



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:23 PM UTC

PDB ID : 5OXO / pdb_00005oxo
Title : PepTSt apo structure
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Deposited on : 2017-09-07
Resolution : 1.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

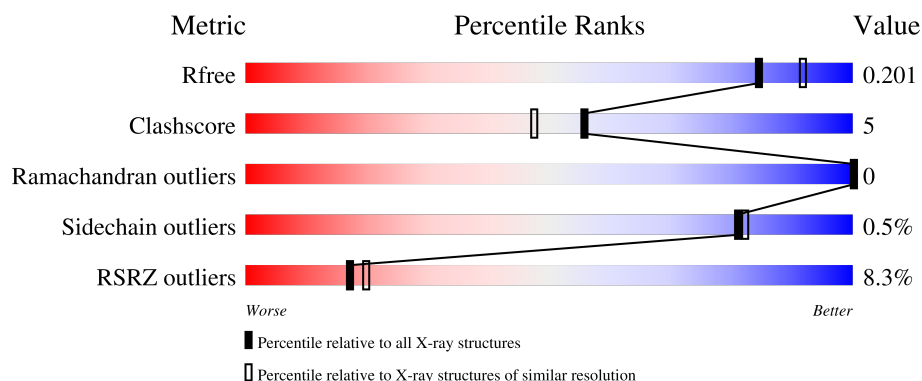
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	490	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4200 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 Di-or tripeptide:H⁺ symporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	6	0
			3546	2391	546	593	16			

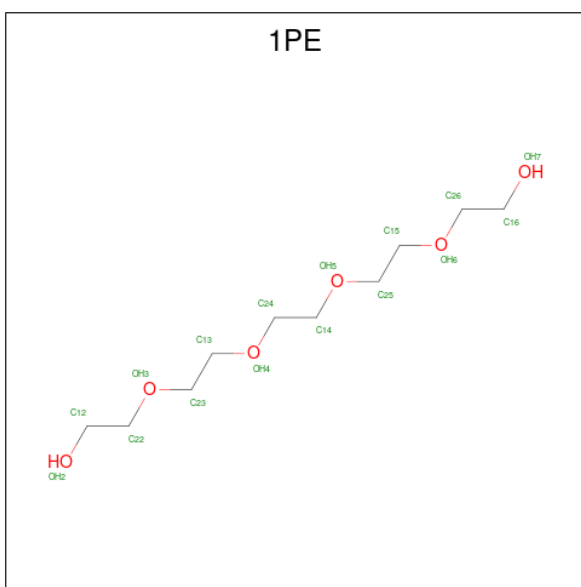
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	484	ALA	-	expression tag	UNP Q5M4H8
A	485	GLU	-	expression tag	UNP Q5M4H8
A	486	ASN	-	expression tag	UNP Q5M4H8
A	487	LEU	-	expression tag	UNP Q5M4H8
A	488	TYR	-	expression tag	UNP Q5M4H8
A	489	PHE	-	expression tag	UNP Q5M4H8
A	490	GLN	-	expression tag	UNP Q5M4H8

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

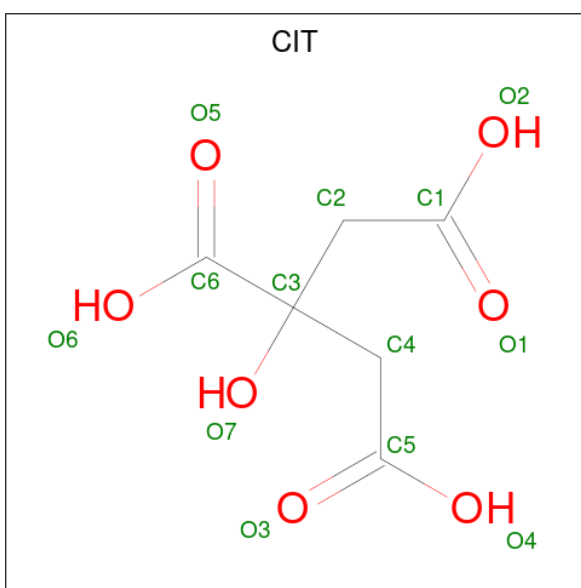
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		
3	A	1	Total	C	O	0	0
			10	6	4		

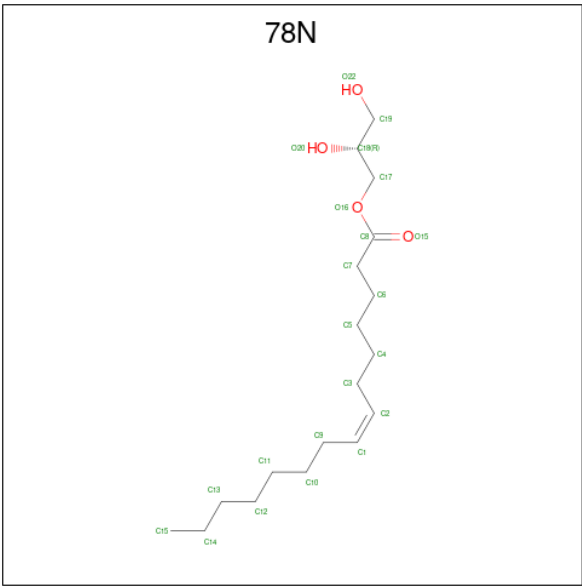
- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is (2R)-2,3-DIHYDROXYPROPYL(7Z)-PENTADEC-7-ENOATE (CCD ID:

78N) (formula: C₁₈H₃₄O₄).



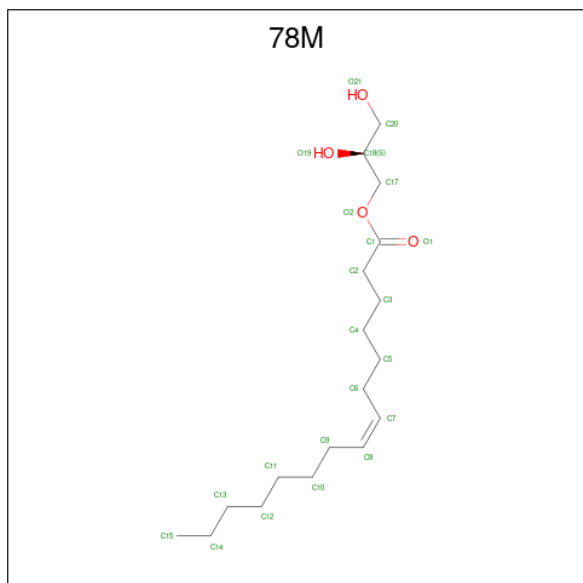
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			22	18	4		
5	A	1	Total	C	O	0	0
			22	18	4		
5	A	1	Total	C	O	0	0
			22	18	4		
5	A	1	Total	C	O	0	0
			22	18	4		
5	A	1	Total	C	O	0	0
			22	18	4		
5	A	1	Total	C	O	0	0
			22	18	4		
5	A	1	Total	C	O	0	0
			22	18	4		
5	A	1	Total	C	O	0	0
			22	18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

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

- Molecule 6 is (2S)-2,3-DIHYDROXYPROPYL(7Z)-PENTADEC-7-ENOATE (CCD ID: 78M) (formula: C₁₈H₃₄O₄).



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

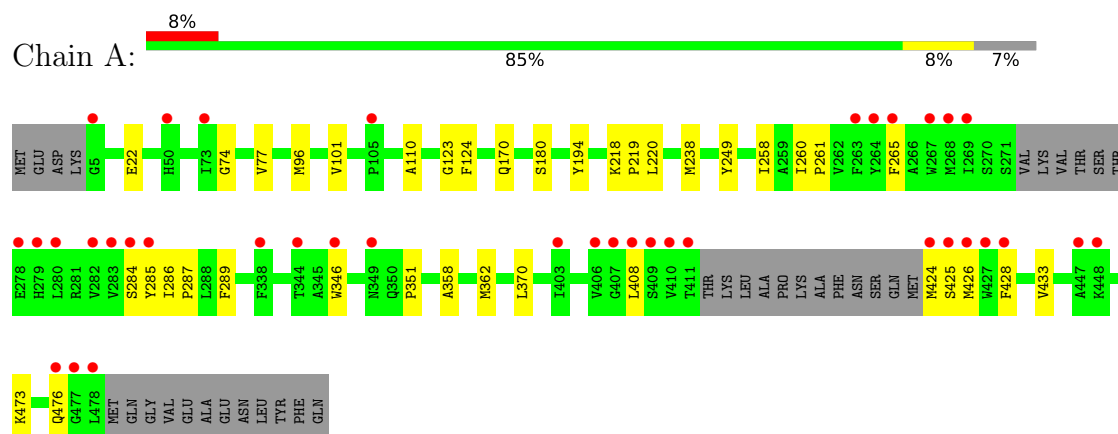
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	177	Total	O	0	0
			177	177		

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: Di- or tripeptide:H⁺ symporter



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	102.10Å 110.30Å 110.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.36 – 1.95 49.36 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.36-1.95) 99.6 (49.36-1.95)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.180 , 0.197 0.186 , 0.201	Depositor DCC
R_{free} test set	2283 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.1	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	0.96	EDS
Total number of atoms	4200	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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: 1PE, 78M, CIT, 78N, NA

