



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:06 pm BST

PDB ID : 3VW7
Title : Crystal structure of human protease-activated receptor 1 (PAR1) bound with antagonist vorapaxar at 2.2 angstrom
Authors : Zhang, C.; Srinivasan, Y.; Arlow, D.H.; Fung, J.J.; Palmer, D.; Zheng, Y.; Green, H.F.; Pandey, A.; Dror, R.O.; Shaw, D.E.; Weis, W.I.; Coughlin, S.R.; Kobilka, B.K.
Deposited on : 2012-08-07
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

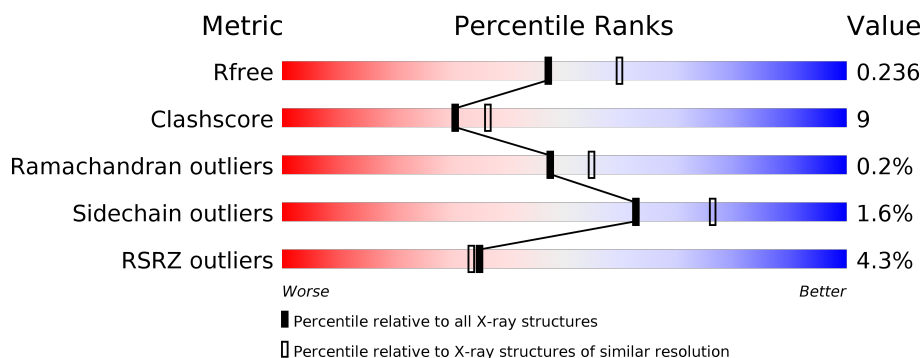
1 Overall quality at a glance

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 on 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	484	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>• 9%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3827 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.

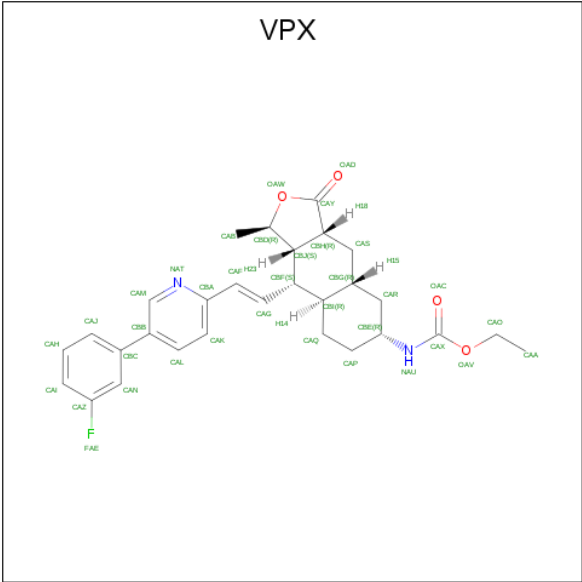
- Molecule 1 is a protein called Proteinase-activated receptor 1, Lysozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	33	1	0
			3473	2271	562	617	23			

There are 20 discrepancies between the modelled and reference sequences:

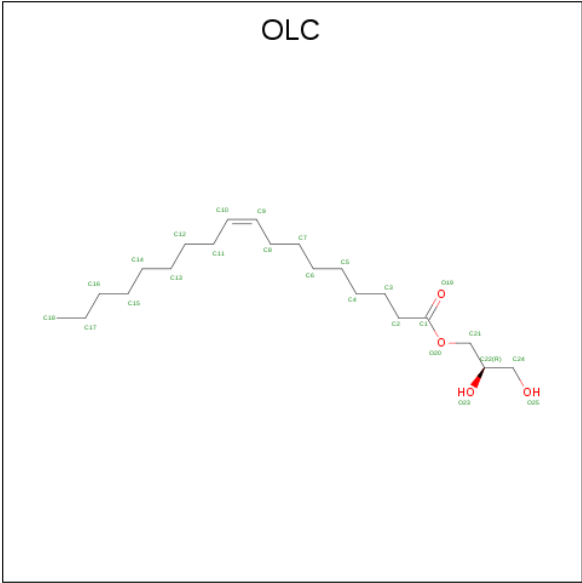
Chain	Residue	Modelled	Actual	Comment	Reference
A	83	SER	-	EXPRESSION TAG	UNP P25116
A	84	GLY	-	EXPRESSION TAG	UNP P25116
A	85	THR	-	EXPRESSION TAG	UNP P25116
A	250	GLY	ASN	ENGINEERED MUTATION	UNP P25116
A	259	SER	ASN	ENGINEERED MUTATION	UNP P25116
A	1020	ASN	ASP	ENGINEERED MUTATION	UNP P00720
A	1054	THR	CYS	ENGINEERED MUTATION	UNP P00720
A	1097	ALA	CYS	ENGINEERED MUTATION	UNP P00720
A	396	CYS	-	EXPRESSION TAG	UNP P25116
A	397	TYR	-	EXPRESSION TAG	UNP P25116
A	398	HIS	-	EXPRESSION TAG	UNP P25116
A	399	HIS	-	EXPRESSION TAG	UNP P25116
A	400	HIS	-	EXPRESSION TAG	UNP P25116
A	401	HIS	-	EXPRESSION TAG	UNP P25116
A	402	HIS	-	EXPRESSION TAG	UNP P25116
A	403	HIS	-	EXPRESSION TAG	UNP P25116
A	404	HIS	-	EXPRESSION TAG	UNP P25116
A	405	HIS	-	EXPRESSION TAG	UNP P25116
A	406	HIS	-	EXPRESSION TAG	UNP P25116
A	407	HIS	-	EXPRESSION TAG	UNP P25116

- Molecule 2 is ethyl [(1R,3aR,4aR,6R,8aR,9S,9aS)-9-{(E)-2-[5-(3-fluorophenyl)pyridin-2-yl]ethenyl}-1-methyl-3-oxododecahydronaphtho[2,3-c]furan-6-yl]carbamate (three-letter code: VPX) (formula: C₂₉H₃₃FN₂O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			36	29	1	2	4		

- Molecule 3 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		3	0
			25	21	4			
3	A	1	Total	C	O		2	0
			25	21	4			

Continued on next page...

Continued from previous page...

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

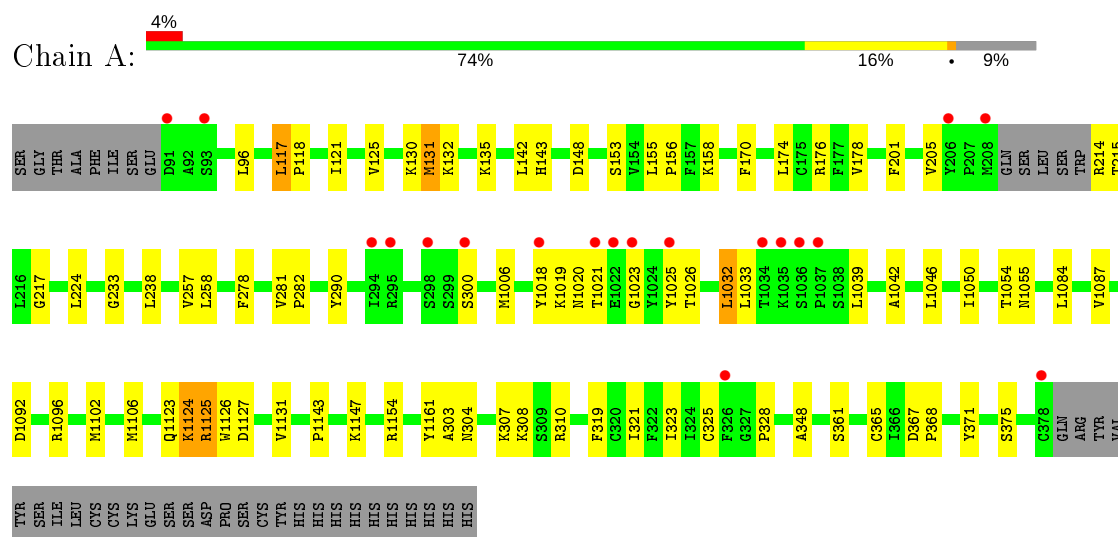
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	91	Total	O	0	0
			91	91		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Proteinase-activated receptor 1, Lysozyme



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.04Å 71.46Å 172.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.27 – 2.20 28.27 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.0 (28.27-2.20) 95.1 (28.27-2.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.7 _650	Depositor
R, R_{free}	0.218 , 0.235 0.215 , 0.236	Depositor DCC
R_{free} test set	1366 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.784	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3827	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, OLC, VPX, CL

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	0.42	1/3556 (0.0%)	0.48	4/4833 (0.1%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1124	LYS	C-N	9.26	1.55	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153[A]	SER	CA-C-O	-5.84	107.83	120.10
1	A	153[B]	SER	CA-C-O	-5.84	107.83	120.10
1	A	153[A]	SER	CA-C-N	5.36	129.00	117.20
1	A	153[B]	SER	CA-C-N	5.36	129.00	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1125	ARG	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3473	0	3537	63	0
2	A	36	0	33	2	0
3	A	225	0	360	9	0
4	A	1	0	0	1	0
5	A	1	0	0	0	0
6	A	91	0	0	1	0
All	All	3827	0	3930	69	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 9.

