



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 2, 2025 – 12:08 pm GMT

PDB ID : 8RWX
Title : Steady state structure of the human adenosine A2A receptor bound to synthetic photoswitch 'StilSwitch3' determined by serial synchrotron crystallography
Authors : Glover, H.; Bertrand, Q.; Weinert, T.
Deposited on : 2024-02-05
Resolution : 3.05 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

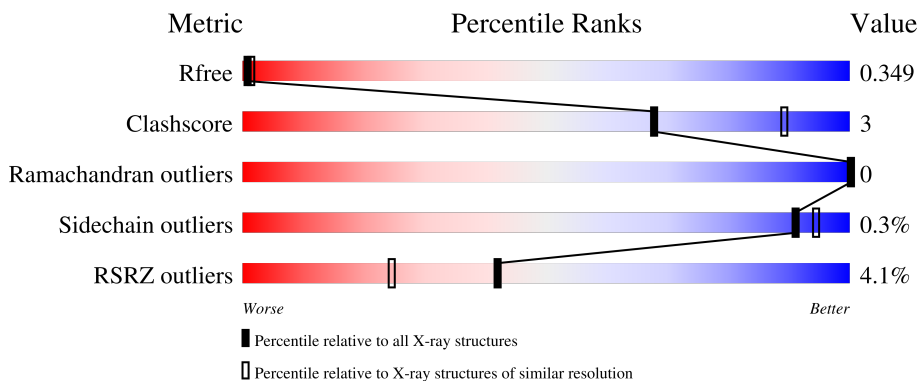
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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}	164625	2258 (3.10-3.02)
Clashscore	180529	2399 (3.10-3.02)
Ramachandran outliers	177936	2269 (3.10-3.02)
Sidechain outliers	177891	2268 (3.10-3.02)
RSRZ outliers	164620	2258 (3.10-3.02)

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 $\leq 5\%$. 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	449	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3170 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	390	2931	1913	484	514	20	0	1	0

There are 48 discrepancies between the modelled and reference sequences:

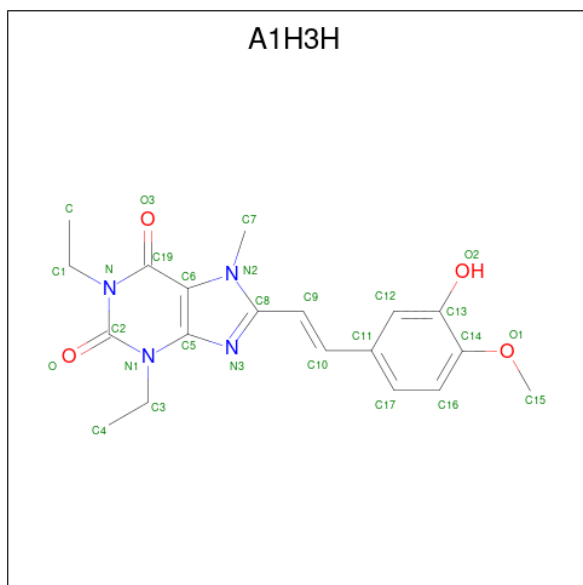
Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP P29274
A	-23	LYS	-	expression tag	UNP P29274
A	-22	THR	-	expression tag	UNP P29274
A	-21	ILE	-	expression tag	UNP P29274
A	-20	ILE	-	expression tag	UNP P29274
A	-19	ALA	-	expression tag	UNP P29274
A	-18	LEU	-	expression 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
A	54	LEU	ALA	engineered mutation	UNP P29274

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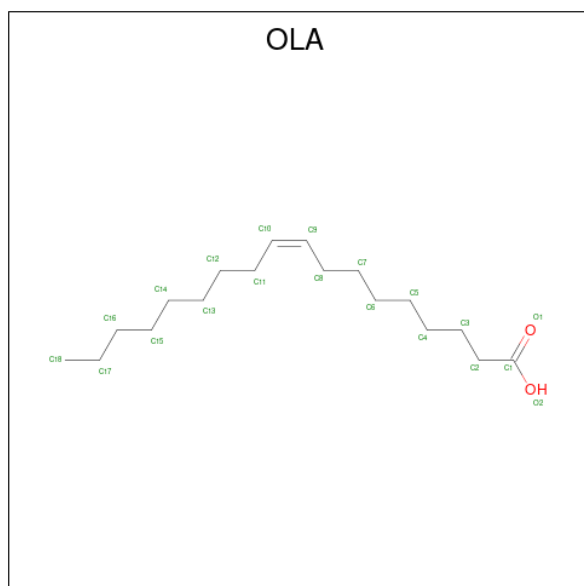
Chain	Residue	Modelled	Actual	Comment	Reference
A	88	ALA	THR	engineered mutation	UNP P29274
A	107	ALA	ARG	engineered mutation	UNP P29274
A	122	ALA	LYS	engineered mutation	UNP P29274
A	154	ALA	ASN	engineered mutation	UNP P29274
A	202	ALA	LEU	engineered mutation	UNP P29274
A	1007	TRP	MET	conflict	UNP P0ABE7
A	1102	ILE	HIS	conflict	UNP P0ABE7
A	1106	LEU	-	linker	UNP P0ABE7
A	235	ALA	LEU	engineered mutation	UNP P29274
A	239	ALA	VAL	engineered mutation	UNP P29274
A	318	ALA	-	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
A	327	HIS	-	expression tag	UNP P29274
A	328	HIS	-	expression tag	UNP P29274

- Molecule 2 is 1,3-diethyl-8-[({E})-2-(4-methoxy-3-oxidanyl-phenyl)ethenyl]-7-methyl-purine-2,6-dione (three-letter code: A1H3H) (formula: C₁₉H₂₂N₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	27	19	4	4	0	0

- Molecule 3 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	19	17	2	0	0
3	A	1	11	11		0	0
3	A	1	18	16	2	0	0
3	A	1	12	10	2	0	0
3	A	1	17	15	2	0	0
3	A	1	16	14	2	0	0
3	A	1	20	18	2	0	0
3	A	1	15	15		0	0
3	A	1	11	9	2	0	0
3	A	1	9	7	2	0	0
3	A	1	8	6	2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 17 15 2	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C O 9 7 2	0	0
3	A	1	Total C O 9 7 2	0	0

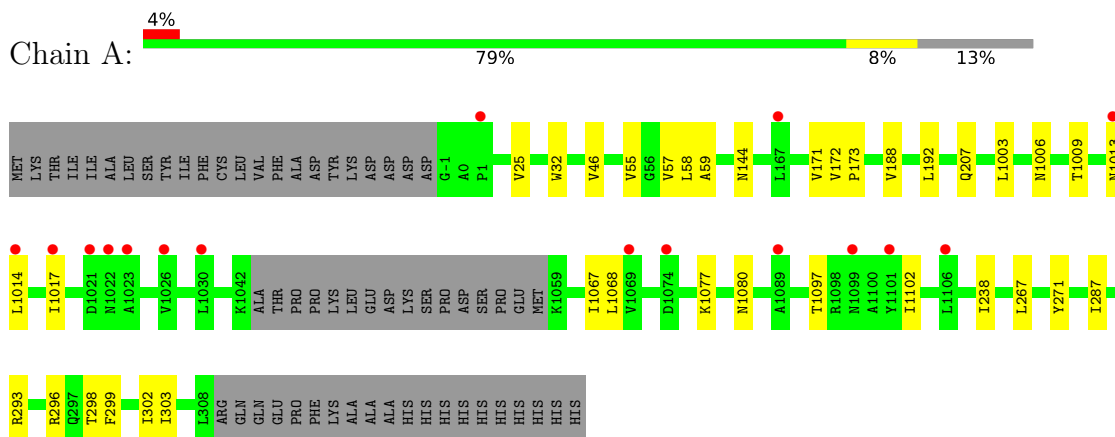
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 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: Adenosine receptor A2a,Soluble cytochrome b562



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	40.55Å 182.54Å 143.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 3.05 19.94 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.94-3.05) 99.5 (19.94-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.98Å)	Xtrriage
Refinement program	PHENIX (1.20_4459: ???)	Depositor
R, R_{free}	0.310 , 0.347 0.310 , 0.349	Depositor DCC
R_{free} test set	10060 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	94.7	Xtrriage
Anisotropy	0.045	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 99.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3170	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.15% 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: OLA, A1H3H, NA

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	0.24	0/2997	0.42	0/4095

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	2931	0	2905	20	0
2	A	27	0	0	0	0
3	A	211	0	296	5	0
4	A	1	0	0	0	0
All	All	3170	0	3201	22	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 3.

