



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:29 pm BST

PDB ID : 5OXP
Title : PepTSt in occluded conformation with phosphate ion bound
Authors : Martinez Molledo, M.; Quistgaard, E.M.; Loew, C.
Deposited on : 2017-09-07
Resolution : 2.37 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

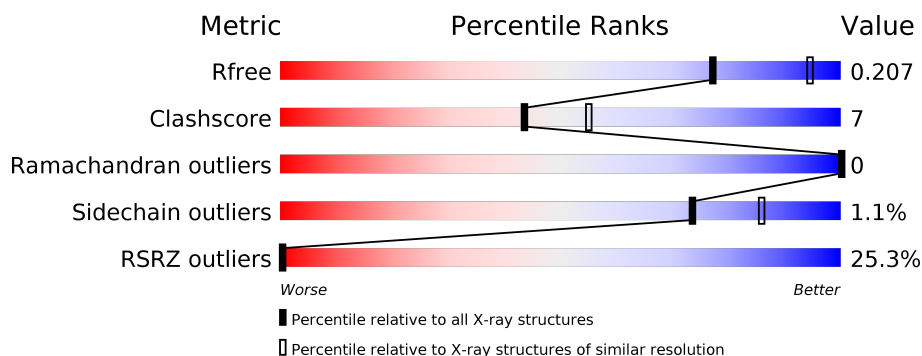
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 on 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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	78N	A	522	-	-	-	X
4	78N	A	523	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4015 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.

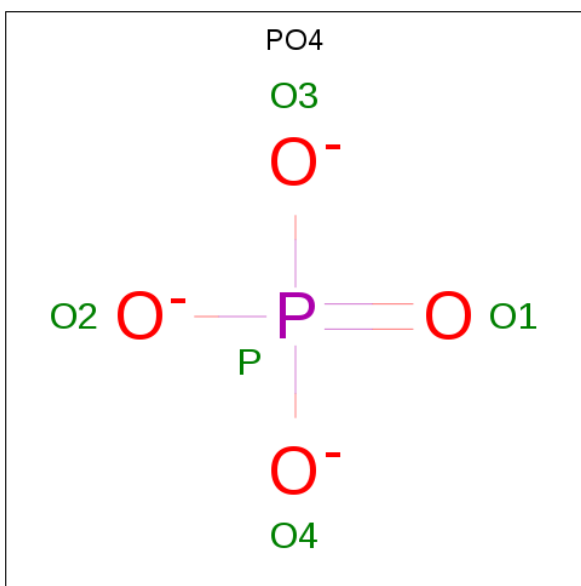
- Molecule 1 is a protein called Di-or tripeptide:H⁺ symporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	462	3572	2403	550	601	18	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

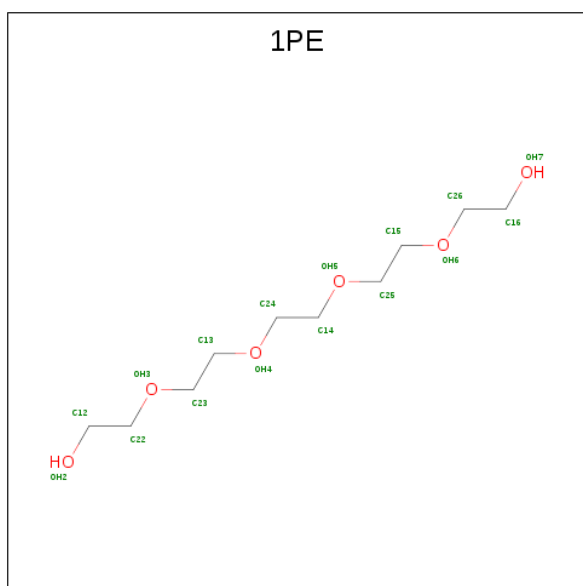
Chain	Residue	Modelled	Actual	Comment	Reference
A	484	ALA	-	expression tag	UNP Q5M4H8
A	485	GLU	-	expression tag	UNP Q5M4H8
A	486	ASN	-	expression tag	UNP Q5M4H8
A	487	LEU	-	expression tag	UNP Q5M4H8
A	488	TYR	-	expression tag	UNP Q5M4H8
A	489	PHE	-	expression tag	UNP Q5M4H8
A	490	GLN	-	expression tag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

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



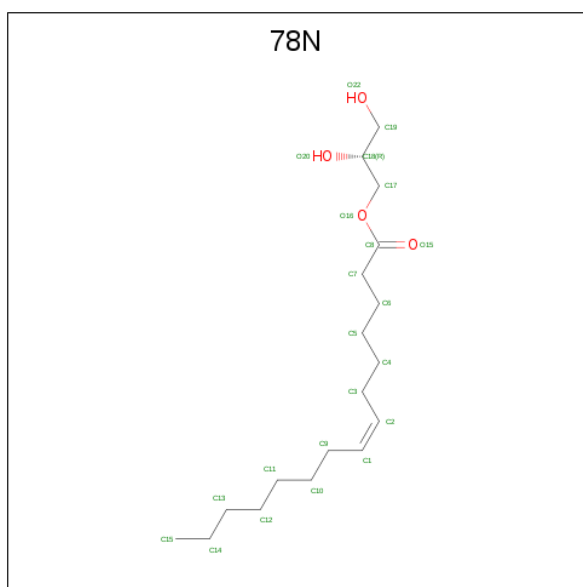
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



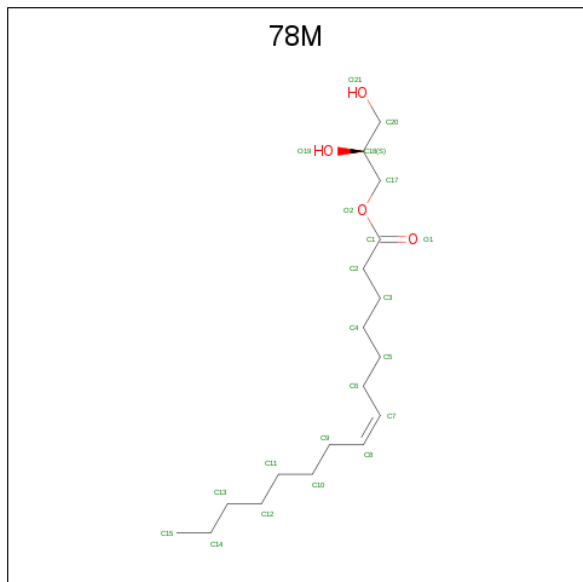
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 8 5	0	0
3	A	1	Total C O 16 10 6	0	0

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



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		
4	A	1	Total	C	O	0	0
			22	18	4		
4	A	1	Total	C	O	0	0
			22	18	4		
4	A	1	Total	C	O	0	0
			22	18	4		
4	A	1	Total	C	O	0	0
			22	18	4		
4	A	1	Total	C	O	0	0
			22	18	4		
4	A	1	Total	C	O	0	0
			22	18	4		
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 (2S)-2,3-DIHYDROXYPROPYL(7Z)-PENTADEC-7-ENOATE (three-letter code: 78M) (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		

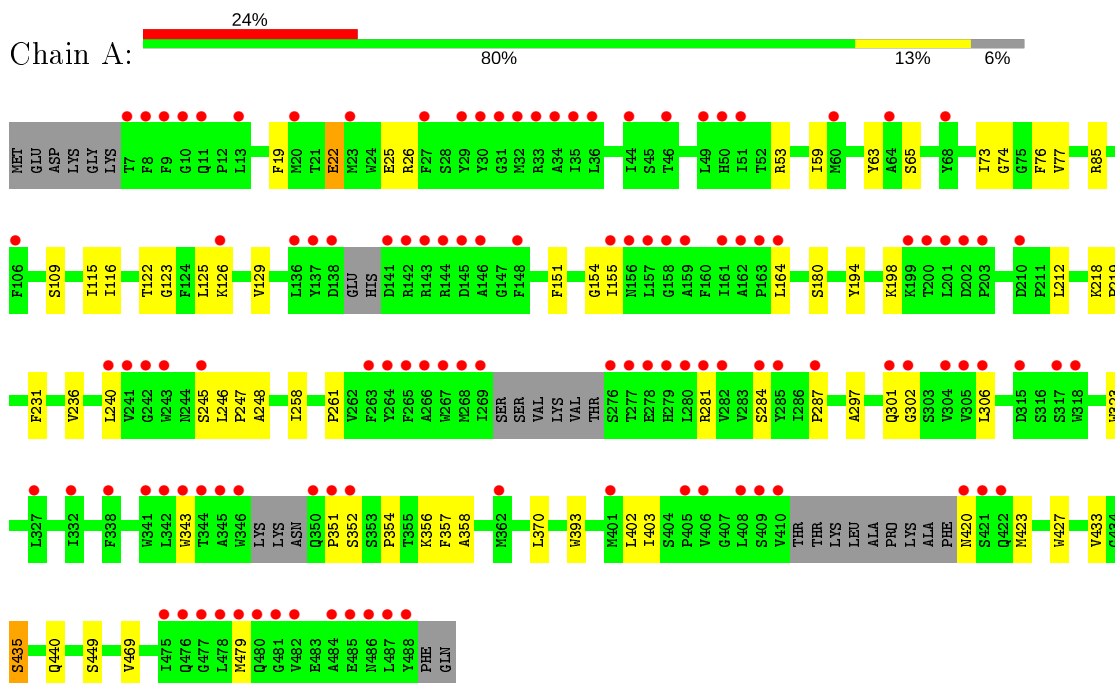
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	37	Total	O		
			37	37	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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	101.60Å 110.10Å 107.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.04 – 2.37 49.04 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.04-2.37) 99.6 (49.04-2.37)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.37Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.194 , 0.208 0.194 , 0.207	Depositor DCC
R_{free} test set	1231 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtrriage
Anisotropy	0.313	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 68.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4015	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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, PO4, 78N, 1PE

