



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:45 pm BST

PDB ID : 5X93
Title : Human endothelin receptor type-B in complex with antagonist K-8794
Authors : Shihoya, W.; Nishizawa, T.; Yamashita, K.; Hirata, K.; Okuta, A.; Tani, K.;
Fujiyoshi, Y.; Doi, T.; Nureki, O.
Deposited on : 2017-03-05
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.11
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) : 2.11

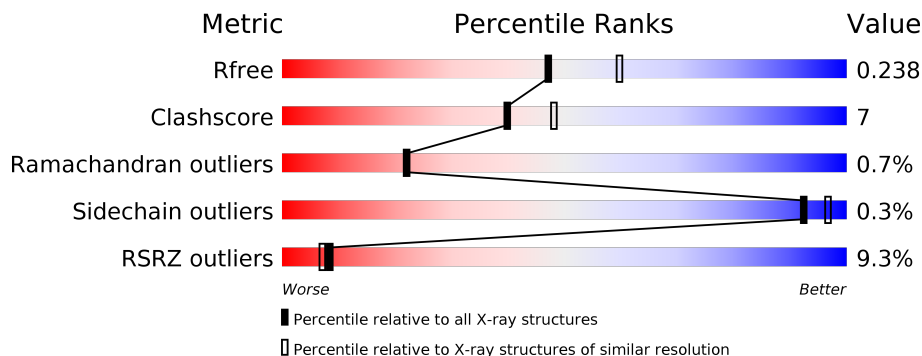
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	464	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OLC	A	1204	-	-	-	X
3	OLC	A	1207	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	A	1216	-	-	X	-

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 3842 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 Endothelin B receptor,Endolysin,Endothelin B receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	430	3372	2211	556	580	25	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

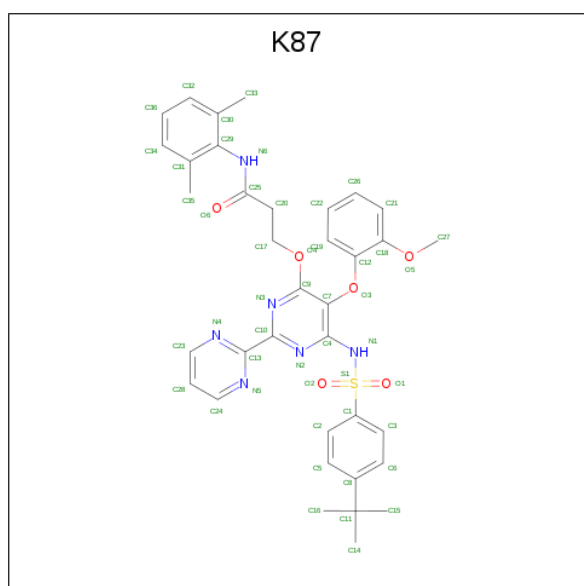
Chain	Residue	Modelled	Actual	Comment	Reference
A	63	GLY	-	expression tag	UNP P24530
A	64	GLY	-	expression tag	UNP P24530
A	65	GLY	-	expression tag	UNP P24530
A	124	TYR	ARG	engineered mutation	UNP P24530
A	154	ALA	ASP	engineered mutation	UNP P24530
A	270	ALA	LYS	engineered mutation	UNP P24530
A	1002	ASN	-	linker	UNP P24530
A	1003	ILE	-	linker	UNP P24530
A	1004	PHE	-	linker	UNP P24530
A	1005	GLU	-	linker	UNP P24530
A	1006	MET	-	linker	UNP P24530
A	1007	LEU	-	linker	UNP P24530
A	1008	ARG	-	linker	UNP P24530
A	1009	ILE	-	linker	UNP P24530
A	1010	ASP	-	linker	UNP P24530
A	1011	GLU	-	linker	UNP P24530
A	1012	GLY	-	linker	UNP P24530
A	1013	GLY	-	linker	UNP P24530
A	1014	GLY	-	linker	UNP P24530
A	1015	SER	-	linker	UNP P24530
A	1016	GLY	-	linker	UNP P24530
A	1017	GLY	-	linker	UNP P24530
A	1054	ALA	CYS	engineered mutation	UNP P00720
A	1094	ARG	ILE	engineered mutation	UNP P00720
A	342	ALA	SER	engineered mutation	UNP P24530
A	381	ALA	ILE	engineered mutation	UNP P24530
A	396	ALA	CYS	engineered mutation	UNP P24530

Continued on next page...

Continued from previous page...

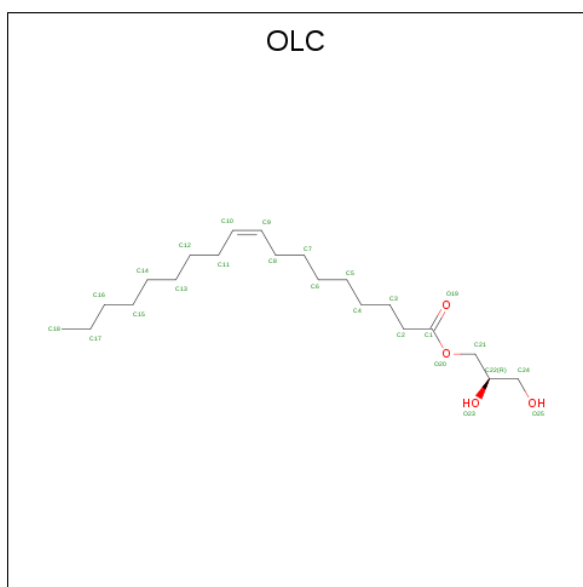
Chain	Residue	Modelled	Actual	Comment	Reference
A	400	ALA	CYS	engineered mutation	UNP P24530
A	405	ALA	CYS	engineered mutation	UNP P24530
A	408	PRO	-	expression tag	UNP P24530
A	409	SER	-	expression tag	UNP P24530
A	410	SER	-	expression tag	UNP P24530
A	411	GLU	-	expression tag	UNP P24530
A	412	ASN	-	expression tag	UNP P24530
A	413	LEU	-	expression tag	UNP P24530
A	414	TYR	-	expression tag	UNP P24530
A	415	PHE	-	expression tag	UNP P24530
A	416	GLN	-	expression tag	UNP P24530

- Molecule 2 is 3-[6-[(4-tert-butylphenyl)sulfonylamino]-5-(2-methoxyphenoxy)-2-pyrimidin-2-yl-pyrimidin-4-yl]oxy-N-(2,6-dimethylphenyl)propanamide (three-letter code: K87) (formula: C₃₆H₃₈N₆O₆S).



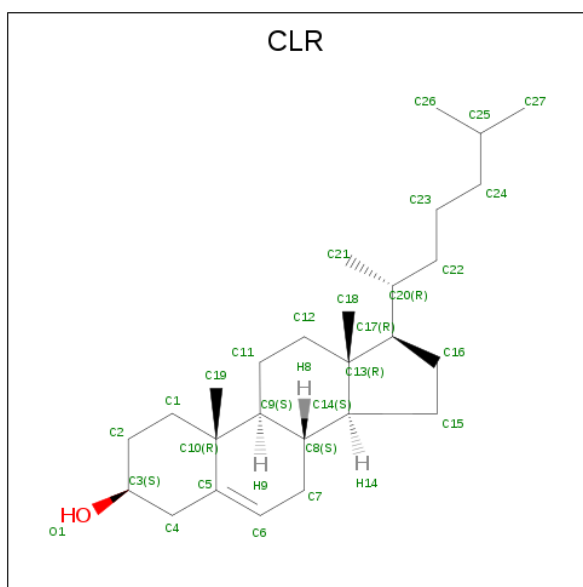
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	49	36	6	6	1	0	0

- Molecule 3 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄).



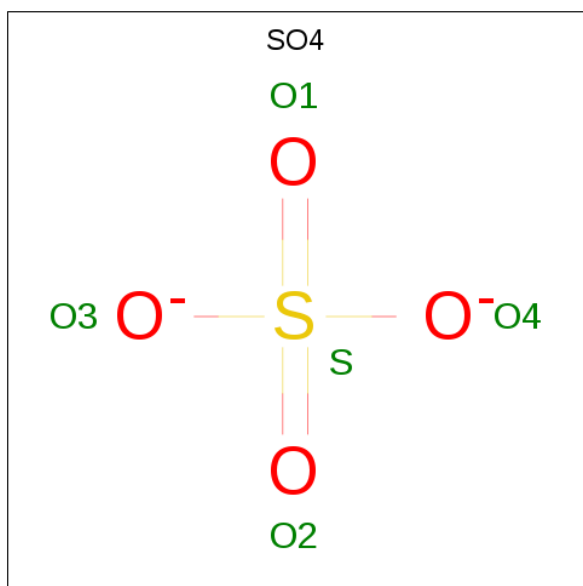
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C 17 17	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C O 20 18 2	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C O 25 21 4	0	0

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



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

- Molecule 5 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O S	0	0
			5	4 1		
5	A	1	Total	O S	0	0
			5	4 1		
5	A	1	Total	O S	0	0
			5	4 1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

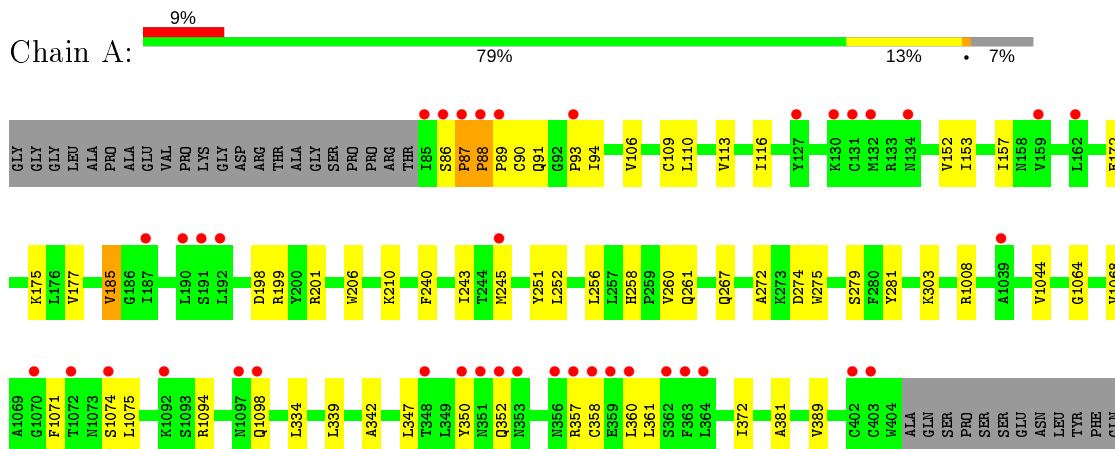
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	106	Total	O	0	0
			106	106		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Endothelin B receptor,Endolysin,Endothelin B receptor



