



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 04:14 AM UTC

PDB ID : 7Z0E / pdb_00007z0e
Title : Crystal structure of the M state of bacteriorhodopsin at 1.22 Angstrom resolution
Authors : Borshchevskiy, V.; Kovalev, K.; Round, E.; Efremov, R.; Bourenkov, G.; Gordeliy, V.
Deposited on : 2022-02-22
Resolution : 1.22 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	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

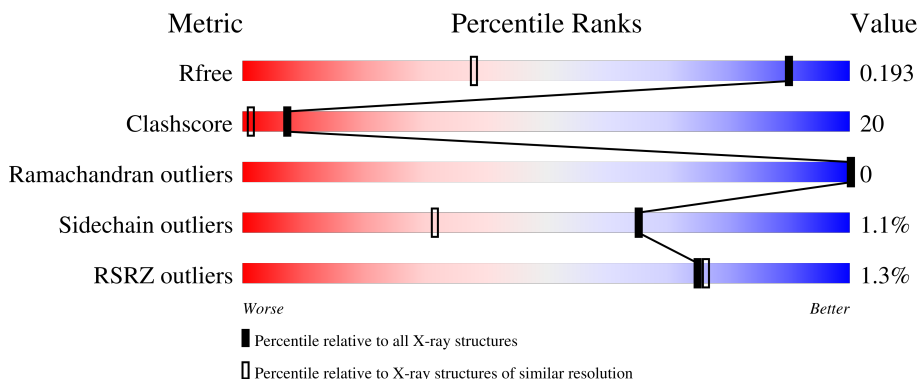
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.22 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	2002 (1.24-1.20)
Clashscore	190562	2061 (1.24-1.20)
Ramachandran outliers	187476	2009 (1.24-1.20)
Sidechain outliers	187428	2008 (1.24-1.20)
RSRZ outliers	180081	2000 (1.24-1.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	P	248	

2 Entry composition [i](#)

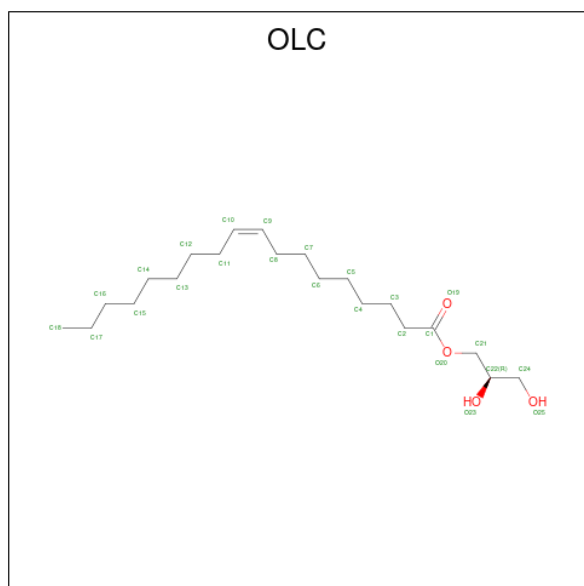
There are 6 unique types of molecules in this entry. The entry contains 6577 atoms, of which 3336 are hydrogens and 0 are deuteriums.

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 Bacteriorhodopsin.

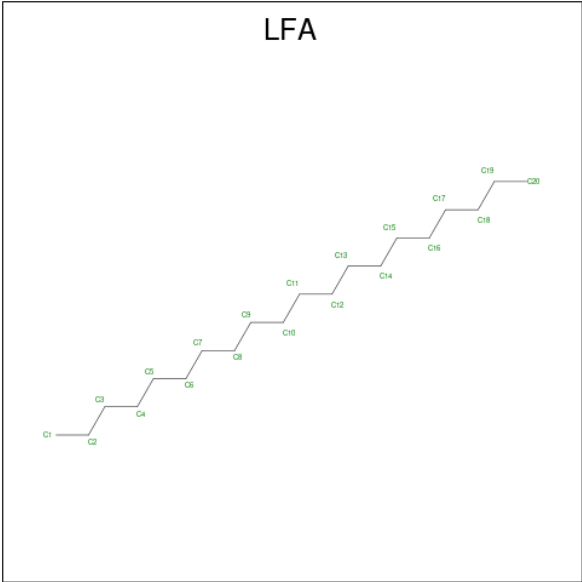
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	P	230	Total	C	H	N	O	S	23	140	0
			5839	1943	2964	425	490	17			

- Molecule 2 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
2	P	1	Total	C	H	O	0	0
			65	21	40	4		

- Molecule 3 is EICOSANE (CCD ID: LFA) (formula: $C_{20}H_{42}$).



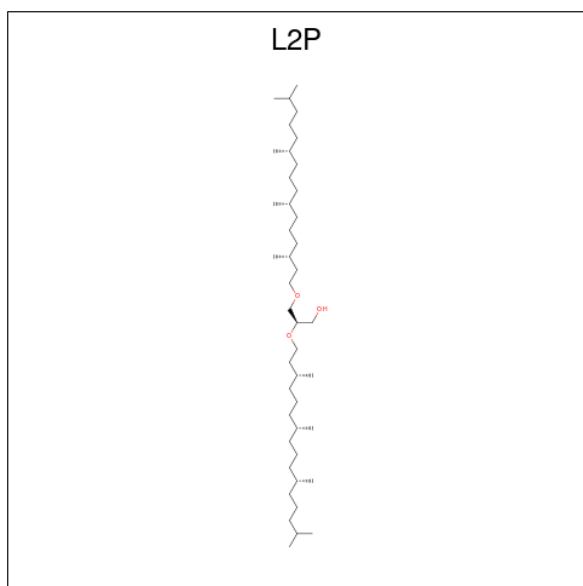
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	1	Total C 9 9	0	0
3	P	1	Total C H 26 12 14	0	0
3	P	1	Total C H 34 12 22	0	0
3	P	1	Total C H 18 10 8	0	0
3	P	1	Total C H 8 6 2	0	0
3	P	1	Total C H 23 11 12	0	0
3	P	1	Total C 6 6	0	0
3	P	1	Total C H 19 9 10	0	0
3	P	1	Total C 3 3	0	0
3	P	1	Total C 7 7	0	0
3	P	1	Total C 6 6	0	0
3	P	1	Total C H 55 18 37	0	0
3	P	1	Total C 5 5	0	0
3	P	1	Total C H 19 9 10	0	0

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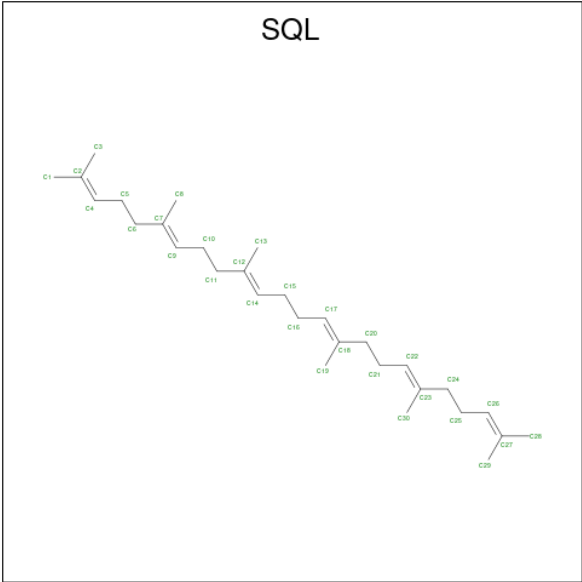
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	P	1	Total	C	H	0	0
			62	20	42		
3	P	1	Total	C	H	0	0
			11	9	2		
3	P	1	Total	C	H	0	0
			46	15	31		
3	P	1	Total	C		0	0
			3	3			
3	P	1	Total	C	H	0	0
			11	7	4		

- Molecule 4 is 2,3-DI-PHYTANYL-GLYCEROL (CCD ID: L2P) (formula: $C_{43}H_{88}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	P	1	Total	C	H	O	0	0
			134	43	88	3		

- Molecule 5 is (6E,10E,14E,18E)-2,6,10,15,19,23-hexamethyltetracos-2,6,10,14,18,22-hexaene (CCD ID: SQL) (formula: $C_{30}H_{50}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	P	1	Total	C	H	0	0
			80	30	50		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	74	Total	O	0	12
			88	88		

- Molecule 1: Bacteriorhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	60.89Å 60.89Å 109.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.45 – 1.22 30.45 – 1.22	Depositor EDS
% Data completeness (in resolution range)	97.7 (30.45-1.22) 97.6 (30.45-1.22)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 1.22Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.182 , 0.195 0.180 , 0.193	Depositor DCC
R_{free} test set	2174 reflections (3.22%)	wwPDB-VP
Wilson B-factor (Å ²)	15.5	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.54 , 110.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.317 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.320 for k,h,-l	Depositor
Outliers	0 of 66432 reflections	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	6577	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.38% 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: LYR, SQL, LFA, OLC, L2P

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	P	0.43	0/3026	0.64	0/4137

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	P	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	32[B]	MET	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	2875	2964	2802	116	0
2	P	25	40	40	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	177	194	293	21	0
4	P	46	88	88	12	0
5	P	30	50	50	14	0
6	P	88	0	0	13	0
All	All	3241	3336	3273	134	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 20.

