Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 12:52 AM JST

PDB ID	:	6KUW
Title	:	Crystal structure of human alpha2C adrenergic G protein-coupled receptor.
Authors	:	Chen, X.Y.; Wu, L.J.; Wu, D.; Zhong, G.S.
Deposited on	:	2019-09-02
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:

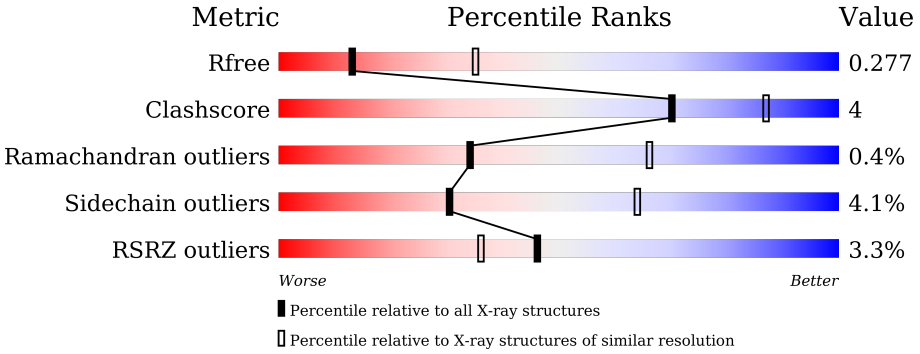
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 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	496	2%, 86%, 9%, •
1	B	496	4%, 82%, 13%, • 5%

2 Entry composition (i)

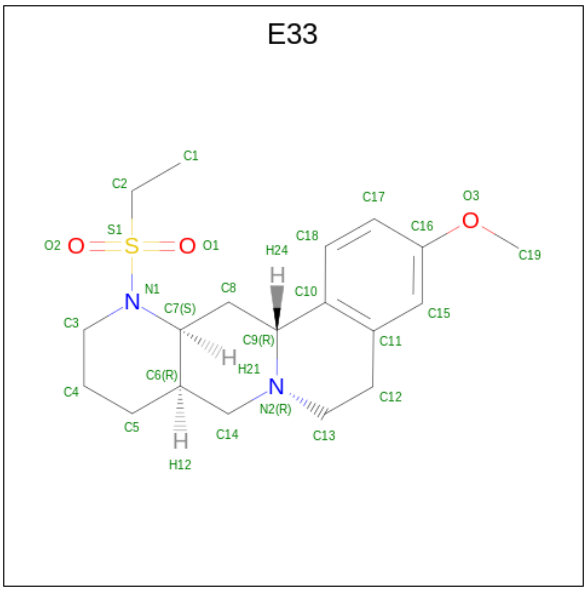
There are 6 unique types of molecules in this entry. The entry contains 7627 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alpha-2C adrenergic receptor.

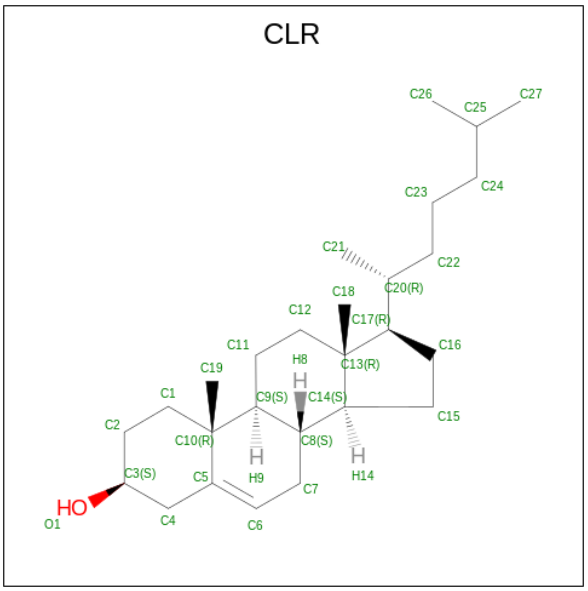
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	474	3696	2426	606	641	23	0	1	0
1	B	472	3686	2417	605	641	23	0	0	0

- Molecule 2 is (8 {a} {R},12 {a} {S},13 {a} {R})-12-ethylsulfonyl-3-methoxy-5,6,8,8 {a}, 9,10,11,12 {a},13,13 {a}-decahydroisoquinolino[2,1-g][1,6]naphthyridine (three-letter code: E33) (formula: $C_{19}H_{28}N_2O_3S$).



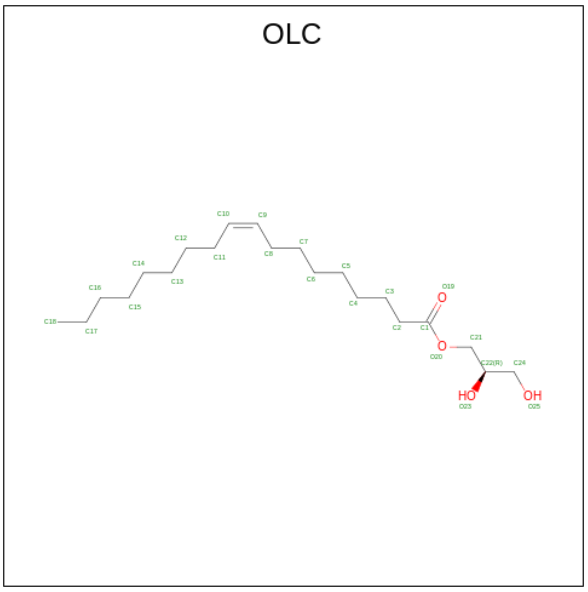
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	25	19	2	3	1	0	0
2	B	1	25	19	2	3	1	0	0

- Molecule 3 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 28 27 1	0	0
3	B	1	Total C O 28 27 1	0	0

- Molecule 4 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
4	A	1	Total C 11 11	0	0

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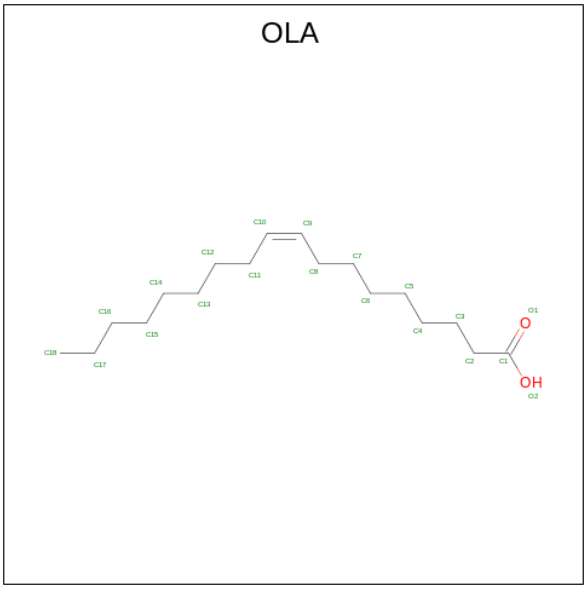
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 22 18 4	0	0
4	A	1	Total C 13 13	0	0
4	A	1	Total C O 13 9 4	0	0
4	A	1	Total C O 18 14 4	0	0
4	B	1	Total C 12 12	0	0
4	B	1	Total C 8 8	0	0

- Molecule 5 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 20 18 2	0	0
5	A	1	Total C O 20 18 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 1 1	0	0

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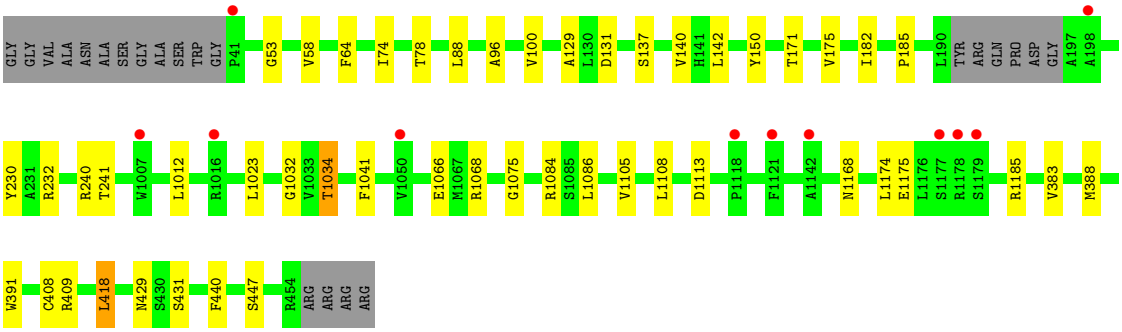
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	B	1	1	1	0	0

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.

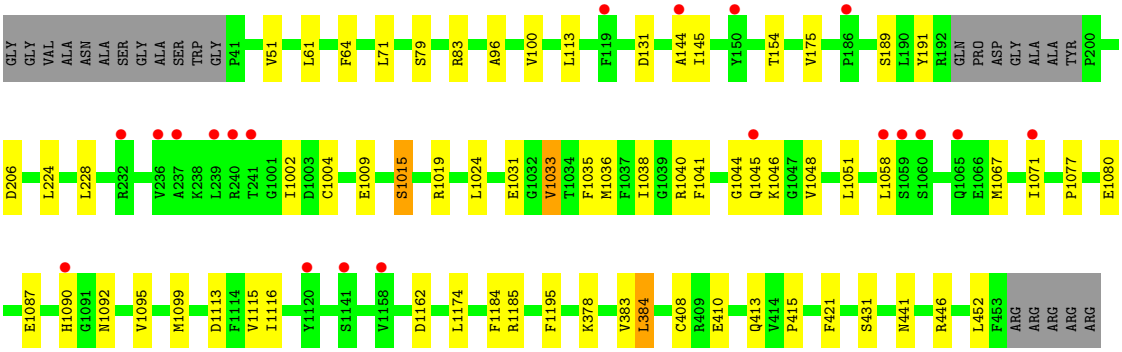
• Molecule 1: Alpha-2C adrenergic receptor

Chain A:



• Molecule 1: Alpha-2C adrenergic receptor

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.48Å 78.74Å 190.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.04 – 2.80 47.04 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.4 (47.04-2.80) 94.4 (47.04-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.213 , 0.262 0.228 , 0.277	Depositor DCC
R_{free} test set	1302 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	70.3	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 67.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7627	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.17% 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, E33, CLR, OLA

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	0.48	0/3790	0.66	0/5150
1	B	0.47	0/3778	0.66	0/5128
All	All	0.48	0/7568	0.66	0/10278

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	3696	0	3683	24	0
1	B	3686	0	3700	27	0
2	A	25	0	0	0	0
2	B	25	0	0	0	0
3	A	28	0	46	1	0
3	B	28	0	46	2	0
4	A	77	0	111	9	0
4	B	20	0	36	0	0
5	A	40	0	66	6	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
All	All	7627	0	7688	55	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 4.