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	74.13Å 147.48Å 108.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.94 – 2.20 41.94 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.94-2.20) 88.5 (41.94-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.211 , 0.239 0.211 , 0.238	Depositor DCC
R_{free} test set	1526 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtrriage
Anisotropy	0.740	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3842	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OLC, SO4, CLR, K87

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	0.29	0/3450	0.44	0/4692

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	3372	0	3451	43	0
2	A	49	0	0	2	0
3	A	262	0	424	19	0
4	A	28	0	46	2	0
5	A	25	0	0	2	0
6	A	106	0	0	0	0
All	All	3842	0	3921	56	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (56) 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:357:ARG:NH1	1:A:358:CYS:SG	2.38	0.95
1:A:90:CYS:SG	1:A:91:GLN:N	2.50	0.85
1:A:352:GLN:HA	1:A:357:ARG:HG3	1.58	0.84
1:A:199:ARG:NH1	5:A:1216:SO4:O1	2.21	0.74
1:A:1044:VAL:HG11	1:A:1075:LEU:HD22	1.73	0.70
1:A:261:GLN:H	1:A:267:GLN:HE21	1.40	0.69
3:A:1208:OLC:H2	3:A:1210:OLC:H7A	1.73	0.69
1:A:272:ALA:HB1	3:A:1202:OLC:H2	1.76	0.66
3:A:1203:OLC:H12	3:A:1205:OLC:H13A	1.83	0.61
1:A:389:VAL:HG23	3:A:1210:OLC:H7	1.83	0.60
1:A:350:TYR:HD1	1:A:360:LEU:HD23	1.65	0.59
1:A:274:ASP:HB3	1:A:347:LEU:HD11	1.85	0.58
1:A:210:LYS:NZ	5:A:1216:SO4:O3	2.35	0.57
1:A:1094:ARG:O	1:A:1098:GLN:HG3	2.06	0.56
1:A:90:CYS:HB2	1:A:357:ARG:NH1	2.21	0.55
1:A:350:TYR:OH	1:A:361:LEU:HD12	2.08	0.54
3:A:1207:OLC:H21A	3:A:1207:OLC:H3A	1.90	0.54
1:A:258:HIS:CE1	1:A:260:VAL:HG22	2.43	0.53
1:A:175:LYS:NZ	1:A:240:PHE:O	2.28	0.53
1:A:275:TRP:CD2	3:A:1212:OLC:H21	2.45	0.52
1:A:93:PRO:HG3	1:A:361:LEU:HD22	1.92	0.52
1:A:152:VAL:HG23	1:A:153:ILE:HG13	1.92	0.52
1:A:206:TRP:CE2	1:A:303:LYS:HE3	2.46	0.51
1:A:245:MET:HE1	1:A:252:LEU:HD12	1.92	0.51
3:A:1204:OLC:O25	3:A:1204:OLC:O20	2.26	0.50
1:A:113:VAL:HG11	4:A:1213:CLR:H263	1.95	0.48
1:A:185:VAL:HG22	1:A:281:TYR:CD1	2.48	0.48
3:A:1208:OLC:H11	3:A:1208:OLC:H8	1.66	0.47
1:A:1071:PHE:HB3	1:A:1074:SER:HB2	1.97	0.47
3:A:1203:OLC:H5	3:A:1205:OLC:H6	1.97	0.46
1:A:381:ALA:HB1	3:A:1210:OLC:H13	1.98	0.46
1:A:106:VAL:HG21	3:A:1209:OLC:H6	1.97	0.46
3:A:1203:OLC:H8A	3:A:1203:OLC:H11	1.65	0.46
1:A:157:ILE:HG21	1:A:177:VAL:HG21	1.98	0.46
3:A:1203:OLC:H7	3:A:1203:OLC:H4	1.52	0.45
3:A:1206:OLC:H8A	3:A:1206:OLC:H11	1.67	0.45
1:A:279:SER:HB3	3:A:1202:OLC:C9	2.46	0.45
3:A:1207:OLC:H8	3:A:1207:OLC:H11	1.74	0.45
1:A:334:LEU:HD12	3:A:1208:OLC:H7	1.97	0.45
1:A:251:TYR:O	1:A:252:LEU:HD23	2.18	0.44
2:A:1201:K87:C1	2:A:1201:K87:N2	2.81	0.43
1:A:198:ASP:OD2	1:A:201:ARG:NH2	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1202:OLC:H8A	3:A:1202:OLC:H11A	1.56	0.43
1:A:1064:GLY:O	1:A:1068:VAL:HG23	2.19	0.42
3:A:1208:OLC:H18A	3:A:1210:OLC:H10	2.00	0.42
1:A:87:PRO:HA	1:A:88:PRO:HD3	1.91	0.42
1:A:90:CYS:O	1:A:94:ILE:HD11	2.19	0.42
1:A:110:LEU:HA	1:A:110:LEU:HD23	1.82	0.41
1:A:243:ILE:HG12	1:A:256:LEU:CD2	2.50	0.41
1:A:86:SER:HA	1:A:87:PRO:HD3	1.68	0.41
1:A:339:LEU:O	1:A:342:ALA:HB3	2.21	0.41
1:A:109:CYS:SG	4:A:1213:CLR:H181	2.61	0.40
1:A:372:ILE:HD13	2:A:1201:K87:C24	2.51	0.40
1:A:113:VAL:O	1:A:116:ILE:HG22	2.21	0.40
1:A:1008:ARG:HA	1:A:1008:ARG:HD3	1.70	0.40
1:A:172:GLU:CD	1:A:172:GLU:H	2.24	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	428/464 (92%)	423 (99%)	2 (0%)	3 (1%)	22 22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	PRO
1	A	88	PRO
1	A	89	PRO

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	360/395 (91%)	359 (100%)	1 (0%)	92 97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	VAL

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

Mol	Chain	Res	Type
1	A	267	GLN
1	A	317	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

18 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	1203	-	24,24,24	0.91	1 (4%)	25,25,25	1.01	1 (4%)
3	OLC	A	1204	-	24,24,24	0.93	1 (4%)	25,25,25	0.81	1 (4%)
3	OLC	A	1207	-	24,24,24	0.95	1 (4%)	25,25,25	0.97	2 (8%)
3	OLC	A	1208	-	24,24,24	0.91	1 (4%)	25,25,25	0.95	1 (4%)
3	OLC	A	1202	-	24,24,24	0.91	1 (4%)	25,25,25	0.89	1 (4%)
5	SO4	A	1216	-	4,4,4	0.14	0	6,6,6	0.06	0
2	K87	A	1201	-	52,53,53	1.02	3 (5%)	71,76,76	0.61	1 (1%)
3	OLC	A	1206	-	16,16,24	0.21	0	15,15,25	0.61	0
3	OLC	A	1210	-	16,19,24	0.23	0	15,19,25	0.57	0
3	OLC	A	1205	-	24,24,24	0.92	1 (4%)	25,25,25	0.86	1 (4%)
3	OLC	A	1211	-	24,24,24	0.92	1 (4%)	25,25,25	0.94	1 (4%)
5	SO4	A	1215	-	4,4,4	0.13	0	6,6,6	0.06	0
3	OLC	A	1209	-	24,24,24	0.94	1 (4%)	25,25,25	0.80	1 (4%)
3	OLC	A	1212	-	24,24,24	0.96	1 (4%)	25,25,25	0.98	2 (8%)
4	CLR	A	1213	-	31,31,31	0.76	1 (3%)	48,48,48	1.04	2 (4%)
5	SO4	A	1214	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	A	1218	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	A	1217	-	4,4,4	0.14	0	6,6,6	0.04	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	1203	-	-	11/24/24/24	-
3	OLC	A	1204	-	-	10/24/24/24	-
3	OLC	A	1207	-	-	9/24/24/24	-
3	OLC	A	1208	-	-	5/24/24/24	-
3	OLC	A	1202	-	-	10/24/24/24	-
2	K87	A	1201	-	-	7/37/37/37	0/5/5/5
3	OLC	A	1206	-	-	5/14/14/24	-
3	OLC	A	1210	-	-	5/15/17/24	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OLC	A	1205	-	-	3/24/24/24	-
3	OLC	A	1211	-	-	6/24/24/24	-
3	OLC	A	1209	-	-	6/24/24/24	-
3	OLC	A	1212	-	-	14/24/24/24	-
4	CLR	A	1213	-	-	1/10/68/68	0/4/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	K87	C4-N1	-4.55	1.32	1.40
3	A	1207	OLC	O20-C1	4.41	1.46	1.33
3	A	1212	OLC	O20-C1	4.39	1.46	1.33
3	A	1209	OLC	O20-C1	4.37	1.46	1.33
3	A	1204	OLC	O20-C1	4.29	1.45	1.33
3	A	1211	OLC	O20-C1	4.28	1.45	1.33
3	A	1205	OLC	O20-C1	4.26	1.45	1.33
3	A	1208	OLC	O20-C1	4.24	1.45	1.33
3	A	1203	OLC	O20-C1	4.21	1.45	1.33
3	A	1202	OLC	O20-C1	4.21	1.45	1.33
2	A	1201	K87	O5-C18	3.93	1.43	1.37
4	A	1213	CLR	C10-C9	-2.26	1.52	1.56
2	A	1201	K87	O4-C9	2.17	1.38	1.35

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1212	OLC	O20-C1-C2	3.09	121.61	111.91
3	A	1207	OLC	O20-C1-C2	3.05	121.48	111.91
3	A	1203	OLC	O20-C1-C2	3.00	121.34	111.91
3	A	1208	OLC	O20-C1-C2	2.92	121.06	111.91
3	A	1211	OLC	O20-C1-C2	2.89	120.99	111.91
3	A	1202	OLC	O20-C1-C2	2.79	120.66	111.91
3	A	1205	OLC	O20-C1-C2	2.64	120.18	111.91
3	A	1209	OLC	O20-C1-C2	2.50	119.75	111.91
3	A	1204	OLC	O20-C1-C2	2.33	119.22	111.91
2	A	1201	K87	O4-C9-N3	-2.21	116.91	120.00
3	A	1207	OLC	O20-C1-O19	-2.15	118.16	123.59
3	A	1212	OLC	O20-C1-O19	-2.12	118.25	123.59
4	A	1213	CLR	C11-C9-C10	-2.10	110.31	113.08
4	A	1213	CLR	C7-C8-C9	2.09	112.25	109.71