The worst 5 of 134 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:P:159:LYS:O	1:P:163:MET:HE3	1.57	1.05
1:P:217[A]:VAL:HG11	5:P:312:SQL:H20	1.39	1.02
1:P:217[C]:VAL:HG11	5:P:312:SQL:H20	1.42	1.02
1:P:194[B]:GLU:OE1	6:P:433[B]:HOH:O	1.78	1.01
2:P:302:OLC:H24A	6:P:429:HOH:O	1.71	0.91

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	P	378/248 (152%)	376 (100%)	2 (0%)	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	P	306/193 (158%)	303 (99%)	3 (1%)	68 36

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

Mol	Chain	Res	Type
1	P	32[A]	MET
1	P	32[B]	MET
1	P	158	SER

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	LYR	P	216[A]	1	27,29,30	2.26	8 (29%)	30,37,39	2.59	11 (36%)
1	LYR	P	216[C]	1	27,29,30	1.66	6 (22%)	30,37,39	3.12	14 (46%)

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	LYR	P	216[A]	1	-	2/22/40/42	0/1/1/1
1	LYR	P	216[C]	1	-	3/22/40/42	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	216[A]	LYR	C17-C11	7.33	1.63	1.53
1	P	216[C]	LYR	C19-C17	-4.24	1.45	1.53
1	P	216[C]	LYR	C12-C11	3.67	1.40	1.34
1	P	216[A]	LYR	C5-C3	-3.58	1.38	1.46
1	P	216[A]	LYR	C18-C17	-3.56	1.47	1.53

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	216[C]	LYR	C18-C17-C11	-10.44	93.87	110.24
1	P	216[A]	LYR	C19-C17-C11	-8.31	97.21	110.24
1	P	216[C]	LYR	C19-C17-C11	-6.82	99.55	110.24
1	P	216[A]	LYR	C1-NZ-CE	5.75	124.52	112.85
1	P	216[C]	LYR	C5-C3-C2	5.28	125.84	118.49

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	P	216[C]	LYR	C2-C1-NZ-CE
1	P	216[C]	LYR	CG-CD-CE-NZ
1	P	216[A]	LYR	C2-C1-NZ-CE
1	P	216[C]	LYR	CD-CE-NZ-C1
1	P	216[A]	LYR	CD-CE-NZ-C1

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	216[A]	LYR	5	0
1	P	216[C]	LYR	7	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
3	LFA	P	320	-	8,8,19	0.15	0	7,7,18	0.42	0
3	LFA	P	317	-	4,4,19	0.25	0	3,3,18	0.27	0
3	LFA	P	321	-	14,14,19	0.25	0	13,13,18	0.81	0
2	OLC	P	302	-	24,24,24	0.85	2 (8%)	25,25,25	1.07	2 (8%)
3	LFA	P	307	-	5,5,19	0.22	0	4,4,18	0.51	0
3	LFA	P	306	-	9,9,19	0.25	0	8,8,18	1.71	2 (25%)
3	LFA	P	309	-	5,5,19	0.13	0	4,4,18	0.37	0
3	LFA	P	303	-	8,8,19	0.44	0	7,7,18	0.94	0
3	LFA	P	315	-	5,5,19	0.21	0	4,4,18	0.42	0
4	L2P	P	310	-	45,45,45	0.36	0	51,53,53	0.81	2 (3%)
3	LFA	P	323	-	6,6,19	0.25	0	5,5,18	0.27	0
5	SQL	P	312	-	29,29,29	2.16	12 (41%)	32,34,34	1.54	7 (21%)
3	LFA	P	313	-	2,2,19	0.24	0	1,1,18	0.01	0
3	LFA	P	319	-	19,19,19	0.12	0	18,18,18	0.71	0
3	LFA	P	316	-	17,17,19	0.29	0	16,16,18	0.87	0
3	LFA	P	308	-	10,10,19	0.26	0	9,9,18	0.53	0
3	LFA	P	318	-	8,8,19	0.15	0	7,7,18	0.75	0
3	LFA	P	304	-	11,11,19	0.47	0	10,10,18	1.02	0
3	LFA	P	305	-	11,11,19	0.22	0	10,10,18	0.59	0
3	LFA	P	322	-	2,2,19	0.07	0	1,1,18	0.11	0
3	LFA	P	311	-	8,8,19	0.19	0	7,7,18	0.52	0
3	LFA	P	314	-	6,6,19	0.32	0	5,5,18	0.43	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
3	LFA	P	320	-	-	5/6/6/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	P	317	-	-	2/2/2/17	-
3	LFA	P	321	-	-	7/12/12/17	-
2	OLC	P	302	-	-	5/24/24/24	-
3	LFA	P	307	-	-	1/3/3/17	-
3	LFA	P	306	-	-	6/7/7/17	-
3	LFA	P	309	-	-	3/3/3/17	-
3	LFA	P	303	-	-	1/6/6/17	-
3	LFA	P	315	-	-	0/3/3/17	-
4	L2P	P	310	-	-	26/51/51/51	-
3	LFA	P	323	-	-	2/4/4/17	-
5	SQL	P	312	-	-	6/31/31/31	-
3	LFA	P	319	-	-	9/17/17/17	-
3	LFA	P	316	-	-	9/15/15/17	-
3	LFA	P	308	-	-	2/8/8/17	-
3	LFA	P	318	-	-	2/6/6/17	-
3	LFA	P	304	-	-	6/9/9/17	-
3	LFA	P	305	-	-	3/9/9/17	-
3	LFA	P	311	-	-	2/6/6/17	-
3	LFA	P	314	-	-	2/4/4/17	-

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	312	SQL	C5-C4	-3.99	1.38	1.50
5	P	312	SQL	C25-C26	-3.73	1.39	1.50
5	P	312	SQL	C15-C14	-3.64	1.39	1.50
5	P	312	SQL	C10-C9	-3.53	1.39	1.50
5	P	312	SQL	C16-C17	-3.46	1.40	1.50

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	306	LFA	C12-C11-C10	2.89	129.00	114.37
3	P	306	LFA	C13-C12-C11	-2.75	100.45	114.37
5	P	312	SQL	C10-C9-C7	-2.66	121.53	127.62
5	P	312	SQL	C29-C27-C28	2.56	120.49	114.59
2	P	302	OLC	O20-C1-C2	2.56	119.63	111.83

There are no chirality outliers.

