



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2022 – 08:20 PM EDT

PDB ID : 5UVI
Title : Serial Millisecond Crystallography of Membrane and Soluble Protein Micro-crystals using Synchrotron Radiation
Authors : Martin-Garcia, J.M.; Conrad, C.E.; Nelson, G.; Stander, N.; Zatsepin, N.A.; Zook, J.; Zhu, L.; Geiger, J.; Chun, E.; Kissick, D.; Hilgart, M.C.; Ogata, C.; Ishchenko, A.; Nagaratnam, N.; Roy-Chowdhury, S.; Coe, J.; Subramanian, G.; Schaffer, A.; James, D.; Ketawala, G.; Venugopalan, N.; Xu, S.; Corcoran, S.; Ferguson, D.; Weierstall, U.; Spence, J.C.H.; Cherezov, V.; Fromme, P.; Fischetti, R.F.; Liu, W.
Deposited on : 2017-02-20
Resolution : 3.20 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	: FAILED
Mogul	: 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	: 1.13
EDS	: FAILED
buster-report	: 1.1.7 (2018)
Percentile statistics	: 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.27

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 3.20 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3130 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 Adenosine receptor A2a,Soluble cytochrome b562,Adenosine receptor A2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			2978	1946	496	515	21			

There are 39 discrepancies between the modelled and reference sequences:

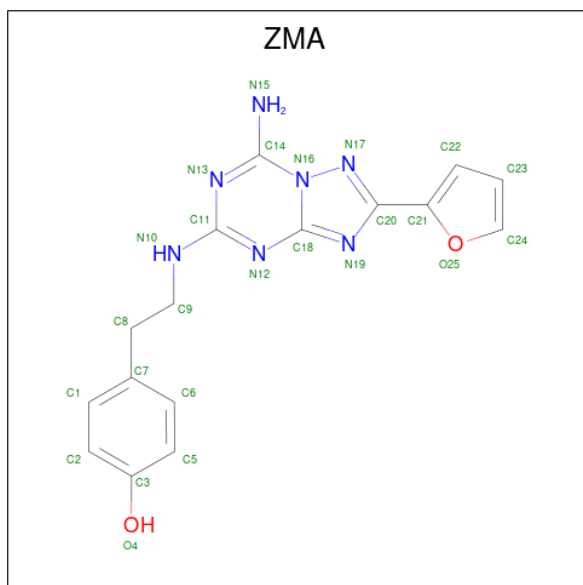
Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP P29274
A	-23	LYS	-	expression tag	UNP P29274
A	-22	THR	-	expression tag	UNP P29274
A	-21	ILE	-	expression tag	UNP P29274
A	-20	ILE	-	expression tag	UNP P29274
A	-19	ALA	-	expression tag	UNP P29274
A	-18	LEU	-	expression tag	UNP P29274
A	-17	SER	-	expression tag	UNP P29274
A	-16	TYR	-	expression tag	UNP P29274
A	-15	ILE	-	expression tag	UNP P29274
A	-14	PHE	-	expression tag	UNP P29274
A	-13	CYS	-	expression tag	UNP P29274
A	-12	LEU	-	expression tag	UNP P29274
A	-11	VAL	-	expression tag	UNP P29274
A	-10	PHE	-	expression tag	UNP P29274
A	-9	ALA	-	expression tag	UNP P29274
A	-8	ASP	-	expression tag	UNP P29274
A	-7	TYR	-	expression tag	UNP P29274
A	-6	LYS	-	expression tag	UNP P29274
A	-5	ASP	-	expression tag	UNP P29274
A	-4	ASP	-	expression tag	UNP P29274
A	-3	ASP	-	expression tag	UNP P29274
A	-2	ASP	-	expression tag	UNP P29274
A	-1	GLY	-	expression tag	UNP P29274
A	0	ALA	-	expression tag	UNP P29274
A	1	PRO	-	expression tag	UNP P29274

