



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 15, 2026 – 10:15 am BST

PDB ID : 9RKG / pdb_00009rkg
Title : Mixed model refinement of beta-2 Adrenergic receptor with photoazolo in dark state and Light state, 10 seconds after light activation, recorded at SwissFEL
Authors : Bertrand, Q.; Stipp, R.; Glover, H.; Stierli, F.; Siedel, H.P.; Mous, S.; Kepa, M.; Weinert, T.; Standfuss, J.
Deposited on : 2025-06-13
Resolution : 2.45 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (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

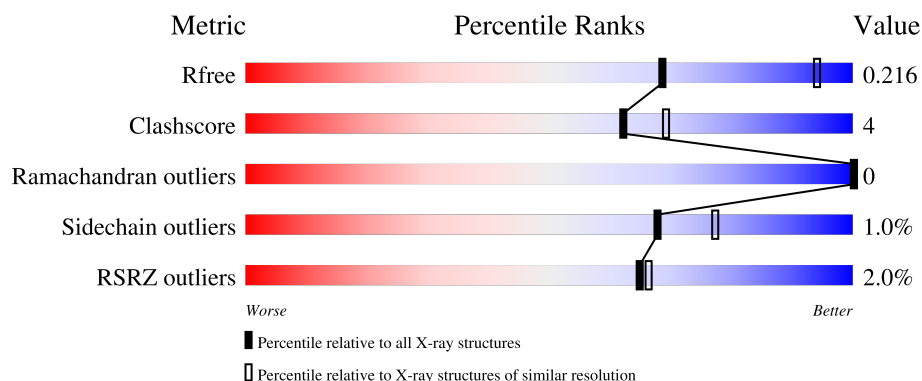
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	443	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	1206[A]	-	-	X	-
8	1PE	A	1225[B]	-	-	-	X
9	EDO	A	1223[B]	-	-	-	X

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 15287 atoms, of which 7480 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.

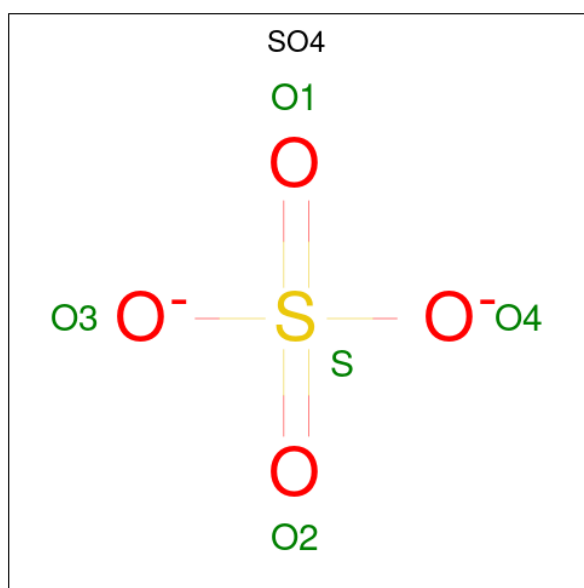
- Molecule 1 is a protein called Beta-2 adrenergic receptor, Endolysin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	443	14337	4647	7230	1183	1229	48	0	443	0

There are 7 discrepancies between the modelled and reference sequences:

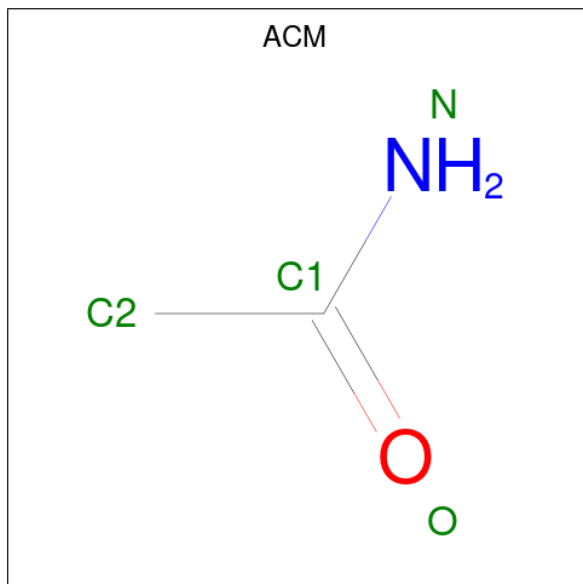
Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ALA	-	expression tag	UNP P07550
A	122	TRP	GLU	conflict	UNP P07550
A	187	GLU	ASN	conflict	UNP P07550
A	1012	GLY	ARG	conflict	UNP P00720
A	1054	THR	CYS	conflict	UNP P00720
A	1097	ALA	CYS	conflict	UNP P00720
A	1137	ARG	ILE	conflict	UNP P00720

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



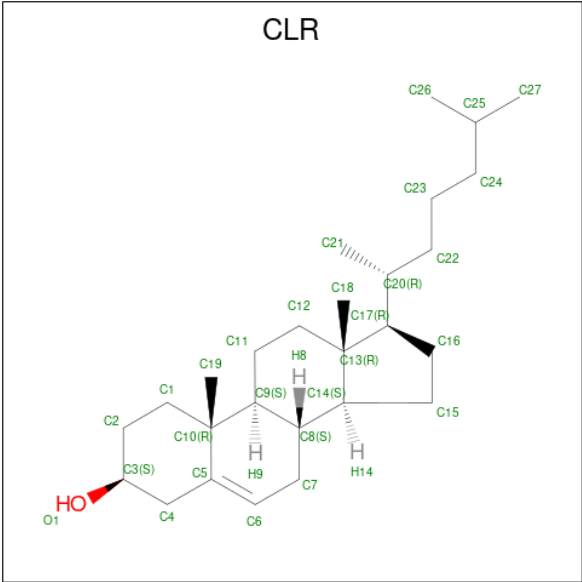
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	1
			10	8	2		
2	A	1	Total	O	S	0	1
			5	4	1		
2	A	1	Total	O	S	0	1
			10	8	2		
2	A	1	Total	O	S	0	1
			10	8	2		
2	A	1	Total	O	S	0	1
			10	8	2		
2	A	1	Total	O	S	0	1
			5	4	1		

- Molecule 3 is ACETAMIDE (CCD ID: ACM) (formula: C₂H₅NO).



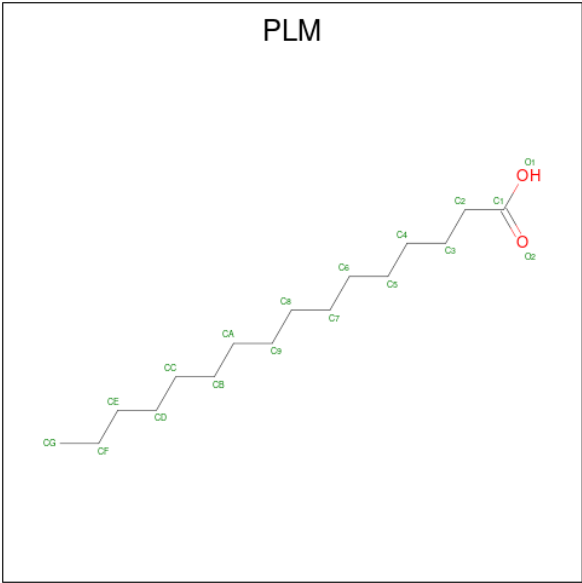
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			8	4	2	2		

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



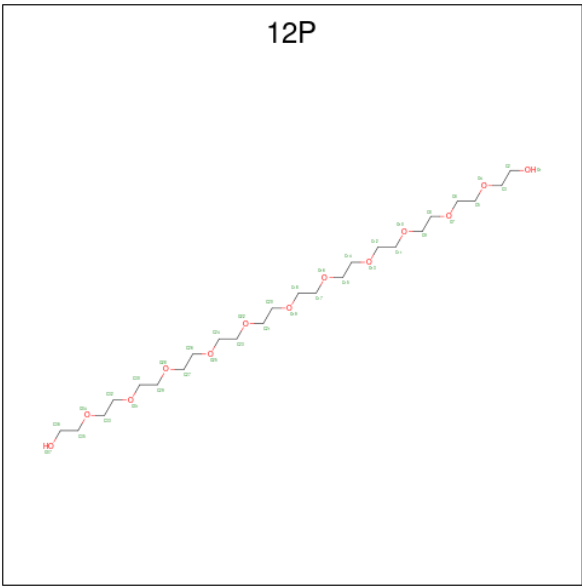
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			56	54	2		
4	A	1	Total	C	O	0	1
			56	54	2		
4	A	1	Total	C	O	0	1
			56	54	2		

- Molecule 5 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



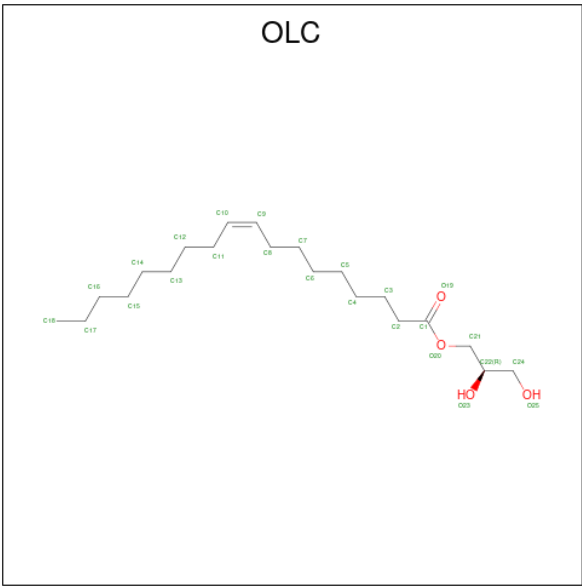
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	1
			34	32	2		

- Molecule 6 is DODECAETHYLENE GLYCOL (CCD ID: 12P) (formula: C₂₄H₅₀O₁₃).



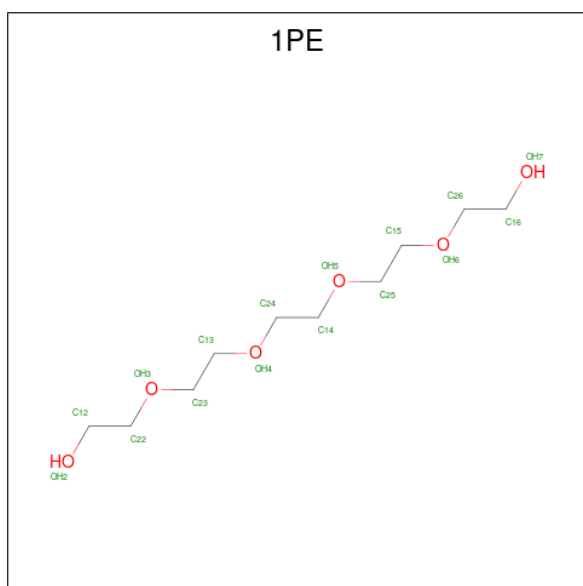
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	1
			34	22	12		
6	A	1	Total	C	O	0	1
			40	26	14		
6	A	1	Total	C	O	0	1
			32	20	12		

- Molecule 7 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C H O 130 42 80 8	0	1
7	A	1	Total C H O 130 42 80 8	0	1
7	A	1	Total C 26 26	0	1
7	A	1	Total C O 50 42 8	0	1
7	A	1	Total C O 38 30 8	0	1

- Molecule 8 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



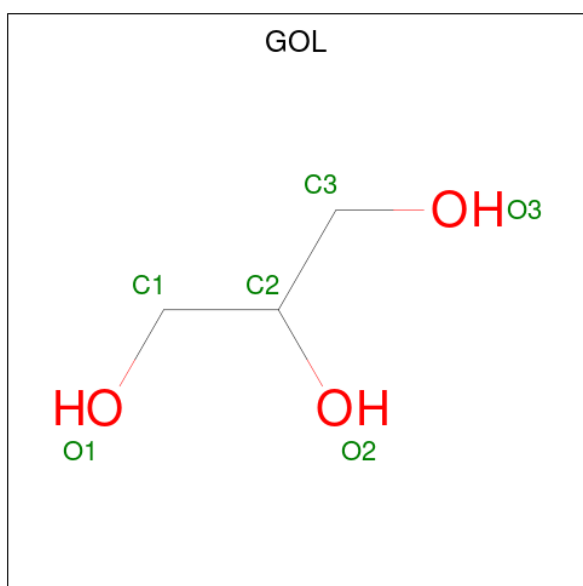
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C H O 46 12 26 8	0	1
8	A	1	Total C O 8 5 3	0	1
8	A	1	Total C O 10 6 4	0	1

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	0	1
			20	4	12	4		
9	A	1	Total	C	O		0	1
			4	2	2			

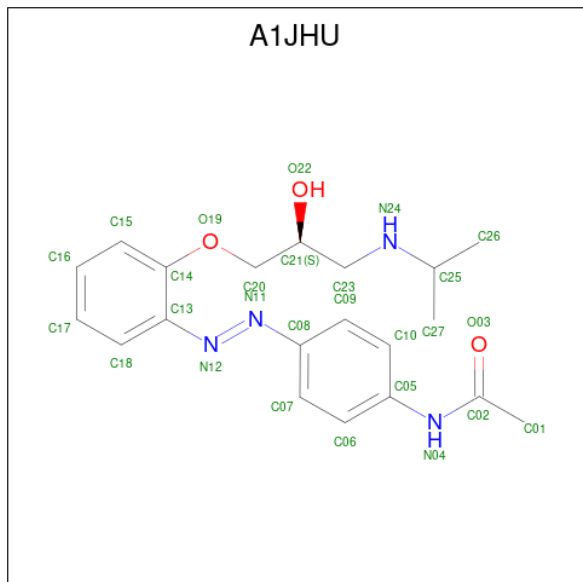
- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	1
			12	6	6		