5 of 99 torsion outliers are listed below:

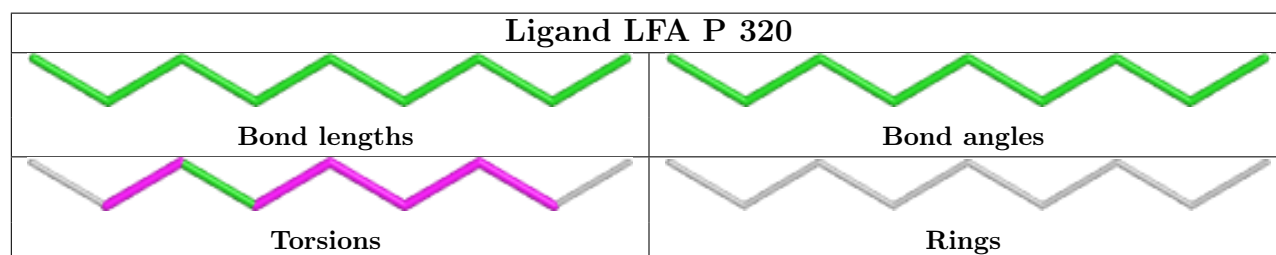
Mol	Chain	Res	Type	Atoms
4	P	310	L2P	C1-C2-C3-O3
4	P	310	L2P	O2-C2-C3-O3
4	P	310	L2P	C41-C42-C43-C44
5	P	312	SQL	C14-C15-C16-C17
5	P	312	SQL	C5-C6-C7-C8

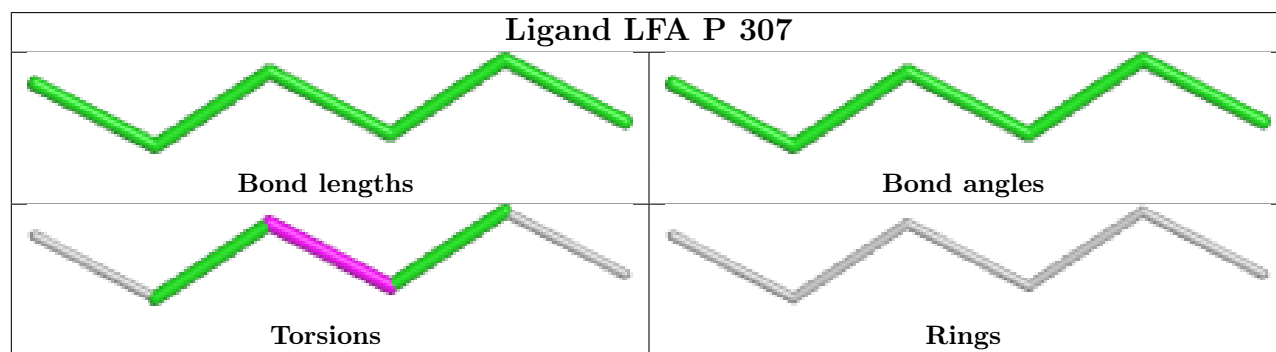
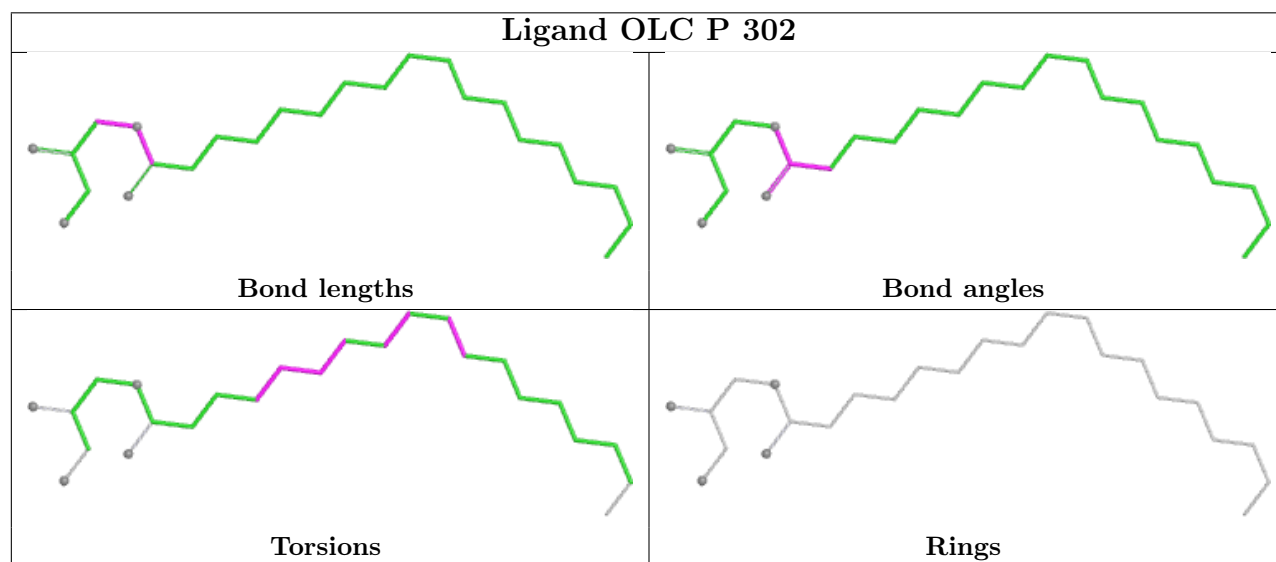
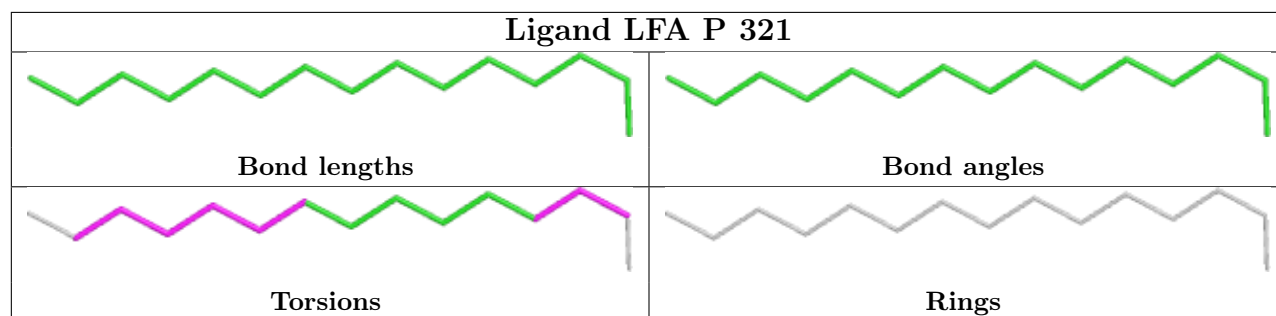
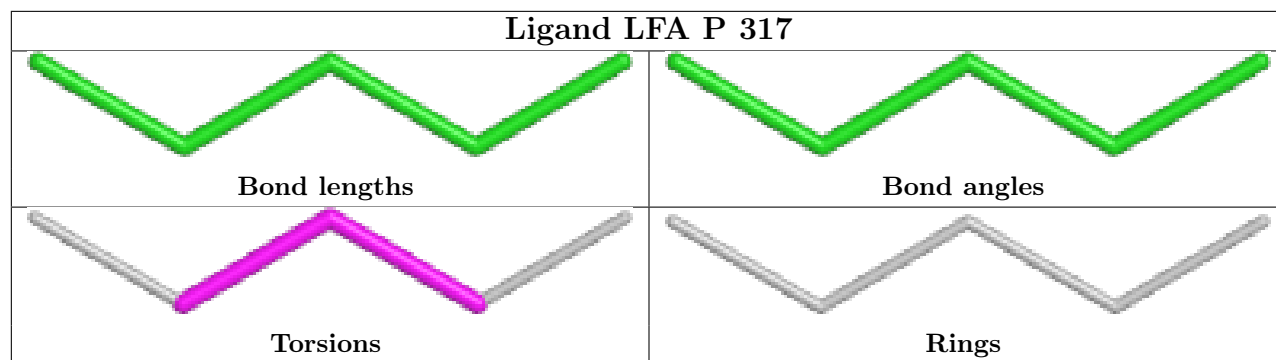
There are no ring outliers.

