



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:35 AM UTC

PDB ID : 7AKX / pdb_00007akx
Title : Crystal structure of the viral rhodopsin OLPVR1 in P1 space group
Authors : Kovalev, K.; Zabelskii, D.; Alekseev, A.; Astashkin, R.; Gordeliy, V.
Deposited on : 2020-10-02
Resolution : 1.60 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

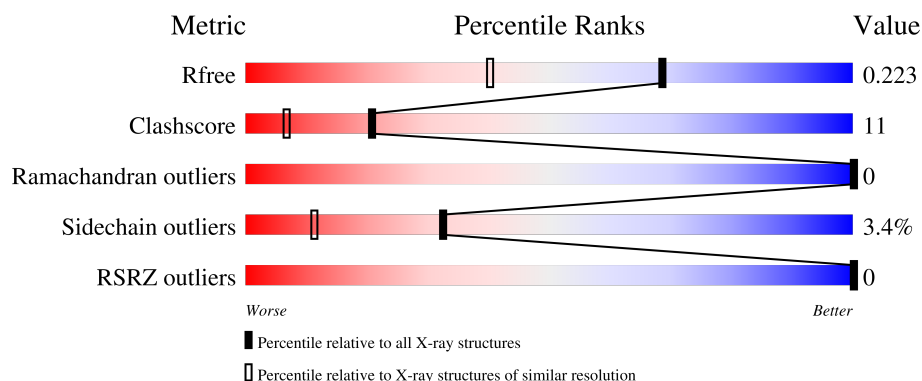
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	231	
1	B	231	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4341 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.

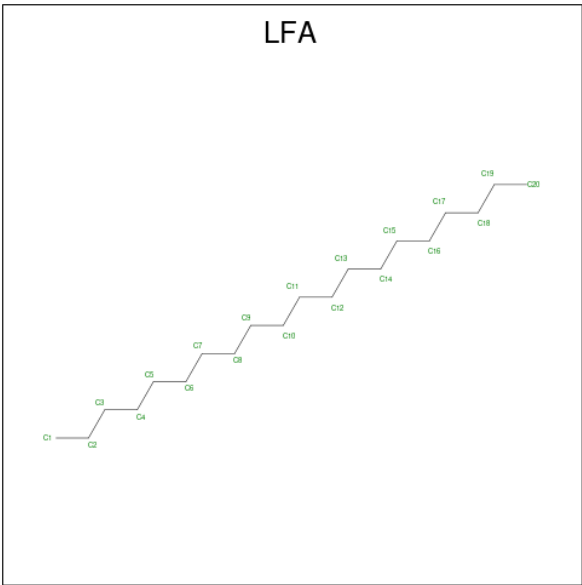
- Molecule 1 is a protein called viral rhodopsin OLPVR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	6	0
			1984	1378	273	321	12			
1	B	224	Total	C	N	O	S	0	7	0
			1971	1364	274	321	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	224	LEU	-	expression tag	UNP F2Y337
A	225	GLU	-	expression tag	UNP F2Y337
A	226	HIS	-	expression tag	UNP F2Y337
A	227	HIS	-	expression tag	UNP F2Y337
A	228	HIS	-	expression tag	UNP F2Y337
A	229	HIS	-	expression tag	UNP F2Y337
A	230	HIS	-	expression tag	UNP F2Y337
A	231	HIS	-	expression tag	UNP F2Y337
B	224	LEU	-	expression tag	UNP F2Y337
B	225	GLU	-	expression tag	UNP F2Y337
B	226	HIS	-	expression tag	UNP F2Y337
B	227	HIS	-	expression tag	UNP F2Y337
B	228	HIS	-	expression tag	UNP F2Y337
B	229	HIS	-	expression tag	UNP F2Y337
B	230	HIS	-	expression tag	UNP F2Y337
B	231	HIS	-	expression tag	UNP F2Y337

- Molecule 2 is EICOSANE (CCD ID: LFA) (formula: C₂₀H₄₂).



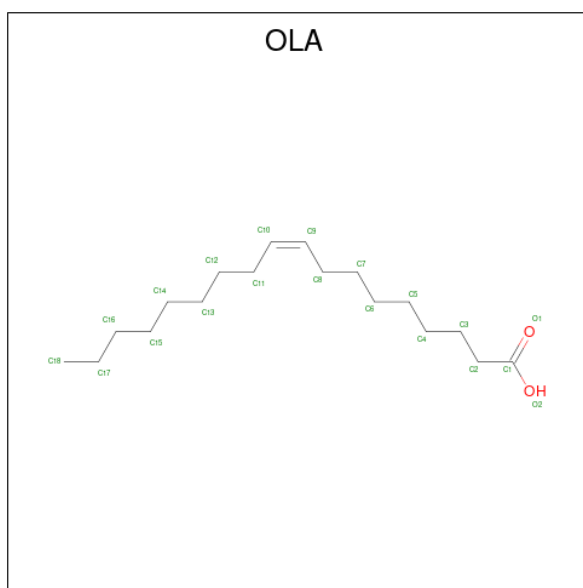
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 14 14	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 4 4	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 11 11	0	0
2	A	1	Total C 4 4	0	0
2	A	1	Total C 13 13	0	0
2	A	1	Total C 3 3	0	0
2	A	1	Total C 5 5	0	0
2	A	1	Total C 4 4	0	0
2	A	1	Total C 11 11	0	0
2	B	1	Total C 20 20	0	0
2	B	1	Total C 8 8	0	0

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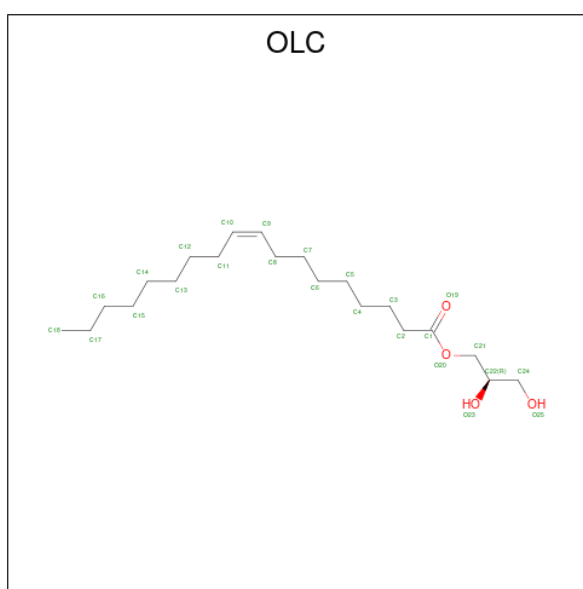
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C 4 4	0	0
2	B	1	Total C 13 13	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 5 5	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C 5 5	0	0
2	B	1	Total C 3 3	0	0
2	B	1	Total C 12 12	0	0
2	B	1	Total C 6 6	0	0
2	B	1	Total C 12 12	0	0
2	B	1	Total C 4 4	0	0
2	B	1	Total C 10 10	0	0

- Molecule 3 is OLEIC ACID (CCD ID: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 9 7 2	0	0
3	A	1	Total C O 11 9 2	0	0
3	B	1	Total C O 9 7 2	0	0
3	B	1	Total C O 11 9 2	0	0

- Molecule 4 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
4	A	1	Total C O 16 12 4	0	0
4	B	1	Total C O 16 12 4	0	0

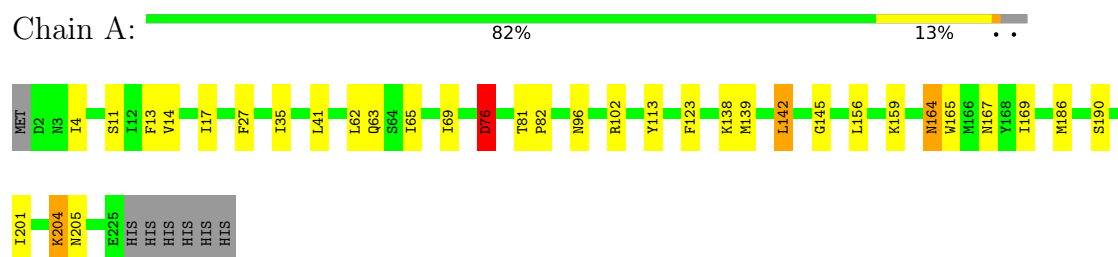
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	47	Total O 47 47	0	0
5	B	51	Total O 51 51	0	0

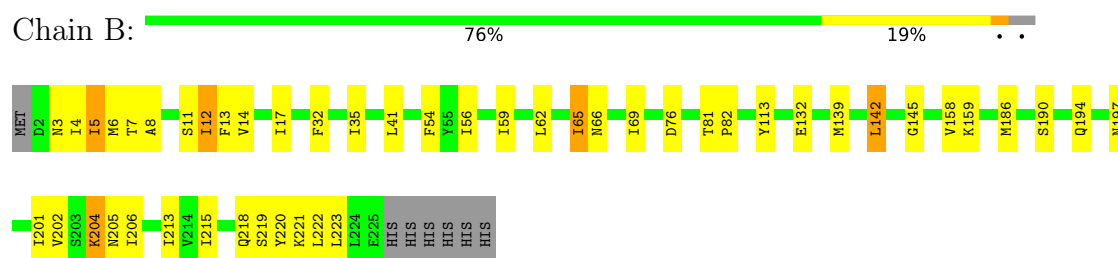
3 Residue-property plots [i](#)

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: viral rhodopsin OLPVR1



- Molecule 1: viral rhodopsin OLPVR1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	40.18Å 56.97Å 62.34Å 113.90° 90.01° 91.49°	Depositor
Resolution (Å)	20.00 – 1.60 20.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	95.2 (20.00-1.60) 95.2 (20.00-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.188 , 0.213 0.201 , 0.223	Depositor DCC
R_{free} test set	3143 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.188 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4341	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OLC, LYR, LFA, OLA

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	0.90	0/2013	1.31	1/2732 (0.0%)
1	B	0.90	0/1998	1.32	1/2714 (0.0%)
All	All	0.90	0/4011	1.31	2/5446 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	76	ASP	CA-CB-CG	5.24	117.84	112.60

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	1984	0	2005	42	0
1	B	1971	0	1998	56	0
2	A	99	0	171	8	0
2	B	117	0	214	12	0
3	A	20	0	24	0	0
3	B	20	0	24	0	0
4	A	16	0	21	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	16	0	21	0	0
5	A	47	0	0	2	0
5	B	51	0	0	2	0
All	All	4341	0	4478	97	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 11.