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	0.40	0/3670	0.71	0/5005

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 [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	3546	0	3649	27	0
2	A	1	0	0	0	0
3	A	23	0	30	2	0
4	A	13	0	5	1	0
5	A	330	0	510	14	0
6	A	110	0	170	10	0
7	A	177	0	0	1	0
All	All	4200	0	4364	39	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 (39) 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)
5:A:508:78N:H122	6:A:509:78M:H101	1.71	0.70
5:A:505:78N:H1	5:A:507:78N:H1	1.73	0.69
1:A:170:GLN:HE22	3:A:502:1PE:H241	1.64	0.63
1:A:261:PRO:HG2	1:A:433:VAL:HG21	1.86	0.56
1:A:96:MET:HE1	6:A:519:78M:H62C	1.86	0.56
6:A:506:78M:H102	5:A:507:78N:H141	1.87	0.56
4:A:504:CIT:O6	7:A:601:HOH:O	2.18	0.54
1:A:473:LYS:HG2	5:A:524:78N:H192	1.91	0.52
1:A:249:TYR:HB3	5:A:515:78N:H41C	1.94	0.49
1:A:101[B]:VAL:HG12	1:A:110:ALA:HB1	1.95	0.49
1:A:425:SER:HA	1:A:428:PHE:HD1	1.79	0.48
1:A:180[B]:SER:OG	5:A:513:78N:H71	2.15	0.47
1:A:220:LEU:HG	5:A:522:78N:H2	1.96	0.47
1:A:258:ILE:O	1:A:261:PRO:HD2	2.15	0.47
5:A:505:78N:H1	5:A:507:78N:C1	2.43	0.46
1:A:260:ILE:HB	1:A:261:PRO:HD3	1.98	0.45
5:A:515:78N:H91C	5:A:515:78N:H32C	1.72	0.45
1:A:265:PHE:CZ	1:A:426:MET:HE1	2.52	0.45
1:A:358:ALA:O	1:A:362:MET:HG3	2.18	0.44
1:A:74:GLY:HA3	1:A:123:GLY:O	2.17	0.43
1:A:194:TYR:CZ	6:A:519:78M:H18	2.54	0.43
1:A:77:VAL:HG11	1:A:124:PHE:HE1	1.83	0.42
1:A:370:LEU:HD11	6:A:509:78M:H32C	2.01	0.42
1:A:96:MET:HE1	6:A:519:78M:C6	2.49	0.42
1:A:285:TYR:CE2	1:A:289:PHE:HB2	2.54	0.42
5:A:512:78N:H112	5:A:512:78N:H142	1.75	0.42
5:A:513:78N:H142	6:A:519:78M:H91C	2.02	0.42
1:A:286:ILE:HB	1:A:287:PRO:HD3	2.02	0.42
1:A:238:MET:HE3	5:A:516:78N:H71	2.02	0.42
1:A:96:MET:HE2	1:A:96:MET:HB3	1.87	0.42
1:A:218:LYS:HB3	1:A:219:PRO:HD3	2.01	0.42
5:A:512:78N:H62C	5:A:512:78N:H31C	1.83	0.42
6:A:518:78M:H112	6:A:518:78M:H8	1.53	0.42
1:A:284:SER:O	1:A:287:PRO:HD2	2.21	0.41
1:A:408:LEU:HD11	1:A:424:MET:HE3	2.02	0.41
1:A:170:GLN:NE2	3:A:502:1PE:H241	2.33	0.41
1:A:346:TRP:CZ2	1:A:351:PRO:HD3	2.56	0.41
5:A:508:78N:H18	6:A:509:78M:H18	2.03	0.41
6:A:521:78M:H8	6:A:521:78M:H112	1.73	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	456/490 (93%)	451 (99%)	5 (1%)	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	373/397 (94%)	371 (100%)	2 (0%)	81	82

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	476	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	A	350	GLN
1	A	476	GLN

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 ⓘ

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 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$
3	1PE	A	502	-	12,12,15	0.54	0	11,11,14	0.53	0
5	78N	A	515	-	21,21,21	0.95	1 (4%)	22,22,22	1.01	1 (4%)
5	78N	A	517	-	21,21,21	0.96	1 (4%)	22,22,22	0.96	1 (4%)
5	78N	A	508	-	21,21,21	0.94	1 (4%)	22,22,22	1.04	1 (4%)
6	78M	A	519	-	21,21,21	1.20	1 (4%)	22,22,22	0.94	1 (4%)
5	78N	A	516	-	21,21,21	0.96	1 (4%)	22,22,22	0.99	1 (4%)
6	78M	A	518	-	21,21,21	1.17	1 (4%)	22,22,22	0.96	1 (4%)
5	78N	A	511	-	21,21,21	0.96	1 (4%)	22,22,22	0.95	1 (4%)
5	78N	A	522	-	21,21,21	0.97	1 (4%)	22,22,22	0.92	1 (4%)
5	78N	A	523	-	21,21,21	0.95	1 (4%)	22,22,22	0.99	1 (4%)
5	78N	A	513	-	21,21,21	0.93	1 (4%)	22,22,22	0.99	1 (4%)
5	78N	A	507	-	21,21,21	0.96	1 (4%)	22,22,22	0.92	1 (4%)
4	CIT	A	504	-	12,12,12	1.32	0	17,17,17	1.32	1 (5%)
5	78N	A	510	-	21,21,21	0.96	1 (4%)	22,22,22	0.94	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	78M	A	521	-	21,21,21	1.17	1 (4%)	22,22,22	1.01	1 (4%)
5	78N	A	512	-	21,21,21	0.97	1 (4%)	22,22,22	1.01	1 (4%)
6	78M	A	506	-	21,21,21	1.17	1 (4%)	22,22,22	0.97	1 (4%)
3	1PE	A	503	-	9,9,15	0.58	0	8,8,14	0.48	0
6	78M	A	509	-	21,21,21	1.14	1 (4%)	22,22,22	0.88	1 (4%)
5	78N	A	524	-	21,21,21	0.96	1 (4%)	22,22,22	0.98	1 (4%)
5	78N	A	514	-	21,21,21	0.98	1 (4%)	22,22,22	0.99	1 (4%)
5	78N	A	520	-	21,21,21	0.94	1 (4%)	22,22,22	1.05	1 (4%)
5	78N	A	505	-	21,21,21	0.92	1 (4%)	22,22,22	1.06	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1PE	A	502	-	-	8/10/10/13	-
5	78N	A	515	-	-	11/21/21/21	-
5	78N	A	517	-	-	12/21/21/21	-
5	78N	A	508	-	-	12/21/21/21	-
6	78M	A	519	-	-	9/21/21/21	-
5	78N	A	516	-	-	8/21/21/21	-
6	78M	A	518	-	-	10/21/21/21	-
5	78N	A	511	-	-	11/21/21/21	-
5	78N	A	522	-	-	8/21/21/21	-
5	78N	A	523	-	-	15/21/21/21	-
5	78N	A	513	-	-	11/21/21/21	-
5	78N	A	507	-	-	8/21/21/21	-
4	CIT	A	504	-	-	0/16/16/16	-
5	78N	A	510	-	-	7/21/21/21	-
6	78M	A	521	-	-	12/21/21/21	-
5	78N	A	512	-	-	9/21/21/21	-
6	78M	A	506	-	-	11/21/21/21	-
3	1PE	A	503	-	-	4/7/7/13	-
6	78M	A	509	-	-	8/21/21/21	-
5	78N	A	524	-	-	12/21/21/21	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	78N	A	514	-	-	9/21/21/21	-
5	78N	A	520	-	-	4/21/21/21	-
5	78N	A	505	-	-	6/21/21/21	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	519	78M	O2-C1	3.37	1.43	1.33
6	A	506	78M	O2-C1	3.35	1.43	1.33
6	A	518	78M	O2-C1	3.35	1.43	1.33
6	A	521	78M	O2-C1	3.25	1.42	1.33
6	A	509	78M	O2-C1	3.21	1.42	1.33
5	A	514	78N	O16-C8	3.02	1.42	1.33
5	A	512	78N	O16-C8	3.02	1.42	1.33
5	A	517	78N	O16-C8	3.01	1.42	1.33
5	A	507	78N	O16-C8	3.00	1.42	1.33
5	A	522	78N	O16-C8	2.99	1.42	1.33
5	A	511	78N	O16-C8	2.98	1.42	1.33
5	A	510	78N	O16-C8	2.96	1.42	1.33
5	A	515	78N	O16-C8	2.95	1.42	1.33
5	A	523	78N	O16-C8	2.94	1.41	1.33
5	A	516	78N	O16-C8	2.92	1.41	1.33
5	A	524	78N	O16-C8	2.90	1.41	1.33
5	A	508	78N	O16-C8	2.89	1.41	1.33
5	A	520	78N	O16-C8	2.84	1.41	1.33
5	A	513	78N	O16-C8	2.79	1.41	1.33
5	A	505	78N	O16-C8	2.77	1.41	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	504	CIT	O6-C6-C3	3.39	119.65	113.14
6	A	521	78M	O2-C1-C2	3.01	121.01	111.83
5	A	508	78N	O16-C8-C7	2.98	120.91	111.83
5	A	514	78N	O16-C8-C7	2.88	120.62	111.83
5	A	512	78N	O16-C8-C7	2.88	120.62	111.83
6	A	519	78M	O2-C1-C2	2.84	120.50	111.83
6	A	506	78M	O2-C1-C2	2.84	120.50	111.83
5	A	516	78N	O16-C8-C7	2.80	120.39	111.83
5	A	520	78N	O16-C8-C7	2.77	120.28	111.83
5	A	524	78N	O16-C8-C7	2.74	120.20	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	515	78N	O16-C8-C7	2.73	120.15	111.83
5	A	523	78N	O16-C8-C7	2.73	120.15	111.83
6	A	518	78M	O2-C1-C2	2.70	120.07	111.83
5	A	517	78N	O16-C8-C7	2.66	119.94	111.83
5	A	511	78N	O16-C8-C7	2.65	119.92	111.83
6	A	509	78M	O2-C1-C2	2.62	119.81	111.83
5	A	505	78N	O16-C8-C7	2.59	119.72	111.83
5	A	510	78N	O16-C8-C7	2.58	119.69	111.83
5	A	522	78N	O16-C8-C7	2.56	119.65	111.83
5	A	513	78N	O16-C8-C7	2.51	119.48	111.83
5	A	507	78N	O16-C8-C7	2.47	119.38	111.83

There are no chirality outliers.