All (22) 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:1068:LEU:HD13	1:A:1102:ILE:HD13	1.74	0.70
1:A:1077:LYS:HA	1:A:1080:ASN:HB2	1.85	0.59
1:A:171:VAL:HG23	1:A:172:VAL:HG23	1.96	0.48
1:A:1067:ILE:HG23	1:A:1097:THR:HG21	1.97	0.47
3:A:1215:OLA:H61	3:A:1215:OLA:H32	1.65	0.47
1:A:32:TRP:CD1	3:A:1202:OLA:H62	2.51	0.45
3:A:1213:OLA:H72	3:A:1213:OLA:H42	1.79	0.44
1:A:144:ASN:HA	1:A:173:PRO:HD3	1.99	0.43
1:A:298:THR:O	1:A:302:ILE:HG13	2.18	0.43
1:A:57:VAL:HG12	1:A:58:LEU:HG	2.01	0.43
1:A:188:VAL:O	1:A:192:LEU:HD13	2.18	0.43
1:A:207:GLN:O	1:A:1003:LEU:HD13	2.20	0.42
1:A:238:ILE:HG13	1:A:287:ILE:HG21	2.00	0.42
1:A:293:ARG:HG2	1:A:296:ARG:NH2	2.35	0.41
1:A:267:LEU:HD22	1:A:271:TYR:HE1	1.84	0.41
1:A:55:VAL:HA	1:A:59:ALA:HB3	2.02	0.41
1:A:25:VAL:HG22	3:A:1202:OLA:H132	2.03	0.41
1:A:1009:THR:O	1:A:1013:ASN:HB2	2.21	0.41
1:A:1014:LEU:O	1:A:1017:ILE:HG12	2.21	0.41
1:A:267:LEU:HD23	1:A:267:LEU:HA	1.88	0.41
1:A:46:VAL:HG11	3:A:1213:OLA:H42	2.03	0.40
1:A:299:PHE:O	1:A:303:ILE:HD12	2.21	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	387/449 (86%)	372 (96%)	15 (4%)	0	100 100

There are no Ramachandran outliers to report.

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	293/368 (80%)	292 (100%)	1 (0%)	91 94

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

Mol	Chain	Res	Type
1	A	1006	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 for Mogul analysis.

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	OLA	A	1213	-	16,16,19	0.86	1 (6%)	16,16,19	0.95	1 (6%)
3	OLA	A	1217	-	8,8,19	0.71	0	8,8,19	1.25	1 (12%)
3	OLA	A	1202	-	18,18,19	0.80	1 (5%)	18,18,19	0.95	1 (5%)
3	OLA	A	1205	-	11,11,19	1.04	1 (9%)	11,11,19	1.17	1 (9%)
3	OLA	A	1209	-	14,14,19	1.03	1 (7%)	13,13,19	1.04	0
3	OLA	A	1210	-	10,10,19	0.62	0	10,10,19	1.21	1 (10%)
2	A1H3H	A	1201	-	26,29,29	0.43	0	30,42,42	1.17	4 (13%)
3	OLA	A	1212	-	7,7,19	0.74	0	7,7,19	1.35	2 (28%)
3	OLA	A	1214	-	9,9,19	0.94	1 (11%)	7,8,19	0.56	0
3	OLA	A	1206	-	16,16,19	0.85	1 (6%)	16,16,19	0.97	0
3	OLA	A	1204	-	17,17,19	0.82	1 (5%)	17,17,19	1.01	2 (11%)
3	OLA	A	1215	-	9,9,19	0.96	1 (11%)	8,8,19	0.66	0
3	OLA	A	1216	-	8,8,19	0.70	0	8,8,19	1.20	0
3	OLA	A	1211	-	8,8,19	0.70	0	8,8,19	1.28	2 (25%)
3	OLA	A	1207	-	15,15,19	0.88	1 (6%)	15,15,19	1.02	1 (6%)
3	OLA	A	1208	-	19,19,19	0.80	1 (5%)	19,19,19	0.92	2 (10%)
3	OLA	A	1203	-	10,10,19	0.79	1 (10%)	9,9,19	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
3	OLA	A	1213	-	-	9/14/14/17	-
3	OLA	A	1217	-	-	5/6/6/17	-
3	OLA	A	1202	-	-	9/16/16/17	-
3	OLA	A	1205	-	-	6/9/9/17	-
3	OLA	A	1209	-	-	6/12/12/17	-
3	OLA	A	1210	-	-	5/8/8/17	-
2	A1H3H	A	1201	-	-	3/9/11/11	0/3/3/3
3	OLA	A	1212	-	-	4/5/5/17	-
3	OLA	A	1214	-	-	4/7/7/17	-
3	OLA	A	1206	-	-	8/14/14/17	-
3	OLA	A	1204	-	-	8/15/15/17	-
3	OLA	A	1215	-	-	5/7/7/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OLA	A	1216	-	-	5/6/6/17	-
3	OLA	A	1211	-	-	5/6/6/17	-
3	OLA	A	1207	-	-	7/13/13/17	-
3	OLA	A	1208	-	-	8/17/17/17	-
3	OLA	A	1203	-	-	3/8/8/17	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1209	OLA	C10-C9	3.64	1.52	1.31
3	A	1205	OLA	C10-C9	2.79	1.47	1.28
3	A	1215	OLA	C10-C9	2.79	1.47	1.28
3	A	1208	OLA	C10-C9	2.73	1.47	1.31
3	A	1213	OLA	C10-C9	2.72	1.47	1.31
3	A	1214	OLA	C10-C9	2.71	1.47	1.31
3	A	1206	OLA	C10-C9	2.71	1.47	1.31
3	A	1202	OLA	C10-C9	2.70	1.47	1.31
3	A	1207	OLA	C10-C9	2.70	1.47	1.31
3	A	1204	OLA	C10-C9	2.69	1.47	1.31
3	A	1203	OLA	C10-C9	2.39	1.47	1.29

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	A1H3H	C6-N2-C8	-3.42	106.28	109.81
2	A	1201	A1H3H	C5-N1-C2	-3.39	119.02	122.22
2	A	1201	A1H3H	C6-C19-N	-2.39	111.61	113.58
3	A	1210	OLA	C3-C2-C1	-2.22	108.87	114.47
3	A	1211	OLA	O2-C1-C2	2.06	120.66	114.03
3	A	1205	OLA	O2-C1-C2	2.06	120.65	114.03
3	A	1212	OLA	O2-C1-C2	2.06	120.64	114.03
2	A	1201	A1H3H	C7-N2-C6	2.03	126.72	124.49
3	A	1204	OLA	C3-C2-C1	-2.03	109.36	114.47
3	A	1207	OLA	O2-C1-C2	2.03	120.55	114.03
3	A	1204	OLA	O2-C1-C2	2.02	120.53	114.03
3	A	1208	OLA	O2-C1-C2	2.02	120.51	114.03
3	A	1212	OLA	C3-C2-C1	-2.01	109.39	114.47
3	A	1217	OLA	O2-C1-C2	2.01	120.50	114.03
3	A	1202	OLA	O2-C1-C2	2.01	120.49	114.03
3	A	1213	OLA	O2-C1-C2	2.00	120.47	114.03
3	A	1208	OLA	C3-C2-C1	-2.00	109.42	114.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1211	OLA	C3-C2-C1	-2.00	109.43	114.47

