



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:51 PM UTC

PDB ID : 4XNV / pdb_00004xnv
Title : The human P2Y1 receptor in complex with BPTU
Authors : Zhang, D.; Gao, Z.; Jacobson, K.; Han, G.W.; Stevens, R.; Zhao, Q.; Wu, B.;
GPCR Network (GPCR)
Deposited on : 2015-01-16
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2022.3.0, CSD as543be (2022)
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

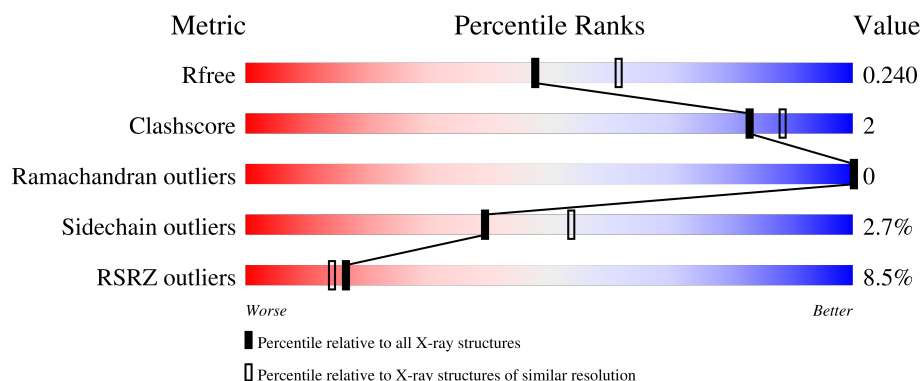
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	421	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 3114 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.

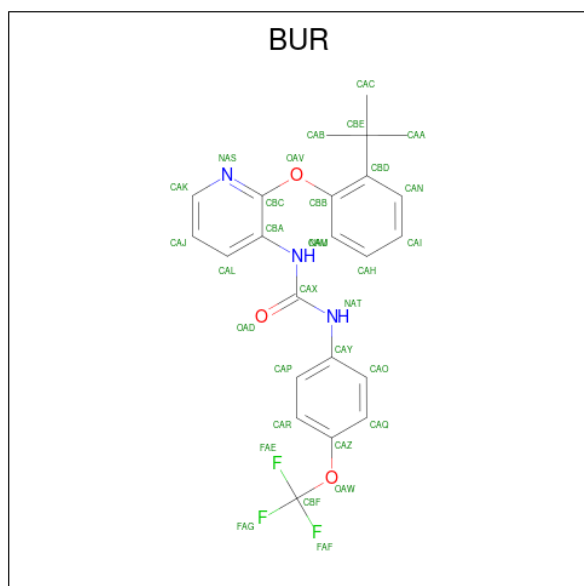
- Molecule 1 is a protein called P2Y purinoceptor 1, Rubredoxin, P2Y purinoceptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2713	1803	426	460	24			

There is a discrepancy between the modelled and reference sequences:

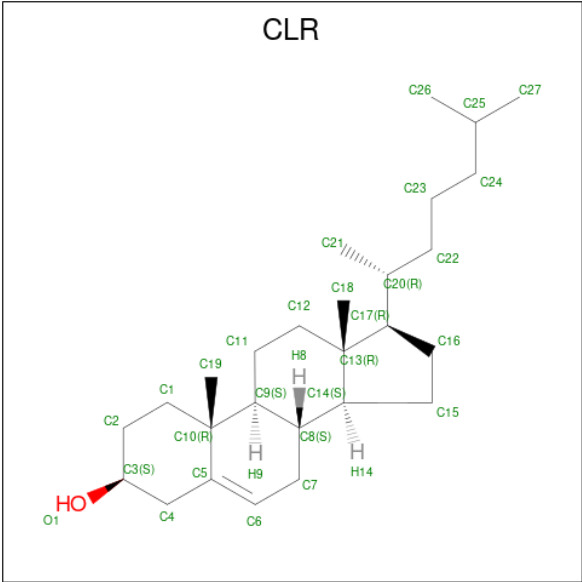
Chain	Residue	Modelled	Actual	Comment	Reference
A	320	ASN	ASP	engineered mutation	UNP P47900

- Molecule 2 is 1-[2-(2-tert-butylphenoxy)pyridin-3-yl]-3-[4-(trifluoromethoxy)phenyl]urea (CCD ID: BUR) (formula: C₂₃H₂₂F₃N₃O₃).



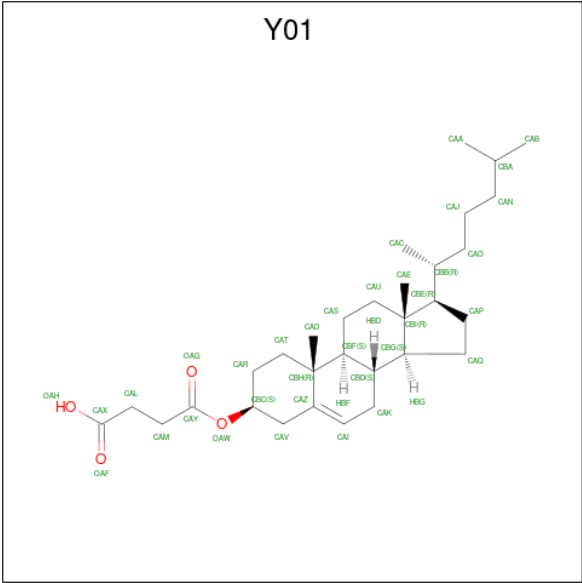
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			32	23	3	3	3		

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



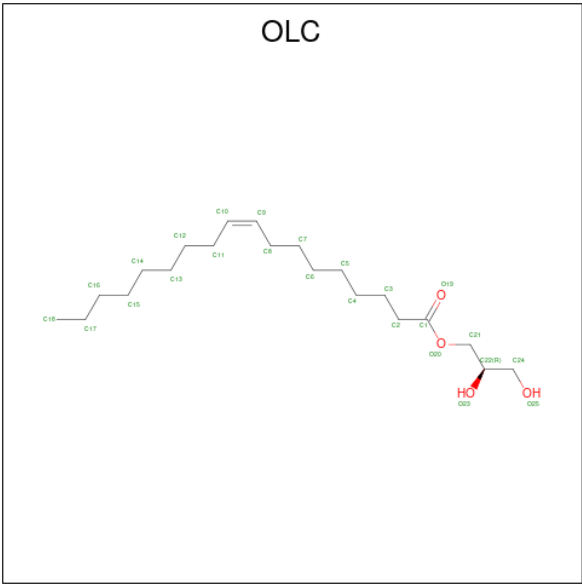
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			28	27	1		

- Molecule 4 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$).



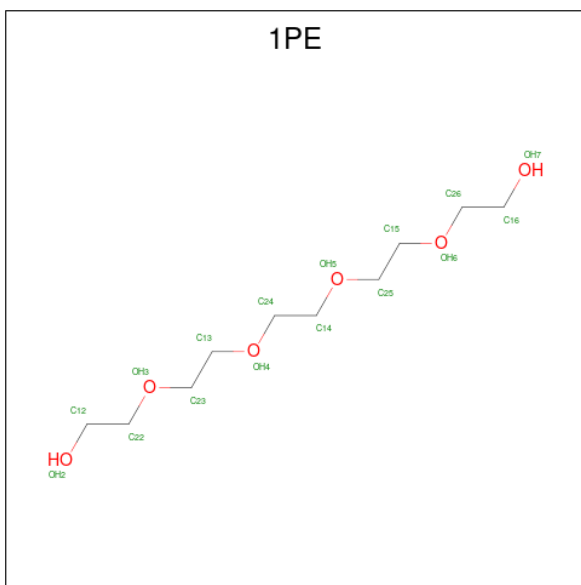
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			35	31	4		
4	A	1	Total	C	O	0	0
			35	31	4		
4	A	1	Total	C	O	0	0
			35	31	4		

- Molecule 5 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			21	17	4		
5	A	1	Total	C	O	0	0
			21	17	4		
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			25	21	4		
5	A	1	Total	C	O	0	0
			22	18	4		
5	A	1	Total	C	O	0	0
			25	21	4		

- Molecule 6 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	C O	0	0
			16	10 6		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Zn	0	0
			1	1		

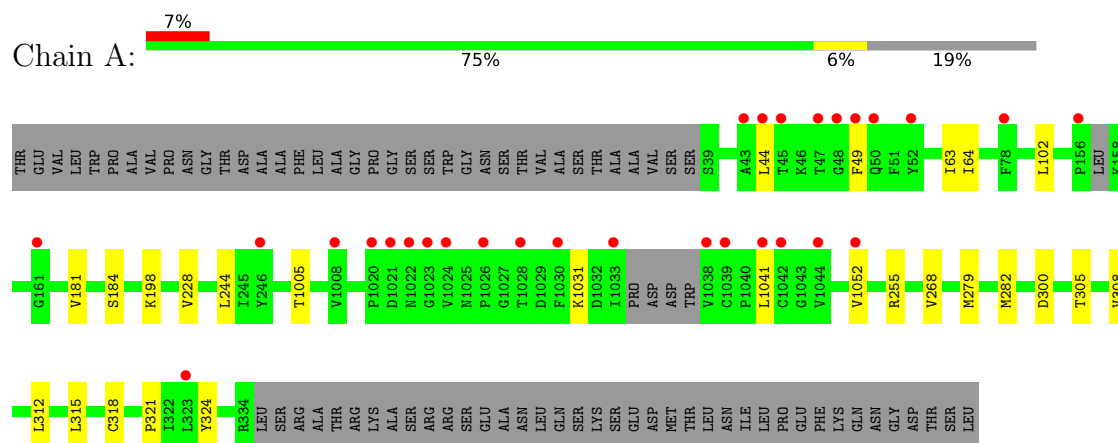
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	30	Total	O	0	0
			30	30		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: P2Y purinoceptor 1, Rubredoxin, P2Y purinoceptor 1



