Full wwPDB X-ray Structure Validation Report (i)

Jan 6, 2024 – 07:55 pm GMT

PDB ID	:	5OXQ
Title	:	PepTSt in complex with HEPES (300 mM)
Authors	:	Martinez Molledo, M.; Quistgaard, E.M.; Loew, C.
Deposited on	:	2017-09-07
Resolution	:	2.19 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:

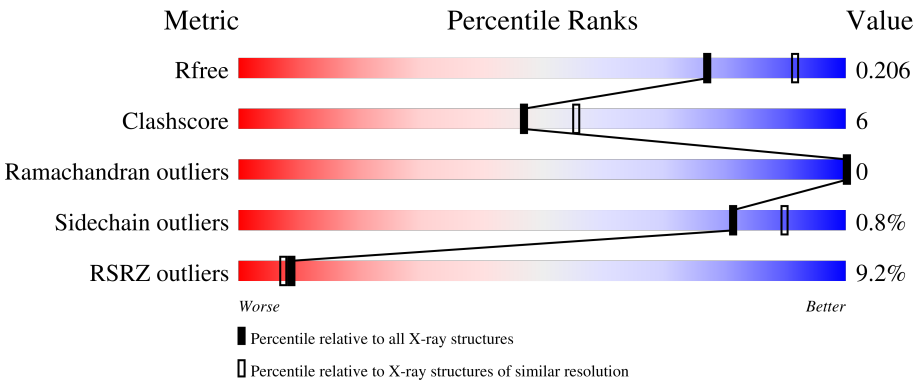
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	490	9% 81% 12% 7%

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
7	78M	A	523	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 4074 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	455	3519	2371	543	588	17	0	0	0

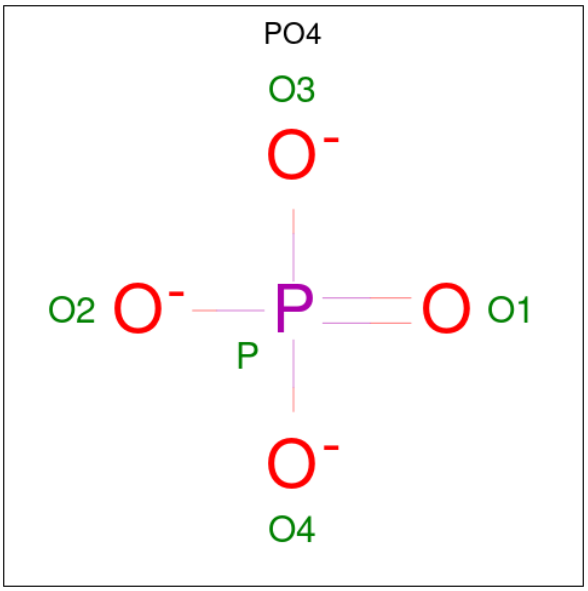
There are 7 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

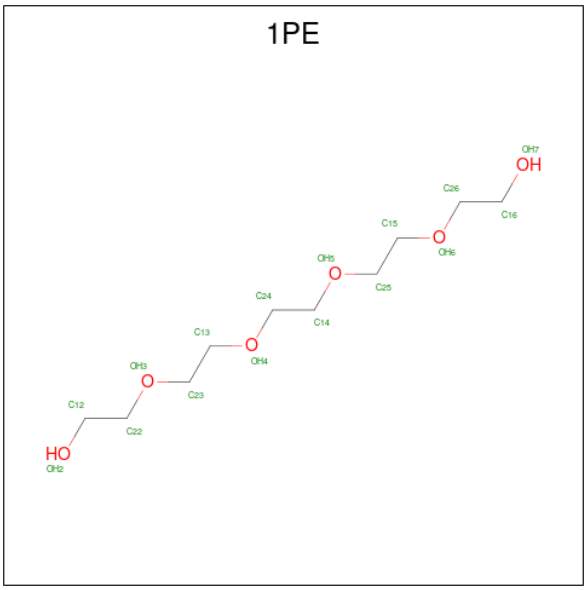
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	1	1	1	0	0

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



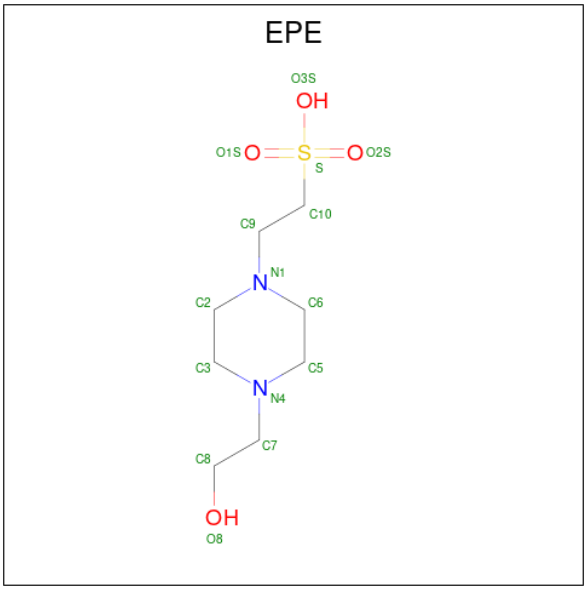
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0

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



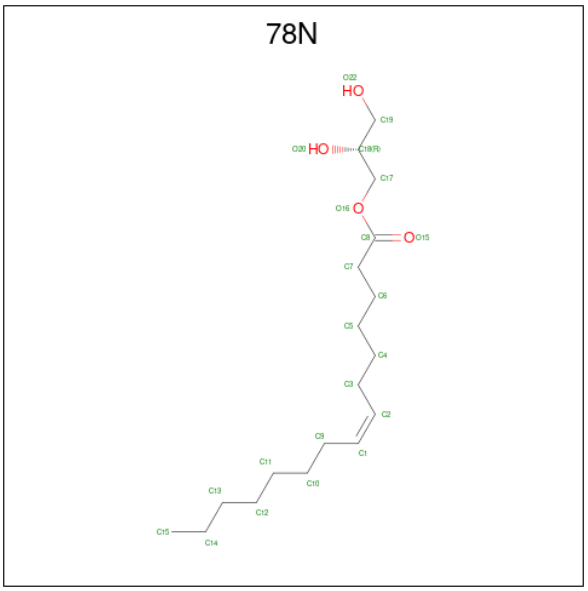
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	10	6	4	0	0

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



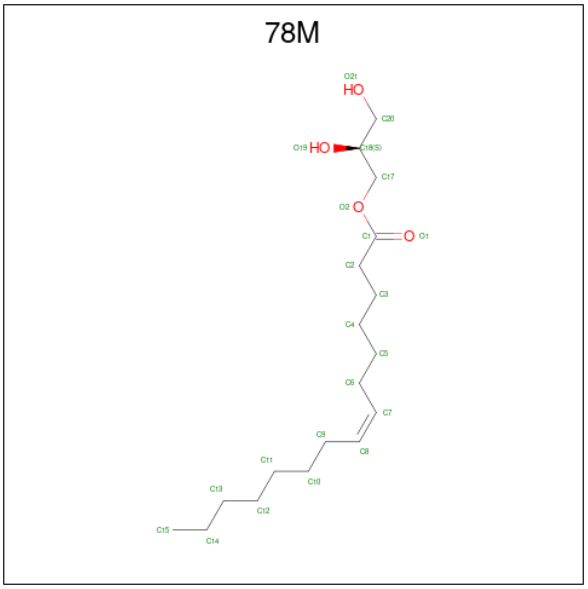
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	A	1	15	8	2	4	1	0	0
			Total	C	N	O	S		
5	A	1	15	8	2	4	1	0	0

- Molecule 6 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		
6	A	1	22	18	4	0	0
			Total	C	O		
6	A	1	22	18	4	0	0
			Total	C	O		
6	A	1	22	18	4	0	0
			Total	C	O		
6	A	1	22	18	4	0	0
			Total	C	O		
6	A	1	22	18	4	0	0
			Total	C	O		
6	A	1	22	18	4	0	0
			Total	C	O		
6	A	1	22	18	4	0	0
			Total	C	O		
6	A	1	22	18	4	0	0
			Total	C	O		
6	A	1	22	18	4	0	0
			Total	C	O		
6	A	1	22	18	4	0	0
			Total	C	O		
6	A	1	22	18	4	0	0
			Total	C	O		
6	A	1	22	18	4	0	0
			Total	C	O		
6	A	1	22	18	4	0	0
			Total	C	O		
6	A	1	22	18	4	0	0

- Molecule 7 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		
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 water.

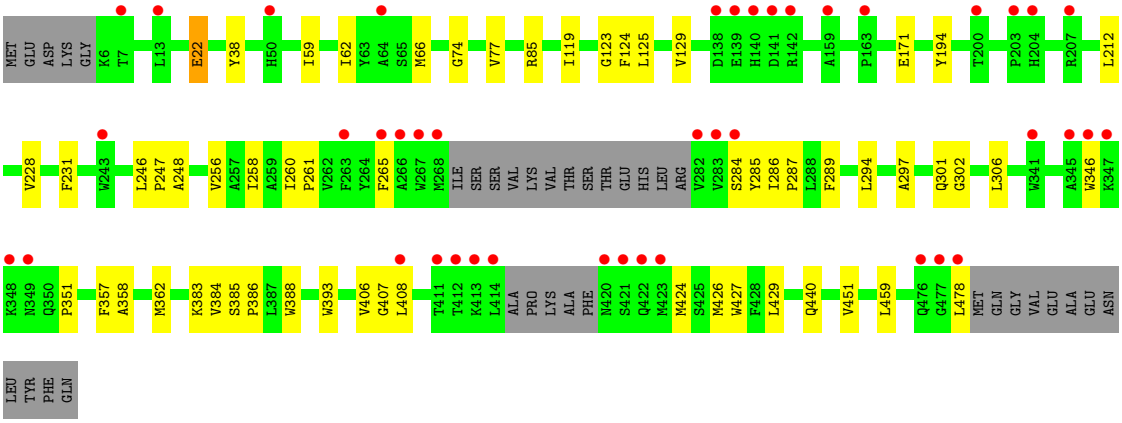
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	98	98	98	0	0

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: 9% 81% 12% 7%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	102.21Å 110.05Å 109.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.31 – 2.19 46.31 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.31-2.19) 99.7 (46.31-2.19)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.190 , 0.205 0.192 , 0.206	Depositor DCC
R_{free} test set	1591 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	45.5	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 58.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4074	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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: 1PE, PO4, EPE, 78N, 78M, NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.46	0/3624	0.52	0/4942

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	3519	0	3609	42	0
2	A	1	0	0	0	0
3	A	20	0	0	0	0
4	A	10	0	13	1	0
5	A	30	0	34	3	0
6	A	308	0	476	21	0
7	A	88	0	136	11	0
8	A	98	0	0	1	0
All	All	4074	0	4268	51	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 6.