All (55) 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:145:ILE:HG21	1:B:384:LEU:HD22	1.60	0.80
1:A:140:VAL:HG13	4:A:1205:OLC:H11A	1.72	0.70
4:A:1207:OLC:H6	5:A:1208:OLA:H51	1.78	0.65
4:A:1207:OLC:H6	5:A:1208:OLA:C5	2.31	0.61
1:B:96:ALA:O	1:B:100:VAL:HG23	2.01	0.61
1:A:230:TYR:CE2	1:A:388:MET:SD	2.95	0.60
1:A:230:TYR:HE2	1:A:388:MET:SD	2.25	0.60
4:A:1207:OLC:H22	1:B:415:PRO:HG3	1.84	0.59
1:B:1040:ARG:HG2	1:B:1046:LYS:HE3	1.86	0.57
1:B:224:LEU:O	1:B:228:LEU:HG	2.04	0.57
1:B:410:GLU:HA	1:B:413:GLN:HE21	1.69	0.57
1:A:129:ALA:HB1	1:A:185:PRO:HB3	1.86	0.56
1:A:74:ILE:O	1:A:78:THR:HG22	2.06	0.56
1:A:142:LEU:HB3	1:A:388:MET:HG2	1.87	0.56
1:B:1035:PHE:CE1	1:B:1067:MET:HG2	2.40	0.55
1:B:51:VAL:HG13	1:B:113:LEU:HD13	1.91	0.53
1:B:1071:ILE:HD11	1:B:1095:VAL:HG22	1.89	0.53
1:A:150:TYR:CE1	1:A:232:ARG:HB3	2.44	0.53
1:A:1113:ASP:HA	1:A:1185:ARG:HH21	1.75	0.52
1:B:144:ALA:HB2	1:B:175:VAL:HG11	1.93	0.51
1:B:1077:PRO:HA	1:B:1080:GLU:HB2	1.91	0.51
1:B:1090:HIS:C	1:B:1092:ASN:H	2.14	0.51
1:A:1034:THR:HG23	1:A:1068:ARG:HB2	1.93	0.51
1:B:383:VAL:HG21	1:B:441:ASN:HB2	1.93	0.51
1:A:53:GLY:HA3	5:A:1208:OLA:H22	1.94	0.50
1:B:1113:ASP:HA	1:B:1185:ARG:HH22	1.77	0.50
1:A:182:ILE:HD11	4:A:1205:OLC:H15	1.94	0.50
1:A:418:LEU:HD11	1:B:421:PHE:HB2	1.93	0.50
1:A:96:ALA:O	1:A:100:VAL:HG23	2.11	0.50
1:A:383:VAL:HG22	1:A:440:PHE:HB3	1.93	0.49
1:B:1033:VAL:HG21	1:B:1174:LEU:HD12	1.93	0.49
1:A:418:LEU:HD21	3:B:1202:CLR:H193	1.94	0.49
1:B:1024:LEU:HD13	1:B:1031:GLU:HA	1.96	0.48
4:A:1207:OLC:H8	5:A:1208:OLA:H72	1.94	0.48
1:A:1105:VAL:HA	1:A:1108:LEU:HD12	1.96	0.47
1:B:79:SER:HB3	1:B:446:ARG:HH22	1.79	0.47
1:B:1041:PHE:HA	1:B:1048:VAL:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1041:PHE:HB2	1:A:1075:GLY:H	1.79	0.47
1:A:88:LEU:HD22	4:A:1206:OLC:H21A	1.96	0.46
1:B:64:PHE:HD2	1:B:431:SER:HB2	1.81	0.46
1:A:64:PHE:CD2	1:A:431:SER:HB2	2.52	0.45
1:B:61:LEU:HD13	3:B:1202:CLR:H25	1.98	0.45
1:B:1015:SER:O	1:B:1019:ARG:HG3	2.18	0.43
4:A:1207:OLC:C8	5:A:1208:OLA:H72	2.49	0.42
1:A:1066:GLU:HB3	1:A:1174:LEU:HD11	2.02	0.42
1:B:71:LEU:HD11	1:B:452:LEU:HD21	2.02	0.42
1:A:58:VAL:HG22	3:A:1202:CLR:H151	2.02	0.42
1:B:1087:GLU:HB2	1:B:1095:VAL:HG23	2.02	0.41
1:B:1051:LEU:HD13	1:B:1116:ILE:HG21	2.03	0.41
4:A:1207:OLC:H6	5:A:1208:OLA:H52	2.02	0.41
1:A:171:THR:O	1:A:175:VAL:HG13	2.21	0.41
1:B:1036:MET:HG2	1:B:1115:VAL:HG22	2.02	0.41
1:A:1032:GLY:HA3	1:A:1068:ARG:HE	1.86	0.40
1:A:391:TRP:HA	1:A:429:ASN:ND2	2.37	0.40
1:B:1058:LEU:HB3	1:B:1067:MET:HE1	2.01	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	471/496 (95%)	447 (95%)	24 (5%)	0	100	100
1	B	468/496 (94%)	440 (94%)	24 (5%)	4 (1%)	17	46
All	All	939/992 (95%)	887 (94%)	48 (5%)	4 (0%)	34	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1045	GLN
1	B	154	THR
1	B	1044	GLY
1	B	1033	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	387/414 (94%)	372 (96%)	15 (4%)	32	66
1	B	390/414 (94%)	373 (96%)	17 (4%)	28	61
All	All	777/828 (94%)	745 (96%)	32 (4%)	30	64

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	ASP
1	A	137	SER
1	A	240	ARG
1	A	241	THR
1	A	1012	LEU
1	A	1023	LEU
1	A	1034	THR
1	A	1084	ARG
1	A	1086	LEU
1	A	1168	ASN
1	A	1175	GLU
1	A	408	CYS
1	A	409	ARG
1	A	418	LEU
1	A	447	SER
1	B	83	ARG
1	B	131	ASP
1	B	189	SER
1	B	191	TYR
1	B	206	ASP

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Mol	Chain	Res	Type
1	B	1002	ILE
1	B	1004	CYS
1	B	1009	GLU
1	B	1015	SER
1	B	1038	ILE
1	B	1099	MET
1	B	1162	ASP
1	B	1184	PHE
1	B	1195	PHE
1	B	378	LYS
1	B	384	LEU
1	B	408	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	1090	HIS
1	B	413	GLN

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)

13 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	$\#\|Z\| > 2$
4	OLC	A	1203	-	10,10,24	0.43	0	9,9,25	0.41	0
5	OLA	A	1208	-	19,19,19	0.51	0	19,19,19	0.90	2 (10%)
2	E33	B	1201	-	28,28,28	3.45	8 (28%)	35,42,42	4.63	13 (37%)
4	OLC	B	1204	-	7,7,24	0.30	0	6,6,25	0.39	0
3	CLR	B	1202	-	31,31,31	0.41	0	48,48,48	0.62	0
3	CLR	A	1202	-	31,31,31	0.44	0	48,48,48	0.51	0
4	OLC	A	1204	-	21,21,24	0.55	0	22,22,25	0.84	2 (9%)
4	OLC	B	1203	-	11,11,24	0.36	0	9,10,25	0.52	0
4	OLC	A	1205	-	12,12,24	0.35	0	11,11,25	0.44	0
4	OLC	A	1206	-	12,12,24	0.74	1 (8%)	13,13,25	1.34	1 (7%)
2	E33	A	1201	-	28,28,28	3.43	6 (21%)	35,42,42	4.21	17 (48%)
4	OLC	A	1207	-	17,17,24	0.61	0	18,18,25	0.91	2 (11%)
5	OLA	A	1209	-	19,19,19	0.52	0	19,19,19	0.73	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
4	OLC	A	1203	-	-	6/8/8/24	-
5	OLA	A	1208	-	-	11/17/17/17	-
2	E33	B	1201	-	-	9/11/46/46	0/4/4/4
4	OLC	B	1204	-	-	4/5/5/24	-
3	CLR	B	1202	-	-	2/10/68/68	0/4/4/4
3	CLR	A	1202	-	-	1/10/68/68	0/4/4/4
4	OLC	A	1204	-	-	9/21/21/24	-
4	OLC	B	1203	-	-	4/9/9/24	-
4	OLC	A	1205	-	-	3/10/10/24	-
4	OLC	A	1206	-	-	6/12/12/24	-
2	E33	A	1201	-	-	9/11/46/46	0/4/4/4
4	OLC	A	1207	-	-	7/17/17/24	-
5	OLA	A	1209	-	-	10/17/17/17	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	E33	O1-S1	8.88	1.53	1.43
2	A	1201	E33	C10-C9	-8.87	1.38	1.52
2	B	1201	E33	C10-C9	-8.81	1.38	1.52
2	B	1201	E33	O1-S1	7.98	1.52	1.43
2	B	1201	E33	O2-S1	7.86	1.52	1.43
2	A	1201	E33	O2-S1	7.62	1.52	1.43
2	A	1201	E33	C12-C11	-7.26	1.38	1.51
2	B	1201	E33	C12-C11	-7.20	1.38	1.51
2	B	1201	E33	S1-N1	5.27	1.72	1.62
2	A	1201	E33	C2-S1	5.22	1.82	1.76
2	B	1201	E33	C2-S1	4.84	1.82	1.76
2	A	1201	E33	S1-N1	4.67	1.71	1.62
2	B	1201	E33	C7-N1	2.67	1.51	1.48
2	B	1201	E33	C8-C9	2.27	1.56	1.53
4	A	1206	OLC	O20-C1	2.24	1.39	1.33

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1201	E33	O2-S1-O1	-18.97	99.52	118.98
2	A	1201	E33	O2-S1-O1	-14.85	103.75	118.98
2	B	1201	E33	C11-C10-C9	-13.40	106.11	121.57
2	A	1201	E33	C11-C10-C9	-12.84	106.76	121.57
2	B	1201	E33	C13-N2-C14	7.19	123.71	110.29
2	A	1201	E33	C6-C14-N2	6.88	121.24	112.23
2	B	1201	E33	C6-C14-N2	6.83	121.18	112.23
2	A	1201	E33	C13-N2-C14	6.68	122.76	110.29
2	A	1201	E33	C10-C9-N2	4.24	125.29	112.16
2	B	1201	E33	O1-S1-N1	4.00	113.25	107.60
2	B	1201	E33	C10-C9-N2	3.96	124.40	112.16
2	A	1201	E33	C14-N2-C9	3.83	115.71	110.12
2	A	1201	E33	C12-C11-C15	-3.75	112.40	119.91
2	B	1201	E33	C12-C11-C15	-3.60	112.70	119.91
2	A	1201	E33	C15-C11-C10	3.56	124.13	119.50
4	A	1206	OLC	O20-C1-C2	3.55	123.06	111.91
2	A	1201	E33	C16-C15-C11	-3.16	116.08	120.47
2	B	1201	E33	C14-N2-C9	3.00	114.49	110.12
2	A	1201	E33	C14-C6-C7	-2.88	106.82	110.45
2	B	1201	E33	C15-C11-C10	2.81	123.15	119.50
2	A	1201	E33	O1-S1-N1	2.68	111.38	107.60
2	A	1201	E33	C4-C5-C6	2.47	116.15	111.93
2	A	1201	E33	C19-O3-C16	-2.43	112.24	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	E33	C13-N2-C9	-2.39	106.50	111.27
2	A	1201	E33	C17-C18-C10	-2.37	117.14	121.13
2	B	1201	E33	C16-C15-C11	-2.33	117.24	120.47
5	A	1208	OLA	O2-C1-C2	2.32	121.47	114.03
4	A	1204	OLC	O20-C1-C2	2.31	119.15	111.91
2	A	1201	E33	C4-C3-N1	-2.28	106.96	110.31
4	A	1204	OLC	O20-C1-O19	-2.25	117.92	123.59
2	A	1201	E33	C18-C17-C16	2.24	122.48	119.73
4	A	1207	OLC	O20-C1-C2	2.23	118.91	111.91
2	B	1201	E33	O1-S1-C2	2.14	112.25	108.55
2	B	1201	E33	O2-S1-C2	2.08	112.14	108.55
4	A	1207	OLC	C21-O20-C1	2.08	124.81	117.12
5	A	1208	OLA	O2-C1-O1	-2.04	118.22	123.30
2	B	1201	E33	C13-N2-C9	-2.00	107.27	111.27

