



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 09:46 PM BST

PDB ID : 5OXN  
Title : PepTSt in complex with dipeptide Phe-Ala  
Authors : Martinez Molledo, M.; Quistgaard, E.M.; Loew, C.  
Deposited on : 2017-09-07  
Resolution : 2.20 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](mailto: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.

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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 : 2.14.4.dev1  
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) : 2.14.4.dev1

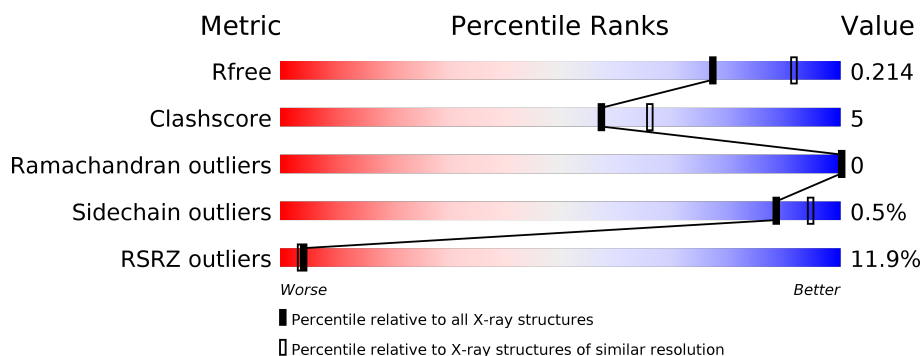
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	<div> <div>11%</div> <div>84%</div> <div>11%</div> <div>6%</div> </div>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 3945 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.

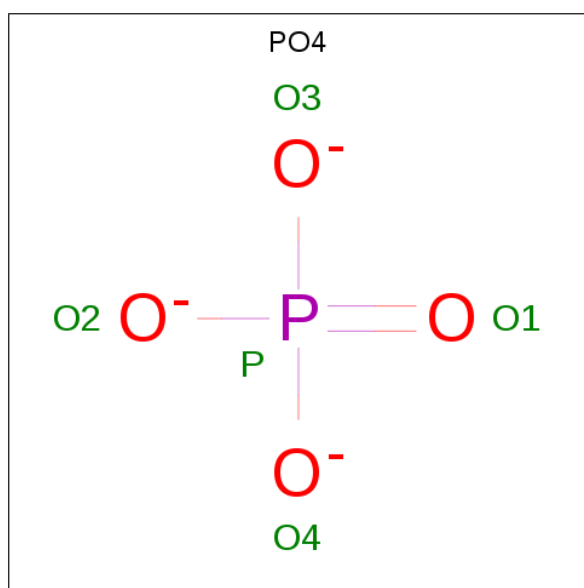
- Molecule 1 is a protein called Di-or tripeptide:H<sup>+</sup> symporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	463	3580	2408	555	600	17	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: O<sub>4</sub>P).

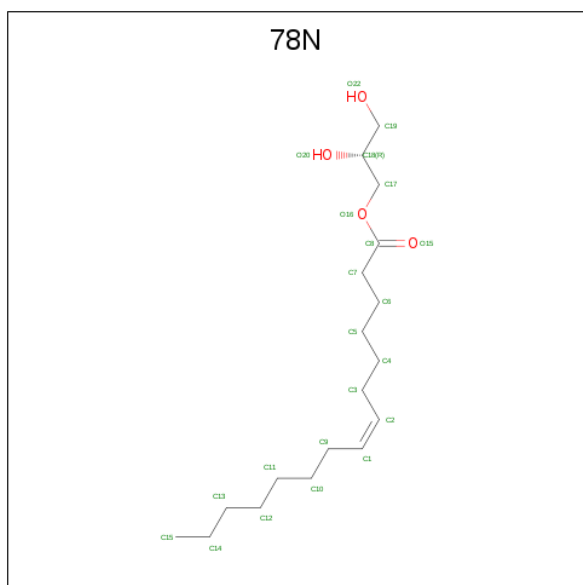


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

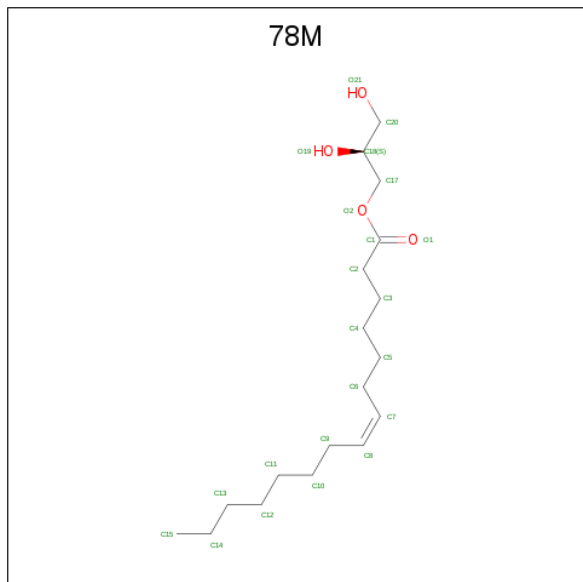
- Molecule 4 is (2R)-2,3-DIHYDROXYPROPYL(7Z)-PENTADEC-7-ENOATE (three-letter code: 78N) (formula: C<sub>18</sub>H<sub>34</sub>O<sub>4</sub>).



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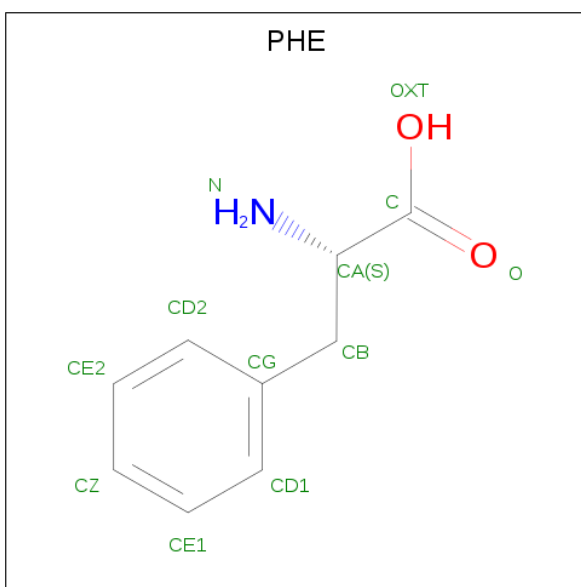
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 22	C 18	O 4	0	0
4	A	1	Total 22	C 18	O 4	0	0
4	A	1	Total 22	C 18	O 4	0	0
4	A	1	Total 22	C 18	O 4	0	0
4	A	1	Total 22	C 18	O 4	0	0

- Molecule 5 is (2S)-2,3-DIHYDROXYPROPYL(7Z)-PENTADEC-7-ENOATE (three-letter code: 78M) (formula: C<sub>18</sub>H<sub>34</sub>O<sub>4</sub>).



