



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:03 AM UTC

PDB ID : 6HLO / pdb_00006hlo
Title : Crystal structure of the Neurokinin 1 receptor in complex with the small molecule antagonist Aprepitant
Authors : Schoppe, J.; Ehrenmann, J.; Klenk, C.; Rucktooa, P.; Schutz, M.; Dore, A.S.; Pluckthun, A.
Deposited on : 2018-09-11
Resolution : 2.40 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

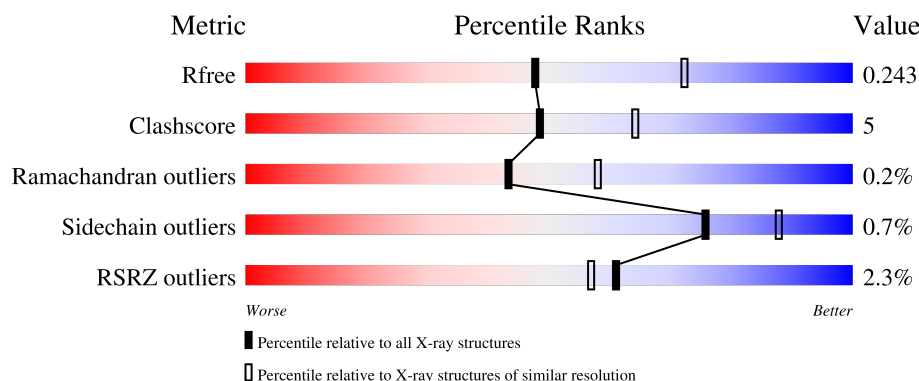
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	520	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4221 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.

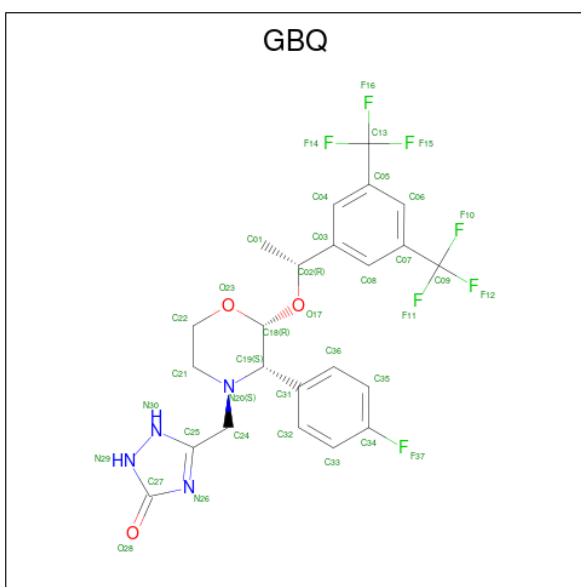
- Molecule 1 is a protein called Substance-P receptor, GlgA glycogen synthase, Substance-P receptor.

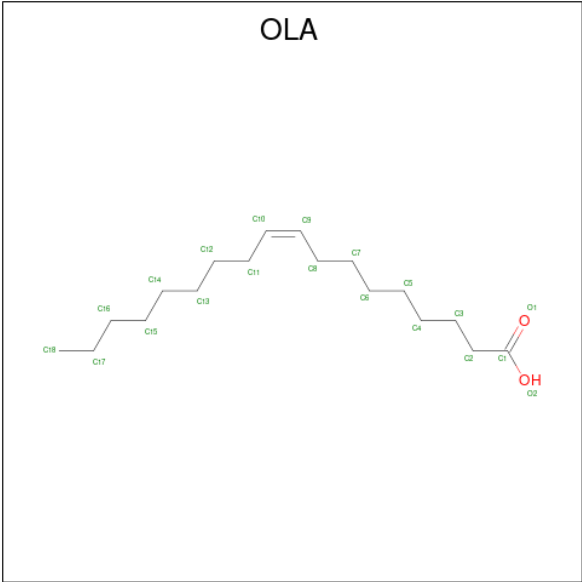
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	0	0
			3832	2524	623	655	30			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ALA	LEU	engineered mutation	UNP P25103
A	116	ILE	VAL	engineered mutation	UNP P25103
A	144	LEU	ALA	engineered mutation	UNP P25103
A	181	LYS	MET	engineered mutation	UNP P25103
A	215	LEU	ALA	engineered mutation	UNP P25103
A	224	ARG	TRP	engineered mutation	UNP P25103
A	1218	GLY	GLU	conflict	UNP P25103
A	243	ALA	LYS	engineered mutation	UNP P25103

- Molecule 2 is 5-[[[(2 {R},3 {S})-2-[(1 {R})-1-[3,5-bis(trifluoromethyl)phenyl]ethoxy]-3-(4-fluorophenyl)morpholin-4-yl]methyl]-1,2-dihydro-1,2,4-triazol-3-one (CCD ID: GBQ) (formula: C₂₃H₂₁F₇N₄O₃).





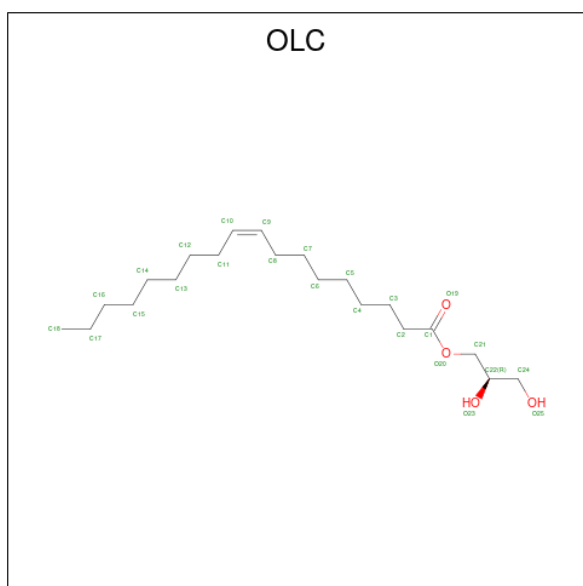
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			14	12	2		
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			10	8	2		
4	A	1	Total	C		0	0
			8	8			
4	A	1	Total	C		0	0
			9	9			
4	A	1	Total	C	O	0	0
			11	9	2		
4	A	1	Total	C	O	0	0
			11	9	2		
4	A	1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

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

- Molecule 5 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			15	11	4		
5	A	1	Total	C	O	0	0
			10	6	4		
5	A	1	Total	C	O	0	0
			25	21	4		

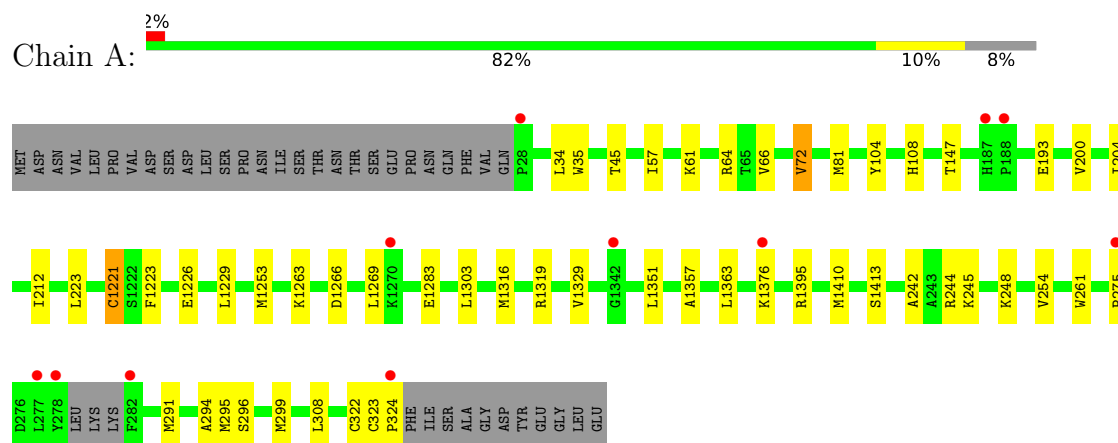
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	74	Total	O	0	0
			74	74		

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: Substance-P receptor,GlgA glycogen synthase,Substance-P receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.19Å 76.45Å 167.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.44 – 2.40 29.44 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.44-2.40) 99.9 (29.44-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.201 , 0.229 0.207 , 0.243	Depositor DCC
R_{free} test set	1658 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	52.1	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.2	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	4221	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.97% 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: CIT, GBQ, OLA, OLC, YCM

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	0.21	0/3910	0.45	1/5304 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1413	SER	O-C-N	13.39	138.74	122.27

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	3832	0	3893	35	0
2	A	37	0	0	1	0
3	A	13	0	5	4	0
4	A	215	0	324	10	0
5	A	50	0	68	3	0
6	A	74	0	0	3	1
All	All	4221	0	4290	46	1

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 5.