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1212	OLC	C21-C22-C24-O25
3	A	1212	OLC	O20-C21-C22-O23
3	A	1207	OLC	O19-C1-O20-C21
3	A	1207	OLC	C2-C1-O20-C21
3	A	1208	OLC	C2-C1-O20-C21
3	A	1208	OLC	O19-C1-O20-C21
4	A	1213	CLR	C21-C20-C22-C23
3	A	1212	OLC	C2-C1-O20-C21
3	A	1212	OLC	O20-C21-C22-C24
3	A	1212	OLC	O19-C1-O20-C21
3	A	1203	OLC	C1-C2-C3-C4
3	A	1212	OLC	C1-C2-C3-C4
3	A	1209	OLC	C1-C2-C3-C4
3	A	1204	OLC	C2-C1-O20-C21
3	A	1203	OLC	C12-C13-C14-C15
3	A	1202	OLC	C4-C5-C6-C7
3	A	1206	OLC	C11-C12-C13-C14
3	A	1204	OLC	O20-C21-C22-O23
3	A	1207	OLC	C4-C5-C6-C7
3	A	1204	OLC	O19-C1-O20-C21
3	A	1206	OLC	C4-C5-C6-C7
3	A	1207	OLC	C3-C4-C5-C6
3	A	1212	OLC	C2-C3-C4-C5
3	A	1203	OLC	C2-C3-C4-C5
3	A	1203	OLC	C3-C4-C5-C6
3	A	1204	OLC	O20-C21-C22-C24
3	A	1210	OLC	C12-C13-C14-C15
3	A	1204	OLC	C14-C15-C16-C17
3	A	1206	OLC	C6-C7-C8-C9
3	A	1211	OLC	C6-C7-C8-C9
3	A	1212	OLC	C12-C13-C14-C15
3	A	1209	OLC	C14-C15-C16-C17
2	A	1201	K87	C2-C1-S1-O2
3	A	1212	OLC	C15-C16-C17-C18
3	A	1209	OLC	C3-C4-C5-C6
3	A	1206	OLC	C10-C11-C12-C13
3	A	1203	OLC	C15-C16-C17-C18
3	A	1203	OLC	C14-C15-C16-C17
3	A	1203	OLC	C11-C12-C13-C14
3	A	1212	OLC	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1210	OLC	C11-C12-C13-C14
3	A	1208	OLC	C13-C14-C15-C16
3	A	1209	OLC	C12-C13-C14-C15
3	A	1203	OLC	C4-C5-C6-C7
3	A	1202	OLC	C3-C4-C5-C6
2	A	1201	K87	C3-C1-S1-O2
3	A	1203	OLC	C5-C6-C7-C8
3	A	1202	OLC	C2-C3-C4-C5
2	A	1201	K87	C17-C20-C25-N6
2	A	1201	K87	C17-C20-C25-O6
3	A	1212	OLC	O23-C22-C24-O25
3	A	1210	OLC	C1-C2-C3-C4
3	A	1206	OLC	C12-C13-C14-C15
3	A	1202	OLC	O20-C21-C22-C24
3	A	1202	OLC	C11-C12-C13-C14
3	A	1204	OLC	C11-C12-C13-C14
3	A	1202	OLC	C6-C7-C8-C9
3	A	1204	OLC	C3-C4-C5-C6
3	A	1207	OLC	C15-C16-C17-C18
3	A	1207	OLC	C5-C6-C7-C8
3	A	1203	OLC	C2-C1-O20-C21
3	A	1208	OLC	C10-C11-C12-C13
3	A	1212	OLC	C10-C11-C12-C13
3	A	1205	OLC	C12-C13-C14-C15
3	A	1204	OLC	C5-C6-C7-C8
3	A	1210	OLC	C7-C8-C9-C10
3	A	1204	OLC	C15-C16-C17-C18
2	A	1201	K87	C2-C1-S1-N1
3	A	1211	OLC	C1-C2-C3-C4
3	A	1211	OLC	C5-C6-C7-C8
3	A	1212	OLC	C13-C14-C15-C16
3	A	1209	OLC	C4-C5-C6-C7
3	A	1203	OLC	O19-C1-O20-C21
3	A	1211	OLC	C9-C10-C11-C12
3	A	1202	OLC	O20-C1-C2-C3
3	A	1209	OLC	C13-C14-C15-C16
3	A	1202	OLC	C15-C16-C17-C18
3	A	1212	OLC	C7-C8-C9-C10
3	A	1211	OLC	C4-C5-C6-C7
3	A	1207	OLC	O20-C21-C22-C24
3	A	1207	OLC	O20-C1-C2-C3
3	A	1204	OLC	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

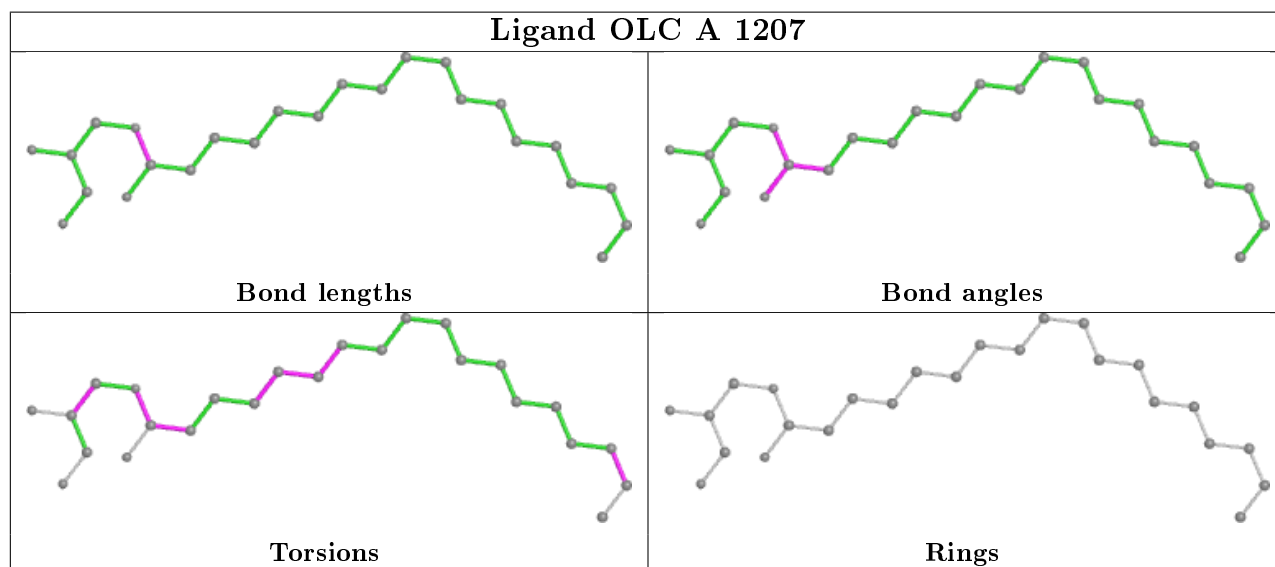
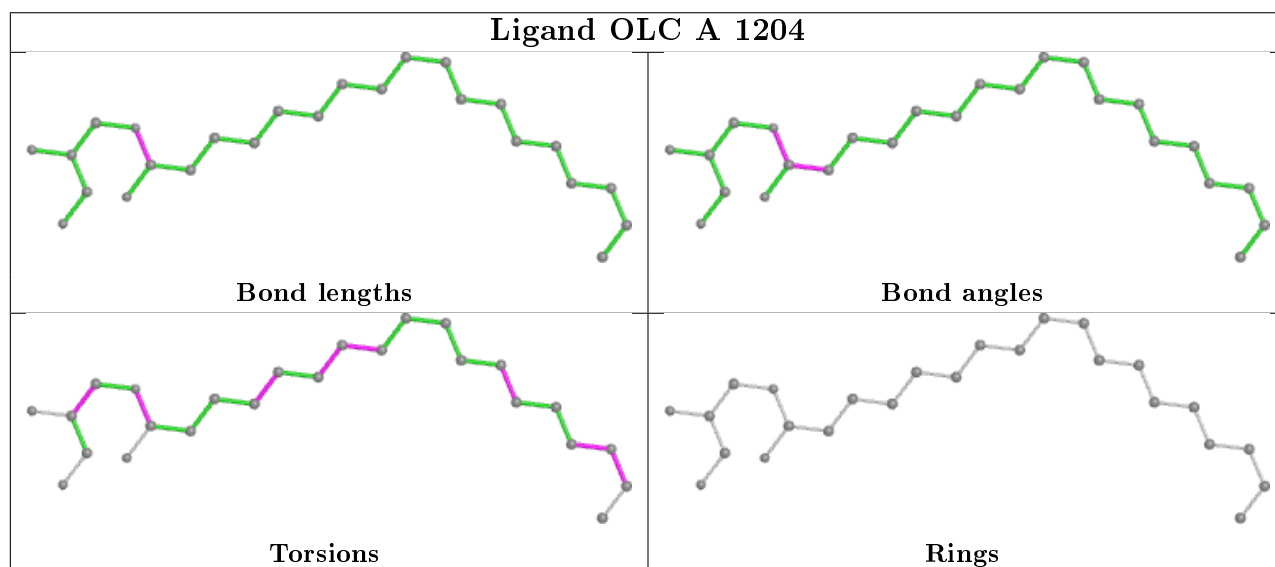
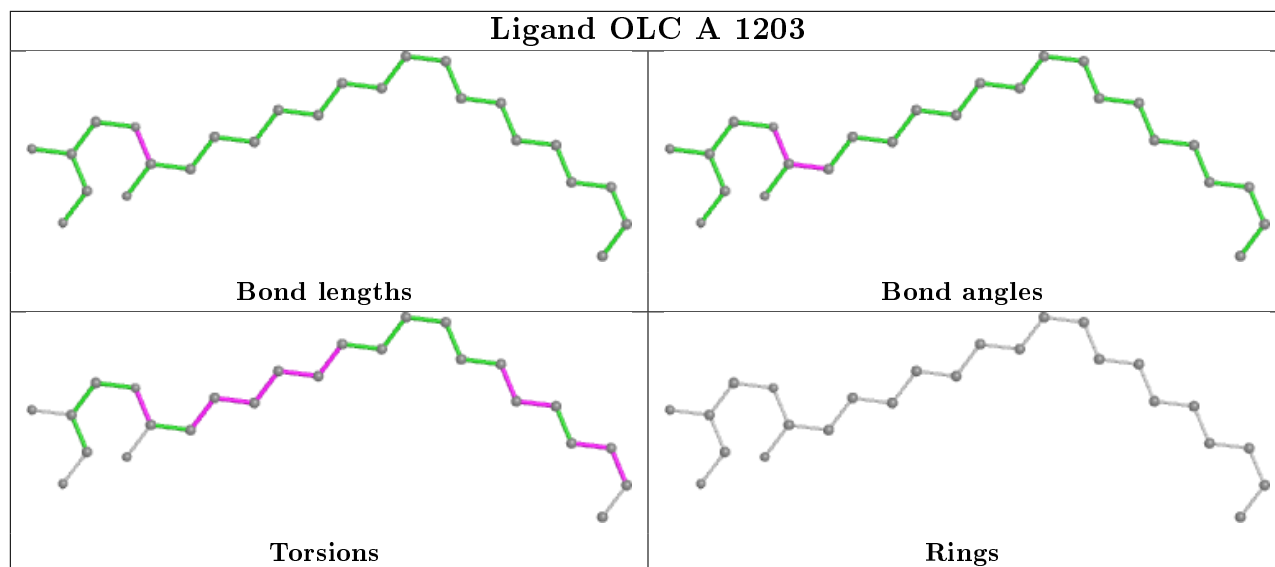
Mol	Chain	Res	Type	Atoms
3	A	1210	OLC	C4-C5-C6-C7
3	A	1211	OLC	C21-C22-C24-O25
3	A	1202	OLC	O20-C21-C22-O23
3	A	1202	OLC	O19-C1-C2-C3
3	A	1205	OLC	C9-C10-C11-C12
2	A	1201	K87	C15-C11-C8-C5
3	A	1205	OLC	C1-C2-C3-C4
3	A	1208	OLC	C5-C6-C7-C8
2	A	1201	K87	C3-C1-S1-N1
3	A	1207	OLC	O19-C1-C2-C3

