



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:34 AM UTC

PDB ID : 6ZDR / pdb_00006zdr
Title : Crystal structure of stabilized A2A adenosine receptor A2AR-StaR2-bRIL in complex with Chromone 4d
Authors : Verdon, G.; Jespers, W.; Azuaje, J.; Majellaro, M.; Keranen, H.; Garcia-mera, X.; Congreve, M.; Deflorian, F.; de Graaf, C.; Zhukov, A.; Dore, A.; Mason, J.; Aqvist, J.; Cooke, R.; Sotelo, E.; Gutierrez-de-Teran, H.
Deposited on : 2020-06-15
Resolution : 1.92 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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

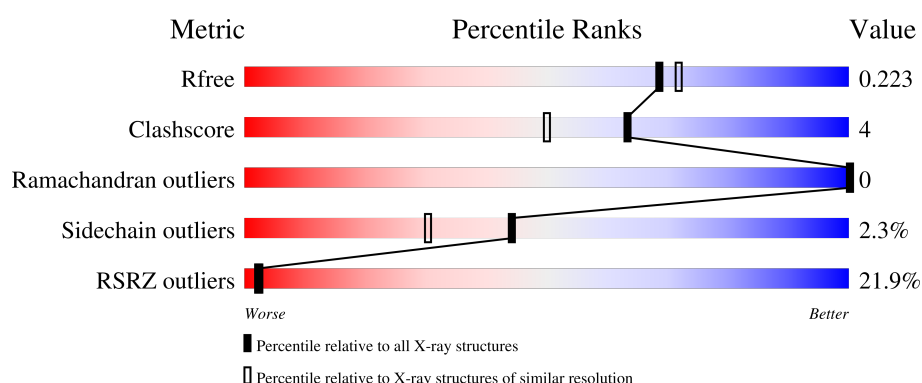
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	433	19% 64% 23% 12%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3426 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Adenosine receptor A2a,Soluble cytochrome b562,Adenosine receptor A2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	6	0
			2995	1956	506	512	21			

There are 33 discrepancies between the modelled and reference sequences:

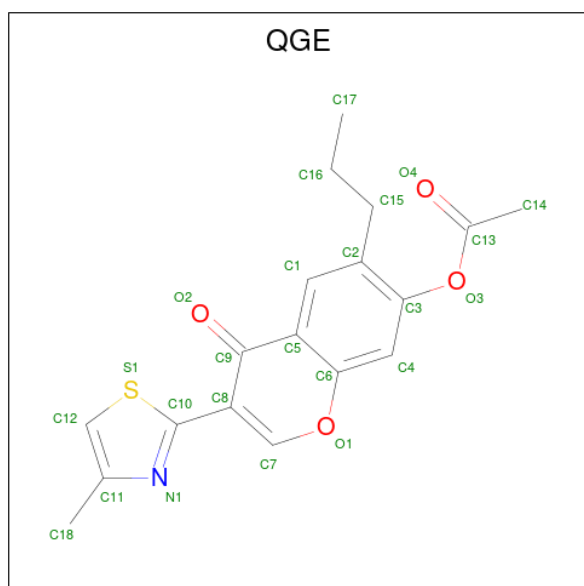
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ASP	-	expression tag	UNP P29274
A	-7	TYR	-	expression tag	UNP P29274
A	-6	LYS	-	expression tag	UNP P29274
A	-5	ASP	-	expression tag	UNP P29274
A	-4	ASP	-	expression tag	UNP P29274
A	-3	ASP	-	expression tag	UNP P29274
A	-2	ASP	-	expression tag	UNP P29274
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	engineered mutation	UNP P29274
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	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	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	277	ALA	SER	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 [3-(4-methyl-1,3-thiazol-2-yl)-4-oxidanylidene-6-propyl-chromen-7-yl] ethanoate (CCD ID: QGE) (formula: C₁₈H₁₇NO₄S) (labeled as "Ligand of Interest" by depositor).

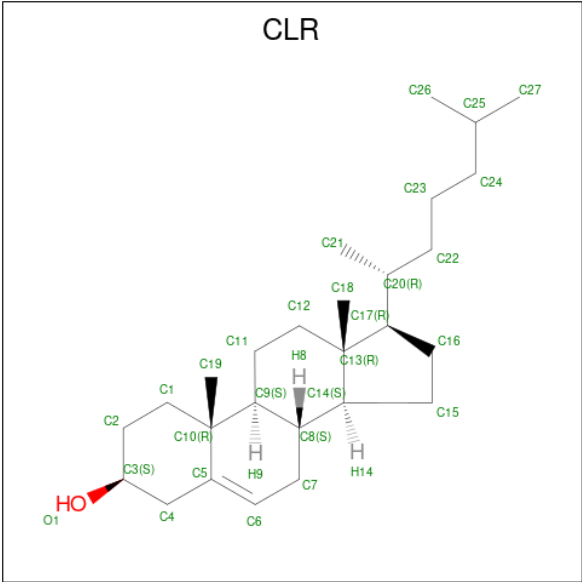


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			24	18	1	4	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

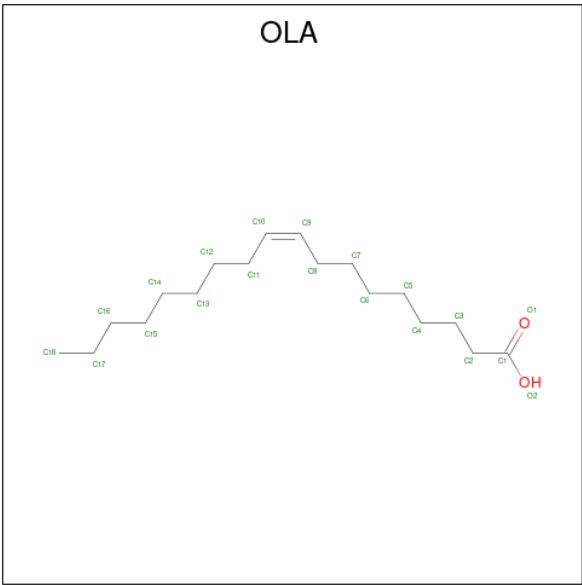
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



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

- Molecule 5 is OLEIC ACID (CCD ID: OLA) (formula: C₁₈H₃₄O₂).



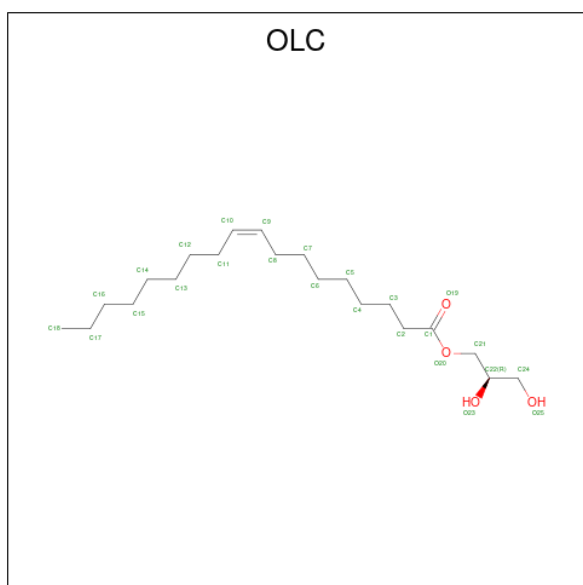
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			15	13	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 5 5	0	0
5	A	1	Total C O 14 12 2	0	0
5	A	1	Total C 8 8	0	0
5	A	1	Total C 16 16	0	0
5	A	1	Total C O 12 10 2	0	0
5	A	1	Total C O 20 18 2	0	0
5	A	1	Total C O 11 9 2	0	0
5	A	1	Total C O 15 13 2	0	0
5	A	1	Total C O 11 9 2	0	0
5	A	1	Total C 9 9	0	0

- Molecule 6 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			19	15	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			20	16	4		
6	A	1	Total	C	O	0	0
			18	14	4		
6	A	1	Total	C	O	0	0
			25	21	4		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	104	Total	O	0	0
			104	104		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	39.26Å 180.23Å 140.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.06 – 1.92 45.06 – 1.92	Depositor EDS
% Data completeness (in resolution range)	84.4 (45.06-1.92) 84.4 (45.06-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.92Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.208 , 0.218 0.214 , 0.223	Depositor DCC
R_{free} test set	1636 reflections (4.22%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3426	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.74	76/3079 (2.5%)	1.38	40/4190 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	188	VAL	C-O	-7.71	1.18	1.24
1	A	138	THR	C-O	-7.25	1.17	1.24
1	A	7[A]	SER	CA-C	7.07	1.61	1.52
1	A	7[B]	SER	CA-C	7.07	1.61	1.52
1	A	247	LEU	C-O	-6.94	1.17	1.24
1	A	9	TYR	C-O	-6.55	1.16	1.24
1	A	92	ILE	C-O	-6.55	1.16	1.24
1	A	55	VAL	C-O	-6.33	1.17	1.24
1	A	252	ILE	C-O	-6.23	1.16	1.24
1	A	176	TYR	C-O	-6.18	1.17	1.24
1	A	293	ARG	CA-C	6.13	1.60	1.52
1	A	178	VAL	C-O	-5.98	1.18	1.24
1	A	60	ILE	C-O	-5.96	1.17	1.24
1	A	187[A]	LEU	CA-C	5.90	1.60	1.52
1	A	187[B]	LEU	CA-C	5.90	1.60	1.52
1	A	205[A]	ARG	CA-C	5.80	1.60	1.52
1	A	205[B]	ARG	CA-C	5.80	1.60	1.52
1	A	274	ILE	C-O	-5.79	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	ASN	C-O	-5.76	1.19	1.24
1	A	79	PHE	C-O	-5.75	1.17	1.24
1	A	51	ALA	C-O	-5.74	1.17	1.24
1	A	83	PHE	C-O	-5.74	1.17	1.24
1	A	75[A]	HIS	CA-C	5.74	1.60	1.52
1	A	75[B]	HIS	CA-C	5.74	1.60	1.52
1	A	249	LEU	C-O	-5.73	1.17	1.24
1	A	49	ALA	C-O	-5.68	1.17	1.24
1	A	147	GLY	C-O	-5.68	1.18	1.24
1	A	56	GLY	C-O	-5.68	1.17	1.23
1	A	59	ALA	C-O	-5.65	1.17	1.24
1	A	29[A]	TRP	CA-C	5.64	1.60	1.52
1	A	29[B]	TRP	CA-C	5.64	1.60	1.52
1	A	133	PHE	C-O	-5.62	1.17	1.24
1	A	22	LEU	C-O	-5.60	1.17	1.24
1	A	6[A]	SER	CA-C	5.60	1.60	1.52
1	A	6[B]	SER	CA-C	5.60	1.60	1.52
1	A	175	ASN	C-O	-5.57	1.17	1.24
1	A	192	LEU	C-O	-5.56	1.17	1.24
1	A	239	ALA	C-O	-5.56	1.17	1.24
1	A	130	VAL	C-O	-5.54	1.17	1.24
1	A	277	ALA	C-O	-5.50	1.17	1.24
1	A	57	VAL	C-O	-5.48	1.17	1.24
1	A	63	ALA	C-O	-5.47	1.17	1.24
1	A	127	ILE	C-O	-5.47	1.17	1.24
1	A	27	VAL	C-O	-5.46	1.18	1.24
1	A	281	SER	C-O	-5.40	1.17	1.24
1	A	243	ALA	C-O	-5.39	1.17	1.24
1	A	11	THR	C-O	-5.38	1.18	1.24
1	A	128	CYS	C-O	-5.35	1.17	1.24
1	A	292	ILE	C-O	-5.35	1.18	1.24
1	A	237	ILE	C-O	-5.34	1.18	1.24
1	A	64	ILE	C-O	-5.32	1.18	1.24
1	A	272	LEU	C-O	-5.30	1.18	1.24
1	A	180	PHE	C-O	-5.27	1.17	1.24
1	A	136	GLY	C-O	-5.25	1.17	1.23
1	A	190	LEU	C-O	-5.20	1.18	1.24
1	A	241	LEU	C-O	-5.19	1.18	1.24
1	A	254	CYS	C-O	-5.18	1.18	1.24
1	A	81	ALA	C-O	-5.17	1.18	1.24
1	A	94	SER	C-O	-5.16	1.18	1.24
1	A	259	CYS	C-O	-5.15	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	ASN	C-O	-5.15	1.18	1.24
1	A	14	LEU	C-O	-5.14	1.18	1.24
1	A	245	CYS	C-O	-5.14	1.17	1.24
1	A	267	LEU	C-O	-5.12	1.18	1.24
1	A	255	PHE	C-O	-5.12	1.18	1.24
1	A	17	ALA	C-O	-5.11	1.18	1.24
1	A	74	CYS	C-O	-5.11	1.18	1.24
1	A	258	PHE	C-O	-5.09	1.17	1.24
1	A	77	CYS	C-O	-5.09	1.18	1.24
1	A	208	LEU	C-N	5.09	1.40	1.33
1	A	189	PRO	C-O	-5.07	1.17	1.24
1	A	91	SER	C-O	-5.03	1.18	1.24
1	A	242	PHE	C-O	-5.03	1.18	1.24
1	A	67	SER	C-O	-5.02	1.17	1.24
1	A	85	LEU	C-O	-5.01	1.17	1.24
1	A	89	GLN	C-O	-5.00	1.18	1.24

