



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:01 AM UTC

PDB ID : 6BD4 / pdb_00006bd4
Title : Crystal structure of human apo-Frizzled4 receptor
Authors : Yang, S.; Wu, Y.; Pu, M.; Chen, Y.; Dong, S.; Guo, Y.; Han, G.Y.; Stevens, R.C.; Zhao, S.; Xu, F.
Deposited on : 2017-10-21
Resolution : 2.40 Å(reported)

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

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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

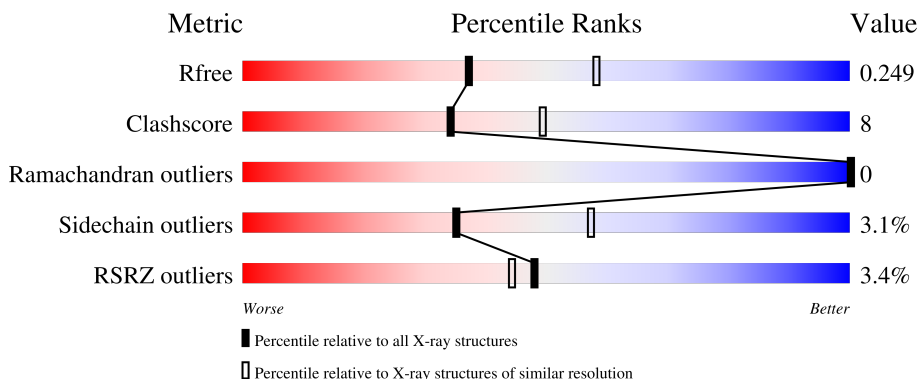
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	420	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3201 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 Frizzled-4/Rubredoxin chimeric protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	1	0
			2996	1972	464	536	24			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	144	ASP	-	expression tag	UNP Q9ULV1
A	145	TYR	-	expression tag	UNP Q9ULV1
A	146	LYS	-	expression tag	UNP Q9ULV1
A	147	ASP	-	expression tag	UNP Q9ULV1
A	148	ASP	-	expression tag	UNP Q9ULV1
A	149	ASP	-	expression tag	UNP Q9ULV1
A	150	ASP	-	expression tag	UNP Q9ULV1
A	151	ALA	-	expression tag	UNP Q9ULV1
A	152	LYS	-	expression tag	UNP Q9ULV1
A	153	LEU	-	expression tag	UNP Q9ULV1
A	154	GLN	-	expression tag	UNP Q9ULV1
A	155	THR	-	expression tag	UNP Q9ULV1
A	156	MET	-	expression tag	UNP Q9ULV1
A	157	HIS	-	expression tag	UNP Q9ULV1
A	158	HIS	-	expression tag	UNP Q9ULV1
A	159	HIS	-	expression tag	UNP Q9ULV1
A	160	HIS	-	expression tag	UNP Q9ULV1
A	161	HIS	-	expression tag	UNP Q9ULV1
A	162	HIS	-	expression tag	UNP Q9ULV1
A	163	HIS	-	expression tag	UNP Q9ULV1
A	164	HIS	-	expression tag	UNP Q9ULV1
A	165	HIS	-	expression tag	UNP Q9ULV1
A	166	HIS	-	expression tag	UNP Q9ULV1
A	167	GLU	-	expression tag	UNP Q9ULV1
A	168	ASN	-	expression tag	UNP Q9ULV1
A	169	LEU	-	expression tag	UNP Q9ULV1
A	170	TYR	-	expression tag	UNP Q9ULV1

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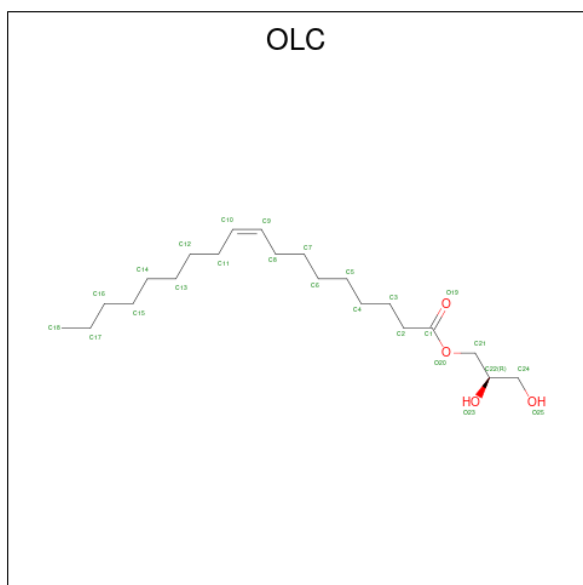
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Chain	Residue	Modelled	Actual	Comment	Reference
A	171	PHE	-	expression tag	UNP Q9ULV1
A	172	GLN	-	expression tag	UNP Q9ULV1
A	173	GLY	-	expression tag	UNP Q9ULV1
A	174	GLY	-	expression tag	UNP Q9ULV1
A	175	THR	-	expression tag	UNP Q9ULV1
A	176	LEU	-	expression tag	UNP Q9ULV1
A	177	GLU	-	expression tag	UNP Q9ULV1
A	309	LEU	MET	engineered mutation	UNP Q9ULV1
A	450	ILE	CYS	engineered mutation	UNP Q9ULV1
A	507	PHE	CYS	engineered mutation	UNP Q9ULV1
A	508	TYR	SER	engineered mutation	UNP Q9ULV1

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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



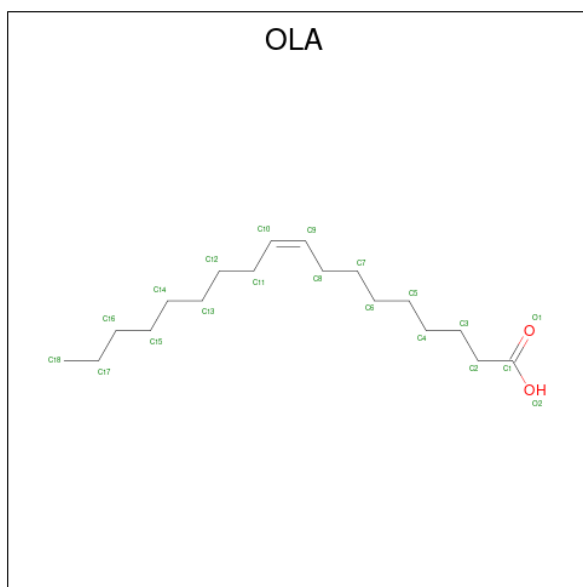
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 8 4	0	0
3	A	1	Total C O 25 21 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			19	15	4		
3	A	1	Total	C	O	0	0
			16	12	4		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			16	14	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			14	12	2		
4	A	1	Total	C	O	0	0
			20	18	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