- Molecule 11 is {N}-[4-[({E})]-[2-[(2 {S})-2-oxidanyl-3-(propan-2-ylamino)propoxy]phenyl]d

iazenyl]phenyl]ethanamide (CCD ID: A1JHU) (formula: $C_{20}H_{26}N_4O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	H	N	O	0	1
			106	40	52	8	6		

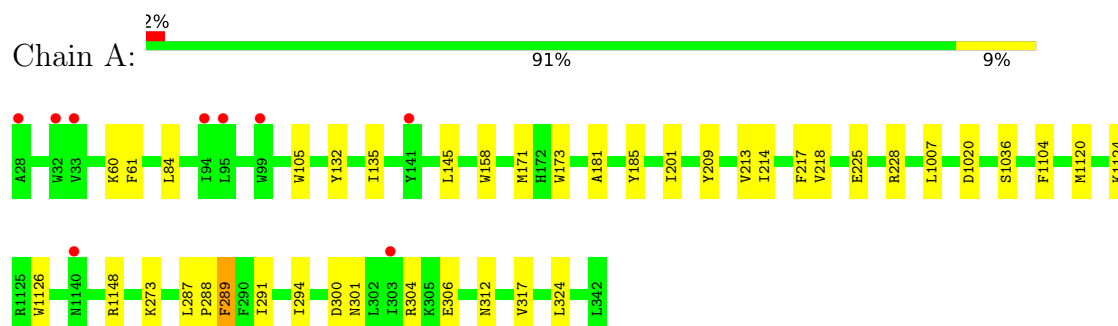
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	4	Total	O	0	0
			4	4		

3 Residue-property plots

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: Beta-2 adrenergic receptor, Endolysin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	111.94Å 172.23Å 41.23Å 90.00° 106.20° 90.00°	Depositor
Resolution (Å)	53.75 – 2.45 53.75 – 2.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (53.75-2.45) 85.5 (53.75-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.20_4459)	Depositor
R, R_{free}	0.183 , 0.217 0.185 , 0.216	Depositor DCC
R_{free} test set	1992 reflections (7.22%)	wwPDB-VP
Wilson B-factor (Å ²)	61.8	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 114.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15287	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OLC, SO4, GOL, PLM, 12P, A1JHU, 1PE, CLR, EDO, ACM

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	0.10	0/7273	0.24	0/9877

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	289[B]	PHE	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7107	7230	7236	34	0
2	A	50	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	8	0	6	0	0
4	A	168	0	276	9	0
5	A	34	0	62	1	0
6	A	106	0	132	12	0
7	A	214	160	330	15	0
8	A	38	26	48	5	0
9	A	12	12	18	0	0
10	A	12	0	16	1	0
11	A	54	52	0	0	0
12	A	4	0	0	2	0
All	All	7807	7480	8124	65	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.

The worst 5 of 65 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)
6:A:1212[B]:12P:H171	8:A:1225[B]:1PE:H252	1.38	1.03
4:A:1208[B]:CLR:H183	4:A:1208[B]:CLR:H212	1.57	0.86
1:A:273[A]:LYS:NZ	2:A:1206[A]:SO4:O1	2.09	0.84
2:A:1202[A]:SO4:O1	2:A:1206[A]:SO4:O1	2.09	0.71
6:A:1212[B]:12P:H262	6:A:1213[B]:12P:H242	1.78	0.64

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	882/443 (199%)	846 (96%)	36 (4%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	766/383 (200%)	758 (99%)	8 (1%)	68 77

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	317[B]	VAL
1	A	317[A]	VAL
1	A	1120[A]	MET
1	A	1036[B]	SER
1	A	1120[B]	MET

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

47 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	SO4	A	1206[A]	-	4,4,4	0.98	0	6,6,6	1.66	1 (16%)
8	1PE	A	1225[B]	-	9,9,15	0.12	0	8,8,14	0.25	0
8	1PE	A	1218[B]	-	9,9,15	0.12	0	8,8,14	0.11	0
7	OLC	A	1214[B]	-	24,24,24	1.06	1 (4%)	25,25,25	1.14	2 (8%)
3	ACM	A	1207[B]	1	3,3,3	0.67	0	3,3,3	0.91	0
2	SO4	A	1203[B]	-	4,4,4	0.12	0	6,6,6	0.05	0
10	GOL	A	1221[A]	-	5,5,5	0.95	0	5,5,5	0.95	0
2	SO4	A	1201[B]	-	4,4,4	0.14	0	6,6,6	0.05	0
9	EDO	A	1219[A]	-	3,3,3	0.47	0	2,2,2	0.28	0
4	CLR	A	1209[B]	-	31,31,31	0.36	0	48,48,48	0.45	0
8	1PE	A	1224[B]	-	7,7,15	0.18	0	6,6,14	0.14	0
7	OLC	A	1220[A]	-	24,24,24	1.04	1 (4%)	25,25,25	1.26	2 (8%)
7	OLC	A	1222[A]	-	18,18,24	1.11	1 (5%)	18,19,25	1.45	2 (11%)
6	12P	A	1217[B]	-	15,15,36	0.53	0	14,14,35	0.22	0
4	CLR	A	1210[A]	-	31,31,31	0.27	0	48,48,48	0.46	0
6	12P	A	1213[B]	-	19,19,36	0.54	0	18,18,35	0.20	0
4	CLR	A	1208[A]	-	31,31,31	0.41	0	48,48,48	0.78	1 (2%)
7	OLC	A	1215[B]	-	24,24,24	1.05	1 (4%)	25,25,25	1.18	2 (8%)
7	OLC	A	1216[A]	-	12,12,24	0.70	0	11,11,25	1.27	1 (9%)
5	PLM	A	1211[A]	1	16,16,17	0.44	0	15,15,17	0.44	0
9	EDO	A	1223[B]	-	3,3,3	0.45	0	2,2,2	0.32	0
2	SO4	A	1205[B]	-	4,4,4	0.14	0	6,6,6	0.06	0
11	A1JHU	A	1226[B]	-	28,28,28	1.28	2 (7%)	36,36,36	2.68	5 (13%)
2	SO4	A	1202[A]	-	4,4,4	0.14	0	6,6,6	0.05	0
3	ACM	A	1207[A]	1	3,3,3	0.68	0	3,3,3	0.89	0
6	12P	A	1212[B]	-	16,16,36	0.53	0	15,15,35	0.19	0
2	SO4	A	1203[A]	-	4,4,4	0.14	0	6,6,6	0.06	0
7	OLC	A	1214[A]	-	24,24,24	1.06	1 (4%)	25,25,25	1.13	2 (8%)
2	SO4	A	1201[A]	-	4,4,4	0.13	0	6,6,6	0.05	0
8	1PE	A	1218[A]	-	9,9,15	0.14	0	8,8,14	0.13	0
4	CLR	A	1209[A]	-	31,31,31	0.35	0	48,48,48	0.47	0
2	SO4	A	1204[B]	-	4,4,4	0.14	0	6,6,6	0.07	0
6	12P	A	1217[A]	-	15,15,36	0.57	0	14,14,35	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	GOL	A	1221[B]	-	5,5,5	0.91	0	5,5,5	0.99	0
6	12P	A	1213[A]	-	19,19,36	0.53	0	18,18,35	0.22	0
9	EDO	A	1219[B]	-	3,3,3	0.45	0	2,2,2	0.29	0
7	OLC	A	1220[B]	-	24,24,24	1.04	1 (4%)	25,25,25	1.24	2 (8%)
7	OLC	A	1222[B]	-	18,18,24	1.14	1 (5%)	18,19,25	1.35	2 (11%)
7	OLC	A	1215[A]	-	24,24,24	1.05	1 (4%)	25,25,25	1.15	2 (8%)
2	SO4	A	1205[A]	-	4,4,4	0.14	0	6,6,6	0.05	0
11	A1JHU	A	1226[A]	-	28,28,28	1.33	2 (7%)	36,36,36	1.14	3 (8%)
4	CLR	A	1210[B]	-	31,31,31	0.34	0	48,48,48	0.85	3 (6%)
6	12P	A	1212[A]	-	16,16,36	0.53	0	15,15,35	0.20	0
5	PLM	A	1211[B]	1	16,16,17	0.32	0	15,15,17	0.36	0
4	CLR	A	1208[B]	-	31,31,31	0.32	0	48,48,48	0.70	1 (2%)
7	OLC	A	1216[B]	-	12,12,24	0.79	0	11,11,25	1.35	1 (9%)
2	SO4	A	1204[A]	-	4,4,4	0.14	0	6,6,6	0.05	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
8	1PE	A	1225[B]	-	-	4/7/7/13	-
8	1PE	A	1218[B]	-	-	3/7/7/13	-
7	OLC	A	1214[B]	-	-	8/24/24/24	-
10	GOL	A	1221[A]	-	-	0/4/4/4	-
9	EDO	A	1219[A]	-	-	0/1/1/1	-
4	CLR	A	1209[B]	-	-	0/10/68/68	0/4/4/4
8	1PE	A	1224[B]	-	-	2/5/5/13	-
7	OLC	A	1220[A]	-	-	17/24/24/24	-
7	OLC	A	1222[A]	-	-	9/18/18/24	-
6	12P	A	1217[B]	-	-	8/13/13/34	-
4	CLR	A	1210[A]	-	-	2/10/68/68	0/4/4/4
6	12P	A	1213[B]	-	-	7/17/17/34	-
4	CLR	A	1208[A]	-	-	5/10/68/68	0/4/4/4
7	OLC	A	1215[B]	-	-	7/24/24/24	-
7	OLC	A	1216[A]	-	-	7/10/10/24	-
5	PLM	A	1211[A]	1	-	2/13/14/15	-
9	EDO	A	1223[B]	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	A1JHU	A	1226[B]	-	-	5/19/19/19	0/2/2/2
6	12P	A	1212[B]	-	-	5/14/14/34	-
8	1PE	A	1218[A]	-	-	3/7/7/13	-
7	OLC	A	1214[A]	-	-	8/24/24/24	-
4	CLR	A	1209[A]	-	-	0/10/68/68	0/4/4/4
6	12P	A	1217[A]	-	-	5/13/13/34	-
10	GOL	A	1221[B]	-	-	2/4/4/4	-
6	12P	A	1213[A]	-	-	9/17/17/34	-
9	EDO	A	1219[B]	-	-	0/1/1/1	-
7	OLC	A	1220[B]	-	-	16/24/24/24	-
7	OLC	A	1222[B]	-	-	11/18/18/24	-
7	OLC	A	1215[A]	-	-	14/24/24/24	-
11	A1JHU	A	1226[A]	-	-	2/19/19/19	0/2/2/2
4	CLR	A	1210[B]	-	-	0/10/68/68	0/4/4/4
6	12P	A	1212[A]	-	-	5/14/14/34	-
5	PLM	A	1211[B]	1	-	2/13/14/15	-
4	CLR	A	1208[B]	-	-	0/10/68/68	0/4/4/4
7	OLC	A	1216[B]	-	-	6/10/10/24	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1226[A]	A1JHU	C02-N04	5.36	1.46	1.36
11	A	1226[B]	A1JHU	C02-N04	4.49	1.44	1.36
7	A	1215[A]	OLC	O20-C1	2.94	1.41	1.33
7	A	1214[B]	OLC	O20-C1	2.94	1.41	1.33
7	A	1220[B]	OLC	O20-C1	2.93	1.41	1.33

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1226[B]	A1JHU	C13-N12-N11	13.99	146.85	114.56
11	A	1226[B]	A1JHU	C05-N04-C02	-4.98	118.95	127.99
7	A	1214[A]	OLC	C8-C9-C10	3.87	154.44	124.73
2	A	1206[A]	SO4	O4-S-O3	3.83	125.39	109.06
7	A	1215[B]	OLC	C8-C9-C10	3.79	153.82	124.73

There are no chirality outliers.