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29[A]	TRP	CA-C-O	12.02	133.79	119.97
1	A	29[B]	TRP	CA-C-O	12.02	133.79	119.97
1	A	293	ARG	N-CA-C	12.01	124.37	111.28
1	A	293	ARG	CA-C-O	11.37	132.61	120.55
1	A	75[A]	HIS	CA-C-O	11.21	132.86	119.97
1	A	75[B]	HIS	CA-C-O	11.21	132.86	119.97
1	A	283	VAL	N-CA-C	11.17	122.00	110.72
1	A	208	LEU	O-C-N	-11.00	108.74	122.27
1	A	205[A]	ARG	CA-C-O	10.98	132.78	119.49
1	A	205[B]	ARG	CA-C-O	10.98	132.78	119.49
1	A	6[A]	SER	CA-C-O	10.27	131.91	119.49
1	A	6[B]	SER	CA-C-O	10.27	131.91	119.49
1	A	208	LEU	CA-C-N	10.07	133.78	120.28
1	A	208	LEU	C-N-CA	10.07	133.78	120.28
1	A	187[A]	LEU	CA-C-O	9.81	131.40	120.90
1	A	187[B]	LEU	CA-C-O	9.81	131.40	120.90
1	A	75[A]	HIS	N-CA-C	9.32	122.63	111.82
1	A	75[B]	HIS	N-CA-C	9.32	122.63	111.82
1	A	205[A]	ARG	N-CA-C	8.15	122.33	112.38
1	A	205[B]	ARG	N-CA-C	8.15	122.33	112.38
1	A	7[A]	SER	CA-C-O	8.06	129.30	119.79
1	A	7[B]	SER	CA-C-O	8.06	129.30	119.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187[A]	LEU	N-CA-C	7.76	120.42	111.11
1	A	187[B]	LEU	N-CA-C	7.76	120.42	111.11
1	A	29[A]	TRP	O-C-N	-7.35	114.33	122.12
1	A	29[B]	TRP	O-C-N	-7.35	114.33	122.12
1	A	29[A]	TRP	N-CA-C	6.76	119.66	111.82
1	A	29[B]	TRP	N-CA-C	6.76	119.66	111.82
1	A	6[A]	SER	N-CA-C	6.54	120.36	112.38
1	A	6[B]	SER	N-CA-C	6.54	120.36	112.38
1	A	184	ALA	N-CA-C	6.31	117.96	111.14
1	A	82	CYS	N-CA-C	6.25	120.90	113.28
1	A	293	ARG	O-C-N	-6.18	115.57	122.12
1	A	6[A]	SER	O-C-N	-5.92	114.69	122.39
1	A	6[B]	SER	O-C-N	-5.92	114.69	122.39
1	A	34	ASN	N-CA-C	5.71	117.96	108.20
1	A	58	LEU	N-CA-C	5.26	119.16	112.12
1	A	1037	ALA	N-CA-C	-5.20	105.22	112.45
1	A	1066	ASP	N-CA-C	-5.17	105.73	111.36
1	A	178	VAL	N-CA-C	5.01	115.30	110.74

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	LEU	Mainchain
1	A	6[A]	SER	Mainchain
1	A	6[B]	SER	Mainchain
1	A	7[B]	SER	Mainchain

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	2995	0	3080	25	0
2	A	24	0	0	2	0
3	A	1	0	0	0	0
4	A	84	0	138	1	0
5	A	136	0	193	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	82	0	111	1	0
7	A	104	0	0	0	0
All	All	3426	0	3522	27	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (27) 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:301:LYS:HB3	1:A:301:LYS:NZ	1.97	0.80
1:A:270:MET:HG3	2:A:1201:QGE:C14	2.13	0.77
1:A:1027:LYS:HE3	1:A:1080:ASN:OD1	1.87	0.74
1:A:1041:GLN:O	1:A:1041:GLN:HG2	1.94	0.66
1:A:270:MET:HE2	2:A:1201:QGE:C14	2.28	0.63
1:A:301:LYS:HB3	1:A:301:LYS:HZ3	1.62	0.63
1:A:1038:LEU:HD21	1:A:1069:VAL:HG21	1.84	0.59
1:A:116:VAL:HG13	5:A:1220:OLA:C10	2.39	0.53
1:A:1017:ILE:HD11	1:A:1030:LEU:HG	1.91	0.52
1:A:55:VAL:HA	1:A:59:ALA:HB3	1.94	0.49
1:A:1038:LEU:HD23	1:A:1038:LEU:N	2.26	0.49
1:A:1007:TRP:CH2	1:A:1103:GLN:HG3	2.49	0.48
1:A:238:ILE:HD11	1:A:287:ILE:HB	1.95	0.48
4:A:1205:CLR:H3	6:A:1211:OLC:H24	1.95	0.48
1:A:301:LYS:NZ	1:A:301:LYS:CB	2.72	0.46
1:A:248:PRO:HG2	1:A:276:LEU:HD23	1.98	0.46
1:A:289:ALA:O	1:A:296:ARG:HD3	2.16	0.46
1:A:208:LEU:CD1	1:A:222:ARG:HG3	2.46	0.45
1:A:32:TRP:CD1	1:A:32:TRP:C	2.95	0.45
1:A:40:VAL:HG11	1:A:116:VAL:CG1	2.47	0.45
1:A:1038:LEU:CD2	1:A:1069:VAL:HG21	2.47	0.44
1:A:1010:LEU:HD23	1:A:1010:LEU:C	2.42	0.44
5:A:1214:OLA:H31	5:A:1215:OLA:H31	1.99	0.44
1:A:0:ALA:HB1	1:A:1:PRO:HD2	2.00	0.43
1:A:208:LEU:HD11	1:A:222:ARG:HG3	2.01	0.43
1:A:187[B]:LEU:HD12	1:A:187[B]:LEU:HA	1.94	0.40
1:A:14:LEU:HD23	1:A:14:LEU:HA	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	385/433 (89%)	383 (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	314/353 (89%)	307 (98%)	7 (2%)	45	32

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	SER
1	A	161	GLU
1	A	1014	LEU
1	A	1039	ASP
1	A	1076	LEU
1	A	275	VAL
1	A	301	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN

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Mol	Chain	Res	Type
1	A	155	HIS
1	A	1025	GLN
1	A	1041	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	$\# Z > 2$
2	QGE	A	1201	-	26,26,26	1.24	3 (11%)	35,37,37	1.90	8 (22%)
4	CLR	A	1204	-	31,31,31	0.69	0	48,48,48	1.07	2 (4%)
6	OLC	A	1212	-	18,18,24	1.11	1 (5%)	18,18,25	1.18	2 (11%)
6	OLC	A	1213	-	17,17,24	1.14	1 (5%)	18,18,25	1.16	2 (11%)
5	OLA	A	1218	-	14,14,19	0.59	0	14,14,19	0.85	0
5	OLA	A	1220	-	8,8,19	0.19	0	7,7,19	0.58	0
5	OLA	A	1217	-	10,10,19	0.71	0	10,10,19	0.84	0
5	OLA	A	1207	-	4,4,19	0.27	0	3,3,19	0.45	0
5	OLA	A	1209	-	7,7,19	0.24	0	6,6,19	0.50	0
4	CLR	A	1205	-	31,31,31	0.64	0	48,48,48	1.30	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	OLA	A	1215	-	19,19,19	0.53	0	19,19,19	0.76	0
5	OLA	A	1210	-	14,14,19	0.27	0	12,12,19	0.46	0
5	OLA	A	1208	-	13,13,19	0.62	0	13,13,19	0.71	0
6	OLC	A	1216	-	24,24,24	0.97	1 (4%)	25,25,25	0.89	2 (8%)
5	OLA	A	1214	-	11,11,19	0.60	0	11,11,19	0.94	0
5	OLA	A	1206	-	14,14,19	0.54	0	14,14,19	0.96	1 (7%)
6	OLC	A	1211	-	18,18,24	0.99	1 (5%)	19,19,25	1.27	2 (10%)
5	OLA	A	1219	-	10,10,19	0.64	0	10,10,19	0.81	0
4	CLR	A	1203	-	31,31,31	0.63	0	48,48,48	1.14	4 (8%)

