



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 06:33 PM UTC

PDB ID : 8E6N / pdb_00008e6n
Title : X-ray structure of the Deinococcus radiodurans Nramp/MntH divalent transition metal transporter G223W mutant in an outward-open, manganese-bound state
Authors : Bozzi, A.T.; Ray, S.; Zimanyi, C.M.; Nicoludis, J.M.; Gaudet, R.
Deposited on : 2022-08-22
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

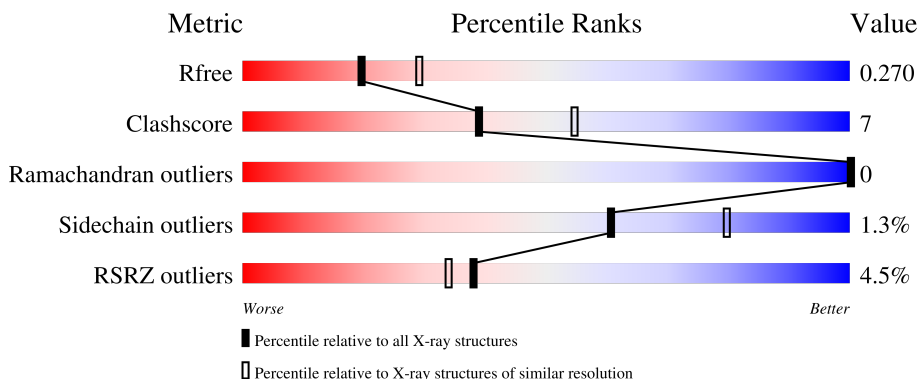
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	411	 4% 83% 13%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3310 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 Divalent metal cation transporter MntH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			3012	1985	505	505	17			

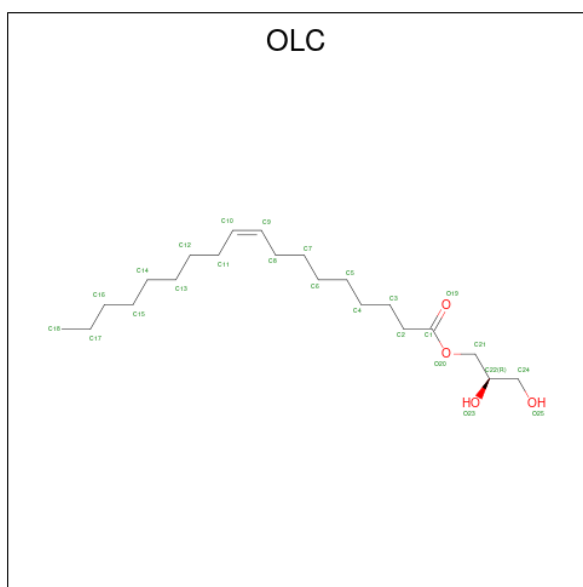
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	expression tag	UNP Q9RTP8
A	27	HIS	-	expression tag	UNP Q9RTP8
A	28	HIS	-	expression tag	UNP Q9RTP8
A	29	HIS	-	expression tag	UNP Q9RTP8
A	30	HIS	-	expression tag	UNP Q9RTP8
A	31	HIS	-	expression tag	UNP Q9RTP8
A	32	HIS	-	expression tag	UNP Q9RTP8
A	33	HIS	-	expression tag	UNP Q9RTP8
A	34	HIS	-	expression tag	UNP Q9RTP8
A	223	TRP	GLY	engineered mutation	UNP Q9RTP8

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		

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



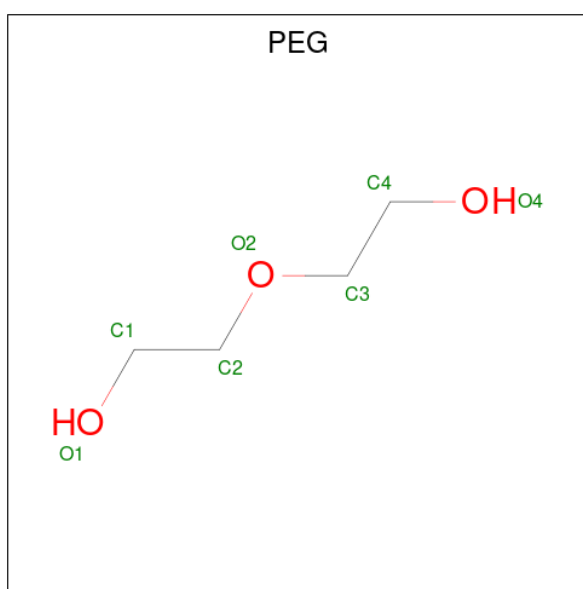
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 18 14 4	0	0
3	A	1	Total C 9 9	0	0
3	A	1	Total C 9 9	0	0
3	A	1	Total C 18 18	0	0
3	A	1	Total C 18 18	0	0
3	A	1	Total C O 14 10 4	0	0
3	A	1	Total C O 16 12 4	0	0
3	A	1	Total C 9 9	0	0
3	A	1	Total C 4 4	0	0
3	A	1	Total C 9 9	0	0
3	A	1	Total C O 18 14 4	0	0
3	A	1	Total C 4 4	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 4 4	0	0

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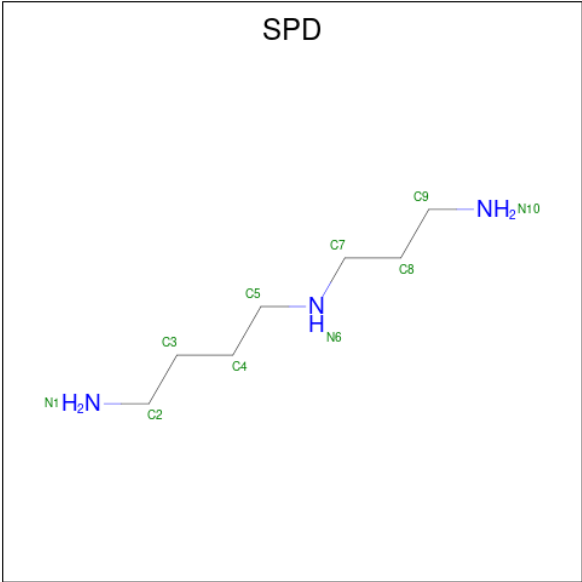
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 11 7 4	0	0
3	A	1	Total C 4 4	0	0
3	A	1	Total C O 16 12 4	0	0
3	A	1	Total C 18 18	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 3 1	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 5 3 2	0	0
4	A	1	Total C O 4 2 2	0	0

- Molecule 5 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			10	7	3		
5	A	1	Total	C	N	0	0
			7	5	2		

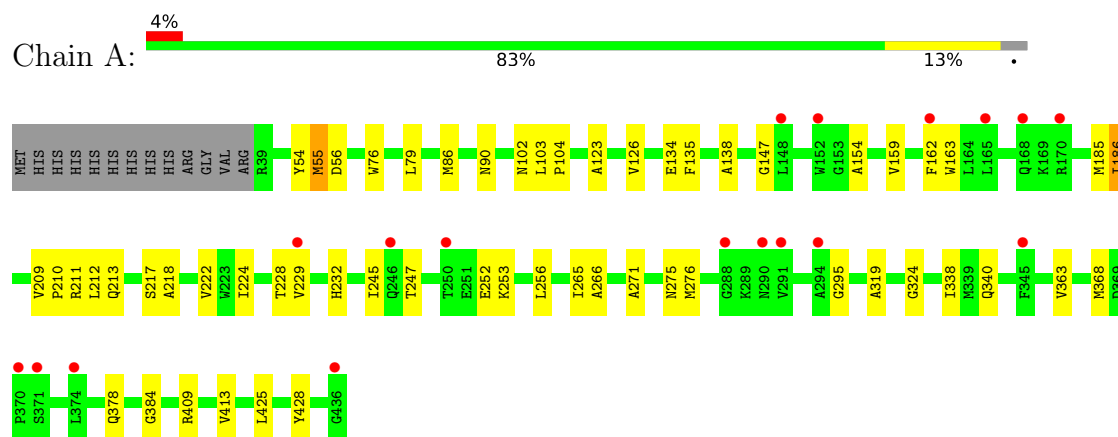
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	54	Total	O	0	0
			54	54		

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: Divalent metal cation transporter MntH



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.76Å 80.39Å 51.75Å 90.00° 94.72° 90.00°	Depositor
Resolution (Å)	39.19 – 2.40 39.19 – 2.40	Depositor EDS
% Data completeness (in resolution range)	82.1 (39.19-2.40) 82.1 (39.19-2.40)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.224 , 0.271 0.224 , 0.270	Depositor DCC
R_{free} test set	701 reflections (4.12%)	wwPDB-VP
Wilson B-factor (Å ²)	58.9	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 57.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3310	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.82% 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, MN, PEG, SPD

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	0.08	0/3080	0.21	0/4209

There are no bond length outliers.

There are no bond angle outliers.

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	3012	0	3167	35	0
2	A	2	0	0	0	0
3	A	205	0	310	15	0
4	A	20	0	22	3	0
5	A	17	0	30	2	0
6	A	54	0	0	3	0
All	All	3310	0	3529	46	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 7.