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	ARG	engineered mutation	UNP P0ABE7
A	317	HIS	-	expression tag	UNP P29274
A	318	HIS	-	expression tag	UNP P29274
A	319	HIS	-	expression tag	UNP P29274
A	320	HIS	-	expression tag	UNP P29274
A	321	HIS	-	expression tag	UNP P29274
A	322	HIS	-	expression tag	UNP P29274
A	323	HIS	-	expression tag	UNP P29274
A	324	HIS	-	expression tag	UNP P29274
A	325	HIS	-	expression tag	UNP P29274
A	326	HIS	-	expression tag	UNP P29274

- Molecule 2 is 4-{2-[(7-amino-2-furan-2-yl)[1,2,4]triazolo[1,5-a][1,3,5]triazin-5-yl)amino]ethyl}phenol (three-letter code: ZMA) (formula: C₁₆H₁₅N₇O₂).



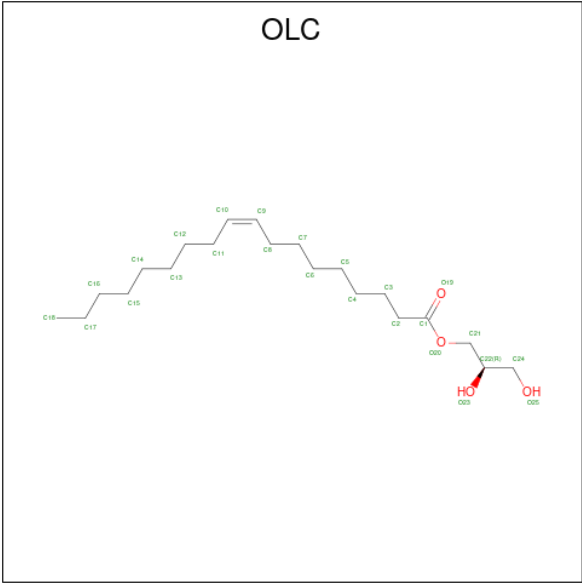
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	16	7	2		

- Molecule 3 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).



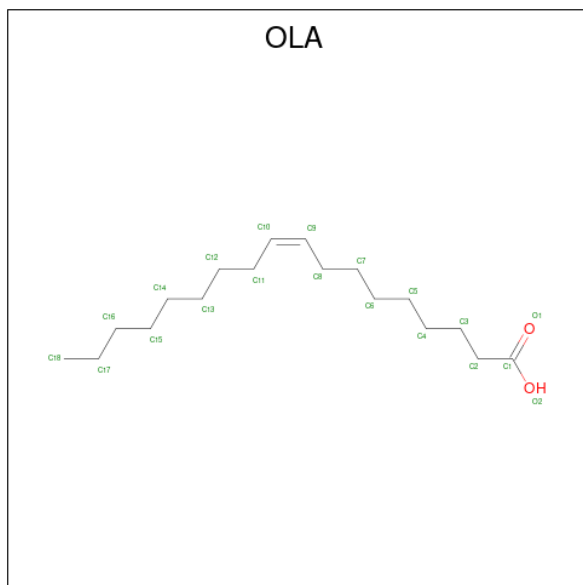
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			28	27	1		
3	A	1	Total	C	O	0	0
			28	27	1		
3	A	1	Total	C	O	0	0
			28	27	1		

- Molecule 4 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	12	4		
4	A	1	Total	C	O	0	0
			18	14	4		

- 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	0	0
			9	7	2		

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	40.30Å 180.30Å 142.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 3.20	Depositor
% Data completeness (in resolution range)	99.8 (45.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.241 , 0.287	Depositor
Wilson B-factor (Å ²)	114.4	Xtriage
Anisotropy	0.117	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3130	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

7 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	1205	-	15,15,24	1.15	1 (6%)	16,16,25	0.99	1 (6%)
4	OLC	A	1206	-	17,17,24	1.08	1 (5%)	18,18,25	1.02	1 (5%)
2	ZMA	A	1201	-	21,28,28	0.49	0	22,39,39	1.80	5 (22%)
5	OLA	A	1207	-	5,8,19	0.24	0	4,8,19	0.56	0
3	CLR	A	1203	-	31,31,31	0.70	0	48,48,48	1.17	5 (10%)
3	CLR	A	1202	-	31,31,31	0.71	0	48,48,48	1.17	5 (10%)
3	CLR	A	1204	-	31,31,31	0.71	0	48,48,48	1.17	5 (10%)

