Full wwPDB X-ray Structure Validation Report ⓘ

Jun 10, 2025 – 04:20 pm BST

PDB ID	:	9H2X / pdb_00009h2x
Title	:	Crystal structure of stabilized A2A adenosine receptor A2AR-StaR2-bRIL in complex with compound 7, a novel nanomolar A2A receptor antagonist from modern hit-finding with structure-guided de novo design
Authors	:	Tian, G.; Maja, N.
Deposited on	:	2024-10-15
Resolution	:	1.75 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:

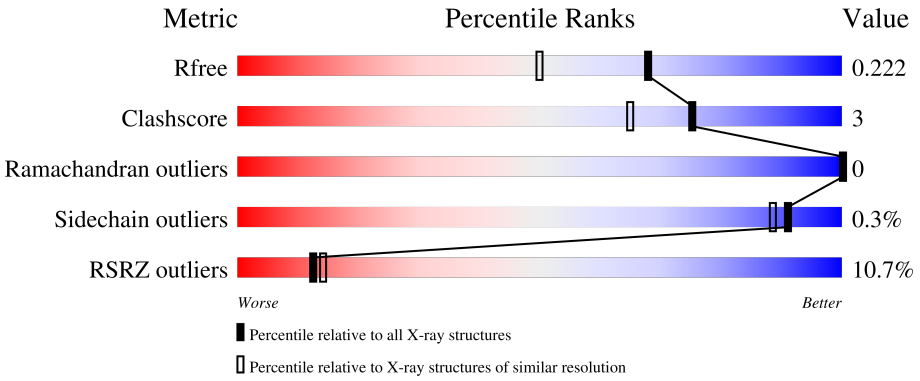
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	2888 (1.76-1.76)
Clashscore	180529	3097 (1.76-1.76)
Ramachandran outliers	177936	3072 (1.76-1.76)
Sidechain outliers	177891	3072 (1.76-1.76)
RSRZ outliers	164620	2887 (1.76-1.76)

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

Mol	Chain	Length	Quality of chain
1	A	433	9% 82% 7% 11%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3586 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	384	3084	2014	517	530	23	0	15	0

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	conflict	UNP P29274
A	88	ALA	THR	conflict	UNP P29274
A	107	ALA	ARG	conflict	UNP P29274
A	122	ALA	LYS	conflict	UNP P29274
A	154	ALA	ASN	conflict	UNP P29274
A	202	ALA	LEU	conflict	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	conflict	UNP P29274
A	239	ALA	VAL	conflict	UNP P29274
A	277	ALA	SER	conflict	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

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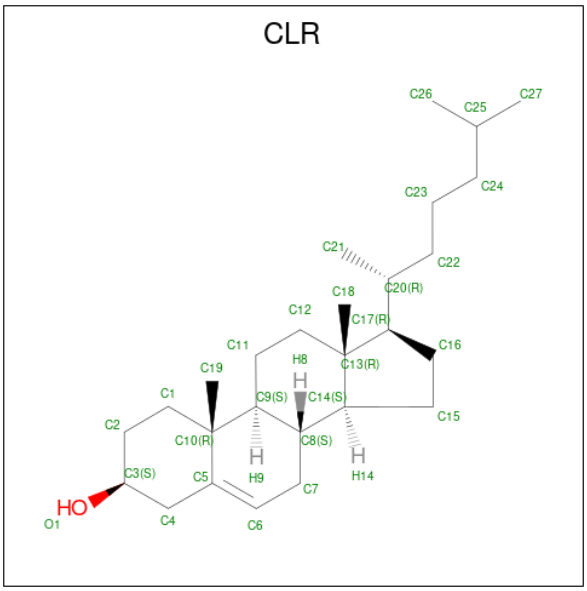
Chain	Residue	Modelled	Actual	Comment	Reference
A	323	HIS	-	expression tag	UNP P29274
A	324	HIS	-	expression tag	UNP P29274
A	325	HIS	-	expression tag	UNP P29274
A	326	HIS	-	expression tag	UNP P29274
A	327	HIS	-	expression tag	UNP P29274
A	328	HIS	-	expression tag	UNP P29274

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

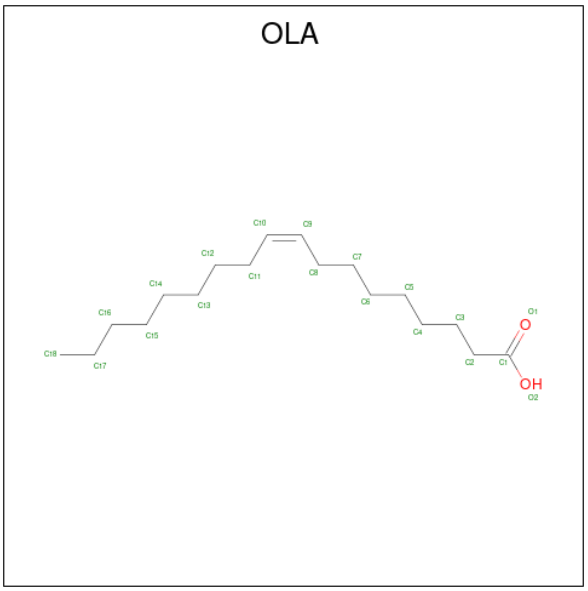
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



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

- Molecule 4 is OLEIC ACID (CCD ID: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 16 14 2	0	0
4	A	1	Total C 11 11	0	0
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 11 9 2	0	0
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 16 14 2	0	0
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C O 11 9 2	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C O 10 8 2	0	0
4	A	1	Total C O 20 18 2	0	0
4	A	1	Total C O 16 14 2	0	0
4	A	1	Total C O 18 16 2	0	0

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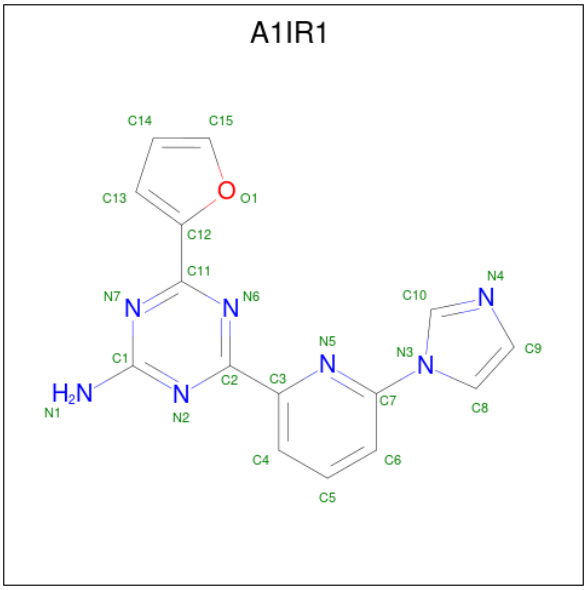
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 18 18	0	0
4	A	1	Total C O 15 13 2	0	0
4	A	1	Total C O 9 7 2	0	0
4	A	1	Total C O 12 10 2	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C O 17 15 2	0	0
4	A	1	Total C O 10 8 2	0	0

- Molecule 5 is 4-(furan-2-yl)-6-(6-imidazol-1-ylpyridin-2-yl)-1,3,5-triazin-2-amine (CCD ID: A1IR1) (formula: $C_{15}H_{11}N_7O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 23 15 7 1	0	0

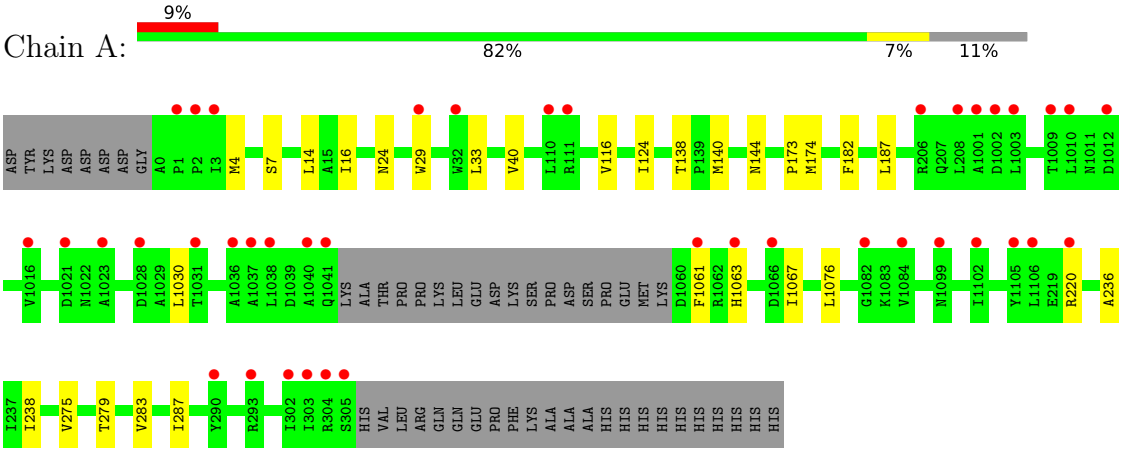
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	116	Total O 116 116	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 (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	39.35Å 179.53Å 140.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.20 – 1.75 25.20 – 1.75	Depositor EDS
% Data completeness (in resolution range)	86.3 (25.20-1.75) 86.3 (25.20-1.75)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 1.75Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.206 , 0.226 0.201 , 0.222	Depositor DCC
R_{free} test set	2200 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	22.6	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3586	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, NA, OLA, A1IR1

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	0.76	0/3156	0.94	2/4295 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	283	VAL	N-CA-C	5.98	118.56	111.09
1	A	24	ASN	CA-CB-CG	-5.48	107.12	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3084	0	3158	20	0
2	A	1	0	0	0	0
3	A	84	0	138	0	0
4	A	278	0	391	5	0
5	A	23	0	0	0	0
6	A	116	0	0	1	0
All	All	3586	0	3687	21	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 (21) 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:29[A]:TRP:NE1	1:A:33:LEU:HD11	2.12	0.65
1:A:29[A]:TRP:HE1	1:A:33:LEU:HD11	1.70	0.56
1:A:1030:LEU:HB3	1:A:1076[B]:LEU:HG	1.88	0.54
1:A:40:VAL:HG11	1:A:116:VAL:CG1	2.40	0.52
1:A:29[A]:TRP:CD1	1:A:33:LEU:CD1	2.92	0.52
1:A:29[A]:TRP:CD1	1:A:33:LEU:HD11	2.46	0.49
1:A:1063:HIS:CD2	1:A:1067:ILE:HD11	2.48	0.49
1:A:174[B]:MET:HG2	6:A:1309:HOH:O	2.14	0.47
1:A:238[B]:ILE:HD11	1:A:287:ILE:HB	1.99	0.45
1:A:14:LEU:HD11	4:A:1208:OLA:C9	2.46	0.45
1:A:124:ILE:HD13	4:A:1221:OLA:H32	1.98	0.45
1:A:1061:PHE:HE2	1:A:220:ARG:HD2	1.83	0.44
1:A:16:ILE:HD11	1:A:275:VAL:HG13	1.99	0.44
1:A:140[A]:MET:HE2	4:A:1214:OLA:H62	2.00	0.43
4:A:1218:OLA:H9	4:A:1218:OLA:H122	1.84	0.43
1:A:144:ASN:HA	1:A:173:PRO:HD3	2.01	0.42
1:A:4:MET:O	1:A:7[B]:SER:OG	2.28	0.42
1:A:40:VAL:HG11	1:A:116:VAL:HG12	2.02	0.42
1:A:236:ALA:HB1	4:A:1206:OLA:H112	2.01	0.42
1:A:182:PHE:CE1	1:A:187[B]:LEU:HG	2.56	0.41
1:A:275:VAL:O	1:A:279[B]:THR:HG23	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	395/433 (91%)	393 (100%)	2 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	324/353 (92%)	323 (100%)	1 (0%)	91 88