All (46) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:VAL:HG21	3:A:509:OLC:H2A	1.61	0.81
1:A:232:HIS:NE2	6:A:601:HOH:O	2.20	0.74
1:A:232:HIS:CE1	6:A:601:HOH:O	2.42	0.72
3:A:503:OLC:H10	3:A:506:OLC:H18	1.75	0.67
1:A:102:ASN:HD21	4:A:522:PEG:H12	1.64	0.63
1:A:271:ALA:O	1:A:275:ASN:ND2	2.30	0.62
1:A:266:ALA:HB2	3:A:511:OLC:H17	1.82	0.60
1:A:222:VAL:HG13	1:A:425:LEU:HD22	1.84	0.60
3:A:510:OLC:H13A	3:A:518:OLC:H14	1.84	0.60
1:A:186:ILE:HD12	1:A:319:ALA:HB1	1.87	0.57
1:A:245:ILE:HB	1:A:256:LEU:HD21	1.86	0.56
3:A:506:OLC:H18B	3:A:506:OLC:H13	1.88	0.56
1:A:247:THR:HG21	1:A:253:LYS:HG3	1.90	0.54
1:A:56:ASP:HB2	1:A:134:GLU:HG2	1.90	0.54
1:A:363:VAL:HG13	1:A:368:MET:HB2	1.91	0.53
1:A:247:THR:HG23	1:A:252:GLU:HB2	1.90	0.53
1:A:126:VAL:HG21	1:A:384:GLY:HA3	1.90	0.53
1:A:55:MET:HE1	1:A:186:ILE:HG21	1.90	0.52
1:A:295:GLY:HA3	5:A:525:SPD:H41	1.92	0.51
1:A:209:VAL:HG12	1:A:211:ARG:HG2	1.93	0.51
1:A:138:ALA:HB2	1:A:324:GLY:HA3	1.96	0.48
1:A:212:LEU:HD13	1:A:218:ALA:HA	1.96	0.47
3:A:512:OLC:H18B	3:A:512:OLC:H15	1.75	0.47
1:A:224:ILE:O	1:A:228:THR:OG1	2.31	0.47
1:A:340:GLN:HG3	4:A:522:PEG:H11	1.97	0.47
3:A:504:OLC:H11A	3:A:504:OLC:H14	1.63	0.46
1:A:86:MET:HE3	1:A:265:ILE:HA	1.98	0.46
3:A:506:OLC:H9	3:A:506:OLC:H6	1.39	0.46
3:A:507:OLC:H16	3:A:507:OLC:H13	1.69	0.45
3:A:503:OLC:H6A	3:A:503:OLC:H3	1.44	0.45
1:A:76:TRP:CE2	1:A:210:PRO:HA	2.52	0.44
1:A:185:MET:HG2	3:A:506:OLC:H13A	2.00	0.43
1:A:147:GLY:HA3	4:A:521:PEG:H21	2.00	0.43
1:A:123:ALA:HB1	1:A:338:ILE:HD13	1.99	0.43
5:A:526:SPD:H101	5:A:526:SPD:H71	1.57	0.42
1:A:79:LEU:HD13	1:A:276:MET:HE1	2.01	0.42
3:A:520:OLC:H13	3:A:520:OLC:H16	1.52	0.42
1:A:54:TYR:HE2	1:A:229:VAL:HA	1.83	0.42
1:A:103:LEU:HB3	1:A:104:PRO:HD3	2.01	0.42
1:A:90:ASN:ND2	6:A:613:HOH:O	2.52	0.41
3:A:508:OLC:H4A	3:A:513:OLC:H4A	2.02	0.41
1:A:135:PHE:HE1	1:A:154:ALA:HB1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:VAL:HA	1:A:162:PHE:HD2	1.85	0.40
1:A:163:TRP:CD1	3:A:505:OLC:H5	2.56	0.40
1:A:428:TYR:HB2	3:A:512:OLC:H12	2.03	0.40
1:A:213:GLN:O	1:A:217:SER:OG	2.38	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	396/411 (96%)	387 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	310/322 (96%)	306 (99%)	4 (1%)	61	80

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	MET
1	A	186	ILE

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Mol	Chain	Res	Type
1	A	378	GLN
1	A	409	ARG

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

Mol	Chain	Res	Type
1	A	82	ASN
1	A	90	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PEG	A	524	-	3,3,6	0.45	0	2,2,5	0.42	0
4	PEG	A	522	-	6,6,6	0.50	0	5,5,5	0.29	0
3	OLC	A	507	-	17,17,24	0.32	0	16,16,25	0.78	0
3	OLC	A	508	-	13,13,24	1.05	2 (15%)	14,14,25	1.15	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OLC	A	517	-	10,10,24	1.21	2 (20%)	11,11,25	1.18	1 (9%)
5	SPD	A	525	-	9,9,9	0.32	0	8,8,8	0.85	0
3	OLC	A	513	-	17,17,24	0.96	2 (11%)	18,18,25	1.10	1 (5%)
3	OLC	A	511	-	3,3,24	0.40	0	2,2,25	0.73	0
3	OLC	A	519	-	15,15,24	1.00	2 (13%)	16,16,25	1.03	1 (6%)
5	SPD	A	526	-	6,6,9	0.41	0	5,5,8	1.16	0
3	OLC	A	520	-	17,17,24	0.33	0	16,16,25	0.74	0
3	OLC	A	504	-	8,8,24	0.30	0	7,7,25	0.79	0
3	OLC	A	505	-	8,8,24	0.30	0	7,7,25	0.81	0
3	OLC	A	509	-	15,15,24	1.00	2 (13%)	16,16,25	1.07	1 (6%)
3	OLC	A	506	-	17,17,24	0.33	0	16,16,25	0.75	0
3	OLC	A	510	-	8,8,24	0.30	0	7,7,25	0.81	0
3	OLC	A	515	-	5,5,24	0.32	0	4,4,25	0.63	0
3	OLC	A	516	-	3,3,24	0.40	0	2,2,25	0.76	0
4	PEG	A	523	-	4,4,6	0.42	0	3,3,5	0.30	0
4	PEG	A	521	-	3,3,6	0.51	0	2,2,5	0.31	0
3	OLC	A	512	-	8,8,24	0.31	0	7,7,25	0.73	0
3	OLC	A	514	-	3,3,24	0.40	0	2,2,25	0.78	0
3	OLC	A	503	-	17,17,24	0.97	2 (11%)	18,18,25	1.00	1 (5%)
3	OLC	A	518	-	3,3,24	0.40	0	2,2,25	0.73	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	524	-	-	0/1/1/4	-
4	PEG	A	522	-	-	1/4/4/4	-
3	OLC	A	507	-	-	7/15/15/24	-
3	OLC	A	508	-	-	8/13/13/24	-
3	OLC	A	517	-	-	5/10/10/24	-
5	SPD	A	525	-	-	3/7/7/7	-
3	OLC	A	513	-	-	13/17/17/24	-
3	OLC	A	511	-	-	1/1/1/24	-
3	OLC	A	519	-	-	10/15/15/24	-
5	SPD	A	526	-	-	1/4/4/7	-
3	OLC	A	520	-	-	8/15/15/24	-
3	OLC	A	504	-	-	4/6/6/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OLC	A	505	-	-	4/6/6/24	-
3	OLC	A	509	-	-	3/15/15/24	-
3	OLC	A	506	-	-	7/15/15/24	-
3	OLC	A	510	-	-	4/6/6/24	-
3	OLC	A	515	-	-	1/3/3/24	-
3	OLC	A	516	-	-	0/1/1/24	-
4	PEG	A	523	-	-	1/2/2/4	-
4	PEG	A	521	-	-	0/0/1/4	-
3	OLC	A	512	-	-	3/6/6/24	-
3	OLC	A	514	-	-	1/1/1/24	-
3	OLC	A	503	-	-	9/17/17/24	-
3	OLC	A	518	-	-	1/1/1/24	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	509	OLC	O20-C1	2.48	1.40	1.33
3	A	517	OLC	O20-C1	2.45	1.40	1.33
3	A	503	OLC	O20-C1	2.42	1.40	1.33
3	A	519	OLC	O20-C1	2.41	1.40	1.33
3	A	508	OLC	O20-C1	2.40	1.40	1.33
3	A	513	OLC	O20-C1	2.39	1.40	1.33
3	A	517	OLC	O20-C21	-2.15	1.40	1.45
3	A	513	OLC	O20-C21	-2.14	1.40	1.45
3	A	519	OLC	O20-C21	-2.14	1.40	1.45
3	A	508	OLC	O20-C21	-2.13	1.40	1.45
3	A	503	OLC	O20-C21	-2.13	1.40	1.45
3	A	509	OLC	O20-C21	-2.12	1.40	1.45

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	508	OLC	O20-C1-C2	2.91	120.71	111.83
3	A	513	OLC	O20-C1-C2	2.90	120.68	111.83
3	A	517	OLC	O20-C1-C2	2.86	120.57	111.83
3	A	509	OLC	O20-C1-C2	2.80	120.36	111.83
3	A	503	OLC	O20-C1-C2	2.76	120.25	111.83
3	A	519	OLC	O20-C1-C2	2.65	119.90	111.83

There are no chirality outliers.