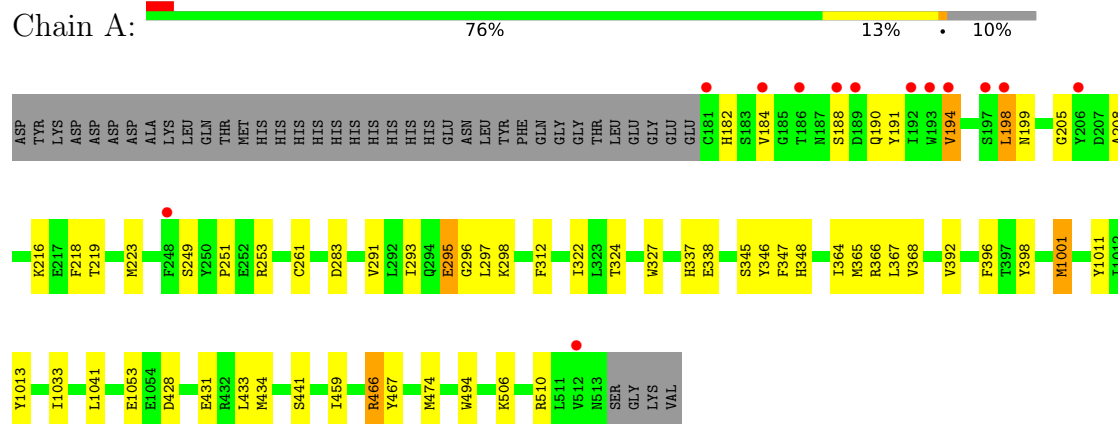
- Molecule 6 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	X	0	0
			4	4		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	23	Total	O	0	0
			23	23		

- Molecule 1: Frizzled-4/Rubredoxin chimeric protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	61.67Å 154.69Å 114.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 30.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-2.40) 99.6 (30.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.210 , 0.233 0.218 , 0.249	Depositor DCC
R_{free} test set	1344 reflections (6.18%)	wwPDB-VP
Wilson B-factor (Å ²)	71.8	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.1	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	0.96	EDS
Total number of atoms	3201	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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, OLA, SO4, UNX, ZN

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	0.13	0/3081	0.32	0/4200

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2996	0	2943	47	0
2	A	1	0	0	0	0
3	A	72	0	99	6	0
4	A	90	0	139	9	0
5	A	15	0	0	2	0
6	A	4	0	0	0	0
7	A	23	0	0	0	0
All	All	3201	0	3181	48	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 8.

All (48) 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:346:TYR:CD1	4:A:1107:OLA:H41	2.04	0.91
1:A:346:TYR:CD1	4:A:1107:OLA:C4	2.69	0.76
1:A:346:TYR:CE1	4:A:1107:OLA:H41	2.28	0.68
1:A:295:GLU:HB2	1:A:298:LYS:HD3	1.82	0.62
1:A:364:ILE:HG21	4:A:1110:OLA:H21	1.81	0.61
1:A:466:ARG:HG3	1:A:467:TYR:CD2	2.37	0.59
1:A:474:MET:HE2	3:A:1103:OLC:H3A	1.87	0.56
1:A:194:VAL:HG21	1:A:291:VAL:HG12	1.89	0.54
1:A:466:ARG:CG	1:A:467:TYR:CE2	2.93	0.52
1:A:396:PHE:HE1	4:A:1108:OLA:H182	1.75	0.51
1:A:346:TYR:CZ	4:A:1107:OLA:O1	2.65	0.50
1:A:431:GLU:HG2	1:A:433:LEU:H	1.77	0.49
1:A:466:ARG:CG	1:A:467:TYR:CD2	2.96	0.49
1:A:494:TRP:HE1	3:A:1102:OLC:H24A	1.78	0.49
1:A:466:ARG:NH1	5:A:1112:SO4:O2	2.45	0.49
1:A:297:LEU:HD12	1:A:366:ARG:HG2	1.94	0.49
1:A:188:SER:C	1:A:190:GLN:H	2.20	0.48
1:A:346:TYR:CD1	4:A:1107:OLA:H42	2.49	0.48
1:A:324:THR:HG22	1:A:441:SER:HB3	1.95	0.48
1:A:205:GLY:O	1:A:216:LYS:NZ	2.41	0.47
1:A:198:LEU:H	1:A:198:LEU:HD22	1.81	0.46
1:A:398:TYR:HE1	4:A:1106:OLA:H142	1.80	0.46
1:A:1011:TYR:HB2	1:A:1041:LEU:HD12	1.96	0.46
1:A:338:GLU:H	1:A:338:GLU:CD	2.25	0.45
1:A:191:TYR:HE1	1:A:208:ALA:HA	1.82	0.45
1:A:466:ARG:HG2	1:A:467:TYR:CE2	2.51	0.45
1:A:249:SER:O	1:A:253:ARG:HG3	2.17	0.44
1:A:346:TYR:CG	4:A:1107:OLA:H42	2.53	0.44
1:A:327:TRP:CD1	1:A:434:MET:HE3	2.54	0.43
1:A:1001:MET:HE2	1:A:1001:MET:HB2	1.72	0.43
1:A:283:ASP:HB2	1:A:293:ILE:HG12	2.00	0.43
1:A:365:MET:HE2	1:A:367:LEU:HD11	2.01	0.43
1:A:322:ILE:HD13	1:A:347:PHE:HB3	2.01	0.43
1:A:327:TRP:HA	1:A:434:MET:HE1	2.00	0.43
1:A:466:ARG:HD2	1:A:467:TYR:CZ	2.53	0.42
1:A:474:MET:CE	3:A:1103:OLC:H3A	2.48	0.42
3:A:1104:OLC:H8	3:A:1104:OLC:H11	1.66	0.42
1:A:261:CYS:HB3	1:A:312:PHE:O	2.20	0.41
1:A:506:LYS:O	1:A:510:ARG:HG2	2.20	0.41
1:A:218:PHE:CZ	3:A:1103:OLC:H4	2.55	0.41
1:A:296:GLY:HA3	1:A:368:VAL:O	2.20	0.41
1:A:345:SER:HB2	5:A:1113:SO4:O3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:VAL:HG21	1:A:459:ILE:HD11	2.02	0.41
1:A:348:HIS:CE1	3:A:1104:OLC:H2A	2.56	0.41
1:A:219:THR:HG22	1:A:223:MET:HE2	2.03	0.40
1:A:191:TYR:CE1	1:A:208:ALA:HA	2.56	0.40
1:A:251:PRO:HG2	1:A:337:HIS:CE1	2.57	0.40
1:A:1013:TYR:CZ	1:A:1033:ILE:HD11	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	378/420 (90%)	360 (95%)	18 (5%)	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	321/363 (88%)	311 (97%)	10 (3%)	35	57