5 of 174 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1220[A]	OLC	C21-C22-C24-O25
7	A	1220[A]	OLC	O20-C21-C22-O23
7	A	1220[B]	OLC	O20-C21-C22-O23
7	A	1222[A]	OLC	C9-C10-C11-C12
7	A	1222[A]	OLC	C21-C22-C24-O25

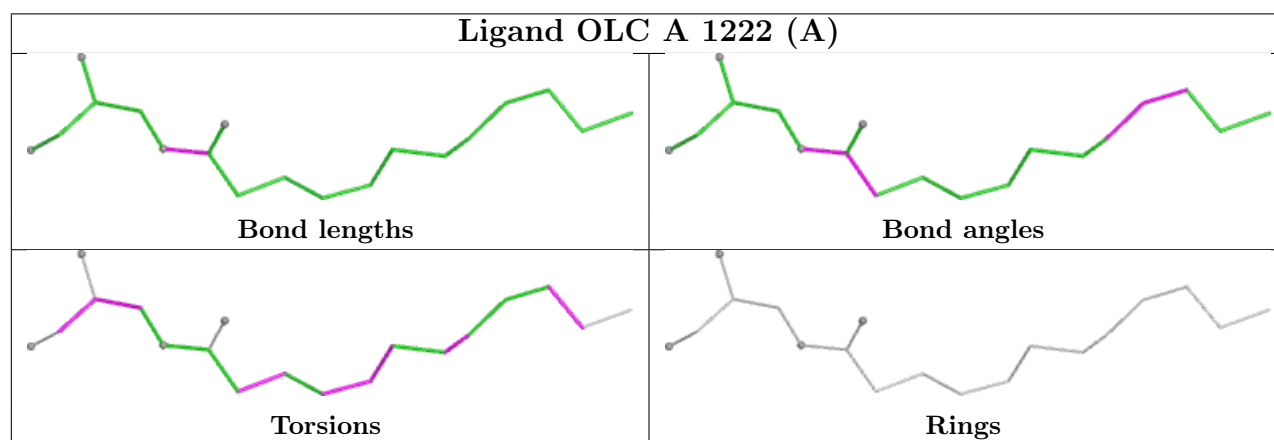
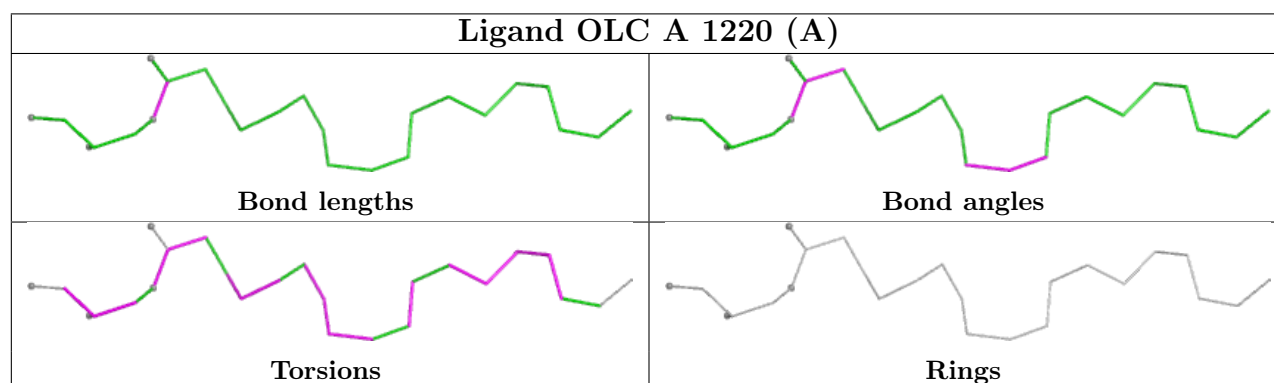
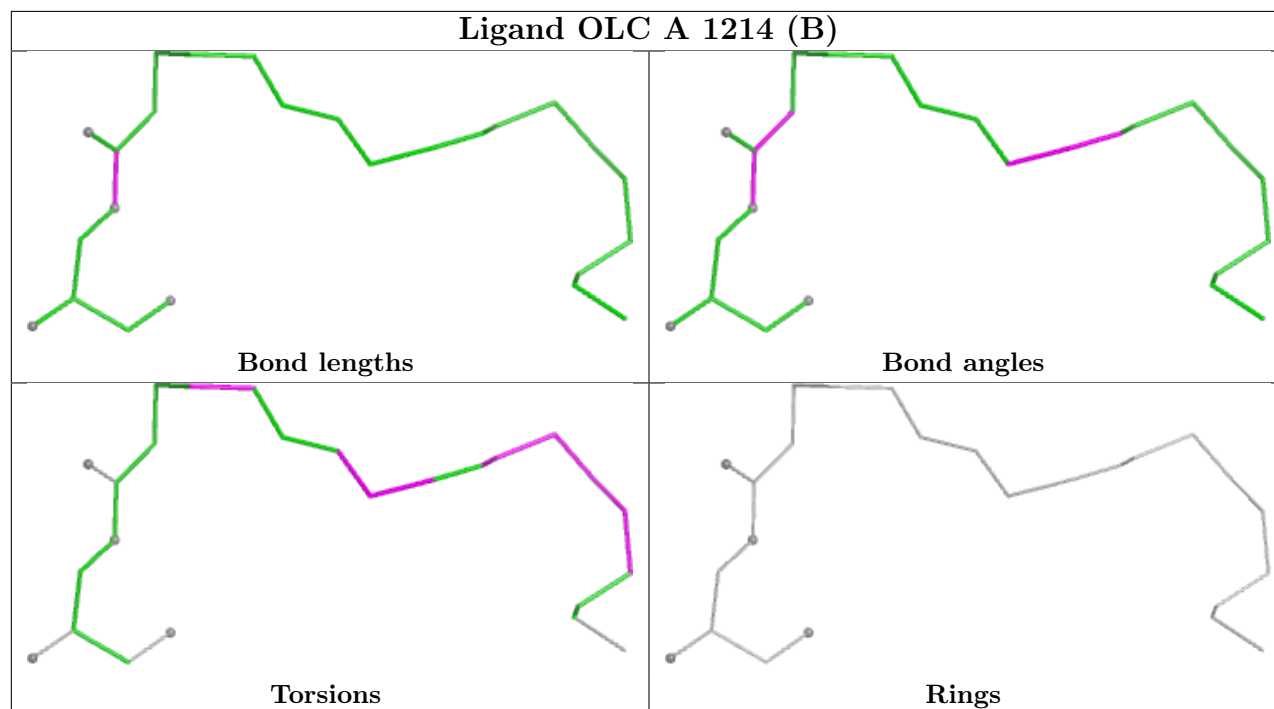
There are no ring outliers.

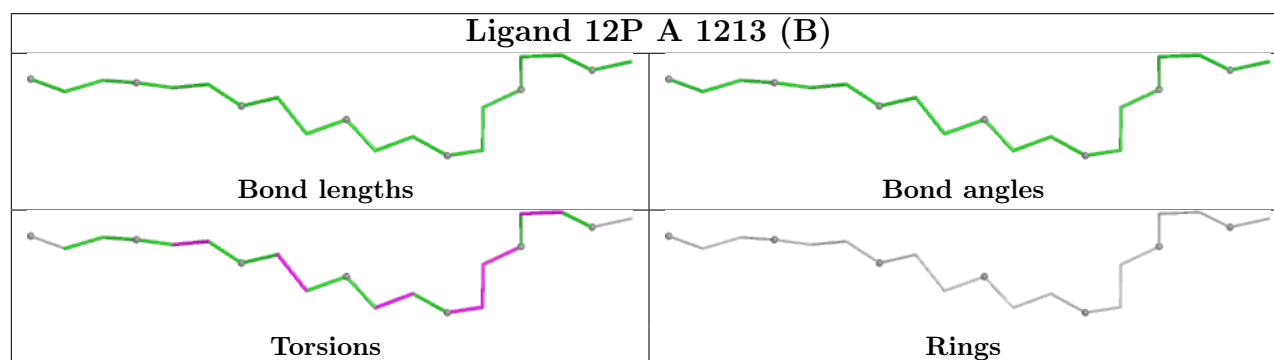
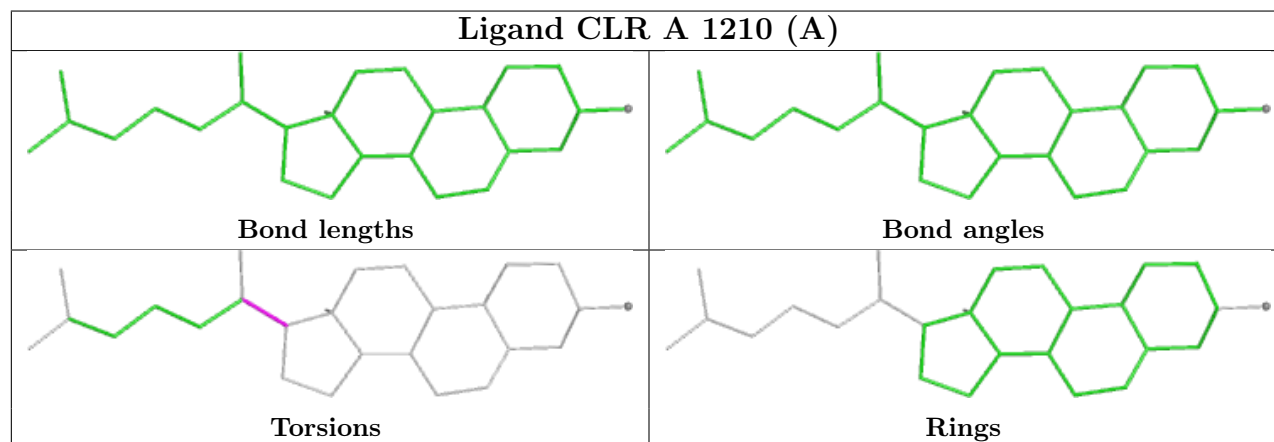
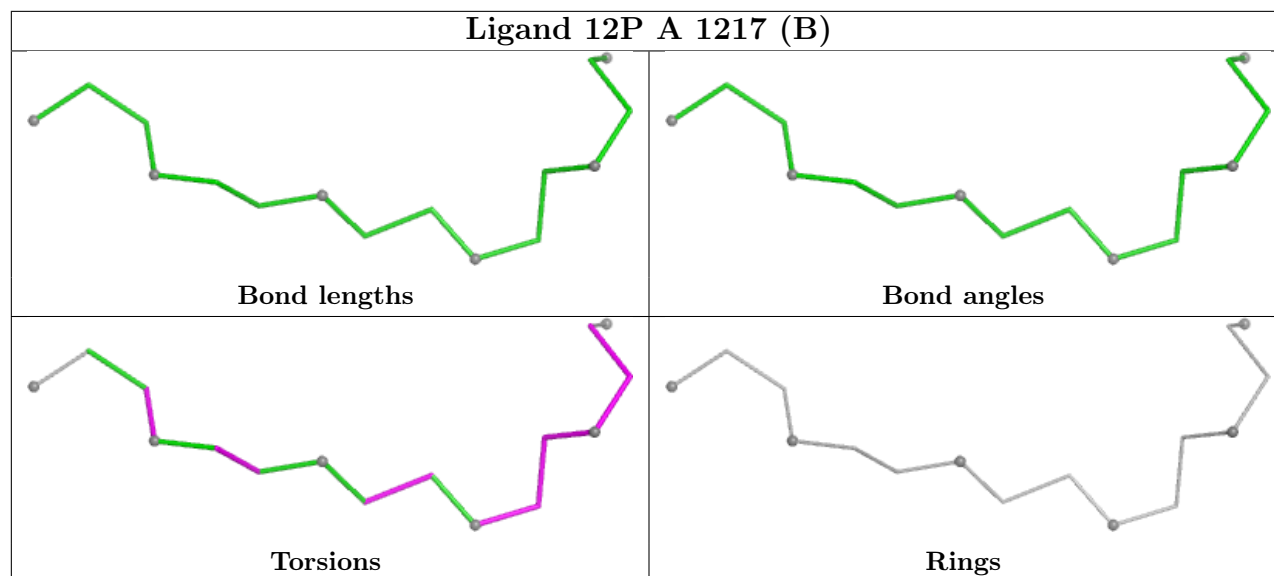
23 monomers are involved in 40 short contacts:

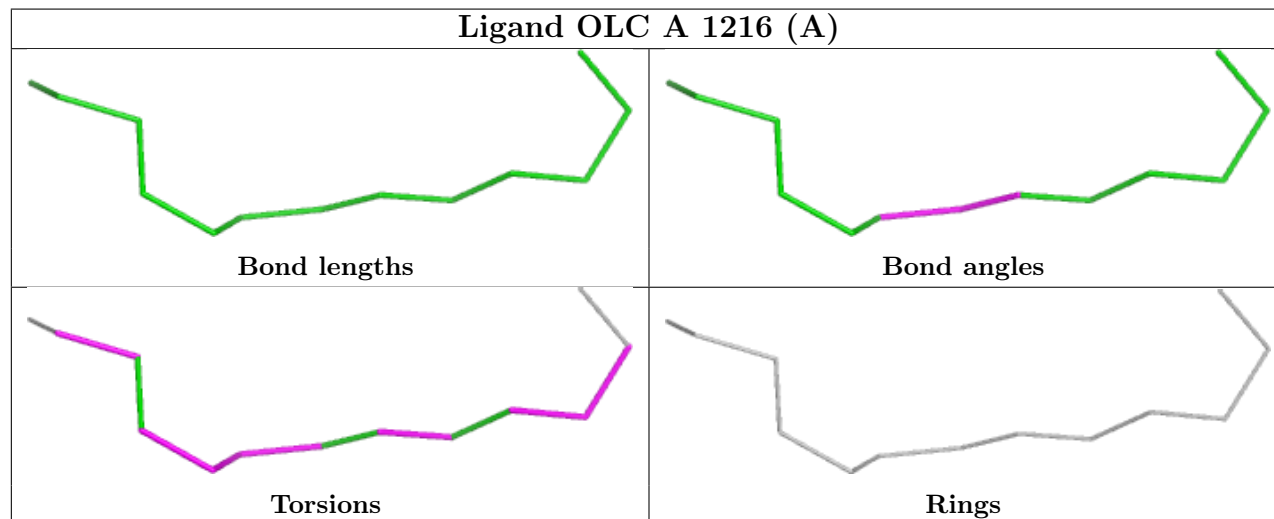
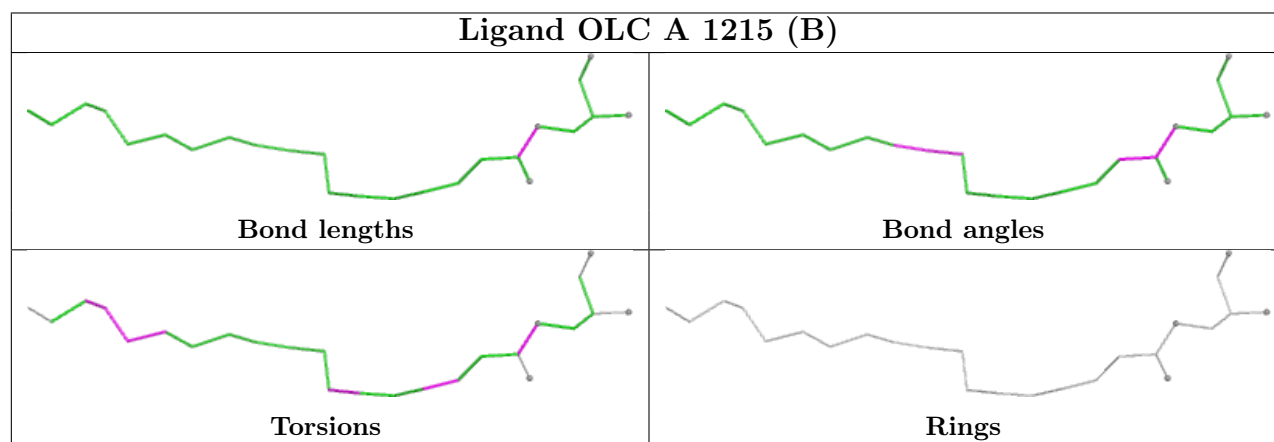
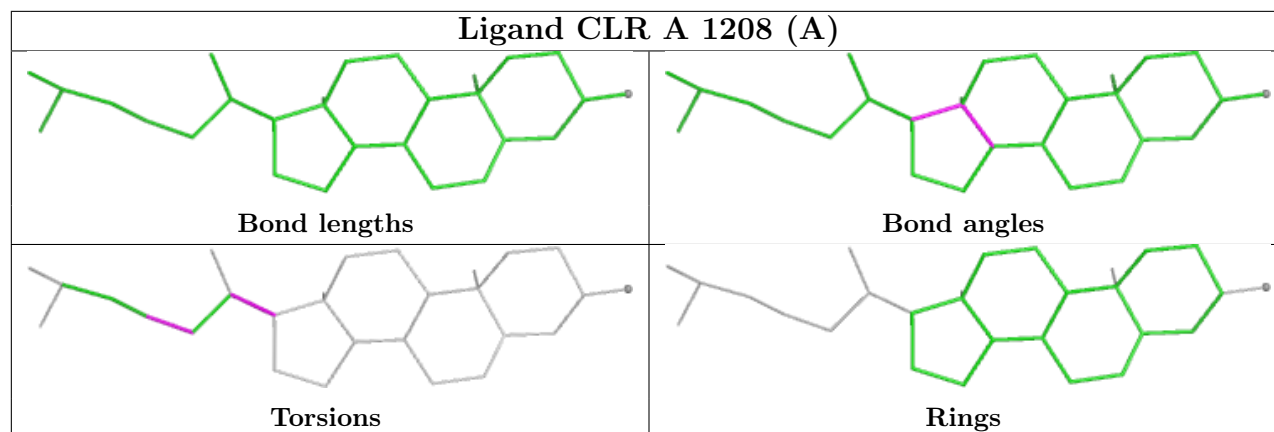
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1206[A]	SO4	2	0
8	A	1225[B]	1PE	4	0
4	A	1209[B]	CLR	1	0
8	A	1224[B]	1PE	1	0
7	A	1220[A]	OLC	3	0
7	A	1222[A]	OLC	2	0
6	A	1217[B]	12P	2	0
4	A	1210[A]	CLR	1	0
6	A	1213[B]	12P	4	0
4	A	1208[A]	CLR	3	0
7	A	1216[A]	OLC	1	0
2	A	1202[A]	SO4	1	0
6	A	1212[B]	12P	5	0
7	A	1214[A]	OLC	1	0
6	A	1217[A]	12P	4	0
10	A	1221[B]	GOL	1	0
6	A	1213[A]	12P	2	0
7	A	1220[B]	OLC	4	0
7	A	1222[B]	OLC	2	0
4	A	1210[B]	CLR	2	0
5	A	1211[B]	PLM	1	0
4	A	1208[B]	CLR	2	0
7	A	1216[B]	OLC	2	0

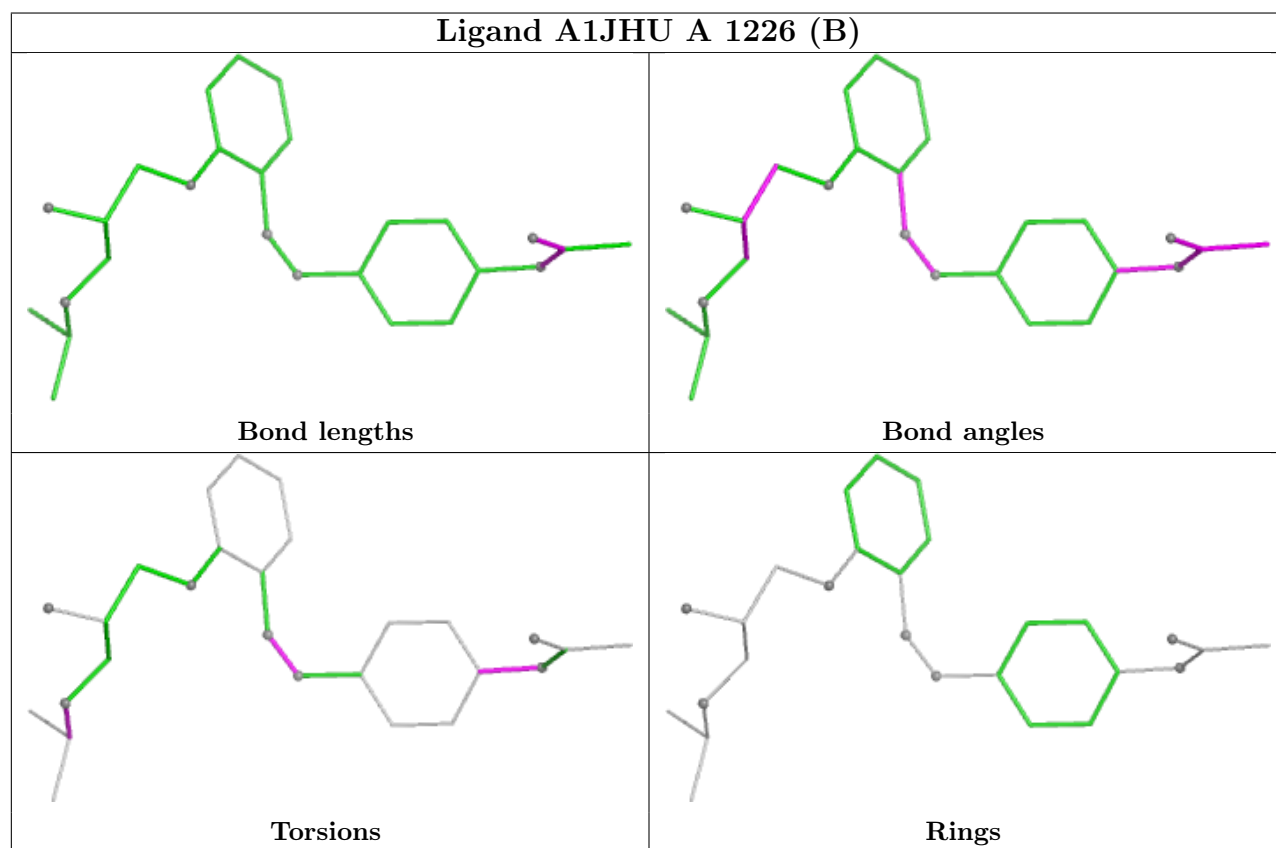
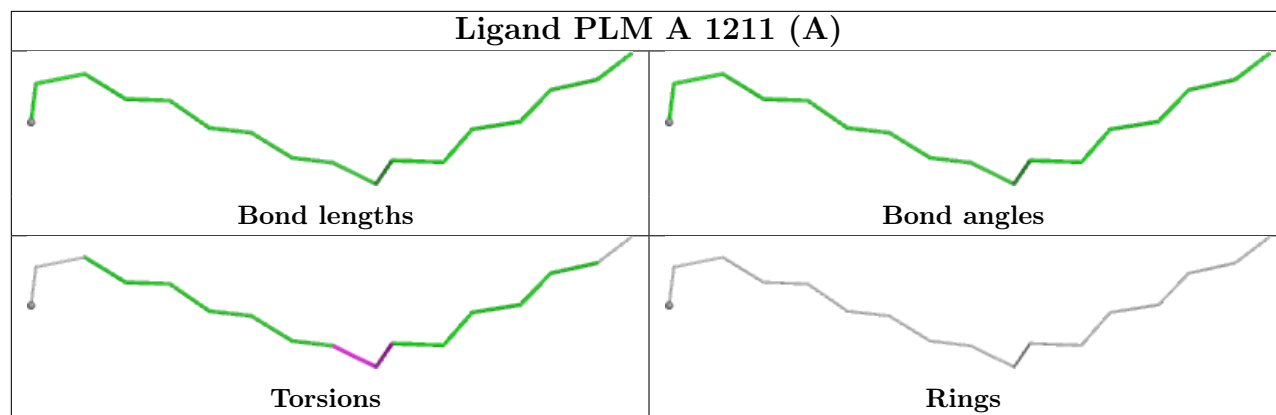
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

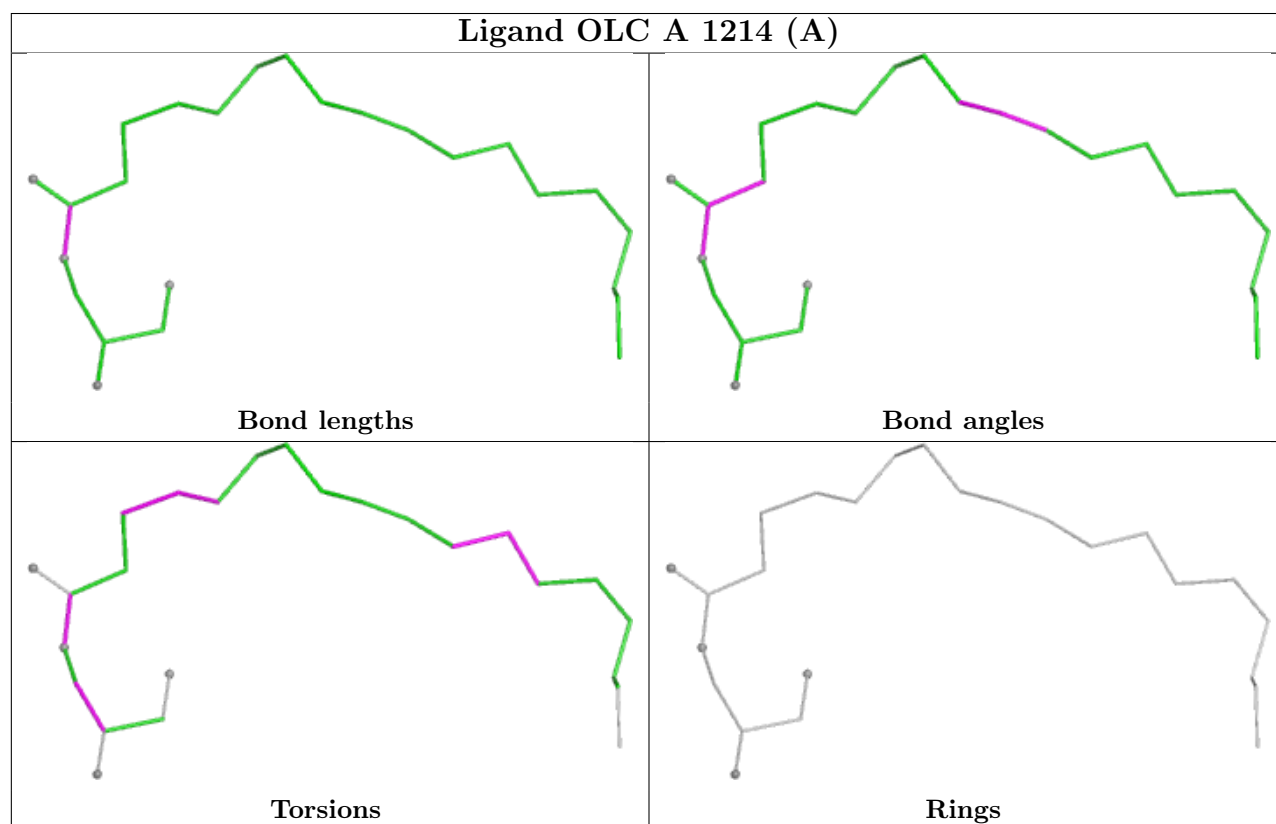
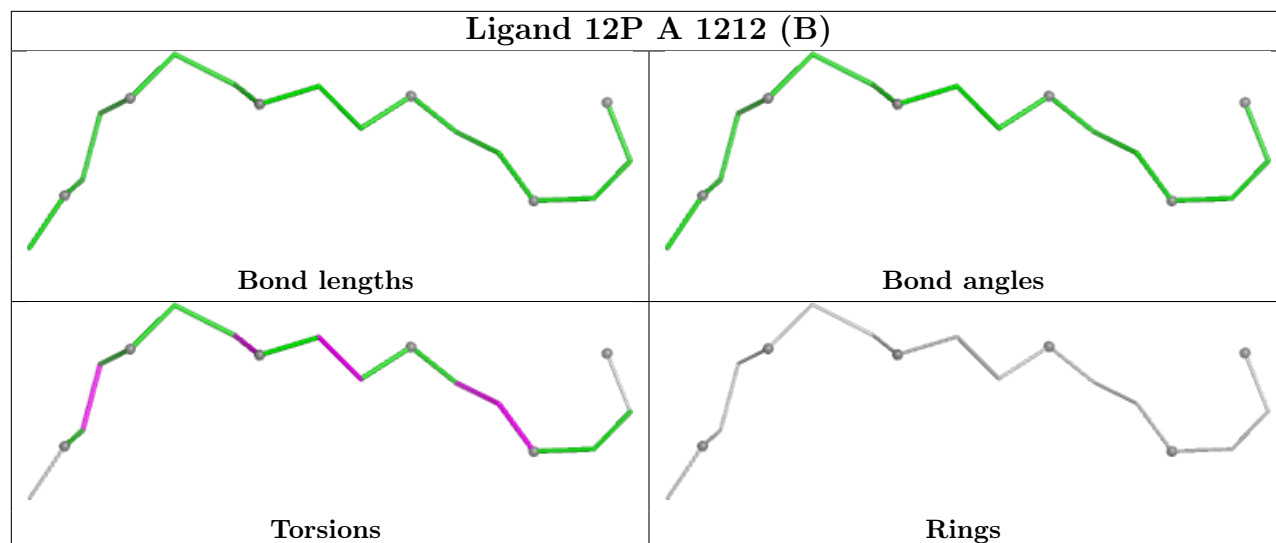
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