All (46) 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:323:CYS:SG	1:A:324:PRO:HD2	2.21	0.81
3:A:1502:CIT:O2	3:A:1502:CIT:O7	2.08	0.70
1:A:34:LEU:HB3	4:A:1511:OLA:H62	1.79	0.64
3:A:1502:CIT:O5	6:A:1601:HOH:O	2.15	0.63
4:A:1504:OLA:H51	4:A:1506:OLA:H72	1.86	0.57
3:A:1502:CIT:O7	3:A:1502:CIT:O3	2.22	0.57
1:A:1266:ASP:N	1:A:1266:ASP:OD1	2.39	0.55
1:A:248:LYS:HG3	5:A:1520:OLC:H2A	1.89	0.54
1:A:323:CYS:SG	1:A:324:PRO:CD	2.95	0.53
1:A:45:THR:HG21	1:A:299:MET:HE3	1.92	0.52
1:A:61:LYS:HG2	1:A:64:ARG:HH12	1.74	0.52
1:A:1283:GLU:OE2	1:A:1395:ARG:NH1	2.38	0.52
1:A:104:TYR:HD1	5:A:1521:OLC:H22	1.75	0.52
1:A:57:ILE:HD12	1:A:72:VAL:HG23	1.90	0.52
3:A:1502:CIT:O2	6:A:1602:HOH:O	2.19	0.51
1:A:66:VAL:HG22	1:A:147:THR:HG21	1.94	0.50
1:A:308:LEU:HD21	4:A:1515:OLA:H31	1.93	0.50
1:A:1223:PHE:CZ	1:A:1319:ARG:HG3	2.47	0.49
1:A:212:ILE:HG21	1:A:254:VAL:HG21	1.93	0.48
1:A:242:ALA:HA	1:A:245:LYS:HE2	1.95	0.48
1:A:1357:ALA:HB1	1:A:1363:LEU:HD13	1.97	0.47
4:A:1512:OLA:H111	4:A:1512:OLA:H82	1.65	0.47
4:A:1504:OLA:H31	4:A:1506:OLA:H42	1.95	0.47
1:A:1229:LEU:HD11	1:A:1351:LEU:HD12	1.98	0.46
1:A:1269:LEU:HD22	1:A:1303:LEU:HD12	1.98	0.46
1:A:61:LYS:HG2	1:A:64:ARG:NH1	2.31	0.45
1:A:45:THR:HG23	4:A:1516:OLA:H31	1.99	0.44
1:A:1221:YCM:HD3	1:A:1221:YCM:HA	1.84	0.44
4:A:1515:OLA:H111	4:A:1515:OLA:H82	1.76	0.44
1:A:66:VAL:HG13	1:A:147:THR:HG21	1.99	0.43
1:A:1221:YCM:OZ1	1:A:1410:MET:HG2	2.19	0.43
1:A:1226:GLU:HG3	1:A:1229:LEU:HD12	2.01	0.43
1:A:296:SER:O	1:A:299:MET:HG2	2.18	0.43
1:A:1263:LYS:HA	1:A:1263:LYS:HD3	1.68	0.43
1:A:291:MET:HE1	6:A:1659:HOH:O	2.19	0.43
1:A:81:MET:HE3	1:A:295:MET:HE3	2.01	0.42
1:A:1376:LYS:HB2	1:A:1376:LYS:HE3	1.81	0.42
4:A:1517:OLA:H82	4:A:1517:OLA:H111	1.61	0.42
1:A:223:LEU:HB3	1:A:244:ARG:HG2	2.01	0.42
5:A:1522:OLC:H8	5:A:1522:OLC:H11	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLU:OE1	2:A:1501:GBQ:N29	2.53	0.42
1:A:1253:MET:HE2	1:A:1329:VAL:HG21	2.02	0.41
1:A:261:TRP:CZ3	1:A:294:ALA:HB1	2.55	0.41
1:A:35:TRP:CE2	4:A:1511:OLA:H31	2.56	0.41
1:A:200:VAL:O	1:A:204:ILE:HG12	2.20	0.41
4:A:1504:OLA:H111	4:A:1504:OLA:H82	1.67	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1610:HOH:O	6:A:1616:HOH:O[3_555]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	473/520 (91%)	467 (99%)	5 (1%)	1 (0%)	43 58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	PRO

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	410/450 (91%)	407 (99%)	3 (1%)	76 88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	VAL
1	A	108	HIS
1	A	1316	MET

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	YCM	A	322	1	7,9,10	1.01	1 (14%)	5,10,12	1.09	0
1	YCM	A	1221	1	7,9,10	1.02	1 (14%)	5,10,12	0.90	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
1	YCM	A	322	1	-	1/6/8/10	-
1	YCM	A	1221	1	-	0/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1221	YCM	CD-SG	-2.04	1.76	1.81
1	A	322	YCM	CD-SG	-2.02	1.76	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	322	YCM	CA-CB-SG-CD

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1221	YCM	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

22 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	$\# Z > 2$
4	OLA	A	1512	-	12,12,19	0.23	0	11,11,19	0.58	0
4	OLA	A	1504	-	13,13,19	0.57	0	13,13,19	0.92	0
4	OLA	A	1508	-	8,8,19	0.21	0	7,7,19	0.56	0
4	OLA	A	1509	-	10,10,19	0.65	0	10,10,19	0.95	0
4	OLA	A	1519	-	9,9,19	0.69	0	9,9,19	1.03	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OLA	A	1503	-	19,19,19	0.50	0	19,19,19	0.77	0
4	OLA	A	1514	-	8,8,19	0.22	0	7,7,19	0.54	0
5	OLC	A	1521	-	9,9,24	1.47	1 (11%)	10,10,25	1.27	1 (10%)
4	OLA	A	1505	-	19,19,19	0.51	0	19,19,19	0.77	0
4	OLA	A	1515	-	19,19,19	0.49	0	19,19,19	0.80	0
4	OLA	A	1506	-	9,9,19	0.64	0	9,9,19	1.07	1 (11%)
4	OLA	A	1516	-	10,10,19	0.64	0	10,10,19	1.01	0
2	GBQ	A	1501	-	38,40,40	1.99	12 (31%)	50,60,60	1.15	1 (2%)
5	OLC	A	1522	-	24,24,24	0.92	1 (4%)	25,25,25	0.89	1 (4%)
4	OLA	A	1510	-	10,10,19	0.65	0	10,10,19	0.98	0
5	OLC	A	1520	-	14,14,24	1.21	1 (7%)	15,15,25	1.15	2 (13%)
4	OLA	A	1518	-	10,10,19	0.65	0	10,10,19	1.02	1 (10%)
4	OLA	A	1513	-	8,8,19	0.22	0	7,7,19	0.52	0
4	OLA	A	1517	-	15,15,19	0.55	0	15,15,19	0.87	0
3	CIT	A	1502	-	12,12,12	1.26	1 (8%)	17,17,17	1.24	2 (11%)
4	OLA	A	1507	-	7,7,19	0.24	0	6,6,19	0.52	0
4	OLA	A	1511	-	12,12,19	0.62	0	12,12,19	1.03	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLA	A	1512	-	-	1/10/10/17	-
4	OLA	A	1504	-	-	5/11/11/17	-
4	OLA	A	1508	-	-	1/6/6/17	-
4	OLA	A	1509	-	-	2/8/8/17	-
4	OLA	A	1519	-	-	1/7/7/17	-
4	OLA	A	1503	-	-	3/17/17/17	-
4	OLA	A	1514	-	-	0/6/6/17	-
5	OLC	A	1521	-	-	4/9/9/24	-
4	OLA	A	1505	-	-	2/17/17/17	-
4	OLA	A	1515	-	-	2/17/17/17	-
4	OLA	A	1506	-	-	2/7/7/17	-
4	OLA	A	1516	-	-	2/8/8/17	-
2	GBQ	A	1501	-	-	2/28/42/42	0/4/4/4
5	OLC	A	1522	-	-	5/24/24/24	-
4	OLA	A	1510	-	-	4/8/8/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OLC	A	1520	-	-	4/14/14/24	-
4	OLA	A	1518	-	-	2/8/8/17	-
4	OLA	A	1513	-	-	0/6/6/17	-
4	OLA	A	1517	-	-	3/13/13/17	-
3	CIT	A	1502	-	-	6/16/16/16	-
4	OLA	A	1507	-	-	0/5/5/17	-
4	OLA	A	1511	-	-	3/10/10/17	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1501	GBQ	C27-N29	4.98	1.44	1.36
5	A	1520	OLC	O20-C1	4.32	1.45	1.33
5	A	1522	OLC	O20-C1	4.28	1.45	1.33
2	A	1501	GBQ	C19-N20	4.27	1.51	1.47
5	A	1521	OLC	O20-C1	4.24	1.45	1.33
2	A	1501	GBQ	C31-C19	3.55	1.57	1.51
2	A	1501	GBQ	C24-C25	3.46	1.53	1.49
2	A	1501	GBQ	C03-C02	3.33	1.58	1.51
2	A	1501	GBQ	C13-C05	2.68	1.55	1.49
2	A	1501	GBQ	C36-C31	2.50	1.43	1.39
3	A	1502	CIT	C3-C6	-2.45	1.50	1.53
2	A	1501	GBQ	C09-C07	2.41	1.54	1.49
2	A	1501	GBQ	C25-N26	2.19	1.38	1.33
2	A	1501	GBQ	C35-C34	2.05	1.41	1.37
2	A	1501	GBQ	N30-N29	2.02	1.42	1.38
2	A	1501	GBQ	C08-C03	2.01	1.42	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1520	OLC	O20-C1-C2	3.12	121.34	111.83
2	A	1501	GBQ	C31-C19-N20	-3.11	106.94	112.50
5	A	1521	OLC	O20-C1-C2	3.08	120.50	111.15
3	A	1502	CIT	O6-C6-C3	2.95	118.80	113.14
5	A	1522	OLC	O20-C1-C2	2.43	119.24	111.83
5	A	1520	OLC	O20-C1-O19	-2.17	118.20	123.63
4	A	1518	OLA	C3-C2-C1	-2.15	108.90	114.51
3	A	1502	CIT	O5-C6-C3	-2.12	117.99	122.09
4	A	1519	OLA	C3-C2-C1	-2.06	109.12	114.51
4	A	1506	OLA	C3-C2-C1	-2.01	109.27	114.51

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1502	CIT	C1-C2-C3-C4
3	A	1502	CIT	C1-C2-C3-C6
5	A	1521	OLC	O19-C1-O20-C21
5	A	1521	OLC	C2-C1-O20-C21
5	A	1522	OLC	O23-C22-C24-O25
4	A	1504	OLA	C1-C2-C3-C4
5	A	1522	OLC	C2-C1-O20-C21
5	A	1520	OLC	C21-C22-C24-O25
5	A	1522	OLC	C21-C22-C24-O25
5	A	1522	OLC	O19-C1-O20-C21
4	A	1516	OLA	C3-C4-C5-C6
4	A	1504	OLA	C6-C7-C8-C9
4	A	1510	OLA	C2-C3-C4-C5
4	A	1503	OLA	C6-C7-C8-C9
3	A	1502	CIT	C1-C2-C3-O7
4	A	1508	OLA	C12-C13-C14-C15
4	A	1505	OLA	C11-C12-C13-C14
4	A	1504	OLA	C2-C3-C4-C5
4	A	1515	OLA	C5-C6-C7-C8
5	A	1520	OLC	C2-C1-O20-C21
5	A	1521	OLC	O20-C21-C22-O23
4	A	1509	OLA	C4-C5-C6-C7
4	A	1510	OLA	C3-C4-C5-C6
4	A	1506	OLA	C3-C4-C5-C6
2	A	1501	GBQ	N20-C24-C25-N30
4	A	1509	OLA	C5-C6-C7-C8
4	A	1511	OLA	C3-C4-C5-C6
5	A	1520	OLC	O19-C1-O20-C21
5	A	1520	OLC	O23-C22-C24-O25
4	A	1517	OLA	C4-C5-C6-C7
2	A	1501	GBQ	N20-C24-C25-N26
4	A	1505	OLA	C5-C6-C7-C8
5	A	1522	OLC	C4-C5-C6-C7
4	A	1503	OLA	C11-C12-C13-C14
4	A	1504	OLA	O1-C1-C2-C3
3	A	1502	CIT	O2-C1-C2-C3
4	A	1516	OLA	C2-C3-C4-C5
4	A	1504	OLA	O2-C1-C2-C3
4	A	1517	OLA	O1-C1-C2-C3
4	A	1517	OLA	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	A	1521	OLC	O20-C21-C22-C24
3	A	1502	CIT	O1-C1-C2-C3
4	A	1510	OLA	O2-C1-C2-C3
3	A	1502	CIT	O7-C3-C4-C5
4	A	1518	OLA	O2-C1-C2-C3
4	A	1503	OLA	C7-C8-C9-C10
4	A	1515	OLA	C11-C12-C13-C14
4	A	1518	OLA	O1-C1-C2-C3
4	A	1510	OLA	O1-C1-C2-C3
4	A	1512	OLA	C12-C13-C14-C15
4	A	1511	OLA	O2-C1-C2-C3
4	A	1519	OLA	O2-C1-C2-C3
4	A	1511	OLA	O1-C1-C2-C3
4	A	1506	OLA	C1-C2-C3-C4

