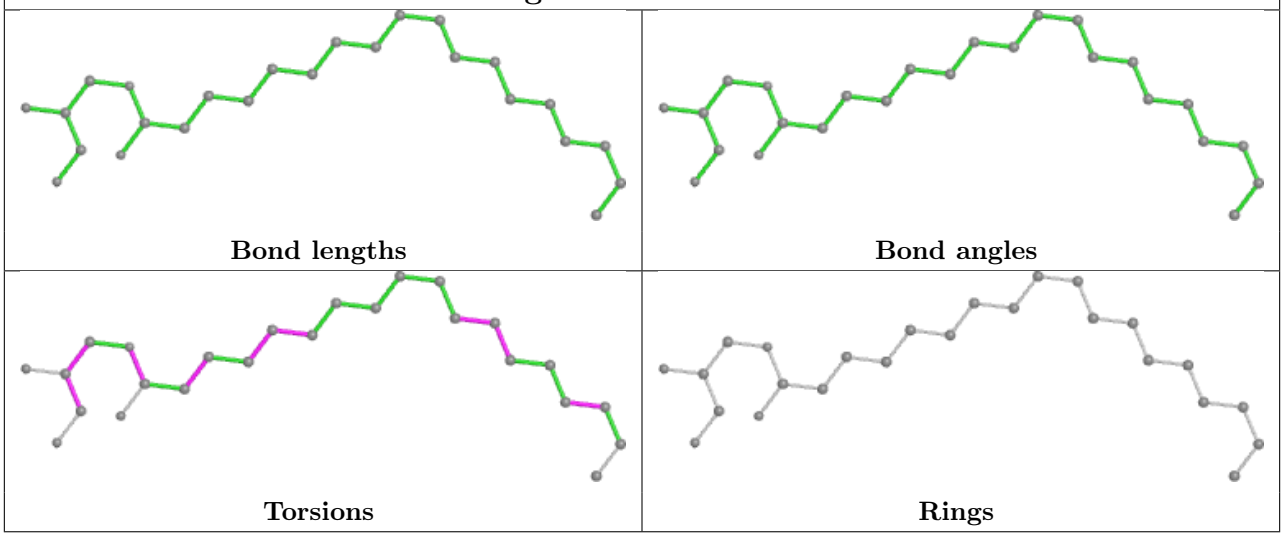
Ligand OLC F 301



Ligand OLC B 201



Ligand OLC A 201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	157/188 (83%)	0.19	3 (1%)	66	59	45, 58, 88, 120	0
1	B	149/188 (79%)	0.28	7 (4%)	31	22	44, 64, 98, 108	0
1	C	149/188 (79%)	0.15	2 (1%)	77	72	44, 58, 96, 128	0
1	D	149/188 (79%)	0.34	10 (6%)	17	10	47, 65, 103, 120	0
2	E	1/5 (20%)	-0.28	0	100	100	53, 53, 53, 53	0
2	F	1/5 (20%)	0.19	0	100	100	53, 53, 53, 53	0
2	G	1/5 (20%)	0.07	0	100	100	66, 66, 66, 66	0
2	H	1/5 (20%)	-0.54	0	100	100	57, 57, 57, 57	0
All	All	608/772 (78%)	0.24	22 (3%)	42	32	44, 60, 98, 128	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	94	GLY	5.9
1	D	93	LYS	3.9
1	B	58	ALA	3.6
1	D	91	LEU	3.0
1	D	60	SER	2.8
1	C	158	PHE	2.8
1	D	55	THR	2.7
1	B	97	TRP	2.7
1	D	56	GLY	2.6
1	B	91	LEU	2.5
1	A	134	TRP	2.5
1	B	59	PHE	2.5
1	C	92	LYS	2.5
1	D	63	ALA	2.4
1	A	157	MET	2.4
1	B	87	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	5	ASP	2.3
1	B	57	ALA	2.3
1	D	88	LEU	2.2
1	B	115	ASP	2.1
1	D	68	TRP	2.1
1	D	57	ALA	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	IIL	E	202	8/9	0.93	0.22	39,48,56,58	0
2	MLE	H	201	9/10	0.94	0.22	55,65,70,71	0
2	IIL	H	202	8/9	0.94	0.20	53,57,59,63	0
2	ALO	H	204	7/8	0.94	0.14	60,64,70,70	0
2	MLE	G	201	9/10	0.95	0.17	52,63,68,71	0
2	IIL	F	202	8/9	0.96	0.21	53,55,60,61	0
2	ALO	E	204	7/8	0.96	0.16	46,49,56,61	0
2	ALO	F	204	7/8	0.96	0.26	52,58,66,70	0
2	ALO	G	204	7/8	0.96	0.19	72,76,86,86	0
2	IIL	G	202	8/9	0.96	0.18	55,64,69,71	0
2	MLE	E	201	9/10	0.97	0.21	51,54,58,59	0
2	MLE	F	201	9/10	0.97	0.20	55,60,63,67	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

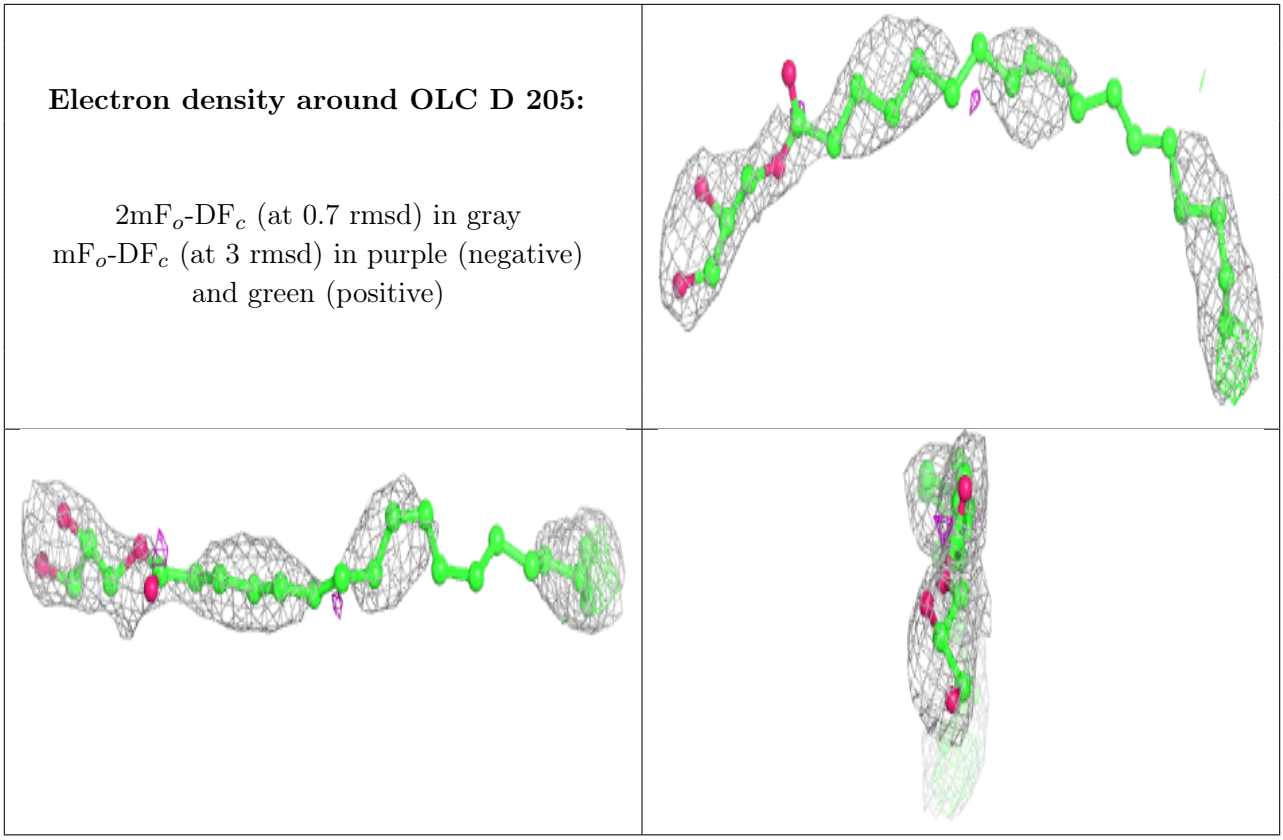
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	OLC	D	205	25/25	0.64	0.41	66,87,112,114	0
3	OLC	D	202	25/25	0.65	0.50	67,99,110,126	0
3	OLC	B	202	25/25	0.67	0.45	77,89,127,131	0
3	OLC	C	204	25/25	0.70	0.60	77,98,120,129	0
3	OLC	F	302	25/25	0.72	0.38	67,90,109,112	0
3	OLC	C	203	25/25	0.74	0.35	72,86,101,106	0
3	OLC	B	203	25/25	0.75	0.34	72,101,119,126	0
3	OLC	D	203	25/25	0.77	0.42	74,103,134,139	0
3	OLC	D	204	25/25	0.77	0.34	67,89,114,118	0
3	OLC	B	206	25/25	0.78	0.34	57,77,115,119	0
3	OLC	A	202	25/25	0.78	0.34	74,84,100,115	0
3	OLC	A	203	25/25	0.80	0.37	80,99,112,118	0
3	OLC	A	206	25/25	0.80	0.36	59,79,95,107	0
3	OLC	C	201	25/25	0.81	0.34	71,95,120,126	0
3	OLC	B	204	25/25	0.82	0.38	67,75,105,119	0
3	OLC	B	207	25/25	0.83	0.30	66,90,103,107	0
3	OLC	A	205	25/25	0.85	0.34	67,77,88,97	0
3	OLC	B	205	25/25	0.85	0.27	60,77,85,102	0
3	OLC	C	202	25/25	0.86	0.47	65,79,105,110	0
3	OLC	A	201	25/25	0.87	0.31	55,71,86,92	0
3	OLC	D	201	25/25	0.88	0.35	53,69,94,95	0
3	OLC	A	204	25/25	0.89	0.37	65,76,89,93	0
3	OLC	F	301	25/25	0.89	0.32	58,69,86,96	0
3	OLC	B	201	25/25	0.89	0.40	52,69,118,125	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.

