Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2024 – 10:08 AM JST

PDB ID	:	8J4C
Title	:	YeeE(TsuA)-YeeD(TsuB) complex for thiosulfate uptake
Authors	:	Ikei, M.; Miyazaki, R.; Monden, K.; Naito, Y.; Takeuchi, A.; Takahashi, Y.S.; Tanaka, Y.; Ichikawa, M.; Tsukazaki, T.
Deposited on	:	2023-04-19
Resolution	:	3.34 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:

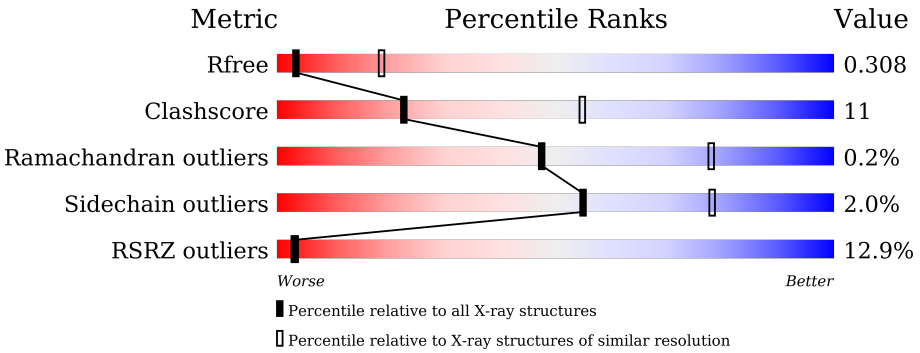
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.34 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	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RSRZ outliers	127900	1028 (3.38-3.30)

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	460	10% 65% 22% · 11%
1	B	460	13% 62% 26% · 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	THJ	A	501	-	-	-	X
2	THJ	B	501	-	-	-	X
3	OLC	A	504	-	-	-	X
3	OLC	A	505	-	-	-	X
3	OLC	A	506	-	-	-	X
3	OLC	A	507	-	-	-	X
3	OLC	A	508	-	-	-	X
3	OLC	A	511	-	-	-	X
3	OLC	B	503	-	-	-	X
3	OLC	B	506	-	-	-	X
3	OLC	B	507	-	-	-	X
3	OLC	B	508	-	-	-	X
3	OLC	B	512	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6675 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 Spirochaeta thermophila YeeE(TsuA)-YeeD(TsuB),UPF0033 domain-containing protein, SirA-like domain-containing protein (chimera).

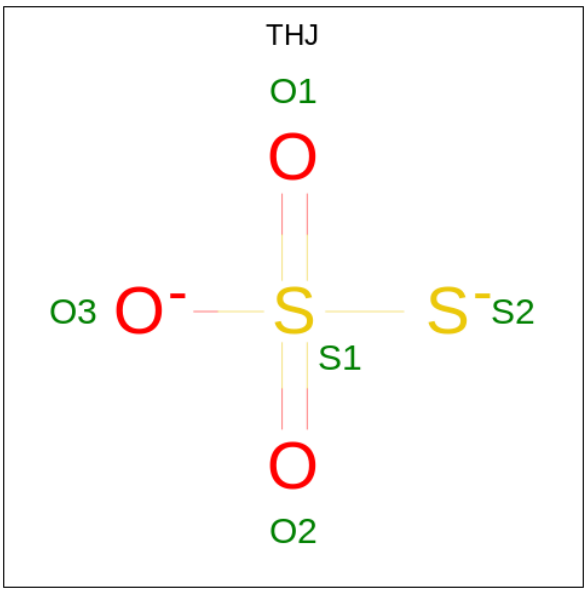
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	408	Total	C	N	O	S	0	0	0
			3119	2065	505	537	12			
1	A	408	Total	C	N	O	S	0	0	0
			3119	2065	505	537	12			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	22	ALA	CYS	engineered mutation	UNP G0GAP6
B	451	GLY	-	expression tag	UNP G0GAP7
B	452	SER	-	expression tag	UNP G0GAP7
B	453	SER	-	expression tag	UNP G0GAP7
B	454	GLY	-	expression tag	UNP G0GAP7
B	455	GLU	-	expression tag	UNP G0GAP7
B	456	ASN	-	expression tag	UNP G0GAP7
B	457	LEU	-	expression tag	UNP G0GAP7
B	458	TYR	-	expression tag	UNP G0GAP7
B	459	PHE	-	expression tag	UNP G0GAP7
B	460	GLN	-	expression tag	UNP G0GAP7
A	22	ALA	CYS	engineered mutation	UNP G0GAP6
A	451	GLY	-	expression tag	UNP G0GAP7
A	452	SER	-	expression tag	UNP G0GAP7
A	453	SER	-	expression tag	UNP G0GAP7
A	454	GLY	-	expression tag	UNP G0GAP7
A	455	GLU	-	expression tag	UNP G0GAP7
A	456	ASN	-	expression tag	UNP G0GAP7
A	457	LEU	-	expression tag	UNP G0GAP7
A	458	TYR	-	expression tag	UNP G0GAP7
A	459	PHE	-	expression tag	UNP G0GAP7
A	460	GLN	-	expression tag	UNP G0GAP7

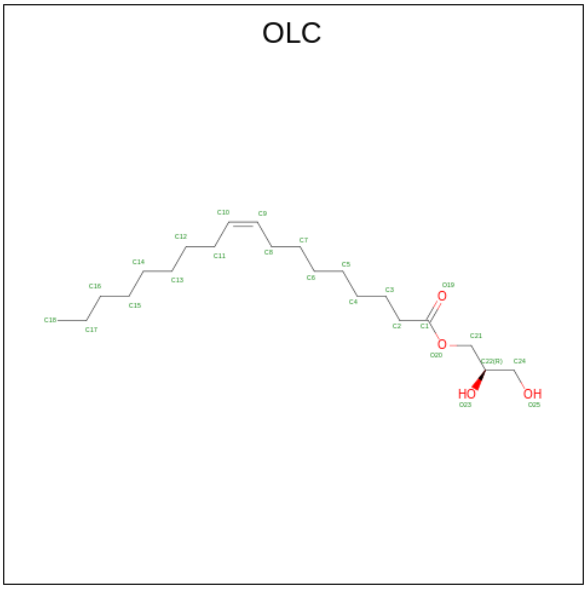
- Molecule 2 is THIOSULFATE (three-letter code: THJ) (formula: O_3S_2) (labeled as "Ligand

of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 3 2	0	0
2	A	1	Total O S 5 3 2	0	0

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

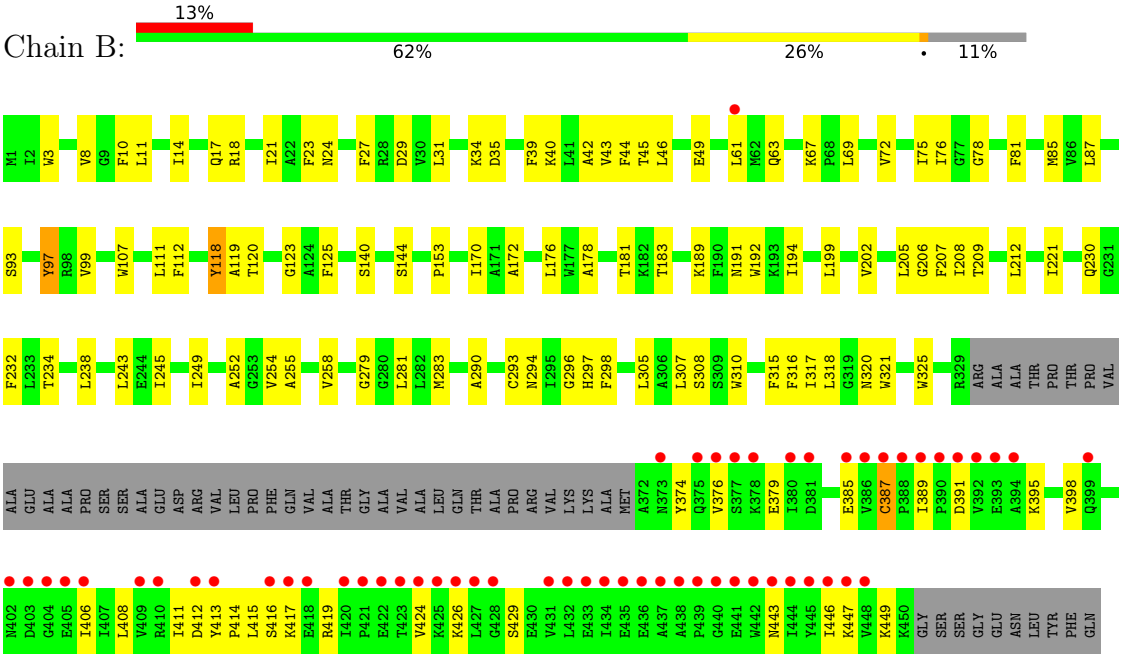


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 25 21 4	0	0
3	B	1	Total C O 25 21 4	0	0
3	B	1	Total C O 20 16 4	0	0
3	B	1	Total C 17 17	0	0
3	B	1	Total C O 17 13 4	0	0
3	B	1	Total C O 25 21 4	0	0
3	B	1	Total C 12 12	0	0
3	B	1	Total C O 25 21 4	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C O 25 21 4	0	0
3	B	1	Total C O 25 21 4	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C 14 14	0	0
3	A	1	Total C 16 16	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C O 11 7 4	0	0
3	A	1	Total C O 12 8 4	0	0

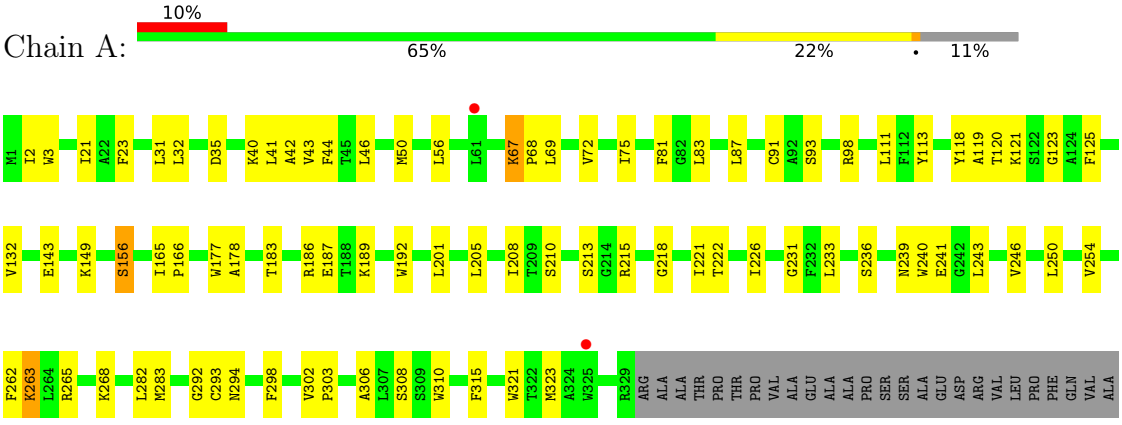
3 Residue-property plots (i)

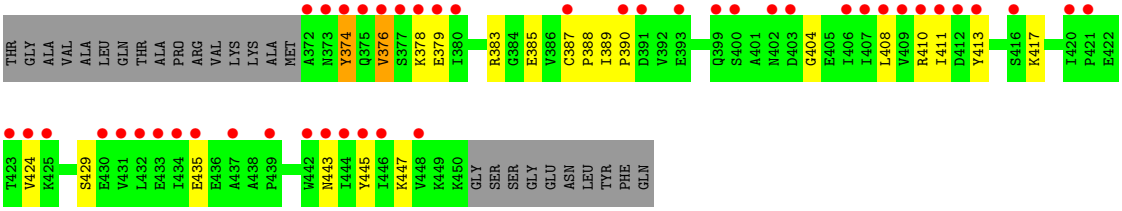
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Spirochaeta thermophila YeeE(TsuA)-YeeD(TsuB),UPF0033 domain-containing protein, SirA-like domain-containing protein (chimera)



• Molecule 1: Spirochaeta thermophila YeeE(TsuA)-YeeD(TsuB),UPF0033 domain-containing protein, SirA-like domain-containing protein (chimera)




THR GLY ALA VAL ALA LEU GLN THR ALA PRO ARG VAL LYS LYS ALA MET
A372 N373 Y374 Q375 V376 S377 K378 E379 I380
R383 G384 E385 V386 C387 P388 I389 P390 D391 V392 E393
Q399 S400 A401 N402 D403 G404 E405 I406 I407 L408 V409 R410 I411 D412 Y413
S416 K417
I420 P421 E422
T423 V424 K425
S429 E430 V431 L432 E433 I434 E435 E436 A437 A438 P439
W442 N443 I444 Y445 I446 K447 V448 K449 K450 GLY SER SER GLY GLU ASN LEU TYR PHE GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	73.98Å 102.44Å 186.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 3.34 49.39 – 3.34	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.39-3.34) 77.1 (49.39-3.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.78 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.265 , 0.311 0.265 , 0.308	Depositor DCC
R_{free} test set	2057 reflections (9.68%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	1.441	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 81.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	6675	wwPDB-VP
Average B, all atoms (Å^2)	66.0	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 43.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6554e-04. 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: OLC, THJ

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	0/3197	0.45	0/4344
1	B	0.26	0/3197	0.45	0/4344
All	All	0.26	0/6394	0.45	0/8688

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	3119	0	3211	69	0
1	B	3119	0	3211	80	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
3	A	203	0	318	13	0
3	B	224	0	356	15	0
All	All	6675	0	7096	158	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 11.