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	E33	C1-C2-S1-O1
2	A	1201	E33	C1-C2-S1-O2
2	A	1201	E33	C1-C2-S1-N1
2	A	1201	E33	C3-N1-S1-C2
2	A	1201	E33	C3-N1-S1-O2
2	A	1201	E33	C7-N1-S1-O2
2	B	1201	E33	C1-C2-S1-O1
2	B	1201	E33	C1-C2-S1-O2
2	B	1201	E33	C1-C2-S1-N1
2	B	1201	E33	C3-N1-S1-C2
2	B	1201	E33	C3-N1-S1-O2
2	B	1201	E33	C7-N1-S1-O2
4	B	1203	OLC	C7-C8-C9-C10
4	A	1206	OLC	O19-C1-O20-C21
4	A	1204	OLC	O19-C1-O20-C21
2	A	1201	E33	C15-C16-O3-C19
2	A	1201	E33	C17-C16-O3-C19
2	B	1201	E33	C15-C16-O3-C19
2	B	1201	E33	C17-C16-O3-C19
4	A	1206	OLC	C2-C1-O20-C21
4	A	1204	OLC	C2-C1-O20-C21
3	B	1202	CLR	C22-C23-C24-C25
4	A	1207	OLC	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
4	B	1204	OLC	C14-C15-C16-C17
4	B	1204	OLC	C13-C14-C15-C16
4	A	1204	OLC	C5-C6-C7-C8
4	A	1205	OLC	C12-C13-C14-C15
4	A	1206	OLC	C1-C2-C3-C4
5	A	1208	OLA	C1-C2-C3-C4
4	A	1204	OLC	C2-C3-C4-C5
4	B	1203	OLC	C13-C14-C15-C16
4	A	1206	OLC	O20-C21-C22-O23
4	A	1206	OLC	C2-C3-C4-C5
5	A	1209	OLA	C2-C3-C4-C5
5	A	1209	OLA	C13-C14-C15-C16
4	B	1203	OLC	C10-C11-C12-C13
5	A	1209	OLA	C10-C11-C12-C13
5	A	1208	OLA	C3-C4-C5-C6
4	A	1204	OLC	C10-C11-C12-C13
4	A	1207	OLC	C2-C3-C4-C5
5	A	1208	OLA	C11-C12-C13-C14
4	B	1203	OLC	C11-C12-C13-C14
4	A	1203	OLC	C10-C11-C12-C13
5	A	1208	OLA	C10-C11-C12-C13
5	A	1209	OLA	C15-C16-C17-C18
4	A	1203	OLC	C11-C12-C13-C14
4	A	1205	OLC	C15-C16-C17-C18
5	A	1208	OLA	C15-C16-C17-C18
4	A	1204	OLC	C4-C5-C6-C7
4	B	1204	OLC	C11-C12-C13-C14
4	A	1206	OLC	C3-C4-C5-C6
3	A	1202	CLR	C22-C23-C24-C25
2	A	1201	E33	C7-N1-S1-C2
4	A	1203	OLC	C12-C13-C14-C15
4	A	1207	OLC	C2-C1-O20-C21
4	A	1203	OLC	C15-C16-C17-C18
5	A	1209	OLA	C1-C2-C3-C4
5	A	1209	OLA	C3-C4-C5-C6
4	A	1207	OLC	O19-C1-O20-C21
5	A	1208	OLA	C5-C6-C7-C8
5	A	1208	OLA	C4-C5-C6-C7
5	A	1208	OLA	C13-C14-C15-C16
5	A	1209	OLA	C11-C12-C13-C14
4	A	1203	OLC	C14-C15-C16-C17
4	B	1204	OLC	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
4	A	1207	OLC	O20-C21-C22-O23
4	A	1204	OLC	C3-C4-C5-C6
3	B	1202	CLR	C20-C22-C23-C24
2	B	1201	E33	C7-N1-S1-C2
4	A	1204	OLC	C1-C2-C3-C4
4	A	1203	OLC	C9-C10-C11-C12
5	A	1208	OLA	C14-C15-C16-C17
5	A	1209	OLA	C5-C6-C7-C8
5	A	1209	OLA	C12-C13-C14-C15
5	A	1208	OLA	O2-C1-C2-C3
4	A	1205	OLC	C9-C10-C11-C12
5	A	1208	OLA	O1-C1-C2-C3
5	A	1209	OLA	C9-C10-C11-C12
4	A	1204	OLC	C6-C7-C8-C9
4	A	1207	OLC	O20-C1-C2-C3
4	A	1207	OLC	O19-C1-C2-C3

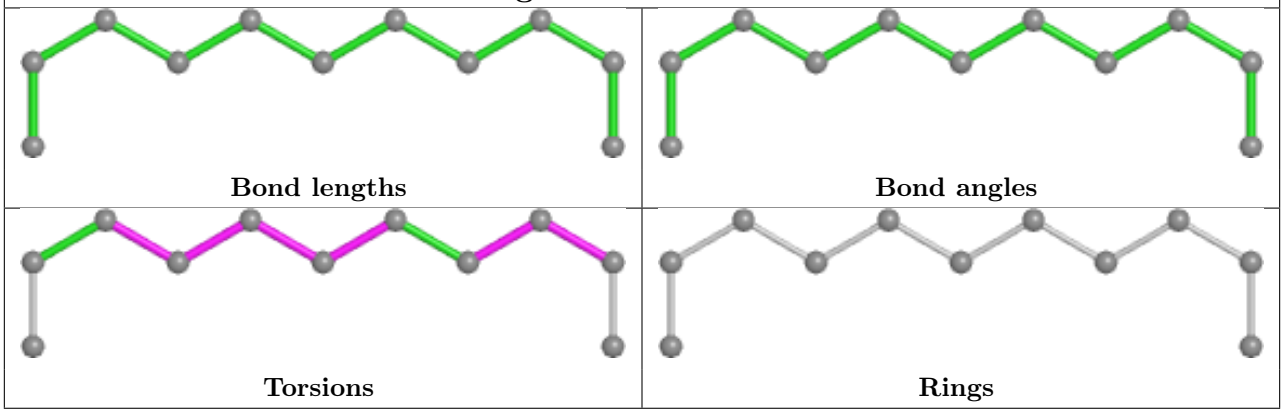
There are no ring outliers.

6 monomers are involved in 13 short contacts:

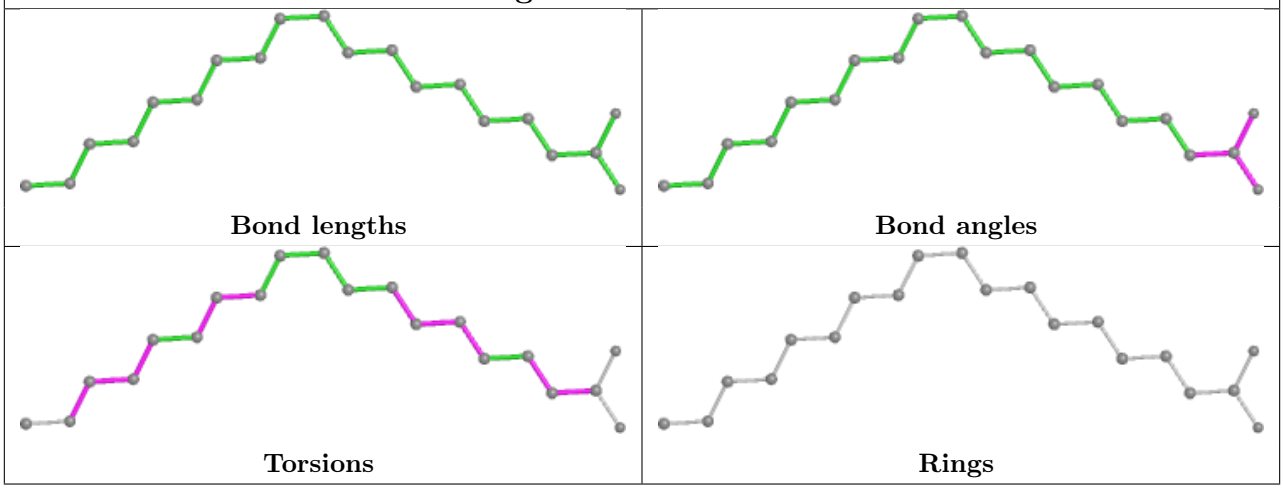
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1208	OLA	6	0
3	B	1202	CLR	2	0
3	A	1202	CLR	1	0
4	A	1205	OLC	2	0
4	A	1206	OLC	1	0
4	A	1207	OLC	6	0

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.

