



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 07:43 pm BST

PDB ID : 5D58
Title : In meso in situ serial X-ray crystallography structure of the PepTSt-Ala-Phe complex at 100 K
Authors : Huang, C.-Y.; Olieric, V.; Diederichs, K.; Wang, M.; Caffrey, M.
Deposited on : 2015-08-10
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

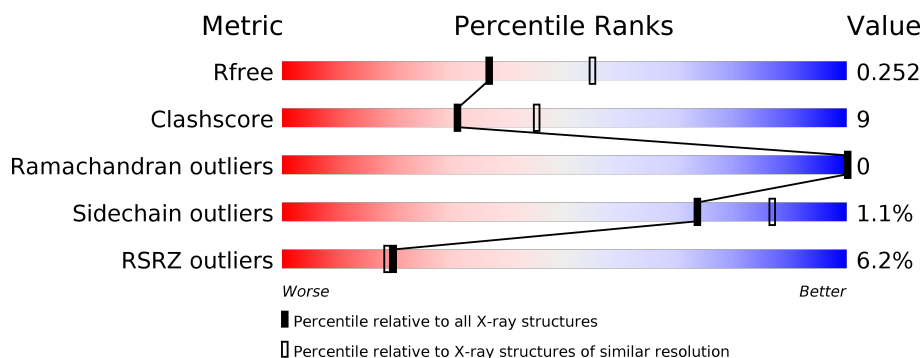
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	483	

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
5	78M	A	523	-	-	-	X

2 Entry composition [i](#)

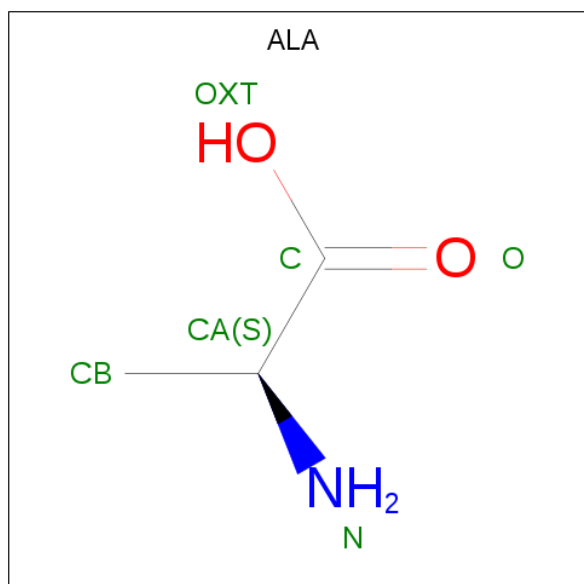
There are 7 unique types of molecules in this entry. The entry contains 4041 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

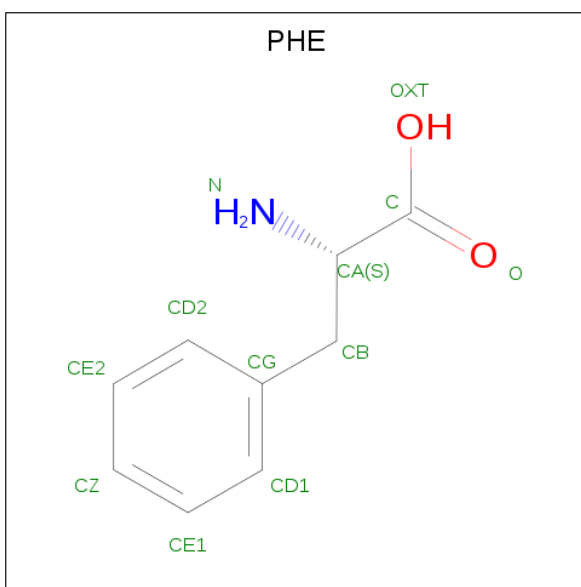
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	448	3475	2342	537	579	17	0	0	0

- Molecule 2 is ALANINE (three-letter code: ALA) (formula: C₃H₇NO₂).



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

- Molecule 3 is PHENYLALANINE (three-letter code: PHE) (formula: C₉H₁₁NO₂).



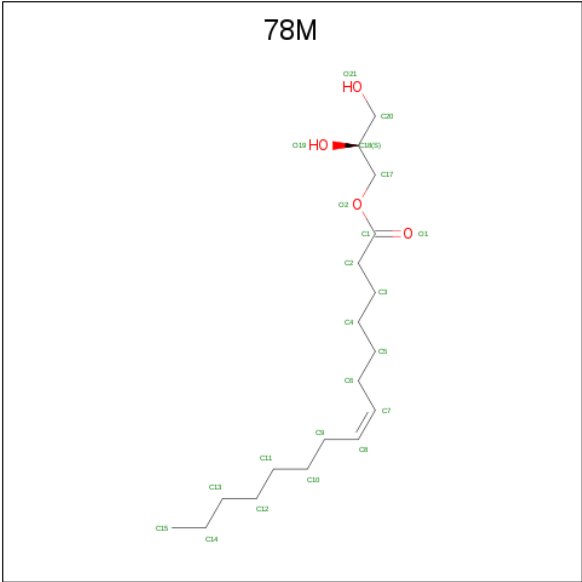
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	9	1	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is (2S)-2,3-DIHYDROXYPROPYL(7Z)-PENTADEC-7-ENOATE (three-letter code: 78M) (formula: $C_{18}H_{34}O_4$).



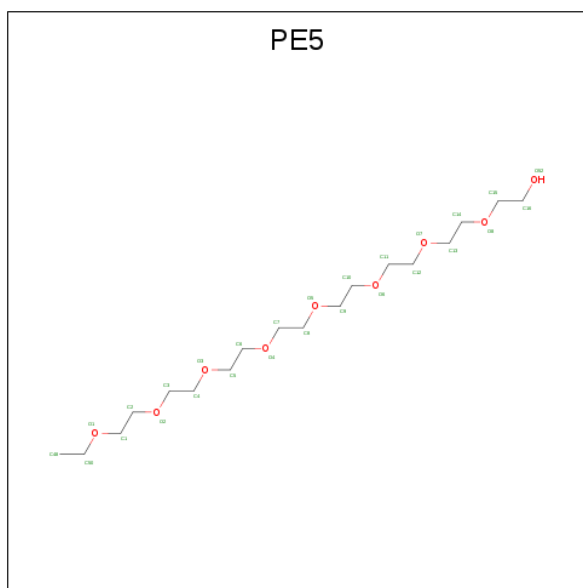
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			22	18	4		
5	A	1	Total	C	O	0	0
			22	18	4		
5	A	1	Total	C	O	0	0
			22	18	4		
5	A	1	Total	C	O	0	0
			22	18	4		
5	A	1	Total	C	O	0	0
			22	18	4		
5	A	1	Total	C	O	0	0
			22	18	4		
5	A	1	Total	C	O	0	0
			22	18	4		
5	A	1	Total	C	O	0	0
			22	18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

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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		
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		

- Molecule 6 is 3,6,9,12,15,18,21,24-OCTAOXAHEXACOSAN-1-OL (three-letter code: PE5) (formula: $C_{18}H_{38}O_9$).



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

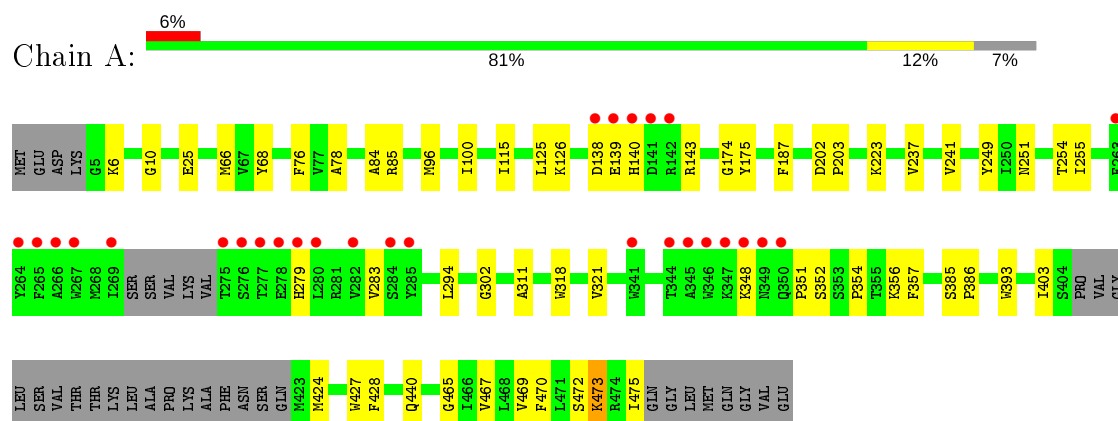
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	64	Total 64	O 64	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	100.16Å 109.52Å 111.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.68 – 2.40 45.68 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.68-2.40) 94.2 (45.68-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.209 , 0.251 0.210 , 0.252	Depositor DCC
R_{free} test set	1218 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.5	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	0.93	EDS
Total number of atoms	4041	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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, PE5

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	0.31	0/3580	0.47	0/4881

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	3475	0	3556	50	0
2	A	5	0	4	0	0
3	A	12	0	9	0	0
4	A	5	0	0	0	0
5	A	462	0	714	42	0
6	A	18	0	20	2	0
7	A	64	0	0	4	0
All	All	4041	0	4303	75	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 9.

All (75) 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:506:78M:H7	5:A:517:78M:H52C	1.75	0.68
1:A:10:GLY:O	1:A:143:ARG:NH1	2.28	0.65
1:A:138:ASP:OD1	1:A:139:GLU:N	2.31	0.64
1:A:175:TYR:H	6:A:525:PE5:H112	1.64	0.63
1:A:352:SER:HB2	1:A:354:PRO:HD2	1.80	0.62
1:A:251:ASN:OD1	1:A:440:GLN:NE2	2.35	0.60
1:A:223:LYS:NZ	7:A:609:HOH:O	2.34	0.60
5:A:514:78M:H112	5:A:519:78M:H41C	1.85	0.59
1:A:302:GLY:HA3	1:A:393:TRP:HH2	1.71	0.56
5:A:513:78M:H111	5:A:516:78M:H7	1.88	0.56
1:A:302:GLY:HA3	1:A:393:TRP:CH2	2.40	0.56
1:A:100:ILE:HD11	5:A:508:78M:H131	1.90	0.54
1:A:66:MET:HG3	5:A:523:78M:H91C	1.91	0.53
1:A:465:GLY:O	1:A:469:VAL:HG23	2.10	0.52
1:A:115:ILE:HD13	5:A:523:78M:H21C	1.93	0.51
1:A:85:ARG:NH2	5:A:514:78M:O21	2.42	0.51
1:A:469:VAL:HA	1:A:472:SER:OG	2.10	0.51
1:A:393:TRP:NE1	7:A:604:HOH:O	2.25	0.51
1:A:25:GLU:HG3	1:A:125:LEU:HD22	1.92	0.50
5:A:511:78M:H131	5:A:517:78M:H121	1.93	0.49
5:A:515:78M:H8	5:A:523:78M:H132	1.95	0.49
1:A:68:TYR:OH	7:A:601:HOH:O	2.16	0.49
1:A:249:TYR:HB3	5:A:518:78M:H32C	1.95	0.48
1:A:96:MET:SD	5:A:508:78M:H132	2.53	0.48
5:A:507:78M:H152	5:A:507:78M:H102	1.96	0.48
1:A:96:MET:HE3	5:A:519:78M:H61C	1.96	0.47
1:A:279:HIS:O	1:A:283:VAL:HG23	2.13	0.47
5:A:506:78M:H131	5:A:513:78M:H62C	1.95	0.47
5:A:506:78M:H152	5:A:513:78M:H112	1.97	0.47
5:A:508:78M:H153	5:A:508:78M:H122	1.64	0.47
1:A:403:ILE:HG22	1:A:427:TRP:HH2	1.80	0.47
1:A:237:VAL:O	1:A:241:VAL:HG23	2.16	0.46
1:A:138:ASP:HB3	1:A:140:HIS:ND1	2.29	0.46
1:A:254:THR:HG21	1:A:440:GLN:OE1	2.15	0.46
1:A:174:GLY:HA3	6:A:525:PE5:H121	1.97	0.46
1:A:469:VAL:O	5:A:511:78M:H18	2.16	0.46
1:A:351:PRO:O	1:A:356:LYS:HE3	2.16	0.45
5:A:507:78M:H8	5:A:520:78M:H52C	1.97	0.45
5:A:524:78M:H111	5:A:524:78M:H142	1.76	0.45
5:A:511:78M:H91C	5:A:511:78M:H62C	1.62	0.45
5:A:514:78M:H91C	5:A:514:78M:H61C	1.63	0.45
1:A:321:VAL:N	7:A:602:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:VAL:HA	1:A:470:PHE:HD2	1.82	0.45
1:A:187:PHE:HE1	5:A:519:78M:H51C	1.81	0.45
1:A:187:PHE:CD1	5:A:508:78M:H152	2.51	0.45
1:A:249:TYR:CE2	5:A:518:78M:H172	2.52	0.44
5:A:509:78M:H42C	5:A:509:78M:H7	1.65	0.44
1:A:202:ASP:HA	1:A:203:PRO:HD2	1.88	0.44
5:A:508:78M:H62C	5:A:508:78M:H91C	1.69	0.44
1:A:386:PRO:HB2	5:A:512:78M:H102	2.00	0.43
5:A:520:78M:H42C	5:A:520:78M:H7	1.63	0.43
5:A:523:78M:H22C	5:A:523:78M:H52C	1.72	0.42
1:A:472:SER:O	1:A:475:ILE:HB	2.20	0.42
5:A:509:78M:C7	5:A:513:78M:H61C	2.49	0.42
1:A:255:ILE:HG12	5:A:524:78M:H22C	2.01	0.42
1:A:473:LYS:HA	1:A:473:LYS:HD2	1.72	0.42
5:A:523:78M:H91C	5:A:523:78M:H62C	1.89	0.42
1:A:311:ALA:HA	1:A:321:VAL:HG21	2.01	0.42
1:A:424:MET:O	1:A:428:PHE:HD1	2.02	0.42
1:A:472:SER:O	1:A:475:ILE:HD12	2.20	0.42
5:A:506:78M:H51C	5:A:517:78M:H31C	2.01	0.42
1:A:76:PHE:CG	5:A:520:78M:H172	2.55	0.42
1:A:78:ALA:HB1	1:A:84:ALA:HA	2.01	0.42
1:A:357:PHE:HE1	1:A:403:ILE:HG23	1.85	0.41
1:A:187:PHE:CE1	5:A:519:78M:H51C	2.55	0.41
1:A:385:SER:HA	1:A:386:PRO:HD3	1.92	0.41
5:A:522:78M:H102	5:A:522:78M:H131	1.76	0.41
1:A:357:PHE:CD1	1:A:403:ILE:HD12	2.54	0.41
1:A:126:LYS:HG2	1:A:428:PHE:CE2	2.56	0.41
1:A:385:SER:CB	5:A:509:78M:H172	2.50	0.41
5:A:505:78M:H92C	5:A:506:78M:H61C	2.02	0.41
5:A:508:78M:H142	5:A:519:78M:C8	2.50	0.41
5:A:505:78M:H91C	5:A:505:78M:H61C	1.87	0.40
5:A:514:78M:H141	5:A:519:78M:H62C	2.03	0.40
1:A:294:LEU:HD21	5:A:510:78M:H121	2.04	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	442/483 (92%)	434 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	361/391 (92%)	357 (99%)	4 (1%)	73	87