All (97) 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:B:201[B]:ILE:HD12	5:B:401:HOH:O	1.63	0.99
1:B:11:SER:OG	1:B:201[B]:ILE:HD11	1.65	0.96
2:A:507:LFA:H201	2:B:316:LFA:C4	2.05	0.86
1:A:96:ASN:HD21	1:A:167:ASN:HD21	1.24	0.84
2:A:507:LFA:H201	2:B:316:LFA:H41	1.60	0.82
1:A:13:PHE:CZ	1:A:17:ILE:HD11	2.18	0.78
1:A:63:GLN:NE2	1:B:221:LYS:HE3	1.99	0.77
1:A:123:PHE:CE2	2:A:502:LFA:C18	2.71	0.74
1:B:65:ILE:HD11	1:B:69:ILE:HG13	1.71	0.72
1:B:11:SER:OG	1:B:201[B]:ILE:CD1	2.40	0.70
1:B:158:VAL:HG12	2:B:303:LFA:H181	1.75	0.69
2:B:310:LFA:H12	2:B:311:LFA:H11	1.73	0.69
1:A:63:GLN:HE22	1:B:221:LYS:HE3	1.59	0.67
1:A:142:LEU:HD21	1:A:186[B]:MET:HG2	1.77	0.67
1:B:5:ILE:HD11	1:B:62:LEU:HB3	1.77	0.66
1:A:35:ILE:HD11	1:A:102:ARG:HD3	1.78	0.65
1:A:123:PHE:CD2	2:A:502:LFA:C18	2.79	0.65
1:A:138:LYS:HE2	5:A:645:HOH:O	1.94	0.65
1:B:222:LEU:C	1:B:222:LEU:HD23	2.21	0.64
1:A:164:ASN:C	1:A:164:ASN:HD22	2.06	0.63
1:B:145:GLY:HA3	1:B:204:LYR:H142	1.81	0.63
1:B:12[B]:ILE:CD1	1:B:59:ILE:HD13	2.29	0.62
1:B:13:PHE:CE2	1:B:17:ILE:HD11	2.34	0.62
1:A:123:PHE:HE2	2:A:502:LFA:C18	2.12	0.60
1:B:204:LYR:H9	1:B:204:LYR:H192	1.82	0.60
1:B:201[B]:ILE:CD1	1:B:201[B]:ILE:N	2.66	0.59
1:B:142:LEU:HD21	1:B:186[B]:MET:HG2	1.84	0.59
1:B:11:SER:CB	1:B:201[B]:ILE:HD11	2.32	0.59
1:B:201[B]:ILE:H	1:B:201[B]:ILE:HD13	1.67	0.58
1:A:142:LEU:HD21	1:A:186[A]:MET:HG2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:PHE:HA	1:B:35:ILE:HD11	1.85	0.58
1:A:204:LYR:H192	1:A:204:LYR:H9	1.83	0.58
1:A:205:ASN:ND2	5:A:602:HOH:O	2.37	0.58
1:B:204:LYR:H9	1:B:204:LYR:H183	1.86	0.58
1:A:145:GLY:HA3	1:A:204:LYR:H142	1.87	0.57
1:B:201[B]:ILE:N	1:B:201[B]:ILE:HD13	2.20	0.56
1:A:138:LYS:HD3	4:A:508:OLC:H24	1.86	0.56
1:A:204:LYR:H9	1:A:204:LYR:H183	1.88	0.56
1:B:6:MET:SD	2:B:306:LFA:H41	2.47	0.55
1:B:4:ILE:HD11	1:B:190[A]:SER:HA	1.88	0.55
1:B:142:LEU:HD21	1:B:186[A]:MET:HG2	1.88	0.55
1:B:4:ILE:HD11	1:B:190[B]:SER:HA	1.88	0.55
1:A:165:TRP:HE3	1:A:169:ILE:HD12	1.71	0.55
1:A:4:ILE:HD11	1:A:190:SER:HA	1.87	0.55
1:A:81:THR:N	1:A:82:PRO:HD2	2.22	0.55
1:B:54:PHE:HA	2:B:301:LFA:H122	1.90	0.54
1:B:4:ILE:HG22	1:B:62:LEU:HD11	1.90	0.53
1:B:12[B]:ILE:HD11	1:B:59:ILE:HD13	1.90	0.52
1:B:113:TYR:CD1	1:B:159:LYS:HD3	2.45	0.52
1:B:81:THR:N	1:B:82:PRO:HD2	2.25	0.52
1:A:27[A]:PHE:CE2	1:B:7:THR:HG21	2.46	0.51
2:A:507:LFA:C20	2:B:316:LFA:C4	2.86	0.50
1:B:222:LEU:C	1:B:222:LEU:CD2	2.84	0.49
1:A:13:PHE:CE1	1:A:17:ILE:HD11	2.47	0.49
1:B:5:ILE:HG13	1:B:62:LEU:HD13	1.95	0.49
1:B:202:VAL:HG21	2:B:316:LFA:C5	2.44	0.48
1:B:32:PHE:HA	1:B:35:ILE:CD1	2.43	0.48
1:B:13:PHE:CZ	1:B:17:ILE:HD11	2.49	0.47
1:B:220:TYR:CD1	2:B:315:LFA:H13	2.49	0.47
2:A:507:LFA:H201	2:B:316:LFA:H42	1.92	0.47
1:B:142:LEU:HD12	1:B:142:LEU:HA	1.84	0.47
1:B:218:GLN:HE22	1:B:221:LYS:NZ	2.13	0.47
1:B:69:ILE:C	1:B:69:ILE:HD12	2.40	0.46
1:B:213:ILE:HG22	2:B:313:LFA:H102	1.97	0.46
1:B:14:VAL:HG11	1:B:201[A]:ILE:HG23	1.98	0.46
1:B:204:LYR:H183	1:B:204:LYR:C9	2.46	0.46
1:A:41:LEU:HD23	1:A:41:LEU:HA	1.83	0.45
1:A:139:MET:HG2	4:A:508:OLC:H2	1.97	0.45
1:B:204:LYR:H192	1:B:204:LYR:C9	2.46	0.45
1:B:41:LEU:HD22	1:B:215:ILE:HD12	1.99	0.45
1:A:165:TRP:CE3	1:A:169:ILE:HD12	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ILE:C	1:A:69:ILE:HD12	2.43	0.44
1:A:204:LYR:H183	1:A:204:LYR:C9	2.48	0.43
1:A:27[A]:PHE:HE2	1:B:7:THR:HG21	1.83	0.43
1:A:113:TYR:CD1	1:A:159:LYS:HD3	2.52	0.43
1:A:27[A]:PHE:CE2	1:B:7:THR:CG2	3.02	0.43
1:B:3:ASN:HB3	1:B:194:GLN:CD	2.44	0.43
1:B:56:ILE:HD13	1:B:59:ILE:HD11	2.00	0.42
1:B:197:ASN:O	1:B:201[B]:ILE:HD13	2.19	0.42
1:A:13:PHE:CE1	1:A:17:ILE:CD1	3.02	0.42
1:A:27[A]:PHE:CZ	1:B:7:THR:CG2	3.02	0.42
1:A:204:LYR:H192	1:A:204:LYR:C9	2.49	0.42
1:A:76:ASP:OD1	1:A:76:ASP:C	2.63	0.42
1:B:11:SER:HA	1:B:201[B]:ILE:HD11	2.02	0.42
1:B:205:ASN:ND2	5:B:401:HOH:O	2.51	0.42
1:A:11:SER:HA	1:A:201:ILE:HD11	2.02	0.41
1:A:27[A]:PHE:HZ	1:B:7:THR:HG22	1.85	0.41
1:A:123:PHE:HD2	2:A:502:LFA:C18	2.28	0.41
1:B:219:SER:O	1:B:222:LEU:HB3	2.20	0.41
2:B:310:LFA:C1	2:B:311:LFA:H11	2.45	0.41
1:A:204:LYR:H6	1:A:204:LYR:H41	1.87	0.41
1:A:4:ILE:HG22	1:A:62:LEU:HD11	2.03	0.41
1:A:186[A]:MET:HE2	1:A:186[A]:MET:HB3	1.93	0.41
1:B:204:LYR:H6	1:B:204:LYR:H41	1.92	0.41
1:B:8:ALA:O	1:B:12[B]:ILE:HG13	2.20	0.41
1:A:14:VAL:HG11	1:A:201:ILE:HG23	2.03	0.40
1:A:142:LEU:HD12	1:A:142:LEU:HA	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	227/231 (98%)	227 (100%)	0	0	100	100
1	B	228/231 (99%)	228 (100%)	0	0	100	100
All	All	455/462 (98%)	455 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	213/220 (97%)	207 (97%)	6 (3%)	38	15
1	B	212/220 (96%)	201 (95%)	11 (5%)	21	5
All	All	425/440 (97%)	408 (96%)	17 (4%)	32	8

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ILE
1	A	76	ASP
1	A	142	LEU
1	A	156[A]	LEU
1	A	156[B]	LEU
1	A	164	ASN
1	B	5	ILE
1	B	12[A]	ILE
1	B	12[B]	ILE
1	B	65	ILE
1	B	66	ASN
1	B	132	GLU
1	B	139[A]	MET
1	B	139[B]	MET
1	B	142	LEU
1	B	206	ILE
1	B	223	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	48	GLN
1	A	63	GLN
1	A	121	ASN
1	A	164	ASN
1	A	167	ASN
1	A	205	ASN
1	A	218	GLN
1	B	15	GLN
1	B	48	GLN
1	B	121	ASN
1	B	135	GLN
1	B	167	ASN
1	B	194	GLN
1	B	205	ASN
1	B	217	ASN
1	B	218	GLN

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	B	204	1	27,29,30	1.23	3 (11%)	30,37,39	2.04	11 (36%)
1	LYR	A	204	1	27,29,30	1.27	4 (14%)	30,37,39	1.87	9 (30%)

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	B	204	1	-	3/22/40/42	0/1/1/1
1	LYR	A	204	1	-	2/22/40/42	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	204	LYR	C2-C3	3.15	1.41	1.33
1	A	204	LYR	C2-C3	2.98	1.40	1.33
1	A	204	LYR	C13-C12	2.12	1.54	1.50
1	B	204	LYR	C7-C80	2.08	1.40	1.35
1	B	204	LYR	C6-C5	2.07	1.40	1.34
1	A	204	LYR	C7-C80	2.02	1.40	1.35
1	A	204	LYR	C6-C5	2.01	1.39	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	204	LYR	C13-C12-C11	-5.52	118.46	124.48
1	A	204	LYR	C13-C12-C11	-4.46	119.61	124.48
1	A	204	LYR	C1-NZ-CE	4.27	121.52	112.85
1	B	204	LYR	C1-NZ-CE	4.27	121.51	112.85
1	B	204	LYR	C6-C7-C80	-3.45	122.44	127.28
1	B	204	LYR	C7-C6-C5	-3.01	114.48	123.20
1	A	204	LYR	C10-C9-C80	-3.01	121.79	126.23
1	B	204	LYR	C10-C9-C80	-2.85	122.02	126.23
1	A	204	LYR	C7-C6-C5	-2.77	115.17	123.20
1	A	204	LYR	C15-C14-C12	-2.76	109.14	114.06
1	B	204	LYR	C15-C14-C12	-2.42	109.75	114.06
1	A	204	LYR	C4-C3-C2	-2.37	119.62	123.73
1	B	204	LYR	C17-C11-C10	2.36	122.06	115.65
1	B	204	LYR	C8-C80-C7	-2.31	119.08	122.82
1	A	204	LYR	C5-C3-C2	2.30	121.70	118.49
1	A	204	LYR	C17-C11-C10	2.29	121.86	115.65
1	B	204	LYR	C4-C3-C2	-2.23	119.86	123.73
1	B	204	LYR	C5-C3-C2	2.20	121.55	118.49
1	A	204	LYR	C6-C7-C80	-2.14	124.28	127.28
1	B	204	LYR	C10-C11-C12	-2.06	116.80	121.56

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	204	LYR	CG-CD-CE-NZ
1	B	204	LYR	CG-CD-CE-NZ
1	B	204	LYR	C2-C1-NZ-CE
1	A	204	LYR	CD-CE-NZ-C1
1	B	204	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	B	204	LYR	6	0
1	A	204	LYR	6	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

32 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$
2	LFA	A	506	-	11,11,19	0.08	0	10,10,18	0.10	0
2	LFA	B	303	-	3,3,19	0.20	0	2,2,18	0.45	0
2	LFA	B	315	-	11,11,19	0.12	0	10,10,18	0.07	0
2	LFA	A	512	-	2,2,19	0.13	0	1,1,18	0.18	0
4	OLC	B	307	-	15,15,24	1.14	1 (6%)	16,16,25	1.00	1 (6%)
2	LFA	B	314	-	5,5,19	0.12	0	4,4,18	0.10	0
2	LFA	B	316	-	3,3,19	0.18	0	2,2,18	0.44	0
2	LFA	A	502	-	9,9,19	0.12	0	8,8,18	0.09	0
4	OLC	A	508	-	15,15,24	1.15	1 (6%)	16,16,25	0.96	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LFA	B	309	-	4,4,19	0.11	0	3,3,18	0.21	0
2	LFA	B	301	-	19,19,19	0.10	0	18,18,18	0.04	0
2	LFA	B	317	-	9,9,19	0.09	0	8,8,18	0.07	0
2	LFA	B	306	-	6,6,19	0.09	0	5,5,18	0.12	0
2	LFA	B	313	-	11,11,19	0.07	0	10,10,18	0.07	0
3	OLA	A	504	-	8,8,19	0.74	0	8,8,19	0.77	0
3	OLA	B	304	-	8,8,19	0.78	0	8,8,19	0.72	0
2	LFA	A	511	-	12,12,19	0.11	0	11,11,18	0.06	0
2	LFA	B	305	-	12,12,19	0.10	0	11,11,18	0.05	0
2	LFA	A	503	-	3,3,19	0.18	0	2,2,18	0.45	0
2	LFA	A	507	-	7,7,19	0.10	0	6,6,18	0.08	0
3	OLA	A	505	-	10,10,19	0.69	0	10,10,19	0.65	0
2	LFA	A	501	-	13,13,19	0.09	0	12,12,18	0.07	0
2	LFA	A	515	-	10,10,19	0.09	0	9,9,18	0.09	0
2	LFA	A	513	-	4,4,19	0.12	0	3,3,18	0.23	0
2	LFA	B	310	-	7,7,19	0.09	0	6,6,18	0.07	0
2	LFA	B	302	-	7,7,19	0.10	0	6,6,18	0.08	0
2	LFA	B	311	-	4,4,19	0.12	0	3,3,18	0.22	0
2	LFA	A	510	-	3,3,19	0.20	0	2,2,18	0.47	0
3	OLA	B	308	-	10,10,19	0.69	0	10,10,19	0.64	0
2	LFA	B	312	-	2,2,19	0.09	0	1,1,18	0.22	0
2	LFA	A	514	-	3,3,19	0.21	0	2,2,18	0.46	0
2	LFA	A	509	-	10,10,19	0.13	0	9,9,18	0.07	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
2	LFA	A	506	-	-	4/9/9/17	-
2	LFA	B	303	-	-	0/1/1/17	-
2	LFA	B	315	-	-	6/9/9/17	-
4	OLC	B	307	-	-	12/15/15/24	-
2	LFA	B	314	-	-	1/3/3/17	-
2	LFA	B	316	-	-	1/1/1/17	-
2	LFA	A	502	-	-	4/7/7/17	-
4	OLC	A	508	-	-	8/15/15/24	-
2	LFA	B	309	-	-	1/2/2/17	-
2	LFA	B	301	-	-	9/17/17/17	-
2	LFA	B	317	-	-	5/7/7/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	B	306	-	-	2/4/4/17	-
2	LFA	B	313	-	-	7/9/9/17	-
3	OLA	A	504	-	-	3/6/6/17	-
3	OLA	B	304	-	-	3/6/6/17	-
2	LFA	A	511	-	-	5/10/10/17	-
2	LFA	B	305	-	-	4/10/10/17	-
2	LFA	A	503	-	-	0/1/1/17	-
2	LFA	A	507	-	-	3/5/5/17	-
3	OLA	A	505	-	-	3/8/8/17	-
2	LFA	A	501	-	-	7/11/11/17	-
2	LFA	A	515	-	-	6/8/8/17	-
2	LFA	A	513	-	-	2/2/2/17	-
2	LFA	B	310	-	-	4/5/5/17	-
2	LFA	B	302	-	-	3/5/5/17	-
2	LFA	B	311	-	-	1/2/2/17	-
2	LFA	A	510	-	-	0/1/1/17	-
3	OLA	B	308	-	-	4/8/8/17	-
2	LFA	A	514	-	-	0/1/1/17	-
2	LFA	A	509	-	-	5/8/8/17	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	508	OLC	O20-C1	4.27	1.45	1.33
4	B	307	OLC	O20-C1	4.22	1.45	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	307	OLC	O20-C1-C2	2.71	120.09	111.83
4	A	508	OLC	O20-C1-C2	2.62	119.82	111.83

There are no chirality outliers.