All (158) 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:201:LEU:HB3	3:A:502:OLC:H13A	1.62	0.82
1:A:435:GLU:HB3	1:A:443:ASN:HB2	1.71	0.72
1:B:424:VAL:HG22	1:B:429:SER:HB2	1.71	0.72
1:B:172:ALA:HB1	3:B:507:OLC:H15	1.72	0.70
1:A:120:THR:HA	1:A:125:PHE:HB2	1.74	0.69
1:B:387:CYS:SG	1:B:419:ARG:NH1	2.66	0.68
1:B:111:LEU:HD13	1:A:111:LEU:HD13	1.76	0.67
3:A:502:OLC:H24A	3:A:506:OLC:H24	1.77	0.66
3:B:504:OLC:H6	3:B:511:OLC:H10	1.76	0.66
1:B:112:PHE:HB3	1:B:281:LEU:HG	1.78	0.65
1:A:143:GLU:HB2	1:A:149:LYS:HB2	1.79	0.63
1:B:17:GLN:HG2	1:B:255:ALA:HB3	1.81	0.62
3:A:502:OLC:H22	3:A:503:OLC:H21	1.80	0.62
1:B:120:THR:HA	1:B:125:PHE:HB2	1.81	0.62
1:B:205:LEU:HD22	3:B:502:OLC:H13A	1.81	0.61
1:A:246:VAL:HG13	3:A:509:OLC:H13	1.82	0.61
1:A:113:TYR:HH	1:A:222:THR:HG1	1.49	0.60
1:A:113:TYR:OH	1:A:222:THR:OG1	2.19	0.60
1:B:305:LEU:HA	1:B:310:TRP:HE1	1.67	0.59
1:B:40:LYS:HD2	1:B:183:THR:HG23	1.85	0.58
1:A:387:CYS:SG	1:A:388:PRO:HD3	2.43	0.57
1:A:69:LEU:HA	1:A:308:SER:HB3	1.86	0.57
1:A:379:GLU:N	1:A:379:GLU:OE1	2.36	0.57
1:A:56:LEU:HD13	1:A:208:ILE:HD11	1.87	0.56
1:A:165:ILE:HB	1:A:166:PRO:HD3	1.88	0.56
1:B:411:ILE:HD12	1:B:412:ASP:H	1.71	0.55
1:A:40:LYS:NZ	1:A:183:THR:OG1	2.38	0.55
1:A:23:PHE:HD2	1:A:294:ASN:HB2	1.71	0.55
1:A:215:ARG:NH2	1:A:218:GLY:O	2.34	0.54
1:B:61:LEU:HB3	1:B:208:ILE:HG12	1.88	0.54
1:B:176:LEU:HD23	3:B:509:OLC:H5A	1.89	0.54
1:B:3:TRP:HA	1:B:243:LEU:HD23	1.89	0.54
1:B:93:SER:HB3	1:B:221:ILE:HG13	1.90	0.53
1:B:67:LYS:NZ	1:B:296:GLY:O	2.42	0.53
1:B:18:ARG:HD3	1:B:255:ALA:HB1	1.91	0.52
1:B:40:LYS:NZ	1:B:181:THR:O	2.41	0.52
1:A:31:LEU:HD13	1:A:321:TRP:CG	2.44	0.52
1:B:294:ASN:O	1:B:298:PHE:HB3	2.09	0.52
1:A:98:ARG:NH1	1:A:413:TYR:OH	2.42	0.52
1:A:410:ARG:NH1	1:A:443:ASN:OD1	2.43	0.51
1:B:69:LEU:HA	1:B:308:SER:HB3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:VAL:HG13	1:B:107:TRP:CD1	2.46	0.51
1:A:46:LEU:HA	1:A:303:PRO:HG3	1.92	0.51
1:B:23:PHE:HD2	1:B:294:ASN:HB2	1.75	0.51
1:B:290:ALA:O	1:B:297:HIS:NE2	2.38	0.51
1:B:415:LEU:HG	1:B:419:ARG:HD3	1.93	0.50
1:A:46:LEU:HD13	1:A:302:VAL:HG11	1.92	0.50
1:A:43:VAL:HG11	1:A:177:TRP:CZ3	2.47	0.50
1:A:205:LEU:HD13	3:A:502:OLC:H18B	1.94	0.50
1:B:63:GLN:NE2	1:B:144:SER:O	2.44	0.50
1:B:447:LYS:HZ2	1:B:449:LYS:HE3	1.75	0.50
1:A:2:ILE:HD13	1:A:213:SER:HB2	1.94	0.50
1:B:81:PHE:CZ	1:B:293:CYS:HB2	2.48	0.49
1:B:119:ALA:HA	1:B:123:GLY:HA3	1.95	0.49
1:B:21:ILE:HD13	1:B:199:LEU:HD22	1.94	0.49
1:A:3:TRP:HA	1:A:243:LEU:HD22	1.94	0.49
1:A:411:ILE:HD11	1:A:417:LYS:HB3	1.94	0.49
1:B:31:LEU:HD13	1:B:321:TRP:CD2	2.47	0.49
1:B:78:GLY:HA2	1:B:316:PHE:CE1	2.47	0.49
1:B:40:LYS:NZ	1:B:178:ALA:O	2.45	0.49
1:A:81:PHE:CZ	1:A:293:CYS:HB2	2.47	0.49
1:B:24:ASN:OD1	1:B:320:ASN:ND2	2.45	0.49
1:B:414:PRO:O	1:B:417:LYS:HG2	2.12	0.49
1:B:45:THR:O	1:B:49:GLU:HG3	2.13	0.49
1:A:210:SER:HB2	1:A:240:TRP:CE2	2.48	0.48
1:B:170:ILE:HD12	1:B:305:LEU:HD21	1.96	0.48
1:A:404:GLY:HA2	1:A:447:LYS:HE2	1.96	0.47
1:A:189:LYS:HE2	3:A:506:OLC:H24A	1.97	0.47
1:A:205:LEU:HD22	3:A:502:OLC:H14A	1.97	0.47
1:B:191:ASN:OD1	1:B:194:ILE:HG22	2.15	0.46
3:B:507:OLC:H11	3:B:509:OLC:H18B	1.97	0.46
1:A:75:ILE:HG12	1:A:315:PHE:CE1	2.51	0.46
1:A:378:LYS:HD3	1:A:379:GLU:H	1.81	0.46
1:A:424:VAL:HG13	1:A:429:SER:HB2	1.97	0.46
1:B:411:ILE:HG13	1:B:413:TYR:H	1.81	0.46
1:B:78:GLY:HA2	1:B:316:PHE:HE1	1.80	0.46
1:A:42:ALA:O	1:A:46:LEU:HG	2.16	0.46
1:A:298:PHE:O	1:A:302:VAL:HB	2.16	0.46
1:A:121:LYS:HD3	1:A:226:ILE:HD13	1.96	0.46
1:B:40:LYS:HZ1	1:B:181:THR:C	2.19	0.46
1:B:44:PHE:HB2	1:B:192:TRP:HZ3	1.80	0.46
3:B:505:OLC:H18B	3:A:509:OLC:H14A	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:VAL:HG11	1:B:446:ILE:HG21	1.98	0.45
1:B:379:GLU:N	1:B:379:GLU:OE1	2.49	0.45
1:A:83:LEU:HB3	1:A:323:MET:HE2	1.97	0.45
3:A:506:OLC:H21A	3:A:506:OLC:H2	1.62	0.45
1:B:8:VAL:HG22	1:B:205:LEU:HG	1.98	0.45
1:B:11:LEU:HD22	3:B:502:OLC:H7	1.97	0.45
1:B:75:ILE:HG23	1:B:315:PHE:CZ	2.52	0.45
1:B:374:TYR:O	1:B:406:ILE:HG21	2.16	0.45
1:B:411:ILE:HG12	1:B:416:SER:OG	2.16	0.45
1:B:391:ASP:HB2	1:B:419:ARG:HH21	1.81	0.45
1:A:50:MET:HG3	1:A:303:PRO:HA	1.99	0.45
1:A:91:CYS:HA	1:A:283:MET:HE3	1.98	0.45
1:B:325:TRP:HB2	3:B:510:OLC:H14	1.99	0.45
1:B:34:LYS:HA	1:B:34:LYS:HD2	1.71	0.44
1:B:385:GLU:HB3	1:B:389:ILE:HB	2.00	0.44
1:A:306:ALA:O	1:A:310:TRP:HD1	2.00	0.44
1:B:10:PHE:O	1:B:14:ILE:HG13	2.17	0.44
3:B:509:OLC:H21A	3:B:509:OLC:H2	1.37	0.44
1:B:153:PRO:HB2	1:B:307:LEU:HD12	1.98	0.44
1:A:156:SER:HB2	1:A:166:PRO:HG2	2.00	0.44
1:B:153:PRO:HG2	1:B:307:LEU:HB2	2.00	0.44
1:A:119:ALA:HA	1:A:123:GLY:HA3	1.98	0.44
3:B:507:OLC:H14A	3:B:507:OLC:H17	1.71	0.44
1:A:374:TYR:O	1:A:376:VAL:N	2.46	0.43
1:B:279:GLY:O	1:B:283:MET:HG3	2.18	0.43
1:A:385:GLU:HG2	1:A:389:ILE:HD12	1.99	0.43
1:B:238:LEU:HG	3:B:506:OLC:O23	2.18	0.43
1:A:231:GLY:HA2	1:A:236:SER:H	1.83	0.43
1:B:29:ASP:HB3	1:B:35:ASP:HB3	2.01	0.43
1:B:315:PHE:CD2	1:B:318:LEU:HD12	2.53	0.43
1:A:292:GLY:HA2	2:A:501:THJ:S2	2.59	0.43
1:B:97:TYR:HB2	1:B:252:ALA:HB2	2.01	0.43
1:B:209:THR:HA	1:B:212:LEU:HD12	2.01	0.42
1:B:189:LYS:HA	1:B:189:LYS:HD2	1.83	0.42
1:B:42:ALA:O	1:B:46:LEU:HG	2.19	0.42
1:A:389:ILE:HB	1:A:390:PRO:HD3	2.01	0.42
1:B:325:TRP:CD1	3:B:510:OLC:H13A	2.54	0.42
1:B:408:LEU:HD21	1:B:443:ASN:ND2	2.35	0.42
1:A:87:LEU:HD12	1:A:282:LEU:HD12	2.02	0.42
1:B:24:ASN:CG	1:B:85:MET:HB3	2.39	0.42
1:B:232:PHE:HB2	3:B:506:OLC:H3A	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:ASP:HB2	1:B:419:ARG:NH2	2.34	0.42
1:A:93:SER:HB3	1:A:221:ILE:HG13	2.02	0.42
1:A:294:ASN:O	1:A:298:PHE:HB3	2.19	0.42
1:B:72:VAL:HG13	1:B:76:ILE:HD12	2.01	0.42
1:A:189:LYS:HE3	1:A:189:LYS:HB3	1.90	0.42
1:A:250:LEU:HD22	3:A:508:OLC:H8	2.02	0.42
1:B:395:LYS:HE3	1:B:395:LYS:HB2	1.80	0.42
1:A:91:CYS:HB2	1:A:294:ASN:CG	2.40	0.42
1:A:408:LEU:HD13	1:A:445:TYR:CE1	2.55	0.42
1:A:21:ILE:HD13	1:A:41:LEU:HD21	2.02	0.41
1:A:43:VAL:HG11	1:A:177:TRP:HZ3	1.83	0.41
3:B:512:OLC:H9	3:B:512:OLC:H6	1.93	0.41
1:A:239:ASN:HD21	1:A:241:GLU:HG2	1.86	0.41
1:A:44:PHE:HB2	1:A:192:TRP:HZ3	1.85	0.41
1:B:87:LEU:HD23	1:B:87:LEU:HA	1.89	0.41
1:B:202:VAL:O	1:B:206:GLY:N	2.49	0.41
1:B:254:VAL:O	1:B:258:VAL:HG23	2.20	0.41
1:A:31:LEU:HD23	1:A:32:LEU:HD23	2.02	0.41
1:B:230:GLN:O	1:B:234:THR:HG22	2.20	0.41
1:A:187:GLU:N	1:A:187:GLU:OE1	2.53	0.41
1:A:262:PHE:CE2	3:A:509:OLC:H5	2.55	0.41
1:A:263:LYS:HZ2	1:A:265:ARG:HG2	1.85	0.41
1:B:39:PHE:O	1:B:43:VAL:HG23	2.20	0.41
1:B:118:TYR:HB3	1:A:233:LEU:HD22	2.03	0.41
3:A:508:OLC:H8A	3:A:509:OLC:H12	2.02	0.41
1:B:27:PHE:HB3	1:B:317:ILE:HG23	2.01	0.41
1:A:40:LYS:HE2	1:A:178:ALA:O	2.21	0.41
1:A:67:LYS:HA	1:A:68:PRO:HD3	1.98	0.41
1:A:383:ARG:HH11	1:A:410:ARG:HH21	1.69	0.40
1:B:17:GLN:HG3	1:B:18:ARG:N	2.35	0.40
1:B:245:ILE:O	1:B:249:ILE:HG13	2.21	0.40
3:B:512:OLC:H5A	3:B:512:OLC:H2	1.88	0.40
1:B:426:LYS:HD2	1:B:426:LYS:HA	1.82	0.40
1:A:72:VAL:HG12	1:A:132:VAL:HG13	2.04	0.40
1:A:254:VAL:HG11	3:A:503:OLC:H7	2.03	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	404/460 (88%)	385 (95%)	18 (4%)	1 (0%)	47 78
1	B	404/460 (88%)	381 (94%)	22 (5%)	1 (0%)	47 78
All	All	808/920 (88%)	766 (95%)	40 (5%)	2 (0%)	47 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	376	VAL
1	A	376	VAL

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	321/359 (89%)	313 (98%)	8 (2%)	47 74
1	B	321/359 (89%)	316 (98%)	5 (2%)	62 81
All	All	642/718 (89%)	629 (98%)	13 (2%)	55 78

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	97	TYR
1	B	118	TYR
1	B	140	SER
1	B	207	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	387	CYS
1	A	35	ASP
1	A	67	LYS
1	A	118	TYR
1	A	156	SER
1	A	186	ARG
1	A	263	LYS
1	A	268	LYS
1	A	374	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	24	ASN
1	B	320	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

23 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	502	-	24,24,24	0.24	0	25,25,25	0.24	0
3	OLC	B	503	-	24,24,24	0.25	0	25,25,25	0.29	0
3	OLC	A	506	-	24,24,24	0.25	0	25,25,25	0.26	0
3	OLC	A	509	-	24,24,24	0.24	0	25,25,25	0.24	0
3	OLC	B	502	-	24,24,24	0.24	0	25,25,25	0.28	0
3	OLC	B	504	-	19,19,24	0.23	0	20,20,25	0.30	0
3	OLC	A	504	-	13,13,24	0.19	0	12,12,25	0.20	0
3	OLC	B	505	-	16,16,24	0.19	0	15,15,25	0.19	0
3	OLC	B	510	-	7,7,24	0.09	0	6,6,25	0.11	0
3	OLC	A	511	-	11,11,24	0.24	0	12,12,25	0.33	0
3	OLC	A	507	-	24,24,24	0.24	0	25,25,25	0.23	0
3	OLC	B	512	-	24,24,24	0.26	0	25,25,25	0.26	0
2	THJ	A	501	-	2,4,4	1.26	0	2,6,6	0.22	0
2	THJ	B	501	-	2,4,4	1.22	0	2,6,6	0.18	0
3	OLC	A	503	-	24,24,24	0.25	0	25,25,25	0.27	0
3	OLC	A	505	-	15,15,24	0.22	0	14,14,25	0.20	0
3	OLC	B	509	-	24,24,24	0.23	0	25,25,25	0.27	0
3	OLC	A	508	-	24,24,24	0.23	0	25,25,25	0.27	0
3	OLC	B	507	-	24,24,24	0.25	0	25,25,25	0.27	0
3	OLC	A	510	-	10,10,24	0.24	0	11,11,25	0.33	0
3	OLC	B	511	-	24,24,24	0.23	0	25,25,25	0.28	0
3	OLC	B	506	-	16,16,24	0.27	0	17,17,25	0.34	0
3	OLC	B	508	-	11,11,24	0.18	0	9,10,25	0.16	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	502	-	-	3/24/24/24	-
3	OLC	B	503	-	-	6/24/24/24	-
3	OLC	A	506	-	-	5/24/24/24	-
3	OLC	A	509	-	-	1/24/24/24	-
3	OLC	B	502	-	-	3/24/24/24	-
3	OLC	B	504	-	-	3/19/19/24	-
3	OLC	A	504	-	-	1/11/11/24	-
3	OLC	B	505	-	-	1/14/14/24	-
3	OLC	B	510	-	-	1/5/5/24	-
3	OLC	A	511	-	-	0/11/11/24	-
3	OLC	A	507	-	-	2/24/24/24	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OLC	B	512	-	-	3/24/24/24	-
3	OLC	A	503	-	-	3/24/24/24	-
3	OLC	A	505	-	-	5/13/13/24	-
3	OLC	B	509	-	-	4/24/24/24	-
3	OLC	A	508	-	-	5/24/24/24	-
3	OLC	B	507	-	-	7/24/24/24	-
3	OLC	A	510	-	-	0/10/10/24	-
3	OLC	B	511	-	-	4/24/24/24	-
3	OLC	B	506	-	-	3/16/16/24	-
3	OLC	B	508	-	-	1/9/9/24	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	506	OLC	O20-C21-C22-O23
3	B	507	OLC	C2-C1-O20-C21
3	B	507	OLC	O19-C1-O20-C21
3	B	509	OLC	C2-C1-O20-C21
3	B	509	OLC	O19-C1-O20-C21
3	A	506	OLC	C2-C1-O20-C21
3	A	506	OLC	O19-C1-O20-C21
3	B	511	OLC	O19-C1-O20-C21
3	B	511	OLC	C2-C1-O20-C21
3	B	507	OLC	O20-C21-C22-O23
3	B	507	OLC	O20-C21-C22-C24
3	B	503	OLC	C1-C2-C3-C4
3	B	512	OLC	O20-C21-C22-O23
3	A	505	OLC	C12-C13-C14-C15
3	B	504	OLC	C2-C3-C4-C5
3	B	502	OLC	C2-C3-C4-C5
3	B	504	OLC	C4-C5-C6-C7
3	B	511	OLC	C1-C2-C3-C4
3	B	503	OLC	C2-C1-O20-C21
3	B	503	OLC	O19-C1-O20-C21
3	A	507	OLC	C1-C2-C3-C4
3	A	508	OLC	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	506	OLC	O20-C21-C22-C24
3	B	506	OLC	C4-C5-C6-C7
3	B	509	OLC	C7-C8-C9-C10
3	A	505	OLC	C9-C10-C11-C12
3	B	508	OLC	C7-C8-C9-C10
3	B	512	OLC	C3-C4-C5-C6
3	A	505	OLC	C13-C14-C15-C16
3	B	503	OLC	C2-C3-C4-C5
3	A	505	OLC	C15-C16-C17-C18
3	B	504	OLC	C1-C2-C3-C4
3	A	507	OLC	C9-C10-C11-C12
3	B	505	OLC	C9-C10-C11-C12
3	A	504	OLC	C7-C8-C9-C10
3	A	505	OLC	C7-C8-C9-C10
3	B	509	OLC	C9-C10-C11-C12
3	A	502	OLC	C14-C15-C16-C17
3	A	502	OLC	C3-C4-C5-C6
3	B	502	OLC	C7-C8-C9-C10
3	B	511	OLC	C9-C10-C11-C12
3	A	506	OLC	C7-C8-C9-C10
3	A	509	OLC	C7-C8-C9-C10
3	A	508	OLC	C11-C12-C13-C14
3	B	502	OLC	C5-C6-C7-C8
3	A	503	OLC	C2-C3-C4-C5
3	B	512	OLC	C14-C15-C16-C17
3	B	507	OLC	C5-C6-C7-C8
3	B	507	OLC	C14-C15-C16-C17
3	B	507	OLC	C7-C8-C9-C10
3	B	503	OLC	C13-C14-C15-C16
3	A	508	OLC	C3-C4-C5-C6
3	A	508	OLC	C7-C8-C9-C10
3	B	510	OLC	C14-C15-C16-C17
3	A	502	OLC	C9-C10-C11-C12
3	A	506	OLC	O20-C1-C2-C3
3	A	503	OLC	C13-C14-C15-C16
3	A	503	OLC	O20-C1-C2-C3
3	A	508	OLC	C1-C2-C3-C4
3	A	506	OLC	C12-C13-C14-C15
3	B	503	OLC	O20-C1-C2-C3

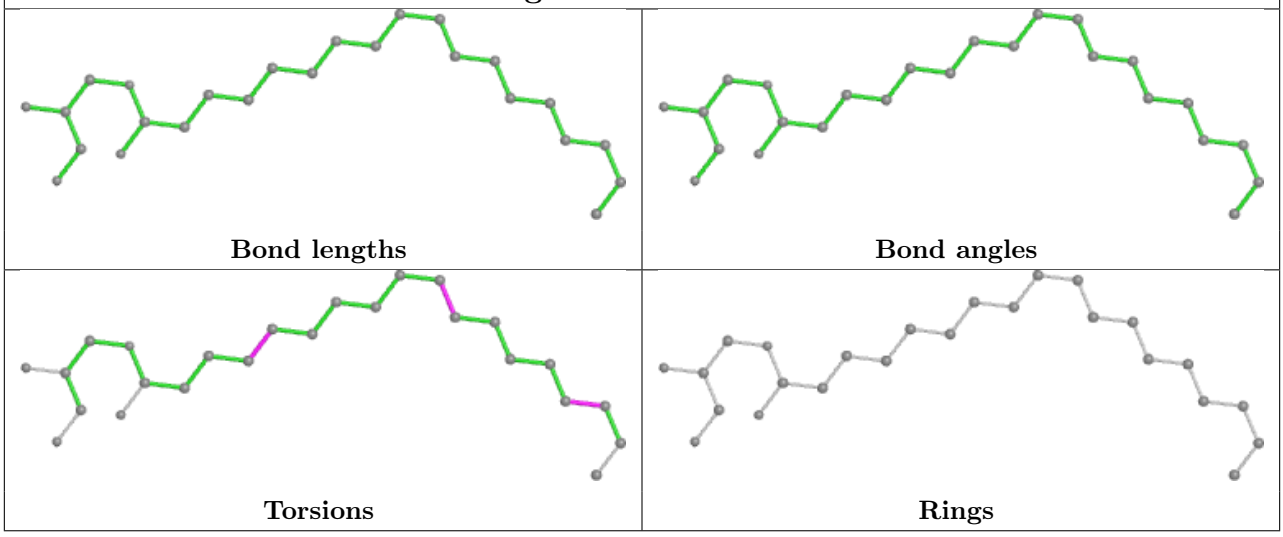
There are no ring outliers.

15 monomers are involved in 28 short contacts:

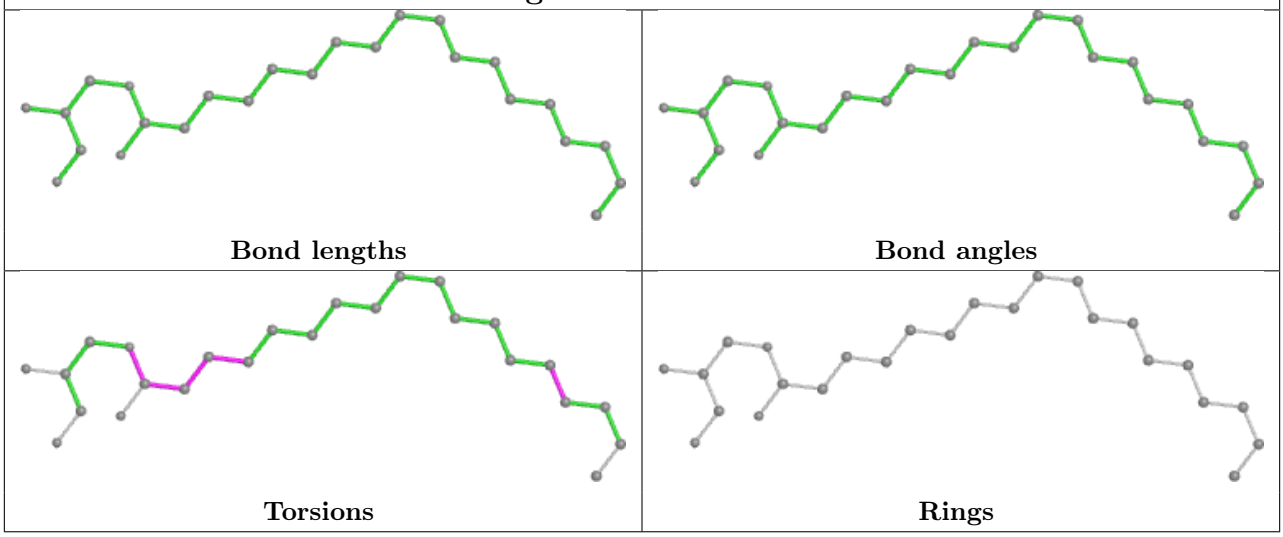
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	OLC	5	0
3	A	506	OLC	3	0
3	A	509	OLC	4	0
3	B	502	OLC	2	0
3	B	504	OLC	1	0
3	B	505	OLC	1	0
3	B	510	OLC	2	0
3	B	512	OLC	2	0
2	A	501	THJ	1	0
3	A	503	OLC	2	0
3	B	509	OLC	3	0
3	A	508	OLC	2	0
3	B	507	OLC	3	0
3	B	511	OLC	1	0
3	B	506	OLC	2	0

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.