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	1205	-	-	10/15/15/24	-
4	OLC	A	1206	-	-	8/17/17/24	-
2	ZMA	A	1201	-	-	2/6/10/10	0/4/4/4
5	OLA	A	1207	-	-	4/4/6/17	-
3	CLR	A	1203	-	-	2/10/68/68	0/4/4/4
3	CLR	A	1202	-	-	1/10/68/68	0/4/4/4
3	CLR	A	1204	-	-	2/10/68/68	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1205	OLC	O20-C1	4.28	1.45	1.33
4	A	1206	OLC	O20-C1	4.21	1.45	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	ZMA	N12-C11-N13	-4.51	119.09	126.23
2	A	1201	ZMA	N15-C14-N16	3.70	120.46	117.97
3	A	1203	CLR	C13-C17-C20	-3.34	114.25	119.49
3	A	1204	CLR	C13-C17-C20	-3.34	114.26	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1202	CLR	C13-C17-C20	-3.31	114.30	119.49
2	A	1201	ZMA	N17-C20-N19	3.03	116.56	114.56
4	A	1205	OLC	O20-C1-C2	2.64	120.18	111.91
2	A	1201	ZMA	N15-C14-N13	2.61	120.46	117.03
3	A	1203	CLR	C11-C12-C13	-2.57	108.38	112.78
3	A	1202	CLR	C11-C12-C13	-2.54	108.42	112.78
3	A	1204	CLR	C11-C12-C13	-2.53	108.45	112.78
3	A	1203	CLR	C13-C14-C8	-2.53	110.64	114.38
4	A	1206	OLC	O20-C1-C2	2.52	119.81	111.91
3	A	1204	CLR	C13-C14-C8	-2.51	110.67	114.38
3	A	1202	CLR	C13-C14-C8	-2.48	110.72	114.38
3	A	1202	CLR	C4-C5-C10	2.26	119.42	116.42
3	A	1202	CLR	C17-C13-C14	2.26	102.75	100.07
3	A	1204	CLR	C4-C5-C10	2.23	119.38	116.42
3	A	1204	CLR	C17-C13-C14	2.21	102.69	100.07
3	A	1203	CLR	C4-C5-C10	2.21	119.35	116.42
3	A	1203	CLR	C17-C13-C14	2.20	102.68	100.07
2	A	1201	ZMA	C9-N10-C11	-2.17	119.99	123.75

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1205	OLC	C21-C22-C24-O25
4	A	1205	OLC	O20-C21-C22-O23
4	A	1206	OLC	C21-C22-C24-O25
5	A	1207	OLA	C1-C2-C3-C4
3	A	1203	CLR	C22-C23-C24-C25
3	A	1204	CLR	C20-C22-C23-C24
3	A	1202	CLR	C22-C23-C24-C25
4	A	1206	OLC	C3-C4-C5-C6
5	A	1207	OLA	C2-C3-C4-C5
4	A	1205	OLC	C3-C4-C5-C6
4	A	1206	OLC	C6-C7-C8-C9
4	A	1205	OLC	C5-C6-C7-C8
4	A	1205	OLC	O23-C22-C24-O25
4	A	1205	OLC	C4-C5-C6-C7
4	A	1205	OLC	O20-C21-C22-C24
4	A	1206	OLC	O23-C22-C24-O25
4	A	1206	OLC	C2-C1-O20-C21
4	A	1205	OLC	C2-C1-O20-C21
4	A	1206	OLC	O19-C1-O20-C21