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
2	QGE	A	1201	-	-	5/11/11/11	0/3/3/3
4	CLR	A	1204	-	-	0/10/68/68	0/4/4/4
6	OLC	A	1212	-	-	6/17/17/24	-
6	OLC	A	1213	-	-	5/17/17/24	-
5	OLA	A	1218	-	-	2/12/12/17	-
5	OLA	A	1220	-	-	1/6/6/17	-
5	OLA	A	1217	-	-	2/8/8/17	-
5	OLA	A	1207	-	-	0/2/2/17	-
5	OLA	A	1209	-	-	3/5/5/17	-
4	CLR	A	1205	-	-	0/10/68/68	0/4/4/4
5	OLA	A	1215	-	-	5/17/17/17	-
5	OLA	A	1210	-	-	3/10/10/17	-
5	OLA	A	1208	-	-	2/11/11/17	-
6	OLC	A	1216	-	-	6/24/24/24	-
5	OLA	A	1214	-	-	1/9/9/17	-
5	OLA	A	1206	-	-	8/12/12/17	-
6	OLC	A	1211	-	-	5/18/18/24	-
5	OLA	A	1219	-	-	1/8/8/17	-
4	CLR	A	1203	-	-	0/10/68/68	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1216	OLC	O20-C1	4.53	1.46	1.33
6	A	1212	OLC	O20-C1	4.46	1.46	1.33
6	A	1213	OLC	O20-C1	4.40	1.46	1.33
6	A	1211	OLC	O20-C1	3.85	1.44	1.33
2	A	1201	QGE	C12-C11	3.68	1.40	1.35
2	A	1201	QGE	C11-N1	-2.71	1.34	1.38
2	A	1201	QGE	C5-C6	-2.01	1.37	1.40

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	QGE	O1-C6-C5	4.96	124.82	121.52
2	A	1201	QGE	O2-C9-C8	4.35	130.07	123.07
4	A	1205	CLR	C4-C5-C6	-3.93	115.24	120.57
2	A	1201	QGE	C11-C12-S1	-3.61	108.70	111.23
6	A	1211	OLC	O20-C1-C2	3.54	122.61	111.83
6	A	1211	OLC	O20-C1-O19	-3.38	115.17	123.63
6	A	1212	OLC	O20-C1-C2	3.30	121.89	111.83
2	A	1201	QGE	C7-C8-C9	3.18	121.89	119.82
2	A	1201	QGE	C9-C8-C10	-3.05	119.37	123.35
6	A	1213	OLC	O20-C1-C2	3.05	121.14	111.83
4	A	1205	CLR	C4-C5-C10	3.04	120.31	116.42
6	A	1212	OLC	O20-C1-O19	-2.91	116.36	123.63
2	A	1201	QGE	C5-C9-C8	-2.80	112.11	115.64
6	A	1216	OLC	O20-C1-C2	2.75	120.23	111.83
6	A	1213	OLC	O20-C1-O19	-2.72	116.82	123.63
4	A	1203	CLR	C4-C5-C10	2.71	119.90	116.42
4	A	1205	CLR	C12-C11-C9	-2.64	108.65	113.14
4	A	1203	CLR	C4-C5-C6	-2.48	117.21	120.57
4	A	1203	CLR	C19-C10-C5	-2.45	104.65	108.38
4	A	1205	CLR	C7-C8-C14	-2.45	107.47	110.93
4	A	1205	CLR	C15-C14-C13	2.40	106.66	103.84
2	A	1201	QGE	O2-C9-C5	-2.36	117.80	121.57
5	A	1206	OLA	C3-C2-C1	-2.20	108.75	114.51
4	A	1204	CLR	C13-C14-C8	-2.16	111.35	114.41
6	A	1216	OLC	O20-C1-O19	-2.06	118.47	123.63
4	A	1205	CLR	C16-C15-C14	-2.06	101.11	105.14
4	A	1203	CLR	C10-C9-C8	-2.04	109.73	112.71
4	A	1204	CLR	C4-C5-C6	-2.03	117.81	120.57
2	A	1201	QGE	C1-C5-C6	2.03	121.03	118.28

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1212	OLC	C21-C22-C24-O25
6	A	1213	OLC	O20-C21-C22-C24
6	A	1213	OLC	O20-C21-C22-O23
2	A	1201	QGE	O4-C13-O3-C3
2	A	1201	QGE	C14-C13-O3-C3
2	A	1201	QGE	C4-C3-O3-C13
5	A	1219	OLA	C1-C2-C3-C4
6	A	1216	OLC	C2-C1-O20-C21
2	A	1201	QGE	C2-C3-O3-C13
6	A	1211	OLC	C21-C22-C24-O25
6	A	1212	OLC	O23-C22-C24-O25
6	A	1216	OLC	O19-C1-O20-C21
6	A	1216	OLC	C11-C12-C13-C14
5	A	1210	OLA	C4-C5-C6-C7
5	A	1209	OLA	C4-C5-C6-C7
6	A	1216	OLC	C2-C3-C4-C5
6	A	1216	OLC	C14-C15-C16-C17
5	A	1215	OLA	C12-C13-C14-C15
6	A	1211	OLC	O23-C22-C24-O25
5	A	1208	OLA	C5-C6-C7-C8
5	A	1206	OLA	C6-C7-C8-C9
5	A	1210	OLA	C11-C12-C13-C14
6	A	1212	OLC	C6-C7-C8-C9
5	A	1206	OLA	C3-C4-C5-C6
6	A	1211	OLC	C5-C6-C7-C8
5	A	1217	OLA	C6-C7-C8-C9
6	A	1213	OLC	C1-C2-C3-C4
5	A	1206	OLA	C1-C2-C3-C4
5	A	1209	OLA	C2-C3-C4-C5
6	A	1211	OLC	O20-C21-C22-C24
5	A	1208	OLA	C9-C10-C11-C12
5	A	1220	OLA	C13-C14-C15-C16
6	A	1213	OLC	C4-C5-C6-C7
6	A	1212	OLC	O20-C21-C22-O23
5	A	1210	OLA	C10-C11-C12-C13
5	A	1215	OLA	C4-C5-C6-C7
6	A	1212	OLC	C3-C4-C5-C6
5	A	1218	OLA	C7-C8-C9-C10
5	A	1214	OLA	C7-C8-C9-C10
5	A	1209	OLA	C3-C4-C5-C6
5	A	1206	OLA	C2-C3-C4-C5
2	A	1201	QGE	C2-C15-C16-C17
5	A	1206	OLA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
5	A	1215	OLA	O2-C1-C2-C3
5	A	1215	OLA	O1-C1-C2-C3
5	A	1206	OLA	O1-C1-C2-C3
6	A	1211	OLC	C7-C8-C9-C10
5	A	1206	OLA	O2-C1-C2-C3
6	A	1212	OLC	C7-C8-C9-C10
5	A	1206	OLA	C9-C10-C11-C12
5	A	1218	OLA	C3-C4-C5-C6
5	A	1215	OLA	C14-C15-C16-C17
6	A	1216	OLC	C7-C8-C9-C10
6	A	1213	OLC	C7-C8-C9-C10
5	A	1217	OLA	O2-C1-C2-C3

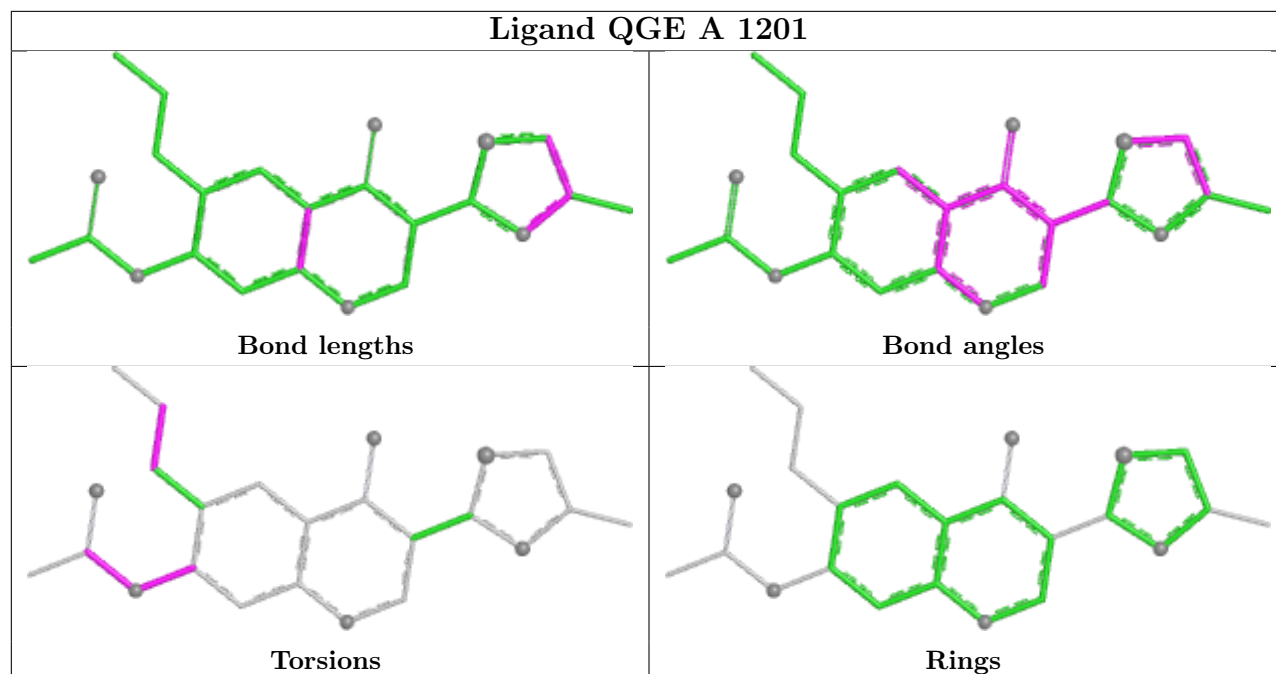
There are no ring outliers.

6 monomers are involved in 5 short contacts:

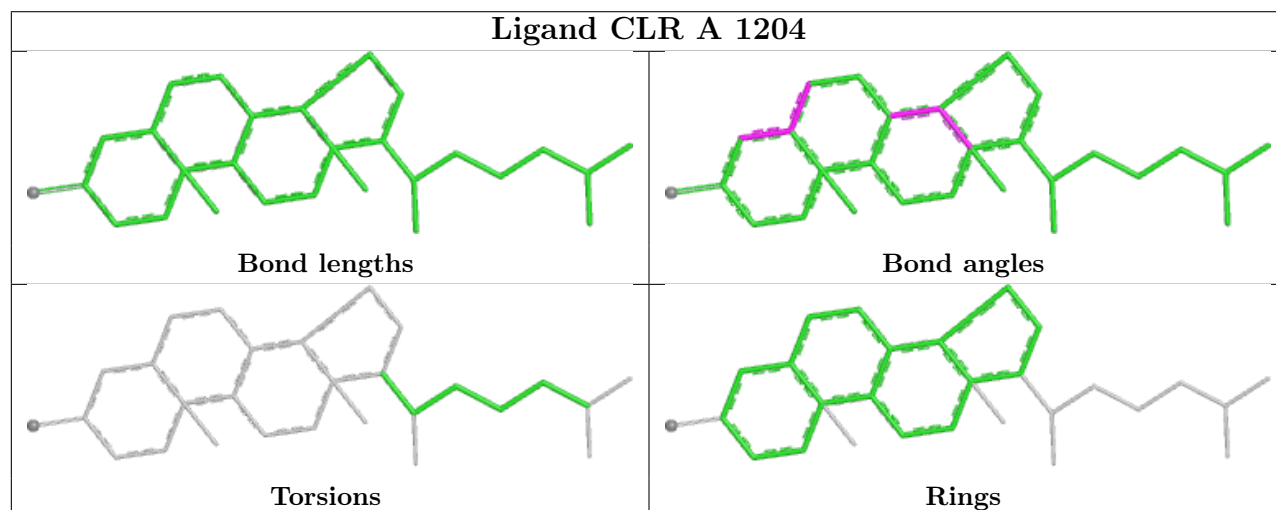
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	QGE	2	0
5	A	1220	OLA	1	0
4	A	1205	CLR	1	0
5	A	1215	OLA	1	0
5	A	1214	OLA	1	0
6	A	1211	OLC	1	0

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.