All (51) 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:384:VAL:HA	5:A:508:EPE:H102	1.64	0.79
1:A:459:LEU:HD13	7:A:510:78M:H22C	1.73	0.69
5:A:508:EPE:O3S	7:A:512:78M:O21	2.07	0.69
1:A:77:VAL:HG11	1:A:124:PHE:HE1	1.59	0.67
1:A:284:SER:HB2	1:A:478:LEU:HD22	1.76	0.67
1:A:385:SER:N	5:A:508:EPE:O1S	2.15	0.66
1:A:228:VAL:HG21	6:A:526:78N:H153	1.83	0.61
1:A:85:ARG:NE	6:A:524:78N:O22	2.31	0.60
1:A:38:TYR:HB3	4:A:506:1PE:H252	1.85	0.59
1:A:231:PHE:HE2	6:A:519:78N:H91C	1.70	0.57
1:A:62:ILE:HG23	6:A:518:78N:H42C	1.87	0.57
1:A:231:PHE:CE2	6:A:519:78N:H91C	2.40	0.56
1:A:248:ALA:HB2	6:A:520:78N:H18	1.88	0.55
6:A:513:78N:H141	6:A:514:78N:H142	1.89	0.55
1:A:451:VAL:HG11	6:A:509:78N:H171	1.89	0.54
7:A:523:78M:H52C	6:A:524:78N:H131	1.92	0.52
1:A:426:MET:HA	1:A:429:LEU:HB2	1.92	0.52
1:A:59:ILE:HD11	1:A:246:LEU:HD21	1.92	0.51
1:A:388:TRP:HZ2	6:A:511:78N:H191	1.75	0.51
1:A:294:LEU:HD21	7:A:522:78M:H52C	1.93	0.50
1:A:194:TYR:CZ	7:A:523:78M:H201	2.47	0.49
1:A:358:ALA:O	1:A:362:MET:HG3	2.12	0.49
1:A:258:ILE:O	1:A:261:PRO:HD2	2.11	0.49
1:A:388:TRP:CZ2	6:A:511:78N:H191	2.50	0.47
7:A:523:78M:H202	6:A:524:78N:C2	2.44	0.47
1:A:74:GLY:HA3	1:A:123:GLY:O	2.14	0.46
1:A:66:MET:HG3	6:A:518:78N:H91C	1.97	0.46
1:A:119:ILE:HD13	6:A:518:78N:H92C	1.97	0.45
1:A:357:PHE:HE1	1:A:406:VAL:HG23	1.81	0.45
1:A:386:PRO:HG2	6:A:515:78N:H192	1.99	0.45
1:A:246:LEU:HB3	1:A:247:PRO:HD3	1.99	0.45
1:A:407:GLY:HA3	1:A:427:TRP:CH2	2.51	0.44
1:A:284:SER:O	1:A:287:PRO:HD2	2.18	0.44
6:A:521:78N:H142	7:A:522:78M:H132	2.00	0.44
1:A:346:TRP:CZ2	1:A:351:PRO:HD3	2.52	0.44
1:A:125:LEU:O	1:A:129:VAL:HG23	2.18	0.43
1:A:265:PHE:CE2	7:A:522:78M:H142	2.54	0.43
1:A:302:GLY:HA2	1:A:306:LEU:HB2	2.00	0.43
1:A:256:VAL:O	1:A:260:ILE:HG13	2.19	0.42
7:A:512:78M:O19	6:A:514:78N:H191	2.19	0.42
1:A:286:ILE:HB	1:A:287:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ALA:O	1:A:301:GLN:HG3	2.20	0.41
1:A:383:LYS:NZ	8:A:616:HOH:O	2.52	0.41
6:A:521:78N:H102	7:A:522:78M:H92C	2.02	0.41
6:A:524:78N:H31C	6:A:524:78N:H91C	1.65	0.41
1:A:285:TYR:CE2	1:A:289:PHE:HB2	2.55	0.40
1:A:22:GLU:HA	1:A:22:GLU:OE2	2.22	0.40
1:A:408:LEU:HD11	1:A:424:MET:HG3	2.02	0.40
1:A:440:GLN:HB3	6:A:521:78N:H71	2.02	0.40
1:A:212:LEU:HD12	6:A:525:78N:H71	2.02	0.40
7:A:523:78M:H31C	7:A:523:78M:H62C	1.88	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	449/490 (92%)	443 (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	367/397 (92%)	364 (99%)	3 (1%)	81 90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	171	GLU
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	350	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 26 ligands modelled in this entry, 1 is monoatomic - leaving 25 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PO4	A	503	-	4,4,4	0.88	0	6,6,6	0.48	0
6	78N	A	521	-	21,21,21	0.97	1 (4%)	22,22,22	1.03	1 (4%)
5	EPE	A	508	-	15,15,15	1.02	0	18,20,20	1.43	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	78N	A	519	-	21,21,21	0.93	1 (4%)	22,22,22	0.97	1 (4%)
7	78M	A	510	-	21,21,21	1.21	1 (4%)	22,22,22	0.79	1 (4%)
6	78N	A	515	-	21,21,21	0.98	1 (4%)	22,22,22	0.94	1 (4%)
7	78M	A	522	-	21,21,21	1.12	1 (4%)	22,22,22	1.02	2 (9%)
7	78M	A	523	-	21,21,21	1.17	1 (4%)	22,22,22	1.10	1 (4%)
6	78N	A	511	-	21,21,21	0.96	1 (4%)	22,22,22	1.00	1 (4%)
6	78N	A	524	-	21,21,21	0.89	1 (4%)	22,22,22	1.17	2 (9%)
6	78N	A	520	-	21,21,21	0.97	1 (4%)	22,22,22	1.01	1 (4%)
6	78N	A	526	-	21,21,21	0.91	2 (9%)	22,22,22	1.15	2 (9%)
3	PO4	A	505	-	4,4,4	0.96	0	6,6,6	0.47	0
3	PO4	A	502	-	4,4,4	0.93	0	6,6,6	0.39	0
6	78N	A	514	-	21,21,21	0.99	1 (4%)	22,22,22	0.94	1 (4%)
6	78N	A	517	-	21,21,21	0.95	1 (4%)	22,22,22	1.03	1 (4%)
5	EPE	A	507	-	15,15,15	0.93	0	18,20,20	1.13	0
6	78N	A	513	-	21,21,21	0.98	1 (4%)	22,22,22	1.08	1 (4%)
6	78N	A	518	-	21,21,21	0.90	1 (4%)	22,22,22	1.08	1 (4%)
6	78N	A	516	-	21,21,21	0.94	1 (4%)	22,22,22	1.05	1 (4%)
7	78M	A	512	-	21,21,21	1.11	1 (4%)	22,22,22	1.01	1 (4%)
4	1PE	A	506	-	9,9,15	0.58	0	8,8,14	0.52	0
6	78N	A	525	-	21,21,21	0.95	1 (4%)	22,22,22	1.04	1 (4%)
6	78N	A	509	-	21,21,21	0.96	1 (4%)	22,22,22	1.08	1 (4%)
3	PO4	A	504	-	4,4,4	0.91	0	6,6,6	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	78N	A	521	-	-	11/21/21/21	-
5	EPE	A	508	-	-	6/9/19/19	0/1/1/1
6	78N	A	519	-	-	9/21/21/21	-
7	78M	A	510	-	-	6/21/21/21	-
6	78N	A	515	-	-	9/21/21/21	-
7	78M	A	522	-	-	10/21/21/21	-
7	78M	A	523	-	-	13/21/21/21	-
6	78N	A	511	-	-	10/21/21/21	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	78N	A	524	-	-	3/21/21/21	-
6	78N	A	520	-	-	9/21/21/21	-
6	78N	A	526	-	-	12/21/21/21	-
6	78N	A	514	-	-	7/21/21/21	-
6	78N	A	517	-	-	11/21/21/21	-
5	EPE	A	507	-	-	2/9/19/19	0/1/1/1
6	78N	A	513	-	-	11/21/21/21	-
6	78N	A	518	-	-	12/21/21/21	-
6	78N	A	516	-	-	11/21/21/21	-
7	78M	A	512	-	-	14/21/21/21	-
4	1PE	A	506	-	-	3/7/7/13	-
6	78N	A	525	-	-	10/21/21/21	-
6	78N	A	509	-	-	10/21/21/21	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	510	78M	O2-C1	3.54	1.43	1.33
6	A	515	78N	O16-C8	3.18	1.42	1.33
6	A	521	78N	O16-C8	3.17	1.42	1.33
6	A	514	78N	O16-C8	3.16	1.42	1.33
7	A	522	78M	O2-C1	3.16	1.42	1.33
7	A	512	78M	O2-C1	3.14	1.42	1.33
7	A	523	78M	O2-C1	3.12	1.42	1.33
6	A	509	78N	O16-C8	3.10	1.42	1.33
6	A	513	78N	O16-C8	3.08	1.42	1.33
6	A	520	78N	O16-C8	3.00	1.42	1.33
6	A	519	78N	O16-C8	2.94	1.41	1.33
6	A	525	78N	O16-C8	2.88	1.41	1.33
6	A	511	78N	O16-C8	2.86	1.41	1.33
6	A	518	78N	O16-C8	2.83	1.41	1.33
6	A	516	78N	O16-C8	2.82	1.41	1.33
6	A	517	78N	O16-C8	2.82	1.41	1.33
6	A	524	78N	O16-C8	2.73	1.41	1.33
6	A	526	78N	O16-C8	2.68	1.41	1.33
6	A	526	78N	O16-C17	-2.01	1.40	1.45

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	523	78M	O2-C1-C2	3.36	122.46	111.91
6	A	513	78N	O16-C8-C7	3.17	121.86	111.91
7	A	522	78M	O2-C1-C2	3.04	121.45	111.91
6	A	521	78N	O16-C8-C7	3.02	121.39	111.91
6	A	516	78N	O16-C8-C7	2.92	121.09	111.91
6	A	509	78N	O16-C8-C7	2.92	121.07	111.91
6	A	520	78N	O16-C8-C7	2.92	121.06	111.91
6	A	511	78N	O16-C8-C7	2.89	120.97	111.91
6	A	514	78N	O16-C8-C7	2.88	120.95	111.91
7	A	512	78M	O2-C1-C2	2.83	120.80	111.91
5	A	508	EPE	O1S-S-C10	-2.83	103.51	106.92
6	A	518	78N	O16-C8-C7	2.73	120.47	111.91
6	A	519	78N	O16-C8-C7	2.70	120.38	111.91
6	A	524	78N	O16-C8-C7	2.66	120.24	111.91
6	A	517	78N	O16-C8-C7	2.65	120.23	111.91
6	A	526	78N	O16-C8-C7	2.63	120.17	111.91
6	A	515	78N	O16-C8-C7	2.59	120.03	111.91
6	A	525	78N	O16-C8-C7	2.59	120.03	111.91
7	A	510	78M	O2-C1-C2	2.41	119.47	111.91
5	A	508	EPE	C7-N4-C5	-2.29	105.38	111.23
7	A	522	78M	O2-C1-O1	-2.13	118.21	123.59
5	A	508	EPE	C6-N1-C2	-2.09	104.12	108.83
6	A	526	78N	C6-C7-C8	-2.09	106.03	113.62
6	A	524	78N	C6-C7-C8	-2.08	106.06	113.62
5	A	508	EPE	C7-N4-C3	-2.06	105.97	111.23

There are no chirality outliers.