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	HIS
1	A	184	VAL
1	A	194	VAL
1	A	198	LEU
1	A	199	ASN
1	A	295	GLU
1	A	1001	MET
1	A	1053	GLU
1	A	428	ASP
1	A	466	ARG

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

Mol	Chain	Res	Type
1	A	182	HIS
1	A	381	ASN
1	A	461	ASN

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 17 ligands modelled in this entry, 1 is monoatomic and 4 are unknown - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	OLC	A	1105	-	15,15,24	1.00	2 (13%)	16,16,25	1.04	1 (6%)
4	OLA	A	1107	-	15,15,19	0.55	0	15,15,19	0.89	0
5	SO4	A	1113	-	4,4,4	0.35	0	6,6,6	0.97	1 (16%)
4	OLA	A	1110	-	19,19,19	0.81	1 (5%)	19,19,19	0.91	1 (5%)
4	OLA	A	1108	-	19,19,19	0.83	1 (5%)	19,19,19	0.94	1 (5%)
5	SO4	A	1111	-	4,4,4	0.24	0	6,6,6	0.06	0
4	OLA	A	1106	-	19,19,19	0.66	1 (5%)	19,19,19	1.10	3 (15%)
5	SO4	A	1112	-	4,4,4	0.43	0	6,6,6	0.08	0
3	OLC	A	1104	-	18,18,24	0.93	2 (11%)	19,19,25	1.08	1 (5%)
4	OLA	A	1109	-	13,13,19	1.01	1 (7%)	13,13,19	1.16	1 (7%)
3	OLC	A	1103	-	24,24,24	0.90	1 (4%)	25,25,25	0.91	2 (8%)
3	OLC	A	1102	-	11,11,24	1.15	2 (18%)	12,12,25	1.12	1 (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
3	OLC	A	1105	-	-	2/15/15/24	-
4	OLA	A	1107	-	-	11/13/13/17	-
4	OLA	A	1110	-	-	11/17/17/17	-
4	OLA	A	1108	-	-	8/17/17/17	-
4	OLA	A	1106	-	-	9/17/17/17	-
3	OLC	A	1104	-	-	0/18/18/24	-
4	OLA	A	1109	-	-	4/11/11/17	-
3	OLC	A	1103	-	-	6/24/24/24	-
3	OLC	A	1102	-	-	1/11/11/24	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1103	OLC	O20-C1	3.90	1.44	1.33
4	A	1108	OLA	O2-C1	-3.03	1.20	1.30
4	A	1110	OLA	C10-C9	2.80	1.47	1.31
4	A	1109	OLA	C10-C9	2.78	1.47	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1102	OLC	O20-C1	2.46	1.40	1.33
3	A	1104	OLC	O20-C1	2.44	1.40	1.33
3	A	1105	OLC	O20-C1	2.43	1.40	1.33
3	A	1104	OLC	O20-C21	-2.16	1.40	1.45
3	A	1105	OLC	O20-C21	-2.14	1.40	1.45
3	A	1102	OLC	O20-C21	-2.10	1.40	1.45
4	A	1106	OLA	O2-C1	-2.10	1.23	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1103	OLC	O20-C1-C2	3.10	121.28	111.83
3	A	1102	OLC	O20-C1-C2	2.79	120.35	111.83
3	A	1103	OLC	O20-C1-O19	-2.79	116.66	123.63
3	A	1104	OLC	O20-C1-C2	2.70	120.06	111.83
3	A	1105	OLC	O20-C1-C2	2.67	119.97	111.83
4	A	1106	OLA	O2-C1-C2	2.53	121.98	114.00
4	A	1106	OLA	O2-C1-O1	-2.32	117.36	123.33
4	A	1106	OLA	C4-C3-C2	2.19	121.17	113.13
4	A	1108	OLA	O2-C1-C2	2.12	120.71	114.00
4	A	1109	OLA	C3-C2-C1	-2.10	109.04	114.51
4	A	1110	OLA	O2-C1-C2	2.06	120.52	114.00
5	A	1113	SO4	O4-S-O1	2.00	120.03	109.56

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1110	OLA	C1-C2-C3-C4
4	A	1107	OLA	C1-C2-C3-C4
4	A	1109	OLA	C1-C2-C3-C4
4	A	1108	OLA	C6-C7-C8-C9
4	A	1110	OLA	C12-C13-C14-C15
4	A	1106	OLA	C12-C13-C14-C15
4	A	1106	OLA	C14-C15-C16-C17
4	A	1107	OLA	C5-C6-C7-C8
4	A	1107	OLA	C2-C3-C4-C5
4	A	1107	OLA	C3-C4-C5-C6
4	A	1109	OLA	C9-C10-C11-C12
4	A	1110	OLA	C11-C12-C13-C14
4	A	1106	OLA	C11-C12-C13-C14
4	A	1108	OLA	C13-C14-C15-C16