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	A1H3H	C11-C10-C9-C8
3	A	1214	OLA	C7-C8-C9-C10
3	A	1205	OLA	C1-C2-C3-C4
3	A	1204	OLA	C1-C2-C3-C4
3	A	1208	OLA	C1-C2-C3-C4
3	A	1213	OLA	C1-C2-C3-C4
3	A	1204	OLA	C11-C10-C9-C8
3	A	1202	OLA	C1-C2-C3-C4
3	A	1210	OLA	C1-C2-C3-C4
3	A	1217	OLA	C1-C2-C3-C4
3	A	1211	OLA	C1-C2-C3-C4
3	A	1213	OLA	C4-C5-C6-C7
3	A	1209	OLA	C11-C10-C9-C8
3	A	1212	OLA	C1-C2-C3-C4
3	A	1215	OLA	C3-C4-C5-C6
3	A	1206	OLA	C11-C12-C13-C14
3	A	1206	OLA	C1-C2-C3-C4
3	A	1205	OLA	C3-C4-C5-C6
3	A	1208	OLA	C3-C4-C5-C6
3	A	1213	OLA	C11-C12-C13-C14
3	A	1204	OLA	C4-C5-C6-C7
3	A	1207	OLA	C4-C5-C6-C7
3	A	1210	OLA	C3-C4-C5-C6
3	A	1205	OLA	C5-C6-C7-C8
3	A	1207	OLA	C1-C2-C3-C4
3	A	1204	OLA	C11-C12-C13-C14
3	A	1213	OLA	C3-C4-C5-C6
3	A	1207	OLA	C3-C4-C5-C6
3	A	1208	OLA	C5-C6-C7-C8
3	A	1216	OLA	C1-C2-C3-C4
3	A	1215	OLA	C1-C2-C3-C4
3	A	1202	OLA	C4-C5-C6-C7
3	A	1209	OLA	C5-C6-C7-C8
3	A	1211	OLA	C3-C4-C5-C6
3	A	1215	OLA	C5-C6-C7-C8
3	A	1202	OLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
3	A	1214	OLA	C11-C10-C9-C8
3	A	1202	OLA	C3-C4-C5-C6
2	A	1201	A1H3H	C4-C3-N1-C2
3	A	1209	OLA	C1-C2-C3-C4
3	A	1215	OLA	C4-C5-C6-C7
3	A	1216	OLA	C4-C5-C6-C7
3	A	1217	OLA	C4-C5-C6-C7
3	A	1208	OLA	C11-C10-C9-C8
3	A	1213	OLA	C11-C10-C9-C8
3	A	1203	OLA	C11-C12-C13-C14
3	A	1202	OLA	C11-C10-C9-C8
3	A	1206	OLA	C11-C10-C9-C8
3	A	1207	OLA	C11-C10-C9-C8
3	A	1209	OLA	C4-C5-C6-C7
3	A	1202	OLA	C11-C12-C13-C14
3	A	1214	OLA	C11-C12-C13-C14
3	A	1211	OLA	C4-C5-C6-C7
3	A	1206	OLA	C4-C5-C6-C7
3	A	1203	OLA	C11-C10-C9-C8
3	A	1212	OLA	C3-C4-C5-C6
3	A	1210	OLA	C5-C6-C7-C8
3	A	1207	OLA	C11-C12-C13-C14
3	A	1205	OLA	C4-C5-C6-C7
3	A	1208	OLA	C12-C13-C14-C15
3	A	1208	OLA	C14-C15-C16-C17
3	A	1206	OLA	C7-C8-C9-C10
3	A	1207	OLA	C7-C8-C9-C10
3	A	1208	OLA	C9-C10-C11-C12
2	A	1201	A1H3H	C13-C14-O1-C15
3	A	1217	OLA	C3-C4-C5-C6
3	A	1204	OLA	O1-C1-C2-C3
3	A	1216	OLA	C3-C4-C5-C6
3	A	1213	OLA	C7-C8-C9-C10
3	A	1202	OLA	O2-C1-C2-C3
3	A	1211	OLA	O2-C1-C2-C3
3	A	1202	OLA	O1-C1-C2-C3
3	A	1211	OLA	O1-C1-C2-C3
3	A	1213	OLA	O1-C1-C2-C3
3	A	1213	OLA	O2-C1-C2-C3
3	A	1204	OLA	O2-C1-C2-C3
3	A	1208	OLA	C4-C5-C6-C7
3	A	1206	OLA	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
3	A	1204	OLA	C9-C10-C11-C12
3	A	1214	OLA	C9-C10-C11-C12
3	A	1212	OLA	O2-C1-C2-C3
3	A	1216	OLA	O2-C1-C2-C3
3	A	1216	OLA	O1-C1-C2-C3
3	A	1212	OLA	O1-C1-C2-C3
3	A	1215	OLA	C7-C8-C9-C10
3	A	1204	OLA	C7-C8-C9-C10
3	A	1203	OLA	C9-C10-C11-C12
3	A	1209	OLA	C7-C8-C9-C10
3	A	1205	OLA	C7-C8-C9-C10
3	A	1206	OLA	O2-C1-C2-C3
3	A	1217	OLA	O2-C1-C2-C3
3	A	1209	OLA	C11-C12-C13-C14
3	A	1202	OLA	C9-C10-C11-C12
3	A	1207	OLA	C9-C10-C11-C12
3	A	1213	OLA	C9-C10-C11-C12
3	A	1206	OLA	O1-C1-C2-C3
3	A	1217	OLA	O1-C1-C2-C3
3	A	1210	OLA	O1-C1-C2-C3
3	A	1205	OLA	O2-C1-C2-C3
3	A	1210	OLA	O2-C1-C2-C3

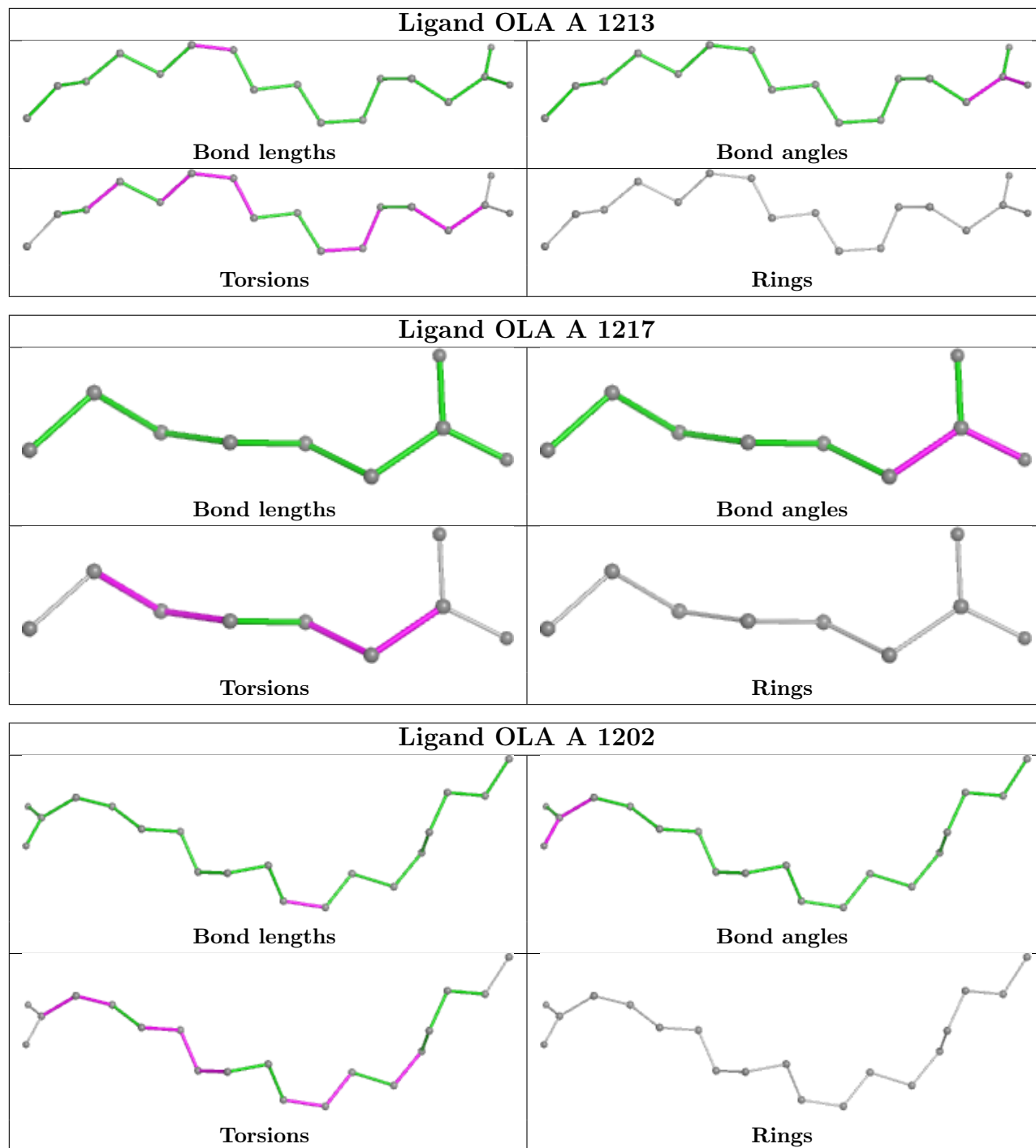
There are no ring outliers.

