



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:04 AM UTC

PDB ID : 4AZL / pdb_00004azl
Title : In meso structure of alginate transporter, AlgE, from *Pseudomonas aeruginosa*, PAO1, crystal form 2.
Authors : Tan, J.; Pye, V.E.; Aragao, D.; Caffrey, M.
Deposited on : 2012-06-26
Resolution : 2.80 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

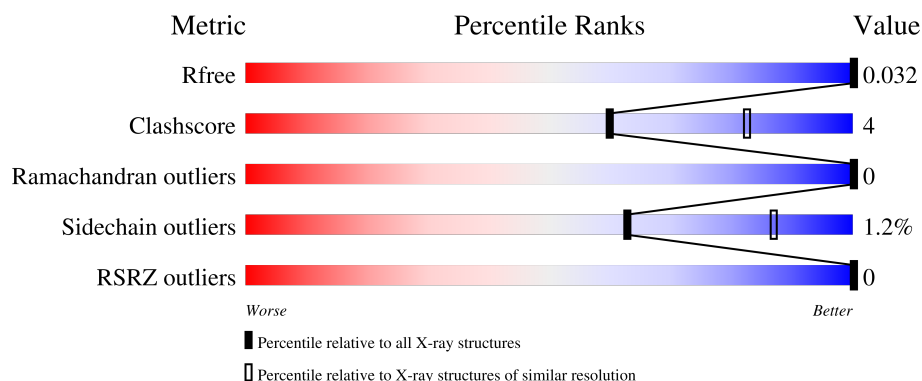
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	458	 81% 9% 9%
1	B	458	 83% 10% 7%

2 Entry composition [i](#)

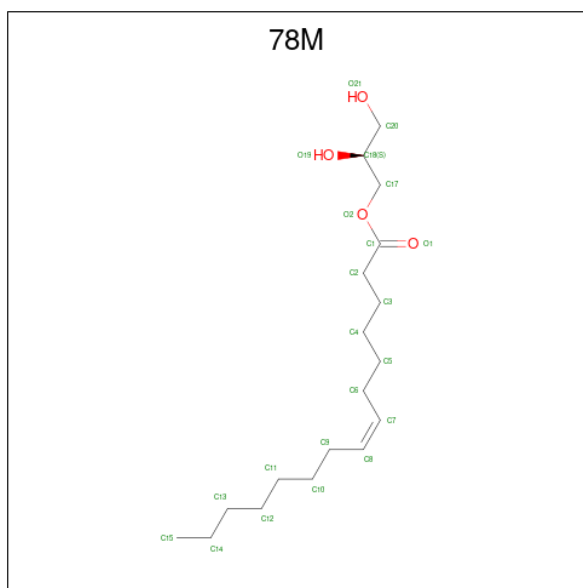
There are 5 unique types of molecules in this entry. The entry contains 6941 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALGINATE PRODUCTION PROTEIN ALGE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3322	2084	588	646	4			
1	B	425	Total	C	N	O	S	0	0	0
			3379	2120	596	659	4			

- Molecule 2 is (2S)-2,3-DIHYDROXYPROPYL(7Z)-PENTADEC-7-ENOATE (CCD ID: 78M) (formula: C₁₈H₃₄O₄).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			8	8		
2	A	1	Total	C	0	0
			11	11		
2	A	1	Total	C	0	0
			13	13		
2	B	1	Total	C	0	0
			9	9		

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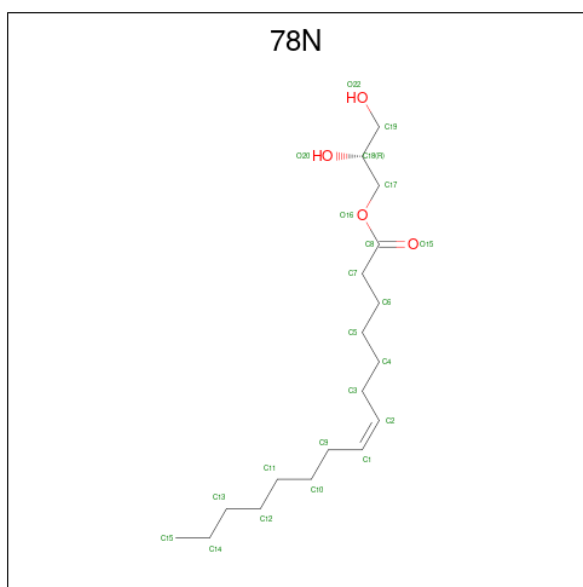
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C 8 8	0	0
2	B	1	Total C 11 11	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 12 12	0	0
2	B	1	Total C O 22 18 4	0	0
2	B	1	Total C O 22 18 4	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0

- Molecule 4 is (2R)-2,3-DIHYDROXYPROPYL(7Z)-PENTADEC-7-ENOATE (CCD ID: 78N) (formula: C₁₈H₃₄O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 22 18 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			22	18	4		
4	A	1	Total	C	O	0	0
			22	18	4		

- Molecule 5 is water.

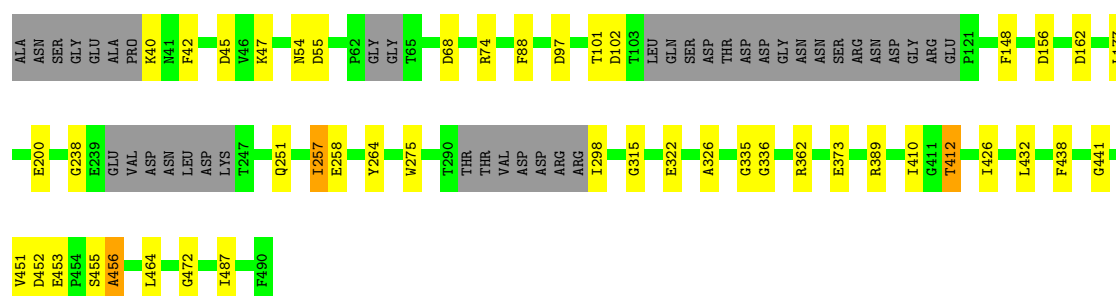
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	19	Total	O	0	0
			19	19		
5	B	30	Total	O	0	0
			30	30		

3 Residue-property plots

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.

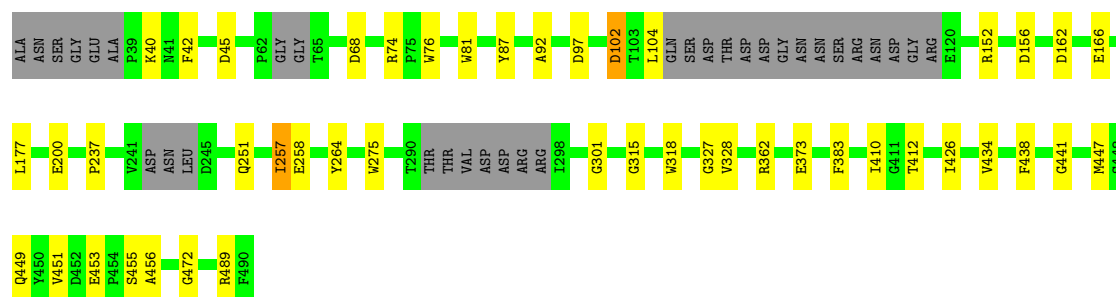
• Molecule 1: ALGINATE PRODUCTION PROTEIN ALGE

Chain A: 



• Molecule 1: ALGINATE PRODUCTION PROTEIN ALGE

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.09Å 245.76Å 47.13Å 90.00° 104.36° 90.00°	Depositor
Resolution (Å)	44.89 – 2.80 44.89 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.3 (44.89-2.80) 93.2 (44.89-2.80)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.237 , 0.280 0.240 , 0.032	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 12.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.180 for l,k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6941	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 78M, CA, 78N

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	0.41	0/3407	0.84	6/4616 (0.1%)
1	B	0.39	0/3465	0.84	2/4695 (0.0%)
All	All	0.40	0/6872	0.84	8/9311 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	472	GLY	CA-C-N	9.79	129.84	119.76
1	A	472	GLY	C-N-CA	9.79	129.84	119.76
1	B	472	GLY	CA-C-N	9.63	129.68	119.76
1	B	472	GLY	C-N-CA	9.63	129.68	119.76
1	A	335	GLY	N-CA-C	5.94	119.81	110.96
1	A	456	ALA	N-CA-C	-5.41	102.99	110.35
1	A	336	GLY	N-CA-C	5.40	120.79	110.86
1	A	389	ARG	CB-CA-C	-5.21	110.55	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3322	0	3088	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3379	0	3144	28	0
2	A	32	0	47	2	0
2	B	91	0	135	7	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	66	0	102	4	0
5	A	19	0	0	0	0
5	B	30	0	0	0	0
All	All	6941	0	6516	57	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 4.

