



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:25 AM UTC

PDB ID : 6EIA / pdb_00006eia
Title : PepTSt in complex with HEPES (100 mM)
Authors : Martinez Molledo, M.; Quistgaard, E.M.; Loew, C.
Deposited on : 2017-09-18
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

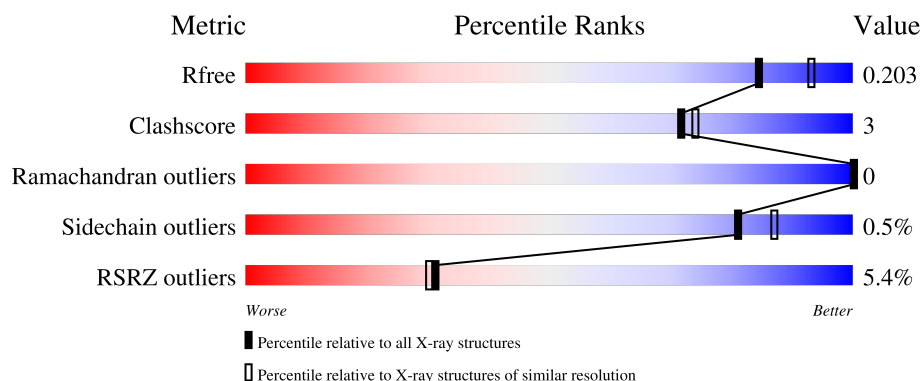
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	490	5% 89% 6% 5%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4182 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.

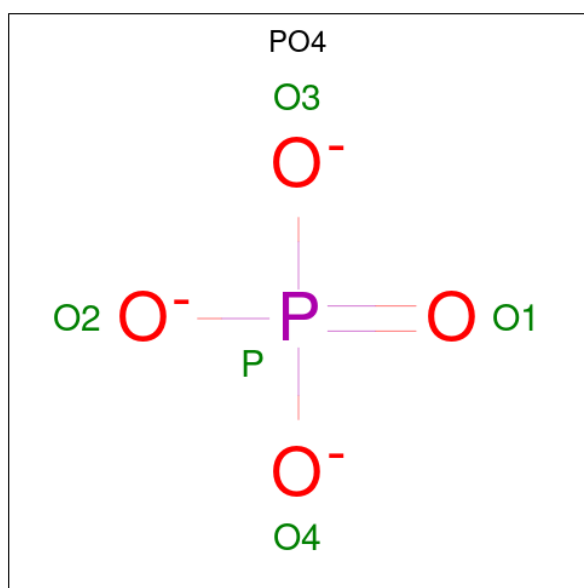
- Molecule 1 is a protein called Di-or tripeptide:H⁺ symporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	464	3601	2422	557	605	17	0	3	0

There are 7 discrepancies between the modelled and reference sequences:

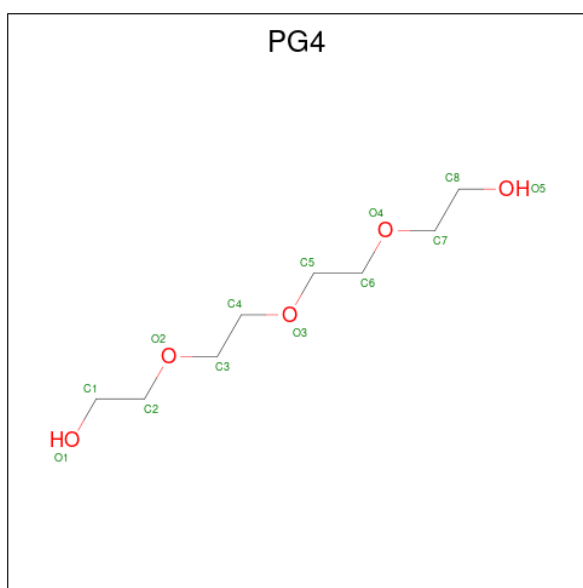
Chain	Residue	Modelled	Actual	Comment	Reference
A	484	ALA	-	expression tag	UNP Q5M4H8
A	485	GLU	-	expression tag	UNP Q5M4H8
A	486	ASN	-	expression tag	UNP Q5M4H8
A	487	LEU	-	expression tag	UNP Q5M4H8
A	488	TYR	-	expression tag	UNP Q5M4H8
A	489	PHE	-	expression tag	UNP Q5M4H8
A	490	GLN	-	expression tag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

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



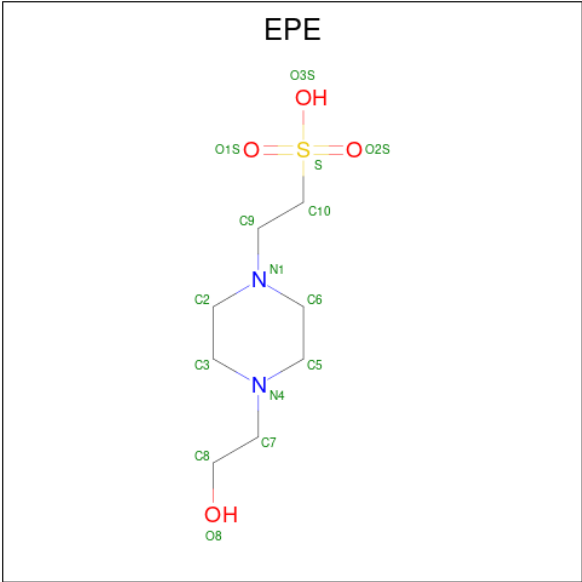
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