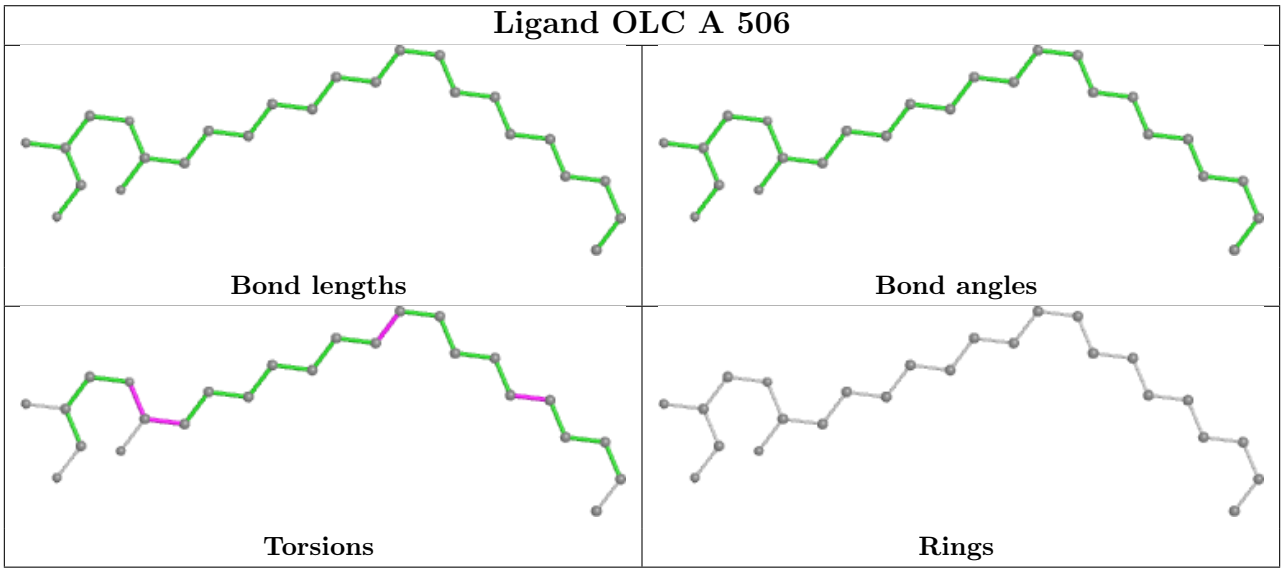
Ligand OLC A 502



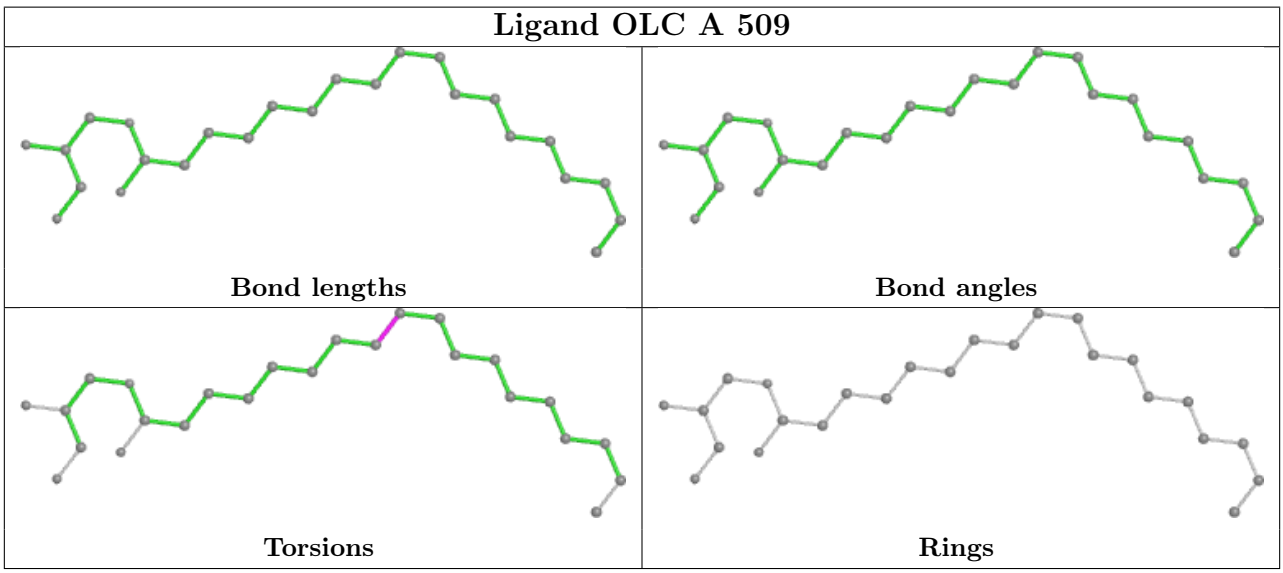
Ligand OLC B 503



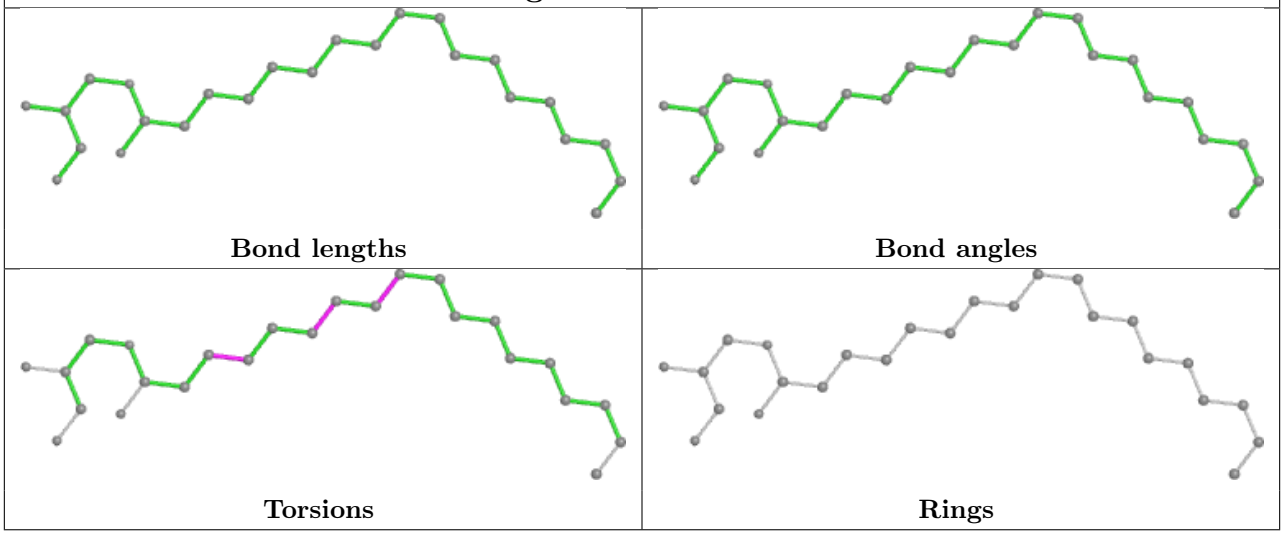
Ligand OLC A 506



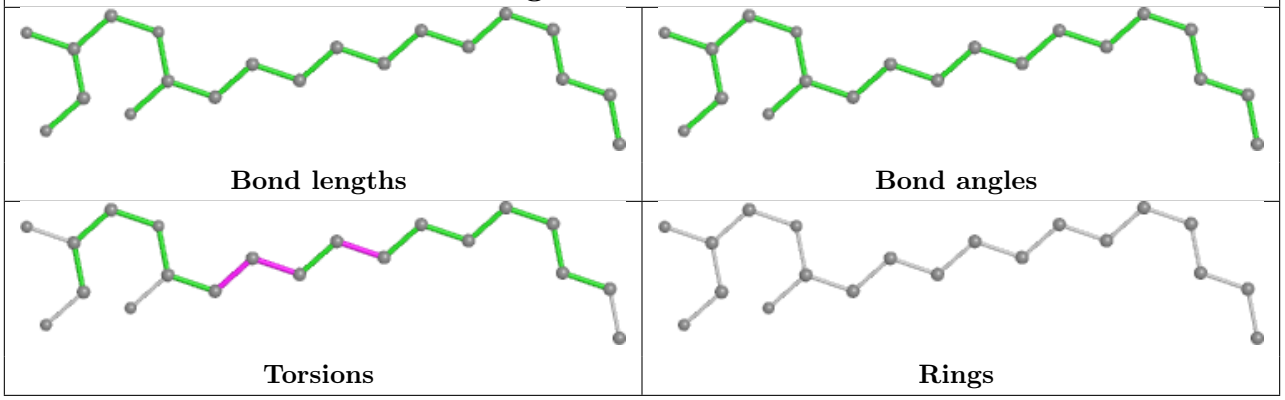
Ligand OLC A 509



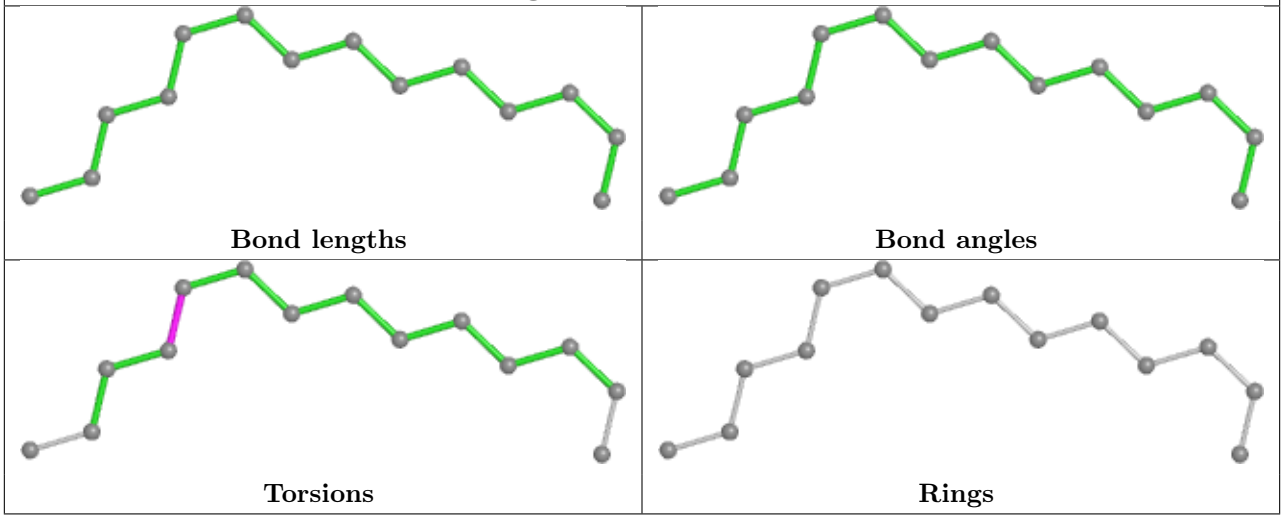
Ligand OLC B 502



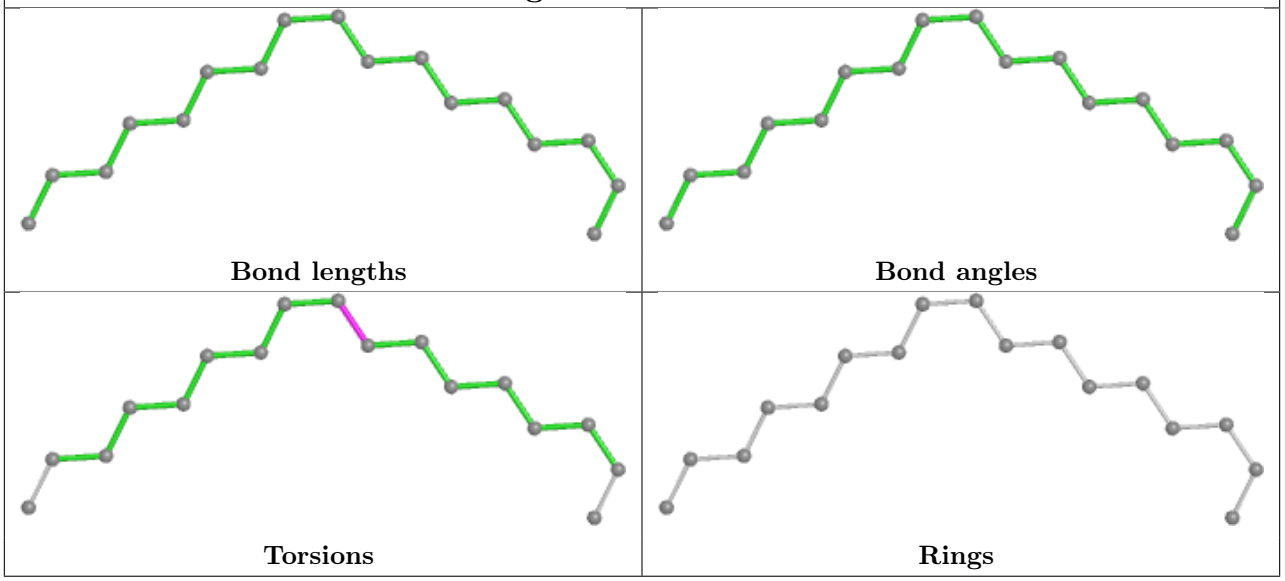
Ligand OLC B 504



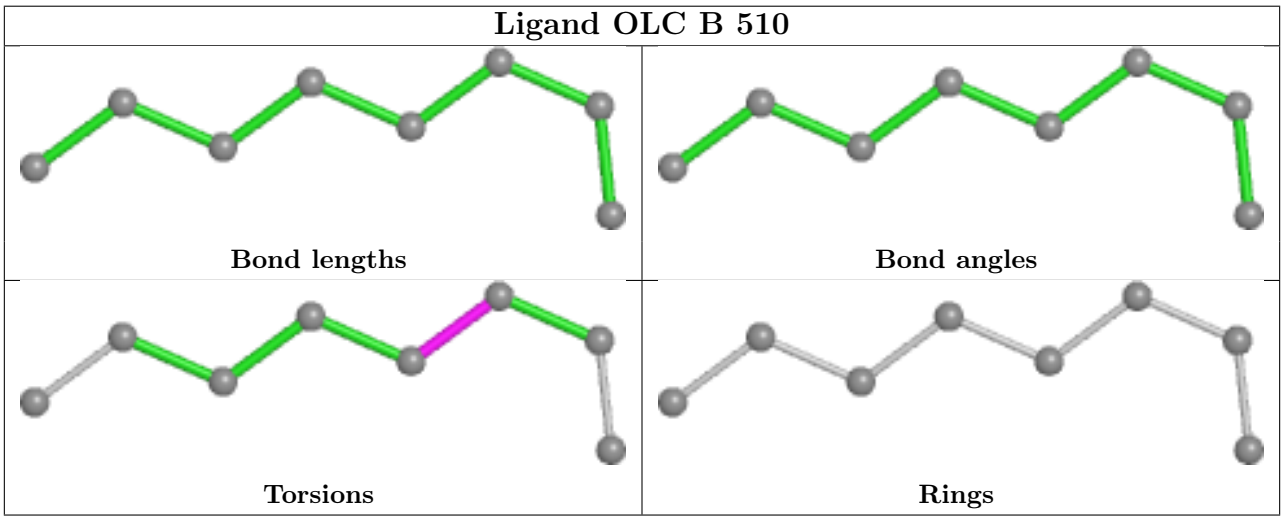
Ligand OLC A 504



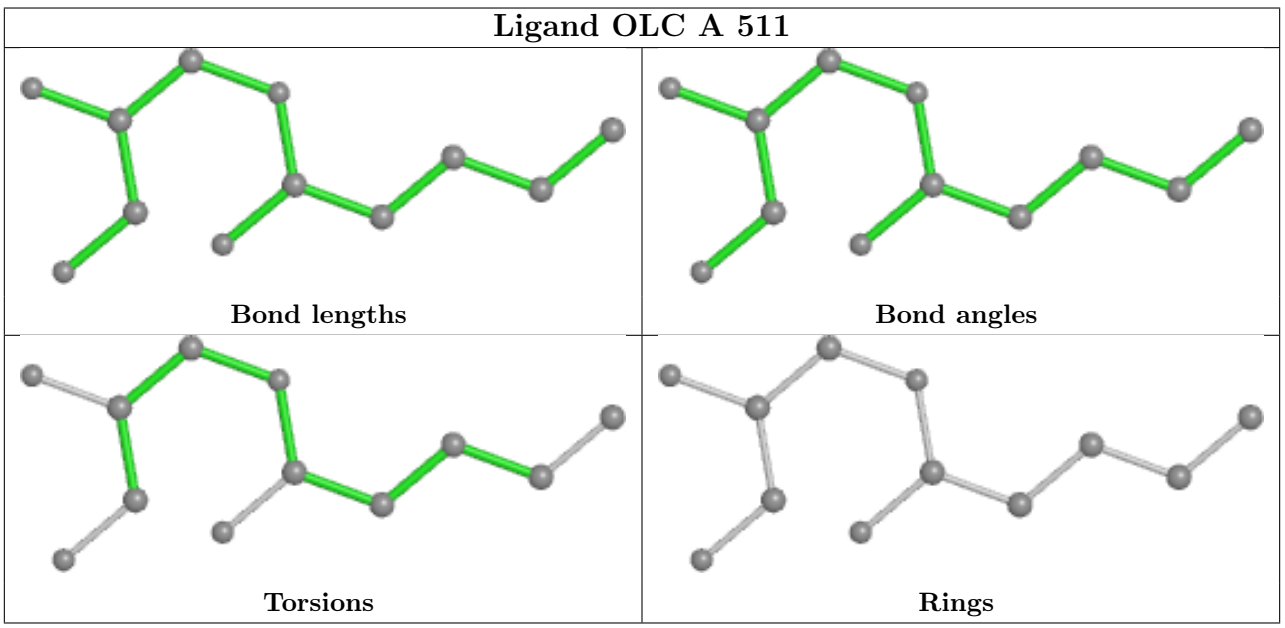
Ligand OLC B 505



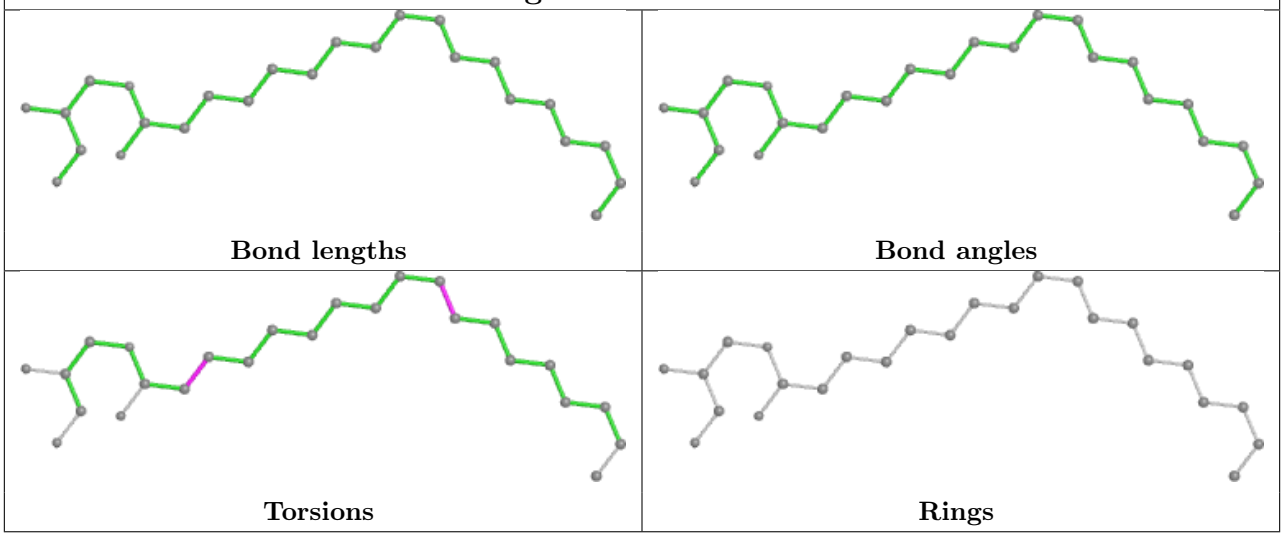
Ligand OLC B 510



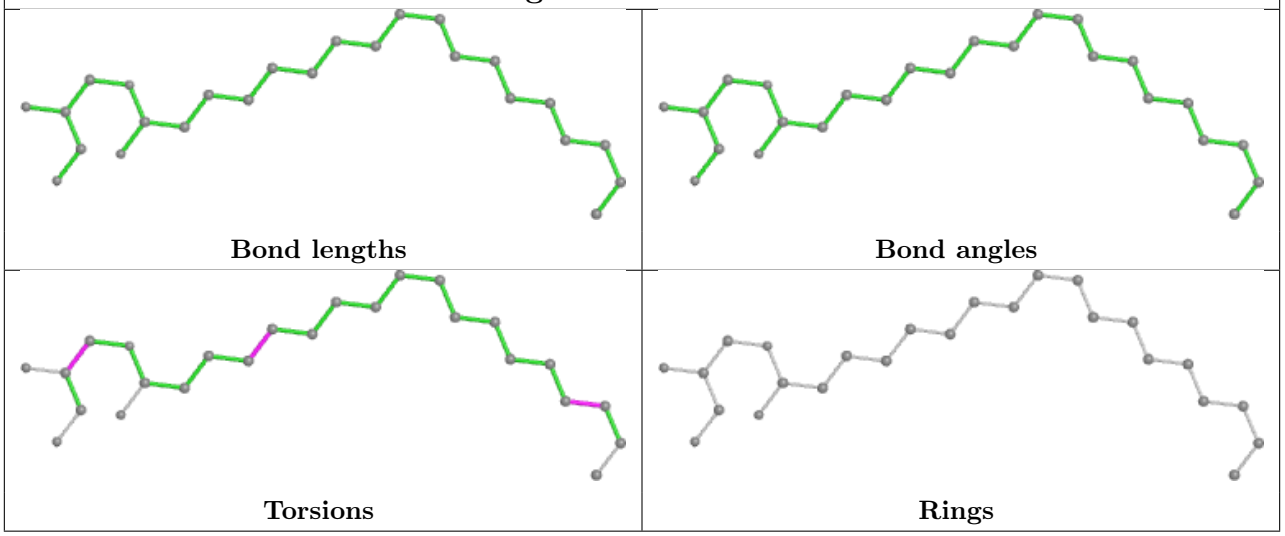
Ligand OLC A 511



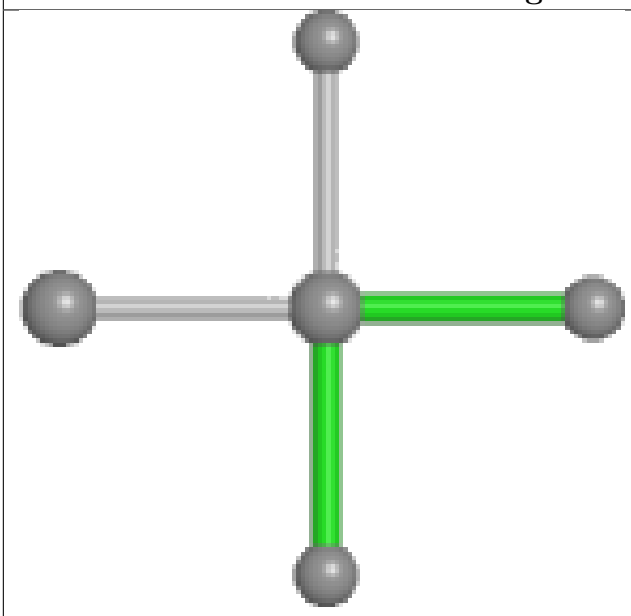
Ligand OLC A 507



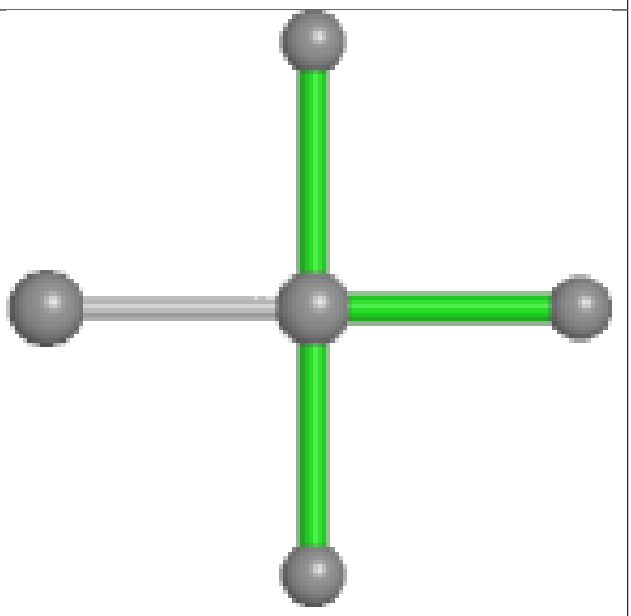
Ligand OLC B 512



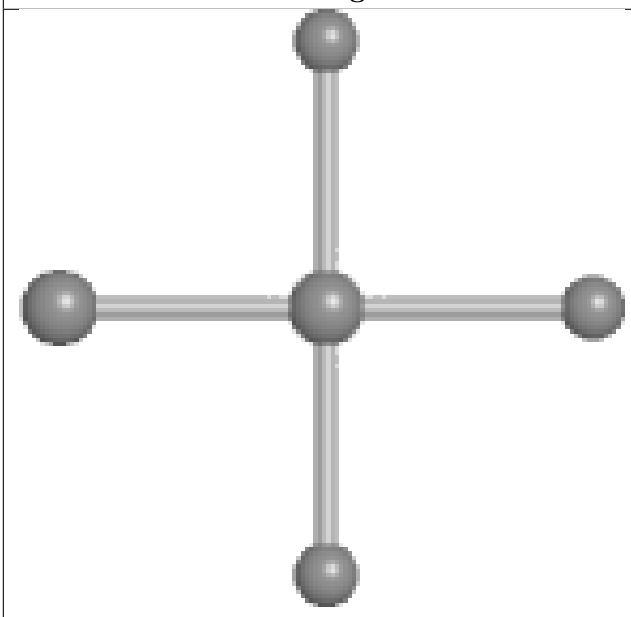
Ligand THJ A 501



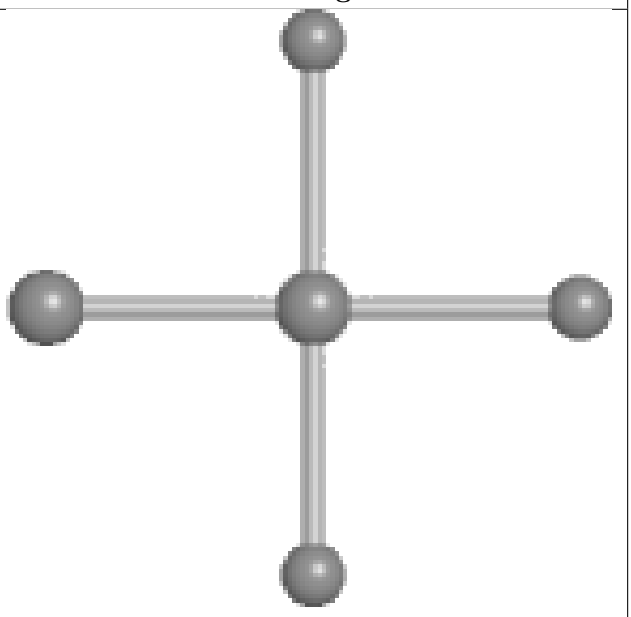
Bond lengths



Bond angles

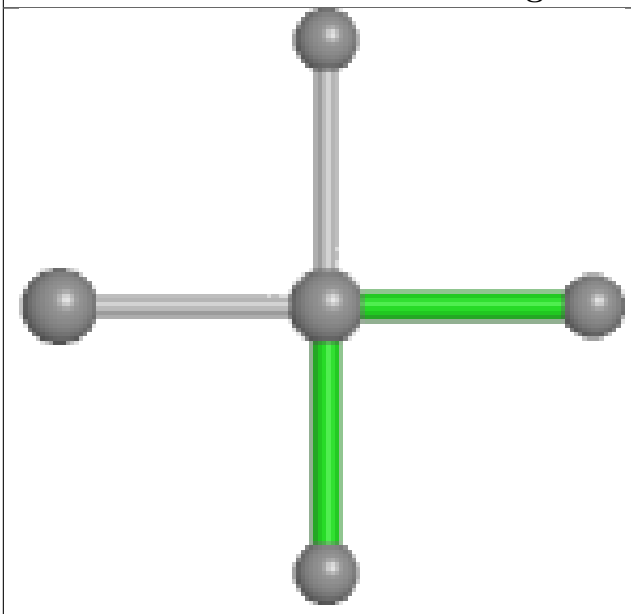


Torsions

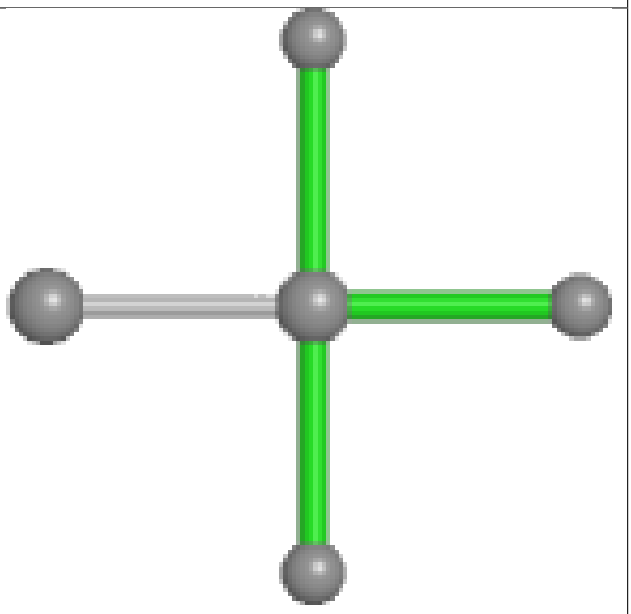


Rings

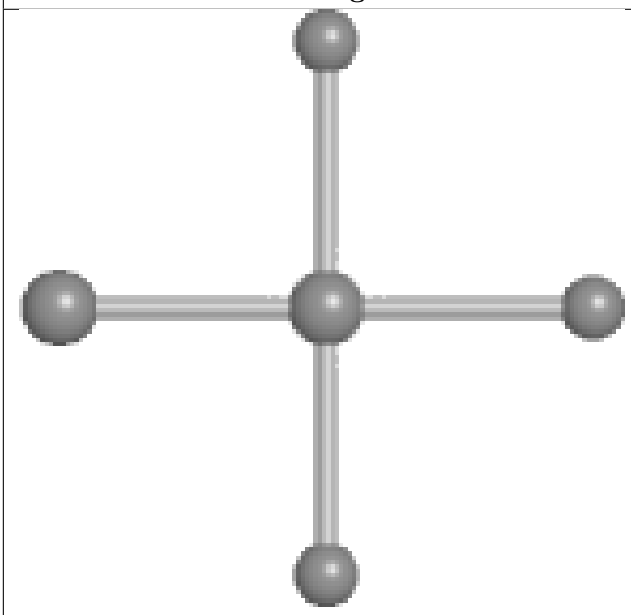
Ligand THJ B 501



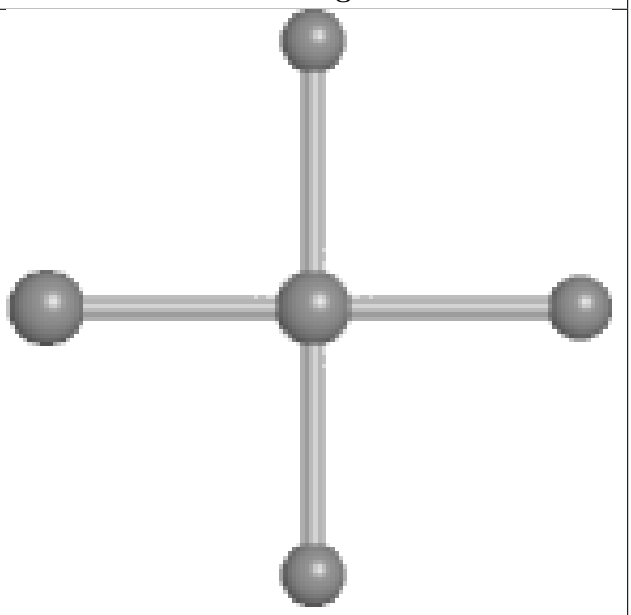
Bond lengths



Bond angles

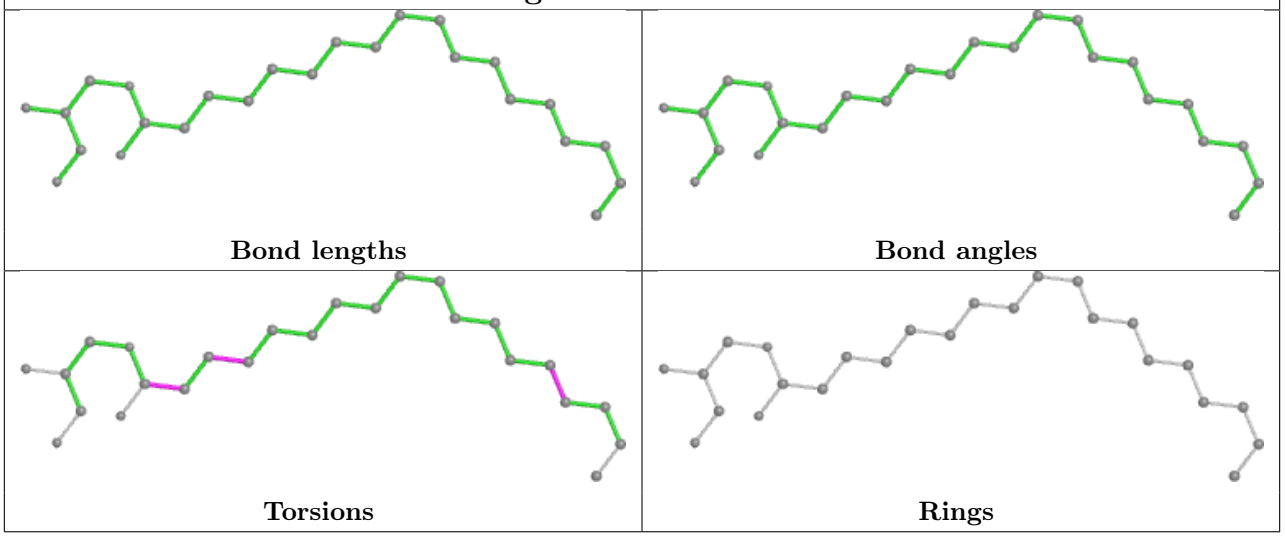


Torsions

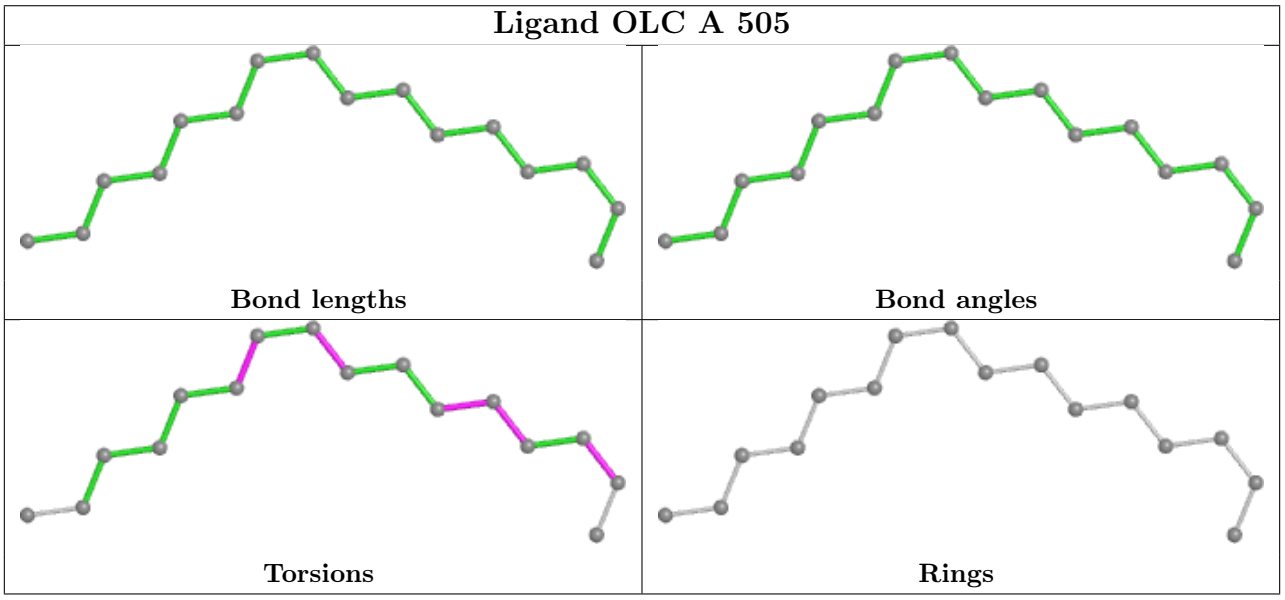


Rings

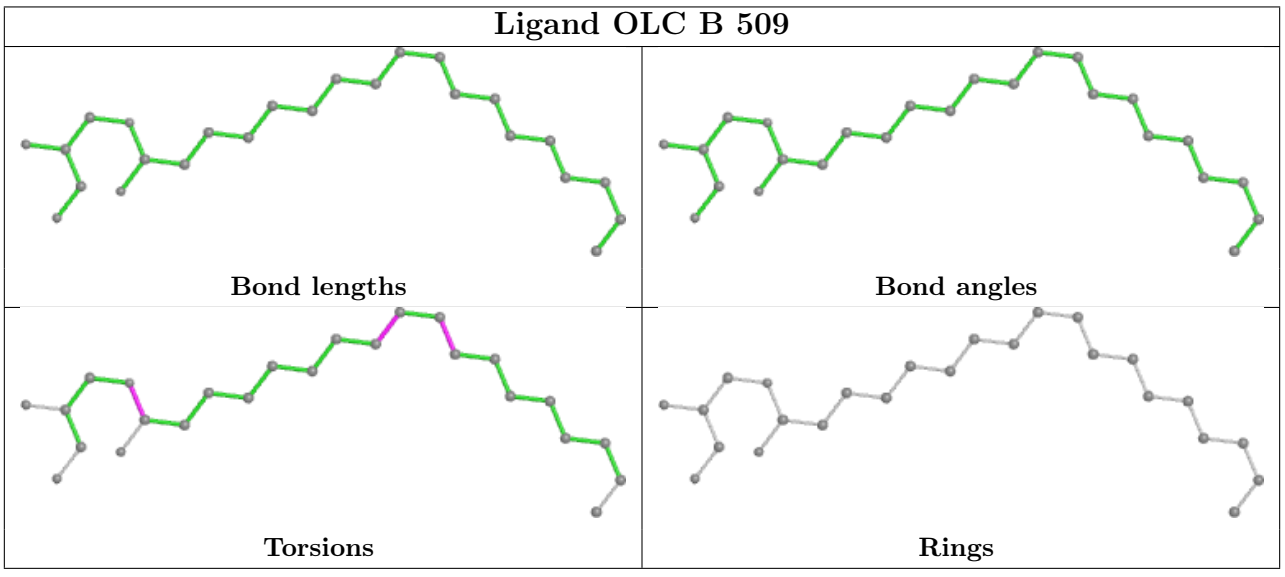
Ligand OLC A 503



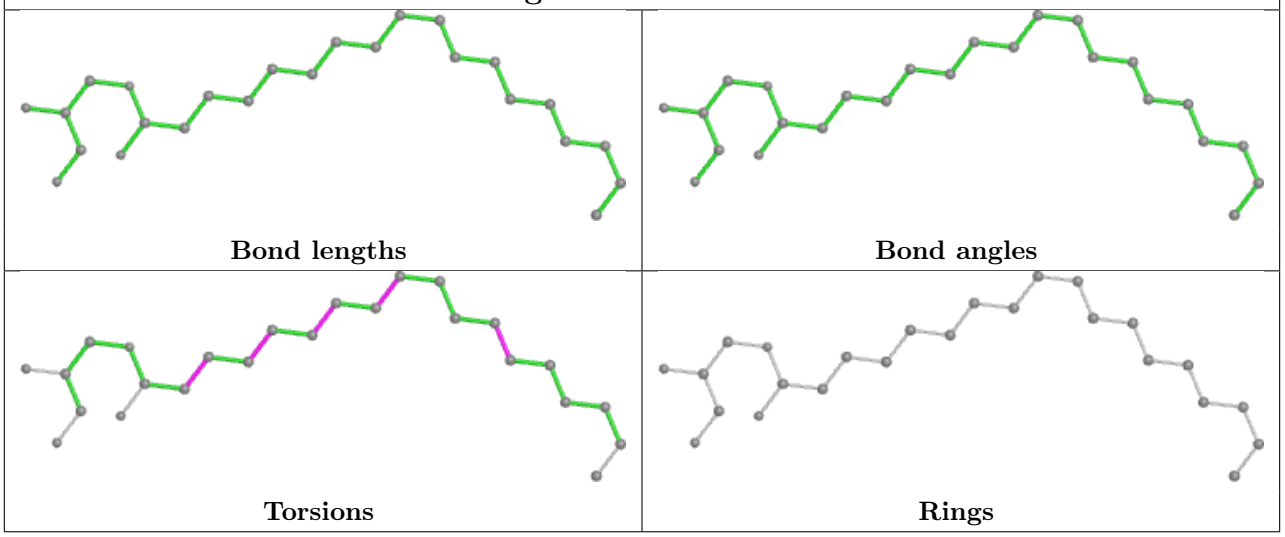
Ligand OLC A 505



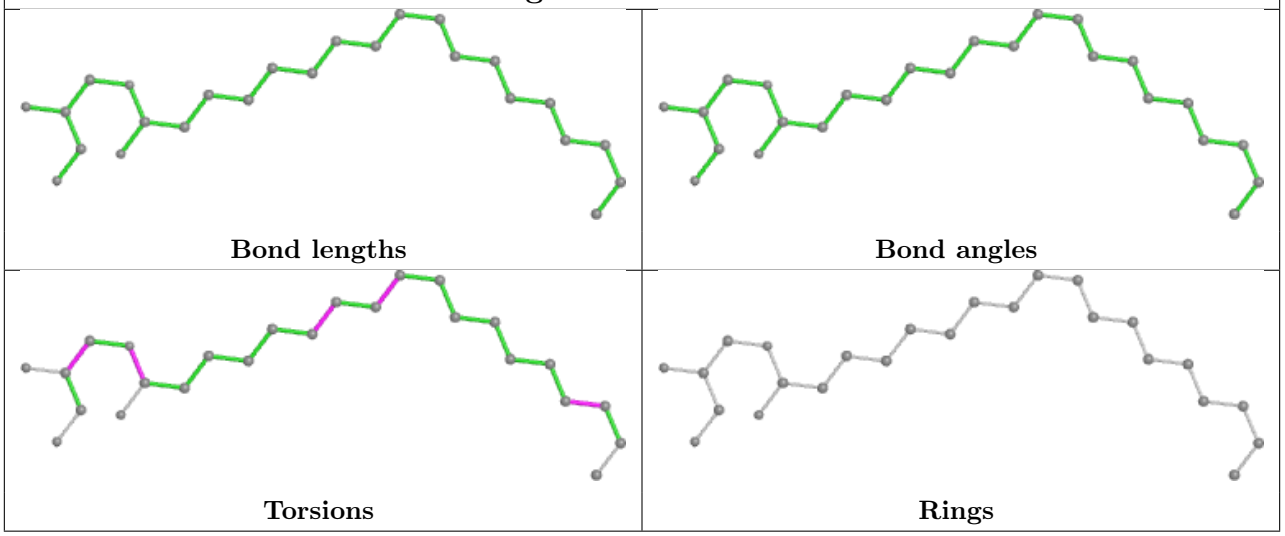
Ligand OLC B 509



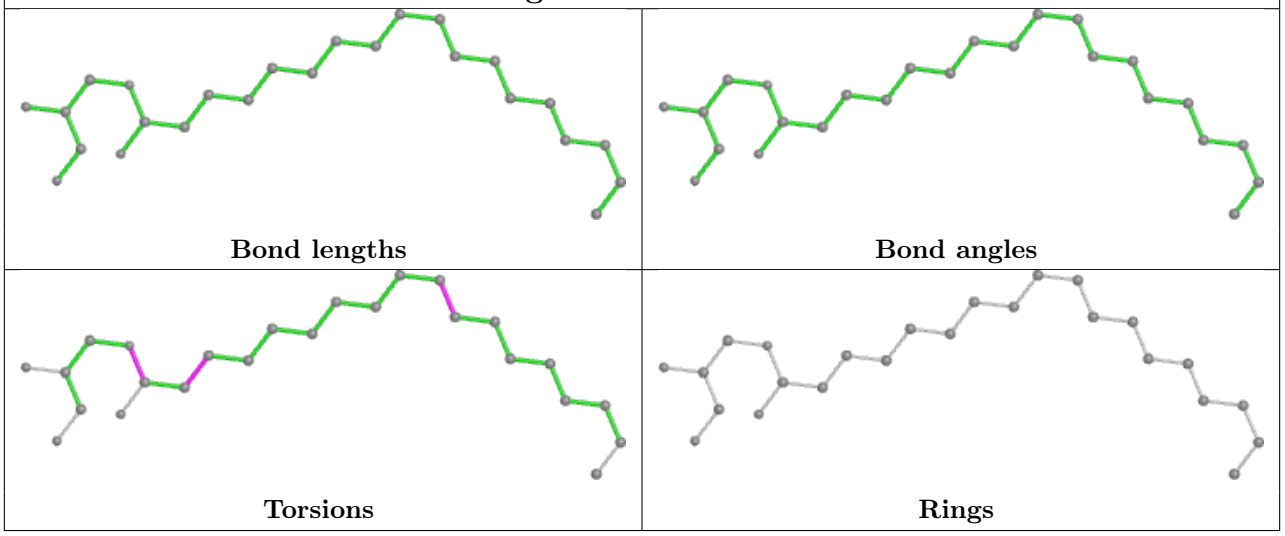
Ligand OLC A 508

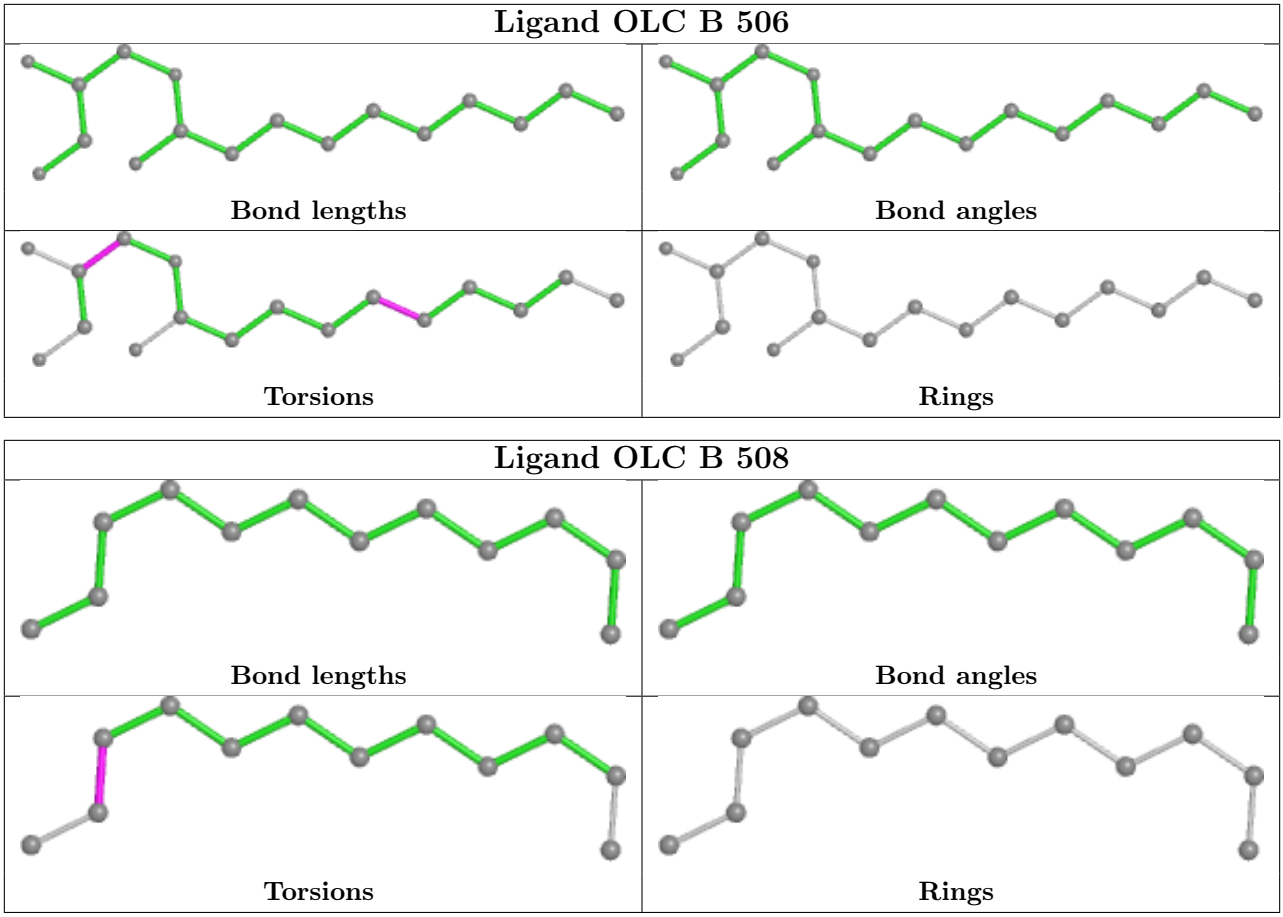


Ligand OLC B 507



Ligand OLC B 511