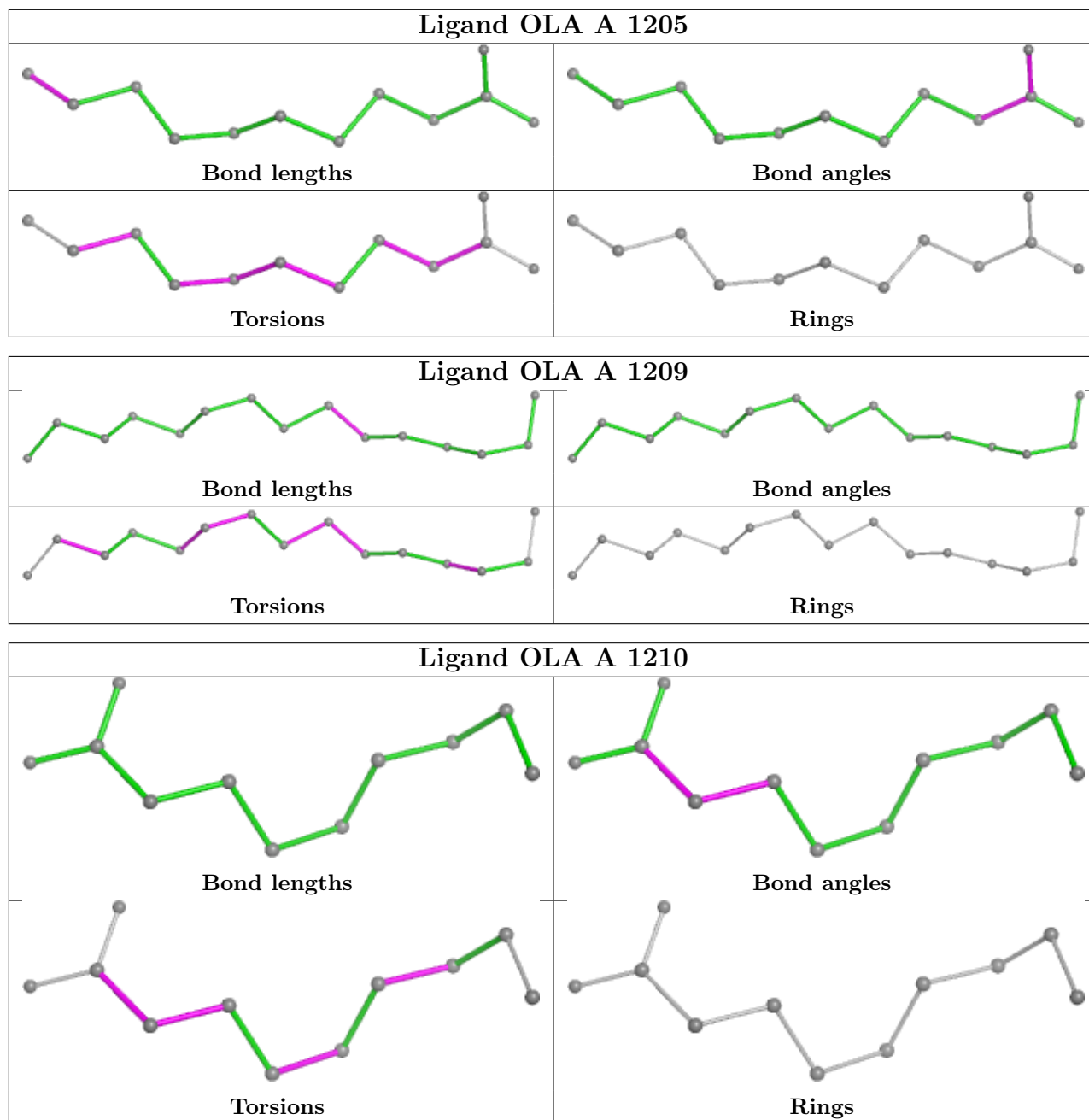
3 monomers are involved in 5 short contacts:

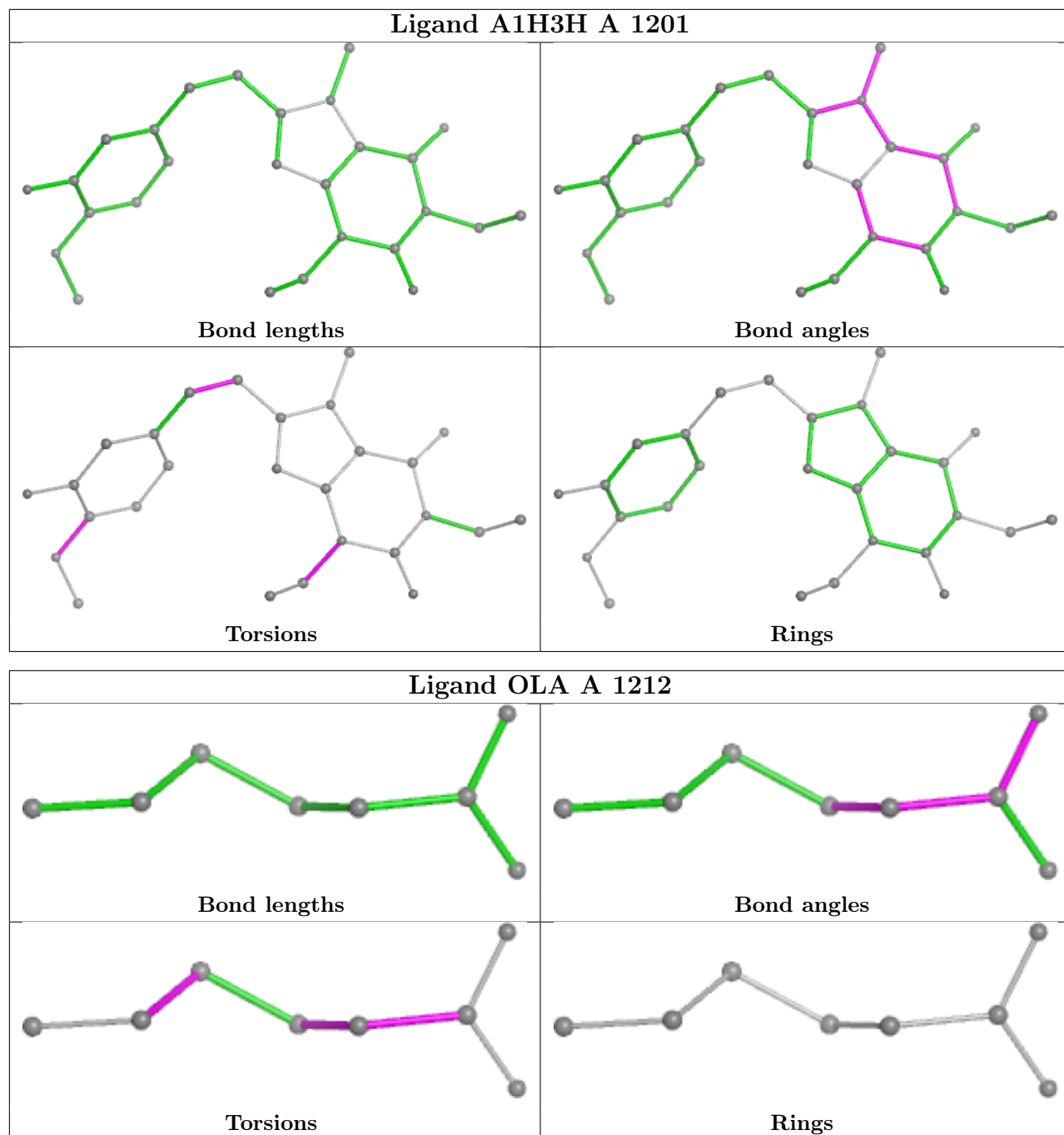
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1213	OLA	2	0
3	A	1202	OLA	2	0
3	A	1215	OLA	1	0