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	OLC	O20-C21-C22-C24
3	A	503	OLC	O20-C21-C22-O23
3	A	509	OLC	C2-C1-O20-C21
3	A	509	OLC	O19-C1-O20-C21
3	A	511	OLC	C15-C16-C17-C18
3	A	514	OLC	C15-C16-C17-C18
3	A	517	OLC	O20-C21-C22-C24
3	A	517	OLC	C2-C1-O20-C21
3	A	517	OLC	O19-C1-O20-C21
3	A	503	OLC	O19-C1-O20-C21
3	A	513	OLC	O19-C1-O20-C21
3	A	503	OLC	C2-C1-O20-C21
3	A	513	OLC	C2-C1-O20-C21
3	A	508	OLC	O20-C21-C22-O23
3	A	517	OLC	O20-C21-C22-O23
3	A	503	OLC	C3-C4-C5-C6
3	A	508	OLC	C2-C1-O20-C21
3	A	519	OLC	C2-C1-O20-C21
5	A	525	SPD	C3-C4-C5-N6
3	A	506	OLC	C6-C7-C8-C9
3	A	519	OLC	O19-C1-O20-C21
3	A	508	OLC	O19-C1-O20-C21
3	A	520	OLC	C13-C14-C15-C16
3	A	508	OLC	O20-C21-C22-C24
3	A	513	OLC	C21-C22-C24-O25
3	A	519	OLC	C21-C22-C24-O25
3	A	507	OLC	C11-C12-C13-C14
3	A	519	OLC	C4-C5-C6-C7
3	A	520	OLC	C14-C15-C16-C17
3	A	520	OLC	C12-C13-C14-C15
3	A	505	OLC	C3-C4-C5-C6
3	A	507	OLC	C12-C13-C14-C15
3	A	513	OLC	C2-C3-C4-C5
5	A	525	SPD	C4-C5-N6-C7
3	A	513	OLC	C1-C2-C3-C4
3	A	519	OLC	C1-C2-C3-C4
3	A	512	OLC	C14-C15-C16-C17
3	A	513	OLC	C4-C5-C6-C7
4	A	522	PEG	O1-C1-C2-O2
3	A	512	OLC	C12-C13-C14-C15
3	A	507	OLC	C13-C14-C15-C16
3	A	508	OLC	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	A	507	OLC	C14-C15-C16-C17
3	A	505	OLC	C4-C5-C6-C7
5	A	526	SPD	C7-C8-C9-N10
3	A	506	OLC	C14-C15-C16-C17
3	A	507	OLC	C3-C4-C5-C6
3	A	508	OLC	C1-C2-C3-C4
3	A	506	OLC	C5-C6-C7-C8
3	A	503	OLC	C5-C6-C7-C8
3	A	510	OLC	C12-C13-C14-C15
3	A	503	OLC	C6-C7-C8-C9
3	A	507	OLC	C6-C7-C8-C9
3	A	503	OLC	C4-C5-C6-C7
3	A	505	OLC	C1-C2-C3-C4
3	A	503	OLC	C2-C3-C4-C5
3	A	506	OLC	C11-C12-C13-C14
3	A	506	OLC	C15-C16-C17-C18
3	A	506	OLC	C12-C13-C14-C15
3	A	519	OLC	C5-C6-C7-C8
3	A	519	OLC	C6-C7-C8-C9
3	A	504	OLC	C13-C14-C15-C16
3	A	508	OLC	C4-C5-C6-C7
3	A	504	OLC	C14-C15-C16-C17
3	A	513	OLC	O23-C22-C24-O25
3	A	510	OLC	C13-C14-C15-C16
3	A	520	OLC	C15-C16-C17-C18
3	A	504	OLC	C12-C13-C14-C15
3	A	510	OLC	C14-C15-C16-C17
3	A	520	OLC	C3-C4-C5-C6
3	A	504	OLC	C11-C12-C13-C14
3	A	512	OLC	C15-C16-C17-C18
3	A	513	OLC	O20-C21-C22-C24
3	A	505	OLC	C5-C6-C7-C8
4	A	523	PEG	C4-C3-O2-C2
3	A	510	OLC	C10-C11-C12-C13
3	A	506	OLC	C7-C8-C9-C10
3	A	520	OLC	C10-C11-C12-C13
3	A	519	OLC	O20-C1-C2-C3
3	A	519	OLC	C2-C3-C4-C5
3	A	509	OLC	C2-C3-C4-C5
3	A	508	OLC	O20-C1-C2-C3
3	A	519	OLC	O23-C22-C24-O25
3	A	507	OLC	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
3	A	513	OLC	C7-C8-C9-C10
3	A	520	OLC	C11-C12-C13-C14
3	A	513	OLC	O20-C1-C2-C3
3	A	513	OLC	C3-C4-C5-C6
3	A	515	OLC	C2-C3-C4-C5
3	A	513	OLC	O20-C21-C22-O23
3	A	517	OLC	C21-C22-C24-O25
3	A	513	OLC	O19-C1-C2-C3
5	A	525	SPD	N1-C2-C3-C4
3	A	518	OLC	C13-C14-C15-C16
3	A	520	OLC	C1-C2-C3-C4

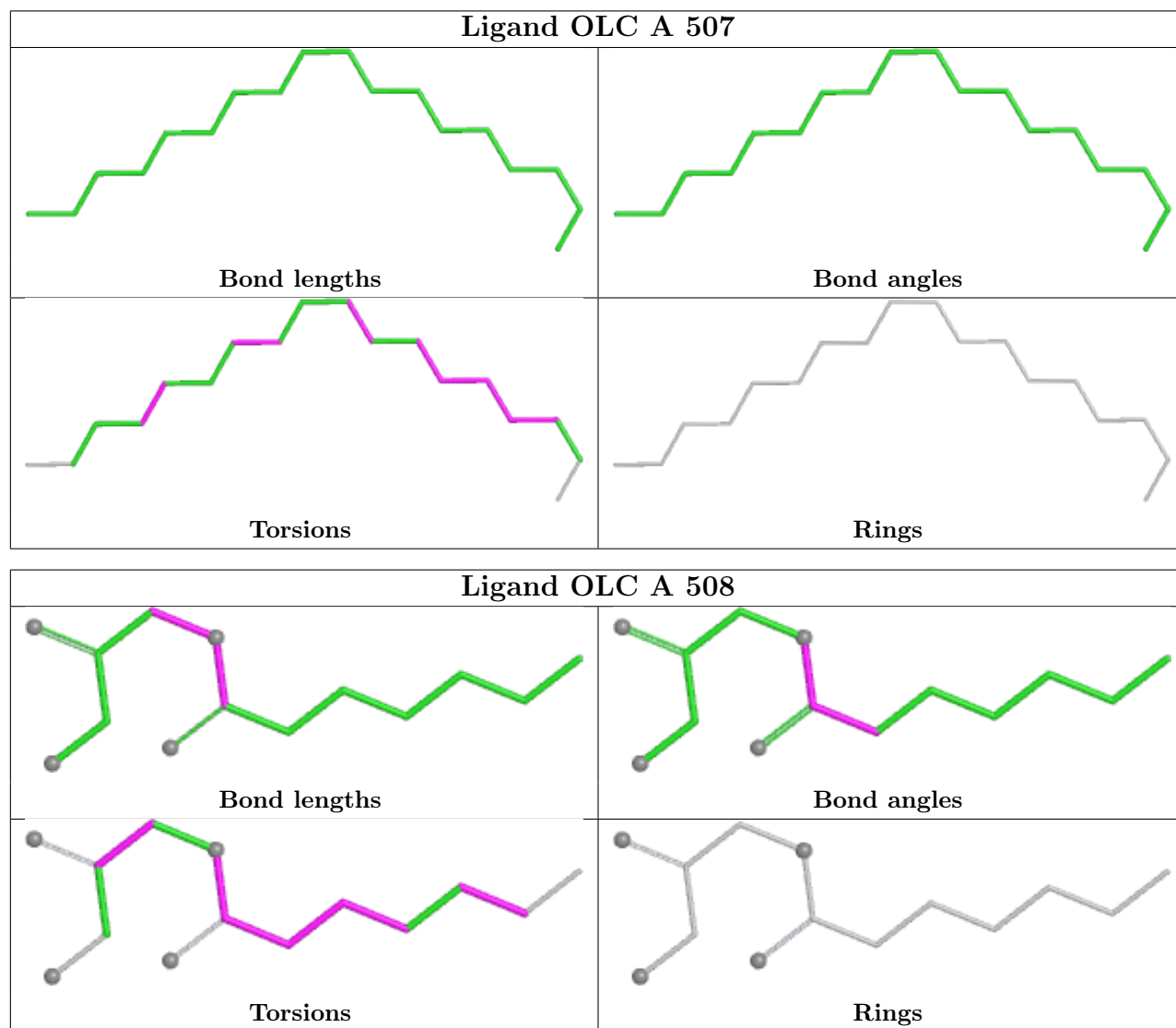
There are no ring outliers.

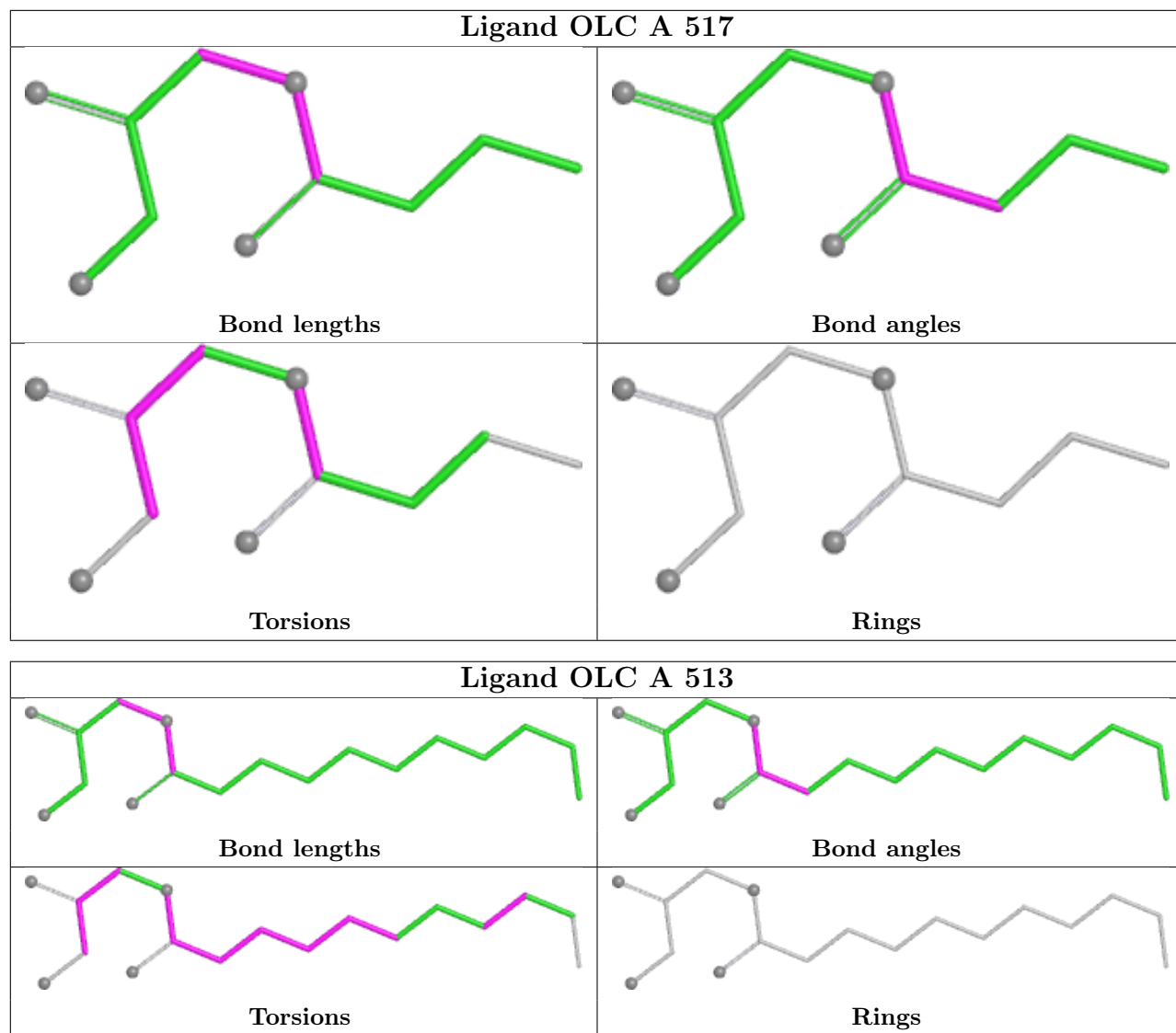
17 monomers are involved in 20 short contacts:

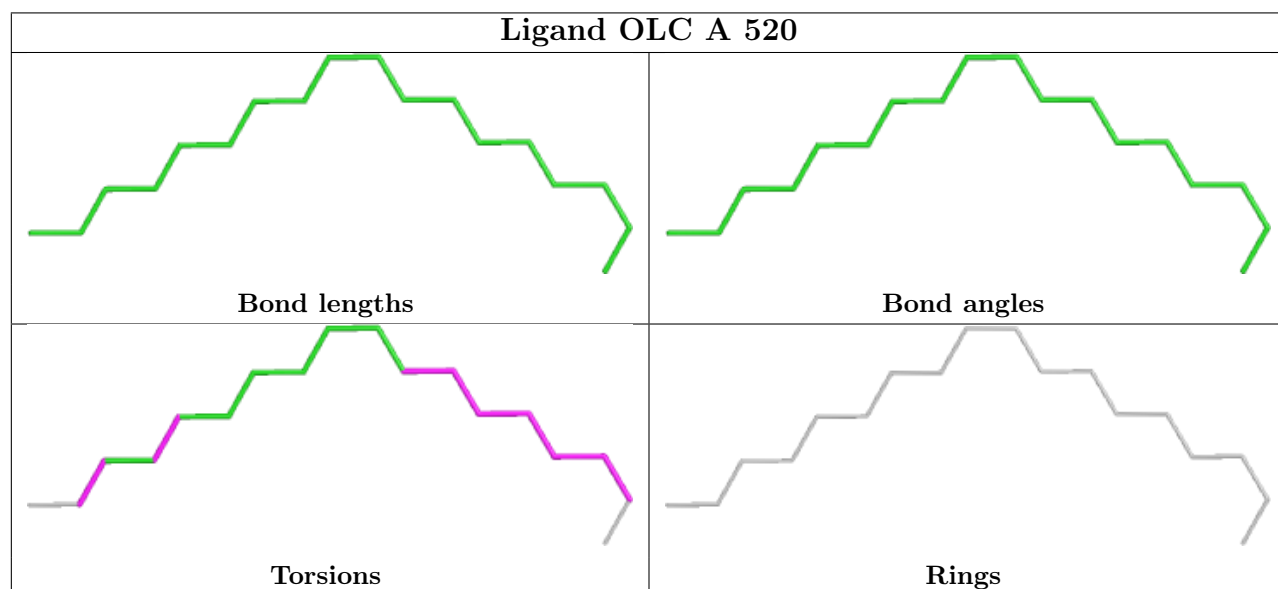
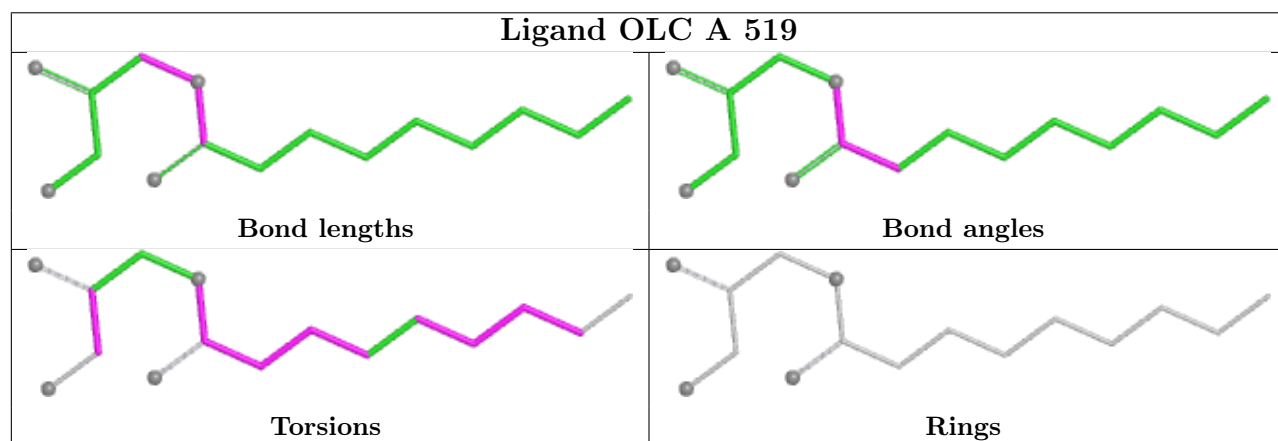
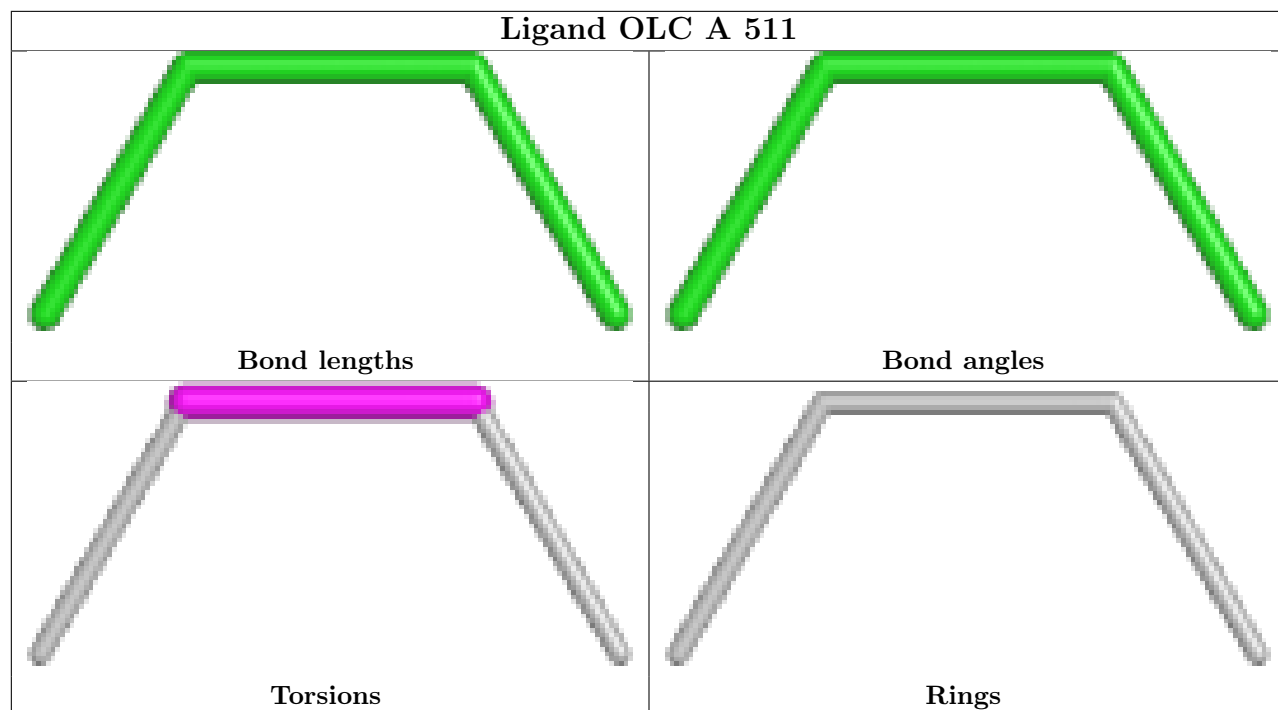
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	522	PEG	2	0
3	A	507	OLC	1	0
3	A	508	OLC	1	0
5	A	525	SPD	1	0
3	A	513	OLC	1	0
3	A	511	OLC	1	0
5	A	526	SPD	1	0
3	A	520	OLC	1	0
3	A	504	OLC	1	0
3	A	505	OLC	1	0
3	A	509	OLC	1	0
3	A	506	OLC	4	0
3	A	510	OLC	1	0
4	A	521	PEG	1	0
3	A	512	OLC	2	0
3	A	503	OLC	2	0
3	A	518	OLC	1	0