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	0.45	0/3676	0.53	0/5012

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	3572	0	3643	50	0
2	A	25	0	0	0	0
3	A	29	0	39	5	0
4	A	308	0	476	16	0
5	A	44	0	68	2	0
6	A	37	0	0	2	0
All	All	4015	0	4226	55	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 (55) 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:26:ARG:NH2	3:A:507:1PE:OH7	2.16	0.78
1:A:19:PHE:CE2	1:A:154:GLY:HA3	2.21	0.74
1:A:22:GLU:HG2	1:A:129:VAL:HG11	1.77	0.67
4:A:514:78N:H2	4:A:515:78N:H71	1.76	0.67
4:A:522:78N:H31C	4:A:522:78N:H112	1.76	0.67
1:A:420:ASN:HB3	1:A:423:MET:HB3	1.77	0.66
1:A:370:LEU:HD21	5:A:510:78M:H8	1.79	0.63
1:A:26:ARG:NH1	3:A:507:1PE:H221	2.14	0.62
1:A:449:SER:HB2	5:A:518:78M:H202	1.80	0.62
1:A:19:PHE:HE2	1:A:154:GLY:HA3	1.66	0.60
1:A:65:SER:HB2	1:A:435:SER:HB3	1.82	0.60
1:A:212:LEU:HB2	4:A:520:78N:H18	1.84	0.59
1:A:26:ARG:HH12	3:A:507:1PE:H221	1.67	0.58
1:A:258:ILE:O	1:A:261:PRO:HD2	2.07	0.55
1:A:25:GLU:HG3	1:A:125:LEU:HD22	1.87	0.55
1:A:351:PRO:HG2	1:A:356:LYS:NZ	2.23	0.54
1:A:358:ALA:HB2	1:A:469:VAL:HB	1.88	0.54
1:A:59:ILE:HD11	1:A:246:LEU:HD21	1.90	0.54
1:A:73:ILE:O	1:A:77:VAL:HG23	2.08	0.53
1:A:248:ALA:HA	4:A:516:78N:H18	1.90	0.53
1:A:402:LEU:O	3:A:506:1PE:H241	2.08	0.52
1:A:151:PHE:CE2	1:A:155:ILE:HD11	2.44	0.52
1:A:194:TYR:CZ	1:A:198:LYS:HE2	2.48	0.48
1:A:427:TRP:CE2	3:A:507:1PE:H252	2.49	0.48
4:A:522:78N:H192	6:A:603:HOH:O	2.14	0.48
1:A:231:PHE:HE2	4:A:515:78N:H1	1.79	0.47
1:A:180:SER:HB2	4:A:512:78N:H52C	1.97	0.47
1:A:245:SER:OG	1:A:247:PRO:HD2	2.15	0.46
1:A:261:PRO:HG2	1:A:433:VAL:HG21	1.98	0.46
1:A:122:THR:HG23	1:A:126:LYS:HG3	1.98	0.46
1:A:236:VAL:O	1:A:240:LEU:HG	2.16	0.45
1:A:420:ASN:ND2	1:A:423:MET:H	2.15	0.45
1:A:85:ARG:HH21	4:A:519:78N:H191	1.83	0.44
1:A:115:ILE:HG21	4:A:514:78N:H101	1.99	0.43
1:A:164:LEU:HA	1:A:323:TRP:CD1	2.53	0.43
4:A:508:78N:H142	4:A:509:78N:H2	2.00	0.43
1:A:281:ARG:HG2	1:A:479:MET:SD	2.59	0.43
1:A:116:ILE:HD11	4:A:514:78N:H141	2.00	0.43
1:A:53:ARG:HD3	6:A:601:HOH:O	2.17	0.43
1:A:74:GLY:HA3	1:A:123:GLY:O	2.19	0.42
1:A:343:TRP:CZ3	1:A:356:LYS:NZ	2.87	0.42
1:A:212:LEU:HD12	4:A:520:78N:H72	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:SER:OG	4:A:513:78N:H192	2.20	0.41
1:A:284:SER:O	1:A:287:PRO:HD2	2.21	0.41
1:A:297:ALA:O	1:A:301:GLN:HG3	2.21	0.41
1:A:440:GLN:HB3	4:A:517:78N:H62C	2.03	0.41
1:A:22:GLU:OE2	1:A:25:GLU:OE1	2.38	0.41
1:A:281:ARG:O	1:A:284:SER:HB3	2.21	0.41
1:A:357:PHE:HA	1:A:403:ILE:HG13	2.03	0.41
1:A:76:PHE:HB2	4:A:522:78N:H191	2.03	0.41
1:A:302:GLY:HA2	1:A:306:LEU:HD12	2.02	0.41
1:A:351:PRO:HG2	1:A:356:LYS:HZ3	1.86	0.40
1:A:352:SER:HB2	1:A:354:PRO:HD2	2.03	0.40
1:A:218:LYS:HB3	1:A:219:PRO:HD3	2.02	0.40
4:A:514:78N:C14	4:A:515:78N:H91C	2.52	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	452/490 (92%)	446 (99%)	6 (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	372/397 (94%)	368 (99%)	4 (1%)	73 86

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

Mol	Chain	Res	Type
1	A	22	GLU
1	A	63	TYR
1	A	393	TRP
1	A	435	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

23 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	A	503	-	4,4,4	0.69	0	6,6,6	0.69	0
4	78N	A	522	-	21,21,21	0.93	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
4	78N	A	523	-	21,21,21	0.98	1 (4%)	22,22,22	0.99	1 (4%)
2	PO4	A	505	-	4,4,4	0.92	0	6,6,6	0.41	0
5	78M	A	510	-	21,21,21	1.15	1 (4%)	22,22,22	0.99	1 (4%)
4	78N	A	517	-	21,21,21	0.99	1 (4%)	22,22,22	1.08	1 (4%)
4	78N	A	516	-	21,21,21	0.98	1 (4%)	22,22,22	1.10	1 (4%)
4	78N	A	514	-	21,21,21	0.90	1 (4%)	22,22,22	1.02	1 (4%)
4	78N	A	519	-	21,21,21	0.94	1 (4%)	22,22,22	1.05	1 (4%)
4	78N	A	521	-	21,21,21	0.91	1 (4%)	22,22,22	1.16	1 (4%)
4	78N	A	508	-	21,21,21	0.94	1 (4%)	22,22,22	0.97	1 (4%)
4	78N	A	512	-	21,21,21	0.98	1 (4%)	22,22,22	0.98	1 (4%)
4	78N	A	515	-	21,21,21	0.96	1 (4%)	22,22,22	0.97	1 (4%)
4	78N	A	513	-	21,21,21	0.96	1 (4%)	22,22,22	1.02	1 (4%)
4	78N	A	509	-	21,21,21	0.96	1 (4%)	22,22,22	1.02	1 (4%)
3	1PE	A	507	-	15,15,15	0.75	0	14,14,14	0.45	0
2	PO4	A	504	-	4,4,4	0.95	0	6,6,6	0.43	0
5	78M	A	518	-	21,21,21	1.17	1 (4%)	22,22,22	0.95	1 (4%)
3	1PE	A	506	-	12,12,15	0.61	0	11,11,14	0.45	0
4	78N	A	511	-	21,21,21	0.94	1 (4%)	22,22,22	1.05	1 (4%)
4	78N	A	520	-	21,21,21	0.91	1 (4%)	22,22,22	0.97	1 (4%)
2	PO4	A	501	-	4,4,4	0.97	0	6,6,6	0.41	0
2	PO4	A	502	-	4,4,4	0.98	0	6,6,6	0.39	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
3	1PE	A	507	-	-	5/13/13/13	-
4	78N	A	521	-	-	11/21/21/21	-
5	78M	A	510	-	-	9/21/21/21	-
4	78N	A	517	-	-	12/21/21/21	-
4	78N	A	516	-	-	10/21/21/21	-
4	78N	A	522	-	-	13/21/21/21	-
5	78M	A	518	-	-	9/21/21/21	-
4	78N	A	512	-	-	11/21/21/21	-
4	78N	A	508	-	-	10/21/21/21	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	78N	A	515	-	-	11/21/21/21	-
4	78N	A	523	-	-	12/21/21/21	-
4	78N	A	511	-	-	6/21/21/21	-
4	78N	A	520	-	-	9/21/21/21	-
4	78N	A	513	-	-	7/21/21/21	-
4	78N	A	514	-	-	9/21/21/21	-
4	78N	A	519	-	-	7/21/21/21	-
4	78N	A	509	-	-	10/21/21/21	-
3	1PE	A	506	-	-	7/10/10/13	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	510	78M	O2-C1	3.66	1.44	1.33
5	A	518	78M	O2-C1	3.45	1.43	1.33
4	A	517	78N	O16-C8	3.24	1.42	1.33
4	A	515	78N	O16-C8	3.16	1.42	1.33
4	A	513	78N	O16-C8	3.09	1.42	1.33
4	A	516	78N	O16-C8	3.08	1.42	1.33
4	A	523	78N	O16-C8	3.07	1.42	1.33
4	A	511	78N	O16-C8	2.98	1.42	1.33
4	A	509	78N	O16-C8	2.97	1.42	1.33
4	A	514	78N	O16-C8	2.95	1.41	1.33
4	A	519	78N	O16-C8	2.93	1.41	1.33
4	A	512	78N	O16-C8	2.92	1.41	1.33
4	A	508	78N	O16-C8	2.91	1.41	1.33
4	A	522	78N	O16-C8	2.85	1.41	1.33
4	A	521	78N	O16-C8	2.81	1.41	1.33
4	A	520	78N	O16-C8	2.74	1.41	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	516	78N	O16-C8-C7	3.34	122.38	111.91
4	A	509	78N	O16-C8-C7	3.14	121.77	111.91
4	A	519	78N	O16-C8-C7	3.13	121.74	111.91
4	A	517	78N	O16-C8-C7	3.08	121.58	111.91
4	A	523	78N	O16-C8-C7	3.07	121.56	111.91
4	A	521	78N	O16-C8-C7	2.96	121.19	111.91
4	A	513	78N	O16-C8-C7	2.88	120.95	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	512	78N	O16-C8-C7	2.82	120.77	111.91
5	A	518	78M	O2-C1-C2	2.82	120.74	111.91
4	A	511	78N	O16-C8-C7	2.81	120.72	111.91
4	A	508	78N	O16-C8-C7	2.78	120.64	111.91
5	A	510	78M	O2-C1-C2	2.76	120.56	111.91
4	A	515	78N	O16-C8-C7	2.59	120.04	111.91
4	A	514	78N	O16-C8-C7	2.57	119.97	111.91
4	A	522	78N	O16-C8-C7	2.42	119.51	111.91
4	A	520	78N	O16-C8-C7	2.33	119.23	111.91

There are no chirality outliers.