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	66.27 Å 66.27 Å 239.07 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.40 – 2.20 41.40 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.40-2.20) 99.9 (41.40-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.20 Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.207 , 0.230 0.211 , 0.240	Depositor DCC
R_{free} test set	1017 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.055 for -h-k,k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3114	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

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: ZN, BUR, Y01, CLR, 1PE, OLC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.76	0/2787	1.32	1/3787 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	228	VAL	N-CA-CB	6.03	115.15	110.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2713	0	2724	11	0
2	A	32	0	22	1	0
3	A	28	0	46	0	0
4	A	105	0	147	2	0
5	A	189	0	289	6	0
6	A	16	0	22	0	0
7	A	1	0	0	0	0
8	A	30	0	0	0	0
All	All	3114	0	3250	15	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 2.

All (15) 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:282:MET:HG2	5:A:1112:OLC:H24A	1.84	0.59
1:A:312:LEU:HA	1:A:315:LEU:HD12	1.87	0.57
1:A:184:SER:HB2	5:A:1110:OLC:H11A	1.88	0.56
1:A:64:ILE:HG22	1:A:318:CYS:HB2	1.93	0.50
1:A:181:VAL:HG13	5:A:1107:OLC:H12	1.95	0.49
2:A:1101:BUR:OAD	2:A:1101:BUR:H4	2.12	0.49
1:A:1005:THR:HB	1:A:1052:VAL:HG22	1.94	0.48
5:A:1108:OLC:H21	5:A:1110:OLC:H2	1.96	0.47
1:A:63:ILE:HG12	4:A:1105:Y01:HAJ1	1.96	0.46
5:A:1107:OLC:H9	5:A:1110:OLC:H7	1.98	0.45
1:A:308:VAL:HG11	5:A:1113:OLC:H2	1.98	0.45
1:A:244:LEU:HD22	1:A:255:ARG:HG3	2.00	0.44
1:A:321:PRO:HA	1:A:324:TYR:CD2	2.54	0.43
1:A:279:MET:HE2	1:A:305:THR:HB	2.00	0.42
4:A:1104:Y01:HAC2	4:A:1104:Y01:HAJ1	1.77	0.41

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	334/421 (79%)	323 (97%)	11 (3%)	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	295/367 (80%)	287 (97%)	8 (3%)	39 53

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	49	PHE
1	A	102	LEU
1	A	198	LYS
1	A	1031	LYS
1	A	1041	LEU
1	A	268	VAL
1	A	300	ASP

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	69	ASN
1	A	134	ASN
1	A	1014	ASN
1	A	316	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	Y01	A	1104	-	38,38,38	1.93	9 (23%)	57,57,57	1.26	4 (7%)
5	OLC	A	1108	-	24,24,24	1.04	1 (4%)	25,25,25	0.73	0
5	OLC	A	1110	-	24,24,24	1.01	1 (4%)	25,25,25	0.69	0
5	OLC	A	1111	-	24,24,24	1.00	1 (4%)	25,25,25	0.77	0
4	Y01	A	1105	-	38,38,38	1.98	9 (23%)	57,57,57	1.45	8 (14%)
6	1PE	A	1114	-	15,15,15	0.55	0	14,14,14	0.48	0
2	BUR	A	1101	-	34,34,34	1.63	6 (17%)	47,49,49	1.12	4 (8%)
4	Y01	A	1103	-	38,38,38	1.96	10 (26%)	57,57,57	1.21	4 (7%)
3	CLR	A	1102	-	31,31,31	1.81	11 (35%)	48,48,48	1.19	6 (12%)
5	OLC	A	1107	-	20,20,24	1.08	1 (5%)	21,21,25	0.64	0
5	OLC	A	1113	-	24,24,24	1.06	1 (4%)	25,25,25	0.79	0
5	OLC	A	1112	-	21,21,24	1.08	1 (4%)	22,22,25	0.60	0
5	OLC	A	1106	-	20,20,24	1.04	1 (5%)	21,21,25	0.75	0
5	OLC	A	1109	-	24,24,24	1.03	1 (4%)	25,25,25	0.75	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	Y01	A	1104	-	-	9/19/77/77	0/4/4/4
5	OLC	A	1108	-	-	11/24/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OLC	A	1110	-	-	13/24/24/24	-
5	OLC	A	1111	-	-	13/24/24/24	-
4	Y01	A	1105	-	-	8/19/77/77	0/4/4/4
6	1PE	A	1114	-	-	8/13/13/13	-
2	BUR	A	1101	-	-	0/23/23/23	0/3/3/3
4	Y01	A	1103	-	-	7/19/77/77	0/4/4/4
3	CLR	A	1102	-	-	4/10/68/68	0/4/4/4
5	OLC	A	1107	-	-	6/20/20/24	-
5	OLC	A	1113	-	-	14/24/24/24	-
5	OLC	A	1112	-	-	12/21/21/24	-
5	OLC	A	1106	-	-	11/20/20/24	-
5	OLC	A	1109	-	-	10/24/24/24	-

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	BUR	CBE-CBD	-5.27	1.46	1.54
4	A	1105	Y01	CAV-CAZ	-5.02	1.41	1.51
4	A	1103	Y01	CAV-CAZ	-4.97	1.41	1.51
4	A	1105	Y01	CAK-CAI	-4.53	1.41	1.50
4	A	1104	Y01	CAV-CAZ	-4.47	1.42	1.51
4	A	1104	Y01	CAK-CAI	-4.45	1.41	1.50
4	A	1103	Y01	CAK-CAI	-4.39	1.41	1.50
5	A	1113	OLC	C9-C10	4.20	1.55	1.31
5	A	1109	OLC	C9-C10	4.17	1.55	1.31
5	A	1110	OLC	C9-C10	4.17	1.55	1.31
5	A	1108	OLC	C9-C10	4.15	1.55	1.31
5	A	1112	OLC	C9-C10	4.12	1.55	1.31
5	A	1111	OLC	C9-C10	4.11	1.55	1.31
4	A	1105	Y01	CAS-CBF	4.07	1.60	1.53
4	A	1103	Y01	CAI-CAZ	4.03	1.41	1.33
5	A	1106	OLC	C9-C10	4.01	1.54	1.31
5	A	1107	OLC	C9-C10	3.97	1.54	1.31
4	A	1104	Y01	CAI-CAZ	3.97	1.41	1.33
4	A	1105	Y01	CAI-CAZ	3.87	1.41	1.33
4	A	1103	Y01	CAS-CBF	3.72	1.59	1.53
4	A	1105	Y01	CBH-CAZ	-3.69	1.45	1.52
4	A	1104	Y01	CBH-CAZ	-3.60	1.46	1.52
4	A	1103	Y01	CBH-CAZ	-3.46	1.46	1.52
2	A	1101	BUR	CAK-NAS	3.45	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1104	Y01	CBD-CBF	3.16	1.59	1.53
4	A	1104	Y01	CAS-CBF	3.09	1.58	1.53
3	A	1102	CLR	C8-C9	3.01	1.59	1.53
4	A	1103	Y01	CBD-CBF	2.91	1.59	1.53
3	A	1102	CLR	C13-C17	2.89	1.60	1.55
3	A	1102	CLR	C13-C14	2.85	1.60	1.55
2	A	1101	BUR	OAW-CBF	2.77	1.46	1.31
3	A	1102	CLR	C10-C9	2.70	1.60	1.56
3	A	1102	CLR	C20-C17	2.69	1.59	1.54
4	A	1105	Y01	CBD-CBF	2.62	1.58	1.53
3	A	1102	CLR	C19-C10	2.58	1.58	1.54
2	A	1101	BUR	CAY-NAT	-2.55	1.36	1.41
3	A	1102	CLR	C11-C9	2.53	1.57	1.53
4	A	1104	Y01	CBH-CBF	2.50	1.60	1.56
2	A	1101	BUR	CBA-NAU	-2.49	1.36	1.41
3	A	1102	CLR	C1-C10	2.46	1.58	1.54
4	A	1105	Y01	CBH-CBF	2.42	1.59	1.56
4	A	1105	Y01	CBI-CBE	2.36	1.59	1.55
2	A	1101	BUR	FAG-CBF	2.32	1.42	1.32
4	A	1104	Y01	CBD-CBG	2.24	1.57	1.53
3	A	1102	CLR	C18-C13	2.23	1.58	1.54
4	A	1103	Y01	CAU-CAS	2.14	1.57	1.53
4	A	1104	Y01	CAU-CBI	2.14	1.57	1.54
4	A	1103	Y01	CAE-CBI	2.14	1.57	1.54
4	A	1103	Y01	CBB-CBE	2.12	1.58	1.54
4	A	1105	Y01	CAU-CAS	2.06	1.57	1.53
3	A	1102	CLR	C4-C3	2.04	1.55	1.52
3	A	1102	CLR	C2-C3	2.04	1.56	1.51
4	A	1103	Y01	CBI-CBE	2.03	1.58	1.55