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

Mol	Chain	Res	Type
1	A	6	LYS
1	A	318	TRP
1	A	348	LYS
1	A	473	LYS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

26 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	$\# Z > 2$
5	78M	A	524	-	21,21,21	0.73	1 (4%)	22,22,22	0.97	1 (4%)
5	78M	A	511	-	21,21,21	0.73	1 (4%)	22,22,22	1.06	1 (4%)
5	78M	A	509	-	21,21,21	0.71	1 (4%)	22,22,22	1.07	1 (4%)
5	78M	A	522	-	21,21,21	0.75	1 (4%)	22,22,22	0.98	1 (4%)
5	78M	A	521	-	21,21,21	0.73	1 (4%)	22,22,22	0.91	1 (4%)
5	78M	A	513	-	21,21,21	0.75	1 (4%)	22,22,22	0.99	1 (4%)
5	78M	A	507	-	21,21,21	0.75	1 (4%)	22,22,22	0.91	1 (4%)
5	78M	A	514	-	21,21,21	0.72	1 (4%)	22,22,22	0.99	1 (4%)
4	PO4	A	503	-	4,4,4	0.85	0	6,6,6	0.42	0
5	78M	A	517	-	21,21,21	0.76	1 (4%)	22,22,22	0.88	1 (4%)
5	78M	A	505	-	21,21,21	0.73	1 (4%)	22,22,22	0.95	1 (4%)
5	78M	A	516	-	21,21,21	0.72	1 (4%)	22,22,22	0.94	1 (4%)
5	78M	A	518	-	21,21,21	0.74	1 (4%)	22,22,22	0.95	1 (4%)
5	78M	A	515	-	21,21,21	0.75	1 (4%)	22,22,22	0.95	1 (4%)
5	78M	A	519	-	21,21,21	0.74	1 (4%)	22,22,22	1.05	1 (4%)
5	78M	A	520	-	21,21,21	0.74	1 (4%)	22,22,22	1.02	1 (4%)
5	78M	A	506	-	21,21,21	0.73	1 (4%)	22,22,22	0.99	1 (4%)
5	78M	A	504	-	21,21,21	0.74	1 (4%)	22,22,22	0.96	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	78M	A	510	-	21,21,21	0.74	1 (4%)	22,22,22	0.95	1 (4%)
6	PE5	A	526	-	9,9,26	0.85	0	8,8,25	0.25	0
6	PE5	A	525	-	7,7,26	0.72	0	6,6,25	0.23	0
5	78M	A	508	-	21,21,21	0.70	1 (4%)	22,22,22	1.04	1 (4%)
5	78M	A	512	-	21,21,21	0.74	1 (4%)	22,22,22	0.92	1 (4%)
5	78M	A	523	-	21,21,21	0.74	1 (4%)	22,22,22	0.94	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
5	78M	A	524	-	-	11/21/21/21	-
5	78M	A	511	-	-	12/21/21/21	-
5	78M	A	509	-	-	10/21/21/21	-
5	78M	A	522	-	-	7/21/21/21	-
5	78M	A	521	-	-	8/21/21/21	-
5	78M	A	513	-	-	12/21/21/21	-
5	78M	A	507	-	-	8/21/21/21	-
5	78M	A	514	-	-	4/21/21/21	-
5	78M	A	515	-	-	13/21/21/21	-
5	78M	A	517	-	-	11/21/21/21	-
5	78M	A	505	-	-	10/21/21/21	-
5	78M	A	516	-	-	9/21/21/21	-
5	78M	A	518	-	-	10/21/21/21	-
5	78M	A	519	-	-	8/21/21/21	-
5	78M	A	520	-	-	11/21/21/21	-
5	78M	A	506	-	-	9/21/21/21	-
5	78M	A	504	-	-	11/21/21/21	-
5	78M	A	510	-	-	9/21/21/21	-
6	PE5	A	526	-	-	5/7/7/24	-
6	PE5	A	525	-	-	5/5/5/24	-
5	78M	A	508	-	-	10/21/21/21	-
5	78M	A	512	-	-	11/21/21/21	-
5	78M	A	523	-	-	13/21/21/21	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	517	78M	O2-C1	2.78	1.41	1.33
5	A	519	78M	O2-C1	2.76	1.41	1.33
5	A	507	78M	O2-C1	2.76	1.41	1.33
5	A	518	78M	O2-C1	2.75	1.41	1.33
5	A	510	78M	O2-C1	2.75	1.41	1.33
5	A	515	78M	O2-C1	2.75	1.41	1.33
5	A	511	78M	O2-C1	2.73	1.41	1.33
5	A	512	78M	O2-C1	2.71	1.41	1.33
5	A	520	78M	O2-C1	2.69	1.41	1.33
5	A	504	78M	O2-C1	2.69	1.41	1.33
5	A	513	78M	O2-C1	2.68	1.41	1.33
5	A	521	78M	O2-C1	2.68	1.41	1.33
5	A	505	78M	O2-C1	2.68	1.41	1.33
5	A	522	78M	O2-C1	2.66	1.41	1.33
5	A	524	78M	O2-C1	2.64	1.41	1.33
5	A	523	78M	O2-C1	2.61	1.41	1.33
5	A	506	78M	O2-C1	2.61	1.41	1.33
5	A	516	78M	O2-C1	2.59	1.40	1.33
5	A	514	78M	O2-C1	2.57	1.40	1.33
5	A	509	78M	O2-C1	2.50	1.40	1.33
5	A	508	78M	O2-C1	2.40	1.40	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	519	78M	O2-C1-C2	3.28	122.20	111.91
5	A	515	78M	O2-C1-C2	2.89	120.99	111.91
5	A	504	78M	O2-C1-C2	2.82	120.77	111.91
5	A	524	78M	O2-C1-C2	2.73	120.48	111.91
5	A	518	78M	O2-C1-C2	2.73	120.46	111.91
5	A	512	78M	O2-C1-C2	2.69	120.34	111.91
5	A	520	78M	O2-C1-C2	2.67	120.30	111.91
5	A	513	78M	O2-C1-C2	2.66	120.26	111.91
5	A	516	78M	O2-C1-C2	2.66	120.26	111.91
5	A	511	78M	O2-C1-C2	2.65	120.22	111.91
5	A	510	78M	O2-C1-C2	2.64	120.19	111.91
5	A	508	78M	O2-C1-C2	2.64	120.18	111.91
5	A	506	78M	O2-C1-C2	2.60	120.08	111.91
5	A	517	78M	O2-C1-C2	2.59	120.03	111.91
5	A	507	78M	O2-C1-C2	2.53	119.85	111.91
5	A	522	78M	O2-C1-C2	2.51	119.79	111.91
5	A	509	78M	O2-C1-C2	2.51	119.78	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	521	78M	O2-C1-C2	2.48	119.70	111.91
5	A	523	78M	O2-C1-C2	2.48	119.70	111.91
5	A	505	78M	O2-C1-C2	2.48	119.67	111.91
5	A	514	78M	O2-C1-C2	2.46	119.62	111.91

There are no chirality outliers.

All (217) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	524	78M	O2-C17-C18-C20
5	A	524	78M	O2-C17-C18-O19
5	A	511	78M	C17-C18-C20-O21
5	A	522	78M	O19-C18-C20-O21
5	A	522	78M	C17-C18-C20-O21
5	A	522	78M	O2-C17-C18-O19
5	A	521	78M	C17-C18-C20-O21
5	A	513	78M	C17-C18-C20-O21
5	A	514	78M	C17-C18-C20-O21
5	A	517	78M	C17-C18-C20-O21
5	A	505	78M	O2-C17-C18-C20
5	A	516	78M	O2-C17-C18-C20
5	A	516	78M	O2-C17-C18-O19
5	A	518	78M	O2-C17-C18-C20
5	A	515	78M	C17-C18-C20-O21
5	A	515	78M	O2-C17-C18-C20
5	A	515	78M	O2-C17-C18-O19
5	A	520	78M	C17-C18-C20-O21
5	A	506	78M	O19-C18-C20-O21
5	A	506	78M	C17-C18-C20-O21
5	A	506	78M	O2-C17-C18-C20
5	A	506	78M	O2-C17-C18-O19
5	A	504	78M	O2-C17-C18-O19
5	A	510	78M	O19-C18-C20-O21
5	A	510	78M	C17-C18-C20-O21
5	A	508	78M	C17-C18-C20-O21
5	A	508	78M	O2-C17-C18-C20
5	A	508	78M	O2-C17-C18-O19
5	A	512	78M	C17-C18-C20-O21
5	A	512	78M	O2-C17-C18-C20
5	A	512	78M	O2-C17-C18-O19
5	A	523	78M	C17-C18-C20-O21
5	A	512	78M	O1-C1-O2-C17