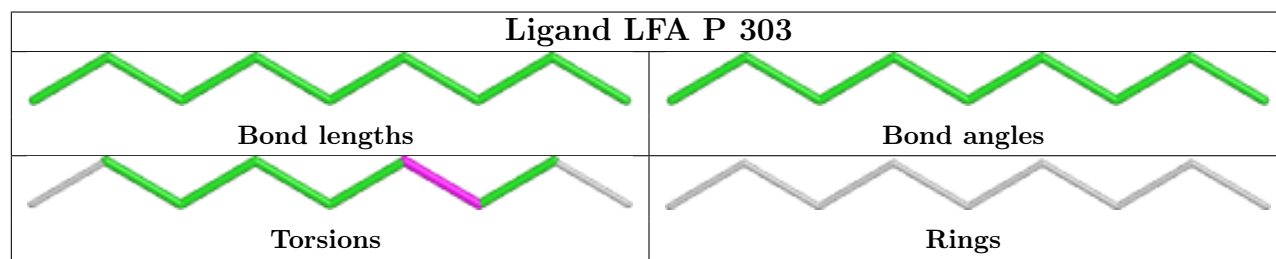
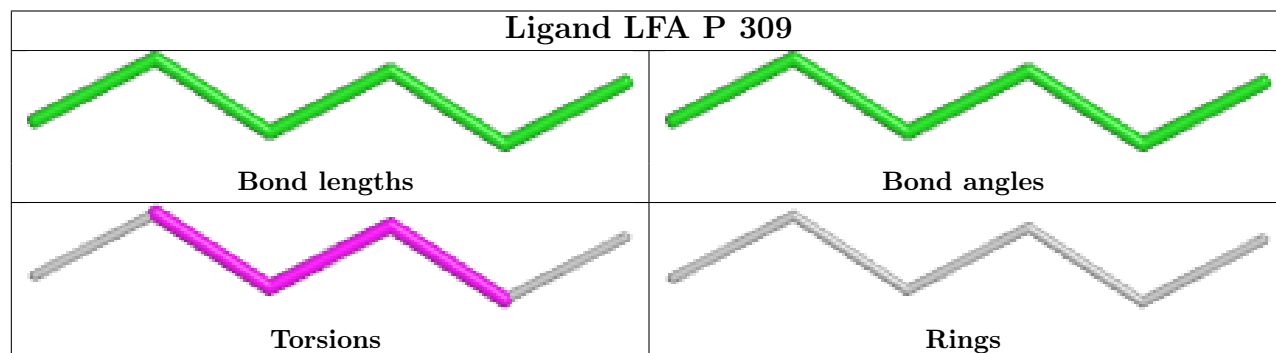
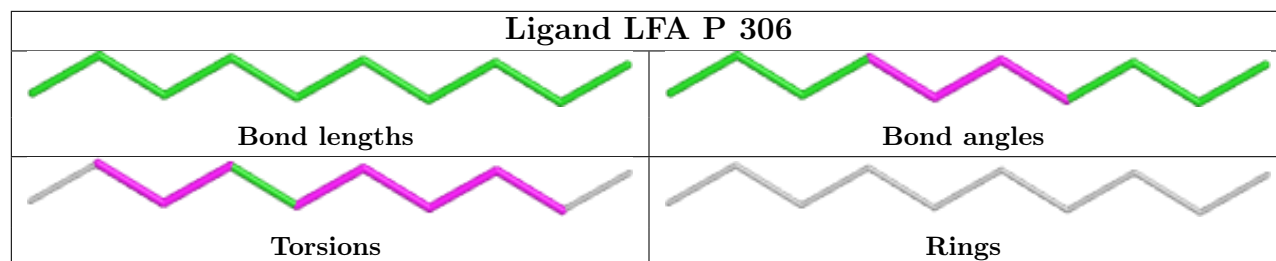
11 monomers are involved in 49 short contacts:

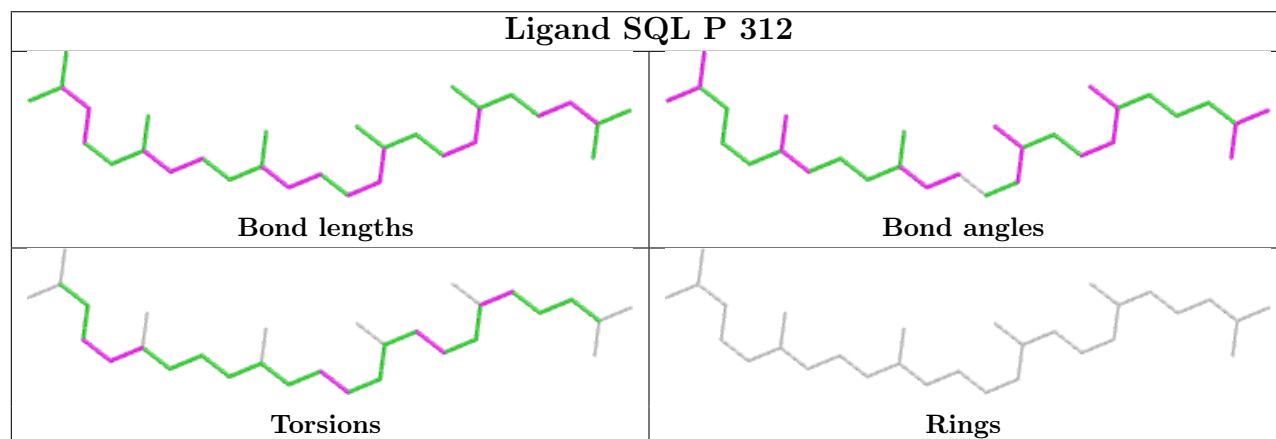
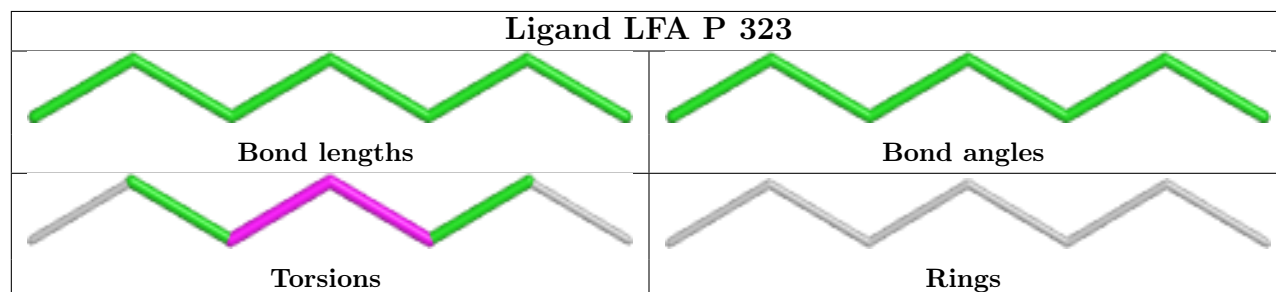
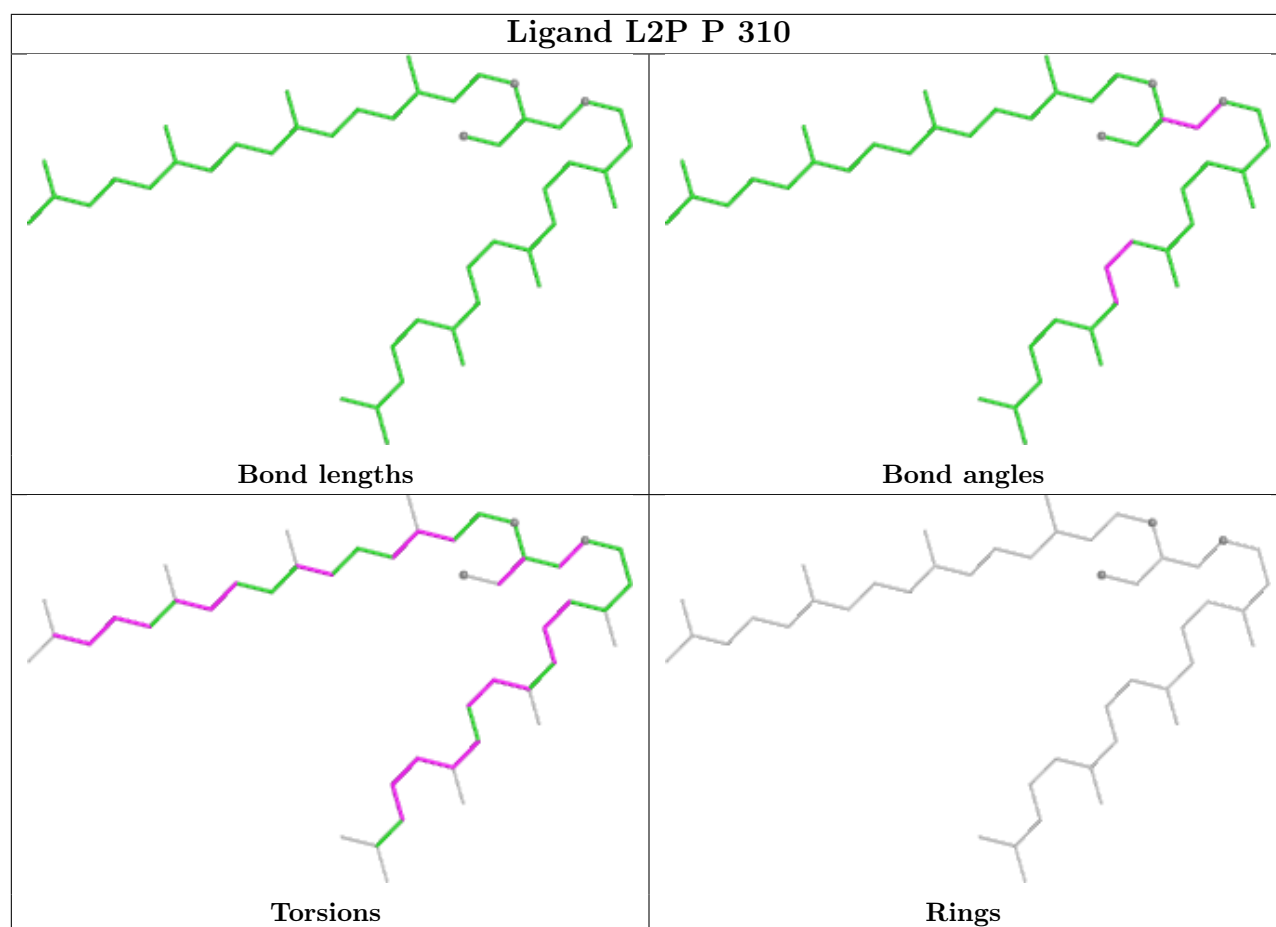
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	320	LFA	2	0
3	P	321	LFA	3	0
2	P	302	OLC	7	0
3	P	303	LFA	7	0
4	P	310	L2P	12	0
5	P	312	SQL	14	0
3	P	313	LFA	2	0
3	P	319	LFA	4	0
3	P	316	LFA	1	0
3	P	308	LFA	3	0
3	P	304	LFA	1	0