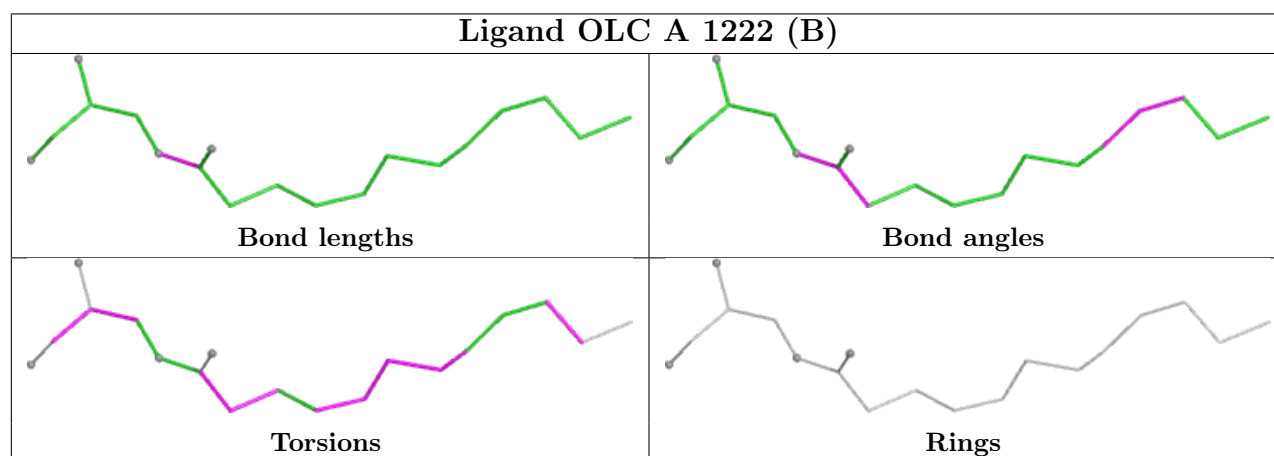
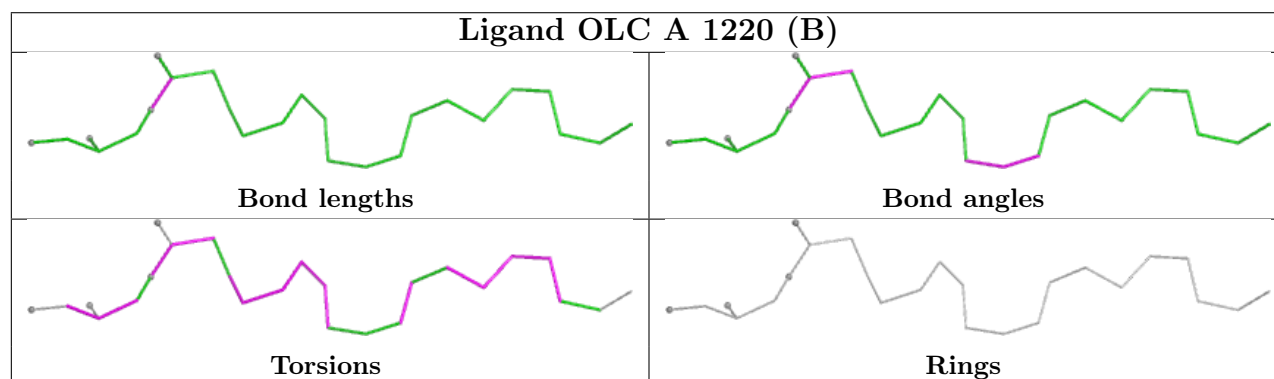
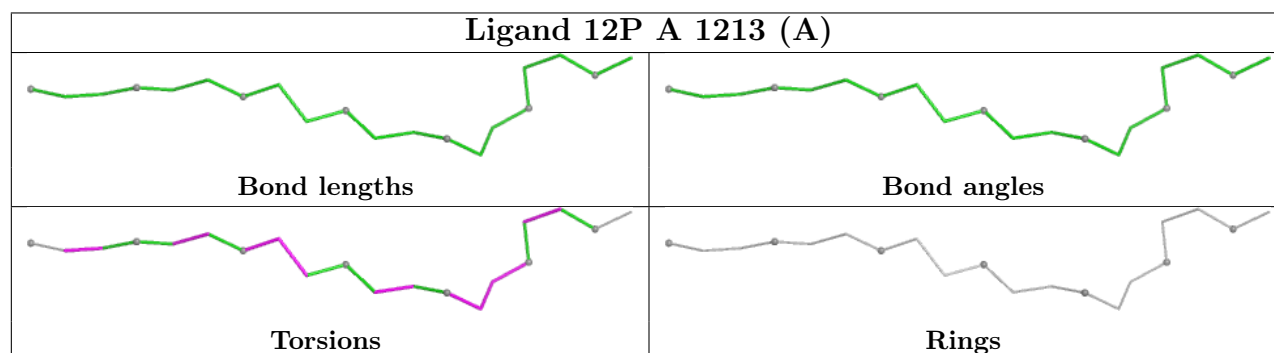
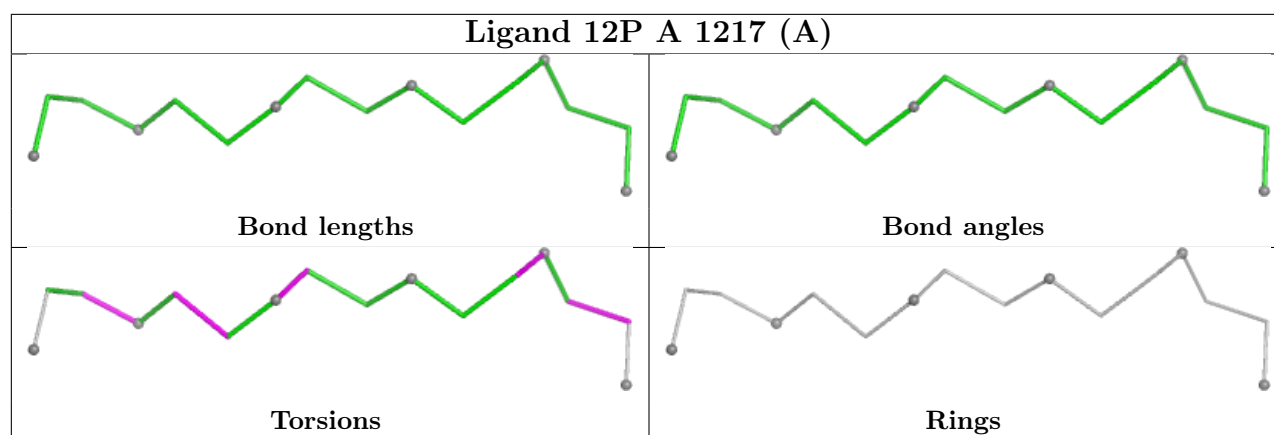


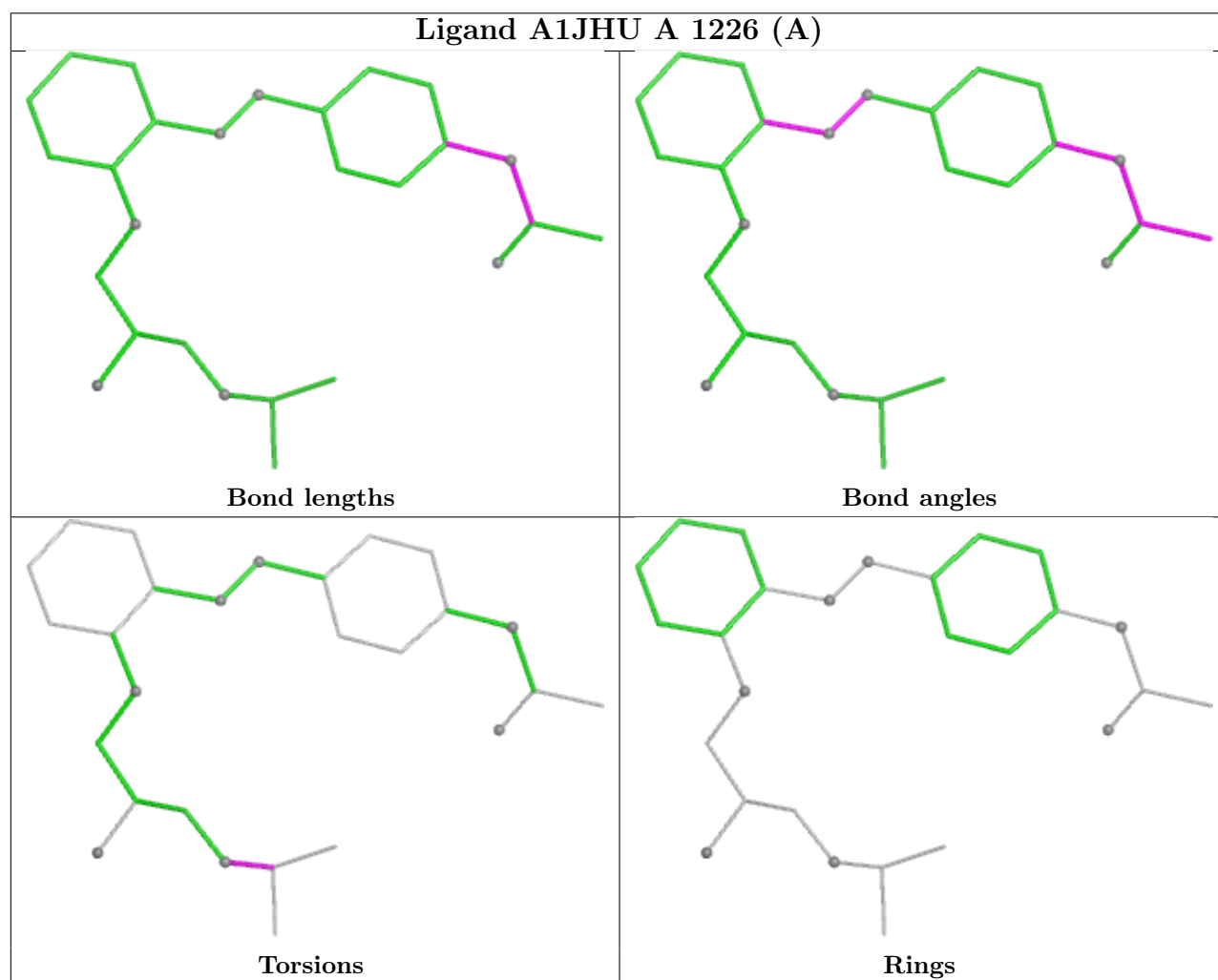
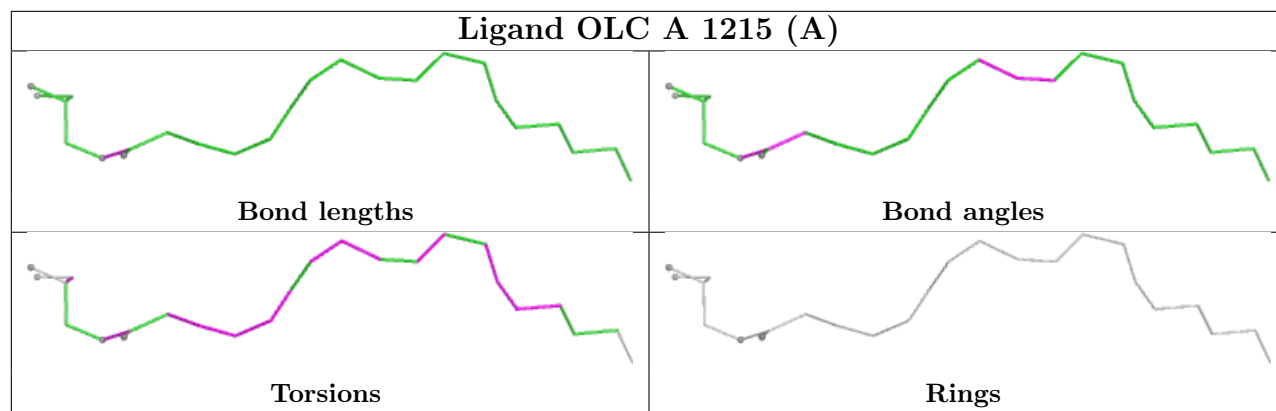




