Full wwPDB X-ray Structure Validation Report (i)

Jan 8, 2024 – 06:11 am GMT

PDB ID	:	6GHJ
Title	:	PepTSt in complex with tripeptide Phe-Ala-Gln
Authors	:	Martinez Molledo, M.; Quistgaard, E.M.; Loew, C.
Deposited on	:	2018-05-08
Resolution	:	2.26 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

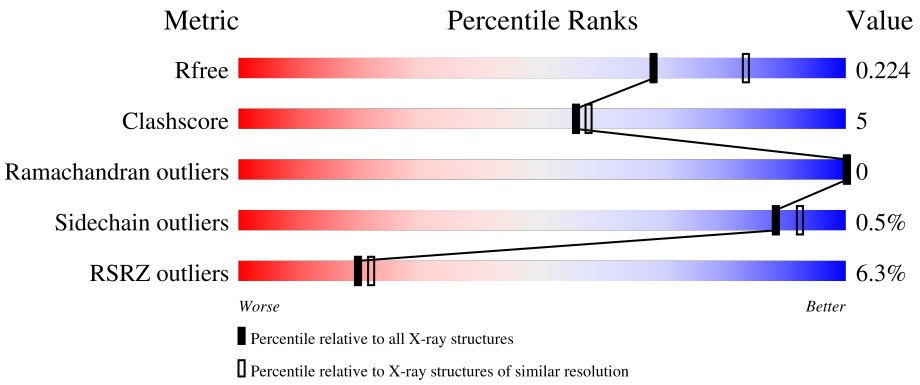
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	6% 84% 10% 5%
2	B	3	67% 33%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 4005 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.

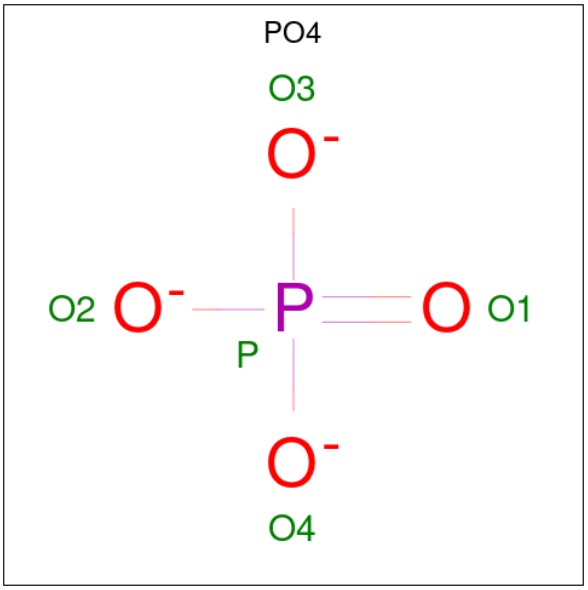
- Molecule 1 is a protein called Di-or tripeptide:H+ symporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	457	3529	2378	545	589	17	0	0	0

- Molecule 2 is a protein called PHE-ALA-GLN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	26	17	4	5	0	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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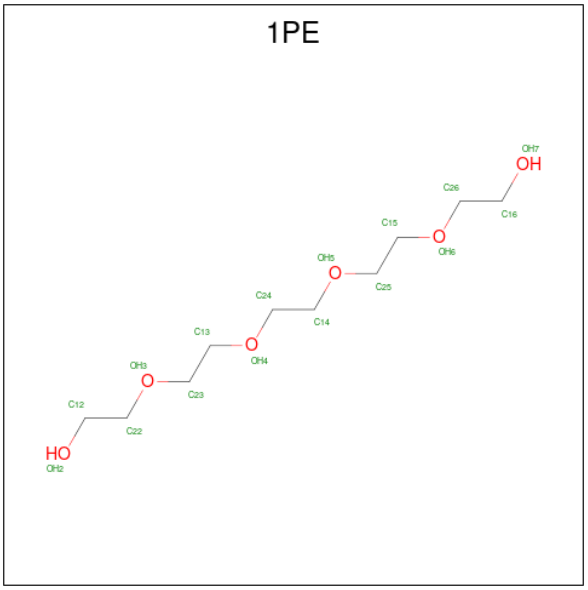
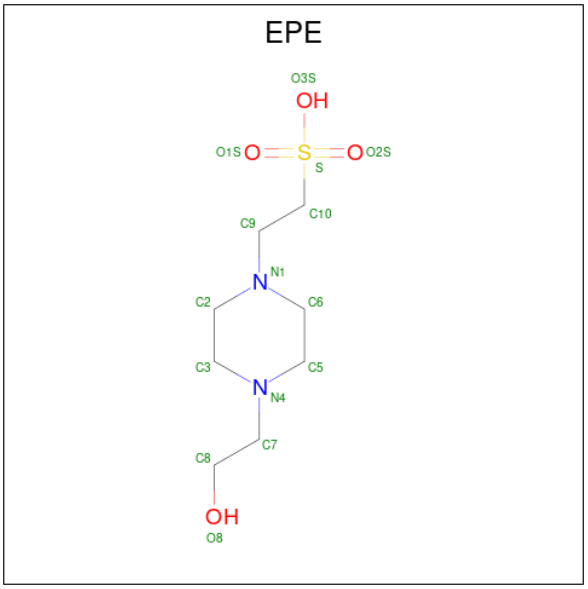
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
3	A	1	5	4	1	0	0

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



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

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).

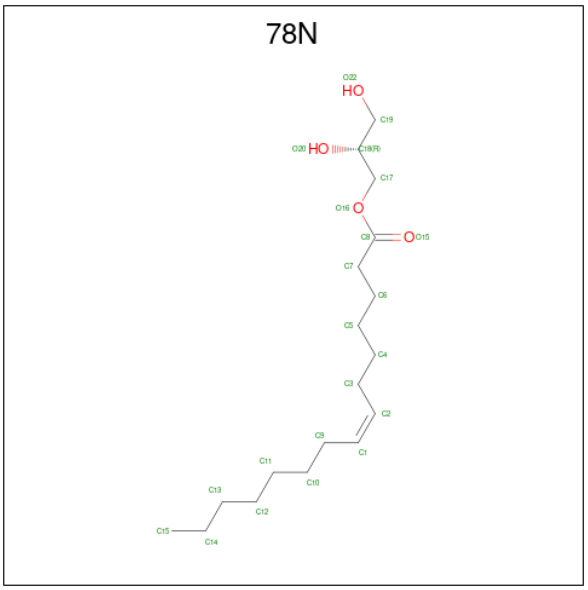


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	A	1	15	8	2	4	1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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



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

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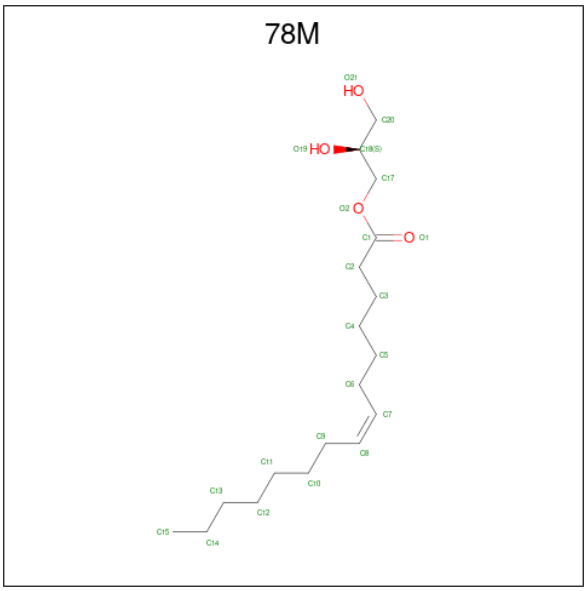
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	22	18	4	0	0
			Total	C	O		
7	A	1	22	18	4	0	0
			Total	C	O		
7	A	1	22	18	4	0	0
			Total	C	O		
7	A	1	22	18	4	0	0

- Molecule 8 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
			Total	C	O		
8	A	1	22	18	4	0	0
			Total	C	O		
8	A	1	22	18	4	0	0
			Total	C	O		
8	A	1	22	18	4	0	0

- Molecule 9 is water.

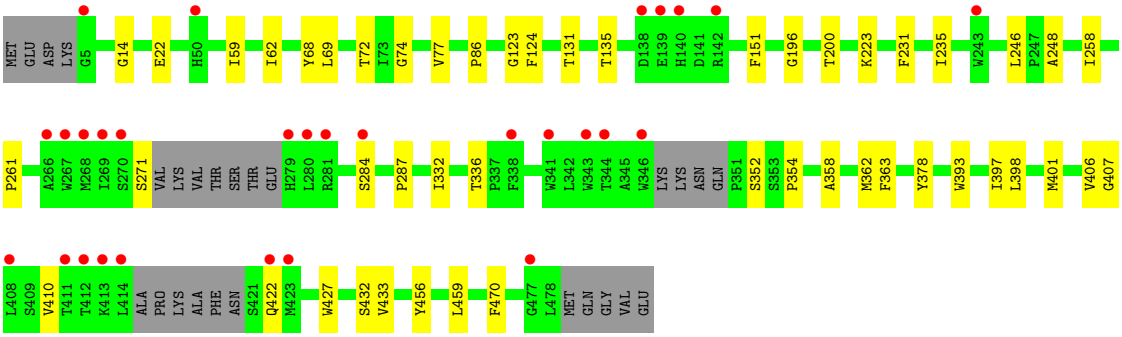
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	100	100	100	0	0
			Total	O		
9	B	1	1	1	0	0

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+ symporter

Chain A:



• Molecule 2: PHE-ALA-GLN

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	101.55Å 108.22Å 111.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.69 – 2.26 48.69 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.69-2.26) 99.7 (48.69-2.26)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.93 (at 2.27Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.191 , 0.222 0.191 , 0.224	Depositor DCC
R_{free} test set	1453 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	40.6	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4005	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NA, PO4, EPE, 78N, 1PE, 78M

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.40	0/3634	0.51	0/4954
2	B	0.58	0/26	0.57	0/32
All	All	0.40	0/3660	0.51	0/4986