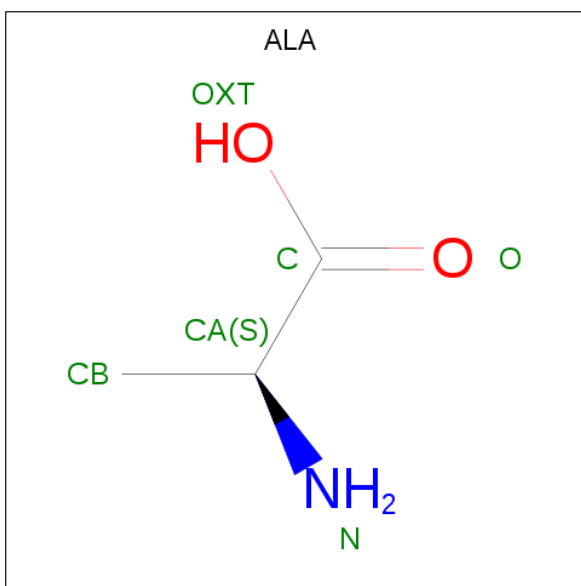
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			22	18	4		

- Molecule 6 is PHENYLALANINE (three-letter code: PHE) (formula:  $\text{C}_9\text{H}_{11}\text{NO}_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 7 is ALANINE (three-letter code: ALA) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			6	3	1	2		

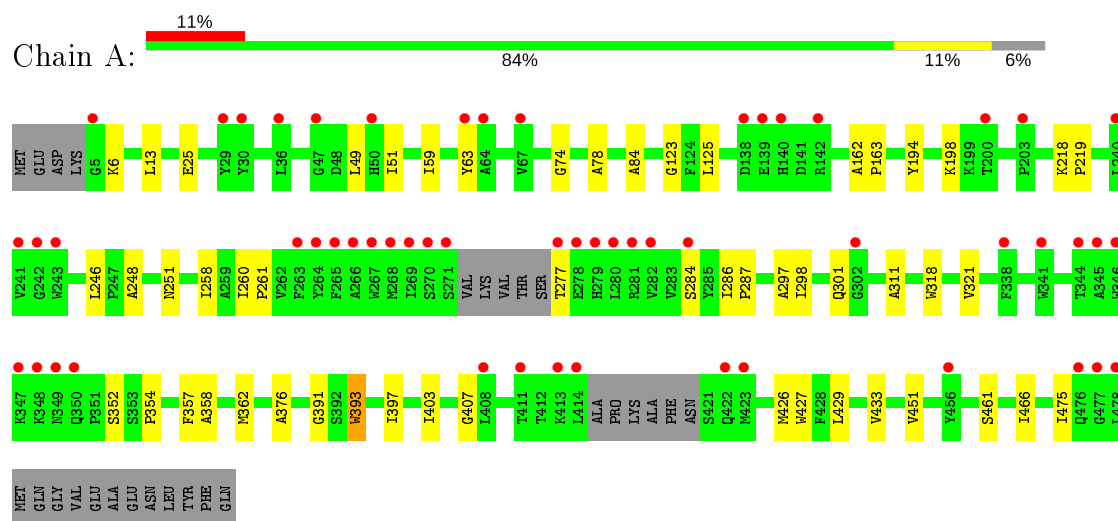
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	73	Total	O	0	0
			73	73		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Di- or tripeptide:H<sup>+</sup> symporter



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.80 Å   107.90 Å   109.80 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	45.80 – 2.20 45.81 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.80-2.20) 99.5 (45.81-2.20)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 2.20 Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.194   ,   0.214 0.196   ,   0.214	Depositor DCC
$R_{free}$ test set	1539 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.2	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3945	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, 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	0.24	0/3686	0.41	0/5025

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	3580	0	3671	34	0
2	A	10	0	0	0	0
3	A	1	0	0	0	0
4	A	242	0	374	12	0
5	A	22	0	34	1	0
6	A	11	0	8	0	0
7	A	6	0	5	0	0
8	A	73	0	0	0	0
All	All	3945	0	4092	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)
1:A:466:ILE:HG21	4:A:515:78N:H2	1.66	0.77
1:A:248:ALA:HA	4:A:511:78N:H172	1.79	0.63
1:A:251:ASN:HD22	4:A:511:78N:H171	1.65	0.61
4:A:509:78N:H1	4:A:510:78N:H92C	1.84	0.60
1:A:59:ILE:HD11	1:A:246:LEU:HD21	1.84	0.59
1:A:6:LYS:HG2	1:A:13:LEU:HD21	1.85	0.58
1:A:391:GLY:HA3	5:A:506:78M:H42C	1.86	0.57
1:A:466:ILE:CG2	4:A:515:78N:H2	2.35	0.54
1:A:318:TRP:HZ2	4:A:507:78N:H191	1.72	0.53
1:A:426:MET:HA	1:A:429:LEU:HB2	1.90	0.52
4:A:509:78N:H2	4:A:510:78N:H32C	1.91	0.51
1:A:260:ILE:HB	1:A:261:PRO:HD3	1.93	0.50
1:A:284:SER:HB3	1:A:475:ILE:HG23	1.93	0.49
1:A:358:ALA:O	1:A:362:MET:HG3	2.12	0.49
1:A:407:GLY:HA3	1:A:427:TRP:CZ2	2.49	0.47
1:A:74:GLY:HA3	1:A:123:GLY:O	2.15	0.47
1:A:261:PRO:HG2	1:A:433:VAL:HG21	1.98	0.45
1:A:357:PHE:HA	1:A:403:ILE:HG12	1.98	0.45
1:A:286:ILE:HB	1:A:287:PRO:HD3	1.98	0.45
1:A:352:SER:HB2	1:A:354:PRO:HD2	1.98	0.45
1:A:284:SER:O	1:A:287:PRO:HD2	2.17	0.45
1:A:376:ALA:HA	4:A:504:78N:H192	1.98	0.45
4:A:512:78N:H91C	4:A:512:78N:H31C	1.70	0.45
1:A:162:ALA:HB3	1:A:163:PRO:HD3	1.99	0.44
4:A:508:78N:H91C	4:A:508:78N:H32C	1.77	0.44
1:A:277:THR:O	1:A:277:THR:OG1	2.26	0.43
1:A:194:TYR:CZ	1:A:198:LYS:HE3	2.54	0.43
1:A:25:GLU:HG3	1:A:125:LEU:HD22	2.01	0.43
1:A:451:VAL:HG11	4:A:504:78N:H171	2.01	0.43
1:A:258:ILE:O	1:A:261:PRO:HD2	2.18	0.43
1:A:311:ALA:HA	1:A:321:VAL:HG21	2.01	0.42
1:A:49:LEU:HG	1:A:51:ILE:HG12	2.00	0.42
1:A:393:TRP:O	1:A:397:ILE:HG12	2.19	0.42
1:A:297:ALA:O	1:A:301:GLN:HG3	2.20	0.41
1:A:218:LYS:HB3	1:A:219:PRO:HD3	2.02	0.41
1:A:261:PRO:HG2	1:A:433:VAL:CG2	2.50	0.41
1:A:78:ALA:HB1	1:A:84:ALA:HA	2.02	0.41
1:A:298:ILE:HD11	1:A:461:SER:OG	2.20	0.40
4:A:507:78N:H62C	4:A:507:78N:H31C	1.69	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	457/490 (93%)	452 (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	374/397 (94%)	372 (100%)	2 (0%)	88	94