All (69) 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:1018:TYR:CE1	1:A:1026:THR:HG21	2.09	0.87
1:A:1020:ASN:O	1:A:1023:GLY:N	2.14	0.80
1:A:1019:LYS:HE3	1:A:1025:TYR:CE1	2.17	0.79
1:A:1018:TYR:CE2	1:A:1026:THR:HG23	2.22	0.75
1:A:1018:TYR:CE1	1:A:1026:THR:CG2	2.71	0.73
1:A:1018:TYR:CZ	1:A:1026:THR:CG2	2.73	0.72
1:A:1018:TYR:CZ	1:A:1026:THR:HG23	2.28	0.67
1:A:1046:LEU:HD12	1:A:1050:ILE:HG12	1.76	0.66
1:A:224:LEU:HD12	3:A:2008:OLC:H8	1.77	0.65
1:A:281:VAL:HB	1:A:282:PRO:HD3	1.79	0.63
1:A:1032:LEU:HD12	1:A:1033:LEU:N	2.15	0.61
1:A:170:PHE:HB3	1:A:174:LEU:HD23	1.81	0.61
1:A:1123:GLN:OE1	1:A:1125:ARG:NH1	2.34	0.60
1:A:1054:THR:O	1:A:1055:ASN:HB2	2.02	0.60
1:A:1018:TYR:CZ	1:A:1026:THR:HG21	2.36	0.60
1:A:1126:TRP:HB3	1:A:1154:ARG:HA	1.85	0.58
1:A:304:ASN:ND2	1:A:307:LYS:HB3	2.19	0.58
1:A:1019:LYS:HE3	1:A:1025:TYR:HE1	1.67	0.57
2:A:2001:VPX:CAG	2:A:2001:VPX:H20	2.35	0.57
1:A:233:GLY:HA2	3:A:2009:OLC:H7A	1.86	0.57
1:A:135:LYS:NZ	4:A:2011:CL:CL	2.77	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1046:LEU:O	1:A:1050:ILE:HG12	2.07	0.54
1:A:1143:PRO:O	1:A:1147:LYS:HG3	2.08	0.54
1:A:1018:TYR:CD2	1:A:1026:THR:HG23	2.43	0.53
1:A:1123:GLN:O	1:A:1124:LYS:HB2	2.08	0.53
1:A:368:PRO:HA	1:A:371:TYR:CD2	2.43	0.53
1:A:201:PHE:CE1	1:A:205:VAL:HG21	2.44	0.52
1:A:348:ALA:HB3	3:A:2007:OLC:H22	1.93	0.51
1:A:215:THR:HG22	1:A:217:GLY:H	1.76	0.50
1:A:131:MET:HE1	1:A:142:LEU:HD22	1.94	0.50
1:A:117:LEU:HB3	1:A:118:PRO:HD3	1.94	0.49
1:A:1092:ASP:O	1:A:1096:ARG:HG3	2.13	0.49
1:A:1046:LEU:HD12	1:A:1046:LEU:O	2.12	0.49
1:A:143:HIS:HE1	3:A:2008:OLC:H2	1.78	0.49
1:A:1006:MET:HG3	1:A:1161:TYR:CE2	2.48	0.48
1:A:1032:LEU:HD12	1:A:1033:LEU:H	1.78	0.48
3:A:2009:OLC:H5A	3:A:2009:OLC:C1	2.43	0.48
1:A:319:PHE:O	1:A:323:ILE:HG12	2.13	0.48
1:A:130:LYS:O	1:A:132:LYS:N	2.47	0.47
1:A:304:ASN:HD21	1:A:307:LYS:HB3	1.79	0.47
1:A:1025:TYR:CD2	1:A:1042:ALA:HB2	2.49	0.47
1:A:131:MET:CE	1:A:142:LEU:HD22	2.44	0.47
3:A:2009:OLC:O19	3:A:2009:OLC:H5A	2.15	0.47
1:A:96:LEU:HD21	1:A:257:VAL:HG21	1.97	0.46
1:A:1127:ASP:O	1:A:1131:VAL:HG23	2.16	0.46
1:A:1084:LEU:O	1:A:1087:VAL:HG12	2.16	0.46
1:A:121:ILE:O	1:A:125:VAL:HG23	2.16	0.46
1:A:176:ARG:HD2	1:A:238:LEU:O	2.16	0.45
1:A:1102:MET:O	1:A:1106:MET:HG2	2.16	0.45
1:A:155:LEU:N	1:A:156:PRO:CD	2.79	0.45
1:A:1018:TYR:O	1:A:1026:THR:HG22	2.16	0.45
1:A:310:ARG:NH2	1:A:375:SER:O	2.36	0.44
3:A:2004:OLC:H15A	3:A:2004:OLC:H12	1.40	0.44
1:A:278:PHE:O	1:A:282:PRO:HG2	2.18	0.44
1:A:170:PHE:CB	1:A:174:LEU:HD23	2.47	0.43
1:A:1018:TYR:CD1	1:A:1026:THR:CG2	3.02	0.43
1:A:158:LYS:HG3	1:A:178:VAL:HG11	2.01	0.43
2:A:2001:VPX:H29	2:A:2001:VPX:H25	1.77	0.43
1:A:1020:ASN:O	1:A:1021:THR:C	2.56	0.43
1:A:361:SER:HB3	6:A:3019:HOH:O	2.18	0.43
1:A:323:ILE:O	1:A:328:PRO:HD3	2.19	0.42
1:A:155:LEU:HD23	1:A:155:LEU:HA	1.90	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ALA:O	1:A:308:LYS:HE2	2.20	0.42
1:A:365:CYS:HB3	3:A:2005:OLC:H13	2.02	0.41
3:A:2009:OLC:H13A	3:A:2009:OLC:H10	1.43	0.41
1:A:304:ASN:O	1:A:308:LYS:HG3	2.20	0.41
1:A:148:ASP:OD1	1:A:367:ASP:OD2	2.39	0.41
1:A:1025:TYR:CE2	1:A:1039:LEU:HA	2.55	0.41
1:A:321:ILE:O	1:A:325:CYS:HB2	2.21	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	439/484 (91%)	428 (98%)	10 (2%)	1 (0%)	47 55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	MET

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	379/418 (91%)	373 (98%)	6 (2%)	62 76

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	LEU
1	A	214	ARG
1	A	258	LEU
1	A	290	TYR
1	A	300	SER
1	A	1032	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	GLN
1	A	304	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	2004	-	24,24,24	0.88	1 (4%)	25,25,25	0.92	1 (4%)
3	OLC	A	2010	-	24,24,24	0.89	1 (4%)	25,25,25	0.90	0
3	OLC	A	2008	-	24,24,24	0.96	1 (4%)	25,25,25	0.94	1 (4%)
3	OLC	A	2002	-	24,24,24	0.90	1 (4%)	25,25,25	0.92	1 (4%)
3	OLC	A	2005	-	24,24,24	0.89	1 (4%)	25,25,25	0.91	1 (4%)
3	OLC	A	2006	-	24,24,24	0.90	1 (4%)	25,25,25	0.92	1 (4%)
3	OLC	A	2009	-	24,24,24	0.90	1 (4%)	25,25,25	0.92	1 (4%)
3	OLC	A	2003	-	24,24,24	0.90	1 (4%)	25,25,25	0.92	1 (4%)
3	OLC	A	2007	-	24,24,24	0.97	1 (4%)	25,25,25	0.95	1 (4%)
2	VPX	A	2001	-	40,40,40	2.08	5 (12%)	49,57,57	2.52	16 (32%)