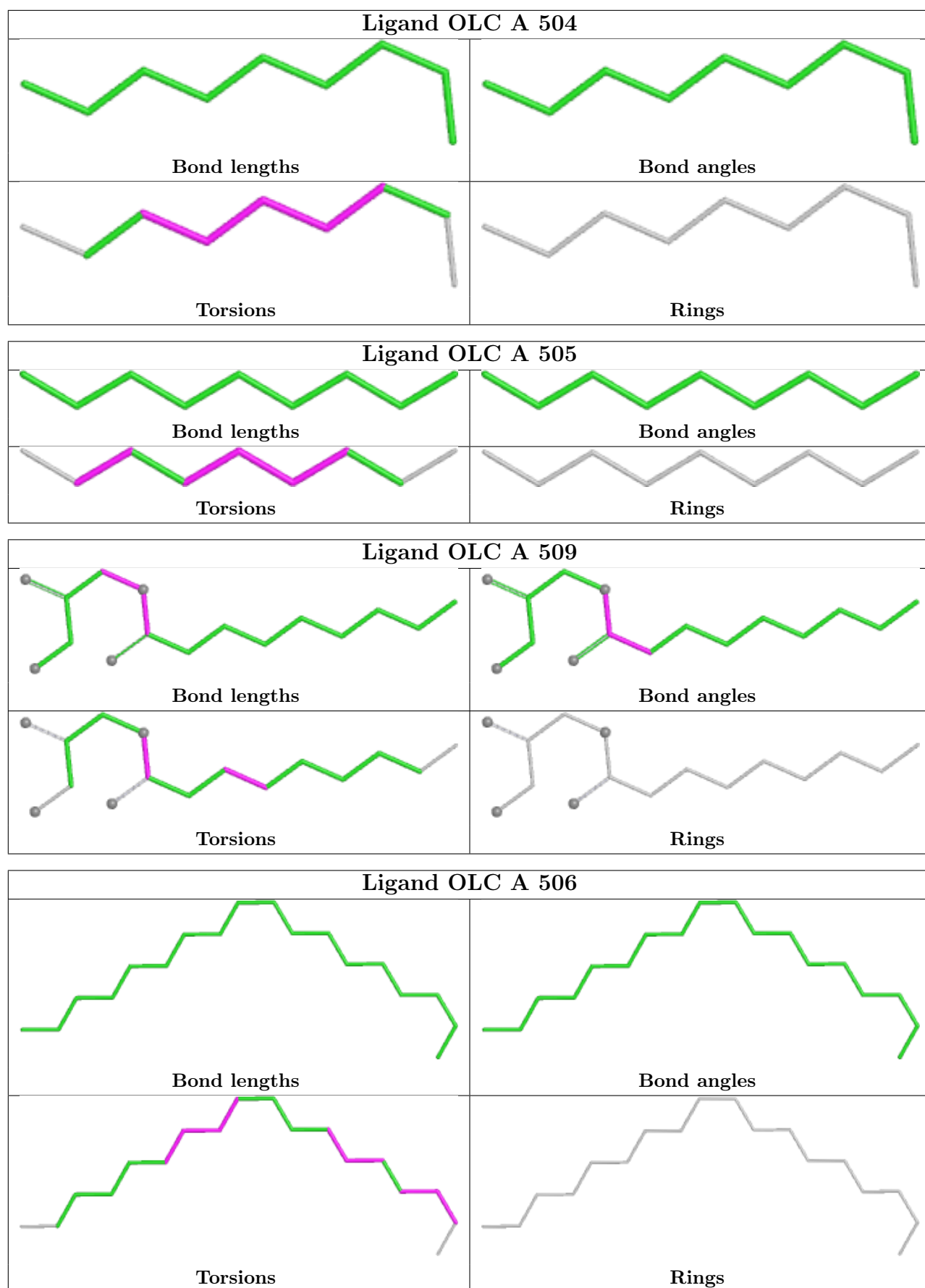
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

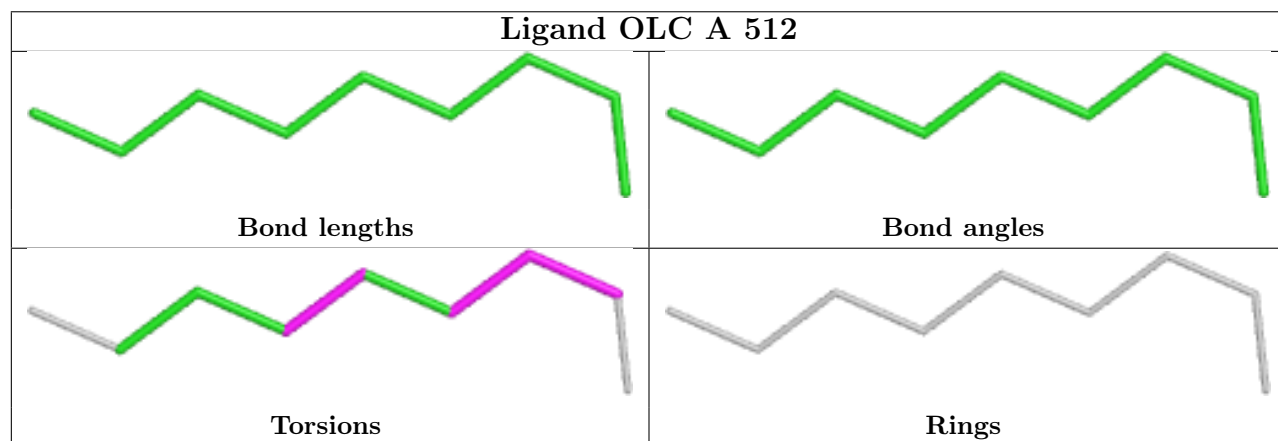
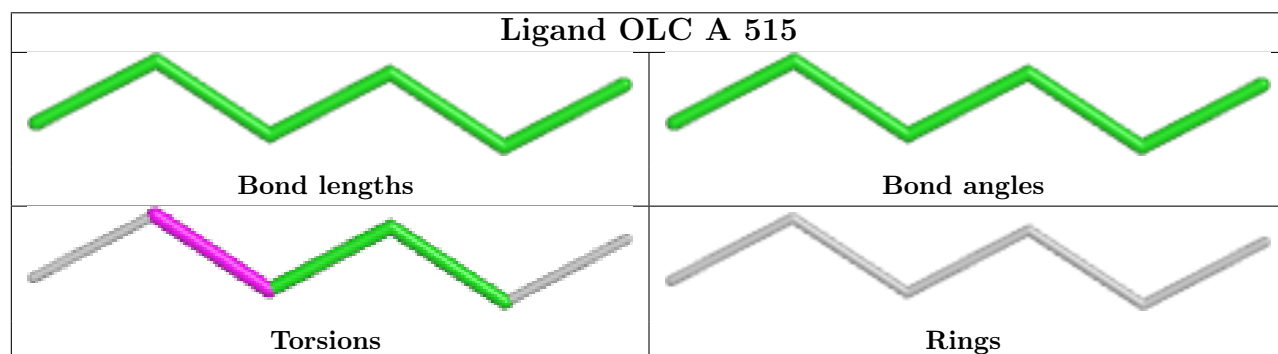
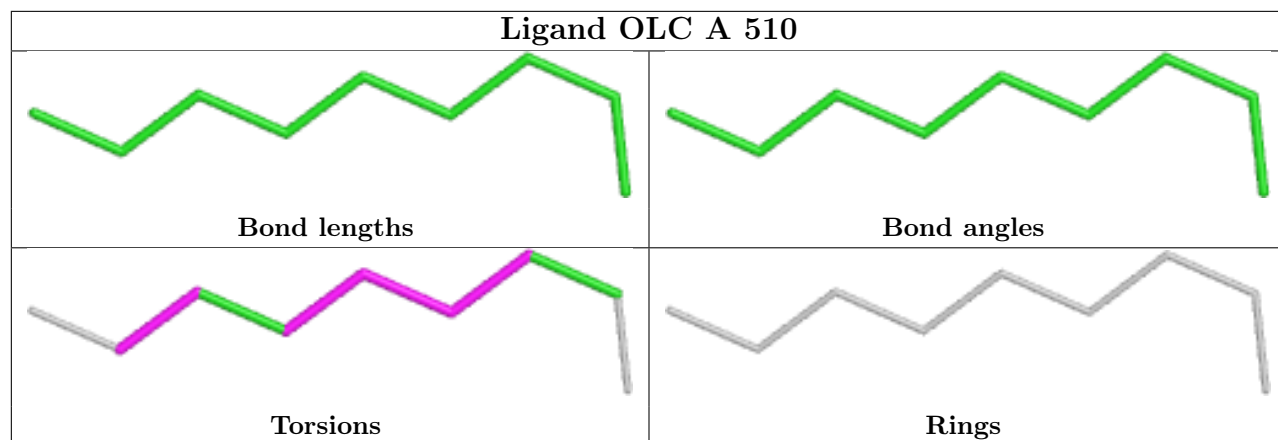
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