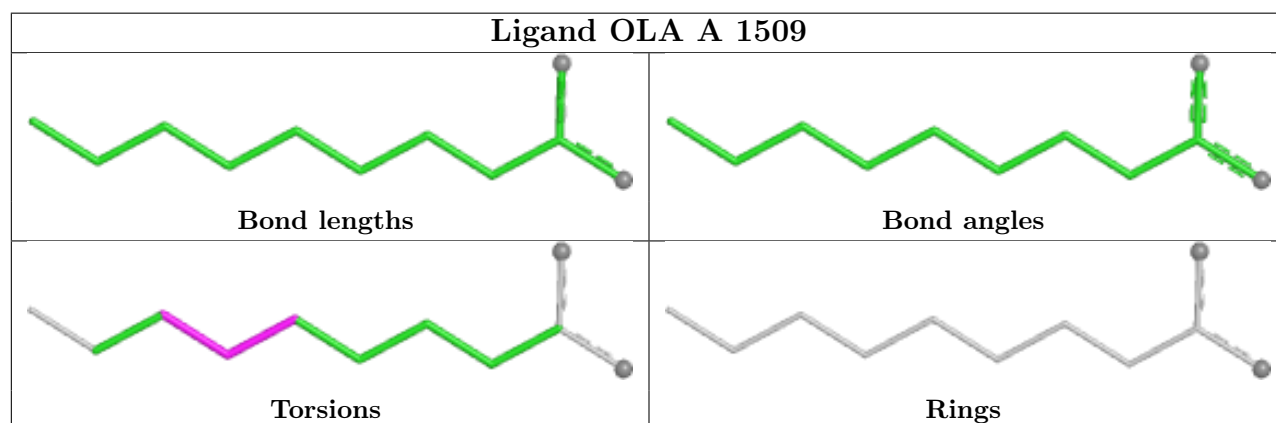
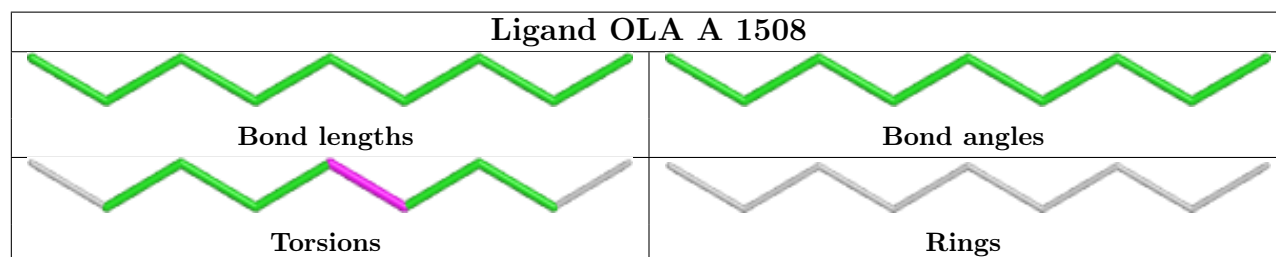
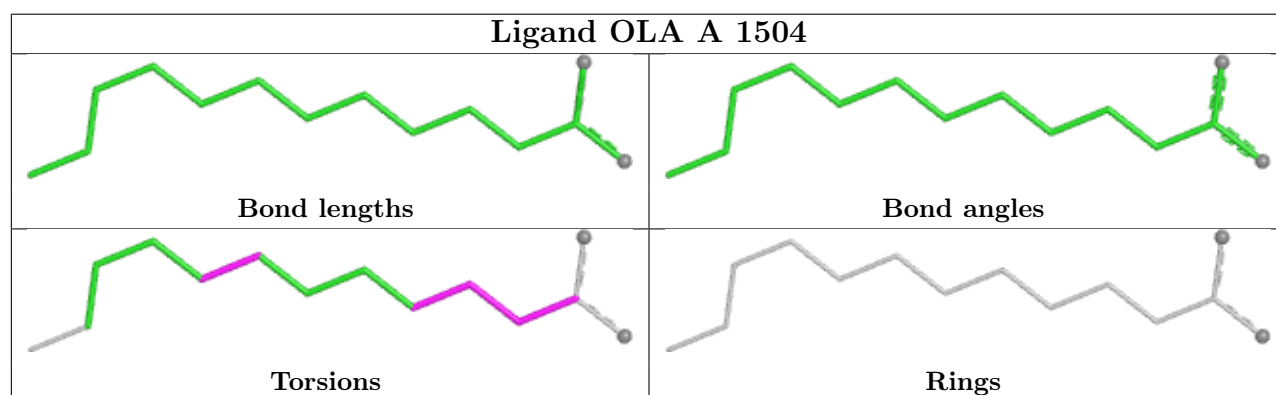
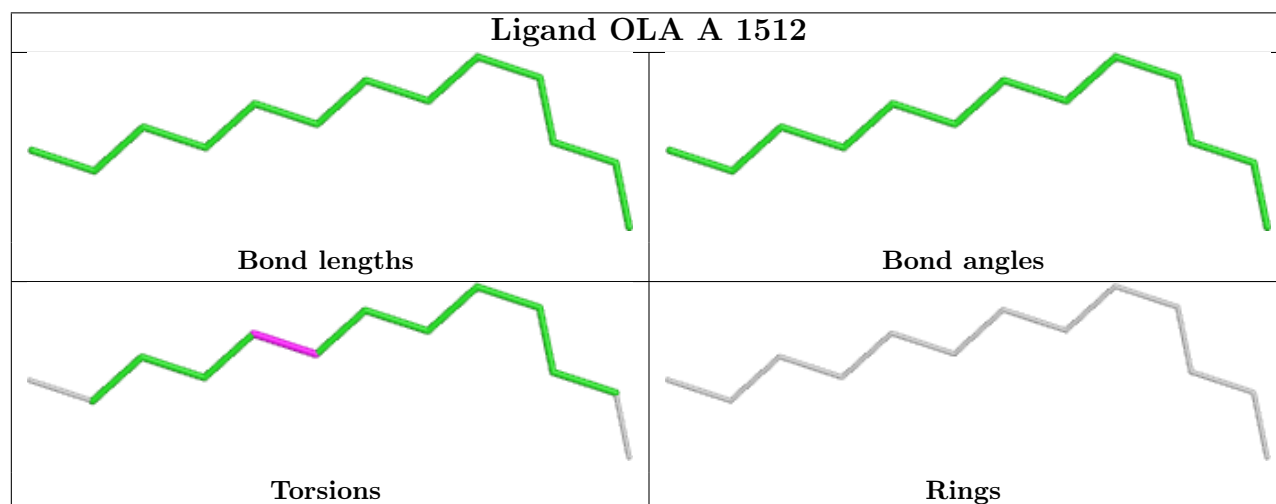
There are no ring outliers.