All (57) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:GLU:HB3	2:B:1493:78M:H91C	1.72	0.71
1:A:362:ARG:NH1	1:A:452:ASP:OD1	2.26	0.68
1:B:40:LYS:HE2	1:B:42:PHE:O	1.94	0.67
1:B:92:ALA:HB1	2:B:1492:78M:H21C	1.79	0.64
1:B:453:GLU:O	1:B:489:ARG:NH2	2.29	0.63
1:A:88:PHE:HB2	4:A:1496:78N:H2	1.81	0.61
1:B:275:TRP:CZ2	1:B:315:GLY:HA3	2.36	0.61
1:A:275:TRP:CZ2	1:A:315:GLY:HA3	2.36	0.60
1:B:74:ARG:NH2	1:B:102:ASP:OD1	2.34	0.60
1:A:362:ARG:HD2	1:A:451:VAL:HG22	1.85	0.59
1:B:373:GLU:HB2	1:B:412:THR:HB	1.87	0.57
1:A:47:LYS:NZ	1:A:101:THR:O	2.30	0.56
1:B:275:TRP:CE2	1:B:315:GLY:HA3	2.42	0.54
1:A:275:TRP:CE2	1:A:315:GLY:HA3	2.43	0.54
1:A:45:ASP:HB2	1:A:74:ARG:HB2	1.90	0.52
1:B:45:ASP:HB2	1:B:74:ARG:HB2	1.91	0.52
1:A:373:GLU:HB2	1:A:412:THR:HB	1.91	0.52
1:A:162:ASP:OD2	1:A:362:ARG:NH2	2.42	0.52
1:B:237:PRO:HG3	1:B:301:GLY:HA2	1.90	0.51
1:B:162:ASP:OD2	1:B:362:ARG:NH2	2.44	0.51
1:B:251:GLN:O	1:B:251:GLN:HG3	2.10	0.50
1:A:251:GLN:O	1:A:251:GLN:HG3	2.11	0.50
1:B:81:TRP:HE1	2:B:1498:78M:H202	1.77	0.49
1:A:410:ILE:HG21	1:A:426:ILE:HD11	1.94	0.48
1:A:326:ALA:HB3	2:A:1492:78M:H92C	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:PHE:HB2	1:A:456:ALA:HB3	1.96	0.48
1:A:40:LYS:HE2	1:A:42:PHE:O	2.14	0.48
1:A:74:ARG:HH22	1:A:102:ASP:HB2	1.80	0.47
1:A:200:GLU:H	1:A:200:GLU:CD	2.23	0.47
1:A:54:ASN:HA	1:A:55:ASP:HA	1.75	0.46
1:B:438:PHE:HB2	1:B:456:ALA:HB3	1.96	0.46
1:B:318:TRP:CD1	2:B:1491:78M:H41C	2.50	0.46
1:A:74:ARG:NH2	1:A:102:ASP:HB2	2.30	0.46
1:A:238:GLY:HA2	1:A:298:ILE:HD11	1.97	0.46
4:A:1495:78N:H121	4:A:1495:78N:H91C	1.64	0.46
1:B:200:GLU:H	1:B:200:GLU:CD	2.23	0.45
1:B:87:TYR:OH	1:B:449:GLN:NE2	2.34	0.45
1:A:148:PHE:CE1	2:A:1491:78M:H51C	2.51	0.45
1:B:328:VAL:HG23	2:B:1497:78M:H8	1.99	0.45
1:A:257:ILE:HG12	1:A:258:GLU:N	2.33	0.44
1:B:257:ILE:HG12	1:B:258:GLU:N	2.33	0.43
1:A:68:ASP:OD2	1:A:97:ASP:HB2	2.19	0.43
1:B:410:ILE:HG21	1:B:426:ILE:HD11	1.99	0.43
1:A:464:LEU:HB2	4:A:1495:78N:H92C	2.01	0.43
2:B:1497:78M:H62C	2:B:1497:78M:H91C	1.59	0.43
1:B:76:TRP:CH2	1:B:447:MET:HE1	2.55	0.42
1:B:152:ARG:NH2	1:B:451:VAL:HG11	2.34	0.42
1:B:156:ASP:HB3	1:B:264:TYR:CD2	2.55	0.42
1:A:156:ASP:HB3	1:A:264:TYR:CD2	2.55	0.42
1:B:434:VAL:HG12	2:B:1494:78M:H51C	2.01	0.41
1:B:327:GLY:HA3	1:B:383:PHE:CZ	2.55	0.41
1:B:68:ASP:OD2	1:B:97:ASP:HB2	2.21	0.41
1:B:441:GLY:O	1:B:455:SER:HA	2.20	0.41
1:A:441:GLY:O	1:A:455:SER:HA	2.22	0.40
1:B:373:GLU:CB	1:B:412:THR:HB	2.50	0.40
1:A:453:GLU:HG2	1:A:487:ILE:HD13	2.03	0.40
1:A:432:LEU:HB2	4:A:1495:78N:H112	2.03	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	408/458 (89%)	395 (97%)	13 (3%)	0	100	100
1	B	415/458 (91%)	404 (97%)	11 (3%)	0	100	100
All	All	823/916 (90%)	799 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	337/370 (91%)	333 (99%)	4 (1%)	63	87
1	B	344/370 (93%)	340 (99%)	4 (1%)	63	87
All	All	681/740 (92%)	673 (99%)	8 (1%)	63	87

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	LEU
1	A	257	ILE
1	A	322	GLU
1	A	412	THR
1	B	102	ASP
1	B	104	LEU
1	B	177	LEU
1	B	257	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN

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Mol	Chain	Res	Type
1	A	169	ASN
1	A	178	ASN
1	A	323	GLN
1	A	428	GLN
1	B	67	ASN
1	B	161	GLN
1	B	178	ASN
1	B	323	GLN