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Mol	Chain	Res	Type	Atoms
5	A	512	78M	C2-C1-O2-C17
5	A	508	78M	C2-C1-O2-C17
5	A	521	78M	O1-C1-O2-C17
5	A	515	78M	O1-C1-O2-C17
5	A	508	78M	O1-C1-O2-C17
5	A	505	78M	O2-C17-C18-O19
5	A	518	78M	O2-C17-C18-O19
5	A	523	78M	O2-C17-C18-O19
5	A	512	78M	C2-C3-C4-C5
5	A	521	78M	C2-C1-O2-C17
5	A	515	78M	C2-C1-O2-C17
5	A	506	78M	C2-C1-O2-C17
5	A	506	78M	O1-C1-O2-C17
5	A	524	78M	C2-C1-O2-C17
5	A	509	78M	C2-C1-O2-C17
5	A	523	78M	C2-C1-O2-C17
5	A	504	78M	C1-C2-C3-C4
5	A	515	78M	C1-C2-C3-C4
5	A	524	78M	O1-C1-O2-C17
5	A	513	78M	O19-C18-C20-O21
5	A	514	78M	O19-C18-C20-O21
5	A	508	78M	O19-C18-C20-O21
5	A	524	78M	C1-C2-C3-C4
5	A	518	78M	C1-C2-C3-C4
6	A	526	PE5	O3-C5-C6-O4
5	A	513	78M	C1-C2-C3-C4
5	A	519	78M	C1-C2-C3-C4
6	A	526	PE5	O4-C7-C8-O5
6	A	526	PE5	C5-C6-O4-C7
5	A	509	78M	O1-C1-O2-C17
5	A	523	78M	O1-C1-O2-C17
5	A	519	78M	C2-C1-O2-C17
5	A	516	78M	C1-C2-C3-C4
6	A	525	PE5	O6-C10-C9-O5
5	A	504	78M	C2-C1-O2-C17
5	A	519	78M	C4-C5-C6-C7
5	A	512	78M	C1-C2-C3-C4
5	A	518	78M	C3-C4-C5-C6
5	A	522	78M	O2-C17-C18-C20
5	A	520	78M	C10-C11-C12-C13
5	A	508	78M	C2-C3-C4-C5
5	A	516	78M	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
5	A	507	78M	C11-C12-C13-C14
5	A	520	78M	C2-C1-O2-C17
5	A	511	78M	C9-C10-C11-C12
5	A	516	78M	C3-C4-C5-C6
5	A	519	78M	O1-C1-O2-C17
5	A	521	78M	C9-C10-C11-C12
5	A	513	78M	C3-C4-C5-C6
5	A	520	78M	C2-C3-C4-C5
5	A	509	78M	C17-C18-C20-O21
5	A	504	78M	C17-C18-C20-O21
5	A	509	78M	O2-C17-C18-O19
5	A	520	78M	O2-C17-C18-O19
5	A	507	78M	C3-C4-C5-C6
5	A	521	78M	C11-C10-C9-C8
5	A	514	78M	C11-C10-C9-C8
6	A	526	PE5	O2-C3-C4-O3
5	A	524	78M	C3-C4-C5-C6
5	A	504	78M	O1-C1-O2-C17
5	A	523	78M	C3-C4-C5-C6
5	A	510	78M	C3-C4-C5-C6
5	A	511	78M	O19-C18-C20-O21
5	A	517	78M	O19-C18-C20-O21
5	A	515	78M	O19-C18-C20-O21
5	A	520	78M	O19-C18-C20-O21
5	A	516	78M	C4-C5-C6-C7
5	A	513	78M	C2-C3-C4-C5
5	A	508	78M	C11-C12-C13-C14
5	A	506	78M	C2-C3-C4-C5
5	A	522	78M	C1-C2-C3-C4
5	A	520	78M	O1-C1-O2-C17
5	A	511	78M	C2-C3-C4-C5
5	A	515	78M	C4-C5-C6-C7
5	A	515	78M	C11-C12-C13-C14
5	A	510	78M	C1-C2-C3-C4
5	A	520	78M	O2-C17-C18-C20
5	A	504	78M	O2-C17-C18-C20
5	A	524	78M	C2-C3-C4-C5
5	A	523	78M	C11-C12-C13-C14
5	A	509	78M	C3-C4-C5-C6
5	A	518	78M	C10-C11-C12-C13
5	A	524	78M	C4-C5-C6-C7
5	A	524	78M	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
5	A	516	78M	C11-C10-C9-C8
5	A	504	78M	C4-C5-C6-C7
5	A	517	78M	C1-C2-C3-C4
5	A	518	78M	C11-C10-C9-C8
5	A	507	78M	C2-C1-O2-C17
5	A	504	78M	C12-C13-C14-C15
5	A	507	78M	C12-C13-C14-C15
5	A	521	78M	O19-C18-C20-O21
5	A	512	78M	O19-C18-C20-O21
5	A	523	78M	O19-C18-C20-O21
5	A	508	78M	C12-C13-C14-C15
5	A	519	78M	C11-C10-C9-C8
5	A	506	78M	C4-C5-C6-C7
5	A	509	78M	O2-C17-C18-C20
5	A	510	78M	C2-C1-O2-C17
5	A	507	78M	O1-C1-O2-C17
5	A	504	78M	C9-C10-C11-C12
5	A	511	78M	C10-C11-C12-C13
5	A	518	78M	C2-C1-O2-C17
5	A	512	78M	C3-C4-C5-C6
5	A	513	78M	C2-C1-O2-C17
5	A	515	78M	C12-C13-C14-C15
5	A	520	78M	C12-C13-C14-C15
5	A	523	78M	C9-C10-C11-C12
5	A	511	78M	O2-C17-C18-C20
5	A	517	78M	C2-C3-C4-C5
5	A	509	78M	O19-C18-C20-O21
5	A	513	78M	C10-C11-C12-C13
5	A	510	78M	O1-C1-O2-C17
5	A	505	78M	C10-C11-C12-C13
5	A	521	78M	C12-C13-C14-C15
6	A	525	PE5	C11-C12-O7-C13
5	A	518	78M	O1-C1-O2-C17
5	A	517	78M	C2-C1-O2-C17
5	A	523	78M	O2-C17-C18-C20
5	A	505	78M	C4-C5-C6-C7
5	A	516	78M	C9-C10-C11-C12
5	A	513	78M	O1-C1-O2-C17
5	A	517	78M	O1-C1-O2-C17
5	A	504	78M	O19-C18-C20-O21
5	A	523	78M	C2-C3-C4-C5
5	A	522	78M	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
5	A	513	78M	C4-C5-C6-C7
6	A	525	PE5	C12-C11-O6-C10
5	A	522	78M	C11-C12-C13-C14
5	A	518	78M	C7-C8-C9-C10
5	A	517	78M	C3-C4-C5-C6
5	A	515	78M	C18-C17-O2-C1
5	A	510	78M	C11-C12-C13-C14
5	A	504	78M	C11-C10-C9-C8
5	A	505	78M	C2-C3-C4-C5
6	A	525	PE5	O6-C11-C12-O7
5	A	505	78M	C3-C4-C5-C6
5	A	523	78M	C11-C10-C9-C8
5	A	508	78M	C10-C11-C12-C13
5	A	523	78M	C12-C13-C14-C15
5	A	524	78M	C10-C11-C12-C13
5	A	505	78M	C1-C2-C3-C4
5	A	507	78M	C7-C8-C9-C10
5	A	511	78M	C11-C12-C13-C14
5	A	513	78M	C7-C8-C9-C10
5	A	516	78M	C5-C6-C7-C8
5	A	519	78M	C2-C3-C4-C5
5	A	517	78M	C10-C11-C12-C13
5	A	517	78M	C9-C10-C11-C12
5	A	514	78M	O2-C1-C2-C3
6	A	526	PE5	C3-C4-O3-C5
6	A	525	PE5	C9-C10-O6-C11
5	A	517	78M	O2-C17-C18-C20
5	A	507	78M	C10-C11-C12-C13
5	A	507	78M	C2-C3-C4-C5
5	A	515	78M	C2-C3-C4-C5
5	A	524	78M	C5-C6-C7-C8
5	A	509	78M	C7-C8-C9-C10
5	A	512	78M	C10-C11-C12-C13
5	A	519	78M	C10-C11-C12-C13
5	A	515	78M	O2-C1-C2-C3
5	A	511	78M	C2-C1-O2-C17
5	A	517	78M	C5-C6-C7-C8
5	A	520	78M	C3-C4-C5-C6
5	A	511	78M	O2-C1-C2-C3
5	A	505	78M	C12-C13-C14-C15
5	A	511	78M	O1-C1-O2-C17
5	A	521	78M	C5-C6-C7-C8

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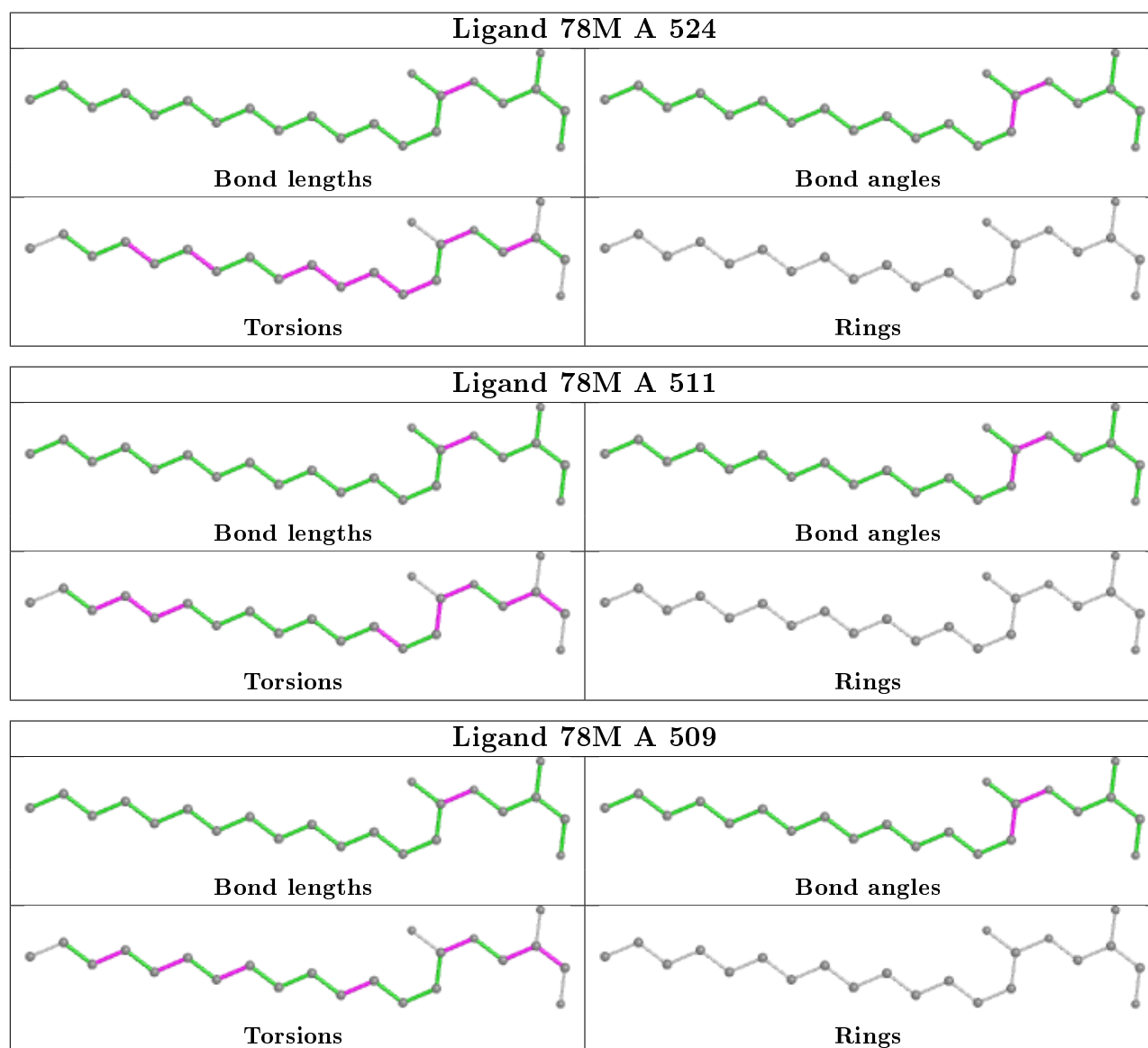
Mol	Chain	Res	Type	Atoms
5	A	513	78M	C5-C6-C7-C8
5	A	523	78M	C5-C6-C7-C8
5	A	518	78M	C11-C12-C13-C14
5	A	519	78M	C5-C6-C7-C8
5	A	506	78M	C5-C6-C7-C8
5	A	505	78M	C5-C6-C7-C8
5	A	520	78M	C5-C6-C7-C8
5	A	511	78M	O2-C17-C18-O19
5	A	509	78M	C11-C12-C13-C14
5	A	512	78M	O2-C1-C2-C3
5	A	511	78M	O1-C1-C2-C3
5	A	510	78M	O2-C1-C2-C3
5	A	509	78M	C9-C10-C11-C12
5	A	505	78M	C11-C12-C13-C14
5	A	510	78M	O1-C1-C2-C3
5	A	513	78M	C11-C12-C13-C14