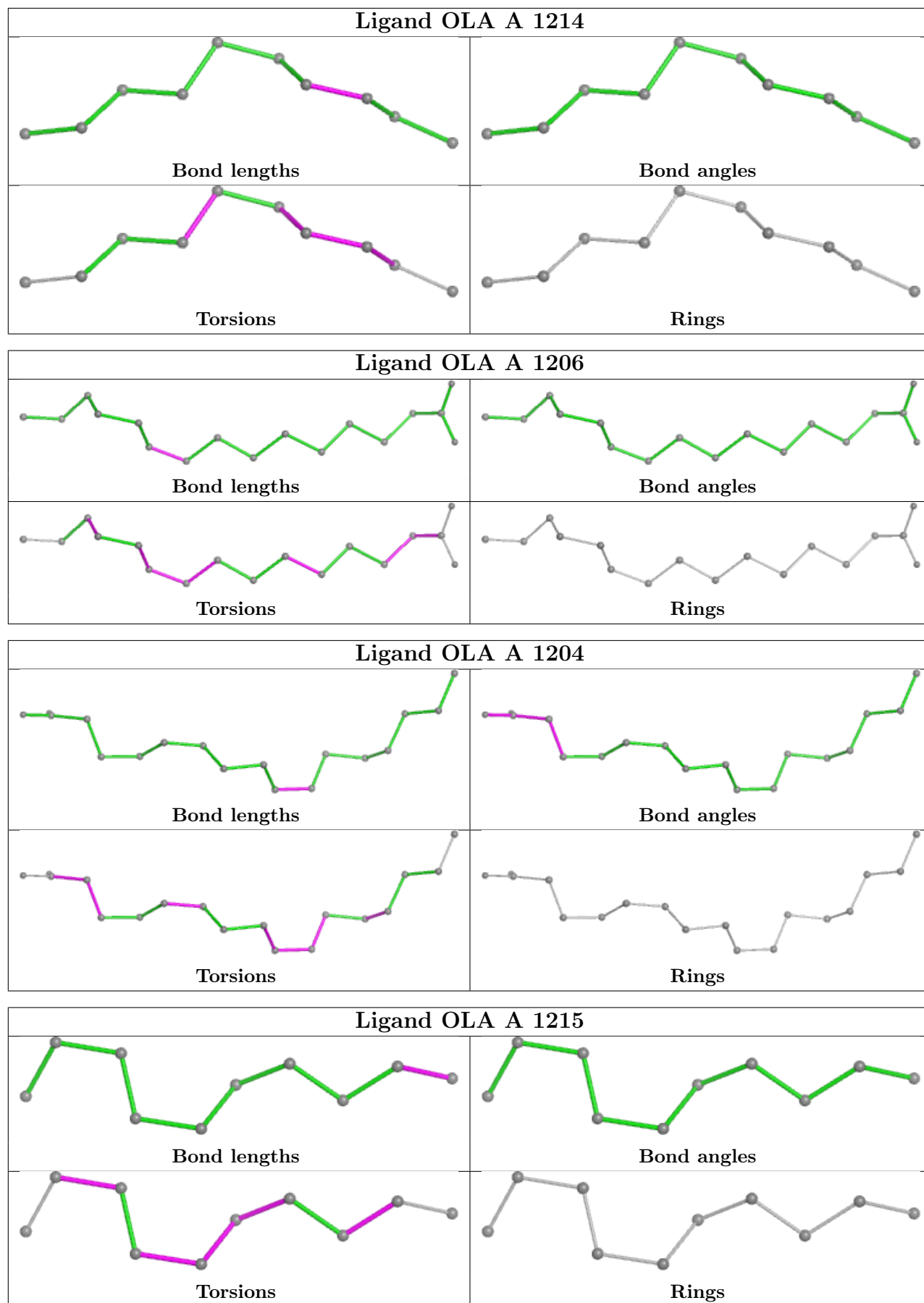
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

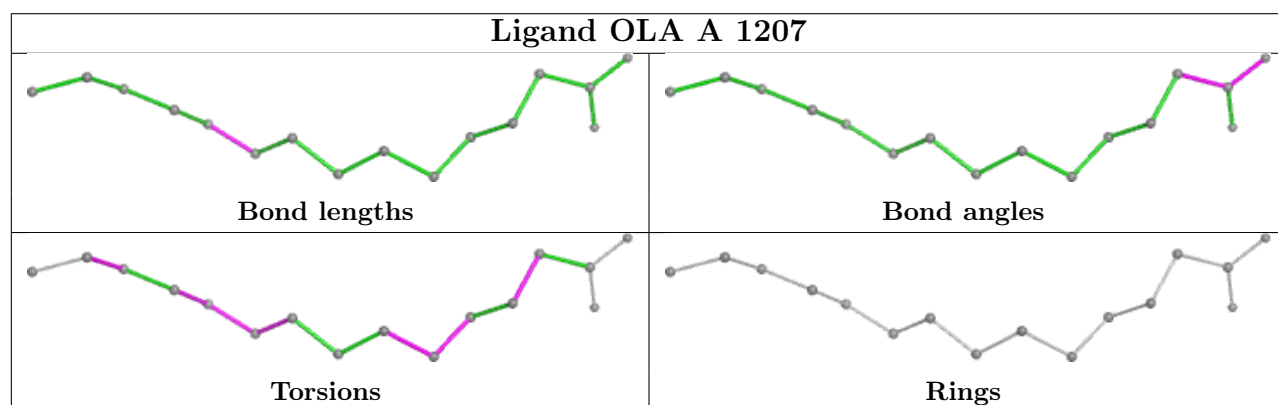
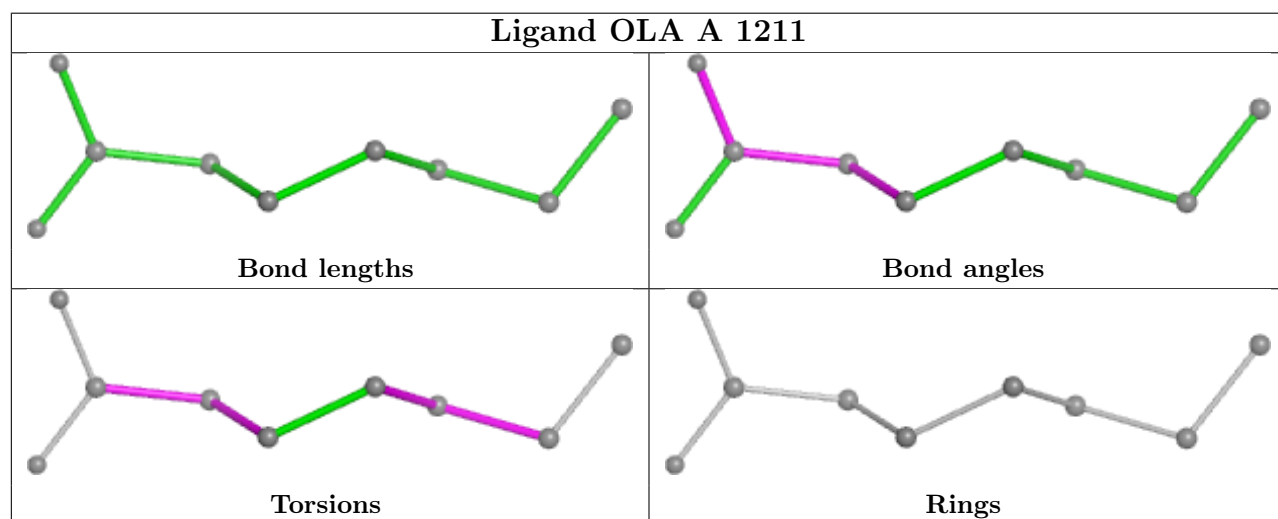
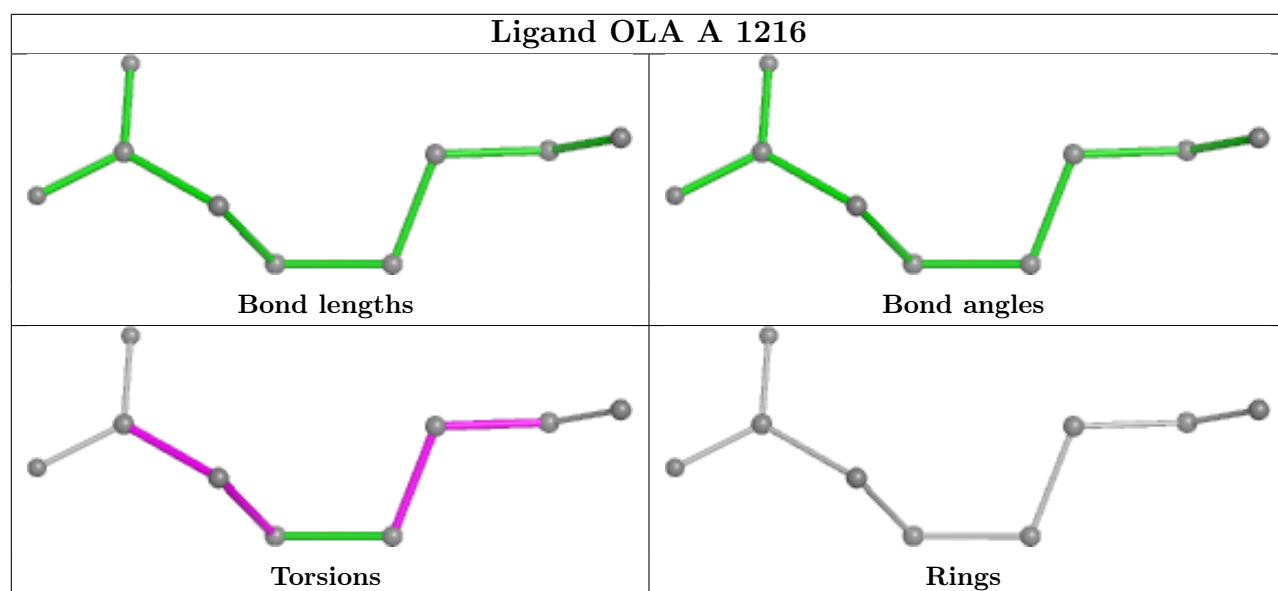
equivalents in the CSD to analyse the geometry.