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	2004	-	-	10/24/24/24	-
3	OLC	A	2010	-	-	17/24/24/24	-
3	OLC	A	2008	-	-	4/24/24/24	-
3	OLC	A	2002	-	-	14/24/24/24	-
3	OLC	A	2005	-	-	10/24/24/24	-
3	OLC	A	2006	-	-	14/24/24/24	-
3	OLC	A	2009	-	-	11/24/24/24	-
3	OLC	A	2003	-	-	13/24/24/24	-
3	OLC	A	2007	-	-	3/24/24/24	-
2	VPX	A	2001	-	-	0/16/57/57	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	VPX	CBH-CAY	-8.71	1.38	1.51
2	A	2001	VPX	CAF-CAG	6.30	1.53	1.31
3	A	2007	OLC	C9-C10	3.88	1.54	1.31
2	A	2001	VPX	CBC-CBB	-3.87	1.39	1.49
3	A	2008	OLC	C9-C10	3.84	1.54	1.31
3	A	2009	OLC	C9-C10	3.74	1.53	1.31
3	A	2005	OLC	C9-C10	3.74	1.53	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2002	OLC	C9-C10	3.74	1.53	1.31
3	A	2006	OLC	C9-C10	3.74	1.53	1.31
3	A	2003	OLC	C9-C10	3.73	1.53	1.31
3	A	2004	OLC	C9-C10	3.72	1.53	1.31
3	A	2010	OLC	C9-C10	3.71	1.53	1.31
2	A	2001	VPX	CBA-CAF	-3.05	1.39	1.47
2	A	2001	VPX	CAM-NAT	2.51	1.39	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	VPX	CBF-CAG-CAF	-10.06	107.82	124.30
2	A	2001	VPX	OAD-CAY-CBH	-5.51	121.22	128.83
2	A	2001	VPX	CBD-OAW-CAY	-5.14	105.36	110.48
2	A	2001	VPX	OAV-CAX-NAU	4.56	119.78	110.50
2	A	2001	VPX	OAW-CAY-CBH	3.63	114.49	110.13
2	A	2001	VPX	CAM-NAT-CBA	3.61	121.09	116.92
2	A	2001	VPX	CBJ-CBH-CAY	-3.38	99.13	103.53
2	A	2001	VPX	CAO-OAV-CAX	-3.27	109.85	116.04
2	A	2001	VPX	CAB-CBD-CBJ	-3.24	109.93	116.71
2	A	2001	VPX	OAC-CAX-NAU	-2.82	120.22	124.85
2	A	2001	VPX	CBB-CAM-NAT	-2.75	119.79	124.32
2	A	2001	VPX	CAS-CBG-CAR	-2.62	108.78	113.05
2	A	2001	VPX	CAI-CAZ-CAN	-2.61	119.90	123.29
3	A	2007	OLC	C3-C2-C1	-2.38	104.96	113.62
2	A	2001	VPX	OAW-CAY-OAD	2.37	124.28	121.29
2	A	2001	VPX	OAV-CAX-OAC	-2.21	120.00	124.25
3	A	2002	OLC	C21-O20-C1	-2.13	109.24	117.12
3	A	2005	OLC	C21-O20-C1	-2.10	109.33	117.12
3	A	2004	OLC	C21-O20-C1	-2.10	109.34	117.12
2	A	2001	VPX	CBF-CBI-CBG	-2.05	108.69	111.74
3	A	2003	OLC	C21-O20-C1	-2.04	109.56	117.12
3	A	2008	OLC	C11-C10-C9	-2.04	109.08	124.73
3	A	2009	OLC	C21-O20-C1	-2.04	109.58	117.12
3	A	2006	OLC	C21-O20-C1	-2.00	109.70	117.12

There are no chirality outliers.

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2004	OLC	C21-C22-C24-O25
3	A	2004	OLC	O23-C22-C24-O25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	2010	OLC	C21-C22-C24-O25
3	A	2006	OLC	C21-C22-C24-O25
3	A	2006	OLC	C2-C1-O20-C21
3	A	2009	OLC	C10-C11-C12-C13
3	A	2009	OLC	C21-C22-C24-O25
3	A	2003	OLC	C21-C22-C24-O25
3	A	2003	OLC	O20-C21-C22-C24
3	A	2006	OLC	O19-C1-O20-C21
3	A	2009	OLC	O19-C1-O20-C21
3	A	2009	OLC	C2-C1-O20-C21
3	A	2008	OLC	O19-C1-O20-C21
3	A	2007	OLC	O19-C1-O20-C21
3	A	2008	OLC	C2-C1-O20-C21
3	A	2007	OLC	C2-C1-O20-C21
3	A	2003	OLC	O20-C21-C22-O23
3	A	2002	OLC	C14-C15-C16-C17
3	A	2010	OLC	C2-C1-O20-C21
3	A	2002	OLC	O20-C21-C22-C24
3	A	2010	OLC	O20-C21-C22-O23
3	A	2002	OLC	O20-C21-C22-O23
3	A	2006	OLC	C1-C2-C3-C4
3	A	2010	OLC	O19-C1-O20-C21
3	A	2004	OLC	C3-C4-C5-C6
3	A	2004	OLC	C12-C13-C14-C15
3	A	2006	OLC	C6-C7-C8-C9
3	A	2010	OLC	C5-C6-C7-C8
3	A	2010	OLC	O20-C21-C22-C24
3	A	2004	OLC	C13-C14-C15-C16
3	A	2005	OLC	C13-C14-C15-C16
3	A	2005	OLC	C10-C11-C12-C13
3	A	2010	OLC	C14-C15-C16-C17
3	A	2010	OLC	C4-C5-C6-C7
3	A	2003	OLC	C4-C5-C6-C7
3	A	2010	OLC	O23-C22-C24-O25
3	A	2009	OLC	O23-C22-C24-O25
3	A	2003	OLC	C11-C12-C13-C14
3	A	2003	OLC	C13-C14-C15-C16
3	A	2010	OLC	C10-C11-C12-C13
3	A	2005	OLC	C6-C7-C8-C9
3	A	2010	OLC	C11-C12-C13-C14
3	A	2004	OLC	C5-C6-C7-C8
3	A	2006	OLC	O20-C21-C22-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	2002	OLC	C4-C5-C6-C7
3	A	2006	OLC	C4-C5-C6-C7
3	A	2010	OLC	C2-C3-C4-C5
3	A	2002	OLC	C11-C12-C13-C14
3	A	2010	OLC	C7-C8-C9-C10
3	A	2008	OLC	C7-C8-C9-C10
3	A	2009	OLC	C11-C12-C13-C14
3	A	2002	OLC	C2-C1-O20-C21
3	A	2006	OLC	C14-C15-C16-C17
3	A	2010	OLC	C13-C14-C15-C16
3	A	2006	OLC	O23-C22-C24-O25
3	A	2003	OLC	O23-C22-C24-O25
3	A	2006	OLC	C10-C11-C12-C13
3	A	2006	OLC	O20-C21-C22-O23
3	A	2002	OLC	C13-C14-C15-C16
3	A	2009	OLC	C5-C6-C7-C8
3	A	2003	OLC	C3-C4-C5-C6
3	A	2002	OLC	O19-C1-O20-C21
3	A	2006	OLC	C5-C6-C7-C8
3	A	2002	OLC	C15-C16-C17-C18
3	A	2003	OLC	C2-C1-O20-C21
3	A	2005	OLC	C5-C6-C7-C8
3	A	2010	OLC	C15-C16-C17-C18
3	A	2005	OLC	C12-C13-C14-C15
3	A	2008	OLC	C9-C10-C11-C12
3	A	2010	OLC	C12-C13-C14-C15
3	A	2003	OLC	O19-C1-O20-C21
3	A	2005	OLC	O23-C22-C24-O25
3	A	2004	OLC	C4-C5-C6-C7
3	A	2009	OLC	C15-C16-C17-C18
3	A	2009	OLC	C1-C2-C3-C4
3	A	2009	OLC	C14-C15-C16-C17
3	A	2003	OLC	C6-C7-C8-C9
3	A	2009	OLC	C6-C7-C8-C9
3	A	2004	OLC	C15-C16-C17-C18
3	A	2002	OLC	C6-C7-C8-C9
3	A	2005	OLC	C11-C12-C13-C14
3	A	2002	OLC	C2-C3-C4-C5
3	A	2005	OLC	C9-C10-C11-C12
3	A	2006	OLC	C7-C8-C9-C10
3	A	2005	OLC	C21-C22-C24-O25
3	A	2004	OLC	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