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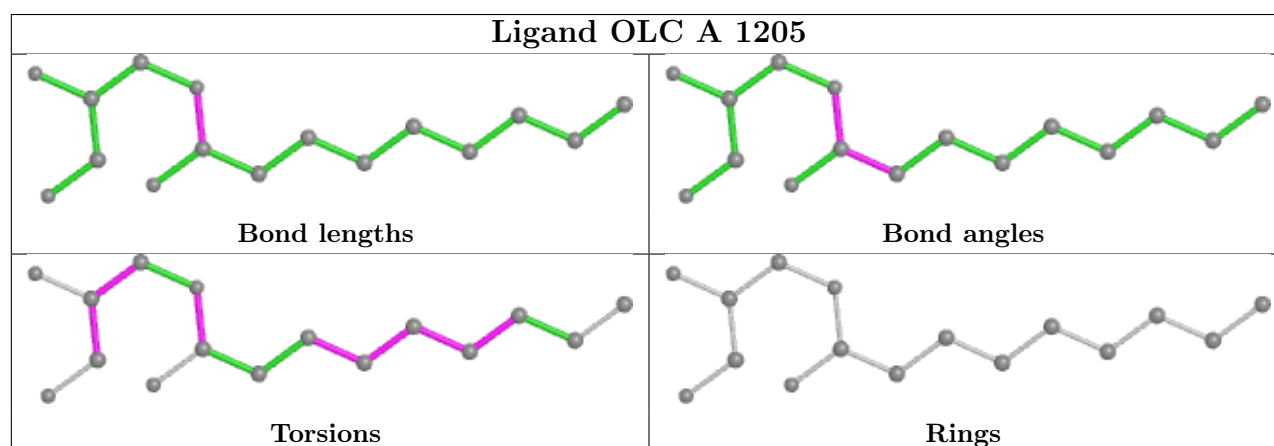
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Mol	Chain	Res	Type	Atoms
4	A	1205	OLC	O19-C1-O20-C21
4	A	1206	OLC	C5-C6-C7-C8
5	A	1207	OLA	C3-C4-C5-C6
3	A	1204	CLR	C22-C23-C24-C25
2	A	1201	ZMA	C1-C7-C8-C9
2	A	1201	ZMA	C6-C7-C8-C9
5	A	1207	OLA	C4-C5-C6-C7
4	A	1206	OLC	C7-C8-C9-C10
4	A	1205	OLC	C2-C3-C4-C5
3	A	1203	CLR	C17-C20-C22-C23

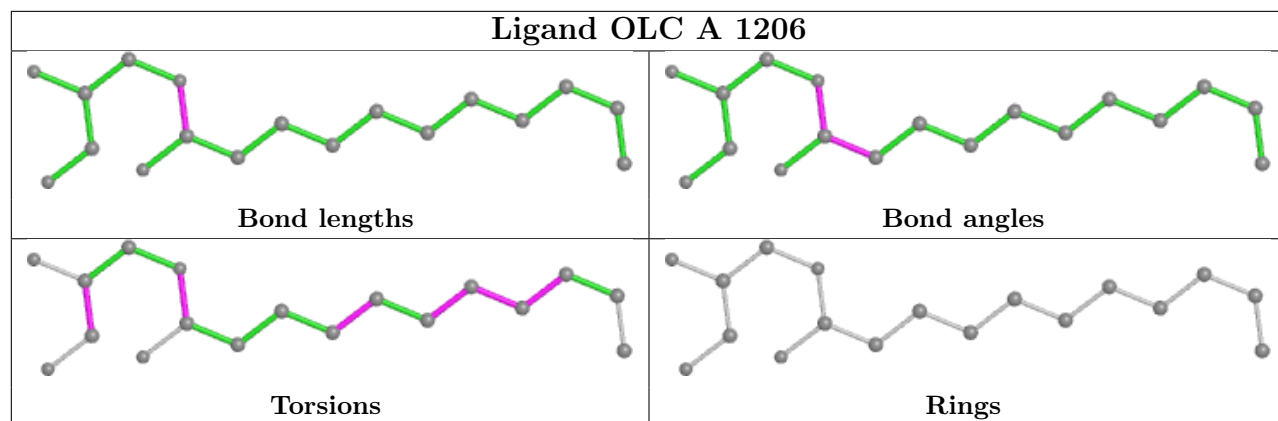
There are no ring outliers.

No monomer is involved in short contacts.