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

Mol	Chain	Res	Type
1	A	138	THR

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

Mol	Chain	Res	Type
1	A	157	GLN
1	A	1006	ASN
1	A	1088	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 26 ligands modelled in this entry, 1 is monoatomic - leaving 25 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	$\#\|Z\| > 2$
4	OLA	A	1205	-	15,15,19	0.59	0	15,15,19	0.56	0
4	OLA	A	1220	-	14,14,19	0.61	0	14,14,19	0.57	0
4	OLA	A	1216	-	19,19,19	0.54	0	19,19,19	0.56	0
4	OLA	A	1217	-	15,15,19	0.60	0	15,15,19	0.59	0
3	CLR	A	1204	-	31,31,31	0.40	0	48,48,48	0.50	0
4	OLA	A	1215	-	9,9,19	0.73	0	9,9,19	0.62	0
4	OLA	A	1224	-	16,16,19	0.57	0	16,16,19	0.51	0
4	OLA	A	1218	-	17,17,19	0.59	0	17,17,19	0.60	0
4	OLA	A	1210	-	15,15,19	0.62	0	15,15,19	0.57	0
4	OLA	A	1213	-	5,5,19	0.17	0	4,4,19	0.18	0
4	OLA	A	1219	-	17,17,19	0.21	0	16,16,19	0.24	0
4	OLA	A	1222	-	10,10,19	0.65	0	9,9,19	0.75	0
4	OLA	A	1223	-	5,5,19	0.30	0	4,4,19	0.18	0
4	OLA	A	1225	-	9,9,19	0.69	0	9,9,19	0.67	0
4	OLA	A	1211	-	19,19,19	0.53	0	19,19,19	0.53	0
4	OLA	A	1212	-	10,10,19	0.64	0	10,10,19	0.67	0
5	A1IR1	A	1226	-	22,26,26	0.51	0	29,36,36	0.77	1 (3%)
4	OLA	A	1214	-	19,19,19	0.50	0	19,19,19	0.53	0
4	OLA	A	1208	-	10,10,19	0.67	0	10,10,19	0.66	0
4	OLA	A	1221	-	8,8,19	0.73	0	8,8,19	0.70	0
3	CLR	A	1202	-	31,31,31	0.42	0	48,48,48	0.51	0
4	OLA	A	1209	-	7,7,19	0.86	0	7,7,19	0.83	0
3	CLR	A	1203	-	31,31,31	0.36	0	48,48,48	0.53	0
4	OLA	A	1206	-	10,10,19	0.24	0	9,9,19	0.32	0
4	OLA	A	1207	-	7,7,19	0.79	0	7,7,19	0.79	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLA	A	1205	-	-	3/13/13/17	-
4	OLA	A	1220	-	-	3/12/12/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLA	A	1216	-	-	7/17/17/17	-
4	OLA	A	1217	-	-	3/13/13/17	-
3	CLR	A	1204	-	-	1/10/68/68	0/4/4/4
4	OLA	A	1215	-	-	2/7/7/17	-
4	OLA	A	1224	-	-	5/14/14/17	-
4	OLA	A	1218	-	-	9/15/15/17	-
4	OLA	A	1210	-	-	2/13/13/17	-
4	OLA	A	1213	-	-	1/3/3/17	-
4	OLA	A	1219	-	-	3/15/15/17	-
4	OLA	A	1222	-	-	3/6/6/17	-
4	OLA	A	1223	-	-	0/3/3/17	-
4	OLA	A	1225	-	-	0/7/7/17	-
4	OLA	A	1211	-	-	5/17/17/17	-
4	OLA	A	1212	-	-	3/8/8/17	-
5	A1IR1	A	1226	-	-	0/8/12/12	0/4/4/4
4	OLA	A	1214	-	-	3/17/17/17	-
4	OLA	A	1208	-	-	2/8/8/17	-
4	OLA	A	1221	-	-	2/6/6/17	-
3	CLR	A	1202	-	-	1/10/68/68	0/4/4/4
4	OLA	A	1209	-	-	2/5/5/17	-
3	CLR	A	1203	-	-	0/10/68/68	0/4/4/4
4	OLA	A	1206	-	-	0/8/8/17	-
4	OLA	A	1207	-	-	2/5/5/17	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1226	A1IR1	C13-C14-C15	-2.03	105.71	112.92

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1224	OLA	C1-C2-C3-C4
4	A	1222	OLA	C9-C10-C11-C12
4	A	1224	OLA	C2-C3-C4-C5
4	A	1218	OLA	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
4	A	1205	OLA	C11-C10-C9-C8
4	A	1220	OLA	C4-C5-C6-C7
4	A	1218	OLA	C11-C12-C13-C14
4	A	1212	OLA	C3-C4-C5-C6
4	A	1218	OLA	C5-C6-C7-C8
4	A	1216	OLA	C11-C10-C9-C8
4	A	1218	OLA	C13-C14-C15-C16
4	A	1205	OLA	C7-C8-C9-C10
4	A	1218	OLA	C7-C8-C9-C10
4	A	1205	OLA	C9-C10-C11-C12
4	A	1211	OLA	C1-C2-C3-C4
4	A	1219	OLA	C11-C10-C9-C8
4	A	1218	OLA	C4-C5-C6-C7
4	A	1216	OLA	C6-C7-C8-C9
3	A	1204	CLR	C22-C23-C24-C25
4	A	1217	OLA	C1-C2-C3-C4
4	A	1224	OLA	C7-C8-C9-C10
4	A	1221	OLA	O1-C1-C2-C3
4	A	1209	OLA	O1-C1-C2-C3
4	A	1215	OLA	O1-C1-C2-C3
4	A	1217	OLA	O2-C1-C2-C3
4	A	1221	OLA	O2-C1-C2-C3
4	A	1211	OLA	C9-C10-C11-C12
4	A	1215	OLA	O2-C1-C2-C3
4	A	1213	OLA	C13-C14-C15-C16
4	A	1219	OLA	C13-C14-C15-C16
4	A	1209	OLA	O2-C1-C2-C3
4	A	1217	OLA	O1-C1-C2-C3
4	A	1224	OLA	C11-C10-C9-C8
4	A	1214	OLA	O2-C1-C2-C3
4	A	1210	OLA	C9-C10-C11-C12
4	A	1212	OLA	O2-C1-C2-C3
4	A	1216	OLA	C5-C6-C7-C8
3	A	1202	CLR	C23-C24-C25-C26
4	A	1208	OLA	O2-C1-C2-C3
4	A	1212	OLA	O1-C1-C2-C3
4	A	1214	OLA	C7-C8-C9-C10
4	A	1224	OLA	C9-C10-C11-C12
4	A	1208	OLA	O1-C1-C2-C3
4	A	1211	OLA	O2-C1-C2-C3
4	A	1210	OLA	C7-C8-C9-C10
4	A	1216	OLA	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	1211	OLA	C3-C4-C5-C6
4	A	1218	OLA	C10-C11-C12-C13
4	A	1219	OLA	C6-C7-C8-C9
4	A	1216	OLA	C14-C15-C16-C17
4	A	1214	OLA	O1-C1-C2-C3
4	A	1222	OLA	O2-C1-C2-C3
4	A	1216	OLA	O1-C1-C2-C3
4	A	1211	OLA	O1-C1-C2-C3
4	A	1218	OLA	C9-C10-C11-C12
4	A	1220	OLA	O2-C1-C2-C3
4	A	1222	OLA	O1-C1-C2-C3
4	A	1207	OLA	O2-C1-C2-C3
4	A	1220	OLA	O1-C1-C2-C3
4	A	1216	OLA	C15-C16-C17-C18
4	A	1207	OLA	O1-C1-C2-C3
4	A	1218	OLA	O2-C1-C2-C3

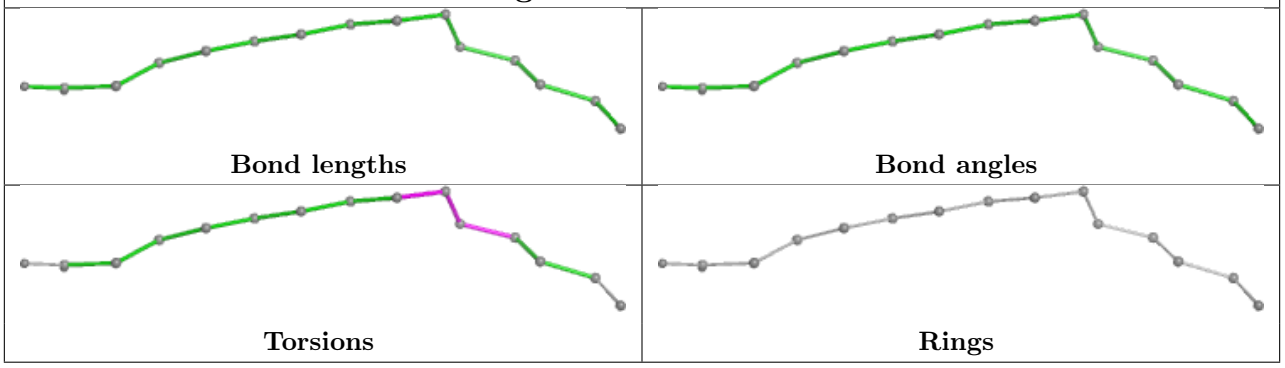
There are no ring outliers.