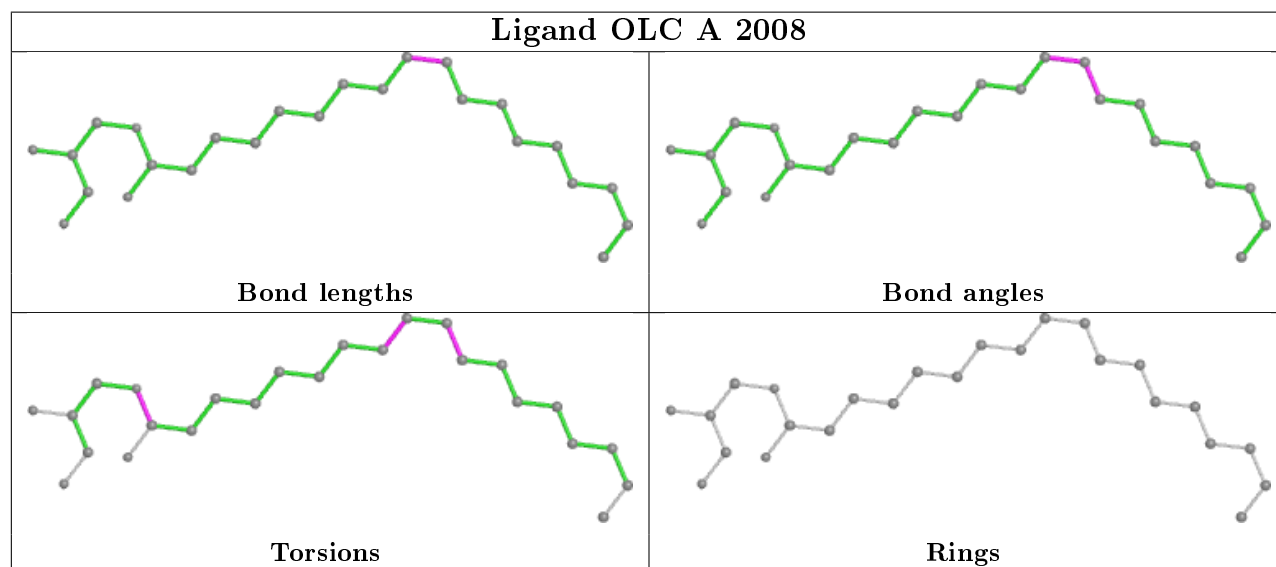
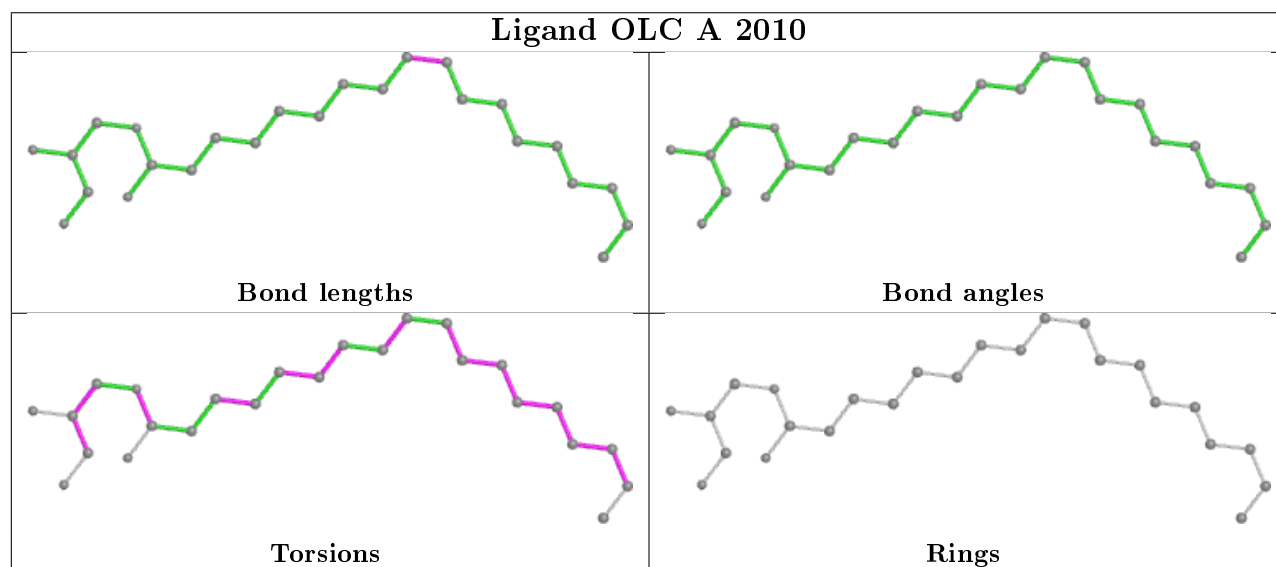
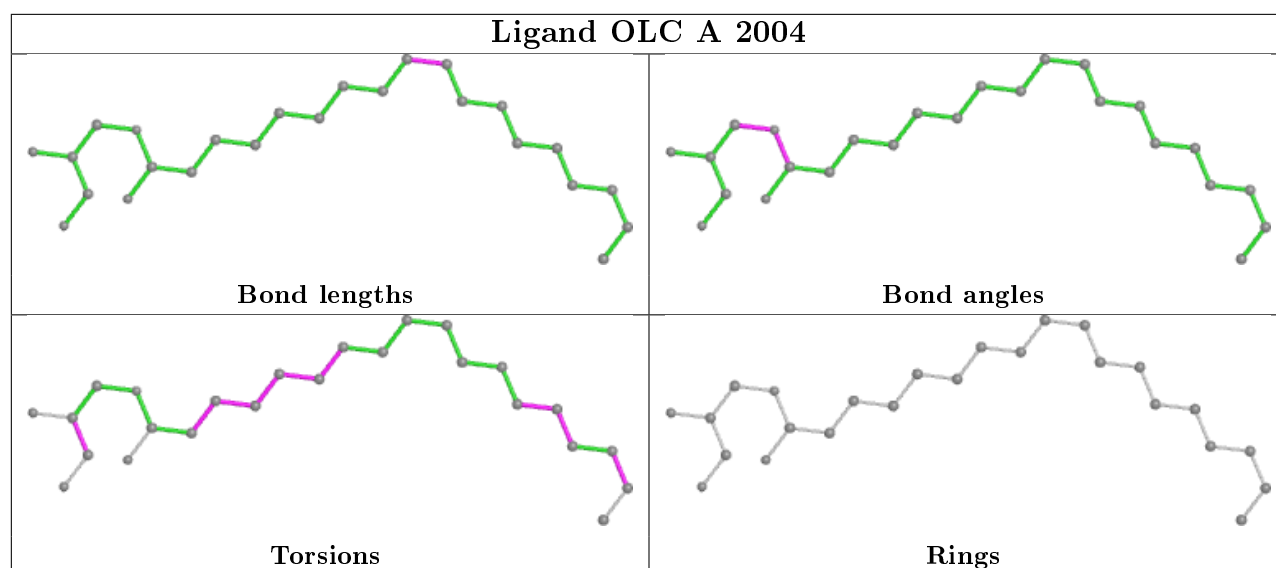
Mol	Chain	Res	Type	Atoms
3	A	2002	OLC	C5-C6-C7-C8
3	A	2003	OLC	C5-C6-C7-C8
3	A	2010	OLC	C9-C10-C11-C12
3	A	2002	OLC	C7-C8-C9-C10
3	A	2007	OLC	C7-C8-C9-C10
3	A	2005	OLC	C15-C16-C17-C18
3	A	2006	OLC	C15-C16-C17-C18
3	A	2002	OLC	C3-C4-C5-C6
3	A	2004	OLC	C1-C2-C3-C4
3	A	2003	OLC	C9-C10-C11-C12