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 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	78N	A	1496	-	21,21,21	1.01	1 (4%)	22,22,22	1.02	1 (4%)
2	78M	B	1498	-	21,21,21	0.99	1 (4%)	22,22,22	0.97	1 (4%)
2	78M	A	1493	-	12,12,21	1.35	2 (16%)	11,11,22	0.90	1 (9%)
2	78M	B	1495	-	11,11,21	1.37	2 (18%)	10,10,22	0.86	0
4	78N	A	1495	-	21,21,21	1.01	1 (4%)	22,22,22	0.96	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	78M	B	1493	-	10,10,21	0.28	0	9,9,22	0.53	0
2	78M	A	1491	-	7,7,21	2.01	2 (28%)	6,6,22	1.31	0
2	78M	A	1492	-	10,10,21	1.47	2 (20%)	9,9,22	0.88	1 (11%)
2	78M	B	1491	-	8,8,21	1.96	2 (25%)	7,7,22	1.61	3 (42%)
2	78M	B	1492	-	7,7,21	1.99	2 (28%)	6,6,22	1.22	1 (16%)
2	78M	B	1497	-	21,21,21	1.02	1 (4%)	22,22,22	1.15	2 (9%)
4	78N	A	1497	-	21,21,21	1.00	1 (4%)	22,22,22	0.93	1 (4%)
2	78M	B	1494	-	6,6,21	0.25	0	5,5,22	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	78N	A	1496	-	-	11/21/21/21	-
2	78M	B	1498	-	-	6/21/21/21	-
2	78M	A	1493	-	-	6/10/10/21	-
2	78M	B	1495	-	-	5/9/9/21	-
4	78N	A	1495	-	-	7/21/21/21	-
2	78M	B	1493	-	-	2/8/8/21	-
2	78M	A	1491	-	-	4/5/5/21	-
2	78M	A	1492	-	-	4/8/8/21	-
2	78M	B	1491	-	-	1/6/6/21	-
2	78M	B	1492	-	-	1/5/5/21	-
2	78M	B	1497	-	-	8/21/21/21	-
4	78N	A	1497	-	-	8/21/21/21	-
2	78M	B	1494	-	-	2/4/4/21	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1497	78M	O2-C1	4.46	1.46	1.33
2	B	1491	78M	C5-C6	-4.43	1.33	1.52
4	A	1496	78N	O16-C8	4.42	1.46	1.33
4	A	1495	78N	O16-C8	4.39	1.46	1.33
4	A	1497	78N	O16-C8	4.32	1.45	1.33
2	B	1498	78M	O2-C1	4.31	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1491	78M	C8-C7	3.73	1.53	1.29
2	B	1492	78M	C8-C7	3.69	1.52	1.29
2	B	1492	78M	C5-C4	-3.68	1.33	1.51
2	A	1491	78M	C5-C4	-3.67	1.33	1.51
2	A	1492	78M	C8-C7	3.48	1.51	1.31
2	A	1493	78M	C8-C7	3.47	1.51	1.31
2	B	1495	78M	C8-C7	3.36	1.50	1.31
2	B	1491	78M	C7-C8	3.18	1.52	1.29
2	A	1493	78M	C9-C8	-3.00	1.33	1.50
2	A	1492	78M	C9-C8	-2.96	1.33	1.50
2	B	1495	78M	C9-C8	-2.92	1.34	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1497	78M	O2-C1-C2	3.60	122.83	111.83
4	A	1495	78N	O16-C8-C7	3.02	121.04	111.83
4	A	1496	78N	O16-C8-C7	2.97	120.90	111.83
2	B	1498	78M	O2-C1-C2	2.92	120.73	111.83
4	A	1497	78N	O16-C8-C7	2.61	119.78	111.83
2	B	1491	78M	C6-C7-C8	-2.31	112.96	130.48
2	B	1491	78M	C9-C8-C7	-2.19	109.29	126.43
2	B	1491	78M	C4-C5-C6	2.15	124.21	113.86
2	B	1492	78M	C6-C7-C8	-2.14	111.08	126.65
2	A	1493	78M	C6-C7-C8	-2.06	109.37	124.83
2	B	1497	78M	O2-C1-O1	-2.05	118.50	123.63
2	A	1492	78M	C6-C7-C8	-2.00	109.82	124.83

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1497	78M	O2-C17-C18-O19
2	B	1498	78M	O2-C17-C18-O19
4	A	1496	78N	O16-C17-C18-O20
2	B	1498	78M	O1-C1-O2-C17
4	A	1495	78N	O15-C8-O16-C17
2	B	1498	78M	C2-C1-O2-C17
4	A	1495	78N	C7-C8-O16-C17
2	B	1497	78M	C2-C1-O2-C17
4	A	1496	78N	O15-C8-O16-C17
2	A	1491	78M	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	B	1497	78M	O1-C1-O2-C17
4	A	1496	78N	C7-C8-O16-C17
4	A	1495	78N	C9-C10-C11-C12
2	B	1498	78M	O2-C17-C18-C20
2	A	1493	78M	C6-C7-C8-C9
2	B	1497	78M	O2-C17-C18-C20
4	A	1496	78N	O16-C17-C18-C19
2	B	1498	78M	C17-C18-C20-O21
4	A	1496	78N	C17-C18-C19-O22
2	B	1497	78M	C11-C12-C13-C14
4	A	1495	78N	C5-C6-C7-C8
2	A	1493	78M	C3-C4-C5-C6
4	A	1497	78N	C9-C10-C11-C12
2	A	1493	78M	C2-C3-C4-C5
4	A	1495	78N	C2-C3-C4-C5
4	A	1497	78N	C4-C5-C6-C7
2	B	1495	78M	C2-C3-C4-C5
4	A	1495	78N	C11-C10-C9-C1
2	B	1497	78M	C3-C4-C5-C6
2	A	1491	78M	C1-C2-C3-C4
4	A	1496	78N	C5-C6-C7-C8
2	B	1497	78M	C10-C11-C12-C13
2	A	1491	78M	C2-C3-C4-C5
2	A	1492	78M	C2-C3-C4-C5
4	A	1497	78N	C11-C12-C13-C14
2	A	1493	78M	C10-C11-C12-C13
2	B	1494	78M	C3-C4-C5-C6
2	A	1493	78M	C1-C2-C3-C4
2	B	1495	78M	C11-C10-C9-C8
4	A	1497	78N	C3-C4-C5-C6
2	B	1492	78M	C4-C5-C6-C7
2	B	1495	78M	C1-C2-C3-C4
4	A	1496	78N	C10-C11-C12-C13
2	A	1492	78M	C7-C8-C9-C10
2	A	1492	78M	C3-C4-C5-C6
2	B	1498	78M	C7-C8-C9-C10
2	B	1495	78M	C7-C8-C9-C10
2	B	1497	78M	C17-C18-C20-O21
4	A	1495	78N	C2-C1-C9-C10
4	A	1497	78N	C6-C7-C8-O16
2	A	1492	78M	C5-C6-C7-C8
4	A	1497	78N	C2-C1-C9-C10