5 monomers are involved in 5 short contacts:

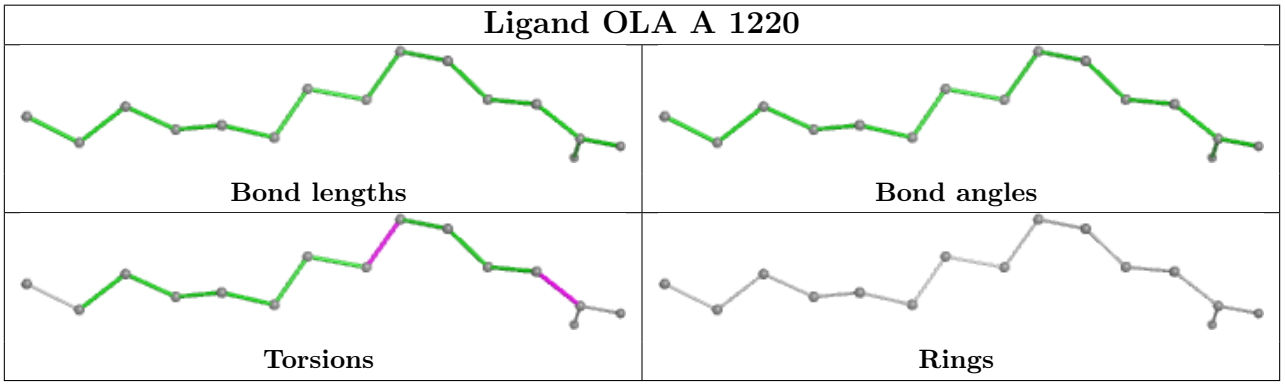
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1218	OLA	1	0
4	A	1214	OLA	1	0
4	A	1208	OLA	1	0
4	A	1221	OLA	1	0
4	A	1206	OLA	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

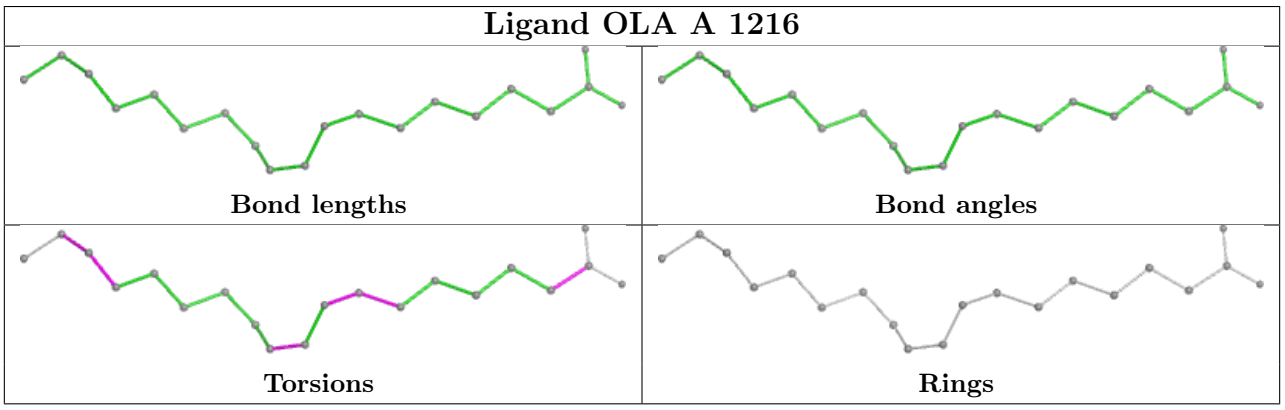
Ligand OLA A 1205



Ligand OLA A 1220



Ligand OLA A 1216



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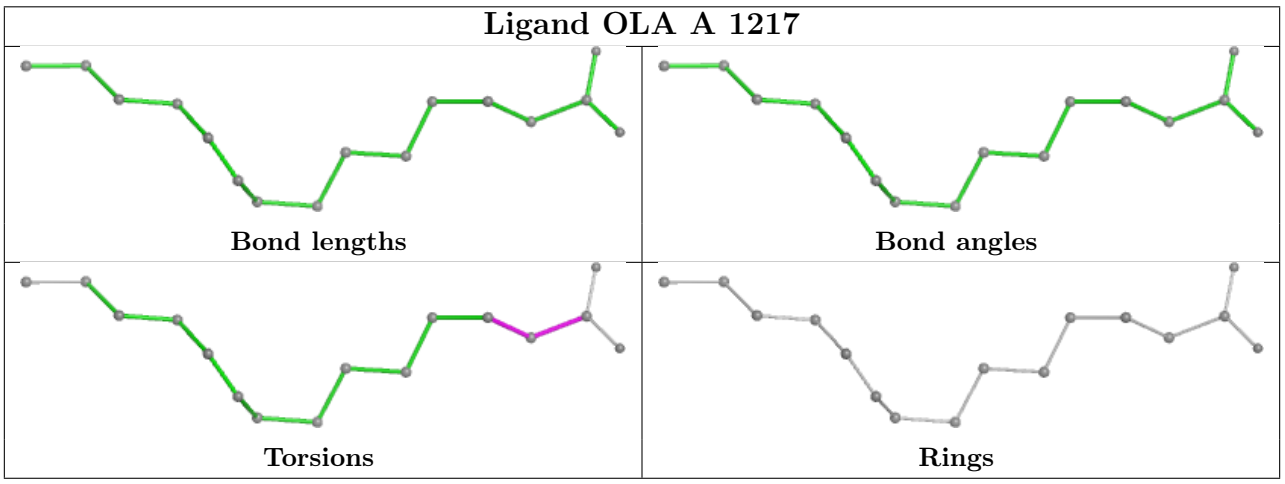
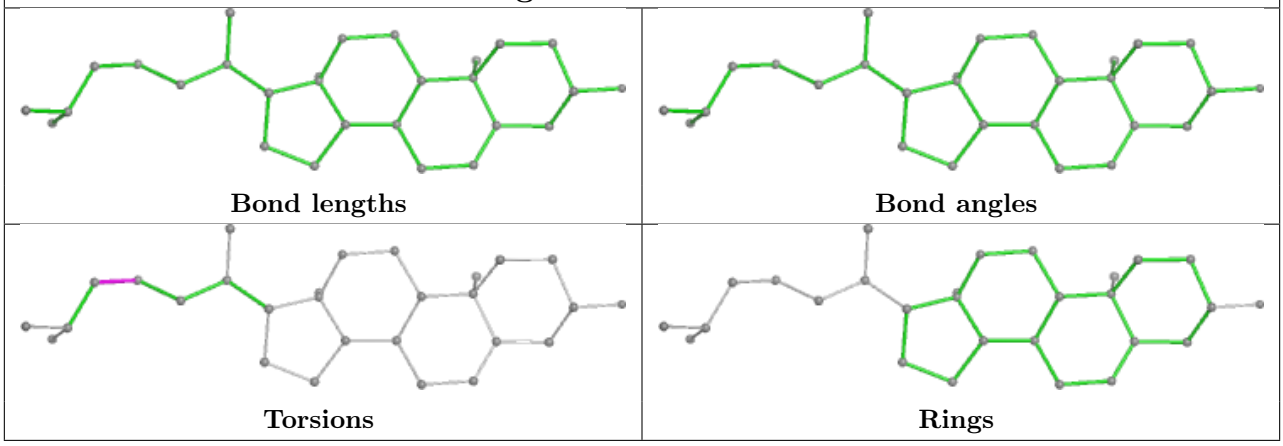
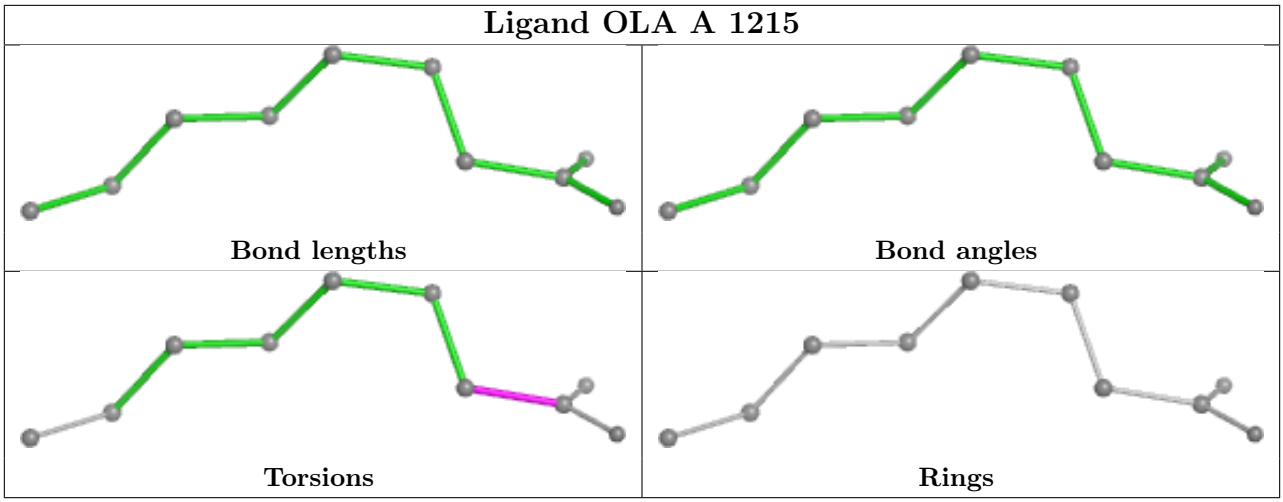


Ligand CLR A 1204



Ligand OLA A 1215



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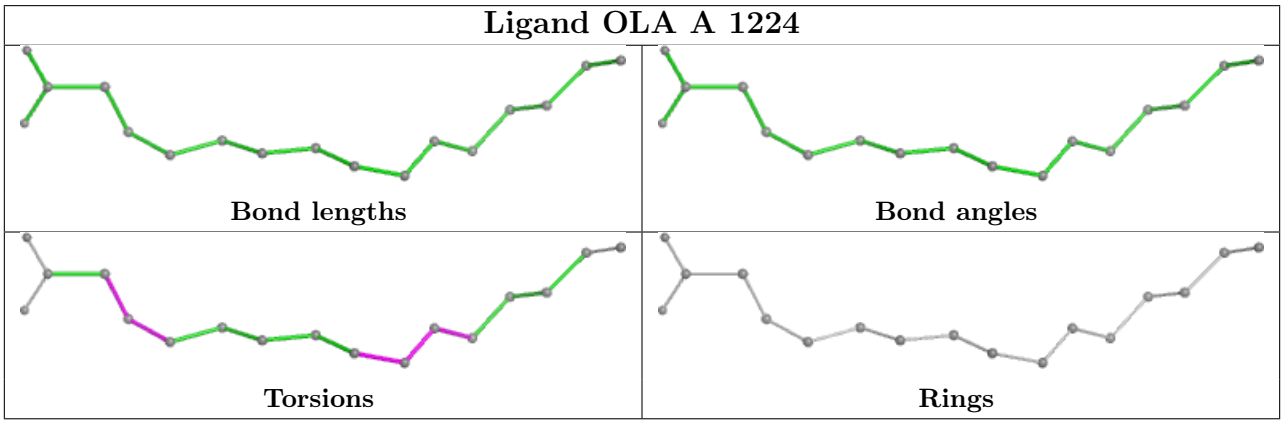