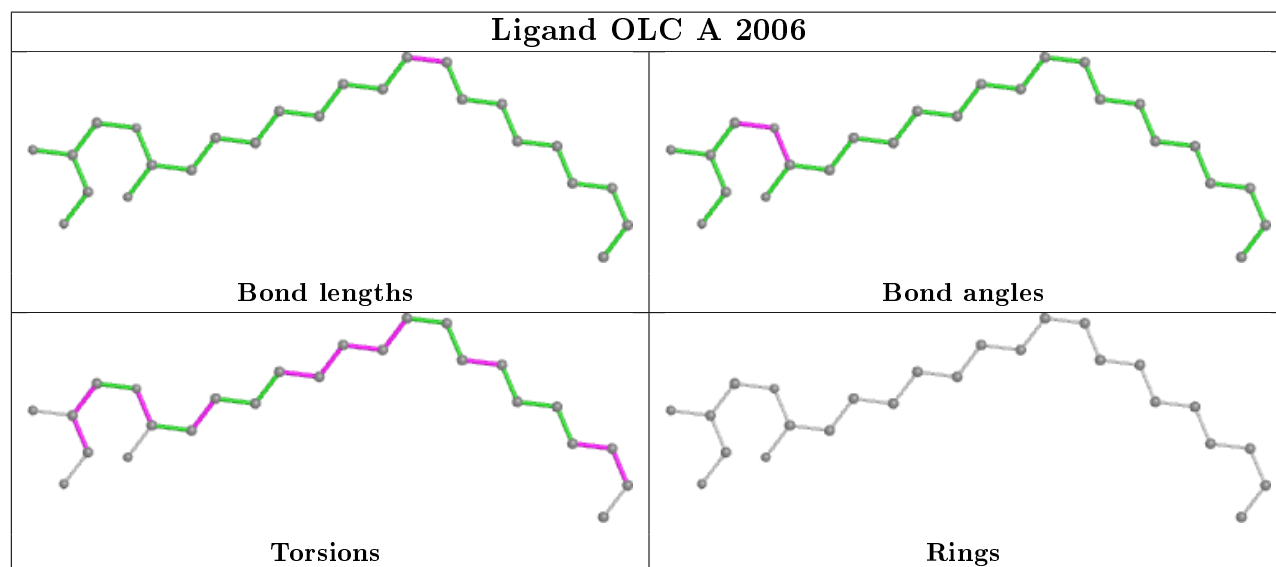
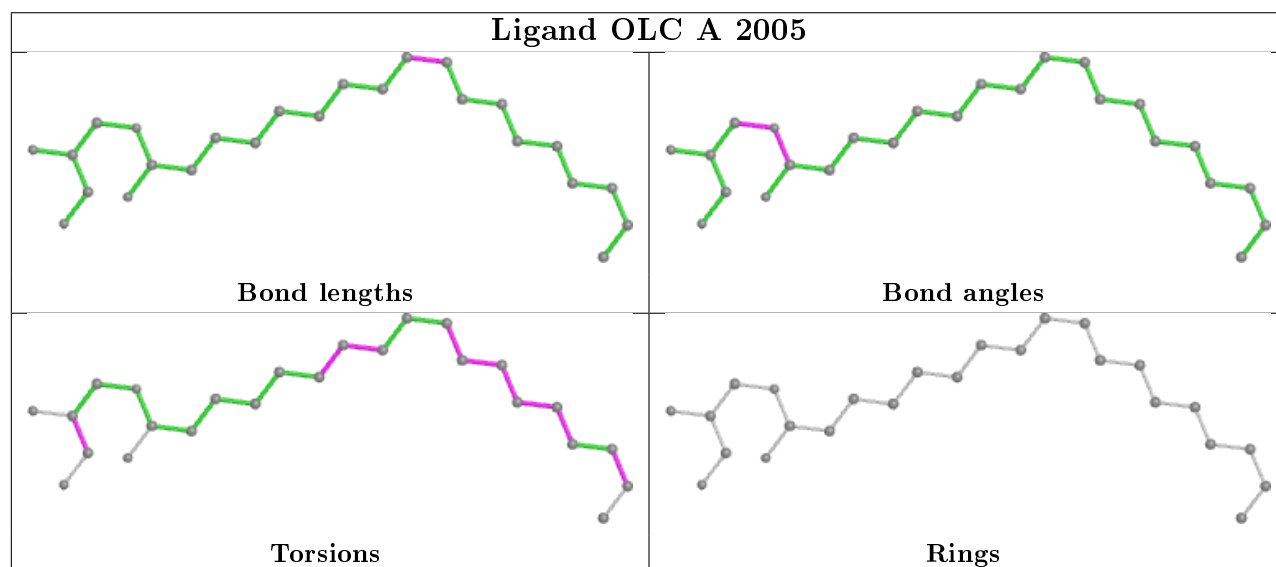
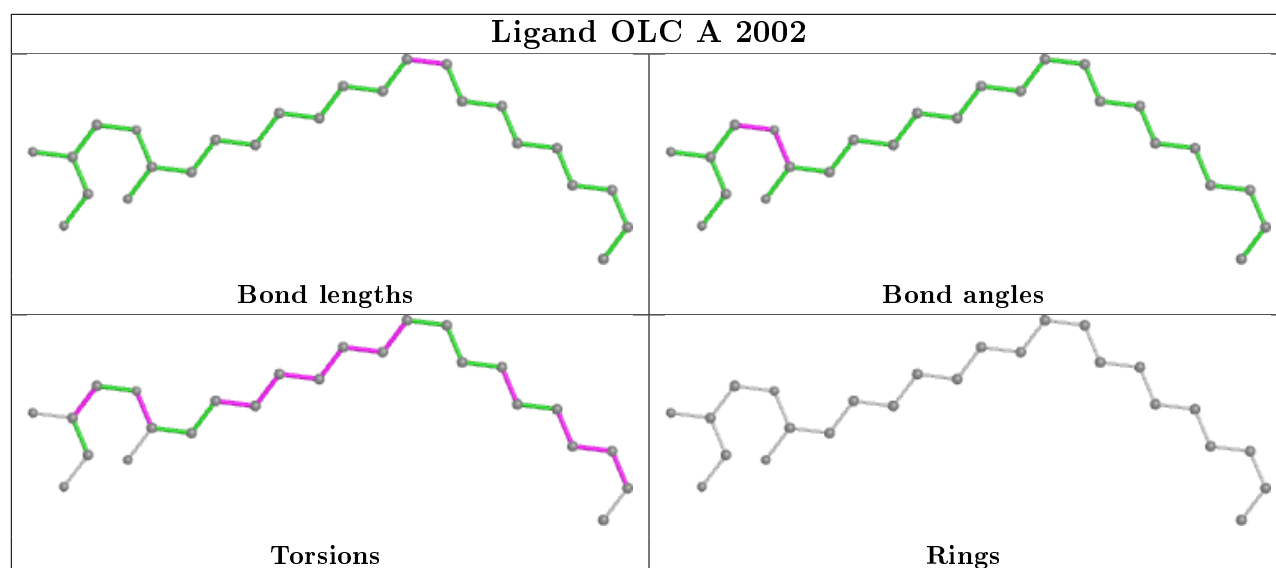
There are no ring outliers.