All (168) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	522	78N	C17-C18-C19-O22
4	A	522	78N	O16-C17-C18-O20
4	A	523	78N	O16-C17-C18-C19
4	A	523	78N	O16-C17-C18-O20
4	A	517	78N	C17-C18-C19-O22
4	A	517	78N	O16-C17-C18-O20
4	A	516	78N	C17-C18-C19-O22
4	A	514	78N	C17-C18-C19-O22
4	A	514	78N	O16-C17-C18-C19
4	A	519	78N	O20-C18-C19-O22
4	A	519	78N	C17-C18-C19-O22
4	A	519	78N	O16-C17-C18-C19
4	A	519	78N	O16-C17-C18-O20
4	A	521	78N	O16-C17-C18-O20
4	A	508	78N	C17-C18-C19-O22
4	A	508	78N	O16-C17-C18-C19
4	A	512	78N	O16-C17-C18-O20
4	A	515	78N	C17-C18-C19-O22
4	A	515	78N	O16-C17-C18-C19
4	A	513	78N	O20-C18-C19-O22
4	A	513	78N	C17-C18-C19-O22
4	A	509	78N	C17-C18-C19-O22
4	A	520	78N	O16-C17-C18-O20
4	A	520	78N	O15-C8-O16-C17
4	A	520	78N	C7-C8-O16-C17
4	A	523	78N	C7-C8-O16-C17
4	A	521	78N	C7-C8-O16-C17
4	A	522	78N	C7-C8-O16-C17

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Mol	Chain	Res	Type	Atoms
4	A	522	78N	O15-C8-O16-C17
4	A	523	78N	O15-C8-O16-C17
4	A	521	78N	O15-C8-O16-C17
4	A	514	78N	O16-C17-C18-O20
4	A	508	78N	O16-C17-C18-O20
4	A	517	78N	C7-C8-O16-C17
3	A	506	1PE	OH5-C14-C24-OH4
4	A	522	78N	O16-C17-C18-C19
3	A	507	1PE	OH6-C15-C25-OH5
4	A	515	78N	O20-C18-C19-O22
4	A	516	78N	C5-C6-C7-C8
4	A	520	78N	C5-C6-C7-C8
4	A	517	78N	C5-C6-C7-C8
4	A	512	78N	C5-C6-C7-C8
4	A	517	78N	O15-C8-O16-C17
5	A	510	78M	O2-C17-C18-O19
4	A	515	78N	O16-C17-C18-O20
5	A	518	78M	O2-C17-C18-O19
4	A	512	78N	C7-C8-O16-C17
3	A	507	1PE	OH5-C14-C24-OH4
4	A	522	78N	C3-C4-C5-C6
5	A	510	78M	O2-C17-C18-C20
4	A	520	78N	O16-C17-C18-C19
4	A	512	78N	C4-C5-C6-C7
5	A	518	78M	C3-C4-C5-C6
4	A	522	78N	C9-C10-C11-C12
4	A	521	78N	C11-C12-C13-C14
4	A	511	78N	C11-C12-C13-C14
4	A	514	78N	C4-C5-C6-C7
4	A	516	78N	C3-C4-C5-C6
4	A	509	78N	C10-C11-C12-C13
4	A	512	78N	O15-C8-O16-C17
4	A	523	78N	C17-C18-C19-O22
5	A	510	78M	C17-C18-C20-O21
5	A	518	78M	C17-C18-C20-O21
5	A	510	78M	C10-C11-C12-C13
4	A	520	78N	C4-C5-C6-C7
4	A	523	78N	C2-C3-C4-C5
4	A	514	78N	C2-C3-C4-C5
4	A	521	78N	C3-C4-C5-C6
4	A	511	78N	C4-C5-C6-C7
3	A	506	1PE	OH2-C12-C22-OH3

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Mol	Chain	Res	Type	Atoms
4	A	523	78N	C3-C4-C5-C6
5	A	510	78M	C11-C12-C13-C14
4	A	519	78N	C10-C11-C12-C13
5	A	510	78M	C9-C10-C11-C12
4	A	522	78N	O20-C18-C19-O22
4	A	517	78N	O20-C18-C19-O22
4	A	516	78N	O20-C18-C19-O22
4	A	514	78N	C9-C10-C11-C12
4	A	517	78N	C9-C10-C11-C12
4	A	508	78N	C4-C5-C6-C7
3	A	506	1PE	OH4-C13-C23-OH3
4	A	516	78N	C9-C10-C11-C12
4	A	513	78N	C11-C12-C13-C14
4	A	517	78N	C10-C11-C12-C13
4	A	517	78N	C2-C3-C4-C5
4	A	516	78N	C11-C10-C9-C1
4	A	509	78N	C2-C3-C4-C5
4	A	521	78N	C9-C10-C11-C12
4	A	508	78N	C10-C11-C12-C13
4	A	509	78N	C4-C5-C6-C7
4	A	521	78N	C11-C10-C9-C1
4	A	515	78N	C9-C10-C11-C12
4	A	508	78N	C2-C3-C4-C5
4	A	508	78N	C11-C12-C13-C14
4	A	514	78N	O20-C18-C19-O22
4	A	508	78N	O20-C18-C19-O22
4	A	509	78N	O20-C18-C19-O22
4	A	523	78N	C11-C10-C9-C1
4	A	511	78N	C2-C3-C4-C5
4	A	520	78N	C2-C3-C4-C5
4	A	522	78N	C5-C6-C7-C8
4	A	512	78N	O16-C17-C18-C19
5	A	510	78M	C12-C13-C14-C15
5	A	518	78M	C10-C11-C12-C13
4	A	516	78N	C7-C8-O16-C17
4	A	512	78N	C3-C4-C5-C6
4	A	514	78N	C10-C11-C12-C13
4	A	520	78N	C3-C4-C5-C6
4	A	511	78N	C10-C11-C12-C13
4	A	523	78N	C10-C11-C12-C13
4	A	521	78N	O16-C17-C18-C19
3	A	506	1PE	C23-C13-OH4-C24

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Mol	Chain	Res	Type	Atoms
4	A	515	78N	C12-C13-C14-C15
4	A	523	78N	C9-C10-C11-C12
3	A	506	1PE	C13-C23-OH3-C22
3	A	507	1PE	C12-C22-OH3-C23
4	A	516	78N	O15-C8-O16-C17
4	A	523	78N	O20-C18-C19-O22
4	A	522	78N	C12-C13-C14-C15
4	A	508	78N	C11-C10-C9-C1
4	A	523	78N	C5-C6-C7-C8
4	A	517	78N	O16-C17-C18-C19
4	A	515	78N	C3-C4-C5-C6
5	A	518	78M	C2-C1-O2-C17
4	A	522	78N	C11-C12-C13-C14
4	A	509	78N	O16-C17-C18-O20
4	A	516	78N	C10-C11-C12-C13
4	A	513	78N	C9-C10-C11-C12
5	A	518	78M	O1-C1-O2-C17
4	A	519	78N	C9-C10-C11-C12
4	A	513	78N	C10-C11-C12-C13
4	A	522	78N	C1-C2-C3-C4
4	A	519	78N	C2-C1-C9-C10
4	A	512	78N	C10-C11-C12-C13
4	A	509	78N	C3-C4-C5-C6
3	A	506	1PE	C12-C22-OH3-C23
5	A	518	78M	O2-C17-C18-C20
4	A	508	78N	C1-C2-C3-C4
4	A	513	78N	C2-C1-C9-C10
4	A	509	78N	C1-C2-C3-C4
4	A	517	78N	C4-C5-C6-C7
4	A	512	78N	C2-C1-C9-C10
4	A	512	78N	C11-C12-C13-C14
4	A	521	78N	C2-C1-C9-C10
5	A	518	78M	C5-C6-C7-C8
5	A	510	78M	C7-C8-C9-C10
4	A	516	78N	C1-C2-C3-C4
4	A	514	78N	C1-C2-C3-C4
4	A	513	78N	C1-C2-C3-C4
5	A	518	78M	C7-C8-C9-C10
4	A	520	78N	C2-C1-C9-C10
5	A	510	78M	C5-C6-C7-C8
4	A	515	78N	C2-C1-C9-C10
4	A	522	78N	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	A	506	1PE	C15-C25-OH5-C14
3	A	507	1PE	C16-C26-OH6-C15
4	A	517	78N	C1-C2-C3-C4
4	A	512	78N	C1-C2-C3-C4
4	A	509	78N	C2-C1-C9-C10
4	A	521	78N	C1-C2-C3-C4
4	A	521	78N	C10-C11-C12-C13
4	A	511	78N	C17-C18-C19-O22
4	A	509	78N	C11-C12-C13-C14
4	A	515	78N	C6-C7-C8-O16
3	A	507	1PE	C13-C23-OH3-C22
4	A	511	78N	C7-C8-O16-C17
4	A	515	78N	O15-C8-O16-C17
4	A	515	78N	C7-C8-O16-C17