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1104	Y01	CAV-CAZ-CBH	4.61	122.32	116.42
4	A	1105	Y01	CAV-CAZ-CAI	-4.40	114.61	120.57
4	A	1105	Y01	CAV-CAZ-CBH	4.24	121.85	116.42
4	A	1103	Y01	CAV-CAZ-CAI	-4.20	114.88	120.57
4	A	1104	Y01	CAV-CAZ-CAI	-4.14	114.96	120.57
4	A	1103	Y01	CAV-CAZ-CBH	3.91	121.43	116.42
4	A	1105	Y01	CAP-CAQ-CBG	-3.26	98.77	105.14
2	A	1101	BUR	OAV-CBC-NAS	3.04	123.53	119.47
4	A	1105	Y01	CBG-CBI-CBE	-2.99	96.67	100.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1105	Y01	CAC-CBB-CAO	-2.92	105.82	110.34
3	A	1102	CLR	C11-C9-C8	2.80	115.69	111.78
4	A	1104	Y01	CBG-CBI-CBE	-2.77	96.92	100.10
4	A	1105	Y01	CAU-CBI-CBE	-2.76	112.54	116.60
3	A	1102	CLR	C11-C9-C10	2.75	116.48	113.08
4	A	1103	Y01	CBG-CBI-CBE	-2.73	96.97	100.10
2	A	1101	BUR	CAJ-CAK-NAS	-2.71	119.13	123.42
2	A	1101	BUR	CBB-OAV-CBC	2.59	121.61	117.86
3	A	1102	CLR	C4-C5-C6	-2.36	117.37	120.57
3	A	1102	CLR	C21-C20-C22	-2.31	106.77	110.34
3	A	1102	CLR	C13-C17-C20	2.24	122.95	119.50
4	A	1104	Y01	CAU-CBI-CBE	-2.23	113.32	116.60
4	A	1105	Y01	CAD-CBH-CAZ	2.21	111.76	108.38
2	A	1101	BUR	CBE-CBD-CBB	2.19	125.07	122.65
4	A	1105	Y01	CAR-CBC-CAV	-2.18	107.94	110.97
4	A	1103	Y01	OAF-CAX-CAL	-2.18	116.19	123.09
3	A	1102	CLR	C18-C13-C14	2.06	115.42	111.68

There are no chirality outliers.

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1106	OLC	C21-C22-C24-O25
5	A	1108	OLC	C21-C22-C24-O25
5	A	1110	OLC	C21-C22-C24-O25
5	A	1110	OLC	O23-C22-C24-O25
5	A	1112	OLC	C21-C22-C24-O25
5	A	1111	OLC	C2-C1-O20-C21
5	A	1110	OLC	C2-C1-O20-C21
5	A	1111	OLC	O19-C1-O20-C21
4	A	1105	Y01	CAJ-CAO-CBB-CBE
5	A	1113	OLC	C2-C1-O20-C21
5	A	1106	OLC	O19-C1-O20-C21
5	A	1108	OLC	O19-C1-O20-C21
5	A	1110	OLC	O19-C1-O20-C21
5	A	1113	OLC	O19-C1-O20-C21
5	A	1108	OLC	C2-C1-O20-C21
5	A	1109	OLC	C2-C1-O20-C21
4	A	1104	Y01	CAJ-CAO-CBB-CBE
5	A	1106	OLC	C2-C1-O20-C21
5	A	1112	OLC	C2-C1-O20-C21
6	A	1114	1PE	OH6-C15-C25-OH5

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Mol	Chain	Res	Type	Atoms
4	A	1103	Y01	CAX-CAL-CAM-CAY
5	A	1112	OLC	O19-C1-O20-C21
5	A	1113	OLC	O20-C21-C22-O23
6	A	1114	1PE	OH5-C14-C24-OH4
5	A	1107	OLC	C2-C1-O20-C21
4	A	1105	Y01	CAJ-CAO-CBB-CAC
5	A	1109	OLC	O19-C1-O20-C21
4	A	1104	Y01	CAN-CAJ-CAO-CBB
5	A	1111	OLC	C1-C2-C3-C4
4	A	1105	Y01	CAO-CAJ-CAN-CBA
5	A	1107	OLC	O19-C1-O20-C21
5	A	1109	OLC	O20-C21-C22-O23
5	A	1106	OLC	C1-C2-C3-C4
5	A	1112	OLC	C1-C2-C3-C4
6	A	1114	1PE	OH2-C12-C22-OH3
5	A	1109	OLC	O20-C21-C22-C24
5	A	1113	OLC	O20-C21-C22-C24
4	A	1104	Y01	CAJ-CAO-CBB-CAC
4	A	1103	Y01	CAJ-CAO-CBB-CBE
5	A	1106	OLC	C2-C3-C4-C5
5	A	1110	OLC	C2-C3-C4-C5
5	A	1111	OLC	C4-C5-C6-C7
5	A	1106	OLC	C4-C5-C6-C7
5	A	1110	OLC	C5-C6-C7-C8
5	A	1106	OLC	O23-C22-C24-O25
5	A	1107	OLC	C4-C5-C6-C7
5	A	1109	OLC	C12-C13-C14-C15
5	A	1109	OLC	C11-C12-C13-C14
4	A	1105	Y01	CAJ-CAN-CBA-CAB
5	A	1112	OLC	C4-C5-C6-C7
6	A	1114	1PE	OH7-C16-C26-OH6
5	A	1109	OLC	C1-C2-C3-C4
5	A	1108	OLC	C2-C3-C4-C5
5	A	1110	OLC	C14-C15-C16-C17
4	A	1105	Y01	CAJ-CAN-CBA-CAA
5	A	1110	OLC	C4-C5-C6-C7
5	A	1110	OLC	C12-C13-C14-C15
5	A	1111	OLC	C12-C13-C14-C15
5	A	1111	OLC	C10-C11-C12-C13
5	A	1111	OLC	C6-C7-C8-C9
5	A	1112	OLC	C10-C11-C12-C13
5	A	1113	OLC	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
5	A	1108	OLC	C1-C2-C3-C4
5	A	1107	OLC	C10-C11-C12-C13
5	A	1108	OLC	C6-C7-C8-C9
5	A	1112	OLC	C3-C4-C5-C6
5	A	1108	OLC	O23-C22-C24-O25
5	A	1112	OLC	C6-C7-C8-C9
5	A	1107	OLC	C1-C2-C3-C4
5	A	1109	OLC	C6-C7-C8-C9
5	A	1113	OLC	C10-C11-C12-C13
5	A	1106	OLC	C10-C11-C12-C13
5	A	1108	OLC	C13-C14-C15-C16
5	A	1111	OLC	C15-C16-C17-C18
5	A	1109	OLC	C10-C11-C12-C13
5	A	1110	OLC	C6-C7-C8-C9
5	A	1110	OLC	C11-C12-C13-C14
5	A	1112	OLC	O23-C22-C24-O25
5	A	1106	OLC	C5-C6-C7-C8
5	A	1106	OLC	C11-C12-C13-C14
5	A	1109	OLC	C15-C16-C17-C18
4	A	1104	Y01	CAO-CAJ-CAN-CBA
5	A	1110	OLC	C1-C2-C3-C4
5	A	1113	OLC	C3-C4-C5-C6
6	A	1114	1PE	C14-C24-OH4-C13
6	A	1114	1PE	C24-C14-OH5-C25
5	A	1108	OLC	C10-C11-C12-C13
5	A	1111	OLC	C13-C14-C15-C16
5	A	1113	OLC	C13-C14-C15-C16
6	A	1114	1PE	C23-C13-OH4-C24
5	A	1112	OLC	C11-C12-C13-C14
4	A	1103	Y01	CAJ-CAN-CBA-CAA
4	A	1103	Y01	CAJ-CAN-CBA-CAB
5	A	1113	OLC	C2-C3-C4-C5
4	A	1103	Y01	CAN-CAJ-CAO-CBB
5	A	1111	OLC	O20-C21-C22-C24
5	A	1111	OLC	C11-C12-C13-C14
4	A	1104	Y01	CAO-CBB-CBE-CBI
5	A	1113	OLC	C14-C15-C16-C17
3	A	1102	CLR	C23-C24-C25-C26
4	A	1104	Y01	CAO-CBB-CBE-CAP
4	A	1103	Y01	CAM-CAL-CAX-OAF
4	A	1104	Y01	CAM-CAL-CAX-OAF
5	A	1107	OLC	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
3	A	1102	CLR	C17-C20-C22-C23
4	A	1105	Y01	CAM-CAL-CAX-OAF
4	A	1104	Y01	CAM-CAL-CAX-OAH
5	A	1111	OLC	C5-C6-C7-C8
5	A	1113	OLC	C9-C10-C11-C12
4	A	1103	Y01	CAM-CAL-CAX-OAH
5	A	1112	OLC	C9-C10-C11-C12
4	A	1105	Y01	CAM-CAL-CAX-OAH
5	A	1112	OLC	C7-C8-C9-C10
5	A	1113	OLC	O23-C22-C24-O25
5	A	1106	OLC	C7-C8-C9-C10
5	A	1113	OLC	C15-C16-C17-C18
5	A	1111	OLC	O20-C21-C22-O23
5	A	1108	OLC	C12-C13-C14-C15
3	A	1102	CLR	C23-C24-C25-C27
4	A	1105	Y01	CAX-CAL-CAM-CAY
5	A	1108	OLC	C11-C12-C13-C14
3	A	1102	CLR	C21-C20-C22-C23
4	A	1104	Y01	CAC-CBB-CBE-CBI
5	A	1113	OLC	C11-C12-C13-C14
6	A	1114	1PE	OH4-C13-C23-OH3
5	A	1110	OLC	C9-C10-C11-C12