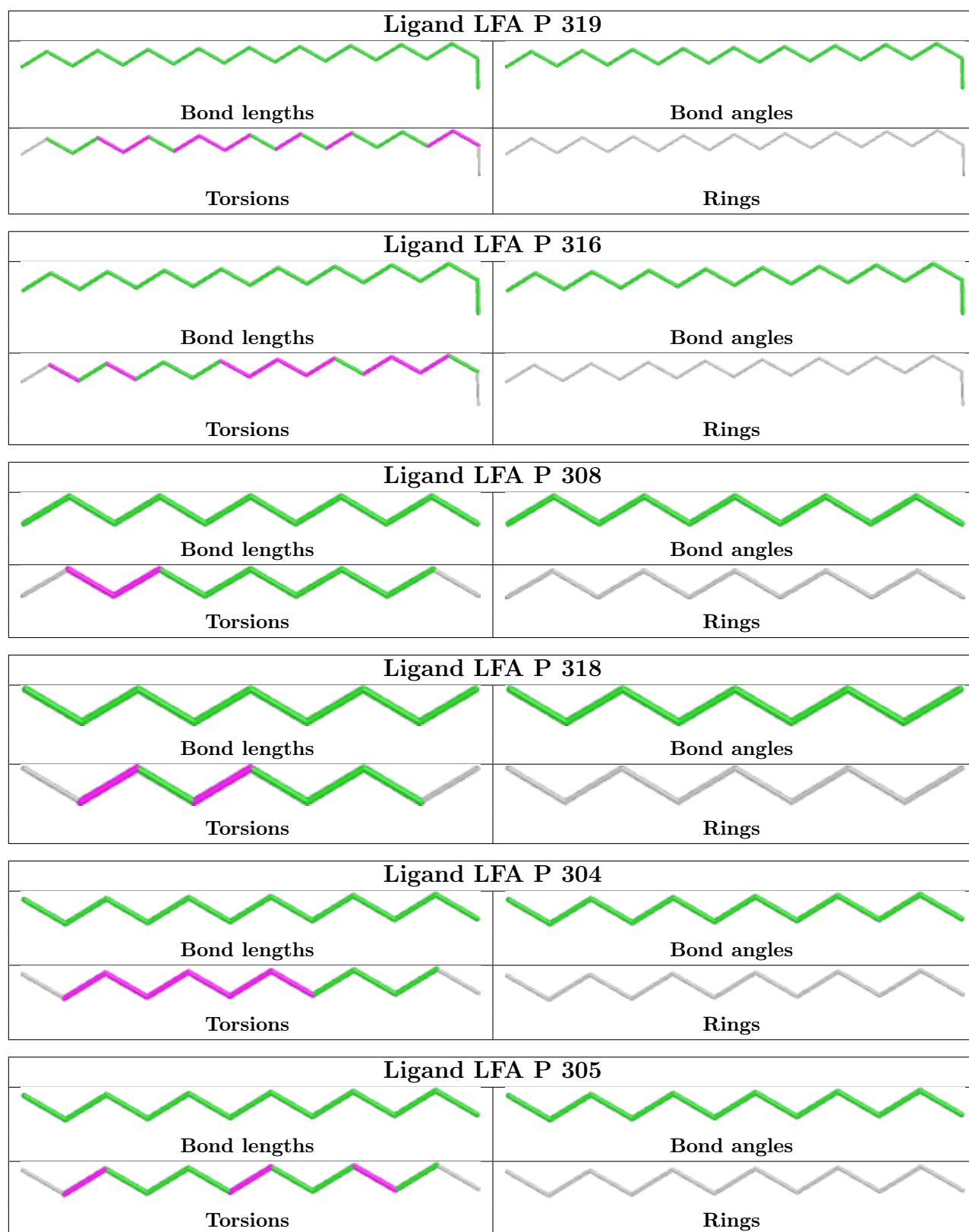
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

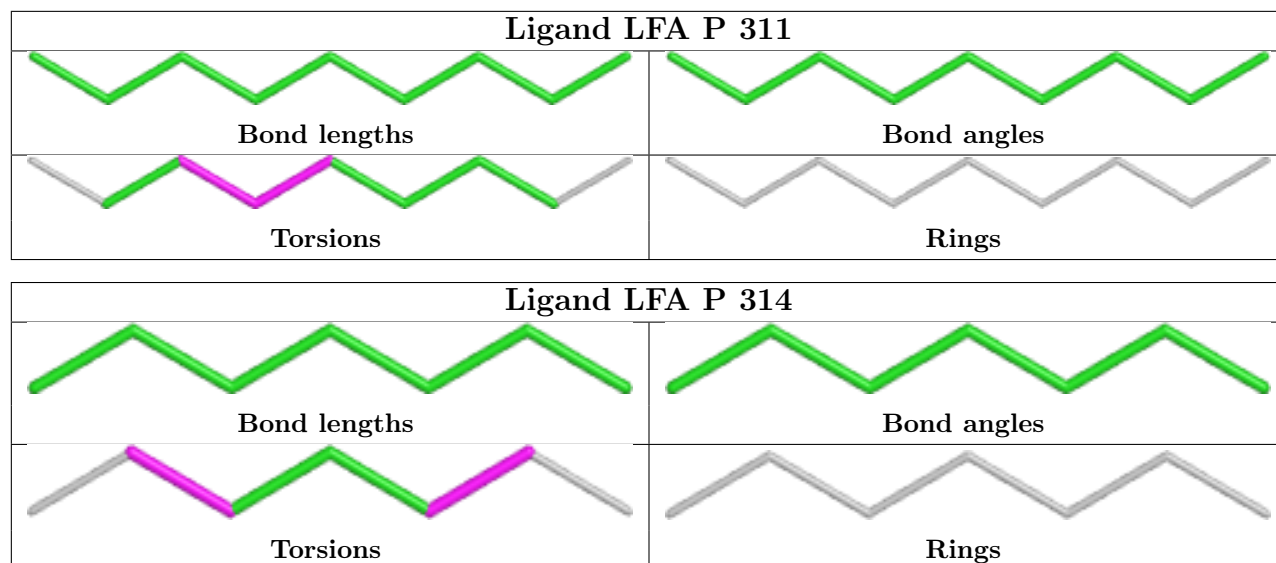












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	P	229/248 (92%)	-0.57	3 (1%) 75 76	5, 13, 50, 107	127 (55%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	224[A]	LEU	2.6
1	P	233	ALA	2.4
1	P	160	ALA	2.2

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

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	LYR	P	216[A]	29/30	0.99	0.04	13,15,19,20	68
1	LYR	P	216[C]	29/30	0.99	0.04	13,15,19,20	68