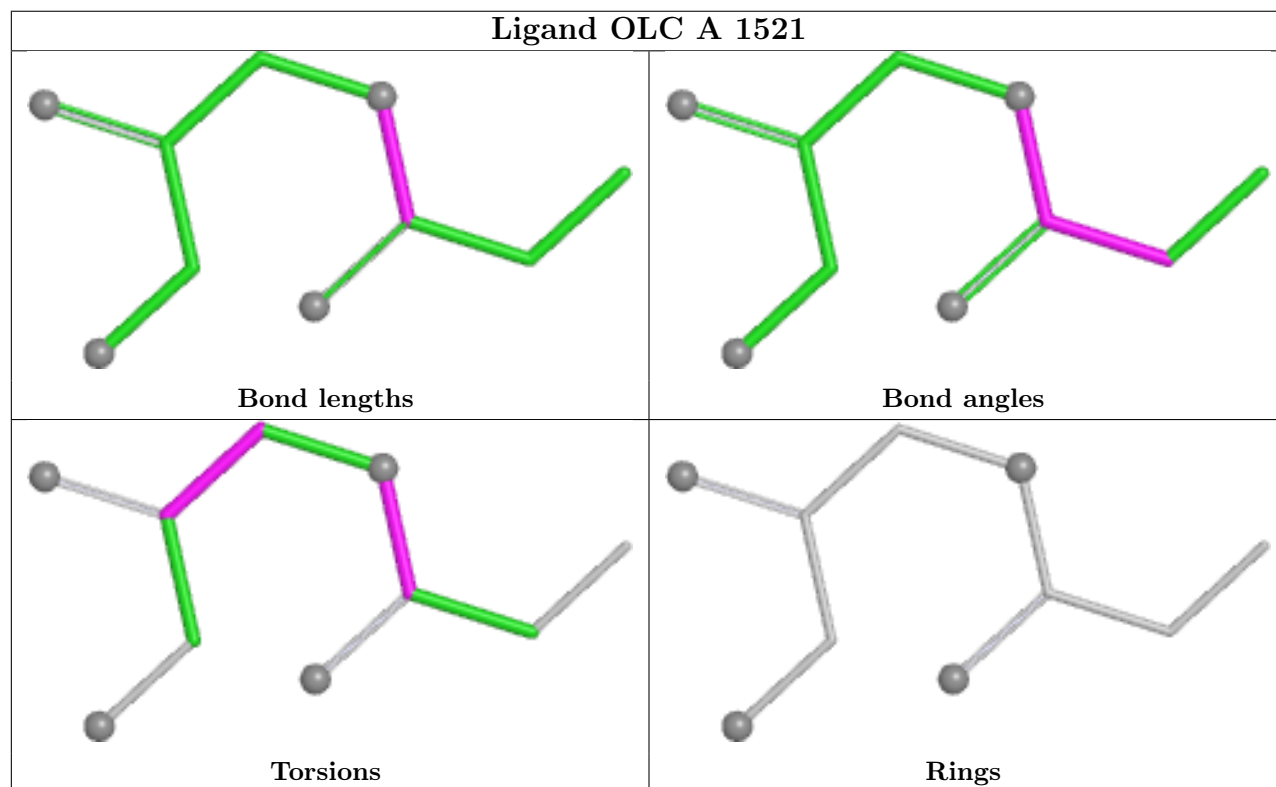
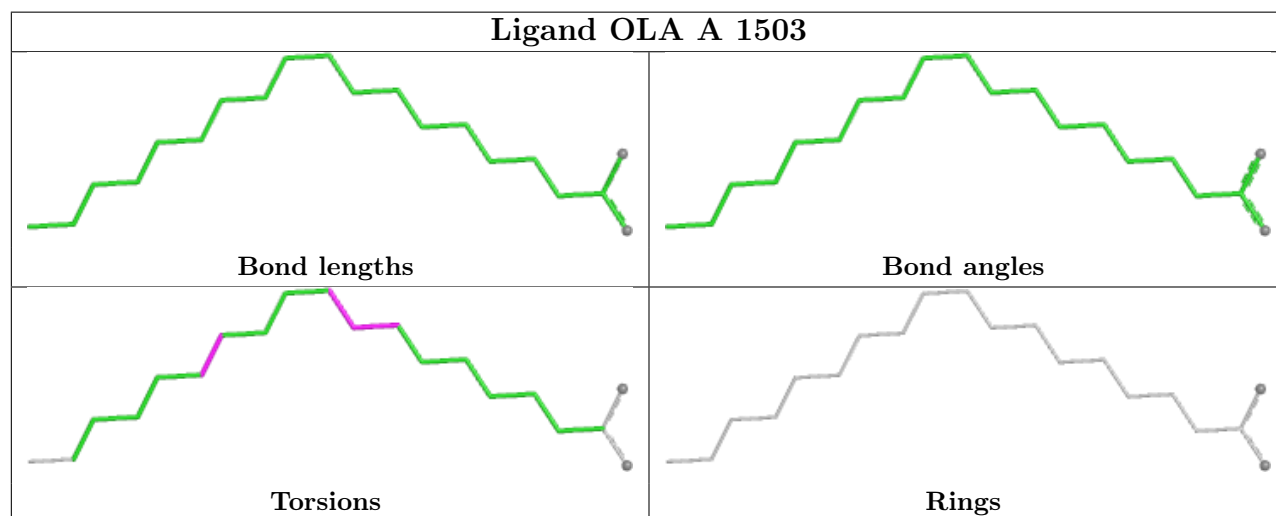
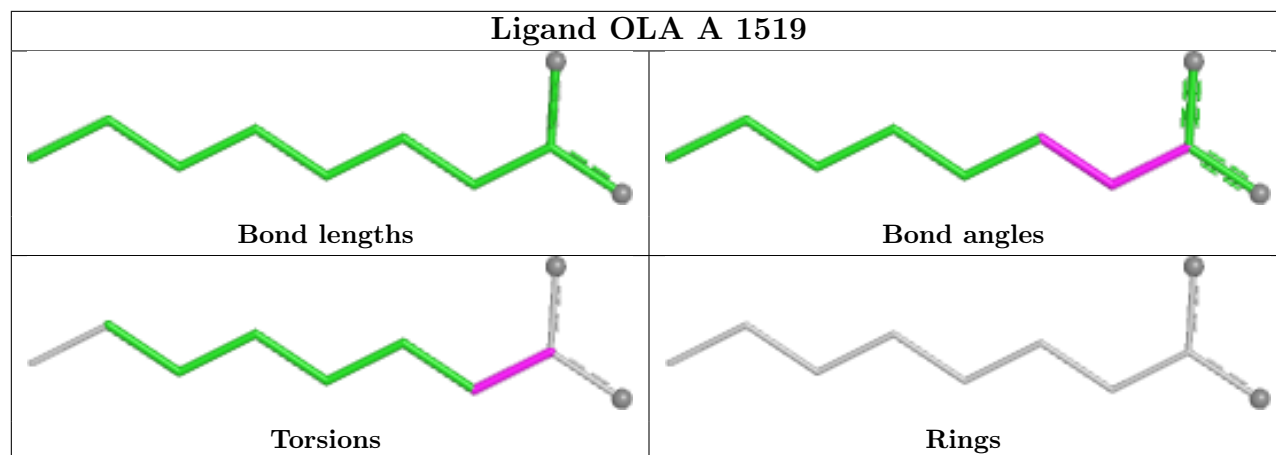
12 monomers are involved in 18 short contacts:

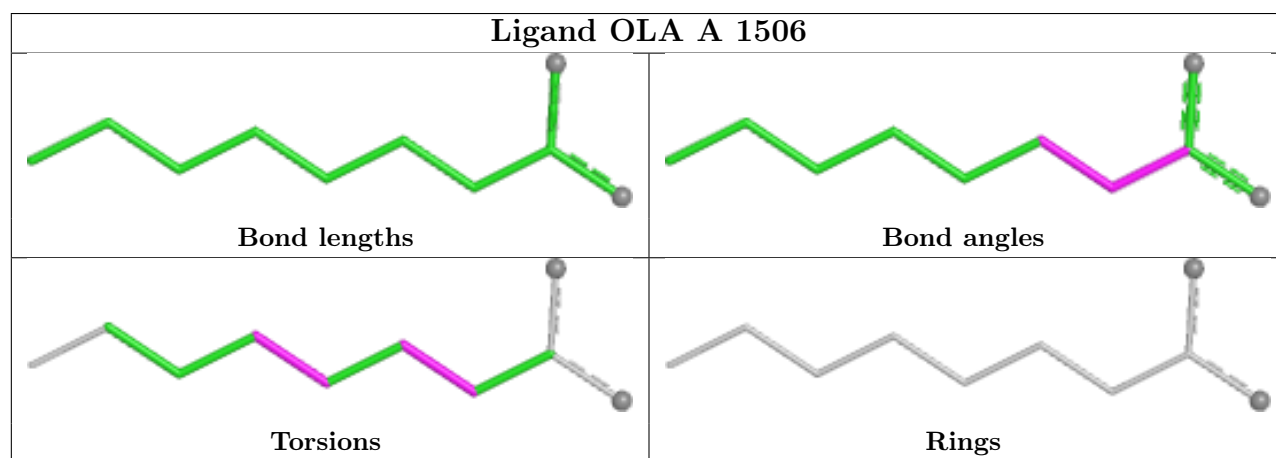
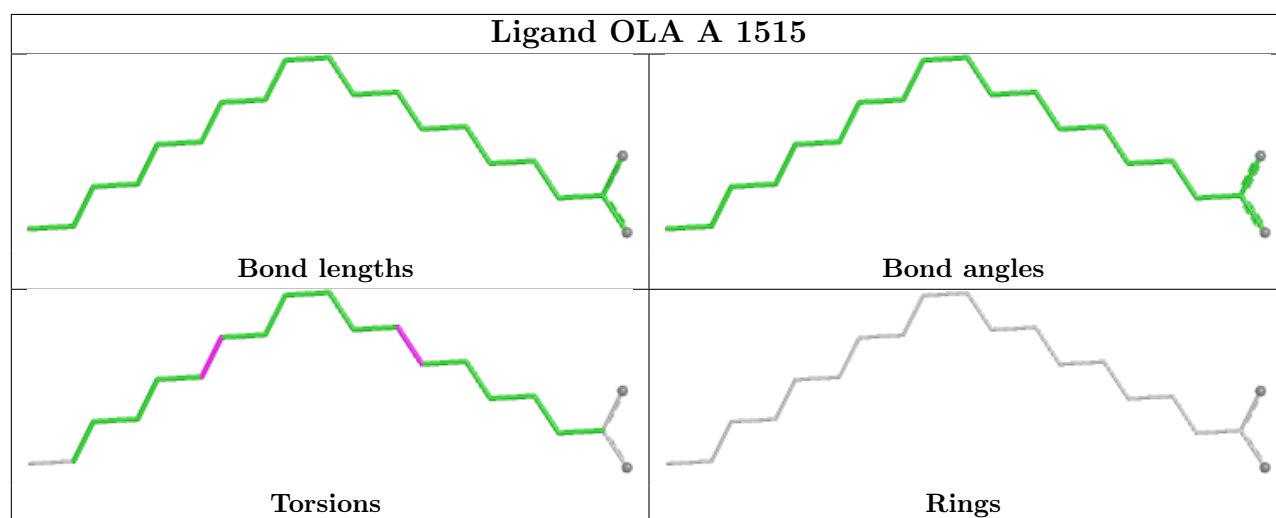
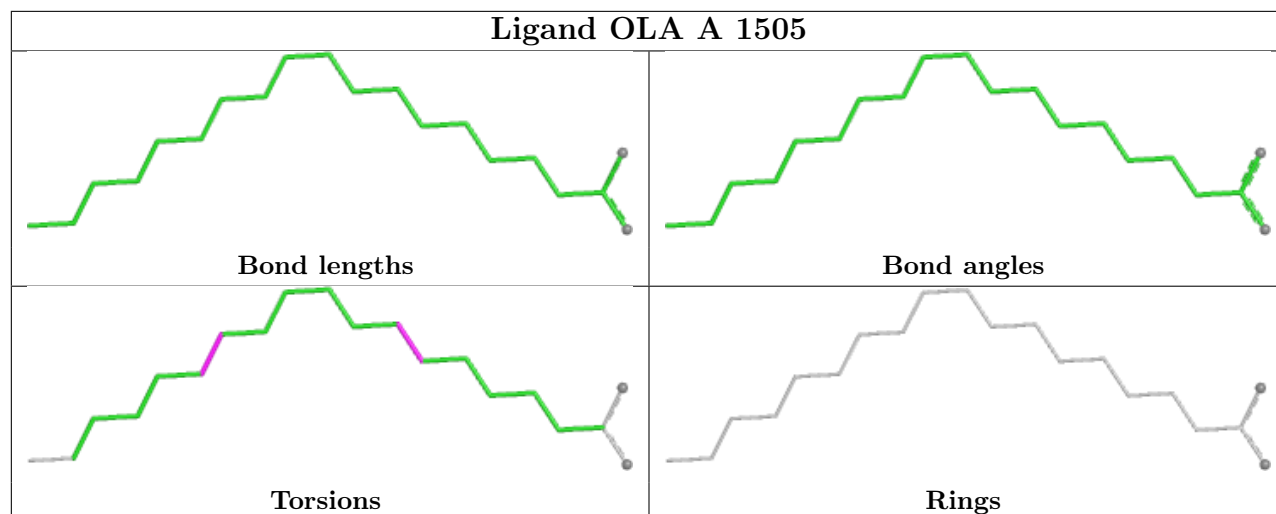
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1512	OLA	1	0
4	A	1504	OLA	3	0
5	A	1521	OLC	1	0
4	A	1515	OLA	2	0
4	A	1506	OLA	2	0
4	A	1516	OLA	1	0
2	A	1501	GBQ	1	0
5	A	1522	OLC	1	0
5	A	1520	OLC	1	0
4	A	1517	OLA	1	0
3	A	1502	CIT	4	0
4	A	1511	OLA	2	0

