



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:36 PM UTC

PDB ID : 5I20 / pdb_00005i20
Title : Crystal structure of protein
Authors : Ishitani, R.; Nureki, O.
Deposited on : 2016-02-08
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

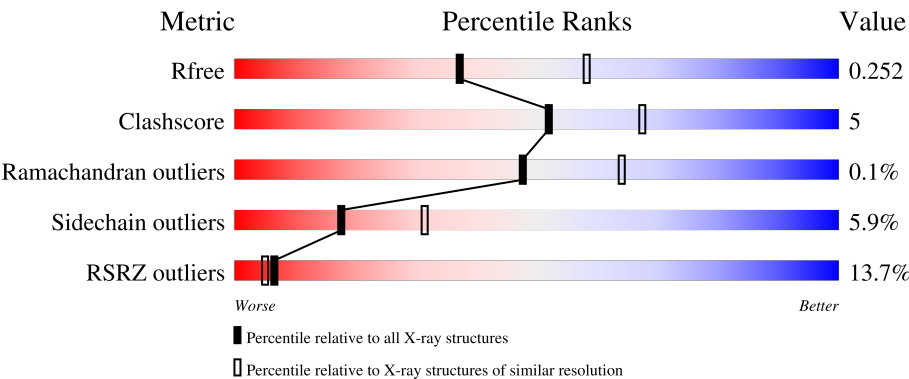
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	298	6% 81% 14% • •
1	B	298	5% 85% 7% • 6%
1	C	298	8% 80% 13% • 5%
1	D	298	11% 83% 9% • 6%
1	E	298	5% 86% 11% • •

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Mol	Chain	Length	Quality of chain
1	F	298	40% 57% 15% • 27%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11923 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2060	1377	333	344	6			
1	B	279	Total	C	N	O	S	0	1	0
			2005	1339	322	338	6			
1	C	282	Total	C	N	O	S	0	0	0
			1993	1332	318	337	6			
1	D	280	Total	C	N	O	S	0	0	0
			1954	1313	303	332	6			
1	E	291	Total	C	N	O	S	0	0	0
			2071	1386	331	348	6			
1	F	219	Total	C	N	O	S	0	0	0
			1480	981	237	257	5			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	288	LEU	-	expression tag	UNP D7A5Q8
A	289	GLU	-	expression tag	UNP D7A5Q8
A	290	SER	-	expression tag	UNP D7A5Q8
A	291	SER	-	expression tag	UNP D7A5Q8
A	292	GLY	-	expression tag	UNP D7A5Q8
A	293	GLU	-	expression tag	UNP D7A5Q8
A	294	ASN	-	expression tag	UNP D7A5Q8
A	295	LEU	-	expression tag	UNP D7A5Q8
A	296	TYR	-	expression tag	UNP D7A5Q8
A	297	PHE	-	expression tag	UNP D7A5Q8
A	298	GLN	-	expression tag	UNP D7A5Q8
B	288	LEU	-	expression tag	UNP D7A5Q8
B	289	GLU	-	expression tag	UNP D7A5Q8
B	290	SER	-	expression tag	UNP D7A5Q8
B	291	SER	-	expression tag	UNP D7A5Q8
B	292	GLY	-	expression tag	UNP D7A5Q8
B	293	GLU	-	expression tag	UNP D7A5Q8

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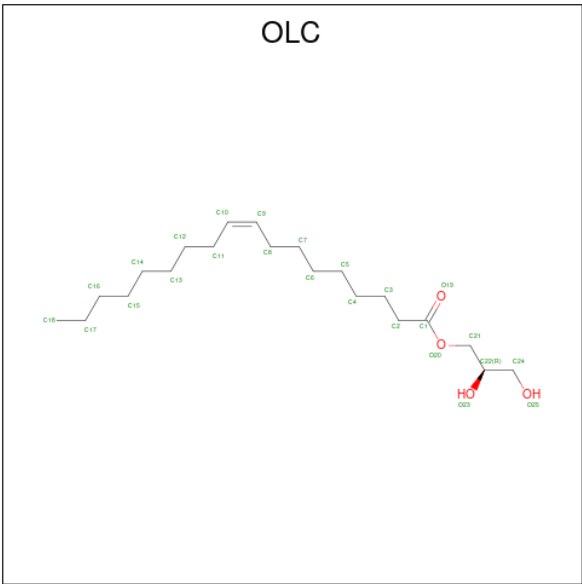
Chain	Residue	Modelled	Actual	Comment	Reference
B	294	ASN	-	expression tag	UNP D7A5Q8
B	295	LEU	-	expression tag	UNP D7A5Q8
B	296	TYR	-	expression tag	UNP D7A5Q8
B	297	PHE	-	expression tag	UNP D7A5Q8
B	298	GLN	-	expression tag	UNP D7A5Q8
C	288	LEU	-	expression tag	UNP D7A5Q8
C	289	GLU	-	expression tag	UNP D7A5Q8
C	290	SER	-	expression tag	UNP D7A5Q8
C	291	SER	-	expression tag	UNP D7A5Q8
C	292	GLY	-	expression tag	UNP D7A5Q8
C	293	GLU	-	expression tag	UNP D7A5Q8
C	294	ASN	-	expression tag	UNP D7A5Q8
C	295	LEU	-	expression tag	UNP D7A5Q8
C	296	TYR	-	expression tag	UNP D7A5Q8
C	297	PHE	-	expression tag	UNP D7A5Q8
C	298	GLN	-	expression tag	UNP D7A5Q8
D	288	LEU	-	expression tag	UNP D7A5Q8
D	289	GLU	-	expression tag	UNP D7A5Q8
D	290	SER	-	expression tag	UNP D7A5Q8
D	291	SER	-	expression tag	UNP D7A5Q8
D	292	GLY	-	expression tag	UNP D7A5Q8
D	293	GLU	-	expression tag	UNP D7A5Q8
D	294	ASN	-	expression tag	UNP D7A5Q8
D	295	LEU	-	expression tag	UNP D7A5Q8
D	296	TYR	-	expression tag	UNP D7A5Q8
D	297	PHE	-	expression tag	UNP D7A5Q8
D	298	GLN	-	expression tag	UNP D7A5Q8
E	288	LEU	-	expression tag	UNP D7A5Q8
E	289	GLU	-	expression tag	UNP D7A5Q8
E	290	SER	-	expression tag	UNP D7A5Q8
E	291	SER	-	expression tag	UNP D7A5Q8
E	292	GLY	-	expression tag	UNP D7A5Q8
E	293	GLU	-	expression tag	UNP D7A5Q8
E	294	ASN	-	expression tag	UNP D7A5Q8
E	295	LEU	-	expression tag	UNP D7A5Q8
E	296	TYR	-	expression tag	UNP D7A5Q8
E	297	PHE	-	expression tag	UNP D7A5Q8
E	298	GLN	-	expression tag	UNP D7A5Q8
F	288	LEU	-	expression tag	UNP D7A5Q8
F	289	GLU	-	expression tag	UNP D7A5Q8
F	290	SER	-	expression tag	UNP D7A5Q8
F	291	SER	-	expression tag	UNP D7A5Q8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	292	GLY	-	expression tag	UNP D7A5Q8
F	293	GLU	-	expression tag	UNP D7A5Q8
F	294	ASN	-	expression tag	UNP D7A5Q8
F	295	LEU	-	expression tag	UNP D7A5Q8
F	296	TYR	-	expression tag	UNP D7A5Q8
F	297	PHE	-	expression tag	UNP D7A5Q8
F	298	GLN	-	expression tag	UNP D7A5Q8

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



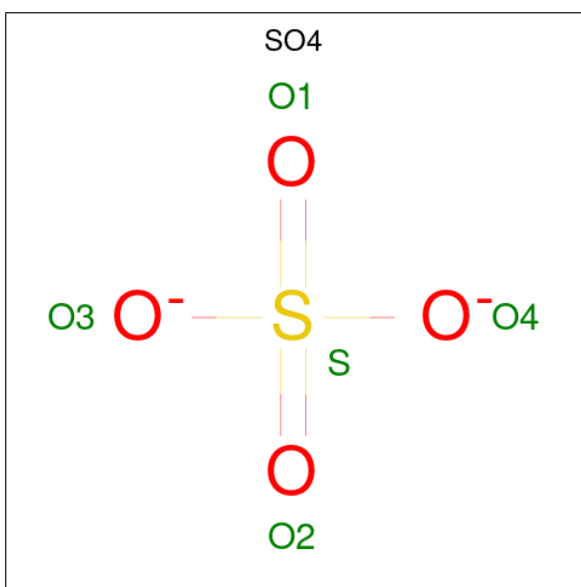
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C 15	0	0
2	A	1	Total	C 10 O 8	0	0
2	A	1	Total	C 8	0	0
2	A	1	Total	C 13 O 11	0	0
2	B	1	Total	C 25 O 21	0	0
2	B	1	Total	C 13 O 11	0	0
2	B	1	Total	C 17 O 13	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C 13 13	0	0
2	B	1	Total C O 17 15 2	0	0
2	C	1	Total C 11 11	0	0
2	C	1	Total C O 24 21 3	0	0
2	C	1	Total C O 13 11 2	0	0
2	D	1	Total C O 25 21 4	0	0
2	D	1	Total C O 7 5 2	0	0
2	D	1	Total C 11 11	0	0
2	D	1	Total C O 16 14 2	0	0
2	D	1	Total C O 13 9 4	0	0
2	E	1	Total C 16 16	0	0
2	E	1	Total C O 25 21 4	0	0
2	E	1	Total C 10 10	0	0
2	E	1	Total C O 14 10 4	0	0
2	E	1	Total C O 14 10 4	0	0
2	E	1	Total C O 14 12 2	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

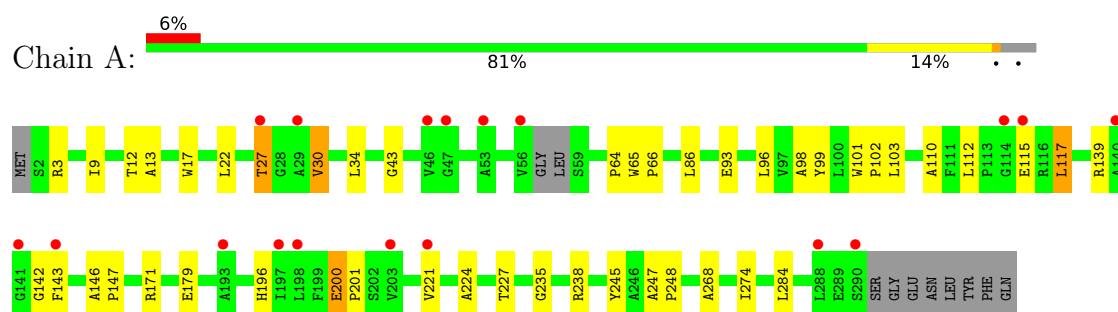
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total	O	0	0
			4	4		
4	C	3	Total	O	0	0
			3	3		
4	D	2	Total	O	0	0
			2	2		
4	E	2	Total	O	0	0
			2	2		

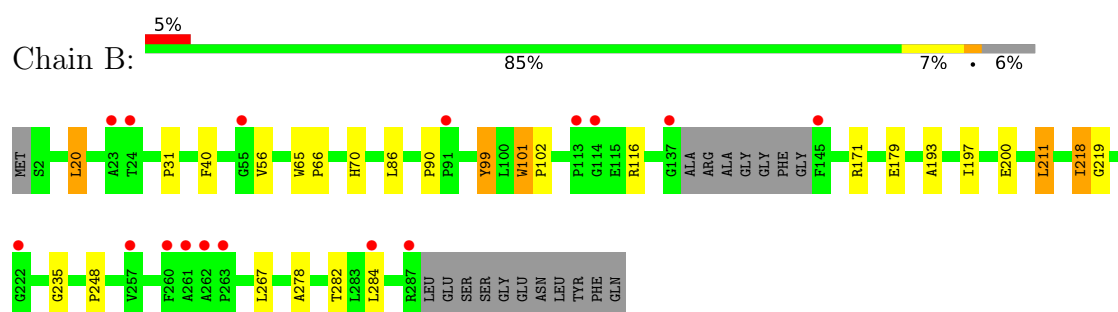
3 Residue-property plots [i](#)

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.

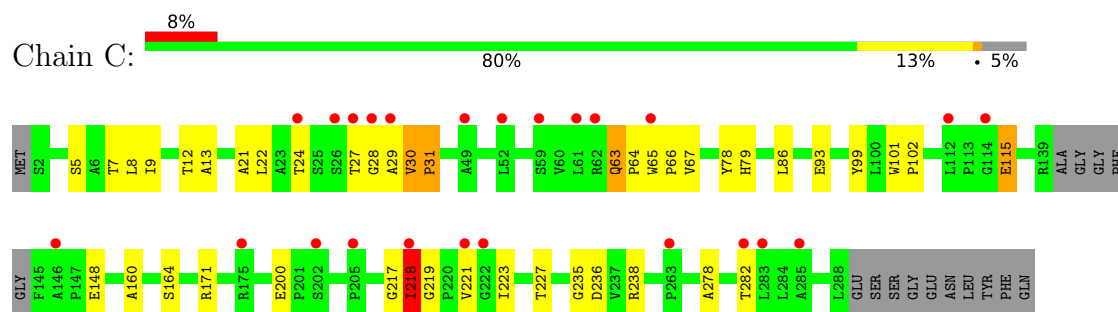
• Molecule 1: Uncharacterized protein



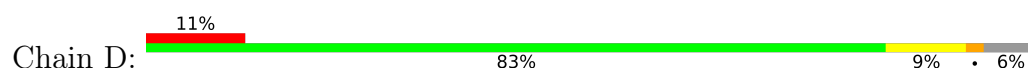
• Molecule 1: Uncharacterized protein

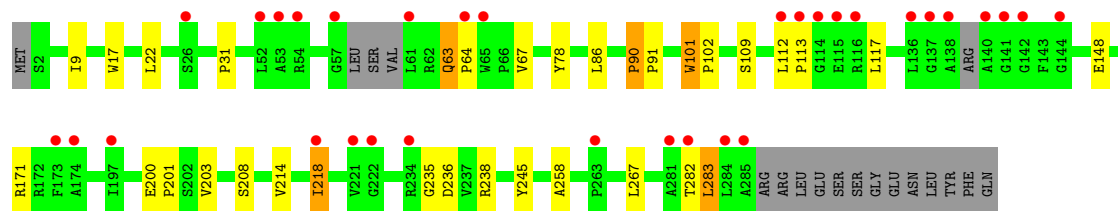


• Molecule 1: Uncharacterized protein

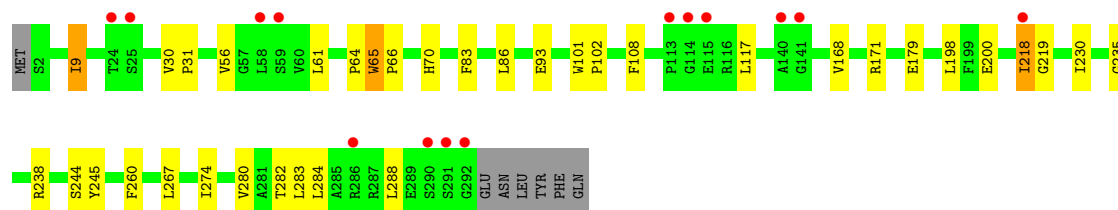
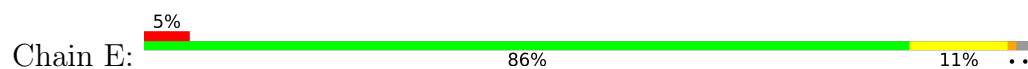