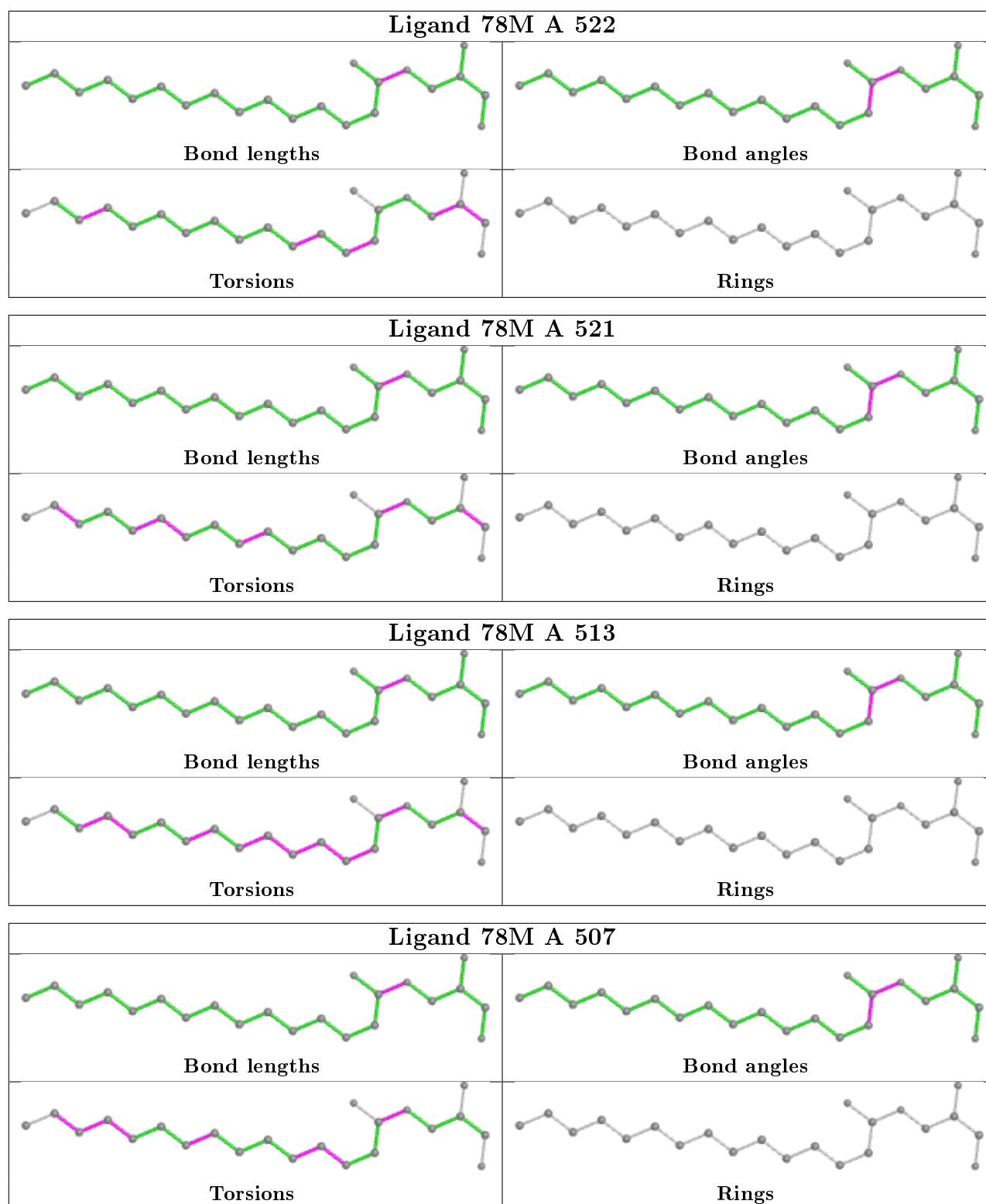
There are no ring outliers.

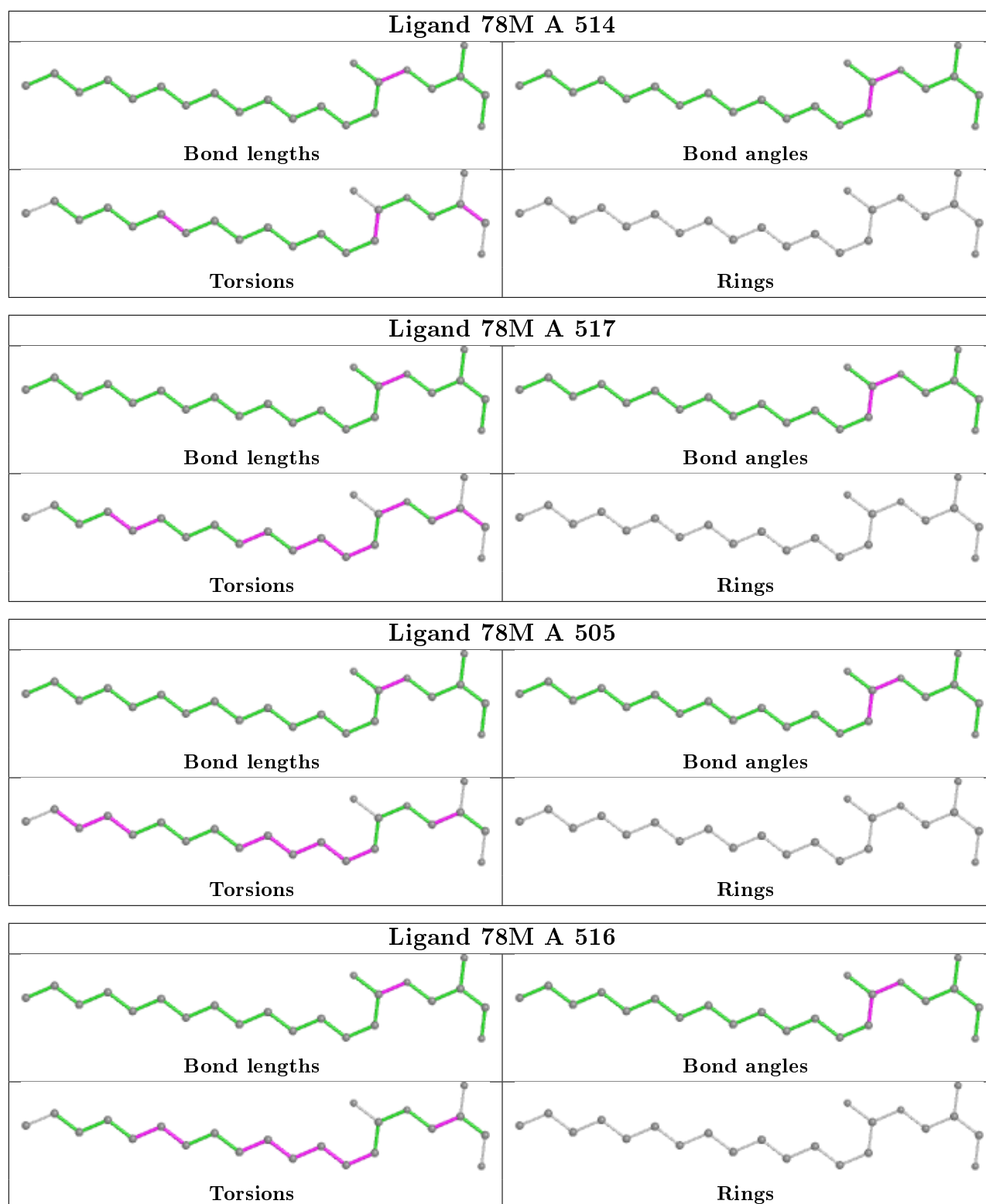
20 monomers are involved in 44 short contacts:

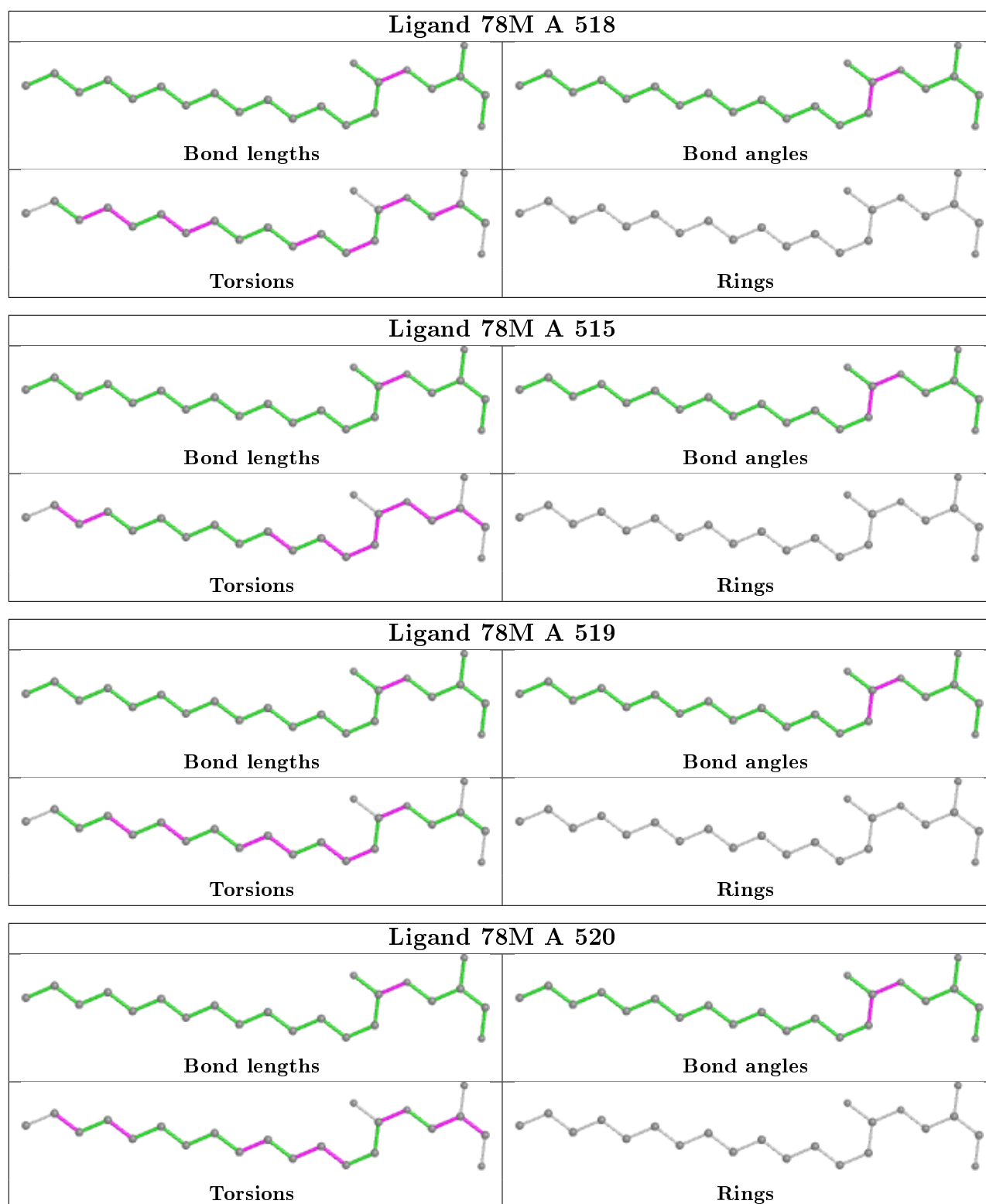
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	524	78M	2	0
5	A	511	78M	3	0
5	A	509	78M	3	0
5	A	522	78M	1	0
5	A	513	78M	4	0
5	A	507	78M	2	0
5	A	514	78M	4	0
5	A	517	78M	3	0
5	A	505	78M	2	0
5	A	516	78M	1	0
5	A	518	78M	2	0
5	A	515	78M	1	0
5	A	519	78M	6	0
5	A	520	78M	3	0
5	A	506	78M	5	0
5	A	510	78M	1	0
6	A	525	PE5	2	0
5	A	508	78M	6	0
5	A	512	78M	1	0
5	A	523	78M	5	0