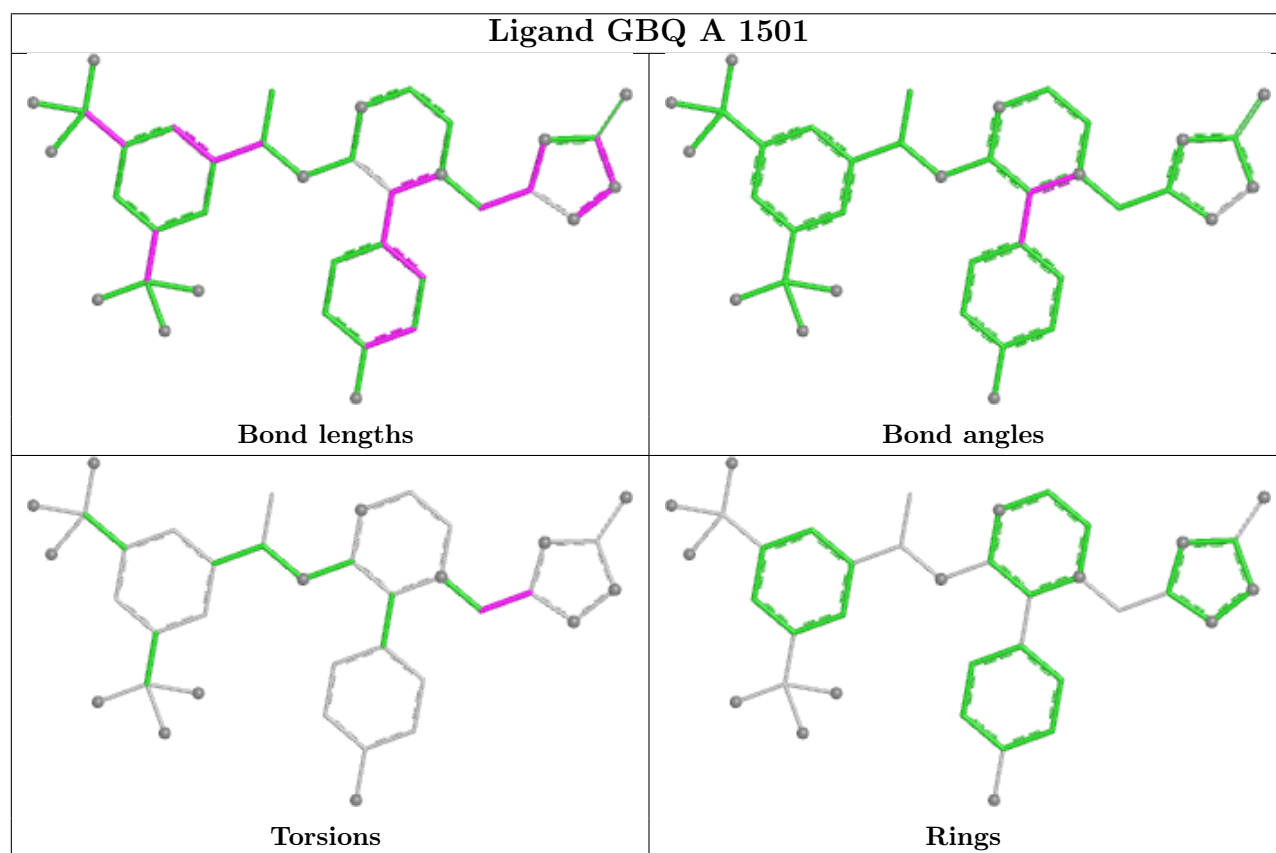
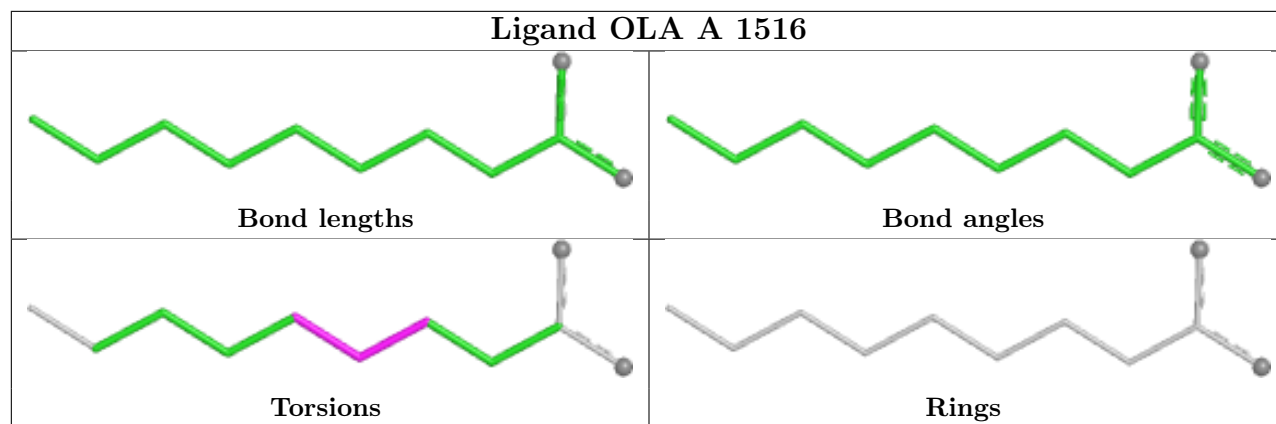
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

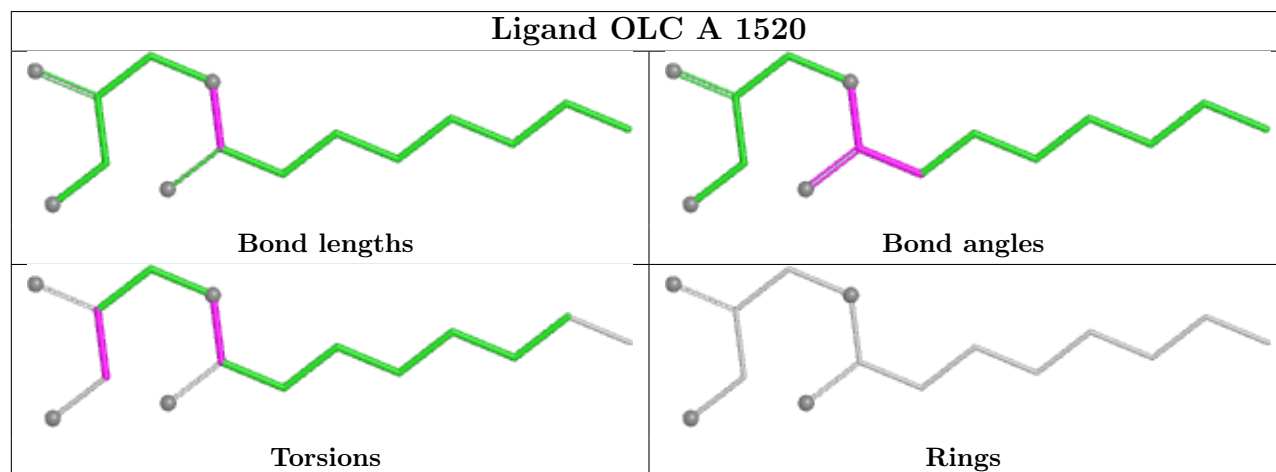
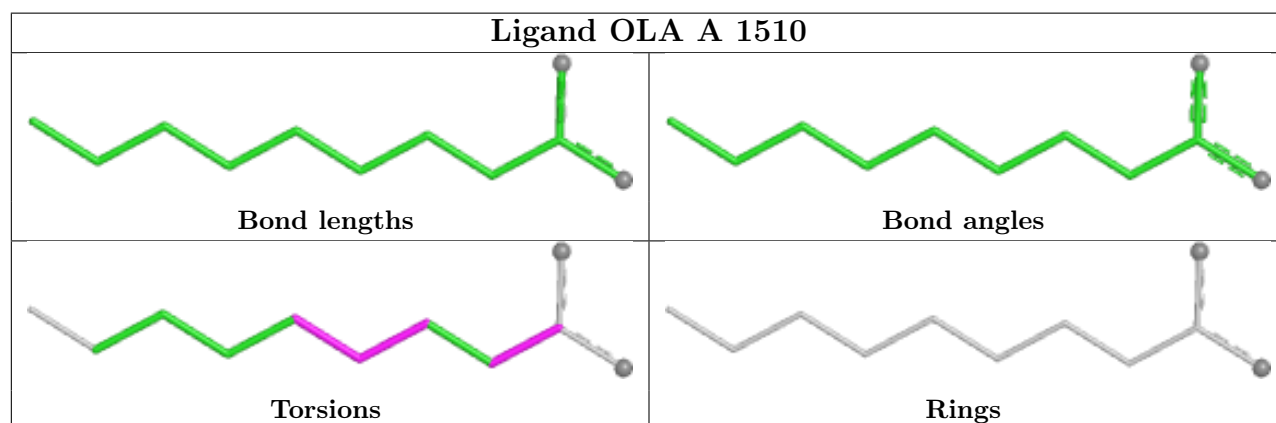
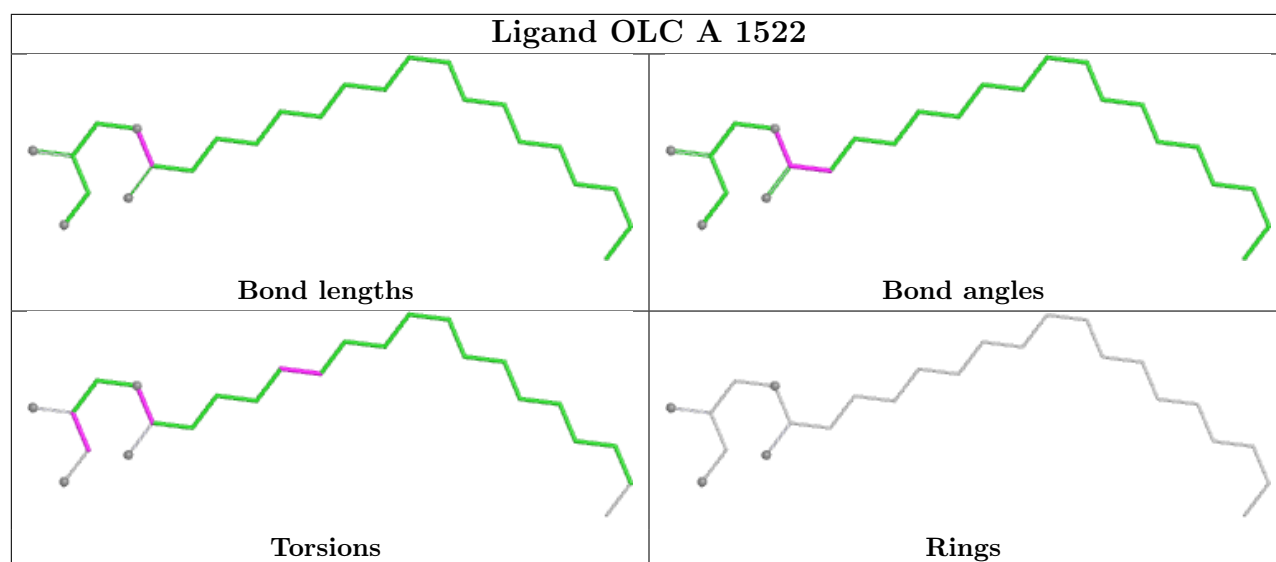
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