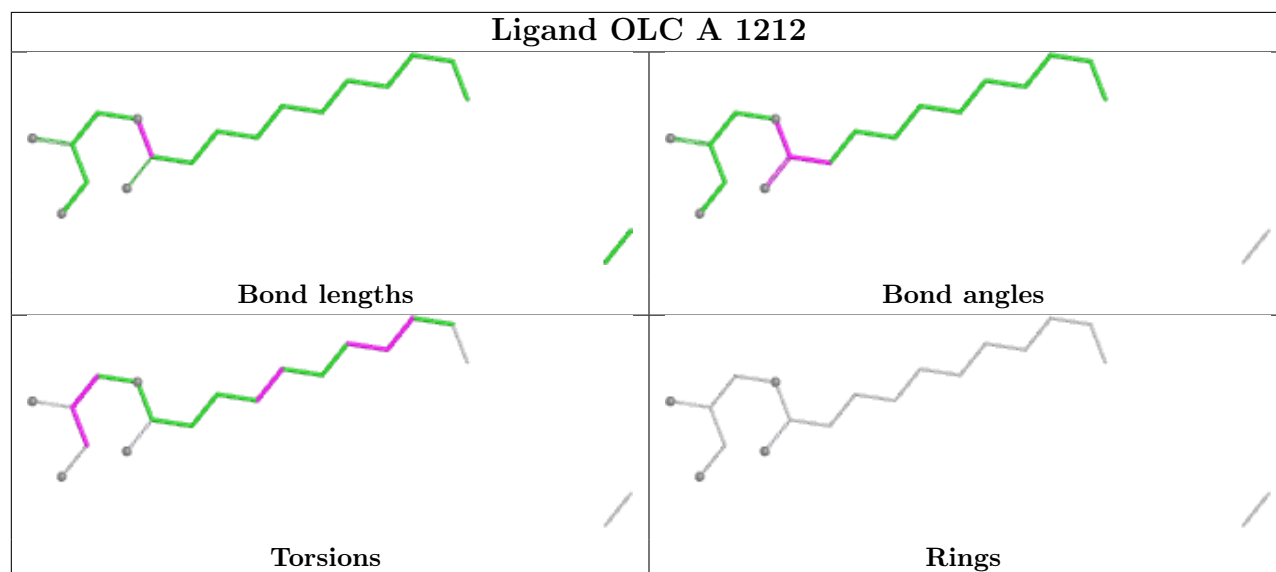
Ligand QGE A 1201

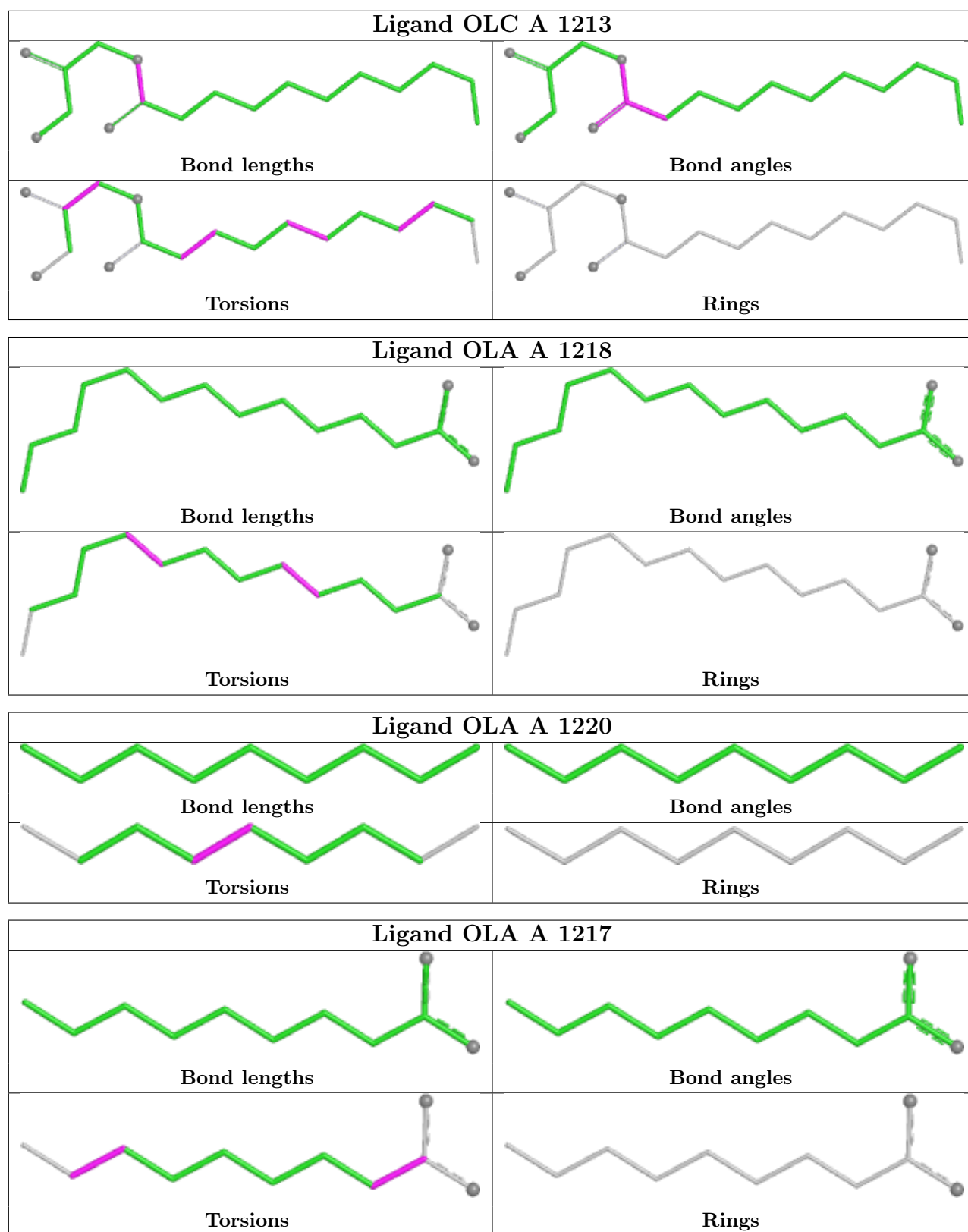


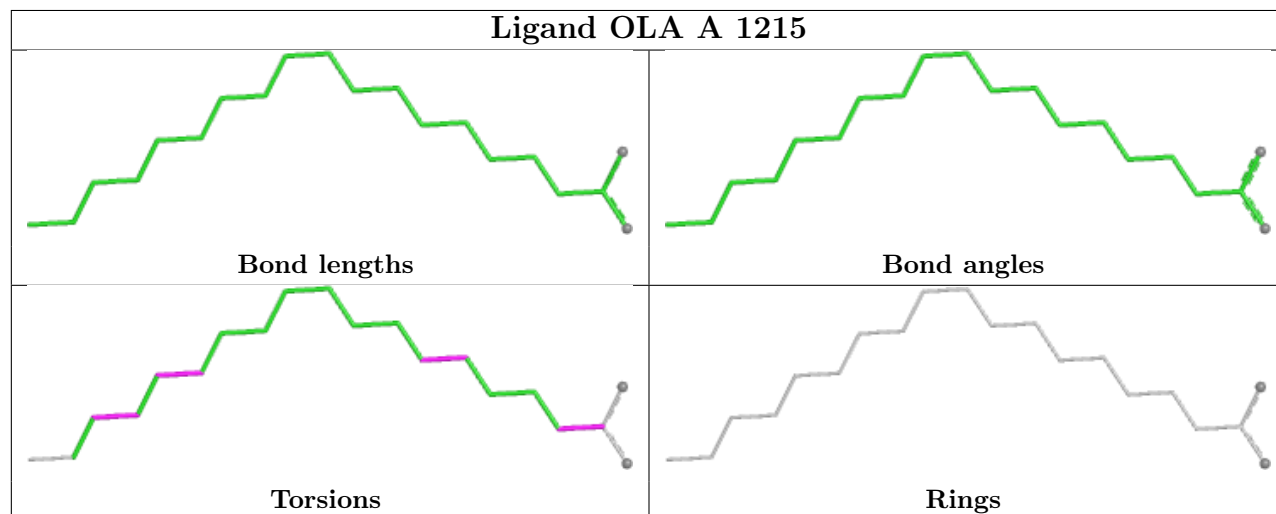
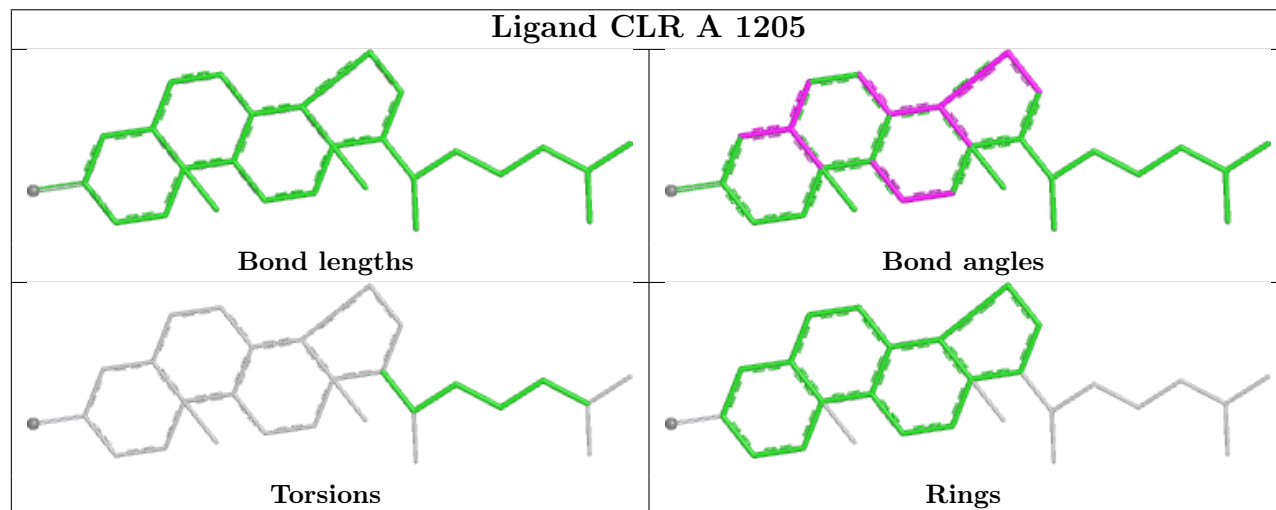
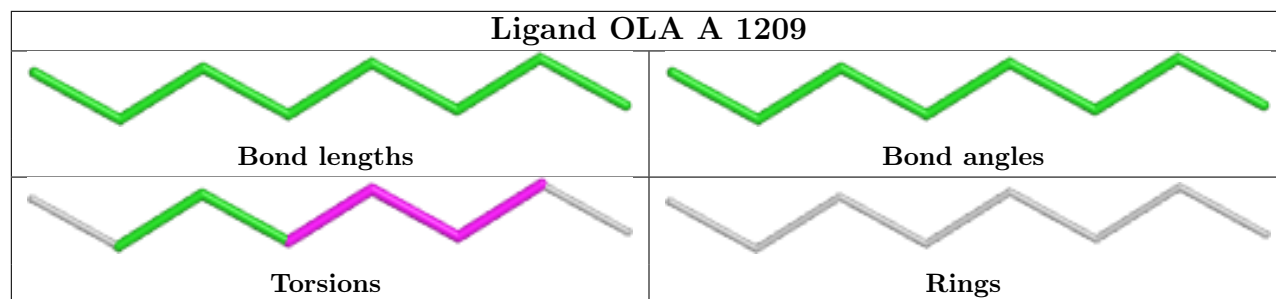
Ligand CLR A 1204