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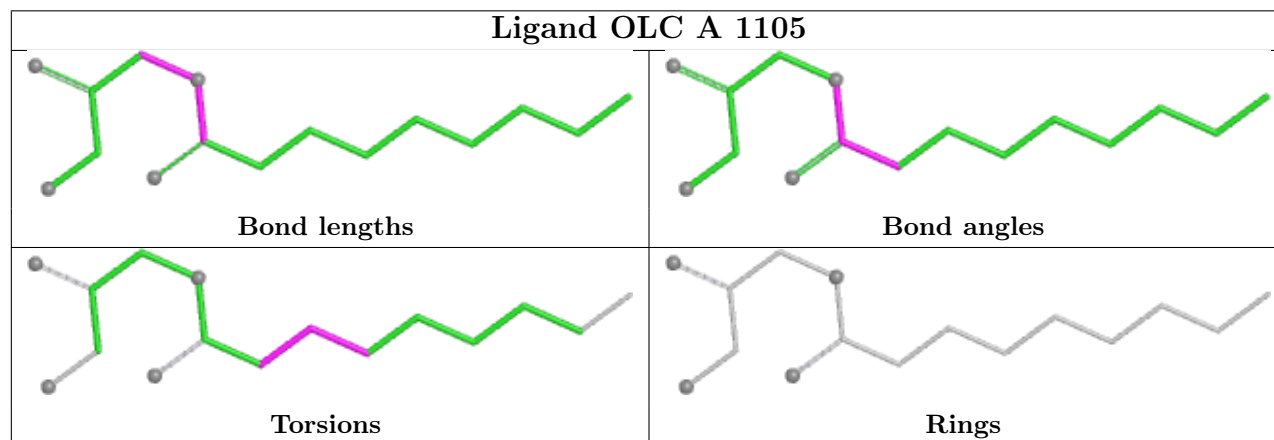
Mol	Chain	Res	Type	Atoms
3	A	1105	OLC	C1-C2-C3-C4
4	A	1108	OLA	C4-C5-C6-C7
4	A	1108	OLA	C14-C15-C16-C17
4	A	1106	OLA	C6-C7-C8-C9
4	A	1107	OLA	C6-C7-C8-C9
4	A	1110	OLA	C11-C10-C9-C8
4	A	1107	OLA	C10-C11-C12-C13
4	A	1110	OLA	C2-C3-C4-C5
4	A	1106	OLA	C3-C4-C5-C6
4	A	1109	OLA	C6-C7-C8-C9
4	A	1109	OLA	C11-C10-C9-C8
3	A	1103	OLC	C15-C16-C17-C18
4	A	1106	OLA	C5-C6-C7-C8
4	A	1110	OLA	C4-C5-C6-C7
3	A	1103	OLC	C6-C7-C8-C9
4	A	1108	OLA	C15-C16-C17-C18
4	A	1106	OLA	C4-C5-C6-C7
4	A	1107	OLA	C4-C5-C6-C7
3	A	1103	OLC	C7-C8-C9-C10
4	A	1107	OLA	C11-C12-C13-C14
4	A	1107	OLA	C7-C8-C9-C10
3	A	1103	OLC	C14-C15-C16-C17
4	A	1110	OLA	O1-C1-C2-C3
4	A	1107	OLA	O2-C1-C2-C3
4	A	1110	OLA	O2-C1-C2-C3
4	A	1107	OLA	O1-C1-C2-C3
4	A	1110	OLA	C13-C14-C15-C16
4	A	1108	OLA	O1-C1-C2-C3
4	A	1108	OLA	O2-C1-C2-C3
3	A	1103	OLC	C13-C14-C15-C16
4	A	1106	OLA	C9-C10-C11-C12
4	A	1108	OLA	C7-C8-C9-C10
4	A	1110	OLA	C9-C10-C11-C12
4	A	1106	OLA	C7-C8-C9-C10
3	A	1103	OLC	O20-C21-C22-O23
3	A	1102	OLC	C2-C3-C4-C5
4	A	1110	OLA	C7-C8-C9-C10
3	A	1105	OLC	C2-C3-C4-C5

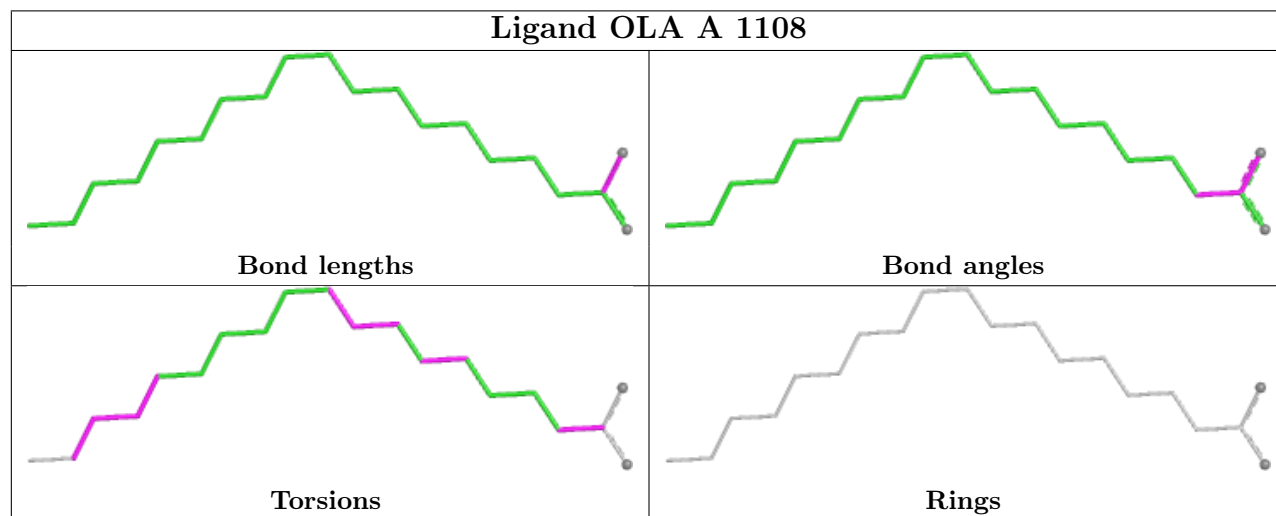
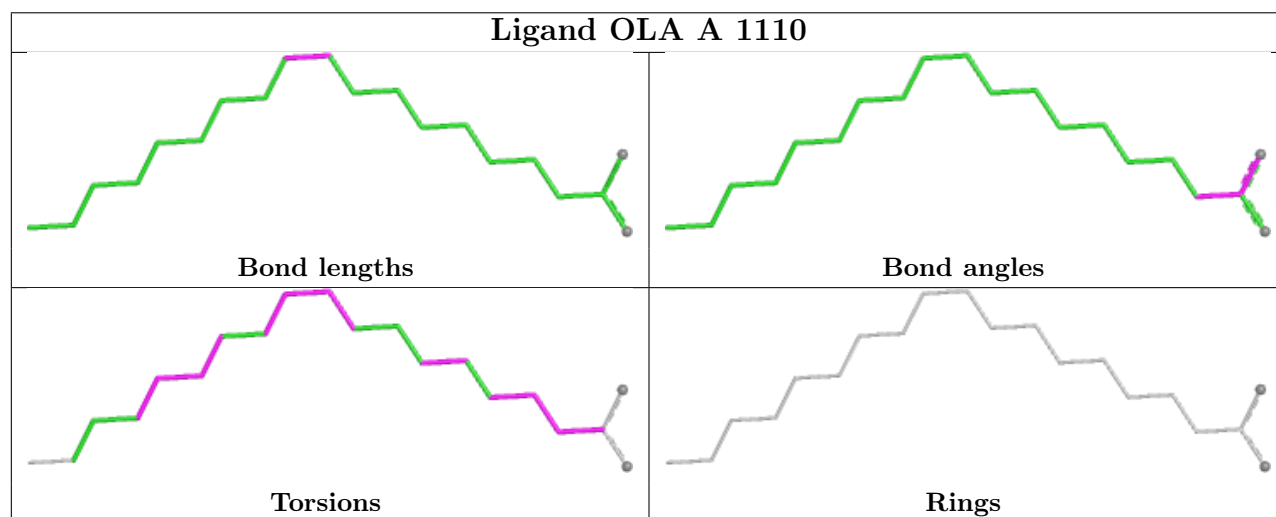
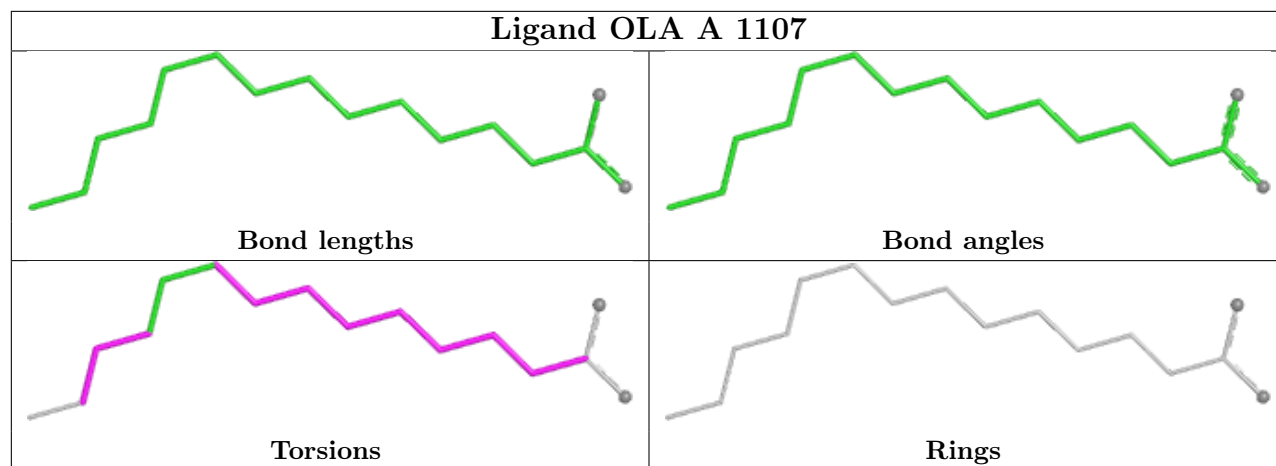
There are no ring outliers.