All (113) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	508	OLC	C21-C22-C24-O25
4	A	508	OLC	O20-C21-C22-C24

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Mol	Chain	Res	Type	Atoms
4	A	508	OLC	O20-C21-C22-O23
4	B	307	OLC	C21-C22-C24-O25
2	A	501	LFA	C9-C10-C11-C12
2	B	305	LFA	C9-C10-C11-C12
4	B	307	OLC	O20-C21-C22-C24
4	B	307	OLC	O23-C22-C24-O25
4	A	508	OLC	C2-C1-O20-C21
4	B	307	OLC	O20-C21-C22-O23
2	B	310	LFA	C4-C5-C6-C7
2	B	301	LFA	C2-C3-C4-C5
2	B	317	LFA	C3-C4-C5-C6
2	B	317	LFA	C6-C7-C8-C9
2	A	509	LFA	C4-C5-C6-C7
3	B	308	OLA	C4-C5-C6-C7
2	B	313	LFA	C11-C10-C9-C8
4	A	508	OLC	O23-C22-C24-O25
2	A	501	LFA	C6-C7-C8-C9
2	B	315	LFA	C6-C7-C8-C9
2	B	310	LFA	C2-C3-C4-C5
2	B	314	LFA	C16-C17-C18-C19
2	A	515	LFA	C7-C8-C9-C10
2	B	313	LFA	C3-C4-C5-C6
2	A	511	LFA	C10-C11-C12-C13
4	A	508	OLC	O19-C1-O20-C21
2	A	515	LFA	C4-C5-C6-C7
2	A	511	LFA	C16-C17-C18-C19
2	A	511	LFA	C9-C10-C11-C12
2	B	317	LFA	C2-C3-C4-C5
4	A	508	OLC	C2-C3-C4-C5
2	A	511	LFA	C11-C12-C13-C14
4	B	307	OLC	C6-C7-C8-C9
2	A	506	LFA	C10-C11-C12-C13
2	B	315	LFA	C4-C5-C6-C7
2	B	301	LFA	C5-C6-C7-C8
3	A	504	OLA	C3-C4-C5-C6
2	B	305	LFA	C16-C17-C18-C19
2	A	507	LFA	C14-C15-C16-C17
2	A	501	LFA	C5-C6-C7-C8
2	A	515	LFA	C5-C6-C7-C8
2	B	313	LFA	C5-C6-C7-C8
4	B	307	OLC	C2-C3-C4-C5
2	A	501	LFA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
2	A	501	LFA	C4-C5-C6-C7
2	B	315	LFA	C11-C10-C9-C8
2	A	502	LFA	C14-C15-C16-C17
2	A	509	LFA	C1-C2-C3-C4
2	A	502	LFA	C10-C11-C12-C13
2	B	301	LFA	C11-C10-C9-C8
2	B	302	LFA	C1-C2-C3-C4
2	B	301	LFA	C1-C2-C3-C4
2	A	502	LFA	C15-C16-C17-C18
2	A	515	LFA	C6-C7-C8-C9
2	B	306	LFA	C2-C3-C4-C5
2	A	507	LFA	C17-C18-C19-C20
2	B	313	LFA	C2-C3-C4-C5
2	B	315	LFA	C9-C10-C11-C12
2	A	507	LFA	C16-C17-C18-C19
2	A	506	LFA	C15-C16-C17-C18
2	B	309	LFA	C2-C3-C4-C5
2	A	502	LFA	C12-C13-C14-C15
2	A	501	LFA	C7-C8-C9-C10
2	A	513	LFA	C2-C3-C4-C5
2	A	501	LFA	C3-C4-C5-C6
2	B	317	LFA	C1-C2-C3-C4
2	B	302	LFA	C2-C3-C4-C5
2	B	310	LFA	C1-C2-C3-C4
2	B	305	LFA	C13-C14-C15-C16
3	A	505	OLA	C4-C5-C6-C7
2	B	301	LFA	C11-C12-C13-C14
2	B	305	LFA	C15-C16-C17-C18
2	B	313	LFA	C7-C8-C9-C10
3	A	505	OLA	C5-C6-C7-C8
2	B	315	LFA	C2-C3-C4-C5
2	B	310	LFA	C3-C4-C5-C6
3	A	505	OLA	C3-C4-C5-C6
2	B	317	LFA	C5-C6-C7-C8
2	B	302	LFA	C4-C5-C6-C7
2	A	509	LFA	C7-C8-C9-C10
4	B	307	OLC	C3-C4-C5-C6
2	B	316	LFA	C2-C3-C4-C5
2	A	506	LFA	C14-C15-C16-C17
2	A	511	LFA	C17-C18-C19-C20
2	B	301	LFA	C12-C13-C14-C15
2	B	301	LFA	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
3	B	304	OLA	C4-C5-C6-C7
2	B	306	LFA	C5-C6-C7-C8
4	A	508	OLC	C5-C6-C7-C8
4	B	307	OLC	C2-C1-O20-C21
2	B	313	LFA	C9-C10-C11-C12
4	B	307	OLC	O19-C1-O20-C21
4	B	307	OLC	C4-C5-C6-C7
3	A	504	OLA	C2-C3-C4-C5
4	B	307	OLC	O20-C1-C2-C3
2	A	515	LFA	C10-C11-C12-C13
2	B	313	LFA	C6-C7-C8-C9
2	B	301	LFA	C6-C7-C8-C9
2	B	315	LFA	C3-C4-C5-C6
4	B	307	OLC	C5-C6-C7-C8
3	B	304	OLA	O1-C1-C2-C3
3	B	304	OLA	O2-C1-C2-C3
3	B	308	OLA	O2-C1-C2-C3
2	A	513	LFA	C3-C4-C5-C6
3	B	308	OLA	O1-C1-C2-C3
3	A	504	OLA	C4-C5-C6-C7
2	B	301	LFA	C4-C5-C6-C7
2	A	509	LFA	C6-C7-C8-C9
2	A	509	LFA	C5-C6-C7-C8
2	A	506	LFA	C11-C12-C13-C14
2	A	515	LFA	C11-C10-C9-C8
2	B	311	LFA	C2-C3-C4-C5
3	B	308	OLA	C2-C3-C4-C5

There are no ring outliers.

11 monomers are involved in 18 short contacts:

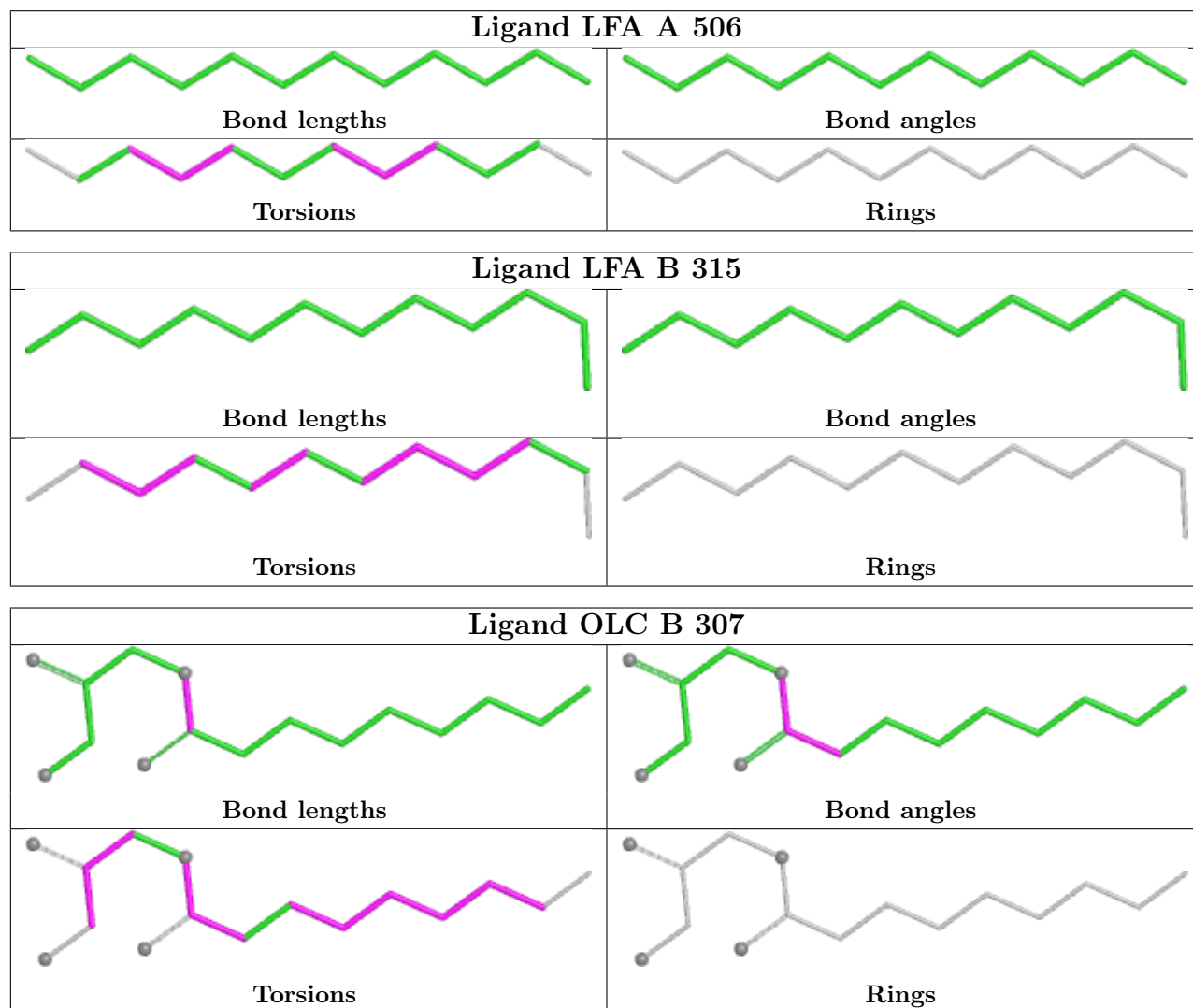
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2	B	315	LFA	1	0
2	B	316	LFA	5	0
2	A	502	LFA	4	0
4	A	508	OLC	2	0
2	B	301	LFA	1	0
2	B	306	LFA	1	0
2	B	313	LFA	1	0
2	A	507	LFA	4	0
2	B	310	LFA	2	0