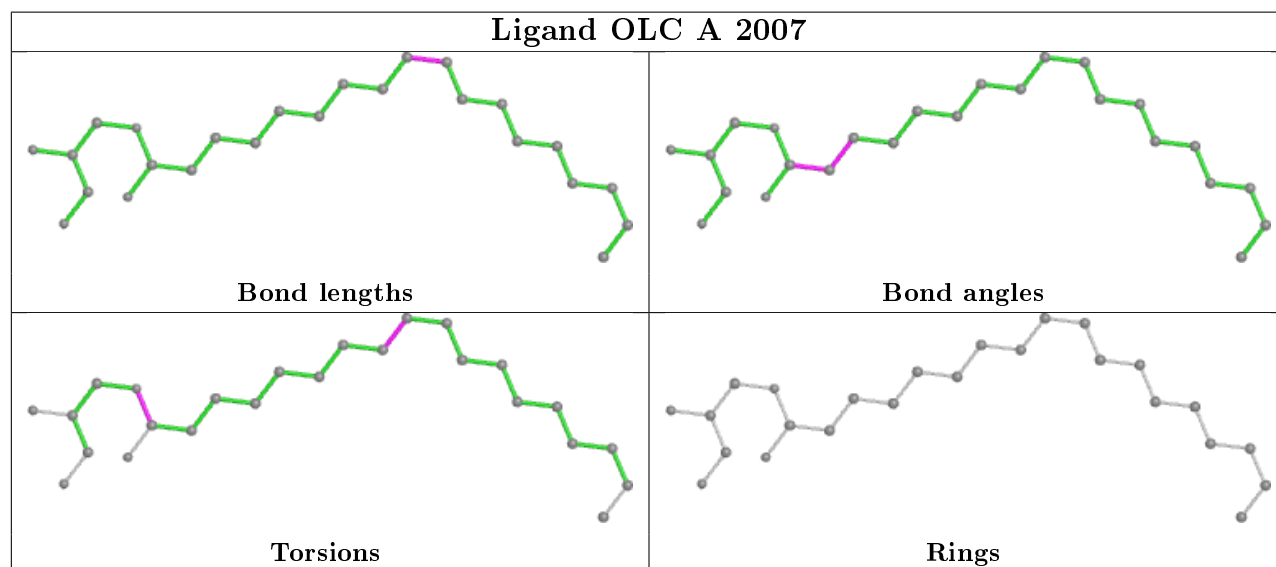
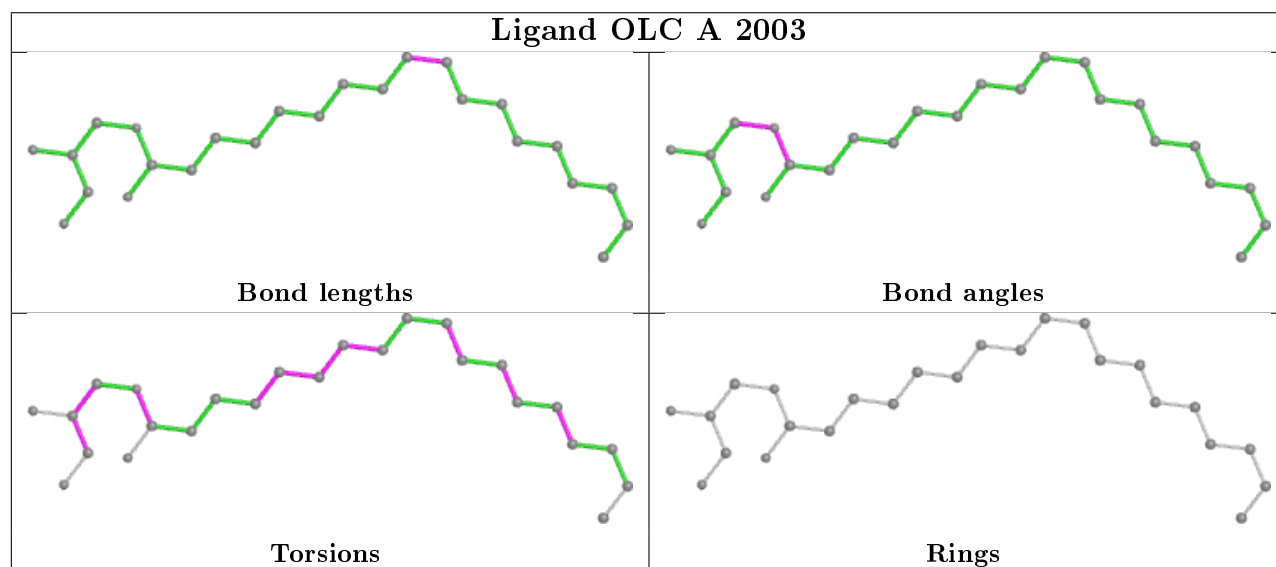
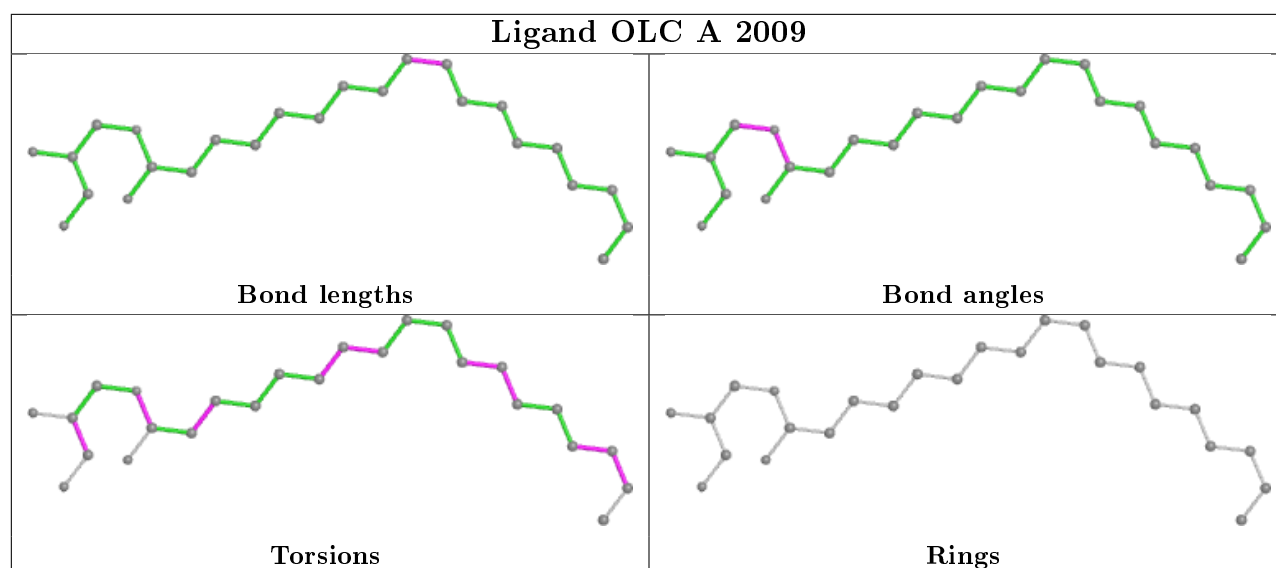
6 monomers are involved in 11 short contacts:

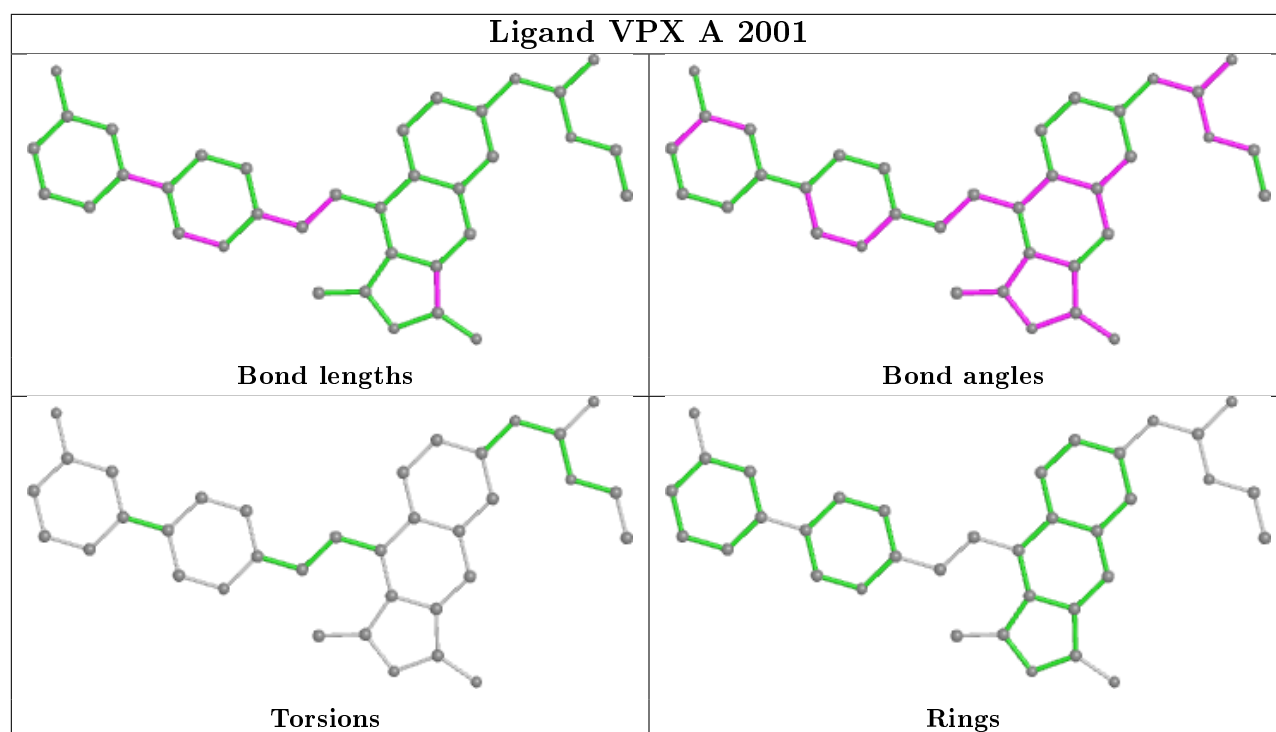
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2004	OLC	1	0
3	A	2008	OLC	2	0
3	A	2005	OLC	1	0
3	A	2009	OLC	4	0
3	A	2007	OLC	1	0
2	A	2001	VPX	2	0

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 ⓘ

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	442/484 (91%)	0.05	19 (4%) 35 33	24, 40, 76, 116	8 (1%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	378	CYS	4.8
1	A	1036	SER	3.8
1	A	1023	GLY	3.8
1	A	298	SER	3.7
1	A	1037	PRO	3.4
1	A	1022	GLU	3.3
1	A	1035	LYS	3.1
1	A	1034	THR	3.0
1	A	206	TYR	2.9
1	A	295	ARG	2.8
1	A	1021	THR	2.8
1	A	208	MET	2.7
1	A	300	SER	2.7
1	A	93	SER	2.4
1	A	1025	TYR	2.4
1	A	1018	TYR	2.2
1	A	294	ILE	2.2
1	A	326	PHE	2.1
1	A	91	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