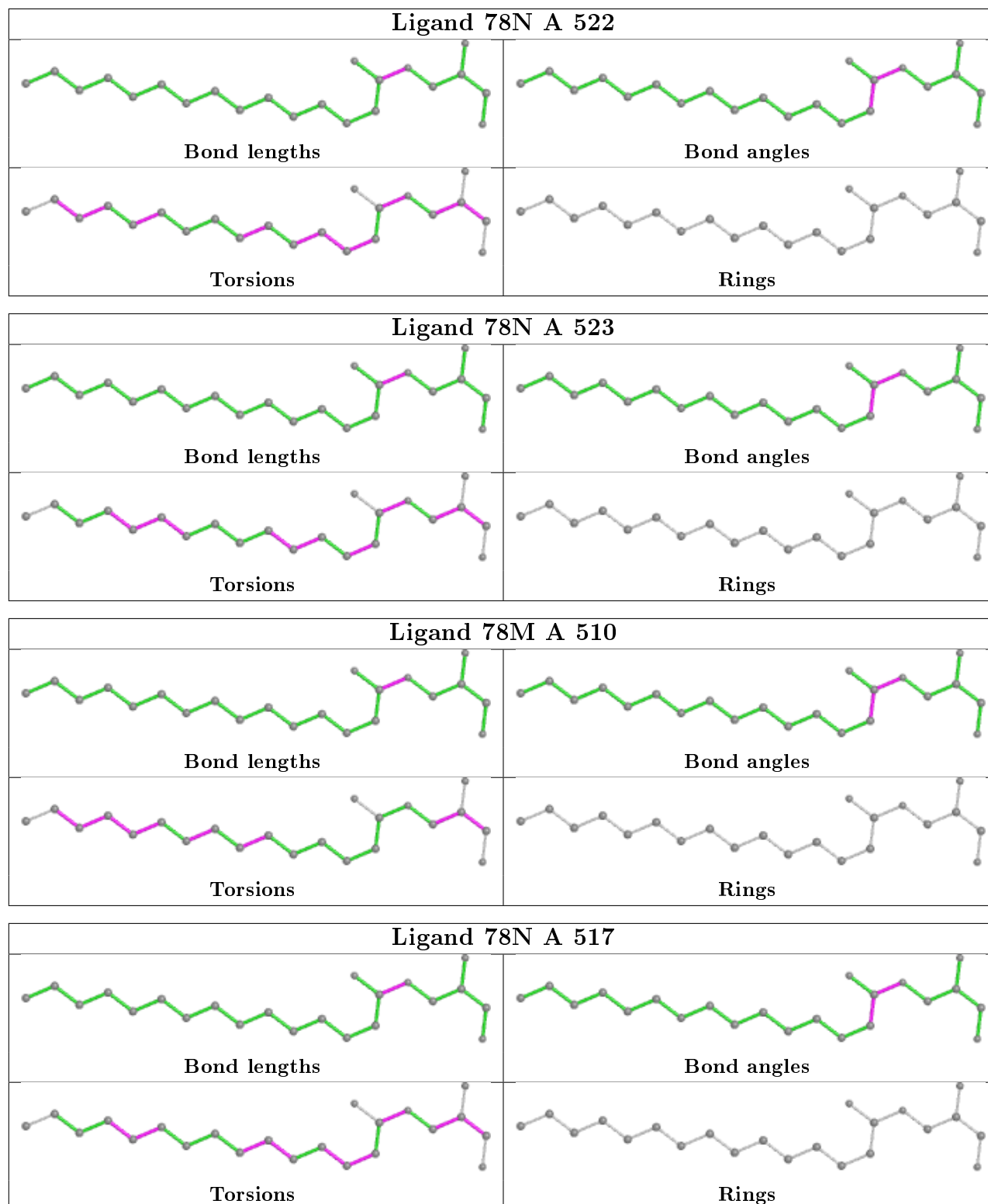
There are no ring outliers.

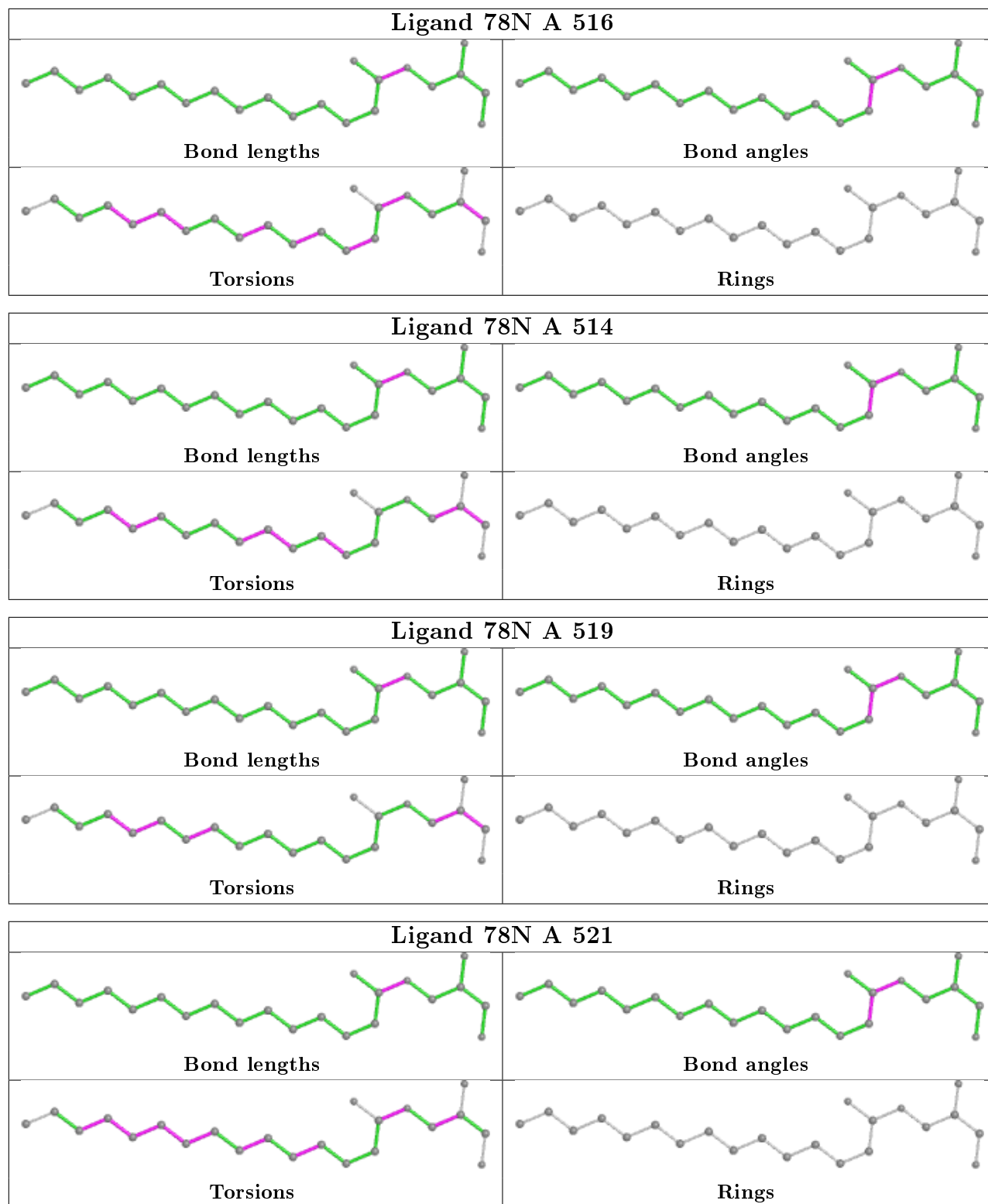
15 monomers are involved in 23 short contacts:

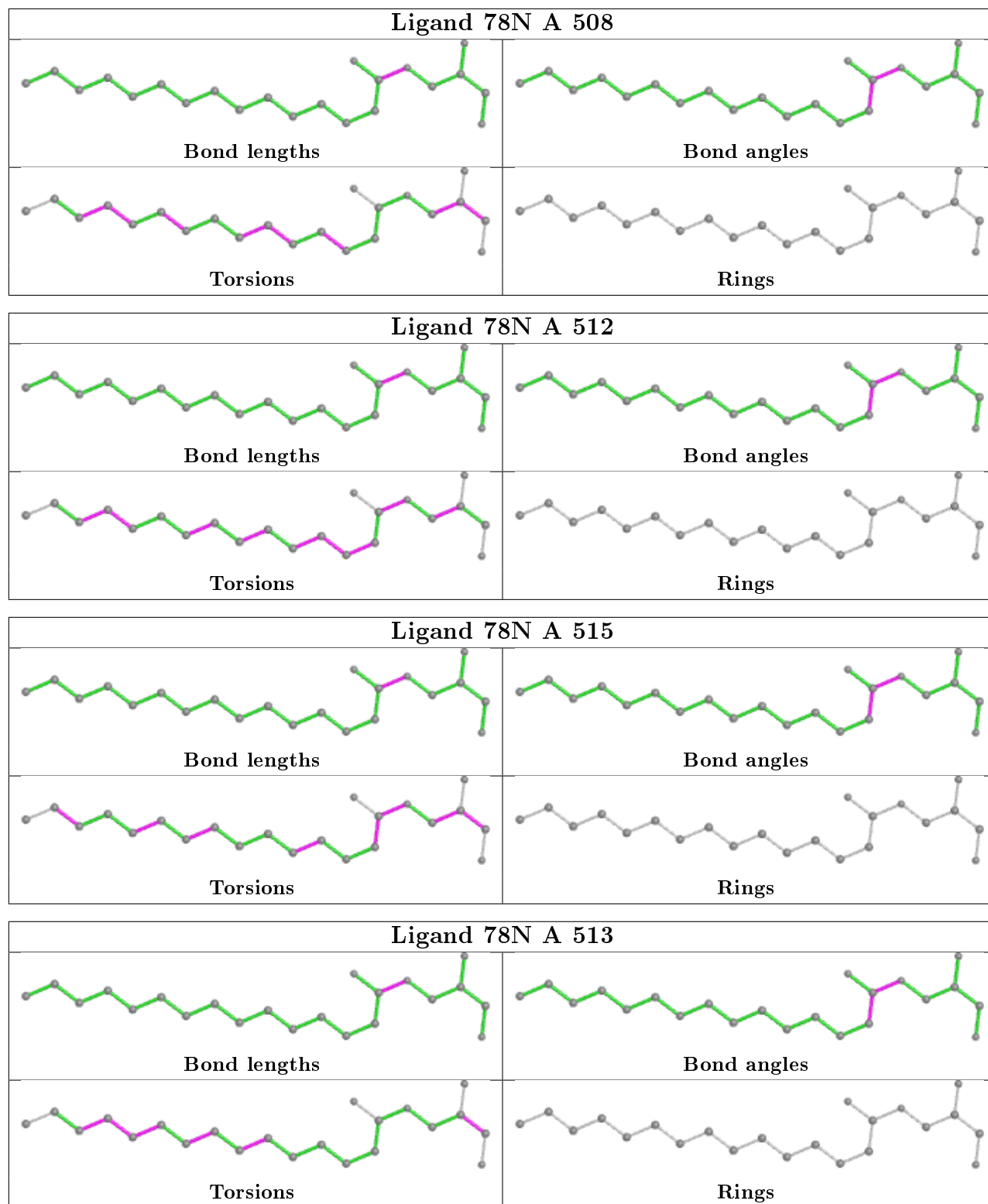
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	522	78N	3	0
5	A	510	78M	1	0
4	A	517	78N	1	0
4	A	516	78N	1	0
4	A	514	78N	4	0
4	A	519	78N	1	0
4	A	508	78N	1	0
4	A	512	78N	1	0
4	A	515	78N	3	0
4	A	513	78N	1	0
4	A	509	78N	1	0
3	A	507	1PE	4	0
5	A	518	78M	1	0
3	A	506	1PE	1	0
4	A	520	78N	2	0