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

Mol	Chain	Res	Type
1	A	63	TYR
1	A	393	TRP

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 ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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	511	-	21,21,21	0.95	1 (4%)	22,22,22	1.02	1 (4%)
4	78N	A	509	-	21,21,21	0.93	1 (4%)	22,22,22	0.89	1 (4%)
4	78N	A	510	-	21,21,21	0.96	1 (4%)	22,22,22	0.95	1 (4%)
2	PO4	A	502	-	4,4,4	0.91	0	6,6,6	0.40	0
6	PHE	A	516	-	10,11,12	0.40	0	10,13,15	0.32	0
4	78N	A	514	-	21,21,21	0.96	1 (4%)	22,22,22	0.92	1 (4%)
2	PO4	A	501	-	4,4,4	0.94	0	6,6,6	0.44	0
4	78N	A	504	-	21,21,21	0.92	1 (4%)	22,22,22	0.98	1 (4%)
4	78N	A	507	-	21,21,21	0.97	1 (4%)	22,22,22	0.91	1 (4%)
7	ALA	A	517	-	2,5,5	0.47	0	2,6,6	0.59	0
4	78N	A	513	-	21,21,21	0.95	1 (4%)	22,22,22	0.96	1 (4%)
4	78N	A	512	-	21,21,21	0.93	1 (4%)	22,22,22	0.96	1 (4%)
4	78N	A	515	-	21,21,21	0.93	1 (4%)	22,22,22	0.97	1 (4%)
4	78N	A	505	-	21,21,21	0.95	1 (4%)	22,22,22	0.97	1 (4%)
4	78N	A	508	-	21,21,21	0.93	1 (4%)	22,22,22	1.03	1 (4%)
5	78M	A	506	-	21,21,21	1.13	1 (4%)	22,22,22	0.90	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
4	78N	A	511	-	-	9/21/21/21	-
4	78N	A	509	-	-	10/21/21/21	-
4	78N	A	510	-	-	10/21/21/21	-
6	PHE	A	516	-	-	2/5/6/8	0/1/1/1
4	78N	A	514	-	-	10/21/21/21	-
4	78N	A	504	-	-	9/21/21/21	-
4	78N	A	507	-	-	11/21/21/21	-
7	ALA	A	517	-	-	0/0/4/4	-
4	78N	A	513	-	-	12/21/21/21	-
4	78N	A	512	-	-	8/21/21/21	-
4	78N	A	515	-	-	8/21/21/21	-
4	78N	A	505	-	-	11/21/21/21	-
4	78N	A	508	-	-	11/21/21/21	-
5	78M	A	506	-	-	14/21/21/21	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	506	78M	O2-C1	3.32	1.43	1.33
4	A	505	78N	O16-C8	3.05	1.42	1.33
4	A	507	78N	O16-C8	3.03	1.42	1.33
4	A	510	78N	O16-C8	3.02	1.42	1.33
4	A	514	78N	O16-C8	3.01	1.42	1.33
4	A	504	78N	O16-C8	3.01	1.42	1.33
4	A	509	78N	O16-C8	3.01	1.42	1.33
4	A	511	78N	O16-C8	2.99	1.42	1.33
4	A	512	78N	O16-C8	2.95	1.42	1.33
4	A	513	78N	O16-C8	2.90	1.41	1.33
4	A	515	78N	O16-C8	2.90	1.41	1.33
4	A	508	78N	O16-C8	2.88	1.41	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	511	78N	O16-C8-C7	2.79	120.65	111.91
4	A	505	78N	O16-C8-C7	2.73	120.46	111.91
4	A	510	78N	O16-C8-C7	2.72	120.44	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	513	78N	O16-C8-C7	2.70	120.38	111.91
4	A	508	78N	O16-C8-C7	2.64	120.20	111.91
4	A	507	78N	O16-C8-C7	2.61	120.10	111.91
4	A	504	78N	O16-C8-C7	2.59	120.04	111.91
4	A	514	78N	O16-C8-C7	2.55	119.90	111.91
4	A	512	78N	O16-C8-C7	2.54	119.88	111.91
5	A	506	78M	O2-C1-C2	2.50	119.77	111.91
4	A	515	78N	O16-C8-C7	2.50	119.76	111.91
4	A	509	78N	O16-C8-C7	2.28	119.08	111.91

There are no chirality outliers.

All (125) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	509	78N	C17-C18-C19-O22
4	A	507	78N	C17-C18-C19-O22
4	A	510	78N	C17-C18-C19-O22
4	A	511	78N	C17-C18-C19-O22
4	A	513	78N	O20-C18-C19-O22
4	A	513	78N	C17-C18-C19-O22
4	A	513	78N	O16-C17-C18-C19
4	A	513	78N	O16-C17-C18-O20
4	A	515	78N	O20-C18-C19-O22
4	A	515	78N	C17-C18-C19-O22
4	A	505	78N	O16-C17-C18-C19
4	A	505	78N	O16-C17-C18-O20
4	A	508	78N	O16-C17-C18-C19
4	A	508	78N	O16-C17-C18-O20
5	A	506	78M	C17-C18-C20-O21
5	A	506	78M	O2-C17-C18-C20
5	A	506	78M	O2-C17-C18-O19
4	A	513	78N	O15-C8-O16-C17
4	A	513	78N	C7-C8-O16-C17
4	A	514	78N	C7-C8-O16-C17
4	A	505	78N	C7-C8-O16-C17
4	A	514	78N	O15-C8-O16-C17
4	A	505	78N	O15-C8-O16-C17
4	A	504	78N	O16-C17-C18-C19
4	A	510	78N	O20-C18-C19-O22
4	A	511	78N	O20-C18-C19-O22
5	A	506	78M	O19-C18-C20-O21
4	A	513	78N	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
4	A	515	78N	C5-C6-C7-C8
4	A	510	78N	O16-C17-C18-O20
4	A	504	78N	O16-C17-C18-O20
4	A	510	78N	C7-C8-O16-C17
4	A	511	78N	C7-C8-O16-C17
4	A	509	78N	C9-C10-C11-C12
4	A	505	78N	C9-C10-C11-C12
5	A	506	78M	C10-C11-C12-C13
4	A	504	78N	C7-C8-O16-C17
4	A	510	78N	O16-C17-C18-C19
5	A	506	78M	C9-C10-C11-C12
4	A	507	78N	C4-C5-C6-C7
4	A	511	78N	C3-C4-C5-C6
4	A	509	78N	C5-C6-C7-C8
4	A	513	78N	C4-C5-C6-C7
4	A	514	78N	C3-C4-C5-C6
4	A	508	78N	C4-C5-C6-C7
4	A	505	78N	C3-C4-C5-C6
5	A	506	78M	C2-C3-C4-C5
4	A	510	78N	O15-C8-O16-C17
4	A	508	78N	C17-C18-C19-O22
4	A	514	78N	C11-C12-C13-C14
4	A	511	78N	C4-C5-C6-C7
4	A	510	78N	C3-C4-C5-C6
4	A	507	78N	O20-C18-C19-O22
5	A	506	78M	C11-C12-C13-C14
4	A	511	78N	O15-C8-O16-C17
4	A	504	78N	O15-C8-O16-C17
4	A	509	78N	C11-C12-C13-C14
4	A	507	78N	C2-C3-C4-C5
4	A	511	78N	C2-C3-C4-C5
4	A	505	78N	C2-C3-C4-C5
4	A	508	78N	C2-C3-C4-C5
4	A	514	78N	C5-C6-C7-C8
4	A	515	78N	C7-C8-O16-C17
4	A	514	78N	C4-C5-C6-C7
4	A	515	78N	C4-C5-C6-C7
4	A	505	78N	C5-C6-C7-C8
4	A	507	78N	C11-C10-C9-C1
4	A	513	78N	C11-C10-C9-C1
4	A	508	78N	C10-C11-C12-C13
4	A	507	78N	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
4	A	507	78N	C3-C4-C5-C6
4	A	509	78N	O20-C18-C19-O22
4	A	508	78N	O20-C18-C19-O22
4	A	515	78N	O15-C8-O16-C17
4	A	509	78N	C12-C13-C14-C15
4	A	512	78N	C12-C13-C14-C15
4	A	508	78N	C7-C8-O16-C17
4	A	512	78N	C4-C5-C6-C7
4	A	505	78N	C4-C5-C6-C7
5	A	506	78M	C3-C4-C5-C6
4	A	512	78N	O16-C17-C18-C19
4	A	508	78N	C12-C13-C14-C15
4	A	509	78N	C2-C3-C4-C5
5	A	506	78M	C1-C2-C3-C4
4	A	508	78N	O15-C8-O16-C17
4	A	513	78N	C12-C13-C14-C15
6	A	516	PHE	CA-CB-CG-CD1
4	A	505	78N	C10-C11-C12-C13
4	A	504	78N	C11-C10-C9-C1
4	A	504	78N	C9-C10-C11-C12
4	A	512	78N	C2-C3-C4-C5
4	A	513	78N	C10-C11-C12-C13
6	A	516	PHE	CA-CB-CG-CD2
5	A	506	78M	C12-C13-C14-C15
4	A	510	78N	C1-C2-C3-C4
4	A	515	78N	C11-C10-C9-C1
4	A	512	78N	C9-C10-C11-C12
4	A	512	78N	C17-C18-C19-O22
4	A	511	78N	C1-C2-C3-C4
5	A	506	78M	C7-C8-C9-C10
4	A	507	78N	C7-C8-O16-C17
4	A	512	78N	O16-C17-C18-O20
4	A	509	78N	C11-C10-C9-C1
4	A	510	78N	C2-C1-C9-C10
4	A	507	78N	O15-C8-O16-C17
4	A	507	78N	C12-C13-C14-C15
4	A	508	78N	C5-C6-C7-C8
4	A	504	78N	C2-C1-C9-C10
4	A	514	78N	C17-C18-C19-O22
4	A	512	78N	C10-C11-C12-C13
4	A	509	78N	C2-C1-C9-C10
4	A	504	78N	C2-C3-C4-C5