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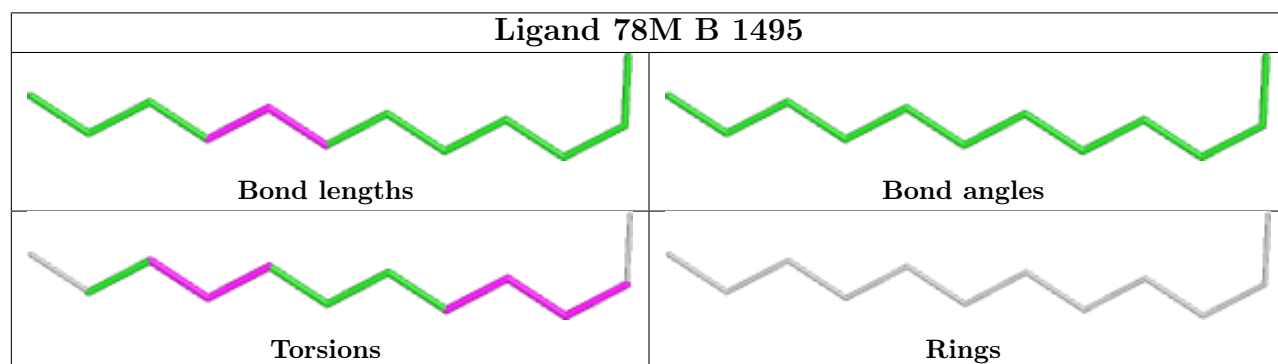
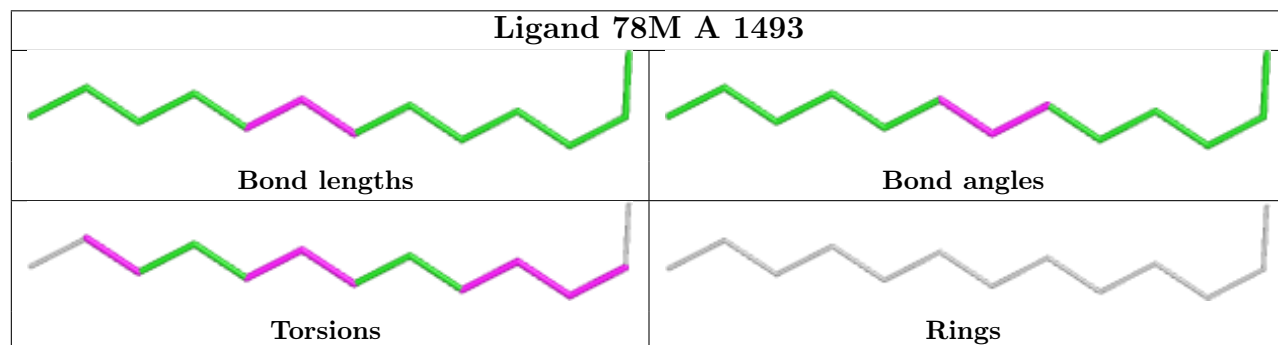
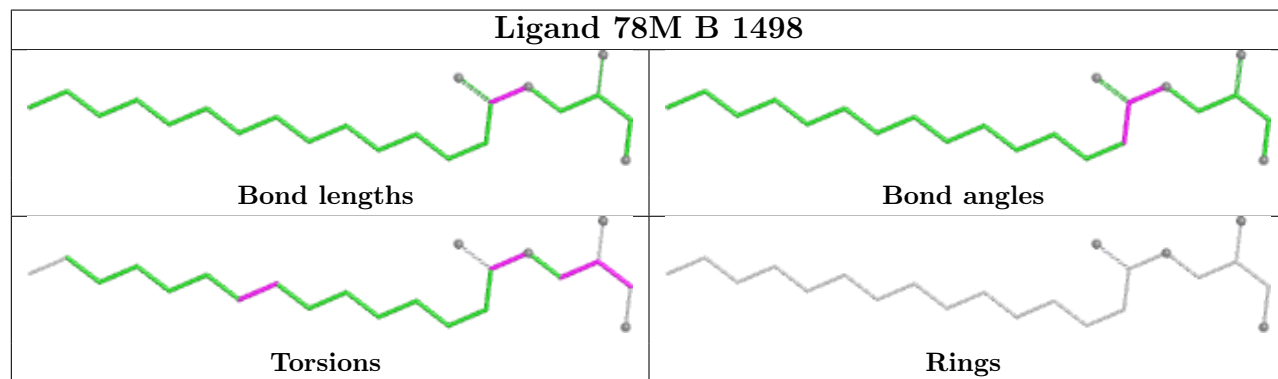
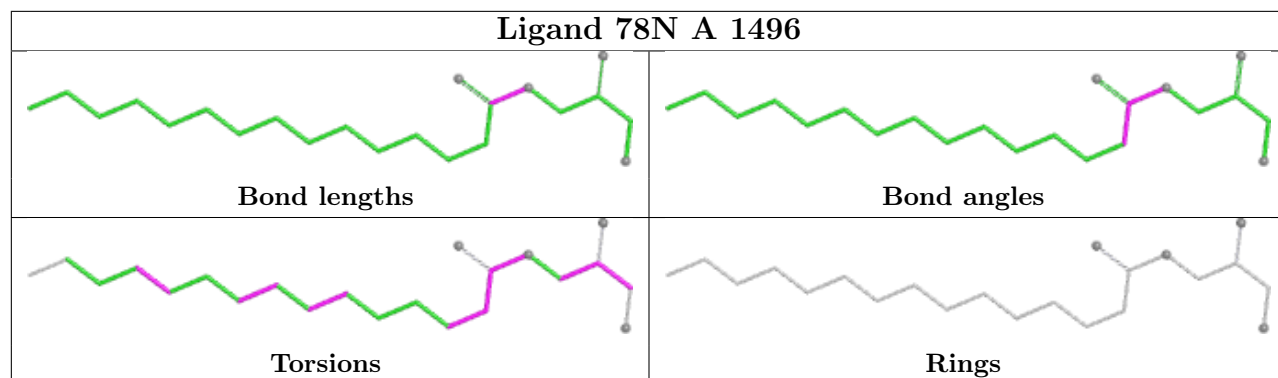
Mol	Chain	Res	Type	Atoms
4	A	1496	78N	C1-C2-C3-C4
2	A	1491	78M	C5-C6-C7-C8
2	B	1493	78M	C11-C10-C9-C8
4	A	1496	78N	O20-C18-C19-O22
4	A	1497	78N	C2-C3-C4-C5
2	B	1491	78M	C5-C6-C7-C8
4	A	1496	78N	C2-C1-C9-C10
2	B	1495	78M	C3-C4-C5-C6
2	B	1493	78M	C5-C6-C7-C8
2	B	1494	78M	C4-C5-C6-C7
4	A	1497	78N	C1-C2-C3-C4
2	A	1493	78M	C7-C8-C9-C10
4	A	1496	78N	C6-C7-C8-O16