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	408/460 (88%)	0.56	47 (11%)	4	4	21, 47, 155, 176	0
1	B	408/460 (88%)	0.65	58 (14%)	2	2	24, 48, 165, 186	0
All	All	816/920 (88%)	0.60	105 (12%)	3	3	21, 48, 161, 186	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	377	SER	6.4
1	B	377	SER	6.3
1	B	391	ASP	6.1
1	B	426	LYS	5.5
1	B	441	GLU	5.3
1	A	432	LEU	5.1
1	B	440	GLY	5.0
1	B	375	GLN	5.0
1	A	391	ASP	4.8
1	B	386	VAL	4.8
1	B	432	LEU	4.7
1	B	390	PRO	4.5
1	B	412	ASP	4.5
1	B	425	LYS	4.5
1	A	431	VAL	4.5
1	B	61	LEU	4.4
1	B	403	ASP	4.3
1	B	444	ILE	4.2
1	B	380	ILE	4.2
1	B	446	ILE	4.2
1	A	407	ILE	4.1
1	B	442	TRP	4.0
1	B	443	ASN	3.9
1	A	373	ASN	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	402	ASN	3.9
1	B	423	THR	3.8
1	A	372	ALA	3.8
1	A	374	TYR	3.5
1	B	393	GLU	3.5
1	B	448	VAL	3.5
1	B	421	PRO	3.5
1	A	434	ILE	3.5
1	A	410	ARG	3.5
1	A	439	PRO	3.5
1	A	446	ILE	3.5
1	B	416	SER	3.4
1	A	444	ILE	3.2
1	A	406	ILE	3.2
1	B	431	VAL	3.2
1	A	380	ILE	3.2
1	B	438	ALA	3.2
1	B	405	GLU	3.1
1	B	417	LYS	3.1
1	B	427	LEU	3.1
1	B	376	VAL	3.1
1	A	61	LEU	3.1
1	A	399	GLN	3.1
1	A	413	TYR	3.0
1	A	437	ALA	3.0
1	A	433	GLU	3.0
1	B	389	ILE	3.0
1	B	445	TYR	2.9
1	B	439	PRO	2.9
1	B	428	GLY	2.9
1	B	436	GLU	2.9
1	A	420	ILE	2.8
1	A	378	LYS	2.8
1	B	410	ARG	2.8
1	A	409	VAL	2.8
1	A	411	ILE	2.8
1	A	375	GLN	2.7
1	B	413	TYR	2.7
1	B	424	VAL	2.7
1	B	404	GLY	2.7
1	A	403	ASP	2.7
1	B	399	GLN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	445	TYR	2.6
1	A	376	VAL	2.6
1	A	393	GLU	2.6
1	A	424	VAL	2.6
1	B	381	ASP	2.6
1	B	373	ASN	2.6
1	B	435	GLU	2.5
1	A	435	GLU	2.5
1	B	392	VAL	2.5
1	A	400	SER	2.5
1	A	430	GLU	2.5
1	A	416	SER	2.5
1	B	378	LYS	2.4