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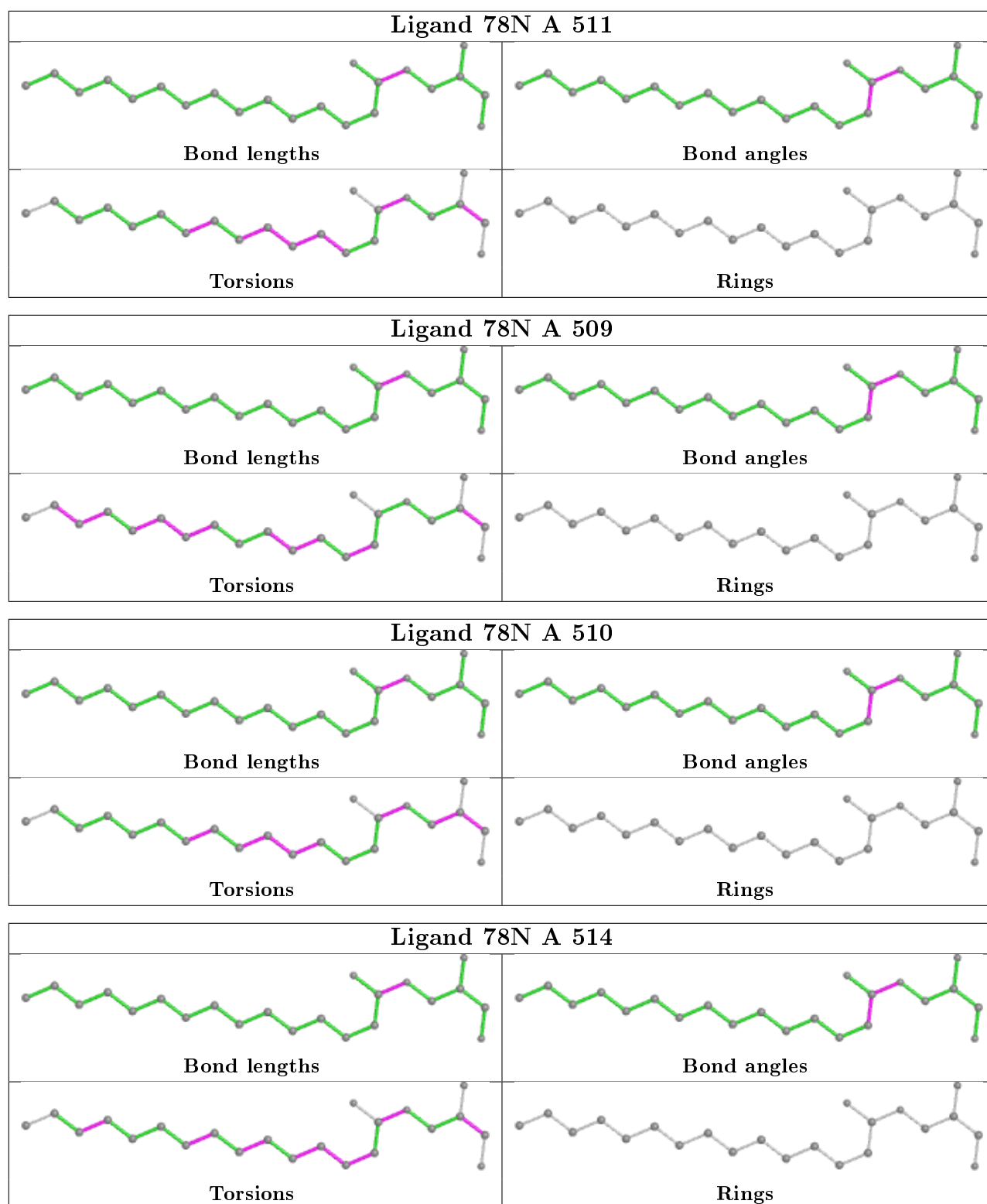
Mol	Chain	Res	Type	Atoms
4	A	514	78N	C1-C2-C3-C4
4	A	505	78N	C2-C1-C9-C10
4	A	509	78N	C3-C4-C5-C6
4	A	515	78N	C10-C11-C12-C13
4	A	514	78N	C2-C1-C9-C10
4	A	513	78N	C11-C12-C13-C14
4	A	507	78N	C11-C12-C13-C14
4	A	511	78N	C2-C1-C9-C10
4	A	504	78N	C10-C11-C12-C13
5	A	506	78M	C4-C5-C6-C7
4	A	514	78N	O20-C18-C19-O22
5	A	506	78M	C5-C6-C7-C8
4	A	510	78N	C2-C3-C4-C5