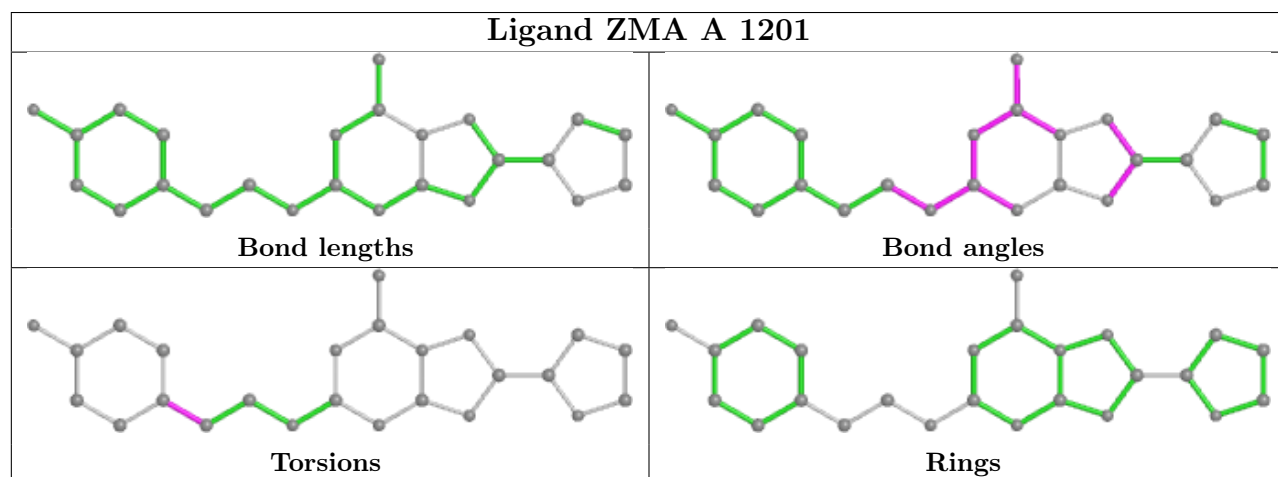
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