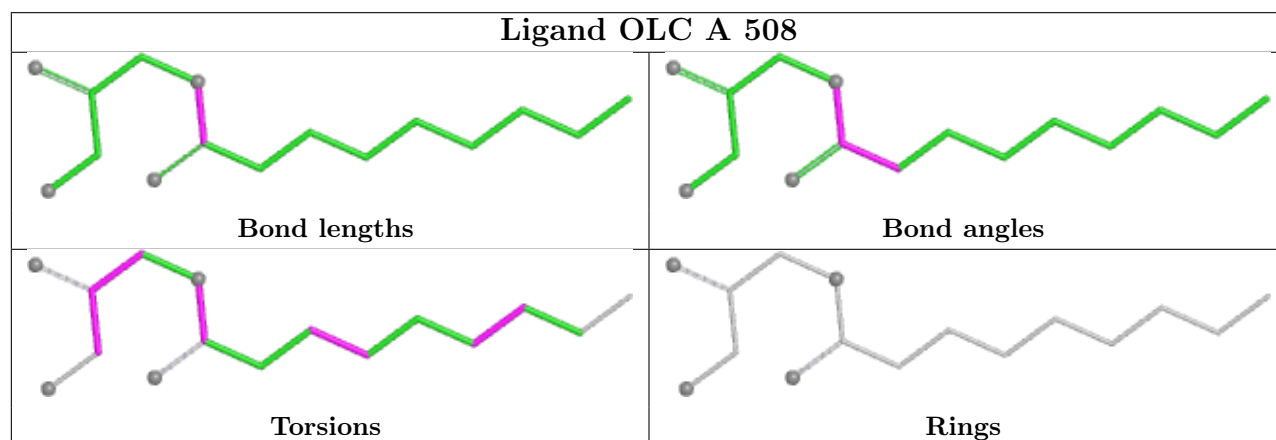
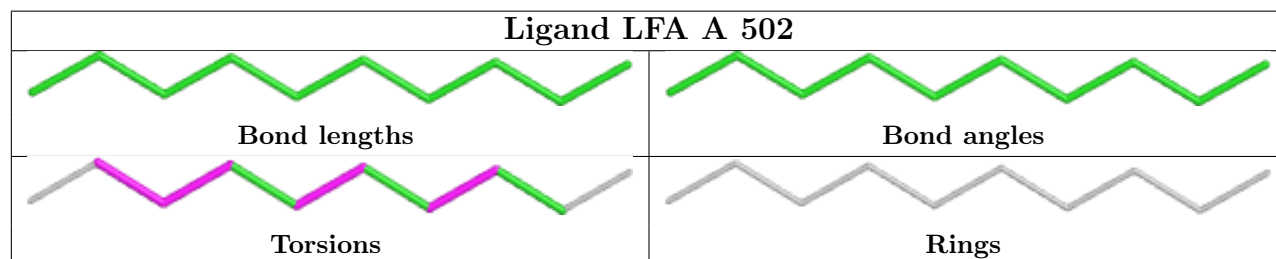
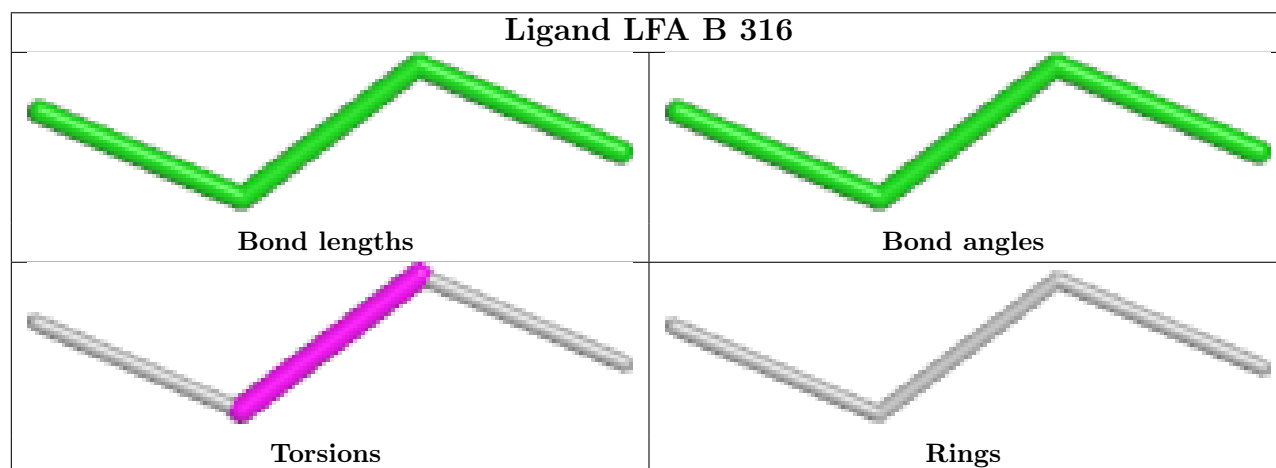
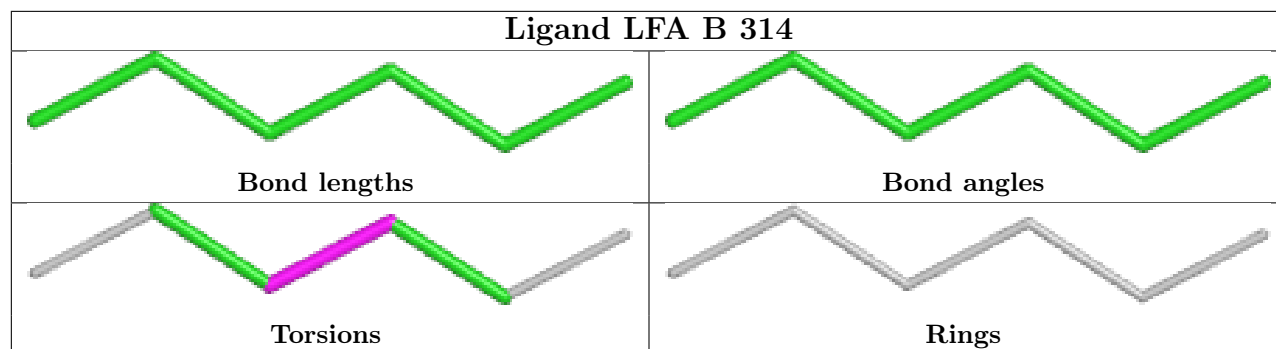
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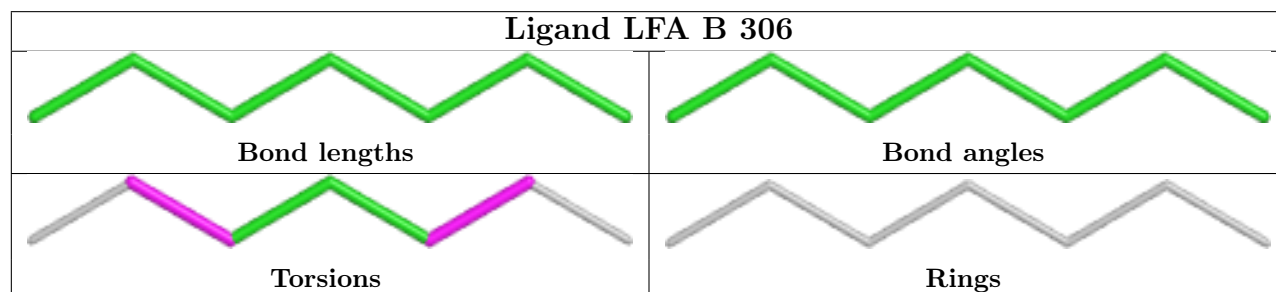
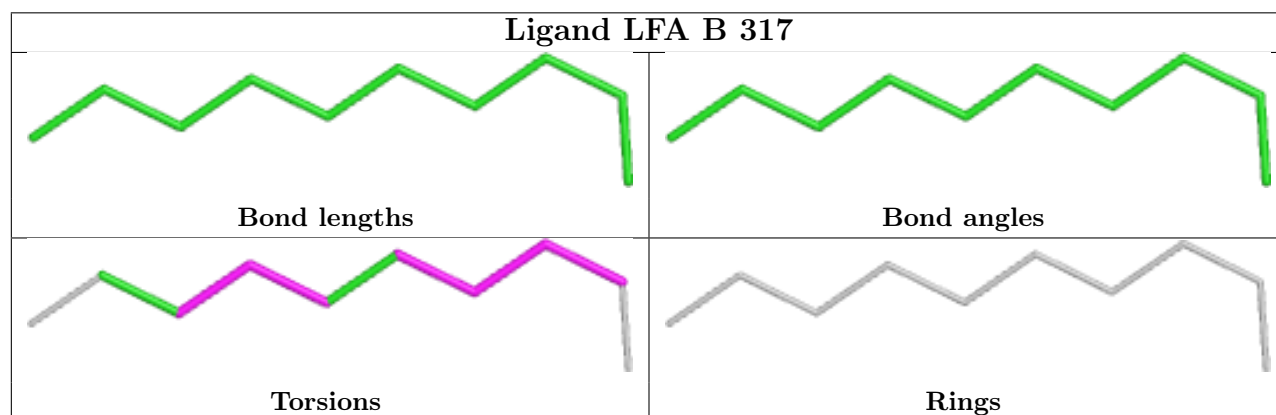
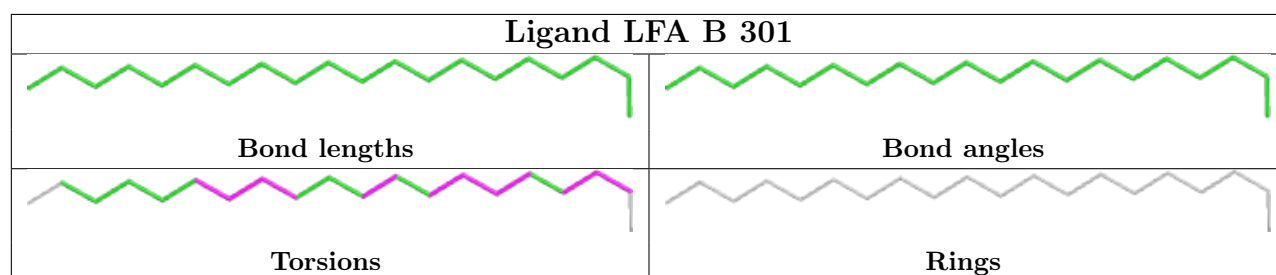
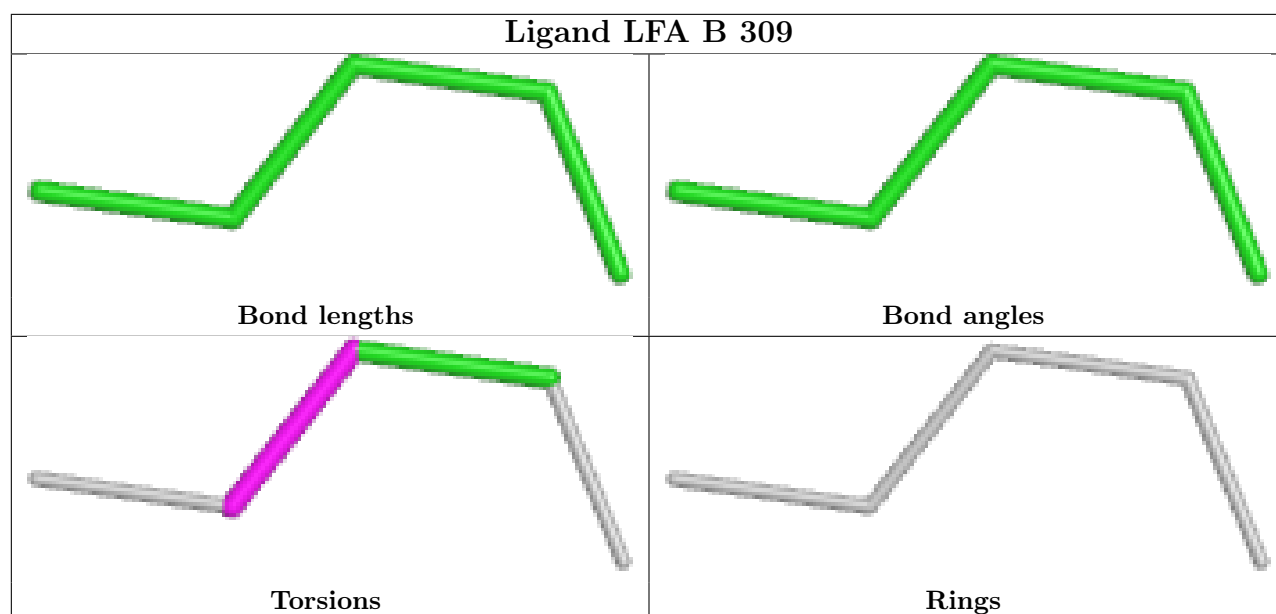
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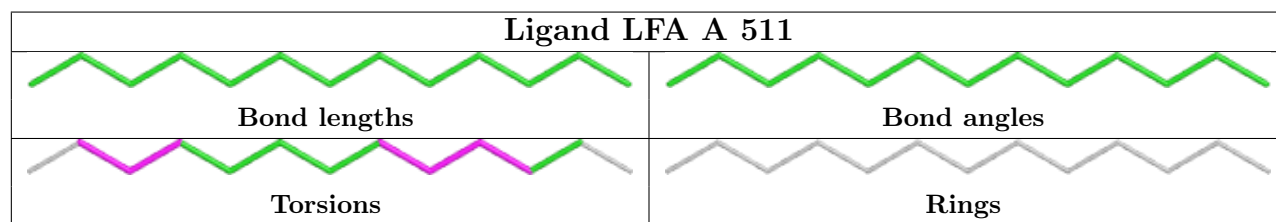
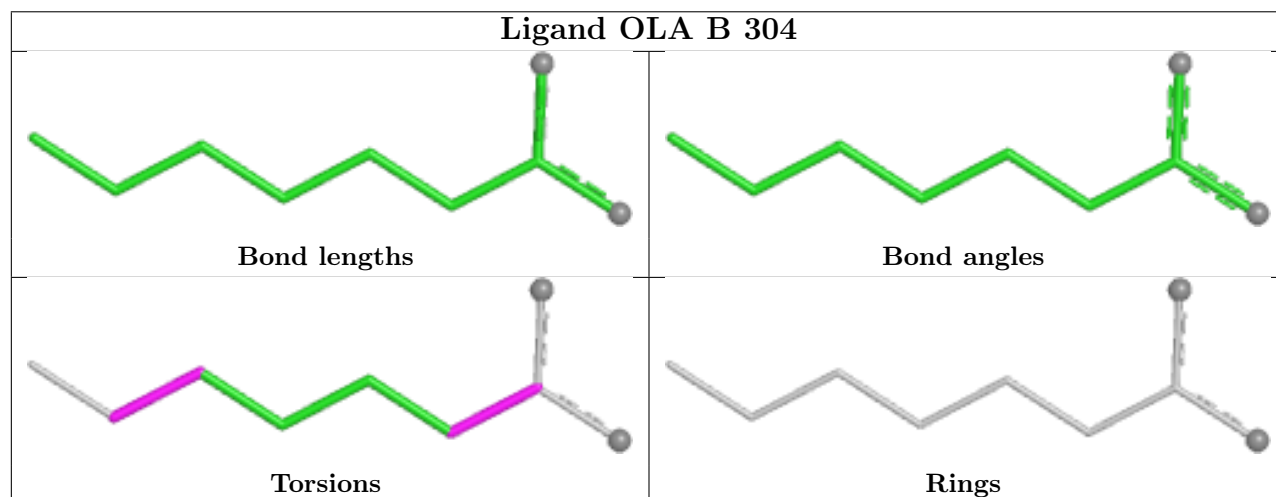
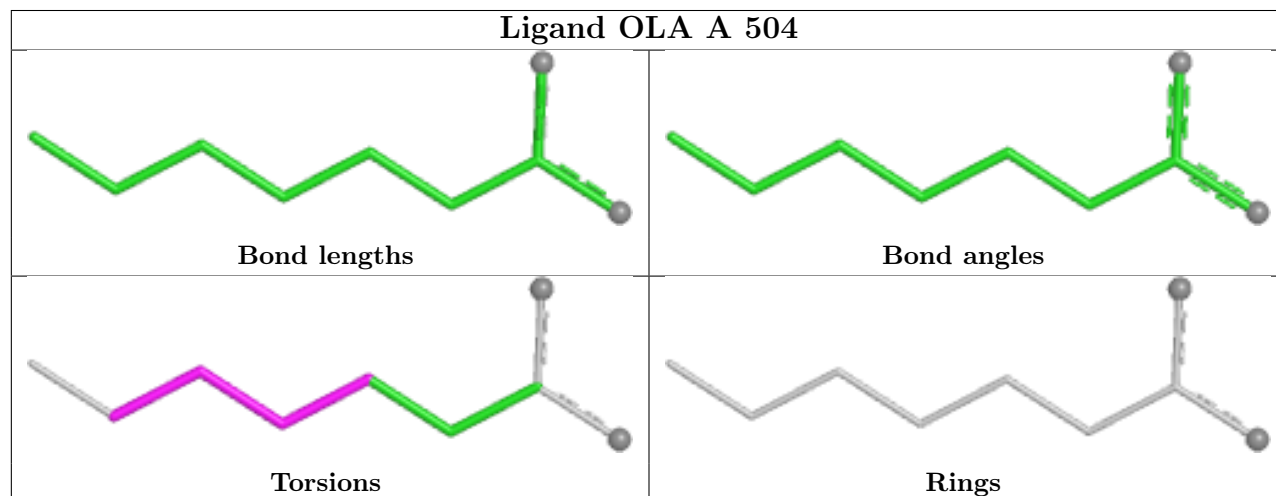
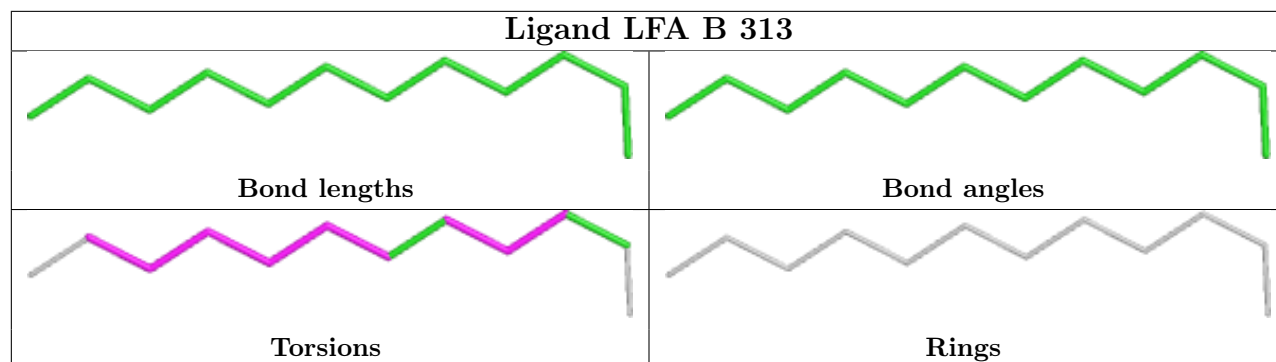
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	311	LFA	2	0