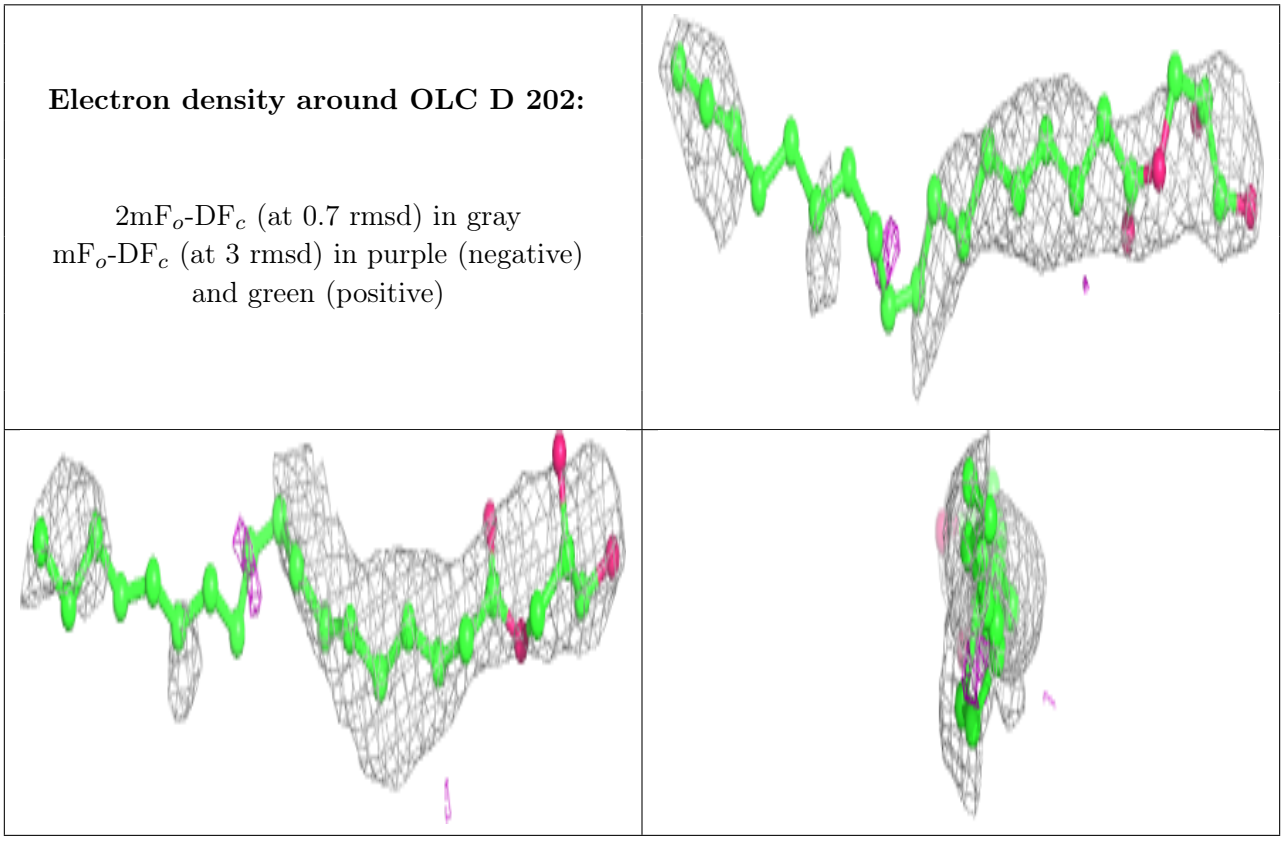
Electron density around OLC D 205:

$2mF_o$-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 D 202:

$2mF_o$-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 202:

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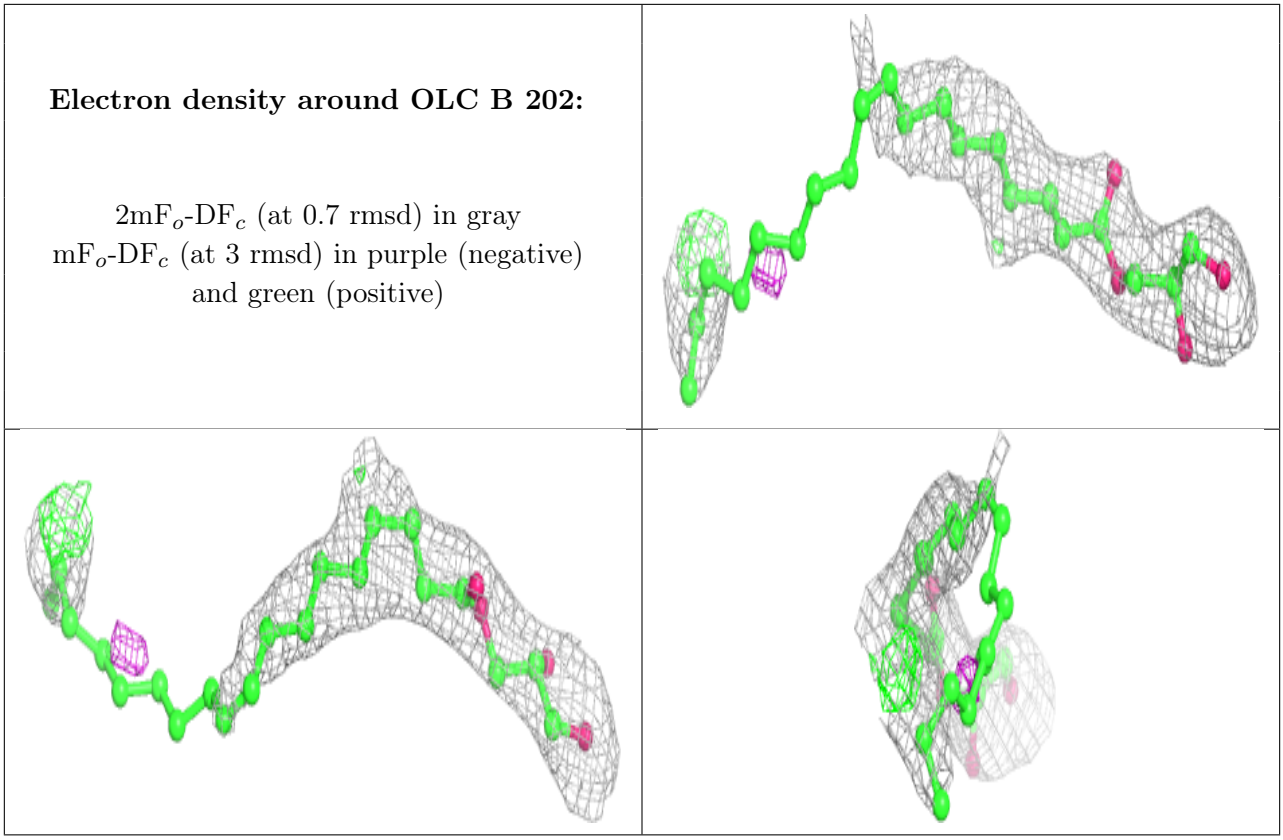
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OLC C 204:

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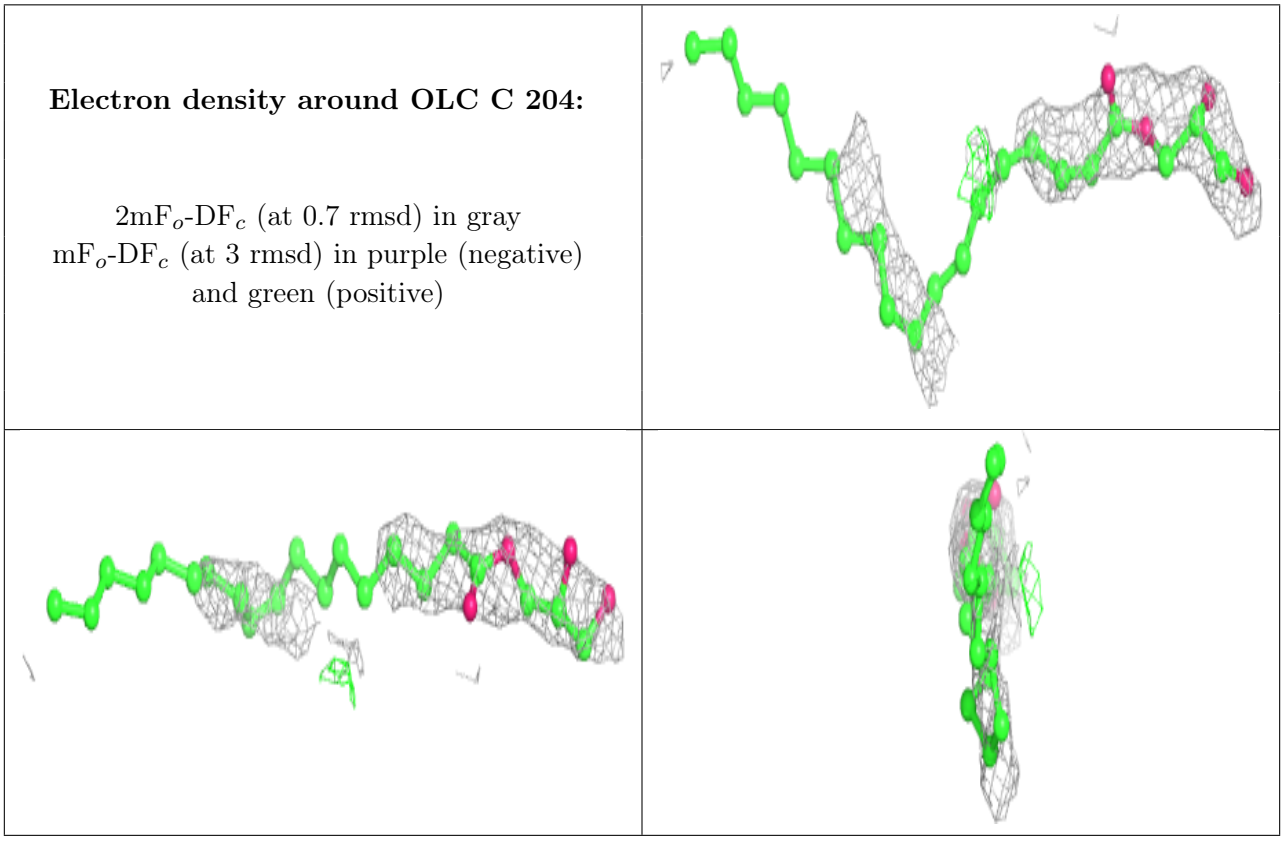
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OLC F 302:

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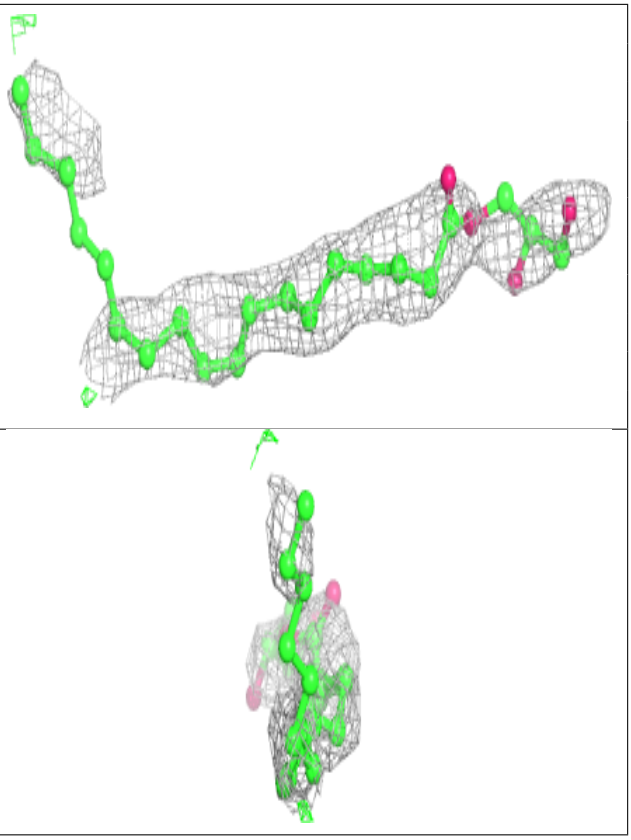
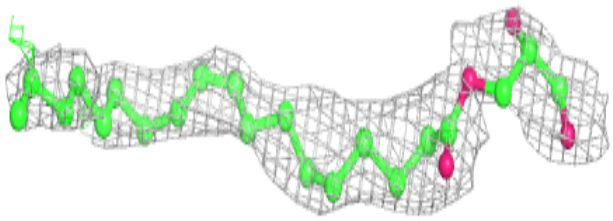
and green (positive)





Electron density around OLC C 203:

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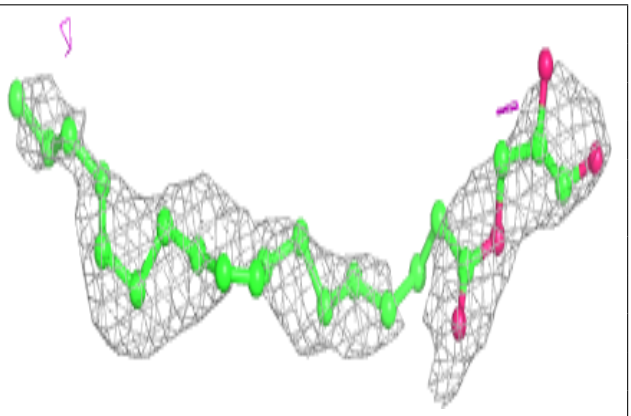

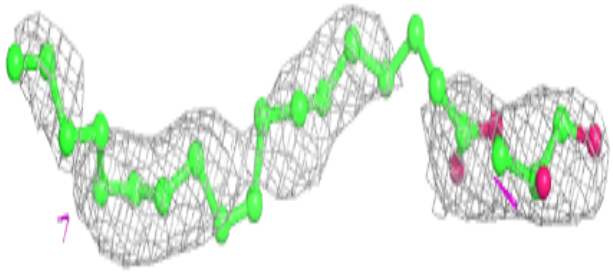

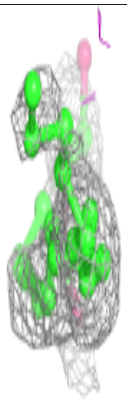

Electron density around OLC B 203:

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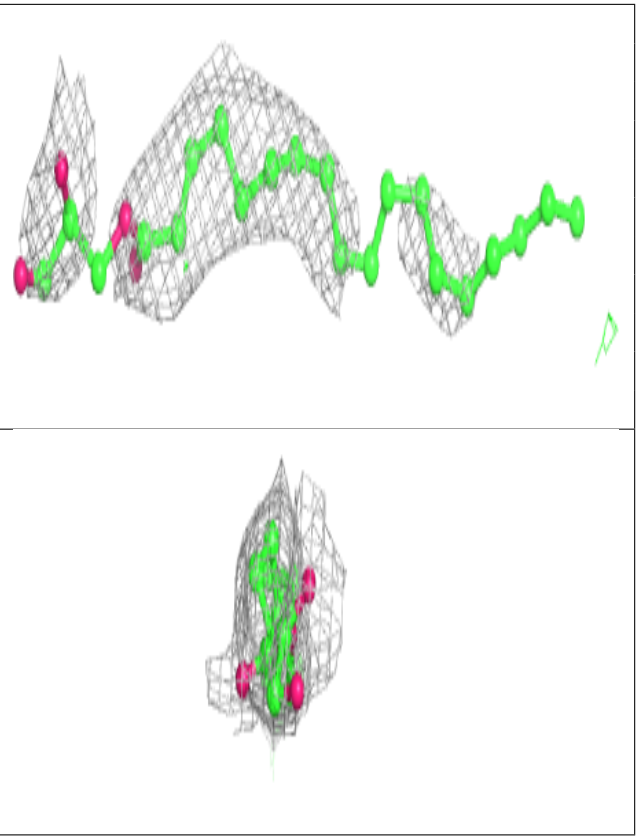

Electron density around OLC D 203:

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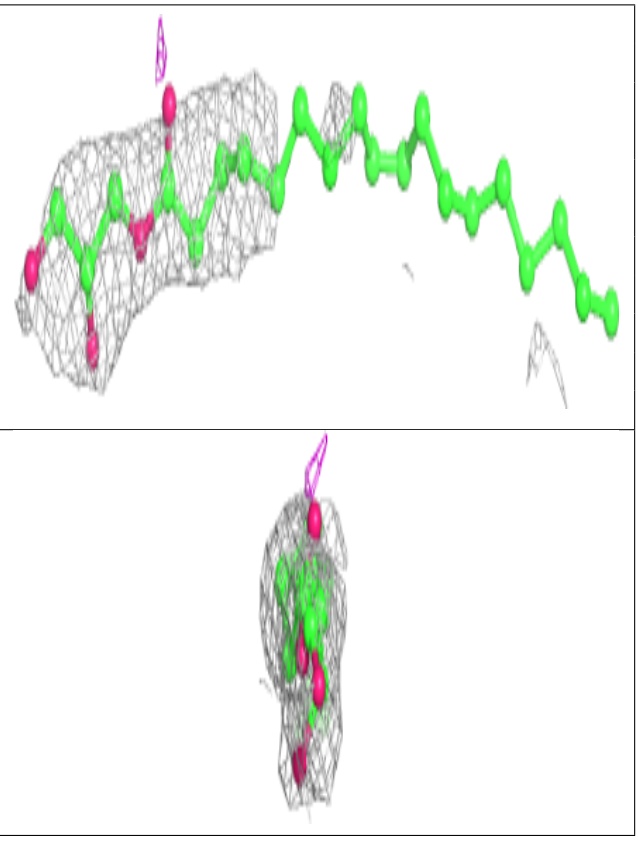
and green (positive)



Electron density around OLC D 204:

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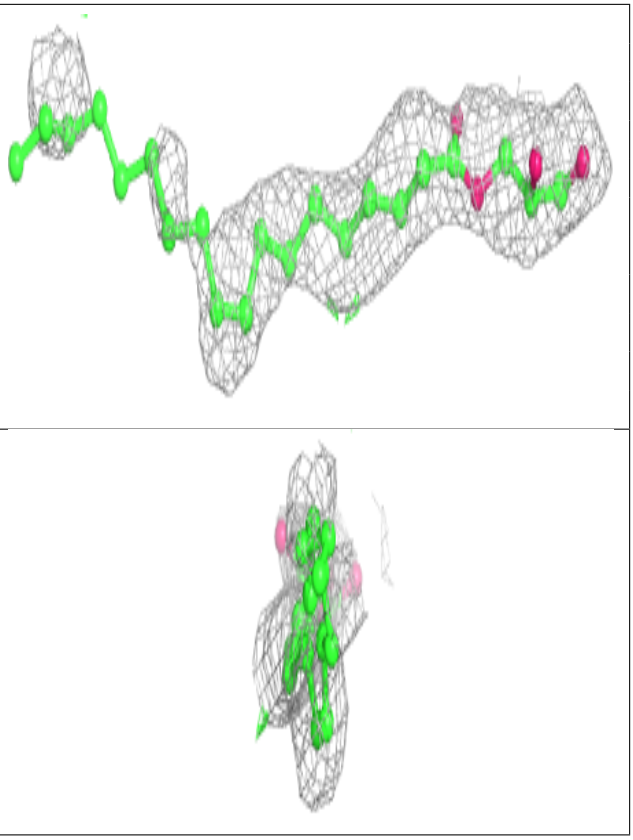
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OLC B 206:

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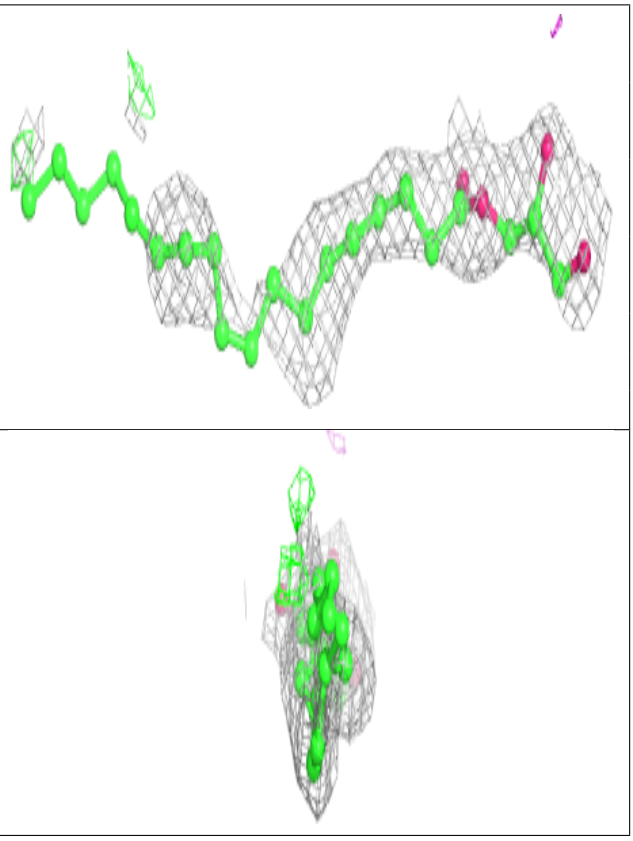
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OLC A 202:

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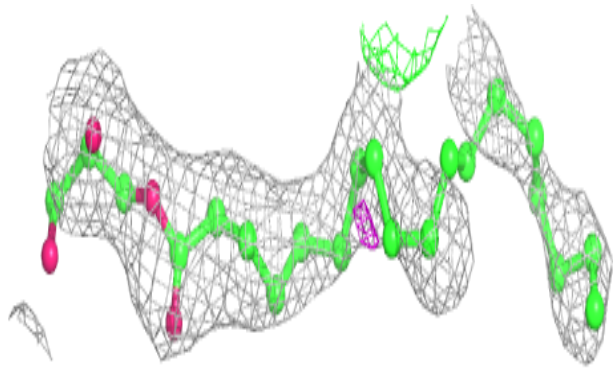
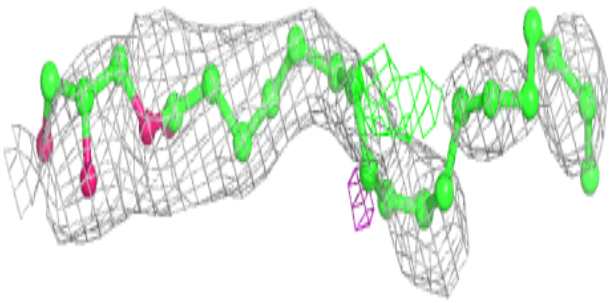
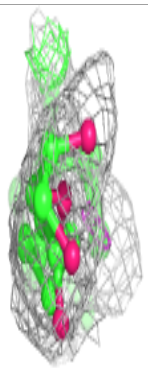
and green (positive)







Electron density around OLC A 203:

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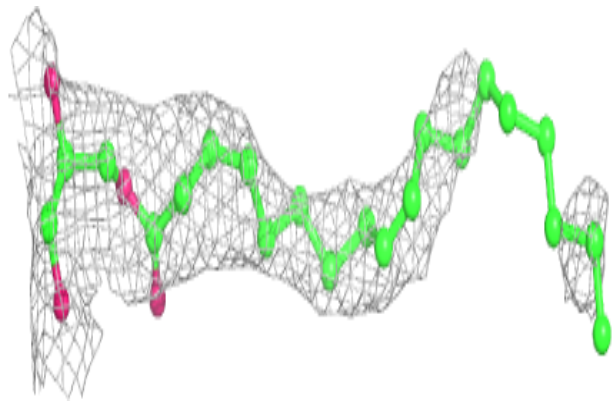
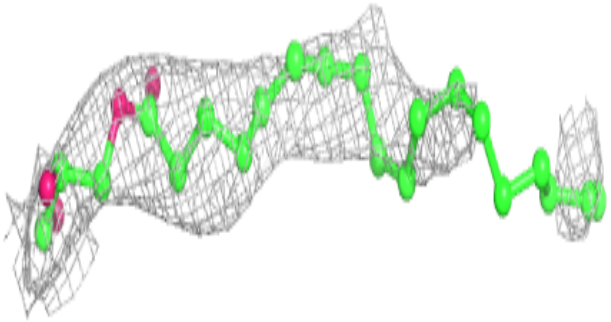
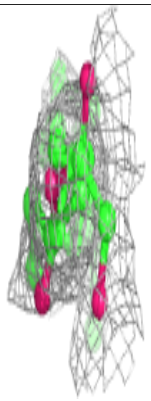
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around OLC A 206:

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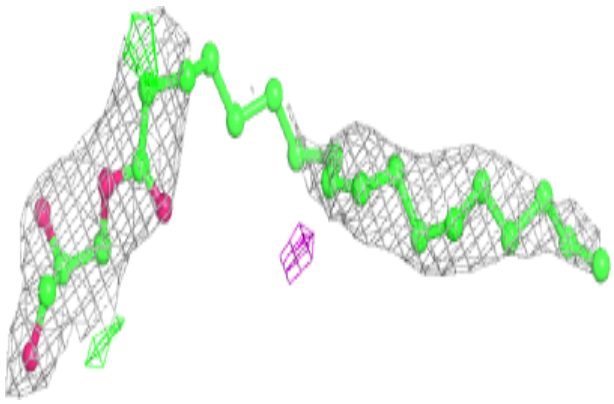
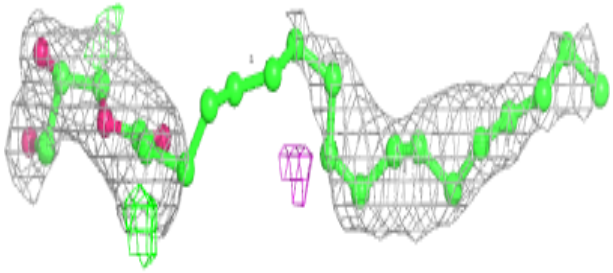
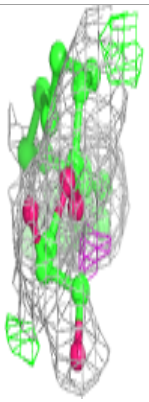
and green (positive)







Electron density around OLC C 201:

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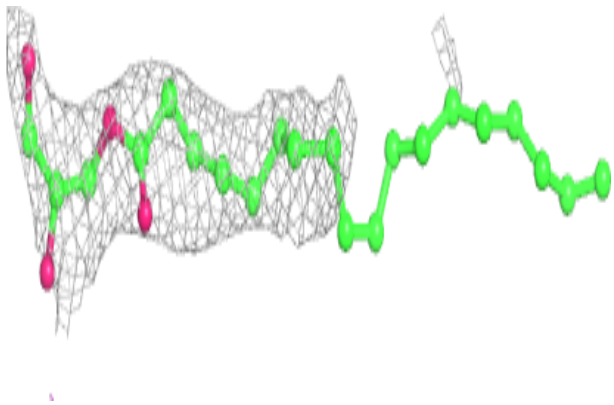
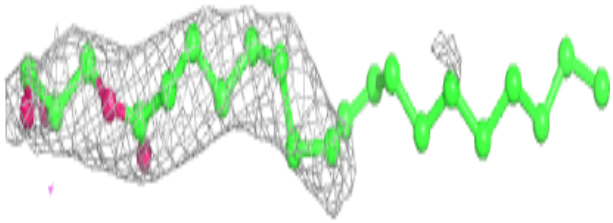
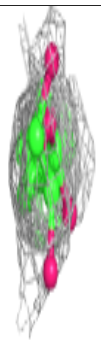
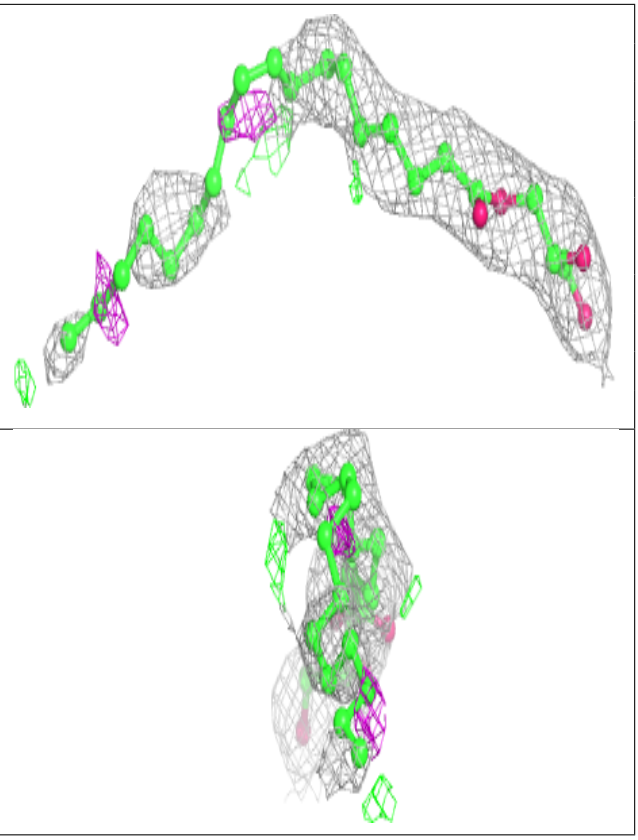