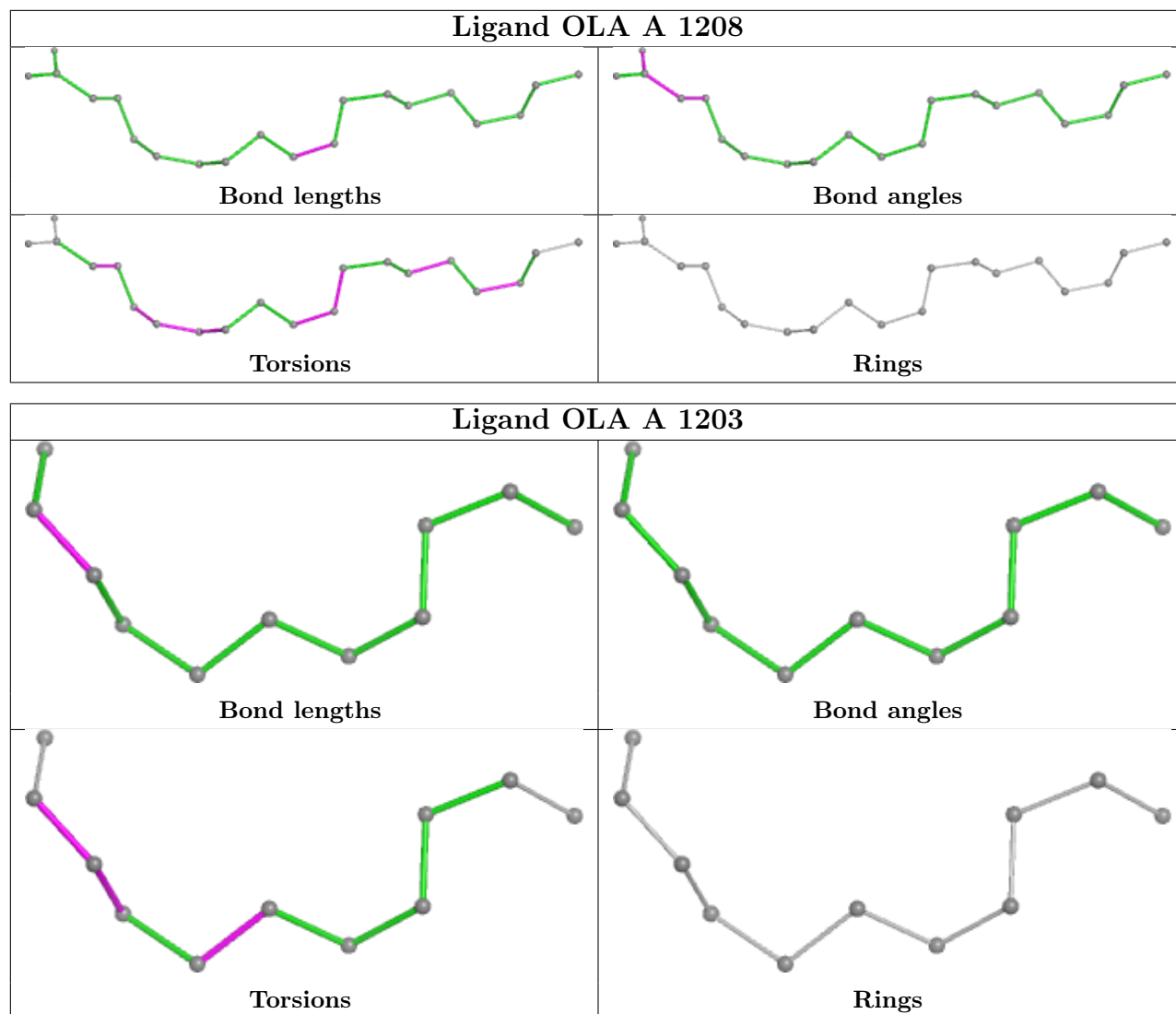












5.7 Other polymers [i](#)

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 [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	390/449 (86%)	0.43	16 (4%) 42 24	45, 86, 146, 171	1 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1099	ASN	3.7
1	A	1014	LEU	3.4
1	A	1023	ALA	3.3
1	A	1069	VAL	3.3
1	A	1026	VAL	3.1
1	A	1013	ASN	2.8
1	A	1021	ASP	2.8
1	A	1	PRO	2.7
1	A	1101	TYR	2.3
1	A	1089	ALA	2.3
1	A	1022	ASN	2.3
1	A	1106	LEU	2.3
1	A	1030	LEU	2.2
1	A	1017	ILE	2.2
1	A	167	LEU	2.0
1	A	1074	ASP	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

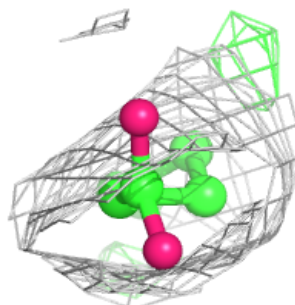
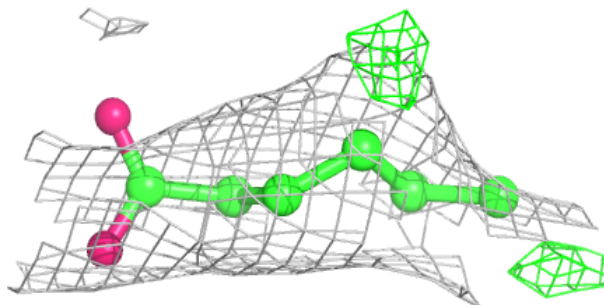
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	OLA	A	1212	8/20	0.48	0.20	86,95,118,128	0
3	OLA	A	1207	16/20	0.52	0.20	67,109,133,140	0
3	OLA	A	1215	10/20	0.58	0.18	61,71,80,80	0
3	OLA	A	1208	20/20	0.61	0.17	55,89,162,162	0
3	OLA	A	1205	12/20	0.65	0.15	73,95,129,139	0
3	OLA	A	1202	19/20	0.66	0.14	66,101,113,114	0
3	OLA	A	1210	11/20	0.68	0.26	72,81,91,97	0
3	OLA	A	1211	9/20	0.73	0.38	74,82,109,111	0
3	OLA	A	1213	17/20	0.75	0.16	72,85,100,104	0
3	OLA	A	1216	9/20	0.75	0.15	61,69,79,89	0
3	OLA	A	1217	9/20	0.75	0.17	71,77,81,86	0
3	OLA	A	1209	15/20	0.76	0.16	75,84,100,101	0
3	OLA	A	1204	18/20	0.76	0.14	64,83,115,122	0
3	OLA	A	1214	10/20	0.78	0.18	67,75,85,88	0
3	OLA	A	1206	17/20	0.81	0.14	62,81,117,120	0
2	A1H3H	A	1201	27/27	0.83	0.15	68,78,94,96	0
3	OLA	A	1203	11/20	0.84	0.15	47,55,67,71	0
4	NA	A	1218	1/1	0.87	0.10	58,58,58,58	0

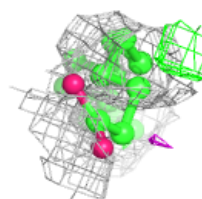
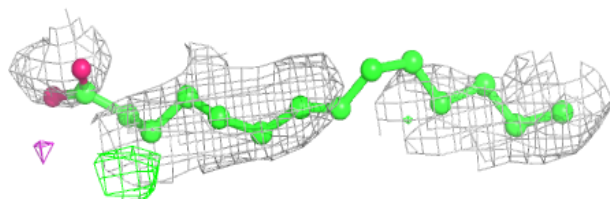
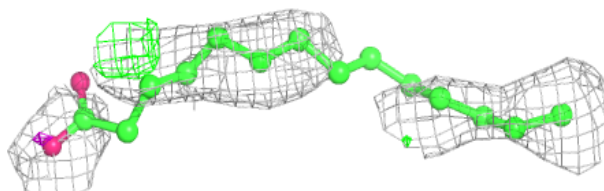
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around OLA A 1212:

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

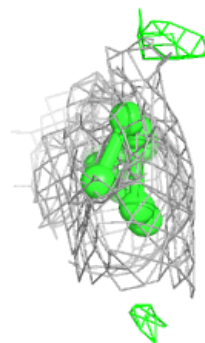
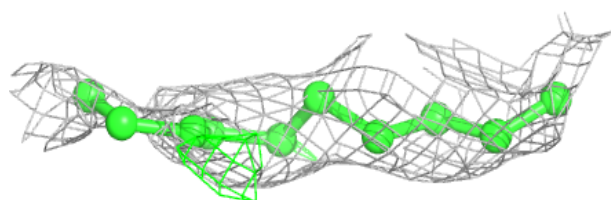
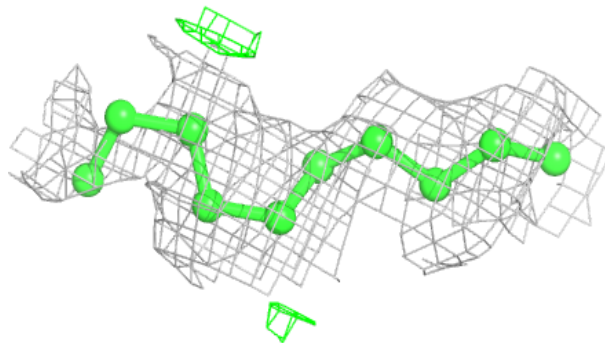
**Electron density around OLA A 1207:**