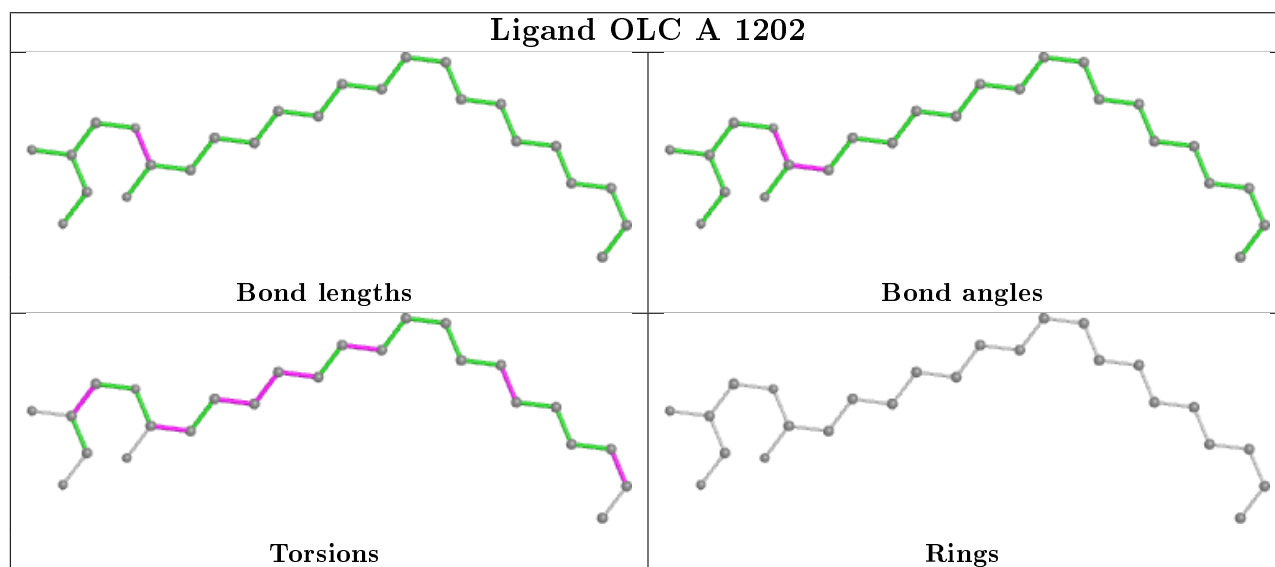
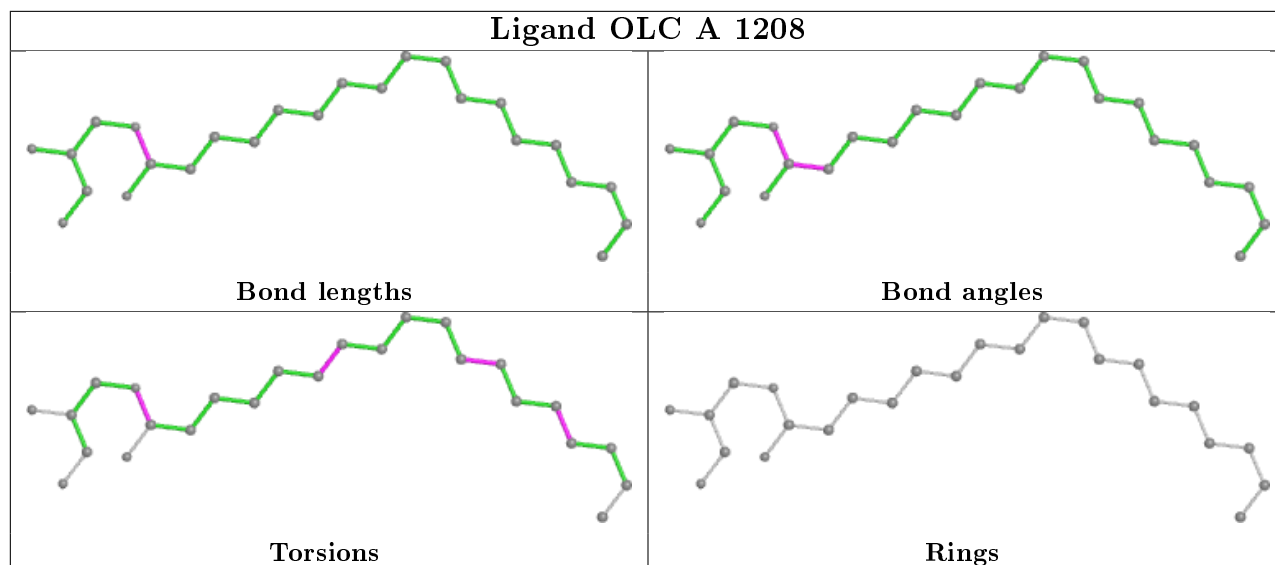
There are no ring outliers.

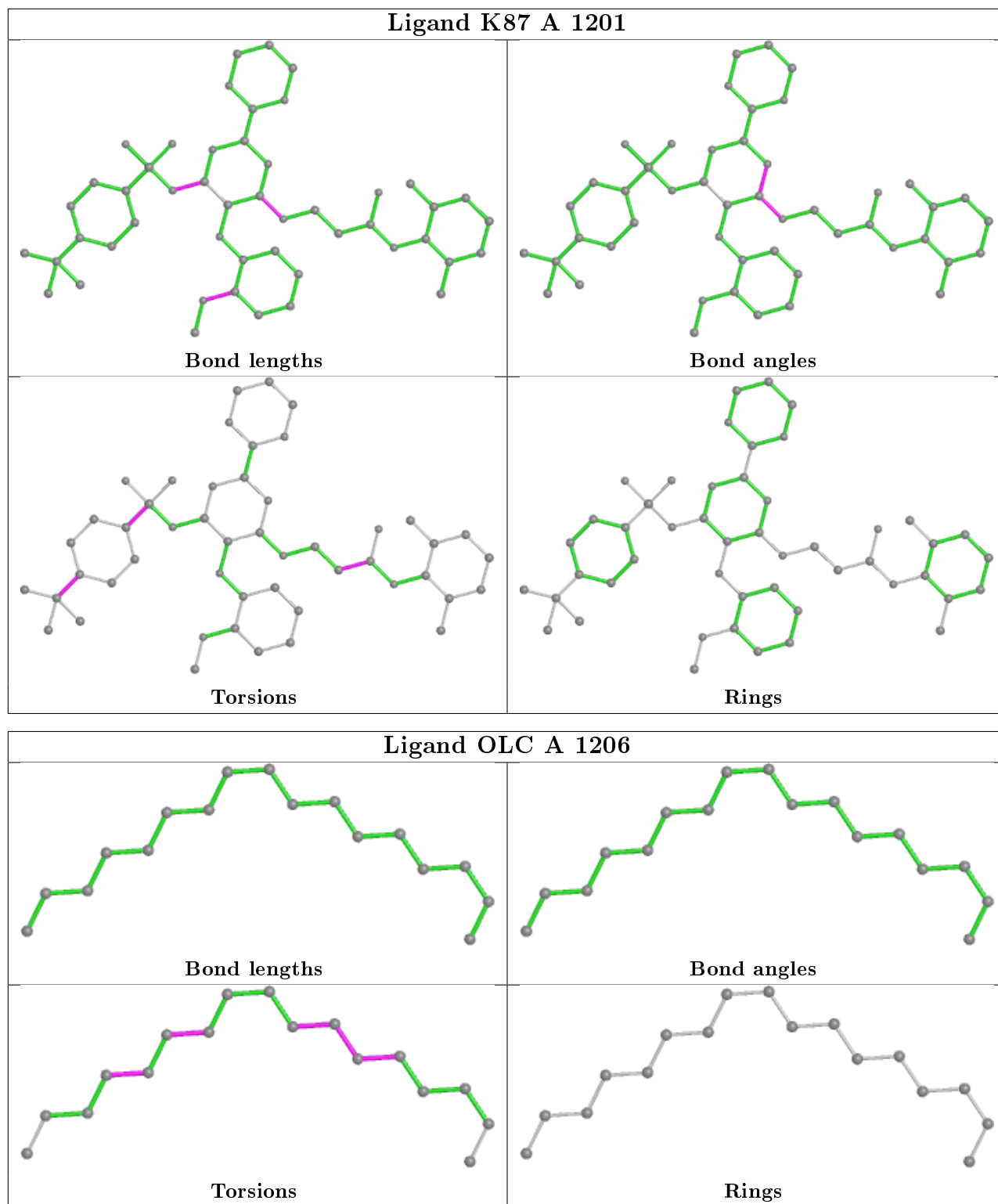
13 monomers are involved in 25 short contacts:

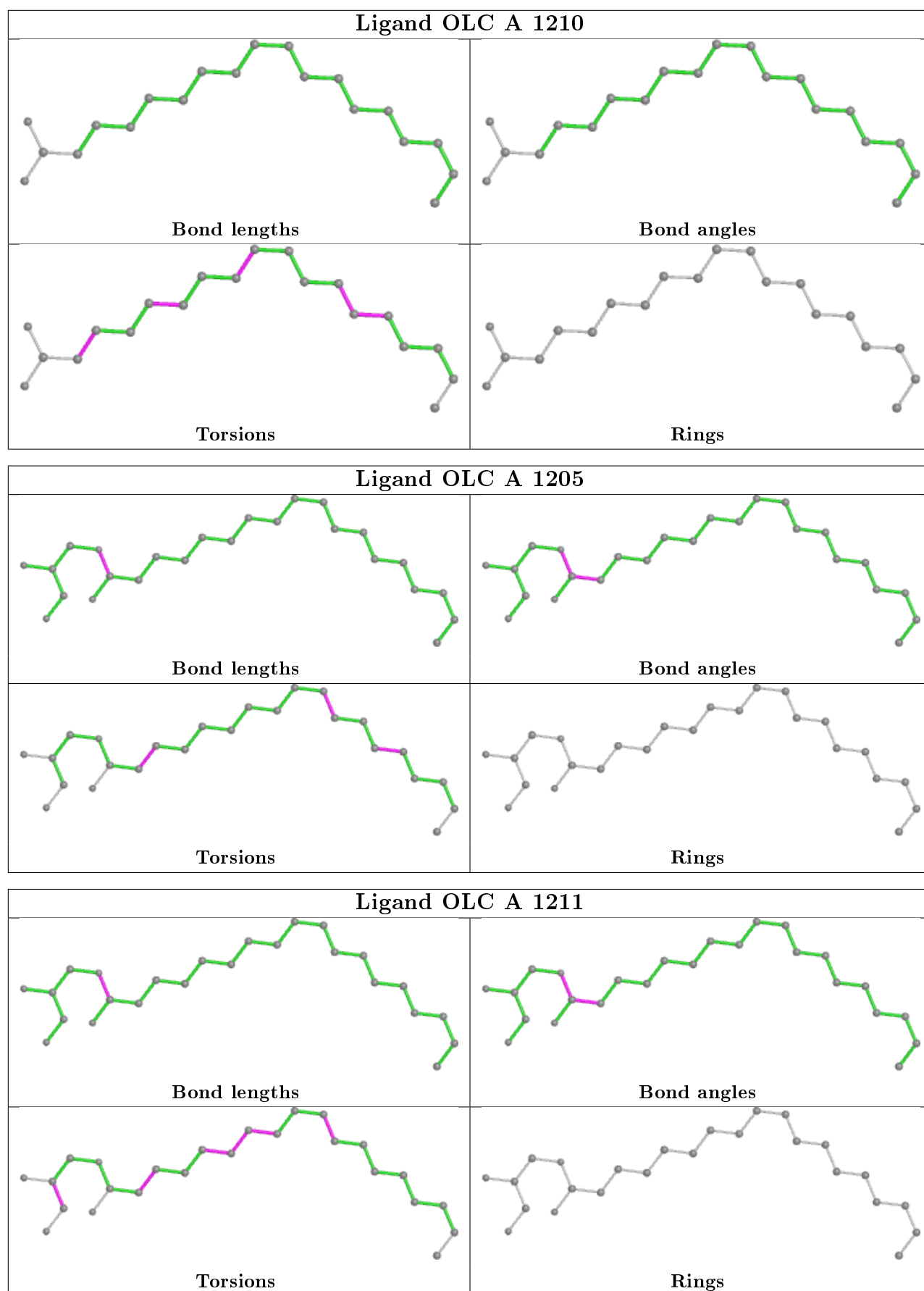
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1203	OLC	4	0
3	A	1204	OLC	1	0
3	A	1207	OLC	2	0
3	A	1208	OLC	4	0
3	A	1202	OLC	3	0
5	A	1216	SO4	2	0
2	A	1201	K87	2	0
3	A	1206	OLC	1	0
3	A	1210	OLC	4	0
3	A	1205	OLC	2	0
3	A	1209	OLC	1	0
3	A	1212	OLC	1	0
4	A	1213	CLR	2	0

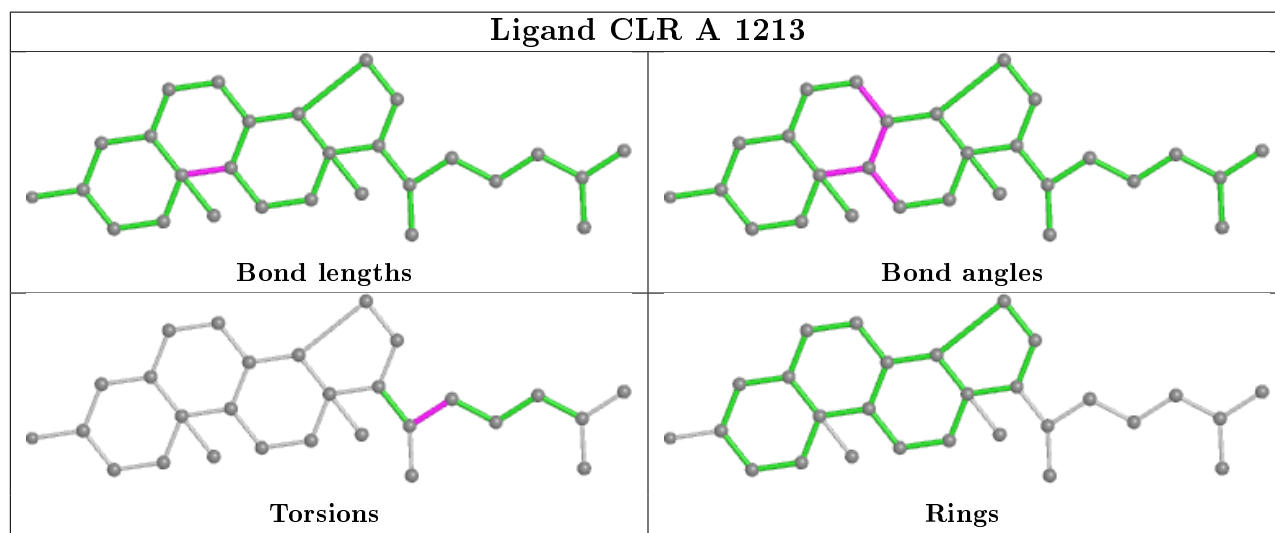
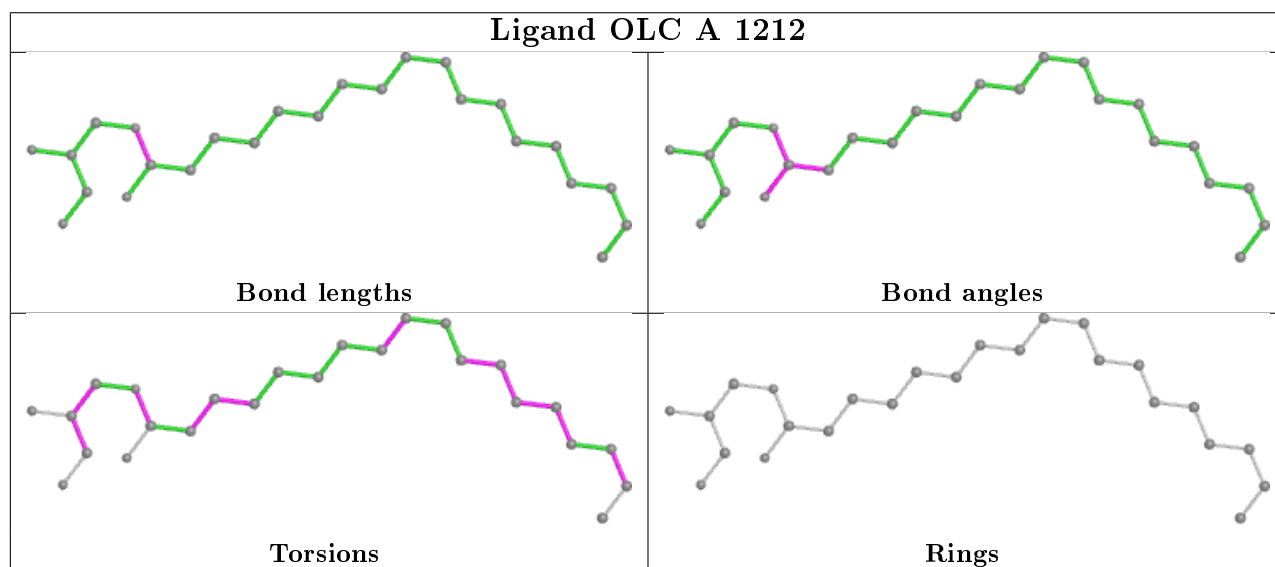
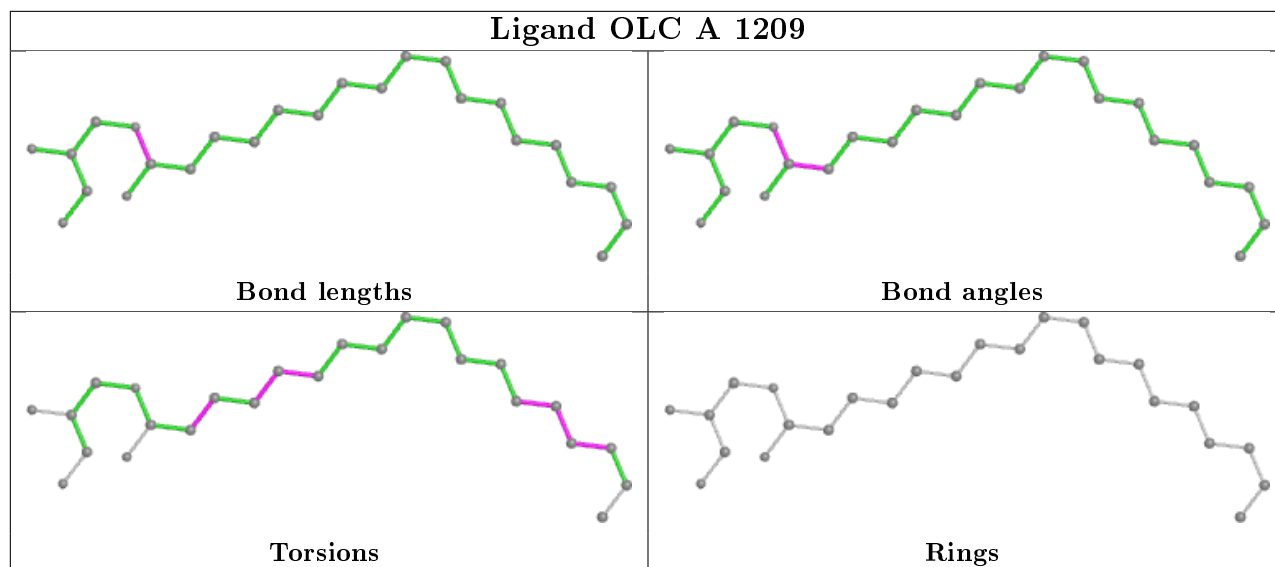
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	430/464 (92%)	0.44	40 (9%) 8 7	30, 50, 93, 129	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	89	PRO	8.3
1	A	131	CYS	6.8
1	A	358	CYS	6.8
1	A	127	TYR	5.4
1	A	357	ARG	5.3
1	A	350	TYR	4.9
1	A	352	GLN	4.5
1	A	403	CYS	4.4
1	A	351	ASN	4.3
1	A	1072	THR	3.9
1	A	88	PRO	3.6
1	A	356	ASN	3.6
1	A	93	PRO	3.5
1	A	363	PHE	3.4
1	A	1074	SER	3.4
1	A	1092	LYS	3.3
1	A	87	PRO	3.2
1	A	132	MET	3.1
1	A	359	GLU	3.0
1	A	86	SER	2.9
1	A	348	THR	2.9
1	A	1098	GLN	2.8
1	A	360	LEU	2.8
1	A	134	ASN	2.8
1	A	362	SER	2.7
1	A	190	LEU	2.6
1	A	192	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	364	LEU	2.5
1	A	402	CYS	2.4
1	A	1097	ASN	2.3
1	A	130	LYS	2.3
1	A	1070	GLY	2.3
1	A	353	ASN	2.2
1	A	85	ILE	2.2
1	A	1039	ALA	2.1
1	A	245	MET	2.1
1	A	159	VAL	2.1
1	A	187	ILE	2.0
1	A	191	SER	2.0
1	A	162	LEU	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 carbohydrates 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.