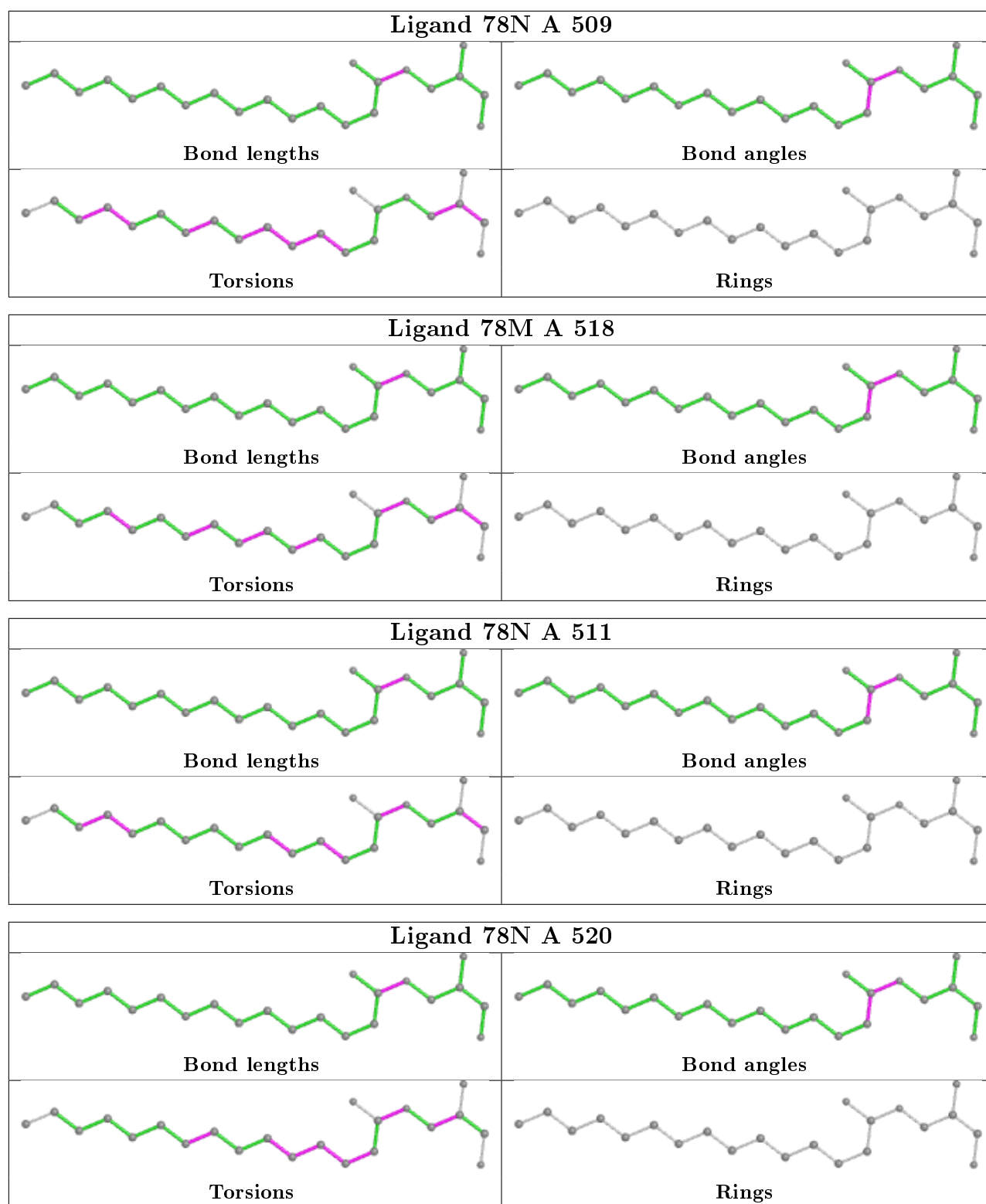
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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	462/490 (94%)	1.51	117 (25%) 0 0	43, 58, 109, 136	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280	LEU	12.2
1	A	341	TRP	9.8
1	A	405	PRO	9.8
1	A	267	TRP	8.6
1	A	346	TRP	7.9
1	A	137	TYR	7.4
1	A	142	ARG	7.3
1	A	269	ILE	7.3
1	A	345	ALA	6.8
1	A	268	MET	6.6
1	A	282	VAL	6.5
1	A	278	GLU	6.5
1	A	265	PHE	6.2
1	A	200	THR	5.9
1	A	263	PHE	5.9
1	A	276	SER	5.7
1	A	350	GLN	5.6
1	A	482	VAL	5.5
1	A	279	HIS	5.5
1	A	479	MET	5.5
1	A	477	GLY	5.3
1	A	410	VAL	5.2
1	A	277	THR	5.2
1	A	478	LEU	5.2
1	A	480	GLN	5.2
1	A	50	HIS	5.1
1	A	475	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	266	ALA	5.1
1	A	318	TRP	5.1
1	A	287	PRO	5.0
1	A	7	THR	5.0
1	A	144	ARG	4.9
1	A	141	ASP	4.8
1	A	281	ARG	4.8
1	A	485	GLU	4.8
1	A	11	GLN	4.8
1	A	406	VAL	4.6
1	A	10	GLY	4.4
1	A	285	TYR	4.3
1	A	8	PHE	4.3
1	A	13	LEU	4.3
1	A	138	ASP	4.2
1	A	362	MET	4.1
1	A	351	PRO	4.1
1	A	136	LEU	4.1
1	A	243	TRP	4.1
1	A	241	VAL	3.9
1	A	161	ILE	3.8
1	A	9	PHE	3.7
1	A	484	ALA	3.7
1	A	421	SER	3.7
1	A	486	ASN	3.6
1	A	338	PHE	3.6
1	A	143	ARG	3.6
1	A	201	LEU	3.5
1	A	159	ALA	3.4
1	A	158	GLY	3.4
1	A	49	LEU	3.4
1	A	145	ASP	3.4
1	A	155	ILE	3.4
1	A	342	LEU	3.3
1	A	481	GLY	3.2
1	A	157	LEU	3.2
1	A	476	GLN	3.2
1	A	344	THR	3.1
1	A	315	ASP	3.0
1	A	29	TYR	3.0
1	A	146	ALA	3.0
1	A	488	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	60	MET	3.0
1	A	36	LEU	3.0
1	A	422	GLN	3.0
1	A	420	ASN	3.0
1	A	317	SER	2.9
1	A	23	MET	2.9
1	A	240	LEU	2.9
1	A	284	SER	2.9
1	A	44	ILE	2.8
1	A	409	SER	2.8
1	A	148	PHE	2.8
1	A	164	LEU	2.8
1	A	163	PRO	2.7
1	A	203	PRO	2.7
1	A	64	ALA	2.7
1	A	306	LEU	2.7
1	A	27	PHE	2.7
1	A	408	LEU	2.7
1	A	51	ILE	2.7
1	A	199	LYS	2.6
1	A	352	SER	2.6
1	A	264	TYR	2.6
1	A	343	TRP	2.5
1	A	305	VAL	2.4
1	A	46	THR	2.4
1	A	20	MET	2.4
1	A	302	GLY	2.4
1	A	30	TYR	2.4
1	A	242	GLY	2.3
1	A	162	ALA	2.3
1	A	106	PHE	2.3
1	A	487	LEU	2.3
1	A	68	TYR	2.3
1	A	332	ILE	2.3
1	A	34	ALA	2.2
1	A	301	GLN	2.2
1	A	33	ARG	2.2
1	A	32	MET	2.2
1	A	327	LEU	2.2
1	A	304	VAL	2.1
1	A	156	ASN	2.1
1	A	245	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	31	GLY	2.1
1	A	202	ASP	2.1
1	A	126	LYS	2.1
1	A	210	ASP	2.0
1	A	35	ILE	2.0
1	A	401	MET	2.0

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 carbohydrates 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.