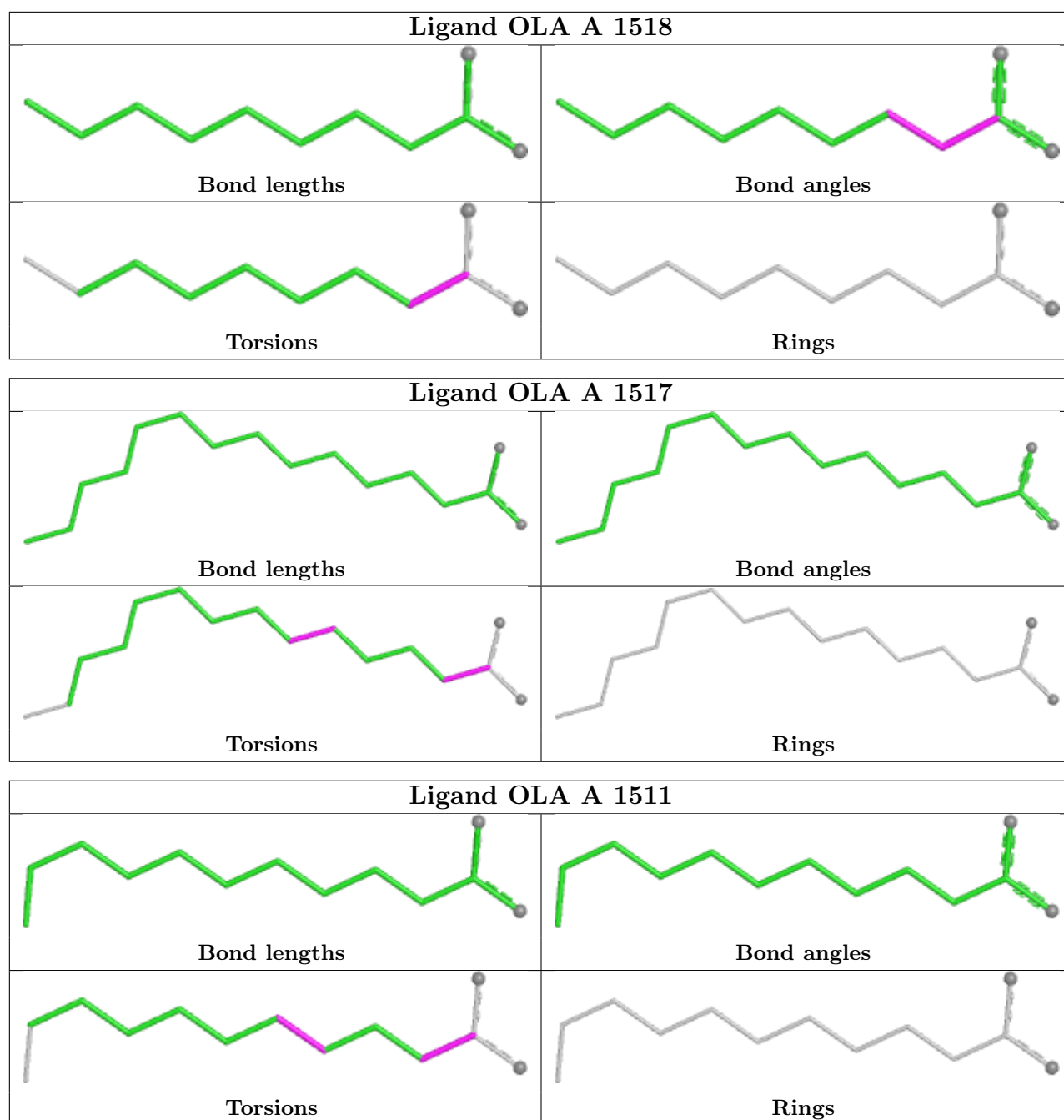












5.7 Other polymers [i](#)

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	477/520 (91%)	0.10	11 (2%) 61 57	42, 56, 97, 170	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	LEU	4.2
1	A	324	PRO	3.9
1	A	28	PRO	3.3
1	A	188	PRO	3.0
1	A	282	PHE	2.8
1	A	278	TYR	2.6
1	A	1270	LYS	2.6
1	A	1342	GLY	2.3
1	A	275	PRO	2.3
1	A	1376	LYS	2.2
1	A	187	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	YCM	A	322	10/11	0.67	0.14	133,147,160,166	0
1	YCM	A	1221	10/11	0.93	0.11	49,59,84,87	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

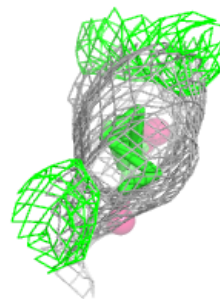
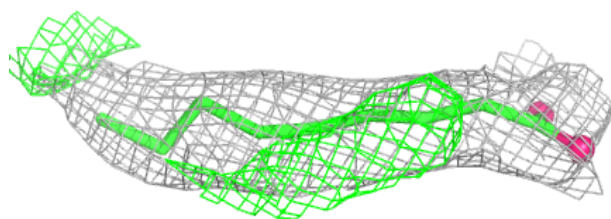
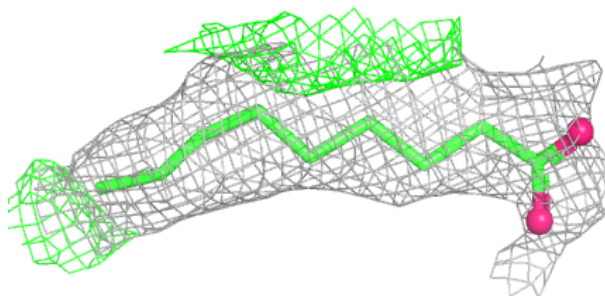
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	OLA	A	1509	11/20	0.73	0.18	74,82,123,127	0
4	OLA	A	1514	9/20	0.74	0.23	73,85,93,93	0
4	OLA	A	1507	8/20	0.76	0.20	64,73,78,83	0
4	OLA	A	1506	10/20	0.79	0.16	65,78,86,88	0
4	OLA	A	1518	11/20	0.79	0.19	78,96,121,122	0
4	OLA	A	1517	16/20	0.80	0.19	73,86,149,151	0
4	OLA	A	1515	20/20	0.80	0.23	70,91,121,122	0
4	OLA	A	1510	11/20	0.81	0.20	83,91,99,103	0
4	OLA	A	1511	13/20	0.81	0.20	91,99,117,120	0
4	OLA	A	1505	20/20	0.82	0.25	82,95,105,108	0
4	OLA	A	1513	9/20	0.82	0.18	71,75,85,85	0
5	OLC	A	1522	25/25	0.83	0.19	79,101,132,137	0
5	OLC	A	1521	10/25	0.84	0.20	90,118,130,136	0
4	OLA	A	1516	11/20	0.85	0.22	81,89,97,100	0
5	OLC	A	1520	15/25	0.85	0.14	58,70,86,96	0
4	OLA	A	1508	9/20	0.86	0.21	67,72,84,84	0
4	OLA	A	1503	20/20	0.87	0.16	69,80,125,127	0
3	CIT	A	1502	13/13	0.87	0.14	61,82,109,113	0
4	OLA	A	1519	10/20	0.87	0.15	67,86,119,122	0
4	OLA	A	1504	14/20	0.88	0.15	65,77,86,87	0
4	OLA	A	1512	13/20	0.89	0.17	71,83,86,87	0
2	GBQ	A	1501	37/37	0.93	0.10	41,52,71,79	0