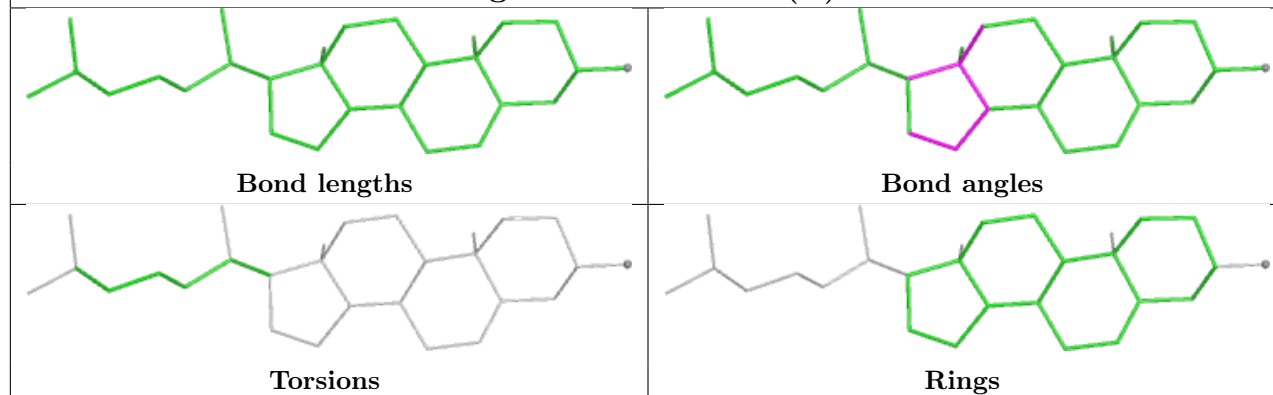




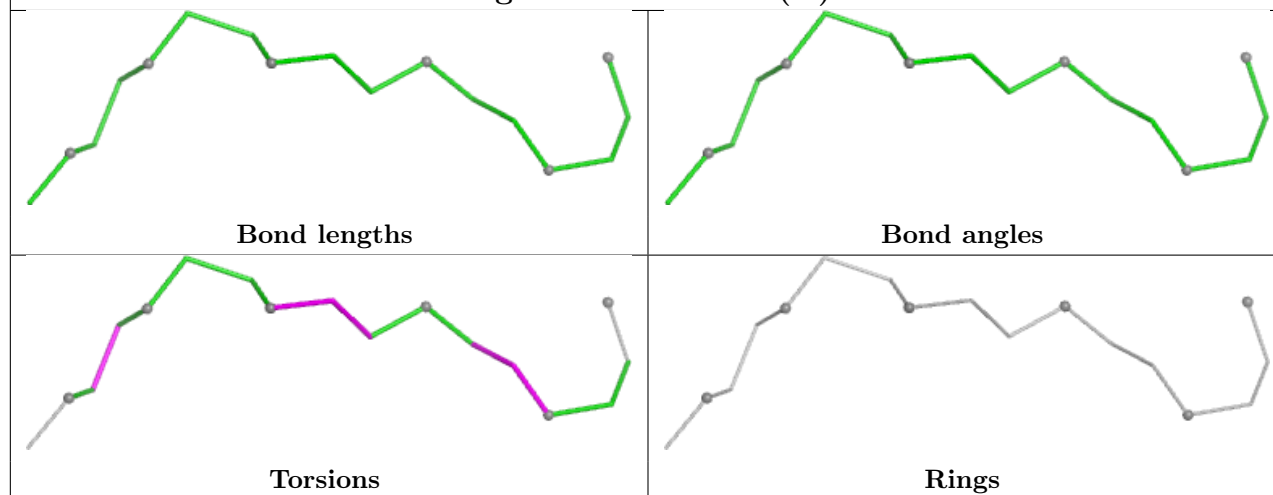




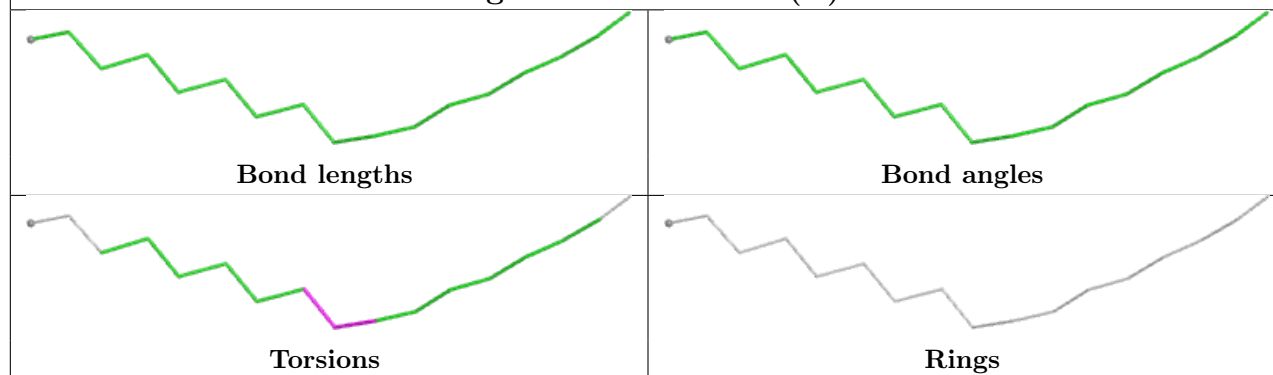
Ligand CLR A 1210 (B)

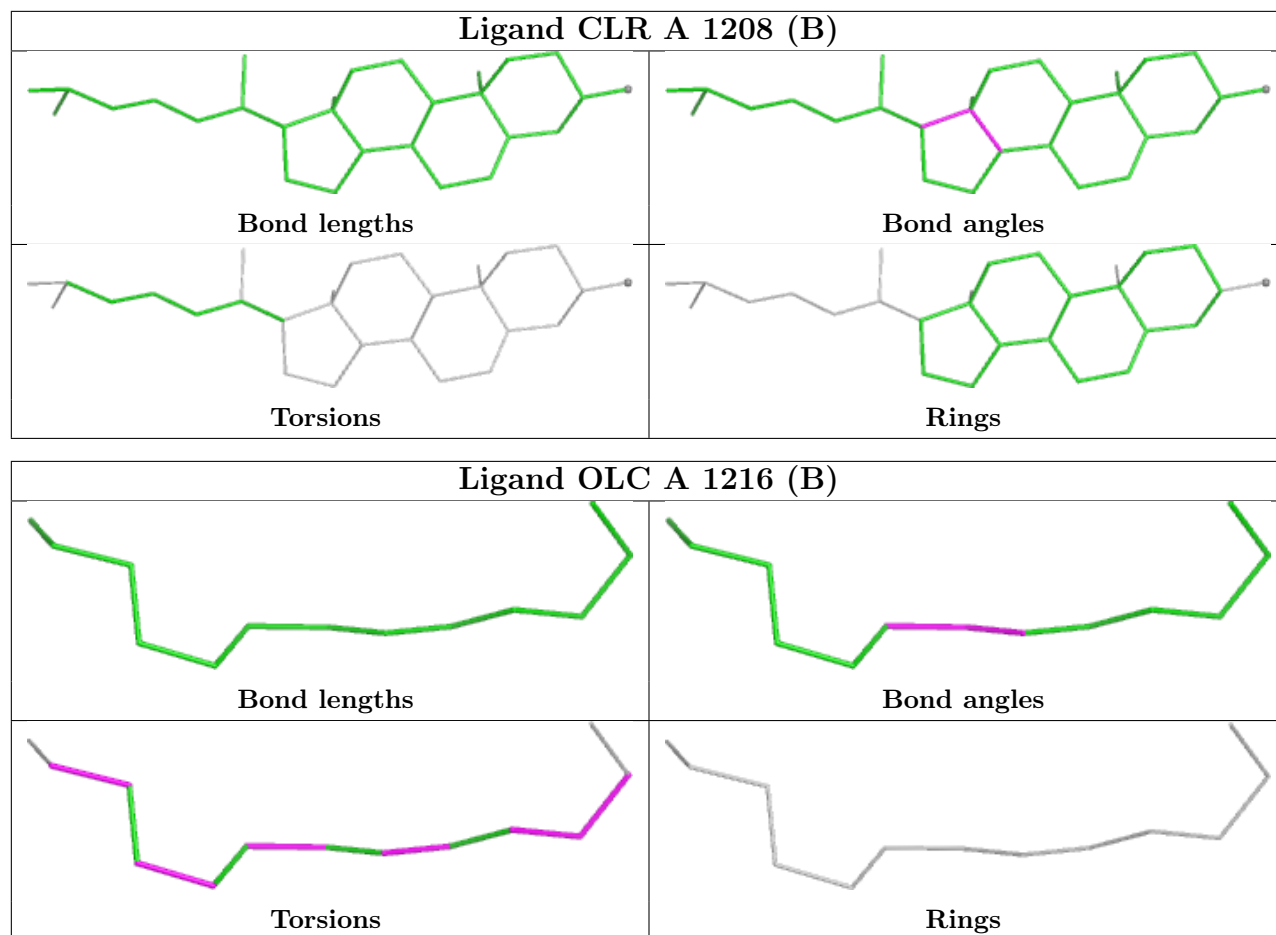


Ligand 12P A 1212 (A)



Ligand PLM A 1211 (B)





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	443/443 (100%)	0.14	9 (2%) 65 66	22, 41, 67, 105	443 (100%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28[A]	ALA	5.5
1	A	95[A]	LEU	2.9
1	A	141[A]	TYR	2.4
1	A	1140[A]	ASN	2.4
1	A	33[A]	VAL	2.3

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(Å ²)	Q<0.9
9	EDO	A	1223[B]	4/4	0.38	1.05	56,58,64,69	4
2	SO4	A	1206[A]	5/5	0.75	0.14	90,95,139,340	5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	1PE	A	1225[B]	10/16	0.77	0.71	32,60,92,113	10
7	OLC	A	1214[A]	25/25	0.78	0.16	83,146,187,198	65
7	OLC	A	1214[B]	25/25	0.78	0.16	62,126,181,188	65
7	OLC	A	1215[A]	25/25	0.79	0.24	84,129,190,201	65
7	OLC	A	1215[B]	25/25	0.79	0.24	69,113,154,178	65
2	SO4	A	1205[B]	5/5	0.81	0.09	71,105,148,158	5
2	SO4	A	1205[A]	5/5	0.81	0.09	93,99,179,183	5
6	12P	A	1213[A]	20/37	0.82	0.18	61,102,120,128	20
6	12P	A	1213[B]	20/37	0.82	0.18	73,94,113,126	20
7	OLC	A	1220[A]	25/25	0.83	0.27	84,112,140,149	25
7	OLC	A	1220[B]	25/25	0.83	0.27	83,106,126,131	25
8	1PE	A	1224[B]	8/16	0.84	0.46	51,66,81,82	8
6	12P	A	1217[A]	16/37	0.84	0.22	70,95,127,134	16
6	12P	A	1217[B]	16/37	0.84	0.22	55,85,102,109	16
10	GOL	A	1221[A]	6/6	0.85	0.23	88,95,109,125	6
10	GOL	A	1221[B]	6/6	0.85	0.23	77,82,96,103	6
4	CLR	A	1210[B]	28/28	0.87	0.22	82,119,146,146	28
4	CLR	A	1210[A]	28/28	0.87	0.22	80,123,161,167	28
7	OLC	A	1222[B]	19/25	0.90	0.20	67,97,124,126	19
7	OLC	A	1222[A]	19/25	0.90	0.20	64,97,137,138	19
9	EDO	A	1219[A]	4/4	0.91	0.19	93,114,139,139	10
9	EDO	A	1219[B]	4/4	0.91	0.19	87,112,135,135	10
5	PLM	A	1211[B]	17/18	0.91	0.17	72,94,117,124	17
2	SO4	A	1202[A]	5/5	0.91	0.12	97,98,130,145	5
5	PLM	A	1211[A]	17/18	0.91	0.17	69,101,139,147	17
6	12P	A	1212[B]	17/37	0.92	0.15	58,81,104,124	17
6	12P	A	1212[A]	17/37	0.92	0.15	54,83,107,134	17
7	OLC	A	1216[B]	13/25	0.93	0.19	60,76,96,104	13
2	SO4	A	1204[B]	5/5	0.93	0.09	68,91,100,113	5
2	SO4	A	1204[A]	5/5	0.93	0.09	66,94,105,120	5
7	OLC	A	1216[A]	13/25	0.93	0.19	60,78,106,116	13
11	A1JHU	A	1226[A]	27/27	0.93	0.13	53,81,107,111	53
11	A1JHU	A	1226[B]	27/27	0.93	0.13	56,82,112,134	53
4	CLR	A	1209[B]	28/28	0.94	0.11	70,95,108,115	28
8	1PE	A	1218[A]	10/16	0.94	0.17	58,107,127,131	23
8	1PE	A	1218[B]	10/16	0.94	0.17	48,97,117,121	23
4	CLR	A	1209[A]	28/28	0.94	0.11	68,95,112,117	28
4	CLR	A	1208[B]	28/28	0.95	0.19	68,99,118,120	28
4	CLR	A	1208[A]	28/28	0.95	0.19	87,100,131,144	28
3	ACM	A	1207[B]	4/4	0.96	0.12	73,78,84,90	4
2	SO4	A	1203[B]	5/5	0.96	0.09	61,76,85,93	5
2	SO4	A	1203[A]	5/5	0.96	0.09	56,64,109,112	5

Continued on next page...

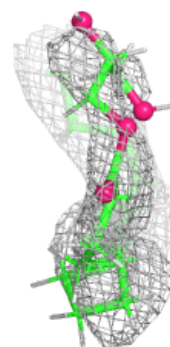
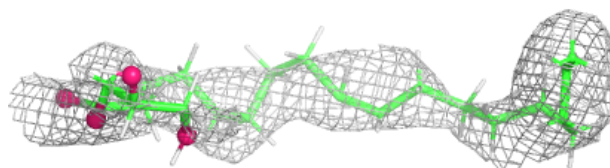
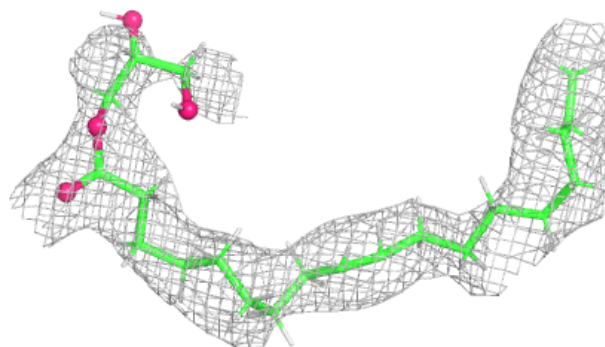
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ACM	A	1207[A]	4/4	0.96	0.12	64,70,80,89	4
2	SO4	A	1201[B]	5/5	0.99	0.05	59,69,72,84	5
2	SO4	A	1201[A]	5/5	0.99	0.05	63,64,83,87	5

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.