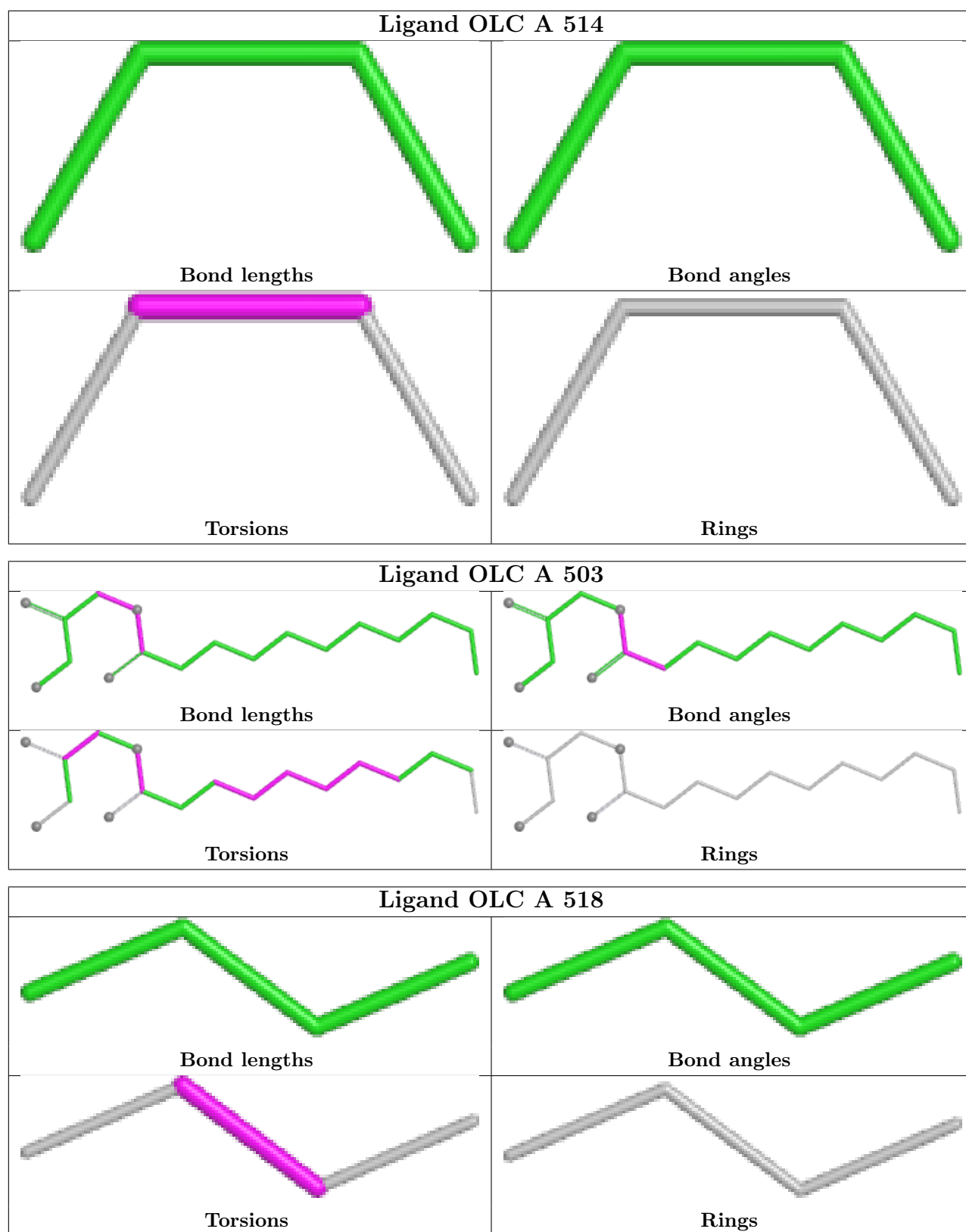












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	398/411 (96%)	0.47	18 (4%) 38 34	51, 65, 121, 193	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	ASN	3.9
1	A	291	VAL	3.6
1	A	374	LEU	2.8
1	A	165	LEU	2.8
1	A	168	GLN	2.8
1	A	148	LEU	2.7
1	A	345	PHE	2.5
1	A	170	ARG	2.5
1	A	370	PRO	2.3
1	A	288	GLY	2.3
1	A	162	PHE	2.2
1	A	371	SER	2.2
1	A	246	GLN	2.2
1	A	250	THR	2.2
1	A	229	VAL	2.1
1	A	294	ALA	2.1
1	A	152	TRP	2.1
1	A	436	GLY	2.1

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 ⓘ

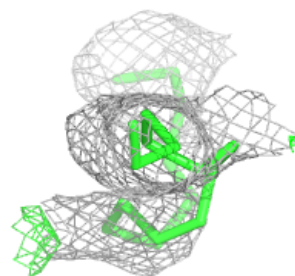
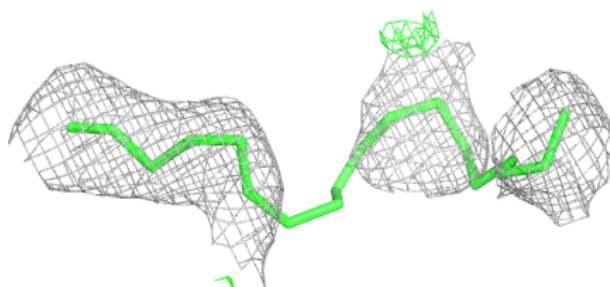
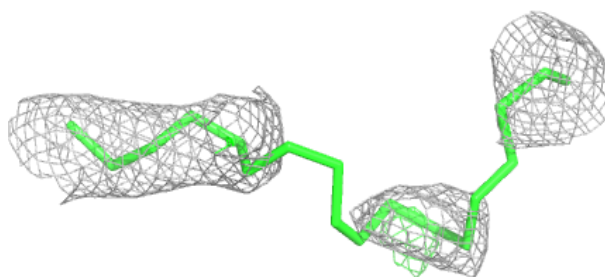
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	OLC	A	520	18/25	0.63	0.16	74,98,112,120	0
3	OLC	A	518	4/25	0.70	0.21	65,68,75,79	0
3	OLC	A	512	9/25	0.70	0.16	71,76,86,86	0
4	PEG	A	521	4/7	0.70	0.21	72,79,85,100	0
3	OLC	A	505	9/25	0.71	0.16	73,81,92,101	0
5	SPD	A	526	7/10	0.71	0.18	64,76,80,89	0
3	OLC	A	519	16/25	0.72	0.13	90,98,111,114	0
3	OLC	A	504	9/25	0.73	0.14	74,78,86,94	0
5	SPD	A	525	10/10	0.76	0.18	84,103,110,110	0
4	PEG	A	522	7/7	0.76	0.17	71,86,92,103	0
3	OLC	A	516	4/25	0.77	0.23	54,63,65,87	0
3	OLC	A	507	18/25	0.77	0.14	72,91,102,103	0
3	OLC	A	503	18/25	0.79	0.14	61,83,97,99	0
3	OLC	A	517	11/25	0.80	0.12	86,97,108,108	0
3	OLC	A	511	4/25	0.80	0.18	75,77,77,77	0
4	PEG	A	523	5/7	0.80	0.09	94,96,104,104	0
3	OLC	A	506	18/25	0.80	0.14	78,90,105,106	0
3	OLC	A	509	16/25	0.80	0.12	74,91,106,118	0
3	OLC	A	514	4/25	0.82	0.17	52,59,64,67	0
3	OLC	A	513	18/25	0.83	0.12	68,87,103,103	0
3	OLC	A	508	14/25	0.84	0.10	63,84,100,104	0
3	OLC	A	515	6/25	0.88	0.13	59,66,74,77	0
4	PEG	A	524	4/7	0.90	0.11	78,79,86,93	0
3	OLC	A	510	9/25	0.91	0.09	70,77,83,83	0
2	MN	A	501	1/1	0.93	0.13	88,88,88,88	1
2	MN	A	502	1/1	0.97	0.07	84,84,84,84	1

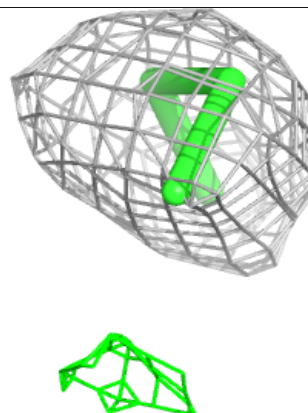
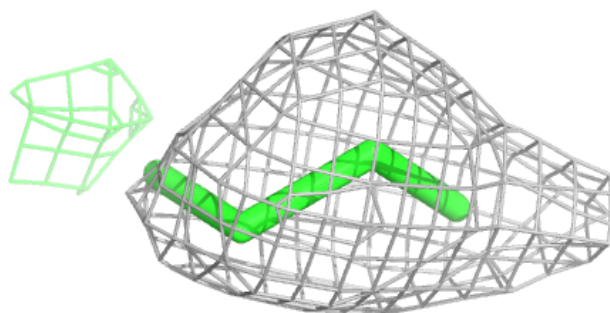
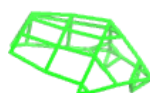
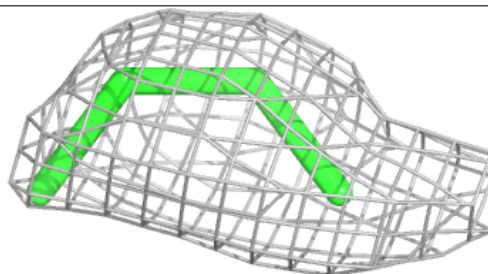
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 520:

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

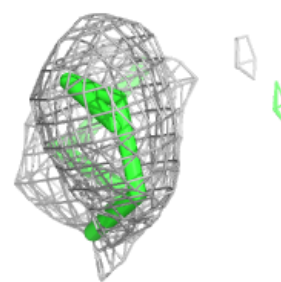
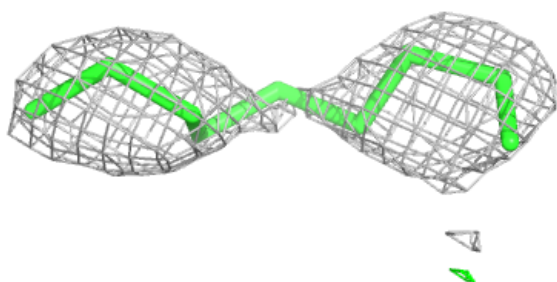
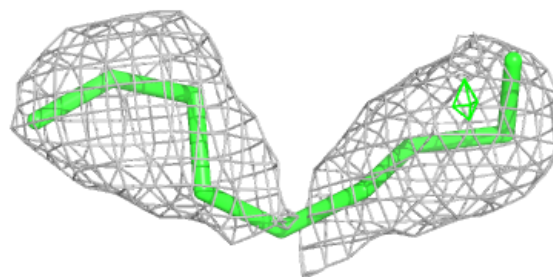
**Electron density around OLC A 518:**