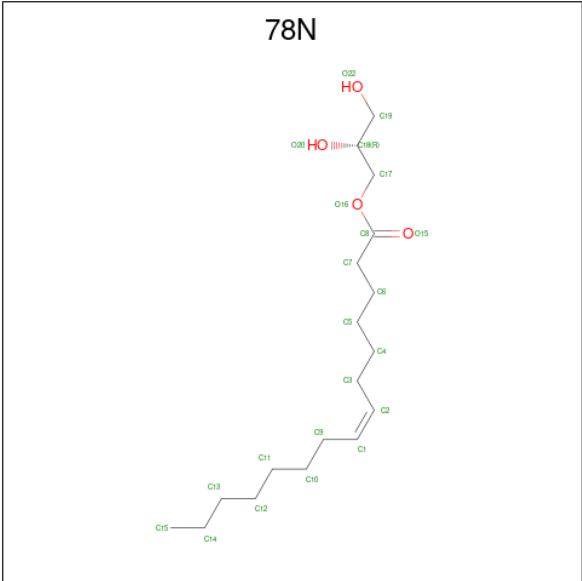
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



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

- Molecule 5 is (2R)-2,3-DIHYDROXYPROPYL(7Z)-PENTADEC-7-ENOATE (CCD ID: 78N) (formula: C₁₈H₃₄O₄).



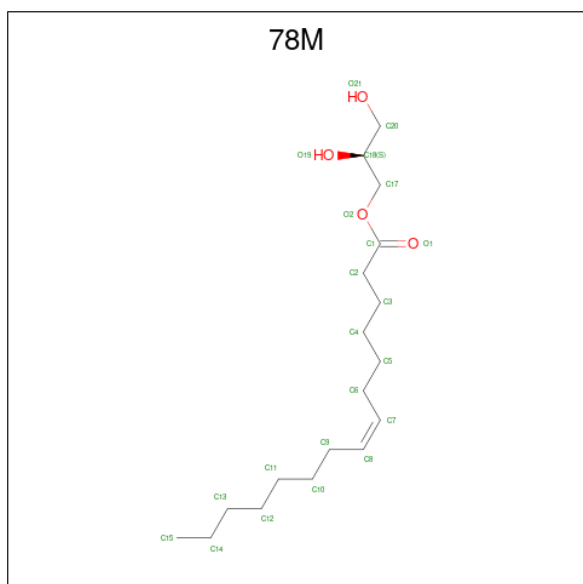
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			22	18	4		

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

- Molecule 6 is (2S)-2,3-DIHYDROXYPROPYL(7Z)-PENTADEC-7-ENOATE (CCD ID: 78M) (formula: C₁₈H₃₄O₄).



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

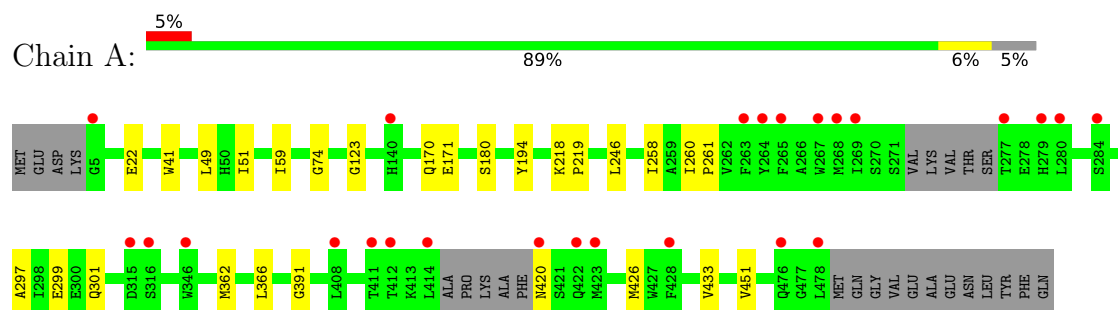
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	122	Total	O	0	0
			122	122		

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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	102.49Å 110.03Å 110.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.25 – 2.00 49.25 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.25-2.00) 99.9 (49.25-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.181 , 0.200 0.186 , 0.203	Depositor DCC
R_{free} test set	2123 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4182	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 78M, EPE, PG4, 78N, PO4

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	0.32	0/3716	0.72	0/5066

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	3601	0	3697	19	0
2	A	20	0	0	0	0
3	A	13	0	18	2	0
4	A	30	0	34	1	0
5	A	286	0	442	11	0
6	A	110	0	170	9	0
7	A	122	0	0	1	0
All	All	4182	0	4361	28	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 3.