All (205) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	508	78N	C17-C18-C19-O22
5	A	511	78N	O16-C17-C18-C19
5	A	511	78N	O16-C17-C18-O20
5	A	512	78N	C17-C18-C19-O22
5	A	513	78N	O20-C18-C19-O22
5	A	513	78N	C17-C18-C19-O22
5	A	513	78N	O16-C17-C18-O20
5	A	514	78N	C17-C18-C19-O22
5	A	514	78N	O16-C17-C18-C19
5	A	514	78N	O16-C17-C18-O20
5	A	524	78N	C17-C18-C19-O22
6	A	509	78M	C17-C18-C20-O21
6	A	518	78M	O19-C18-C20-O21
6	A	518	78M	O2-C17-C18-O19
6	A	521	78M	O19-C18-C20-O21
6	A	521	78M	C17-C18-C20-O21
5	A	517	78N	O15-C8-O16-C17
5	A	517	78N	C7-C8-O16-C17
5	A	505	78N	O15-C8-O16-C17
5	A	513	78N	O15-C8-O16-C17
6	A	521	78M	O1-C1-O2-C17
5	A	513	78N	C7-C8-O16-C17
6	A	521	78M	C2-C1-O2-C17
5	A	505	78N	C7-C8-O16-C17
6	A	521	78M	O2-C17-C18-O19
3	A	502	1PE	OH4-C13-C23-OH3

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Mol	Chain	Res	Type	Atoms
5	A	508	78N	C7-C8-O16-C17
5	A	510	78N	O16-C17-C18-C19
5	A	512	78N	O16-C17-C18-C19
5	A	513	78N	O16-C17-C18-C19
5	A	522	78N	O16-C17-C18-C19
5	A	510	78N	O16-C17-C18-O20
5	A	512	78N	O20-C18-C19-O22
5	A	514	78N	O20-C18-C19-O22
6	A	509	78M	C1-C2-C3-C4
5	A	524	78N	C5-C6-C7-C8
3	A	502	1PE	OH2-C12-C22-OH3
5	A	512	78N	C5-C6-C7-C8
5	A	508	78N	O15-C8-O16-C17
5	A	523	78N	C7-C8-O16-C17
5	A	514	78N	C5-C6-C7-C8
5	A	523	78N	C5-C6-C7-C8
5	A	515	78N	O16-C17-C18-O20
5	A	522	78N	O16-C17-C18-O20
5	A	523	78N	O16-C17-C18-O20
3	A	502	1PE	OH6-C15-C25-OH5
5	A	515	78N	O16-C17-C18-C19
5	A	523	78N	O16-C17-C18-C19
6	A	518	78M	O2-C17-C18-C20
5	A	522	78N	C7-C8-O16-C17
5	A	507	78N	O16-C17-C18-O20
5	A	512	78N	O16-C17-C18-O20
6	A	519	78M	O2-C17-C18-O19
5	A	515	78N	C17-C18-C19-O22
5	A	517	78N	C17-C18-C19-O22
5	A	520	78N	C17-C18-C19-O22
5	A	523	78N	C17-C18-C19-O22
6	A	506	78M	C17-C18-C20-O21
6	A	518	78M	C17-C18-C20-O21
5	A	516	78N	C5-C6-C7-C8
5	A	523	78N	O15-C8-O16-C17
5	A	505	78N	C10-C11-C12-C13
6	A	509	78M	C3-C4-C5-C6
5	A	508	78N	O20-C18-C19-O22
5	A	524	78N	O20-C18-C19-O22
5	A	516	78N	C3-C4-C5-C6
6	A	509	78M	C9-C10-C11-C12
5	A	523	78N	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
5	A	523	78N	C11-C12-C13-C14
5	A	523	78N	C9-C10-C11-C12
3	A	503	1PE	OH5-C14-C24-OH4
5	A	511	78N	C10-C11-C12-C13
5	A	513	78N	C4-C5-C6-C7
5	A	515	78N	C4-C5-C6-C7
6	A	519	78M	C10-C11-C12-C13
5	A	514	78N	C11-C12-C13-C14
5	A	516	78N	C2-C3-C4-C5
5	A	514	78N	C3-C4-C5-C6
5	A	522	78N	O15-C8-O16-C17
5	A	517	78N	C10-C11-C12-C13
5	A	508	78N	C4-C5-C6-C7
5	A	512	78N	C4-C5-C6-C7
6	A	521	78M	C10-C11-C12-C13
5	A	511	78N	C7-C8-O16-C17
5	A	505	78N	C11-C12-C13-C14
6	A	506	78M	C10-C11-C12-C13
5	A	517	78N	C11-C10-C9-C1
6	A	519	78M	C4-C5-C6-C7
6	A	519	78M	C11-C10-C9-C8
5	A	510	78N	C4-C5-C6-C7
5	A	517	78N	C11-C12-C13-C14
5	A	507	78N	C9-C10-C11-C12
5	A	510	78N	C11-C12-C13-C14
6	A	518	78M	C2-C3-C4-C5
6	A	506	78M	C11-C12-C13-C14
5	A	511	78N	C11-C10-C9-C1
5	A	514	78N	C2-C3-C4-C5
5	A	523	78N	C11-C10-C9-C1
5	A	524	78N	C10-C11-C12-C13
5	A	517	78N	C9-C10-C11-C12
5	A	515	78N	O20-C18-C19-O22
6	A	509	78M	O19-C18-C20-O21
5	A	524	78N	C4-C5-C6-C7
5	A	511	78N	C2-C3-C4-C5
6	A	521	78M	C4-C5-C6-C7
5	A	511	78N	O15-C8-O16-C17
5	A	515	78N	C5-C6-C7-C8
5	A	517	78N	C2-C3-C4-C5
5	A	522	78N	C2-C3-C4-C5
5	A	522	78N	C11-C10-C9-C1

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Mol	Chain	Res	Type	Atoms
6	A	509	78M	C11-C10-C9-C8
6	A	518	78M	C4-C5-C6-C7
5	A	524	78N	C7-C8-O16-C17
5	A	522	78N	C3-C4-C5-C6
6	A	521	78M	C3-C4-C5-C6
5	A	515	78N	C10-C11-C12-C13
5	A	508	78N	C9-C10-C11-C12
5	A	523	78N	C3-C4-C5-C6
6	A	521	78M	C1-C2-C3-C4
5	A	520	78N	C10-C11-C12-C13
6	A	506	78M	C2-C1-O2-C17
5	A	524	78N	C12-C13-C14-C15
5	A	515	78N	C11-C12-C13-C14
6	A	519	78M	C2-C1-O2-C17
6	A	506	78M	O19-C18-C20-O21
6	A	509	78M	C2-C3-C4-C5
6	A	506	78M	C4-C5-C6-C7
6	A	518	78M	C11-C12-C13-C14
5	A	524	78N	O15-C8-O16-C17
6	A	518	78M	C11-C10-C9-C8
6	A	506	78M	C12-C13-C14-C15
5	A	507	78N	C3-C4-C5-C6
6	A	506	78M	C1-C2-C3-C4
5	A	510	78N	C12-C13-C14-C15
5	A	510	78N	C11-C10-C9-C1
5	A	515	78N	C7-C8-O16-C17
5	A	507	78N	C11-C12-C13-C14
6	A	506	78M	O1-C1-O2-C17
5	A	524	78N	O16-C17-C18-C19
5	A	524	78N	O16-C17-C18-O20
5	A	507	78N	O20-C18-C19-O22
5	A	523	78N	O20-C18-C19-O22
6	A	519	78M	C2-C3-C4-C5
3	A	503	1PE	C16-C26-OH6-C15
5	A	523	78N	C12-C13-C14-C15
6	A	518	78M	C3-C4-C5-C6
5	A	511	78N	C5-C6-C7-C8
5	A	505	78N	C11-C10-C9-C1
5	A	517	78N	C12-C13-C14-C15
6	A	519	78M	O1-C1-O2-C17
5	A	511	78N	C11-C12-C13-C14
5	A	515	78N	O15-C8-O16-C17

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Mol	Chain	Res	Type	Atoms
5	A	514	78N	C12-C13-C14-C15
5	A	516	78N	C10-C11-C12-C13
6	A	521	78M	C9-C10-C11-C12
5	A	522	78N	C9-C10-C11-C12
5	A	524	78N	C11-C12-C13-C14
5	A	516	78N	O16-C17-C18-C19
5	A	516	78N	C9-C10-C11-C12
5	A	508	78N	C12-C13-C14-C15
6	A	519	78M	C11-C12-C13-C14
5	A	517	78N	O20-C18-C19-O22
3	A	502	1PE	OH5-C14-C24-OH4
3	A	503	1PE	C24-C14-OH5-C25
5	A	520	78N	C11-C12-C13-C14
3	A	502	1PE	C15-C25-OH5-C14
5	A	508	78N	C11-C10-C9-C1
5	A	508	78N	O16-C17-C18-O20
6	A	521	78M	O2-C17-C18-C20
5	A	515	78N	C3-C4-C5-C6
5	A	513	78N	C2-C1-C9-C10
3	A	502	1PE	C24-C14-OH5-C25
5	A	520	78N	C6-C7-C8-O16
5	A	523	78N	C10-C11-C12-C13
5	A	516	78N	O16-C17-C18-O20
3	A	502	1PE	C23-C13-OH4-C24
5	A	512	78N	C3-C4-C5-C6
5	A	507	78N	C11-C10-C9-C1
3	A	502	1PE	C14-C24-OH4-C13
5	A	517	78N	C2-C1-C9-C10
5	A	505	78N	C9-C10-C11-C12
5	A	511	78N	C9-C10-C11-C12
5	A	508	78N	C1-C2-C3-C4
3	A	503	1PE	OH6-C15-C25-OH5
5	A	523	78N	C2-C1-C9-C10
5	A	524	78N	C1-C2-C3-C4
6	A	506	78M	C7-C8-C9-C10
5	A	513	78N	C5-C6-C7-C8
5	A	507	78N	C1-C2-C3-C4
5	A	507	78N	C2-C1-C9-C10
5	A	508	78N	C2-C3-C4-C5
5	A	512	78N	C12-C13-C14-C15
5	A	508	78N	C2-C1-C9-C10
5	A	510	78N	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
5	A	511	78N	C1-C2-C3-C4
6	A	506	78M	C5-C6-C7-C8
6	A	519	78M	C7-C8-C9-C10
5	A	512	78N	C1-C2-C3-C4
5	A	516	78N	C1-C2-C3-C4
6	A	521	78M	C7-C8-C9-C10
6	A	509	78M	C12-C13-C14-C15
5	A	513	78N	C6-C7-C8-O16
5	A	513	78N	C6-C7-C8-O15
5	A	517	78N	C6-C7-C8-O16
6	A	518	78M	C7-C8-C9-C10