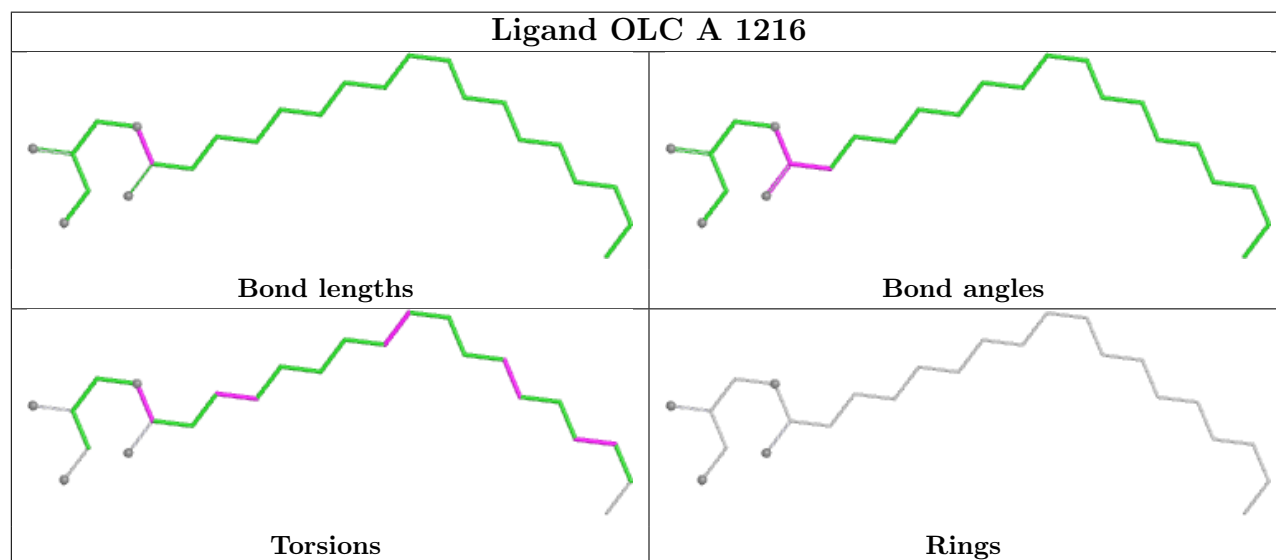
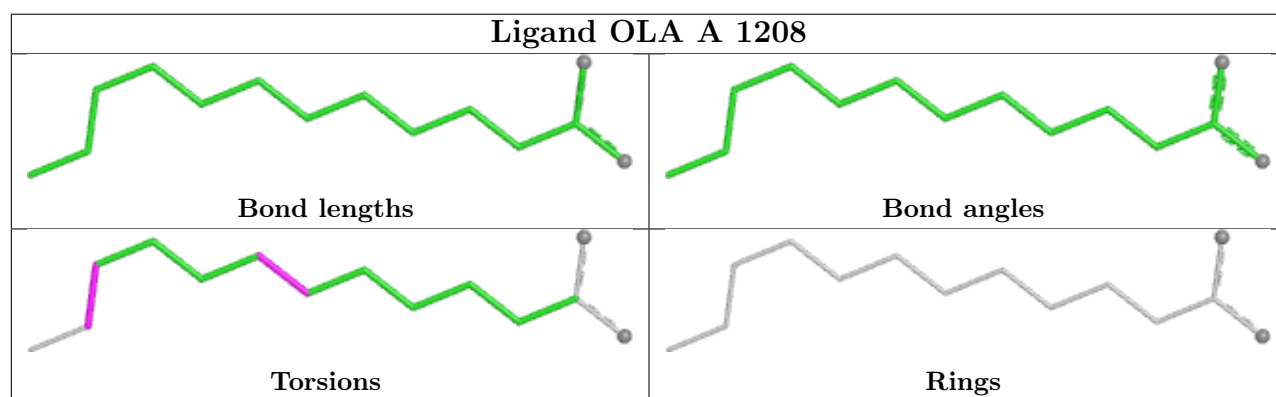
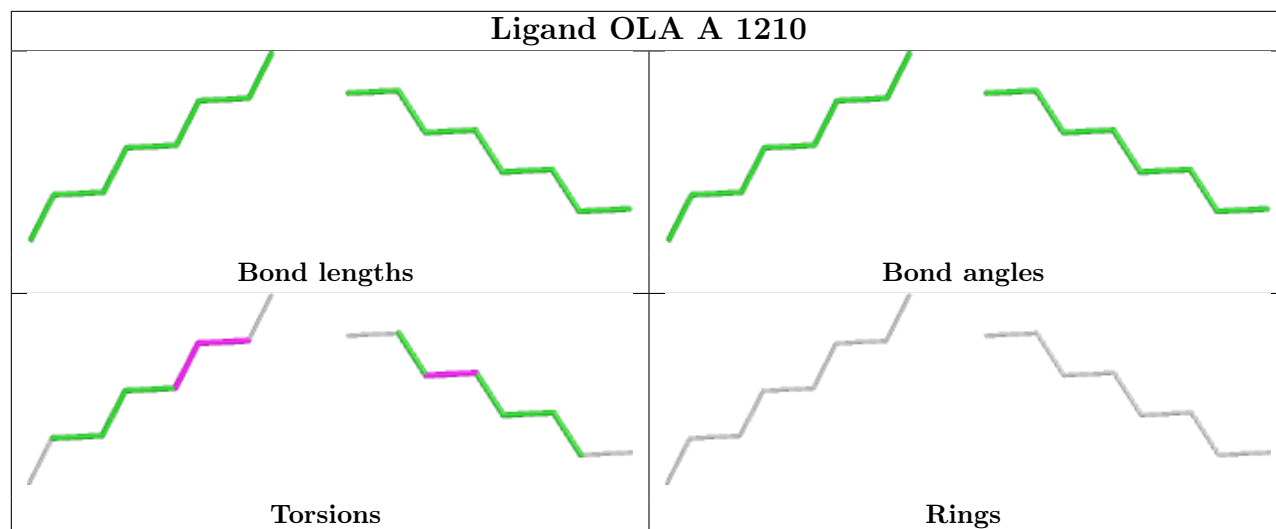