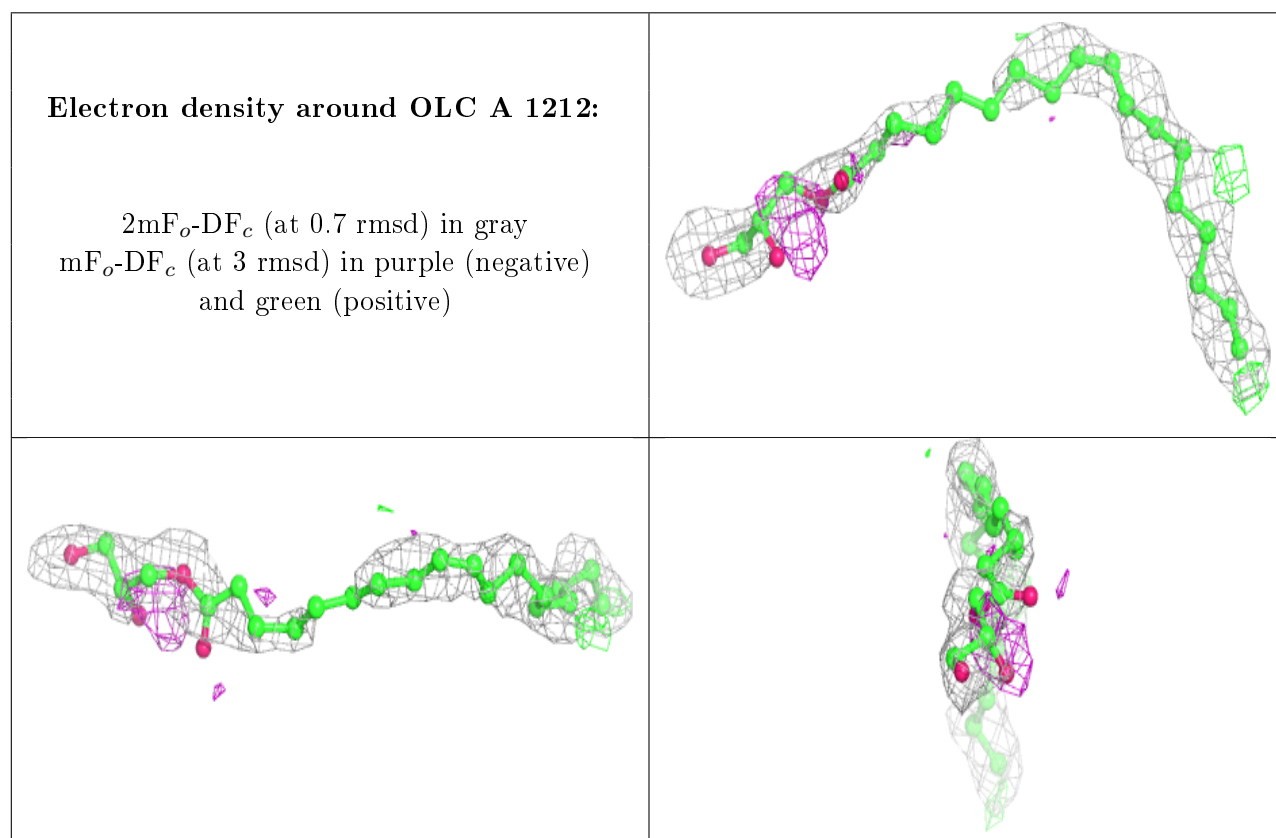
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	OLC	A	1212	25/25	0.57	0.34	45,68,82,87	0
3	OLC	A	1207	25/25	0.60	0.40	62,78,114,118	0
3	OLC	A	1211	25/25	0.68	0.29	57,79,104,107	0
3	OLC	A	1204	25/25	0.69	0.40	51,83,121,123	0
3	OLC	A	1209	25/25	0.70	0.31	57,72,85,90	0
3	OLC	A	1205	25/25	0.70	0.30	61,81,98,99	0
3	OLC	A	1208	25/25	0.71	0.36	62,78,89,93	0
3	OLC	A	1202	25/25	0.76	0.27	47,58,84,85	0
3	OLC	A	1203	25/25	0.77	0.28	41,72,85,92	0
3	OLC	A	1206	17/25	0.82	0.20	44,51,77,83	0

Continued on next page...

Continued from previous page...

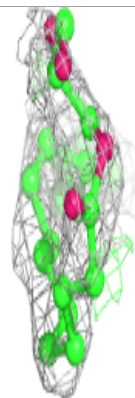
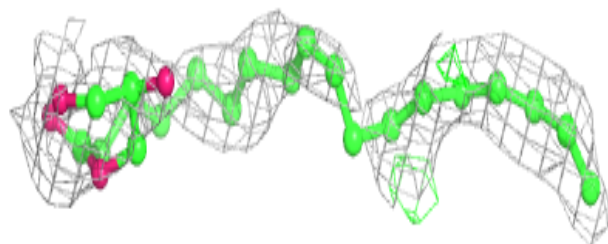
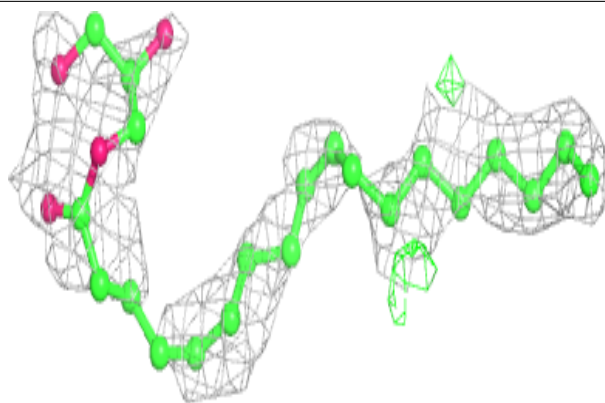
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	A	1218	5/5	0.84	0.18	89,89,93,96	5
3	OLC	A	1210	20/25	0.85	0.19	52,69,77,81	0
5	SO4	A	1217	5/5	0.85	0.36	105,110,113,119	0
4	CLR	A	1213	28/28	0.86	0.22	42,51,58,65	0
5	SO4	A	1216	5/5	0.91	0.15	75,86,95,96	0
2	K87	A	1201	49/49	0.96	0.17	26,37,47,53	0
5	SO4	A	1215	5/5	0.97	0.09	73,75,78,79	0
5	SO4	A	1214	5/5	0.97	0.12	67,70,74,79	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.