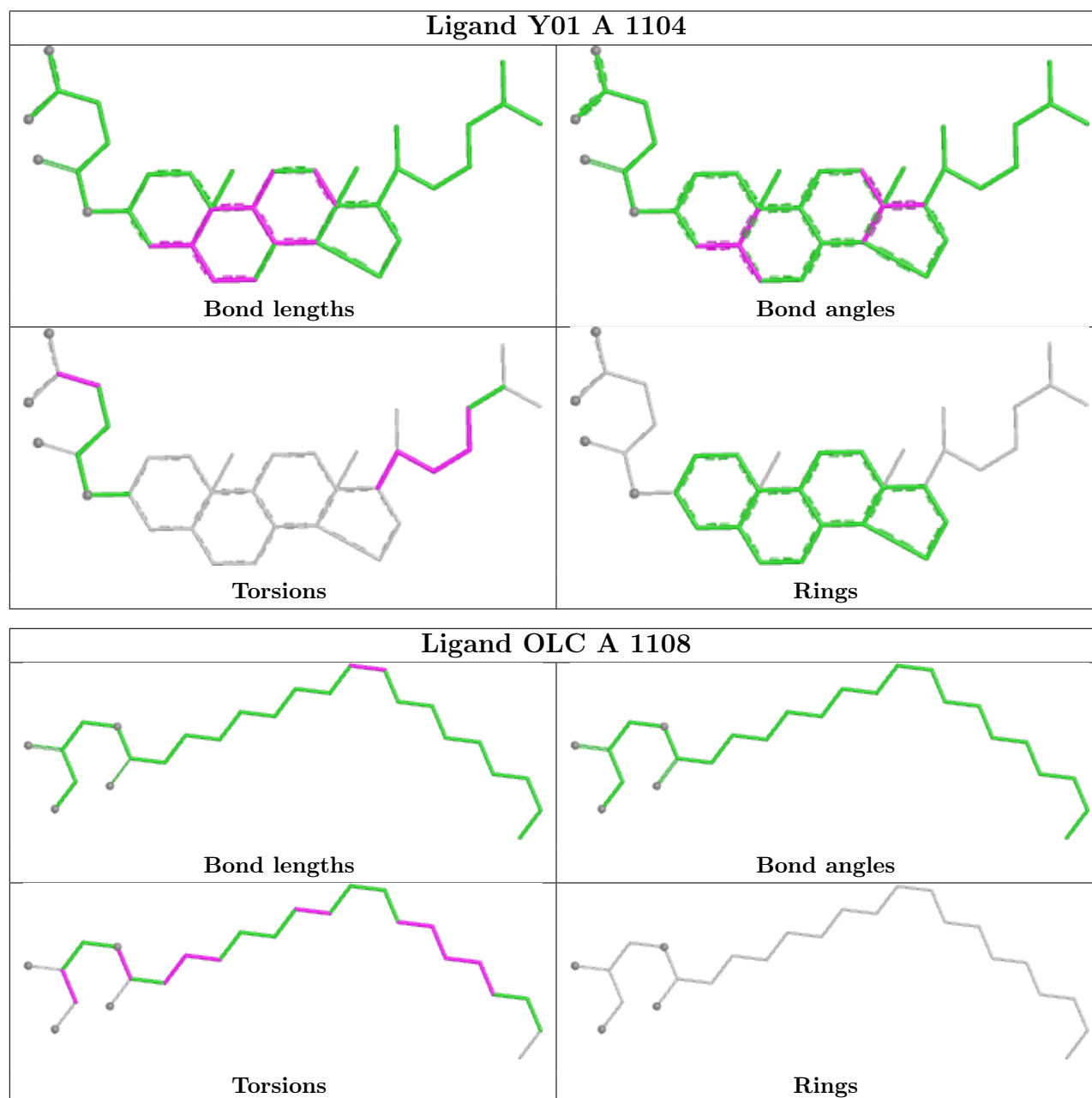
There are no ring outliers.

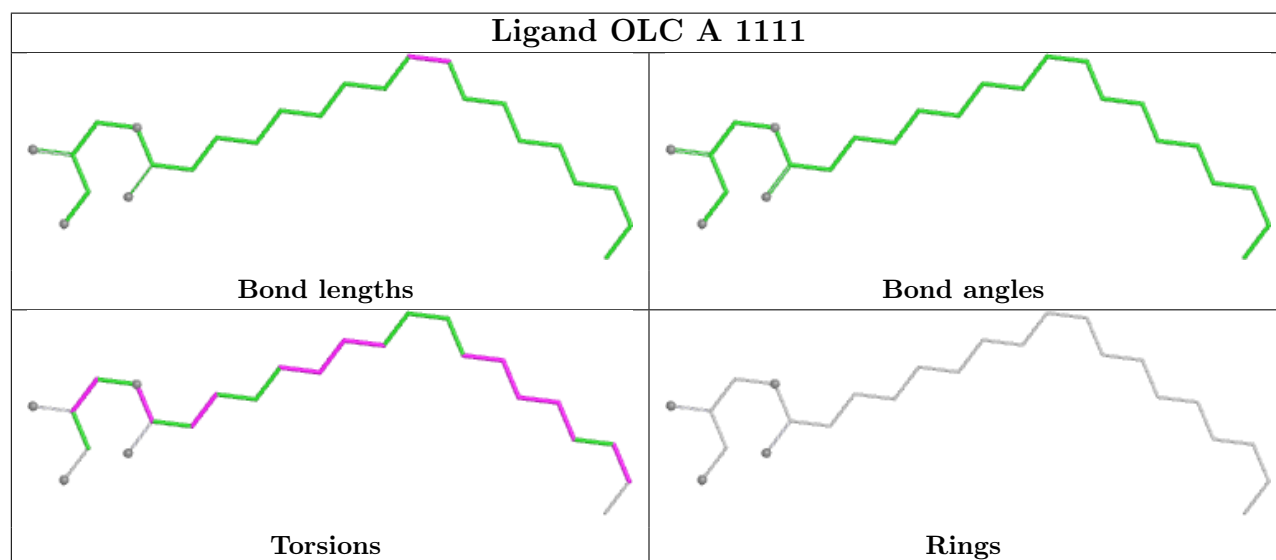
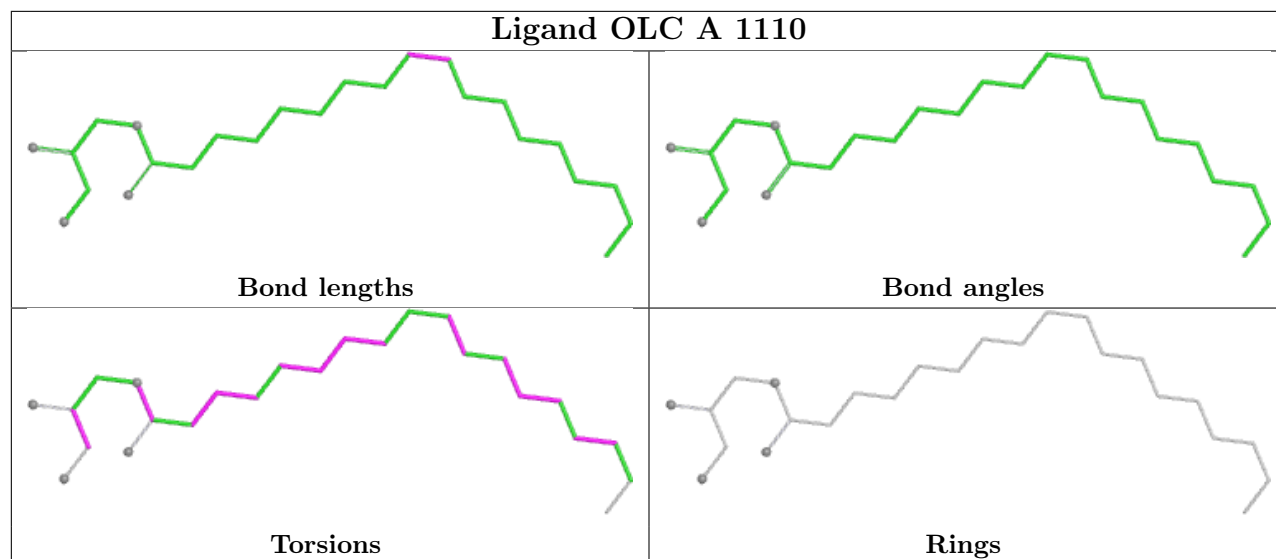
8 monomers are involved in 9 short contacts:

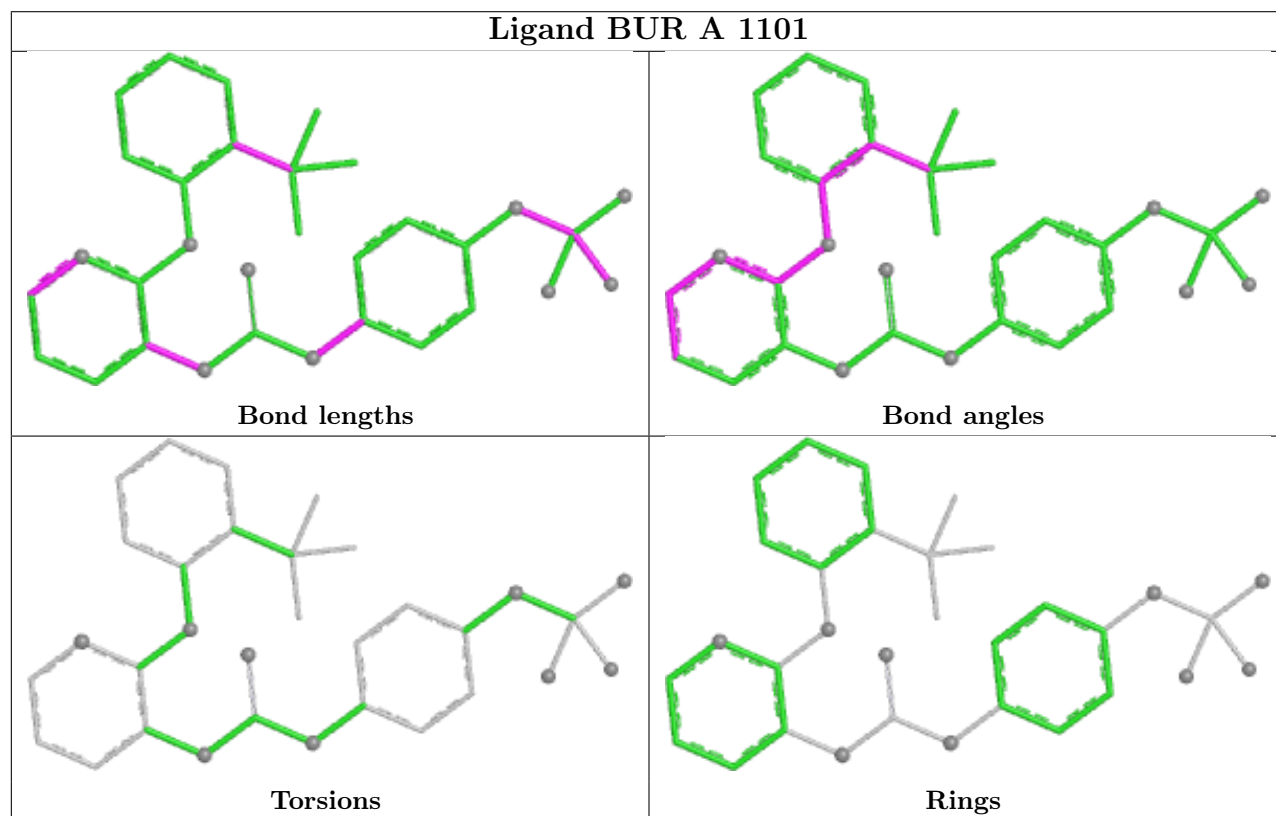
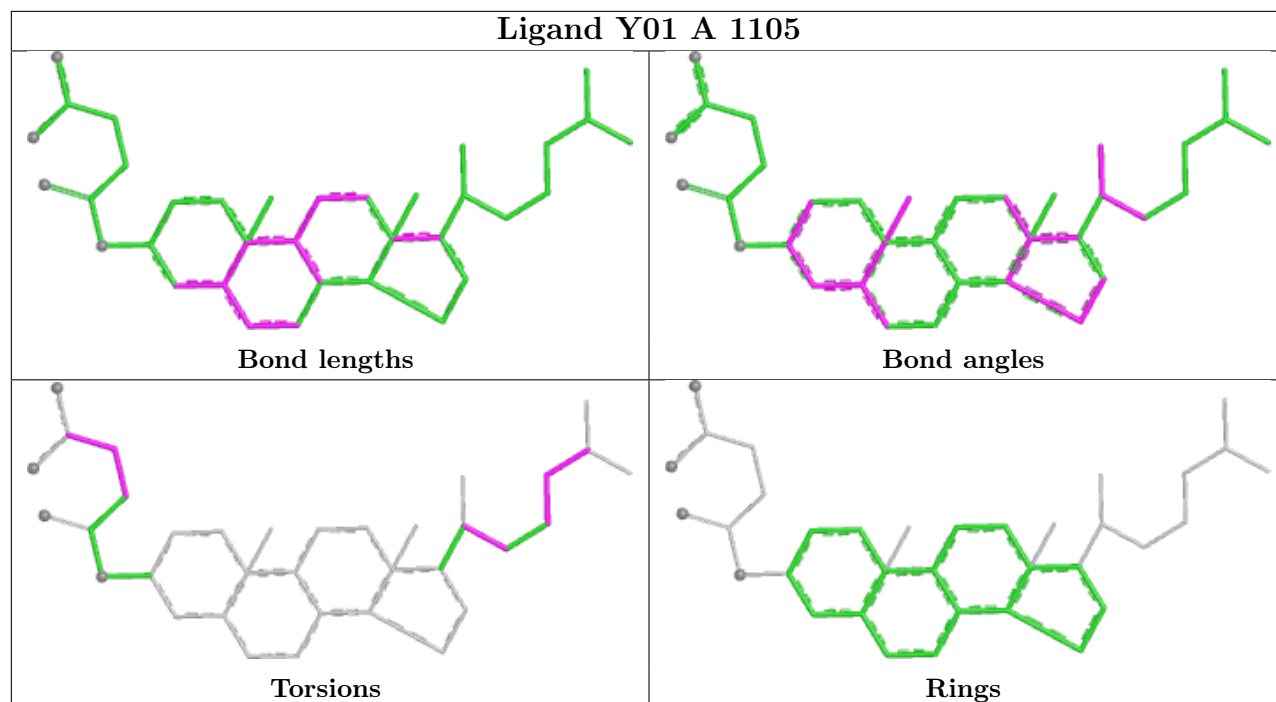
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1104	Y01	1	0
5	A	1108	OLC	1	0
5	A	1110	OLC	3	0
4	A	1105	Y01	1	0
2	A	1101	BUR	1	0
5	A	1107	OLC	2	0
5	A	1113	OLC	1	0
5	A	1112	OLC	1	0

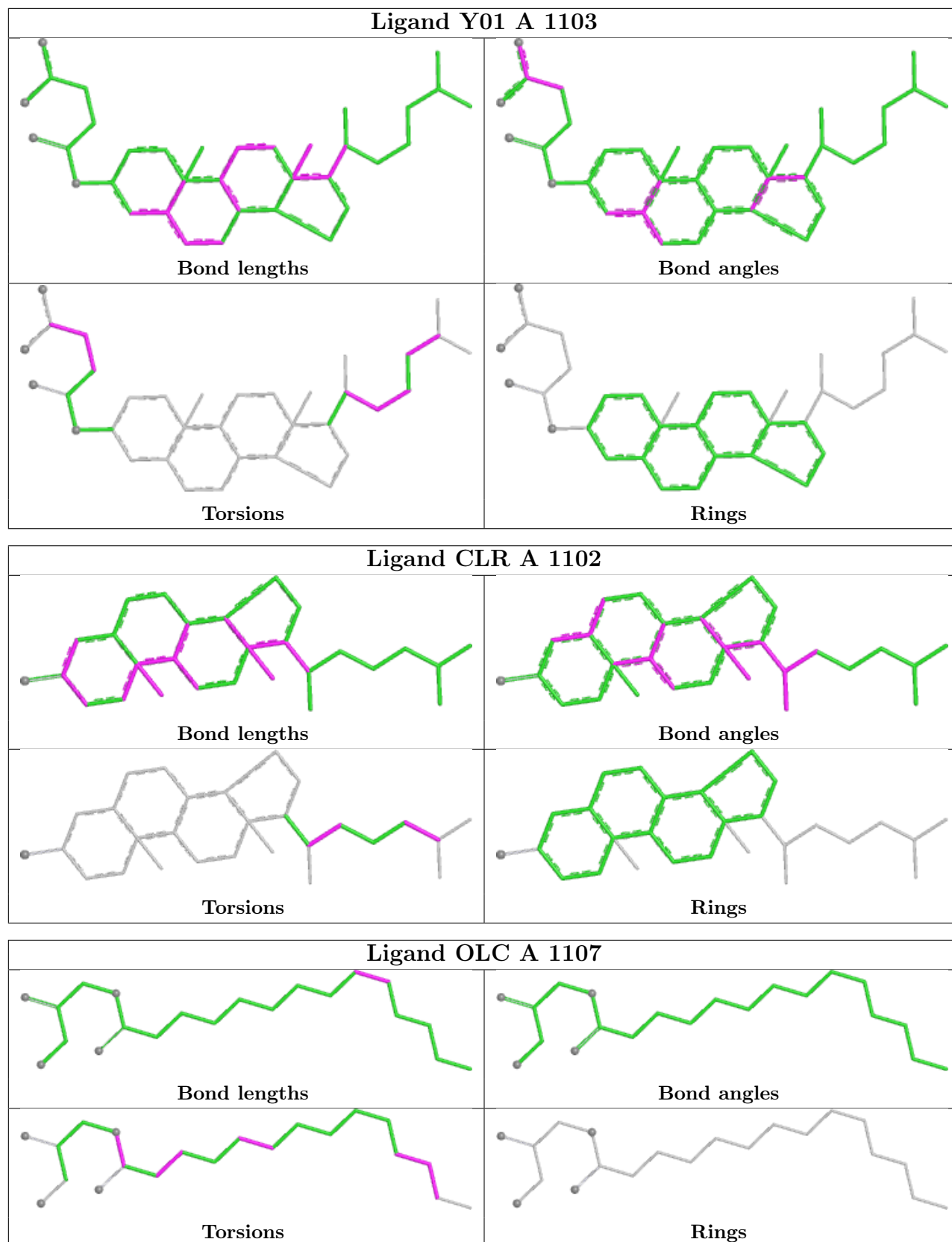
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