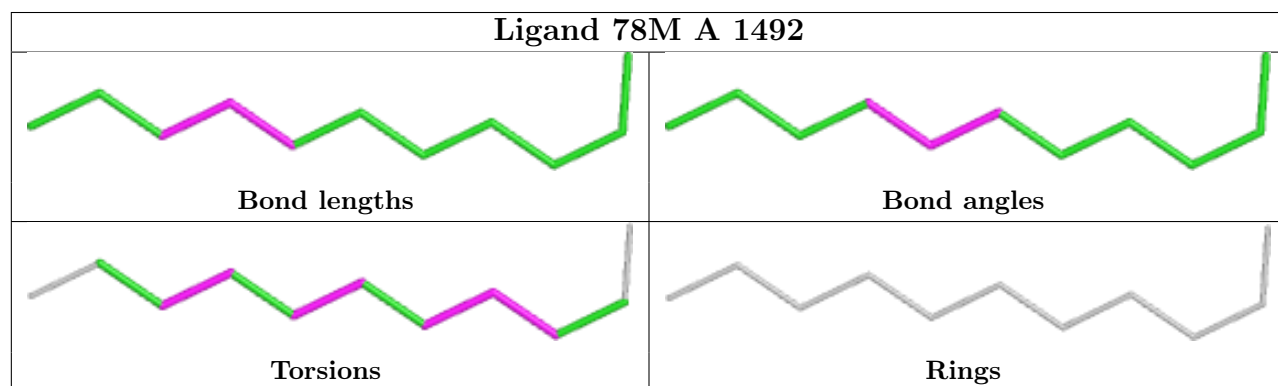
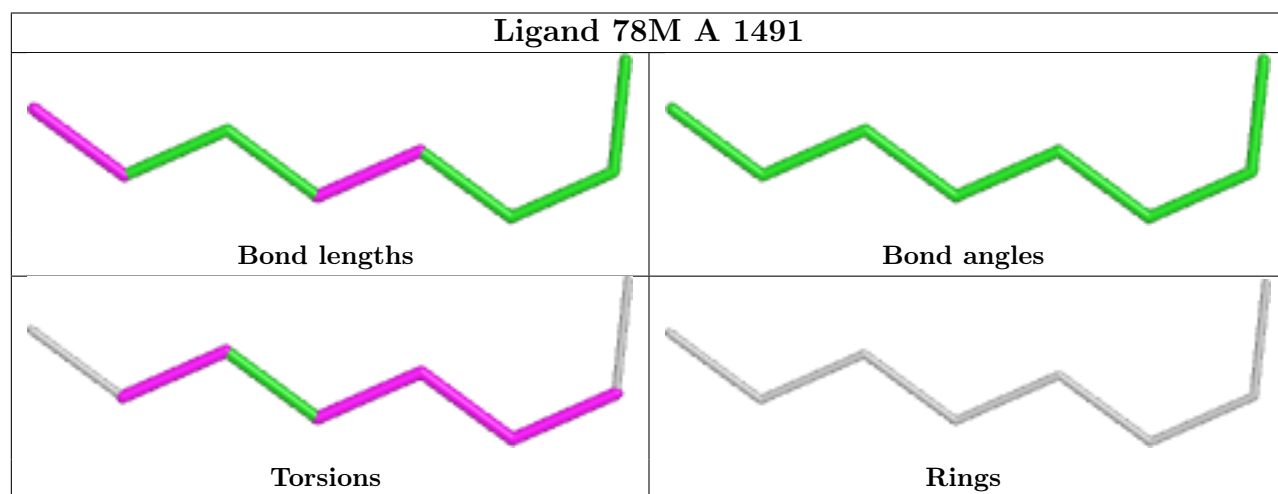
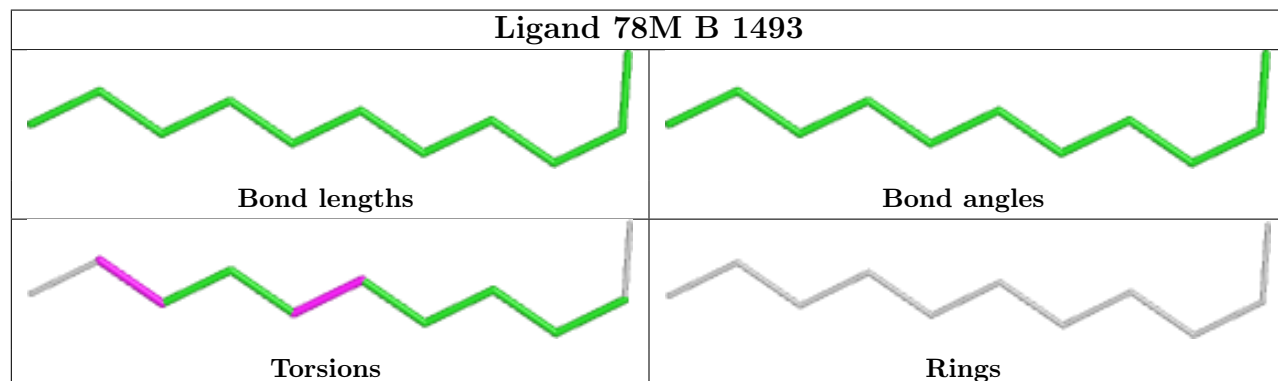
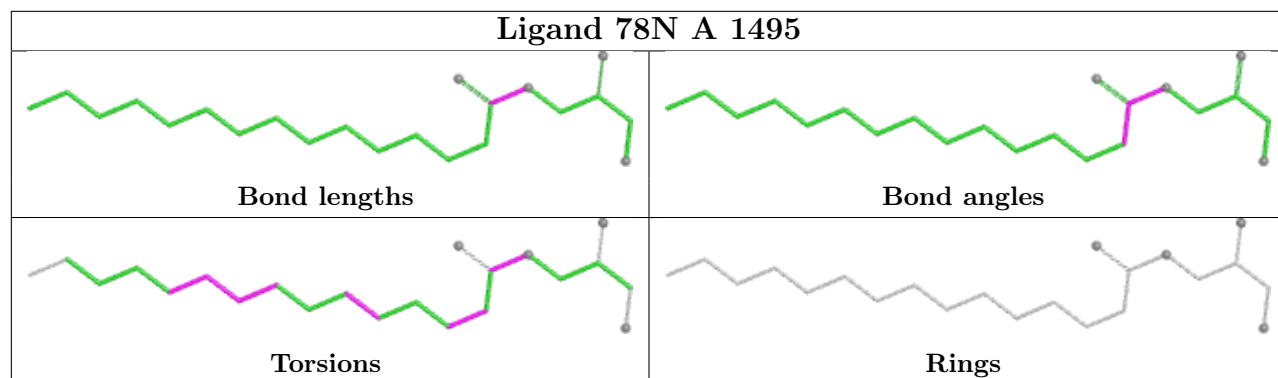
There are no ring outliers.

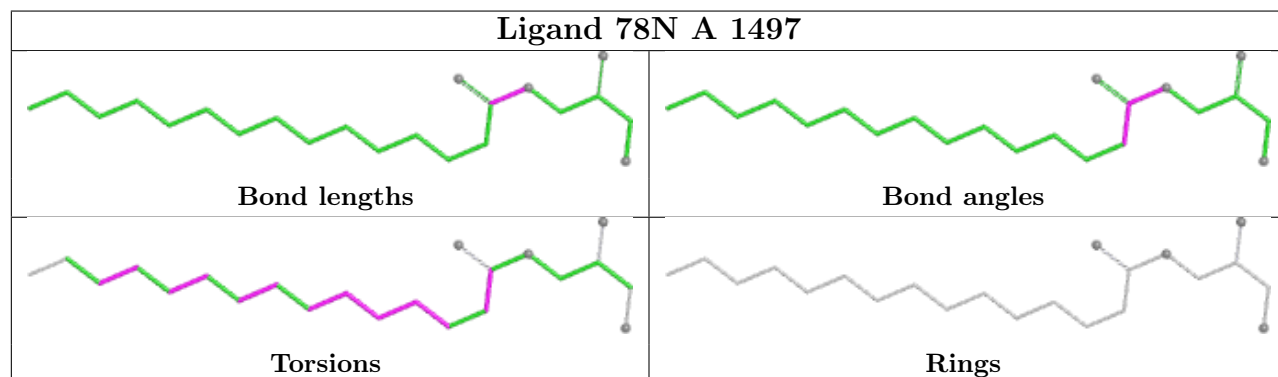
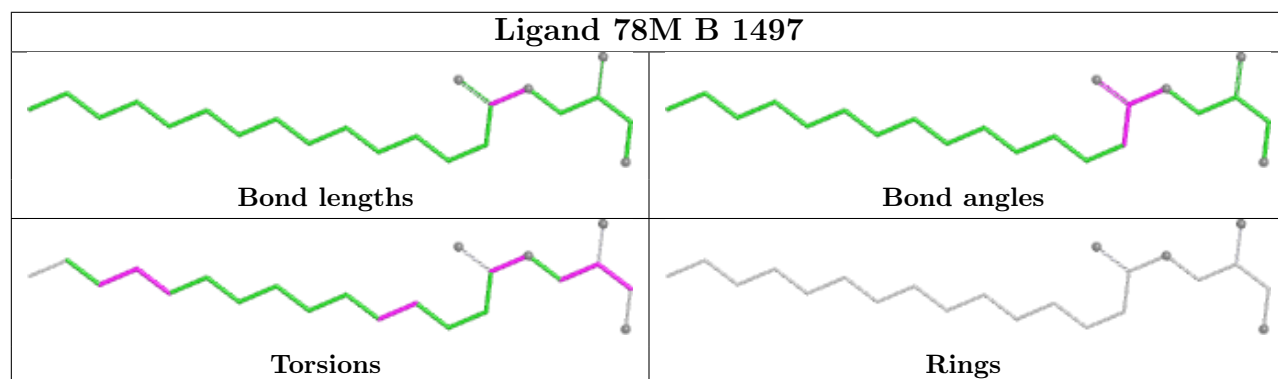
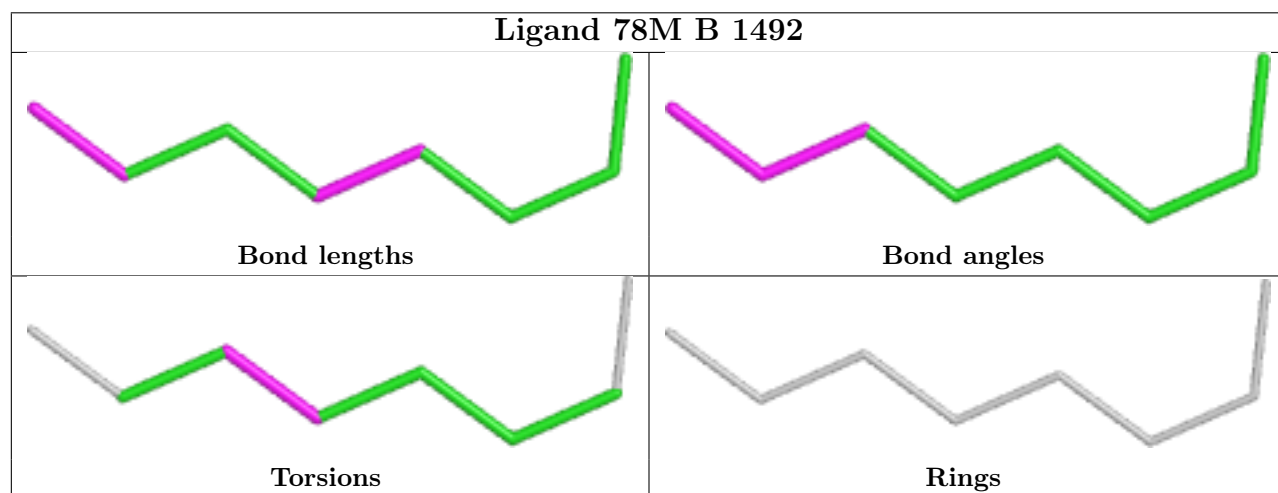
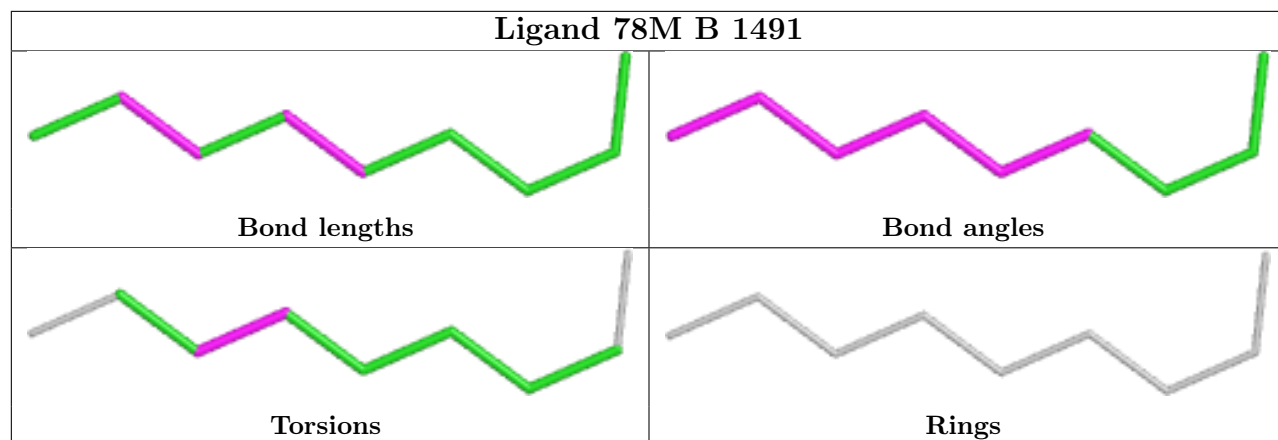
10 monomers are involved in 13 short contacts:

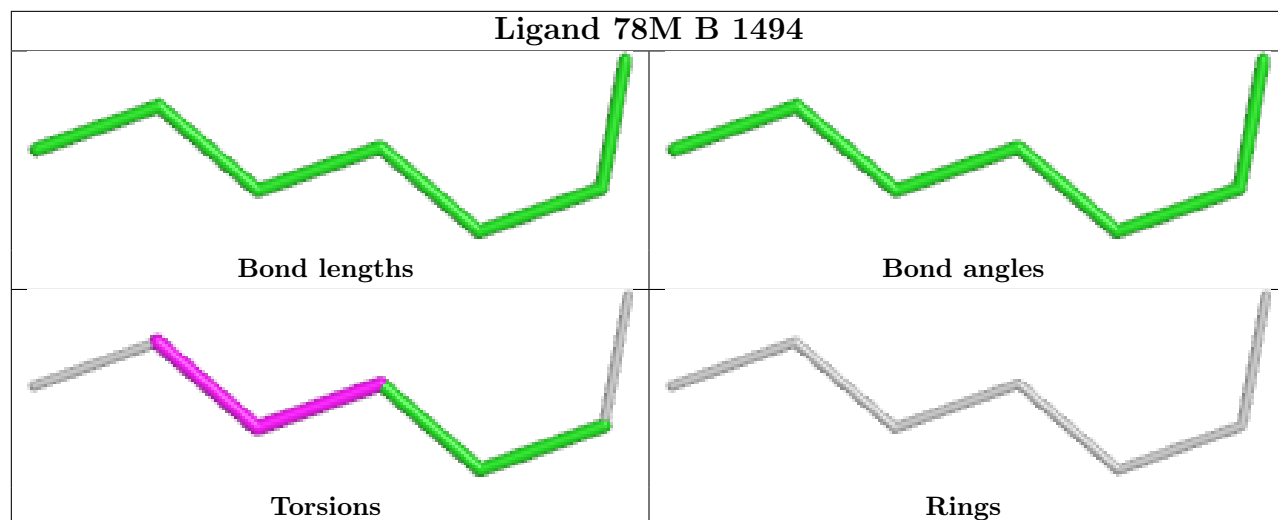
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1496	78N	1	0
2	B	1498	78M	1	0
4	A	1495	78N	3	0
2	B	1493	78M	1	0
2	A	1491	78M	1	0
2	A	1492	78M	1	0
2	B	1491	78M	1	0
2	B	1492	78M	1	0
2	B	1497	78M	2	0
2	B	1494	78M	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	418/458 (91%)	-1.41	0 100 100	7, 38, 91, 143	0
1	B	425/458 (92%)	-1.41	0 100 100	7, 39, 95, 174	0
All	All	843/916 (92%)	-1.41	0 100 100	7, 39, 94, 174	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

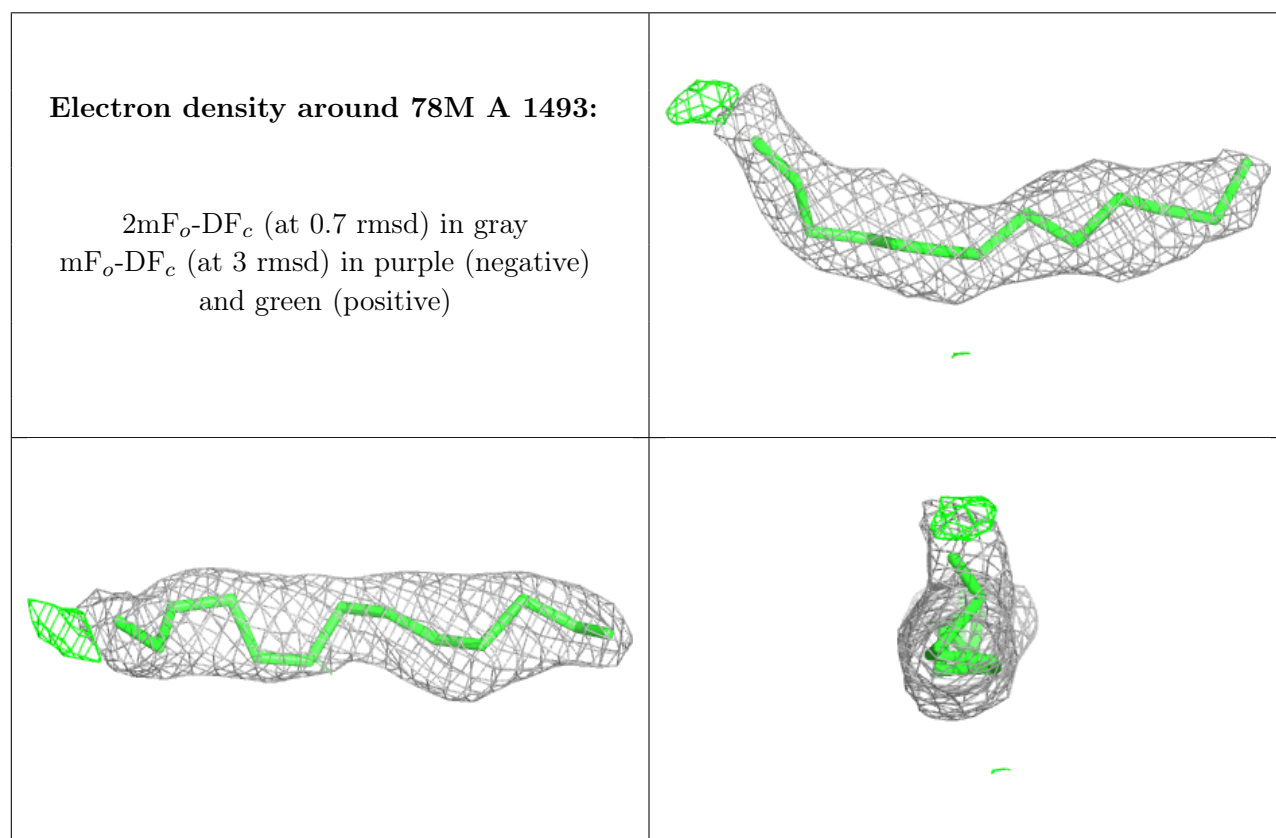
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	78M	A	1493	13/22	0.98	0.06	42,42,42,42	0
2	78M	B	1492	8/22	0.98	0.08	38,38,38,38	0
2	78M	B	1493	11/22	0.98	0.08	40,40,40,40	0
4	78N	A	1496	22/22	0.98	0.07	41,41,41,41	0
4	78N	A	1497	22/22	0.98	0.06	54,54,54,54	0
2	78M	A	1491	8/22	0.99	0.07	35,35,35,35	0
2	78M	B	1494	7/22	0.99	0.07	33,33,33,33	0