All (189) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	509	78N	O16-C17-C18-C19
6	A	511	78N	O16-C17-C18-C19
6	A	513	78N	O16-C17-C18-C19
6	A	516	78N	C17-C18-C19-O22
6	A	517	78N	C17-C18-C19-O22
6	A	517	78N	O16-C17-C18-C19
6	A	518	78N	C17-C18-C19-O22
6	A	518	78N	O16-C17-C18-O20
6	A	520	78N	O16-C17-C18-C19
6	A	520	78N	O16-C17-C18-O20
6	A	521	78N	O16-C17-C18-C19
6	A	521	78N	O16-C17-C18-O20
6	A	521	78N	O15-C8-O16-C17

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Mol	Chain	Res	Type	Atoms
6	A	521	78N	C7-C8-O16-C17
6	A	526	78N	O16-C17-C18-C19
7	A	512	78M	O2-C17-C18-C20
7	A	512	78M	O2-C17-C18-O19
7	A	523	78M	C17-C18-C20-O21
7	A	523	78M	O2-C17-C18-C20
6	A	520	78N	O15-C8-O16-C17
6	A	520	78N	C7-C8-O16-C17
6	A	525	78N	C7-C8-O16-C17
6	A	526	78N	C7-C8-O16-C17
6	A	511	78N	O16-C17-C18-O20
6	A	526	78N	O16-C17-C18-O20
6	A	525	78N	O15-C8-O16-C17
6	A	526	78N	O15-C8-O16-C17
6	A	516	78N	O16-C17-C18-C19
6	A	509	78N	O16-C17-C18-O20
6	A	513	78N	O16-C17-C18-O20
6	A	516	78N	O16-C17-C18-O20
7	A	523	78M	O2-C17-C18-O19
7	A	523	78M	C1-C2-C3-C4
6	A	513	78N	C5-C6-C7-C8
6	A	525	78N	C5-C6-C7-C8
6	A	526	78N	C5-C6-C7-C8
7	A	512	78M	C1-C2-C3-C4
6	A	518	78N	C7-C8-O16-C17
6	A	517	78N	O16-C17-C18-O20
5	A	508	EPE	C9-C10-S-O3S
6	A	516	78N	C9-C10-C11-C12
6	A	525	78N	C11-C12-C13-C14
6	A	513	78N	C4-C5-C6-C7
6	A	509	78N	C7-C8-O16-C17
6	A	526	78N	C3-C4-C5-C6
6	A	518	78N	C9-C10-C11-C12
7	A	523	78M	C10-C11-C12-C13
6	A	521	78N	C10-C11-C12-C13
7	A	512	78M	C9-C10-C11-C12
7	A	512	78M	C17-C18-C20-O21
7	A	512	78M	C3-C4-C5-C6
6	A	514	78N	C4-C5-C6-C7
6	A	519	78N	C9-C10-C11-C12
7	A	523	78M	C11-C12-C13-C14
6	A	517	78N	C7-C8-O16-C17

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Mol	Chain	Res	Type	Atoms
6	A	518	78N	O15-C8-O16-C17
6	A	516	78N	O20-C18-C19-O22
6	A	516	78N	C11-C12-C13-C14
6	A	514	78N	C11-C10-C9-C1
6	A	516	78N	C11-C10-C9-C1
7	A	512	78M	C11-C12-C13-C14
6	A	518	78N	C11-C12-C13-C14
6	A	525	78N	C10-C11-C12-C13
6	A	515	78N	C3-C4-C5-C6
7	A	522	78M	C9-C10-C11-C12
6	A	509	78N	O15-C8-O16-C17
4	A	506	1PE	OH5-C14-C24-OH4
6	A	511	78N	C4-C5-C6-C7
7	A	522	78M	C3-C4-C5-C6
6	A	526	78N	C4-C5-C6-C7
6	A	517	78N	O15-C8-O16-C17
7	A	522	78M	C2-C1-O2-C17
6	A	526	78N	C11-C12-C13-C14
7	A	510	78M	C2-C3-C4-C5
6	A	524	78N	C9-C10-C11-C12
6	A	521	78N	C9-C10-C11-C12
6	A	518	78N	C11-C10-C9-C1
7	A	510	78M	C11-C10-C9-C8
7	A	523	78M	C11-C10-C9-C8
6	A	525	78N	C2-C3-C4-C5
7	A	512	78M	C11-C10-C9-C8
6	A	513	78N	C10-C11-C12-C13
6	A	511	78N	C3-C4-C5-C6
6	A	521	78N	C11-C12-C13-C14
6	A	514	78N	C12-C13-C14-C15
6	A	521	78N	C12-C13-C14-C15
7	A	522	78M	O1-C1-O2-C17
6	A	509	78N	C9-C10-C11-C12
6	A	517	78N	O20-C18-C19-O22
6	A	518	78N	O20-C18-C19-O22
6	A	509	78N	C2-C3-C4-C5
6	A	515	78N	C11-C10-C9-C1
6	A	515	78N	C7-C8-O16-C17
7	A	523	78M	C12-C13-C14-C15
6	A	518	78N	C12-C13-C14-C15
6	A	519	78N	C3-C4-C5-C6
6	A	525	78N	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
6	A	517	78N	C12-C13-C14-C15
7	A	523	78M	C2-C1-O2-C17
7	A	510	78M	O2-C17-C18-O19
6	A	521	78N	C4-C5-C6-C7
5	A	508	EPE	S-C10-C9-N1
6	A	513	78N	C11-C12-C13-C14
6	A	520	78N	C9-C10-C11-C12
6	A	515	78N	O15-C8-O16-C17
5	A	507	EPE	C10-C9-N1-C2
5	A	507	EPE	C10-C9-N1-C6
6	A	513	78N	C7-C8-O16-C17
6	A	518	78N	O16-C17-C18-C19
6	A	516	78N	C4-C5-C6-C7
7	A	523	78M	O19-C18-C20-O21
7	A	510	78M	C11-C12-C13-C14
6	A	516	78N	C10-C11-C12-C13
6	A	515	78N	O16-C17-C18-O20
7	A	512	78M	C2-C3-C4-C5
6	A	525	78N	C9-C10-C11-C12
7	A	522	78M	C2-C3-C4-C5
6	A	513	78N	O15-C8-O16-C17
7	A	523	78M	O1-C1-O2-C17
6	A	519	78N	C11-C12-C13-C14
6	A	526	78N	C9-C10-C11-C12
6	A	514	78N	C7-C8-O16-C17
5	A	508	EPE	C9-C10-S-O1S
5	A	508	EPE	C9-C10-S-O2S
6	A	518	78N	C3-C4-C5-C6
6	A	513	78N	C11-C10-C9-C1
7	A	522	78M	C11-C12-C13-C14
6	A	514	78N	O15-C8-O16-C17
7	A	512	78M	C12-C13-C14-C15
6	A	511	78N	C9-C10-C11-C12
6	A	524	78N	C6-C7-C8-O16
7	A	510	78M	C12-C13-C14-C15
6	A	509	78N	C10-C11-C12-C13
6	A	519	78N	C12-C13-C14-C15
6	A	511	78N	C11-C10-C9-C1
6	A	511	78N	C12-C13-C14-C15
6	A	520	78N	C2-C3-C4-C5
7	A	512	78M	O1-C1-O2-C17
7	A	512	78M	C2-C1-O2-C17

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Mol	Chain	Res	Type	Atoms
4	A	506	1PE	C16-C26-OH6-C15
6	A	511	78N	C2-C1-C9-C10
6	A	514	78N	C1-C2-C3-C4
5	A	508	EPE	C8-C7-N4-C3
6	A	525	78N	C12-C13-C14-C15
6	A	516	78N	C12-C13-C14-C15
6	A	517	78N	C3-C4-C5-C6
6	A	511	78N	C10-C11-C12-C13
6	A	519	78N	C1-C2-C3-C4
6	A	526	78N	C1-C2-C3-C4
6	A	520	78N	C12-C13-C14-C15
6	A	520	78N	C2-C1-C9-C10
6	A	525	78N	C2-C1-C9-C10
7	A	512	78M	O19-C18-C20-O21
6	A	509	78N	C11-C10-C9-C1
7	A	522	78M	C7-C8-C9-C10
6	A	521	78N	C2-C3-C4-C5
7	A	523	78M	C4-C5-C6-C7
6	A	515	78N	O16-C17-C18-C19
6	A	511	78N	C1-C2-C3-C4
6	A	513	78N	C1-C2-C3-C4
6	A	517	78N	C1-C2-C3-C4
6	A	521	78N	C2-C1-C9-C10
7	A	523	78M	C5-C6-C7-C8
6	A	509	78N	C2-C1-C9-C10
6	A	517	78N	C2-C1-C9-C10
6	A	519	78N	C2-C1-C9-C10
5	A	508	EPE	C8-C7-N4-C5
6	A	509	78N	C1-C2-C3-C4
6	A	518	78N	C2-C1-C9-C10
7	A	512	78M	C5-C6-C7-C8
7	A	522	78M	C4-C5-C6-C7
6	A	526	78N	O20-C18-C19-O22
6	A	519	78N	C7-C8-O16-C17
7	A	522	78M	O2-C17-C18-O19
4	A	506	1PE	OH6-C15-C25-OH5
6	A	513	78N	C2-C1-C9-C10
7	A	510	78M	C5-C6-C7-C8
7	A	522	78M	O2-C17-C18-C20
6	A	515	78N	C5-C6-C7-C8
6	A	516	78N	C2-C1-C9-C10
6	A	519	78N	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
6	A	526	78N	C17-C18-C19-O22
6	A	520	78N	C11-C12-C13-C14
6	A	519	78N	O15-C8-O16-C17
6	A	524	78N	C10-C11-C12-C13
6	A	515	78N	O20-C18-C19-O22
6	A	515	78N	C2-C1-C9-C10
6	A	514	78N	C9-C10-C11-C12
6	A	517	78N	C11-C12-C13-C14

There are no ring outliers.

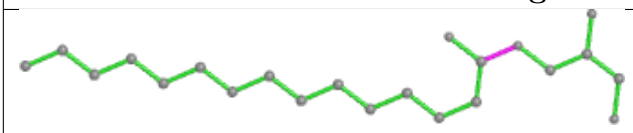
18 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	521	78N	3	0
5	A	508	EPE	3	0
6	A	519	78N	2	0
7	A	510	78M	1	0
6	A	515	78N	1	0
7	A	522	78M	4	0
7	A	523	78M	4	0
6	A	511	78N	2	0
6	A	524	78N	4	0
6	A	520	78N	1	0
6	A	526	78N	1	0
6	A	514	78N	2	0
6	A	513	78N	1	0
6	A	518	78N	3	0
7	A	512	78M	2	0
4	A	506	1PE	1	0
6	A	525	78N	1	0
6	A	509	78N	1	0

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

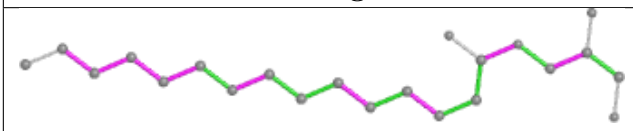
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 78N A 521

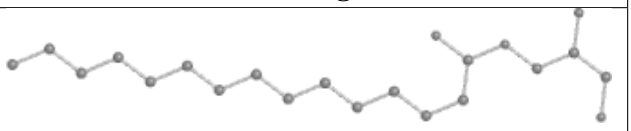


Bond lengths

Bond angles

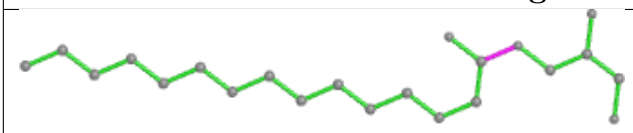


Torsions



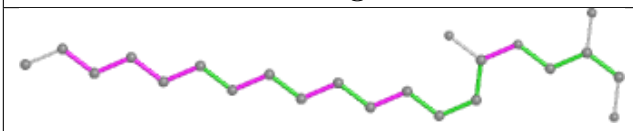
Rings

Ligand 78N A 519

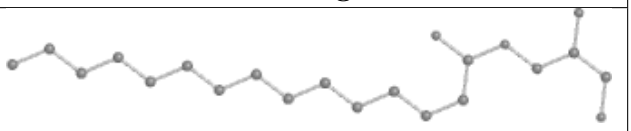


Bond lengths

Bond angles

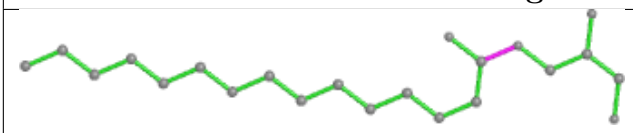


Torsions

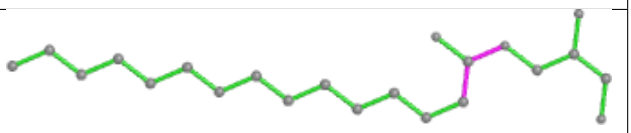


Rings

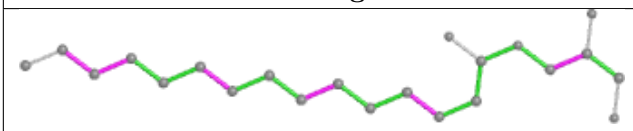
Ligand 78M A 510



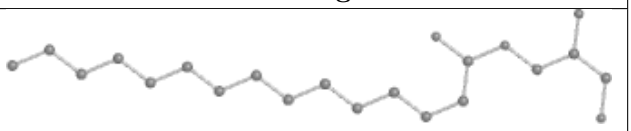
Bond lengths



Bond angles

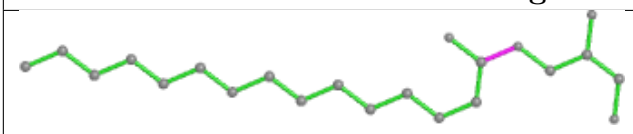


Torsions



Rings

Ligand 78N A 515



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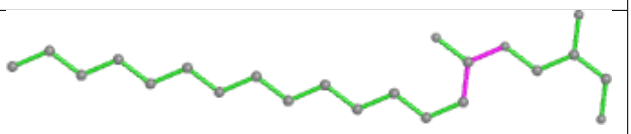
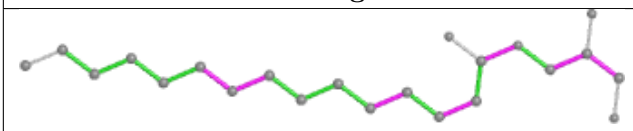