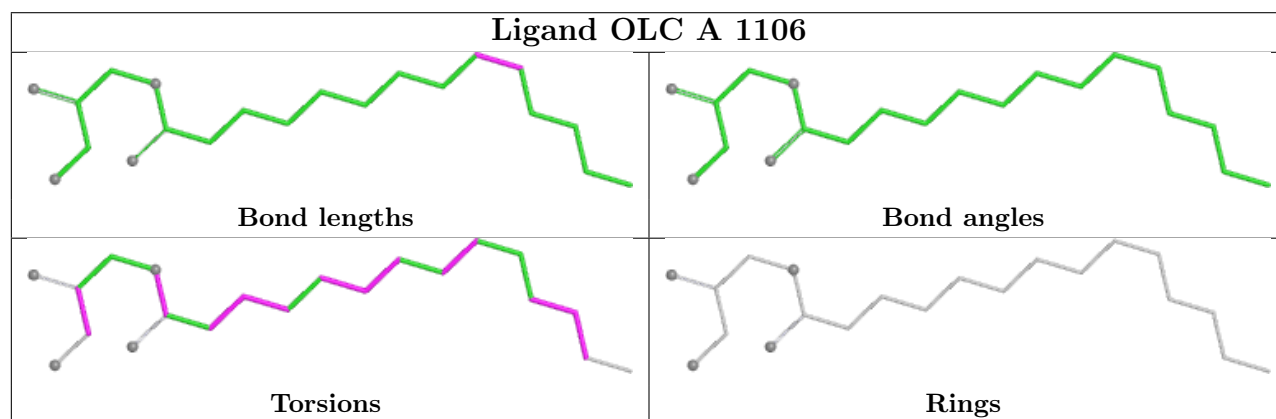
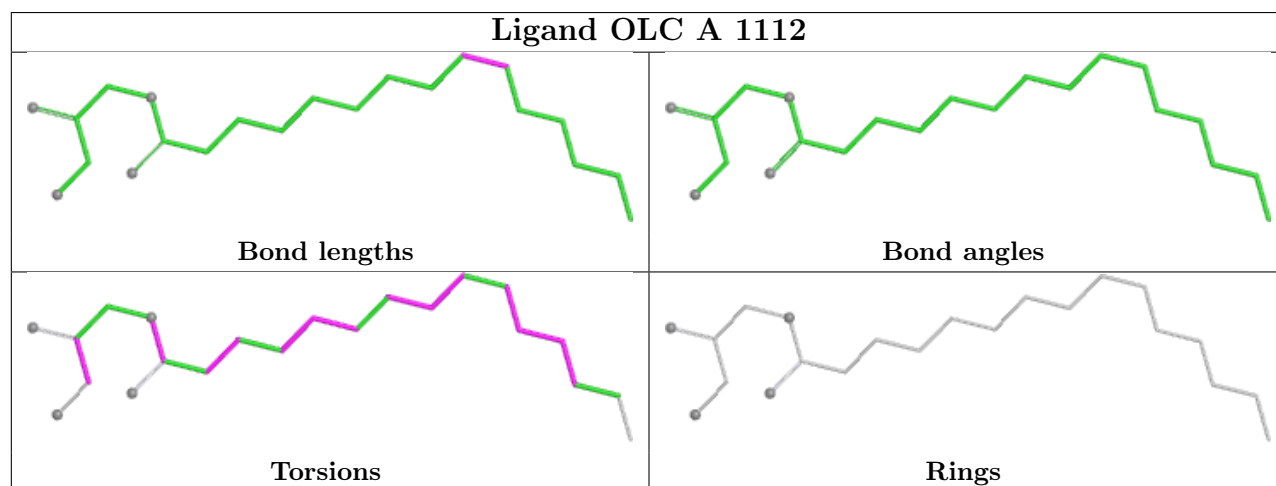
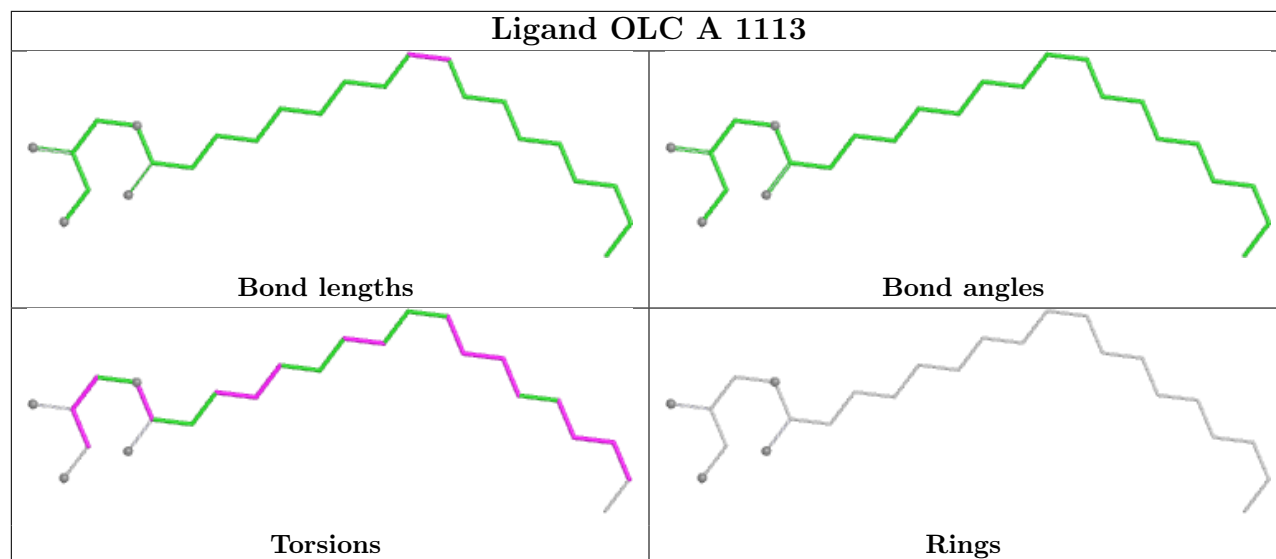
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