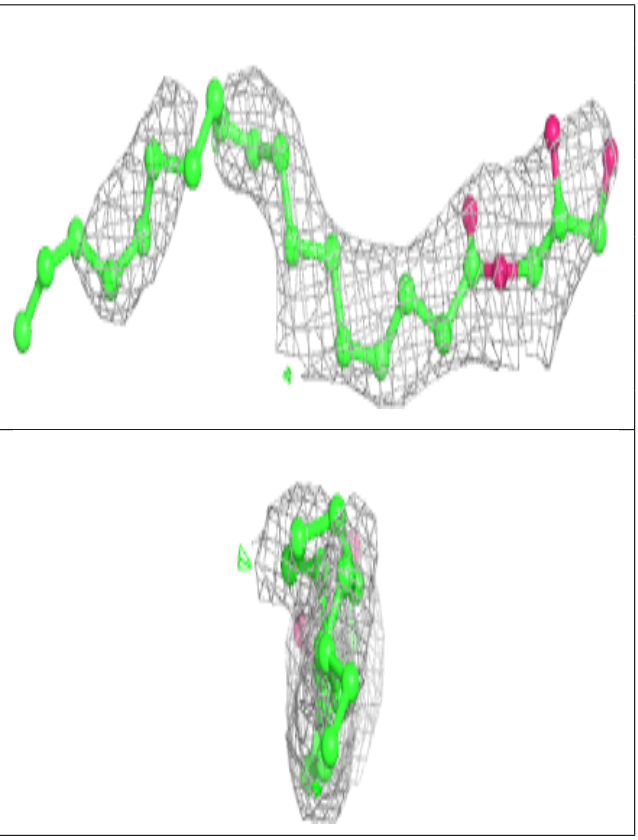
Electron density around OLC B 204:

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



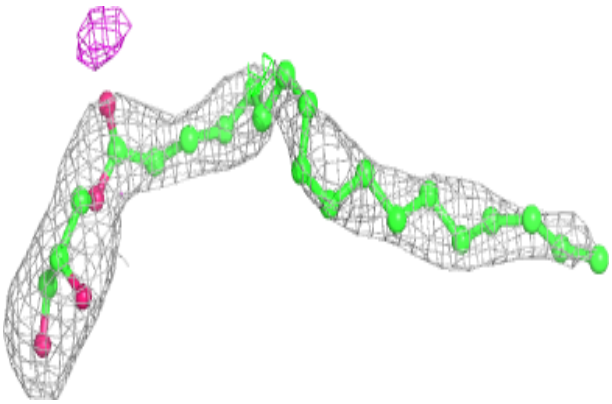
Electron density around OLC B 207:

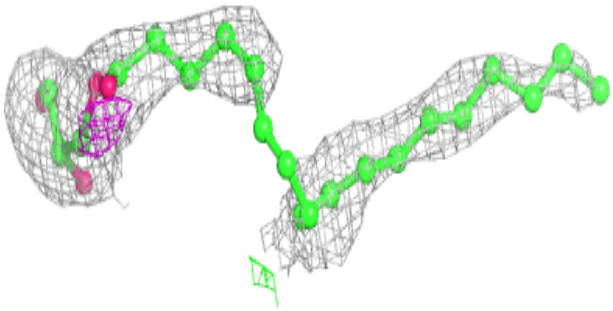
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

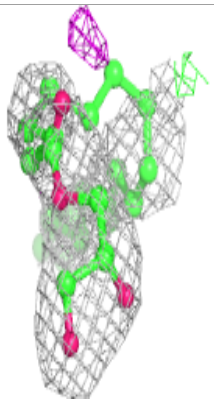


Electron density around OLC A 205:

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

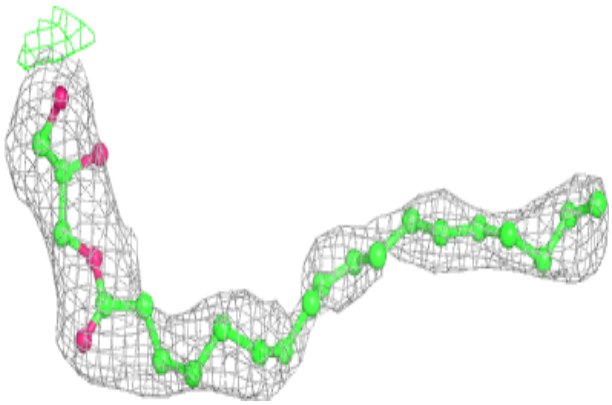


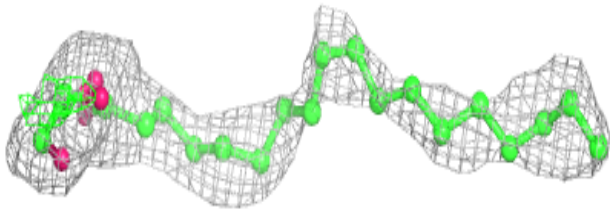


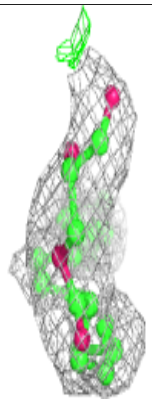


Electron density around OLC B 205:

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

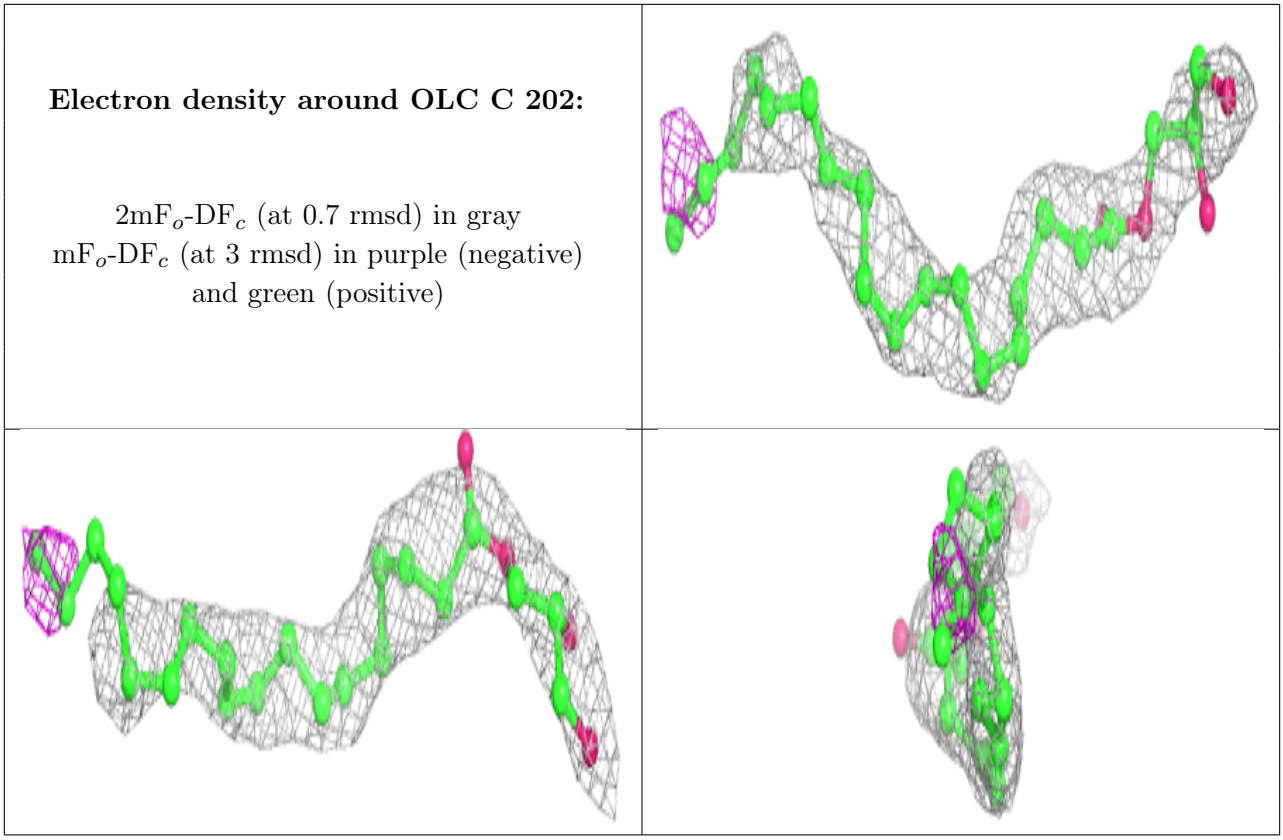






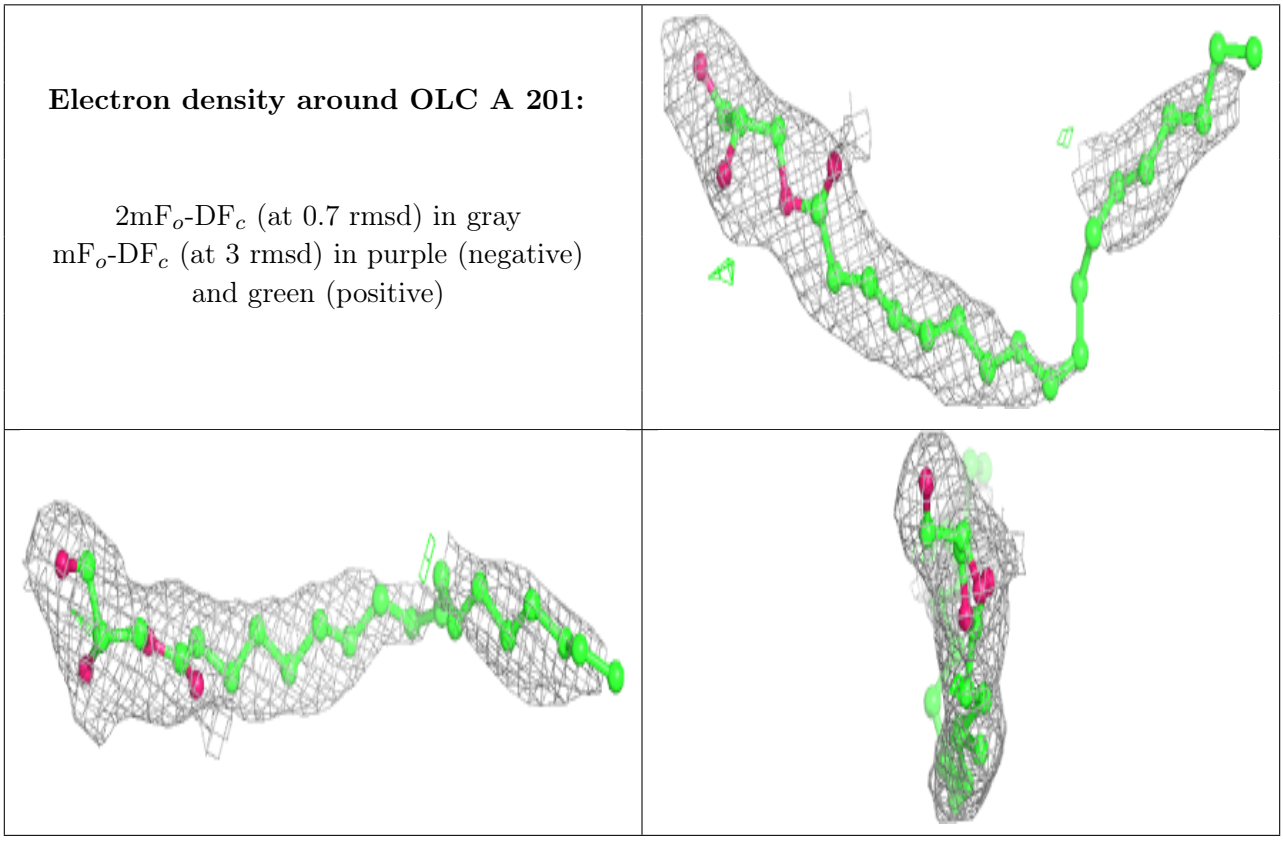
Electron density around OLC C 202:

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



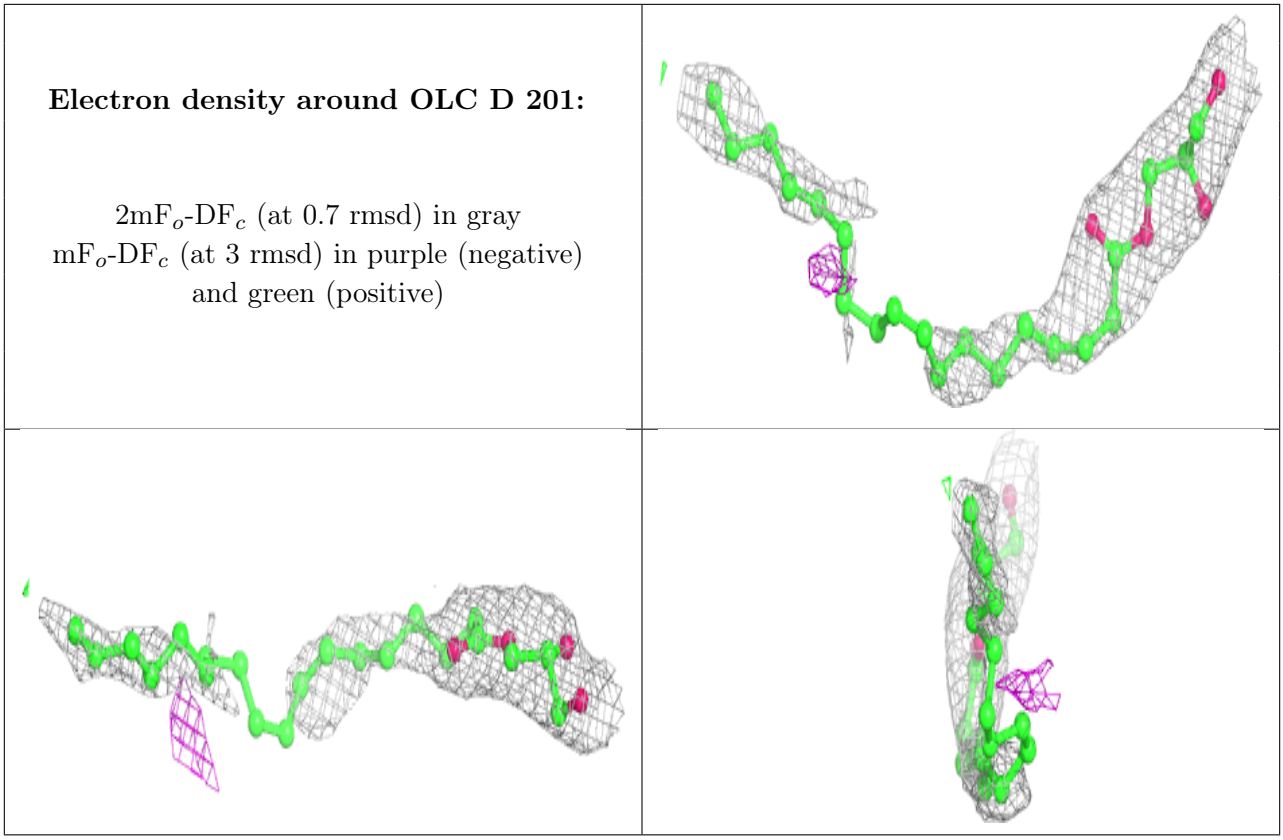
Electron density around OLC A 201:

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



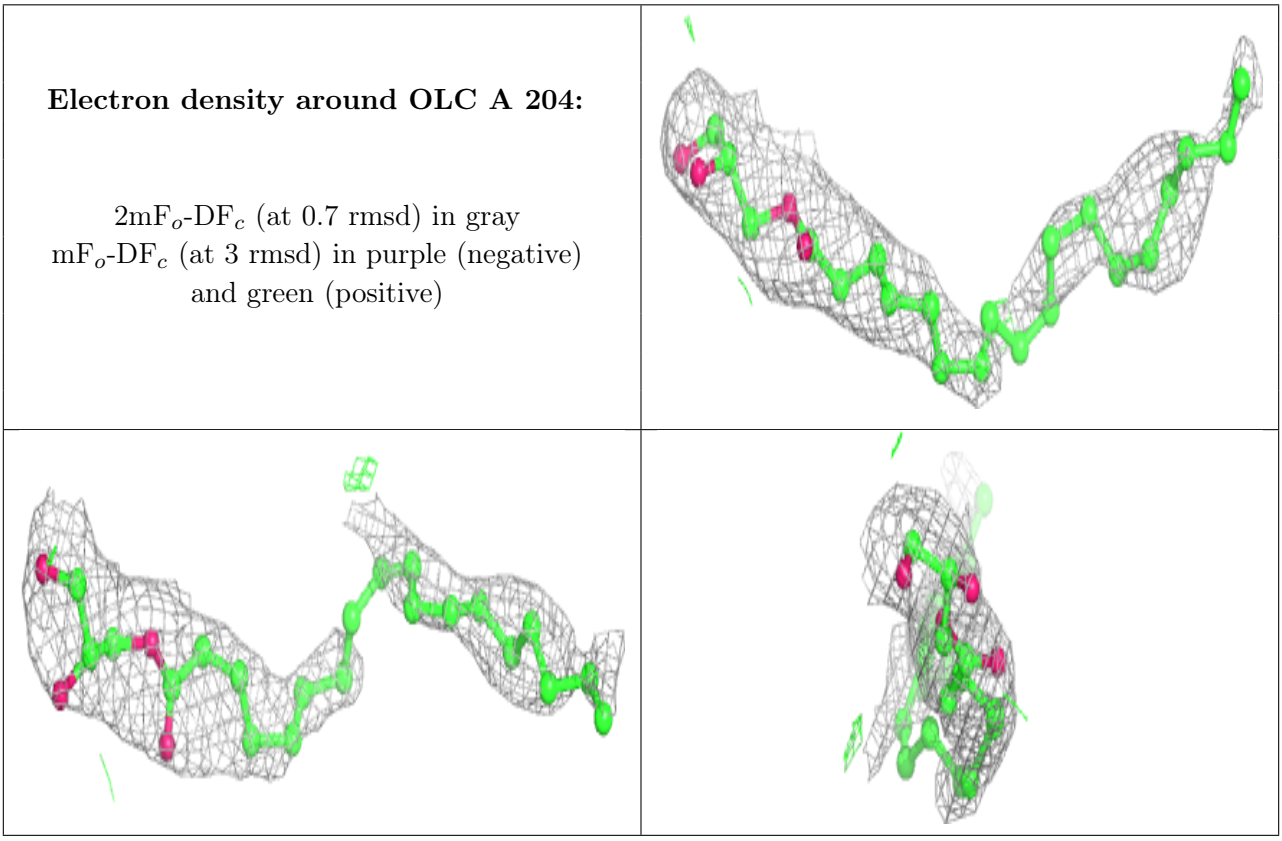
Electron density around OLC D 201:

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



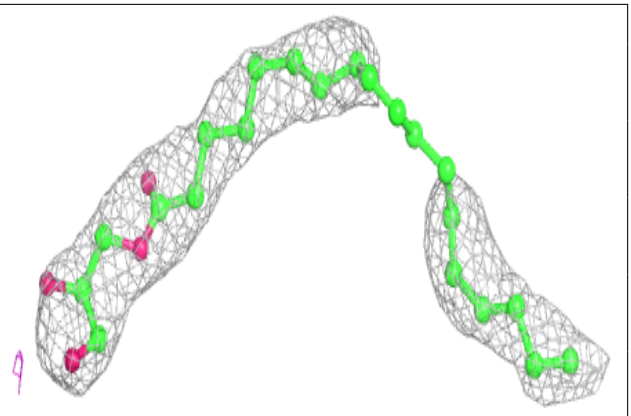
Electron density around OLC A 204:

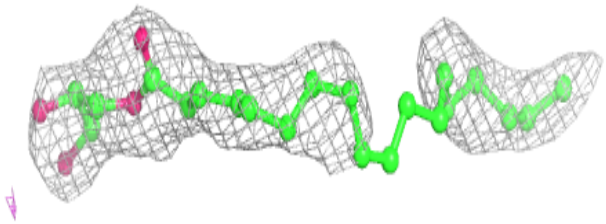
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

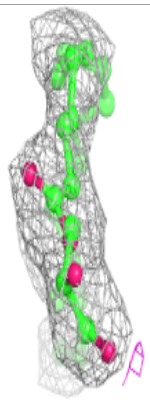


Electron density around OLC F 301:

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

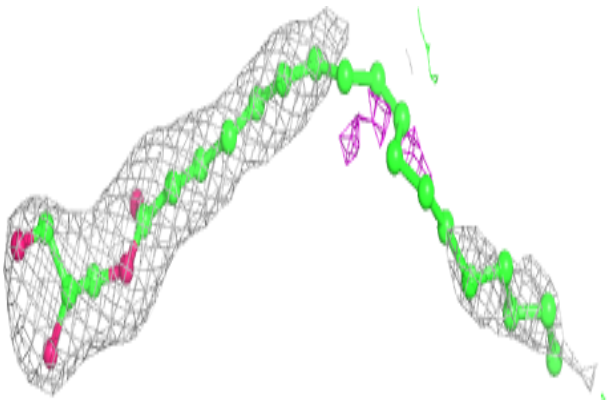


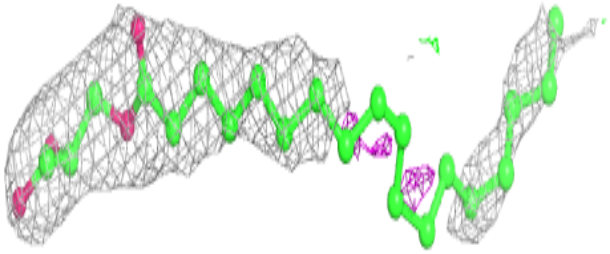


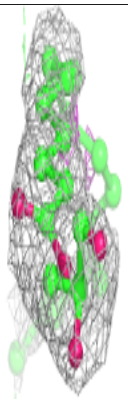


Electron density around OLC B 201:

$2mF_o$-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.