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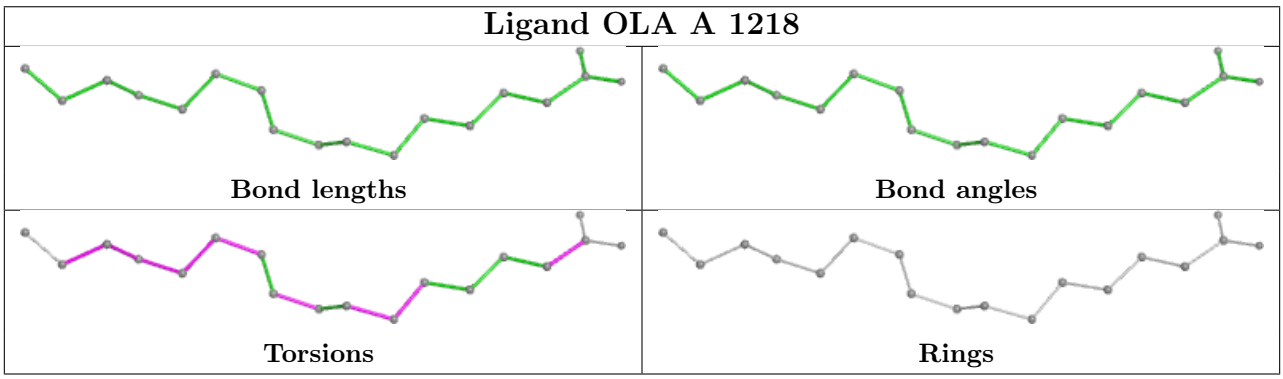

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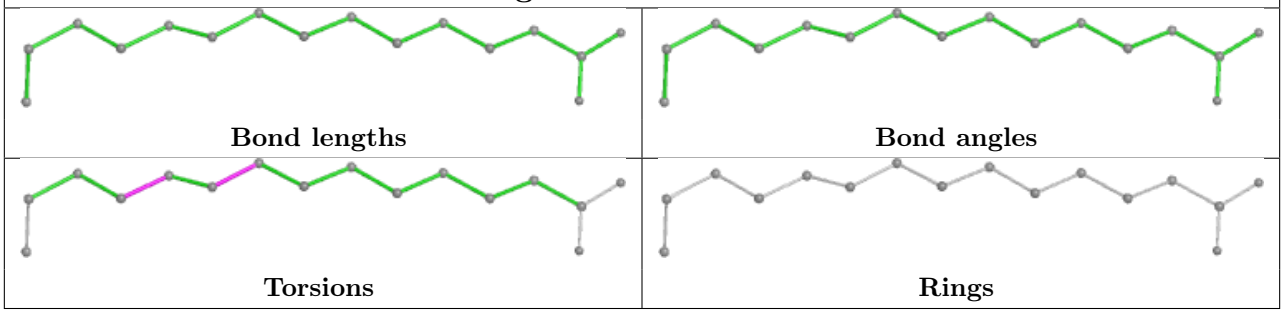

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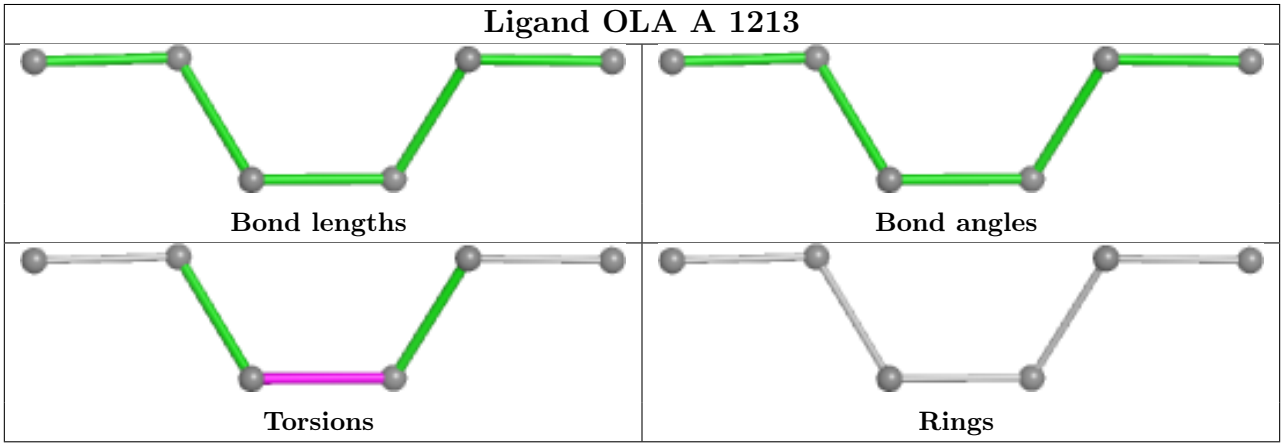

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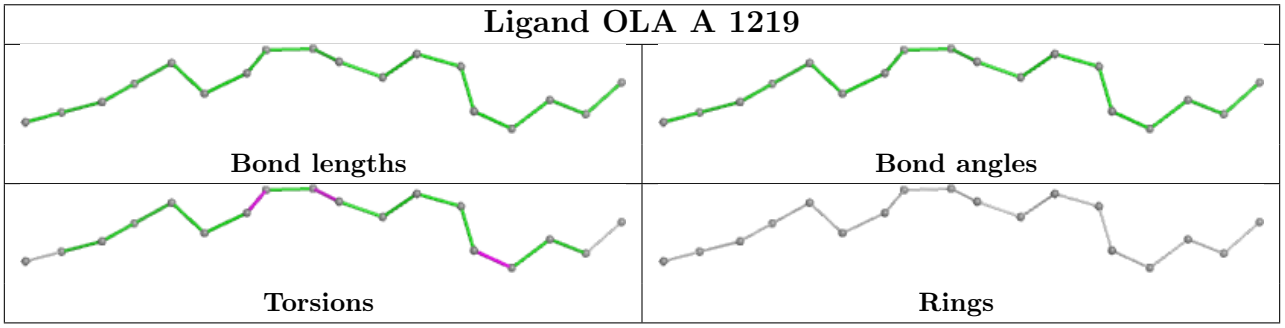

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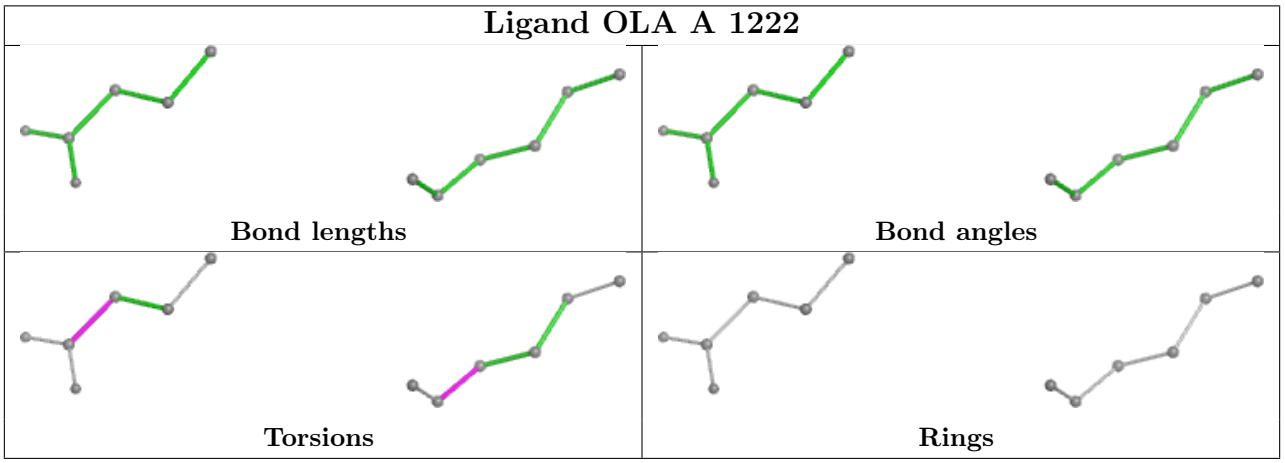
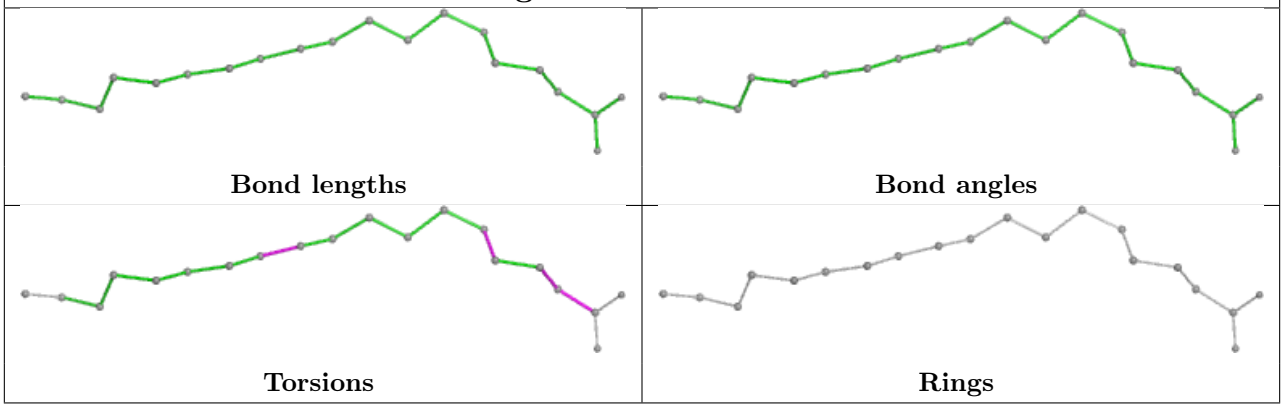
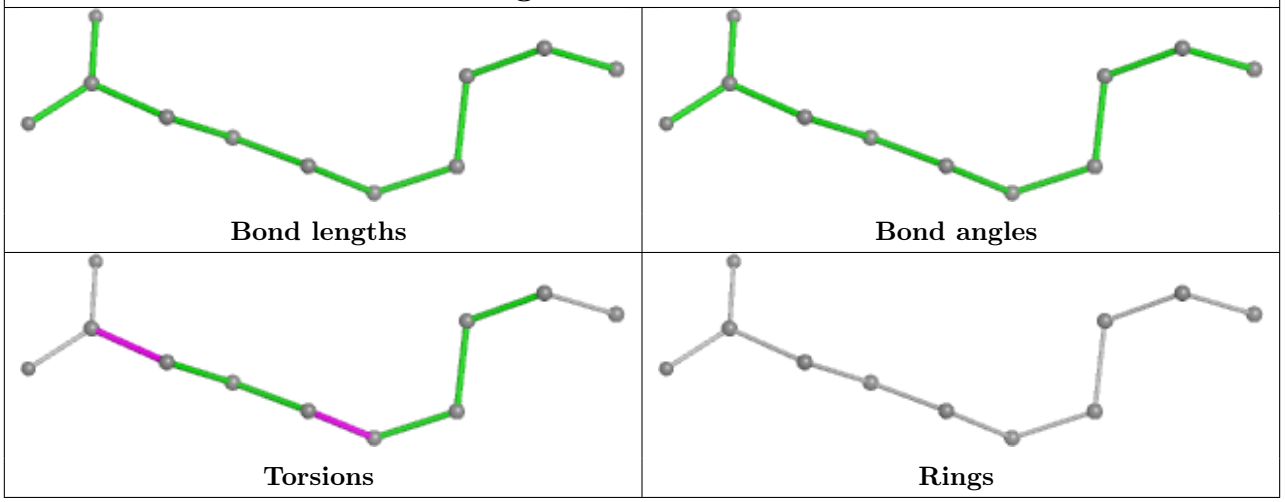