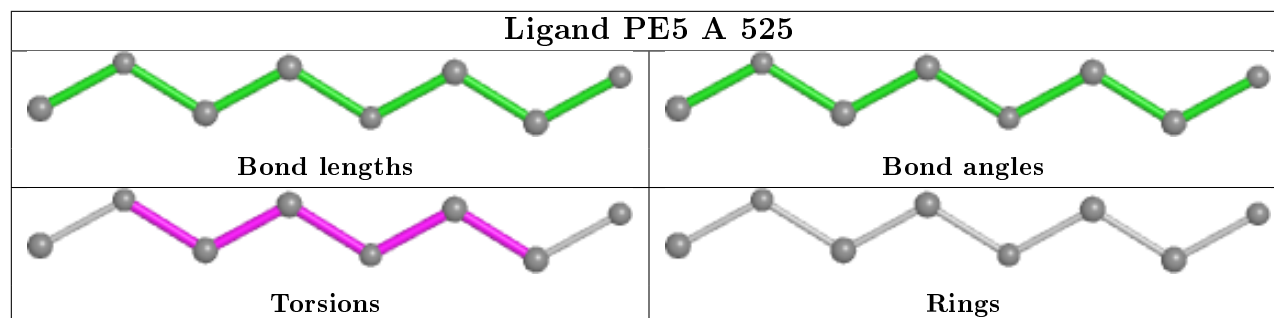
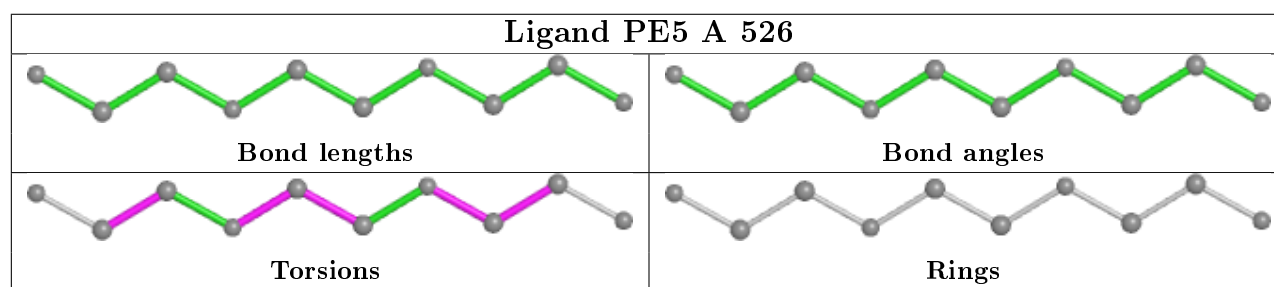
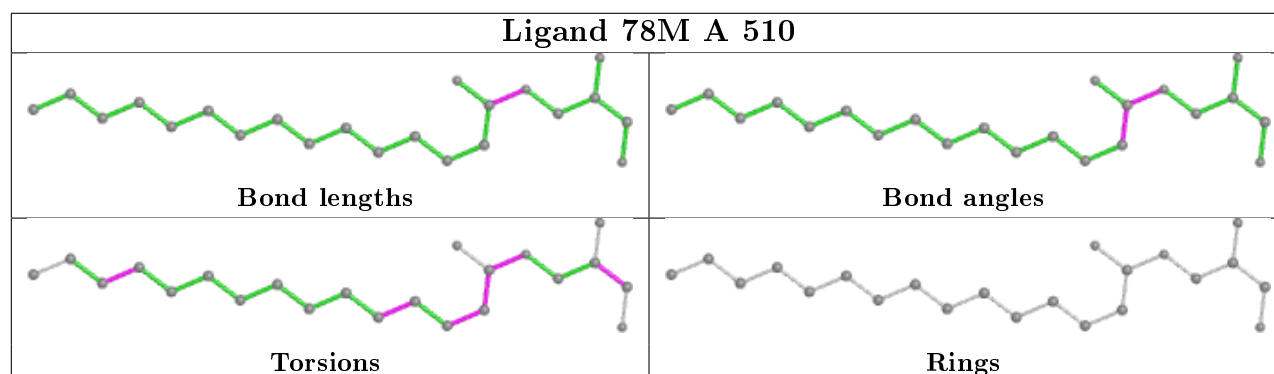
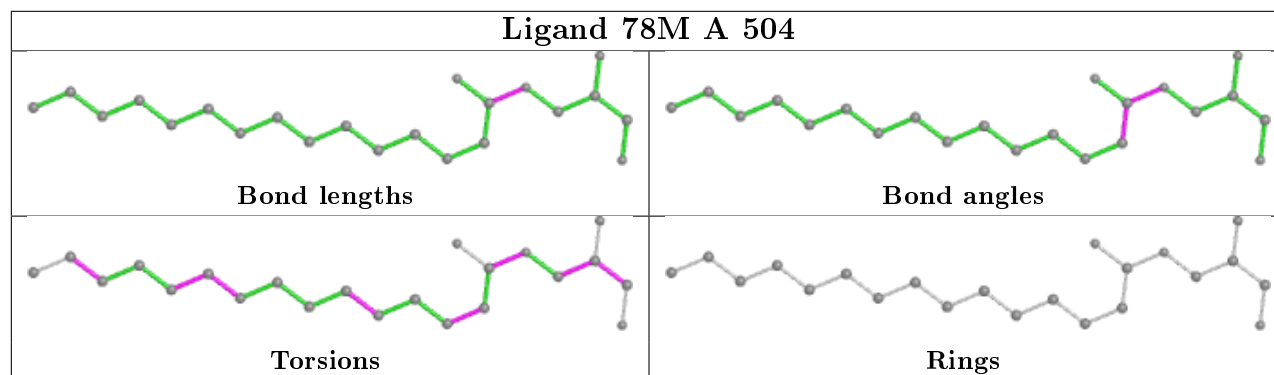
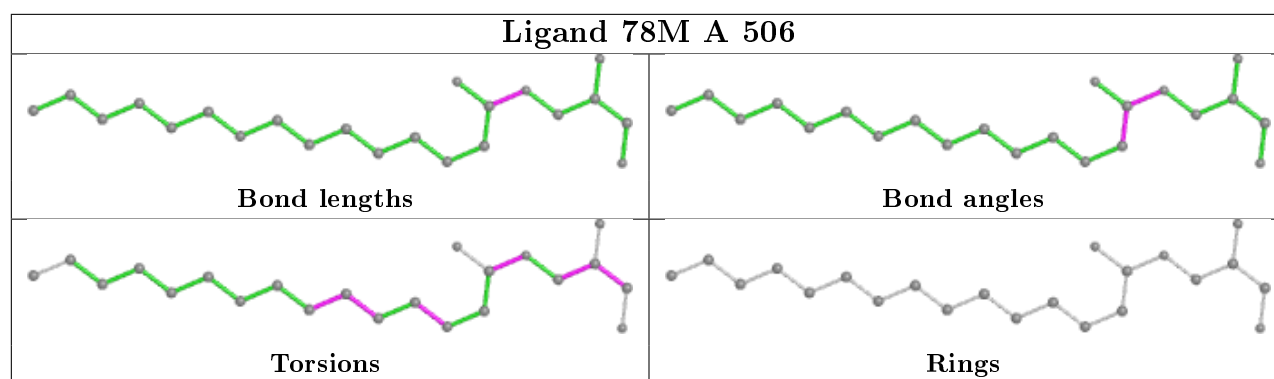
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

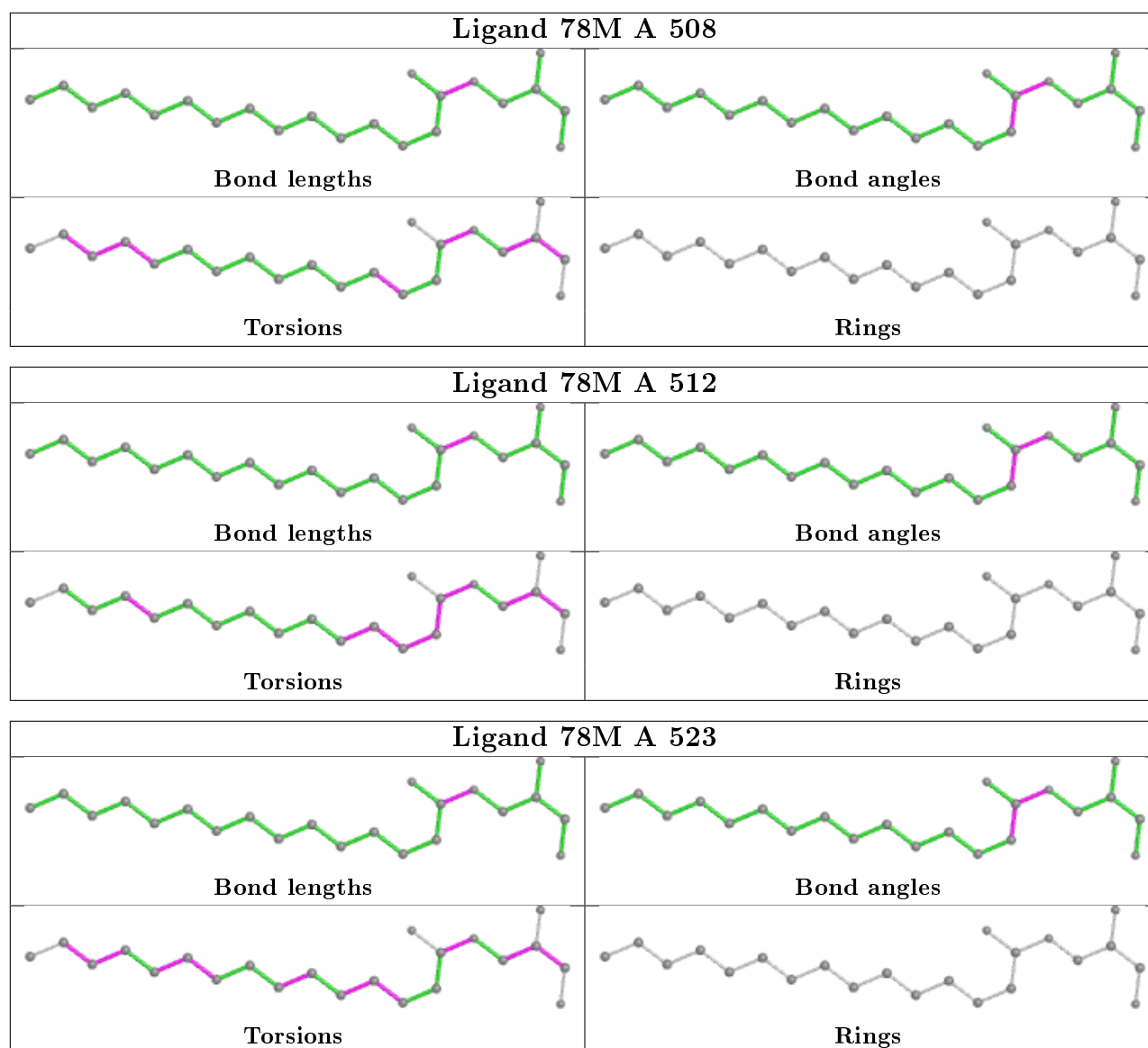












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	448/483 (92%)	0.13	28 (6%) 20 18	33, 49, 96, 117	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	275	THR	8.7
1	A	277	THR	6.5
1	A	280	LEU	6.1
1	A	140	HIS	5.8
1	A	266	ALA	5.6
1	A	267	TRP	5.1
1	A	276	SER	5.1
1	A	279	HIS	5.0
1	A	269	ILE	5.0
1	A	347	LYS	4.7
1	A	346	TRP	4.6
1	A	350	GLN	4.5
1	A	345	ALA	4.1
1	A	142	ARG	4.0
1	A	282	VAL	4.0
1	A	278	GLU	3.8
1	A	348	LYS	3.6
1	A	285	TYR	3.5
1	A	265	PHE	3.2
1	A	284	SER	3.2
1	A	344	THR	3.0
1	A	264	TYR	2.7
1	A	139	GLU	2.6
1	A	138	ASP	2.5
1	A	341	TRP	2.4
1	A	141	ASP	2.4
1	A	263	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	349	ASN	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 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
5	78M	A	523	22/22	0.68	0.45	61,70,82,96	22
5	78M	A	512	22/22	0.70	0.19	47,72,88,93	0
5	78M	A	524	22/22	0.72	0.36	60,73,84,101	22
5	78M	A	518	22/22	0.75	0.29	57,71,83,88	22
5	78M	A	521	22/22	0.76	0.32	60,78,88,94	0
5	78M	A	507	22/22	0.78	0.27	59,75,87,93	0
5	78M	A	515	22/22	0.80	0.29	54,73,91,100	0
6	PE5	A	526	10/27	0.80	0.18	65,69,78,81	0
4	PO4	A	503	5/5	0.80	0.38	89,95,108,122	5
5	78M	A	522	22/22	0.80	0.27	49,71,94,98	0
5	78M	A	506	22/22	0.81	0.21	53,61,76,91	0
5	78M	A	519	22/22	0.81	0.42	48,61,84,85	22
5	78M	A	510	22/22	0.82	0.26	46,71,89,97	0
5	78M	A	511	22/22	0.82	0.27	61,76,83,95	22
5	78M	A	520	22/22	0.83	0.31	60,78,85,96	0
5	78M	A	516	22/22	0.83	0.23	61,68,87,90	22
5	78M	A	517	22/22	0.83	0.26	67,74,84,86	0
5	78M	A	505	22/22	0.84	0.26	53,69,78,85	0
5	78M	A	513	22/22	0.85	0.33	49,69,94,99	0
5	78M	A	509	22/22	0.86	0.20	49,63,81,85	0
5	78M	A	508	22/22	0.88	0.26	49,66,81,87	0
6	PE5	A	525	8/27	0.89	0.14	56,66,74,82	0