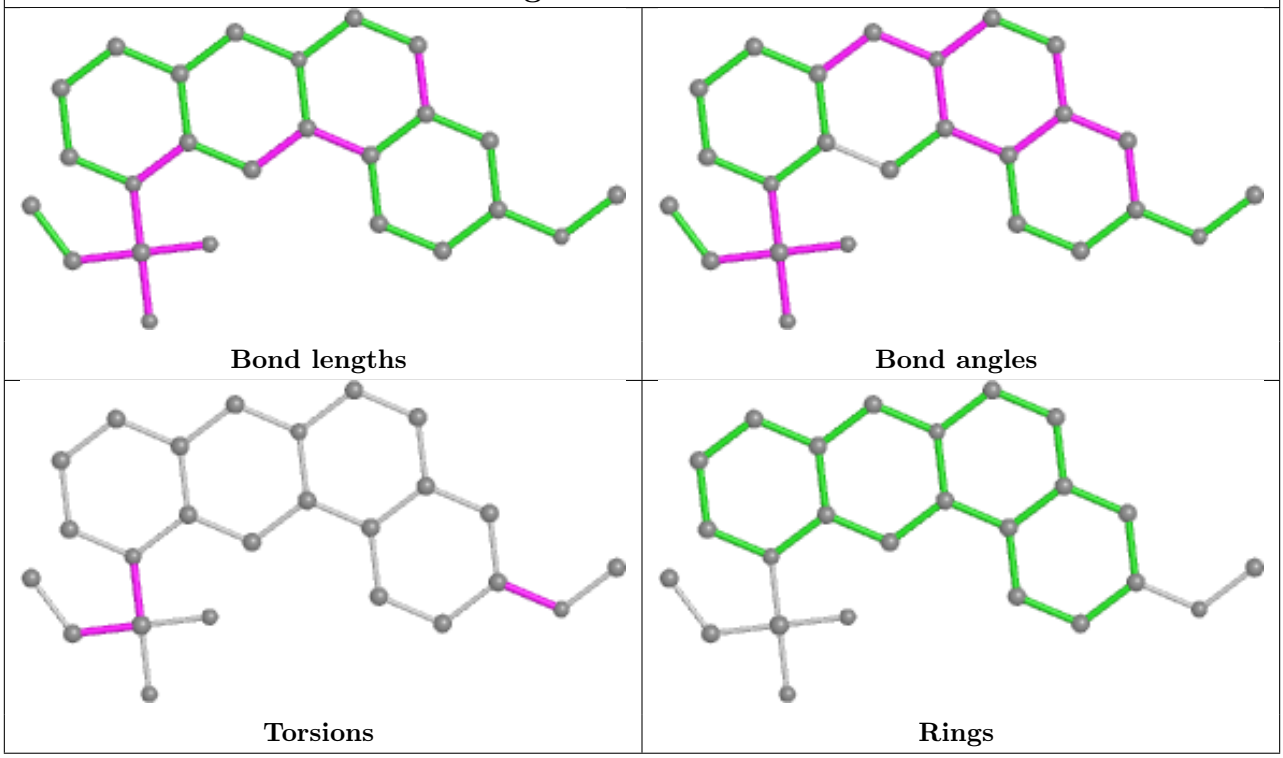
Ligand OLC A 1203



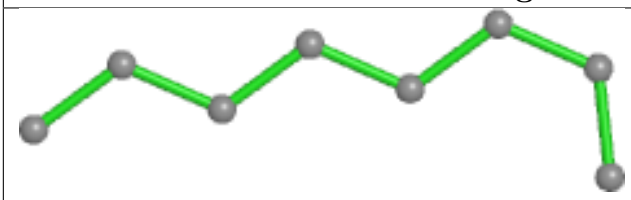
Ligand OLA A 1208



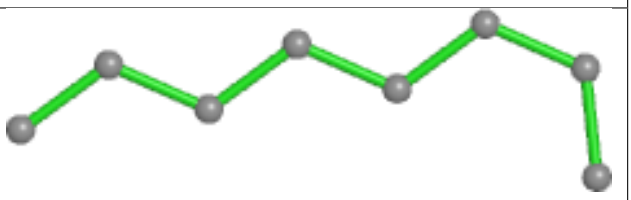
Ligand E33 B 1201



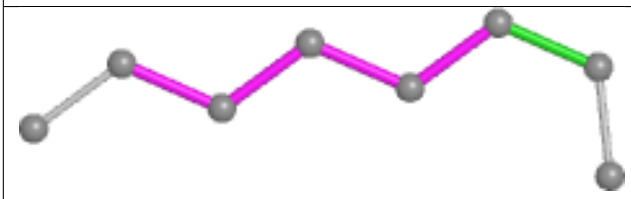
Ligand OLC B 1204



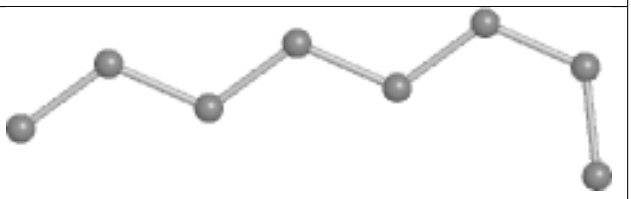
Bond lengths



Bond angles

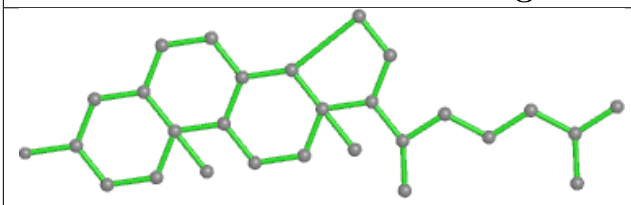


Torsions

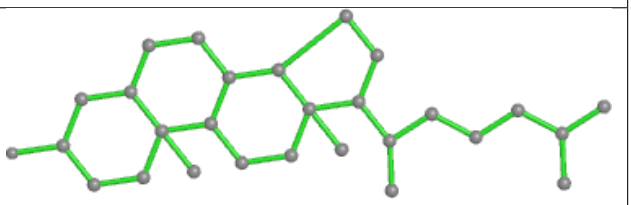


Rings

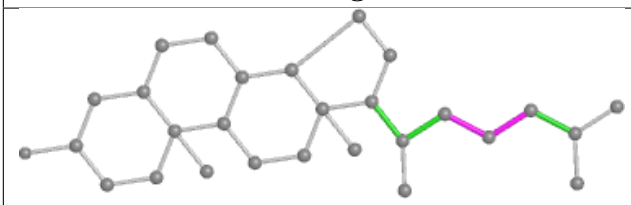
Ligand CLR B 1202



Bond lengths



Bond angles



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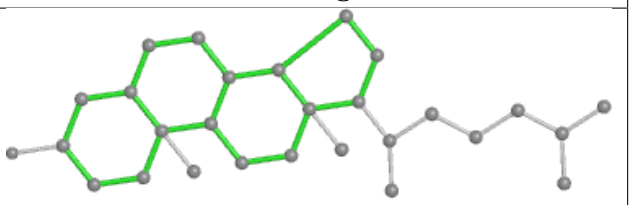
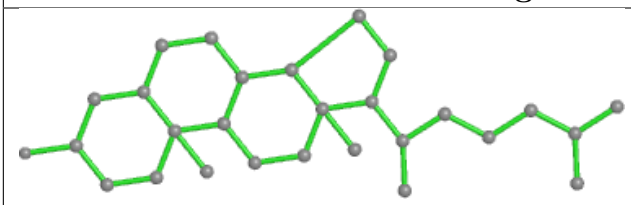
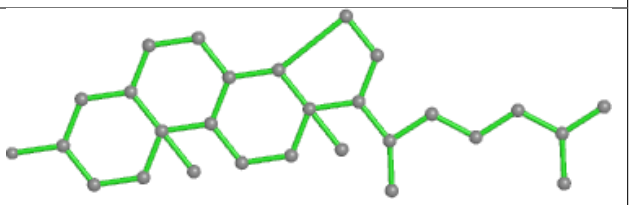