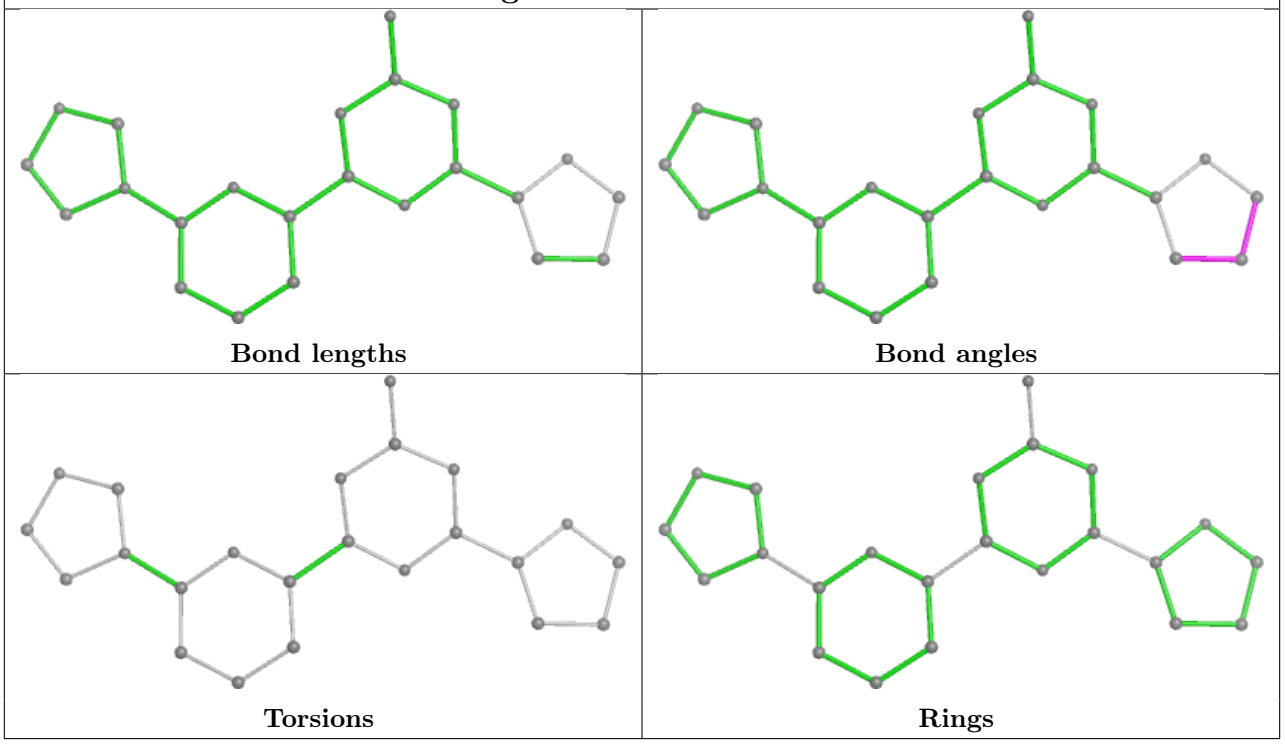
Ligand OLA A 1211



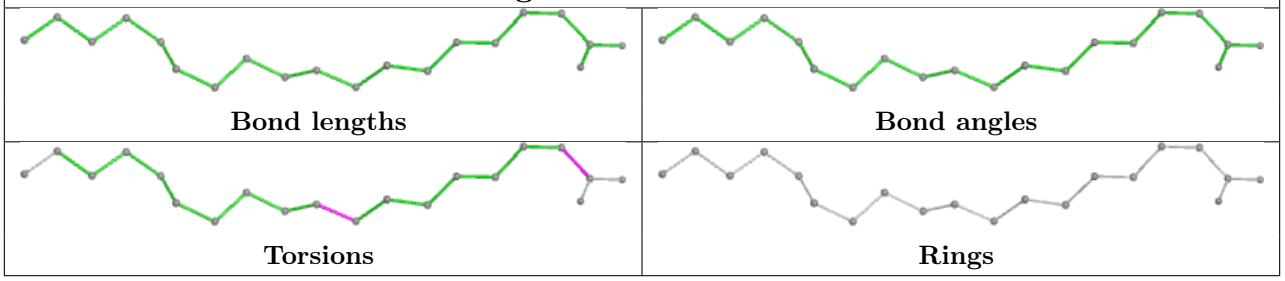
Ligand OLA A 1212



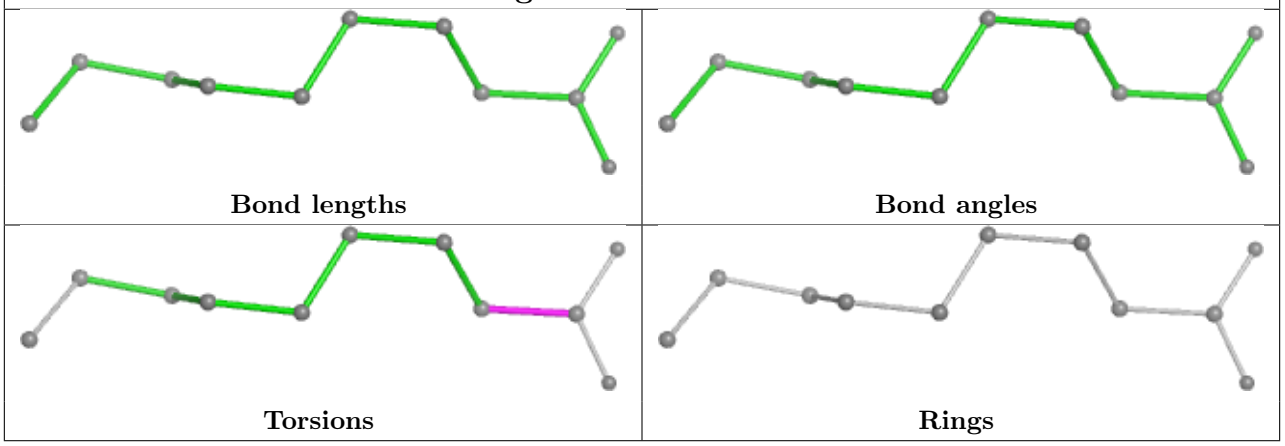
Ligand A1IR1 A 1226



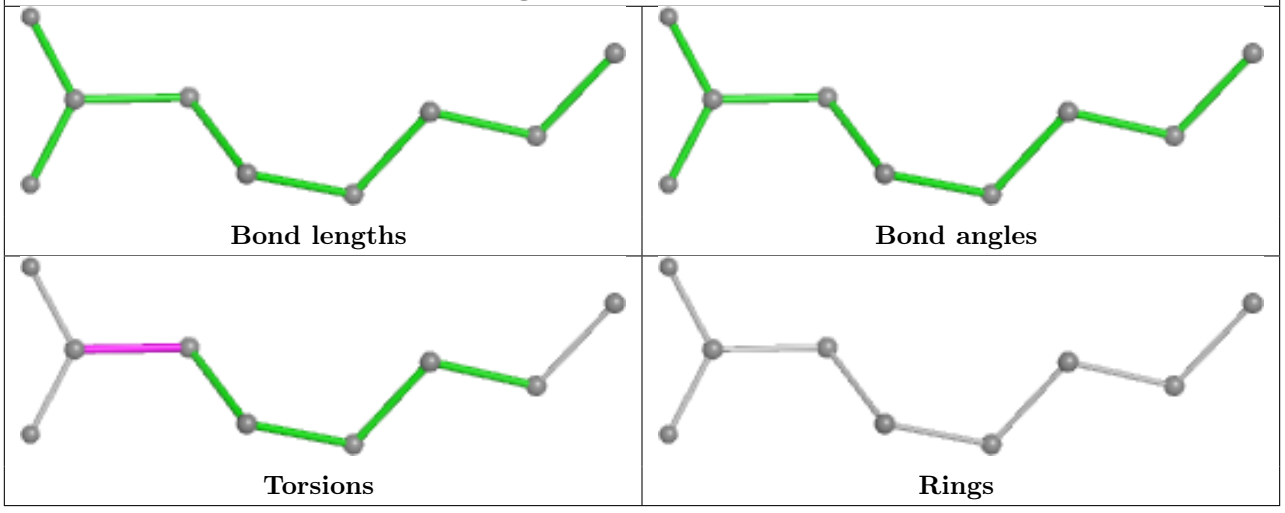
Ligand OLA A 1214



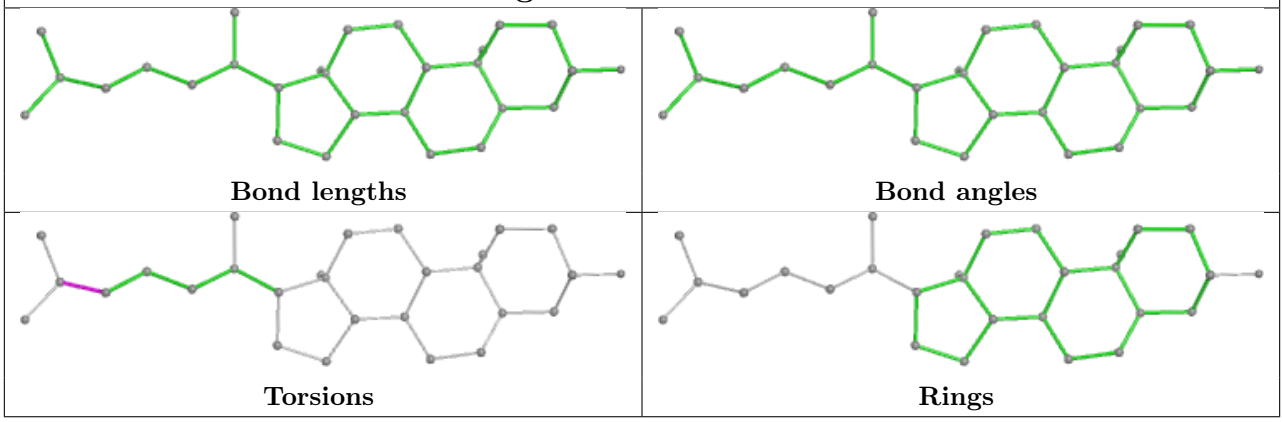
Ligand OLA A 1208



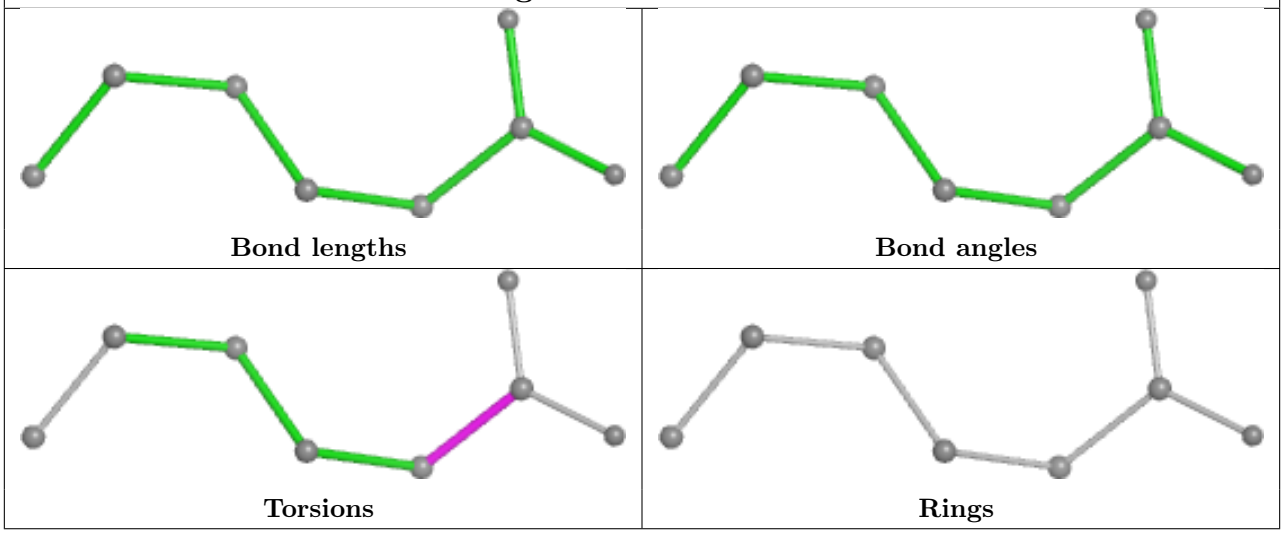
Ligand OLA A 1221



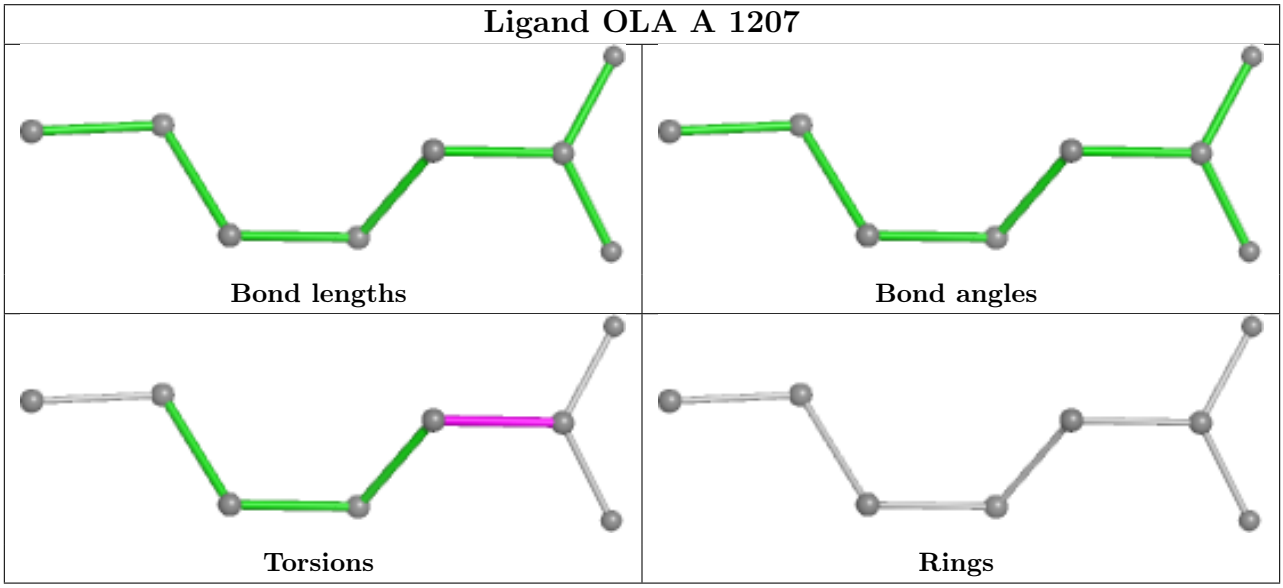
Ligand CLR A 1202



Ligand OLA A 1209



Ligand OLA A 1207



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	384/433 (88%)	0.49	41 (10%)	12	14	7, 27, 51, 72	15 (3%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1021	ASP	5.3
1	A	1061	PHE	5.0
1	A	290	TYR	4.1
1	A	1	PRO	3.7
1	A	1040	ALA	3.7
1	A	303	ILE	3.5
1	A	1066	ASP	3.4
1	A	1036	ALA	3.2
1	A	110	LEU	3.0
1	A	2	PRO	2.9
1	A	1082	GLY	2.8
1	A	1037	ALA	2.8
1	A	32	TRP	2.7
1	A	305	SER	2.7
1	A	1016	VAL	2.6
1	A	304	ARG	2.5
1	A	1023	ALA	2.5
1	A	29[A]	TRP	2.4
1	A	1105	TYR	2.4
1	A	1041	GLN	2.4
1	A	1038	LEU	2.4
1	A	1002	ASP	2.4
1	A	220	ARG	2.3
1	A	1028	ASP	2.3
1	A	1084	VAL	2.3
1	A	1106	LEU	2.3
1	A	1102	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1001	ALA	2.3
1	A	1003	LEU	2.3
1	A	1063	HIS	2.3
1	A	208	LEU	2.3
1	A	206	ARG	2.2
1	A	1010	LEU	2.2
1	A	3	ILE	2.2
1	A	302	ILE	2.2
1	A	1031	THR	2.2
1	A	293	ARG	2.2
1	A	111	ARG	2.1
1	A	1012	ASP	2.1
1	A	1009	THR	2.1
1	A	1099	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	OLA	A	1207	8/20	0.50	0.26	66,66,67,67	0
4	OLA	A	1214	20/20	0.67	0.23	64,64,67,67	0
4	OLA	A	1213	6/20	0.69	0.22	42,42,43,43	0