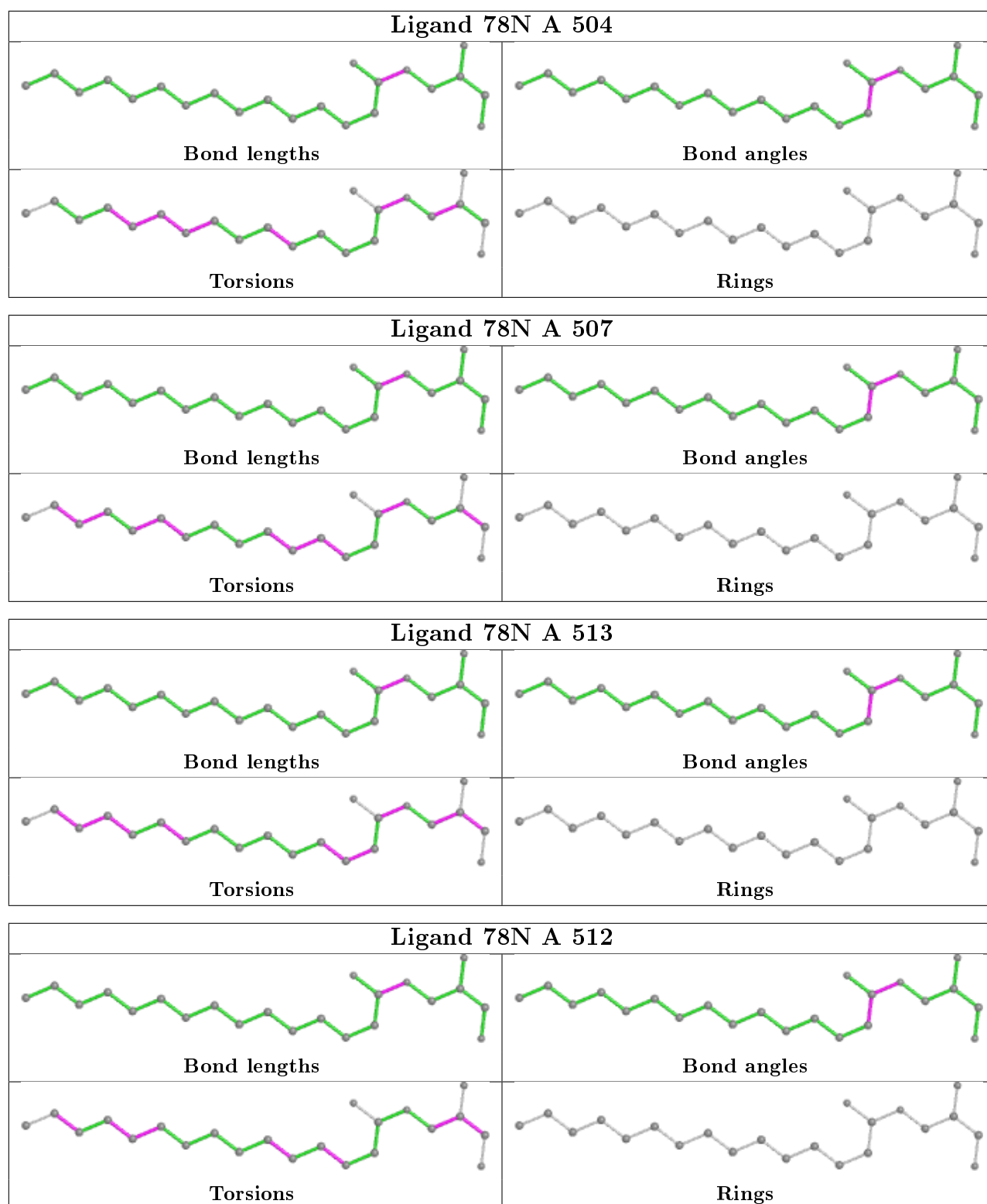
There are no ring outliers.

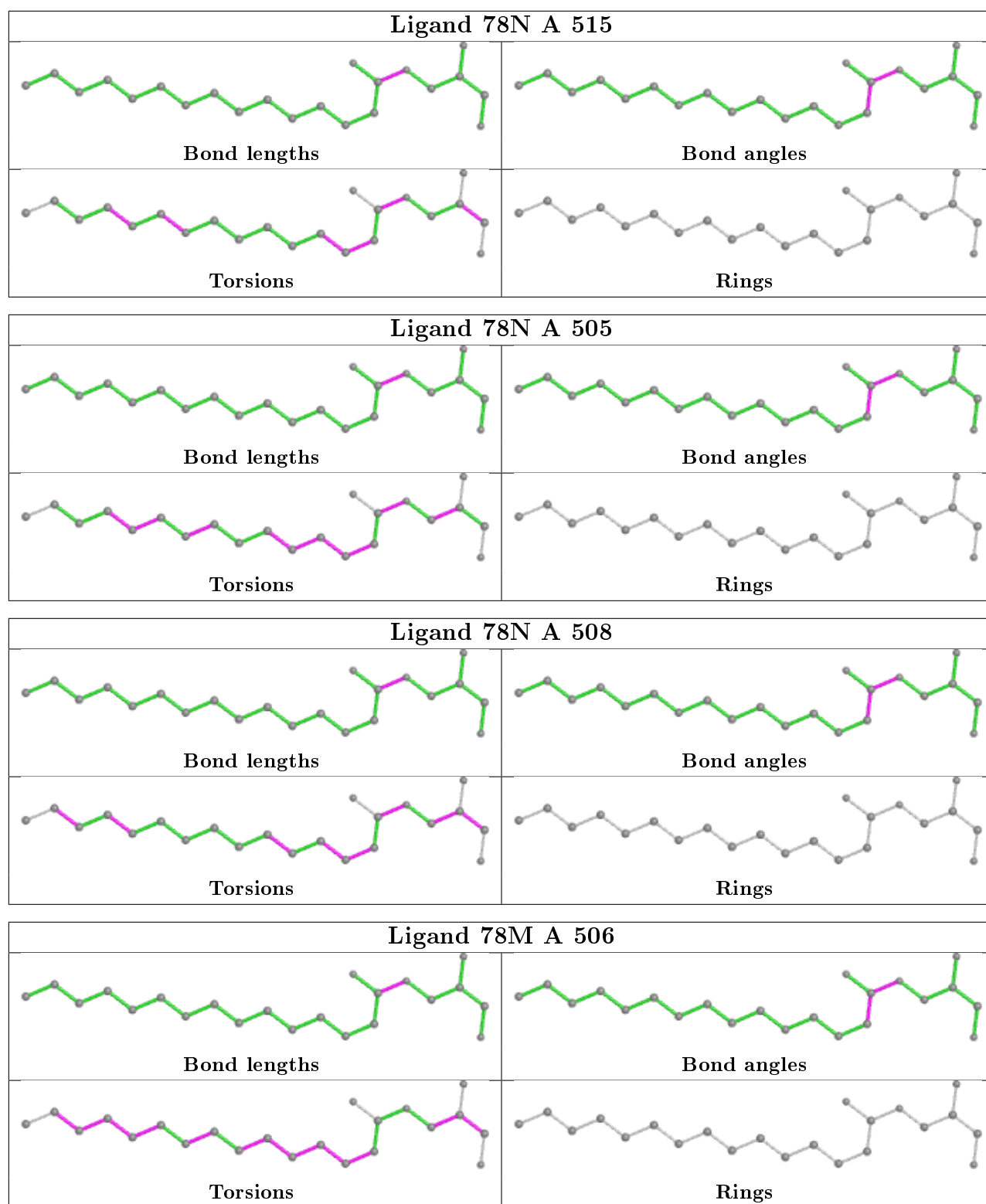
9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	511	78N	2	0
4	A	509	78N	2	0
4	A	510	78N	2	0
4	A	504	78N	2	0
4	A	507	78N	2	0
4	A	512	78N	1	0
4	A	515	78N	2	0
4	A	508	78N	1	0
5	A	506	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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	463/490 (94%)	0.67	55 (11%) 4 4	36, 50, 94, 121	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	348	LYS	10.4
1	A	280	LEU	6.9
1	A	349	ASN	6.8
1	A	140	HIS	6.3
1	A	269	ILE	5.9
1	A	341	TRP	5.8
1	A	278	GLU	5.7
1	A	142	ARG	5.3
1	A	50	HIS	4.8
1	A	346	TRP	4.5
1	A	347	LYS	4.4
1	A	268	MET	4.4
1	A	284	SER	4.4
1	A	422	GLN	4.3
1	A	267	TRP	4.3
1	A	138	ASP	4.3
1	A	350	GLN	4.3
1	A	5	GLY	4.2
1	A	281	ARG	4.2
1	A	423	MET	4.1
1	A	270	SER	4.1
1	A	413	LYS	4.0
1	A	414	LEU	4.0
1	A	338	PHE	3.8
1	A	279	HIS	3.5
1	A	200	THR	3.4
1	A	408	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	265	PHE	3.3
1	A	64	ALA	3.3
1	A	411	THR	3.3
1	A	240	LEU	3.3
1	A	139	GLU	3.2
1	A	344	THR	3.1
1	A	277	THR	3.0
1	A	47	GLY	2.9
1	A	30	TYR	2.8
1	A	264	TYR	2.7
1	A	477	GLY	2.7
1	A	478	LEU	2.7
1	A	29	TYR	2.5
1	A	203	PRO	2.5
1	A	266	ALA	2.5
1	A	271	SER	2.5
1	A	263	PHE	2.5
1	A	476	GLN	2.5
1	A	456	TYR	2.4
1	A	242	GLY	2.4
1	A	243	TRP	2.3
1	A	345	ALA	2.3
1	A	67	VAL	2.3
1	A	282	VAL	2.3
1	A	241	VAL	2.2
1	A	302	GLY	2.1
1	A	63	TYR	2.1
1	A	36	LEU	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 monosaccharides 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,