Bond angles



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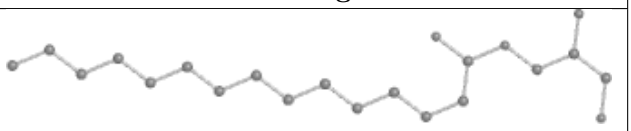
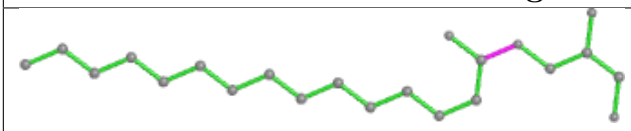
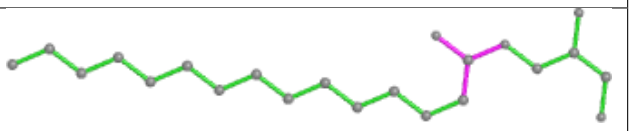
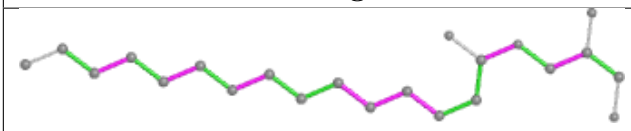
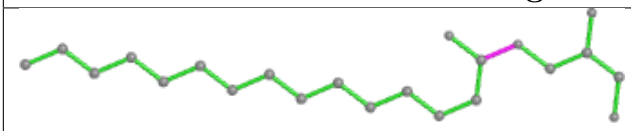
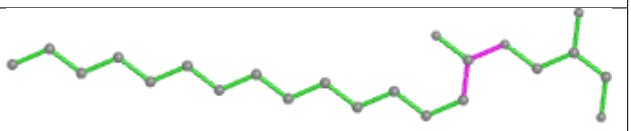
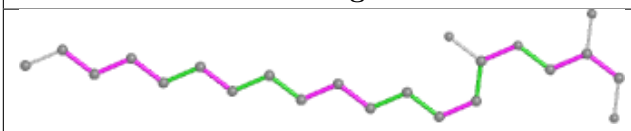
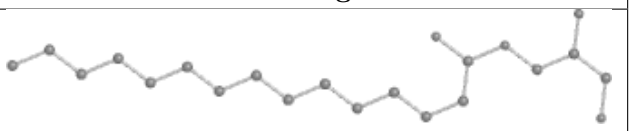
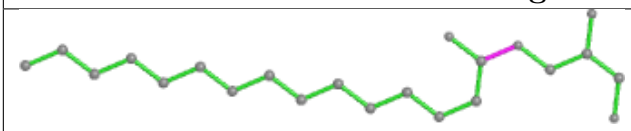
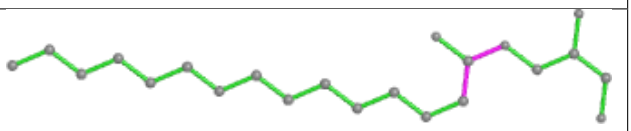
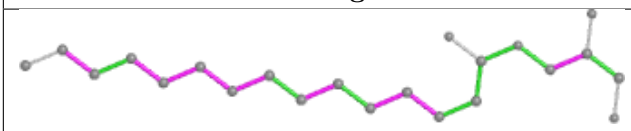
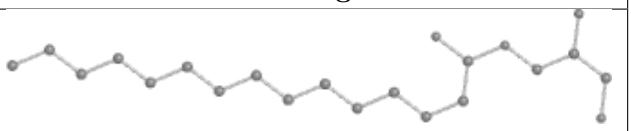


Rings

Ligand 78M A 522	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand 78M A 523	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 78N A 511	
 Bond lengths	 Bond angles
 Torsions	 Rings

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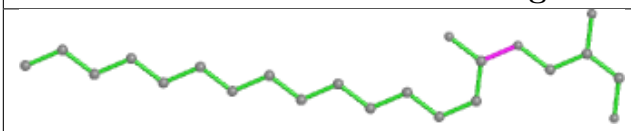
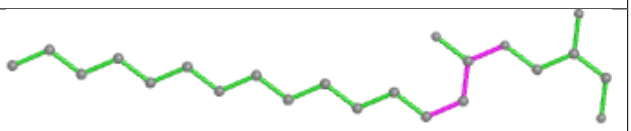
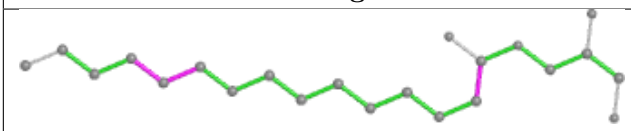
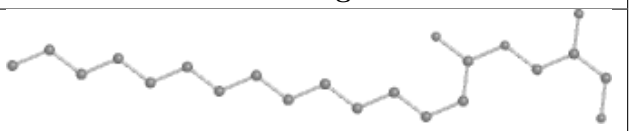
 Bond lengths	 Bond angles
 Torsions	 Rings

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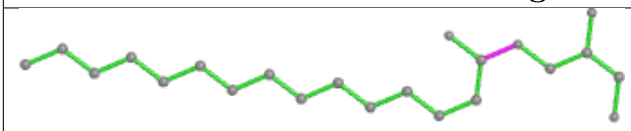
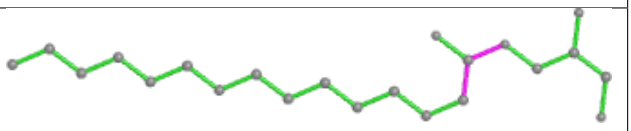
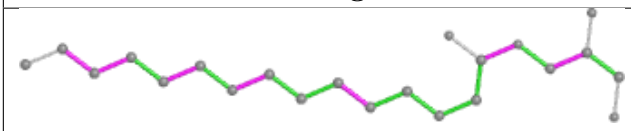
 Bond lengths	 Bond angles
 Torsions	Rings

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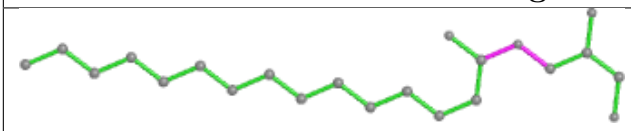
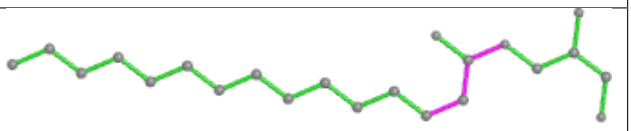
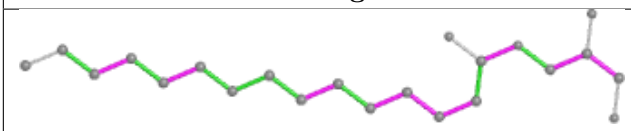
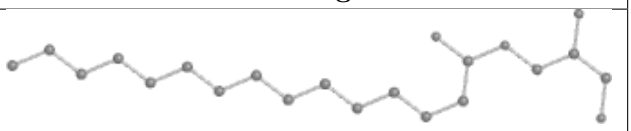
 Bond lengths	 Bond angles
 Torsions	 Rings

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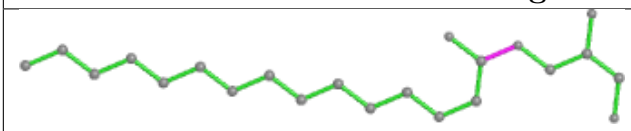
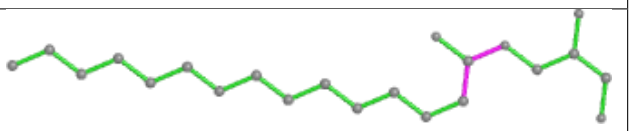
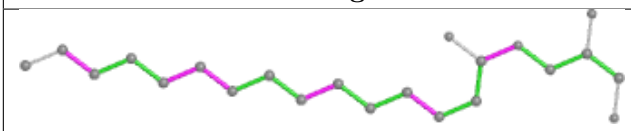
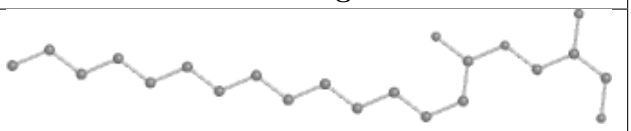
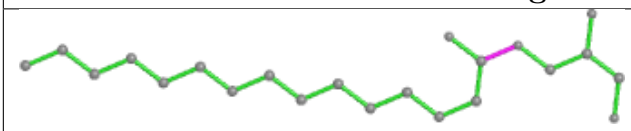
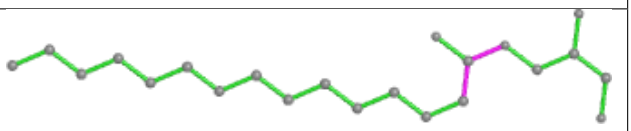
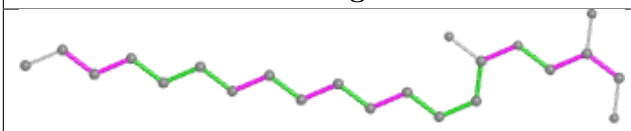
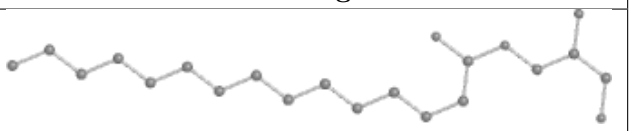
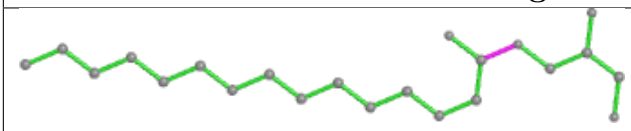
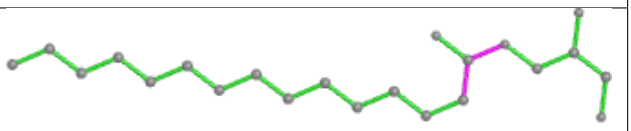
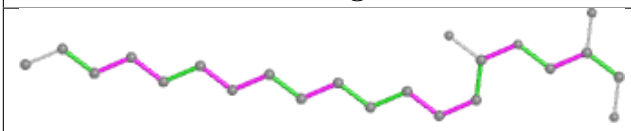
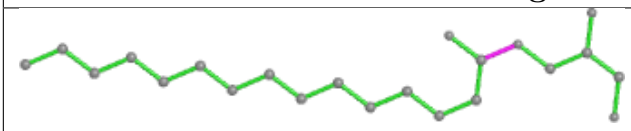
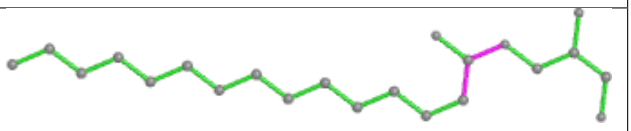
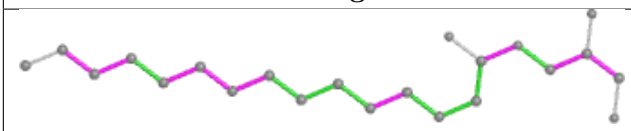
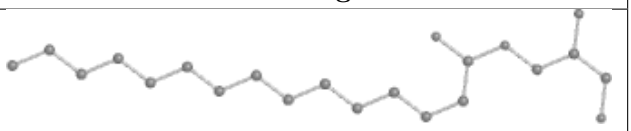
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 78N A 517	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 78N A 513	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand 78N A 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