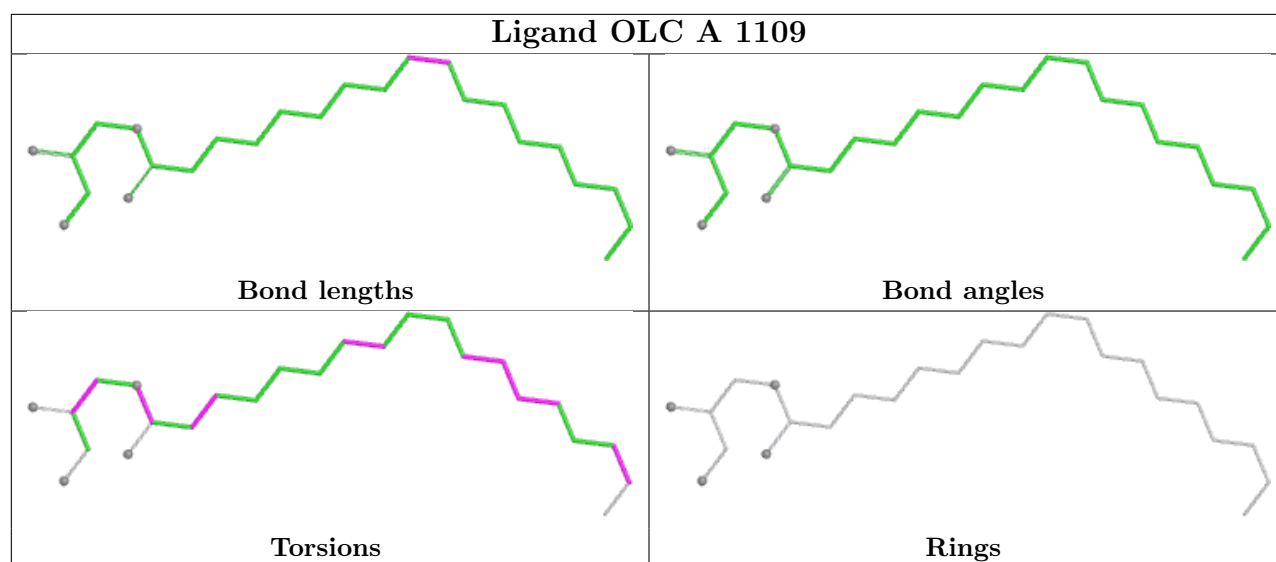












5.7 Other polymers [i](#)

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	340/421 (80%)	0.52	29 (8%) 16 14	28, 50, 149, 200	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1033	ILE	4.1
1	A	1041	LEU	3.6
1	A	1030	PHE	3.3
1	A	1044	VAL	3.2
1	A	1038	VAL	3.0
1	A	1042	CYS	2.9
1	A	43	ALA	2.9
1	A	161	GLY	2.7
1	A	1020	PRO	2.7
1	A	49	PHE	2.5
1	A	50	GLN	2.5
1	A	1052	VAL	2.4
1	A	1024	VAL	2.4
1	A	44	LEU	2.4
1	A	45	THR	2.4
1	A	1028	THR	2.3
1	A	1023	GLY	2.3
1	A	78	PHE	2.3
1	A	1021	ASP	2.3
1	A	47	THR	2.3
1	A	1008	VAL	2.3
1	A	323	LEU	2.1
1	A	1022	ASN	2.0
1	A	52	TYR	2.0
1	A	246	TYR	2.0
1	A	48	GLY	2.0
1	A	1039	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	156	PRO	2.0
1	A	1026	PRO	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](#)

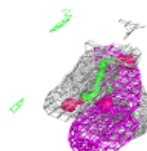
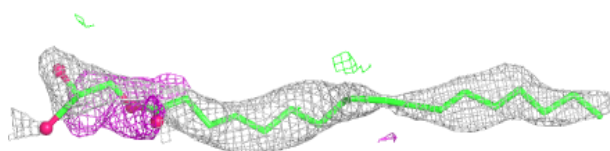
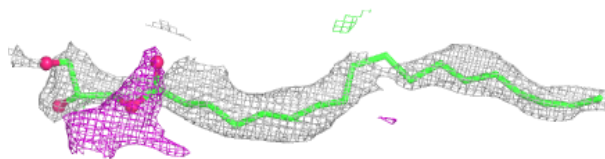
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	OLC	A	1113	25/25	0.74	0.21	63,70,81,82	0
5	OLC	A	1111	25/25	0.75	0.20	71,77,87,91	0
5	OLC	A	1108	25/25	0.79	0.19	78,85,88,88	0
5	OLC	A	1109	25/25	0.79	0.21	66,73,83,83	0
5	OLC	A	1112	22/25	0.80	0.19	43,63,83,84	0
5	OLC	A	1110	25/25	0.81	0.19	60,63,72,72	0
4	Y01	A	1105	35/35	0.81	0.17	65,70,88,89	0
6	1PE	A	1114	16/16	0.82	0.20	84,88,91,92	0
5	OLC	A	1107	21/25	0.83	0.19	57,62,82,85	0
2	BUR	A	1101	32/32	0.86	0.11	44,47,68,70	0
5	OLC	A	1106	21/25	0.87	0.16	50,54,74,75	0
4	Y01	A	1103	35/35	0.92	0.09	35,41,59,62	0
4	Y01	A	1104	35/35	0.92	0.10	41,48,55,58	0
3	CLR	A	1102	28/28	0.92	0.10	32,39,52,53	0
7	ZN	A	1115	1/1	0.97	0.05	87,87,87,87	0

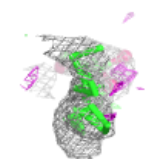
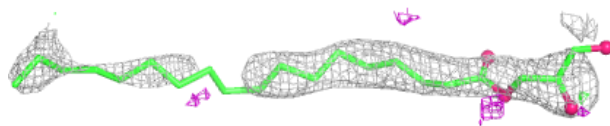
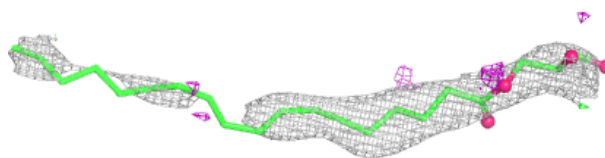
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 1113:

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

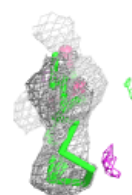
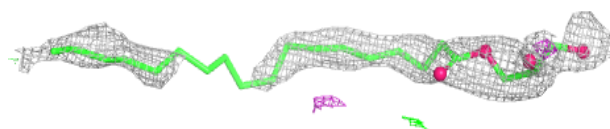
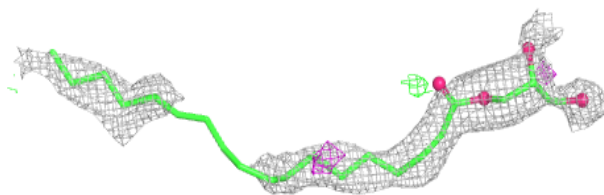
**Electron density around OLC A 1111:**

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

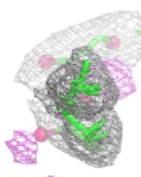
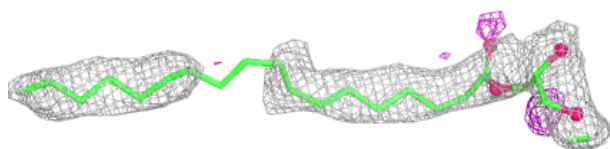
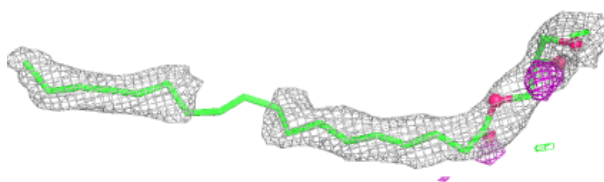


Electron density around OLC A 1108:

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

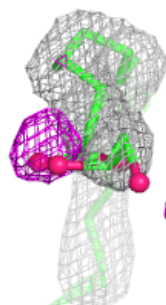
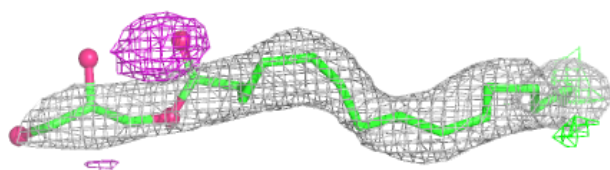
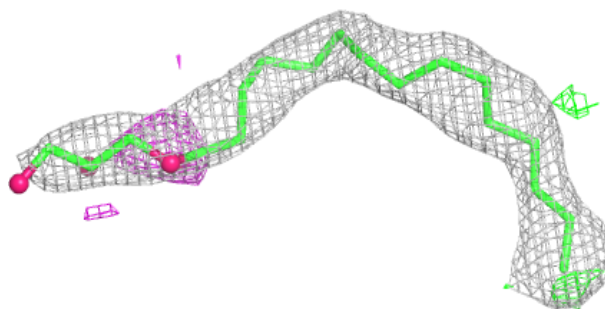
**Electron density around OLC A 1109:**

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

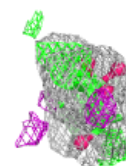
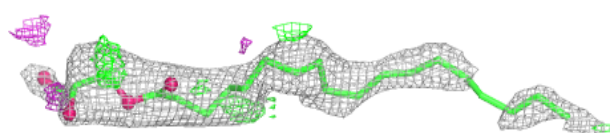
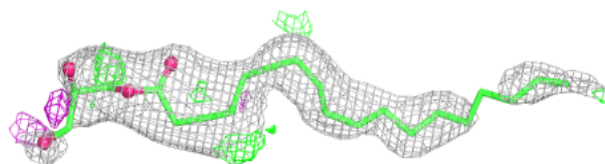


Electron density around OLC A 1112:

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

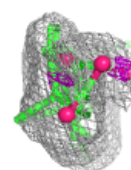
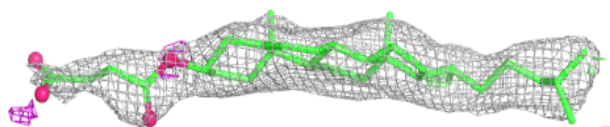
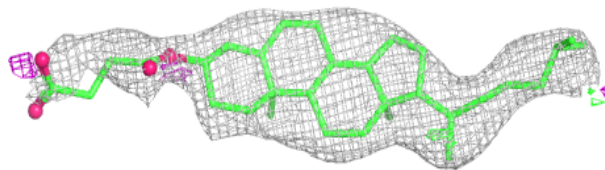
**Electron density around OLC A 1110:**