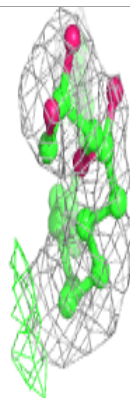
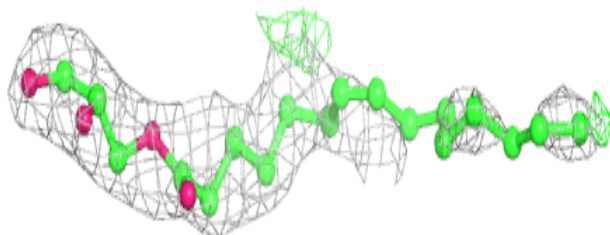
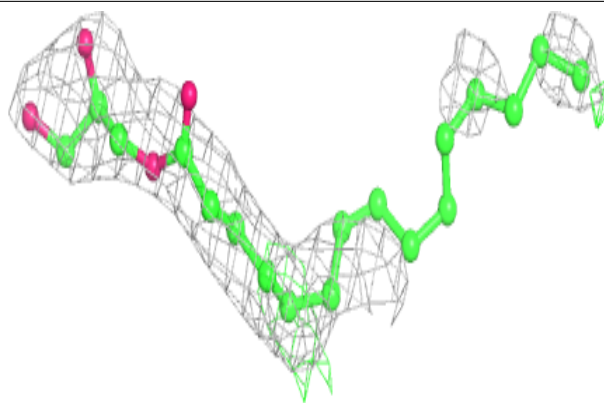
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	78N	A	510	22/22	0.68	0.26	78,100,104,106	0
4	78N	A	511	22/22	0.69	0.28	71,88,93,98	0
4	78N	A	505	22/22	0.76	0.27	75,95,106,107	0
2	PO4	A	502	5/5	0.77	0.33	95,100,109,109	0
4	78N	A	515	22/22	0.78	0.30	80,93,97,99	0
5	78M	A	506	22/22	0.78	0.28	67,90,105,109	0
4	78N	A	514	22/22	0.79	0.32	72,84,96,97	0
4	78N	A	513	22/22	0.81	0.28	76,85,97,100	0
3	NA	A	503	1/1	0.82	0.09	80,80,80,80	0
6	PHE	A	516	11/12	0.83	0.33	60,78,89,91	0
7	ALA	A	517	6/6	0.83	0.46	93,99,100,104	0
4	78N	A	509	22/22	0.83	0.25	68,85,90,96	0
4	78N	A	507	22/22	0.86	0.23	71,81,95,96	0
4	78N	A	504	22/22	0.88	0.21	49,70,90,92	0
4	78N	A	512	22/22	0.90	0.22	44,70,83,85	0
4	78N	A	508	22/22	0.93	0.26	64,75,84,84	0
2	PO4	A	501	5/5	0.95	0.17	68,77,82,88	0

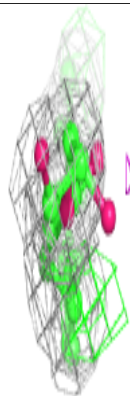
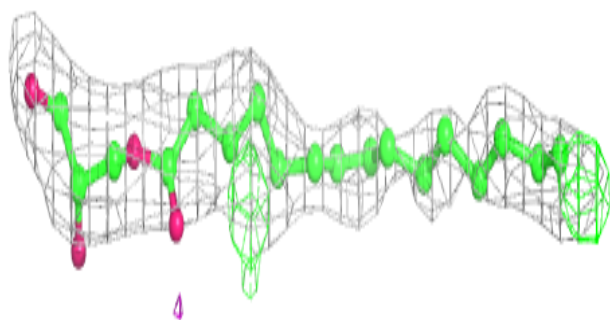
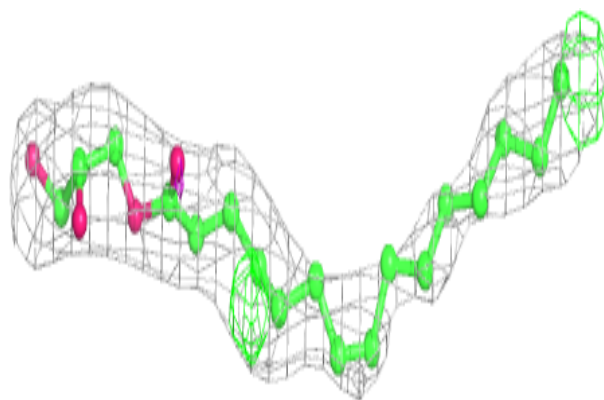
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

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

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

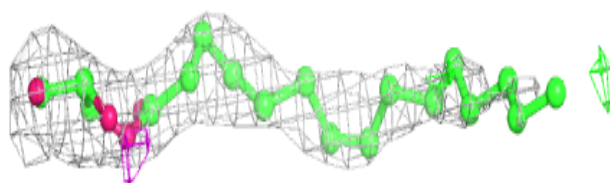
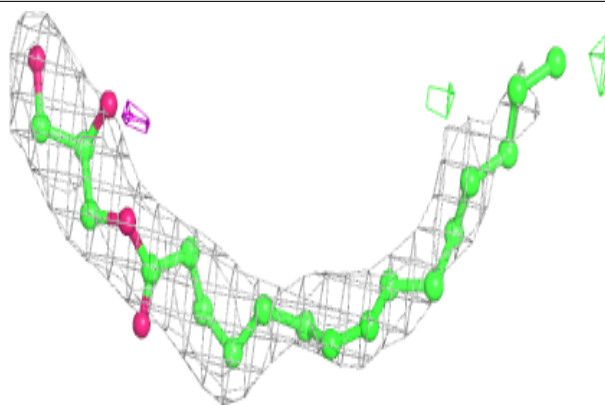
**Electron density around 78N A 511:**