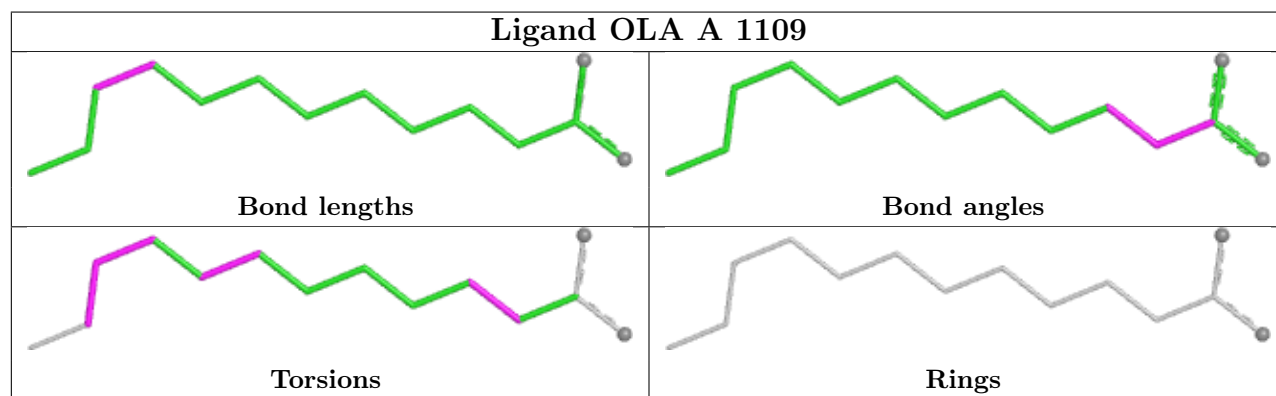
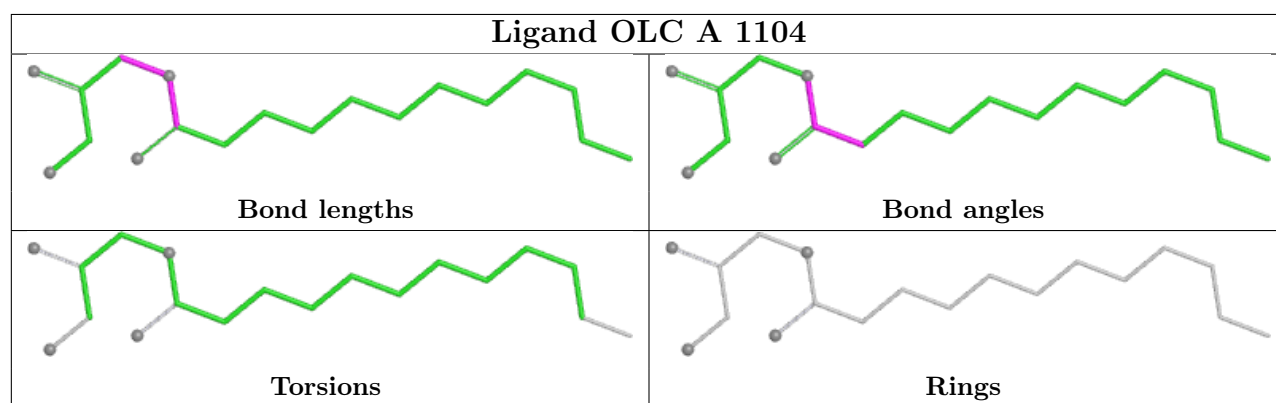
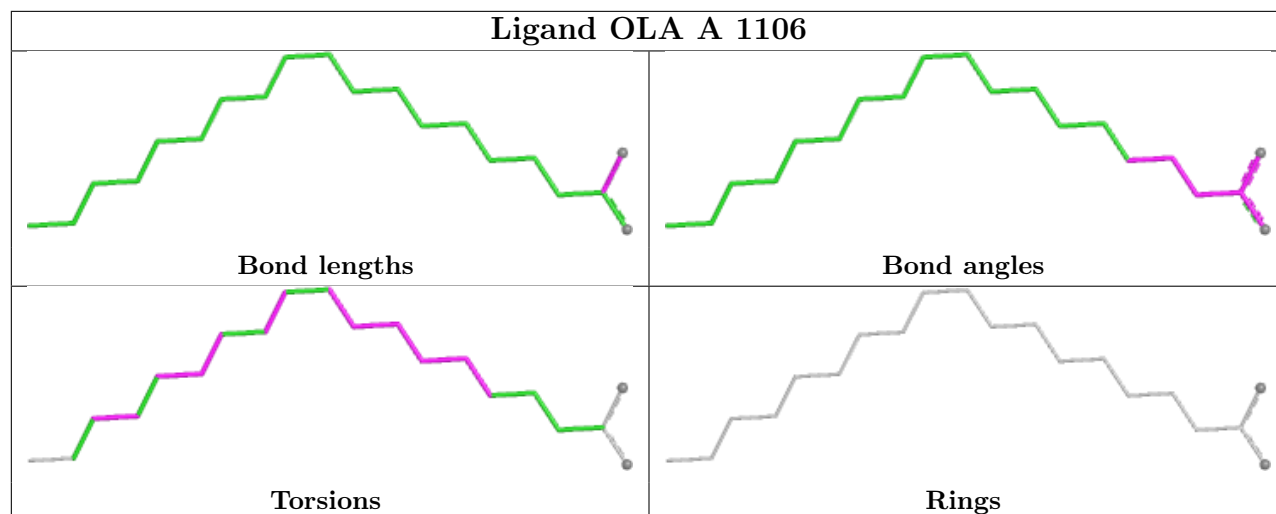
9 monomers are involved in 17 short contacts:

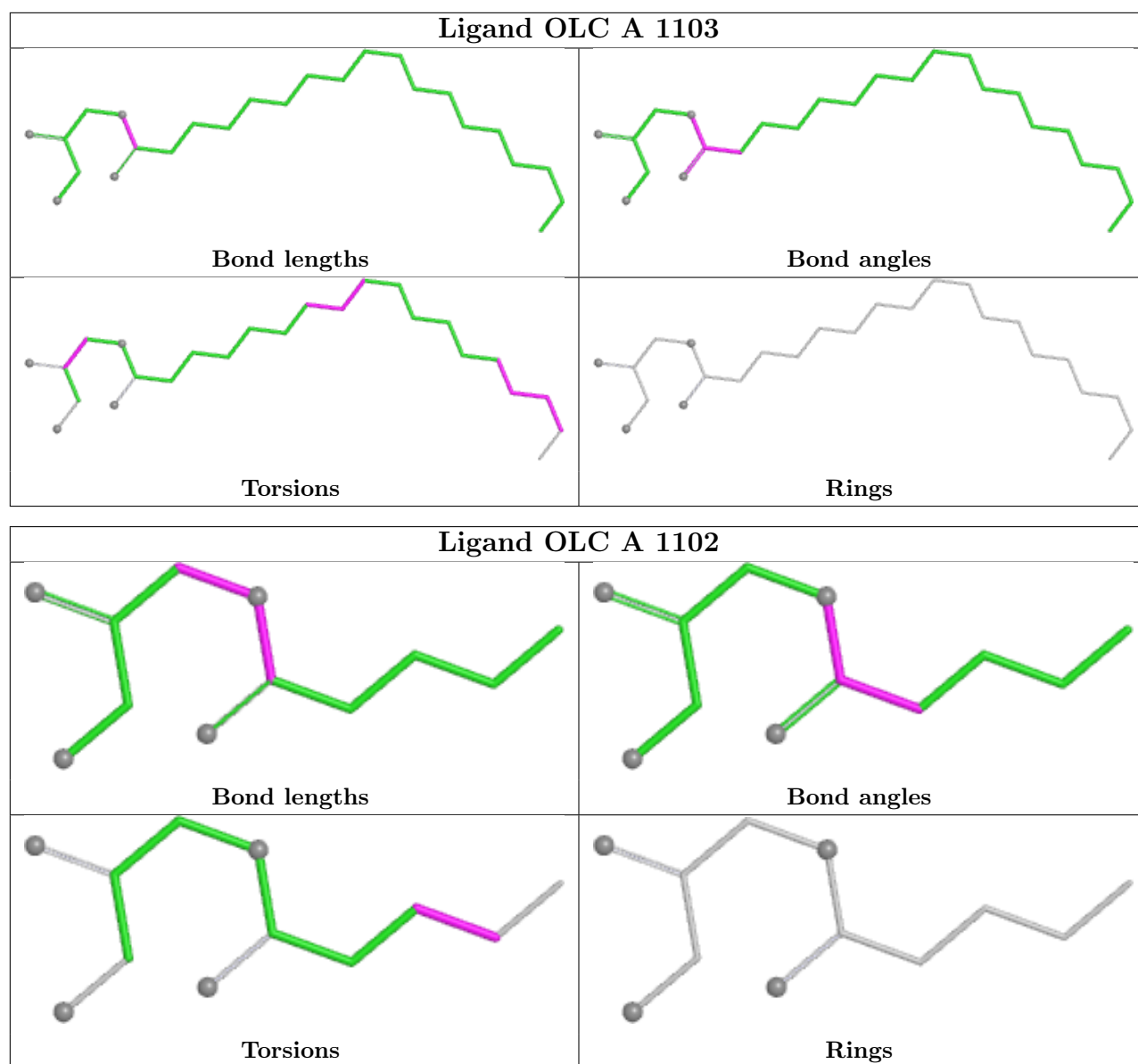
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1107	OLA	6	0
5	A	1113	SO4	1	0
4	A	1110	OLA	1	0
4	A	1108	OLA	1	0
4	A	1106	OLA	1	0
5	A	1112	SO4	1	0
3	A	1104	OLC	2	0
3	A	1103	OLC	3	0
3	A	1102	OLC	1	0

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 [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	379/420 (90%)	0.19	13 (3%)	48 44	62, 87, 143, 176	1 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	192	ILE	4.4
1	A	188	SER	3.5
1	A	206	TYR	3.2
1	A	193	TRP	3.0
1	A	197	SER	2.6
1	A	198	LEU	2.6
1	A	186	THR	2.6
1	A	512	VAL	2.5
1	A	194	VAL	2.4
1	A	181	CYS	2.3
1	A	248	PHE	2.2
1	A	189	ASP	2.2
1	A	184	VAL	2.1