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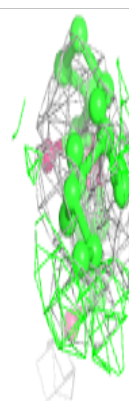
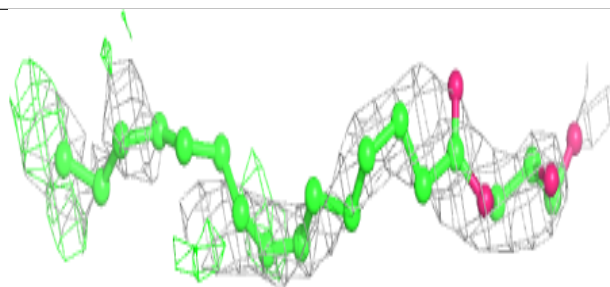
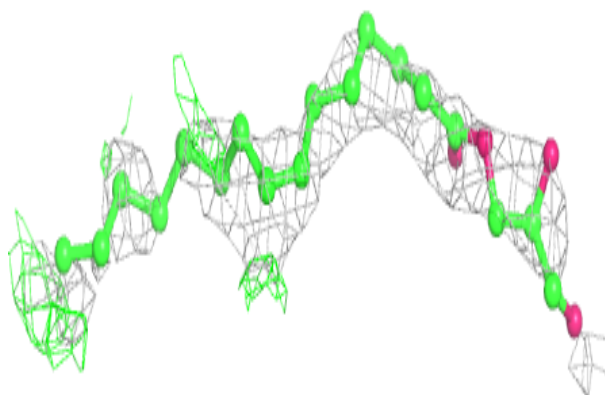
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PHE	A	502	12/12	0.90	0.27	48,60,70,71	12
5	78M	A	504	22/22	0.90	0.35	59,71,88,91	22
2	ALA	A	501	5/6	0.92	0.26	45,47,56,61	0
5	78M	A	514	22/22	0.94	0.15	42,59,70,72	0

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

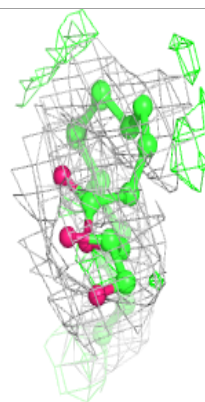
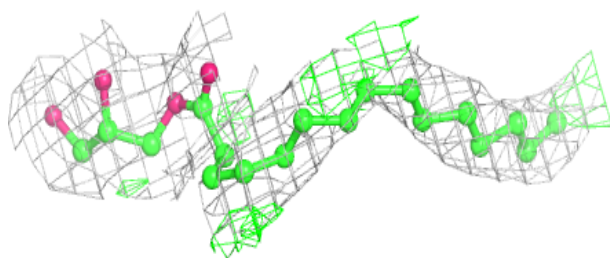
Electron density around 78M A 523:

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

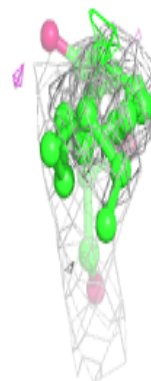
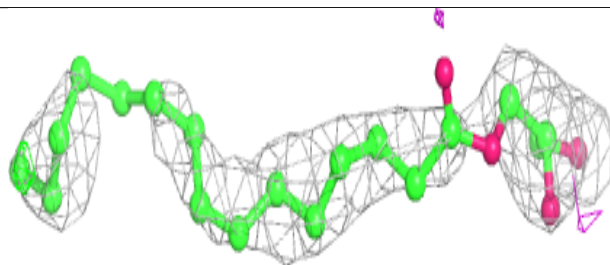
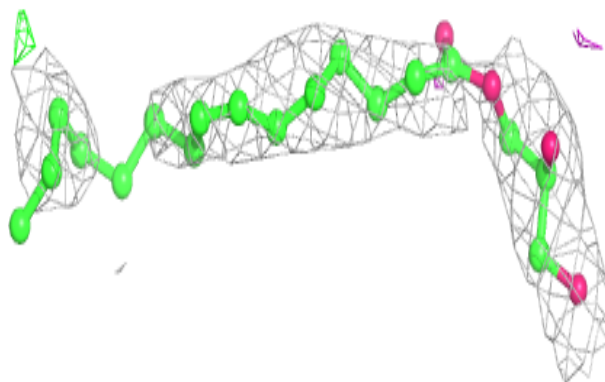


Electron density around 78M A 512:

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and green (positive)

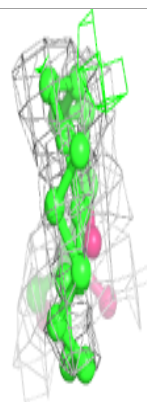
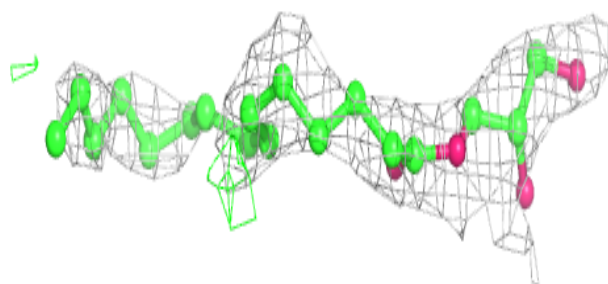
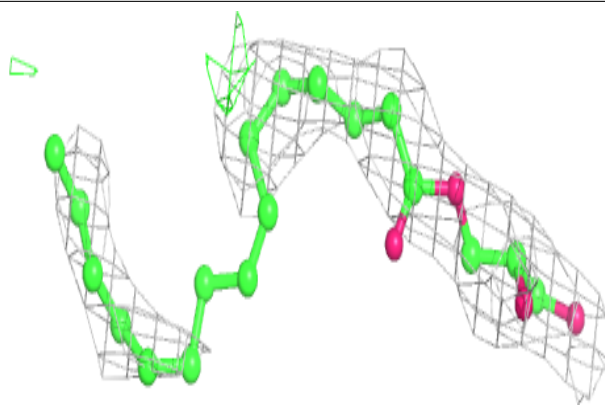
**Electron density around 78M A 524:**

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

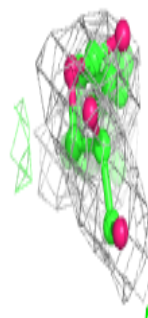
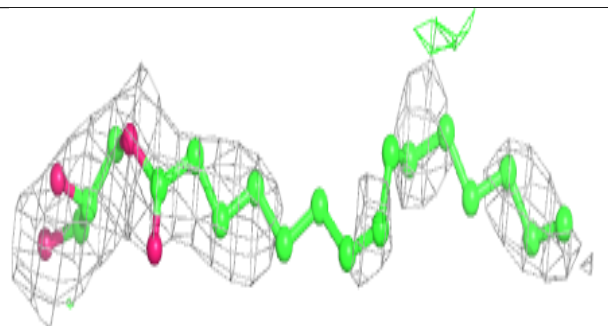
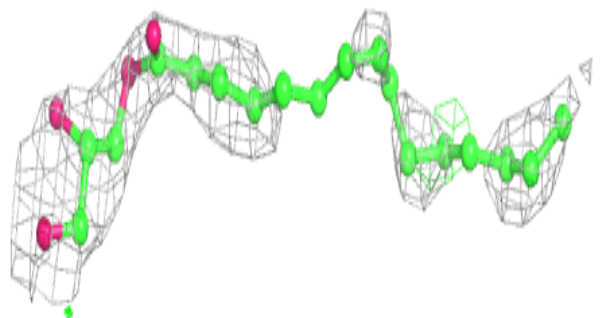


Electron density around 78M A 518:

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and green (positive)

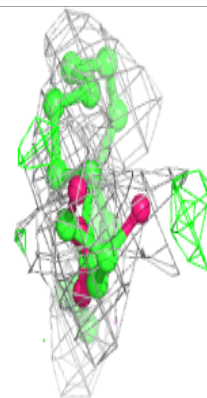
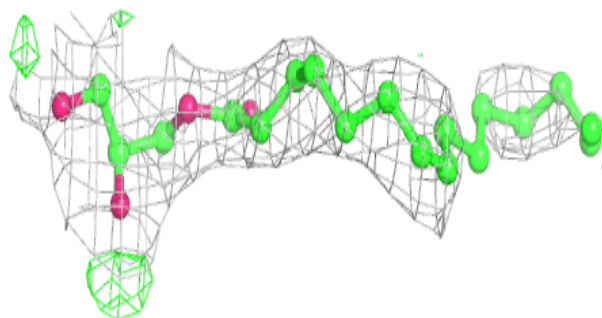
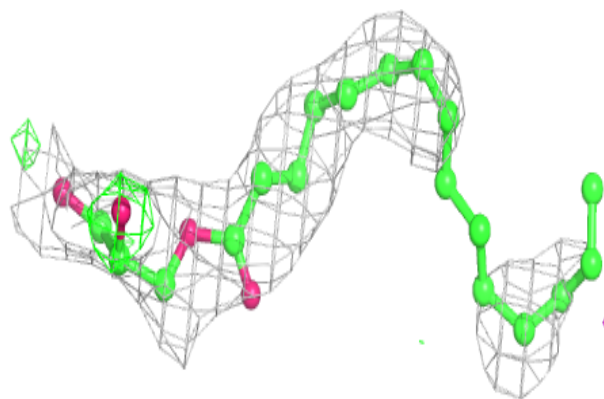
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and green (positive)

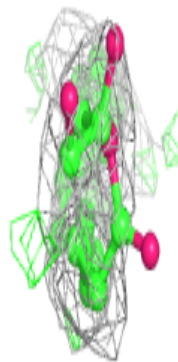
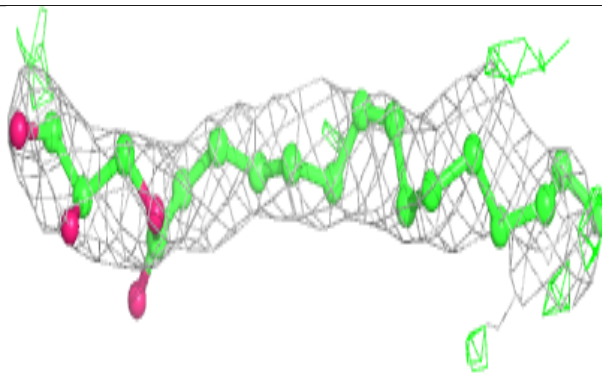
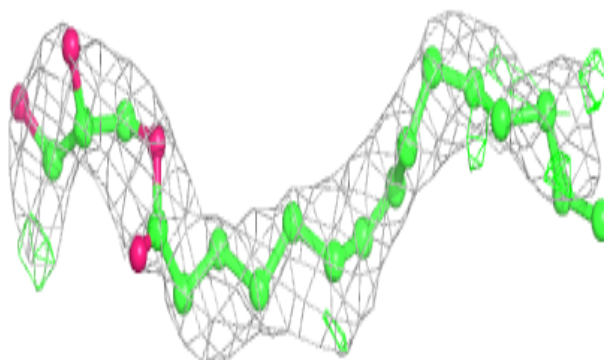


Electron density around 78M A 507:

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

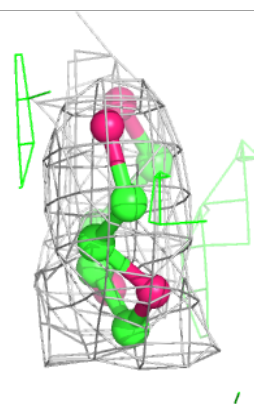
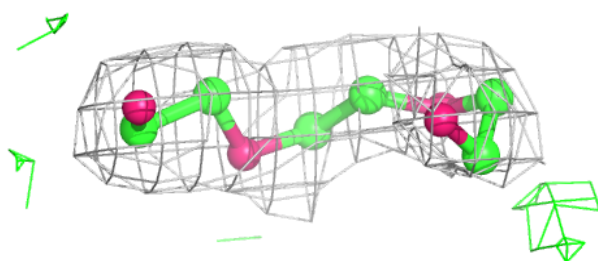
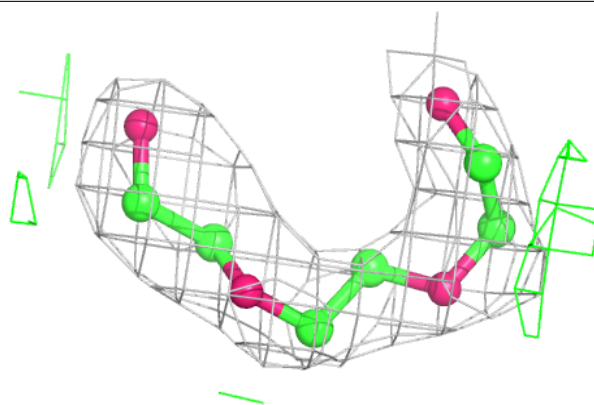
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and green (positive)