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

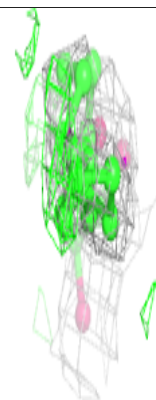
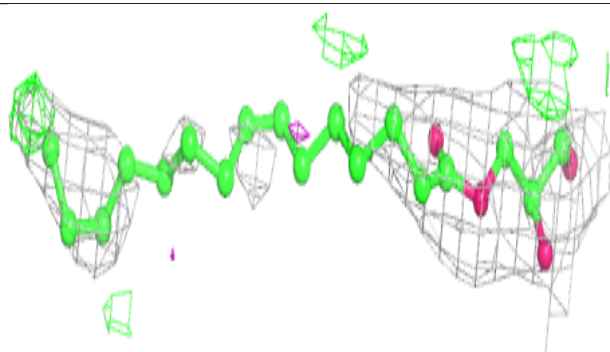
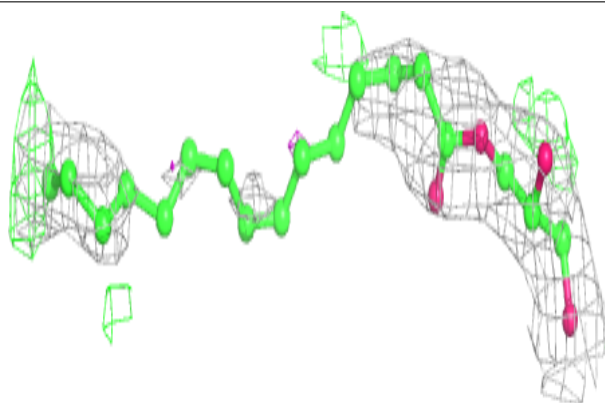


**Electron density around 78N A 505:**

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

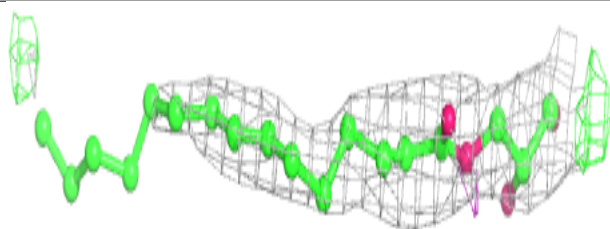
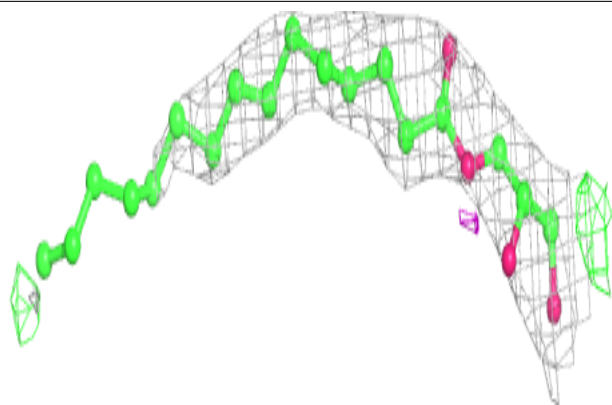
**Electron density around 78N A 515:**

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

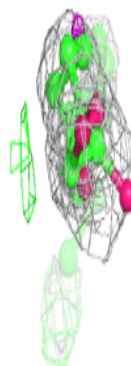
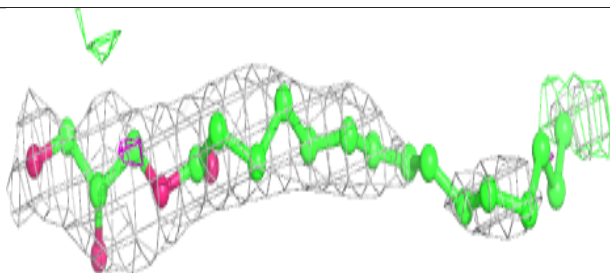
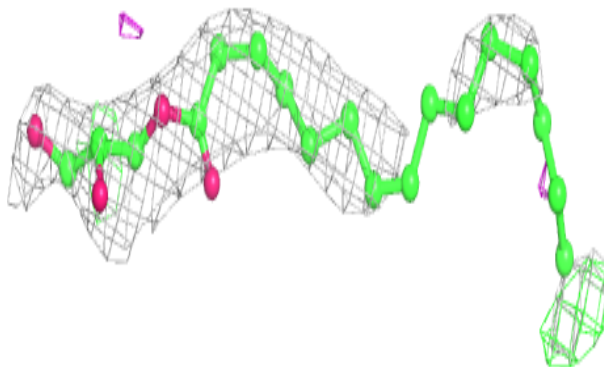


**Electron density around 78M A 506:**

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

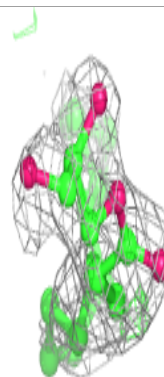
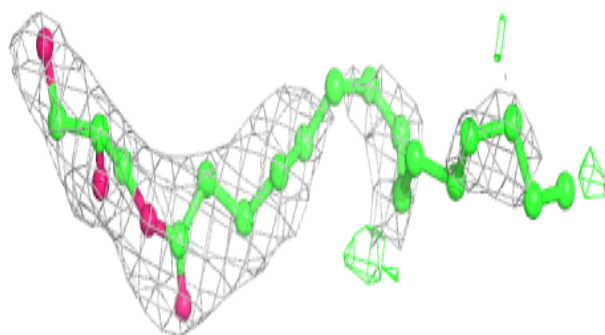
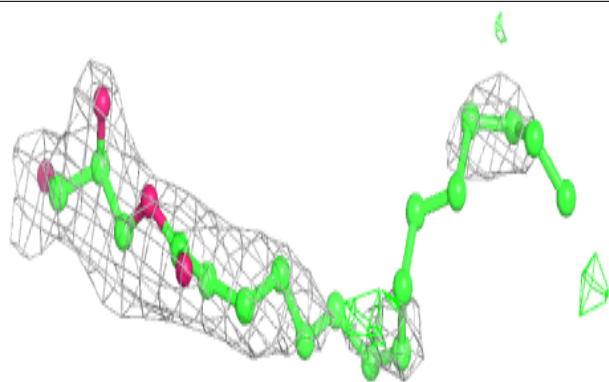
**Electron density around 78N A 514:**

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

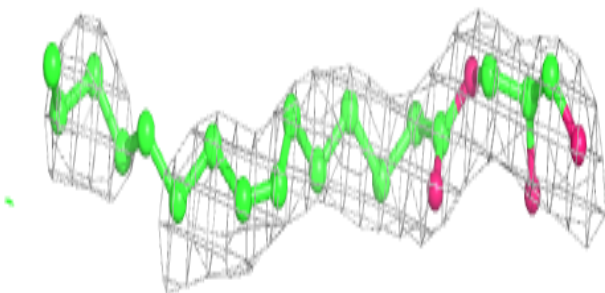
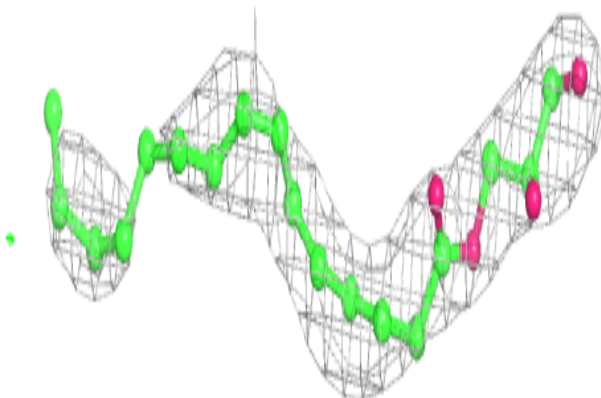