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	3529	0	3618	35	0
2	B	26	0	24	1	0
3	A	15	0	0	0	0
4	A	10	0	13	1	0
5	A	15	0	17	1	0
6	A	1	0	0	0	0
7	A	242	0	374	10	0
8	A	66	0	102	6	0
9	A	100	0	0	1	0
9	B	1	0	0	0	0
All	All	4005	0	4148	41	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 (41) 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:332:ILE:O	1:A:336:THR:HG23	1.89	0.73
1:A:459:LEU:HD13	8:A:508:78M:H22C	1.72	0.70
1:A:22:GLU:HG3	1:A:151:PHE:CZ	2.26	0.69
1:A:246:LEU:HD11	7:A:513:78N:H71	1.75	0.69
7:A:509:78N:H31C	8:A:510:78M:H7	1.74	0.68
1:A:62:ILE:HG23	7:A:513:78N:H42C	1.79	0.64
1:A:77:VAL:HG11	1:A:124:PHE:HE1	1.62	0.64
1:A:248:ALA:HA	7:A:515:78N:H172	1.82	0.62
1:A:69:LEU:O	1:A:72:THR:HG22	2.01	0.61
1:A:196:GLY:O	1:A:200:THR:HG22	2.00	0.60
1:A:248:ALA:HB2	7:A:515:78N:H191	1.85	0.59
7:A:509:78N:H91C	8:A:510:78M:H92C	1.90	0.53
1:A:456:TYR:CE1	8:A:520:78M:H31C	2.44	0.52
1:A:378:TYR:CE2	5:A:505:EPE:H102	2.46	0.50
1:A:422:GLN:H	1:A:422:GLN:CD	2.14	0.50
1:A:406:VAL:O	1:A:410:VAL:HG23	2.12	0.49
1:A:284:SER:O	1:A:287:PRO:HD2	2.15	0.46
1:A:363:PHE:CE1	1:A:398:LEU:HD23	2.51	0.46
1:A:407:GLY:HA3	1:A:427:TRP:CH2	2.51	0.46
1:A:59:ILE:HD11	1:A:246:LEU:HD21	1.99	0.45
1:A:131:THR:O	1:A:135:THR:HG23	2.16	0.45
1:A:231:PHE:CE2	1:A:235:ILE:HD11	2.52	0.45
1:A:68:TYR:HE1	2:B:3:GLN:HG2	1.83	0.44
1:A:258:ILE:O	1:A:261:PRO:HD2	2.17	0.44
1:A:336:THR:HG22	1:A:401:MET:HE1	1.99	0.44
7:A:514:78N:H132	7:A:514:78N:H101	1.79	0.44
1:A:398:LEU:HD12	1:A:398:LEU:HA	1.89	0.43
1:A:470:PHE:CE1	7:A:519:78N:H52C	2.54	0.42
1:A:14:GLY:HA2	1:A:200:THR:HG21	1.99	0.42
1:A:86:PRO:HA	7:A:516:78N:H171	2.02	0.42
4:A:504:1PE:H151	9:A:675:HOH:O	2.18	0.42
1:A:352:SER:HB2	1:A:354:PRO:HD2	2.02	0.42
1:A:223:LYS:HE3	1:A:223:LYS:HB2	1.73	0.41
1:A:358:ALA:O	1:A:362:MET:HG3	2.21	0.41
1:A:398:LEU:HD22	8:A:510:78M:H142	2.02	0.41
1:A:68:TYR:HB2	1:A:432:SER:HB2	2.03	0.41
1:A:397:ILE:O	1:A:401:MET:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:PRO:HG2	1:A:433:VAL:HG21	2.02	0.40
1:A:74:GLY:HA3	1:A:123:GLY:O	2.21	0.40
8:A:508:78M:H111	8:A:508:78M:H8	1.93	0.40
7:A:517:78N:H72	7:A:518:78N:H62C	2.03	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	449/483 (93%)	443 (99%)	6 (1%)	0	100	100
2	B	1/3 (33%)	1 (100%)	0	0	100	100
All	All	450/486 (93%)	444 (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	368/391 (94%)	366 (100%)	2 (0%)	88	92
2	B	2/2 (100%)	2 (100%)	0	100	100
All	All	370/393 (94%)	368 (100%)	2 (0%)	88	92

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

Mol	Chain	Res	Type
1	A	271	SER
1	A	393	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	$\#\|Z\| > 2$
8	78M	A	508	-	21,21,21	1.16	1 (4%)	22,22,22	0.98	1 (4%)
7	78N	A	514	-	21,21,21	0.93	1 (4%)	22,22,22	1.00	1 (4%)
5	EPE	A	505	-	15,15,15	0.88	0	18,20,20	1.45	2 (11%)
3	PO4	A	502	-	4,4,4	0.84	0	6,6,6	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	78M	A	510	-	21,21,21	1.16	1 (4%)	22,22,22	1.06	1 (4%)
7	78N	A	512	-	21,21,21	0.91	1 (4%)	22,22,22	1.07	1 (4%)
7	78N	A	517	-	21,21,21	0.94	1 (4%)	22,22,22	1.08	1 (4%)
4	1PE	A	504	-	9,9,15	0.57	0	8,8,14	0.50	0
7	78N	A	511	-	21,21,21	0.95	1 (4%)	22,22,22	0.97	1 (4%)
7	78N	A	516	-	21,21,21	1.05	1 (4%)	22,22,22	0.84	1 (4%)
8	78M	A	520	-	21,21,21	1.20	1 (4%)	22,22,22	1.00	1 (4%)
7	78N	A	515	-	21,21,21	0.99	1 (4%)	22,22,22	1.05	1 (4%)
7	78N	A	513	-	21,21,21	0.94	1 (4%)	22,22,22	1.02	1 (4%)
7	78N	A	518	-	21,21,21	0.91	1 (4%)	22,22,22	1.08	1 (4%)
7	78N	A	519	-	21,21,21	0.98	1 (4%)	22,22,22	1.12	2 (9%)
3	PO4	A	503	-	4,4,4	0.90	0	6,6,6	0.46	0
7	78N	A	507	-	21,21,21	0.95	1 (4%)	22,22,22	1.06	1 (4%)
3	PO4	A	501	-	4,4,4	0.95	0	6,6,6	0.53	0
7	78N	A	509	-	21,21,21	0.91	1 (4%)	22,22,22	1.24	2 (9%)

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
7	78N	A	518	-	-	13/21/21/21	-
7	78N	A	512	-	-	12/21/21/21	-
8	78M	A	508	-	-	7/21/21/21	-
8	78M	A	510	-	-	11/21/21/21	-
7	78N	A	517	-	-	12/21/21/21	-
4	1PE	A	504	-	-	3/7/7/13	-
7	78N	A	511	-	-	12/21/21/21	-
7	78N	A	514	-	-	12/21/21/21	-
7	78N	A	509	-	-	12/21/21/21	-
7	78N	A	516	-	-	10/21/21/21	-
7	78N	A	519	-	-	14/21/21/21	-
8	78M	A	520	-	-	14/21/21/21	-
7	78N	A	515	-	-	8/21/21/21	-
5	EPE	A	505	-	-	3/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	78N	A	513	-	-	10/21/21/21	-
7	78N	A	507	-	-	6/21/21/21	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	510	78M	O2-C1	3.69	1.44	1.33
8	A	520	78M	O2-C1	3.60	1.43	1.33
8	A	508	78M	O2-C1	3.49	1.43	1.33
7	A	516	78N	O16-C8	3.45	1.43	1.33
7	A	519	78N	O16-C8	3.20	1.42	1.33
7	A	515	78N	O16-C8	3.11	1.42	1.33
7	A	511	78N	O16-C8	3.07	1.42	1.33
7	A	513	78N	O16-C8	3.04	1.42	1.33
7	A	514	78N	O16-C8	3.01	1.42	1.33
7	A	507	78N	O16-C8	2.99	1.42	1.33
7	A	517	78N	O16-C8	2.92	1.41	1.33
7	A	518	78N	O16-C8	2.80	1.41	1.33
7	A	509	78N	O16-C8	2.76	1.41	1.33
7	A	512	78N	O16-C8	2.64	1.41	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	509	78N	O16-C8-C7	3.31	122.29	111.91
7	A	519	78N	O16-C8-C7	3.05	121.49	111.91
7	A	515	78N	O16-C8-C7	3.03	121.42	111.91
5	A	505	EPE	O1S-S-C10	-3.01	103.29	106.92
8	A	520	78M	O2-C1-C2	2.94	121.12	111.91
7	A	513	78N	O16-C8-C7	2.92	121.08	111.91
7	A	512	78N	O16-C8-C7	2.91	121.05	111.91
7	A	507	78N	O16-C8-C7	2.89	120.97	111.91
8	A	508	78M	O2-C1-C2	2.81	120.73	111.91
8	A	510	78M	O2-C1-C2	2.79	120.67	111.91
7	A	514	78N	O16-C8-C7	2.78	120.65	111.91
7	A	518	78N	O16-C8-C7	2.75	120.55	111.91
7	A	511	78N	O16-C8-C7	2.72	120.45	111.91
7	A	517	78N	O16-C8-C7	2.66	120.25	111.91
5	A	505	EPE	C9-N1-C6	-2.35	105.21	111.23
7	A	516	78N	O16-C8-C7	2.30	119.12	111.91
7	A	519	78N	C6-C7-C8	-2.26	105.39	113.62
7	A	509	78N	C6-C7-C8	-2.21	105.57	113.62

There are no chirality outliers.