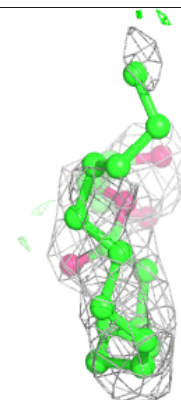
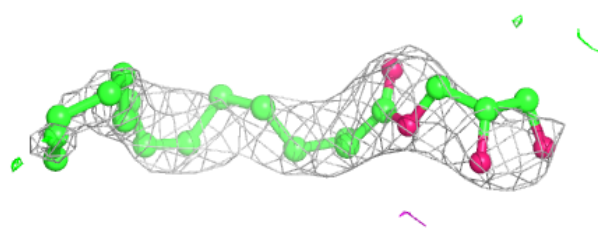
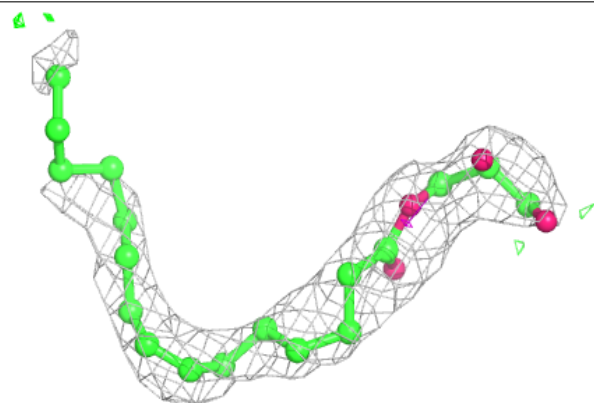


Electron density around PE5 A 526:

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and green (positive)

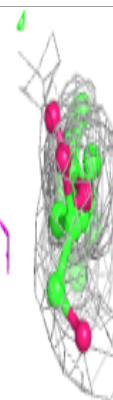
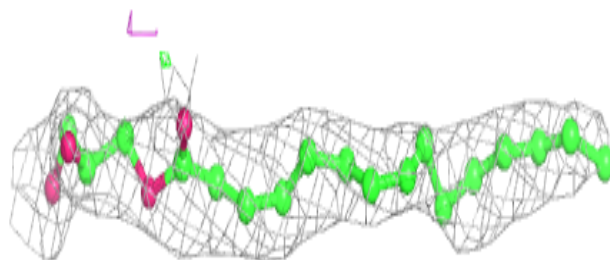
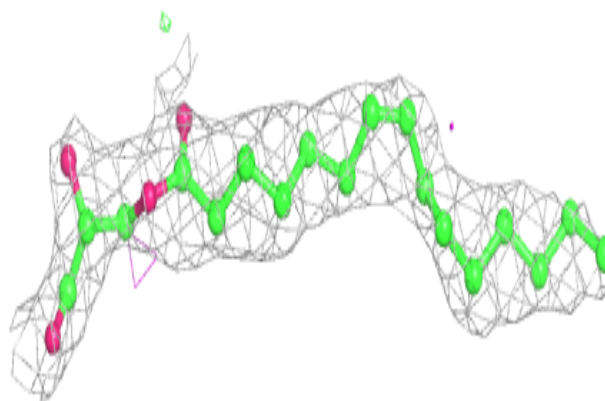
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and green (positive)

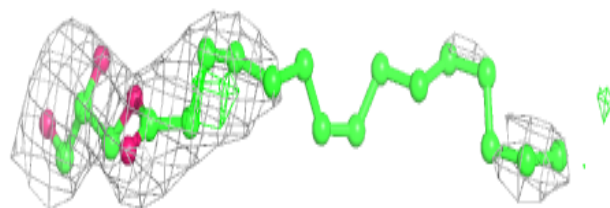
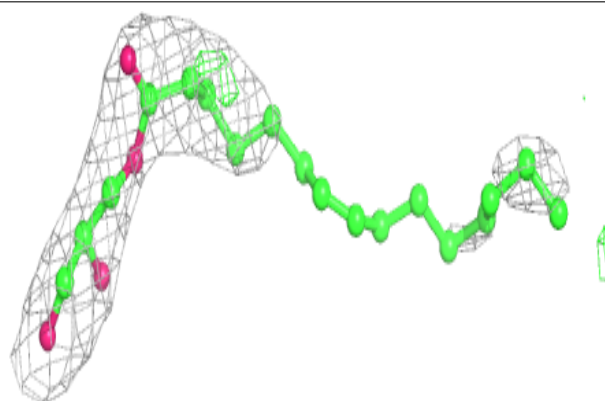


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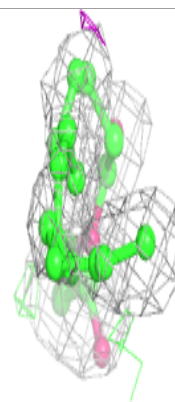
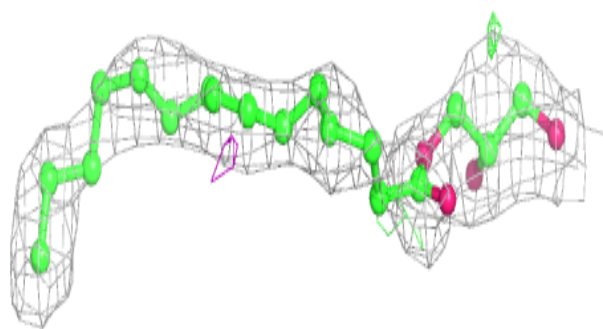
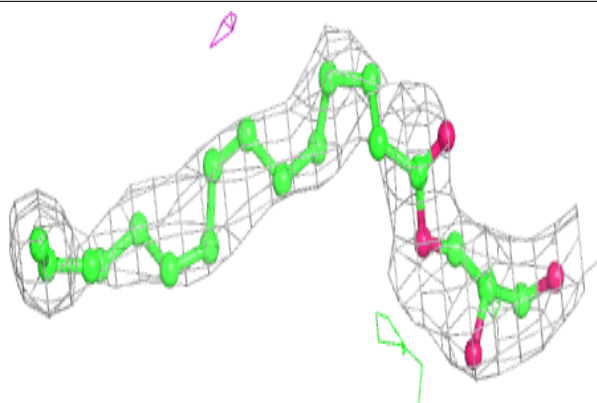
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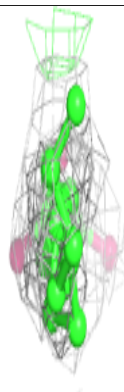
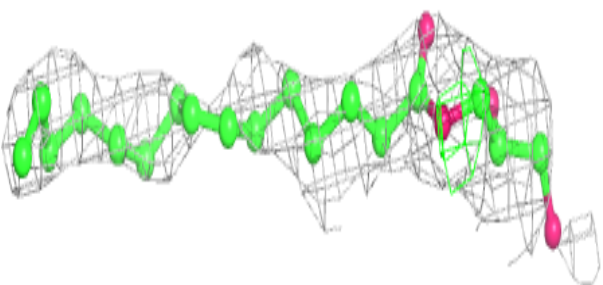
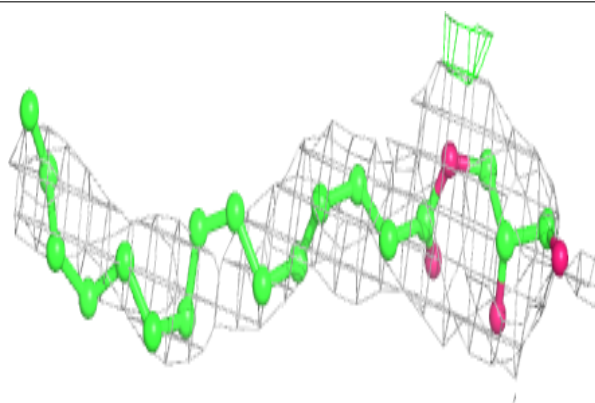


Electron density around 78M A 510:

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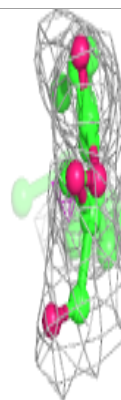
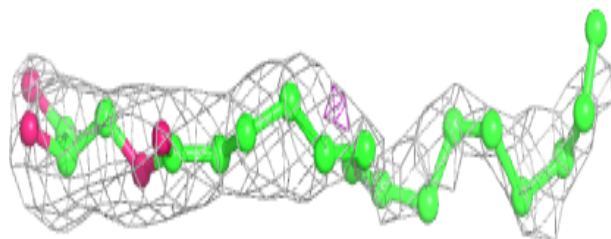
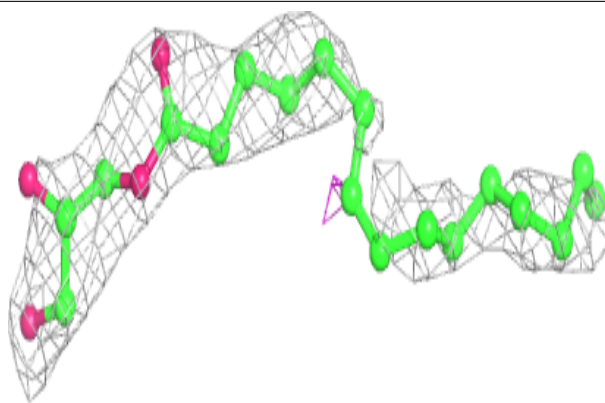
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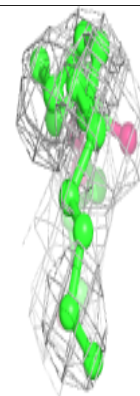
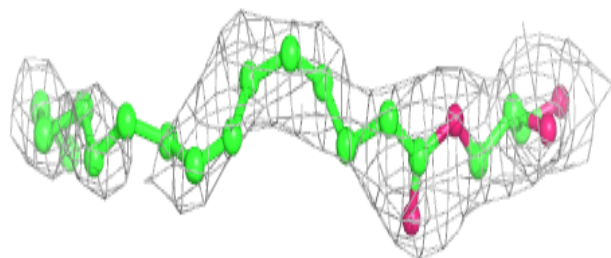
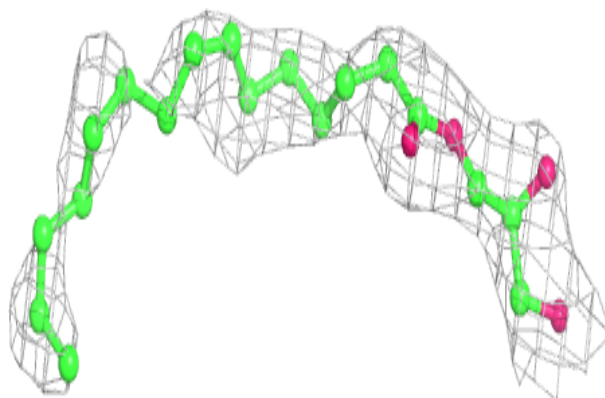


Electron density around 78M A 520:

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and green (positive)

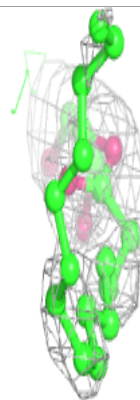
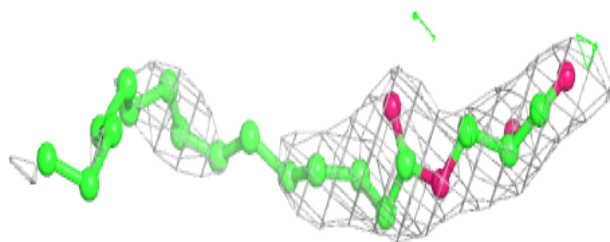
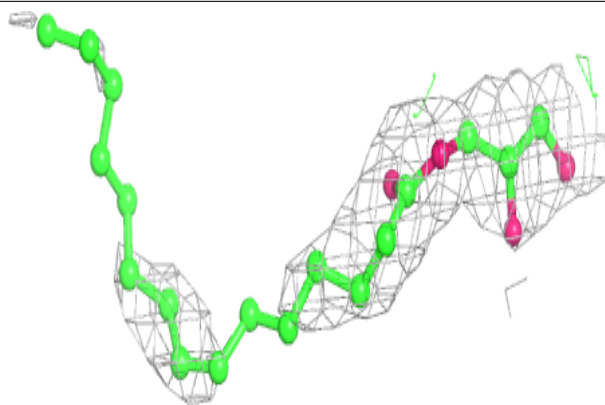
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and green (positive)