Rings

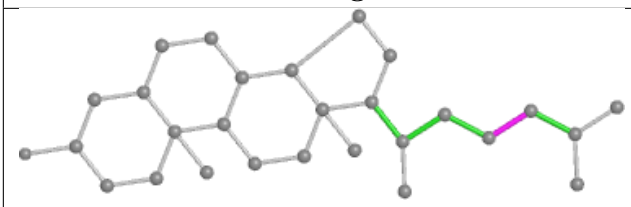
Ligand CLR A 1202



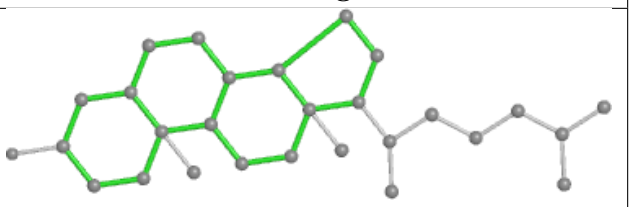
Bond lengths



Bond angles

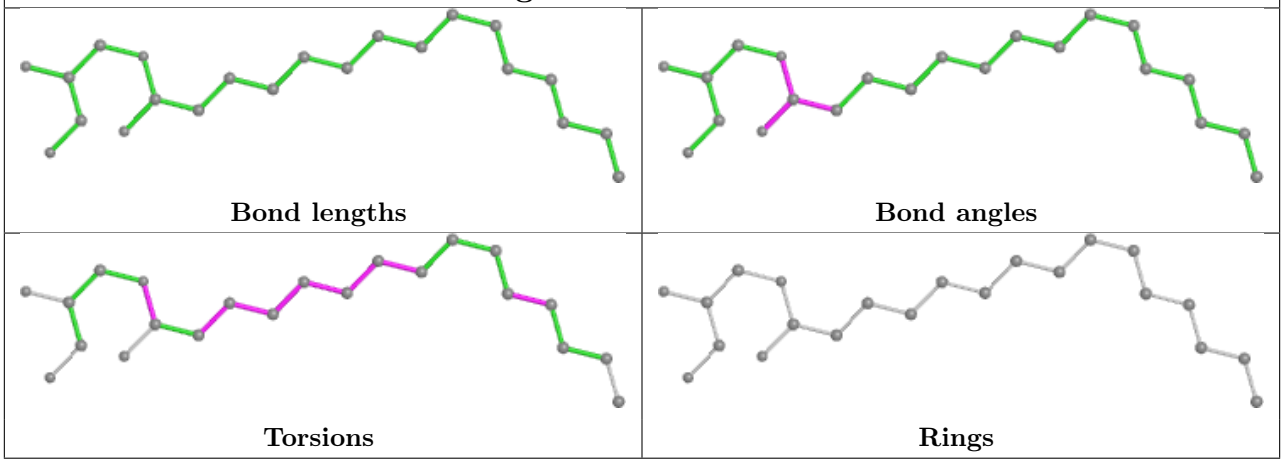


Torsions

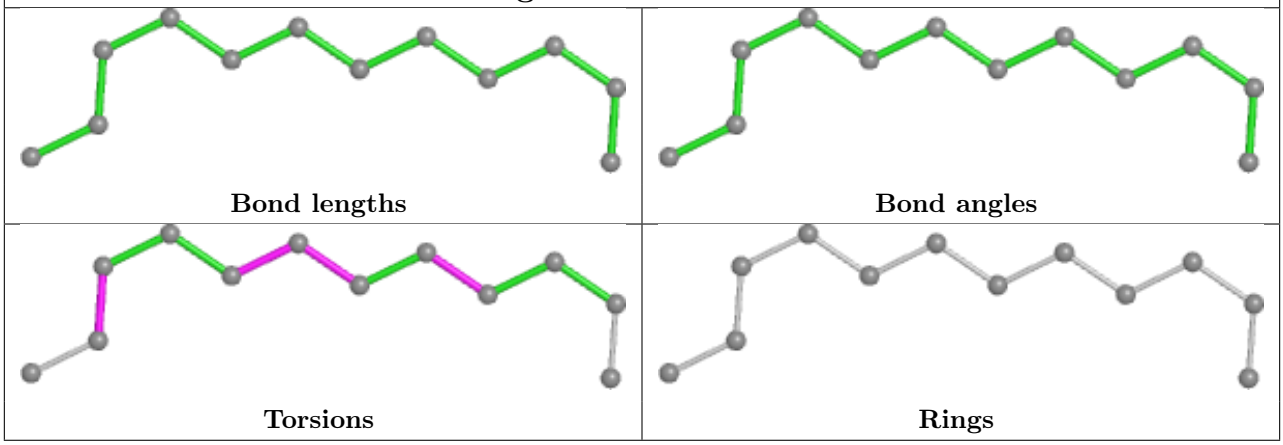


Rings

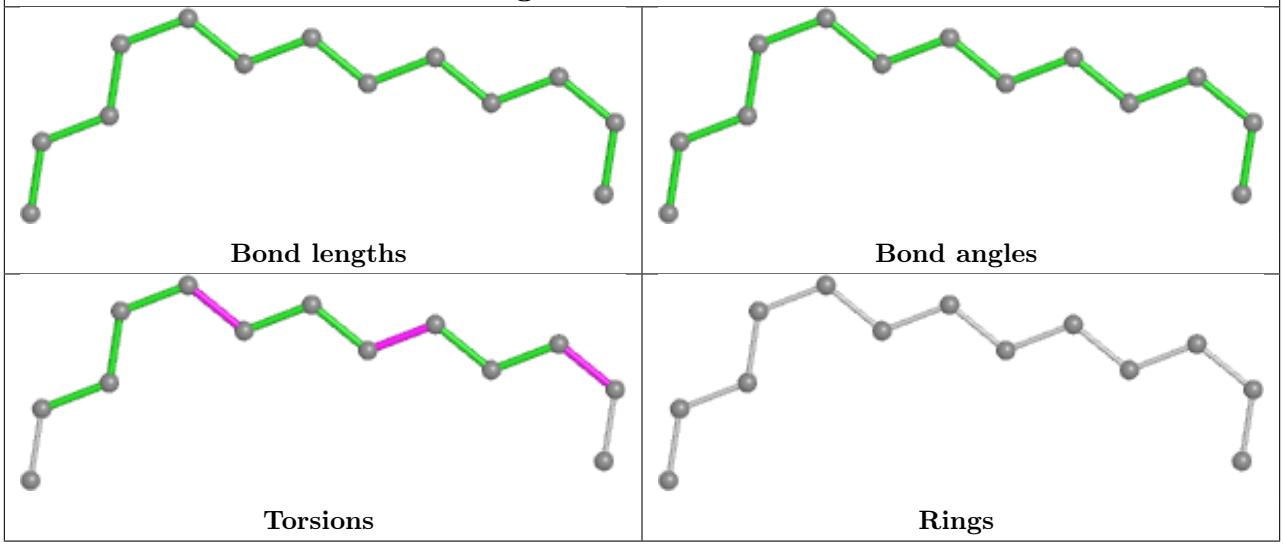
Ligand OLC A 1204



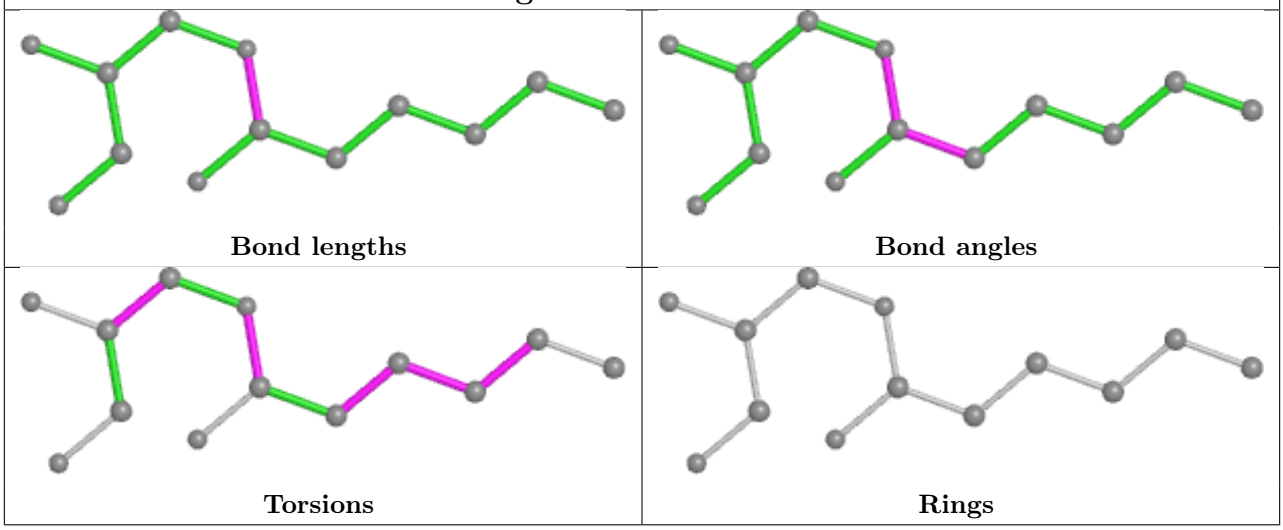
Ligand OLC B 1203



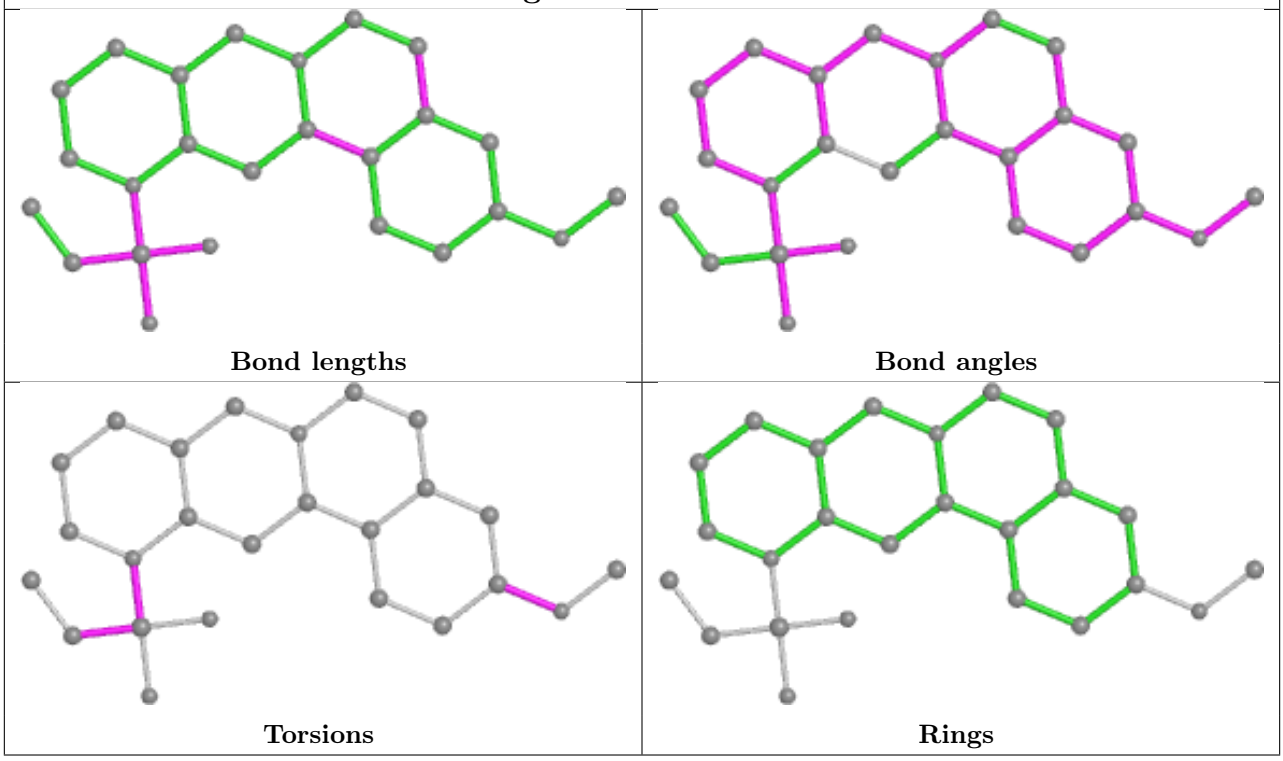
Ligand OLC A 1205



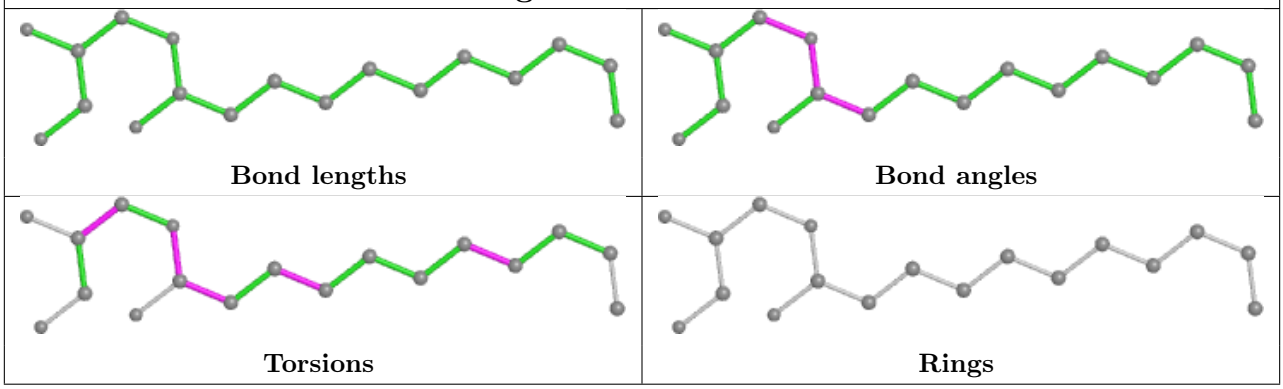
Ligand OLC A 1206

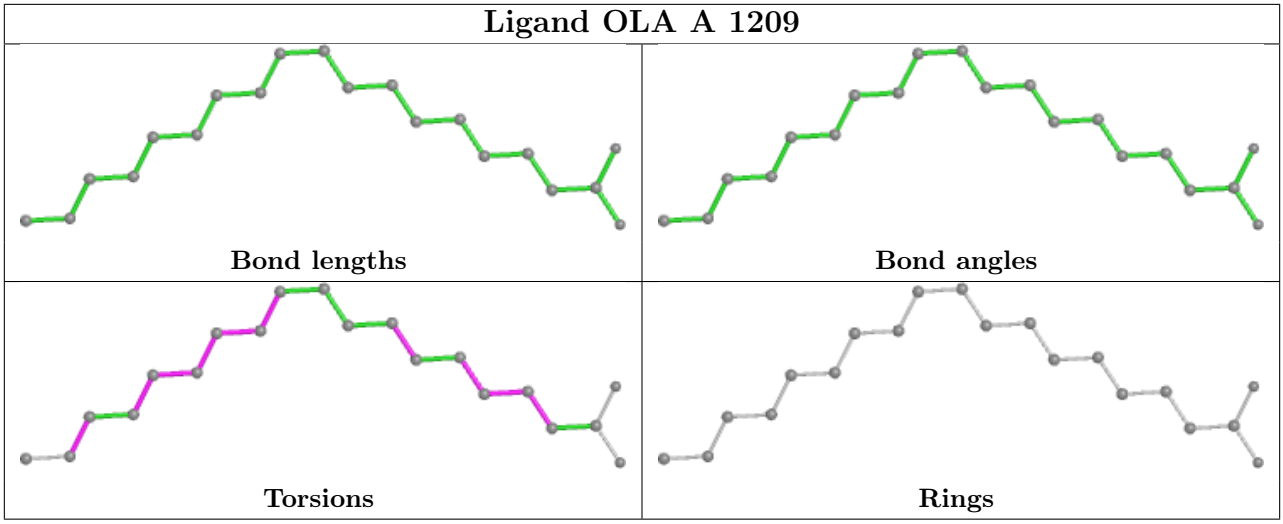


Ligand E33 A 1201



Ligand OLC A 1207





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	474/496 (95%)	0.08	11 (2%)	60	51	41, 75, 145, 179	0
1	B	472/496 (95%)	0.18	20 (4%)	36	26	48, 91, 148, 172	0
All	All	946/992 (95%)	0.13	31 (3%)	46	36	41, 86, 145, 179	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1178	ARG	5.4
1	A	198	ALA	4.3
1	B	1045	GLN	4.1
1	A	1179	SER	3.9
1	A	1142	ALA	3.7
1	B	236	VAL	3.4
1	B	240	ARG	3.3
1	B	1120	TYR	3.2
1	B	1058	LEU	3.2
1	B	186	PRO	3.1
1	A	1016	ARG	3.0
1	B	241	THR	2.9
1	B	150	TYR	2.7
1	B	1090	HIS	2.6
1	A	1177	SER	2.6
1	B	1158	VAL	2.5
1	B	232	ARG	2.4
1	B	1141	SER	2.4
1	A	1121	PHE	2.4
1	A	41	PRO	2.4
1	A	1118	PRO	2.3
1	B	119	PHE	2.2
1	B	239	LEU	2.2
1	B	237	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1059	SER	2.1
1	A	1050	VAL	2.1
1	B	1060	SER	2.1
1	B	1071	ILE	2.1
1	A	1007	TRP	2.1
1	B	144	ALA	2.1
1	B	1065	GLN	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, 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.