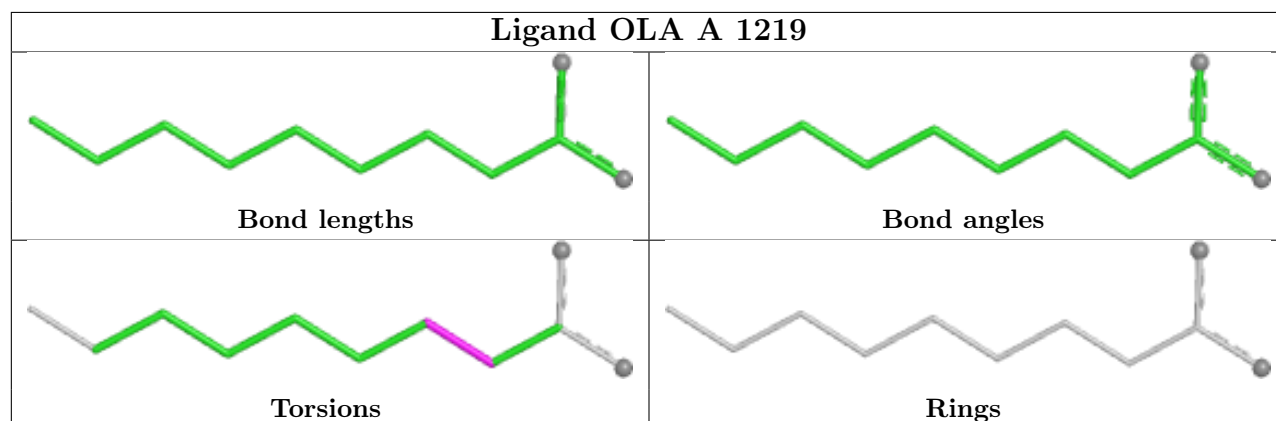
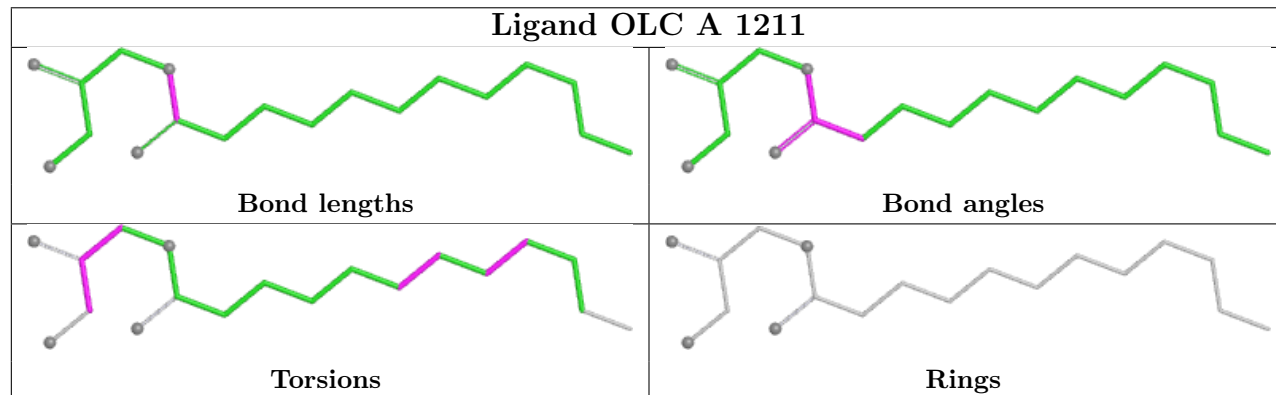
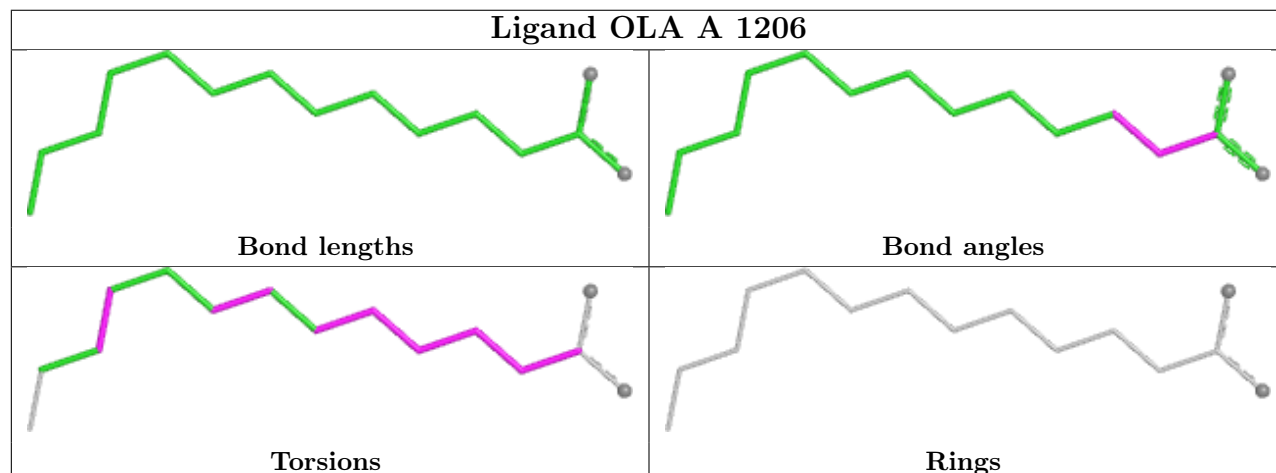
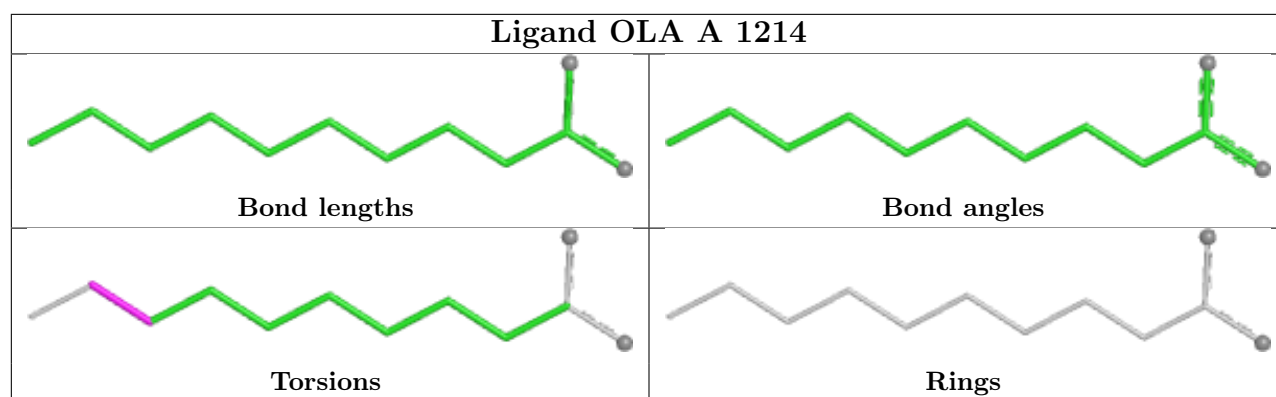
Ligand OLC A 1212

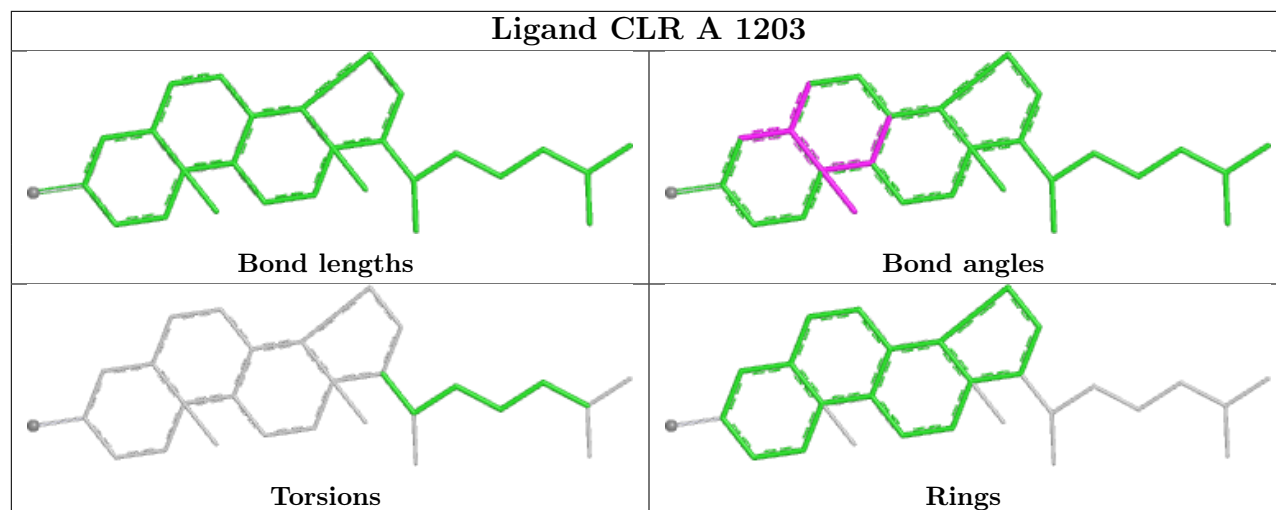












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	383/433 (88%)	1.00	84 (21%) 2 2	14, 40, 94, 143	6 (1%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1016	VAL	6.0
1	A	1063	HIS	4.9
1	A	208	LEU	4.7
1	A	1019	LYS	4.7
1	A	29[A]	TRP	4.7
1	A	205[A]	ARG	4.5
1	A	221	ALA	4.4
1	A	302	ILE	4.4
1	A	1038	LEU	4.3
1	A	1106	LEU	3.8
1	A	148	GLN	3.7
1	A	1023	ALA	3.7
1	A	1093	GLN	3.6
1	A	1012	ASP	3.6
1	A	225	LEU	3.6
1	A	303	ILE	3.6
1	A	110	LEU	3.6
1	A	290	TYR	3.5
1	A	1017	ILE	3.5
1	A	1035	ALA	3.5
1	A	1067	ILE	3.4
1	A	1015	LYS	3.4
1	A	162	GLY	3.4
1	A	305	SER	3.3
1	A	0	ALA	3.3
1	A	1022	ASN	3.3
1	A	1026	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	1084	VAL	3.3
1	A	220	ARG	3.3
1	A	1082	GLY	3.3
1	A	1031	THR	3.2
1	A	1077	LYS	3.2
1	A	1021	ASP	3.2
1	A	1105	TYR	3.1
1	A	160	GLY	3.1
1	A	206	ARG	3.1
1	A	1	PRO	3.1
1	A	1032	LYS	3.0
1	A	111	ARG	2.9
1	A	1005	ASP	2.9
1	A	32	TRP	2.9
1	A	108	ILE	2.8
1	A	116	VAL	2.8
1	A	1020	ALA	2.8
1	A	1081	GLU	2.8
1	A	1024	ALA	2.8
1	A	1075	ALA	2.8
1	A	1092	GLU	2.8
1	A	1039	ASP	2.8
1	A	3	ILE	2.7
1	A	1001	ALA	2.7
1	A	204	ALA	2.7
1	A	1101	TYR	2.6
1	A	1100	ALA	2.6
1	A	1080	ASN	2.6
1	A	119	THR	2.6
1	A	222	ARG	2.5
1	A	1025	GLN	2.5
1	A	33	LEU	2.5
1	A	106	ILE	2.5
1	A	229	VAL	2.5
1	A	226	GLN	2.5
1	A	1096	THR	2.5
1	A	1036	ALA	2.5
1	A	1073	ASP	2.4
1	A	1037	ALA	2.4
1	A	223	SER	2.4
1	A	1027	LYS	2.4
1	A	1062	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	107	ALA	2.4
1	A	1087	ALA	2.4
1	A	224	THR	2.3
1	A	1085	LYS	2.3
1	A	207	GLN	2.2
1	A	230	HIS	2.2
1	A	1003	LEU	2.2
1	A	1064	GLY	2.2
1	A	1089	ALA	2.2
1	A	109	PRO	2.1
1	A	115	LEU	2.1
1	A	1010	LEU	2.1
1	A	293	ARG	2.1
1	A	286	PHE	2.0
1	A	1069	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

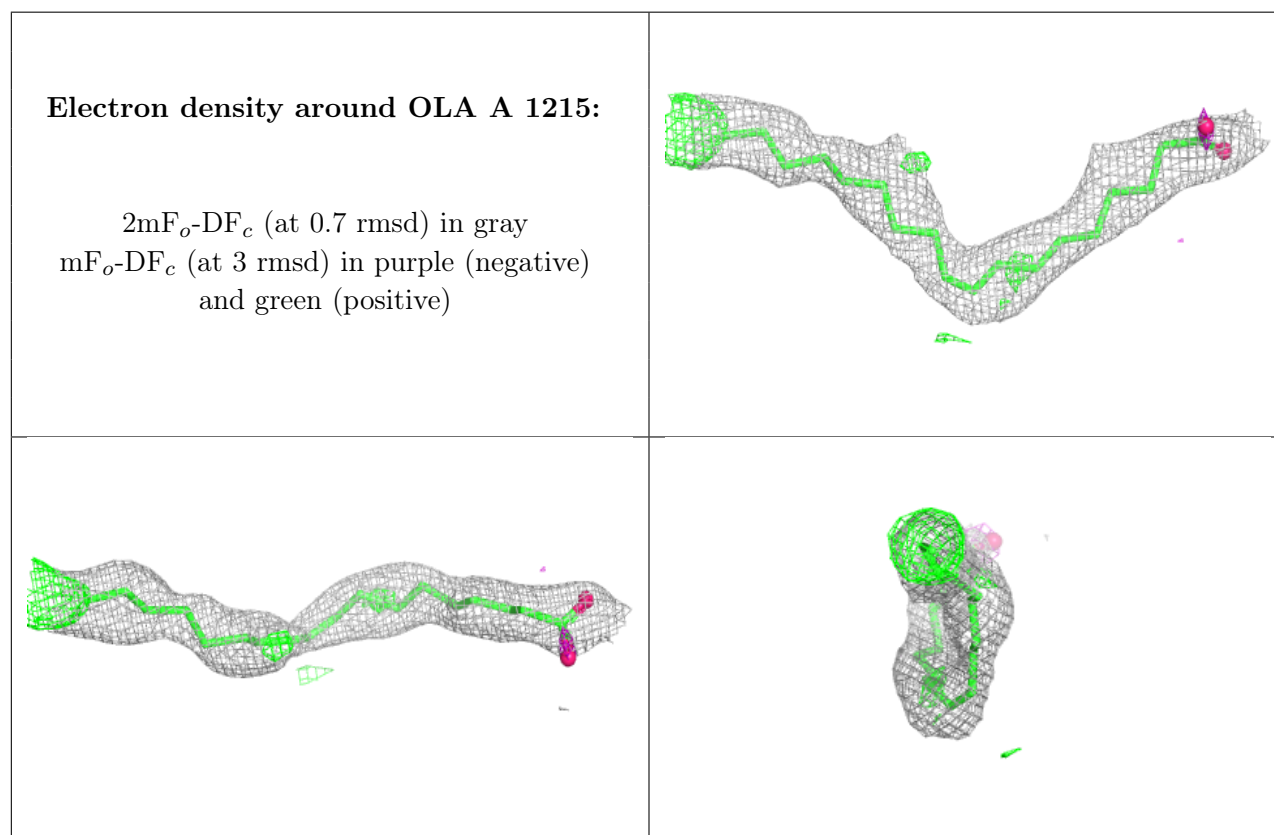
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	OLA	A	1215	20/20	0.74	0.23	56,57,60,60	0
6	OLC	A	1216	25/25	0.75	0.25	60,62,67,68	0
5	OLA	A	1218	15/20	0.77	0.21	60,60,65,65	0
5	OLA	A	1219	11/20	0.79	0.22	52,54,57,57	0
6	OLC	A	1212	20/25	0.79	0.20	43,57,62,62	0
5	OLA	A	1208	14/20	0.79	0.22	68,70,72,72	0
5	OLA	A	1217	11/20	0.80	0.21	55,56,60,60	0
6	OLC	A	1211	19/25	0.80	0.21	52,54,56,56	0