All (159) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	505	EPE	S-C10-C9-N1
7	A	512	78N	O16-C17-C18-C19
7	A	513	78N	C17-C18-C19-O22
7	A	513	78N	O16-C17-C18-C19
7	A	513	78N	O16-C17-C18-O20
7	A	518	78N	C17-C18-C19-O22
8	A	510	78M	C17-C18-C20-O21
8	A	520	78M	O2-C17-C18-C20
8	A	520	78M	O2-C17-C18-O19
7	A	512	78N	O16-C17-C18-O20
7	A	519	78N	O16-C17-C18-O20
7	A	517	78N	O16-C17-C18-C19
7	A	519	78N	O16-C17-C18-C19
7	A	511	78N	O16-C17-C18-O20
7	A	518	78N	C7-C8-O16-C17
7	A	516	78N	C5-C6-C7-C8
7	A	518	78N	C5-C6-C7-C8
7	A	512	78N	O20-C18-C19-O22
7	A	512	78N	C5-C6-C7-C8
7	A	517	78N	C5-C6-C7-C8
8	A	510	78M	C1-C2-C3-C4
7	A	507	78N	O16-C17-C18-O20
7	A	509	78N	O16-C17-C18-O20
7	A	517	78N	O16-C17-C18-O20
8	A	520	78M	C1-C2-C3-C4
7	A	513	78N	C7-C8-O16-C17
4	A	504	1PE	OH7-C16-C26-OH6
7	A	509	78N	C9-C10-C11-C12
7	A	517	78N	C9-C10-C11-C12
7	A	507	78N	O16-C17-C18-C19
7	A	509	78N	O16-C17-C18-C19
7	A	511	78N	O16-C17-C18-C19
7	A	515	78N	C3-C4-C5-C6
7	A	518	78N	C10-C11-C12-C13
7	A	512	78N	C9-C10-C11-C12
7	A	514	78N	C9-C10-C11-C12
7	A	515	78N	C4-C5-C6-C7
7	A	518	78N	O15-C8-O16-C17
7	A	516	78N	C9-C10-C11-C12
7	A	519	78N	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
7	A	518	78N	C9-C10-C11-C12
7	A	511	78N	C17-C18-C19-O22
7	A	512	78N	C17-C18-C19-O22
7	A	517	78N	C17-C18-C19-O22
8	A	520	78M	C17-C18-C20-O21
7	A	517	78N	C3-C4-C5-C6
8	A	510	78M	C11-C12-C13-C14
8	A	520	78M	C11-C12-C13-C14
7	A	507	78N	C2-C3-C4-C5
7	A	518	78N	C11-C10-C9-C1
7	A	509	78N	C4-C5-C6-C7
7	A	511	78N	C9-C10-C11-C12
8	A	520	78M	C2-C3-C4-C5
7	A	513	78N	O20-C18-C19-O22
7	A	517	78N	O20-C18-C19-O22
8	A	510	78M	O19-C18-C20-O21
7	A	512	78N	C3-C4-C5-C6
7	A	509	78N	C2-C3-C4-C5
7	A	513	78N	O15-C8-O16-C17
7	A	516	78N	C10-C11-C12-C13
7	A	515	78N	C5-C6-C7-C8
7	A	509	78N	C7-C8-O16-C17
7	A	516	78N	C4-C5-C6-C7
7	A	519	78N	C4-C5-C6-C7
7	A	513	78N	C11-C10-C9-C1
7	A	509	78N	C11-C12-C13-C14
7	A	518	78N	C3-C4-C5-C6
8	A	510	78M	C2-C3-C4-C5
7	A	513	78N	C3-C4-C5-C6
8	A	520	78M	C3-C4-C5-C6
7	A	512	78N	C11-C10-C9-C1
7	A	517	78N	C11-C10-C9-C1
7	A	518	78N	C4-C5-C6-C7
7	A	509	78N	O15-C8-O16-C17
7	A	516	78N	C2-C3-C4-C5
7	A	519	78N	C12-C13-C14-C15
7	A	518	78N	C12-C13-C14-C15
7	A	518	78N	O20-C18-C19-O22
7	A	509	78N	C11-C10-C9-C1
7	A	514	78N	C11-C10-C9-C1
7	A	515	78N	C2-C3-C4-C5
7	A	517	78N	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
8	A	508	78M	C2-C1-O2-C17
4	A	504	1PE	C16-C26-OH6-C15
8	A	520	78M	C9-C10-C11-C12
7	A	507	78N	C7-C8-O16-C17
8	A	510	78M	C10-C11-C12-C13
8	A	510	78M	C3-C4-C5-C6
7	A	514	78N	C12-C13-C14-C15
7	A	515	78N	C7-C8-O16-C17
7	A	507	78N	O15-C8-O16-C17
7	A	519	78N	C3-C4-C5-C6
8	A	508	78M	C2-C3-C4-C5
8	A	508	78M	C3-C4-C5-C6
7	A	514	78N	C6-C7-C8-O16
7	A	519	78N	C11-C12-C13-C14
7	A	514	78N	C7-C8-O16-C17
8	A	508	78M	O1-C1-O2-C17
7	A	519	78N	C7-C8-O16-C17
7	A	514	78N	C3-C4-C5-C6
7	A	514	78N	C2-C3-C4-C5
7	A	517	78N	C12-C13-C14-C15
7	A	515	78N	O15-C8-O16-C17
7	A	511	78N	C11-C10-C9-C1
7	A	519	78N	C5-C6-C7-C8
7	A	511	78N	C7-C8-O16-C17
7	A	517	78N	C10-C11-C12-C13
7	A	511	78N	O15-C8-O16-C17
7	A	514	78N	O15-C8-O16-C17
7	A	519	78N	O15-C8-O16-C17
4	A	504	1PE	C15-C25-OH5-C14
8	A	510	78M	O2-C17-C18-O19
7	A	512	78N	C7-C8-O16-C17
7	A	514	78N	O16-C17-C18-C19
7	A	507	78N	C10-C11-C12-C13
7	A	511	78N	O20-C18-C19-O22
7	A	519	78N	C11-C10-C9-C1
7	A	514	78N	C10-C11-C12-C13
7	A	512	78N	O15-C8-O16-C17
7	A	516	78N	C3-C4-C5-C6
7	A	513	78N	C9-C10-C11-C12
5	A	505	EPE	C10-C9-N1-C2
5	A	505	EPE	C10-C9-N1-C6
7	A	512	78N	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
7	A	509	78N	C12-C13-C14-C15
7	A	511	78N	C2-C3-C4-C5
7	A	517	78N	C1-C2-C3-C4
8	A	520	78M	C7-C8-C9-C10
7	A	516	78N	C7-C8-O16-C17
7	A	509	78N	C1-C2-C3-C4
7	A	511	78N	C1-C2-C3-C4
7	A	516	78N	O15-C8-O16-C17
7	A	516	78N	C1-C2-C3-C4
7	A	514	78N	C6-C7-C8-O15
7	A	515	78N	C1-C2-C3-C4
7	A	519	78N	C1-C2-C3-C4
8	A	520	78M	O2-C1-C2-C3
8	A	510	78M	O1-C1-O2-C17
8	A	510	78M	C2-C1-O2-C17
7	A	516	78N	C2-C1-C9-C10
8	A	520	78M	C10-C11-C12-C13
7	A	518	78N	C2-C3-C4-C5
8	A	508	78M	C4-C5-C6-C7
7	A	509	78N	C2-C1-C9-C10
8	A	508	78M	C5-C6-C7-C8
7	A	511	78N	C2-C1-C9-C10
7	A	513	78N	C2-C1-C9-C10
7	A	519	78N	C2-C1-C9-C10
8	A	508	78M	C7-C8-C9-C10
7	A	519	78N	C2-C3-C4-C5
8	A	510	78M	C9-C10-C11-C12
7	A	515	78N	C2-C1-C9-C10
7	A	518	78N	C2-C1-C9-C10
8	A	520	78M	C5-C6-C7-C8
8	A	520	78M	O19-C18-C20-O21
7	A	514	78N	O16-C17-C18-O20
8	A	520	78M	O1-C1-C2-C3
7	A	512	78N	C2-C1-C9-C10
7	A	511	78N	C4-C5-C6-C7

There are no ring outliers.

13 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	508	78M	2	0
7	A	514	78N	1	0

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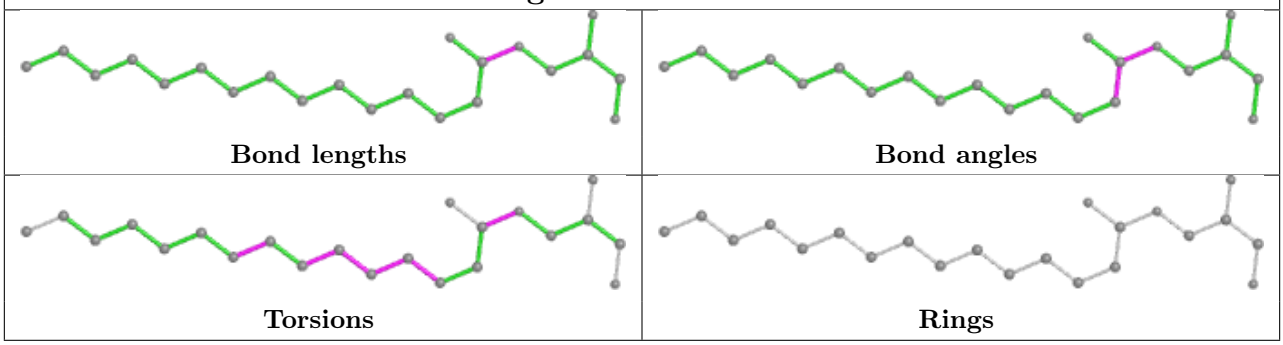
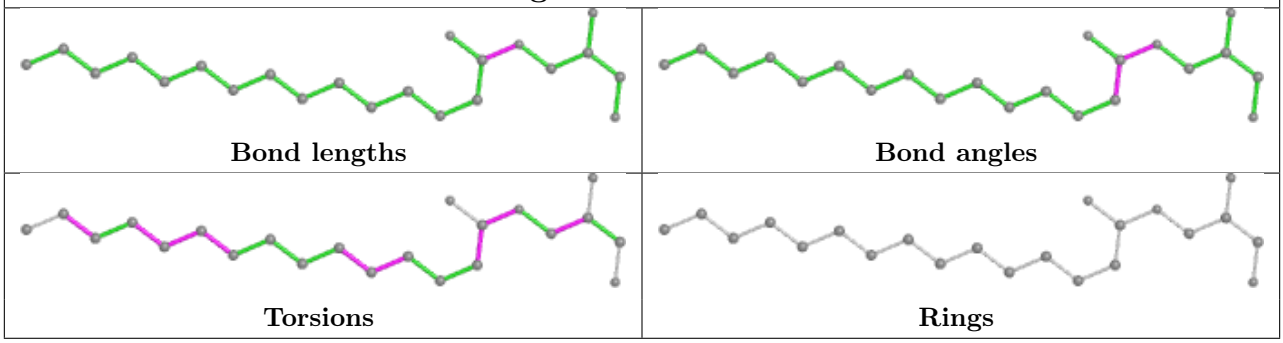
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	505	EPE	1	0
8	A	510	78M	3	0
7	A	517	78N	1	0
4	A	504	1PE	1	0
7	A	516	78N	1	0
8	A	520	78M	1	0
7	A	515	78N	2	0
7	A	513	78N	2	0
7	A	518	78N	1	0
7	A	519	78N	1	0
7	A	509	78N	2	0

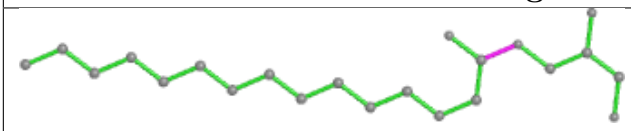
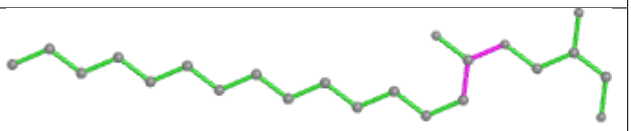
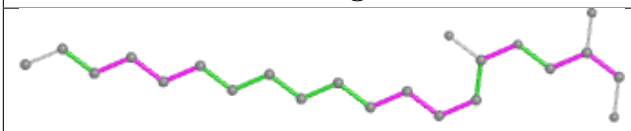
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand 78M A 508



Ligand 78N A 514



Ligand 78M A 510	
 Bond lengths	 Bond angles
 Torsions	Rings

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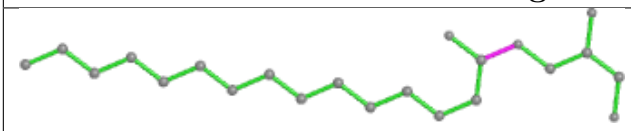
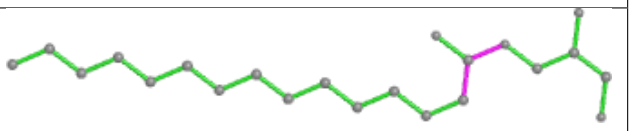
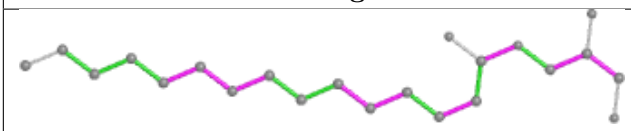
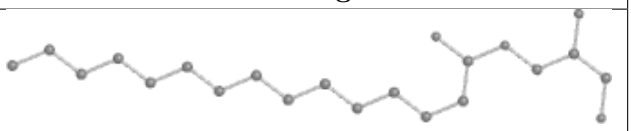
 Bond lengths	 Bond angles
 Torsions	 Rings