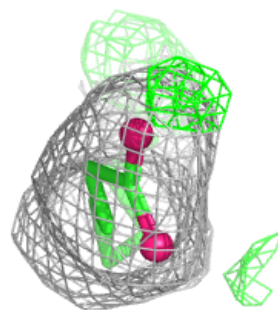
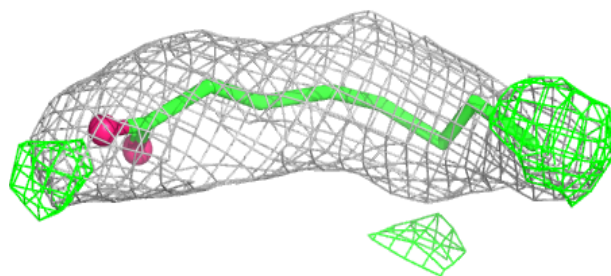
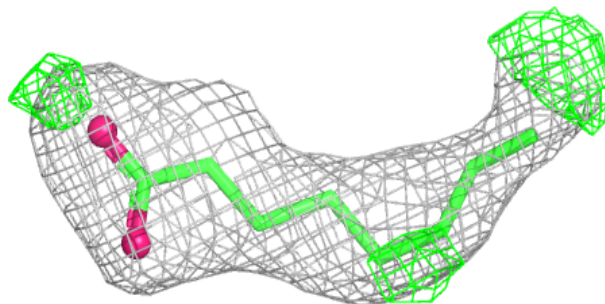
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA A 1509:

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

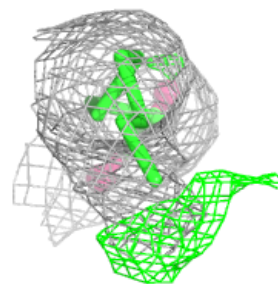
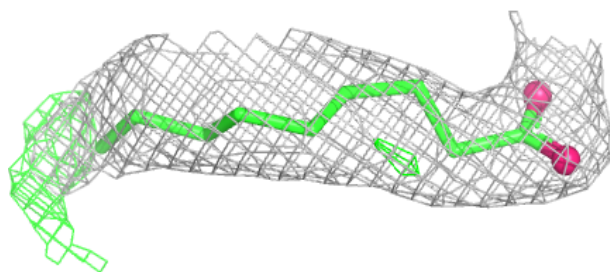
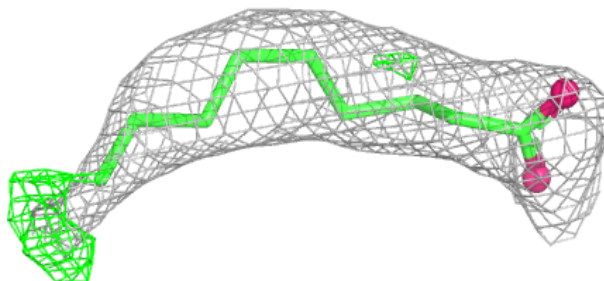
**Electron density around OLA A 1506:**

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

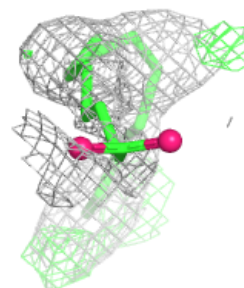
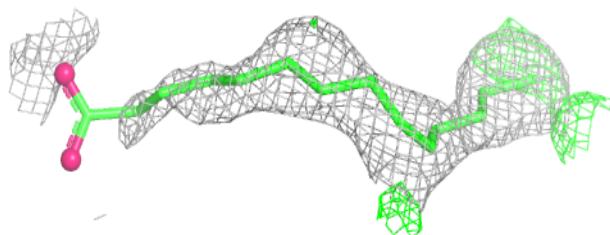
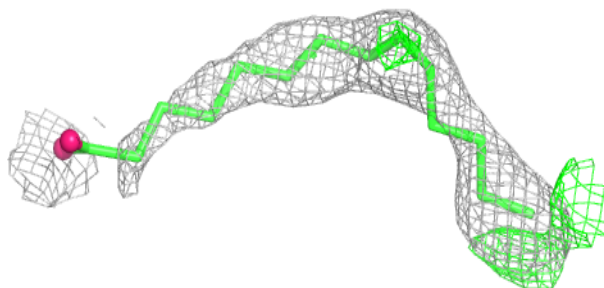


Electron density around OLA A 1518:

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and green (positive)

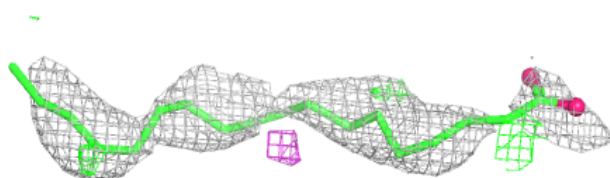
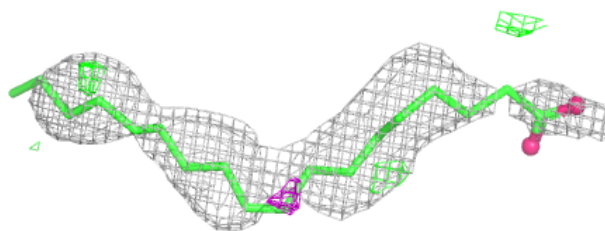
**Electron density around OLA A 1517:**

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

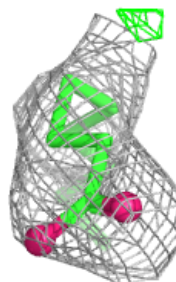
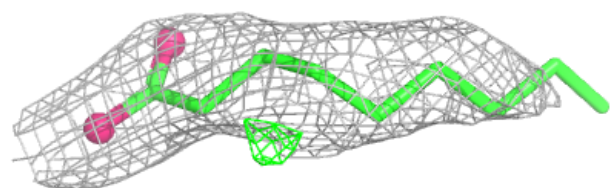
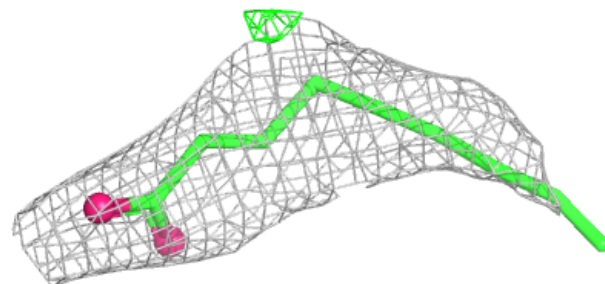


Electron density around OLA A 1515:

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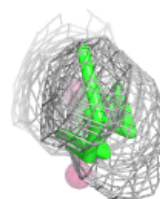
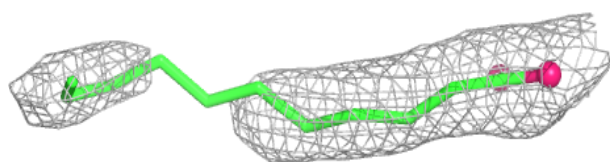
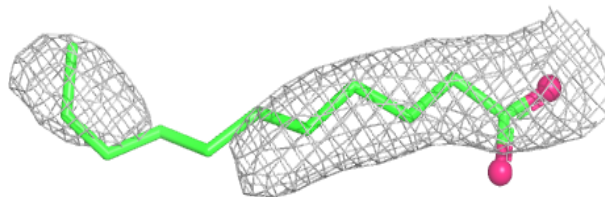
**Electron density around OLA A 1510:**

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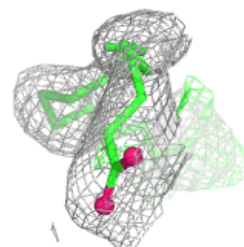
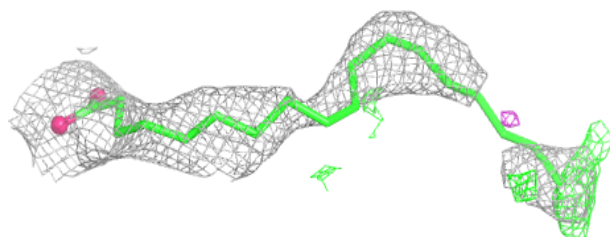
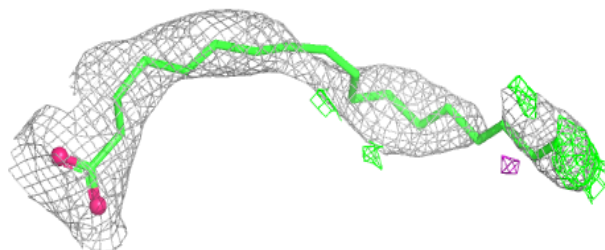


Electron density around OLA A 1511:

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

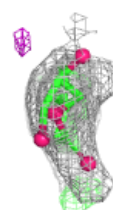
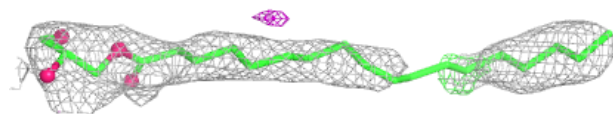
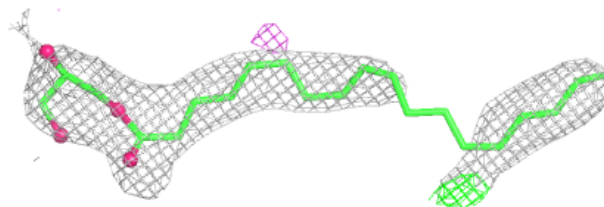
**Electron density around OLA A 1505:**

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

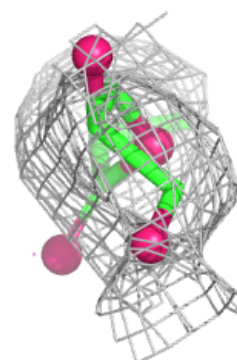
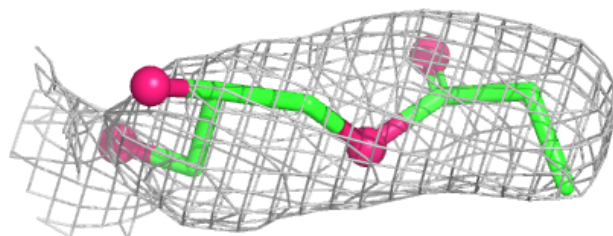
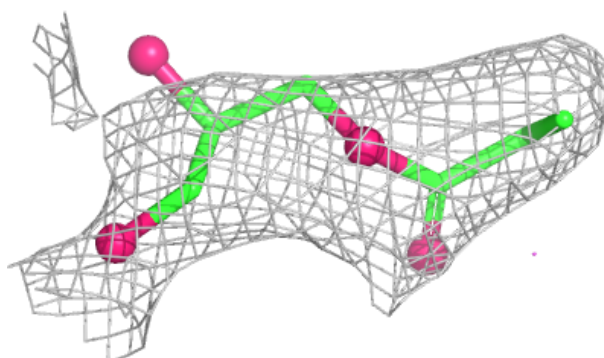