• Molecule 1: Uncharacterized protein

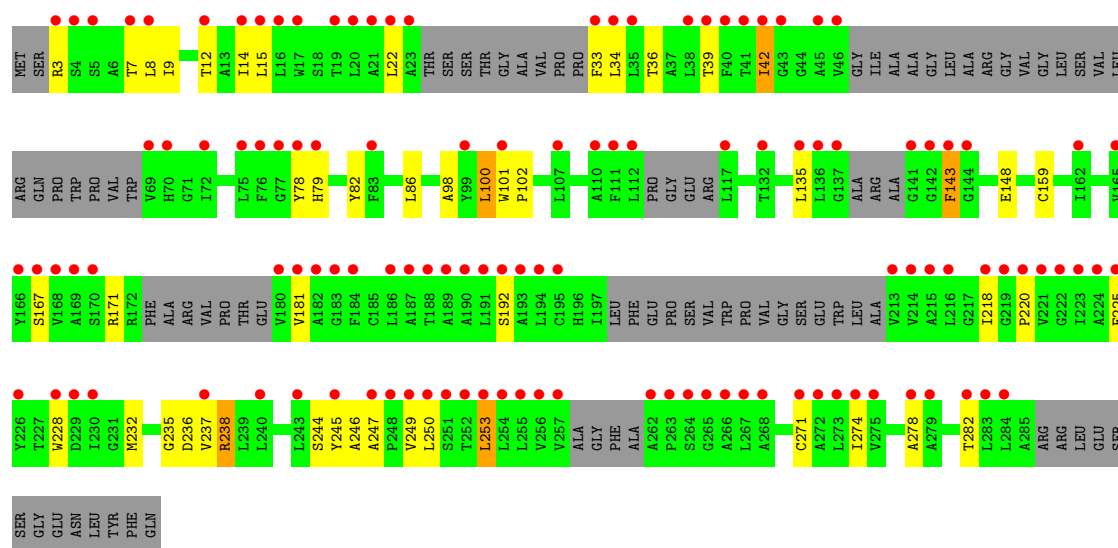




● Molecule 1: Uncharacterized protein



● Molecule 1: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.84Å 84.65Å 112.25Å 90.00° 108.46° 90.00°	Depositor
Resolution (Å)	45.97 – 2.40 45.97 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.97-2.40) 93.9 (45.97-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.8.3_1479	Depositor
R, R_{free}	0.226 , 0.249 0.230 , 0.252	Depositor DCC
R_{free} test set	3642 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.1	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	0.93	EDS
Total number of atoms	11923	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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: OLC, SO4

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	0.34	0/2119	0.79	4/2912 (0.1%)
1	B	0.35	0/2062	0.79	5/2838 (0.2%)
1	C	0.35	0/2050	0.80	5/2825 (0.2%)
1	D	0.34	0/2012	0.80	5/2775 (0.2%)
1	E	0.36	0/2131	0.81	1/2931 (0.0%)
1	F	0.33	0/1512	0.78	2/2071 (0.1%)
All	All	0.34	0/11886	0.80	22/16352 (0.1%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	ILE	N-CA-C	8.34	118.91	110.82
1	E	218	ILE	N-CA-C	7.53	118.45	111.45
1	A	30	VAL	CA-C-N	6.42	124.28	119.66
1	A	30	VAL	C-N-CA	6.42	124.28	119.66
1	C	218	ILE	N-CA-C	6.34	117.69	111.67
1	F	101	TRP	CA-C-N	-5.71	113.14	119.19
1	F	101	TRP	C-N-CA	-5.71	113.14	119.19
1	C	30	VAL	CA-C-N	5.54	123.70	119.66
1	C	30	VAL	C-N-CA	5.54	123.70	119.66
1	C	31	PRO	CA-C-N	5.27	124.89	119.05
1	C	31	PRO	C-N-CA	5.27	124.89	119.05
1	D	218	ILE	N-CA-C	5.26	115.40	110.30
1	A	65	TRP	CA-C-N	-5.24	114.27	119.56
1	A	65	TRP	C-N-CA	-5.24	114.27	119.56
1	B	101	TRP	CA-C-N	-5.19	113.69	119.19
1	B	101	TRP	C-N-CA	-5.19	113.69	119.19
1	D	90	PRO	CA-C-N	5.13	124.92	119.28
1	D	90	PRO	C-N-CA	5.13	124.92	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	PRO	CA-C-N	5.05	124.83	119.28
1	B	90	PRO	C-N-CA	5.05	124.83	119.28
1	D	101	TRP	CA-C-N	-5.02	113.47	119.05
1	D	101	TRP	C-N-CA	-5.02	113.47	119.05

There are no chirality outliers.

There are no planarity outliers.

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	2060	0	2105	24	0
1	B	2005	0	2047	16	0
1	C	1993	0	2010	23	0
1	D	1954	0	1956	17	0
1	E	2071	0	2116	17	0
1	F	1480	0	1413	26	0
2	A	46	0	64	4	0
2	B	85	0	122	6	0
2	C	48	0	69	3	0
2	D	72	0	99	3	0
2	E	93	0	135	5	0
3	A	5	0	0	0	0
4	B	4	0	0	0	0
4	C	3	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
All	All	11923	0	12136	123	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 5.

All (123) 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:C:115:GLU:O	1:C:238:ARG:NH2	2.22	0.73
1:E:9:ILE:HD11	1:E:230:ILE:HB	1.70	0.72
1:E:56:VAL:HG21	1:E:179:GLU:HG2	1.71	0.72
1:C:9:ILE:O	1:C:227:THR:OG1	2.08	0.71
1:D:282:THR:HG23	1:D:283:LEU:HD13	1.74	0.69
1:B:171:ARG:NH2	1:B:235:GLY:O	2.26	0.69
1:B:116:ARG:HD3	1:F:143:PHE:H	1.56	0.68
1:E:70:HIS:HB2	2:E:305:OLC:H24A	1.76	0.67
1:D:171:ARG:NH2	1:D:235:GLY:O	2.27	0.67
1:C:171:ARG:NH1	1:C:235:GLY:O	2.28	0.67
1:F:181:VAL:HG11	1:F:225:PHE:HB3	1.78	0.66
1:A:171:ARG:NH2	1:A:235:GLY:O	2.31	0.63
1:A:268:ALA:HB2	2:A:303:OLC:H3	1.81	0.63
1:F:171:ARG:NH1	1:F:235:GLY:O	2.33	0.61
1:C:7:THR:HG22	1:C:236:ASP:H	1.66	0.60
1:C:13:ALA:HB2	1:C:227:THR:HG23	1.83	0.60
2:D:301:OLC:H22	2:D:301:OLC:H3A	1.84	0.59
1:F:33:PHE:O	1:F:192:SER:OG	2.21	0.58
1:A:9:ILE:O	1:A:227:THR:OG1	2.21	0.58
1:B:66:PRO:HB3	2:B:305:OLC:H3	1.87	0.57
1:A:3:ARG:NH1	1:A:115:GLU:OE2	2.38	0.57
1:F:102:PRO:HG2	1:F:245:TYR:CZ	2.40	0.56
1:C:217:GLY:HA2	1:C:221:VAL:HB	1.87	0.56
1:D:236:ASP:OD1	1:D:238:ARG:NH1	2.38	0.56
1:A:13:ALA:HB2	1:A:227:THR:HG23	1.87	0.55
1:F:135:LEU:HD22	1:F:249:VAL:HG22	1.88	0.55
1:C:278:ALA:O	1:C:282:THR:HG22	2.06	0.55
1:F:36:THR:HA	1:F:39:THR:HG22	1.87	0.55
1:B:31:PRO:HB2	1:B:200:GLU:CD	2.31	0.55
1:A:112:LEU:HD13	1:A:171:ARG:HD2	1.89	0.54
1:E:283:LEU:HB2	1:E:284:LEU:HD12	1.89	0.54
1:F:7:THR:HG22	1:F:236:ASP:H	1.73	0.53
1:B:211:LEU:HD13	1:D:258:ALA:HB2	1.91	0.53
1:C:31:PRO:HB2	1:C:200:GLU:CD	2.34	0.52
1:E:171:ARG:NH2	1:E:235:GLY:O	2.40	0.52
1:C:218:ILE:N	1:C:219:GLY:HA3	2.24	0.51
1:A:43:GLY:HA3	1:A:221:VAL:HG12	1.92	0.51
1:D:214:VAL:O	1:D:218:ILE:HG12	2.11	0.51
1:F:9:ILE:O	1:F:12:THR:OG1	2.28	0.51
1:F:232:MET:HE1	1:F:237:VAL:HG13	1.92	0.51
1:F:14:ILE:HG23	1:F:247:ALA:HB2	1.93	0.51
1:A:110:ALA:HB2	1:A:117:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:167:SER:HB3	1:F:232:MET:HE2	1.93	0.50
1:B:278:ALA:O	1:B:282:THR:HG22	2.12	0.50
1:A:64:PRO:HB2	1:A:66:PRO:HD2	1.94	0.50
1:C:218:ILE:H	1:C:219:GLY:HA3	1.77	0.50
1:D:63:GLN:HG2	1:D:67:VAL:HG11	1.94	0.50
1:D:17:TRP:CE2	2:D:301:OLC:H9	2.48	0.49
1:C:5:SER:O	1:C:9:ILE:HG12	2.13	0.49
1:E:70:HIS:HA	2:E:305:OLC:H21	1.94	0.49
1:E:218:ILE:N	1:E:219:GLY:HA3	2.28	0.49
1:F:102:PRO:HB3	1:F:244:SER:HB2	1.94	0.49
1:A:27:THR:HG23	1:A:30:VAL:HB	1.94	0.48
1:B:218:ILE:N	1:B:219:GLY:HA3	2.28	0.48
1:E:64:PRO:HB2	1:E:66:PRO:HD2	1.95	0.48
1:D:102:PRO:HB2	1:D:245:TYR:CE2	2.49	0.48
1:E:31:PRO:HB2	1:E:200:GLU:CD	2.39	0.48
1:B:40:PHE:HE1	2:B:301:OLC:H2A	1.79	0.48
1:C:160:ALA:O	1:C:164:SER:OG	2.25	0.48
1:A:139:ARG:HG3	1:A:142:GLY:H	1.79	0.47
1:E:280:VAL:HA	1:E:284:LEU:HD13	1.95	0.47
1:F:246:ALA:O	1:F:250:LEU:N	2.37	0.47
1:C:64:PRO:HB2	1:C:66:PRO:HD2	1.96	0.47
1:C:28:GLY:HA2	1:C:29:ALA:HA	1.52	0.47
1:D:63:GLN:HG3	1:D:64:PRO:HD2	1.96	0.47
1:E:102:PRO:HB2	1:E:245:TYR:CE2	2.50	0.47
1:A:103:LEU:HD21	2:E:301:OLC:H11	1.97	0.46
1:A:200:GLU:HG3	1:A:201:PRO:HD2	1.96	0.46
1:B:99:TYR:CZ	1:B:248:PRO:HG3	2.50	0.46
1:C:24:THR:HA	1:C:27:THR:HG23	1.97	0.46
1:F:82:TYR:HB2	1:F:159:CYS:SG	2.55	0.46
2:E:302:OLC:H15A	2:E:302:OLC:H12	1.67	0.46
1:B:65:TRP:HB3	2:B:303:OLC:H21	1.98	0.46
1:B:70:HIS:HB2	2:B:305:OLC:H7A	1.97	0.45
1:F:278:ALA:O	1:F:282:THR:HG22	2.16	0.45
1:A:196:HIS:HA	1:A:200:GLU:HB2	1.98	0.45
1:A:12:THR:HB	2:A:304:OLC:H9	1.98	0.45
1:A:224:ALA:HA	1:A:227:THR:HG22	1.98	0.45
1:F:228:TRP:O	1:F:232:MET:HG2	2.17	0.45
1:A:34:LEU:HB2	1:A:196:HIS:ND1	2.32	0.45
1:F:42:ILE:HD11	1:F:218:ILE:HG12	1.99	0.45
1:C:218:ILE:O	1:C:223:ILE:HG13	2.17	0.45
1:C:101:TRP:CG	1:C:102:PRO:HD3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:TYR:OH	2:D:301:OLC:H8A	2.17	0.44
1:F:3:ARG:O	1:F:7:THR:HG23	2.17	0.44
1:C:63:GLN:HG2	1:C:67:VAL:HG11	2.00	0.44
1:A:101:TRP:CG	1:A:102:PRO:HD3	2.53	0.44
1:B:65:TRP:CG	1:B:66:PRO:HD3	2.52	0.44
1:C:21:ALA:O	1:C:24:THR:HG22	2.17	0.43
1:F:238:ARG:HE	1:F:238:ARG:HB2	1.43	0.43
1:D:112:LEU:HA	1:D:113:PRO:HD3	1.88	0.43
1:E:65:TRP:CD1	1:E:65:TRP:C	2.96	0.43
1:E:101:TRP:CG	1:E:102:PRO:HD3	2.54	0.43
1:E:102:PRO:HB3	1:E:244:SER:HB2	2.01	0.43
1:F:250:LEU:HA	1:F:253:LEU:HD11	1.99	0.43
1:D:90:PRO:HA	1:D:91:PRO:HD3	1.82	0.43
1:F:82:TYR:CE2	1:F:86:LEU:HD11	2.54	0.43
1:D:101:TRP:CG	1:D:102:PRO:HD3	2.53	0.43
1:A:96:LEU:HD22	1:A:143:PHE:CE2	2.54	0.43
1:F:14:ILE:HG12	1:F:244:SER:HA	2.00	0.43
1:F:15:LEU:HD23	1:F:250:LEU:HD21	2.01	0.43
1:C:12:THR:HB	2:C:301:OLC:H6A	2.01	0.42
1:B:101:TRP:CG	1:B:102:PRO:HD3	2.55	0.42
1:C:223:ILE:O	1:C:227:THR:HG22	2.19	0.42
1:A:17:TRP:CD2	2:A:301:OLC:H9	2.54	0.42
1:C:78:TYR:OH	2:C:302:OLC:H6A	2.20	0.42
1:E:30:VAL:HA	1:E:31:PRO:HD2	1.93	0.42
1:E:83:PHE:CZ	2:E:302:OLC:H22	2.55	0.42
1:A:98:ALA:HB1	2:A:301:OLC:H14	2.01	0.42
1:A:102:PRO:HB2	1:A:245:TYR:CE2	2.55	0.42
1:D:31:PRO:HD3	1:D:203:VAL:HB	2.01	0.42
1:D:200:GLU:HA	1:D:201:PRO:HD3	1.93	0.42
1:A:146:ALA:HA	1:A:147:PRO:HD3	1.94	0.42
1:F:98:ALA:C	1:F:100:LEU:H	2.28	0.42
1:B:193:ALA:O	1:B:197:ILE:HG13	2.20	0.41
1:D:31:PRO:HB2	1:D:200:GLU:CD	2.46	0.41
1:A:247:ALA:HB3	1:A:248:PRO:HD3	2.03	0.41
1:B:20:LEU:HD21	2:B:301:OLC:H5A	2.02	0.41
1:B:211:LEU:HD21	1:D:22:LEU:HD22	2.02	0.41
1:E:108:PHE:HB2	1:E:168:VAL:HG21	2.03	0.41
1:C:79:HIS:NE2	2:C:302:OLC:H2	2.35	0.40
2:B:305:OLC:H8	2:B:305:OLC:H11	1.88	0.40
1:F:271:CYS:HA	1:F:274:ILE:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	283/298 (95%)	275 (97%)	8 (3%)	0	100	100
1	B	276/298 (93%)	271 (98%)	5 (2%)	0	100	100
1	C	278/298 (93%)	275 (99%)	3 (1%)	0	100	100
1	D	274/298 (92%)	270 (98%)	4 (2%)	0	100	100
1	E	289/298 (97%)	286 (99%)	3 (1%)	0	100	100
1	F	203/298 (68%)	195 (96%)	7 (3%)	1 (0%)	24	37
All	All	1603/1788 (90%)	1572 (98%)	30 (2%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	220	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	195/212 (92%)	184 (94%)	11 (6%)	19	33
1	B	192/212 (91%)	183 (95%)	9 (5%)	23	41
1	C	186/212 (88%)	175 (94%)	11 (6%)	18	31
1	D	181/212 (85%)	172 (95%)	9 (5%)	22	38
1	E	196/212 (92%)	183 (93%)	13 (7%)	15	26
1	F	124/212 (58%)	113 (91%)	11 (9%)	9	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1074/1272 (84%)	1010 (94%)	64 (6%)	18	31