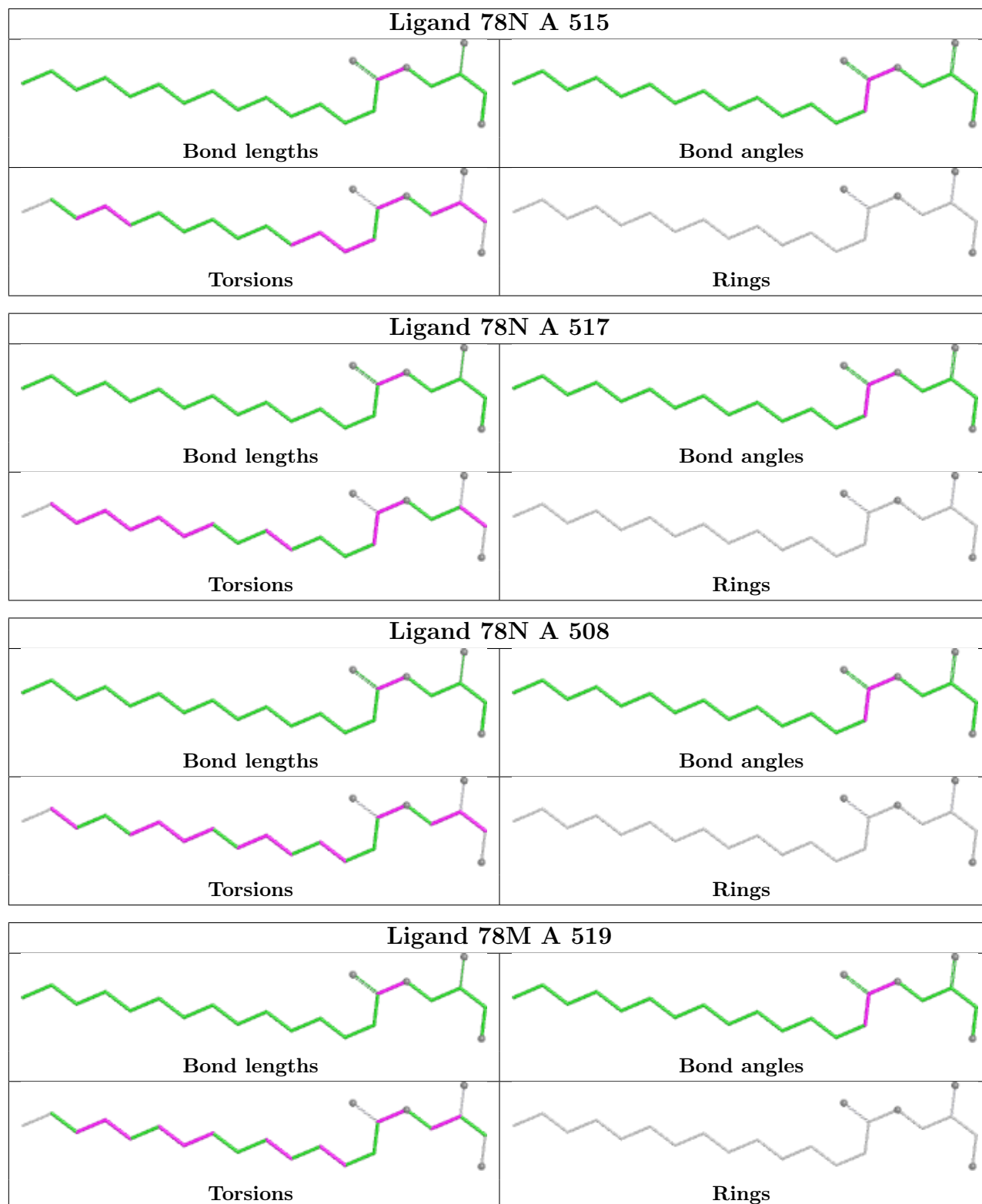
There are no ring outliers.

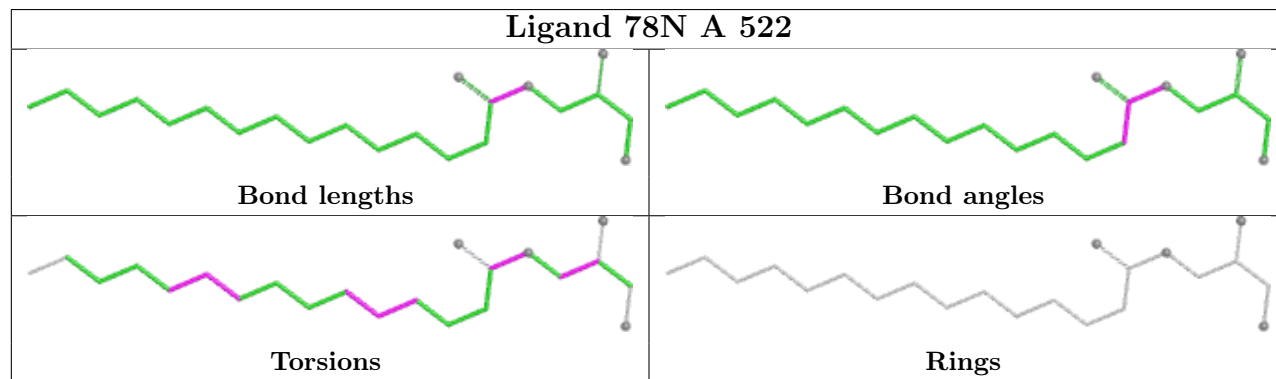
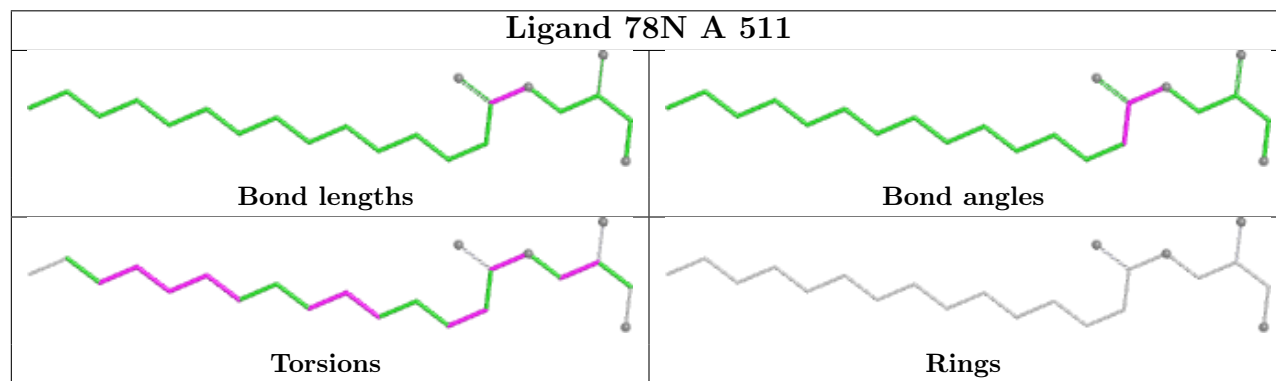
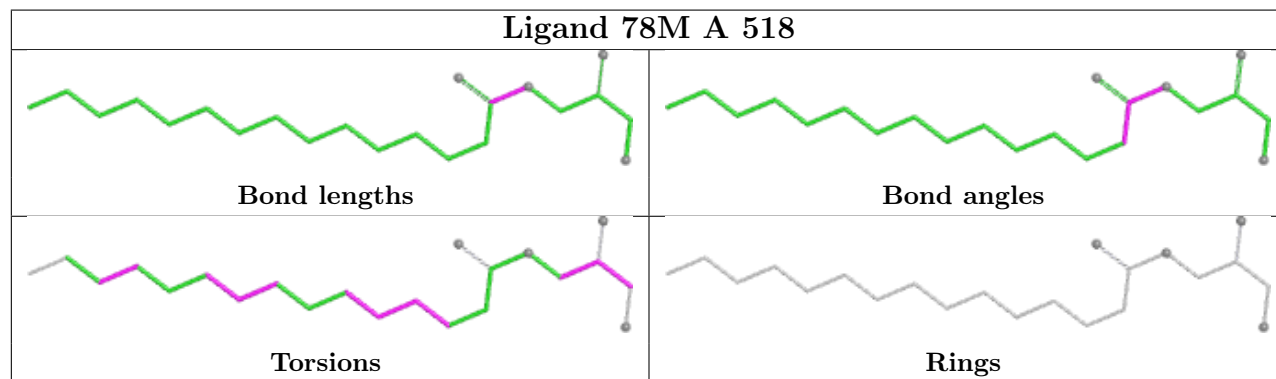
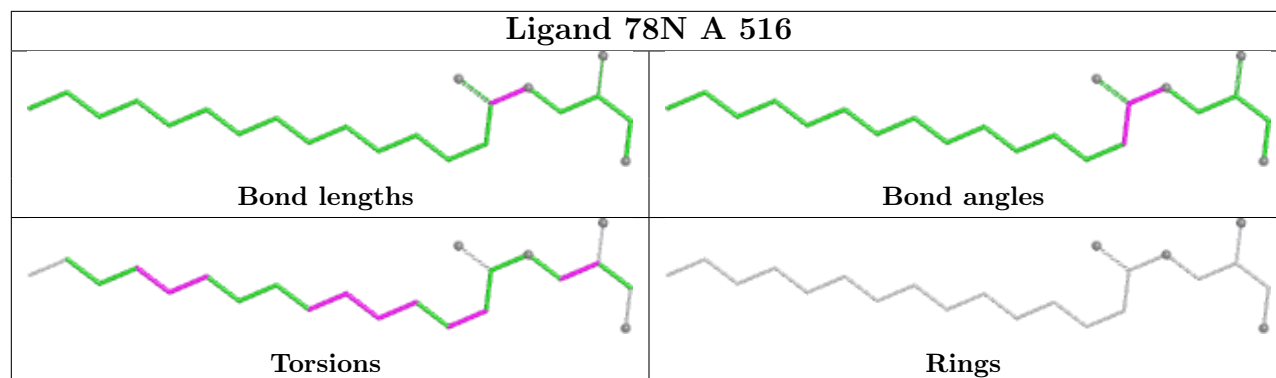
16 monomers are involved in 23 short contacts:

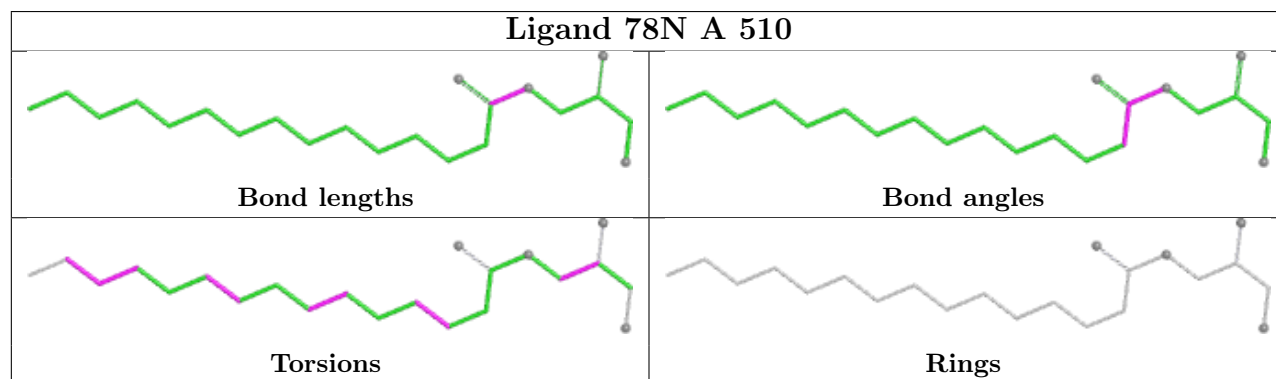
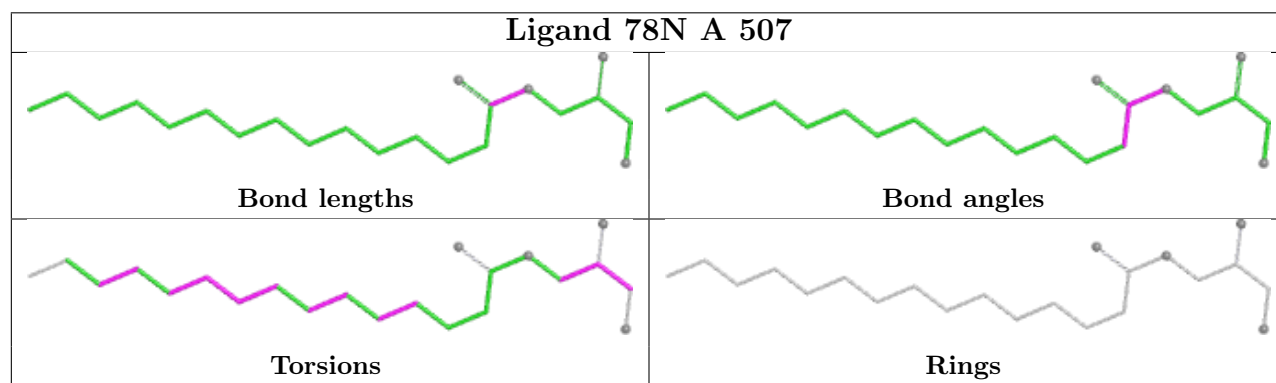
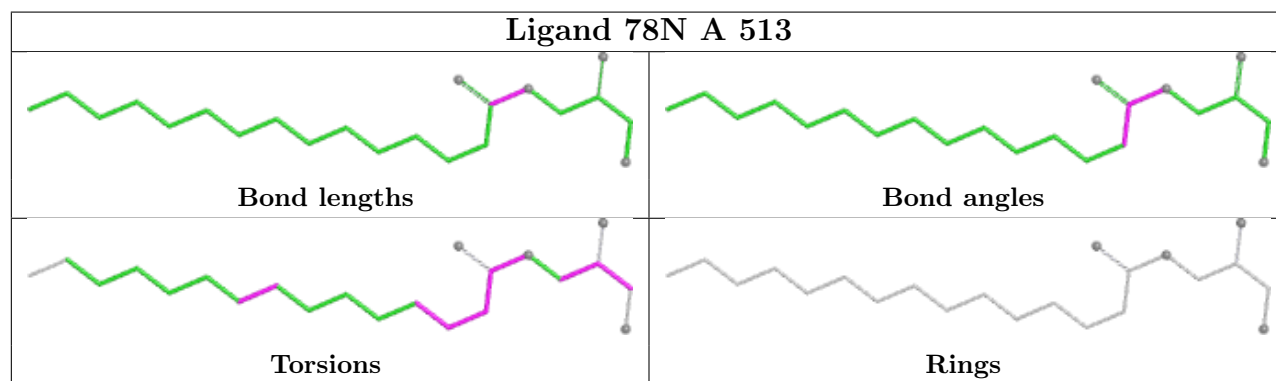
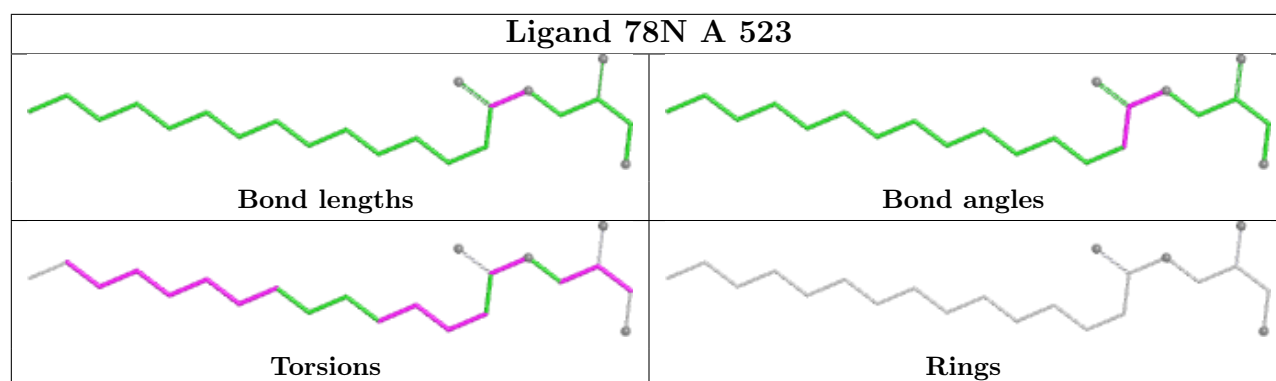
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	1PE	2	0
5	A	515	78N	2	0
5	A	508	78N	2	0
6	A	519	78M	4	0
5	A	516	78N	1	0
6	A	518	78M	1	0
5	A	522	78N	1	0
5	A	513	78N	2	0
5	A	507	78N	3	0
4	A	504	CIT	1	0
6	A	521	78M	1	0
5	A	512	78N	2	0
6	A	506	78M	1	0
6	A	509	78M	3	0
5	A	524	78N	1	0
5	A	505	78N	2	0

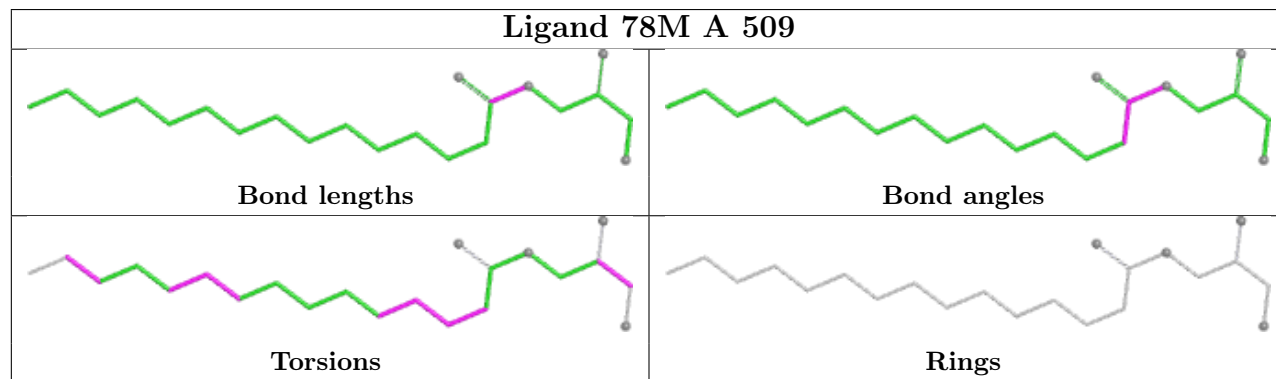
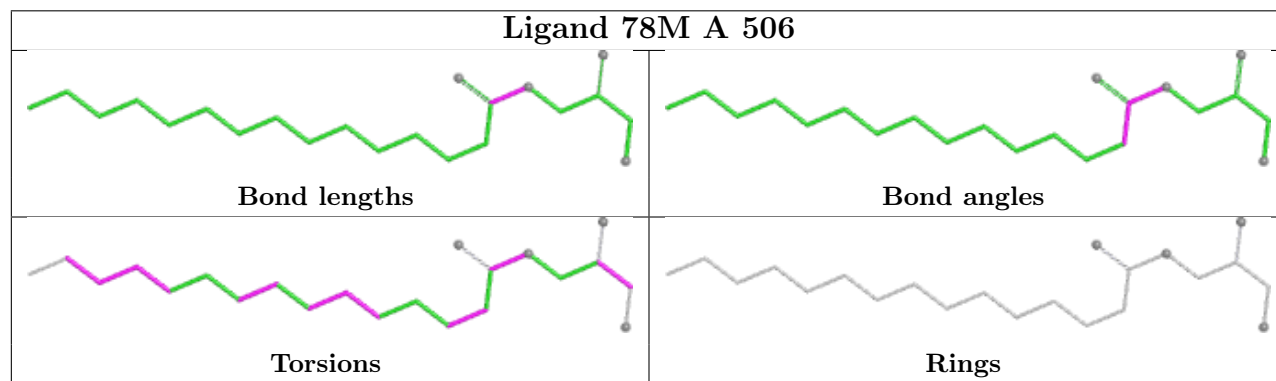
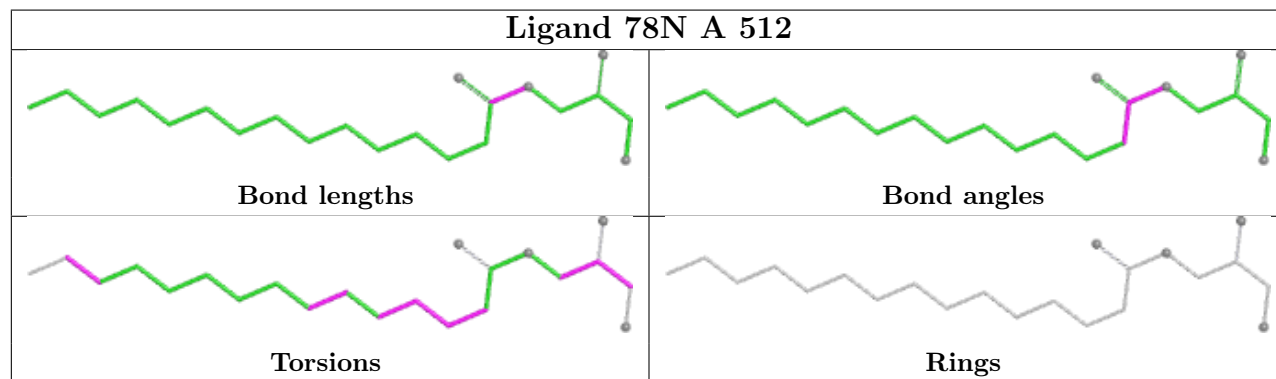
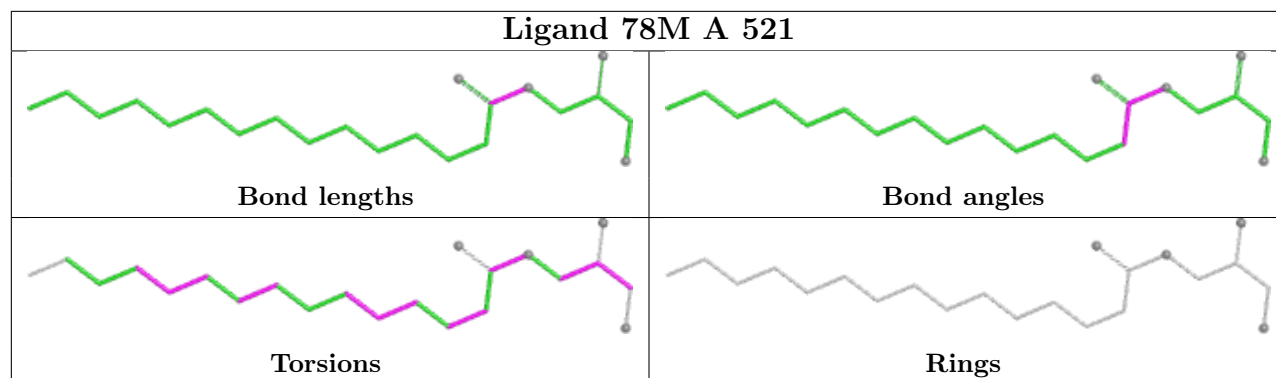
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