Electron density around OLC A 1522:

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

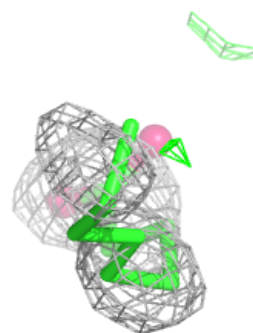
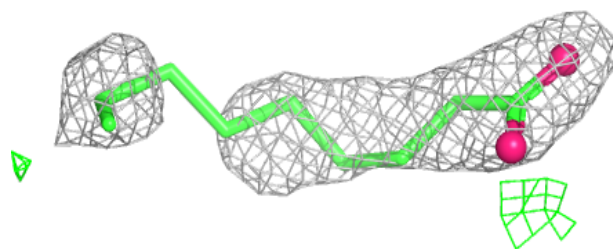
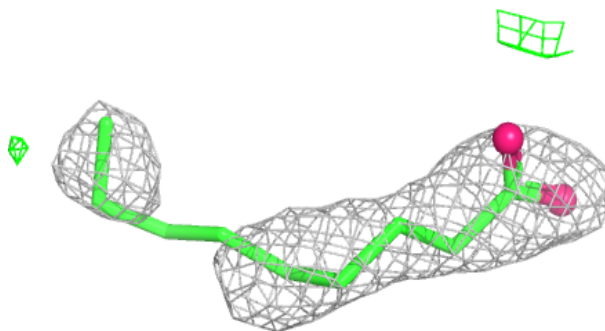
**Electron density around OLC A 1521:**

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

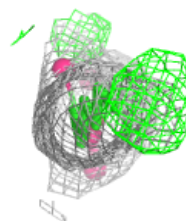
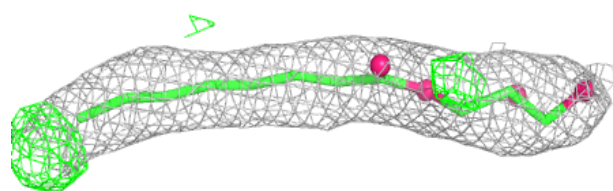
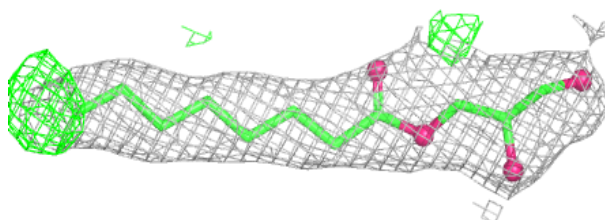


Electron density around OLA A 1516:

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

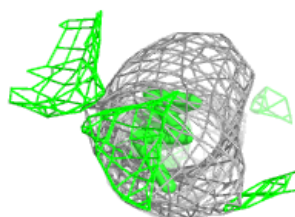
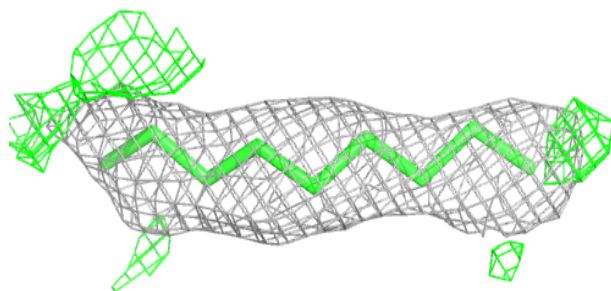
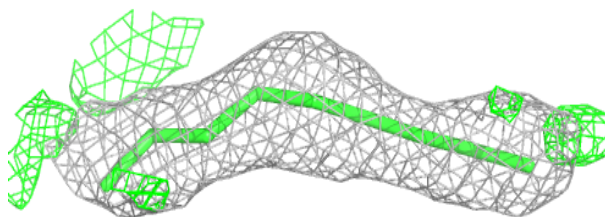
**Electron density around OLC A 1520:**

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

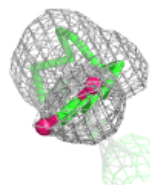
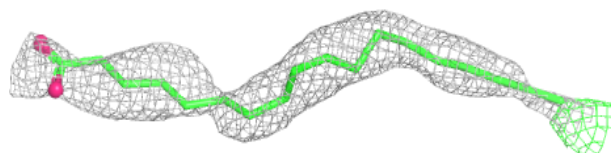
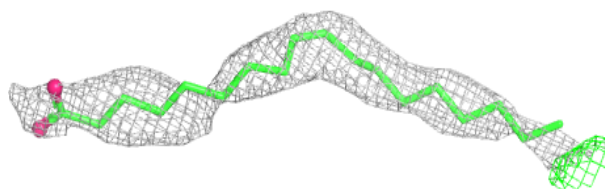


Electron density around OLA A 1508:

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

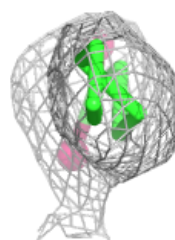
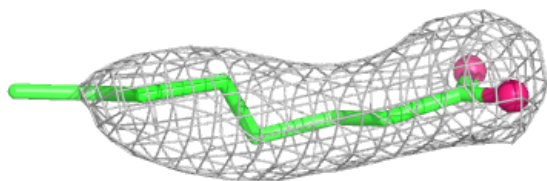
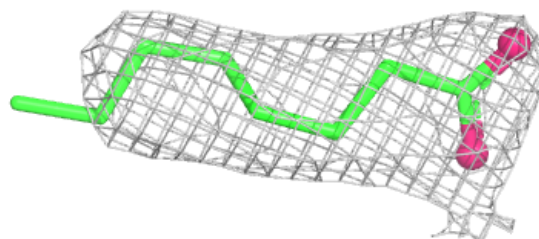
**Electron density around OLA A 1503:**

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

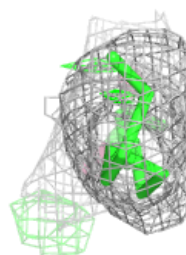
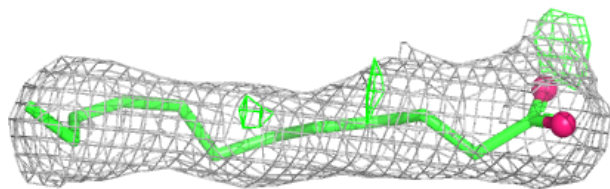
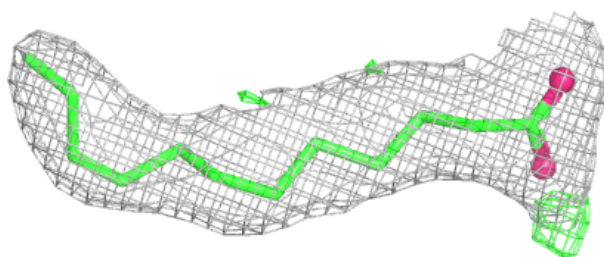


Electron density around OLA A 1519:

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

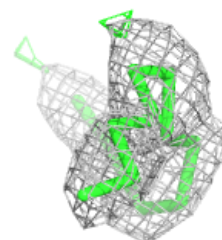
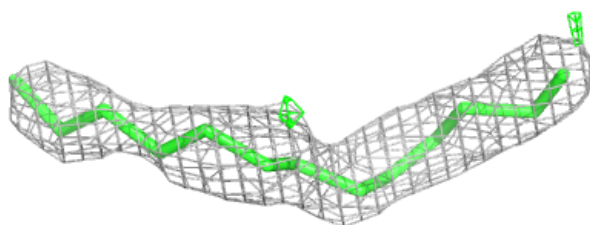
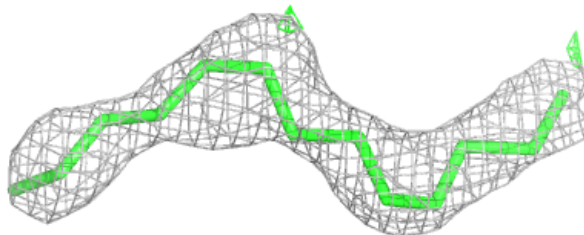
**Electron density around OLA A 1504:**

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

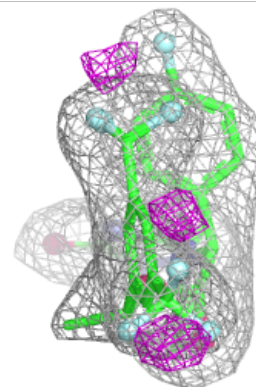
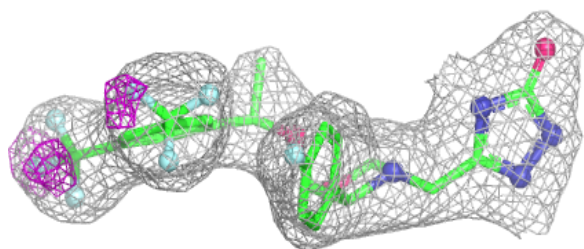
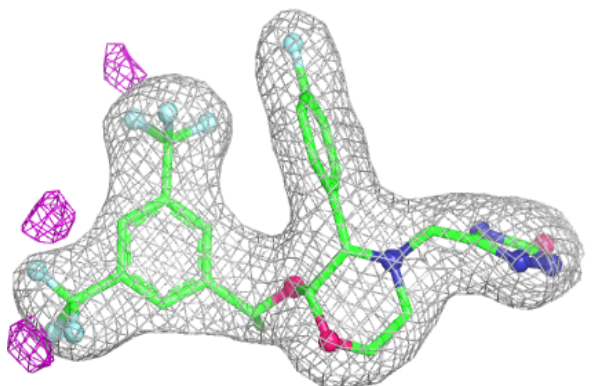


Electron density around OLA A 1512:

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

**Electron density around GBQ A 1501:**

$2mF_o-DF_c$ (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.