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

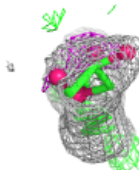
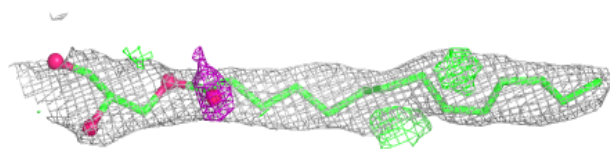
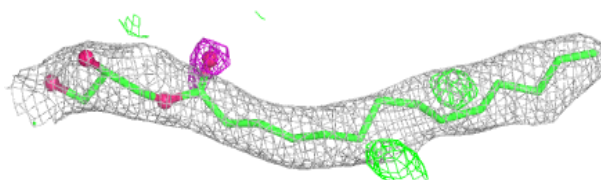


Electron density around Y01 A 1105:

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

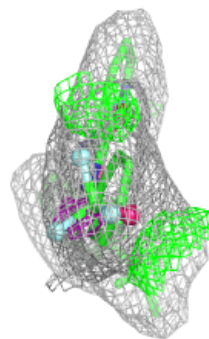
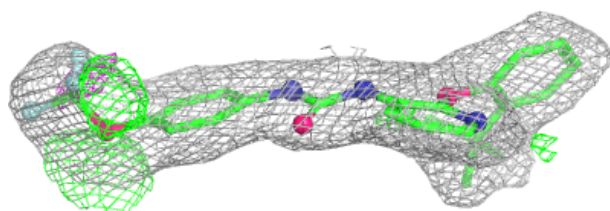
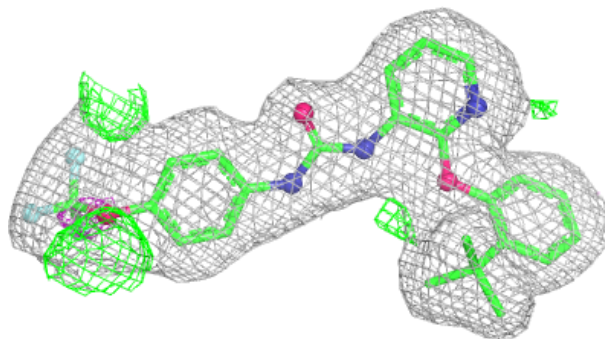
**Electron density around OLC A 1107:**

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

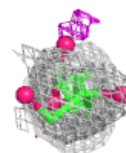
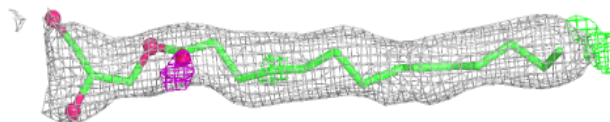
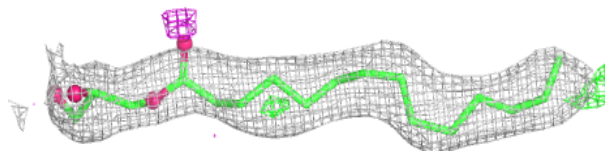


Electron density around BUR A 1101:

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

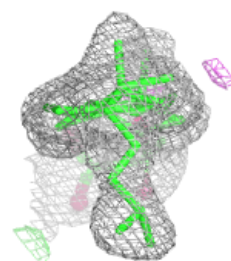
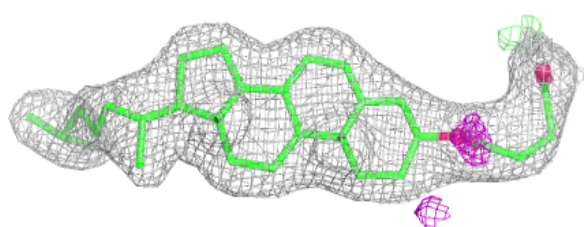
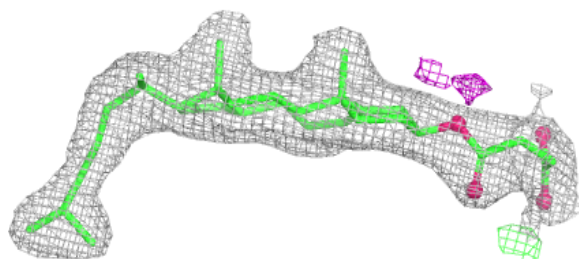
**Electron density around OLC A 1106:**

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

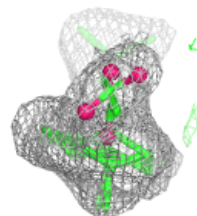
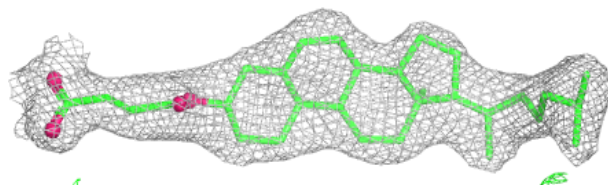
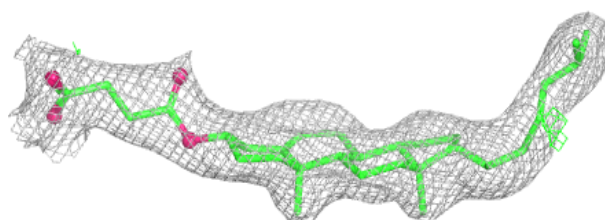


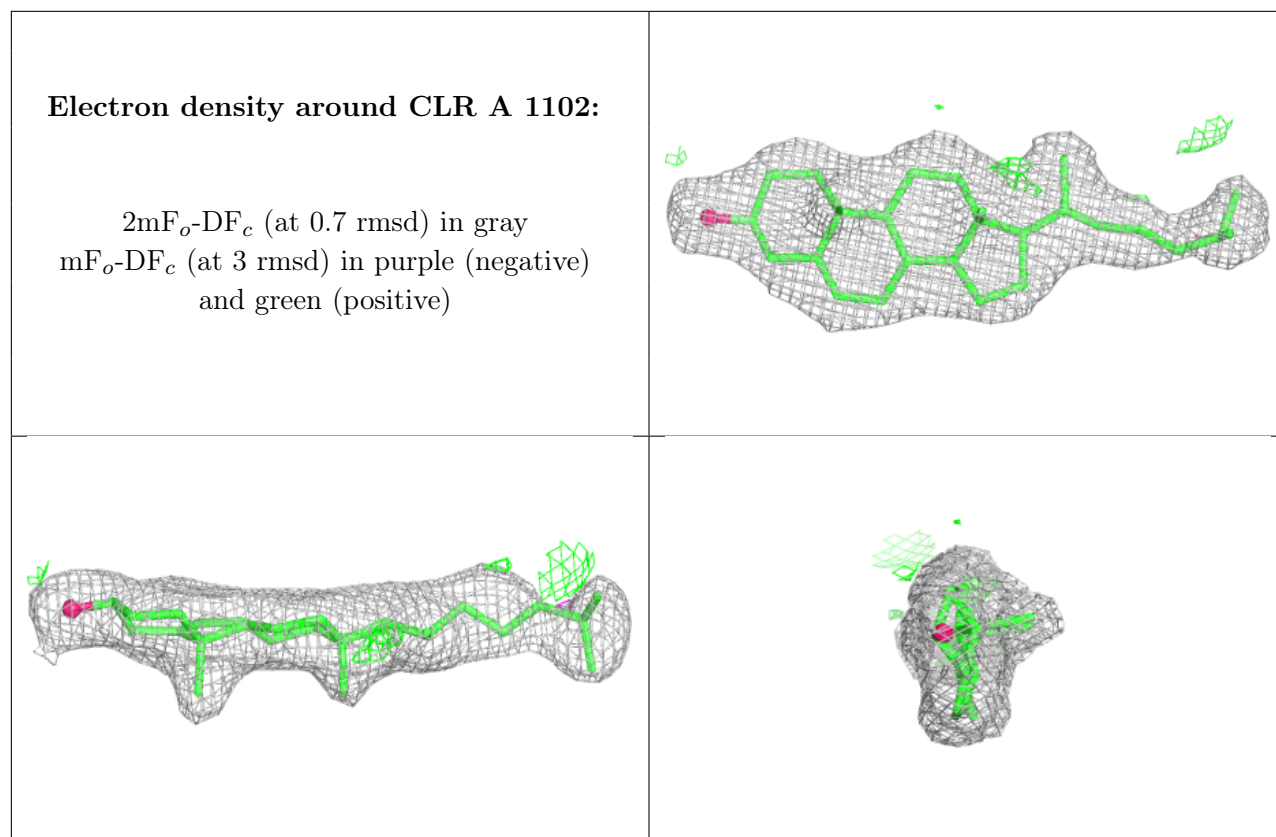
Electron density around Y01 A 1103:

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

**Electron density around Y01 A 1104:**

$2mF_o-DF_c$ (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.