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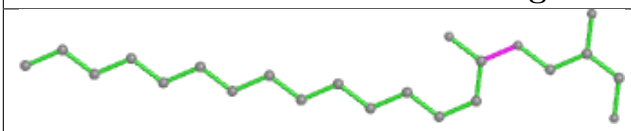
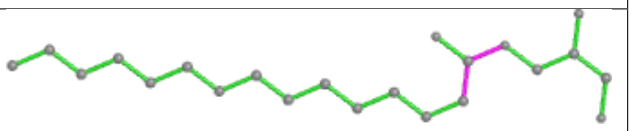
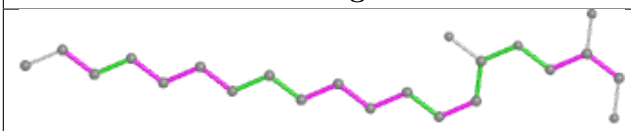
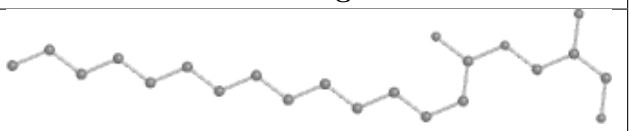
 Bond lengths	 Bond angles
 Torsions	 Rings

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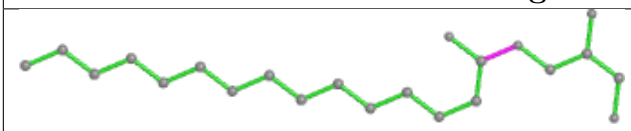
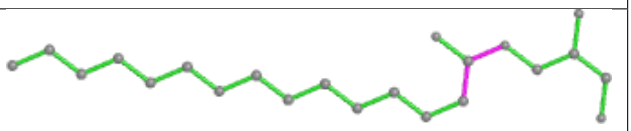
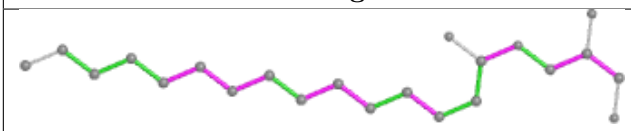
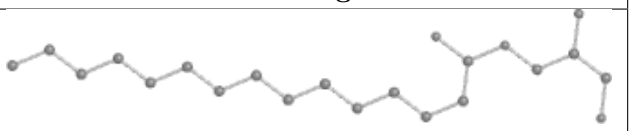
 Bond lengths	 Bond angles
 Torsions	 Rings

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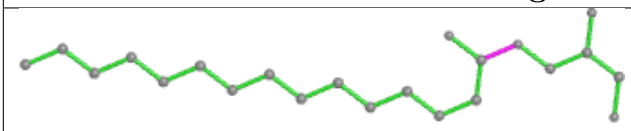
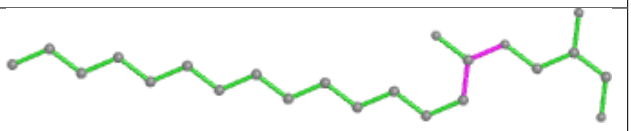
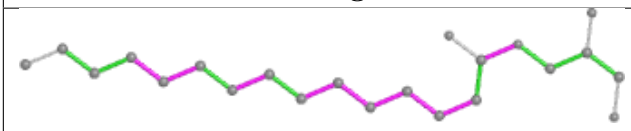
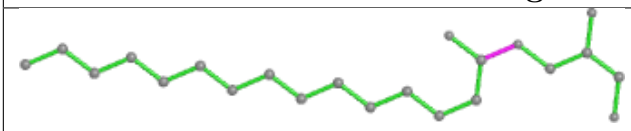
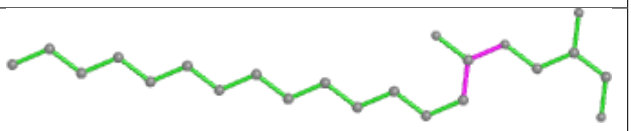
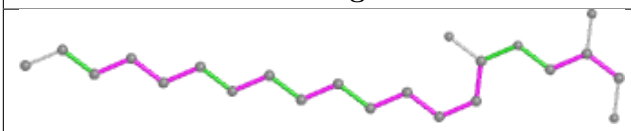
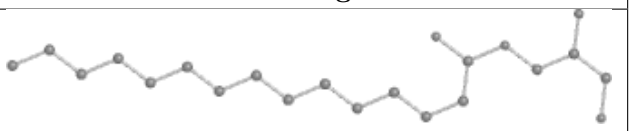
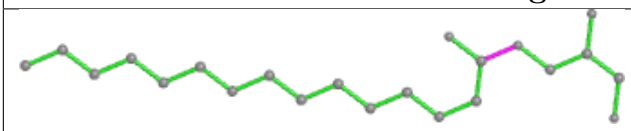
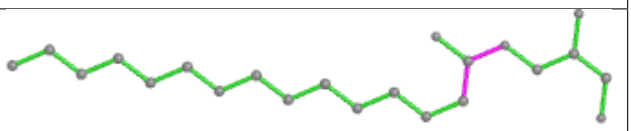
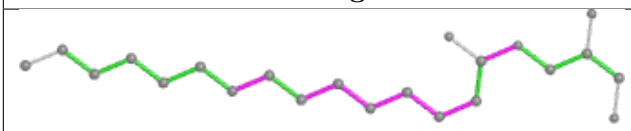
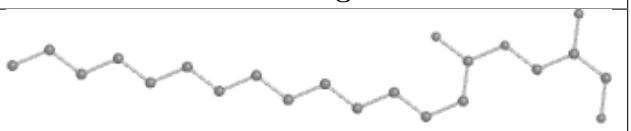
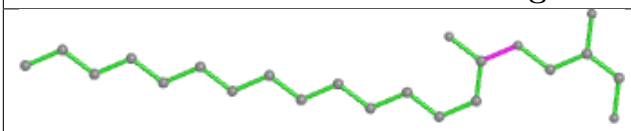
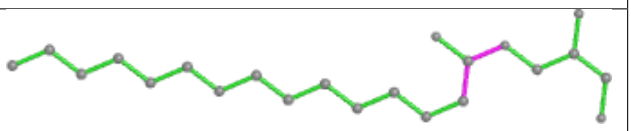
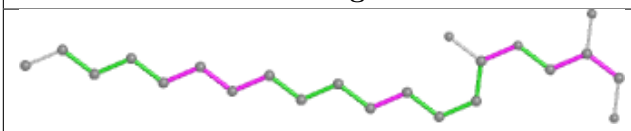
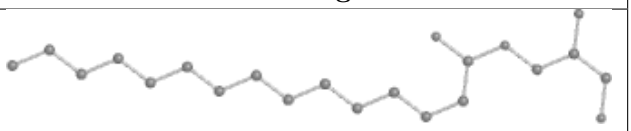
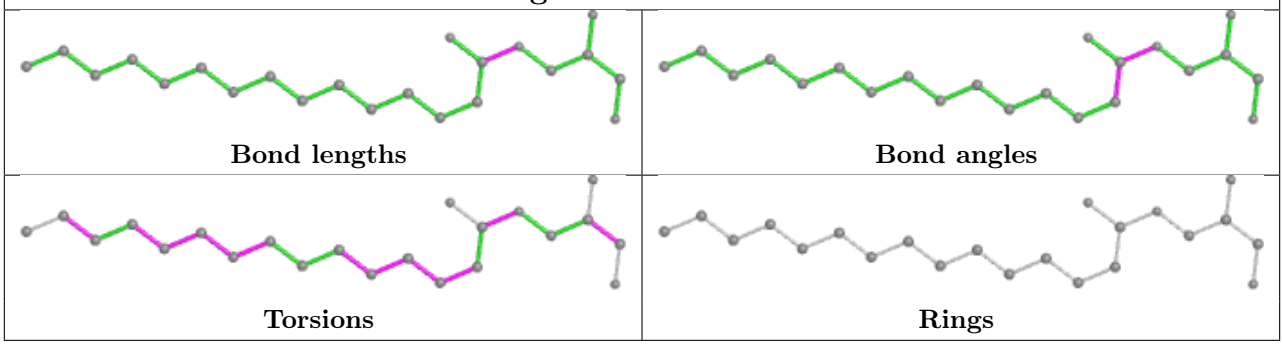
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand 78M A 520	
 Bond lengths	 Bond angles
 Torsions	 Rings

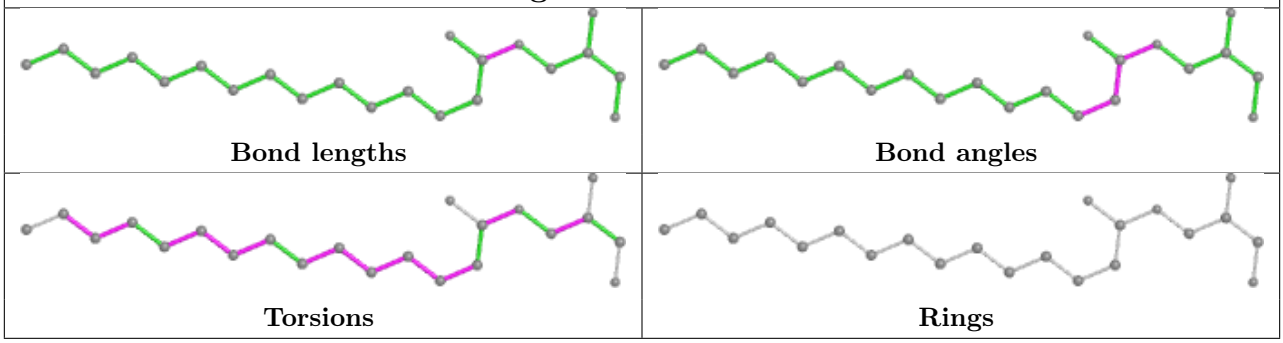
Ligand 78N A 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 78N A 513	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 78N A 518