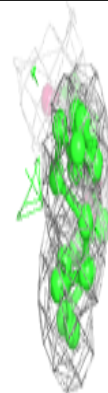
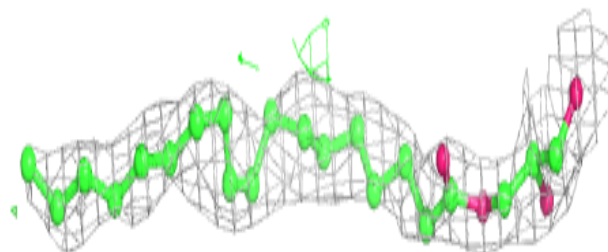
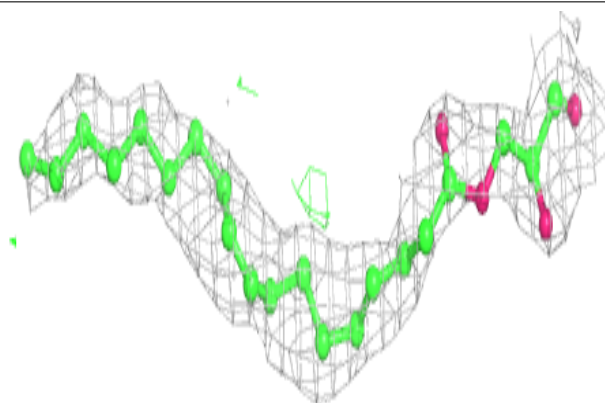


Electron density around OLC A 1207:

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

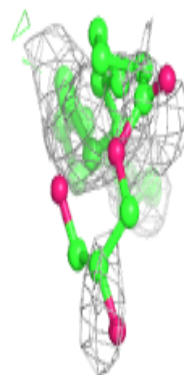
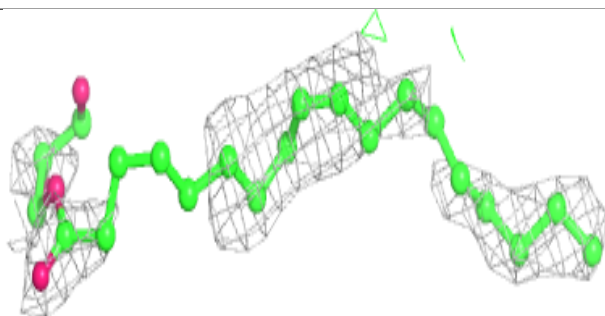
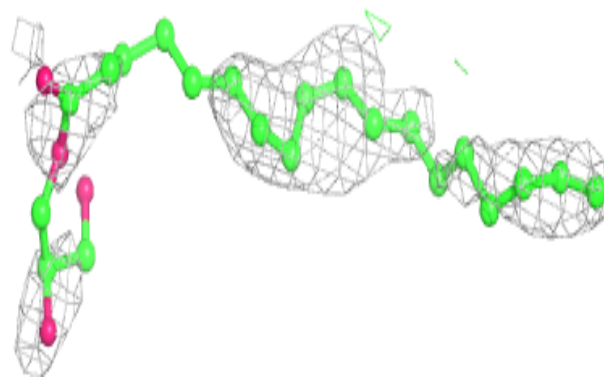
**Electron density around OLC A 1211:**

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

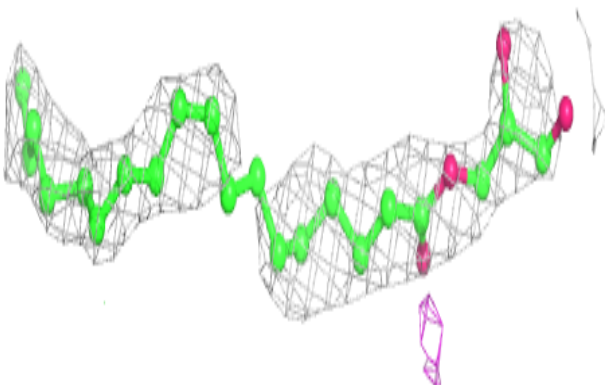
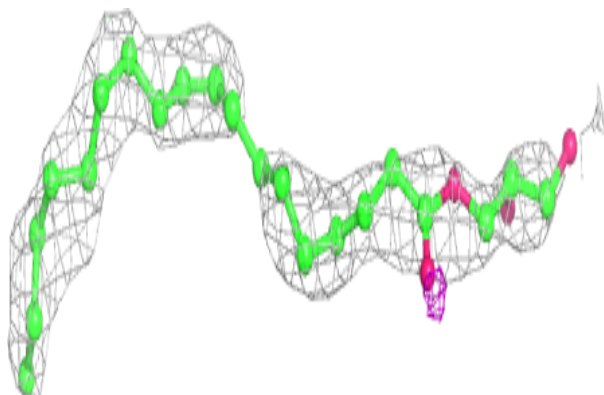


Electron density around OLC A 1204:

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

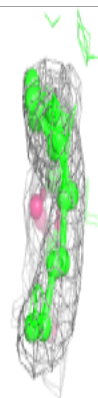
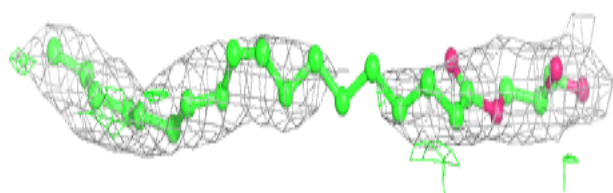
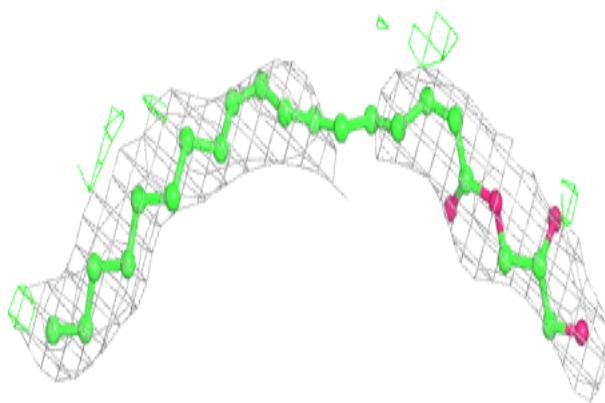
**Electron density around OLC A 1209:**

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

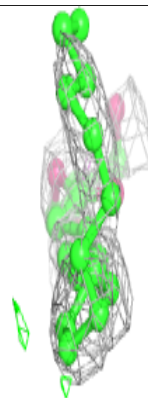
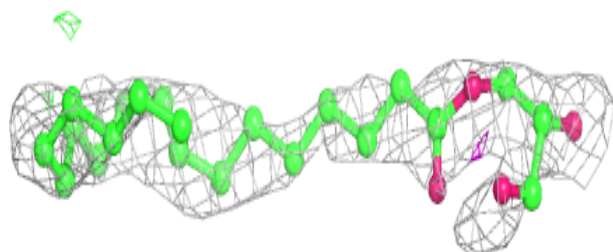
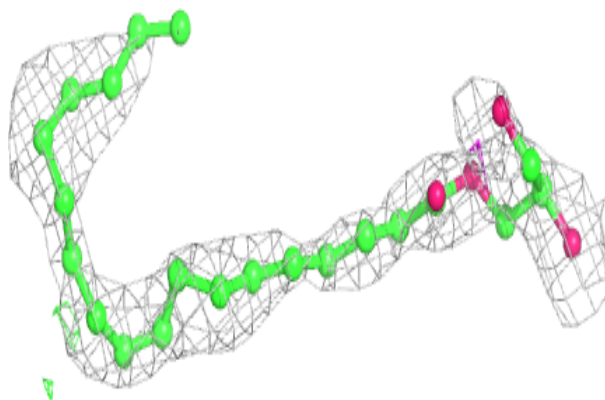


Electron density around OLC A 1205:

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

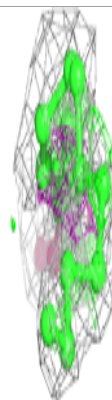
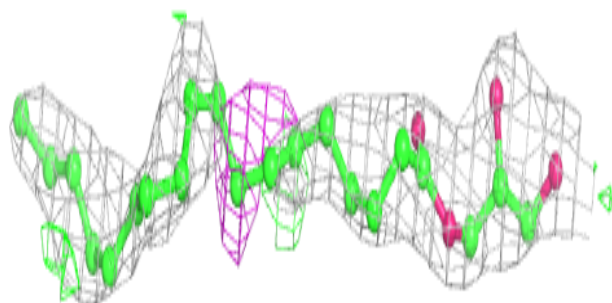
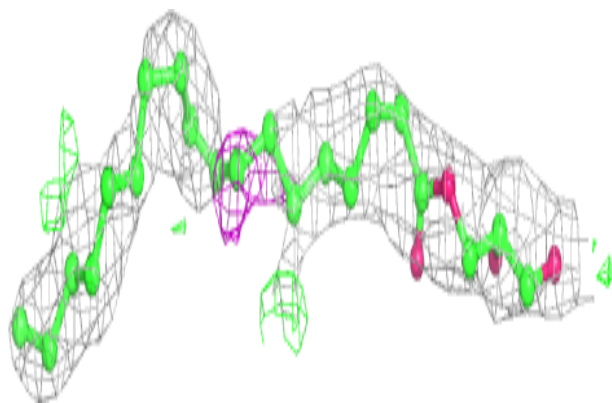
**Electron density around OLC A 1208:**

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

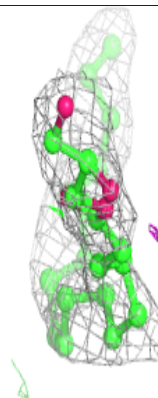
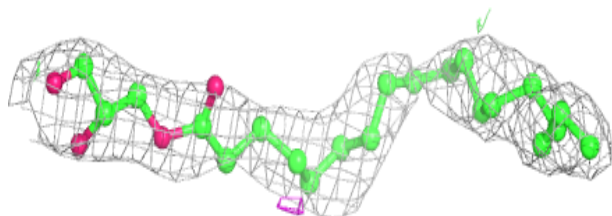
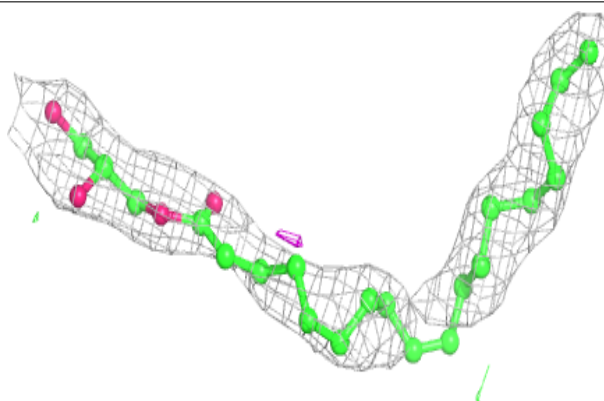


Electron density around OLC A 1202:

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

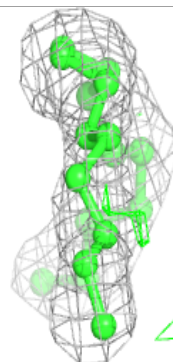
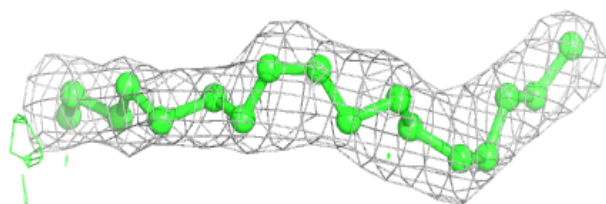
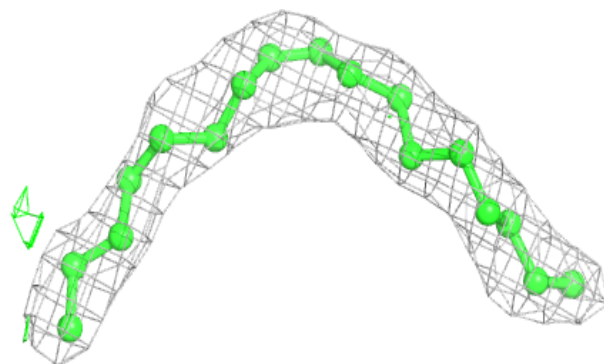
**Electron density around OLC A 1203:**

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

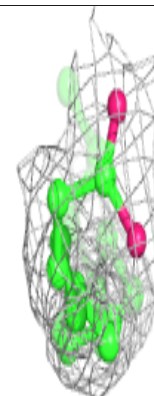
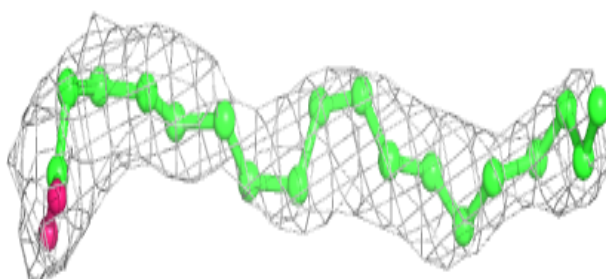
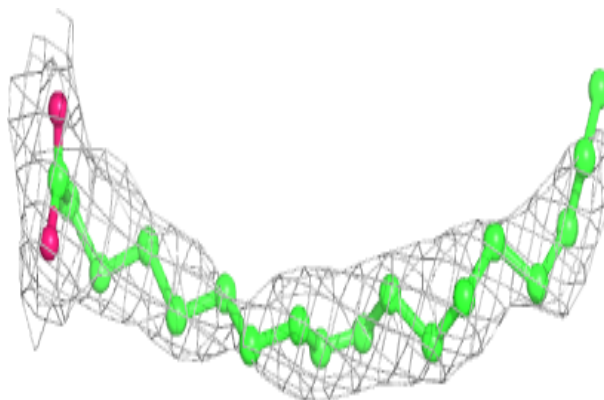


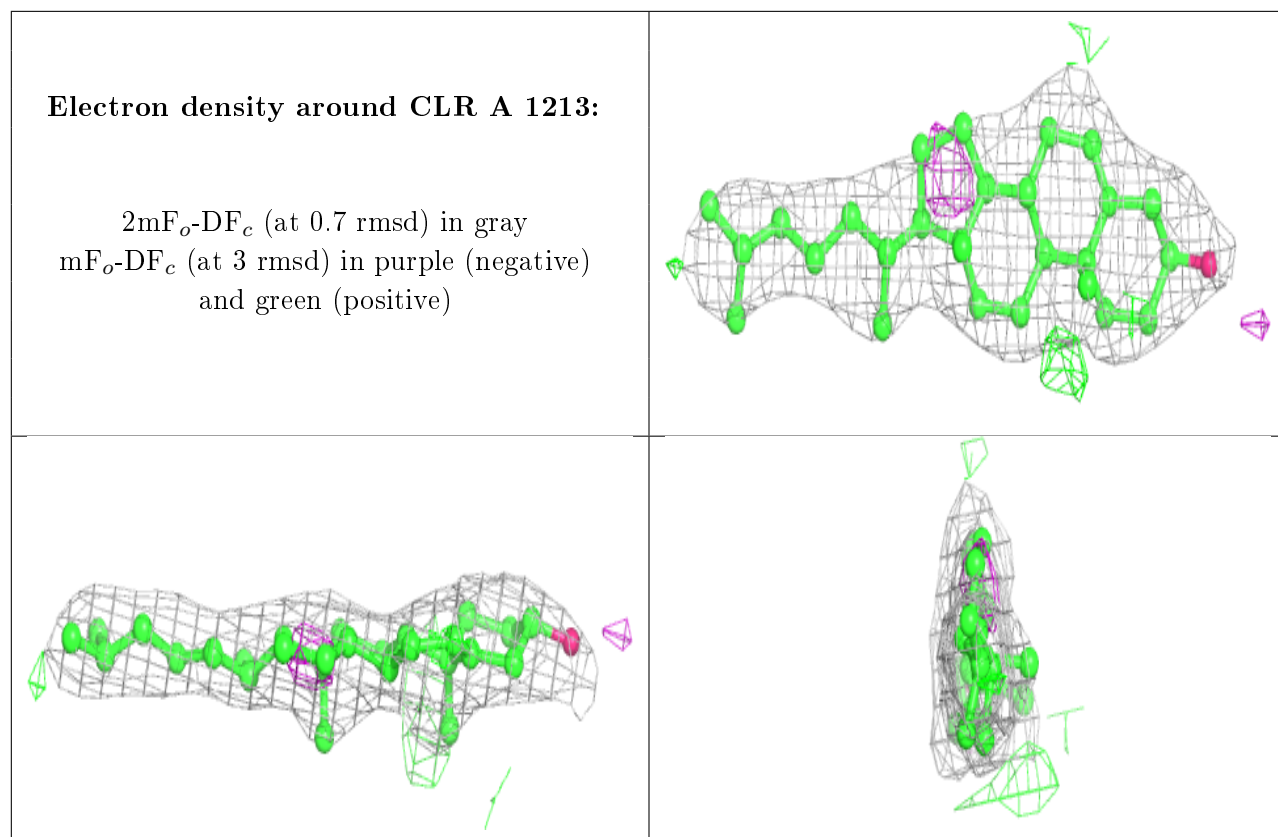
Electron density around OLC A 1206:

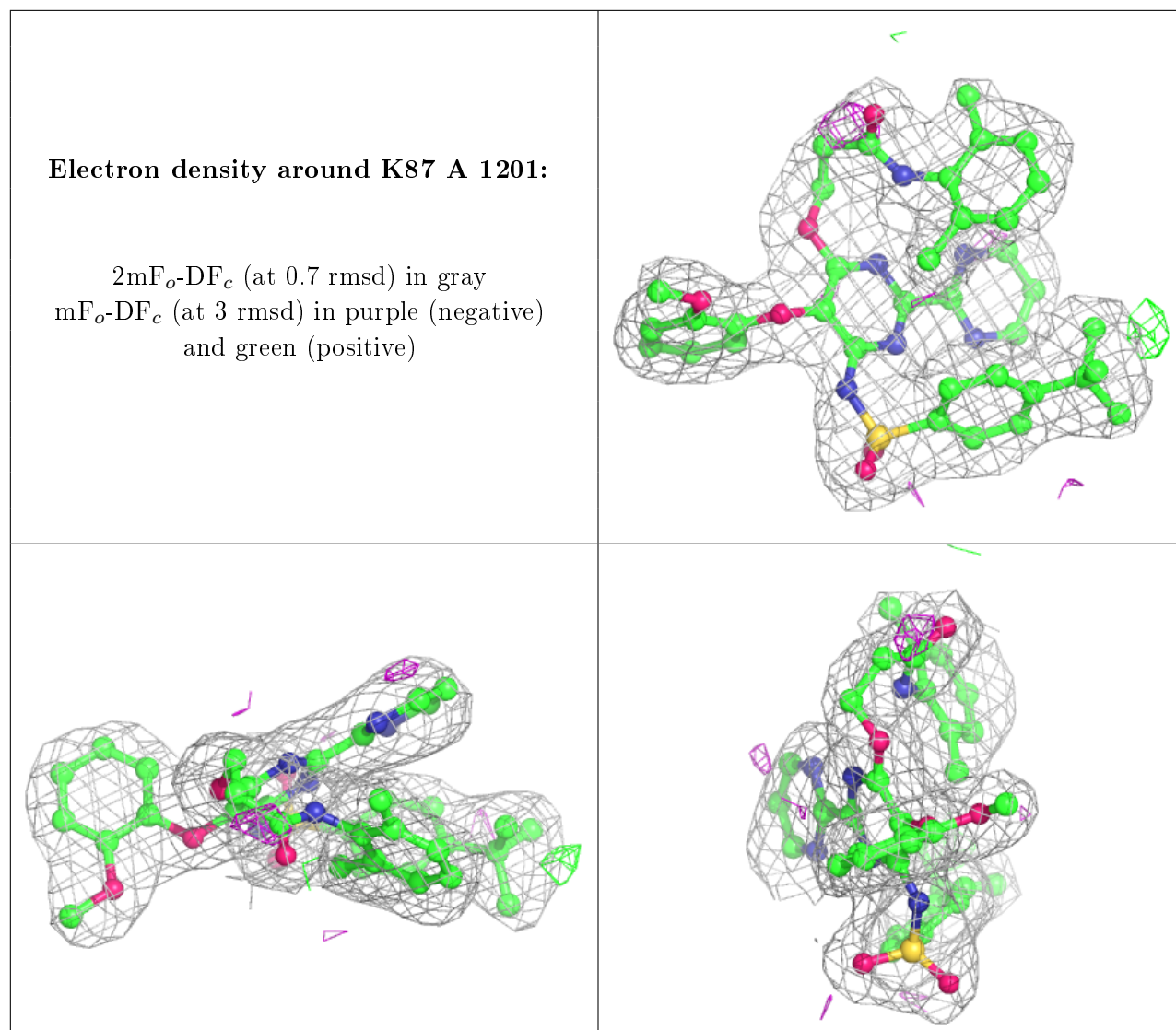
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around OLC A 1210:**

$2mF_o-DF_c$ (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.