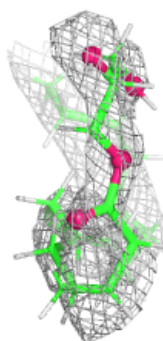
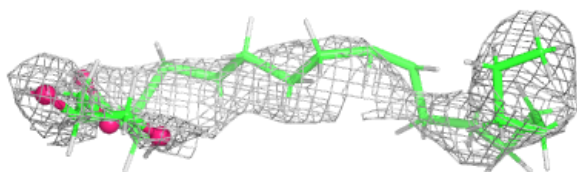
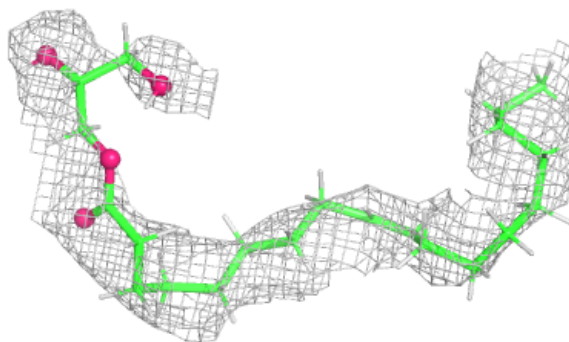
Electron density around OLC A 1214 (A):

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

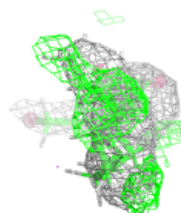
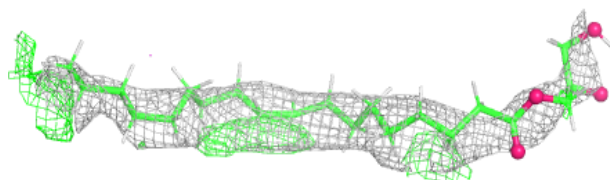
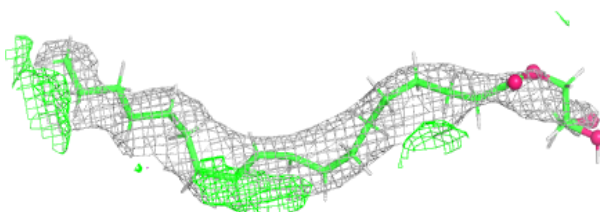


Electron density around OLC A 1214 (B):

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

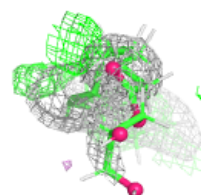
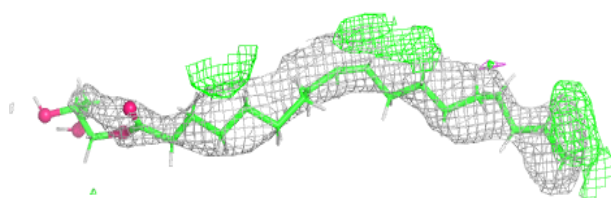
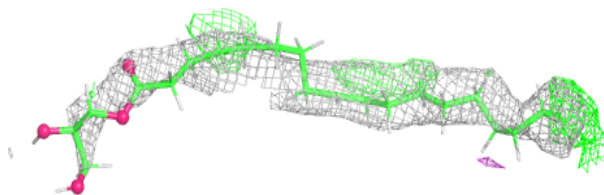
**Electron density around OLC A 1215 (A):**

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

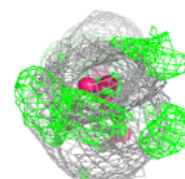
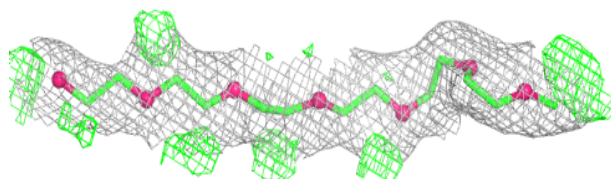
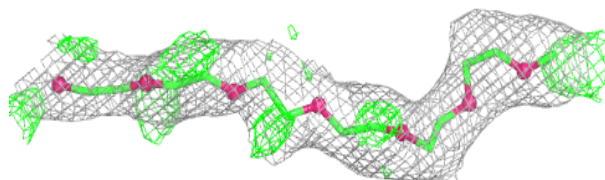


Electron density around OLC A 1215 (B):

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

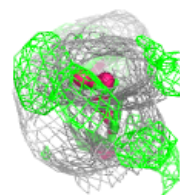
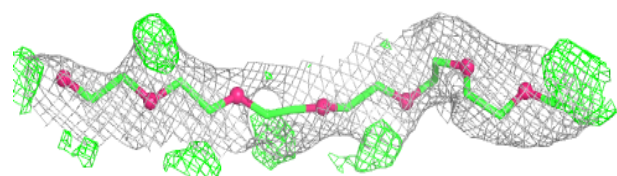
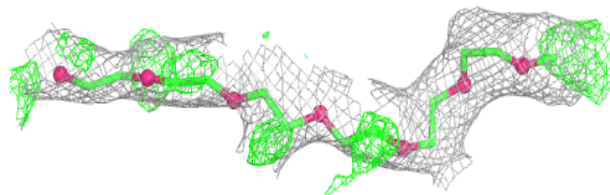
**Electron density around 12P A 1213 (A):**

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

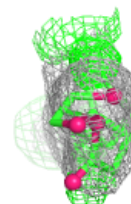
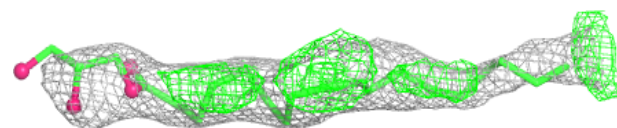
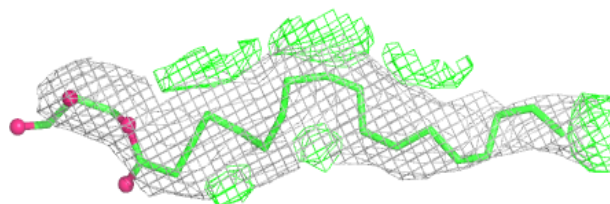


Electron density around 12P A 1213 (B):

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

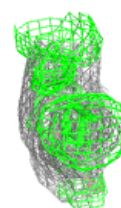
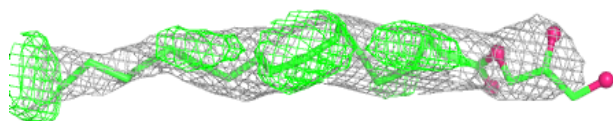
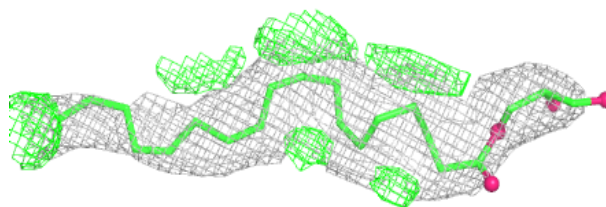
**Electron density around OLC A 1220 (A):**

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

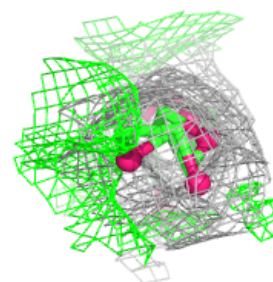
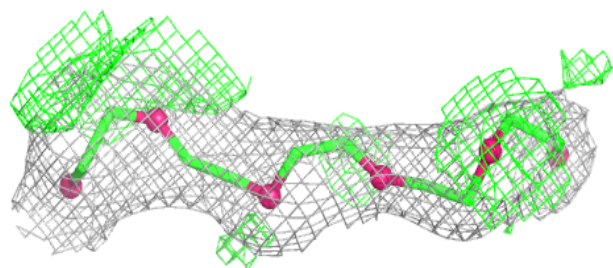
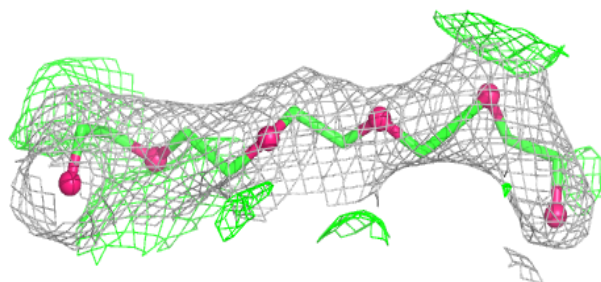


Electron density around OLC A 1220 (B):

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

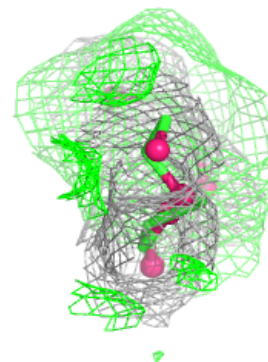
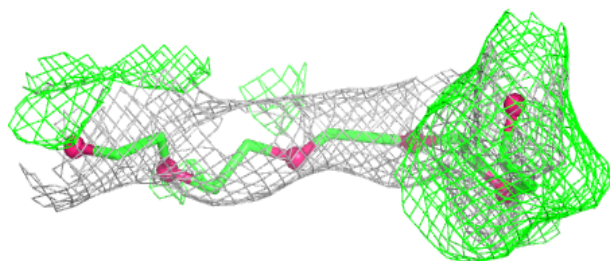
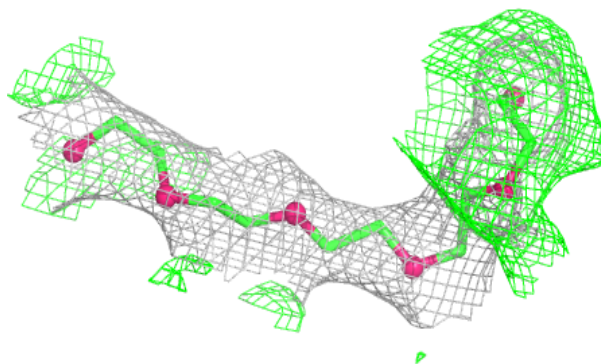
**Electron density around 12P A 1217 (A):**

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

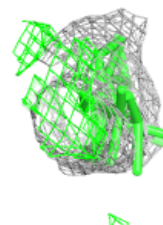
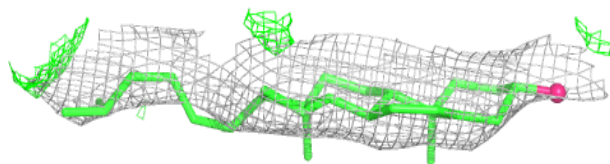
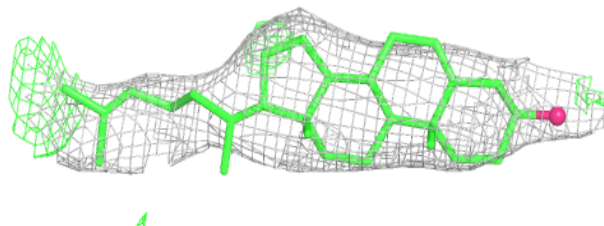


Electron density around 12P A 1217 (B):

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

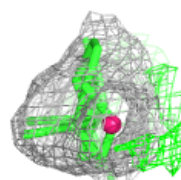
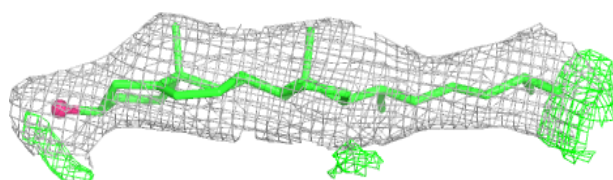
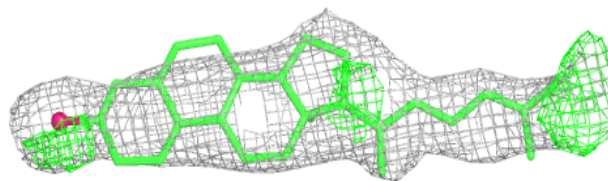
**Electron density around CLR A 1210 (B):**

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

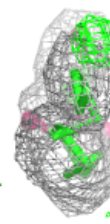
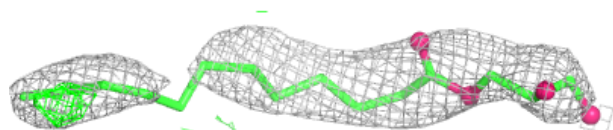
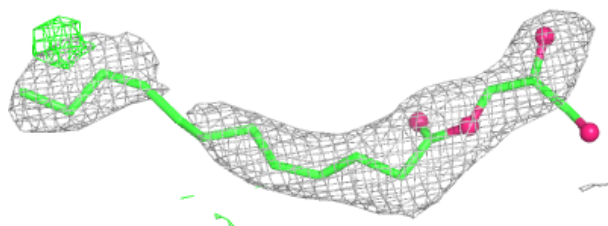


Electron density around CLR A 1210 (A):