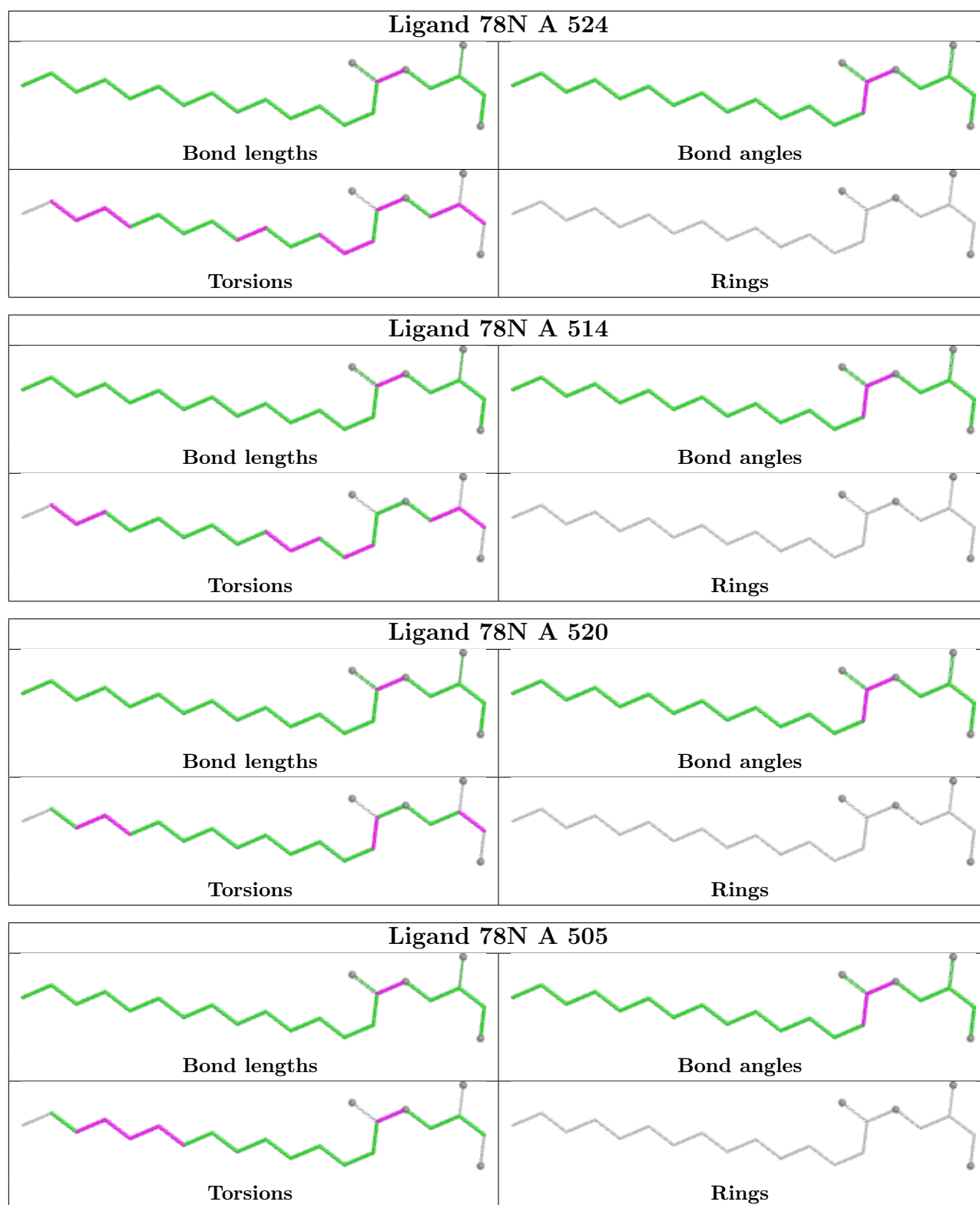
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers ⓘ

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	456/490 (93%)	0.29	38 (8%) 17 20	18, 34, 83, 132	6 (1%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	408	LEU	6.1
1	A	349	ASN	4.2
1	A	407	GLY	4.2
1	A	280	LEU	4.1
1	A	427	TRP	4.0
1	A	285	TYR	3.9
1	A	406	VAL	3.8
1	A	264	TYR	3.8
1	A	478	LEU	3.7
1	A	426	MET	3.7
1	A	284	SER	3.6
1	A	410	VAL	3.5
1	A	428	PHE	3.3
1	A	409	SER	3.2
1	A	282	VAL	3.2
1	A	411	THR	3.0
1	A	476	GLN	3.0
1	A	265	PHE	2.9
1	A	278	GLU	2.9
1	A	268	MET	2.9
1	A	5	GLY	2.8
1	A	283	VAL	2.8
1	A	425	SER	2.7
1	A	424	MET	2.6
1	A	346	TRP	2.5
1	A	338	PHE	2.4
1	A	403	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	279	HIS	2.3
1	A	344	THR	2.3
1	A	447	ALA	2.3
1	A	263	PHE	2.2
1	A	269	ILE	2.2
1	A	448	LYS	2.2
1	A	267	TRP	2.1
1	A	477	GLY	2.1
1	A	73	ILE	2.1
1	A	50	HIS	2.1
1	A	105	PRO	2.1

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
5	78N	A	507	22/22	0.72	0.23	81,87,96,97	0
5	78N	A	515	22/22	0.74	0.23	68,93,96,98	0
6	78M	A	506	22/22	0.75	0.20	70,78,103,108	0
5	78N	A	517	22/22	0.76	0.22	65,85,91,94	0
6	78M	A	519	22/22	0.76	0.24	70,85,122,123	0
5	78N	A	511	22/22	0.77	0.22	61,89,112,114	0
6	78M	A	521	22/22	0.77	0.23	67,72,90,91	0
5	78N	A	524	22/22	0.78	0.27	79,90,101,103	0
5	78N	A	516	22/22	0.79	0.19	59,74,79,79	0
6	78M	A	518	22/22	0.79	0.20	47,80,94,95	0
5	78N	A	522	22/22	0.80	0.24	63,76,109,112	0
5	78N	A	508	22/22	0.81	0.20	61,81,107,108	0

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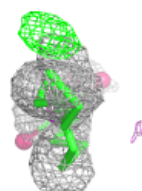
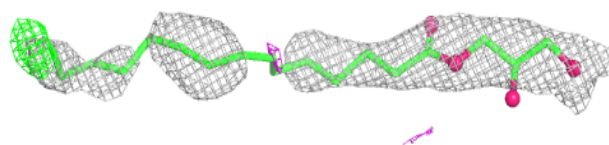
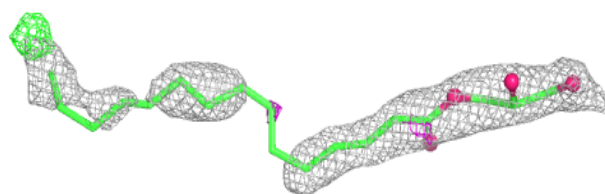
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	78N	A	510	22/22	0.81	0.21	84,87,117,118	0
4	CIT	A	504	13/13	0.84	0.17	82,90,98,100	0
3	1PE	A	503	10/16	0.85	0.23	72,79,89,89	0
5	78N	A	505	22/22	0.86	0.18	41,58,73,74	0
3	1PE	A	502	13/16	0.86	0.23	70,73,79,80	0
6	78M	A	509	22/22	0.87	0.19	56,69,101,102	0
5	78N	A	514	22/22	0.87	0.23	55,77,86,87	0
5	78N	A	513	22/22	0.87	0.19	52,66,73,77	0
5	78N	A	520	22/22	0.87	0.16	38,56,77,78	0
5	78N	A	512	22/22	0.88	0.17	48,74,87,88	0
5	78N	A	523	22/22	0.90	0.19	52,76,91,92	0
2	NA	A	501	1/1	0.95	0.15	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.