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 ⓘ

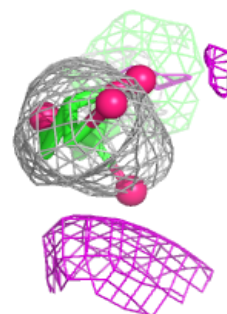
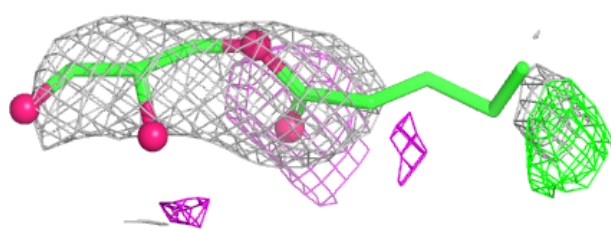
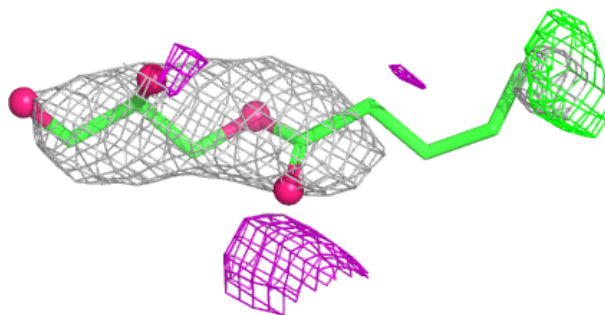
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	A	1112	5/5	0.76	0.11	127,128,134,135	0
3	OLC	A	1102	12/25	0.77	0.24	114,119,125,125	0
4	OLA	A	1106	20/20	0.79	0.22	88,106,121,122	0
4	OLA	A	1107	16/20	0.79	0.18	109,125,147,148	0
3	OLC	A	1103	25/25	0.79	0.16	98,109,140,149	0
5	SO4	A	1113	5/5	0.82	0.14	187,188,190,190	0
6	UNX	A	1114	1/1	0.82	0.29	95,95,95,95	0
3	OLC	A	1105	16/25	0.84	0.14	101,116,138,139	0
3	OLC	A	1104	19/25	0.85	0.22	88,108,139,140	0
4	OLA	A	1110	20/20	0.86	0.17	79,92,114,115	0
6	UNX	A	1115	1/1	0.88	0.24	97,97,97,97	0
6	UNX	A	1117	1/1	0.88	0.30	71,71,71,71	0
6	UNX	A	1116	1/1	0.89	0.25	81,81,81,81	0
4	OLA	A	1109	14/20	0.89	0.18	92,108,113,115	0
4	OLA	A	1108	20/20	0.91	0.17	74,81,111,115	0
5	SO4	A	1111	5/5	0.91	0.10	151,153,156,156	0
2	ZN	A	1101	1/1	0.99	0.03	81,81,81,81	0

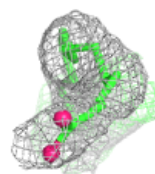
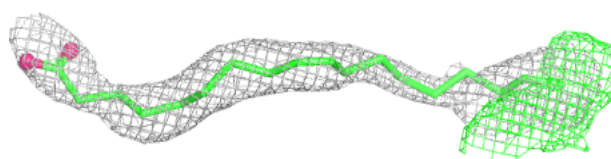
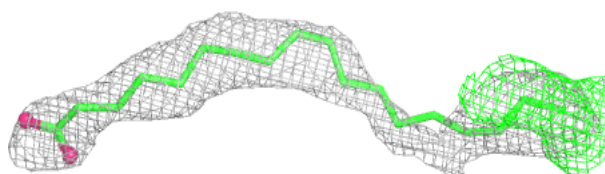
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 1102:

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

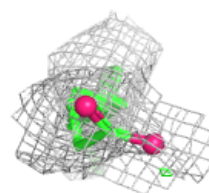
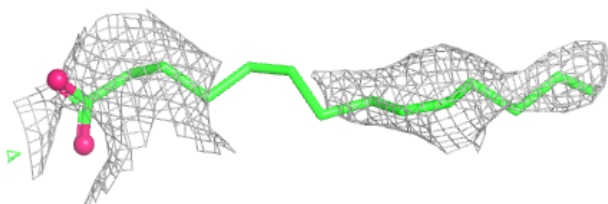
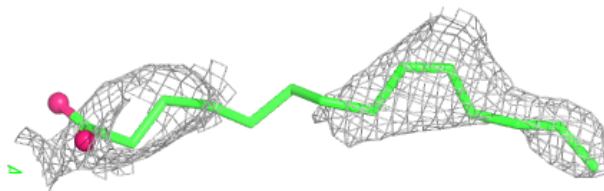
**Electron density around OLA A 1106:**

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

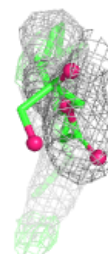
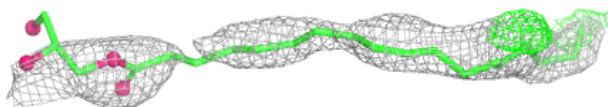
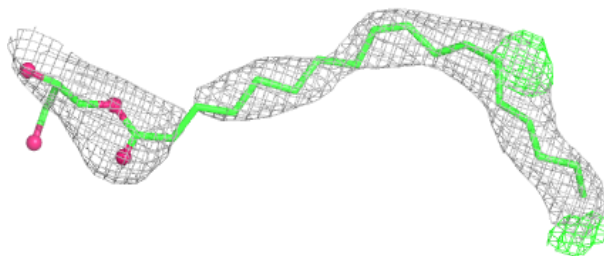


Electron density around OLA A 1107:

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

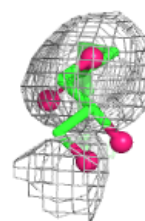
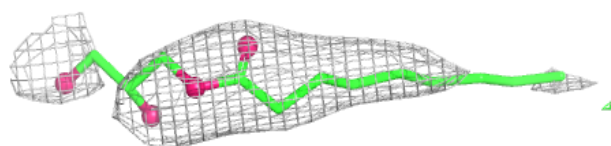
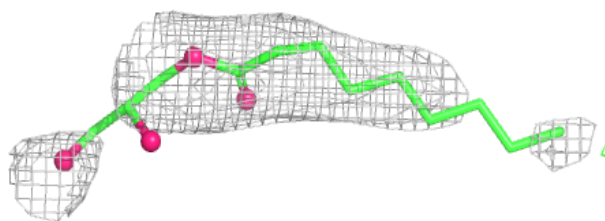
**Electron density around OLC A 1103:**

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

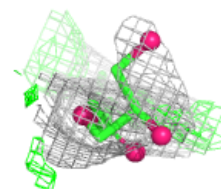
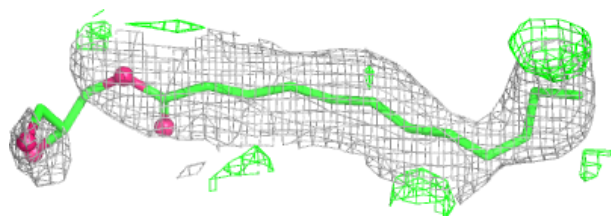
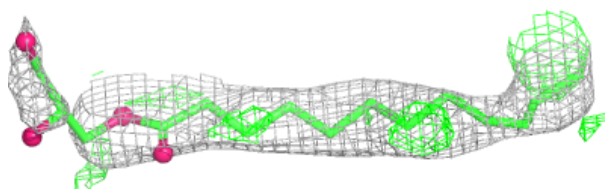