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	27	THR
1	A	86	LEU
1	A	93	GLU
1	A	99	TYR
1	A	117	LEU
1	A	179	GLU
1	A	200	GLU
1	A	238	ARG
1	A	274	ILE
1	A	284	LEU
1	B	20	LEU
1	B	56	VAL
1	B	86	LEU
1	B	99	TYR
1	B	179[A]	GLU
1	B	179[B]	GLU
1	B	211	LEU
1	B	267	LEU
1	B	284	LEU
1	C	8	LEU
1	C	22	LEU
1	C	30	VAL
1	C	63	GLN
1	C	65	TRP
1	C	86	LEU
1	C	93	GLU
1	C	99	TYR
1	C	115	GLU
1	C	148	GLU
1	C	218	ILE
1	D	9	ILE
1	D	63	GLN
1	D	86	LEU
1	D	109	SER
1	D	117	LEU
1	D	148	GLU

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Mol	Chain	Res	Type
1	D	208	SER
1	D	267	LEU
1	D	283	LEU
1	E	9	ILE
1	E	61	LEU
1	E	65	TRP
1	E	86	LEU
1	E	93	GLU
1	E	117	LEU
1	E	198	LEU
1	E	238	ARG
1	E	260	PHE
1	E	267	LEU
1	E	274	ILE
1	E	282	THR
1	E	288	LEU
1	F	8	LEU
1	F	22	LEU
1	F	34	LEU
1	F	42	ILE
1	F	78	TYR
1	F	79	HIS
1	F	100	LEU
1	F	143	PHE
1	F	148	GLU
1	F	238	ARG
1	F	253	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	C	70	HIS
1	D	121	HIS
1	F	196	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

24 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	OLC	A	303	-	7,7,24	0.34	0	6,6,25	0.71	0
2	OLC	E	306	-	13,13,24	1.13	2 (15%)	13,13,25	1.13	0
2	OLC	D	302	-	6,6,24	0.96	1 (16%)	6,6,25	1.28	0
2	OLC	B	302	-	12,12,24	1.80	3 (25%)	12,12,25	1.28	1 (8%)
2	OLC	D	305	-	12,12,24	1.21	1 (8%)	13,13,25	1.05	1 (7%)
2	OLC	D	303	-	10,10,24	1.05	1 (10%)	9,9,25	0.72	0
2	OLC	D	301	-	24,24,24	1.10	2 (8%)	25,25,25	0.98	1 (4%)
2	OLC	E	301	-	15,15,24	0.89	1 (6%)	14,14,25	0.70	0
2	OLC	E	303	-	9,9,24	1.10	1 (11%)	8,8,25	0.80	0
2	OLC	C	303	-	12,12,24	1.09	2 (16%)	12,12,25	1.25	1 (8%)
2	OLC	B	301	-	24,24,24	1.11	2 (8%)	25,25,25	0.99	1 (4%)
2	OLC	E	302	-	24,24,24	1.07	2 (8%)	25,25,25	0.96	1 (4%)
2	OLC	B	304	-	12,12,24	0.98	1 (8%)	11,11,25	0.67	0
2	OLC	B	305	-	16,16,24	1.03	2 (12%)	16,16,25	1.03	0
2	OLC	D	304	-	15,15,24	1.07	2 (13%)	15,15,25	1.09	0
2	OLC	E	304	-	13,13,24	1.15	1 (7%)	14,14,25	1.13	1 (7%)
2	OLC	A	301	-	14,14,24	0.91	1 (7%)	13,13,25	0.72	0
3	SO4	A	305	-	4,4,4	0.23	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLC	A	302	-	9,9,24	0.83	1 (11%)	9,9,25	1.22	1 (11%)
2	OLC	B	303	-	16,16,24	1.34	2 (12%)	17,17,25	1.05	1 (5%)
2	OLC	C	302	-	23,23,24	1.07	2 (8%)	24,24,25	0.99	1 (4%)
2	OLC	E	305	-	13,13,24	1.16	1 (7%)	14,14,25	1.08	1 (7%)
2	OLC	C	301	-	10,10,24	1.06	1 (10%)	9,9,25	0.78	0
2	OLC	A	304	-	12,12,24	1.80	3 (25%)	12,12,25	1.21	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	OLC	A	303	-	-	3/5/5/24	-
2	OLC	E	306	-	-	3/11/11/24	-
2	OLC	D	302	-	-	1/4/4/24	-
2	OLC	B	302	-	-	5/10/10/24	-
2	OLC	D	305	-	-	5/12/12/24	-
2	OLC	D	303	-	-	1/8/8/24	-
2	OLC	D	301	-	-	12/24/24/24	-
2	OLC	E	301	-	-	9/13/13/24	-
2	OLC	E	303	-	-	3/7/7/24	-
2	OLC	C	303	-	-	2/10/10/24	-
2	OLC	B	301	-	-	13/24/24/24	-
2	OLC	E	302	-	-	12/24/24/24	-
2	OLC	B	304	-	-	5/10/10/24	-
2	OLC	B	305	-	-	3/14/14/24	-
2	OLC	D	304	-	-	6/13/13/24	-
2	OLC	E	304	-	-	6/13/13/24	-
2	OLC	A	301	-	-	5/12/12/24	-
2	OLC	A	302	-	-	2/7/7/24	-
2	OLC	B	303	-	-	6/16/16/24	-
2	OLC	C	302	-	-	10/22/22/24	-
2	OLC	E	305	-	-	3/13/13/24	-
2	OLC	C	301	-	-	4/8/8/24	-
2	OLC	A	304	-	-	3/10/10/24	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	304	OLC	O19-C1	4.84	1.37	1.22
2	B	302	OLC	O19-C1	4.83	1.37	1.22
2	B	303	OLC	C10-C9	3.18	1.49	1.29
2	C	301	OLC	C9-C10	3.17	1.49	1.31
2	E	302	OLC	C9-C10	3.16	1.49	1.31
2	D	304	OLC	C9-C10	3.15	1.49	1.31
2	B	304	OLC	C9-C10	3.15	1.49	1.31
2	B	305	OLC	C9-C10	3.15	1.49	1.31
2	E	301	OLC	C9-C10	3.15	1.49	1.31
2	D	303	OLC	C9-C10	3.15	1.49	1.31
2	E	303	OLC	C9-C10	3.13	1.49	1.31
2	E	306	OLC	C9-C10	3.12	1.49	1.31
2	D	301	OLC	C9-C10	3.12	1.49	1.31
2	B	301	OLC	C9-C10	3.12	1.49	1.31
2	A	301	OLC	C9-C10	3.11	1.49	1.31
2	C	302	OLC	C9-C10	3.10	1.49	1.31
2	D	305	OLC	O20-C21	-3.08	1.38	1.45
2	B	303	OLC	O20-C21	-3.06	1.38	1.45
2	C	302	OLC	O20-C21	-3.03	1.38	1.45
2	D	301	OLC	O20-C21	-2.99	1.38	1.45
2	E	304	OLC	O20-C21	-2.99	1.38	1.45
2	B	301	OLC	O20-C21	-2.98	1.38	1.45
2	E	305	OLC	O20-C21	-2.97	1.38	1.45
2	E	302	OLC	O20-C21	-2.92	1.38	1.45
2	C	303	OLC	C9-C10	2.78	1.49	1.29
2	A	304	OLC	C9-C10	2.77	1.49	1.29
2	B	302	OLC	C9-C10	2.72	1.49	1.29
2	A	304	OLC	O20-C1	-2.44	1.22	1.30
2	B	302	OLC	O20-C1	-2.44	1.22	1.30
2	E	306	OLC	O20-C1	2.18	1.38	1.30
2	D	302	OLC	O20-C1	2.17	1.38	1.30
2	B	305	OLC	O20-C1	2.16	1.38	1.30
2	C	303	OLC	O20-C1	2.15	1.37	1.30
2	D	304	OLC	O20-C1	2.15	1.37	1.30
2	A	302	OLC	O20-C1	2.14	1.37	1.30

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	302	OLC	O20-C1-C2	2.86	120.54	111.83
2	C	302	OLC	O20-C1-C2	2.79	120.33	111.83
2	E	304	OLC	O20-C1-C2	2.65	119.90	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	OLC	O20-C1-C2	2.56	119.64	111.83
2	E	305	OLC	O20-C1-C2	2.54	119.57	111.83
2	D	305	OLC	O20-C1-C2	2.53	119.54	111.83
2	B	301	OLC	O20-C1-C2	2.52	119.53	111.83
2	B	303	OLC	O20-C1-C2	2.31	118.88	111.83
2	C	303	OLC	C3-C2-C1	-2.17	108.85	114.51
2	B	302	OLC	C3-C2-C1	-2.14	108.93	114.51
2	A	302	OLC	C3-C2-C1	-2.05	109.17	114.51

There are no chirality outliers.

All (122) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	302	OLC	O20-C21-C22-C24
2	C	302	OLC	O20-C21-C22-O23
2	C	302	OLC	O19-C1-O20-C21
2	D	301	OLC	O20-C21-C22-C24
2	D	305	OLC	C21-C22-C24-O25
2	D	305	OLC	O20-C21-C22-C24
2	E	302	OLC	O20-C21-C22-C24
2	E	302	OLC	O20-C21-C22-O23
2	E	304	OLC	C21-C22-C24-O25
2	E	304	OLC	O23-C22-C24-O25
2	E	304	OLC	O20-C21-C22-O23
2	E	305	OLC	C21-C22-C24-O25
2	E	304	OLC	C2-C1-O20-C21
2	E	304	OLC	O19-C1-O20-C21
2	C	302	OLC	C2-C1-O20-C21
2	E	302	OLC	C2-C1-O20-C21
2	E	302	OLC	O19-C1-O20-C21
2	B	301	OLC	C2-C1-O20-C21
2	B	301	OLC	O19-C1-O20-C21
2	D	305	OLC	O20-C21-C22-O23
2	B	303	OLC	O19-C1-O20-C21
2	B	303	OLC	C2-C1-O20-C21
2	D	301	OLC	O19-C1-O20-C21
2	D	301	OLC	O20-C21-C22-O23
2	A	302	OLC	C1-C2-C3-C4
2	D	301	OLC	C1-C2-C3-C4
2	D	301	OLC	C2-C1-O20-C21
2	D	302	OLC	C1-C2-C3-C4
2	E	304	OLC	O20-C21-C22-C24

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Mol	Chain	Res	Type	Atoms
2	D	305	OLC	O23-C22-C24-O25
2	E	305	OLC	O23-C22-C24-O25
2	A	301	OLC	C12-C13-C14-C15
2	D	301	OLC	C5-C6-C7-C8
2	B	301	OLC	C11-C12-C13-C14
2	B	301	OLC	O20-C21-C22-O23
2	C	302	OLC	C11-C12-C13-C14
2	E	303	OLC	C11-C12-C13-C14
2	B	305	OLC	C10-C11-C12-C13
2	C	301	OLC	C11-C10-C9-C8
2	A	303	OLC	C5-C6-C7-C8
2	A	301	OLC	C5-C6-C7-C8
2	D	301	OLC	C13-C14-C15-C16
2	E	302	OLC	C11-C12-C13-C14
2	B	301	OLC	C2-C3-C4-C5
2	C	301	OLC	C9-C10-C11-C12
2	E	303	OLC	C7-C8-C9-C10
2	E	306	OLC	C9-C10-C11-C12
2	D	301	OLC	C3-C4-C5-C6
2	A	304	OLC	C4-C5-C6-C7
2	E	302	OLC	C4-C5-C6-C7
2	B	304	OLC	C6-C7-C8-C9
2	D	301	OLC	C6-C7-C8-C9
2	B	301	OLC	C4-C5-C6-C7
2	C	301	OLC	C3-C4-C5-C6
2	D	304	OLC	C2-C3-C4-C5
2	E	301	OLC	C14-C15-C16-C17
2	A	304	OLC	C5-C6-C7-C8
2	B	304	OLC	C10-C11-C12-C13
2	E	301	OLC	C10-C11-C12-C13
2	E	301	OLC	C5-C6-C7-C8
2	D	301	OLC	C22-C21-O20-C1
2	E	302	OLC	C12-C13-C14-C15
2	B	301	OLC	O20-C21-C22-C24
2	E	302	OLC	C1-C2-C3-C4
2	D	304	OLC	C5-C6-C7-C8
2	C	302	OLC	C11-C10-C9-C8
2	B	301	OLC	C10-C11-C12-C13
2	D	304	OLC	C10-C11-C12-C13
2	E	301	OLC	C12-C13-C14-C15
2	B	301	OLC	C6-C7-C8-C9
2	B	301	OLC	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
2	E	302	OLC	C3-C4-C5-C6
2	E	301	OLC	C11-C12-C13-C14
2	A	303	OLC	C2-C3-C4-C5
2	B	304	OLC	C5-C6-C7-C8
2	A	301	OLC	C13-C14-C15-C16
2	A	303	OLC	C6-C7-C8-C9
2	E	301	OLC	C4-C5-C6-C7
2	C	302	OLC	C5-C6-C7-C8
2	D	301	OLC	C2-C3-C4-C5
2	E	301	OLC	C15-C16-C17-C18
2	C	302	OLC	C6-C7-C8-C9
2	C	303	OLC	C3-C4-C5-C6
2	B	301	OLC	C14-C15-C16-C17
2	D	304	OLC	C4-C5-C6-C7
2	E	302	OLC	C5-C6-C7-C8
2	C	302	OLC	C3-C4-C5-C6
2	C	301	OLC	C7-C8-C9-C10
2	D	304	OLC	C9-C10-C11-C12
2	E	301	OLC	C11-C10-C9-C8
2	C	302	OLC	C9-C10-C11-C12
2	D	303	OLC	C7-C8-C9-C10
2	A	301	OLC	C11-C12-C13-C14
2	B	301	OLC	C3-C4-C5-C6
2	E	302	OLC	C15-C16-C17-C18
2	B	302	OLC	O20-C1-C2-C3
2	B	303	OLC	C7-C8-C9-C10
2	B	302	OLC	O19-C1-C2-C3
2	C	303	OLC	C7-C8-C9-C10
2	E	305	OLC	O20-C1-C2-C3
2	B	302	OLC	C7-C8-C9-C10
2	E	303	OLC	C9-C10-C11-C12
2	E	306	OLC	O20-C1-C2-C3
2	E	301	OLC	C9-C10-C11-C12
2	B	302	OLC	C11-C10-C9-C8
2	A	304	OLC	C3-C4-C5-C6
2	B	305	OLC	C3-C4-C5-C6
2	D	301	OLC	C12-C13-C14-C15
2	B	304	OLC	C7-C8-C9-C10
2	E	306	OLC	C7-C8-C9-C10
2	D	304	OLC	C11-C10-C9-C8
2	B	304	OLC	C12-C13-C14-C15
2	B	301	OLC	C9-C10-C11-C12