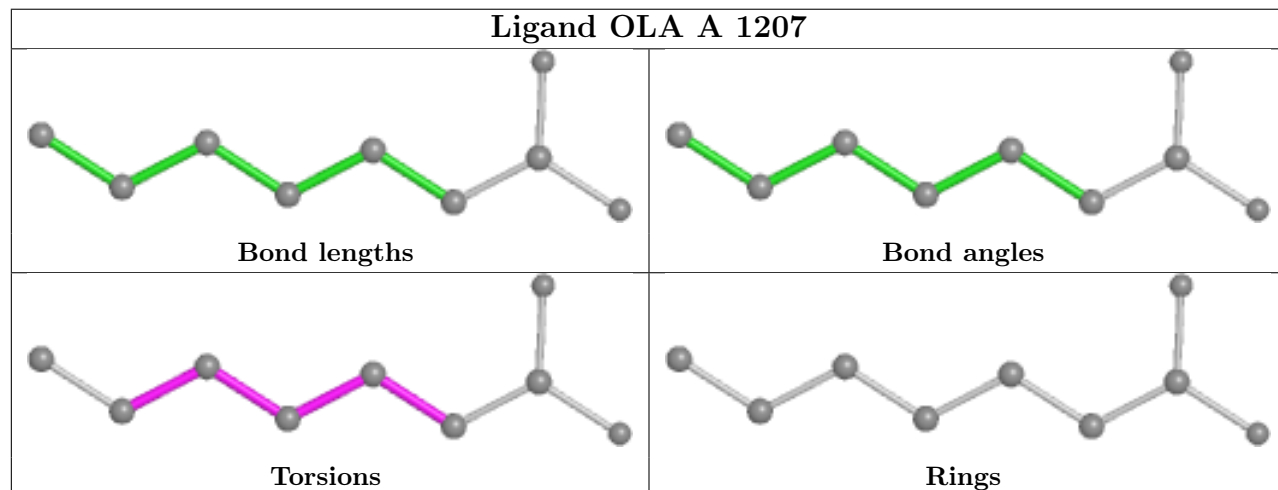
Ligand OLC A 1206

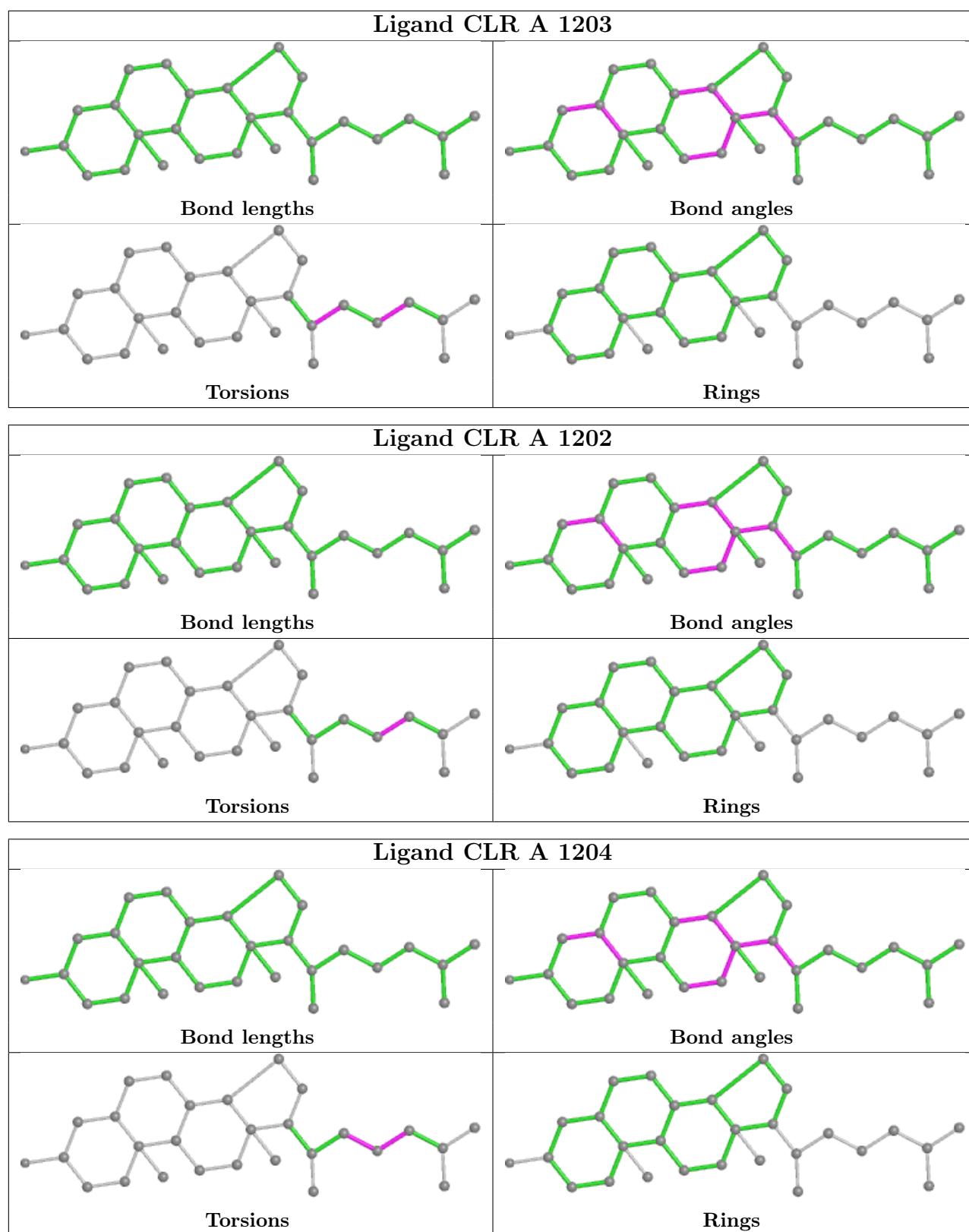


Ligand ZMA A 1201



Ligand OLA A 1207





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

5.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.