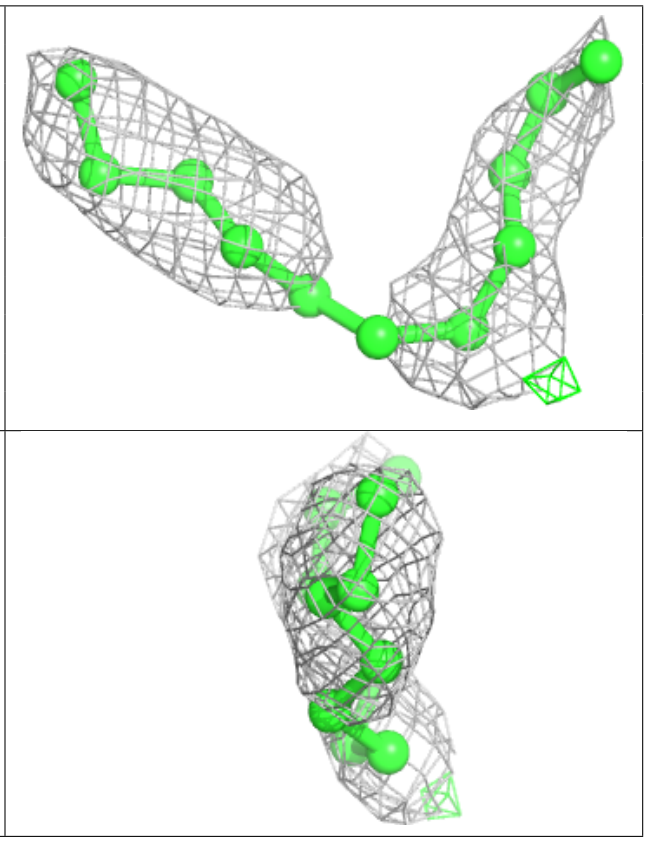
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	OLC	A	1203	11/25	0.70	0.33	71,80,82,82	0
4	OLC	A	1207	18/25	0.74	0.33	69,84,99,102	0
4	OLC	A	1206	13/25	0.77	0.21	73,87,92,92	0
4	OLC	B	1204	8/25	0.77	0.30	79,82,83,83	0
5	OLA	A	1209	20/20	0.80	0.39	78,83,93,94	0
5	OLA	A	1208	20/20	0.82	0.33	56,70,85,85	0
4	OLC	B	1203	12/25	0.83	0.25	63,74,92,92	0
3	CLR	B	1202	28/28	0.85	0.29	85,92,96,98	0
4	OLC	A	1205	13/25	0.85	0.24	58,62,64,65	0
4	OLC	A	1204	22/25	0.87	0.26	70,75,98,99	0
2	E33	B	1201	25/25	0.94	0.16	56,64,74,75	0
3	CLR	A	1202	28/28	0.94	0.25	65,68,69,70	0
2	E33	A	1201	25/25	0.95	0.19	45,64,81,81	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

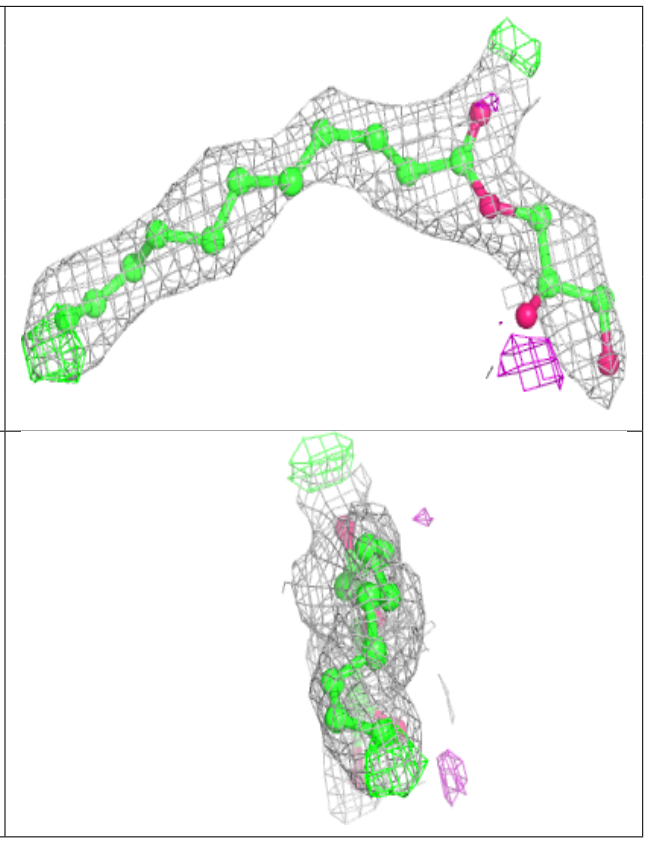
Electron density around OLC A 1203:

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



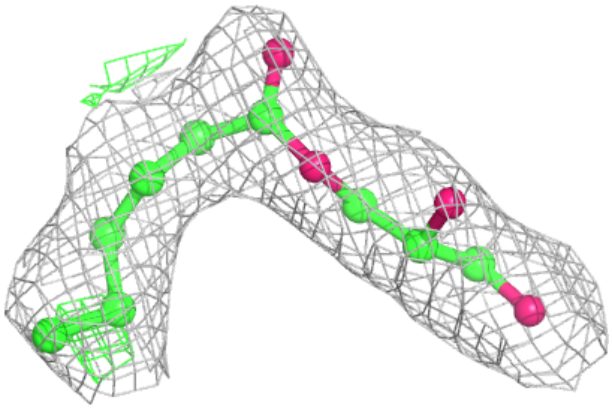
Electron density around OLC A 1207:

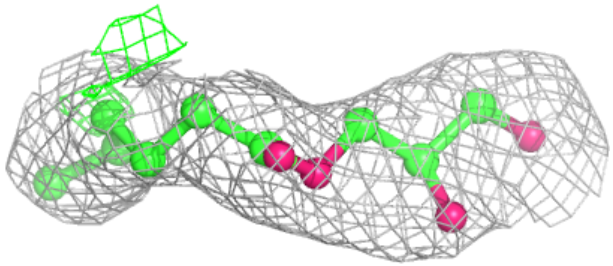
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

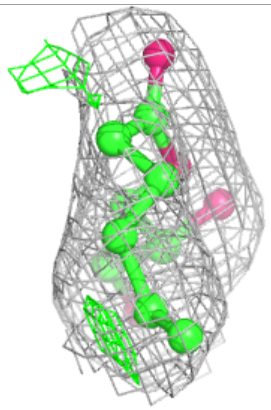


Electron density around OLC A 1206:

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

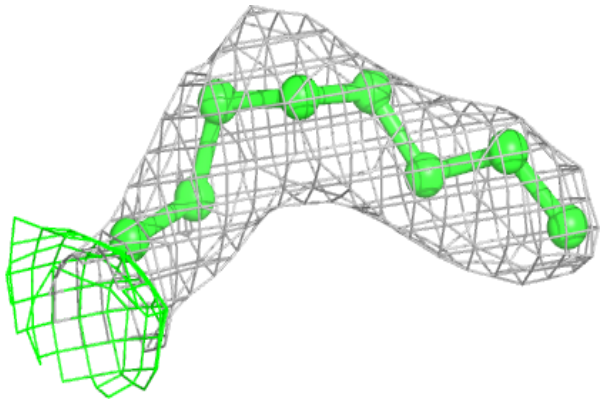


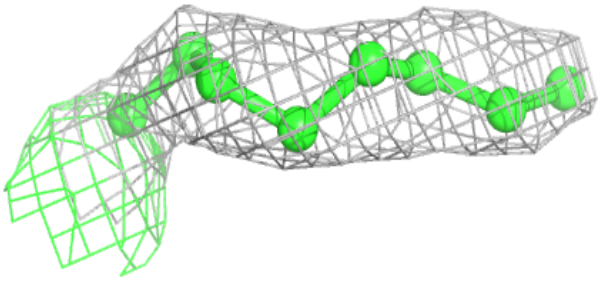


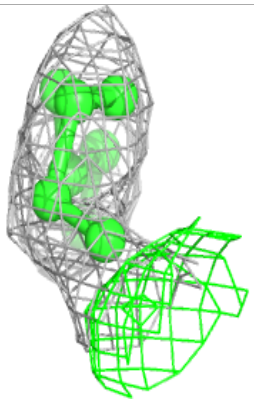


Electron density around OLC B 1204:

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

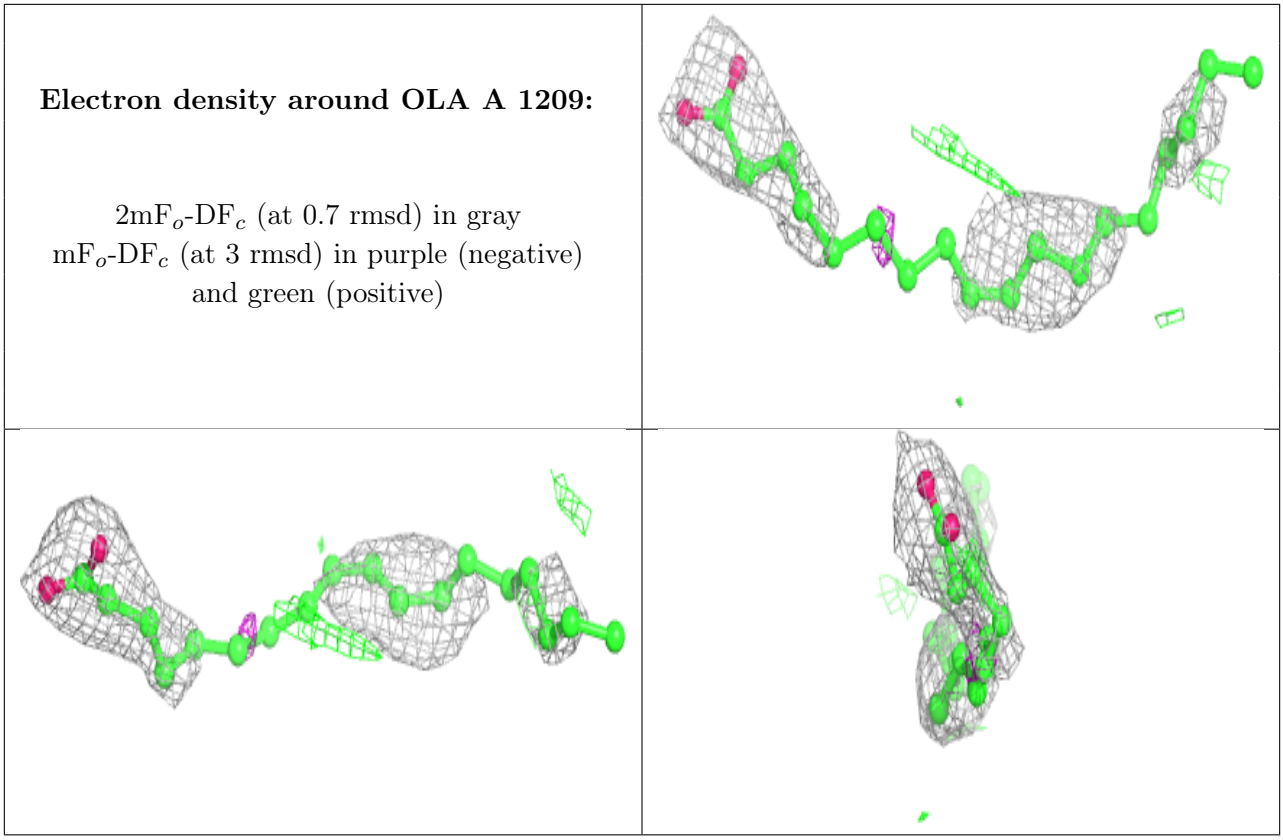






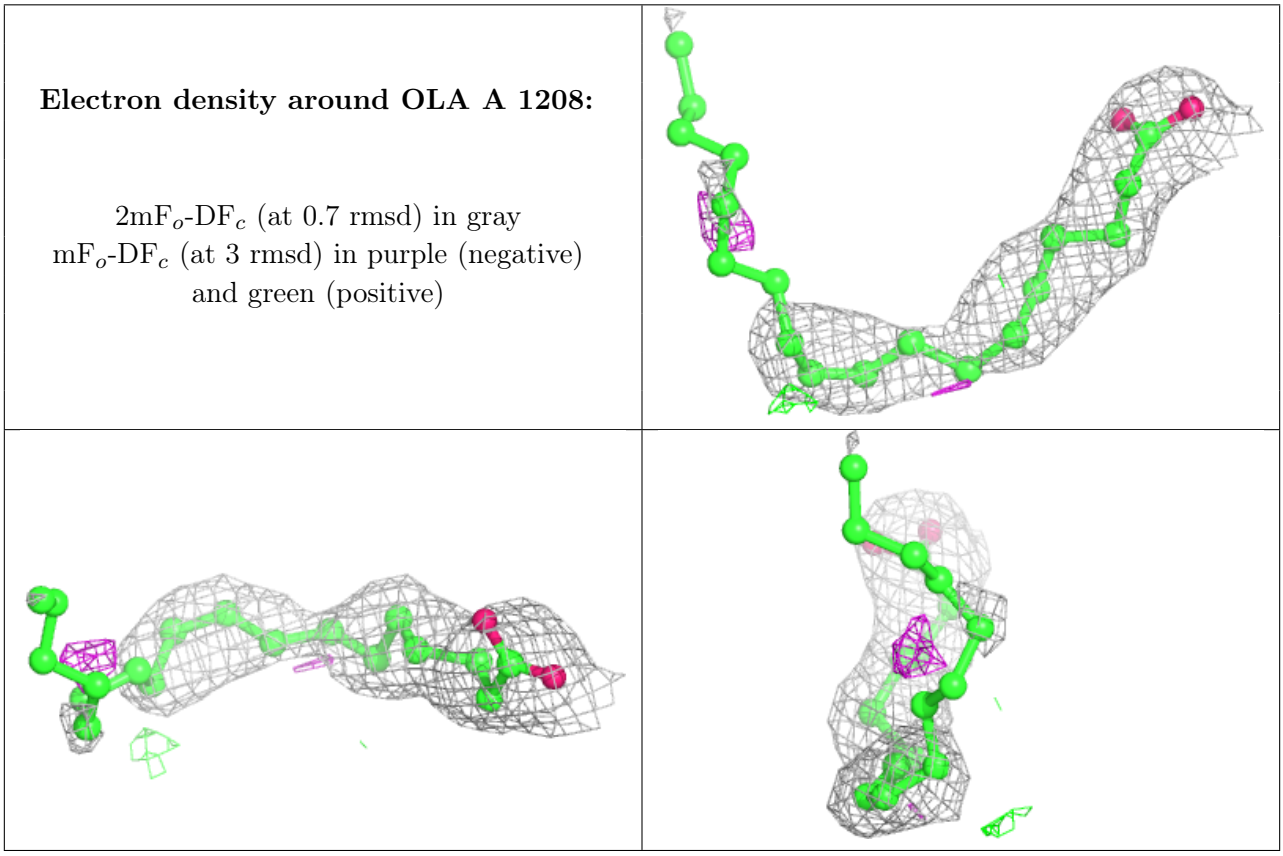
Electron density around OLA A 1209:

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



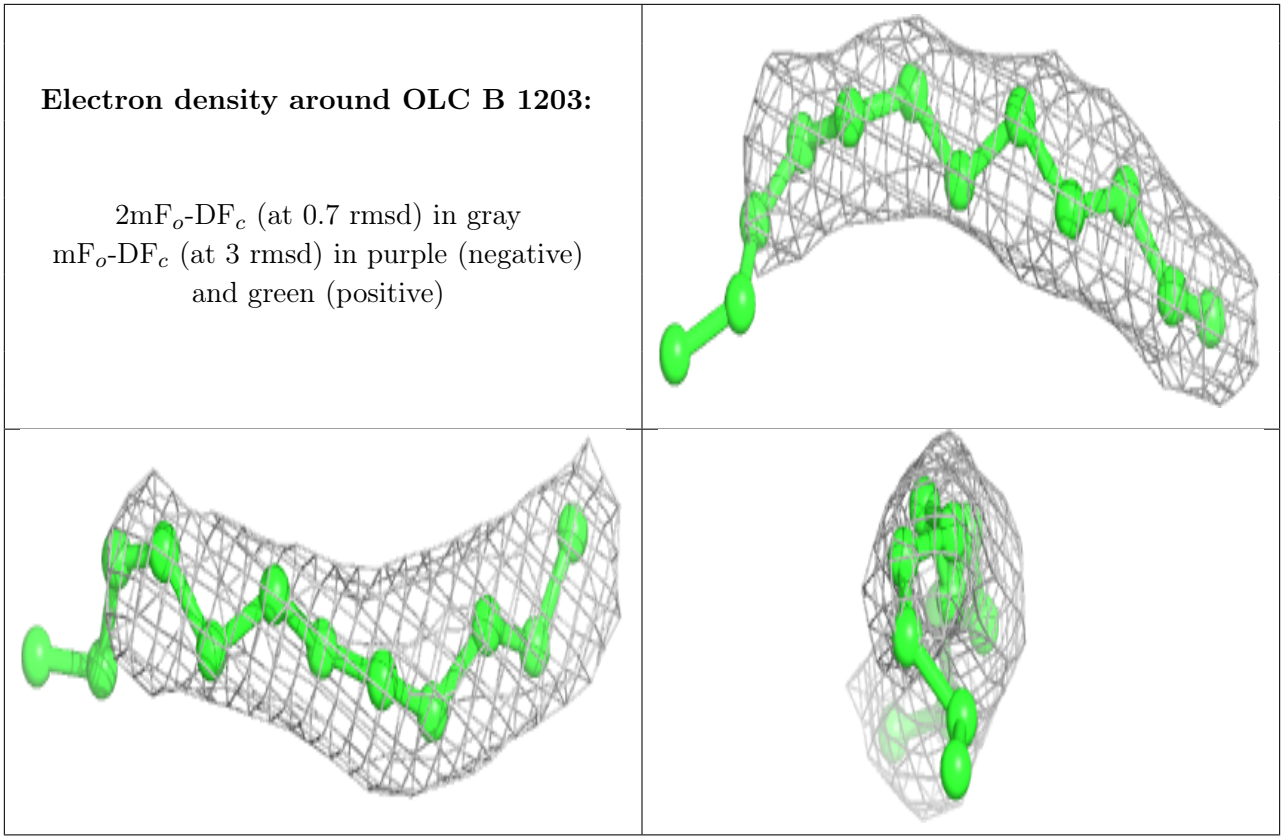
Electron density around OLA A 1208:

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



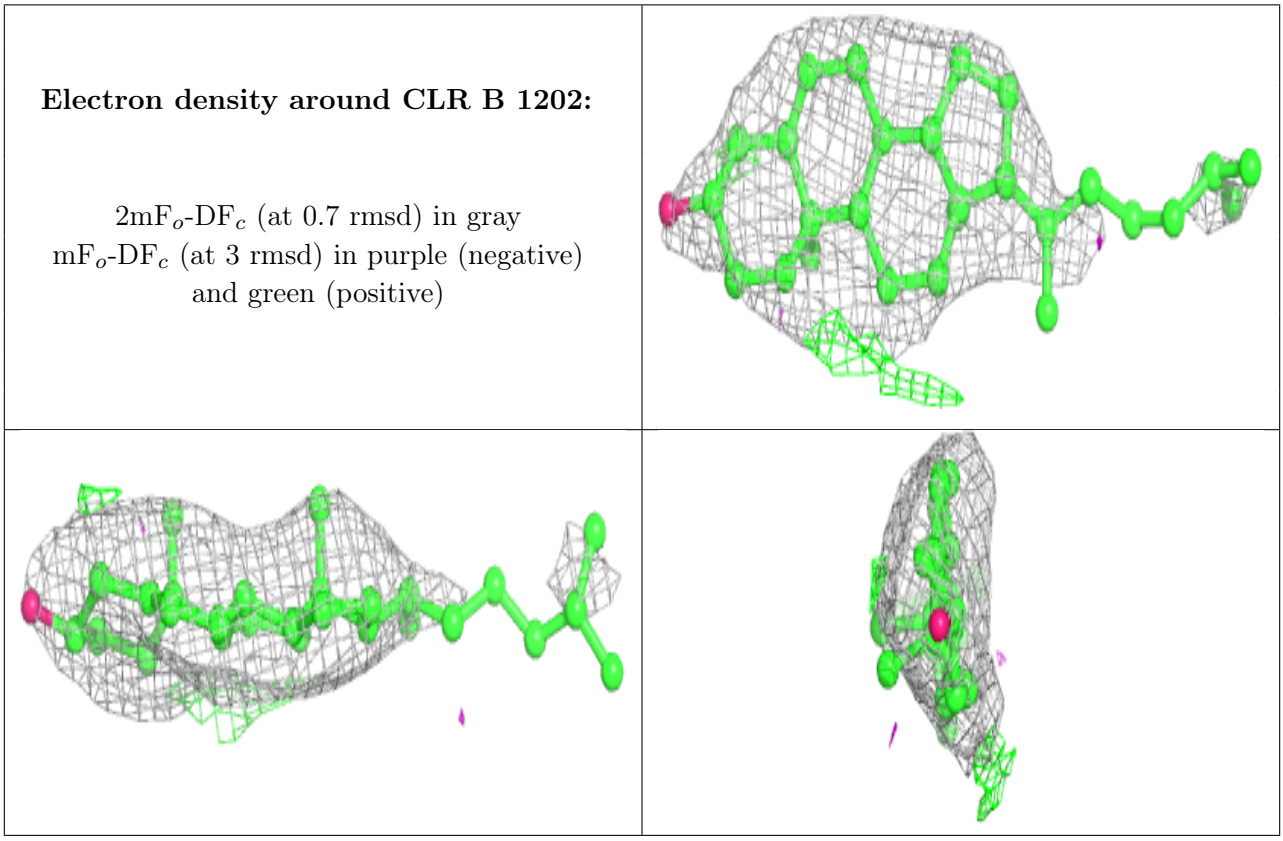
Electron density around OLC B 1203:

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



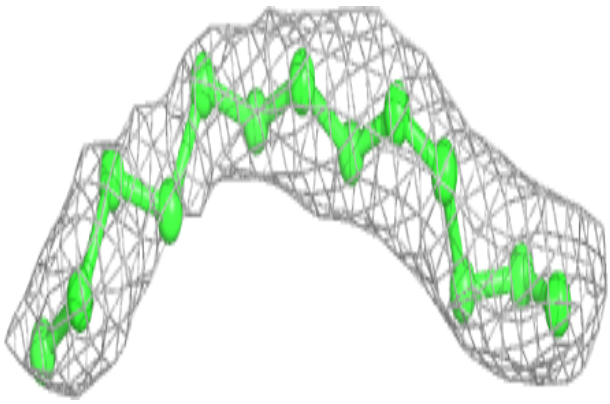
Electron density around CLR B 1202:

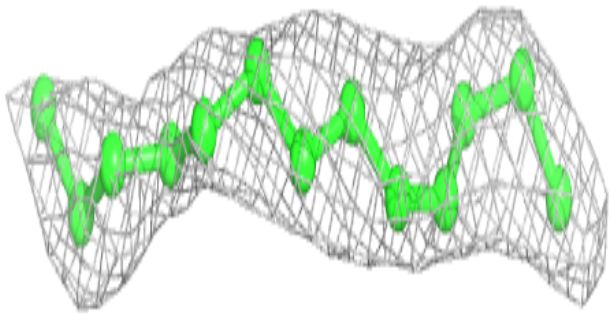
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

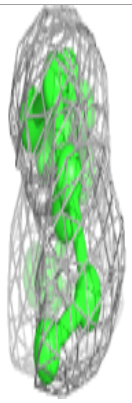


Electron density around OLC A 1205:

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

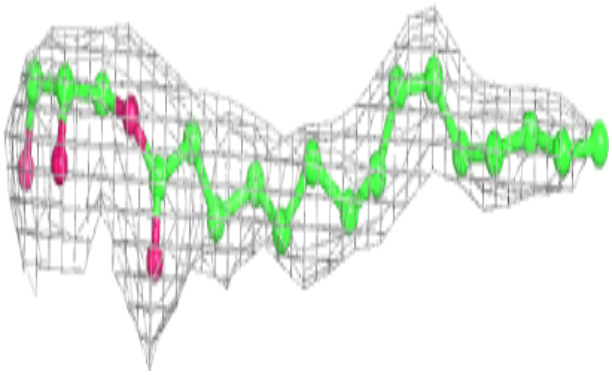


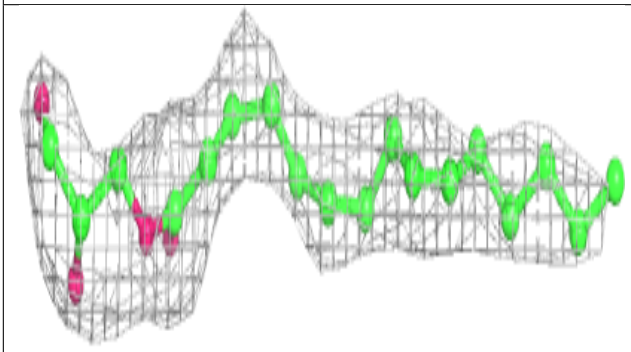


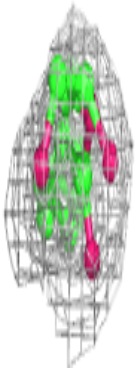


Electron density around OLC A 1204:

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

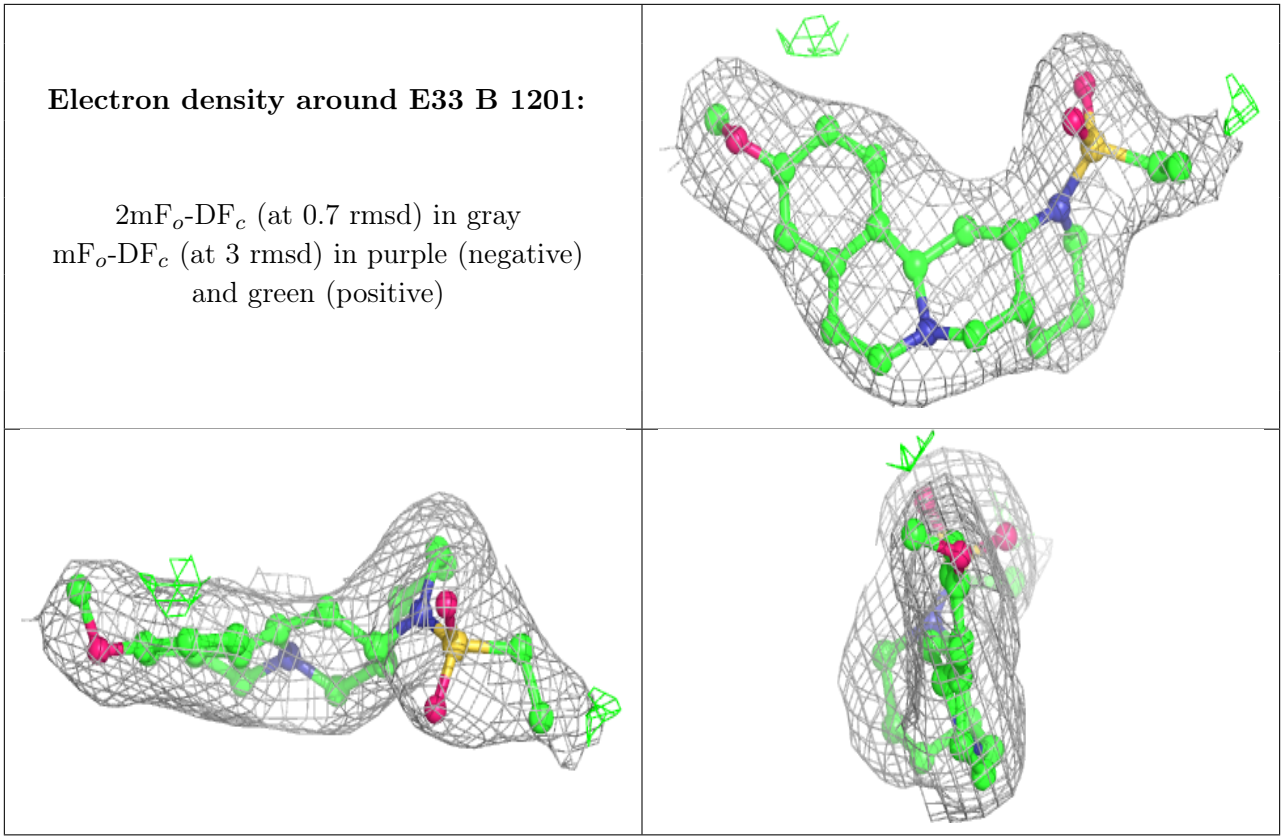






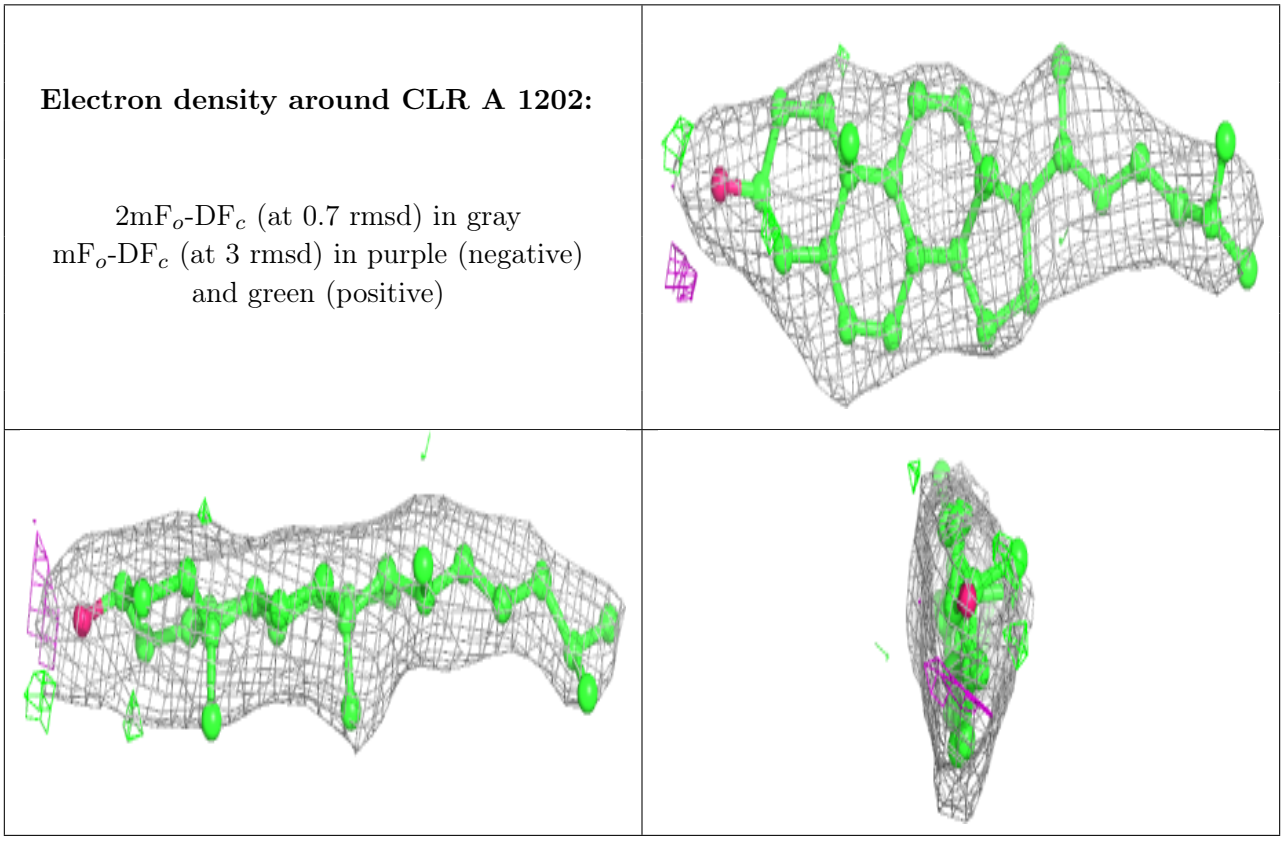
Electron density around E33 B 1201:

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



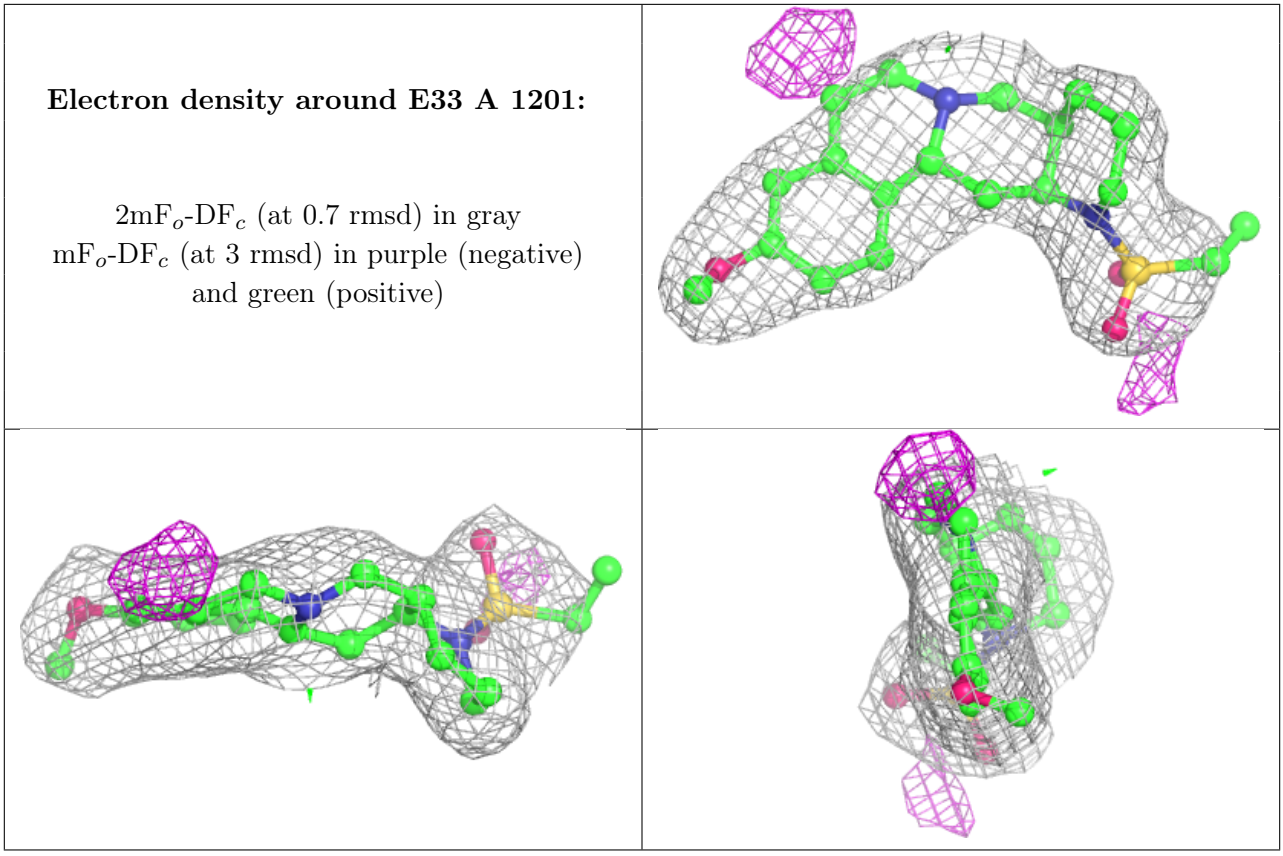
Electron density around CLR A 1202:

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



Electron density around E33 A 1201:

$2mF_o$-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.