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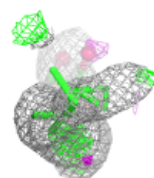
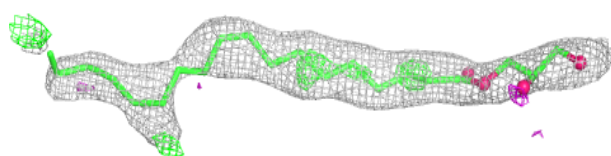
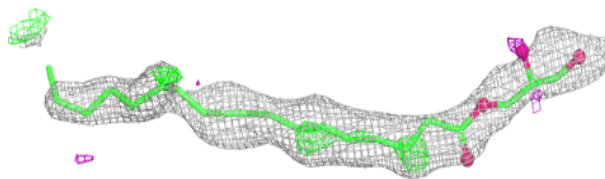
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	OLA	A	1209	8/20	0.82	0.17	46,48,49,49	0
6	OLC	A	1213	18/25	0.85	0.16	47,50,56,56	0
5	OLA	A	1206	15/20	0.86	0.17	61,62,64,65	0
5	OLA	A	1210	16/20	0.86	0.18	50,50,58,59	0
5	OLA	A	1214	12/20	0.88	0.16	48,50,53,53	0
2	QGE	A	1201	24/24	0.90	0.14	27,32,45,47	0
5	OLA	A	1220	9/20	0.90	0.15	51,51,52,52	0
4	CLR	A	1203	28/28	0.92	0.09	36,37,42,43	0
4	CLR	A	1205	28/28	0.92	0.10	31,32,39,40	0
5	OLA	A	1207	5/20	0.93	0.13	45,45,46,46	0
4	CLR	A	1204	28/28	0.94	0.08	28,30,41,42	0
3	NA	A	1202	1/1	0.96	0.15	41,41,41,41	0

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

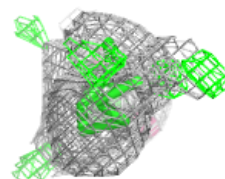
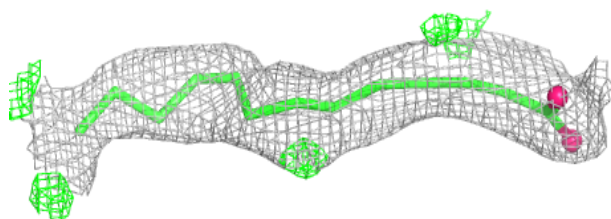
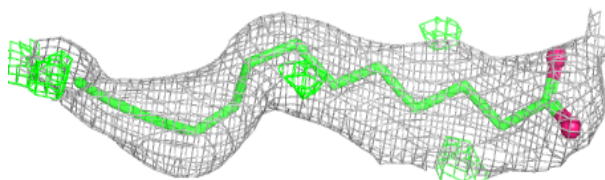


Electron density around OLC A 1216:

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

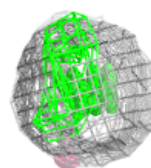
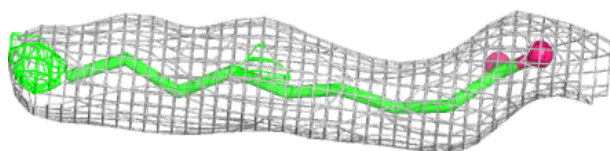
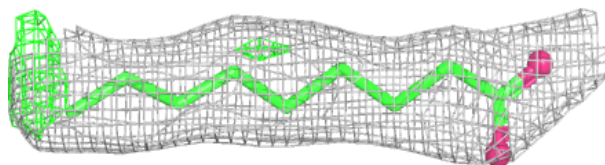
**Electron density around OLA A 1218:**

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

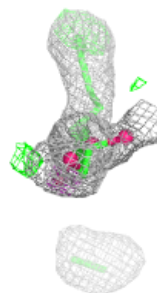
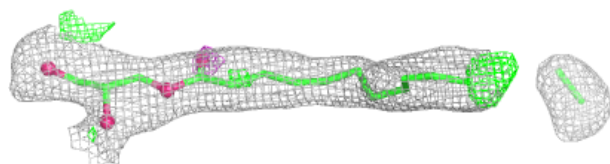
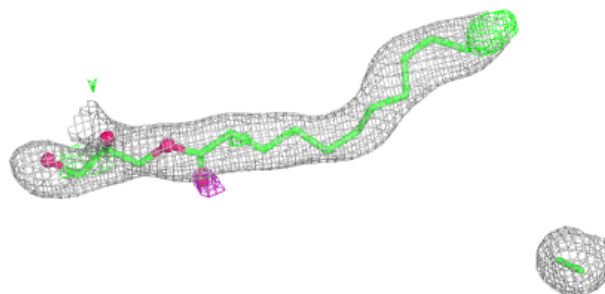


Electron density around OLA A 1219:

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

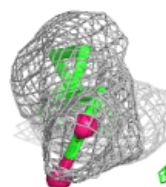
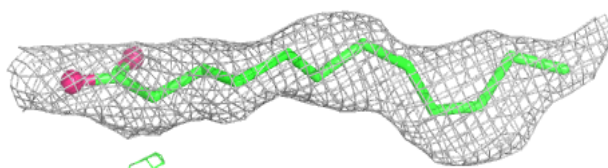
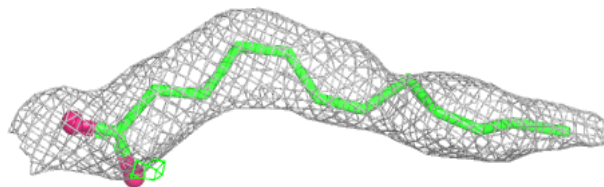
**Electron density around OLC A 1212:**

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

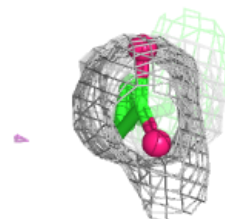
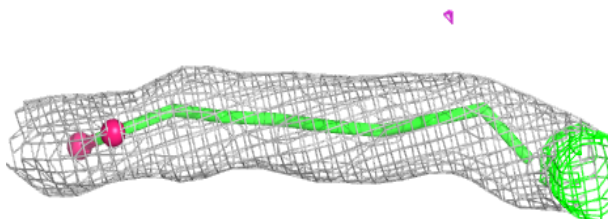
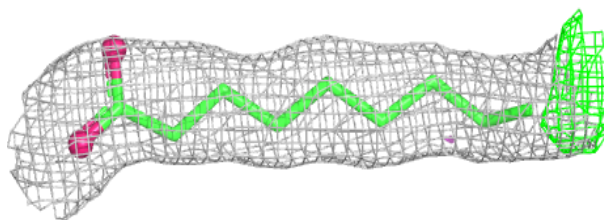


Electron density around OLA A 1208:

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

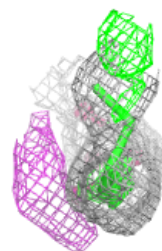
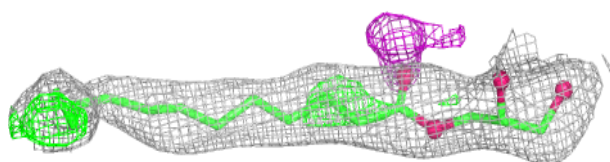
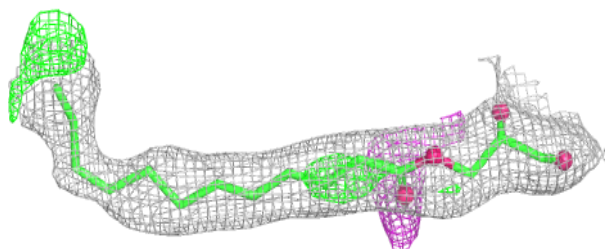
**Electron density around OLA A 1217:**

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

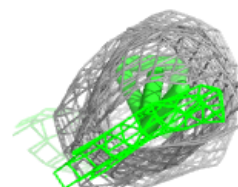
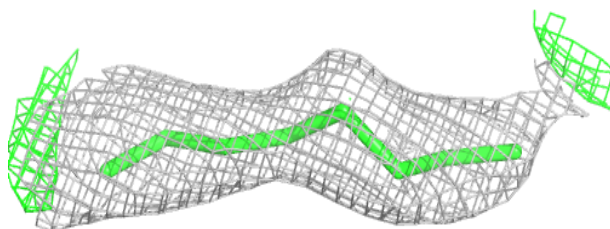
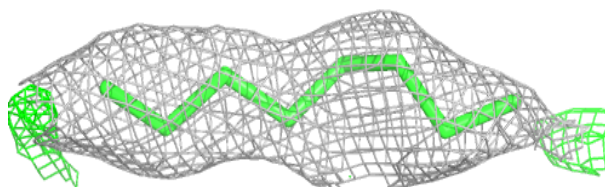


Electron density around OLC A 1211:

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

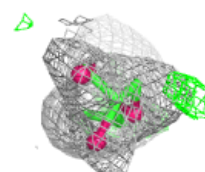
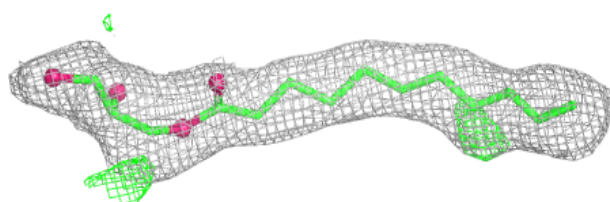
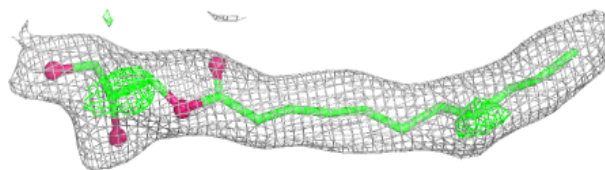
**Electron density around OLA A 1209:**

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

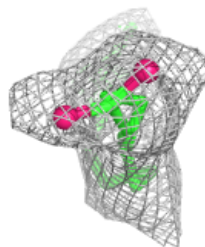
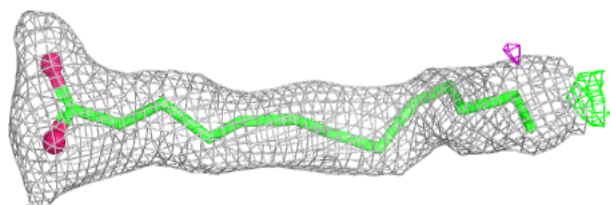
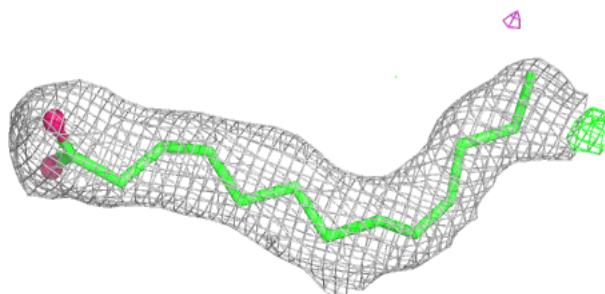


Electron density around OLC A 1213:

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

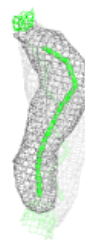
**Electron density around OLA A 1206:**

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

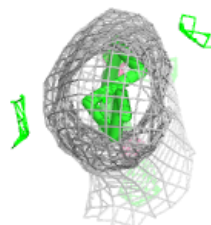
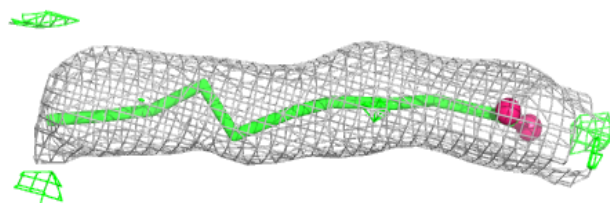
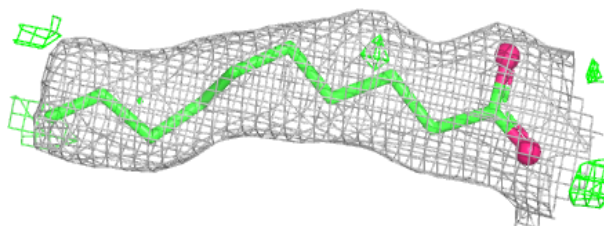


Electron density around OLA A 1210:

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

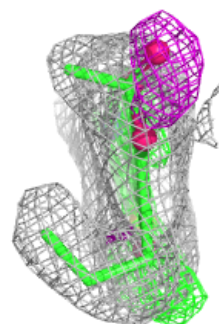
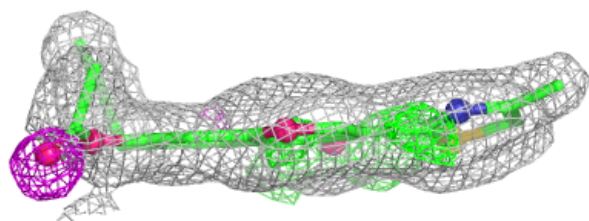
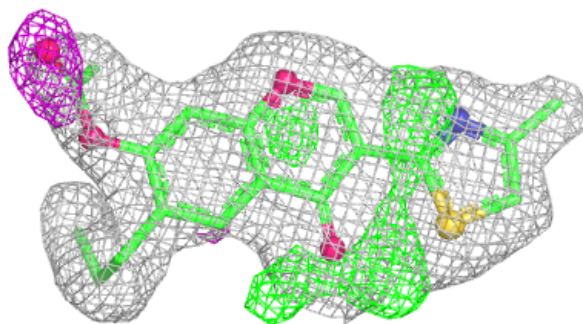
**Electron density around OLA A 1214:**

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

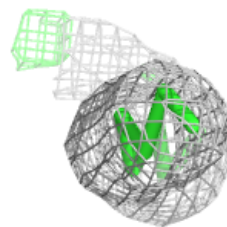
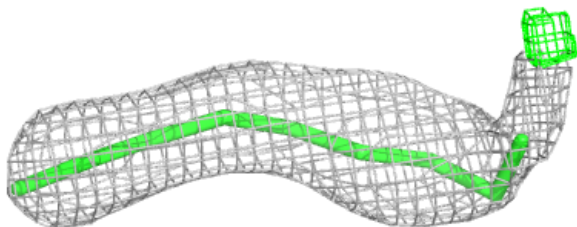
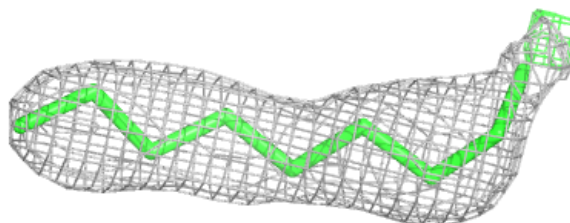


Electron density around QGE A 1201:

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

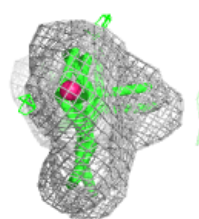
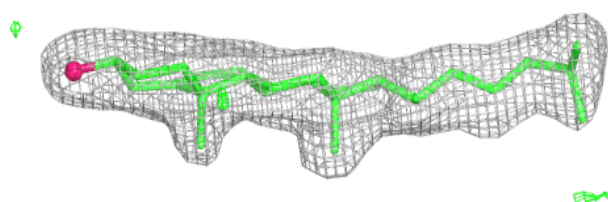
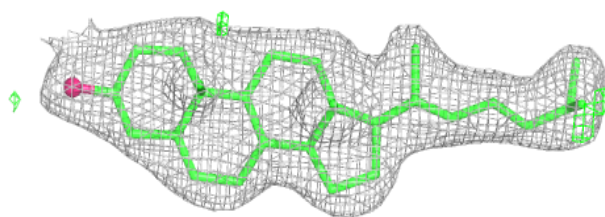
**Electron density around OLA A 1220:**

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

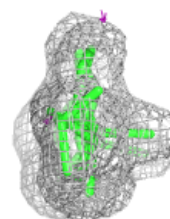
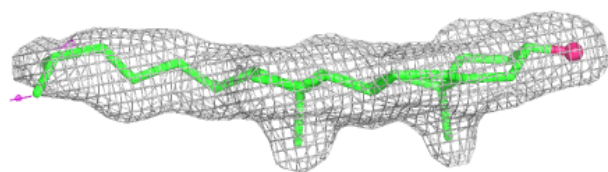
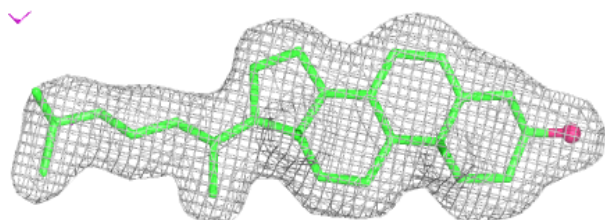


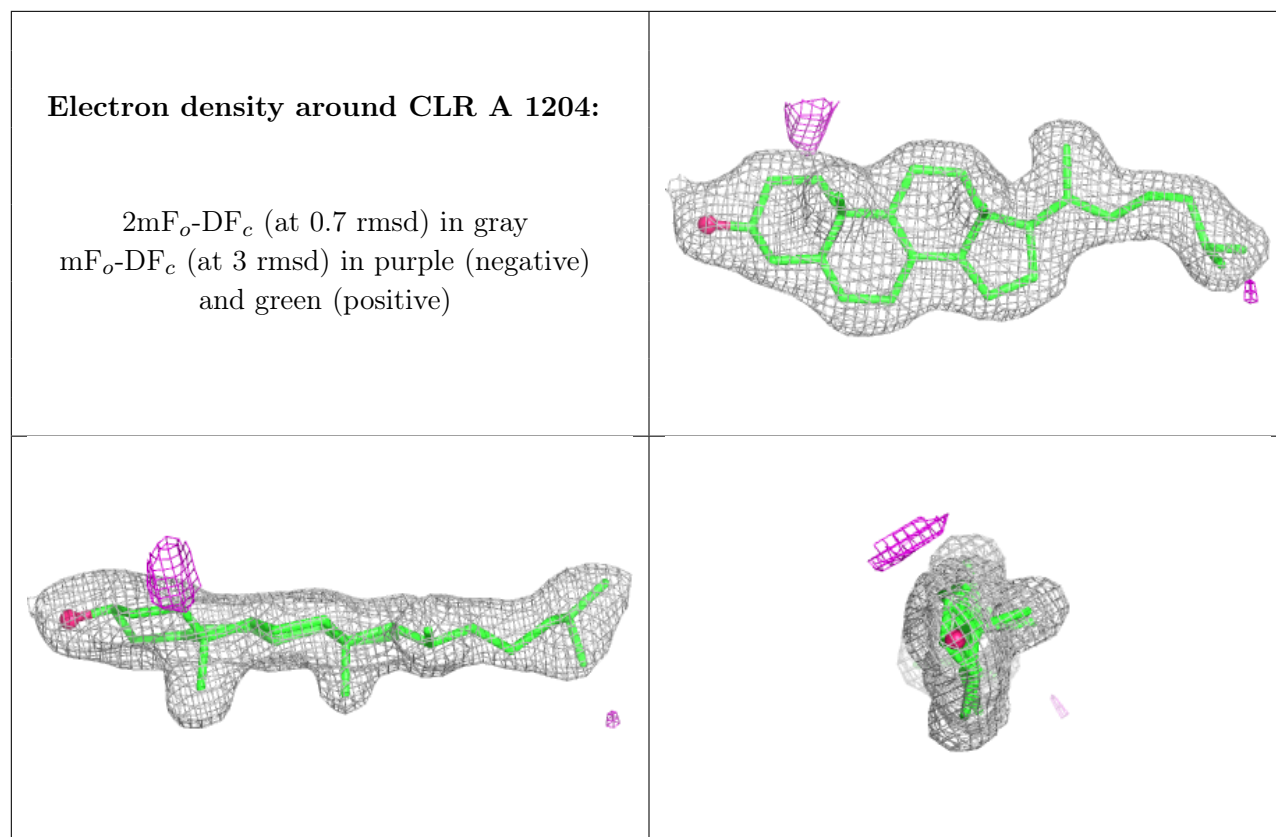
Electron density around CLR A 1203:

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

**Electron density around CLR 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.