4	OLA	A	1222	12/20	0.70	0.20	44,44,62,62	0
4	OLA	A	1215	10/20	0.72	0.25	64,64,64,64	0
4	OLA	A	1209	8/20	0.75	0.24	57,59,61,61	0
4	OLA	A	1217	16/20	0.76	0.21	64,64,65,65	0
4	OLA	A	1210	16/20	0.77	0.18	34,38,43,43	0
4	OLA	A	1208	11/20	0.77	0.22	68,69,69,69	0

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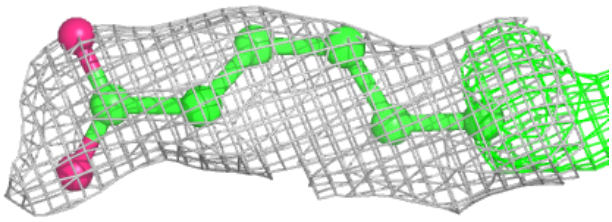
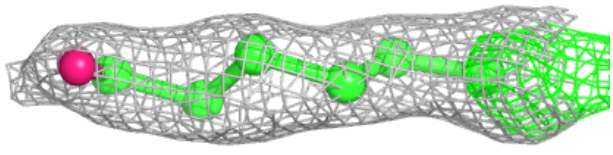
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	OLA	A	1206	11/20	0.77	0.20	46,47,48,48	0
4	OLA	A	1212	11/20	0.78	0.18	50,50,53,53	0
4	OLA	A	1216	20/20	0.78	0.18	49,51,55,55	0
4	OLA	A	1223	6/20	0.78	0.26	52,53,53,53	0
4	OLA	A	1211	20/20	0.79	0.17	43,46,54,54	0
4	OLA	A	1220	15/20	0.80	0.16	44,47,54,54	0
4	OLA	A	1219	18/20	0.81	0.17	44,48,49,49	0
4	OLA	A	1225	10/20	0.81	0.15	51,52,54,54	0
4	OLA	A	1224	17/20	0.82	0.20	48,49,51,51	0
4	OLA	A	1221	9/20	0.82	0.19	47,48,51,52	0
4	OLA	A	1205	16/20	0.83	0.15	40,42,45,45	0
4	OLA	A	1218	18/20	0.85	0.16	46,47,50,50	0
3	CLR	A	1203	28/28	0.91	0.09	23,24,30,32	0
3	CLR	A	1202	28/28	0.93	0.07	20,23,32,33	0
3	CLR	A	1204	28/28	0.95	0.07	17,20,36,37	0
2	NA	A	1201	1/1	0.95	0.13	36,36,36,36	0
5	A1IR1	A	1226	23/23	0.97	0.05	13,14,23,25	0

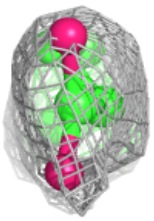
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA A 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 1214:

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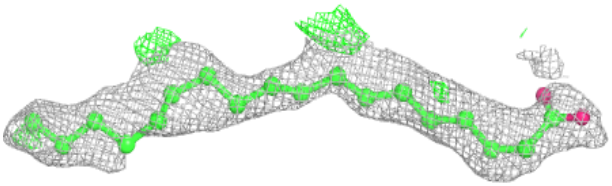
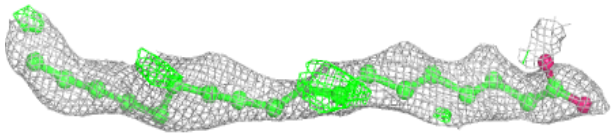
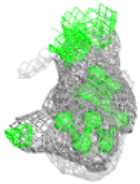
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