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

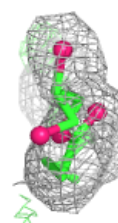
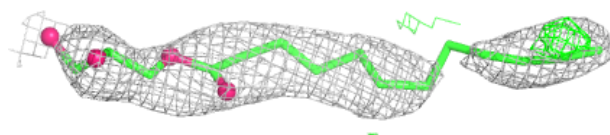
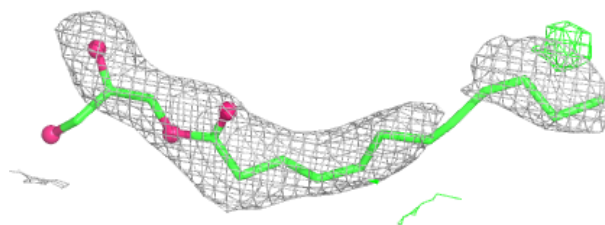
**Electron density around OLC A 1222 (B):**

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

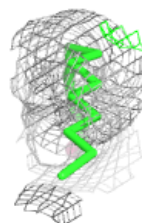
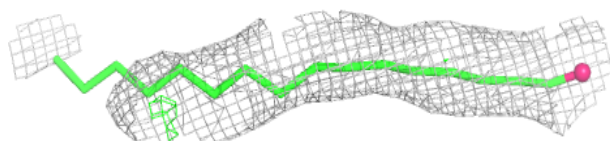
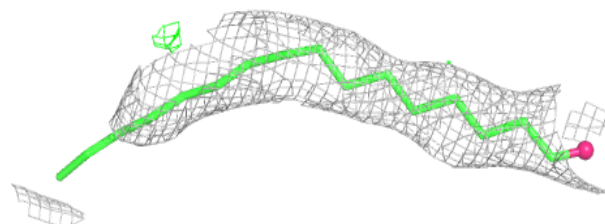


Electron density around OLC A 1222 (A):

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

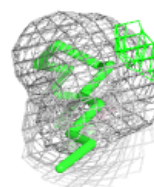
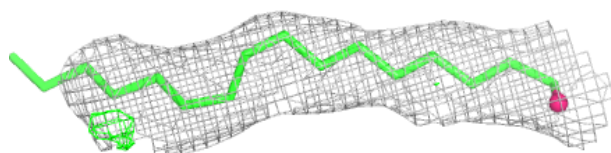
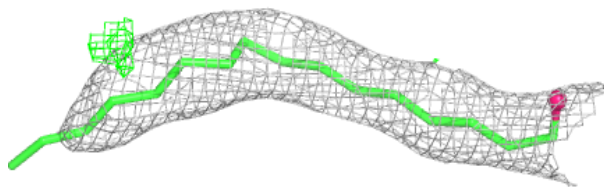
**Electron density around PLM A 1211 (B):**

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

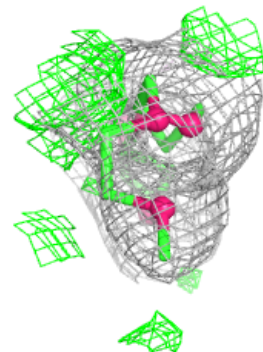
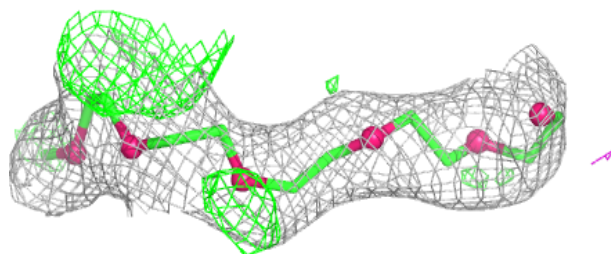
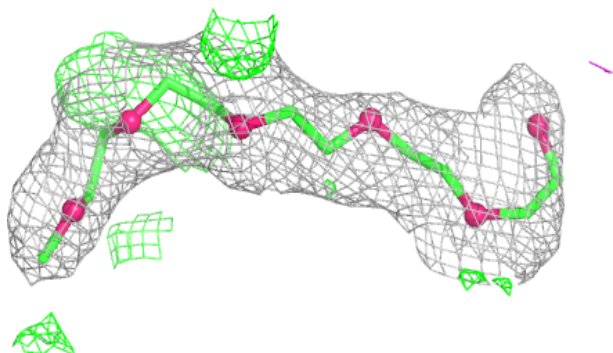


Electron density around PLM A 1211 (A):

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

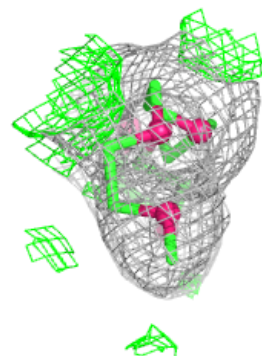
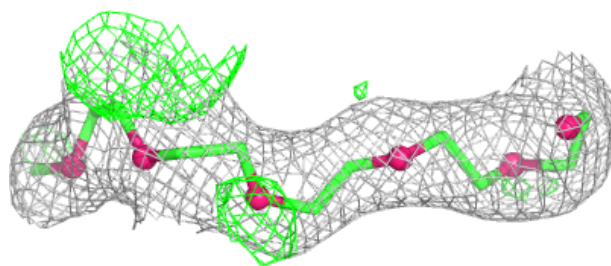
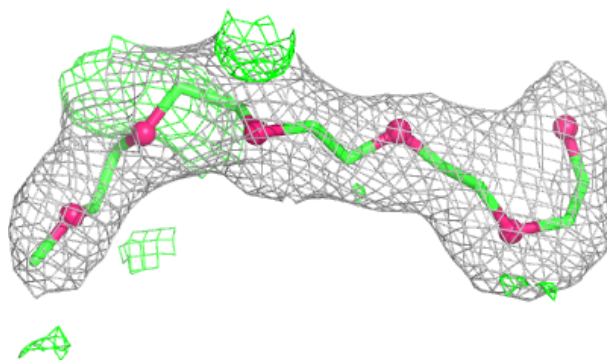
**Electron density around 12P A 1212 (B):**

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

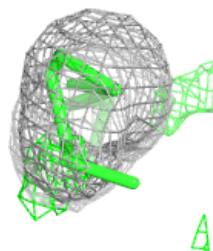
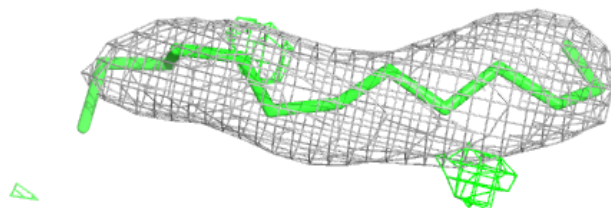
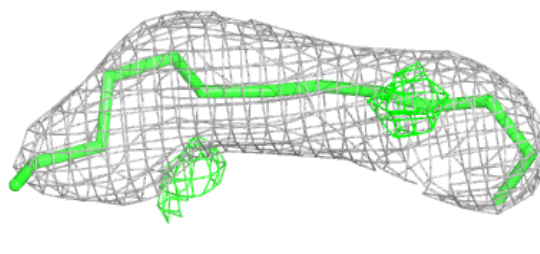


Electron density around 12P A 1212 (A):

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

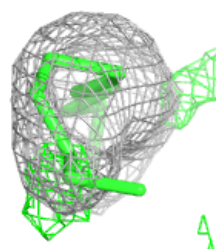
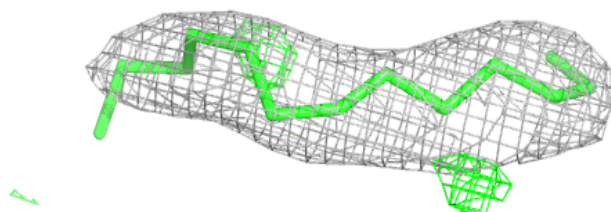
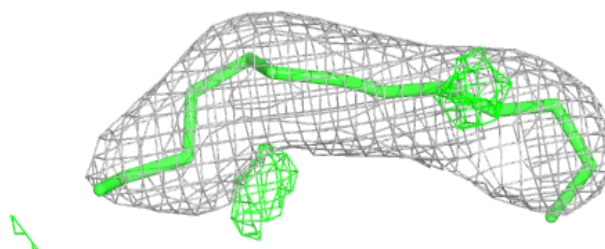
**Electron density around OLC A 1216 (B):**

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

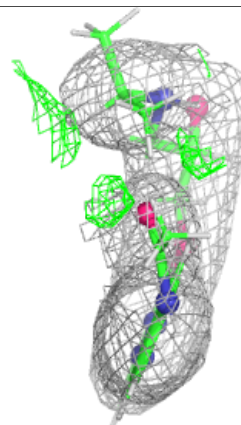
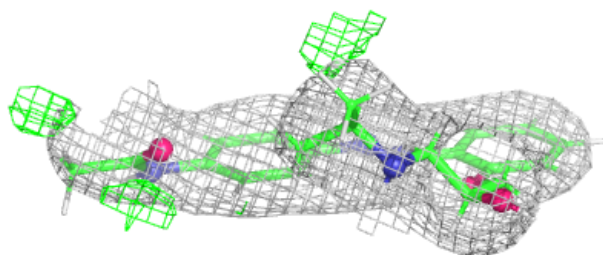
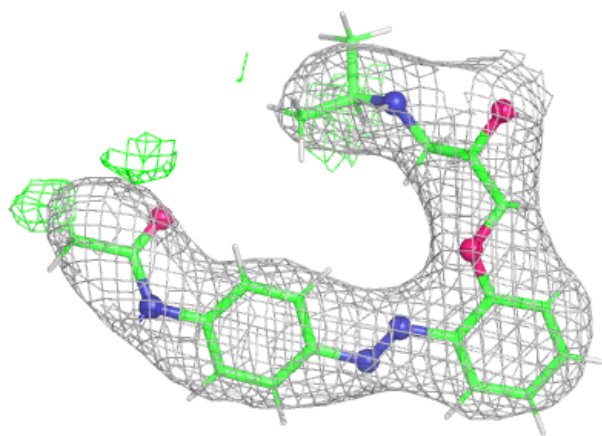


Electron density around OLC A 1216 (A):

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

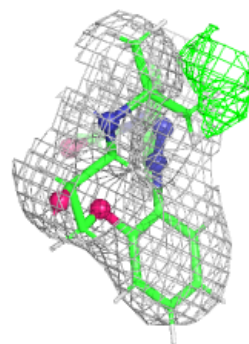
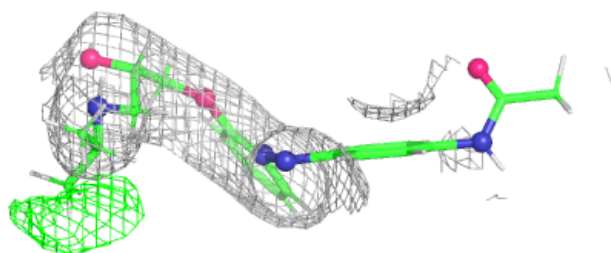
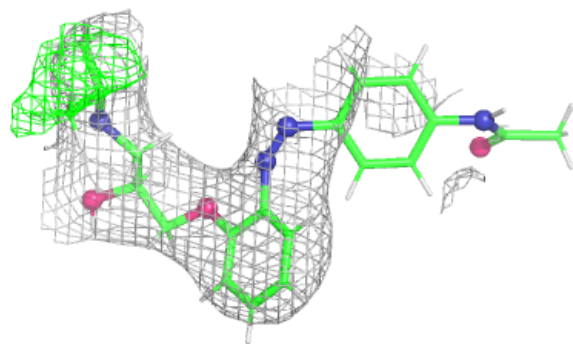
**Electron density around A1JHU A 1226 (A):**

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

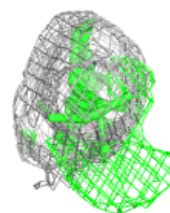
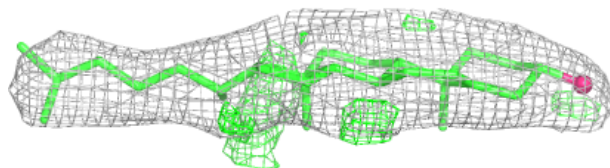
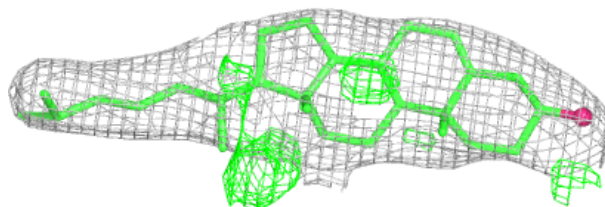


Electron density around A1JHU A 1226 (B):

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

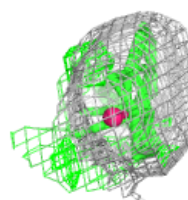
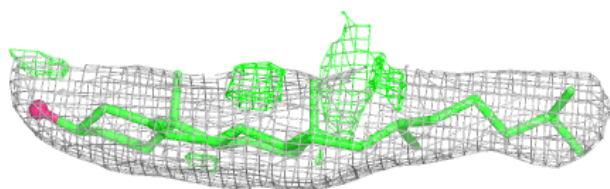
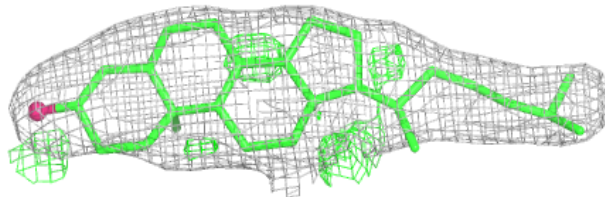
**Electron density around CLR A 1208 (B):**

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



Electron density around CLR A 1208 (A):

$2mF_o-DF_c$ (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.