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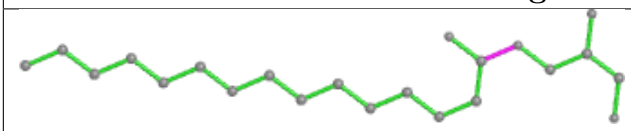
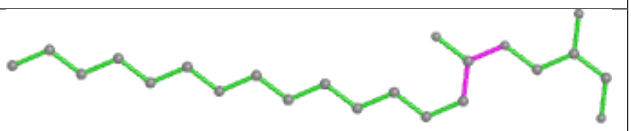
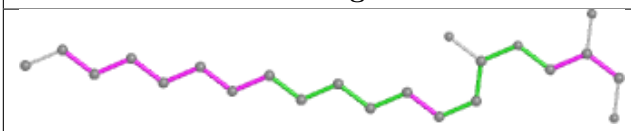
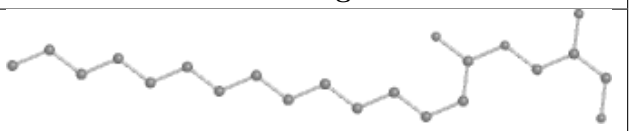
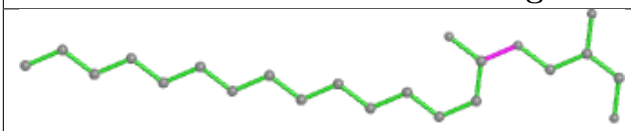
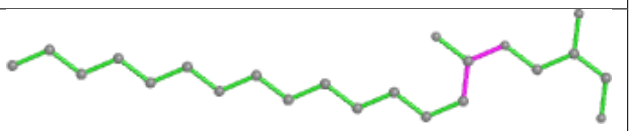
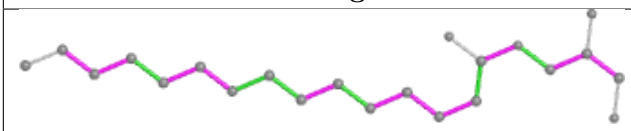
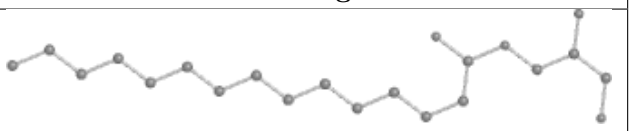
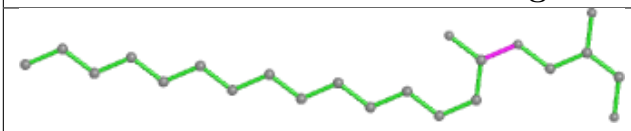
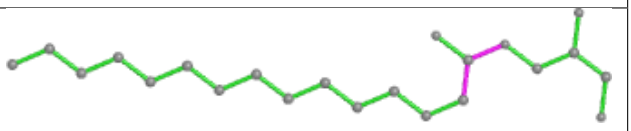
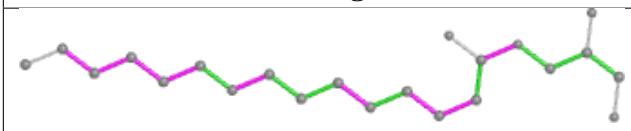
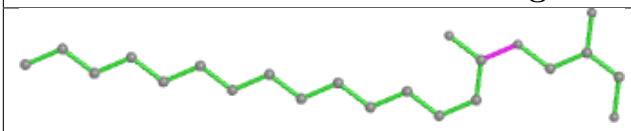
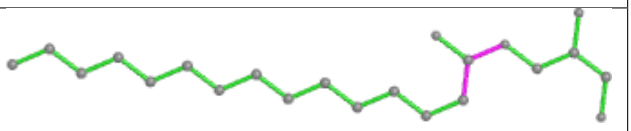
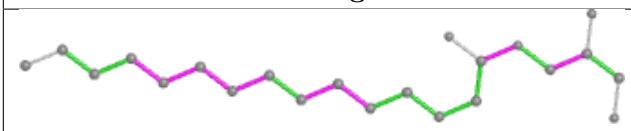
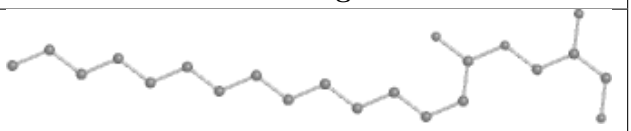
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 78M A 512	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 78N A 525	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand 78N A 509	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	455/490 (92%)	0.42	42 (9%) 9 7	36, 50, 100, 124	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	HIS	8.4
1	A	142	ARG	7.5
1	A	413	LYS	7.0
1	A	265	PHE	6.3
1	A	267	TRP	6.0
1	A	411	THR	5.7
1	A	347	LYS	5.6
1	A	412	THR	5.5
1	A	346	TRP	5.5
1	A	284	SER	5.4
1	A	348	LYS	5.4
1	A	341	TRP	5.2
1	A	414	LEU	4.8
1	A	423	MET	4.7
1	A	349	ASN	4.6
1	A	345	ALA	4.4
1	A	282	VAL	4.3
1	A	422	GLN	4.0
1	A	478	LEU	3.8
1	A	476	GLN	3.8
1	A	243	TRP	3.8
1	A	268	MET	3.5
1	A	139	GLU	3.5
1	A	283	VAL	3.4
1	A	50	HIS	3.3
1	A	421	SER	3.3
1	A	138	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	477	GLY	2.9
1	A	263	PHE	2.8
1	A	203	PRO	2.8
1	A	141	ASP	2.6
1	A	266	ALA	2.6
1	A	200	THR	2.4
1	A	420	ASN	2.4
1	A	408	LEU	2.4
1	A	159	ALA	2.3
1	A	7	THR	2.3
1	A	207	ARG	2.3
1	A	64	ALA	2.2
1	A	13	LEU	2.2
1	A	204	HIS	2.1
1	A	163	PRO	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
6	78N	A	521	22/22	0.62	0.30	72,94,99,99	0
7	78M	A	523	22/22	0.64	0.61	79,105,131,142	0
6	78N	A	514	22/22	0.68	0.33	79,94,116,116	0
7	78M	A	510	22/22	0.70	0.34	83,90,106,139	0
4	1PE	A	506	10/16	0.70	0.20	82,83,84,85	0
7	78M	A	522	22/22	0.72	0.32	79,84,103,103	0
6	78N	A	518	22/22	0.72	0.26	67,76,105,105	0
5	EPE	A	508	15/15	0.75	0.31	113,114,130,130	0

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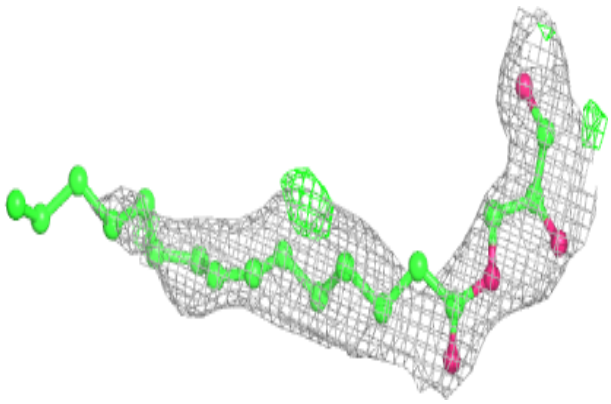
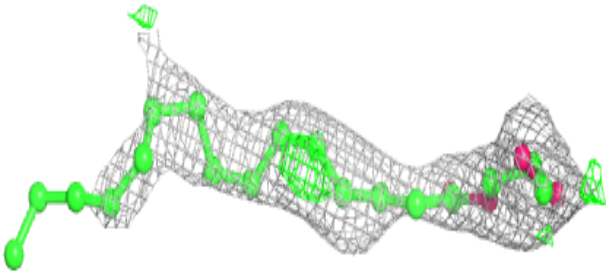
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	78N	A	519	22/22	0.75	0.24	78,96,142,142	0
6	78N	A	511	22/22	0.76	0.26	70,83,110,110	0
6	78N	A	520	22/22	0.76	0.28	75,86,89,90	0
6	78N	A	525	22/22	0.80	0.30	64,79,117,117	0
6	78N	A	513	22/22	0.80	0.32	86,92,131,132	0
7	78M	A	512	22/22	0.81	0.22	55,82,100,100	0
6	78N	A	517	22/22	0.82	0.19	80,89,95,96	0
6	78N	A	515	22/22	0.87	0.20	67,85,91,91	0
6	78N	A	526	22/22	0.87	0.24	68,81,120,126	0
6	78N	A	516	22/22	0.89	0.21	63,79,83,84	0
3	PO4	A	503	5/5	0.89	0.12	104,105,105,106	0
6	78N	A	509	22/22	0.89	0.19	55,67,77,78	0
2	NA	A	501	1/1	0.90	0.17	65,65,65,65	0
6	78N	A	524	22/22	0.92	0.15	51,63,95,96	0
5	EPE	A	507	15/15	0.93	0.29	61,62,89,90	0
3	PO4	A	504	5/5	0.93	0.24	104,105,106,106	0
3	PO4	A	505	5/5	0.95	0.13	82,82,83,83	0
3	PO4	A	502	5/5	0.98	0.09	76,77,77,78	0

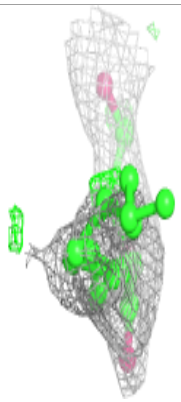
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 78N A 521:

$2mF_o$-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 523:

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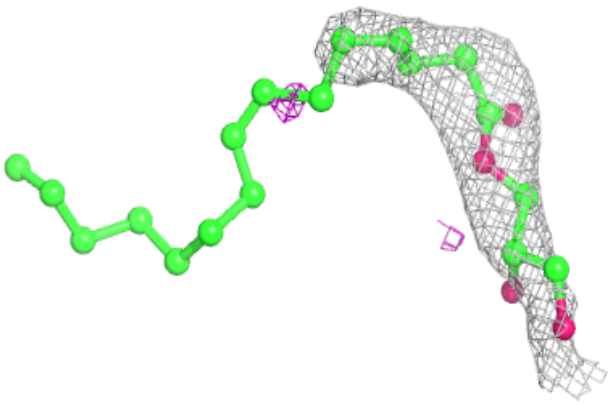
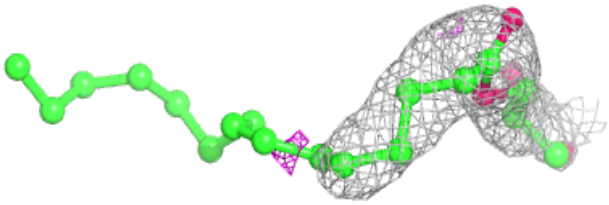
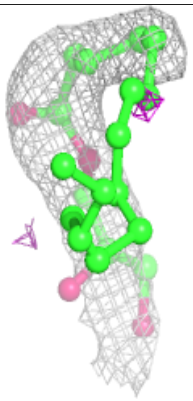
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around 78N A 514:

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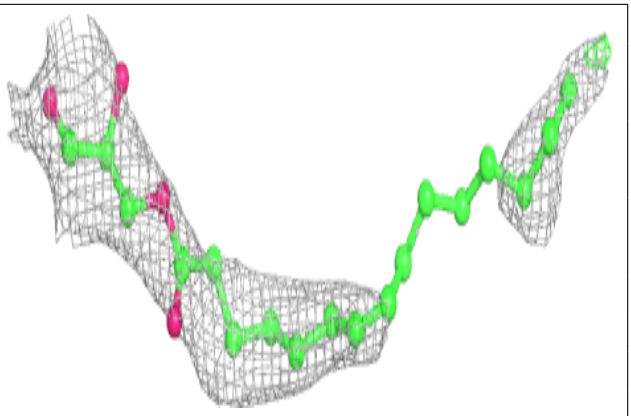
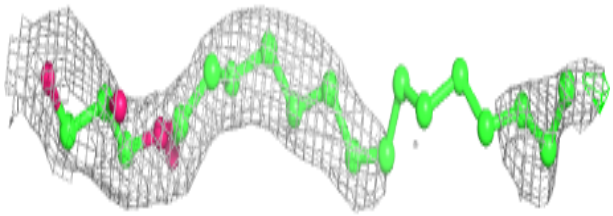
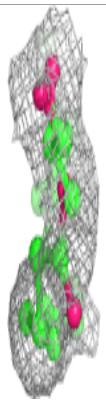
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around 78M A 510:

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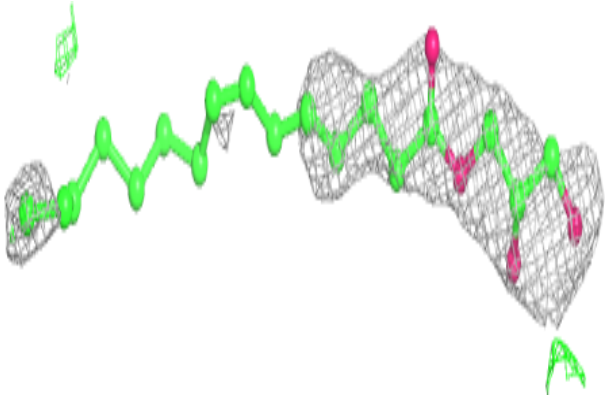
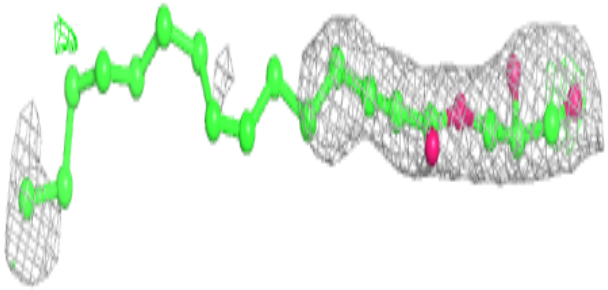
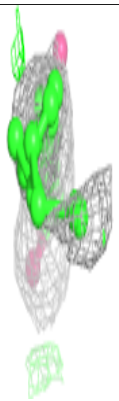
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around 78M A 522:

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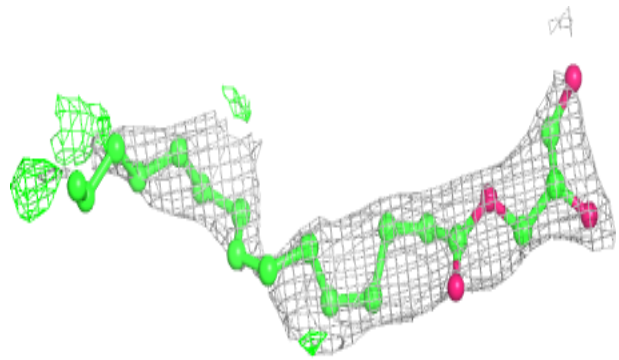
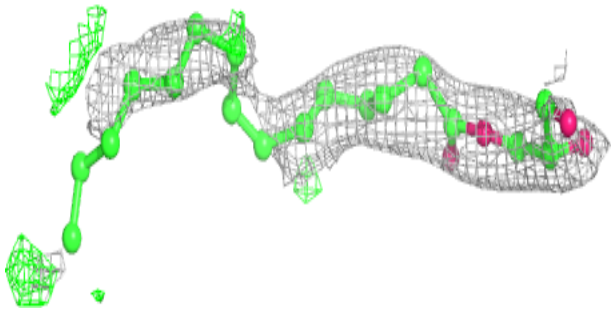
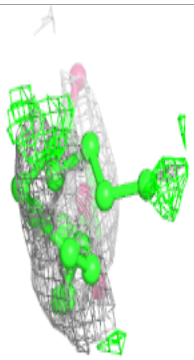
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

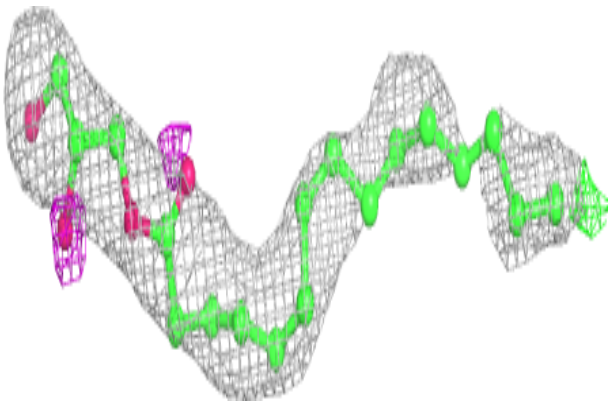


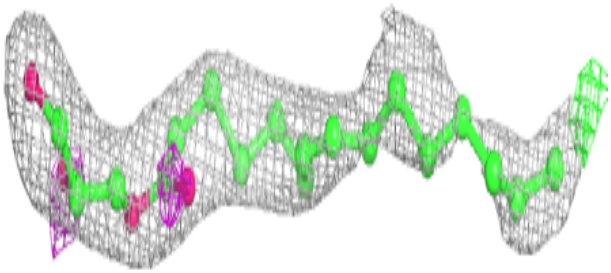


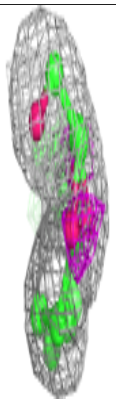


Electron density around 78N A 518:

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

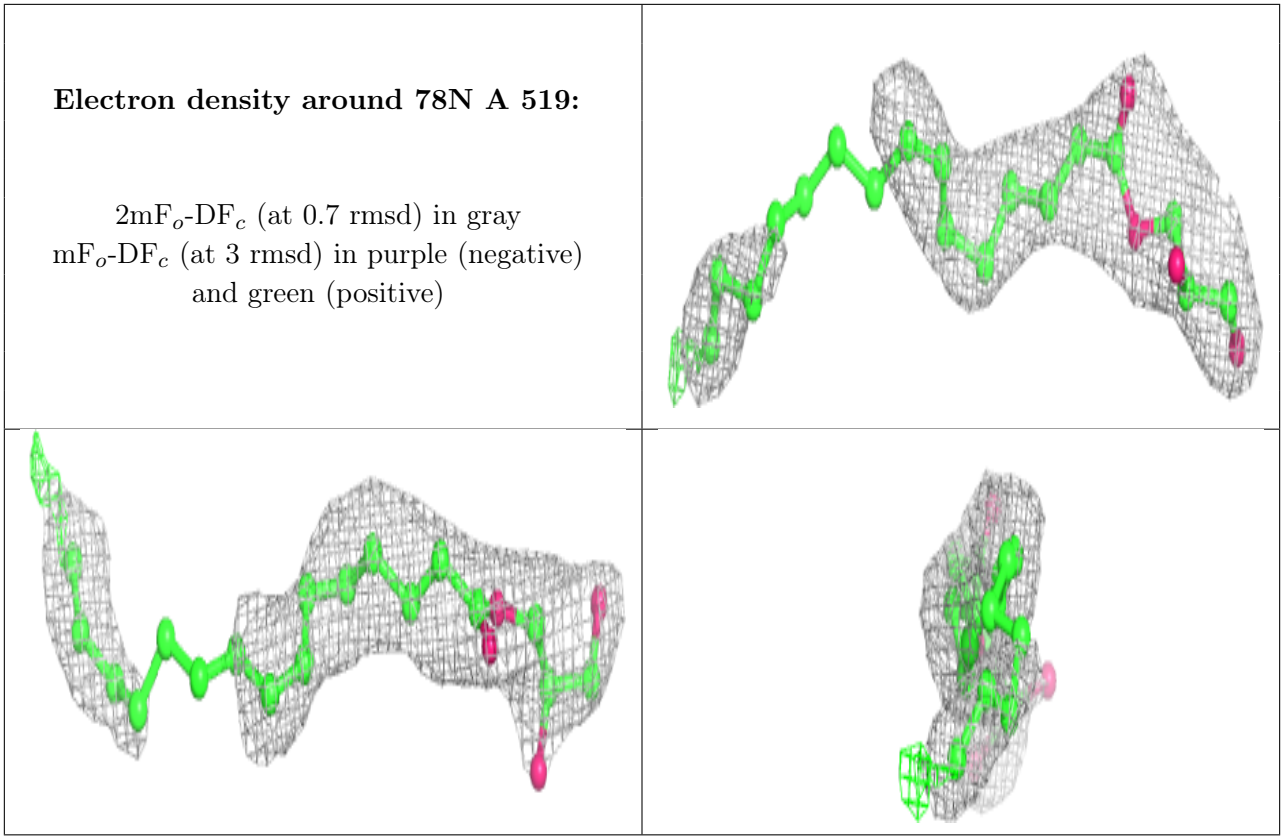






Electron density around 78N A 519:

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



Electron density around 78N A 511:

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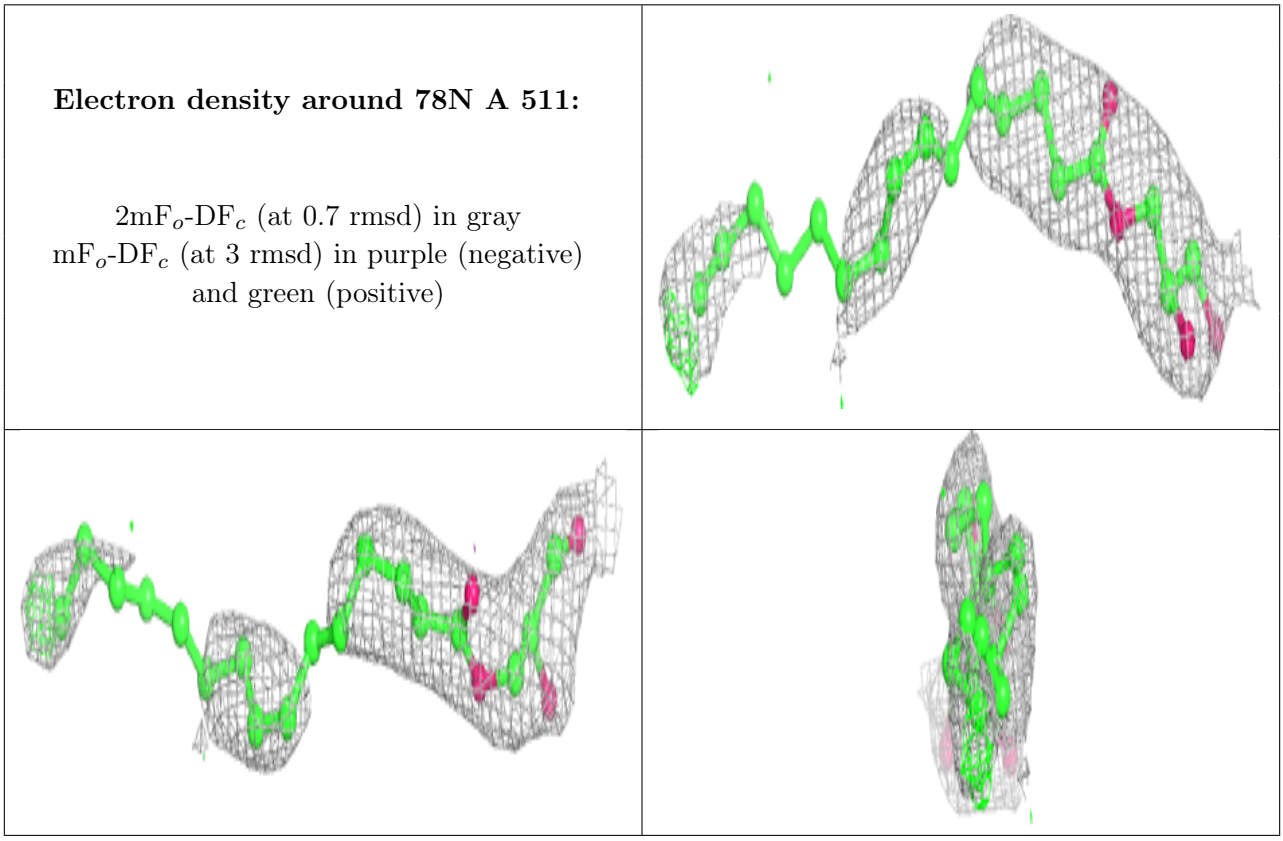
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 78N A 520:

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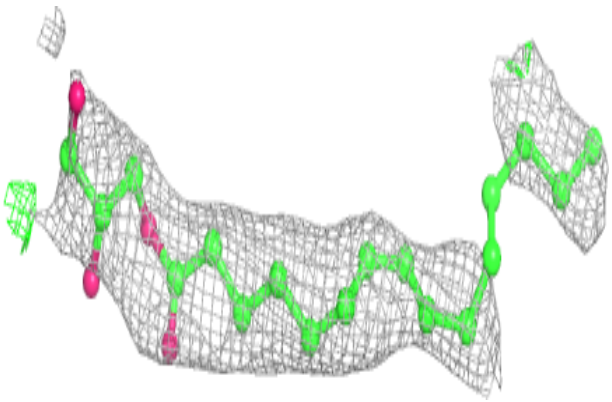
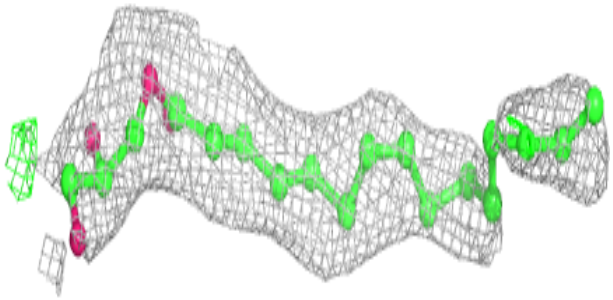
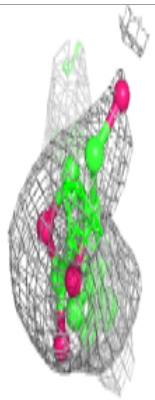
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around 78N A 525:

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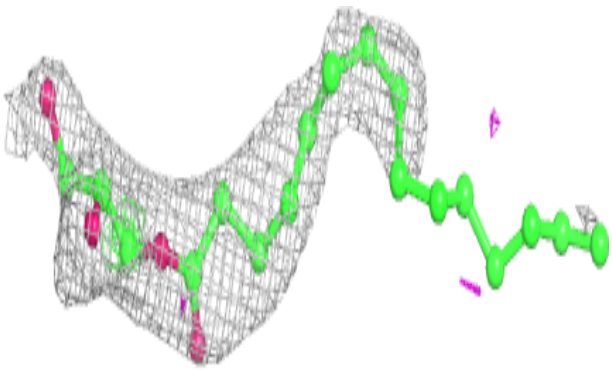
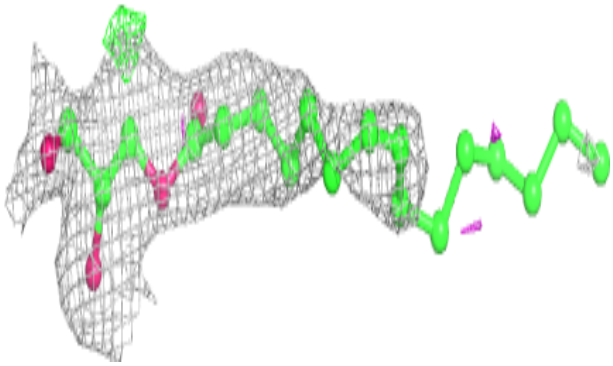
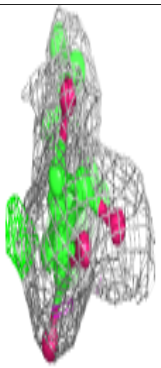
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around 78N A 513:

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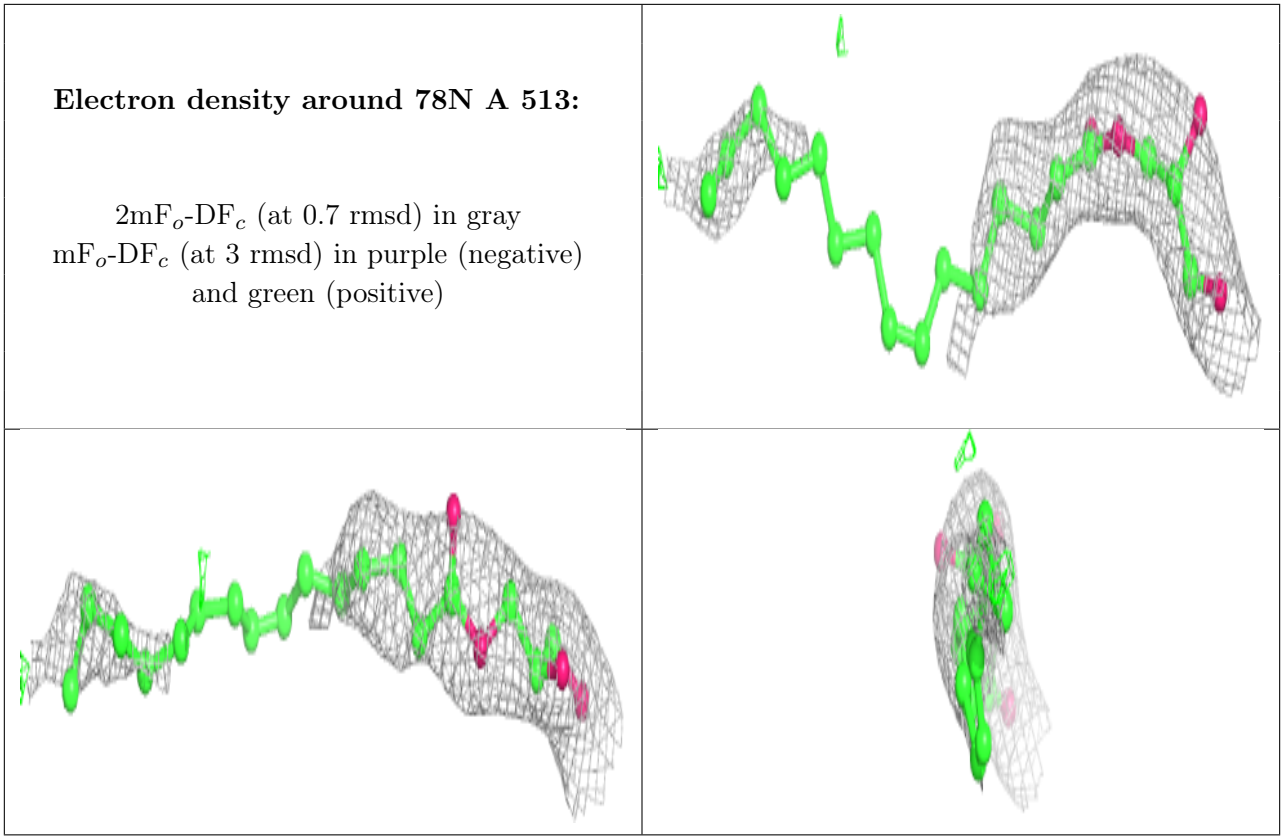
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 78M A 512:

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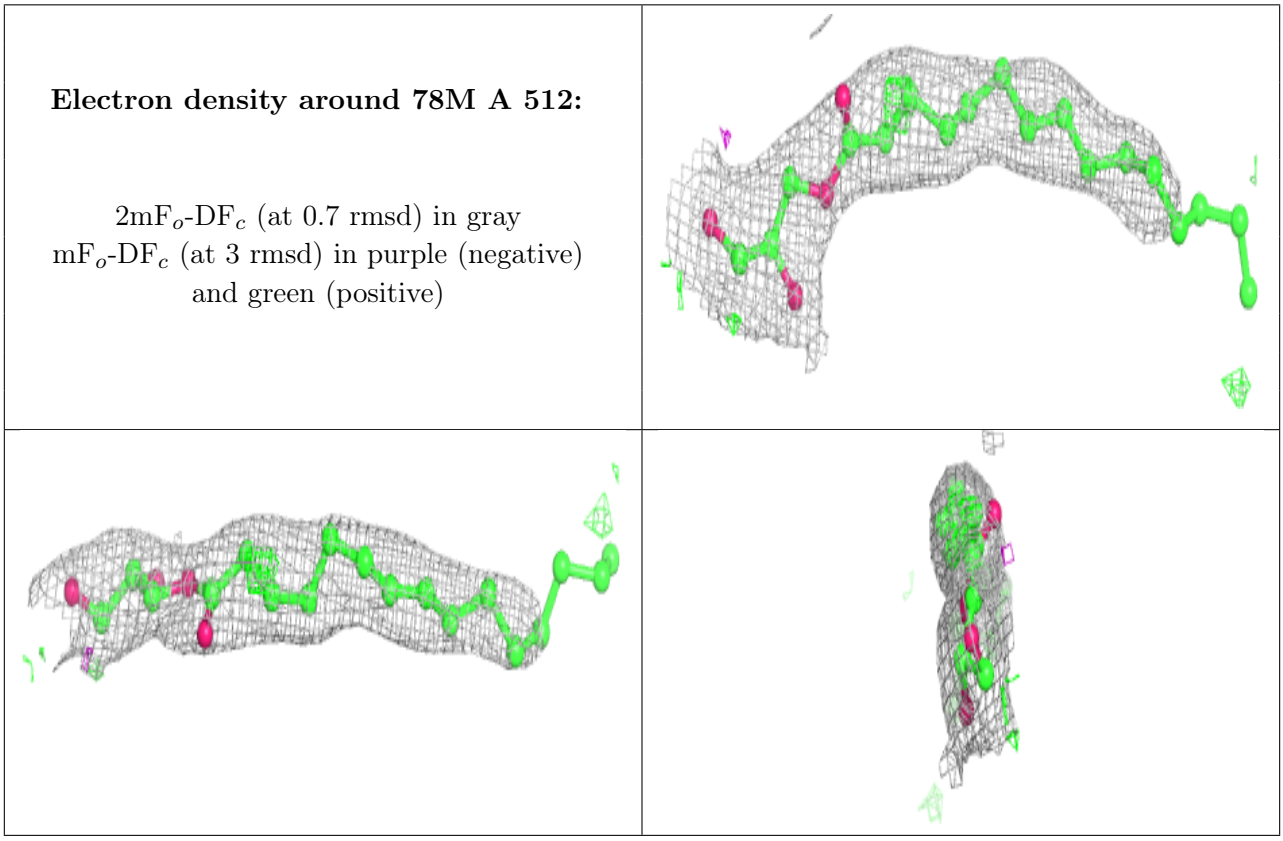
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 78N A 517:

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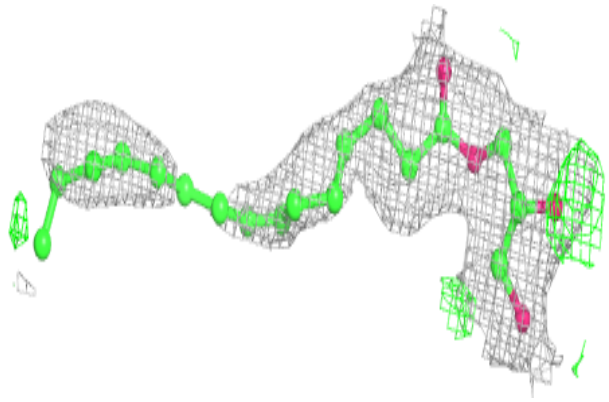
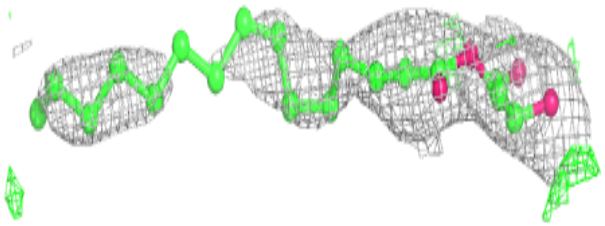
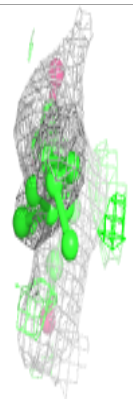
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

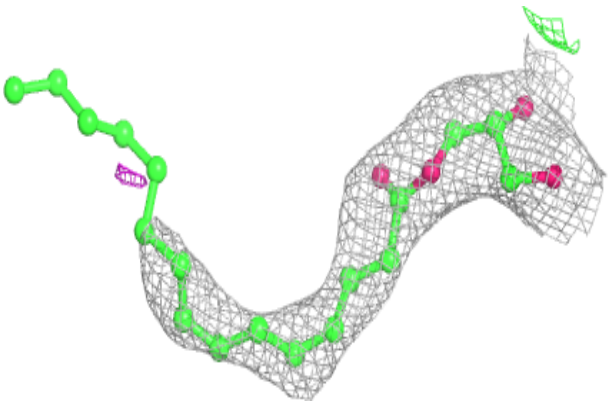


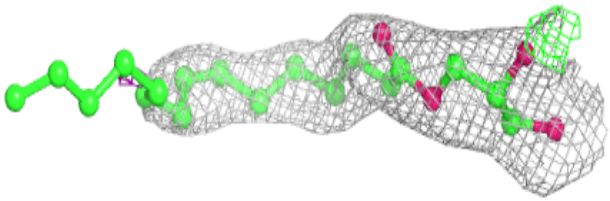


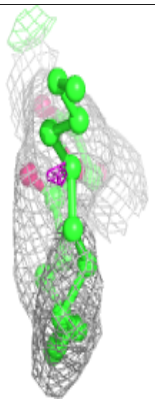


Electron density around 78N A 515:

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

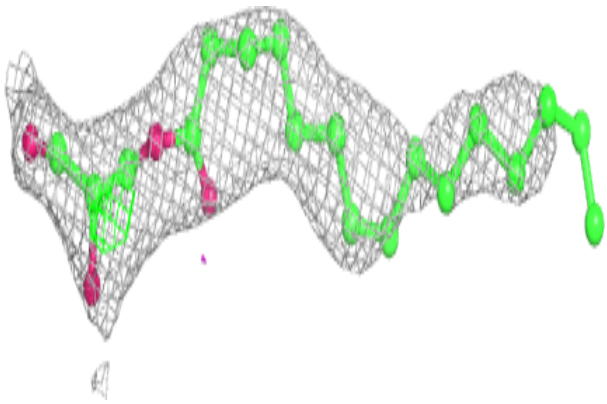


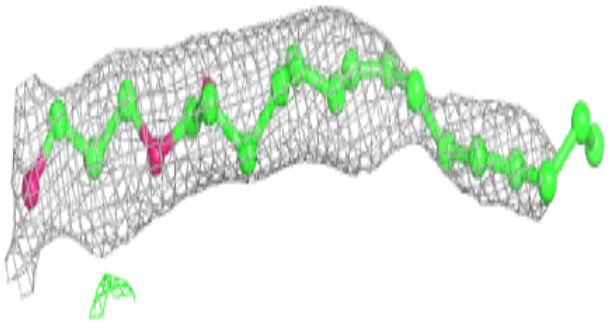


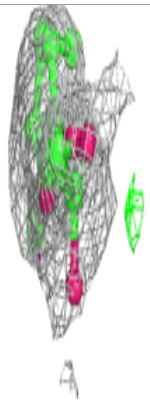


Electron density around 78N A 526:

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

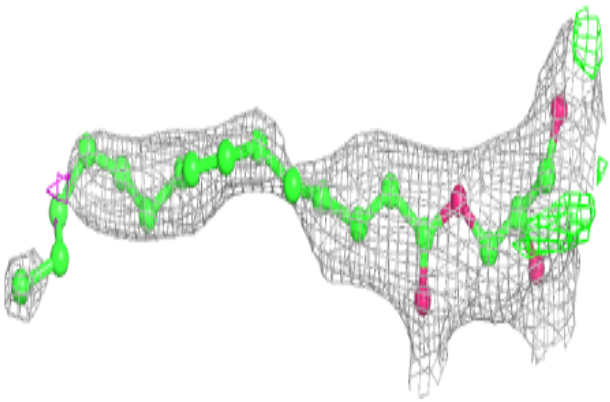


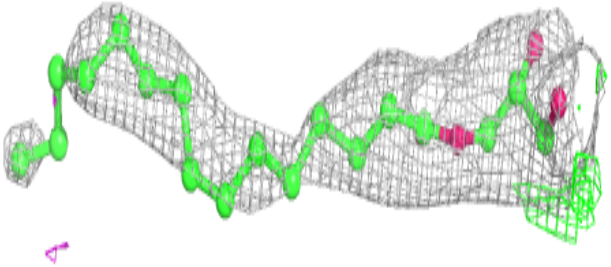


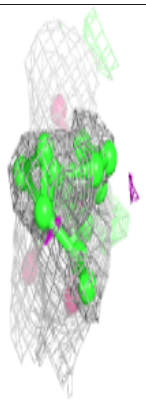


Electron density around 78N A 516:

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

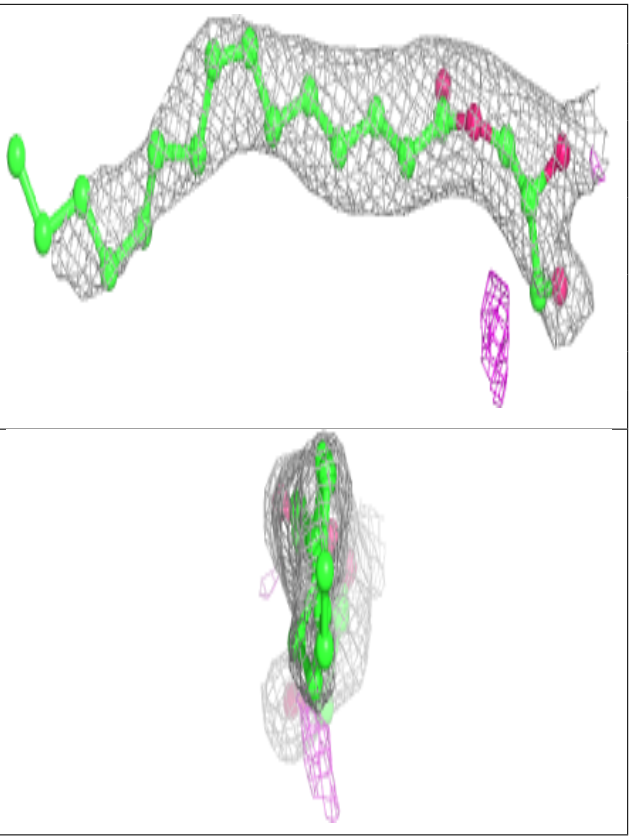


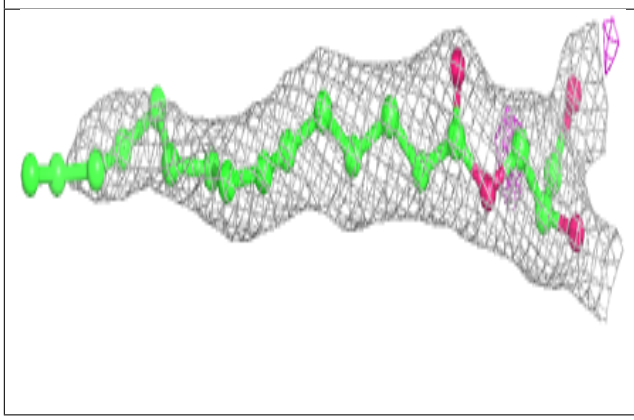




Electron density around 78N A 509:

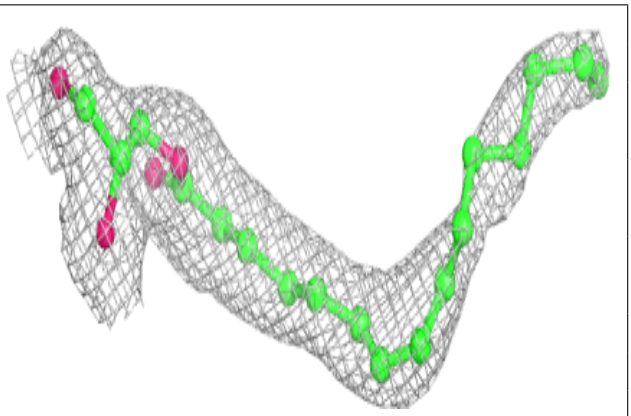
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

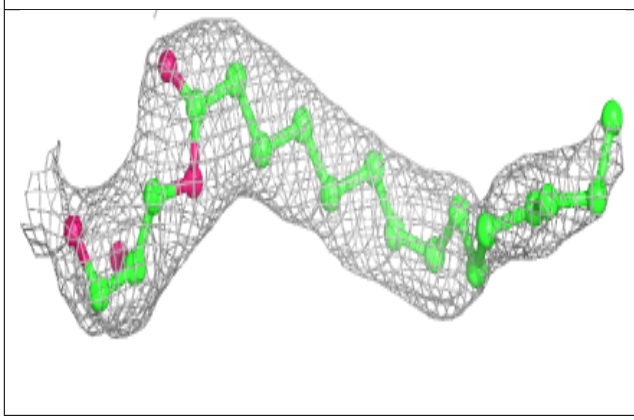


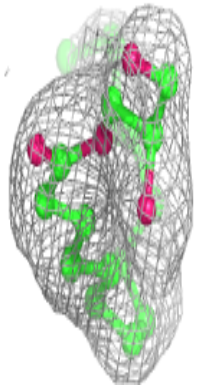


Electron density around 78N A 524:

$2mF_o$-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.