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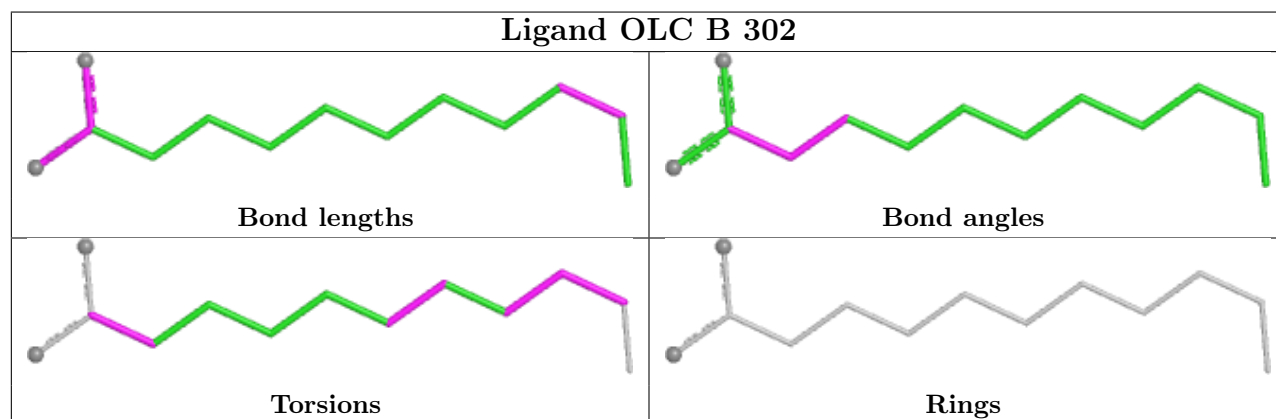
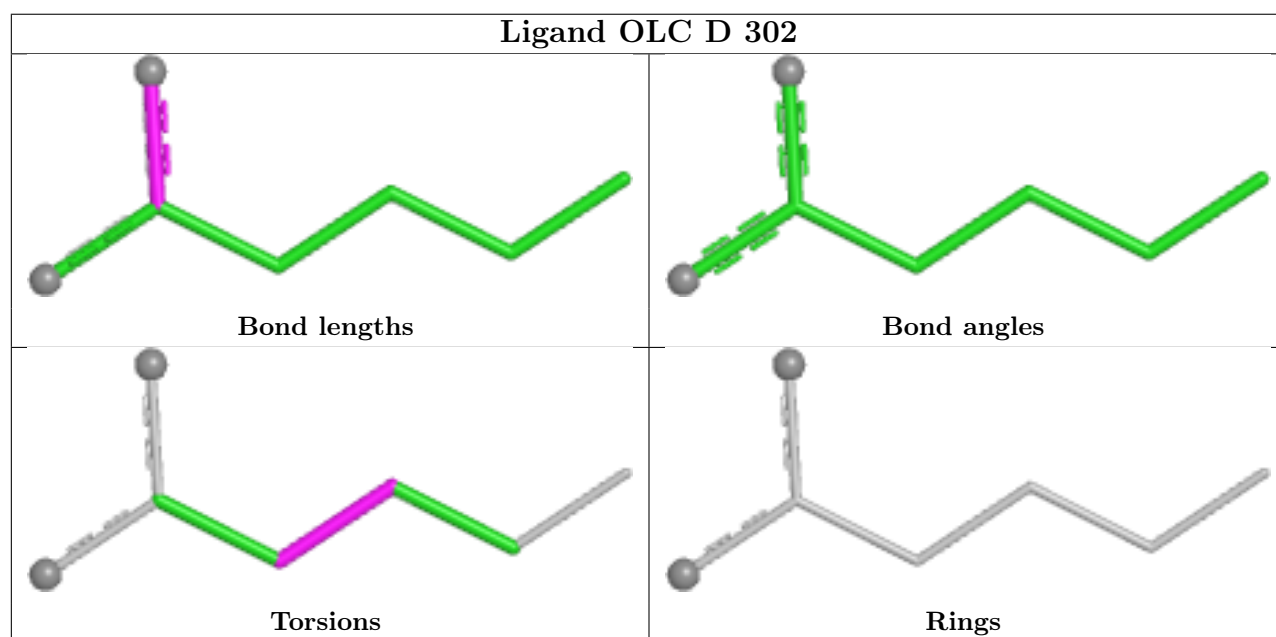
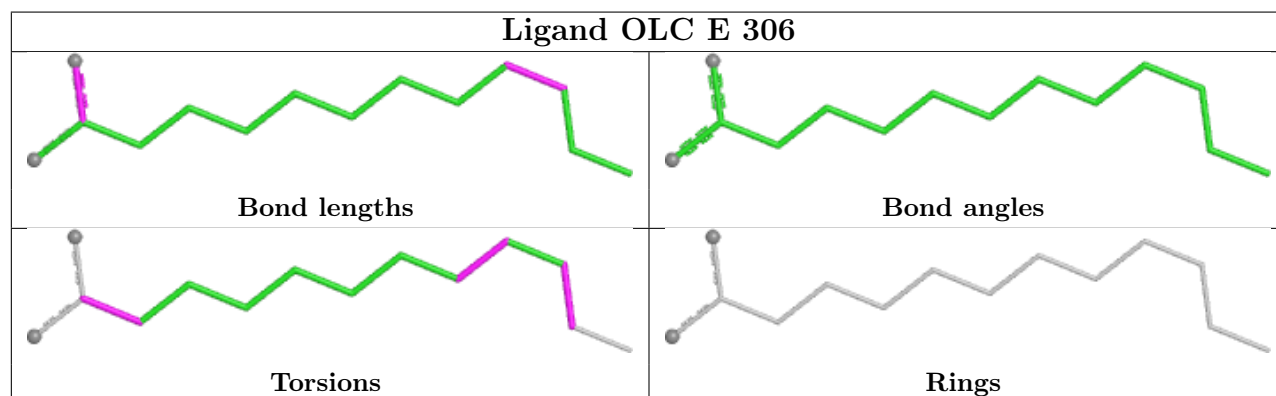
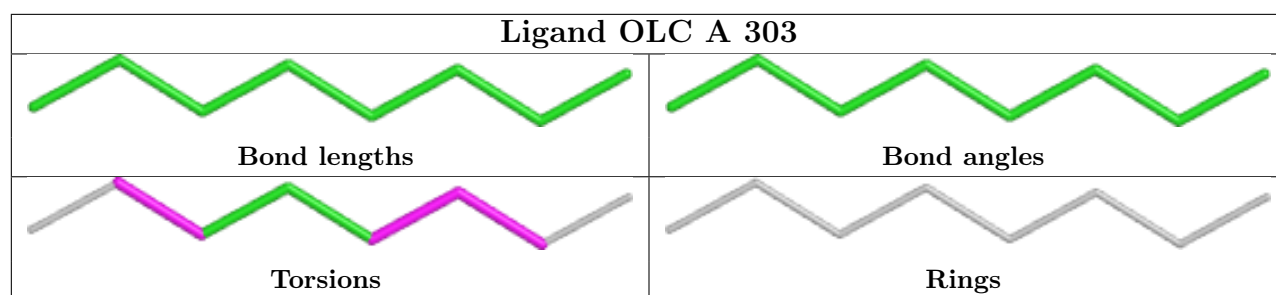
Mol	Chain	Res	Type	Atoms
2	B	305	OLC	C5-C6-C7-C8
2	B	303	OLC	C21-C22-C24-O25
2	B	303	OLC	O19-C1-C2-C3
2	B	302	OLC	C5-C6-C7-C8
2	E	302	OLC	C7-C8-C9-C10
2	A	302	OLC	O20-C1-C2-C3
2	A	301	OLC	C10-C11-C12-C13
2	B	303	OLC	O20-C1-C2-C3
2	D	305	OLC	O20-C1-C2-C3

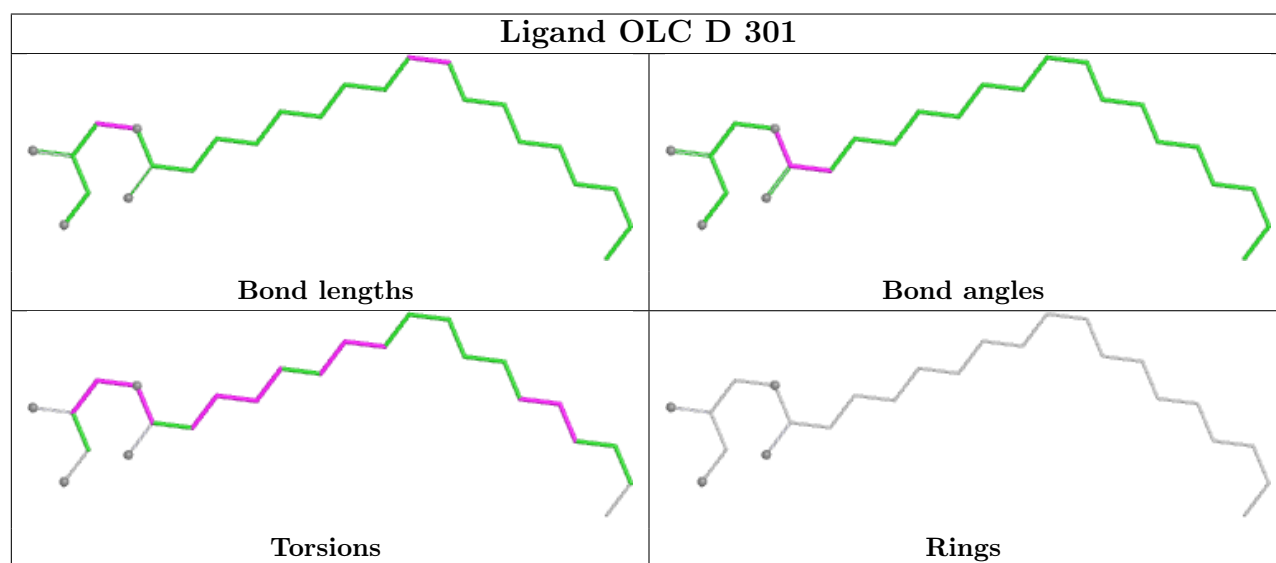
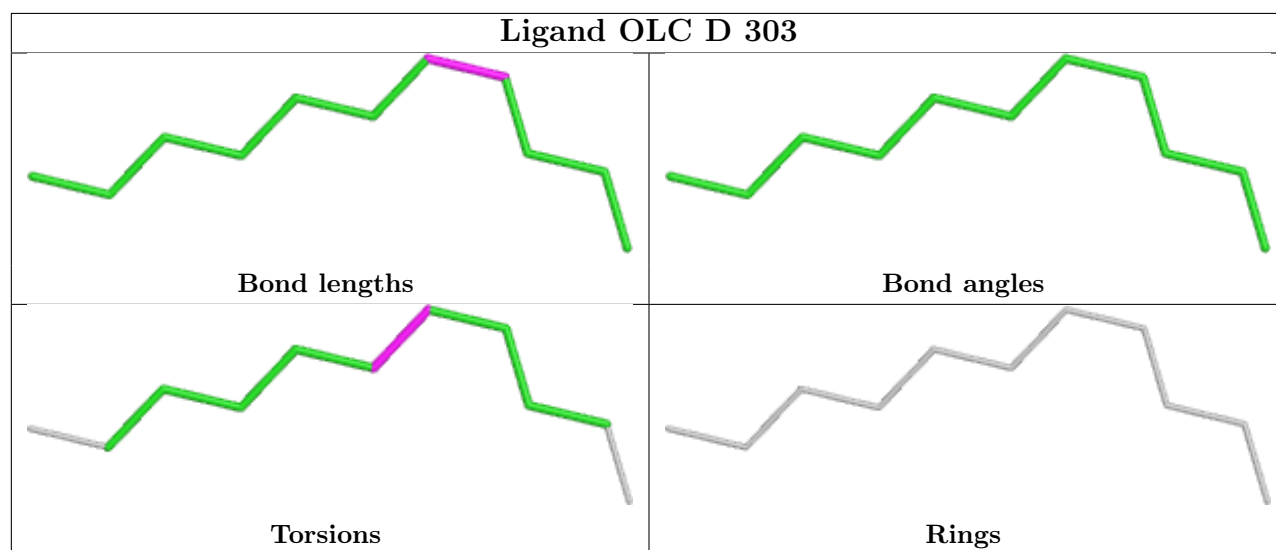
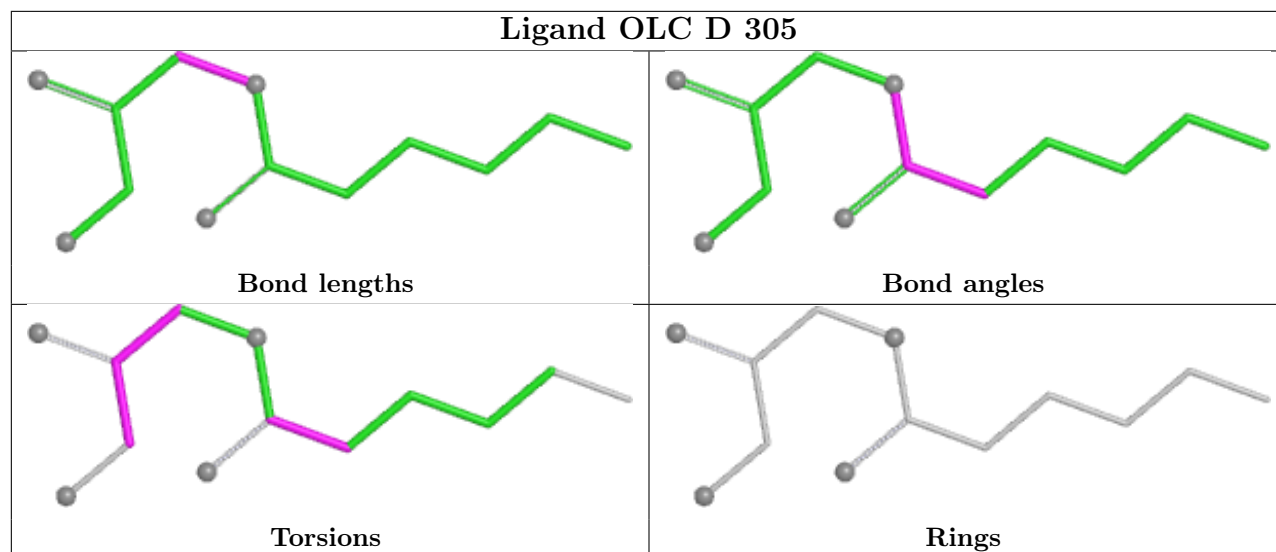
There are no ring outliers.

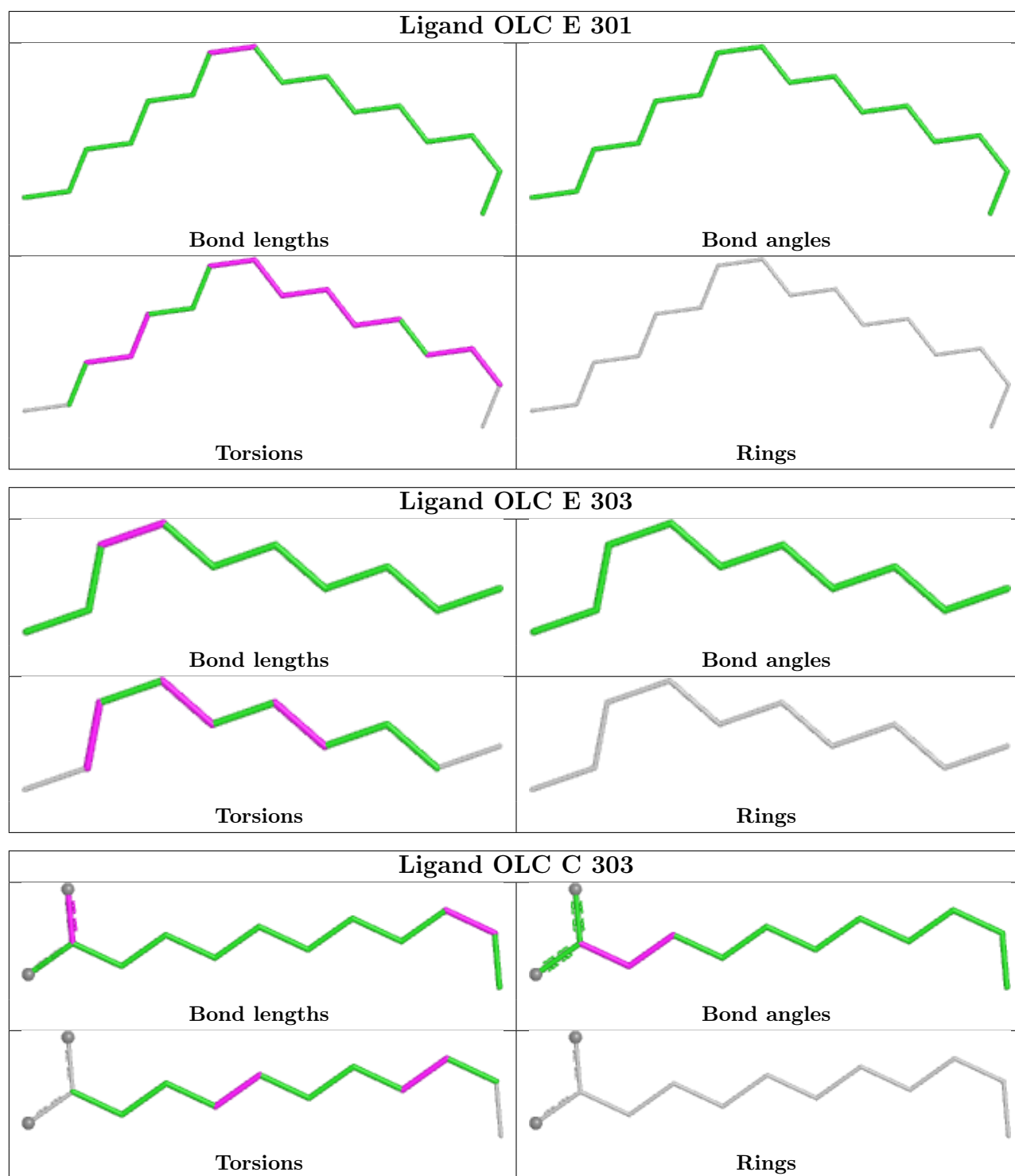
12 monomers are involved in 21 short contacts:

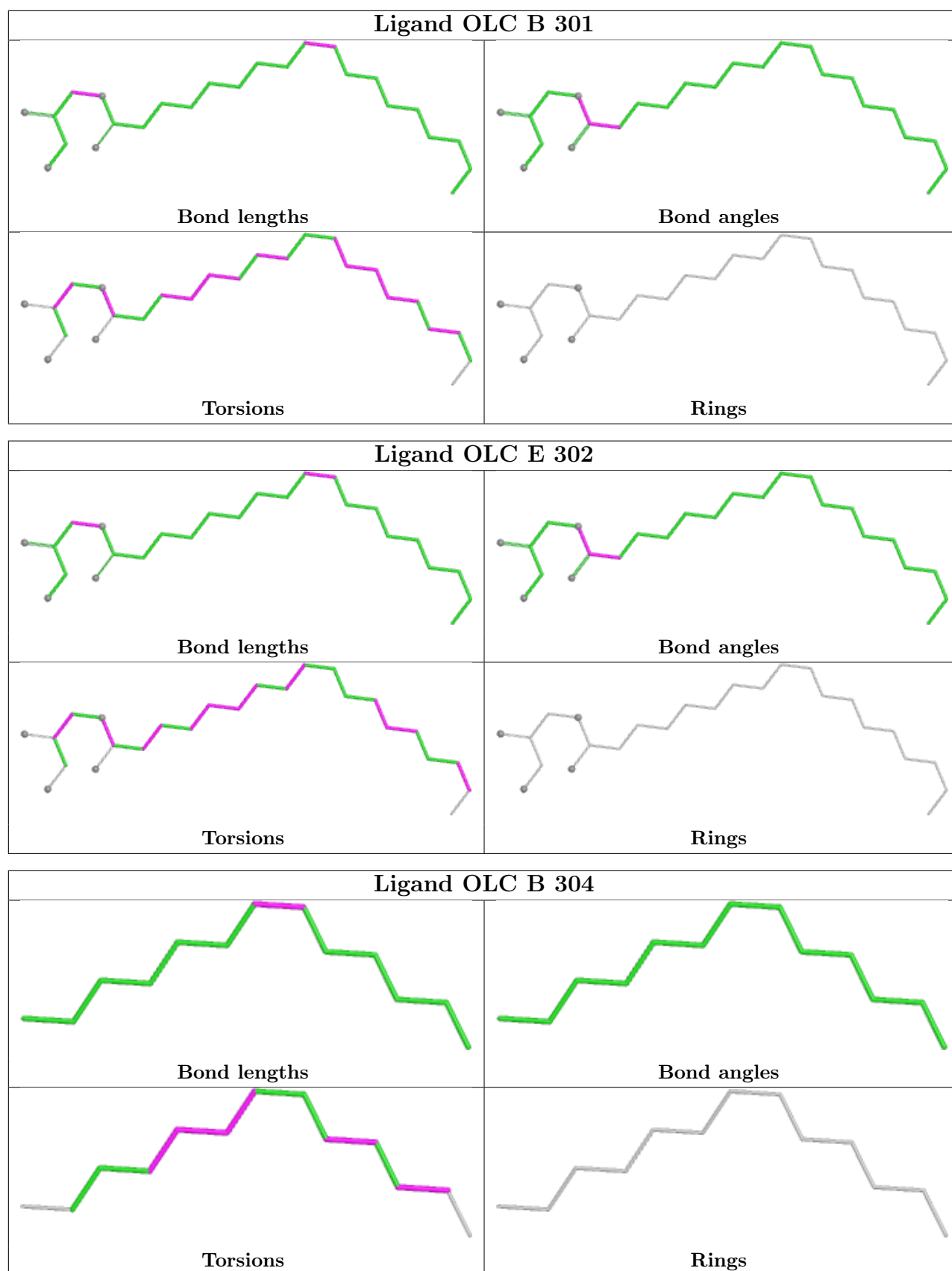
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	303	OLC	1	0
2	D	301	OLC	3	0
2	E	301	OLC	1	0
2	B	301	OLC	2	0
2	E	302	OLC	2	0
2	B	305	OLC	3	0
2	A	301	OLC	2	0
2	B	303	OLC	1	0
2	C	302	OLC	2	0
2	E	305	OLC	2	0
2	C	301	OLC	1	0
2	A	304	OLC	1	0

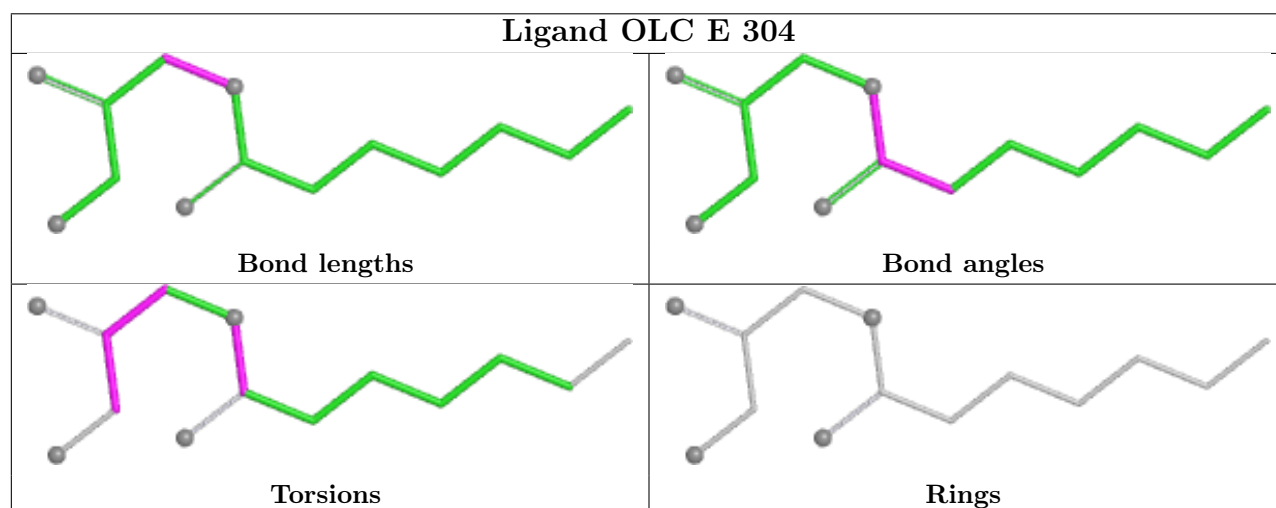
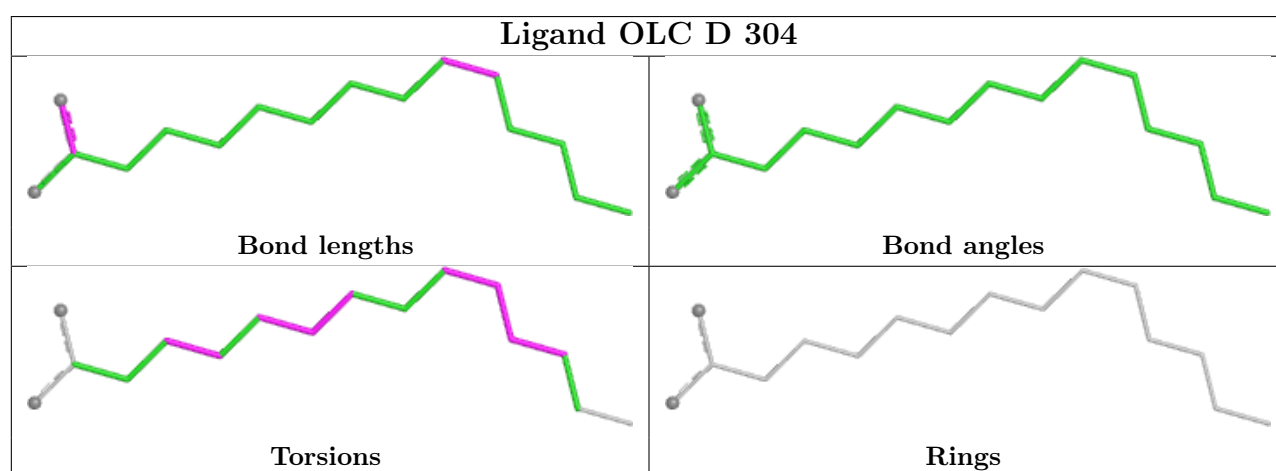
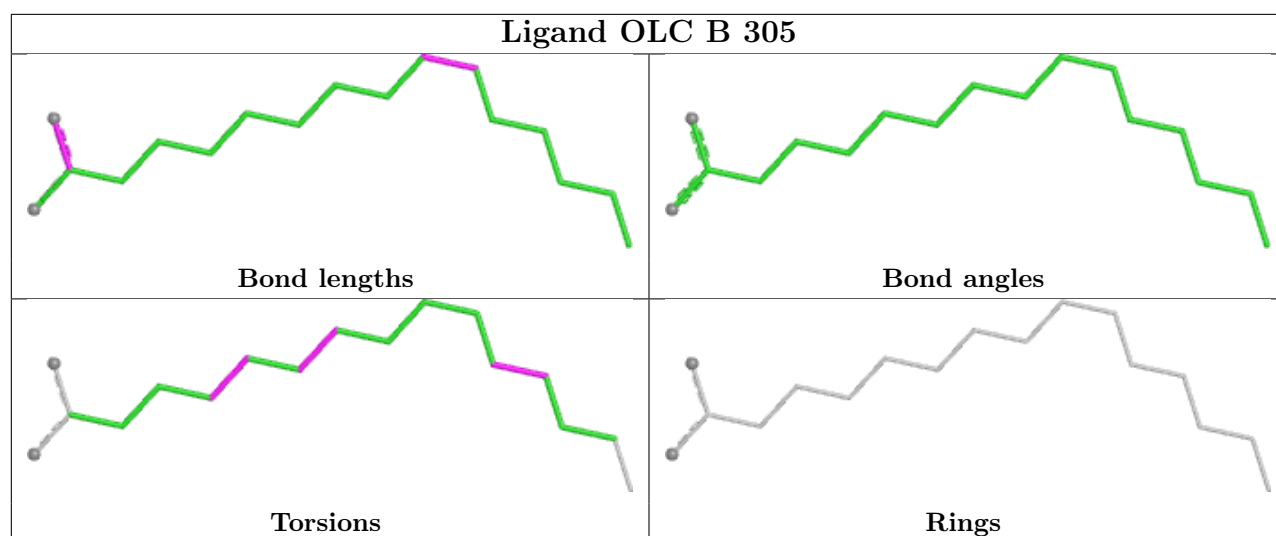
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

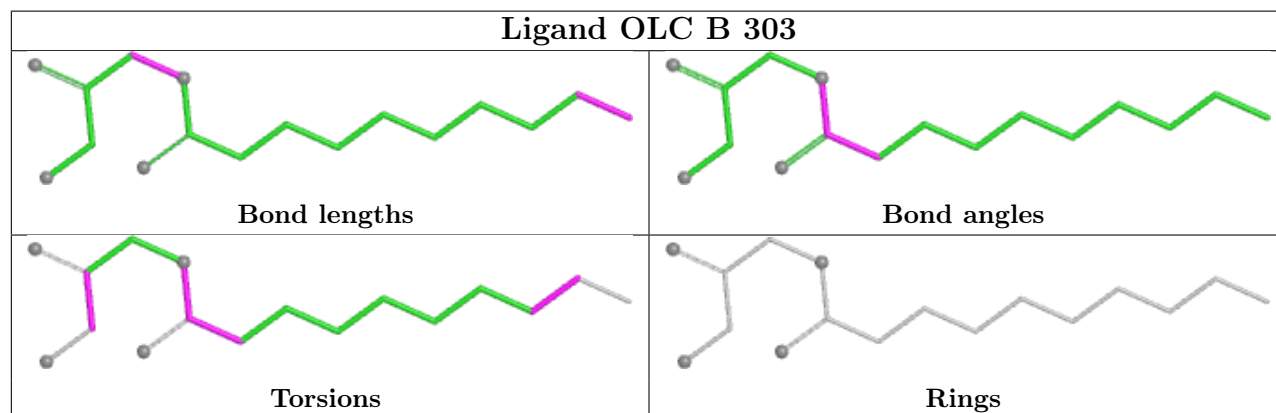
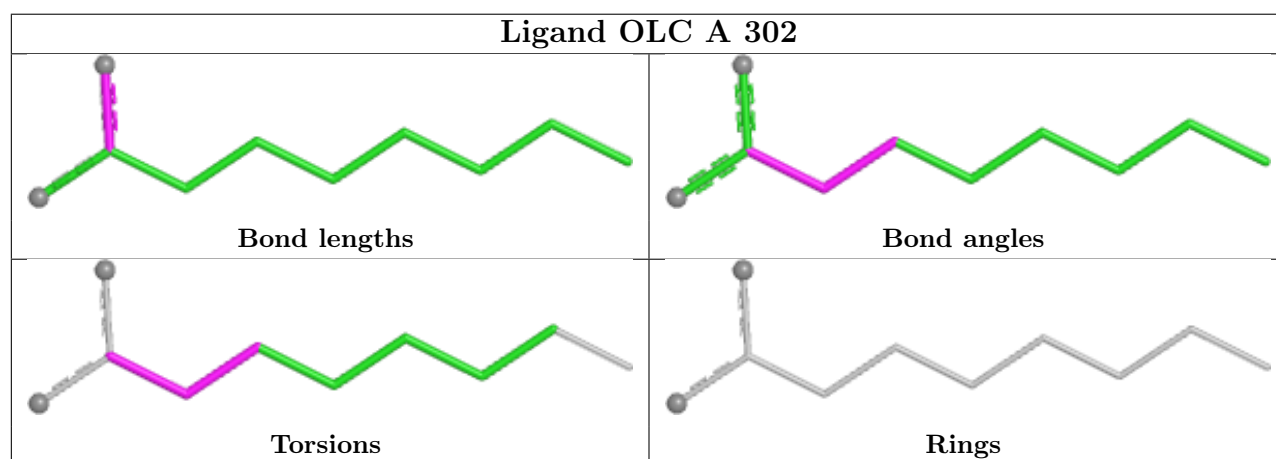
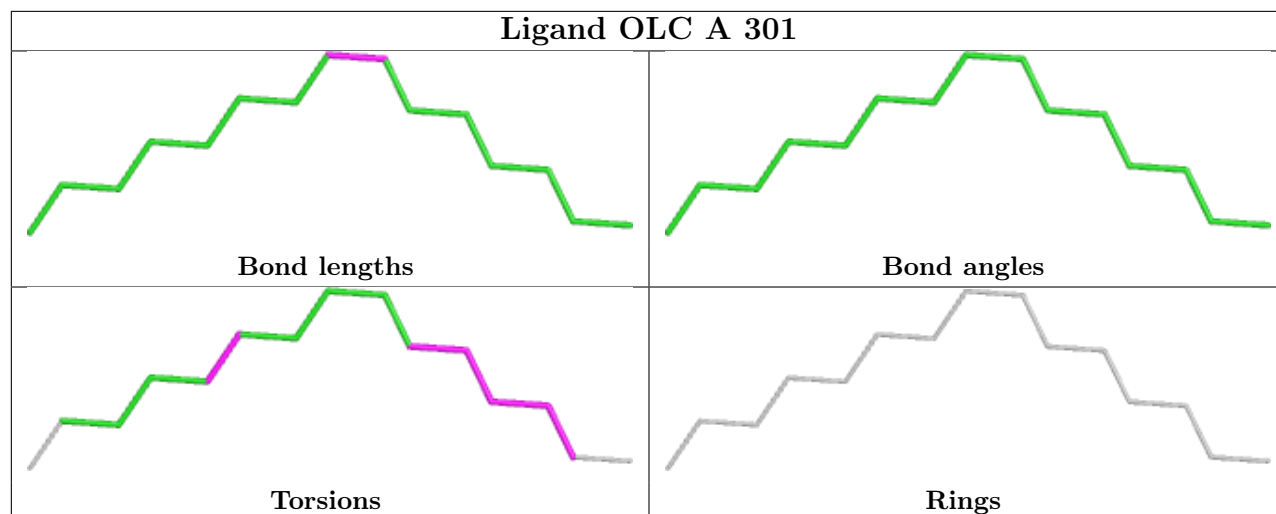