**Electron density around 78N A 513:**

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

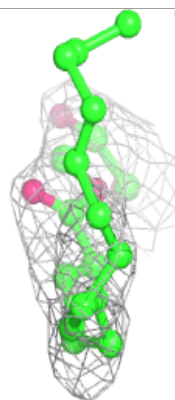
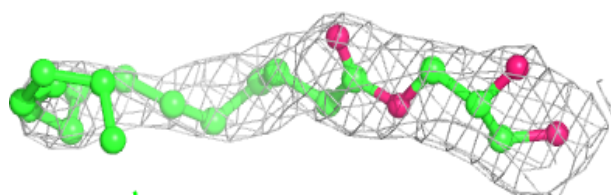
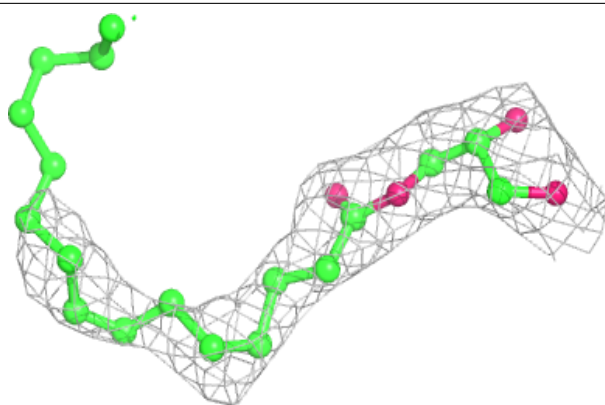
**Electron density around 78N A 509:**

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

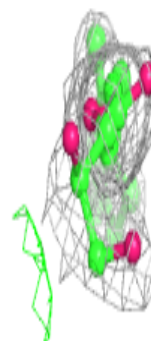
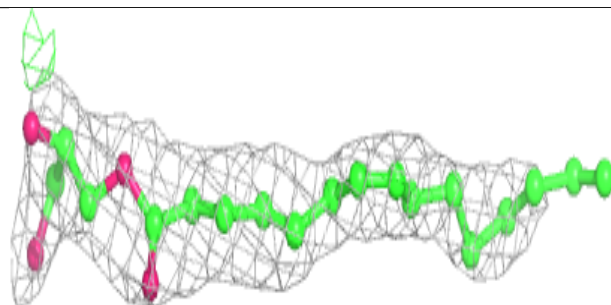
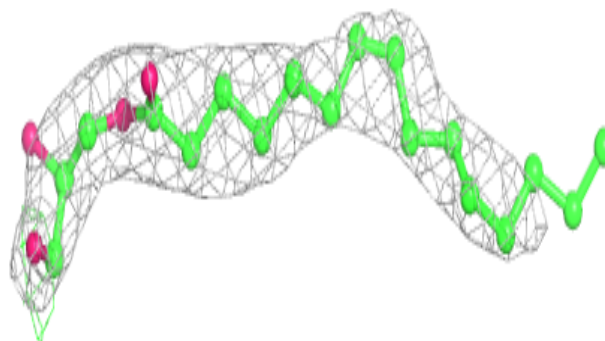


**Electron density around 78N A 507:**

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

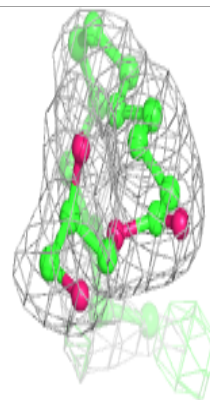
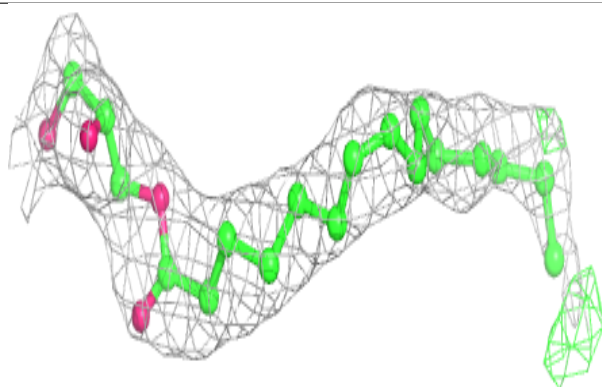
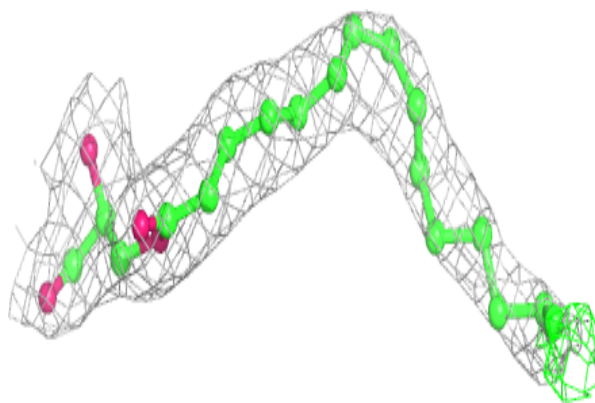
**Electron density around 78N A 504:**

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

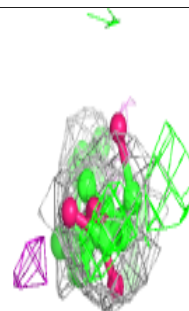
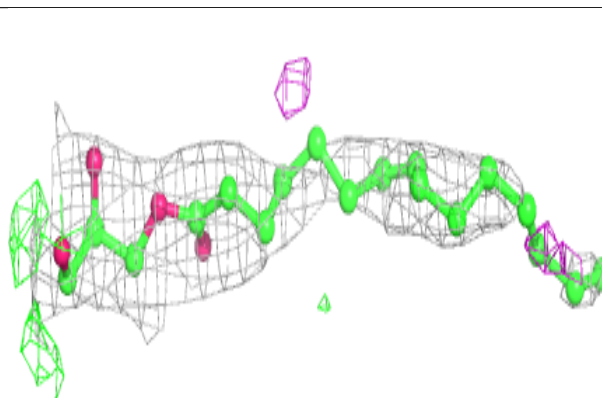
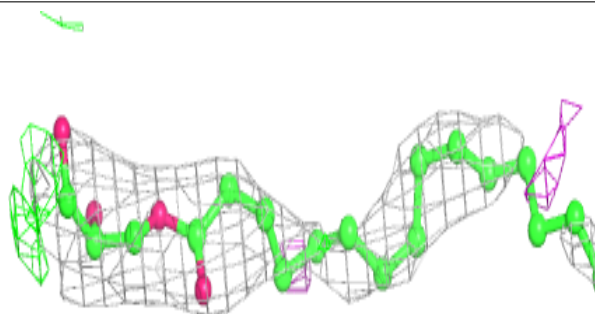


**Electron density around 78N A 512:**

$2mF_o-DF_c$  (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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.