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

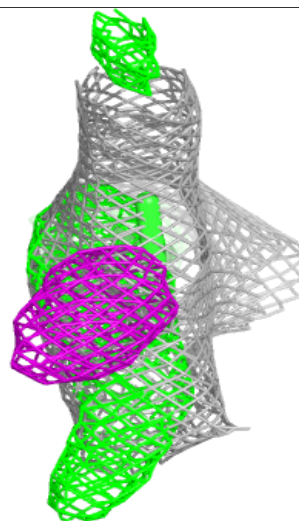
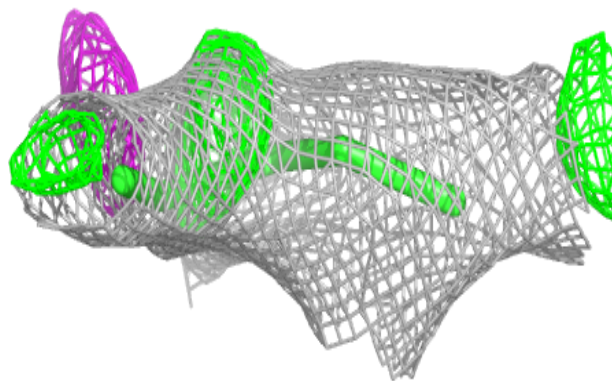
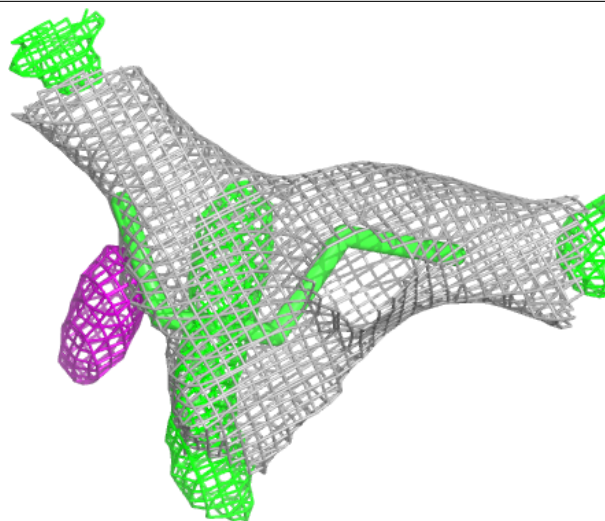
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
3	LFA	P	317	5/20	0.89	0.10	42,43,43,43	0
3	LFA	P	311	9/20	0.90	0.10	42,42,43,46	0
3	LFA	P	318	9/20	0.91	0.08	43,44,47,47	0
3	LFA	P	308	11/20	0.93	0.10	42,47,55,55	0
3	LFA	P	319	20/20	0.94	0.07	42,45,51,51	0
3	LFA	P	316	18/20	0.95	0.08	43,54,61,63	0
3	LFA	P	304	12/20	0.95	0.07	42,45,53,53	0
3	LFA	P	305	12/20	0.95	0.05	43,47,54,54	0
3	LFA	P	313	3/20	0.95	0.09	43,43,43,43	0
3	LFA	P	315	6/20	0.96	0.07	43,43,48,53	0
3	LFA	P	303	9/20	0.96	0.09	42,43,49,51	0
3	LFA	P	306	10/20	0.96	0.07	42,43,44,44	0
3	LFA	P	307	6/20	0.96	0.07	42,42,43,44	0
3	LFA	P	314	7/20	0.96	0.09	42,43,49,49	0
3	LFA	P	320	9/20	0.96	0.06	42,43,43,47	0
4	L2P	P	310	46/46	0.96	0.08	42,48,56,57	0
5	SQL	P	312	30/30	0.96	0.07	42,50,57,59	0
3	LFA	P	322	3/20	0.97	0.06	42,42,42,43	0
3	LFA	P	323	7/20	0.97	0.07	42,43,46,54	0
2	OLC	P	302	25/25	0.97	0.07	42,43,50,54	0
3	LFA	P	321	15/20	0.97	0.07	42,47,54,56	0
3	LFA	P	309	6/20	0.98	0.05	42,42,43,43	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.

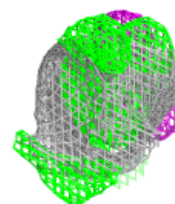
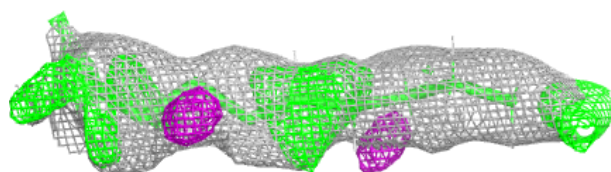
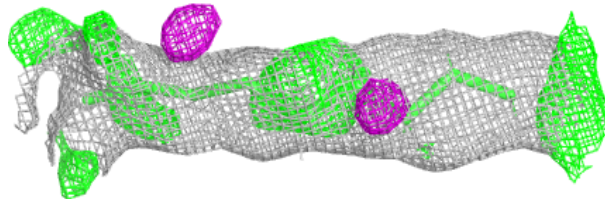
Electron density around LFA P 317:

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

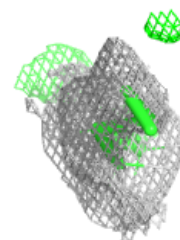
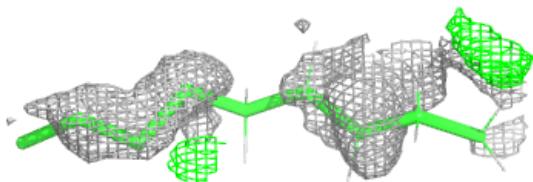
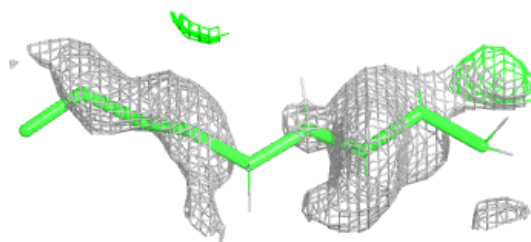


Electron density around LFA P 311:

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

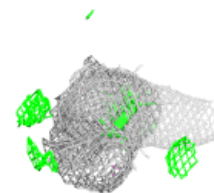
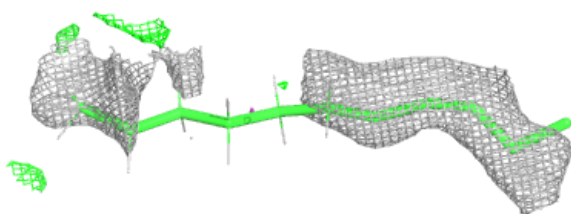
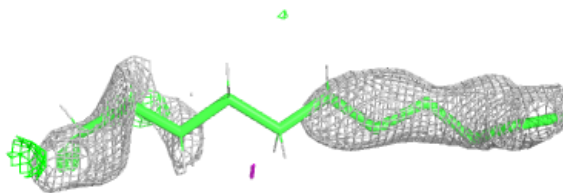
**Electron density around LFA P 318:**

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

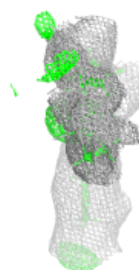
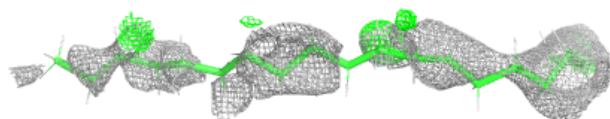
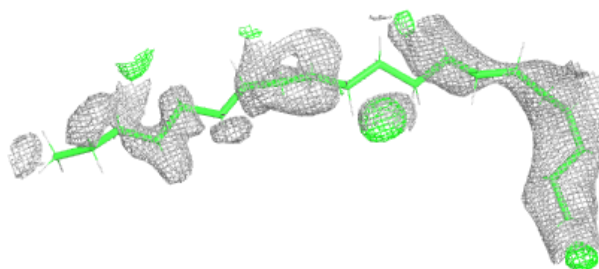


Electron density around LFA P 308:

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

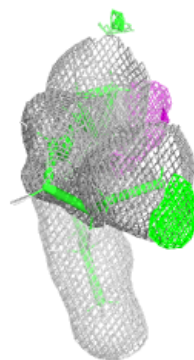
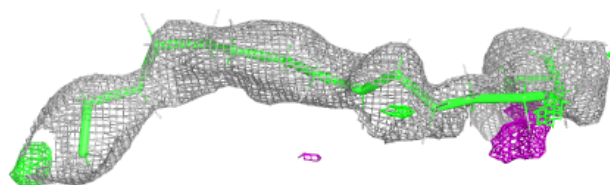
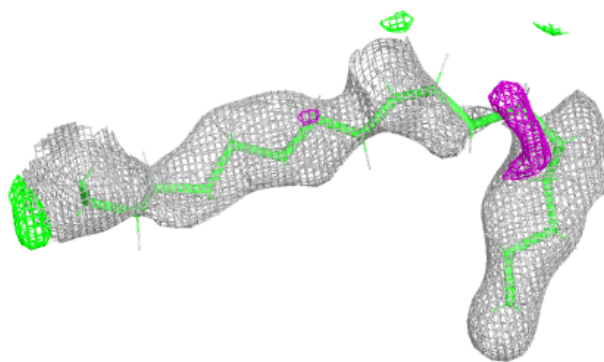
**Electron density around LFA P 319:**

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

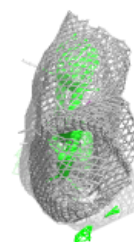
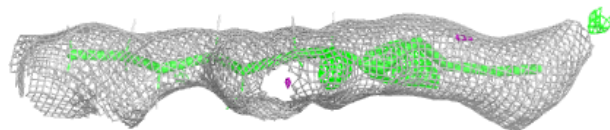
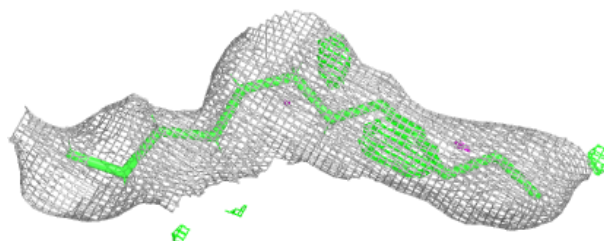


Electron density around LFA P 316:

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

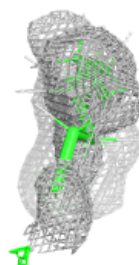
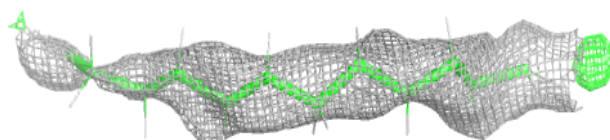
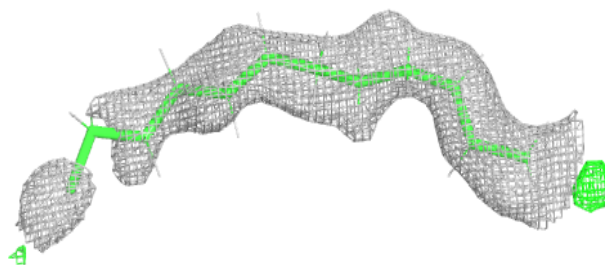
**Electron density around LFA P 304:**

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

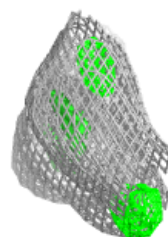
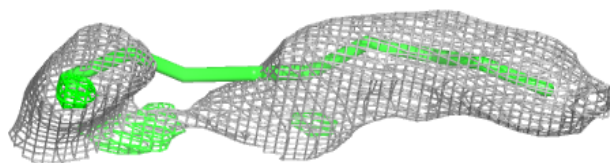
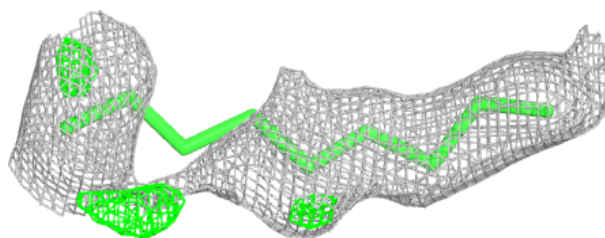


Electron density around LFA P 305:

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and green (positive)

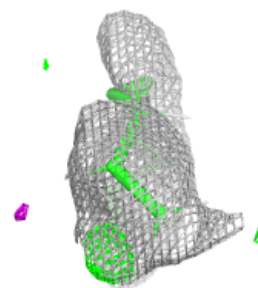
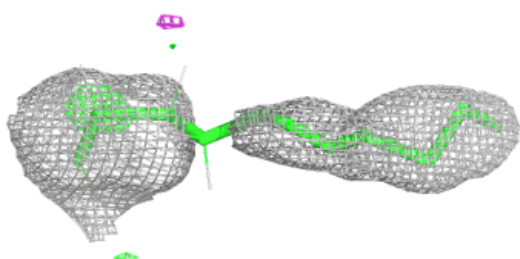
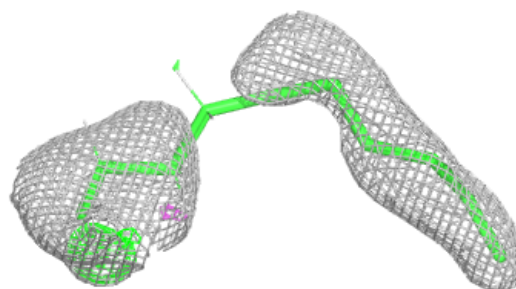
**Electron density around LFA P 303:**

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

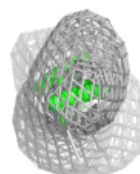
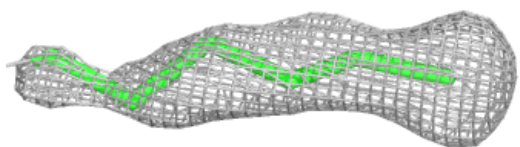
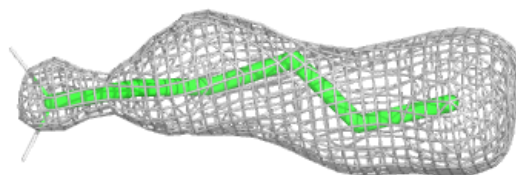


Electron density around LFA P 306:

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

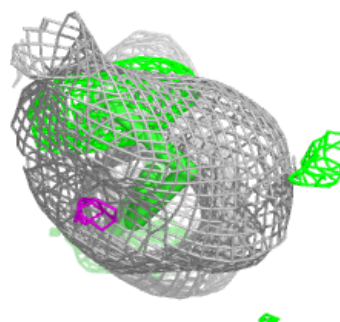
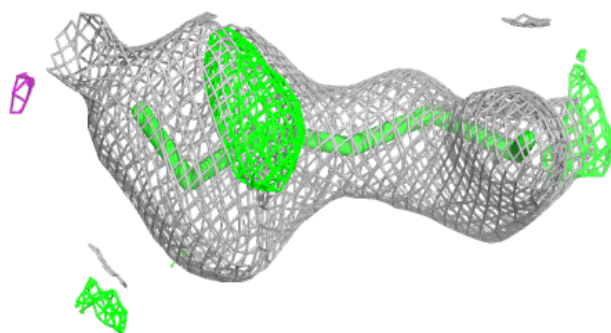
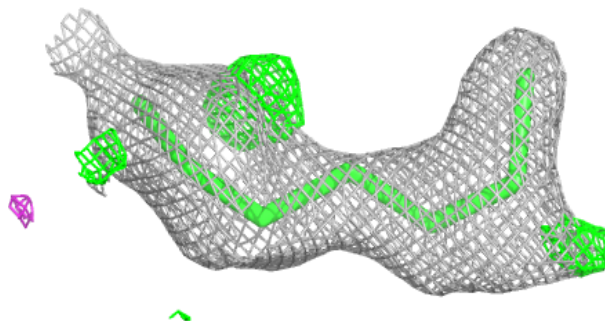
**Electron density around LFA P 307:**

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

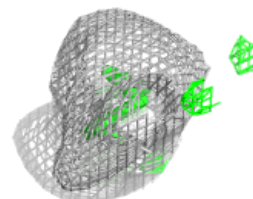
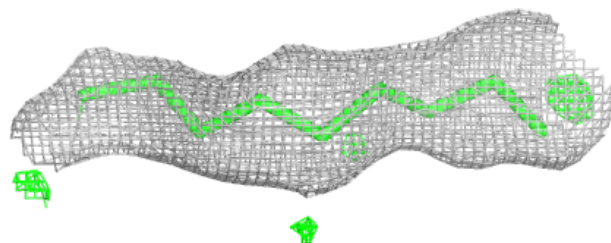
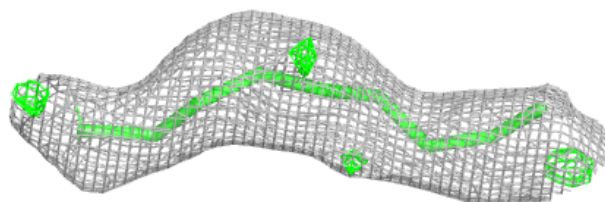