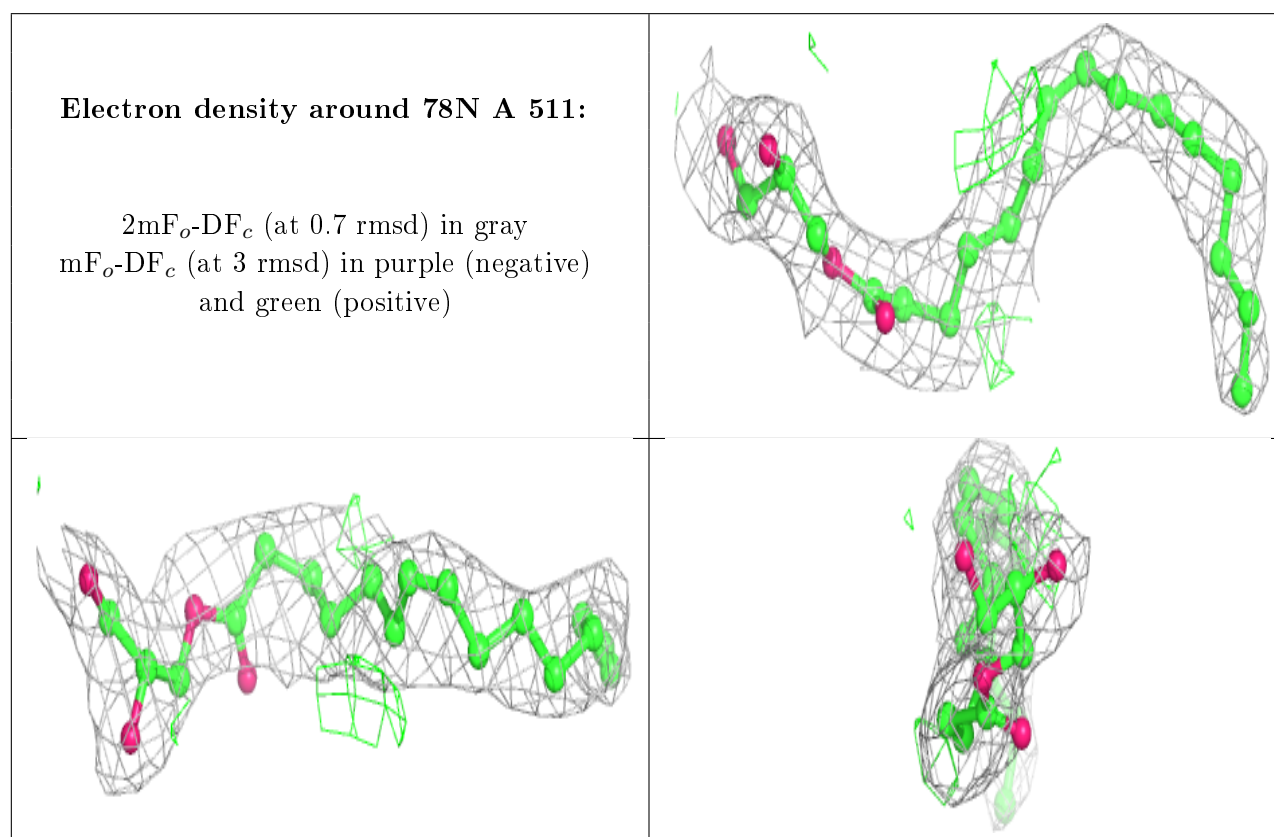
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	78N	A	511	22/22	0.55	0.31	68,95,101,106	0
4	78N	A	523	22/22	0.64	0.42	92,106,110,115	0
3	1PE	A	506	13/16	0.65	0.27	111,111,116,117	0
4	78N	A	522	22/22	0.66	0.41	86,98,108,110	0
4	78N	A	514	22/22	0.69	0.29	61,98,115,117	0
4	78N	A	516	22/22	0.70	0.30	86,91,97,98	0
4	78N	A	517	22/22	0.70	0.20	85,92,100,103	0
4	78N	A	515	22/22	0.72	0.35	92,98,109,110	0
4	78N	A	520	22/22	0.72	0.32	70,99,125,129	0
5	78M	A	518	22/22	0.73	0.29	67,95,110,111	0
4	78N	A	519	22/22	0.77	0.25	69,90,95,96	0
4	78N	A	512	22/22	0.78	0.26	73,84,113,113	0
4	78N	A	508	22/22	0.78	0.25	55,77,87,91	0
5	78M	A	510	22/22	0.80	0.21	62,73,115,116	0
2	PO4	A	504	5/5	0.80	0.35	149,150,151,155	0
4	78N	A	509	22/22	0.81	0.27	60,77,127,129	0
3	1PE	A	507	16/16	0.83	0.46	70,76,105,105	0

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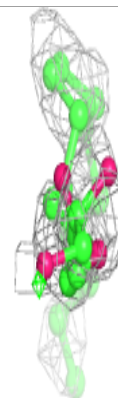
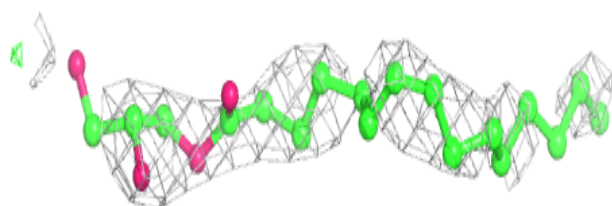
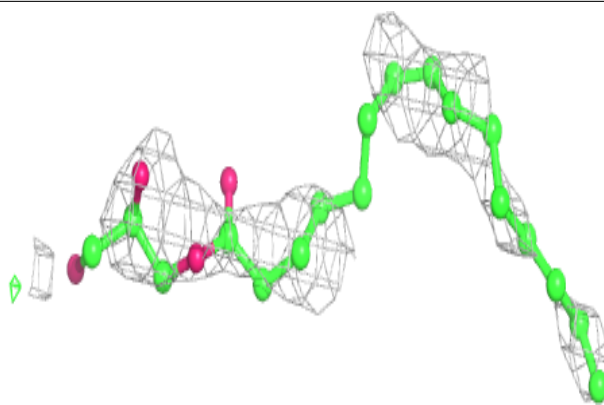
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	78N	A	513	22/22	0.84	0.21	77,97,105,108	0
2	PO4	A	505	5/5	0.84	0.33	147,147,148,148	0
4	78N	A	521	22/22	0.85	0.25	69,87,95,97	0
2	PO4	A	502	5/5	0.85	0.32	138,138,139,142	0
2	PO4	A	501	5/5	0.96	0.10	73,76,78,84	0
2	PO4	A	503	5/5	0.97	0.17	56,57,61,65	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.

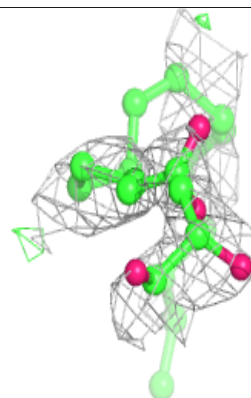
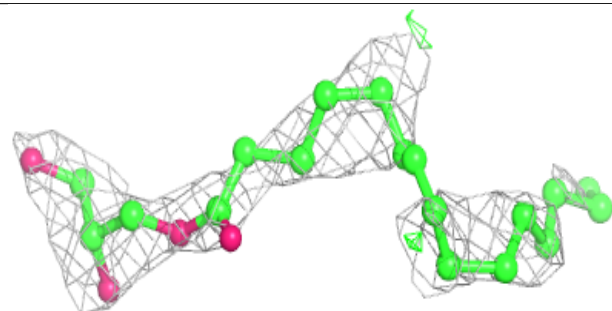
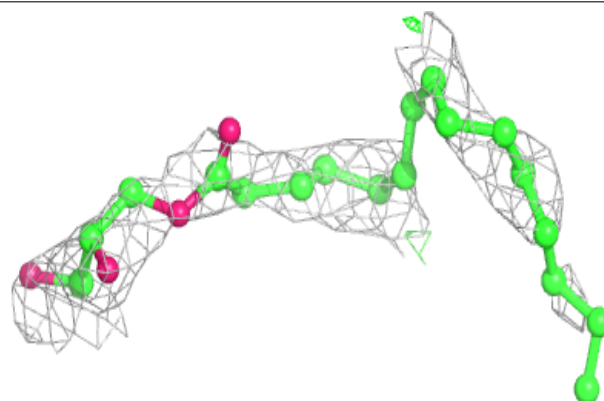


Electron density around 78N A 523:

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

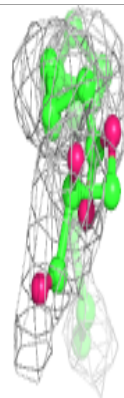
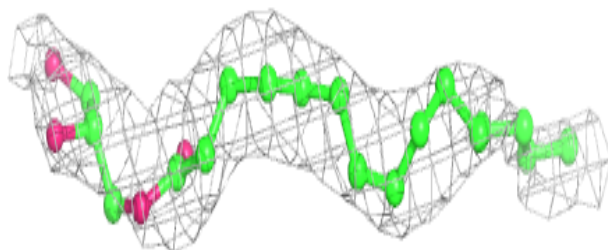
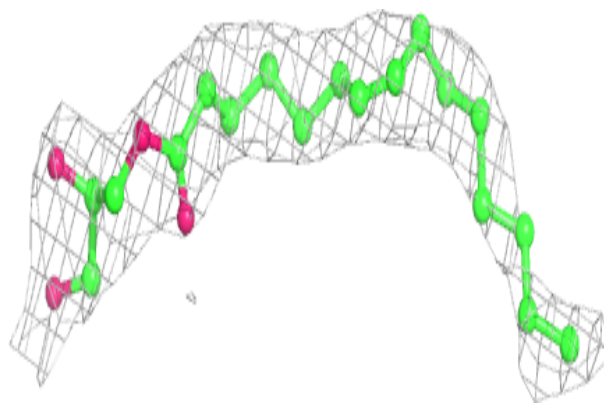
**Electron density around 78N A 522:**

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

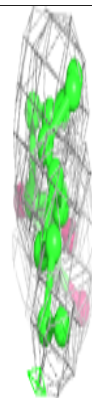
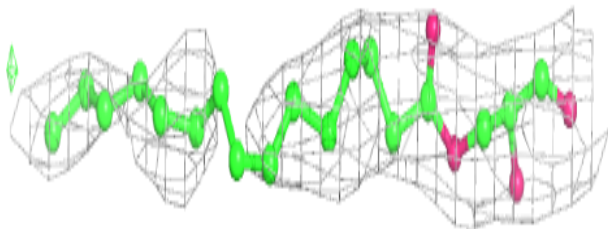
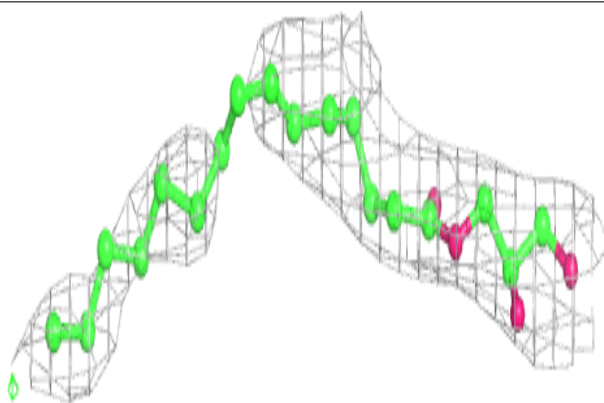