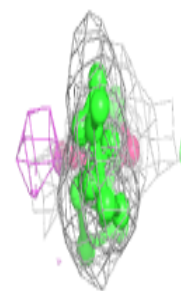
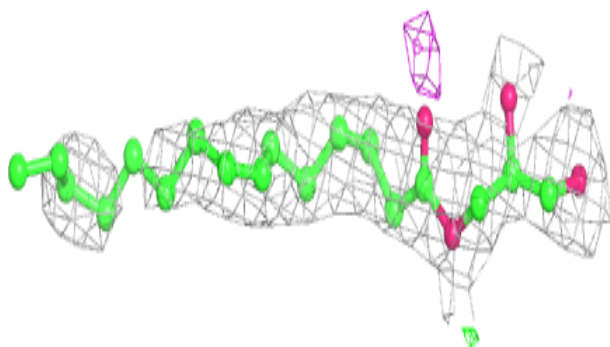
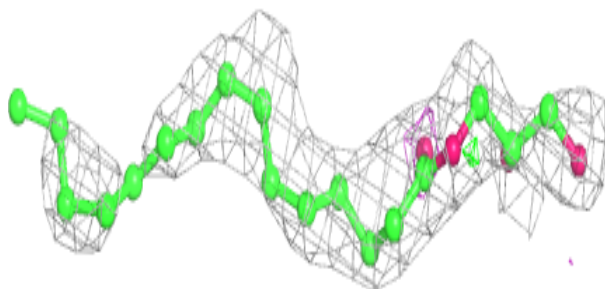


Electron density around 78M A 517:

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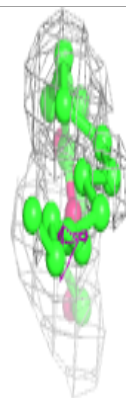
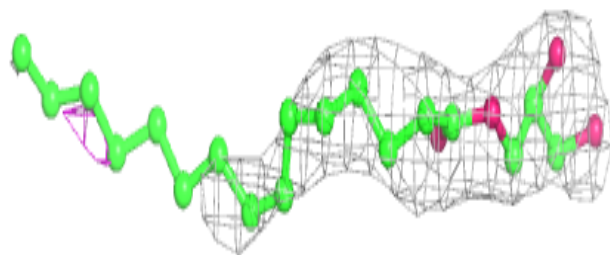
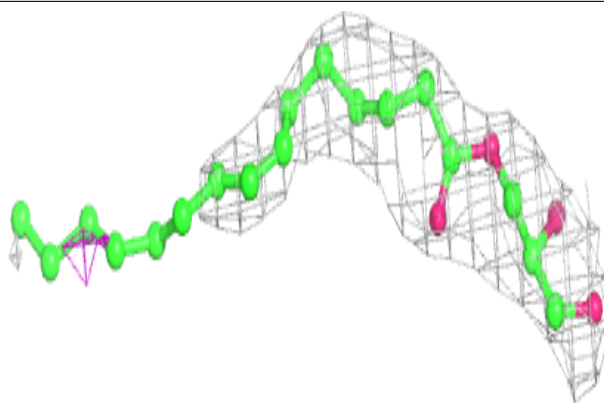
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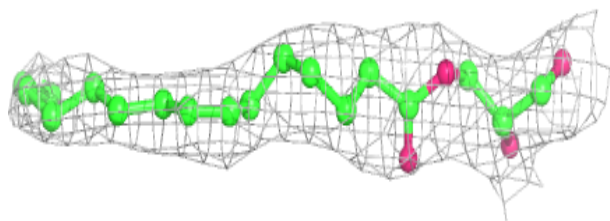
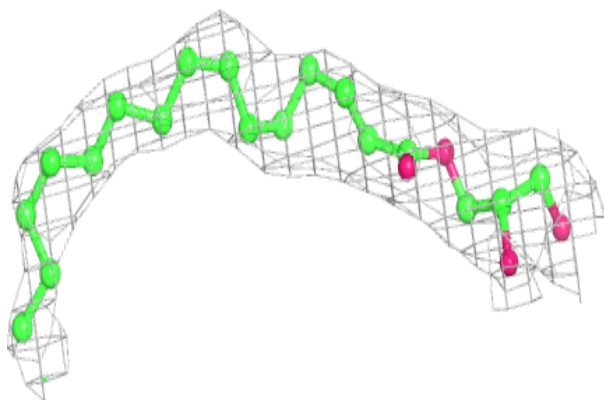


Electron density around 78M A 513:

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and green (positive)

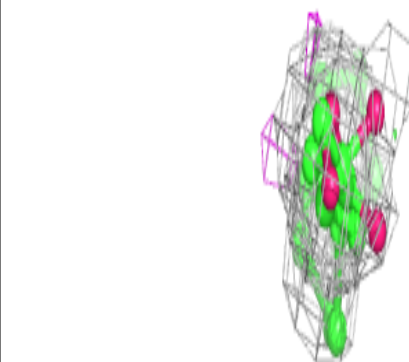
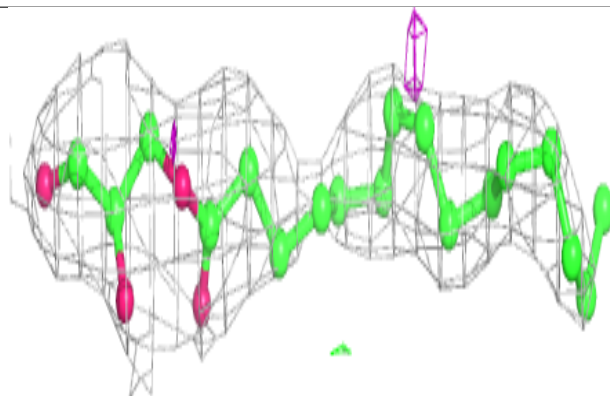
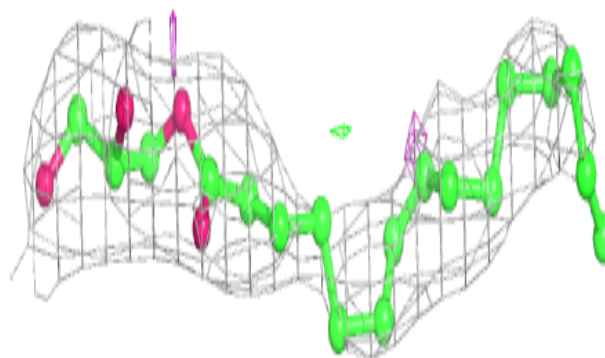
**Electron density around 78M A 509:**

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and green (positive)

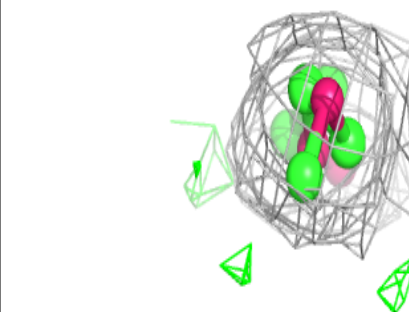
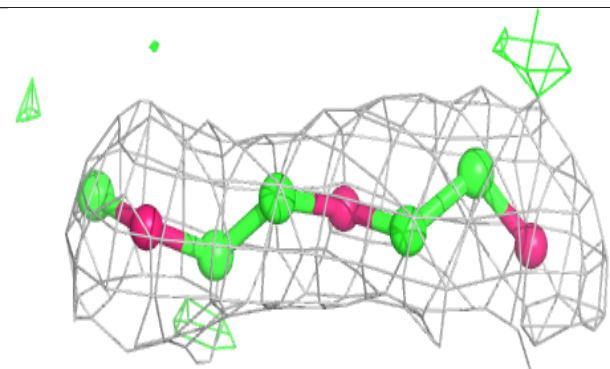
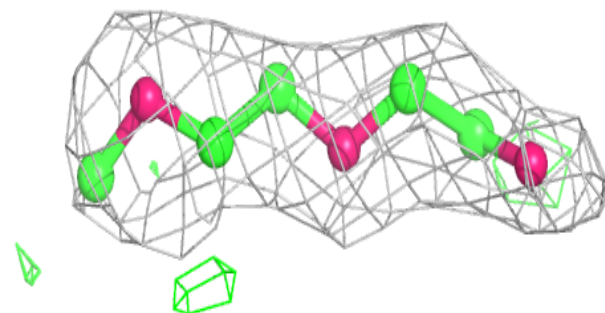


Electron density around 78M A 508:

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

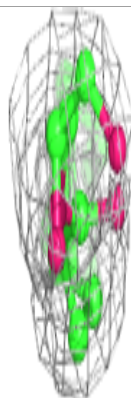
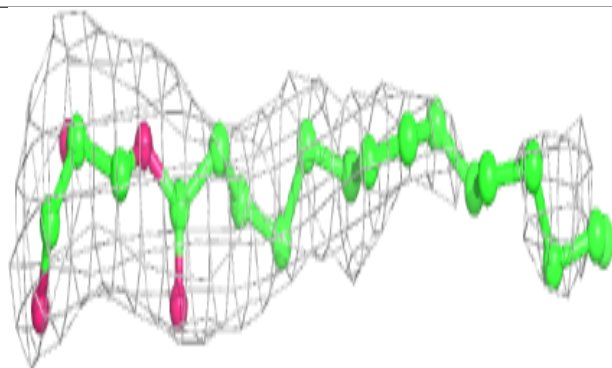
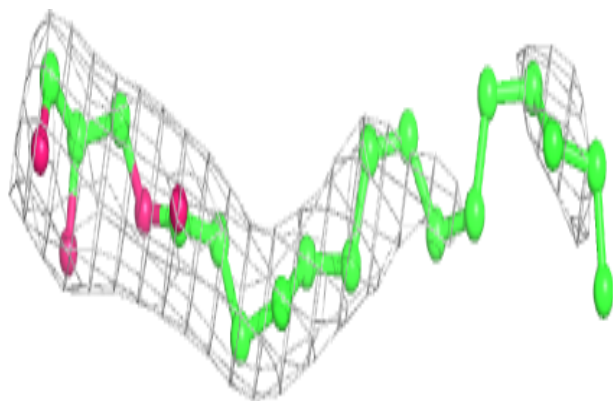
**Electron density around PE5 A 525:**

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

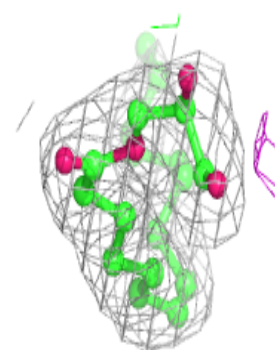
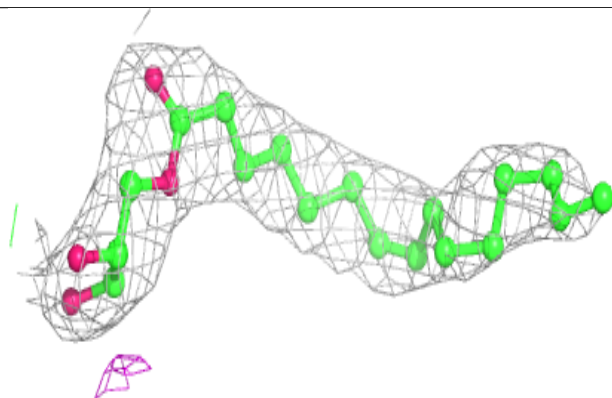
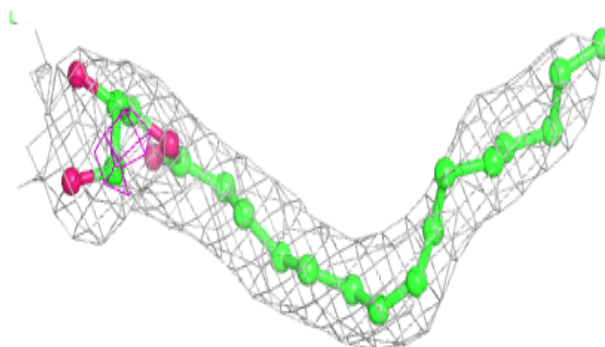


Electron density around 78M A 504:

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

**Electron density around 78M 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.