Electron density around OLC A 1105:

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

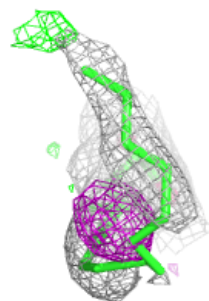
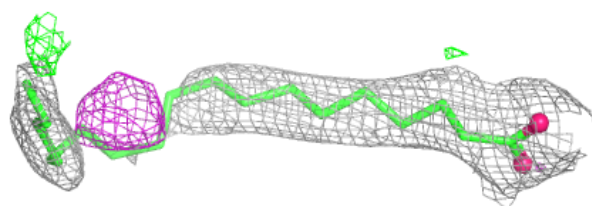
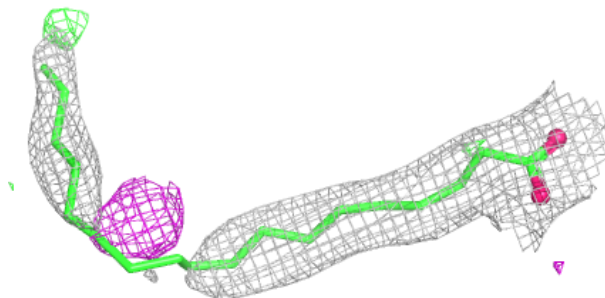
**Electron density around OLC A 1104:**

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

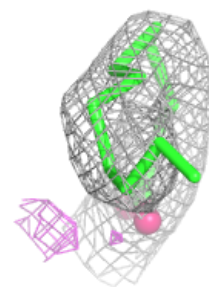
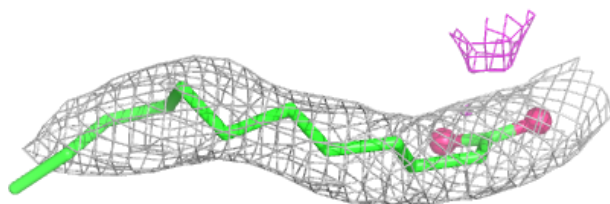
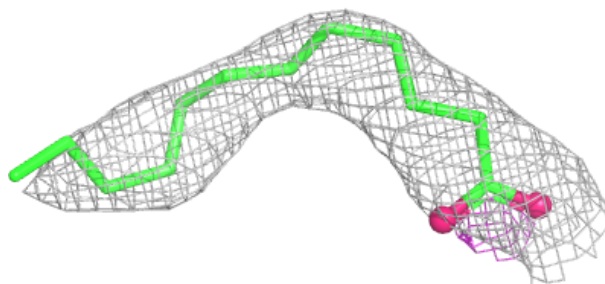


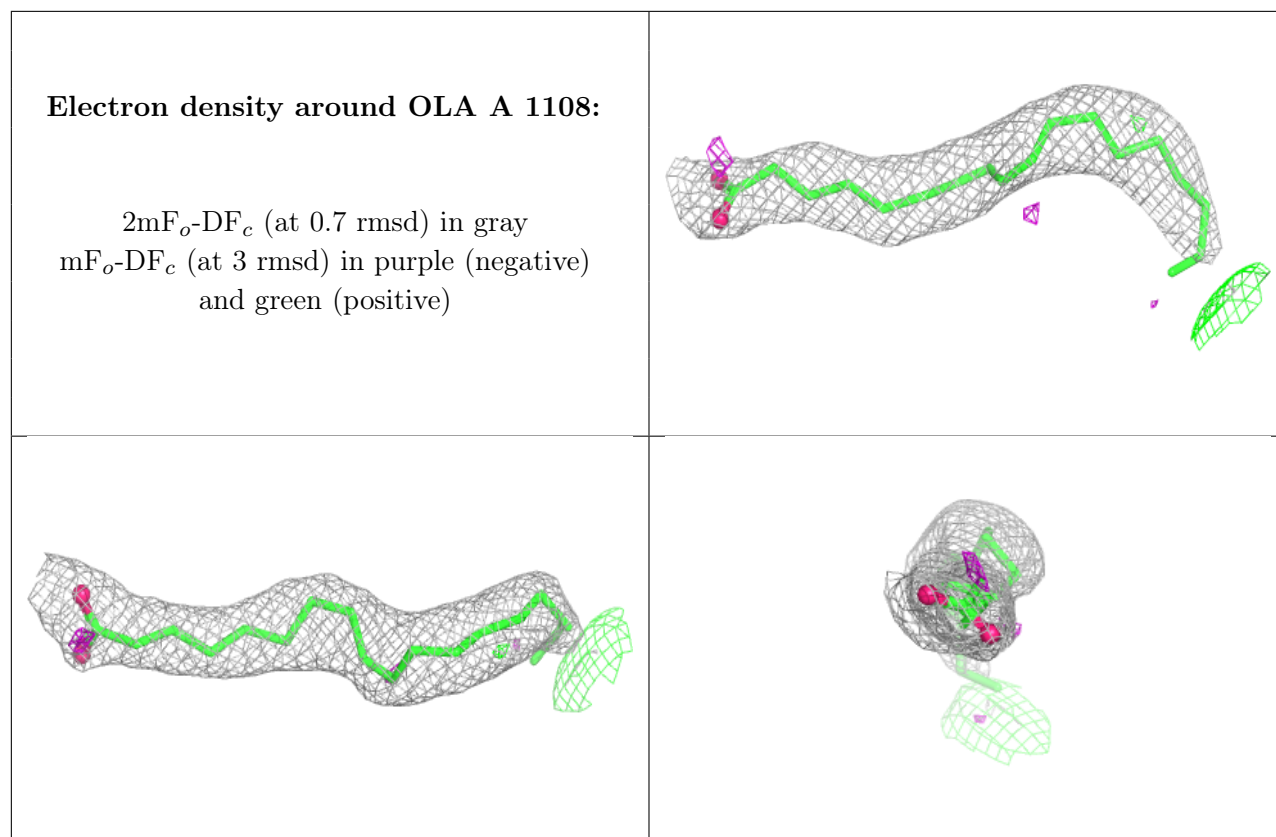
Electron density around OLA A 1110:

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

**Electron density around OLA 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.