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

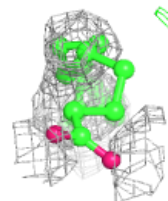
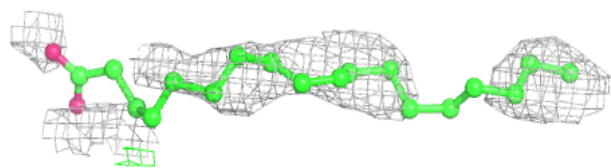
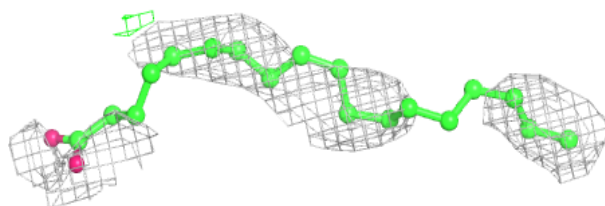


Electron density around OLA A 1215:

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

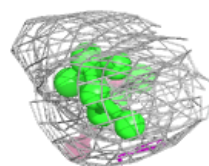
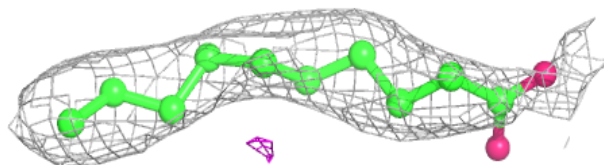
**Electron density around OLA A 1208:**

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

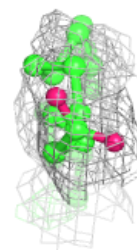
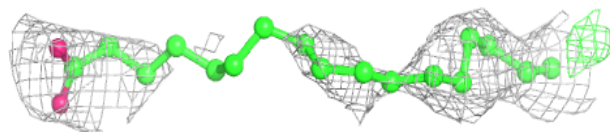
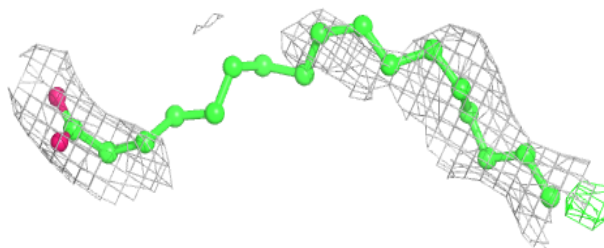


Electron density around OLA A 1205:

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

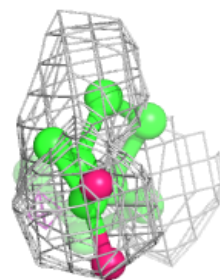
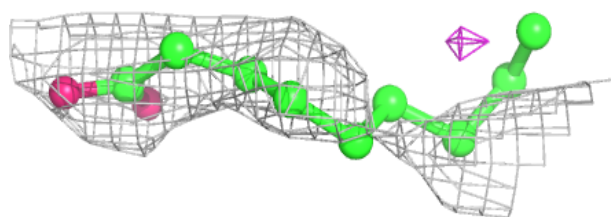
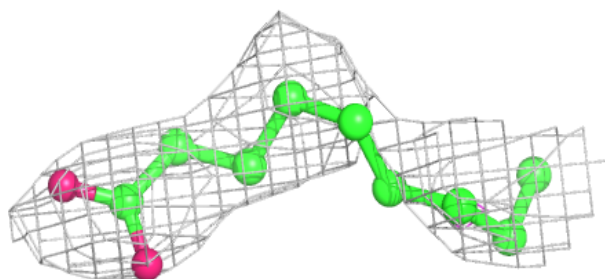
**Electron density around OLA A 1202:**

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

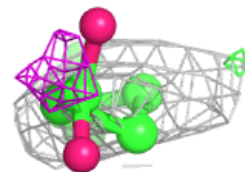
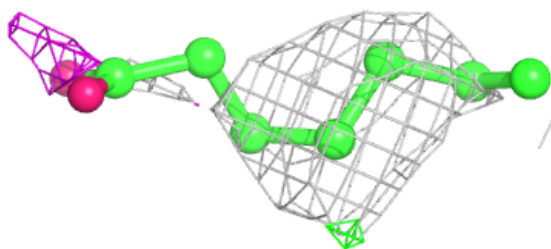
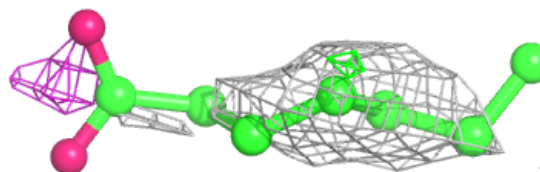


Electron density around OLA A 1210:

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

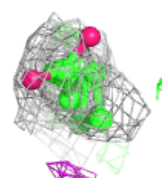
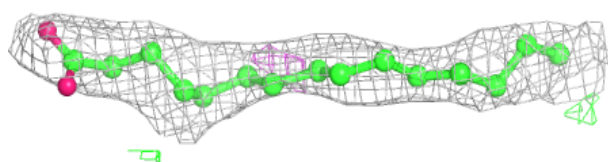
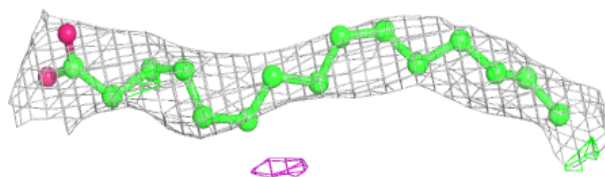
**Electron density around OLA A 1211:**

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

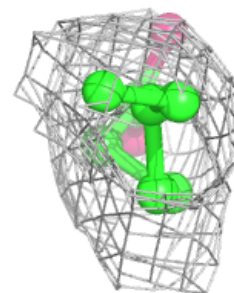
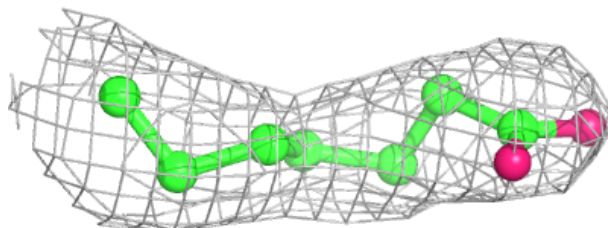
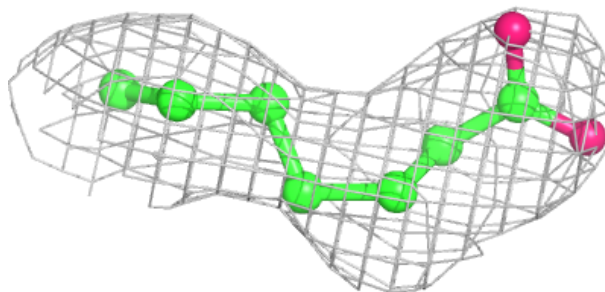


Electron density around OLA A 1213:

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

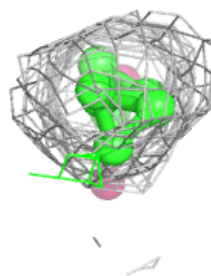
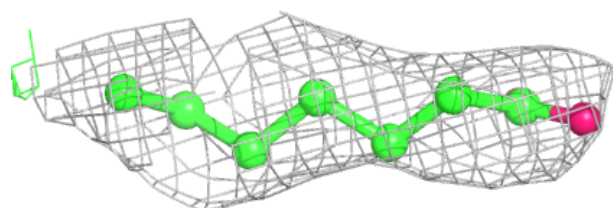
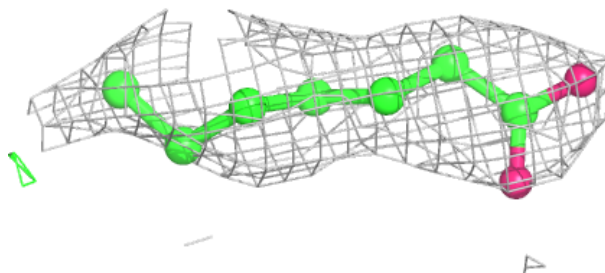
**Electron density around OLA A 1216:**