1	A	412	ASP	2.4
1	B	409	VAL	2.4
1	B	447	LYS	2.4
1	A	387	CYS	2.4
1	A	390	PRO	2.4
1	B	394	ALA	2.4
1	A	408	LEU	2.4
1	A	448	VAL	2.4
1	A	443	ASN	2.4
1	A	423	THR	2.3
1	B	388	PRO	2.3
1	B	420	ILE	2.3
1	A	425	LYS	2.3
1	B	422	GLU	2.3
1	B	437	ALA	2.3
1	B	434	ILE	2.3
1	A	379	GLU	2.3
1	A	421	PRO	2.3
1	A	325	TRP	2.2
1	B	387	CYS	2.2
1	B	385	GLU	2.1
1	B	433	GLU	2.1
1	A	442	TRP	2.1
1	B	418	GLU	2.0
1	B	402	ASN	2.0
1	B	406	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.

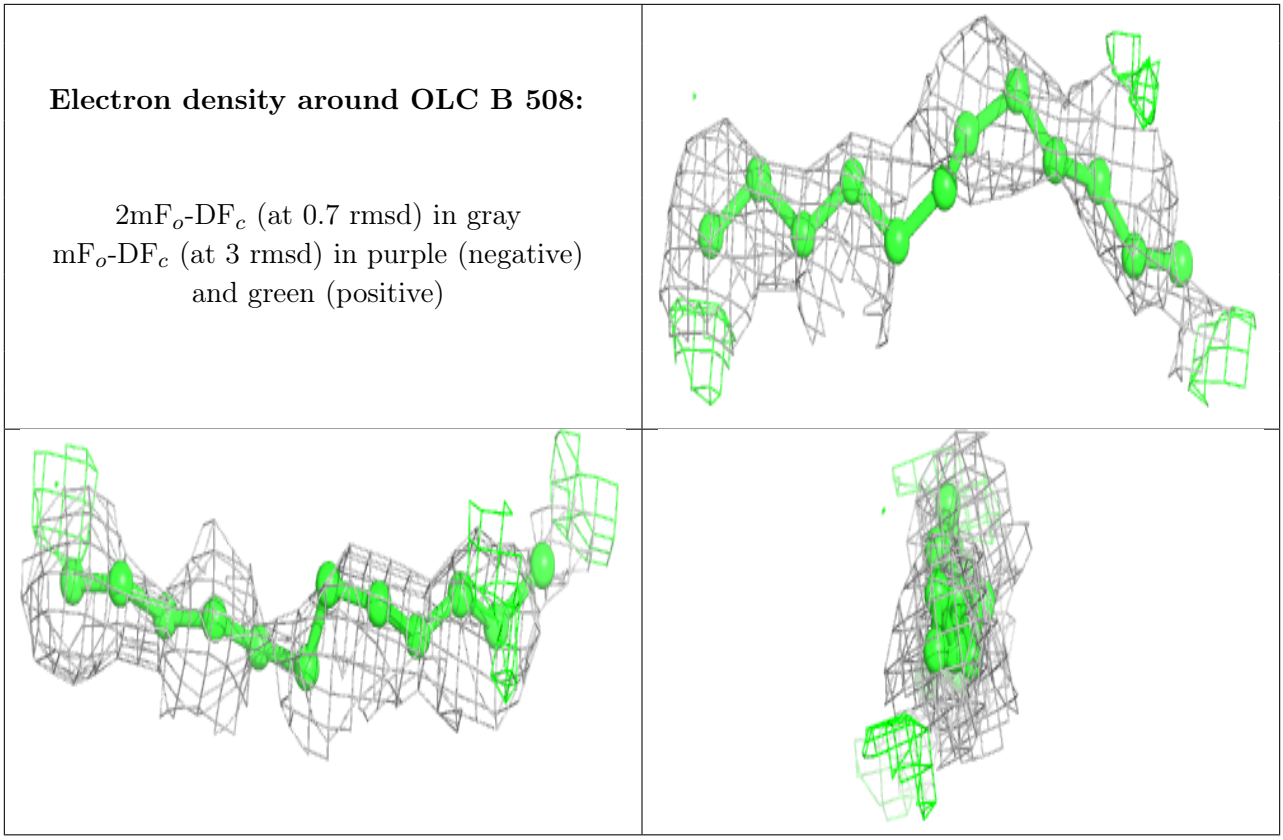
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	OLC	B	508	12/25	0.52	0.55	29,40,55,63	0
2	THJ	A	501	5/5	0.53	0.49	42,43,96,115	0
3	OLC	A	504	14/25	0.64	0.42	33,47,61,63	0
3	OLC	A	507	25/25	0.68	0.61	24,54,93,101	0
2	THJ	B	501	5/5	0.69	0.45	47,57,76,114	0
3	OLC	B	509	25/25	0.69	0.37	32,54,90,98	0
3	OLC	A	508	25/25	0.69	0.54	20,59,114,116	0
3	OLC	B	506	17/25	0.71	0.44	20,31,47,51	0
3	OLC	A	505	16/25	0.71	0.44	8,22,44,57	0
3	OLC	B	511	25/25	0.72	0.37	24,41,88,111	0
3	OLC	B	507	25/25	0.73	0.59	37,51,70,75	0
3	OLC	A	506	25/25	0.74	0.49	10,39,82,90	0
3	OLC	B	512	25/25	0.76	0.53	9,35,69,75	0
3	OLC	A	511	12/25	0.77	0.44	18,43,69,75	0
3	OLC	A	510	11/25	0.78	0.33	6,37,56,65	0
3	OLC	B	503	25/25	0.79	0.45	17,33,46,48	0
3	OLC	B	505	17/25	0.80	0.36	13,34,69,76	0
3	OLC	B	504	20/25	0.81	0.53	31,50,62,71	0
3	OLC	A	509	25/25	0.81	0.47	13,26,80,109	0
3	OLC	A	503	25/25	0.85	0.41	13,24,57,69	0
3	OLC	B	502	25/25	0.86	0.42	13,25,46,49	0
3	OLC	A	502	25/25	0.90	0.42	12,30,49,58	0
3	OLC	B	510	8/25	0.90	0.36	3,14,15,17	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.