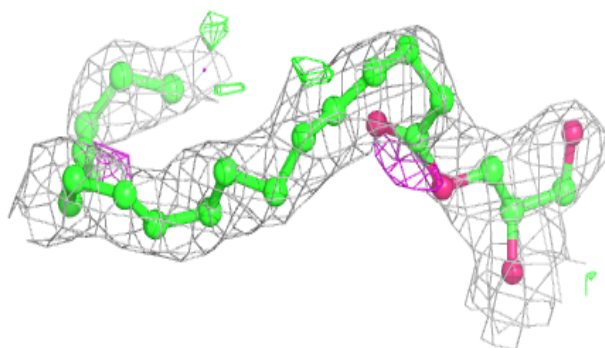
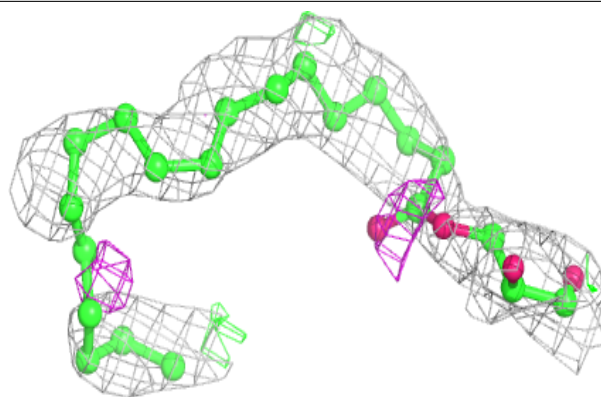
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	OLC	A	2009	25/25	0.58	0.29	51,61,82,83	0
3	OLC	A	2007	25/25	0.69	0.32	49,67,102,102	0
3	OLC	A	2005	25/25	0.70	0.27	53,70,88,88	0
3	OLC	A	2006	25/25	0.71	0.25	58,66,87,90	1
3	OLC	A	2008	25/25	0.73	0.32	75,80,83,84	0
3	OLC	A	2002	25/25	0.74	0.23	71,72,77,82	3
3	OLC	A	2010	25/25	0.78	0.26	51,56,67,68	4
3	OLC	A	2003	25/25	0.79	0.18	44,57,80,83	2
3	OLC	A	2004	25/25	0.81	0.30	45,53,79,83	3
5	NA	A	2012	1/1	0.89	0.09	35,35,35,35	0
4	CL	A	2011	1/1	0.93	0.11	71,71,71,71	0
2	VPX	A	2001	36/36	0.96	0.15	24,29,39,43	0

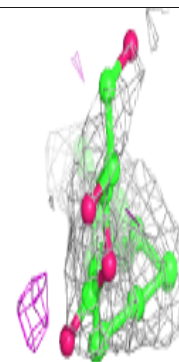
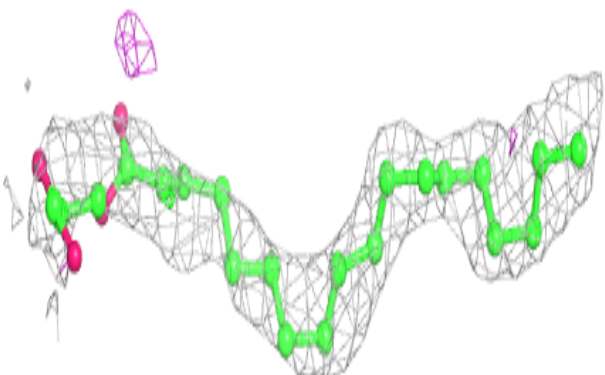
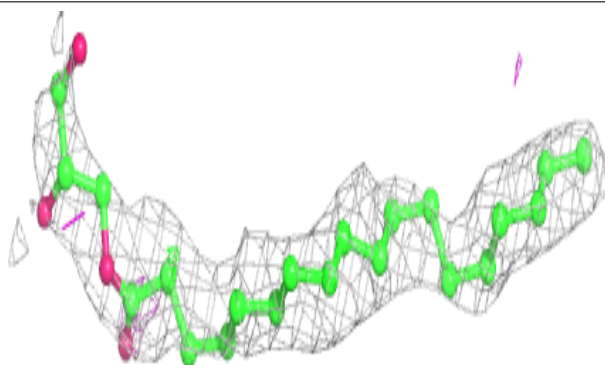
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 2009:

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

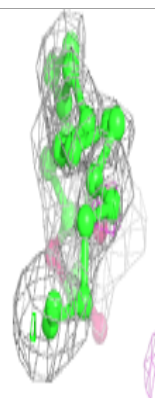
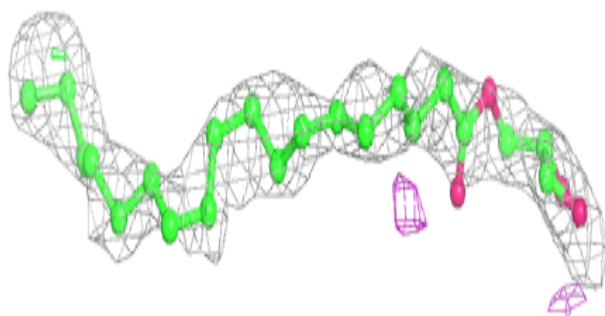
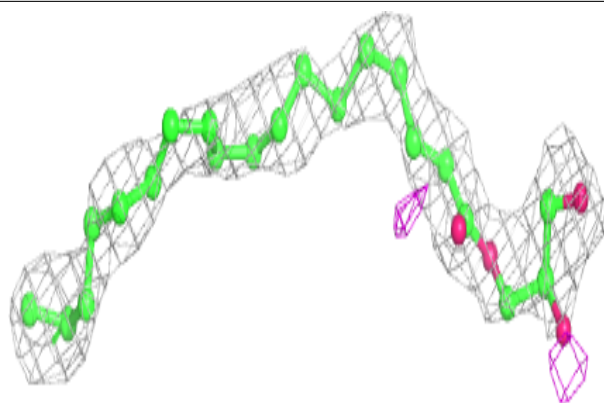
**Electron density around OLC A 2007:**

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

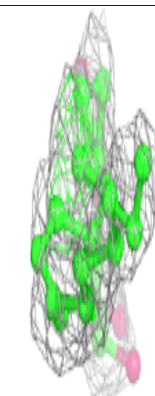
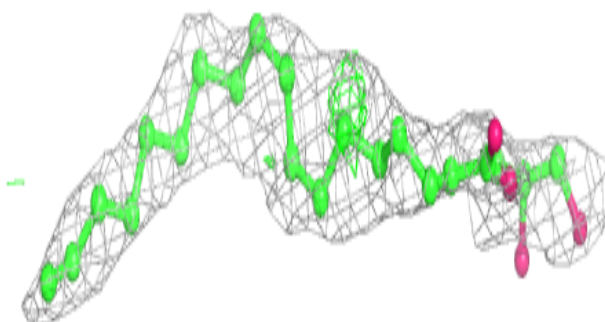
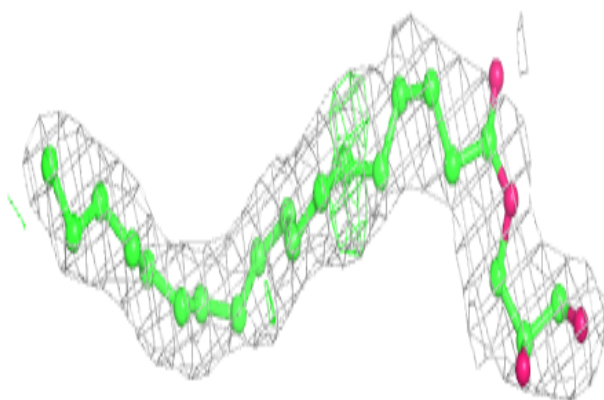


Electron density around OLC A 2005:

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

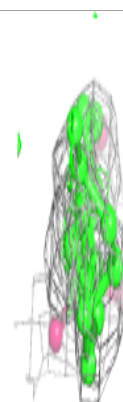
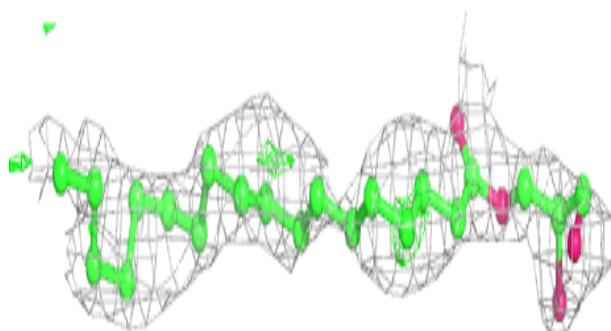
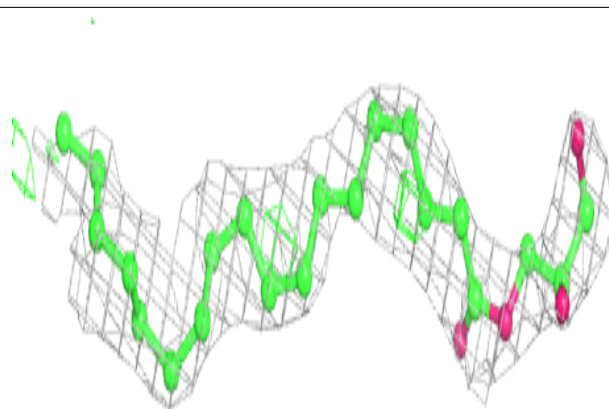
**Electron density around OLC A 2006:**