Electron density around 78N A 514:

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

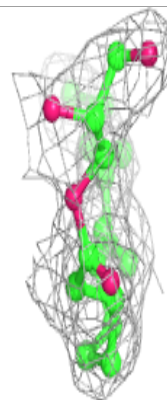
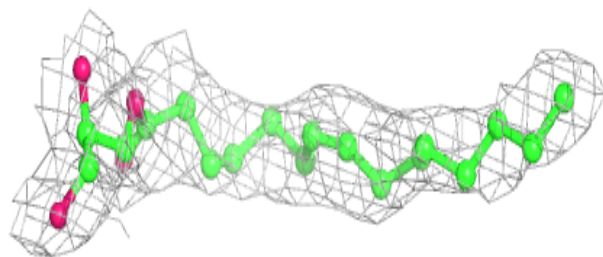
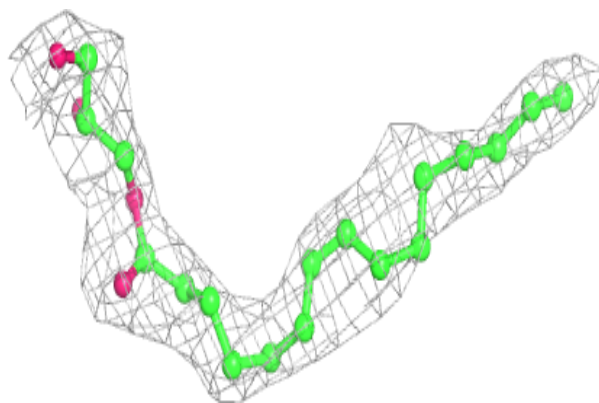
**Electron density around 78N A 516:**

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

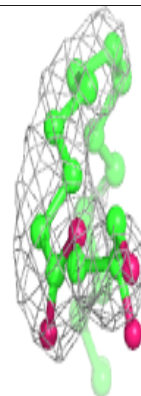
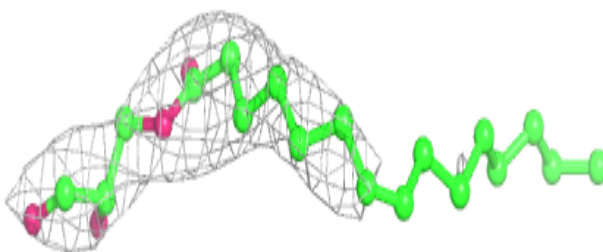
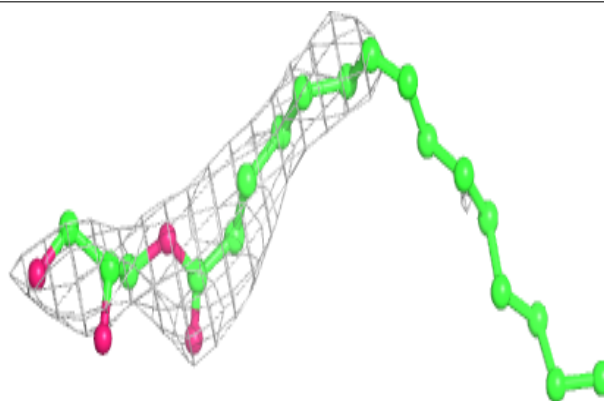


Electron density around 78N A 517:

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

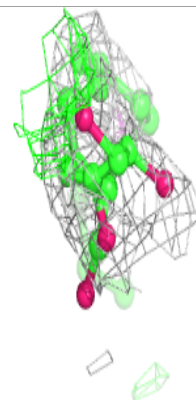
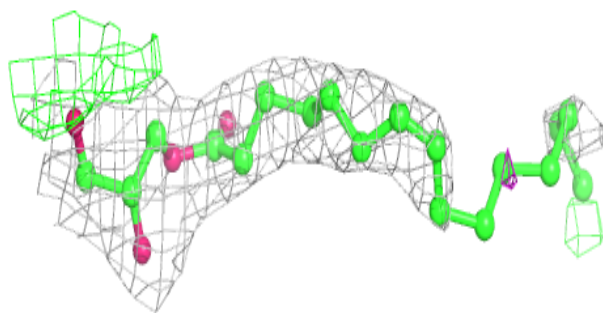
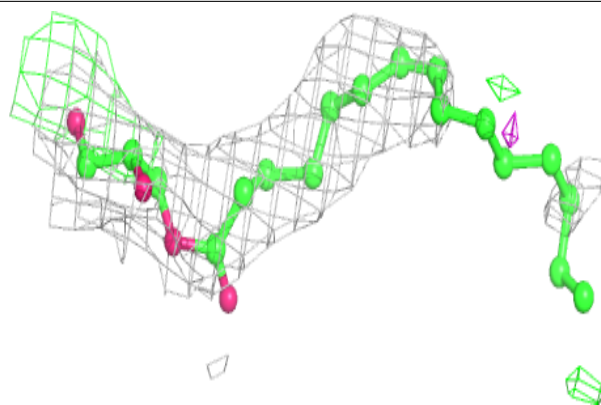
**Electron density around 78N A 515:**

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

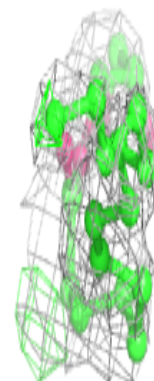
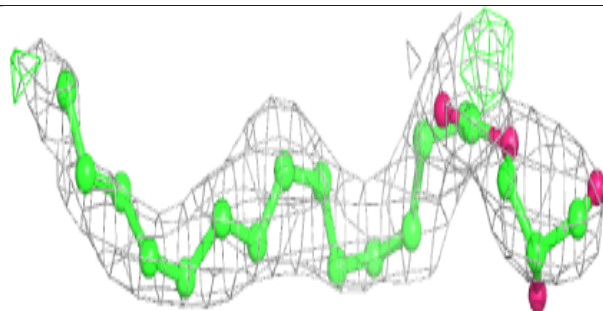
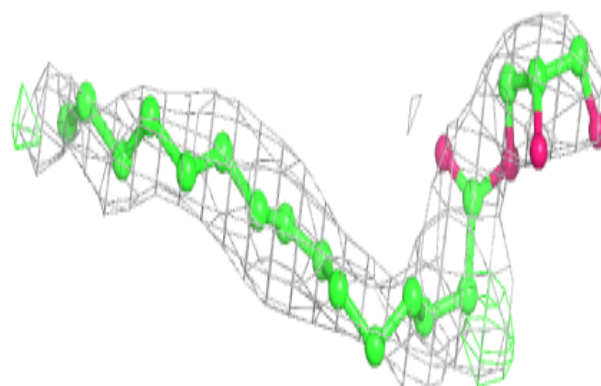


Electron density around 78N A 520:

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

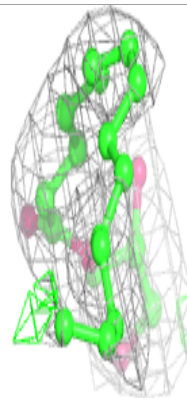
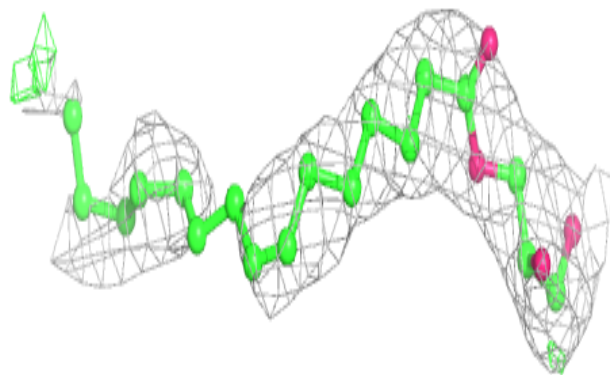
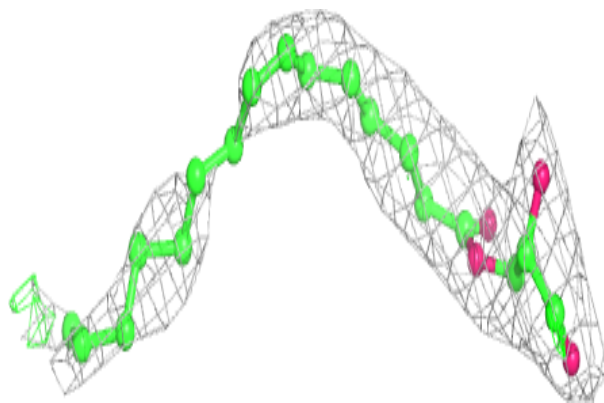
**Electron density around 78M A 518:**

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

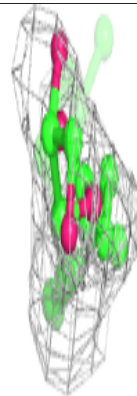
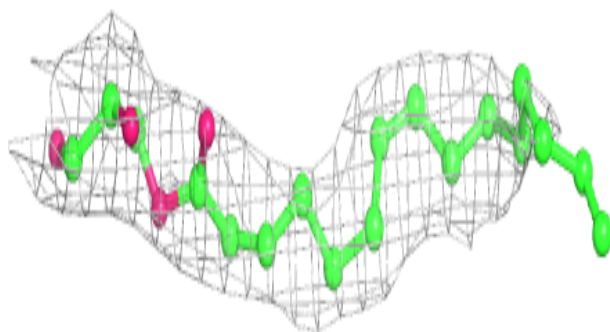
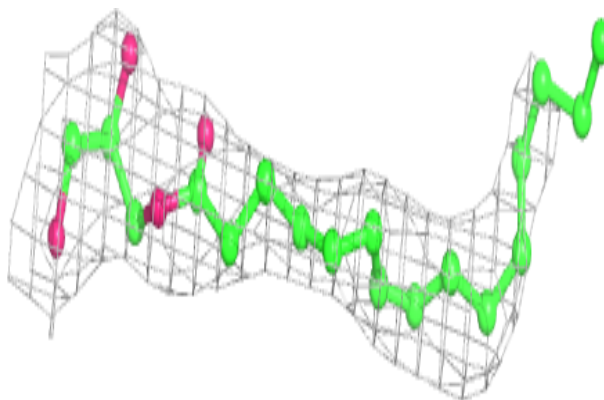