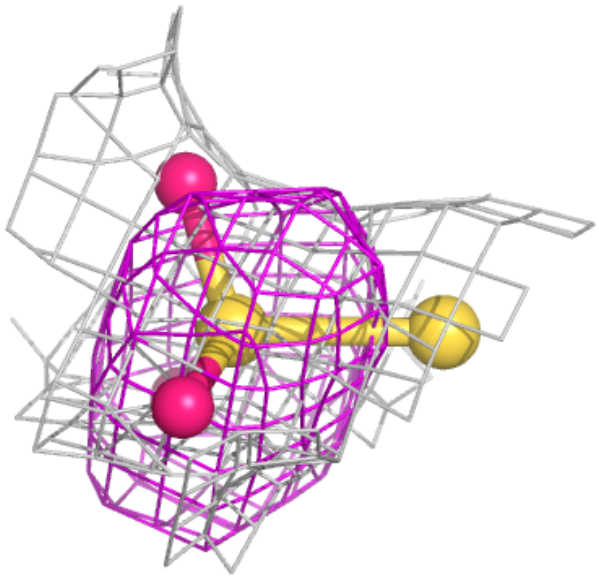
Electron density around OLC B 508:

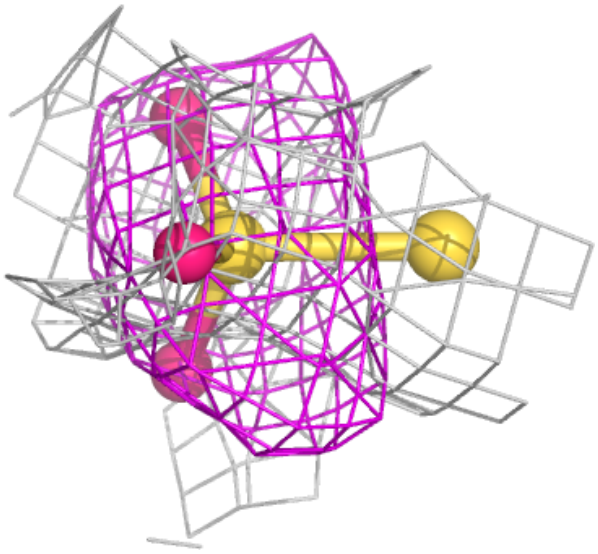
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

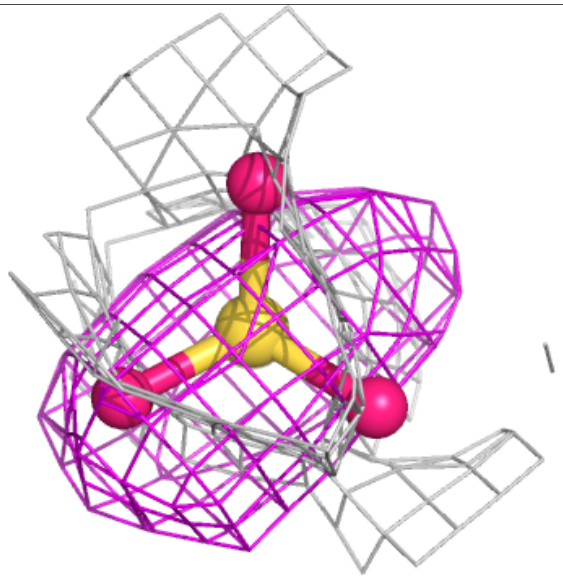


Electron density around THJ A 501:

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

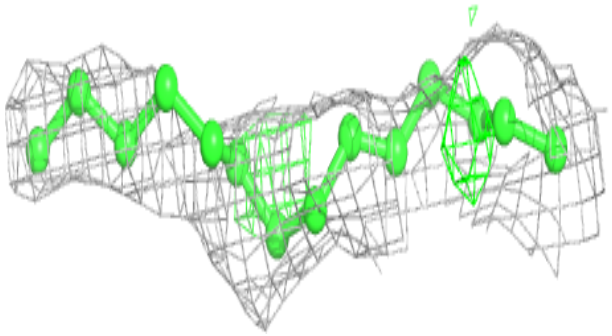


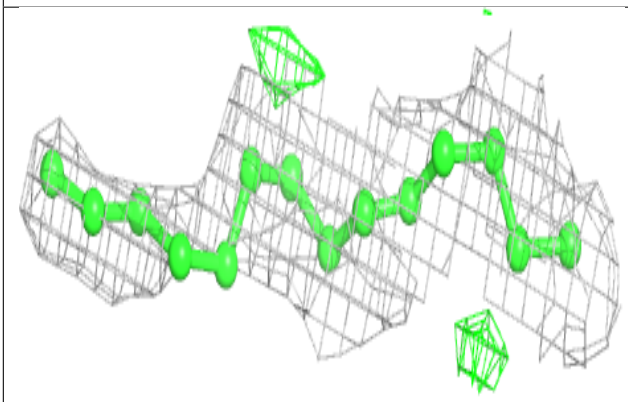


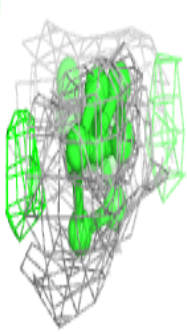


Electron density around OLC A 504:

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

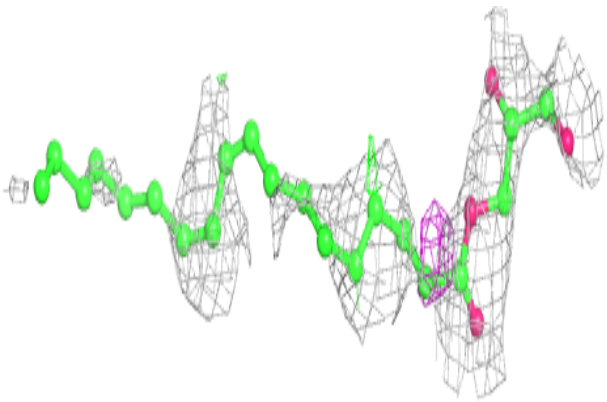


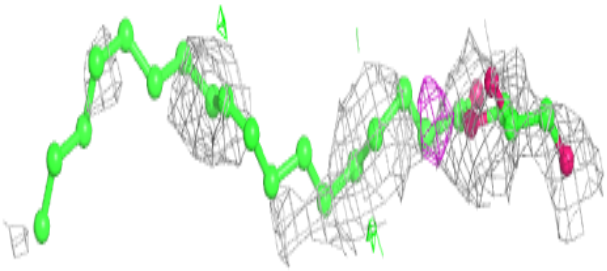




Electron density around OLC A 507:

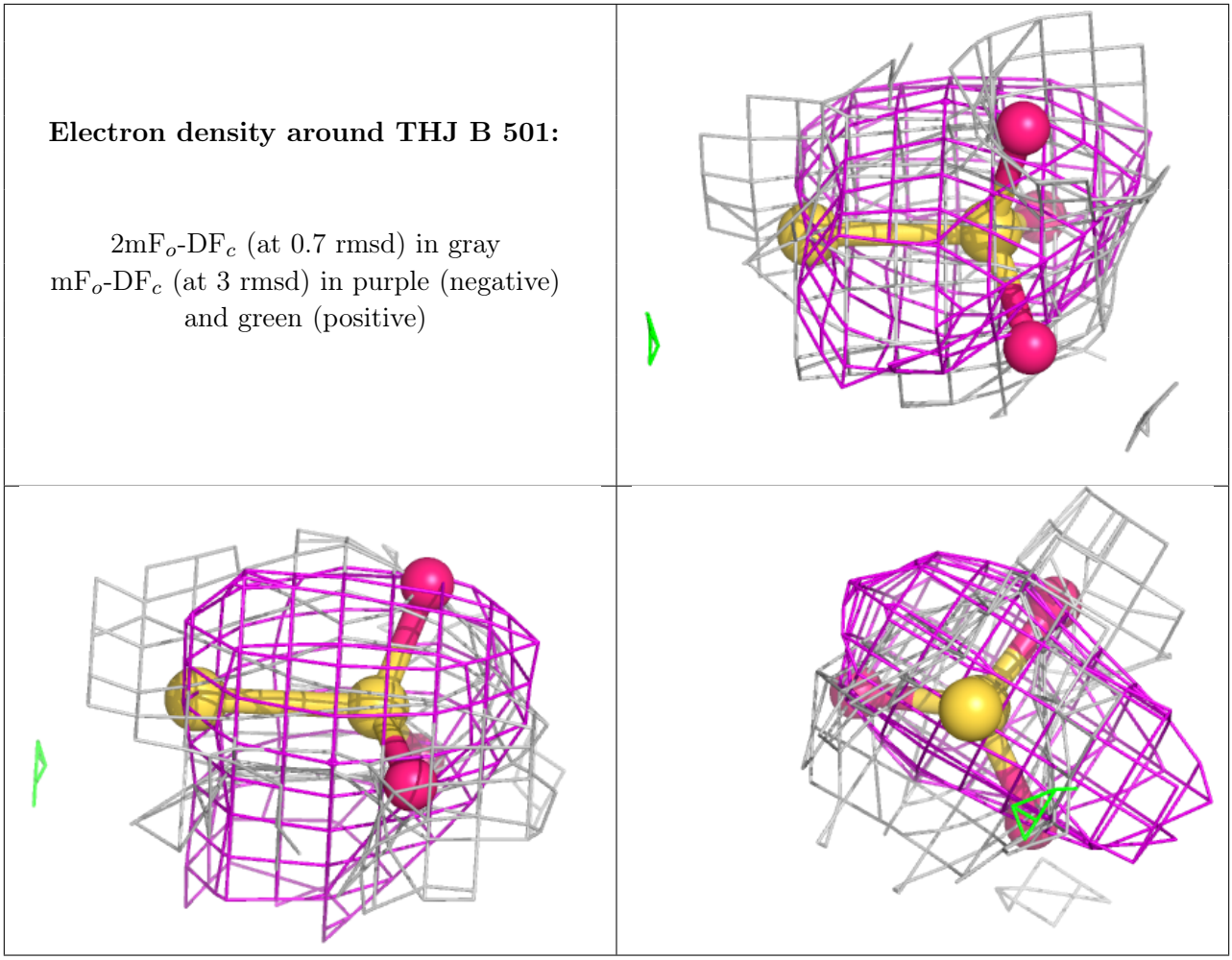
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





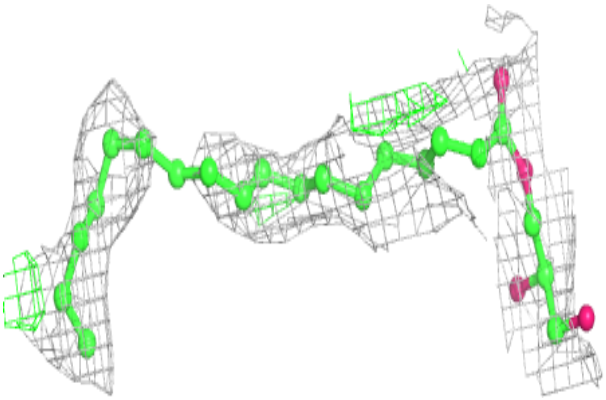
Electron density around THJ B 501:

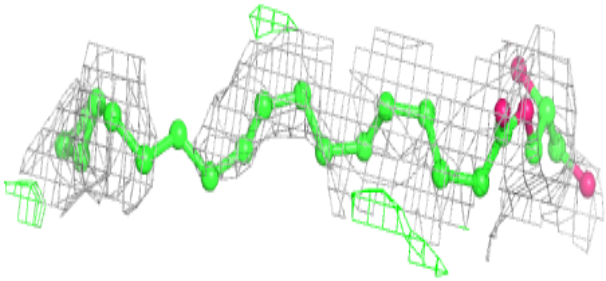
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

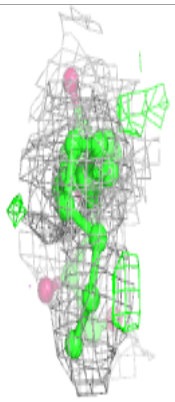


Electron density around OLC B 509:

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

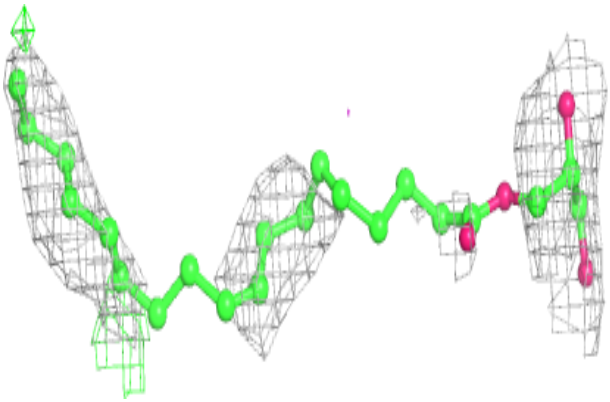


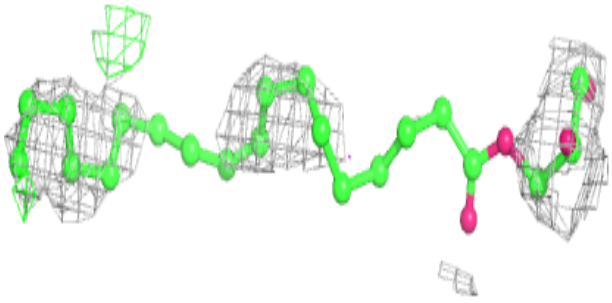


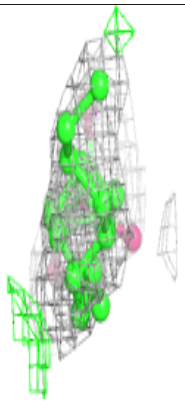


Electron density around OLC A 508:

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

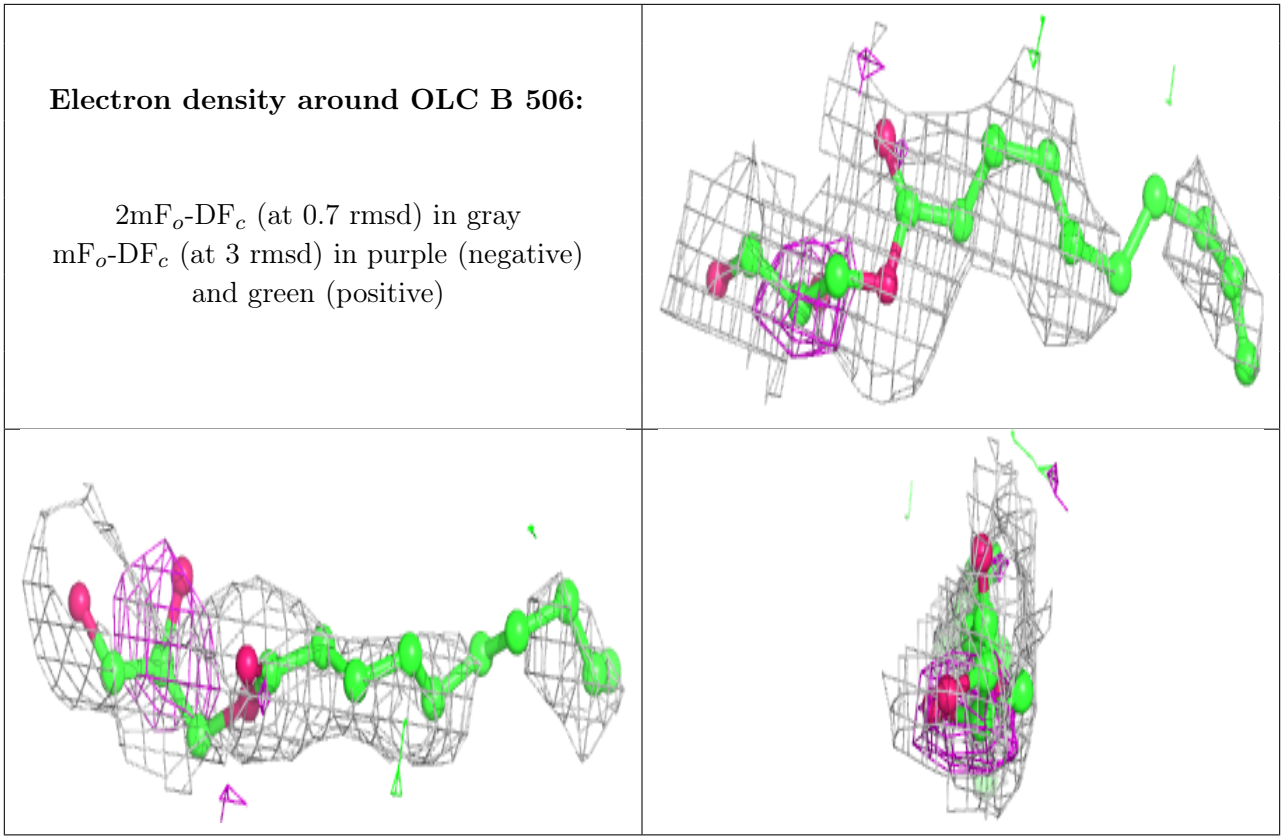






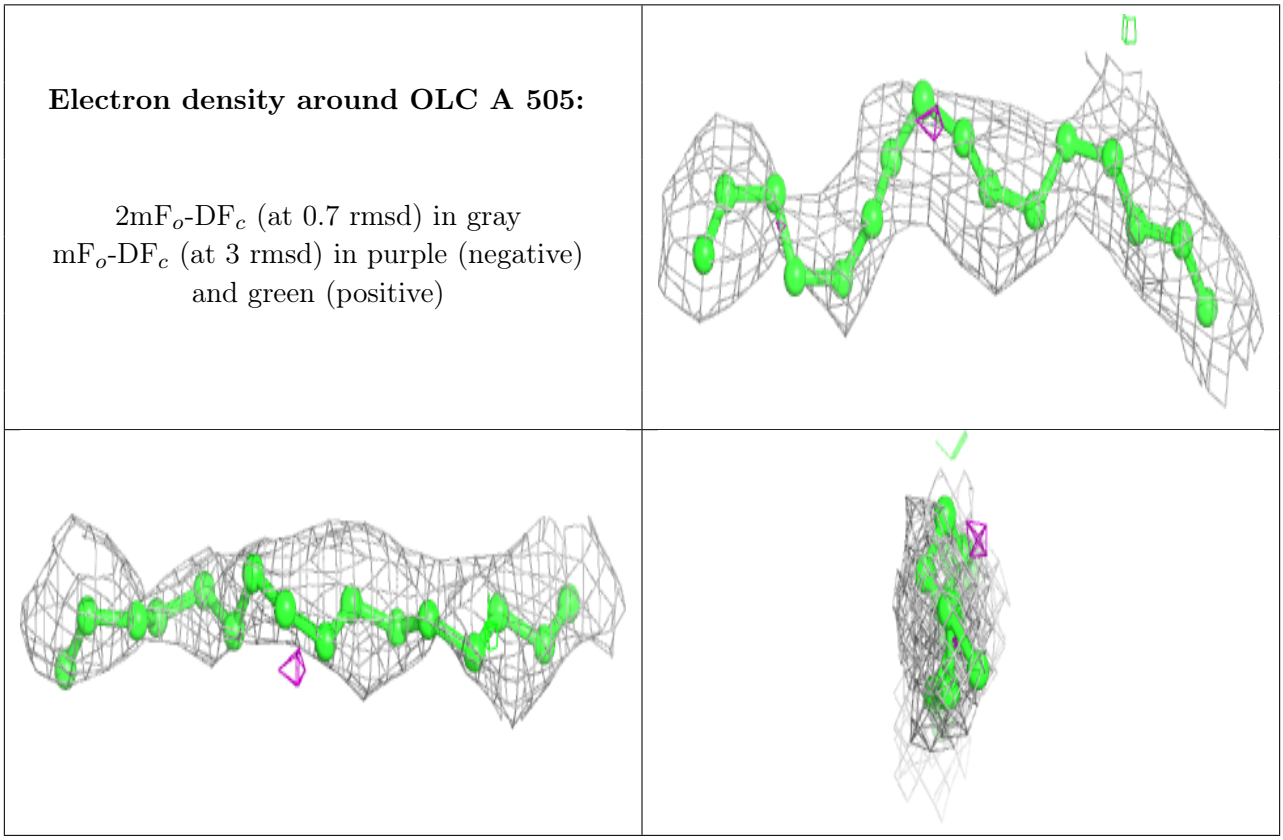
Electron density around OLC B 506:

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



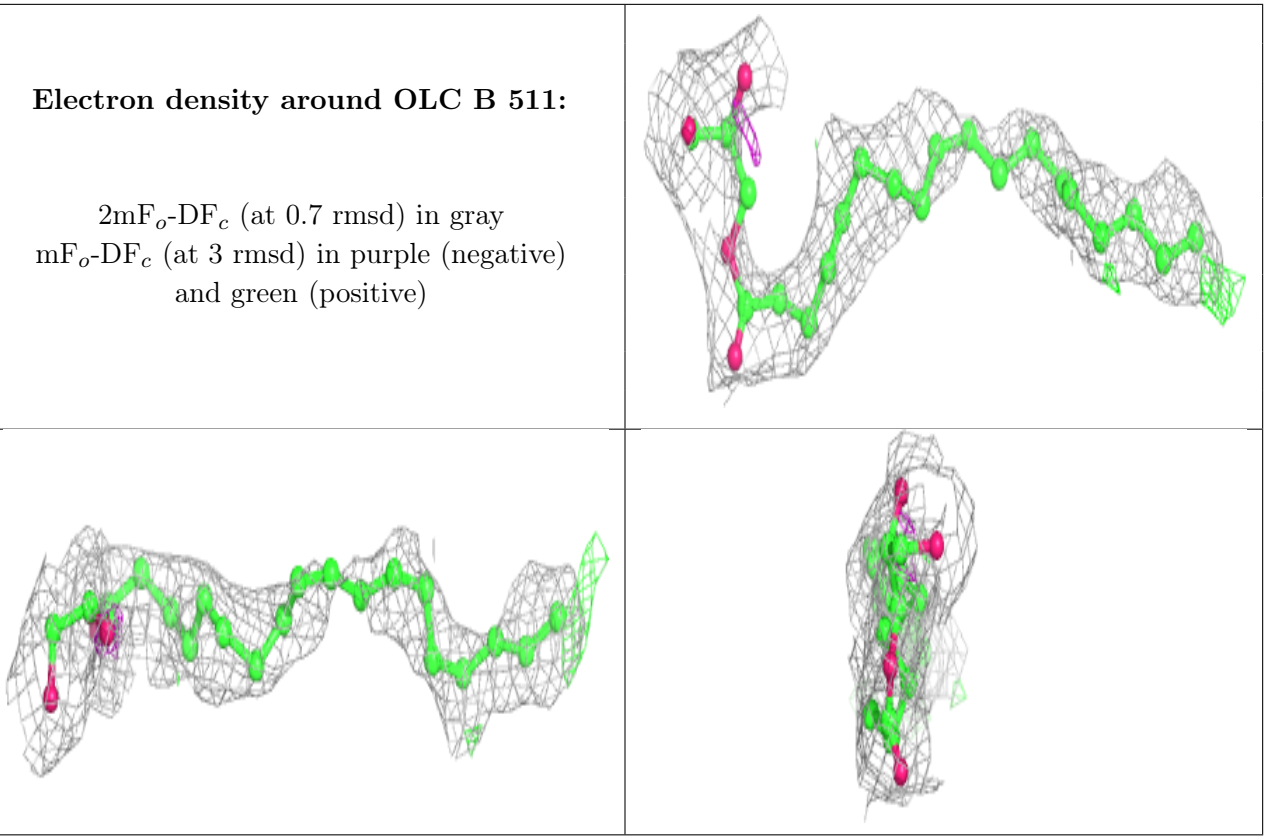
Electron density around OLC A 505:

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



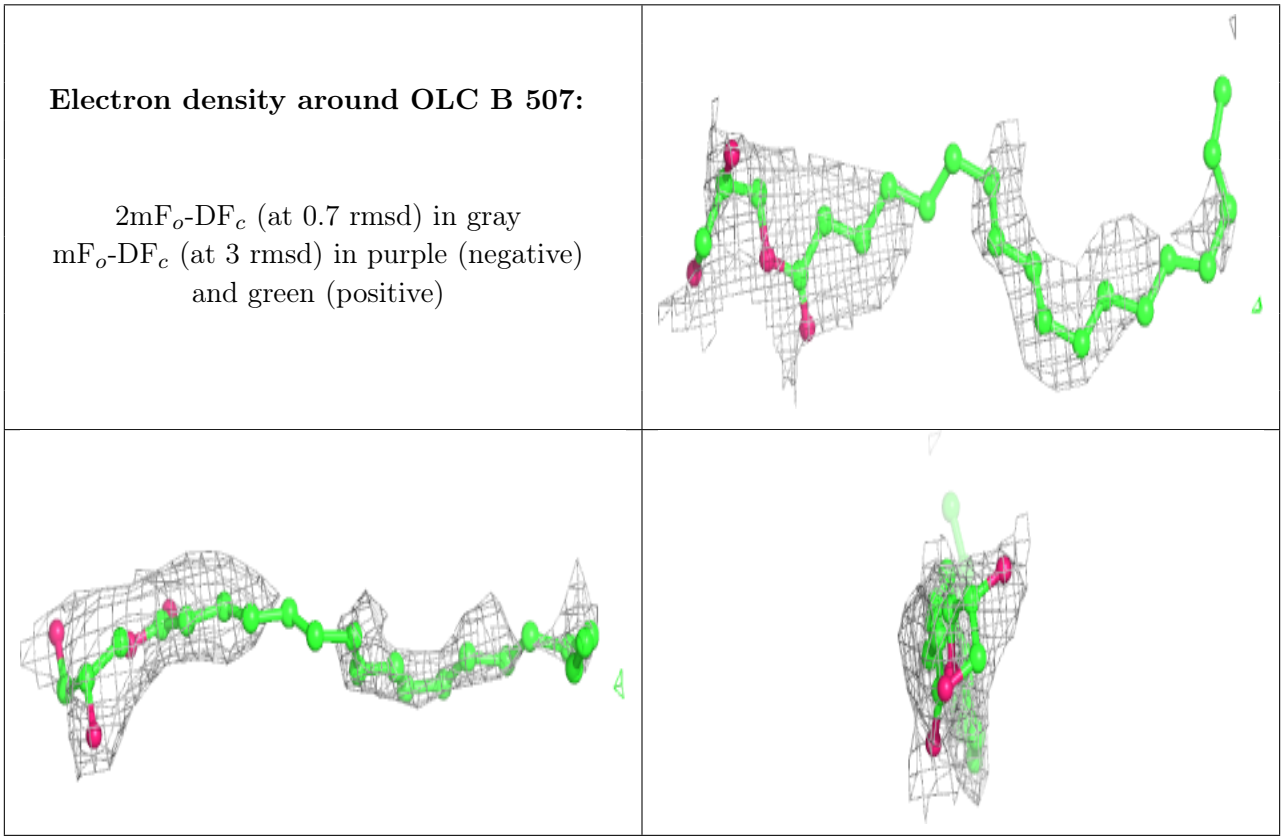
Electron density around OLC B 511:

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



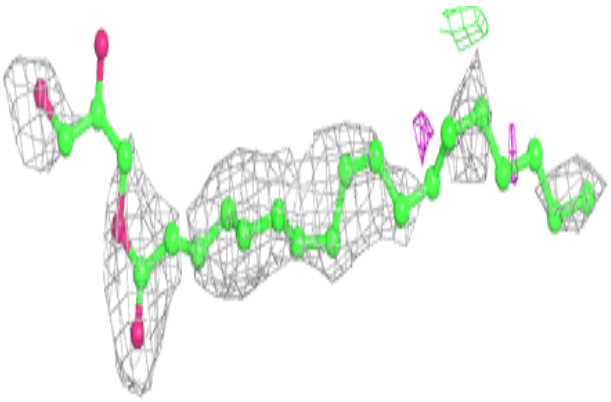
Electron density around OLC B 507:

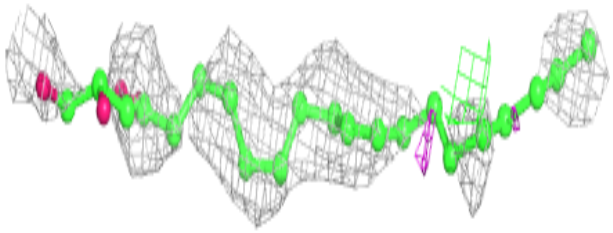
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

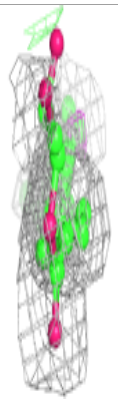


Electron density around OLC A 506:

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

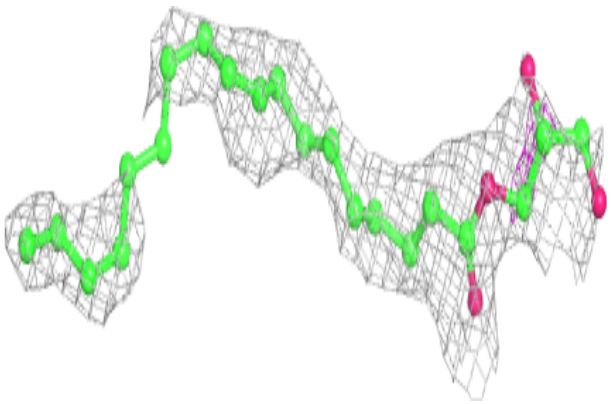


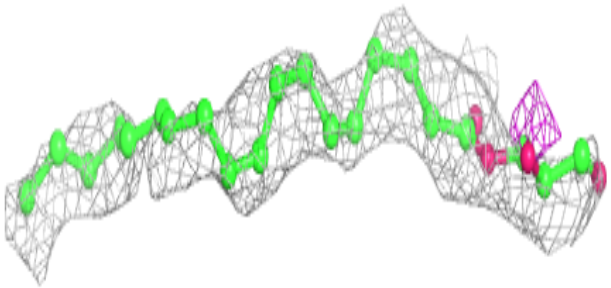


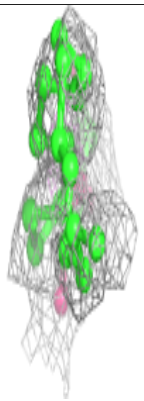


Electron density around OLC B 512:

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

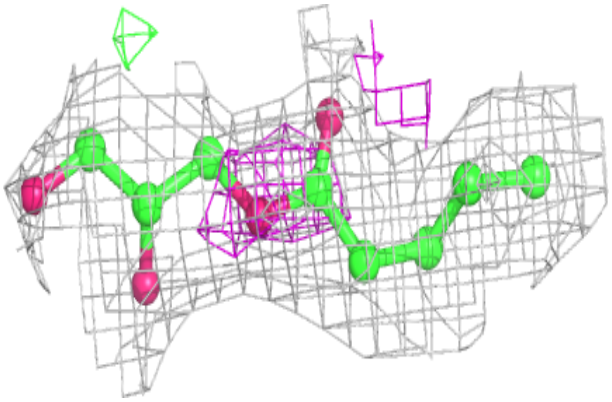


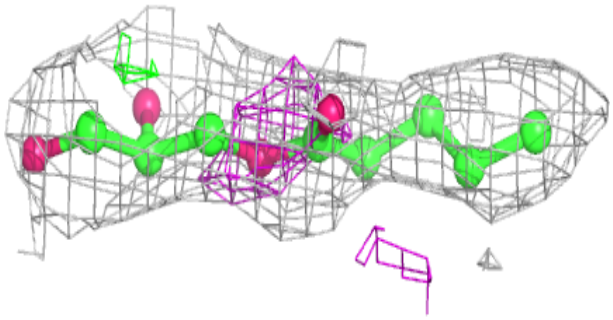


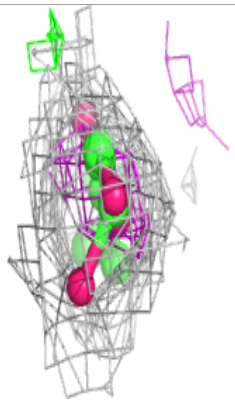


Electron density around OLC A 511:

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

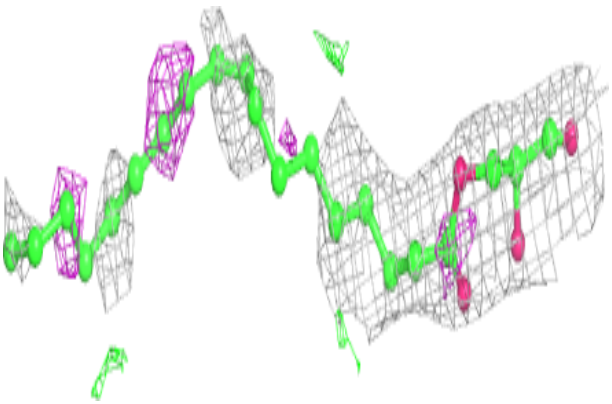


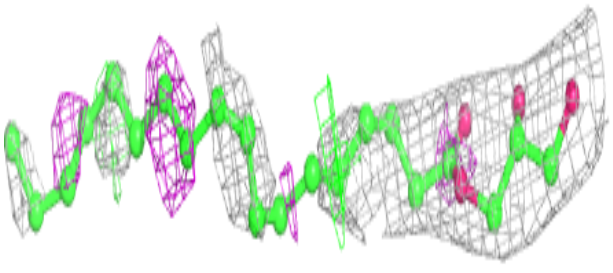


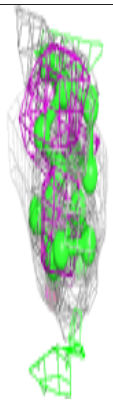


Electron density around OLC B 503:

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

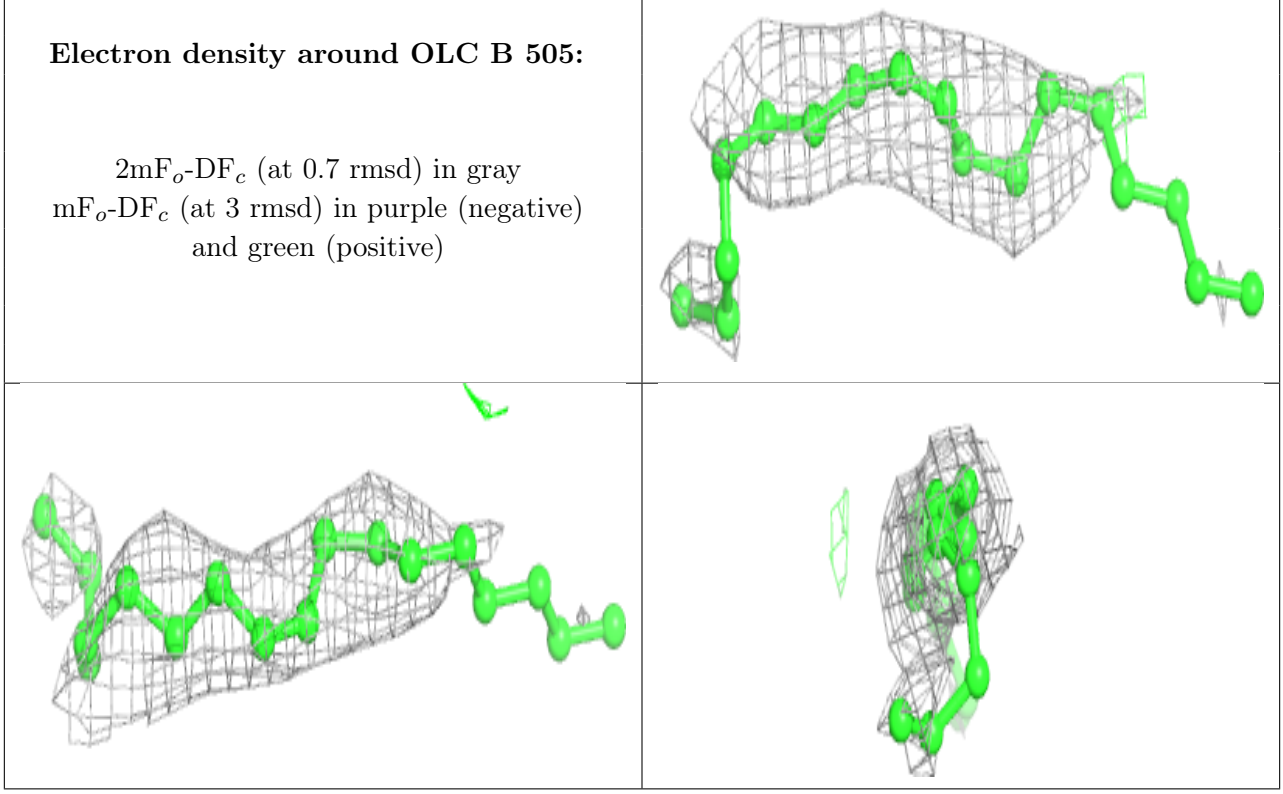






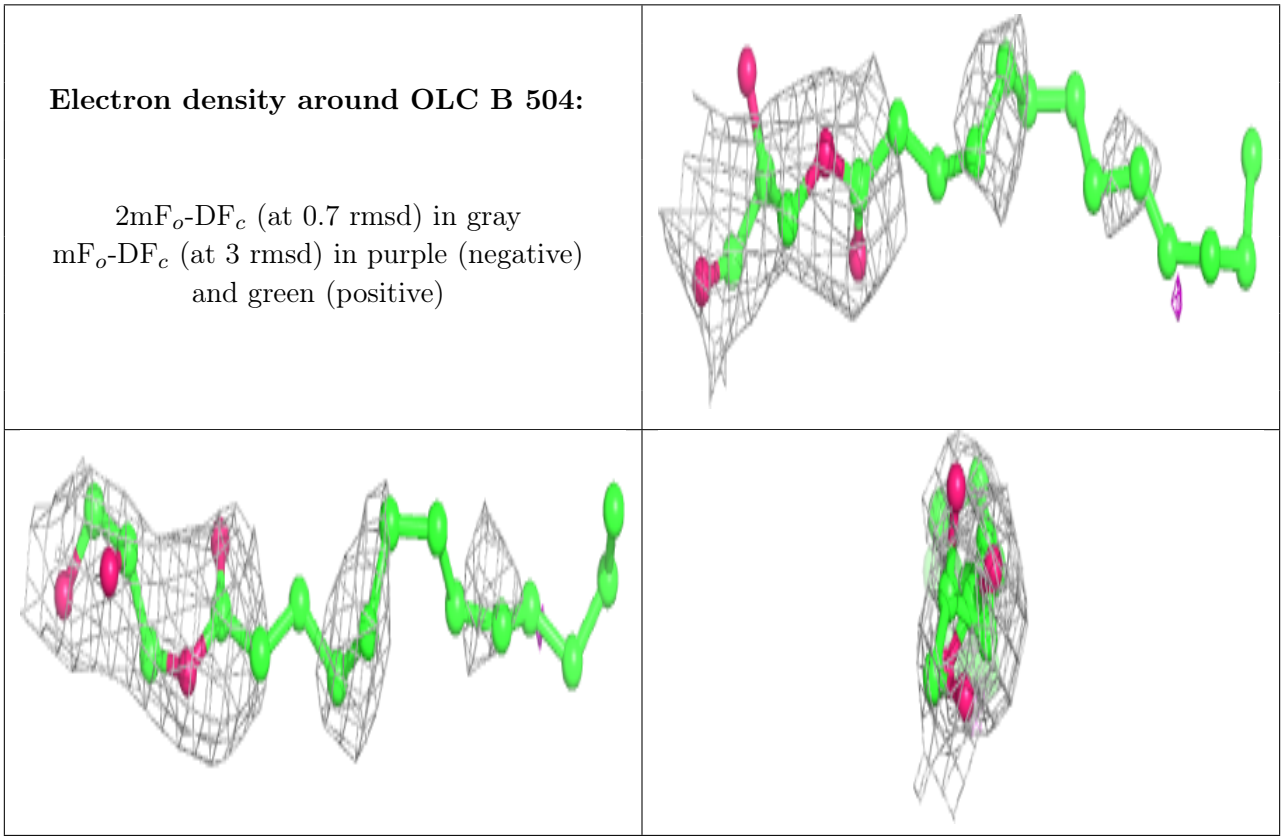
Electron density around OLC B 505:

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



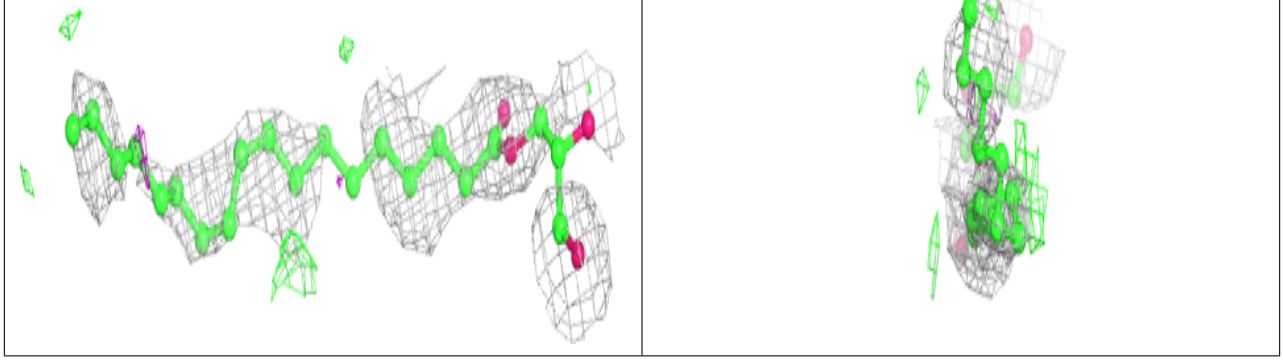
Electron density around OLC B 504:

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



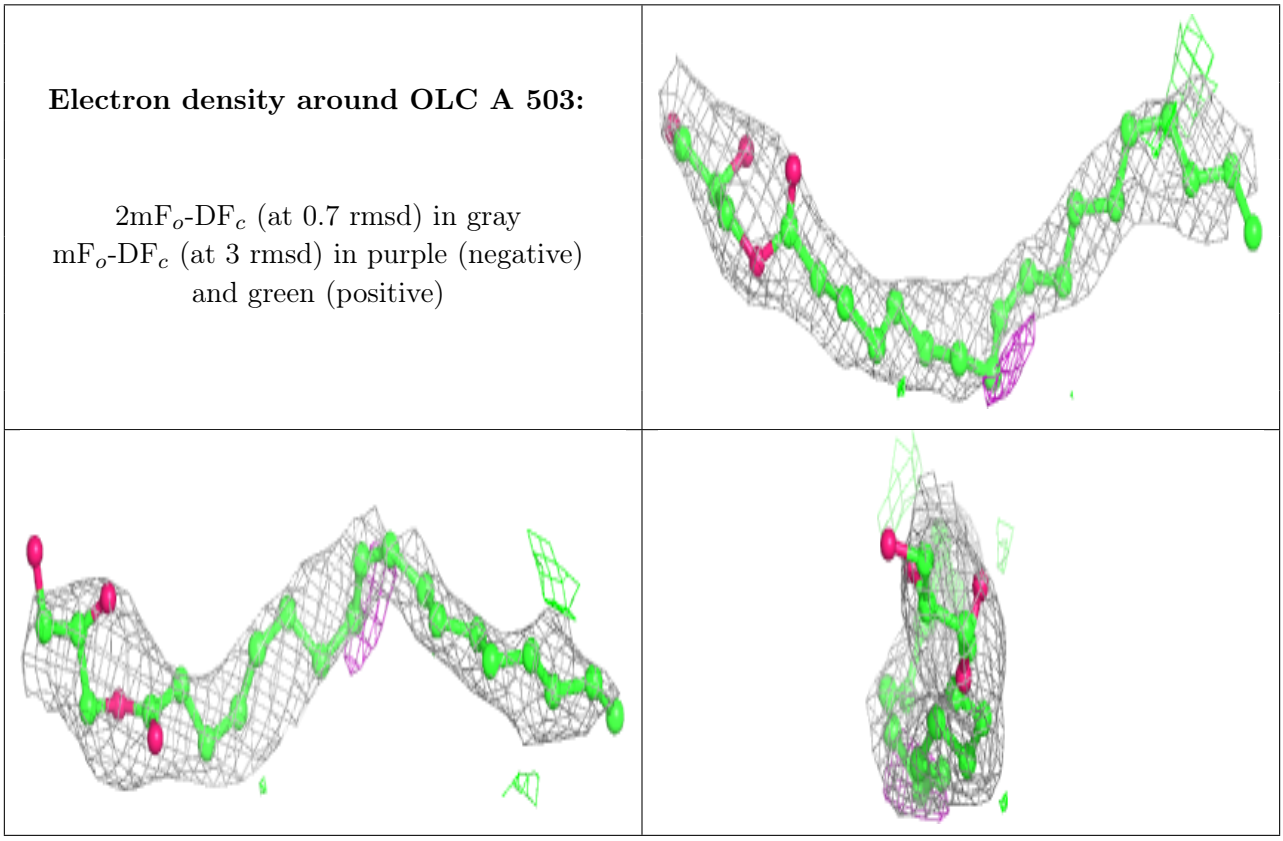
Electron density around OLC A 509:

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



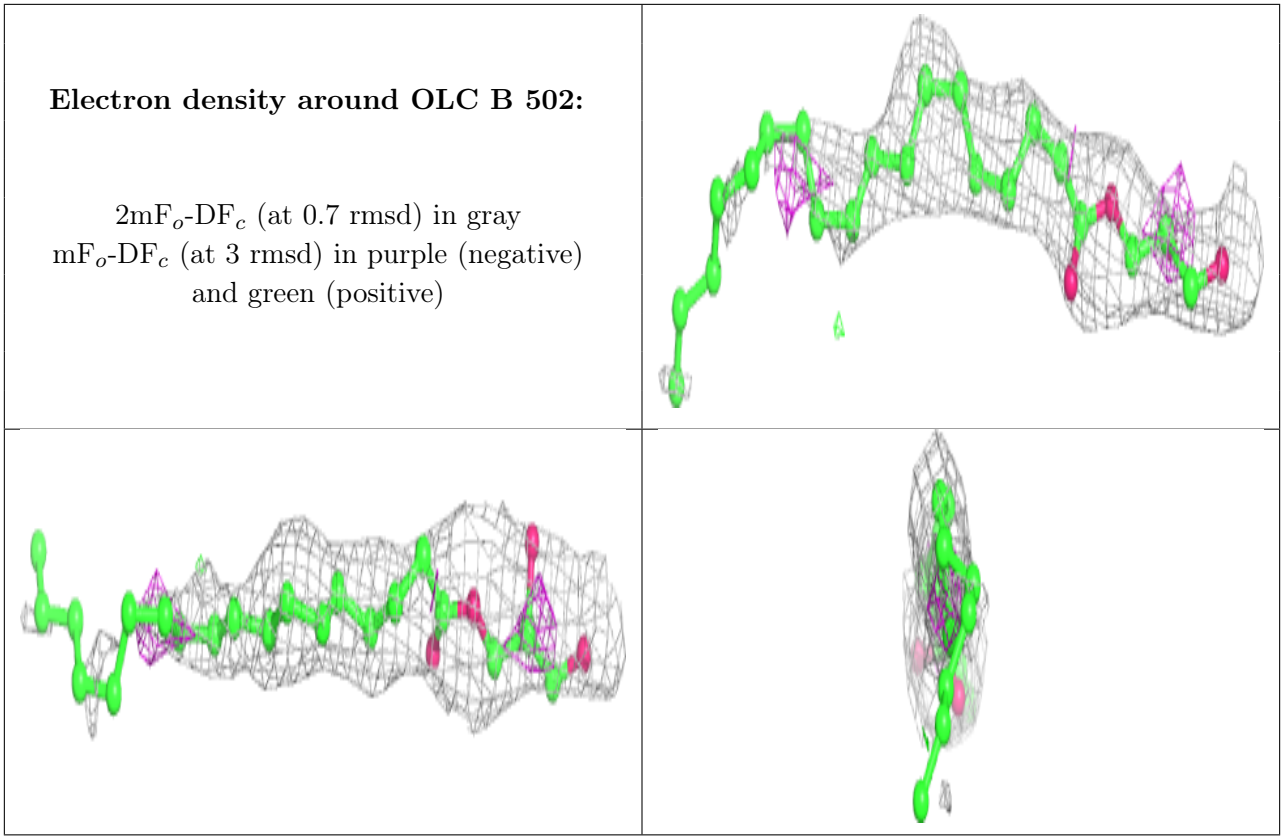
Electron density around OLC A 503:

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



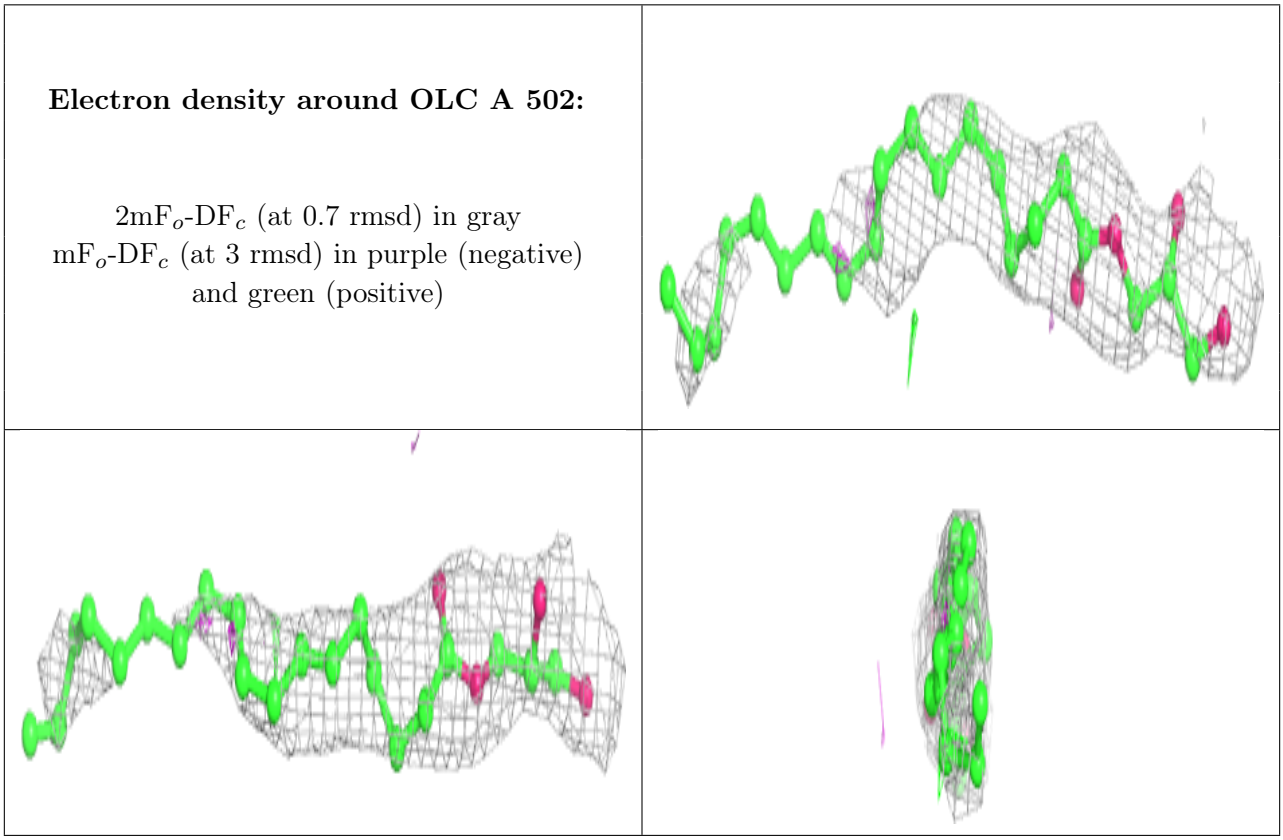
Electron density around OLC B 502:

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



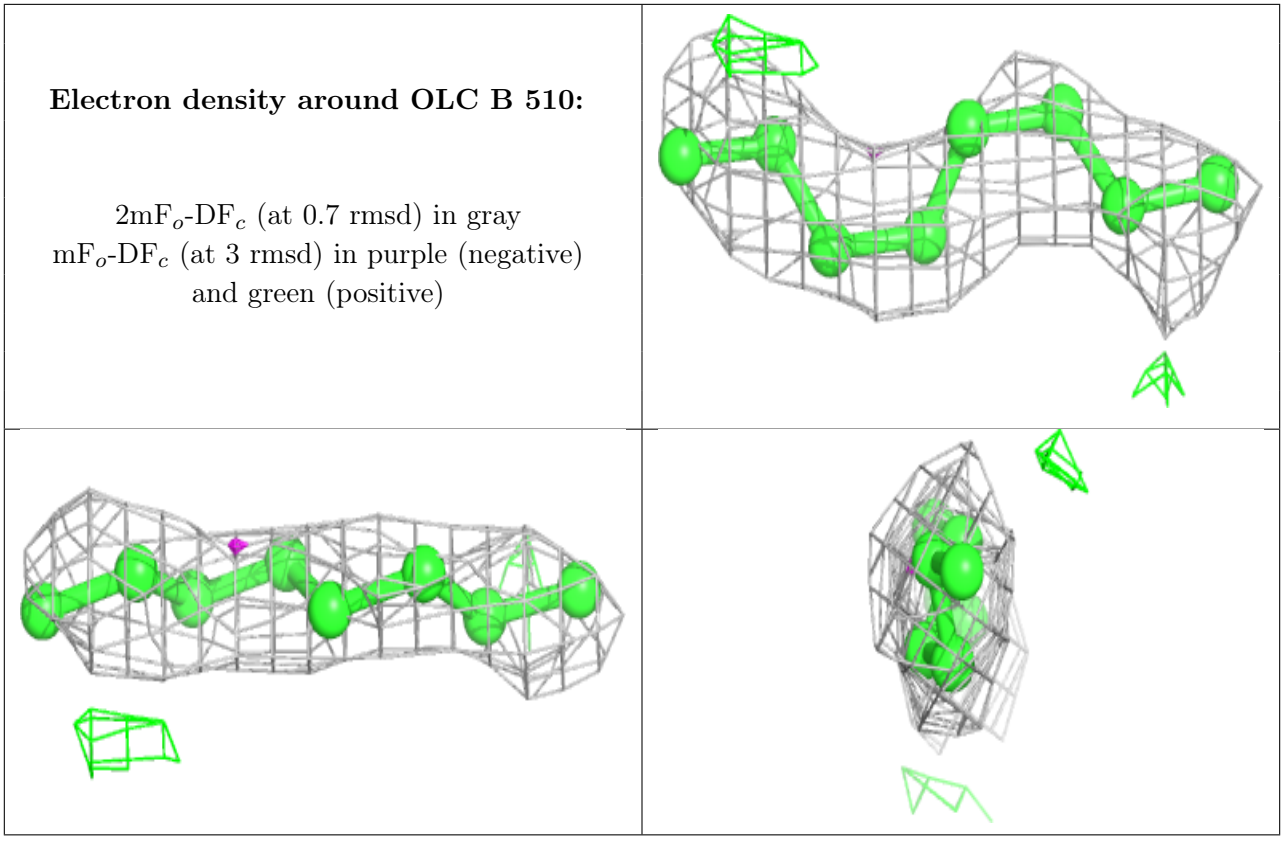
Electron density around OLC A 502:

$2mF_o$-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 510:

$2mF_o$-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.