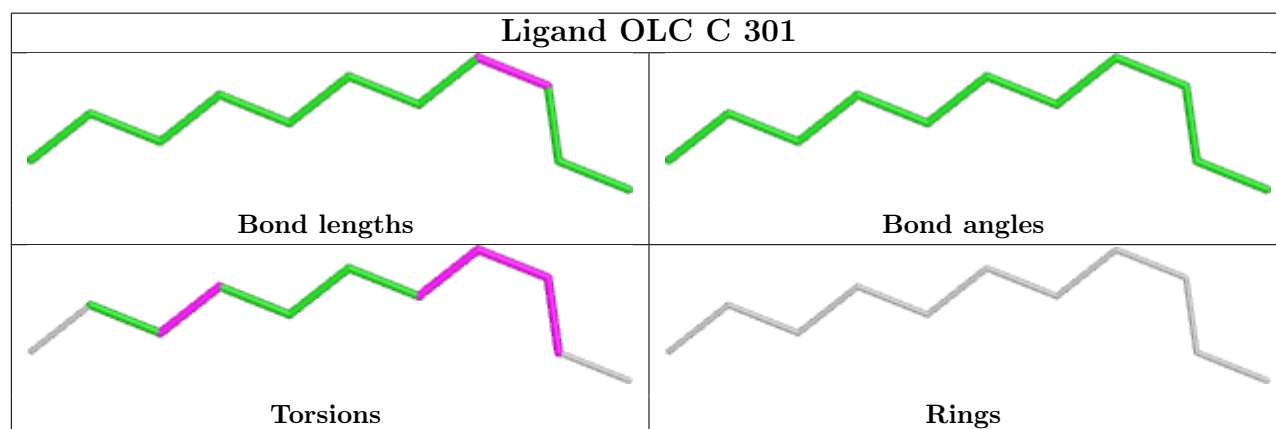
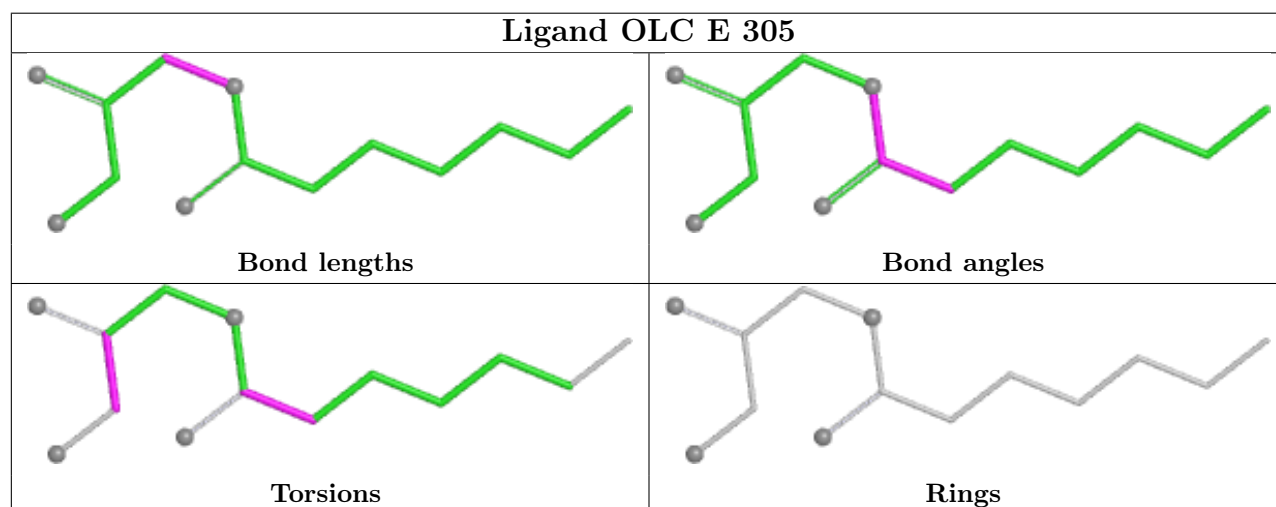
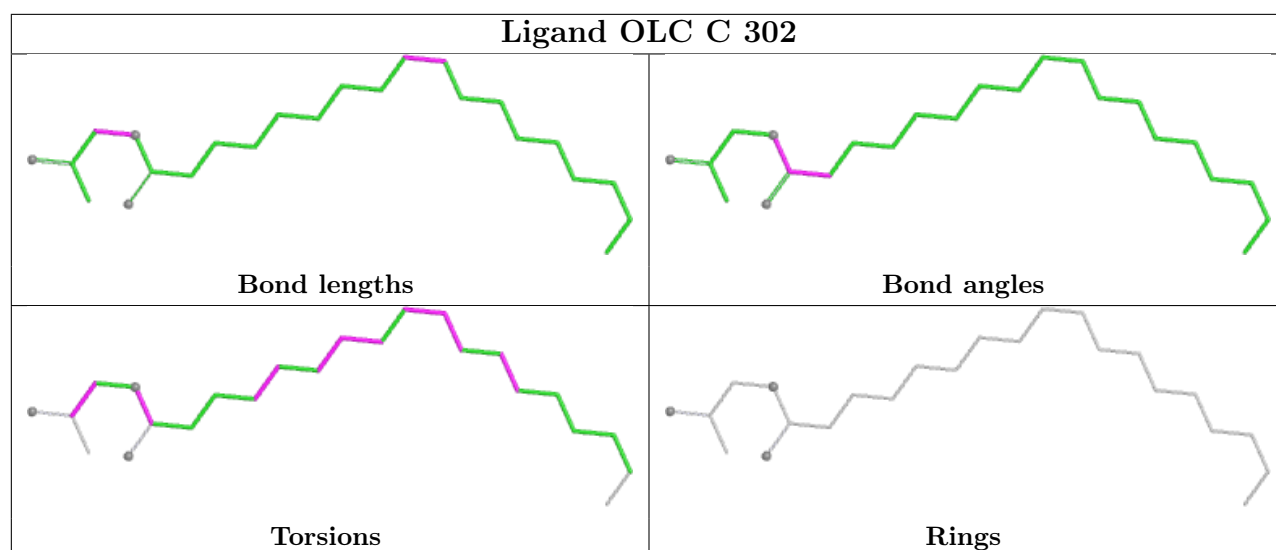


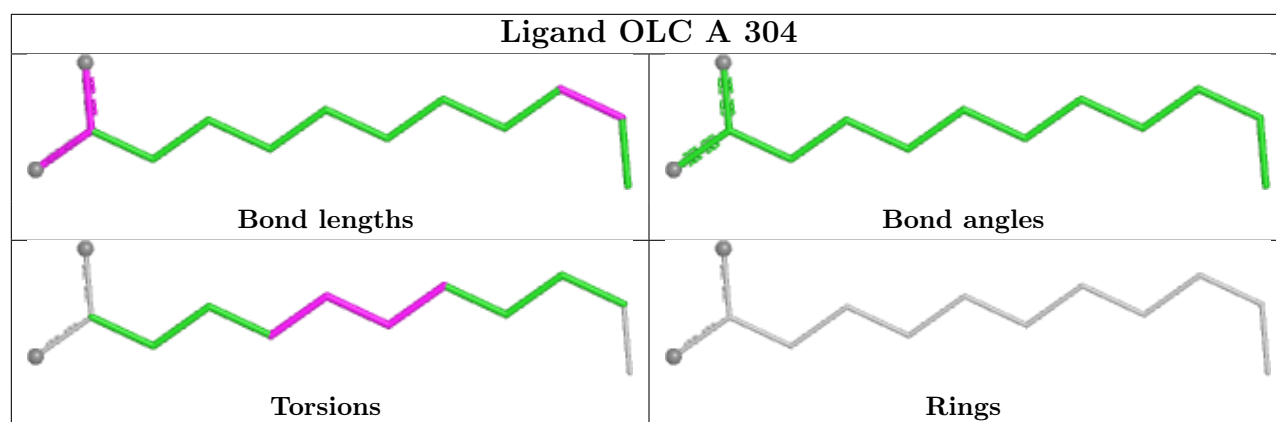












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	287/298 (96%)	0.43	18 (6%) 26 22	35, 54, 96, 123	0
1	B	279/298 (93%)	0.45	16 (5%) 29 25	27, 54, 95, 135	1 (0%)
1	C	282/298 (94%)	0.63	24 (8%) 16 13	42, 61, 100, 123	0
1	D	280/298 (93%)	0.67	32 (11%) 10 7	40, 60, 107, 131	0
1	E	291/298 (97%)	0.33	14 (4%) 35 32	34, 51, 95, 118	0
1	F	219/298 (73%)	2.21	120 (54%) 0 0	62, 107, 152, 201	0
All	All	1638/1788 (91%)	0.73	224 (13%) 6 5	27, 60, 118, 201	1 (0%)

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	20	LEU	6.3
1	E	114	GLY	6.0
1	F	251	SER	5.3
1	F	33	PHE	5.3
1	F	195	CYS	5.0
1	F	221	VAL	4.9
1	F	142	GLY	4.9
1	F	19	THR	4.7
1	F	226	TYR	4.7
1	F	35	LEU	4.6
1	F	41	THR	4.6
1	F	223	ILE	4.5
1	D	57	GLY	4.4
1	F	169	ALA	4.4
1	F	42	ILE	4.3
1	F	278	ALA	4.3
1	B	145	PHE	4.3
1	F	247	ALA	4.3
1	F	218	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	69	VAL	4.2
1	F	254	LEU	4.2
1	F	216	LEU	4.1
1	D	197	ILE	4.0
1	F	75	LEU	4.0
1	F	46	VAL	4.0
1	D	140	ALA	4.0
1	D	285	ALA	3.9
1	F	213	VAL	3.9
1	D	142	GLY	3.8
1	F	144	GLY	3.8
1	D	136	LEU	3.7
1	D	284	LEU	3.7
1	F	214	VAL	3.7
1	F	72	ILE	3.7
1	A	288	LEU	3.6
1	B	114	GLY	3.6
1	F	17	TRP	3.6
1	D	115	GLU	3.6
1	F	16	LEU	3.6
1	F	193	ALA	3.5
1	C	282	THR	3.5
1	F	252	THR	3.5
1	A	140	ALA	3.5
1	A	290	SER	3.5
1	F	224	ALA	3.4
1	C	218	ILE	3.4
1	A	56	VAL	3.4
1	F	8	LEU	3.4
1	F	135	LEU	3.4
1	F	240	LEU	3.4
1	E	25	SER	3.4
1	F	188	THR	3.4
1	F	255	LEU	3.4
1	A	143	PHE	3.3
1	C	65	TRP	3.3
1	F	283	LEU	3.3
1	C	27	THR	3.3
1	F	257	VAL	3.3
1	E	292	GLY	3.3
1	F	222	GLY	3.3
1	F	282	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	114	GLY	3.2
1	F	78	TYR	3.2
1	B	261	ALA	3.2
1	D	61	LEU	3.2
1	D	144	GLY	3.2
1	E	291	SER	3.1
1	F	228	TRP	3.1
1	C	62	ARG	3.1
1	D	282	THR	3.0
1	F	225	PHE	3.0
1	C	175	ARG	3.0
1	C	52	LEU	3.0
1	F	107	LEU	3.0
1	F	250	LEU	3.0
1	F	190	ALA	3.0
1	C	146	ALA	3.0
1	F	262	ALA	3.0
1	F	220	PRO	3.0
1	F	5	SER	3.0
1	C	283	LEU	2.9
1	D	222	GLY	2.9
1	F	15	LEU	2.9
1	F	38	LEU	2.9
1	F	99	TYR	2.9
1	B	137	GLY	2.9
1	F	43	GLY	2.9
1	F	23	ALA	2.9
1	F	268	ALA	2.9
1	F	166	TYR	2.9
1	F	243	LEU	2.9
1	E	140	ALA	2.8
1	F	45	ALA	2.8
1	E	113	PRO	2.8
1	F	186	LEU	2.8
1	F	76	PHE	2.8
1	F	184	PHE	2.8
1	F	219	GLY	2.8
1	F	274	ILE	2.8
1	F	180	VAL	2.8
1	F	110	ALA	2.8
1	B	284	LEU	2.7
1	F	229	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	265	GLY	2.7
1	C	205	PRO	2.7
1	A	203	VAL	2.7
1	F	112	LEU	2.7
1	F	70	HIS	2.7
1	C	222	GLY	2.7
1	D	137	GLY	2.7
1	D	138	ALA	2.7
1	F	215	ALA	2.7
1	F	83	PHE	2.7
1	D	221	VAL	2.7
1	F	167	SER	2.7
1	F	284	LEU	2.7
1	B	24	THR	2.7
1	A	141	GLY	2.6
1	F	248	PRO	2.6
1	F	34	LEU	2.6
1	F	165	VAL	2.6
1	B	263	PRO	2.6
1	D	113	PRO	2.6
1	C	112	LEU	2.6
1	F	117	LEU	2.6
1	E	290	SER	2.6
1	F	256	VAL	2.6
1	F	279	ALA	2.6
1	F	263	PRO	2.5
1	E	115	GLU	2.5
1	F	253	LEU	2.5
1	C	29	ALA	2.5
1	F	132	THR	2.5
1	D	64	PRO	2.5
1	E	141	GLY	2.5
1	D	52	LEU	2.5
1	F	245	TYR	2.5
1	A	197	ILE	2.5
1	D	218	ILE	2.5
1	E	218	ILE	2.5
1	F	191	LEU	2.5
1	B	287	ARG	2.5
1	F	266	ALA	2.5
1	F	141	GLY	2.5
1	F	7	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	275	VAL	2.4
1	C	49	ALA	2.4
1	C	285	ALA	2.4
1	B	260	PHE	2.4
1	B	262	ALA	2.4
1	D	281	ALA	2.4
1	F	21	ALA	2.4
1	F	267	LEU	2.4
1	B	257	VAL	2.4
1	F	187	ALA	2.4
1	B	113	PRO	2.4
1	A	114	GLY	2.4
1	F	271	CYS	2.4
1	F	136	LEU	2.3
1	A	29	ALA	2.3
1	F	39	THR	2.3
1	C	26	SER	2.3
1	F	143	PHE	2.3
1	D	53	ALA	2.3
1	F	272	ALA	2.3
1	F	4	SER	2.3
1	F	192	SER	2.3
1	D	174	ALA	2.3
1	C	28	GLY	2.3
1	D	26	SER	2.3
1	F	264	SER	2.3
1	B	91	PRO	2.3
1	F	79	HIS	2.2
1	C	59	SER	2.2
1	A	115	GLU	2.2
1	C	221	VAL	2.2
1	F	168	VAL	2.2
1	F	249	VAL	2.2
1	A	53	ALA	2.2
1	F	22	LEU	2.2
1	F	170	SER	2.2
1	F	40	PHE	2.2
1	B	23	ALA	2.2
1	F	182	ALA	2.2
1	E	24	THR	2.2
1	A	198	LEU	2.2
1	D	141	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	286	ARG	2.2
1	F	3	ARG	2.2
1	F	194	LEU	2.2
1	F	162	ILE	2.2
1	F	111	PHE	2.2
1	C	24	THR	2.1
1	D	114	GLY	2.1
1	F	12	THR	2.1
1	F	230	ILE	2.1
1	C	202	SER	2.1
1	D	116	ARG	2.1
1	D	263	PRO	2.1
1	A	221	VAL	2.1
1	F	181	VAL	2.1
1	F	237	VAL	2.1
1	F	189	ALA	2.1
1	F	137	GLY	2.1
1	F	183	GLY	2.1
1	A	46	VAL	2.1
1	D	65	TRP	2.1
1	C	61	LEU	2.1
1	D	173	PHE	2.1
1	F	273	LEU	2.1
1	A	27	THR	2.1
1	E	59	SER	2.1
1	C	263	PRO	2.1
1	A	193	ALA	2.0
1	E	58	LEU	2.0
1	B	55	GLY	2.0
1	F	77	GLY	2.0
1	F	101	TRP	2.0
1	F	14	ILE	2.0
1	D	54	ARG	2.0
1	D	234	ARG	2.0
1	D	112	LEU	2.0
1	A	47	GLY	2.0
1	B	222	GLY	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