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

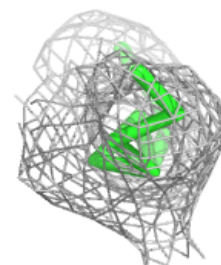
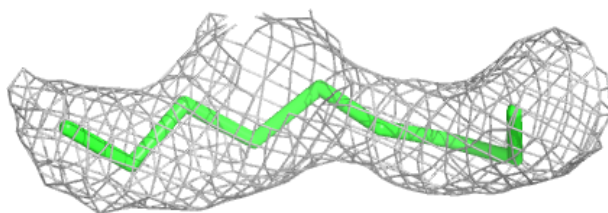
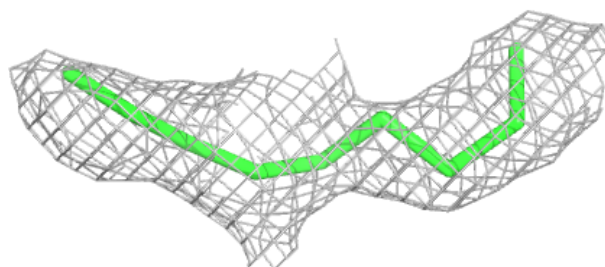


Electron density around OLC A 512:

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

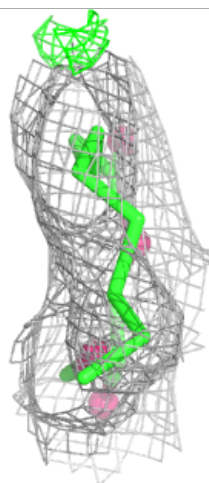
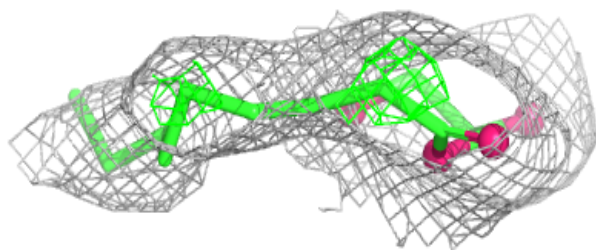
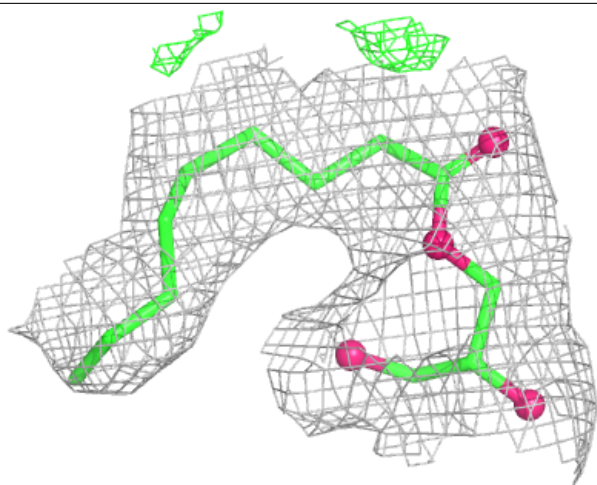
**Electron density around OLC A 505:**

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



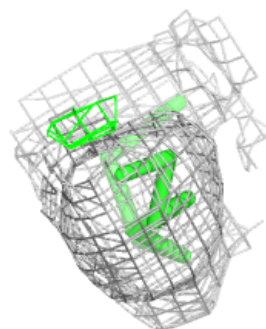
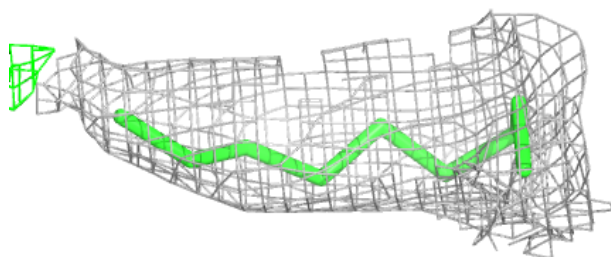
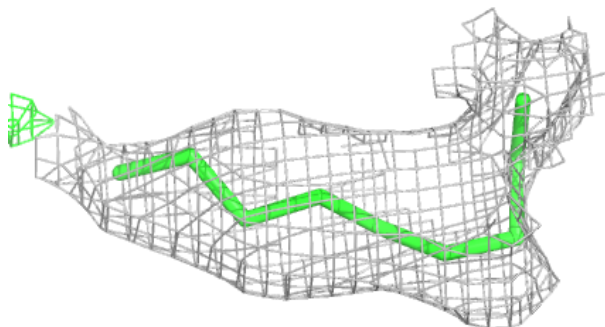
Electron density around OLC A 519:

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

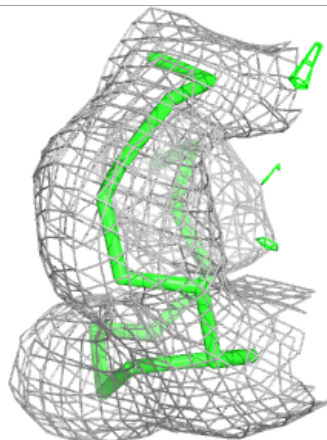
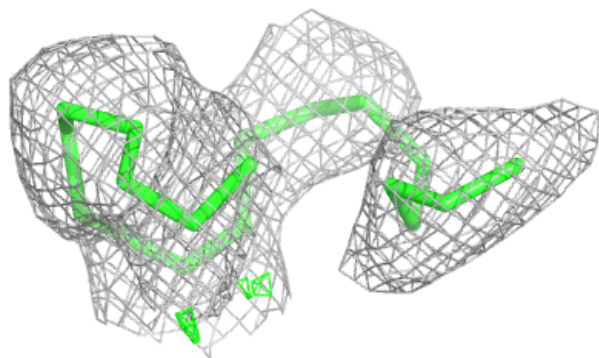
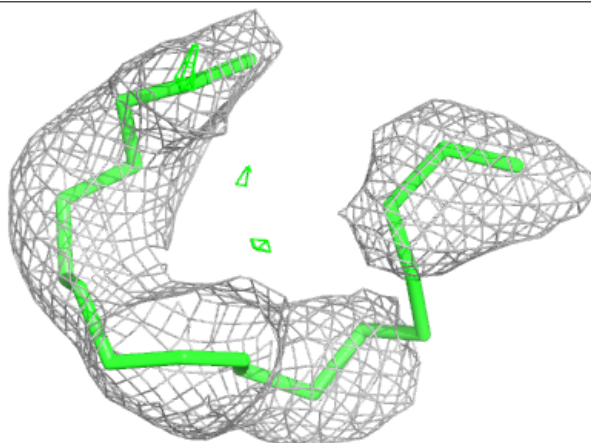


Electron density around OLC A 504:

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

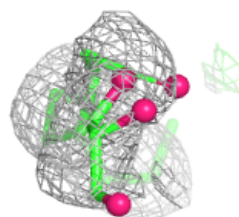
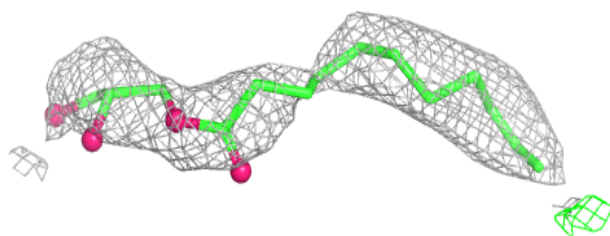
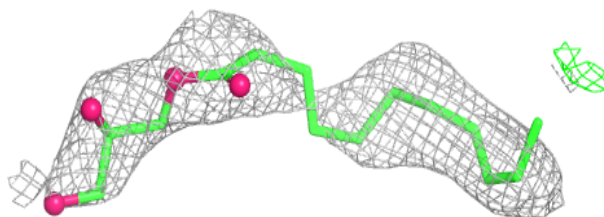
**Electron density around OLC A 507:**

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

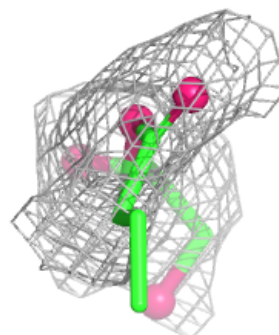
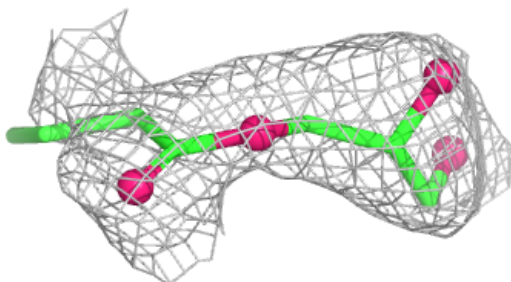
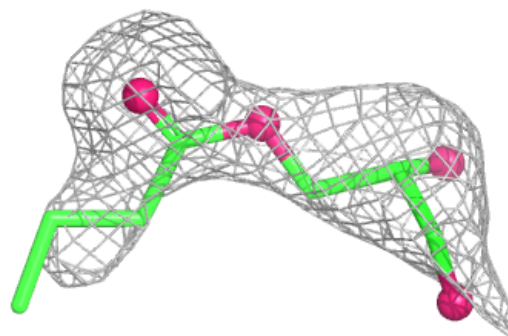


Electron density around OLC A 503:

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

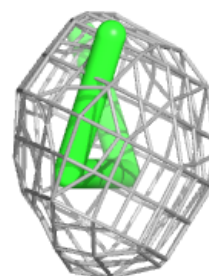
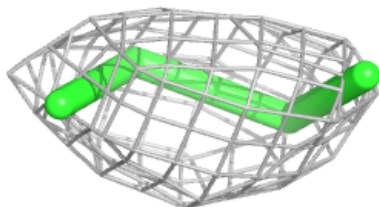
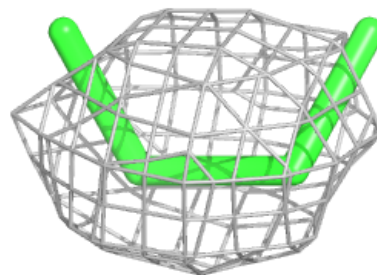
**Electron density around OLC A 517:**

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

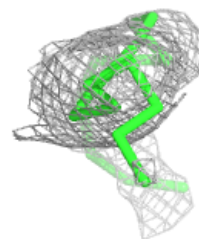
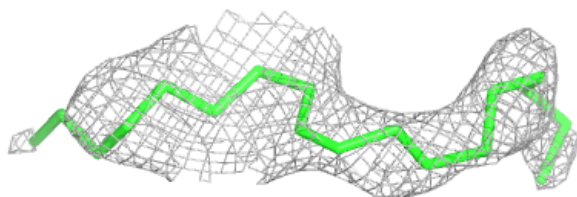
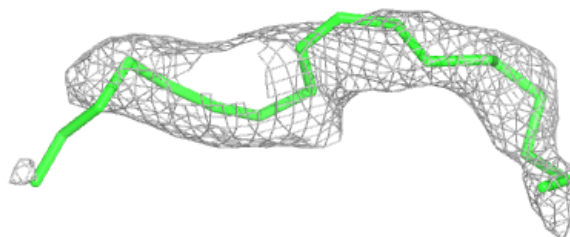


Electron density around OLC A 511:

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

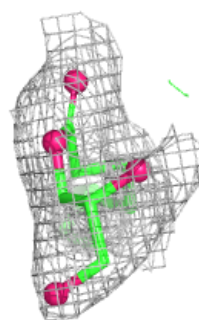
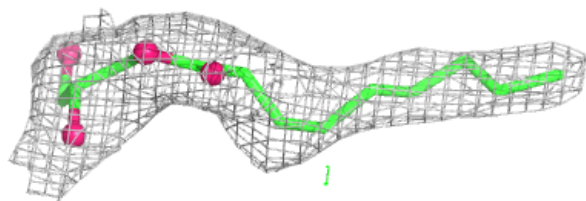
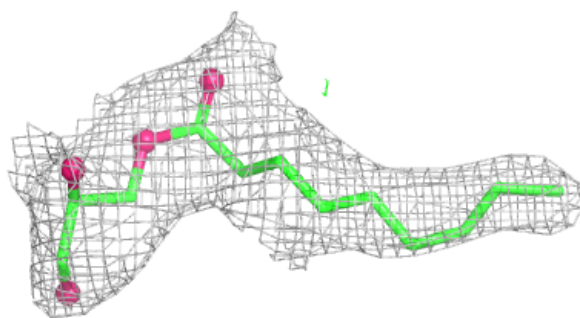
**Electron density around OLC A 506:**

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



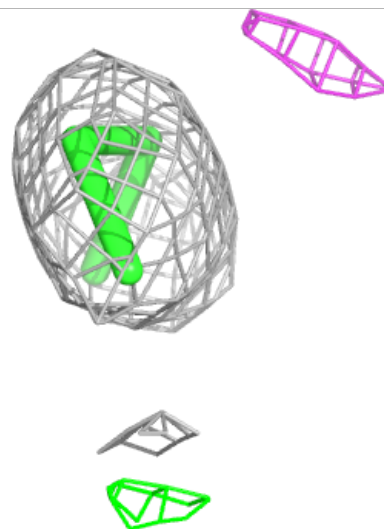
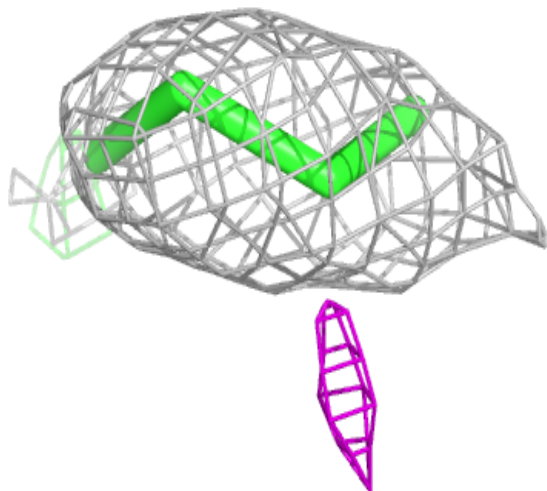
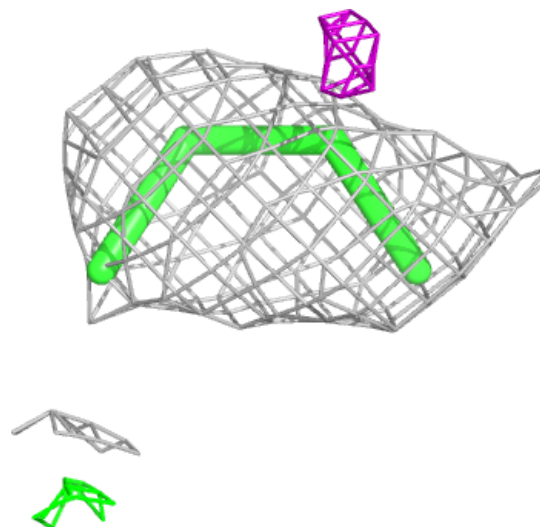
Electron density around OLC A 509:

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



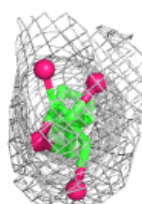
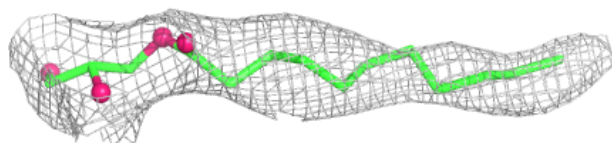
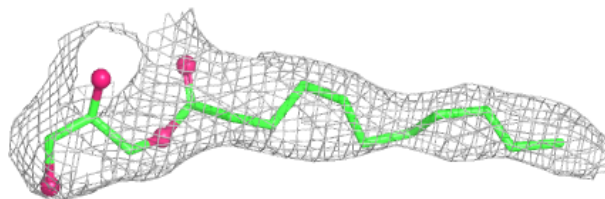
Electron density around OLC A 514:

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

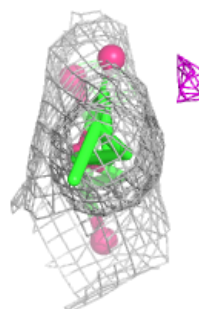
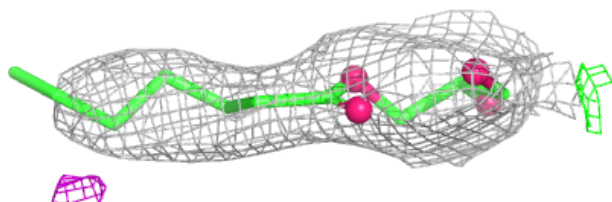


Electron density around OLC A 513:

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

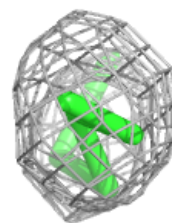
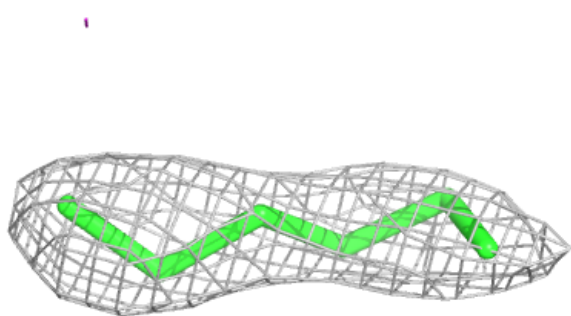
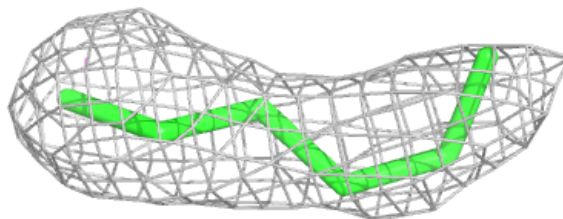
**Electron density around OLC A 508:**

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

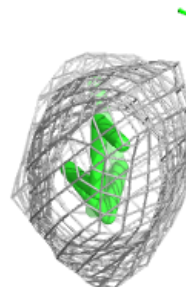
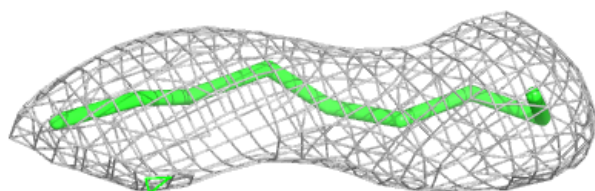
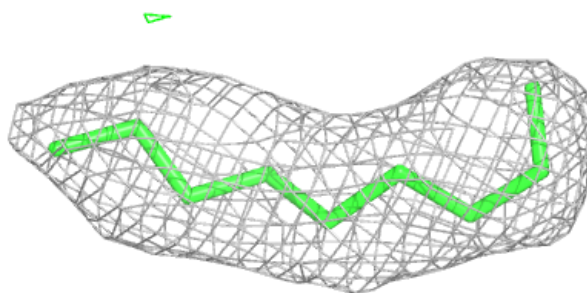


Electron density around OLC A 515:

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

**Electron density around OLC A 510:**

$2mF_o-DF_c$ (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.