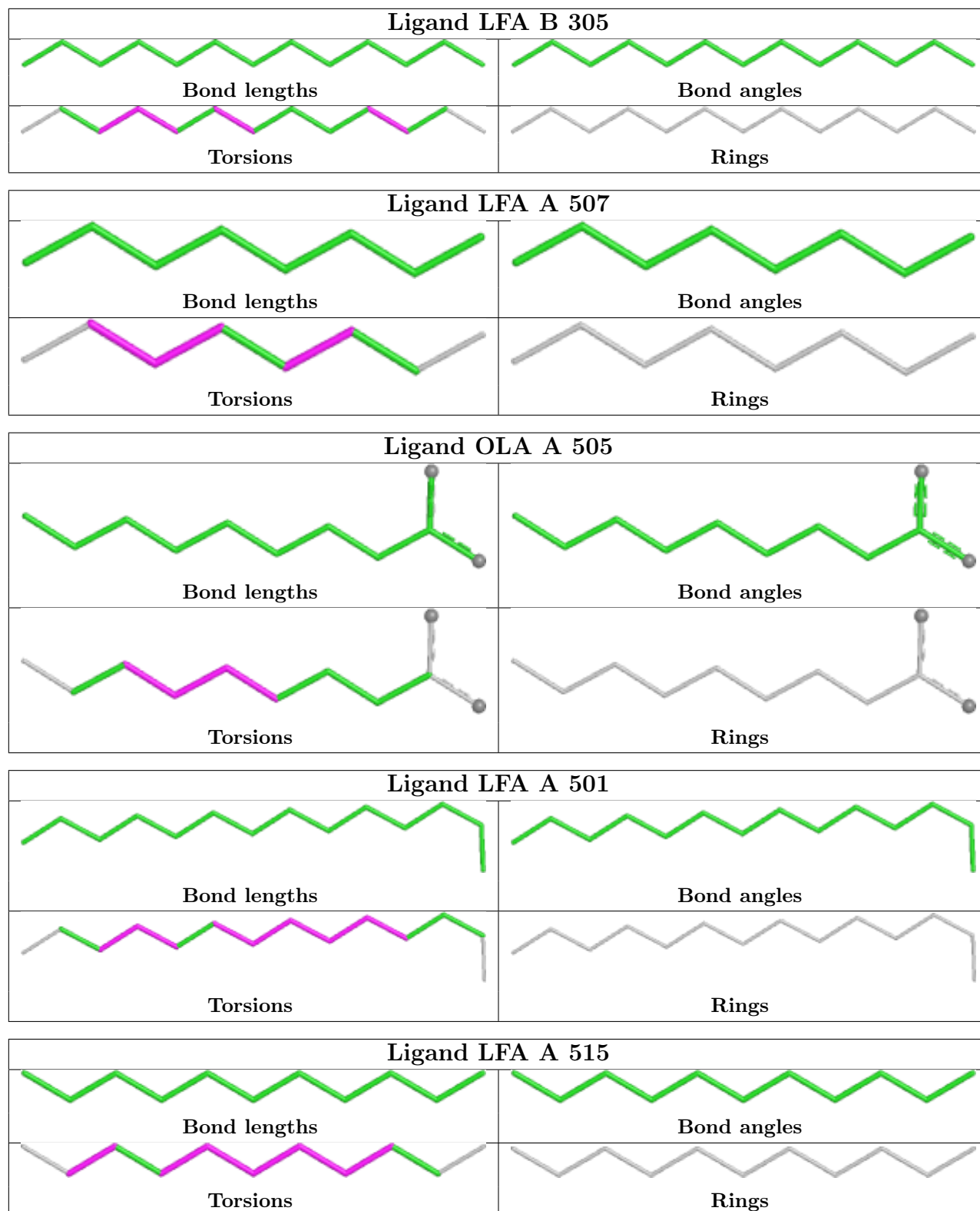
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