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

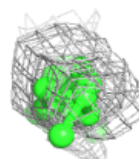
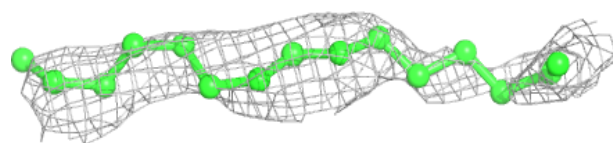
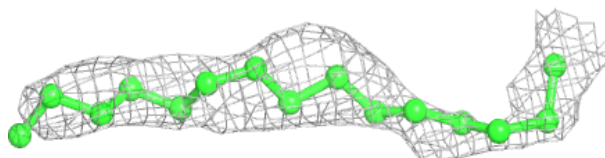


Electron density around OLA A 1217:

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

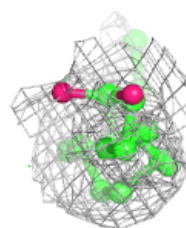
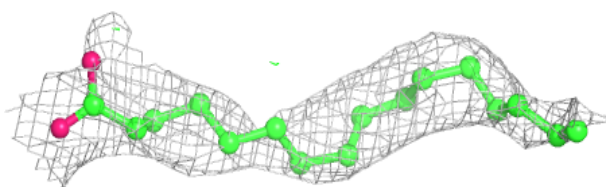
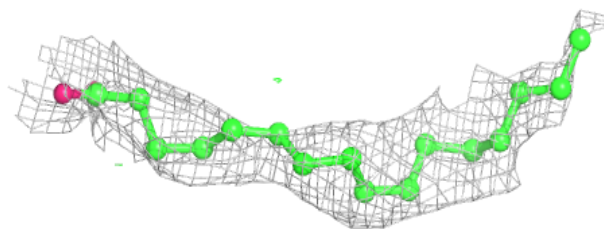
**Electron density around OLA A 1209:**

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

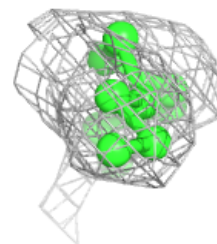
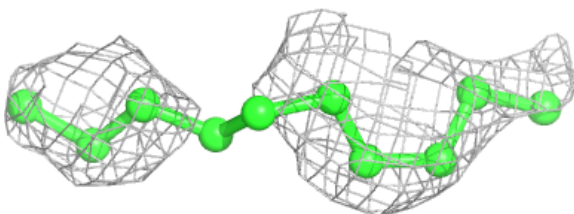
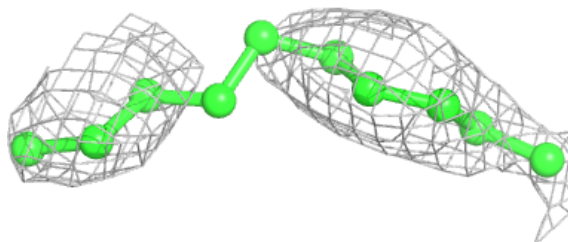


Electron density around OLA A 1204:

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

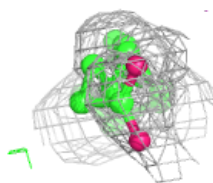
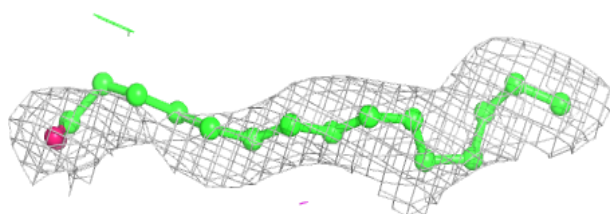
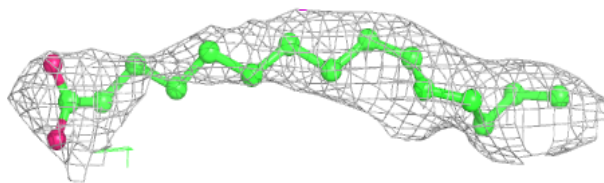
**Electron density around OLA A 1214:**

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

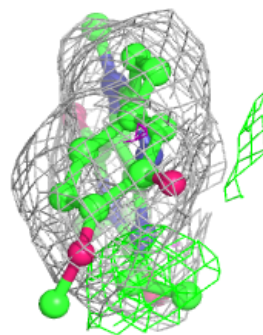
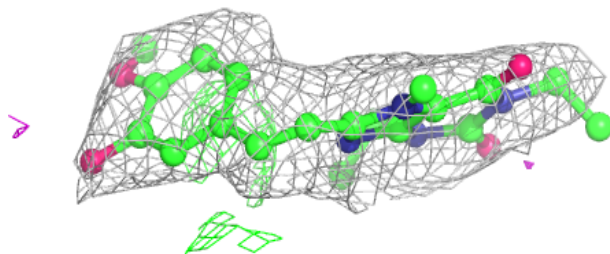
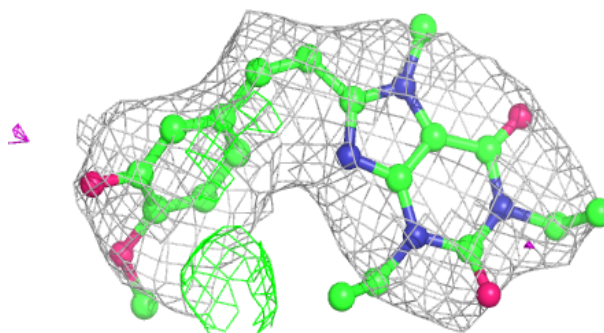


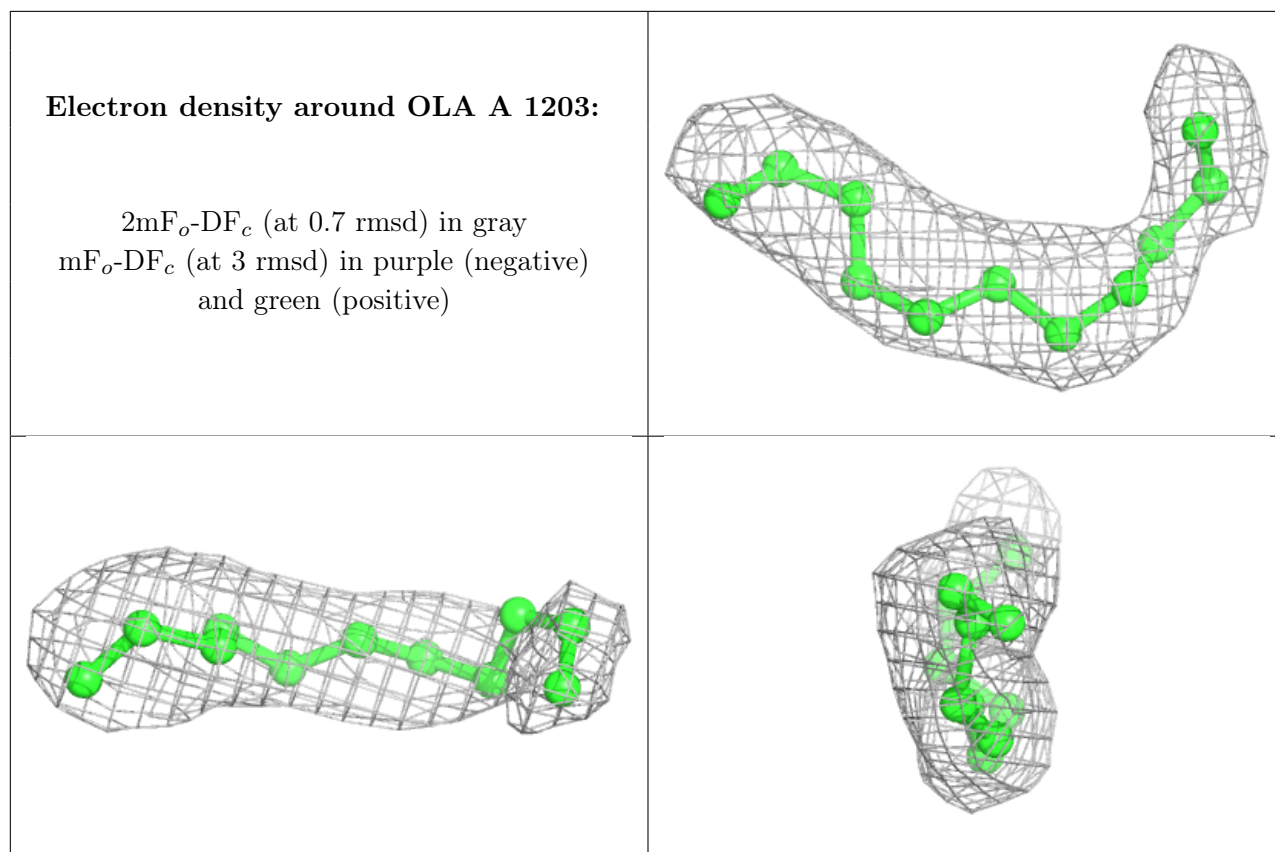
Electron density around OLA A 1206:

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

**Electron density around A1H3H 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.