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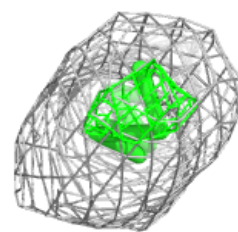
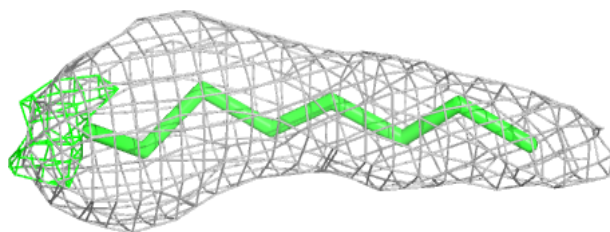
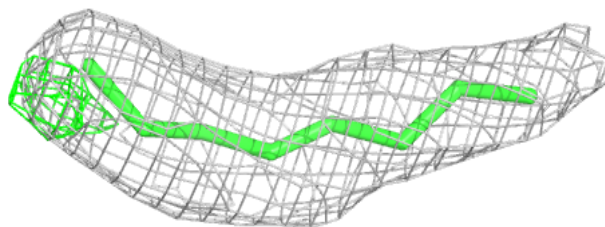
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	78M	B	1497	22/22	0.99	0.04	56,56,56,56	0
2	78M	B	1498	22/22	0.99	0.04	44,44,44,44	0
3	CA	A	1494	1/1	0.99	0.04	64,64,64,64	0
3	CA	B	1496	1/1	0.99	0.04	67,67,67,67	0
4	78N	A	1495	22/22	0.99	0.05	55,55,55,55	0
2	78M	B	1491	9/22	0.99	0.03	23,23,23,23	0
2	78M	A	1492	11/22	0.99	0.05	37,37,37,37	0
2	78M	B	1495	12/22	1.00	0.03	34,34,34,34	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.

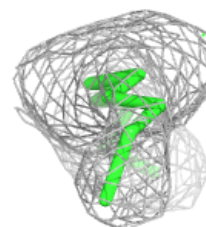
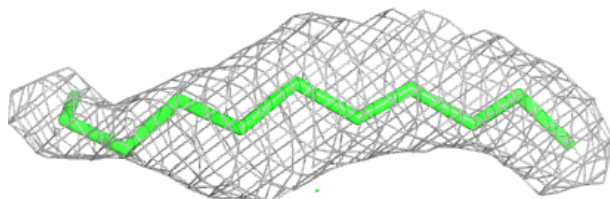
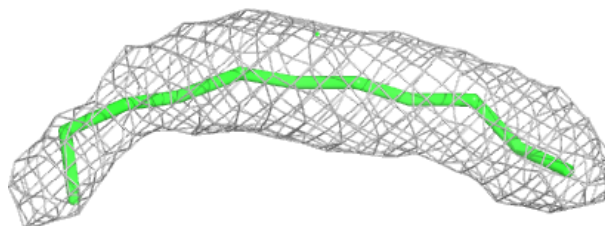


Electron density around 78M B 1492:

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

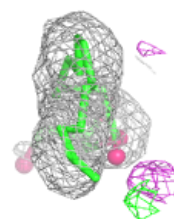
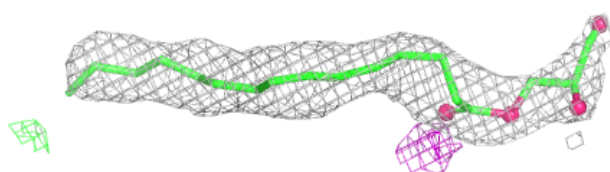
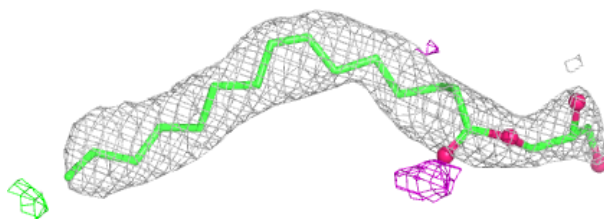
**Electron density around 78M B 1493:**

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

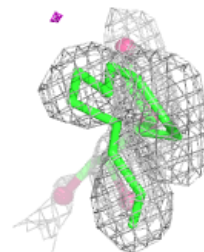
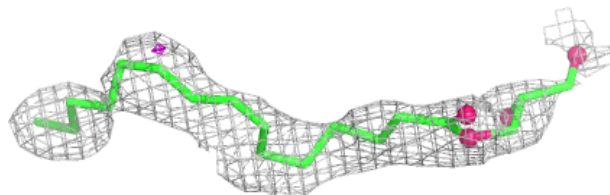
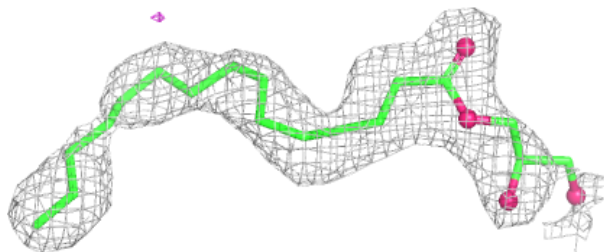


Electron density around 78N A 1496:

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

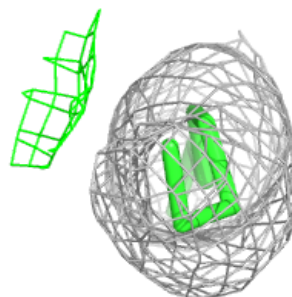
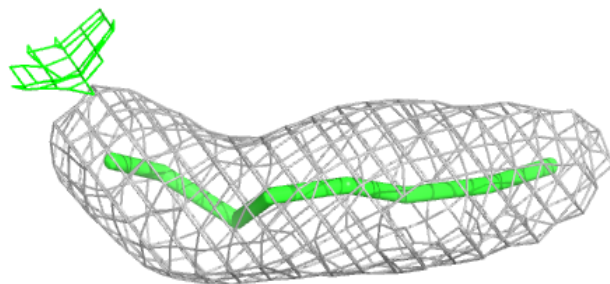
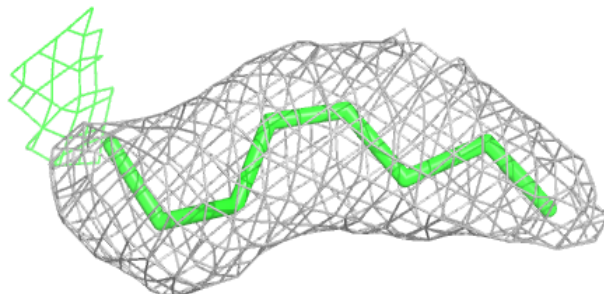
**Electron density around 78N A 1497:**