Electron density around 78N A 519:

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

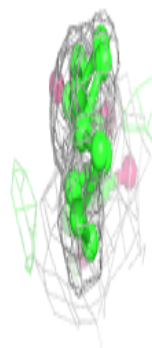
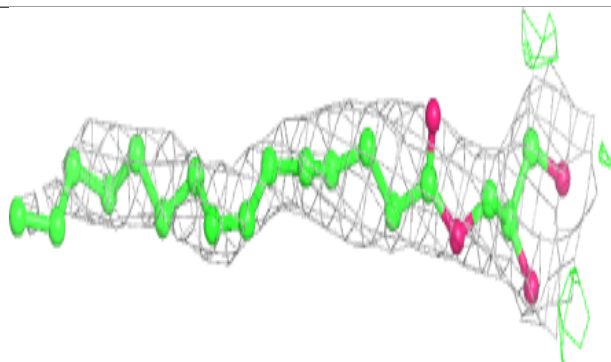
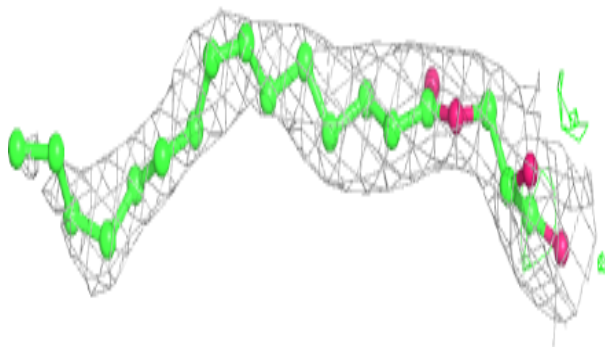
**Electron density around 78N A 512:**

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

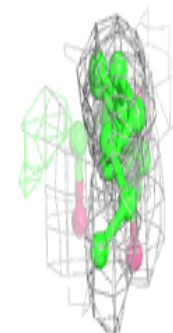
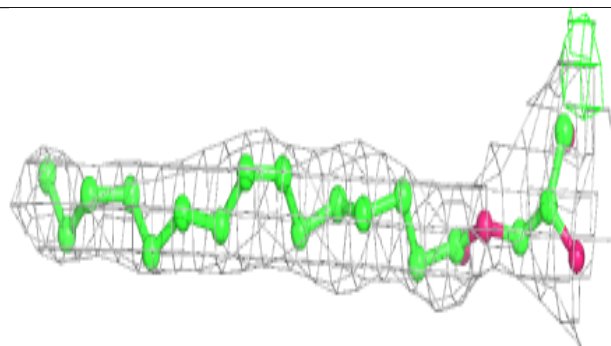
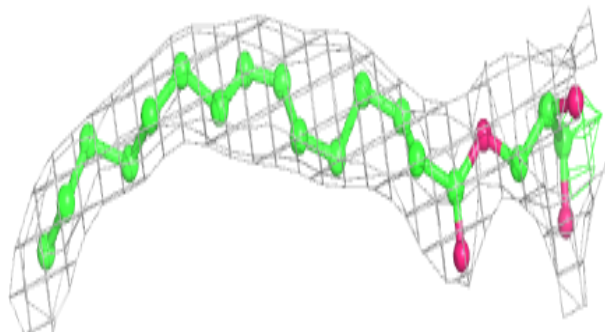


Electron density around 78N A 508:

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

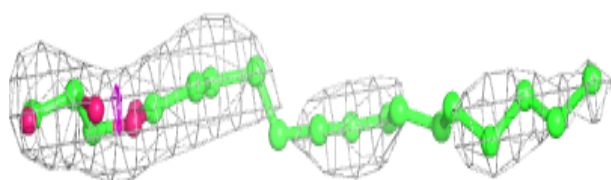
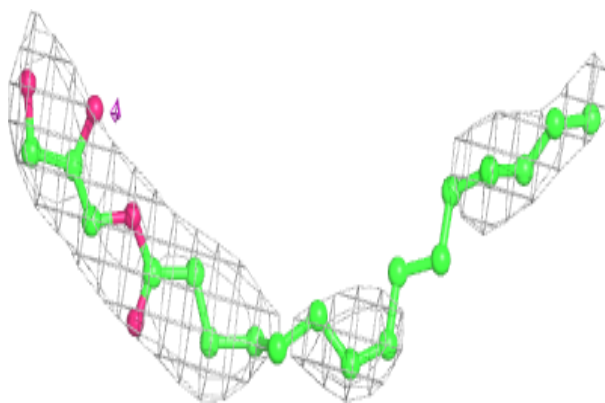
**Electron density around 78M A 510:**

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

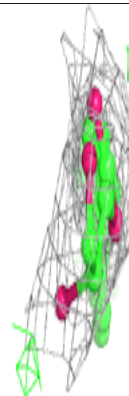
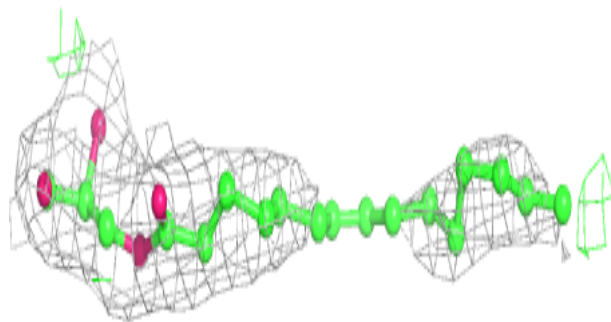
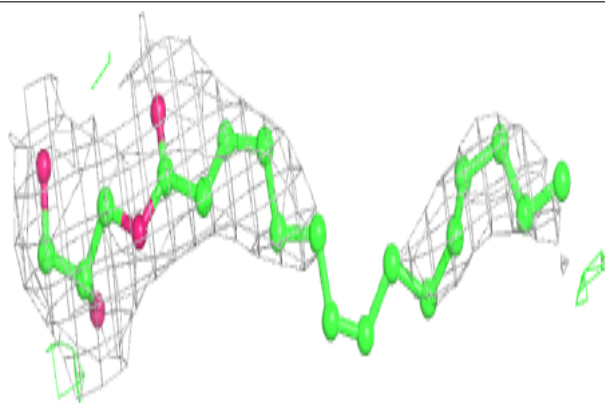


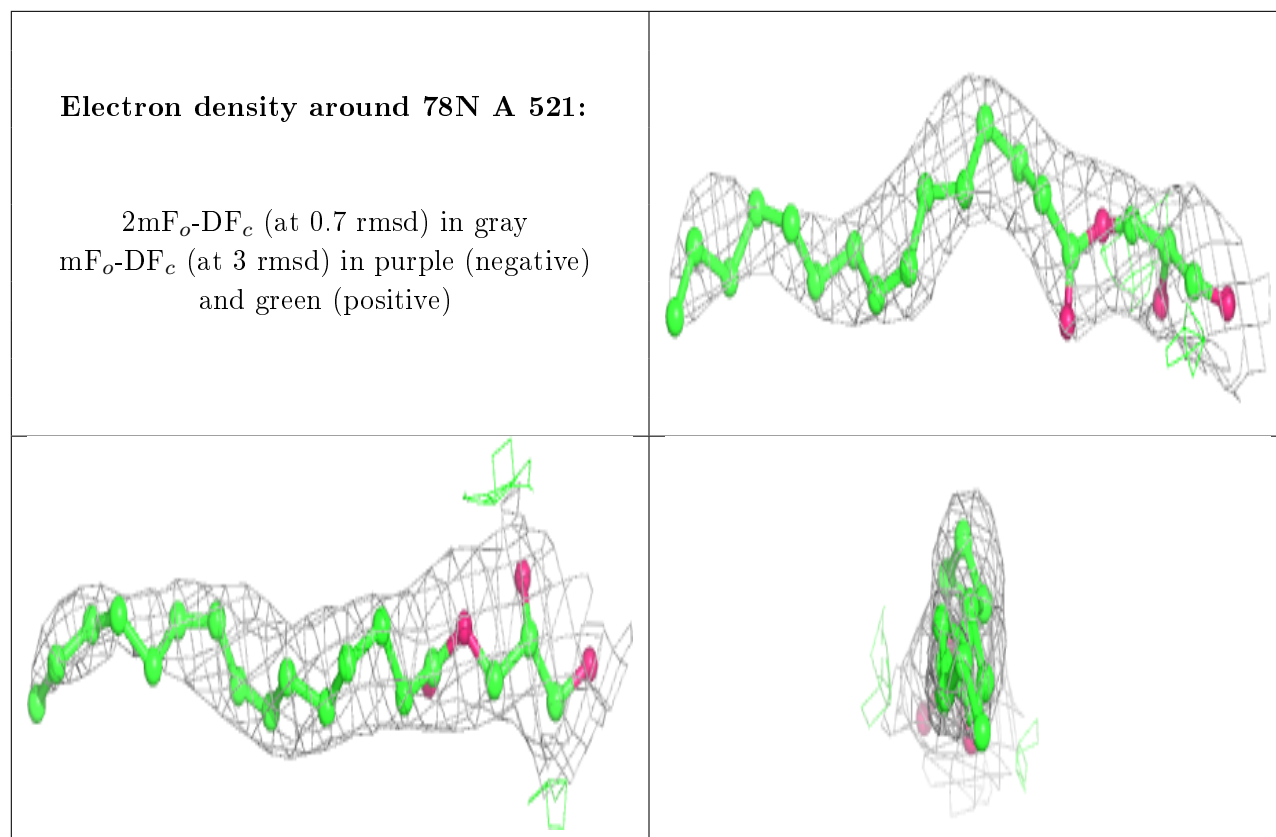
Electron density around 78N A 509:

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

**Electron density around 78N 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.