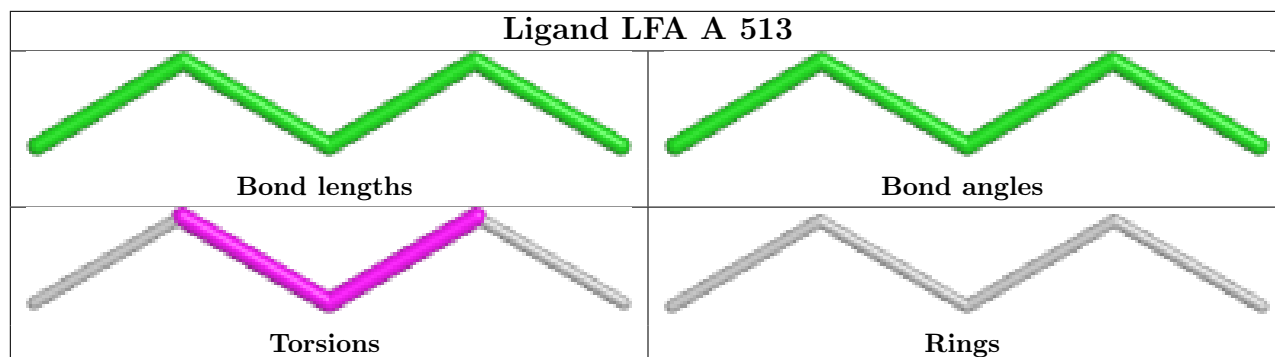




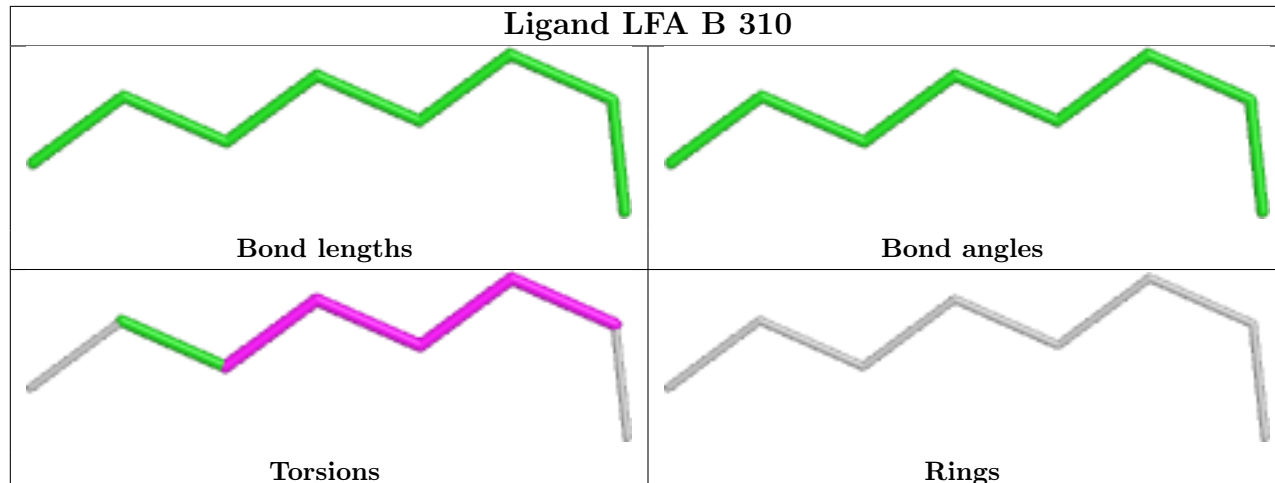




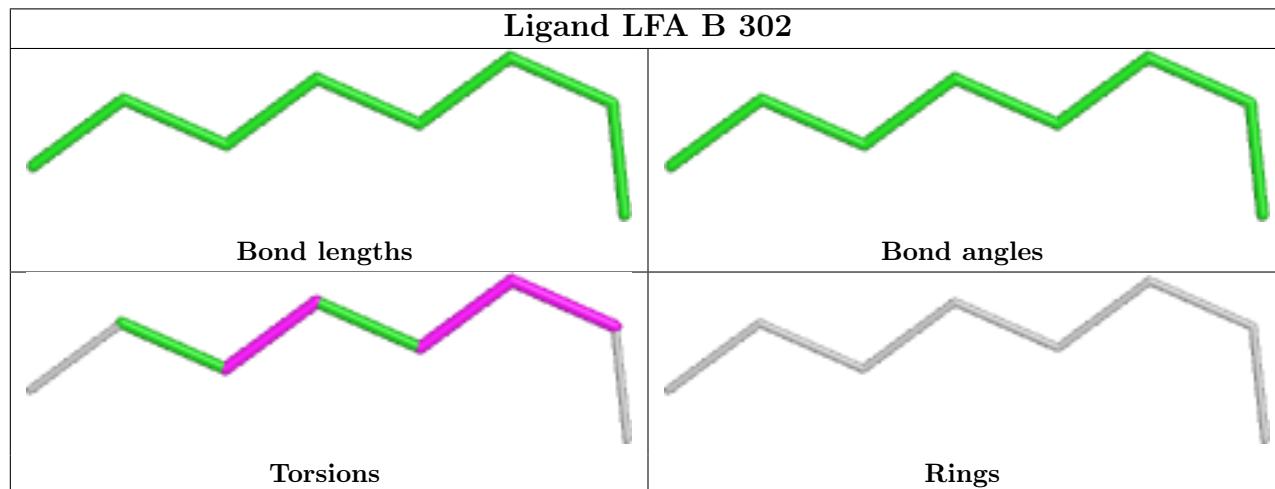
Ligand LFA A 513

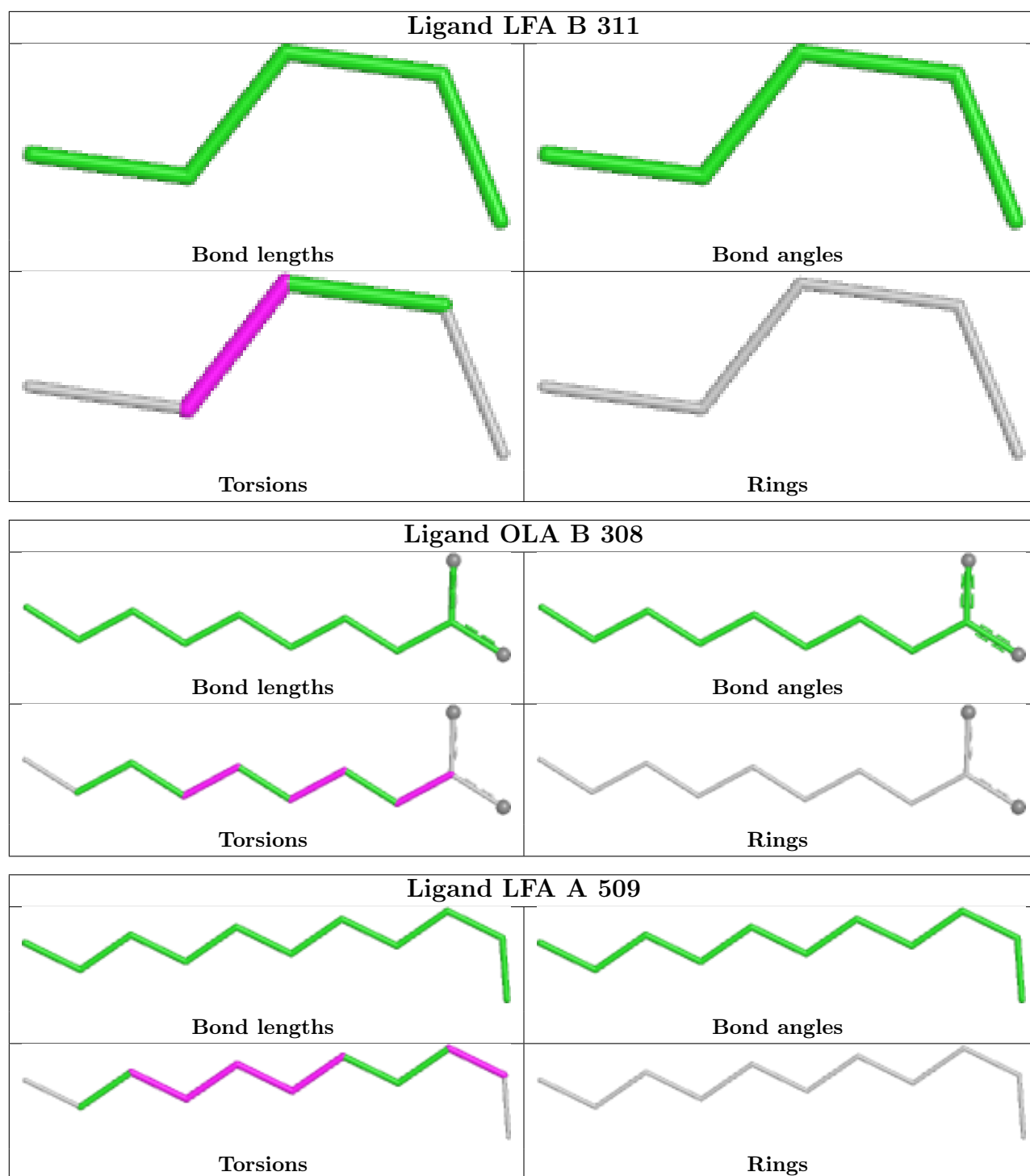


Ligand LFA B 310



Ligand LFA B 302





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	223/231 (96%)	-0.91	0 100 100	13, 28, 50, 78	6 (2%)
1	B	223/231 (96%)	-0.91	0 100 100	12, 28, 50, 99	7 (3%)
All	All	446/462 (96%)	-0.91	0 100 100	12, 28, 50, 99	13 (2%)

There are no RSRZ outliers to report.

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	LYR	A	204	29/30	0.99	0.03	19,22,27,29	0
1	LYR	B	204	29/30	0.99	0.03	19,23,27,30	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

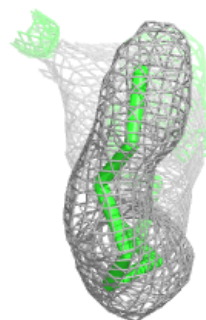
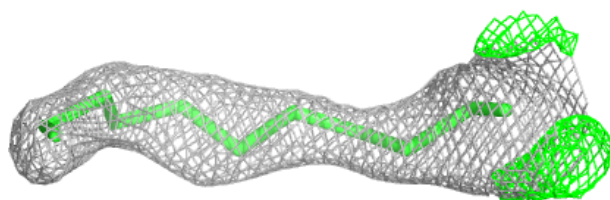
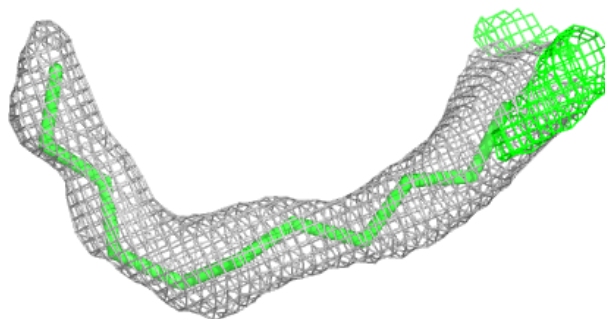
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LFA	A	515	11/20	0.95	0.09	51,56,61,62	0
2	LFA	B	303	4/20	0.95	0.08	48,48,49,54	0
2	LFA	B	316	4/20	0.95	0.10	48,51,51,52	0
2	LFA	A	510	4/20	0.96	0.09	46,47,49,50	0
2	LFA	B	306	7/20	0.96	0.08	57,63,73,75	0
2	LFA	B	311	5/20	0.96	0.09	39,42,47,52	0
2	LFA	B	313	12/20	0.96	0.08	41,46,59,59	0
2	LFA	A	509	11/20	0.96	0.07	44,46,52,55	0
3	OLA	B	308	11/20	0.96	0.07	52,55,62,62	0
2	LFA	A	507	8/20	0.97	0.08	43,57,65,69	0
2	LFA	B	305	13/20	0.97	0.06	43,52,56,59	0
2	LFA	A	501	14/20	0.97	0.07	42,51,59,60	0
2	LFA	B	309	5/20	0.97	0.08	55,58,62,64	0
2	LFA	A	502	10/20	0.97	0.07	44,48,53,59	0
2	LFA	B	312	3/20	0.97	0.08	38,38,43,51	0
2	LFA	A	511	13/20	0.97	0.09	47,60,65,65	0
2	LFA	B	315	12/20	0.97	0.08	46,56,62,64	0
2	LFA	A	503	4/20	0.97	0.07	40,44,44,44	0
2	LFA	B	317	10/20	0.97	0.09	54,60,65,65	0
3	OLA	A	504	9/20	0.97	0.07	48,54,60,62	0
3	OLA	A	505	11/20	0.97	0.06	54,59,80,81	0
3	OLA	B	304	9/20	0.97	0.07	40,48,55,57	0
2	LFA	B	302	8/20	0.97	0.06	41,47,54,55	0
4	OLC	A	508	16/25	0.97	0.07	35,46,52,53	8
4	OLC	B	307	16/25	0.97	0.07	41,48,56,60	8
2	LFA	B	310	8/20	0.98	0.07	46,48,58,60	0
2	LFA	A	512	3/20	0.98	0.07	39,39,44,52	0
2	LFA	A	513	5/20	0.98	0.05	38,39,41,44	0
2	LFA	A	514	4/20	0.98	0.07	42,51,52,55	0
2	LFA	B	314	6/20	0.98	0.09	55,58,59,59	0
2	LFA	A	506	12/20	0.98	0.08	45,49,56,60	0
2	LFA	B	301	20/20	0.98	0.07	49,55,66,74	0

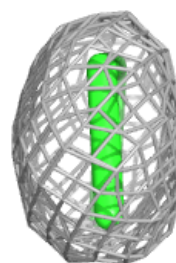
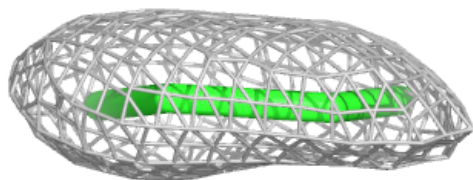
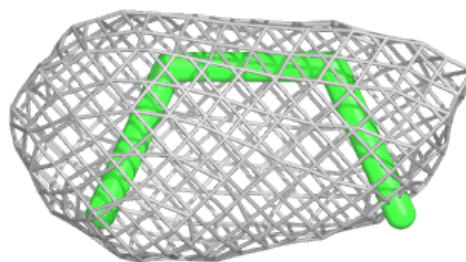
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LFA A 515:

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

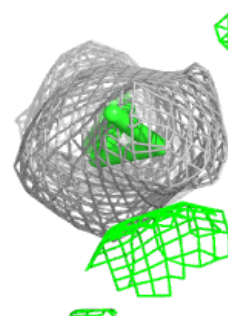
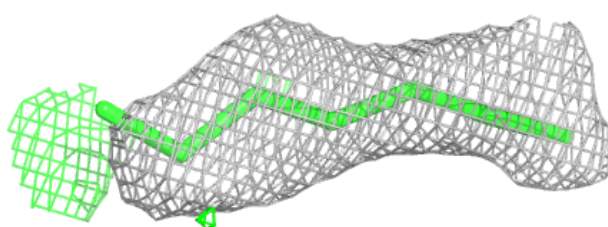
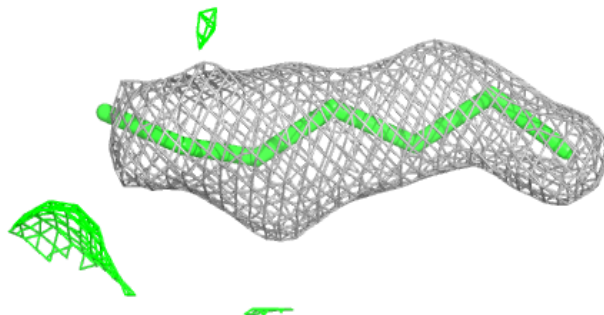
**Electron density around LFA B 316:**

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

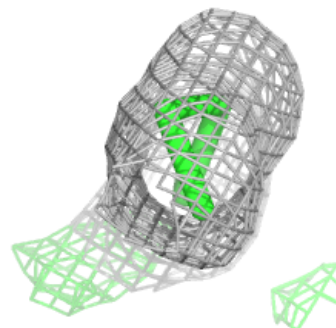
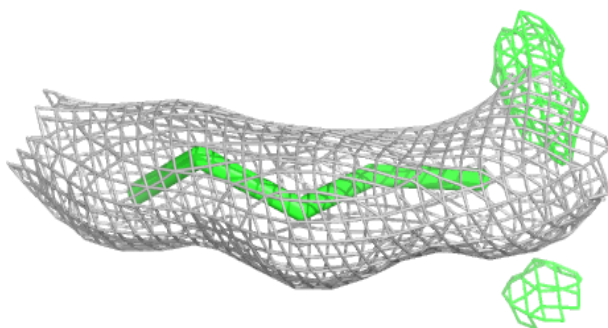
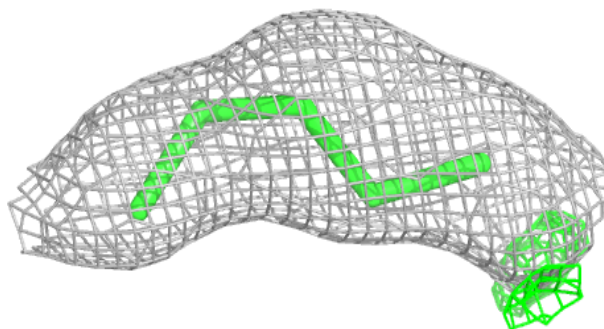


Electron density around LFA B 306:

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

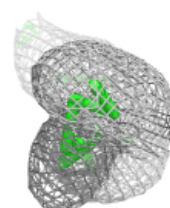
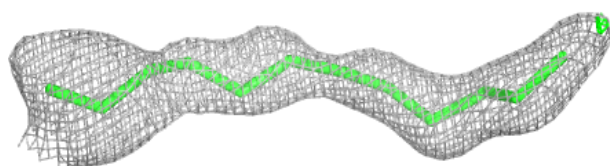
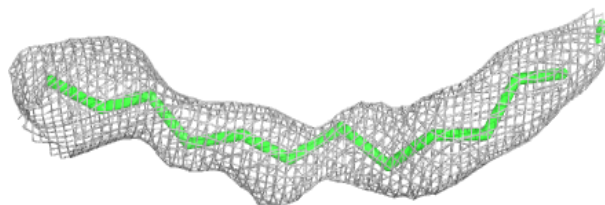
**Electron density around LFA B 311:**