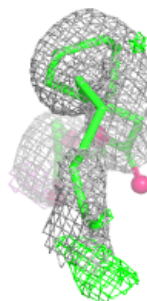
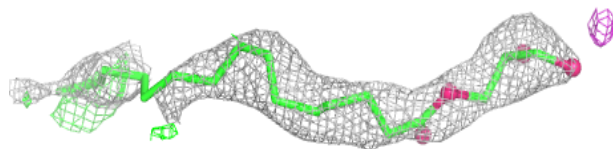
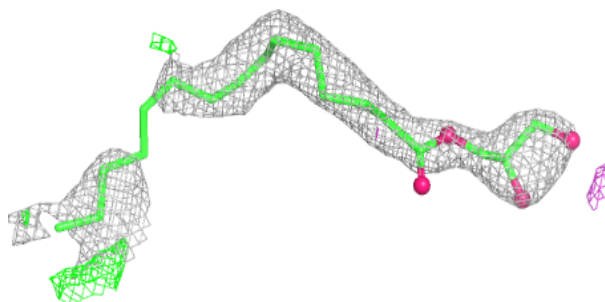
Electron density around 78N A 507:

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

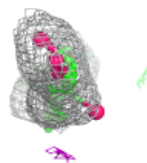
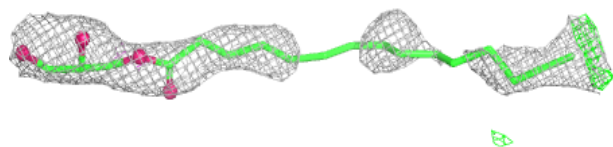
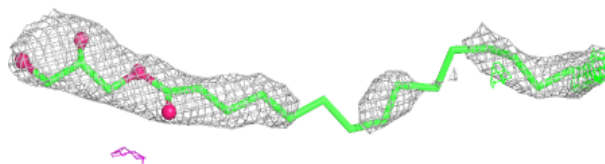


Electron density around 78N A 515:

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

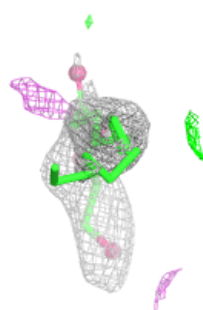
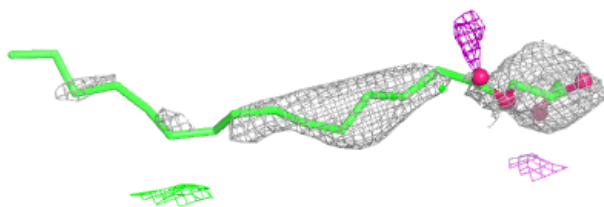
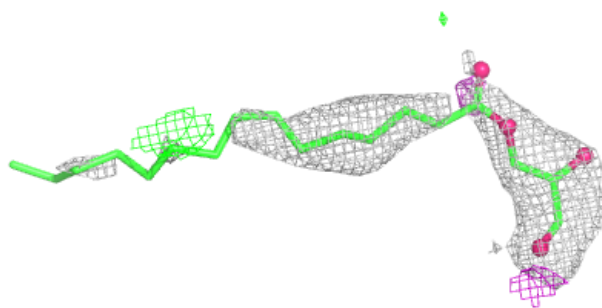
**Electron density around 78M A 506:**

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

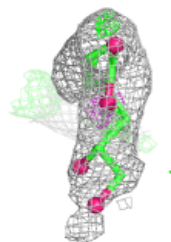
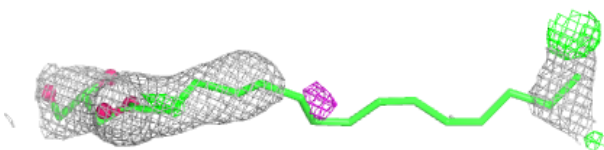
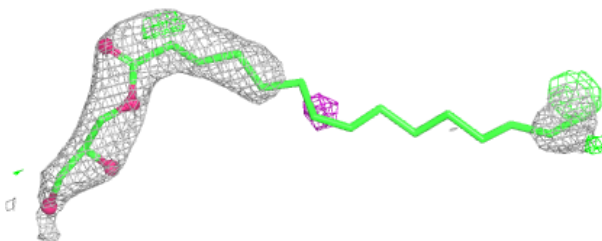


Electron density around 78N A 517:

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

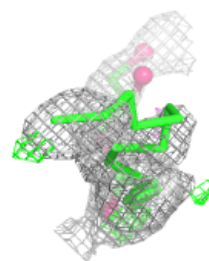
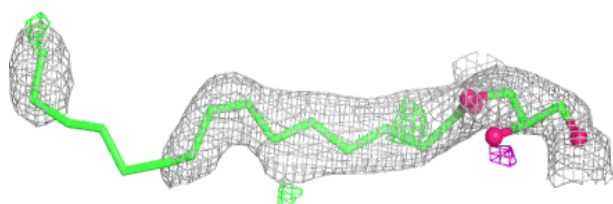
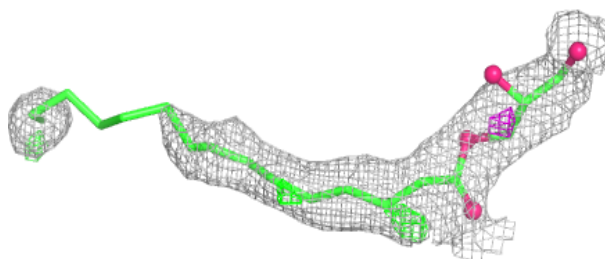
**Electron density around 78M A 519:**

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

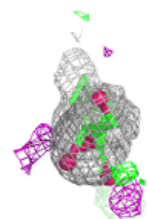
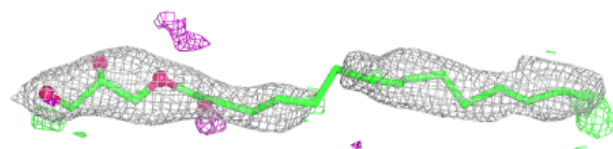
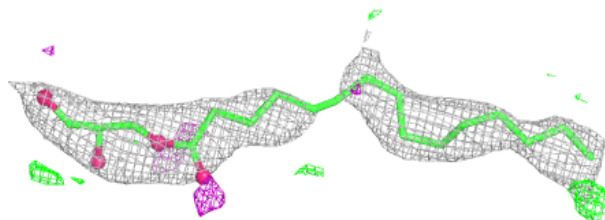


Electron density around 78N A 511:

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

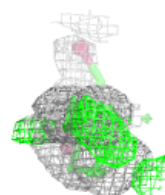
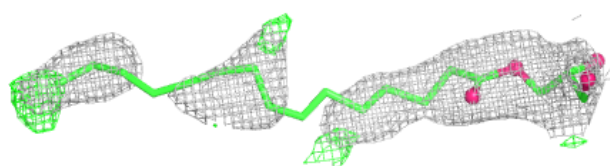
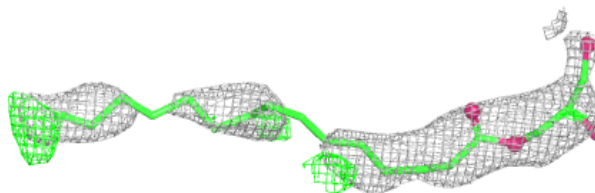
**Electron density around 78M A 521:**

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

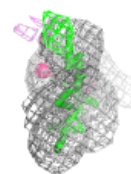
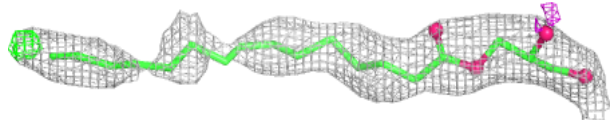
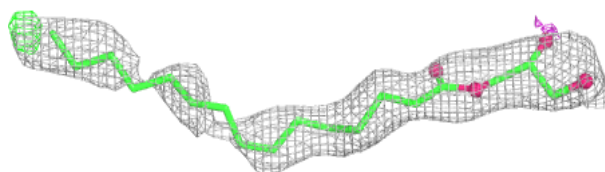


Electron density around 78N A 524:

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and green (positive)

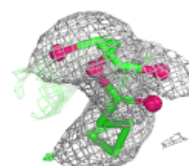
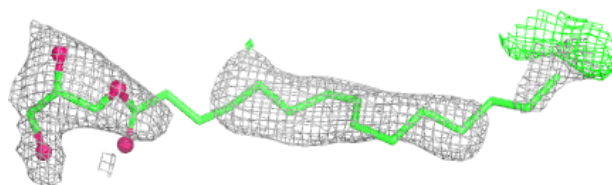
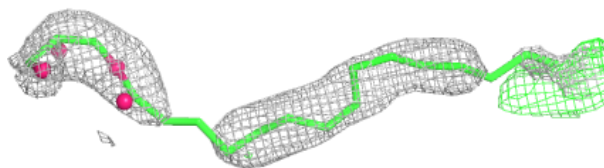
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and green (positive)

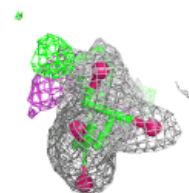
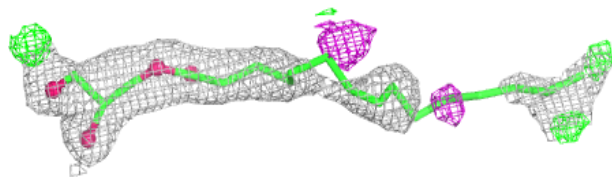
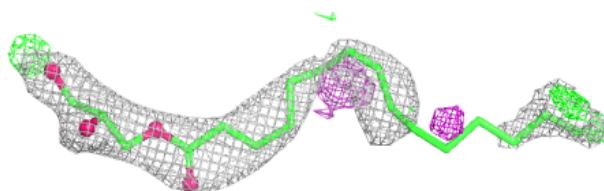


Electron density around 78M A 518:

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

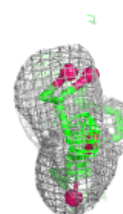
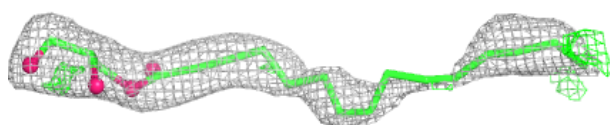
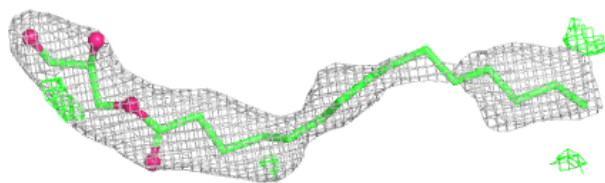
**Electron density around 78N A 522:**

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and green (positive)