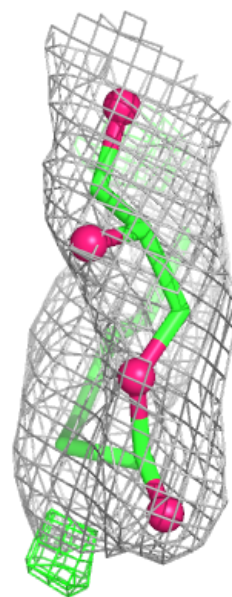
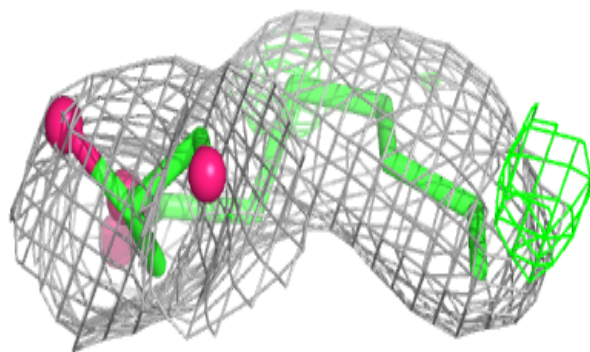
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	OLC	E	304	14/25	0.78	0.18	54,81,94,97	0
2	OLC	E	305	14/25	0.78	0.22	62,74,85,91	0
2	OLC	E	306	14/25	0.80	0.17	71,73,88,88	0
2	OLC	D	304	16/25	0.81	0.16	62,70,83,85	0
2	OLC	D	303	11/25	0.81	0.19	65,72,76,77	0
2	OLC	B	303	17/25	0.82	0.16	64,71,86,89	0
2	OLC	A	304	13/25	0.83	0.17	64,68,78,79	0
2	OLC	B	305	17/25	0.84	0.18	64,72,82,82	0
2	OLC	C	301	11/25	0.85	0.16	60,62,70,70	0
2	OLC	C	303	13/25	0.85	0.17	62,64,72,72	0
2	OLC	D	301	25/25	0.85	0.21	45,63,106,110	0
2	OLC	B	301	25/25	0.85	0.21	37,62,81,84	0
2	OLC	B	304	13/25	0.86	0.19	60,63,66,68	0
2	OLC	A	301	15/25	0.86	0.17	36,50,66,70	0
2	OLC	E	301	16/25	0.87	0.19	58,63,71,71	0
2	OLC	A	303	8/25	0.87	0.21	61,61,63,65	0
2	OLC	C	302	24/25	0.87	0.18	40,69,92,94	0
2	OLC	D	305	13/25	0.87	0.18	62,78,92,93	0
2	OLC	E	302	25/25	0.88	0.17	34,60,76,80	0
2	OLC	A	302	10/25	0.88	0.14	60,68,76,77	0
2	OLC	B	302	13/25	0.89	0.13	55,62,81,83	0
2	OLC	E	303	10/25	0.90	0.16	64,67,72,72	0
2	OLC	D	302	7/25	0.93	0.11	61,64,67,68	0
3	SO4	A	305	5/5	0.93	0.10	84,84,85,91	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.

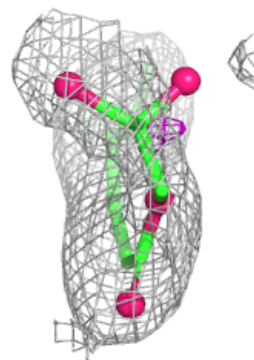
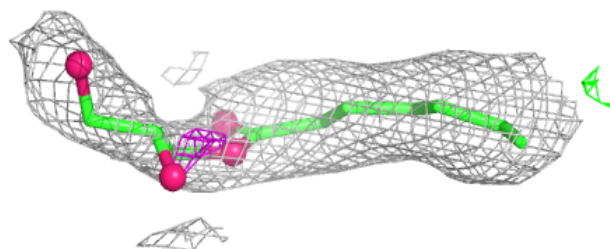
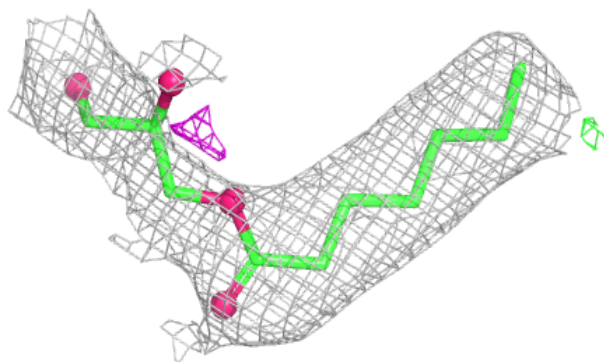
Electron density around OLC E 304:

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

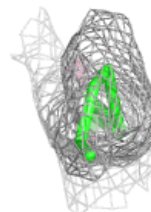
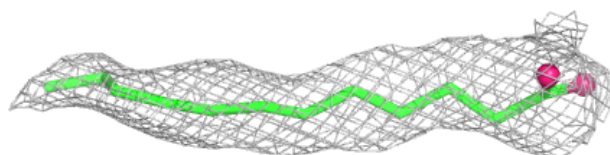
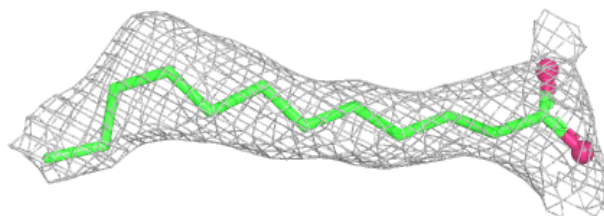


Electron density around OLC E 305:

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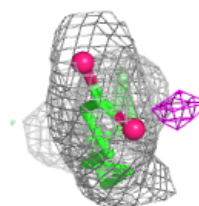
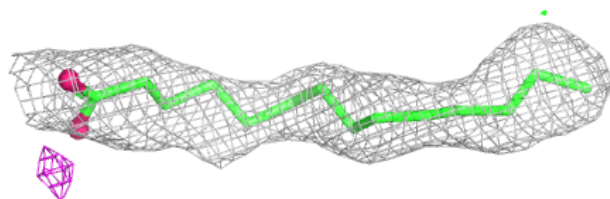
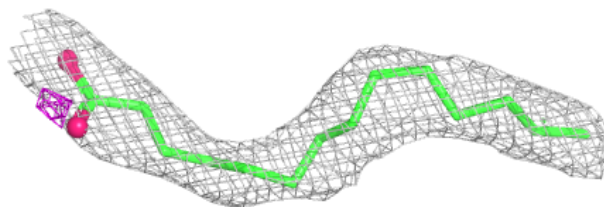
**Electron density around OLC E 306:**

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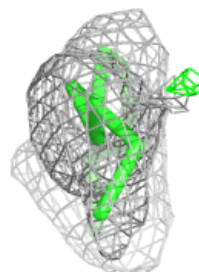
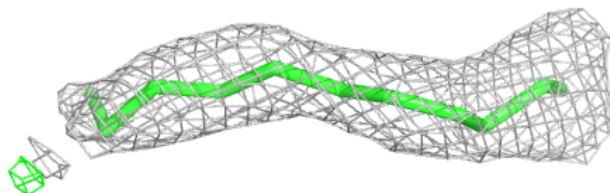
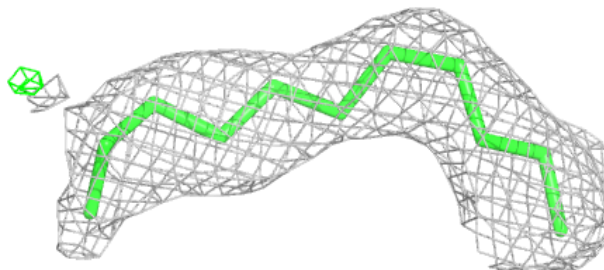


Electron density around OLC D 304:

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and green (positive)

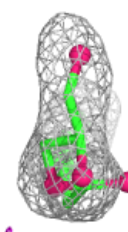
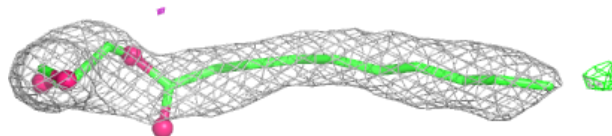
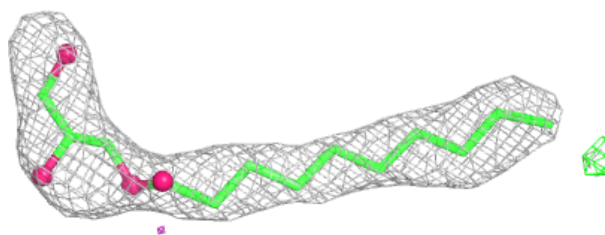
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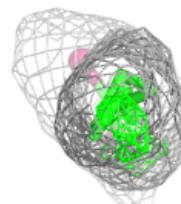
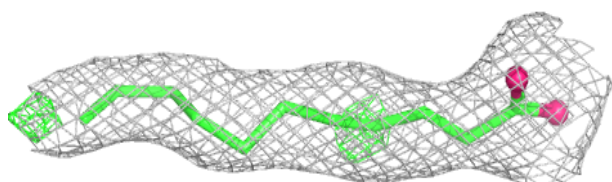
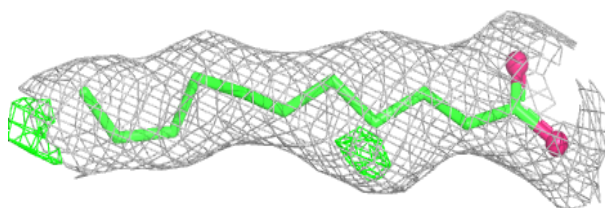


Electron density around OLC B 303:

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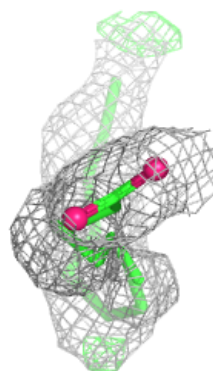
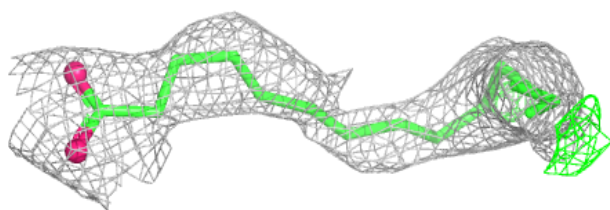
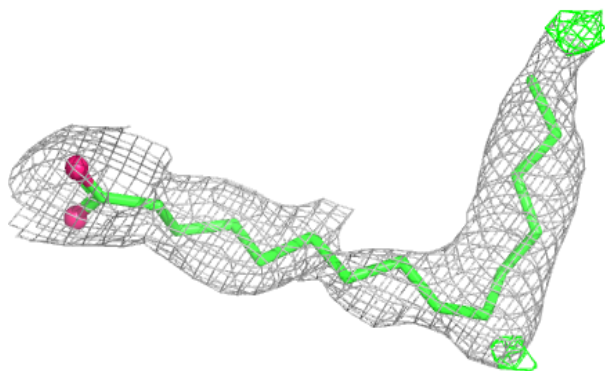
**Electron density around OLC A 304:**

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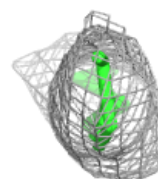
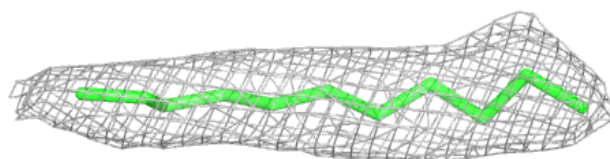
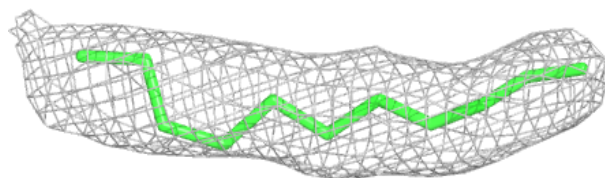


Electron density around OLC B 305:

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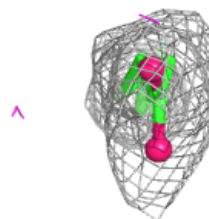
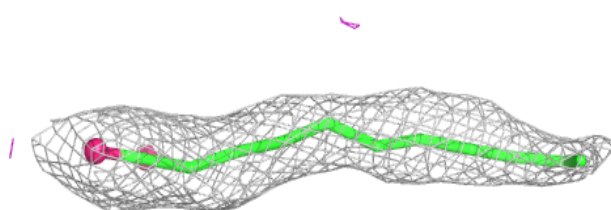
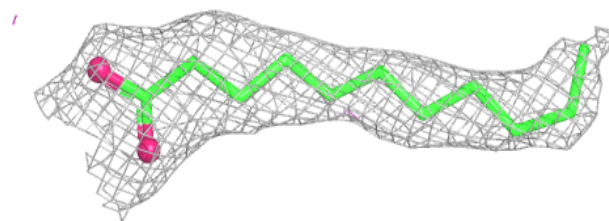
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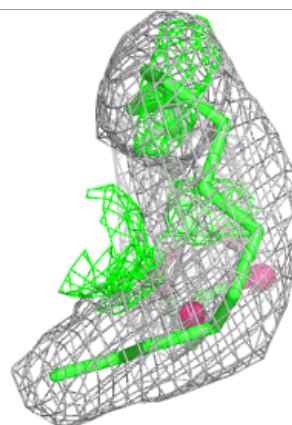
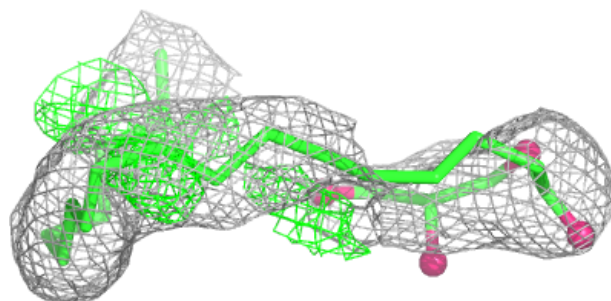
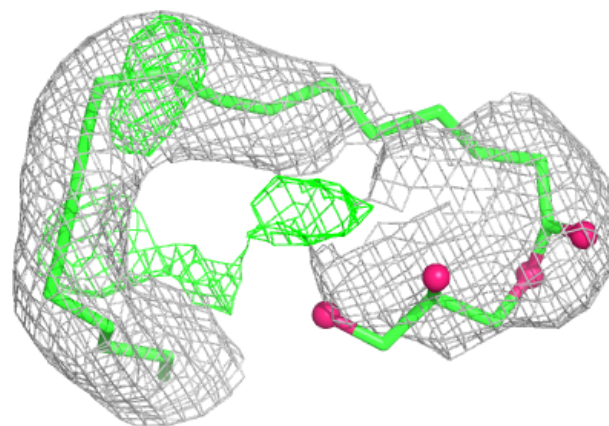