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

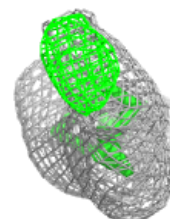
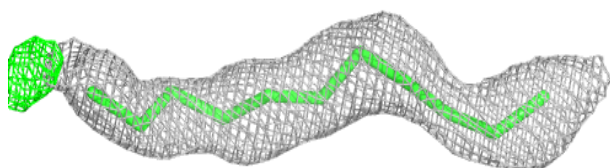
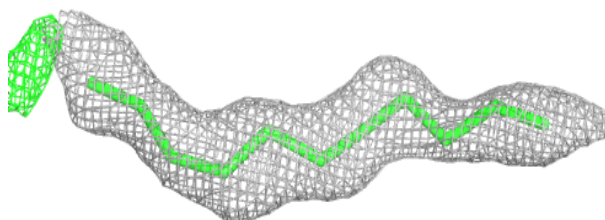


Electron density around LFA B 313:

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

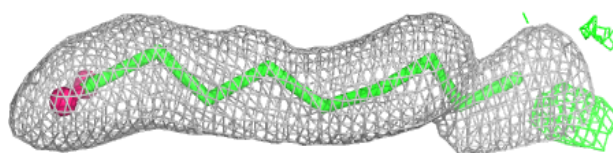
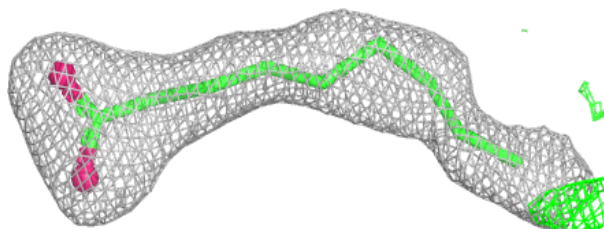
**Electron density around LFA A 509:**

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

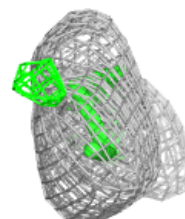
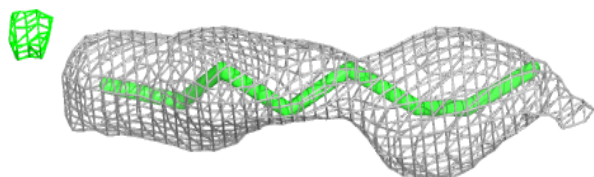
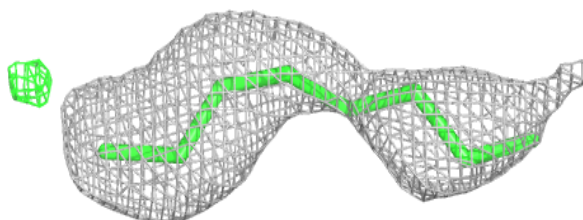


Electron density around OLA B 308:

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

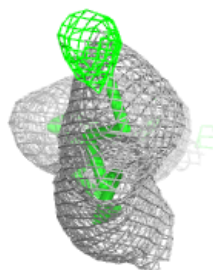
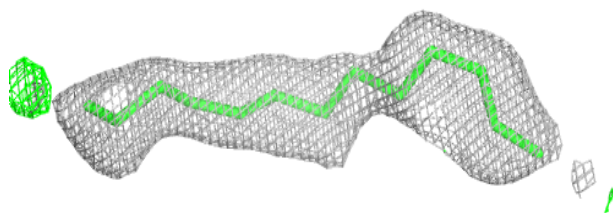
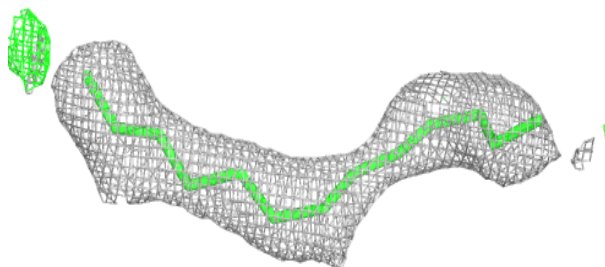
**Electron density around LFA A 507:**

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

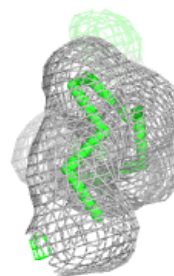
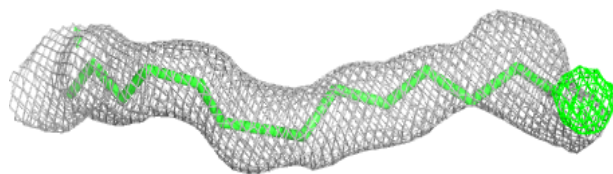
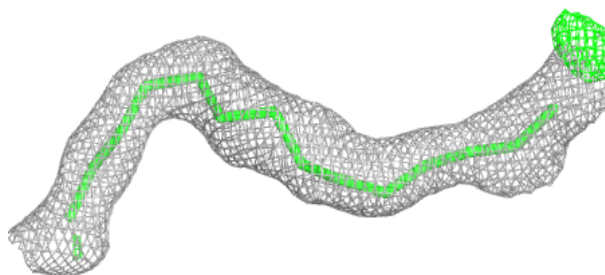


Electron density around LFA B 305:

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

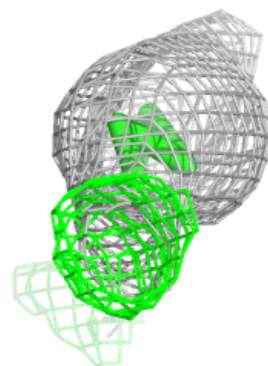
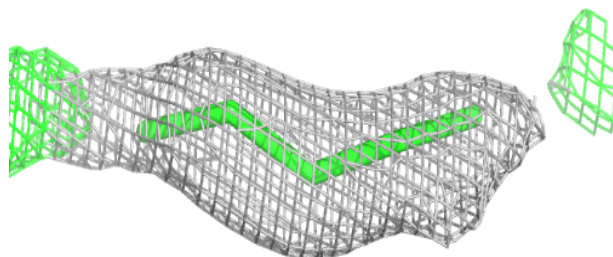
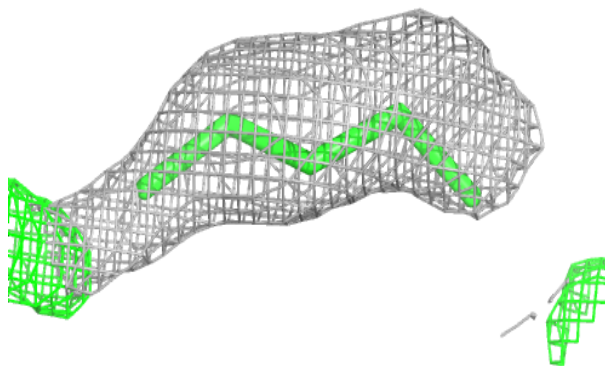
**Electron density around LFA A 501:**

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

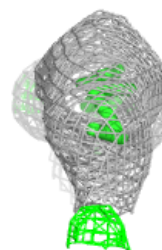
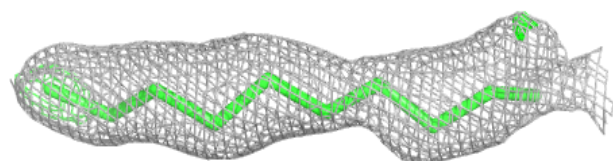
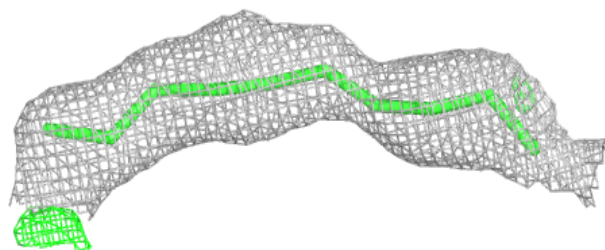


Electron density around LFA B 309:

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

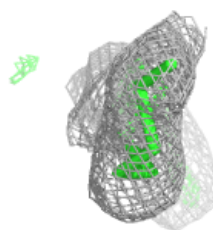
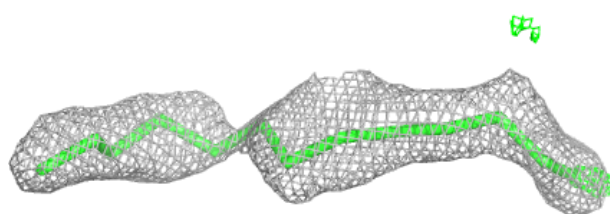
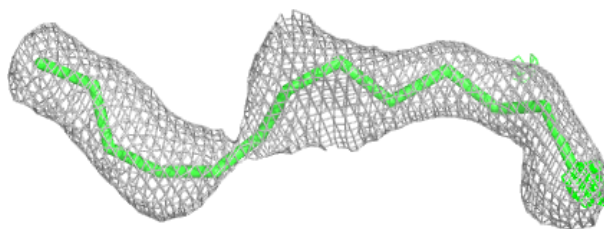
**Electron density around LFA A 502:**

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

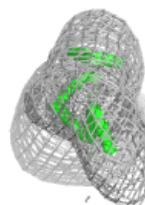
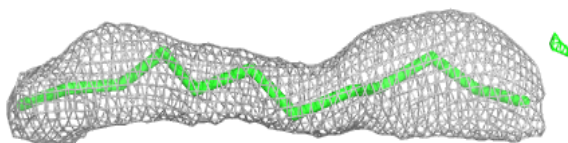
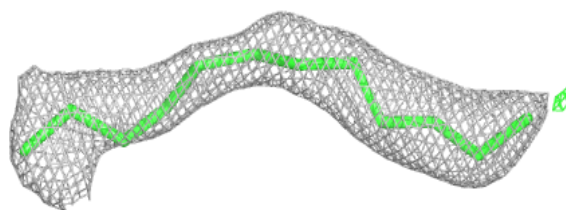


Electron density around LFA A 511:

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

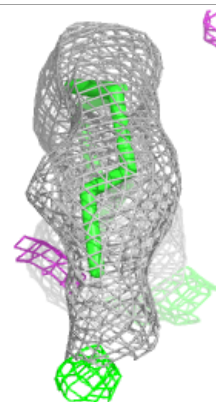
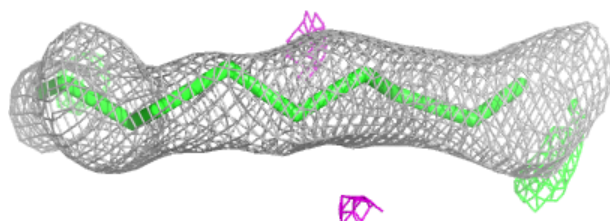
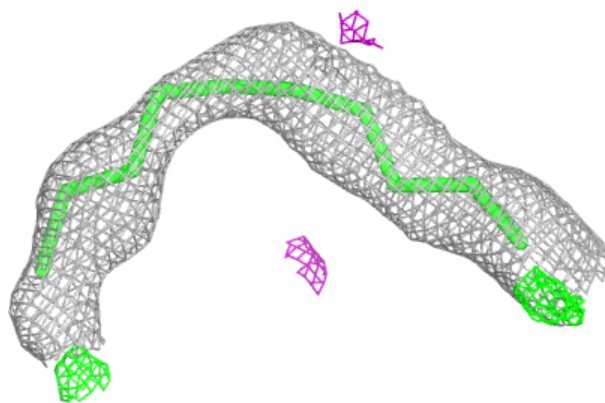
**Electron density around LFA B 315:**

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

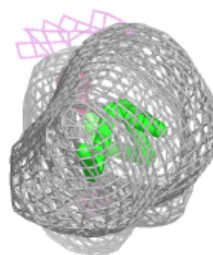
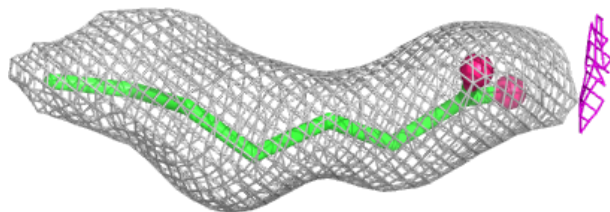
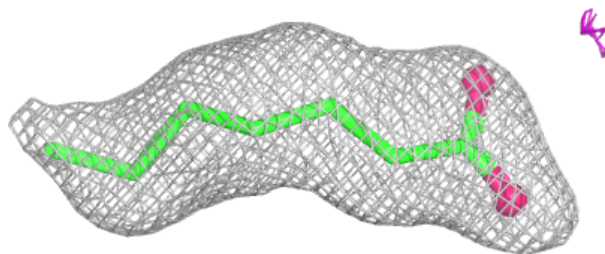


Electron density around LFA B 317:

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and green (positive)