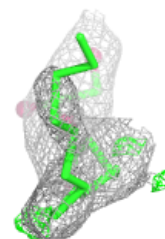
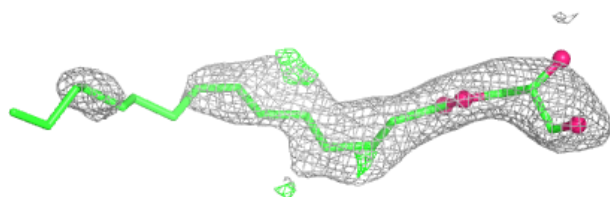
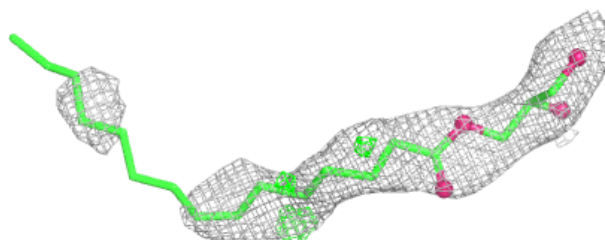


Electron density around 78N A 508:

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

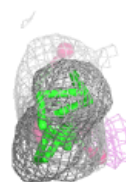
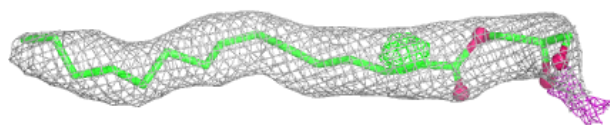
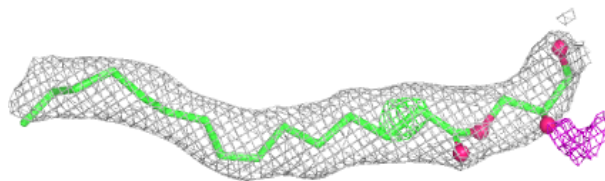
**Electron density around 78N A 510:**

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and green (positive)

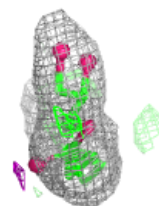
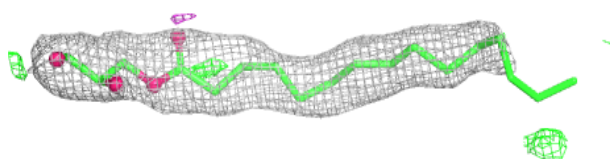
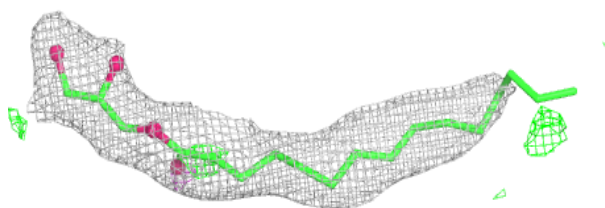


Electron density around 78N A 505:

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

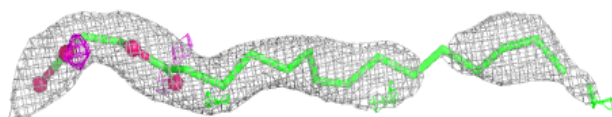
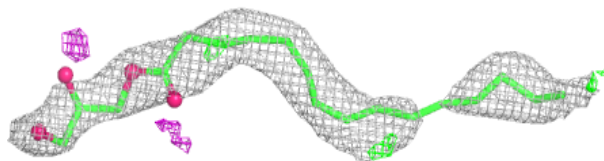
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and green (positive)

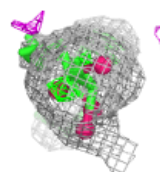
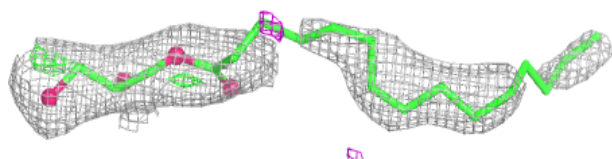
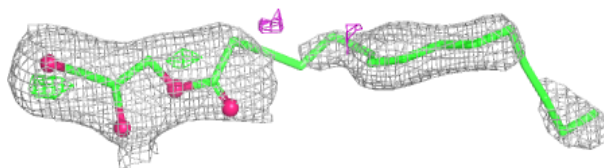


Electron density around 78N A 514:

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and green (positive)

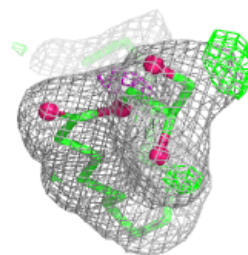
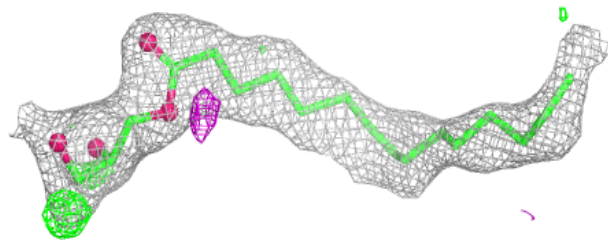
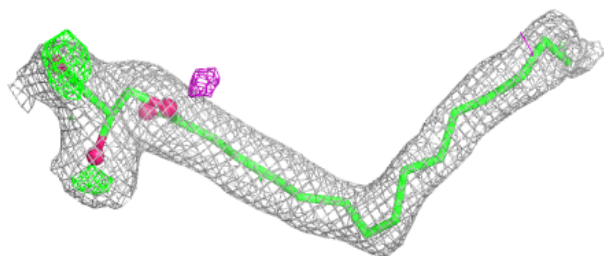
**Electron density around 78N A 513:**

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and green (positive)

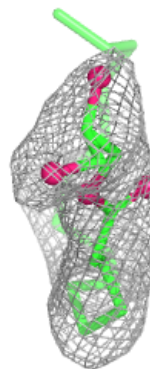
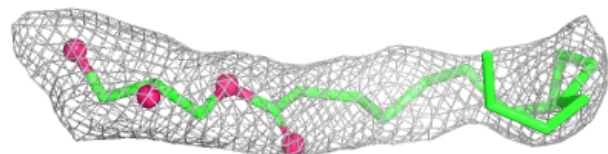
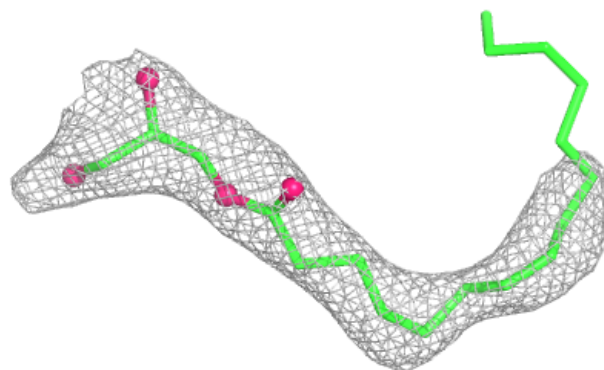


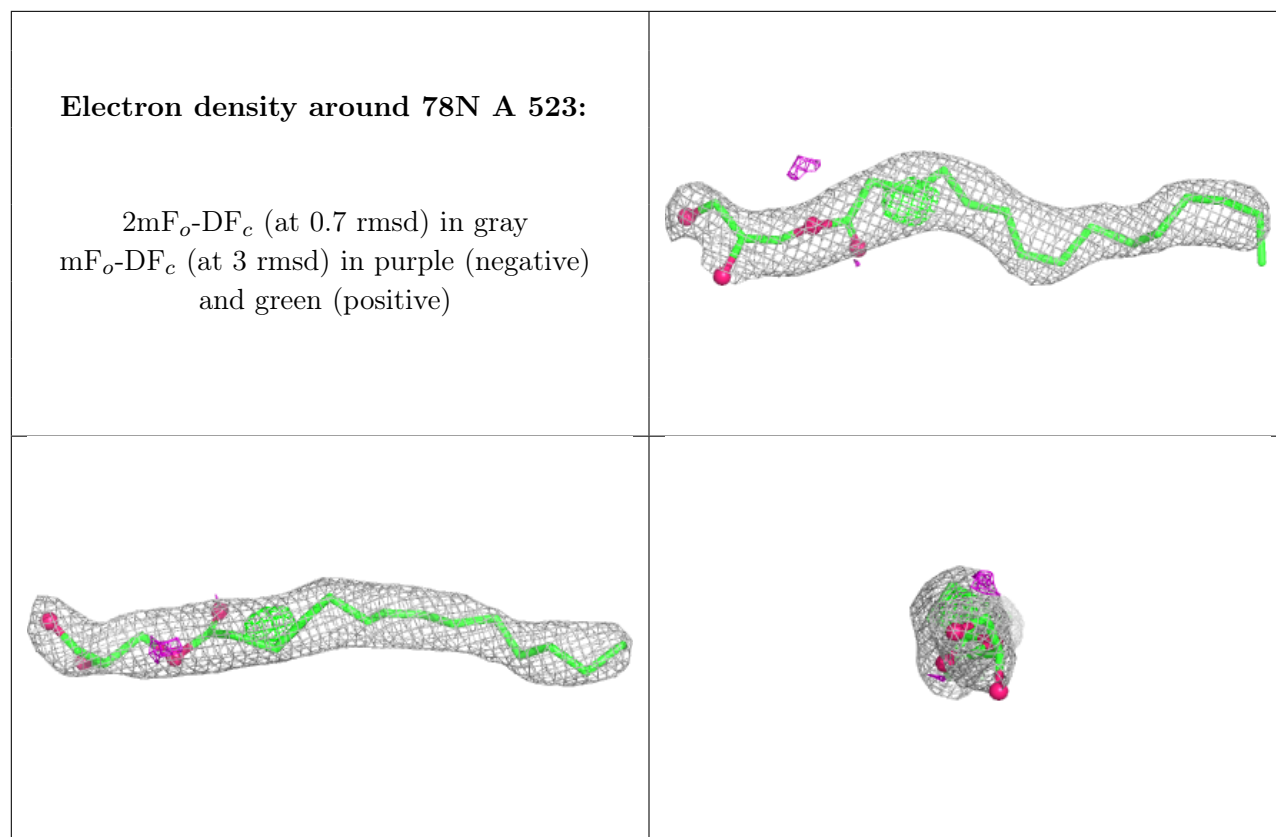
Electron density around 78N A 520:

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

**Electron density around 78N 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.