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

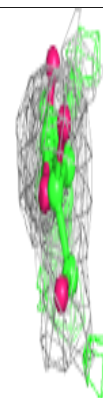
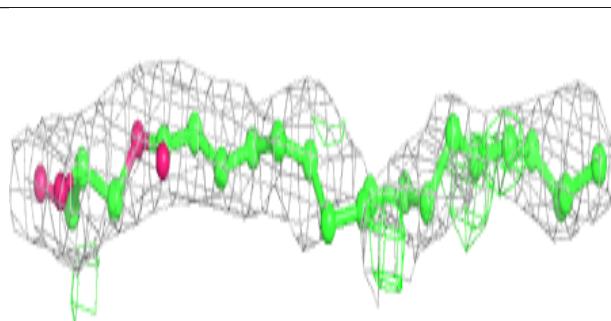
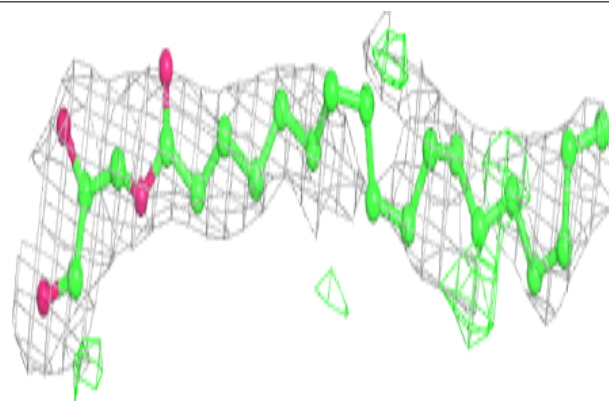


Electron density around OLC A 2008:

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

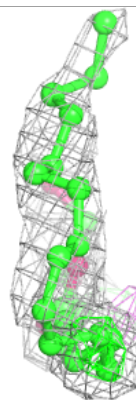
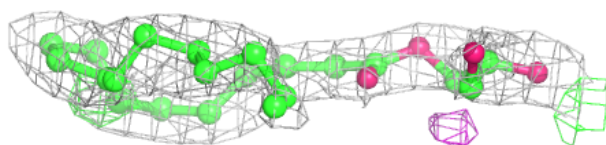
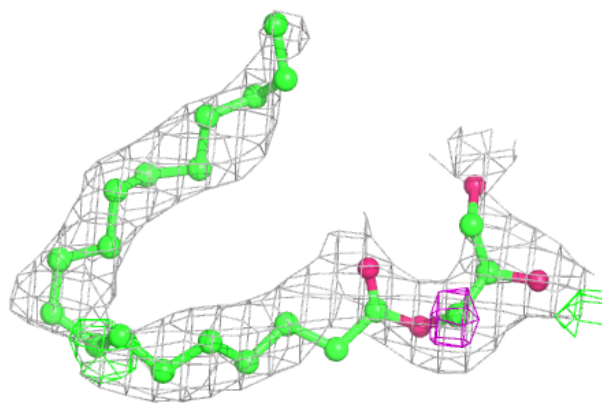
**Electron density around OLC A 2002:**

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

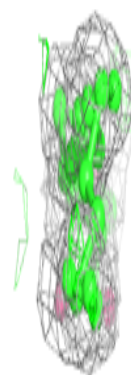
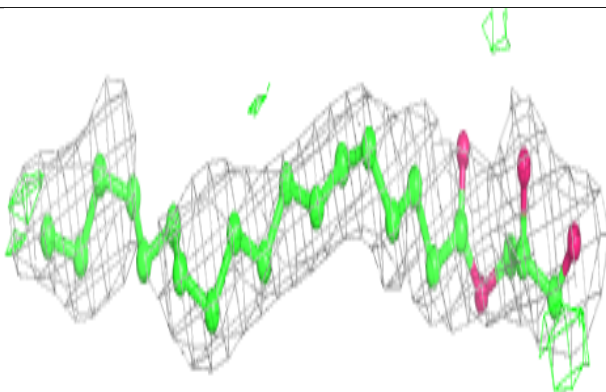
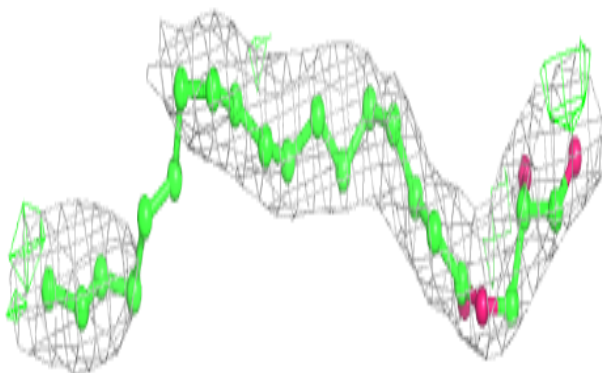


Electron density around OLC A 2010:

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

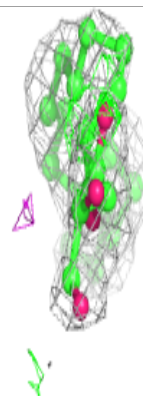
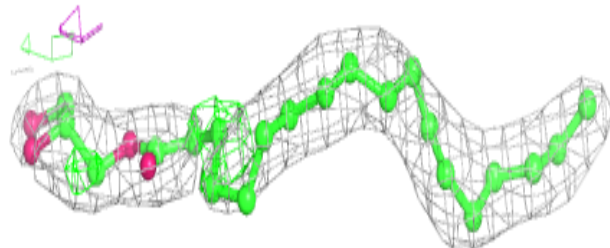
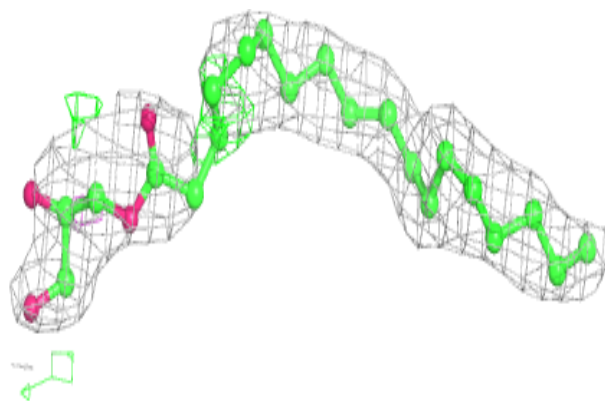
**Electron density around OLC A 2003:**

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

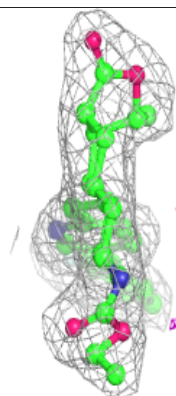
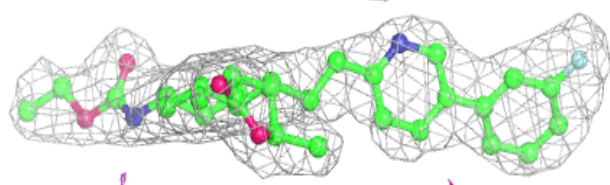
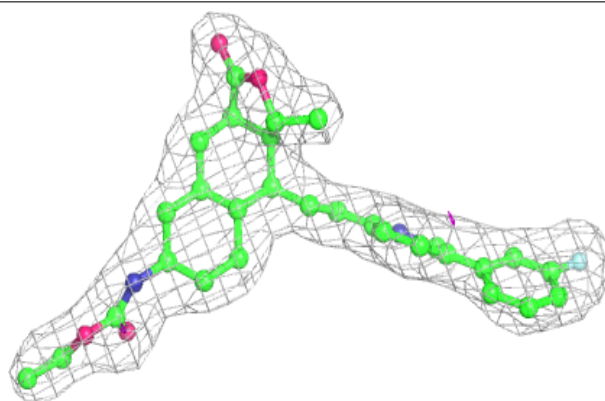


Electron density around OLC A 2004:

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

**Electron density around VPX A 2001:**

$2mF_o-DF_c$ (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.