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

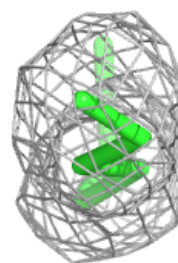
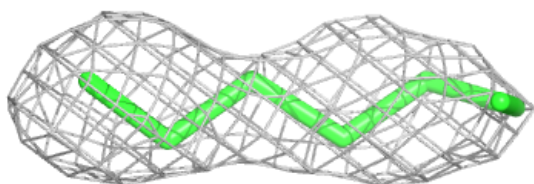
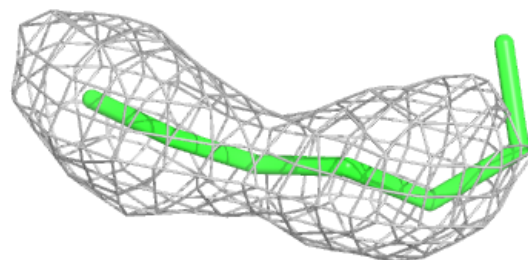


Electron density around 78M A 1491:

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

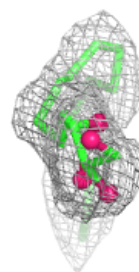
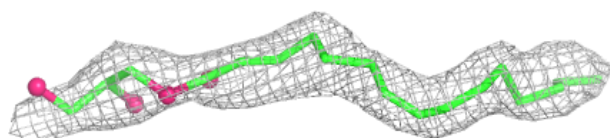
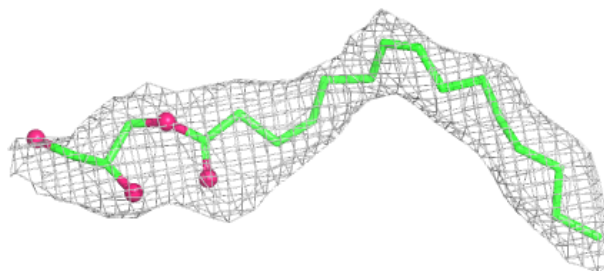
**Electron density around 78M B 1494:**

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and green (positive)

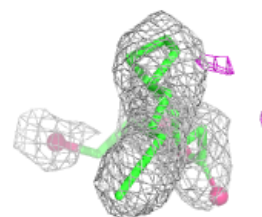
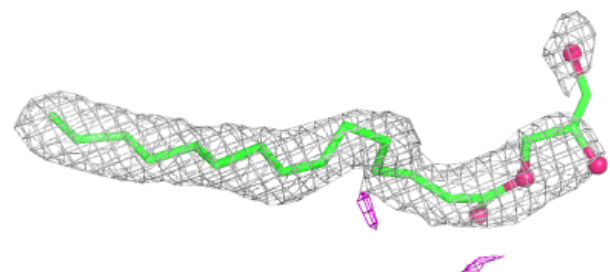
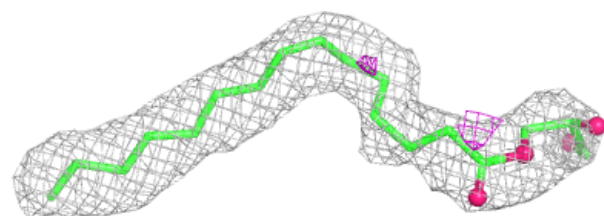


Electron density around 78M B 1497:

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and green (positive)

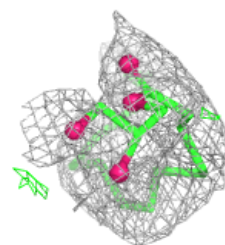
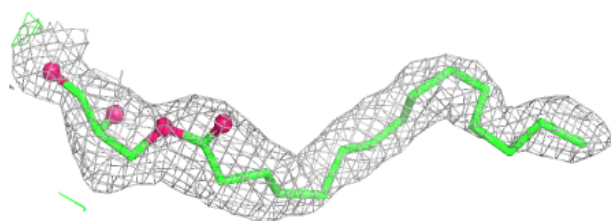
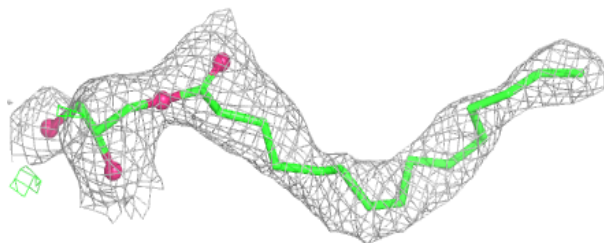
**Electron density around 78M B 1498:**

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

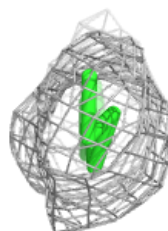
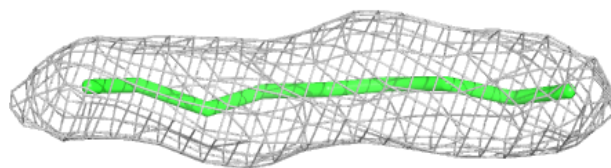
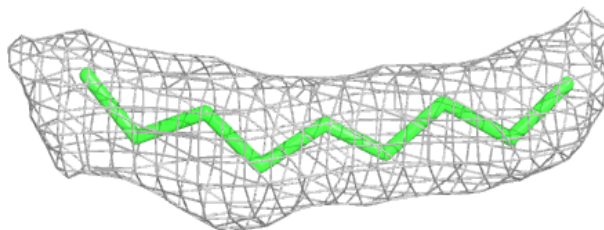


Electron density around 78N A 1495:

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and green (positive)

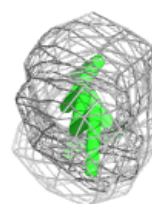
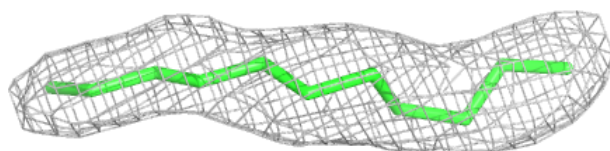
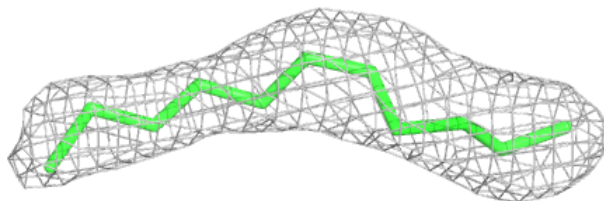
**Electron density around 78M B 1491:**

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

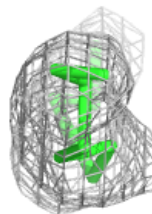
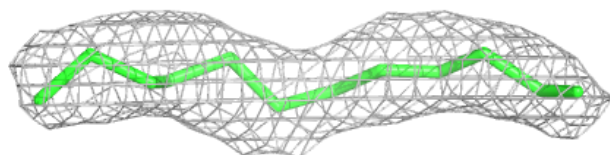
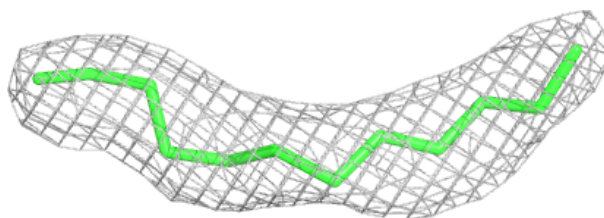


Electron density around 78M A 1492:

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

**Electron density around 78M B 1495:**

$2mF_o-DF_c$ (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.