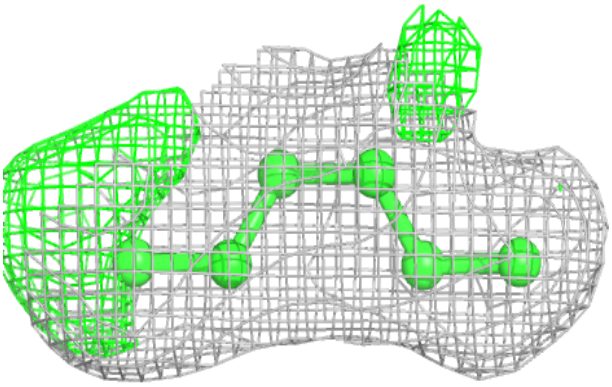


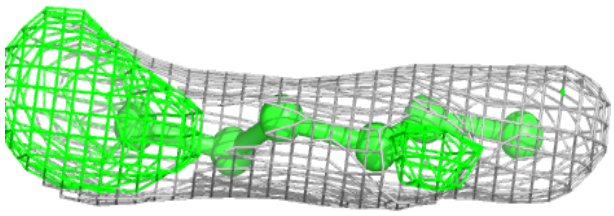


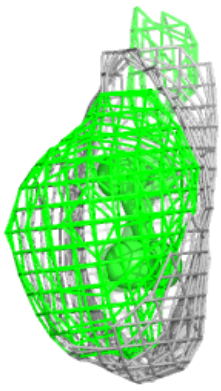


Electron density around OLA A 1213:

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

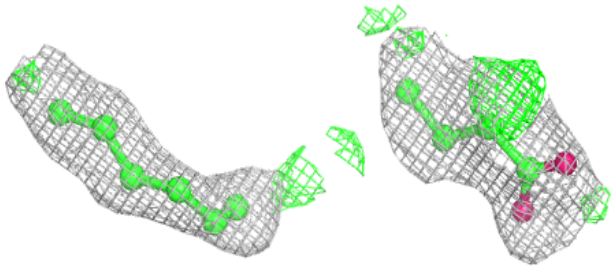


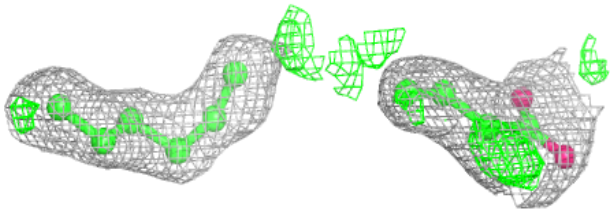


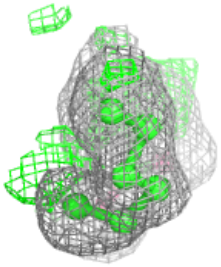


Electron density around OLA A 1222:

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

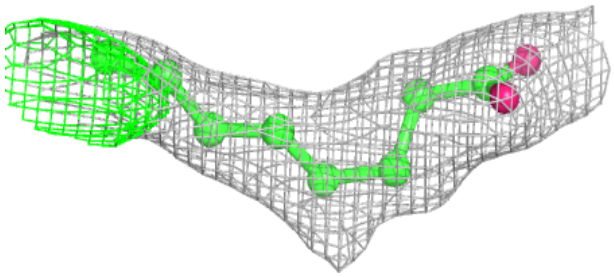


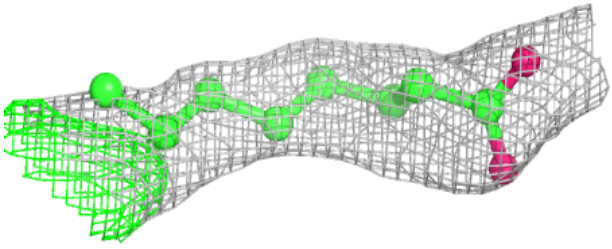


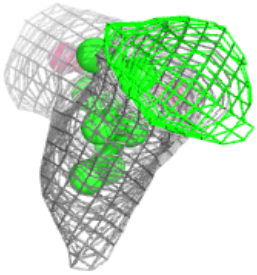


Electron density around OLA A 1215:

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

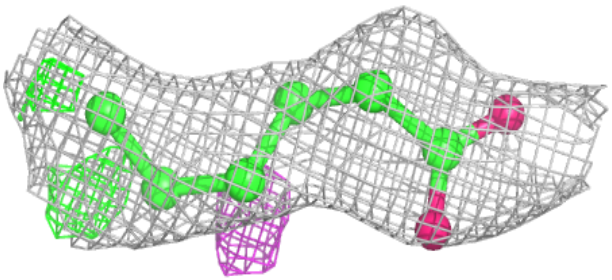


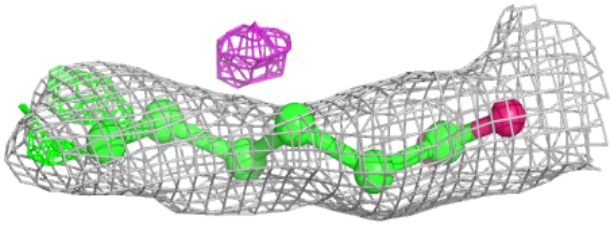


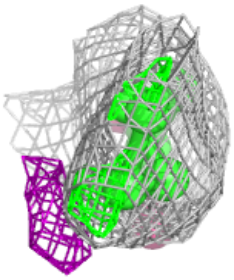


Electron density around OLA A 1209:

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

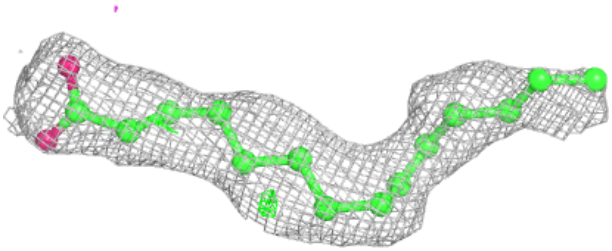


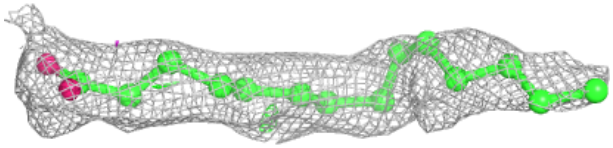


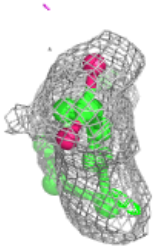


Electron density around OLA A 1217:

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

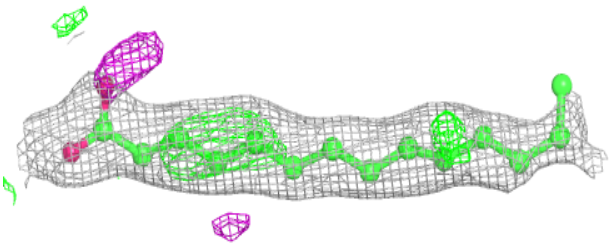


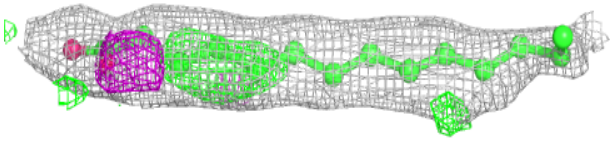


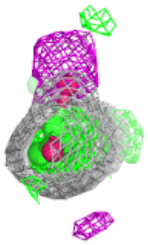


Electron density around OLA A 1210:

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

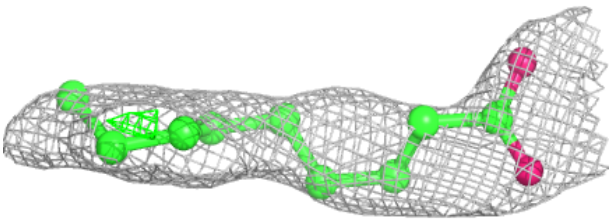


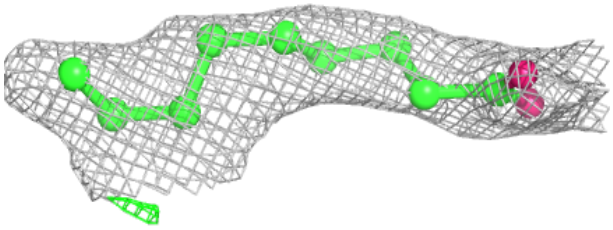


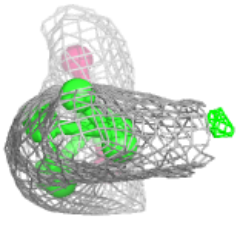


Electron density around OLA A 1208:

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

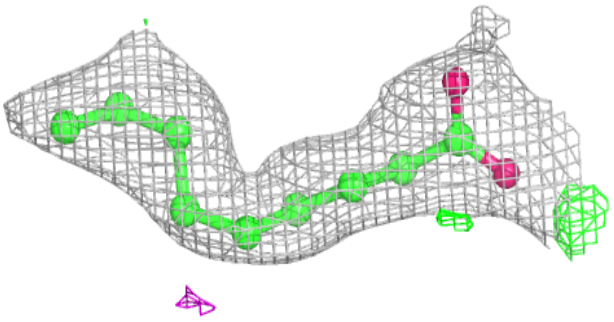


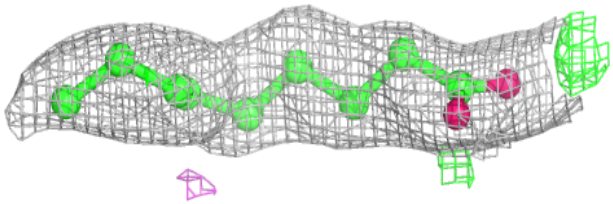


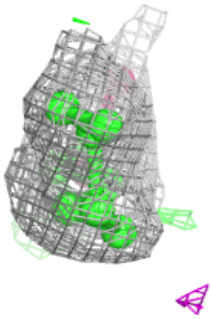


Electron density around OLA A 1212:

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

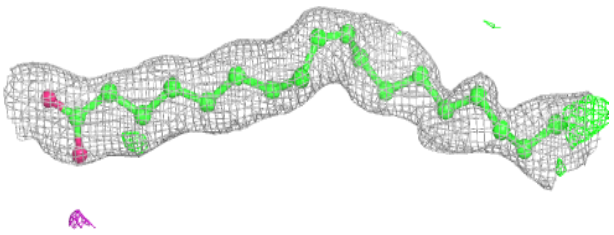


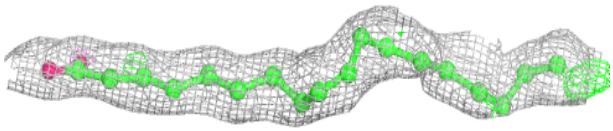


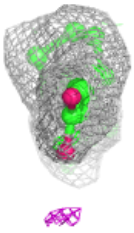


Electron density around OLA A 1216:

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

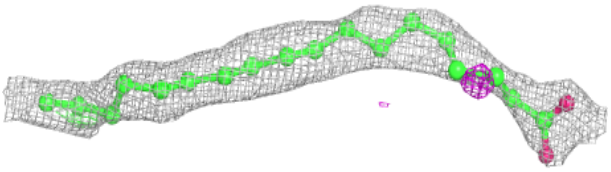


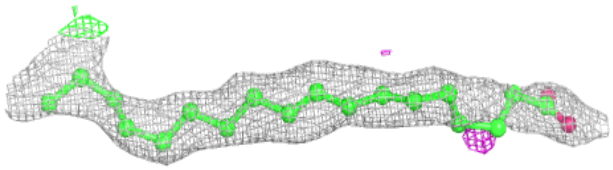


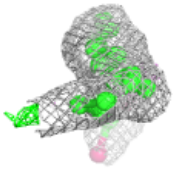


Electron density around OLA A 1211:

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

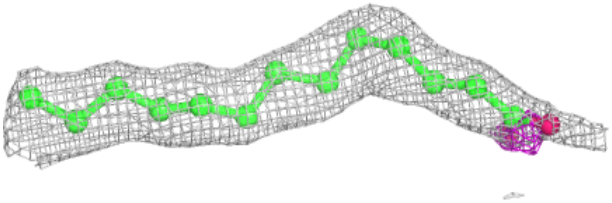


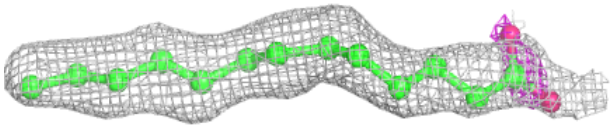


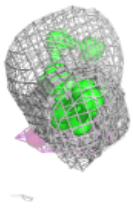


Electron density around OLA A 1220:

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

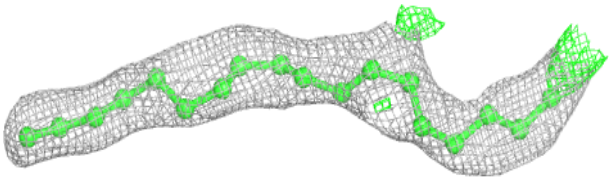


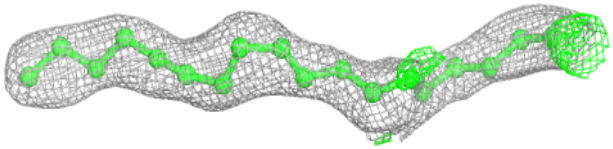


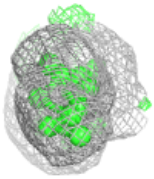


Electron density around OLA A 1219:

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

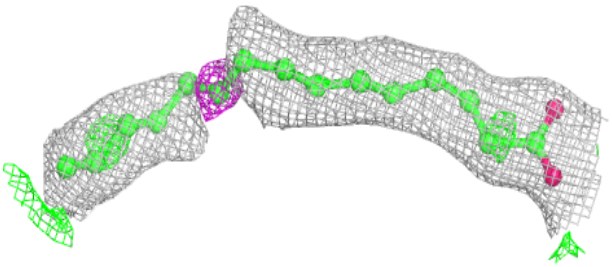


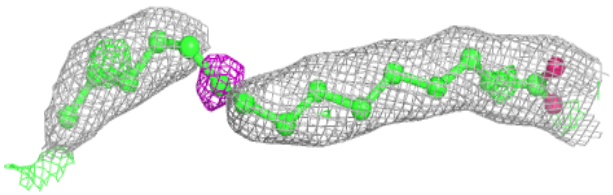


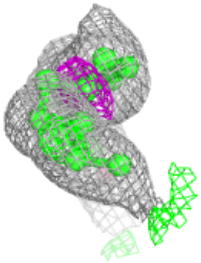


Electron density around OLA A 1224:

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

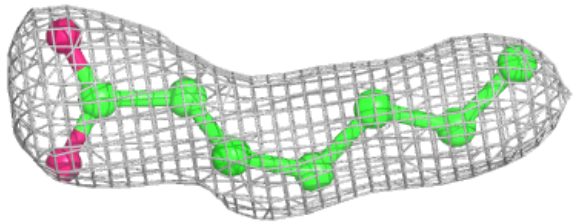


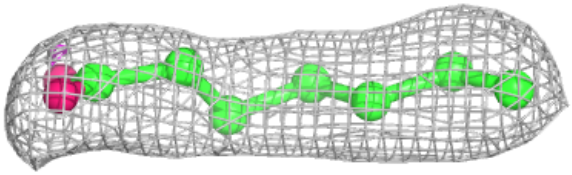


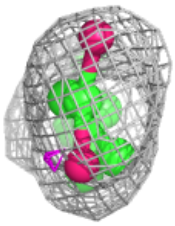


Electron density around OLA A 1221:

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

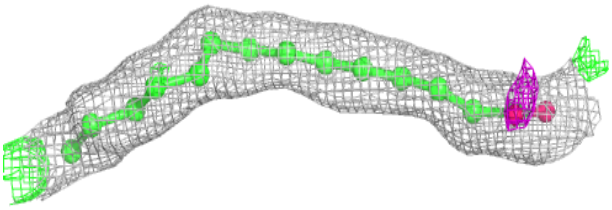


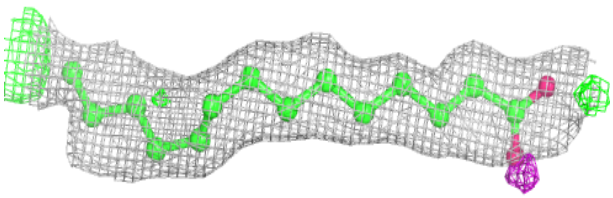


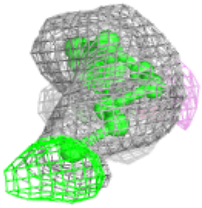


Electron density around OLA A 1205:

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

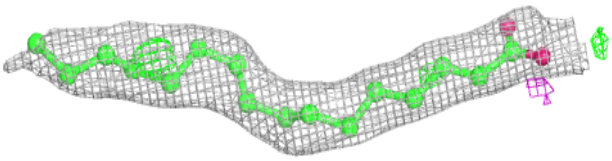


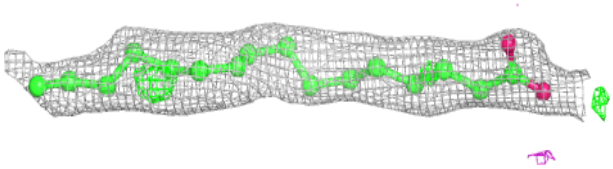


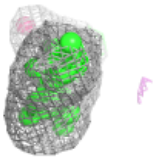


Electron density around OLA A 1218:

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

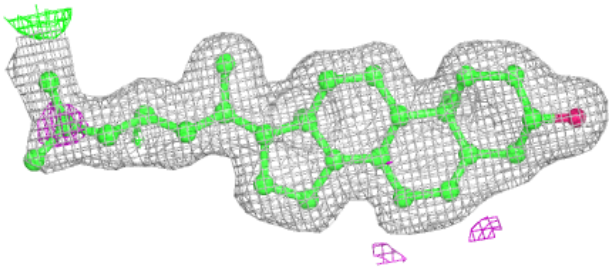


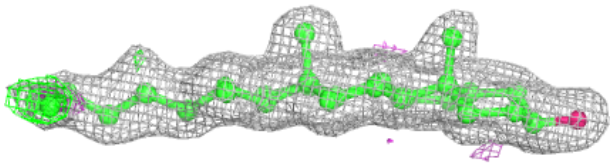


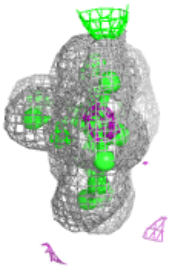


Electron density around CLR A 1202:

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

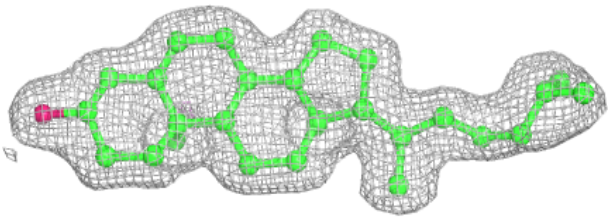


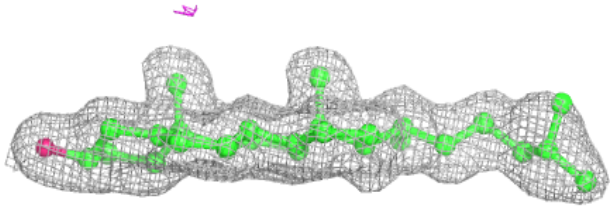


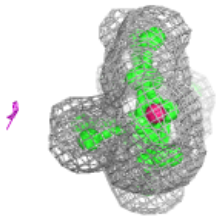


Electron density around CLR A 1204:

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

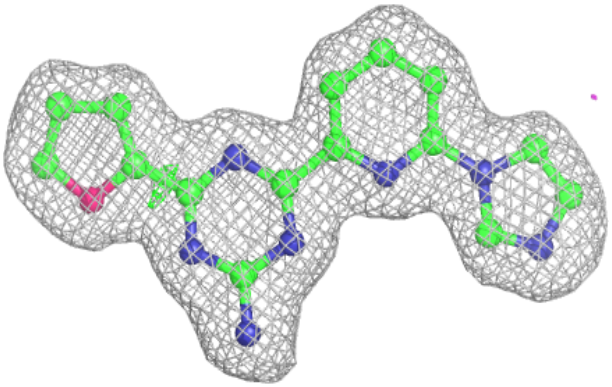


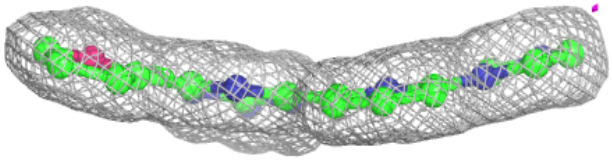


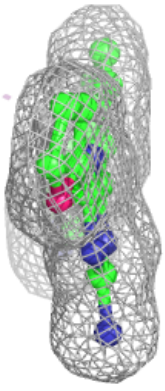


Electron density around A1IR1 A 1226:

$2mF_o$-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.