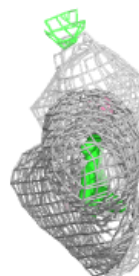
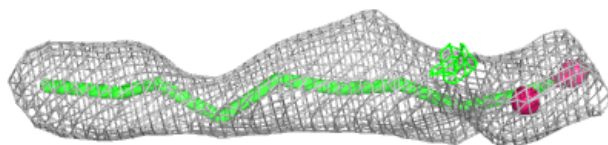
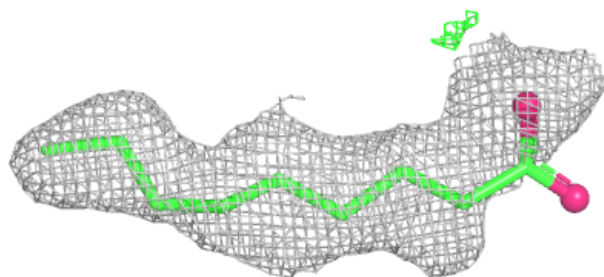
**Electron density around OLA A 504:**

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

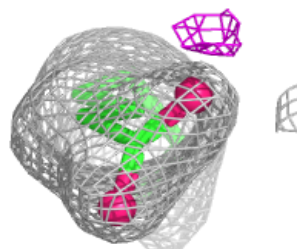
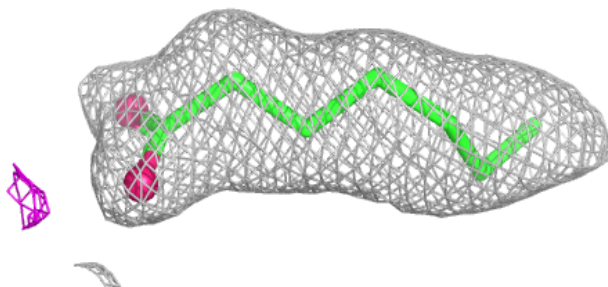
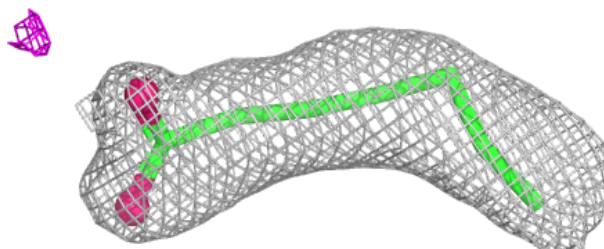


Electron density around OLA A 505:

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

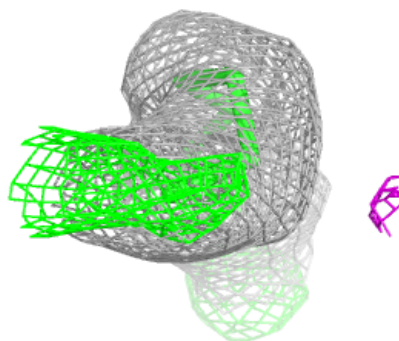
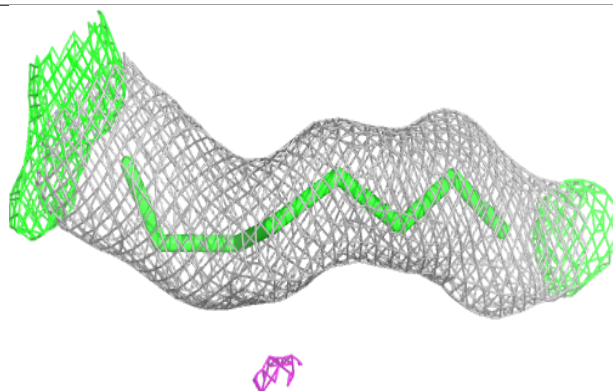
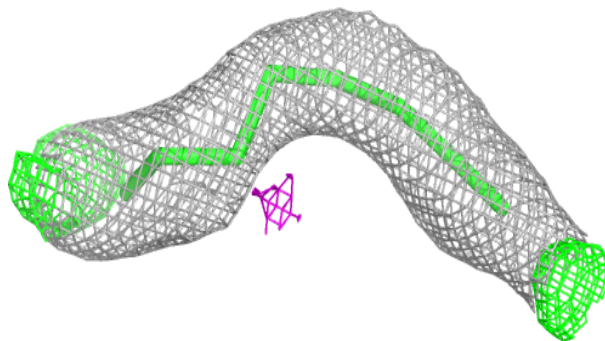
**Electron density around OLA B 304:**

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

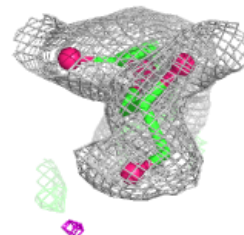
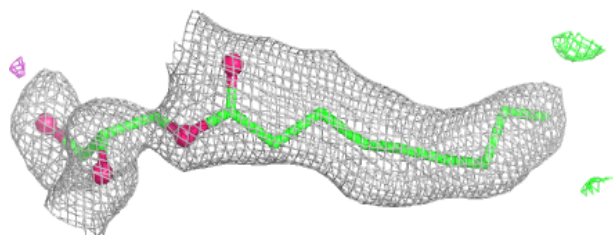
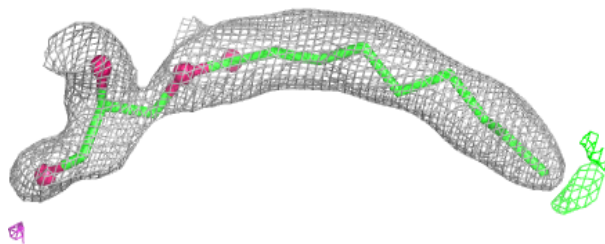


Electron density around LFA B 302:

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

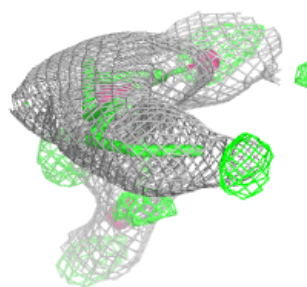
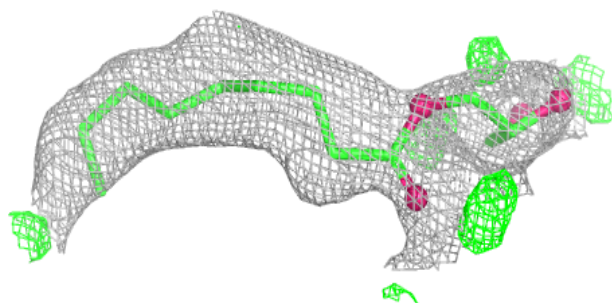
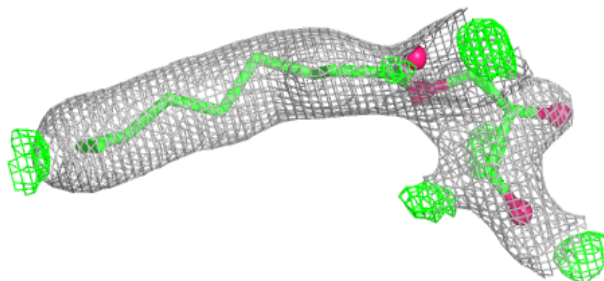
**Electron density around OLC A 508:**

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

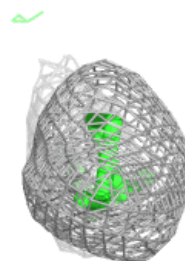
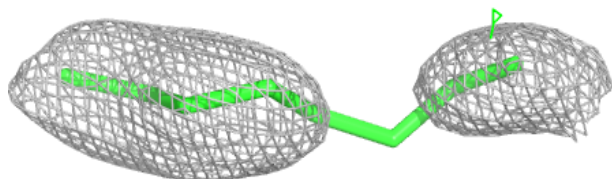
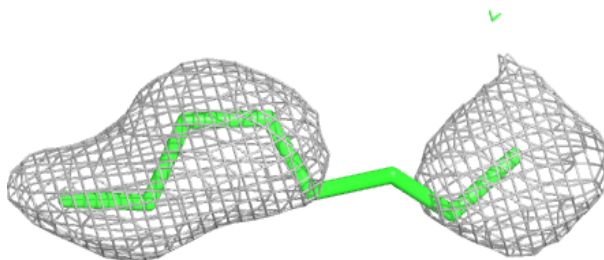


Electron density around OLC B 307:

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

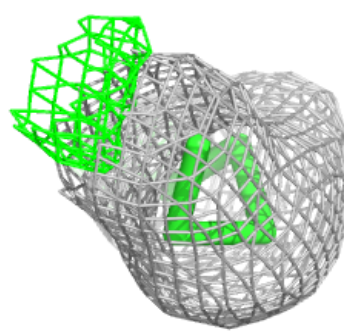
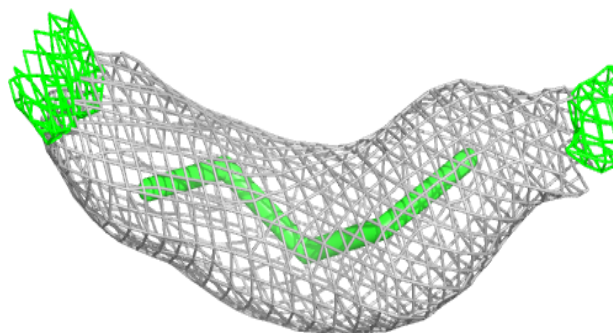
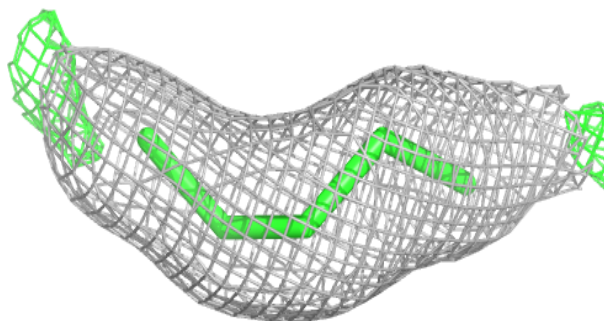
**Electron density around LFA B 310:**

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

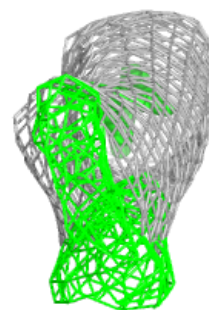
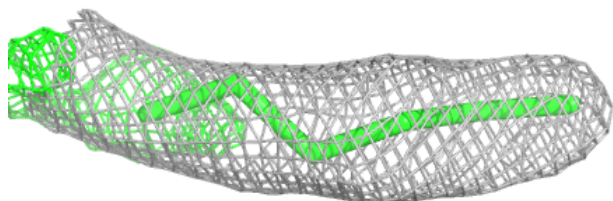
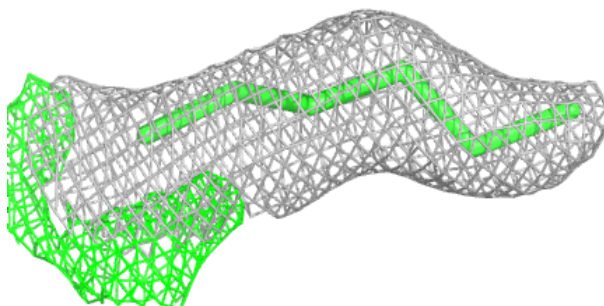


Electron density around LFA A 513:

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

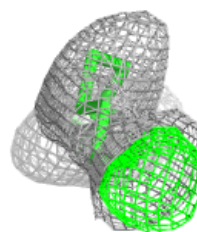
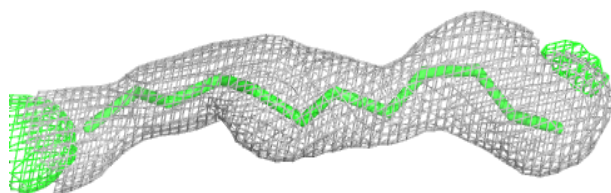
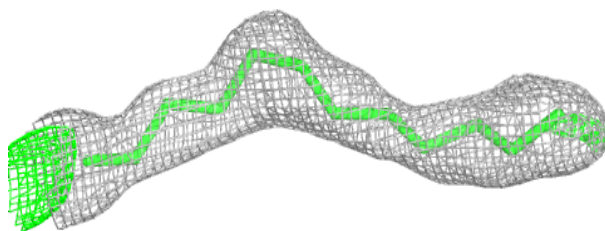
**Electron density around LFA B 314:**

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

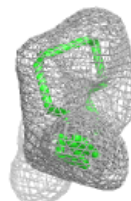
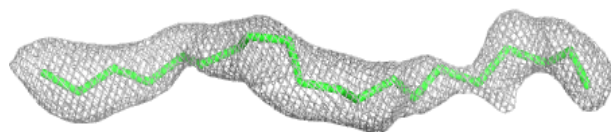
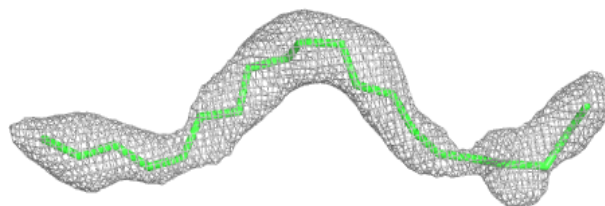


Electron density around LFA A 506:

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

**Electron density around LFA B 301:**

$2mF_o-DF_c$ (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.