Electron density around LFA P 314:

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and green (positive)

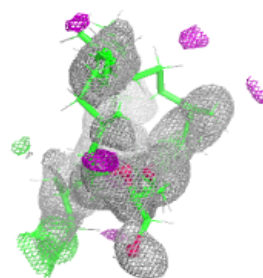
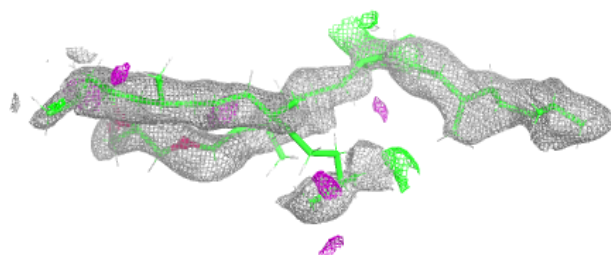
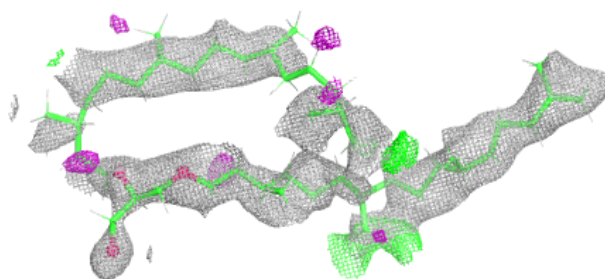
**Electron density around LFA P 320:**

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

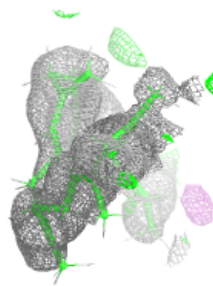
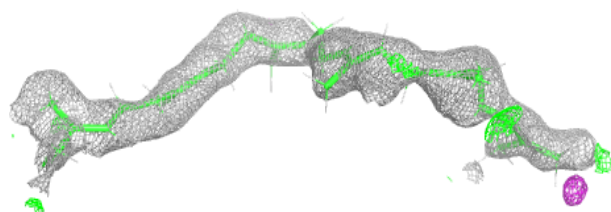
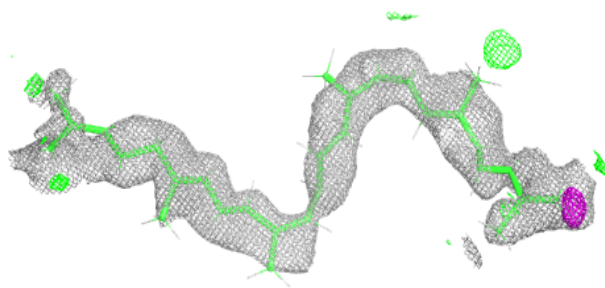


Electron density around L2P P 310:

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

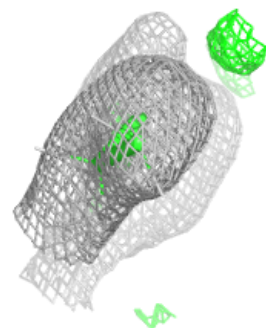
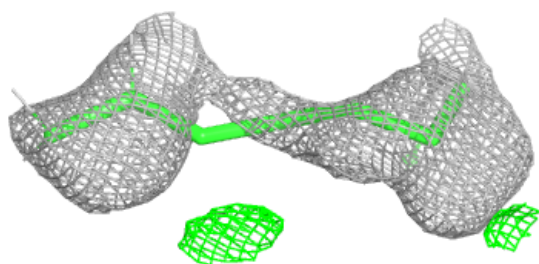
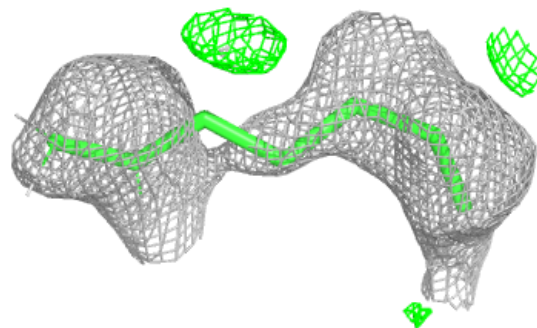
**Electron density around SQL P 312:**

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

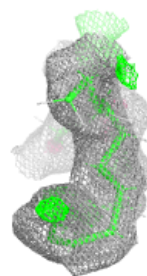
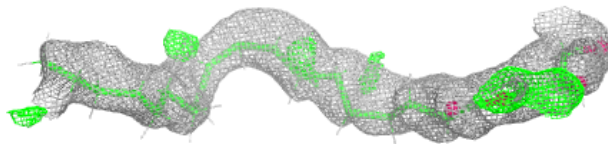
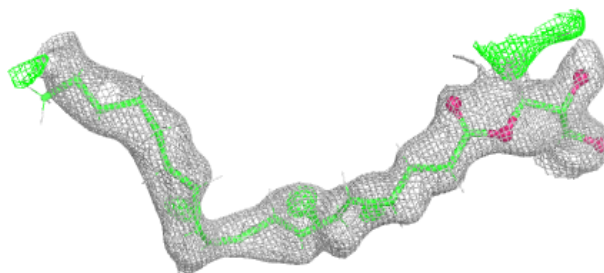


Electron density around LFA P 323:

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and green (positive)

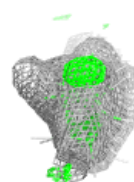
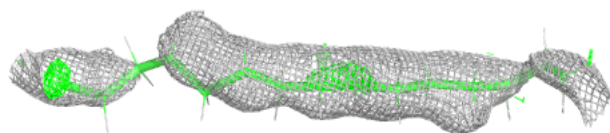
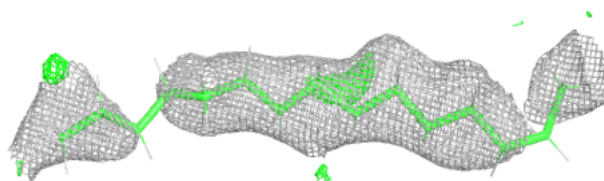
**Electron density around OLC P 302:**

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and green (positive)

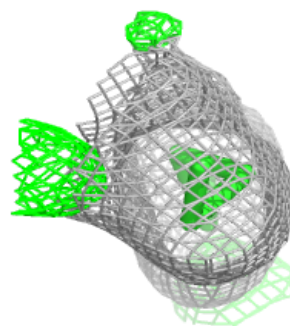
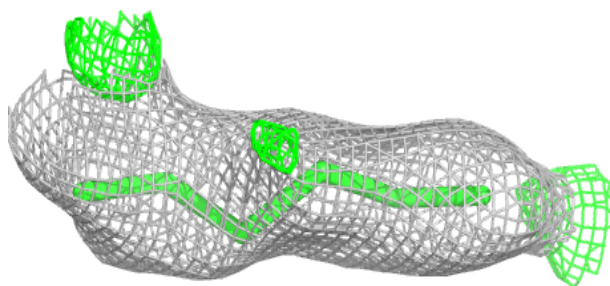
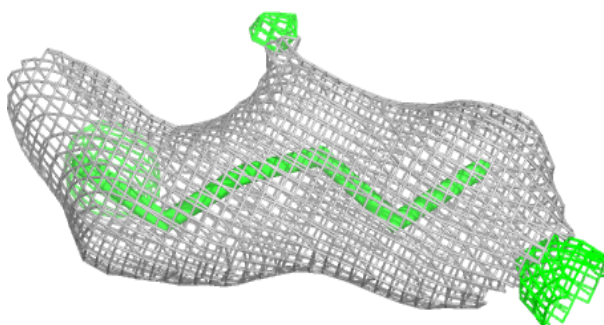


Electron density around LFA P 321:

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

**Electron density around LFA P 309:**

$2mF_o-DF_c$ (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.