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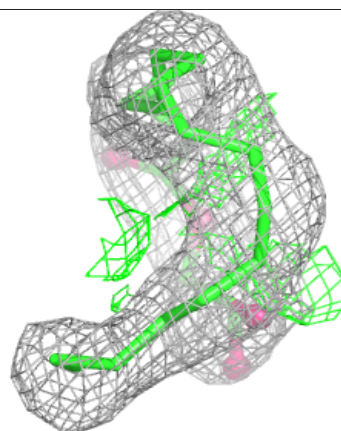
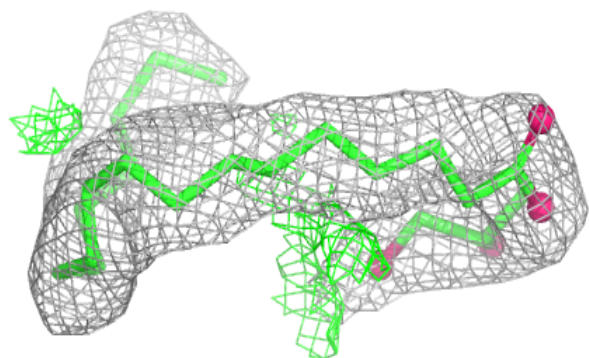
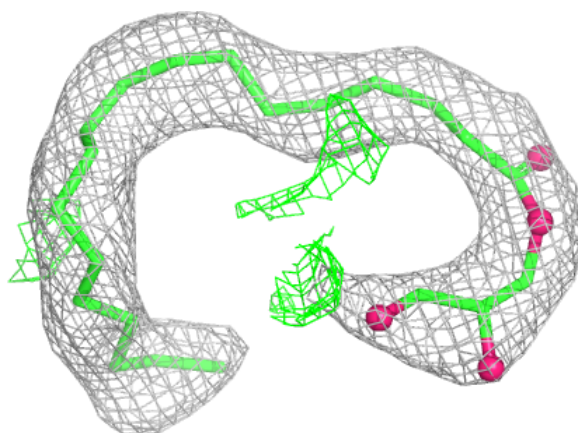
**Electron density around OLC D 301:**

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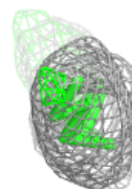
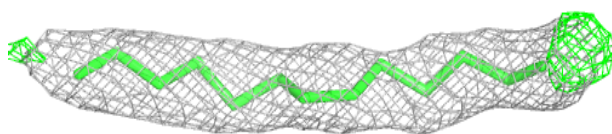
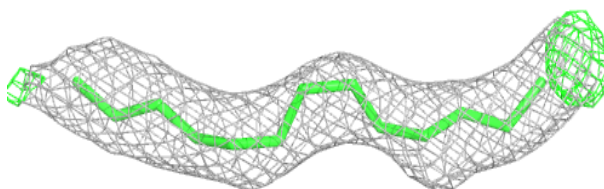


Electron density around OLC B 301:

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and green (positive)

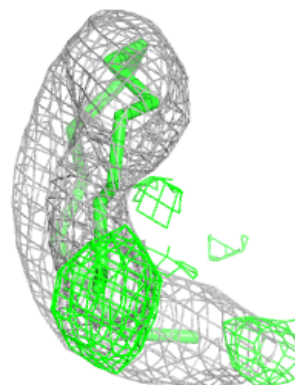
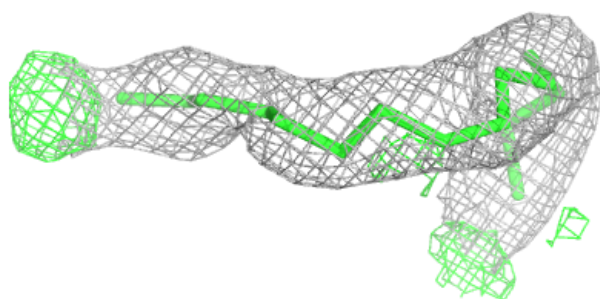
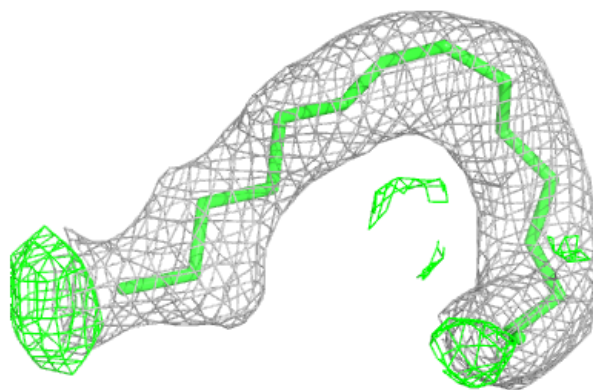
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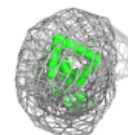
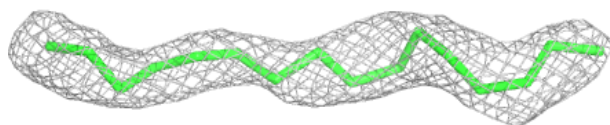
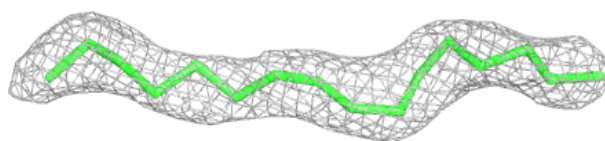


Electron density around OLC A 301:

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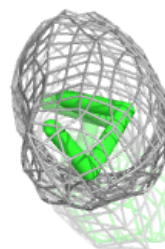
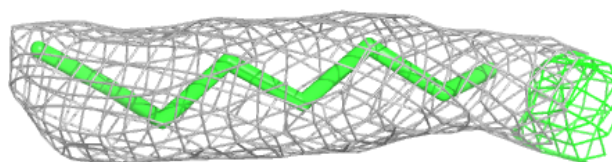
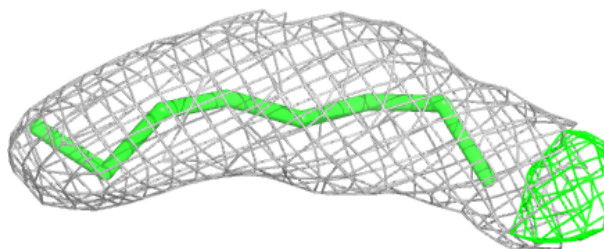
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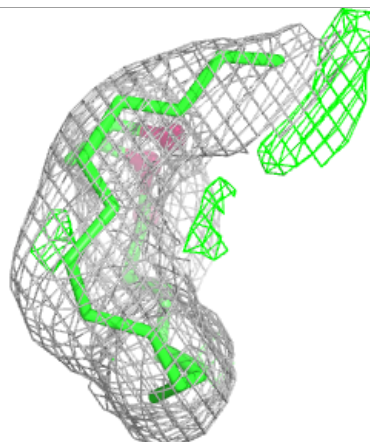
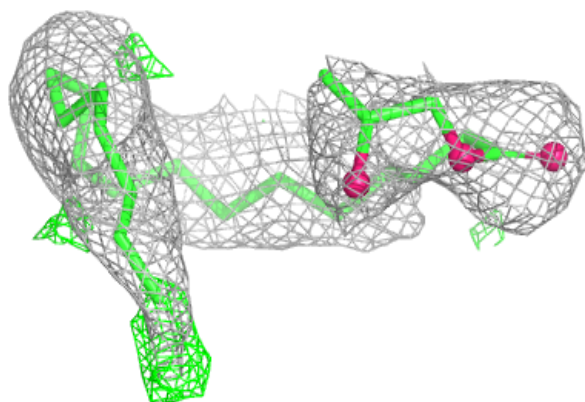
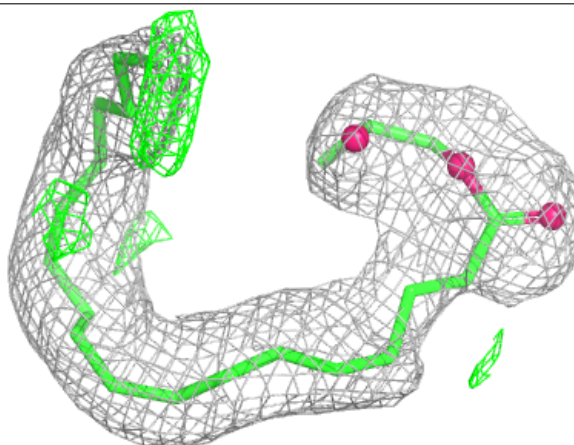


Electron density around OLC A 303:

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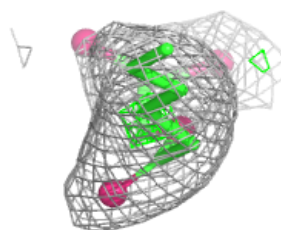
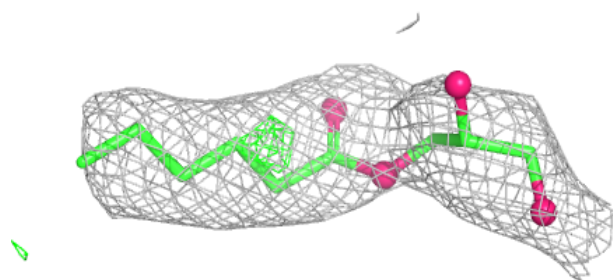
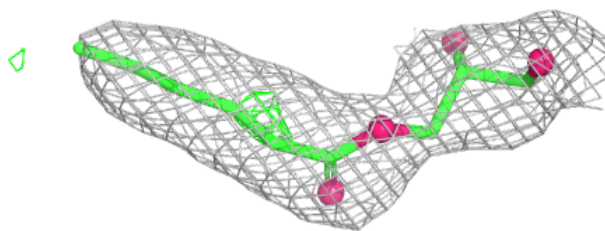
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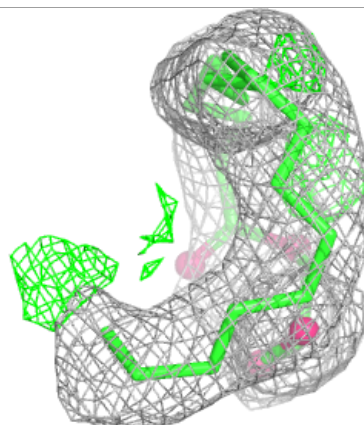
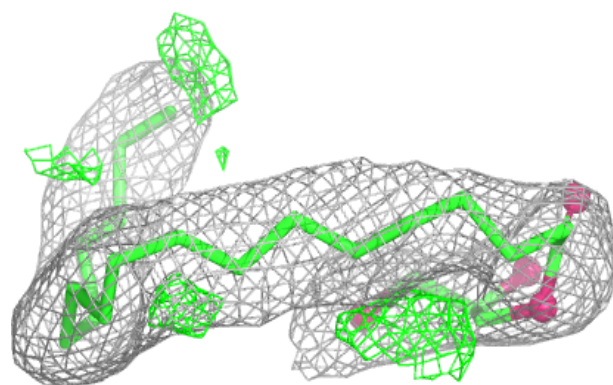
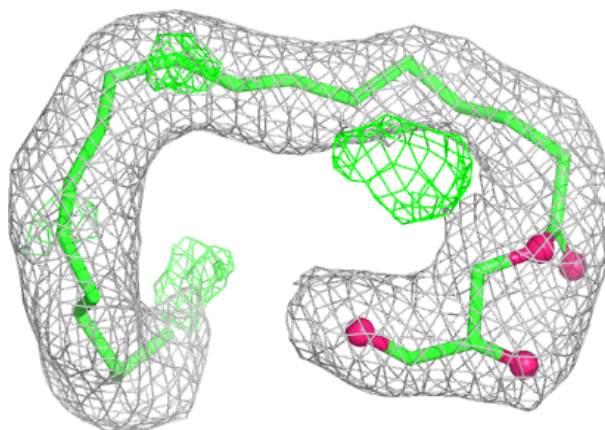


Electron density around OLC D 305:

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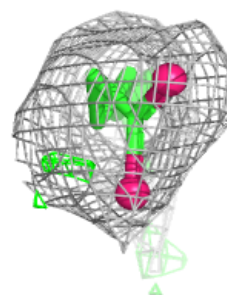
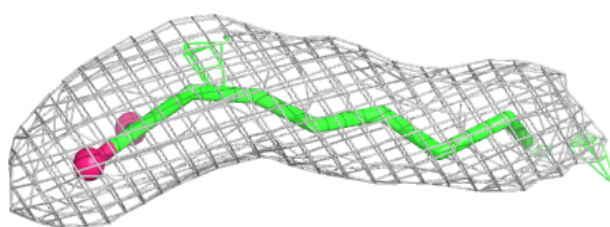
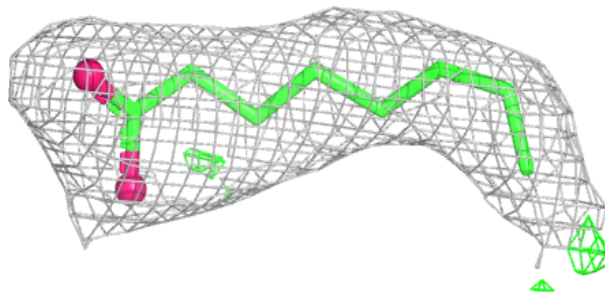
**Electron density around OLC E 302:**

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and green (positive)

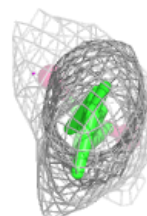
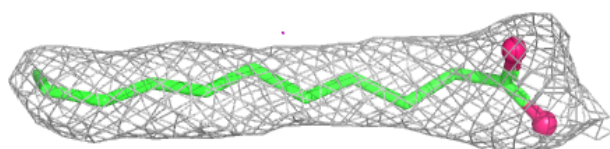
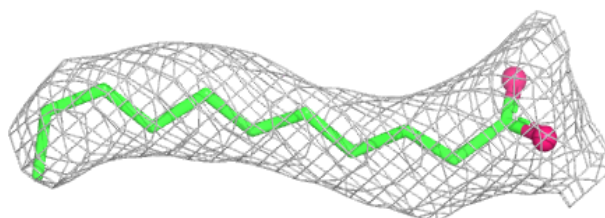


Electron density around OLC A 302:

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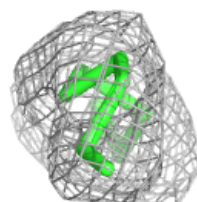
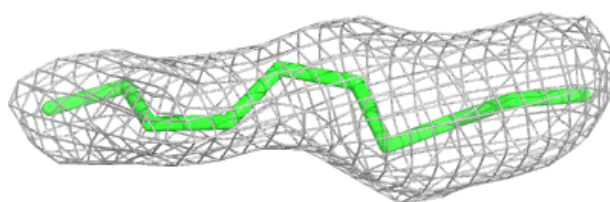
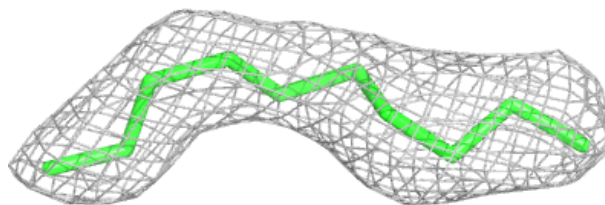
**Electron density around OLC B 302:**

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and green (positive)

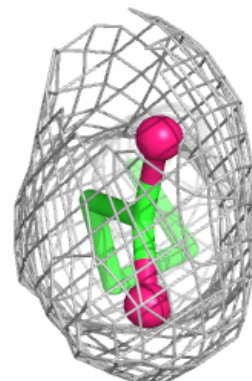
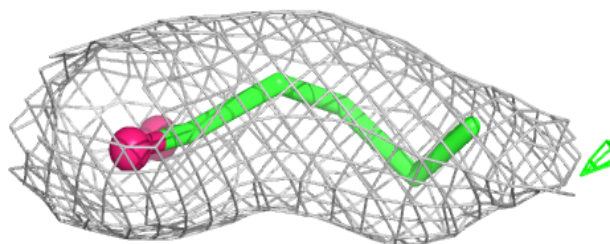
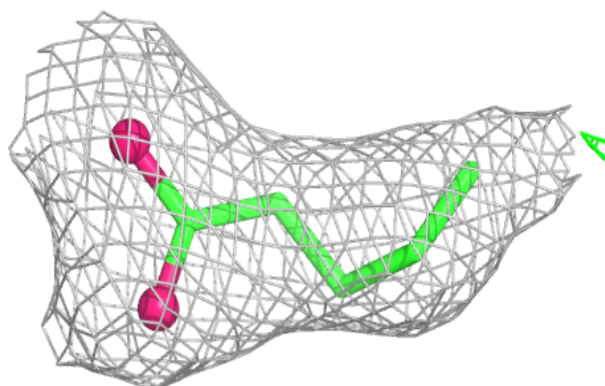


Electron density around OLC E 303:

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and green (positive)

**Electron density around OLC D 302:**

$2mF_o-DF_c$ (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.