Ligand 78N A 519



Ligand 78N A 507

Ligand 78N A 509

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	457/483 (94%)	0.07	29 (6%) 20 22	32, 43, 82, 101	0
2	B	3/3 (100%)	0.48	0 100 100	39, 39, 50, 54	0
All	All	460/486 (94%)	0.07	29 (6%) 20 22	32, 43, 82, 101	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	HIS	6.7
1	A	413	LYS	6.6
1	A	269	ILE	6.1
1	A	280	LEU	4.8
1	A	279	HIS	4.6
1	A	414	LEU	4.2
1	A	281	ARG	4.1
1	A	50	HIS	3.9
1	A	138	ASP	3.8
1	A	268	MET	3.7
1	A	142	ARG	3.6
1	A	5	GLY	3.6
1	A	422	GLN	3.5
1	A	423	MET	3.5
1	A	267	TRP	3.4
1	A	338	PHE	3.4
1	A	412	THR	3.2
1	A	139	GLU	3.1
1	A	408	LEU	3.1
1	A	270	SER	3.0
1	A	344	THR	3.0
1	A	346	TRP	2.7
1	A	284	SER	2.5
1	A	341	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	266	ALA	2.2
1	A	343	TRP	2.1
1	A	243	TRP	2.1
1	A	477	GLY	2.0
1	A	411	THR	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, 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
7	78N	A	514	22/22	0.70	0.30	77,90,113,118	0
8	78M	A	520	22/22	0.70	0.25	65,72,78,85	0
7	78N	A	513	22/22	0.72	0.29	62,72,82,82	0
7	78N	A	516	22/22	0.73	0.32	45,70,77,79	0
7	78N	A	515	22/22	0.74	0.25	61,68,75,82	0
7	78N	A	517	22/22	0.76	0.34	67,78,100,103	0
8	78M	A	508	22/22	0.78	0.33	76,86,108,113	0
7	78N	A	509	22/22	0.80	0.32	65,76,89,93	0
5	EPE	A	505	15/15	0.81	0.36	104,108,114,115	0
4	1PE	A	504	10/16	0.82	0.17	59,62,66,70	0
7	78N	A	511	22/22	0.83	0.30	57,73,84,95	0
7	78N	A	518	22/22	0.84	0.25	63,79,97,104	0
7	78N	A	512	22/22	0.85	0.23	52,64,71,76	0
3	PO4	A	502	5/5	0.86	0.15	98,98,100,102	0
8	78M	A	510	22/22	0.87	0.23	54,70,88,89	0
7	78N	A	507	22/22	0.88	0.23	47,61,67,74	0
7	78N	A	519	22/22	0.90	0.14	73,77,80,81	0
3	PO4	A	503	5/5	0.95	0.18	74,76,81,82	0

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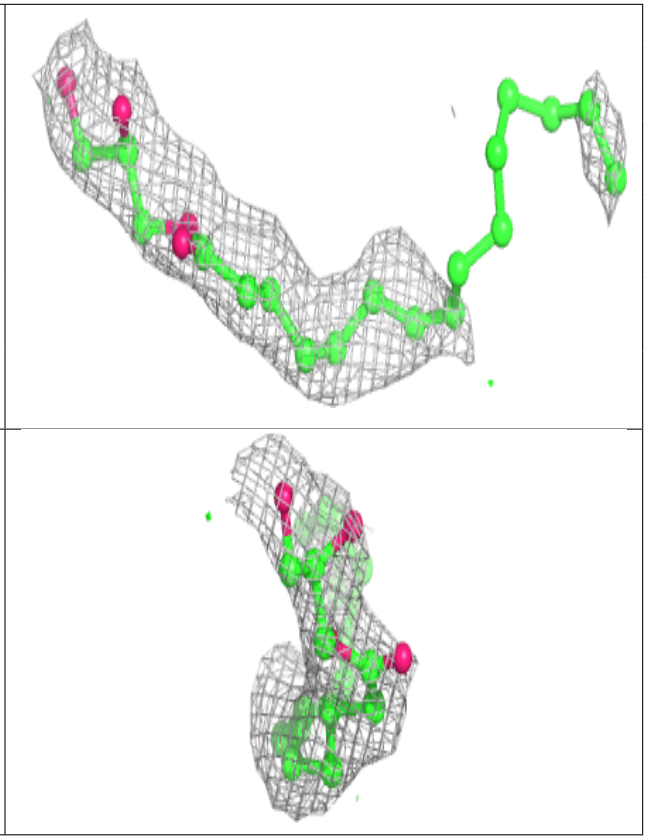
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PO4	A	501	5/5	0.96	0.22	67,68,70,84	0
6	NA	A	506	1/1	0.98	0.17	46,46,46,46	0

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.

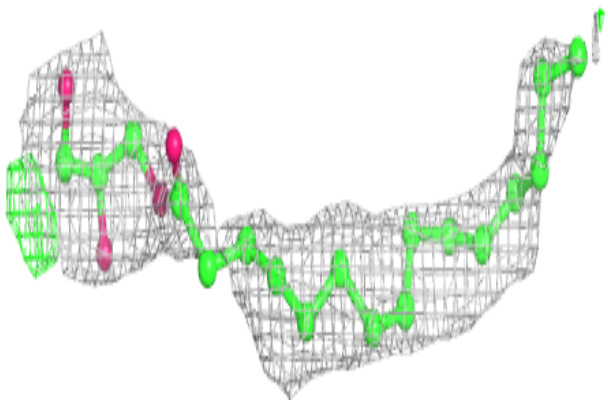
Electron density around 78N A 514:

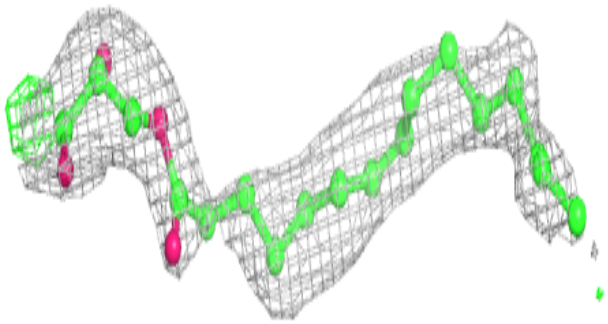
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

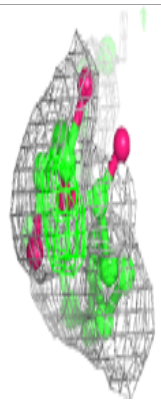


Electron density around 78M A 520:

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

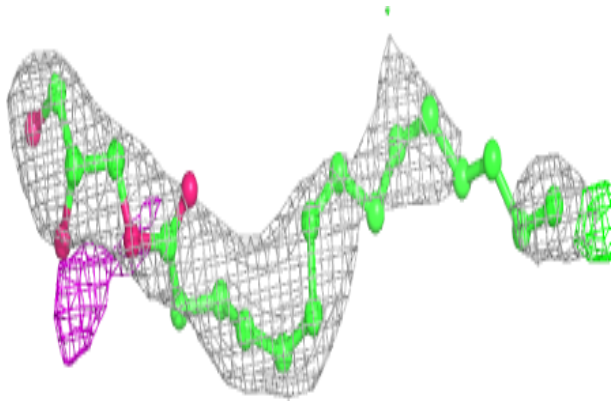


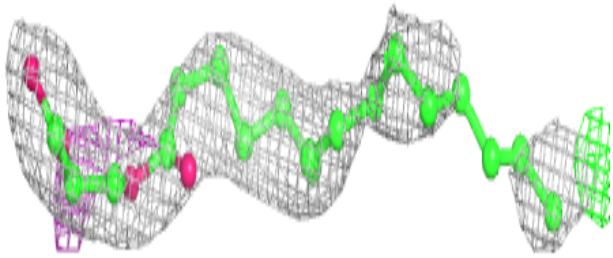


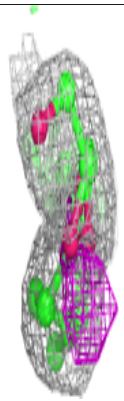


Electron density around 78N A 513:

$2mF_o$-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 516:

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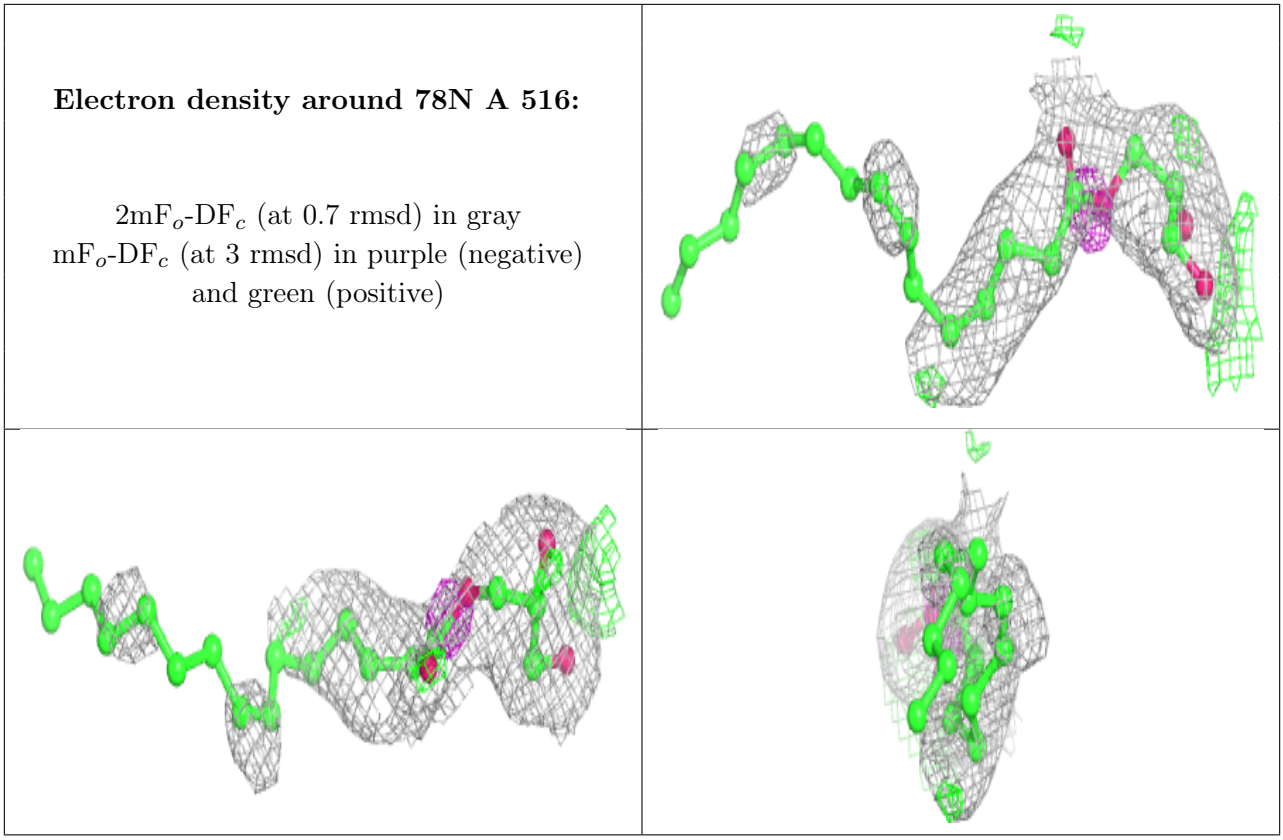
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 78N A 515:

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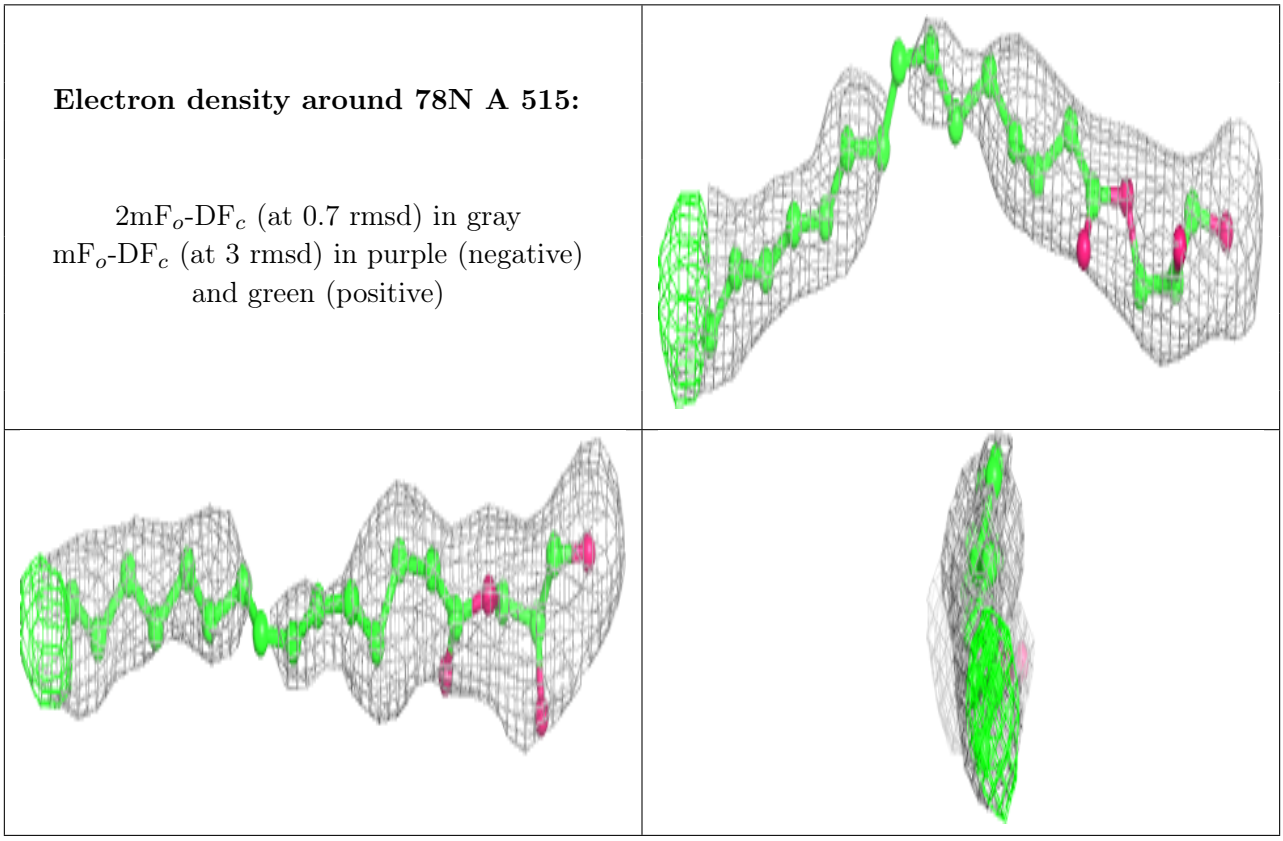
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 78N A 517:

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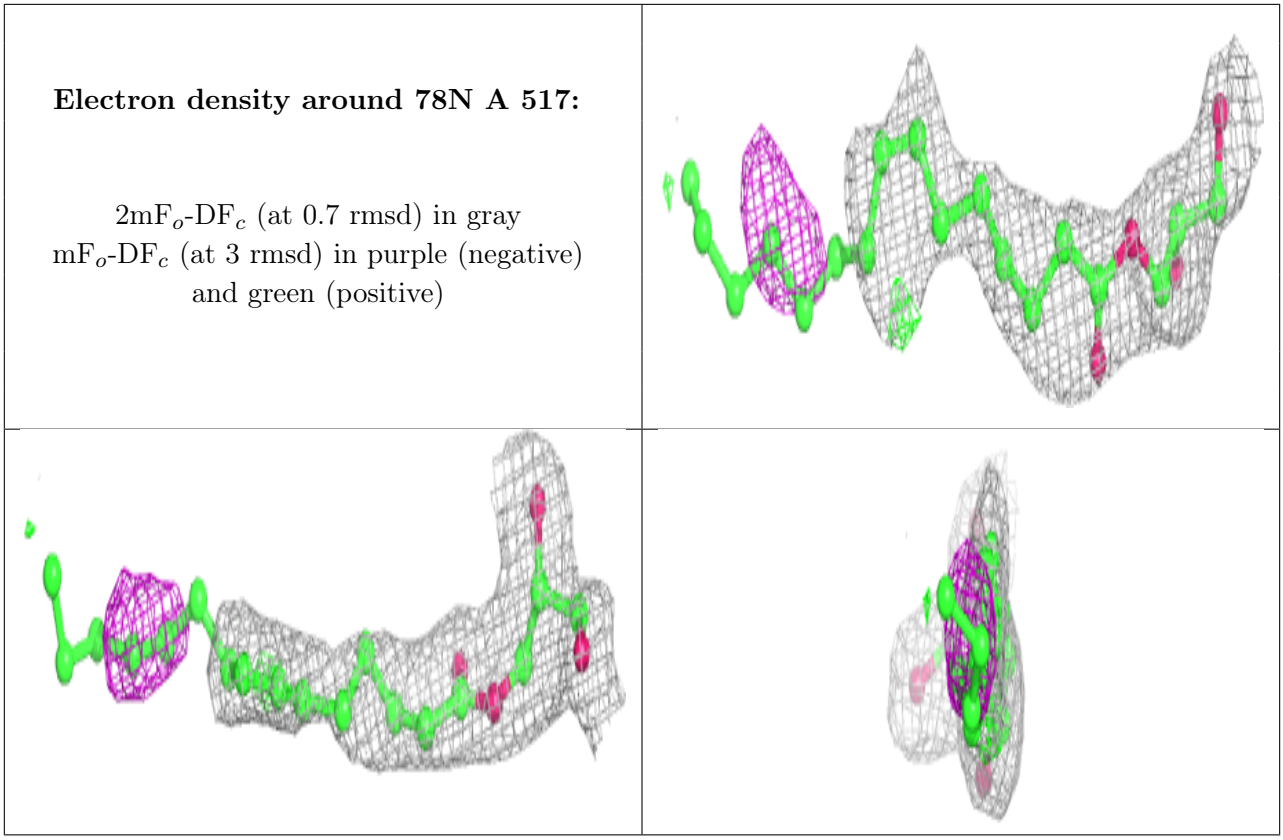
and green (positive)



Electron density around 78M A 508:

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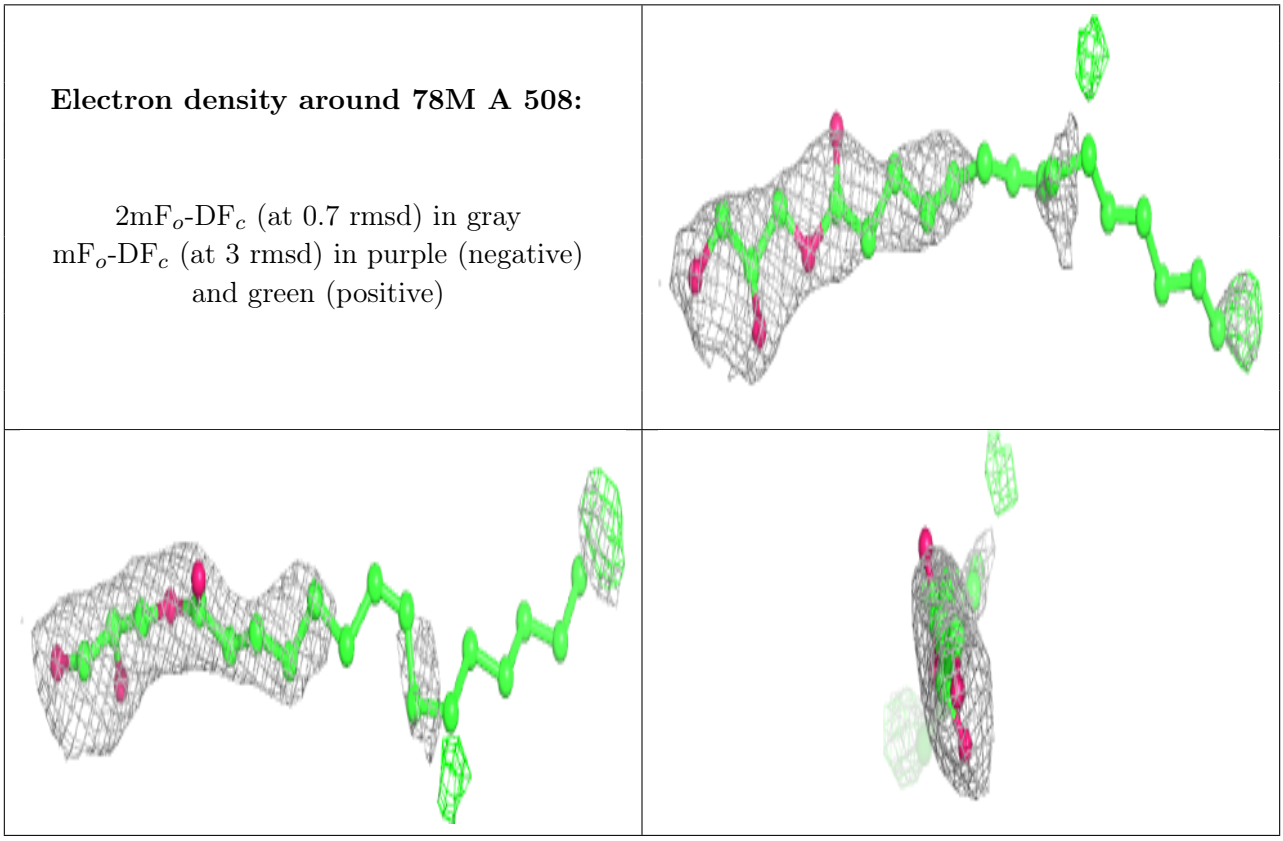
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 78N A 509:

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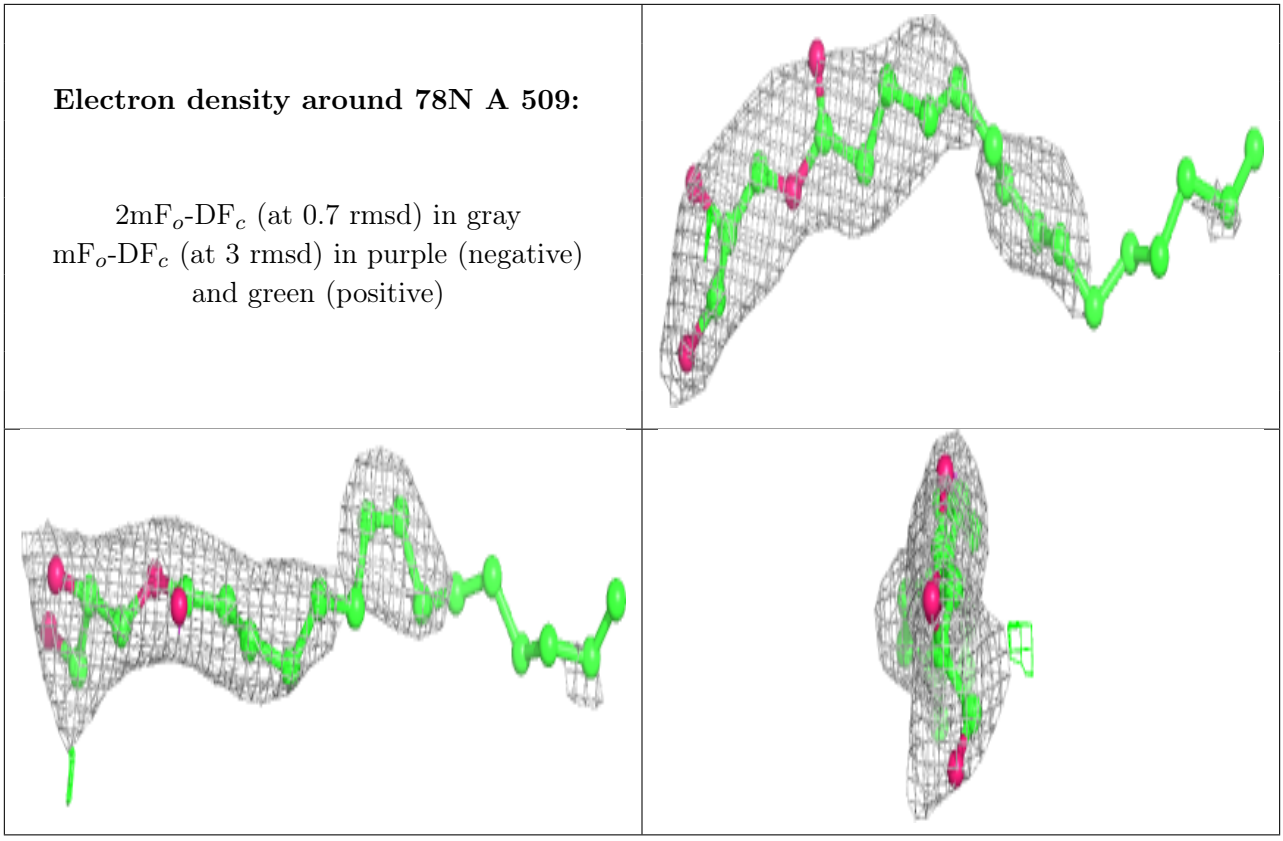
and green (positive)



Electron density around 78N A 511:

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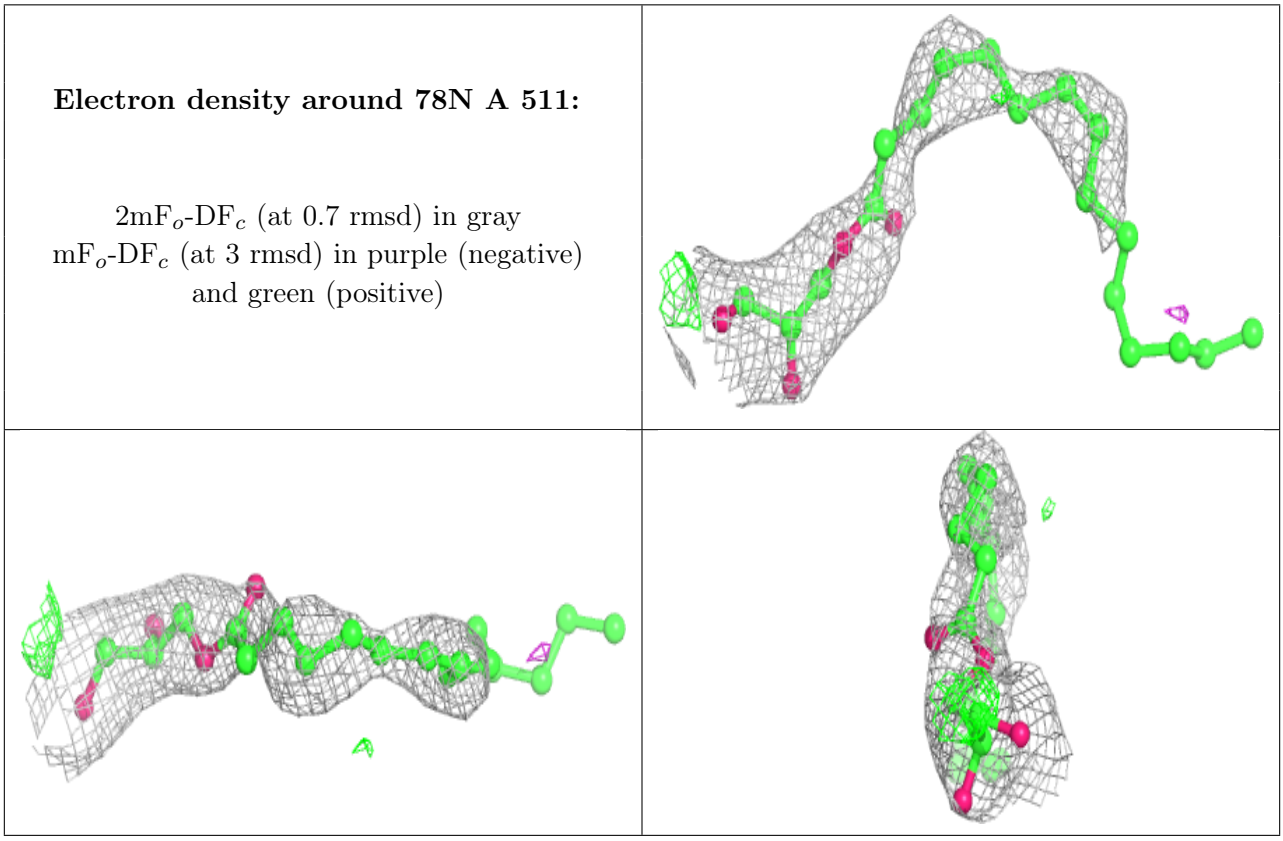
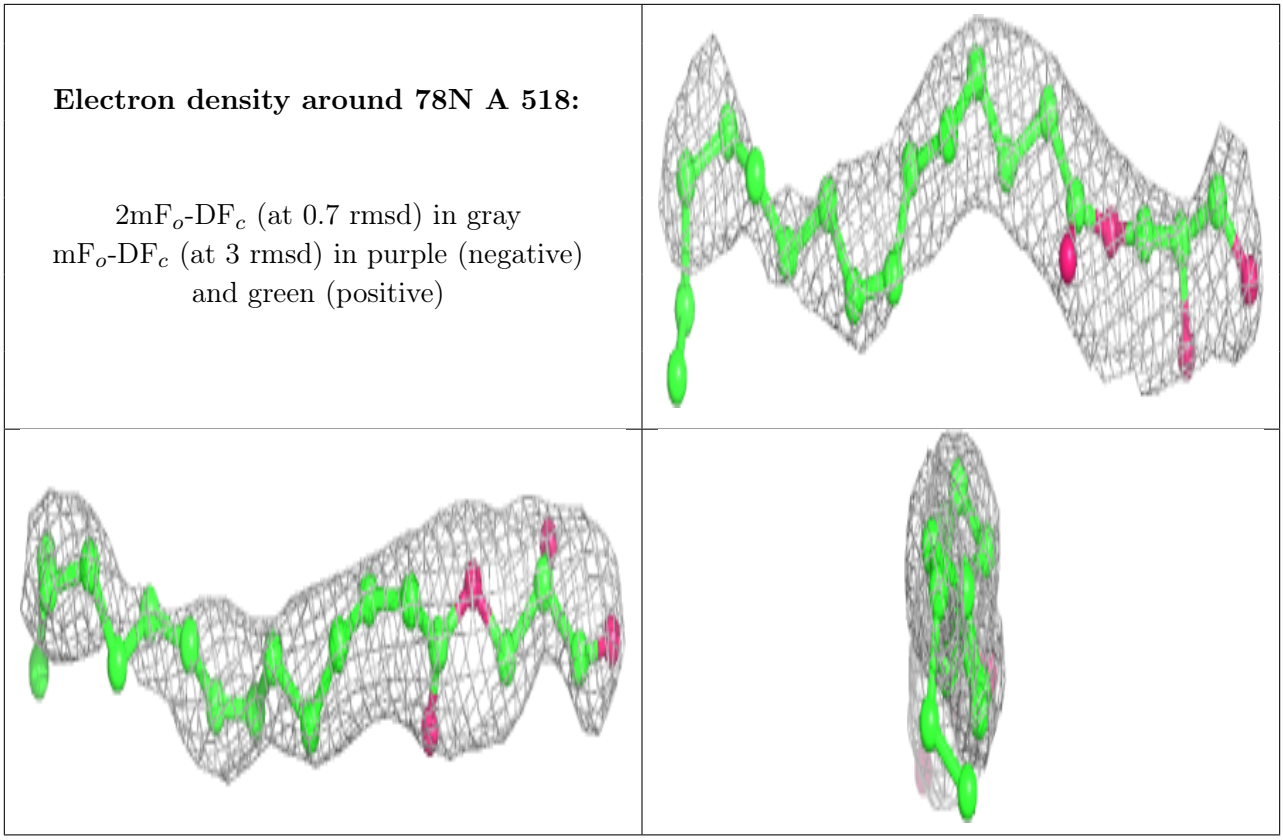
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 78N 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 512:

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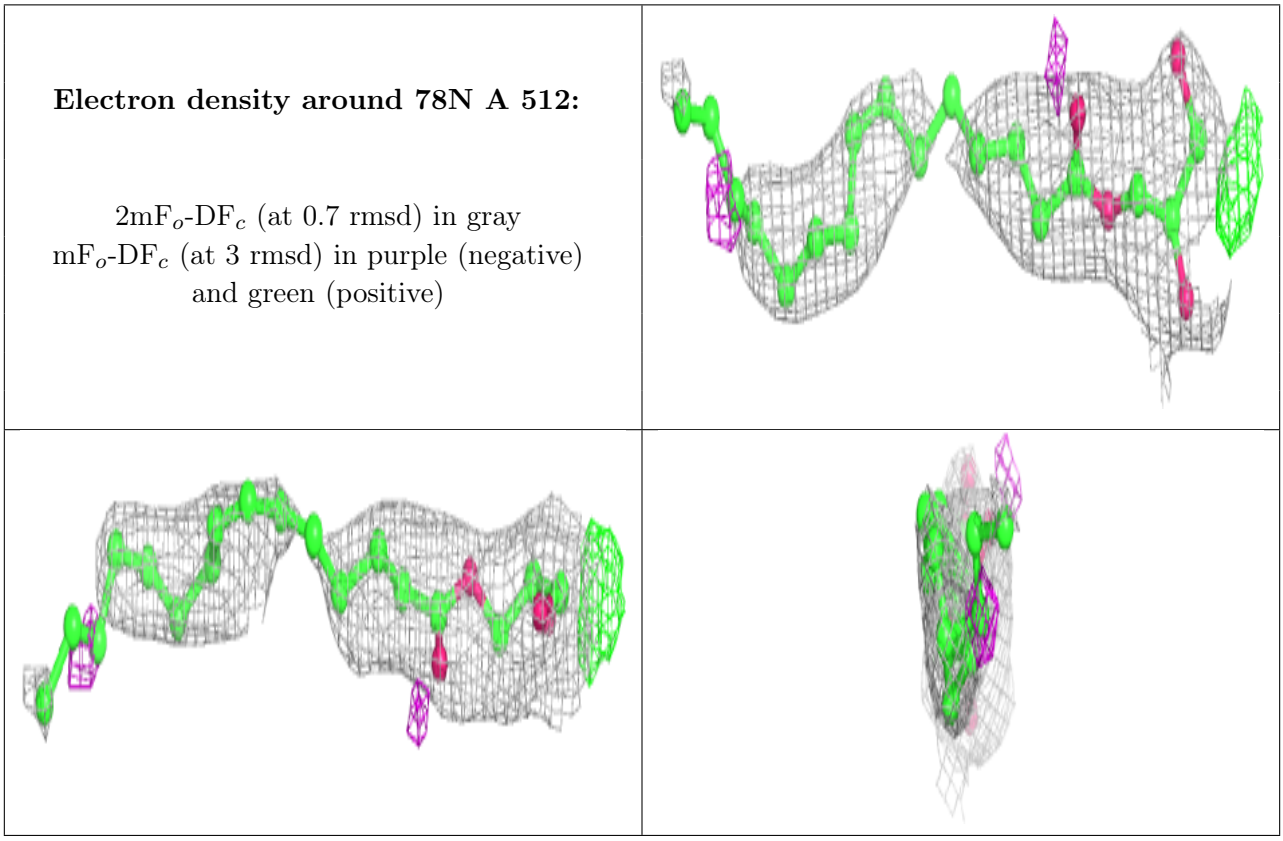
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 78M A 510:

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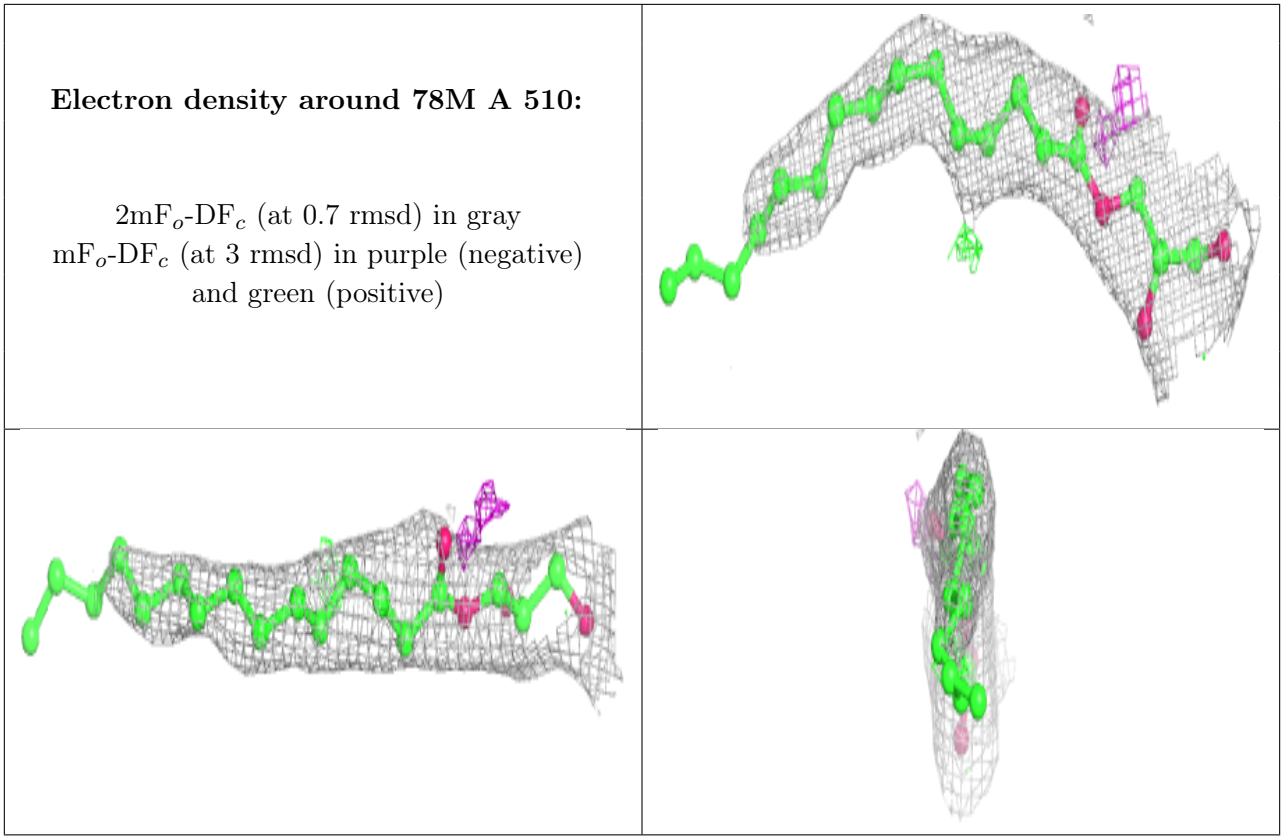
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 78N A 507:

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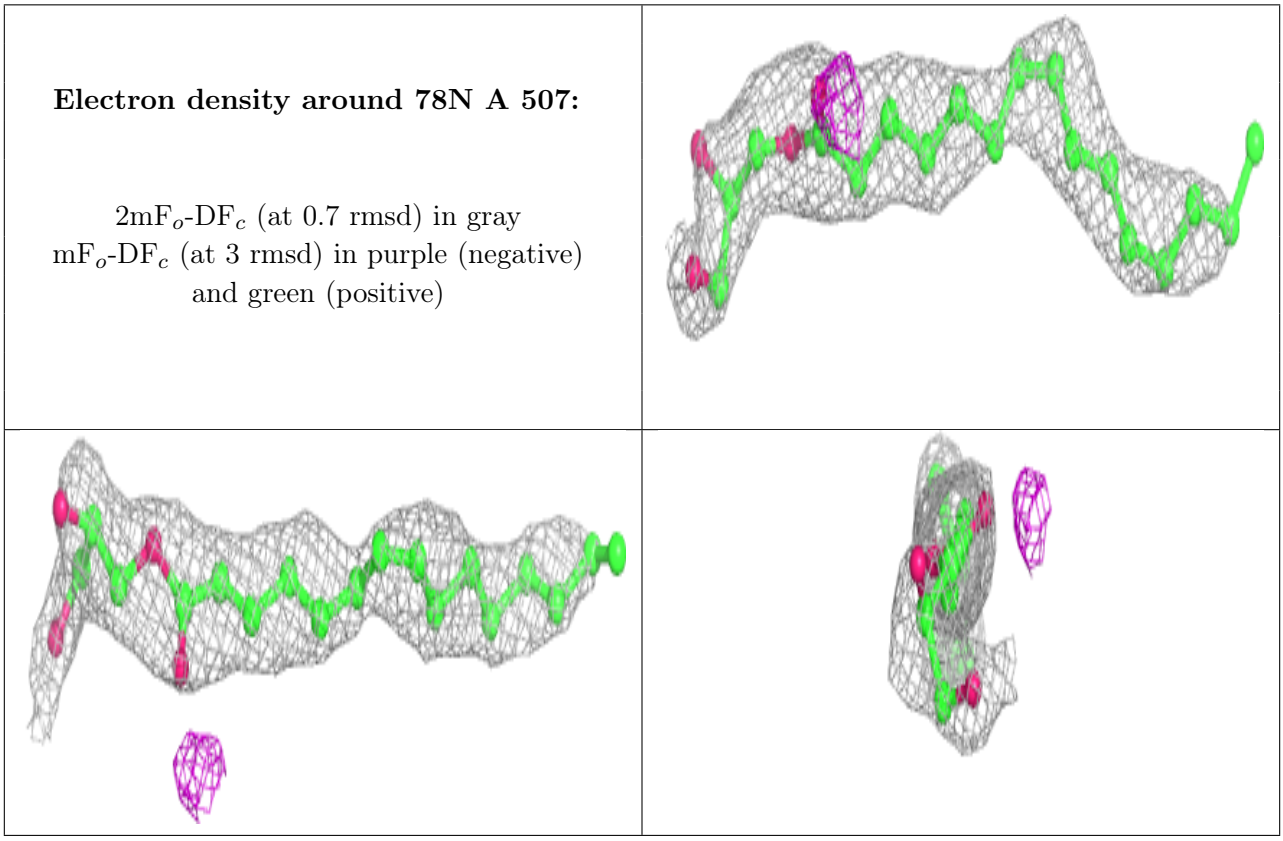
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 78N A 519:

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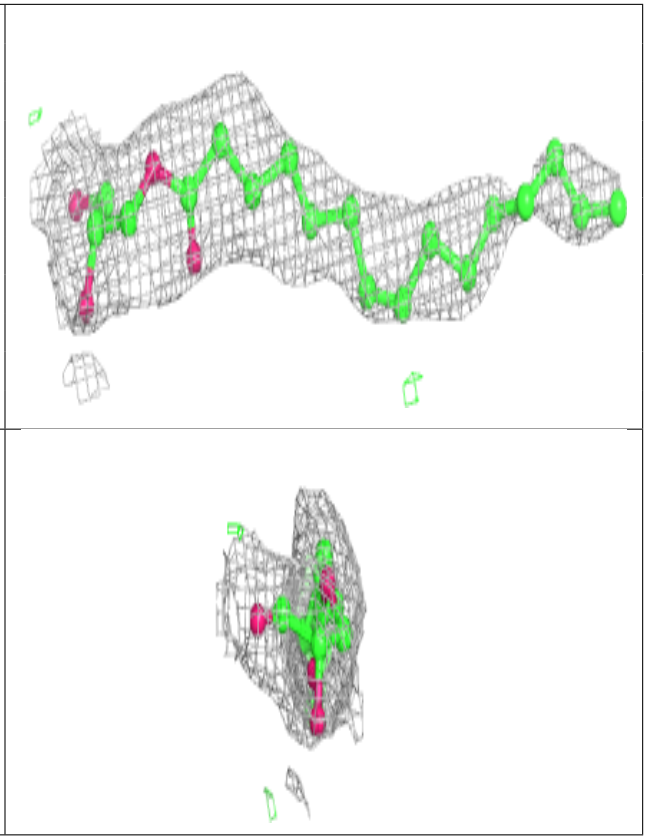
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.