All (28) 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)
6:A:512:78M:H121	5:A:514:78N:H1	1.80	0.63
1:A:180:SER:HB2	5:A:516:78N:H2	1.85	0.58
1:A:366:LEU:HD13	5:A:508:78N:H152	1.87	0.57
1:A:59:ILE:HD11	1:A:246:LEU:HD21	1.91	0.53
1:A:170:GLN:HE22	3:A:505:PG4:H81	1.73	0.53
6:A:509:78M:H102	5:A:510:78N:H142	1.92	0.51
1:A:261:PRO:HG2	1:A:433:VAL:HG21	1.94	0.50
1:A:171:GLU:OE2	7:A:601:HOH:O	2.19	0.50
5:A:517:78N:H1	5:A:518:78N:H92C	1.93	0.50
1:A:451:VAL:HG11	5:A:508:78N:H171	1.95	0.49
5:A:511:78N:H122	6:A:512:78M:H101	1.95	0.48
5:A:516:78N:H2	5:A:516:78N:H52C	1.62	0.47
1:A:194:TYR:CZ	6:A:521:78M:H171	2.49	0.47
1:A:391:GLY:HA3	6:A:512:78M:H42C	1.96	0.47
1:A:49:LEU:HG	1:A:51:ILE:HG12	1.97	0.47
6:A:520:78M:H112	6:A:520:78M:H8	1.56	0.46
6:A:512:78M:H91C	5:A:514:78N:H2	1.98	0.44
1:A:258:ILE:O	1:A:261:PRO:HD2	2.17	0.44
1:A:362:MET:HE2	6:A:509:78M:H112	1.99	0.44
1:A:218:LYS:HB3	1:A:219:PRO:HD3	1.98	0.44
1:A:41:TRP:HE3	3:A:505:PG4:H22	1.83	0.44
1:A:297:ALA:O	1:A:301:GLN:HG3	2.18	0.43
1:A:299:GLU:OE2	4:A:506:EPE:N1	2.52	0.42
1:A:74:GLY:HA3	1:A:123:GLY:O	2.19	0.42
1:A:260:ILE:HB	1:A:261:PRO:HD3	2.01	0.42
1:A:426:MET:HE2	1:A:426:MET:HB3	1.96	0.41
6:A:521:78M:O21	5:A:522:78N:H2	2.20	0.41
5:A:515:78N:H31C	5:A:515:78N:H62C	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	461/490 (94%)	458 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	378/397 (95%)	376 (100%)	2 (0%)	81	87

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

Mol	Chain	Res	Type
1	A	22	GLU
1	A	420	ASN

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	440	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

25 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	A	503	-	4,4,4	0.96	0	6,6,6	0.43	0
5	78N	A	508	-	21,21,21	0.95	1 (4%)	22,22,22	0.96	1 (4%)
5	78N	A	518	-	21,21,21	0.97	1 (4%)	22,22,22	0.99	1 (4%)
5	78N	A	525	-	21,21,21	0.95	1 (4%)	22,22,22	0.98	1 (4%)
6	78M	A	509	-	21,21,21	1.15	1 (4%)	22,22,22	0.97	1 (4%)
5	78N	A	513	-	21,21,21	0.96	1 (4%)	22,22,22	1.00	1 (4%)
6	78M	A	523	-	21,21,21	1.18	1 (4%)	22,22,22	0.97	1 (4%)
3	PG4	A	505	-	12,12,12	0.58	0	11,11,11	0.48	0
5	78N	A	524	-	21,21,21	0.98	1 (4%)	22,22,22	0.96	1 (4%)
5	78N	A	522	-	21,21,21	0.95	1 (4%)	22,22,22	1.03	1 (4%)
5	78N	A	515	-	21,21,21	0.96	1 (4%)	22,22,22	1.00	1 (4%)
6	78M	A	512	-	21,21,21	1.14	1 (4%)	22,22,22	0.96	1 (4%)
6	78M	A	521	-	21,21,21	1.16	1 (4%)	22,22,22	0.96	1 (4%)
2	PO4	A	502	-	4,4,4	0.94	0	6,6,6	0.45	0
5	78N	A	519	-	21,21,21	0.98	1 (4%)	22,22,22	1.06	1 (4%)
5	78N	A	514	-	21,21,21	0.97	1 (4%)	22,22,22	0.93	1 (4%)
5	78N	A	517	-	21,21,21	0.97	1 (4%)	22,22,22	0.95	1 (4%)
4	EPE	A	507	-	15,15,15	0.97	1 (6%)	19,20,20	1.24	2 (10%)
6	78M	A	520	-	21,21,21	1.16	1 (4%)	22,22,22	0.97	1 (4%)
5	78N	A	510	-	21,21,21	0.97	1 (4%)	22,22,22	0.92	1 (4%)
2	PO4	A	501	-	4,4,4	0.99	0	6,6,6	0.49	0
5	78N	A	516	-	21,21,21	0.96	1 (4%)	22,22,22	0.98	1 (4%)
5	78N	A	511	-	21,21,21	0.96	1 (4%)	22,22,22	1.00	1 (4%)
2	PO4	A	504	-	4,4,4	0.98	0	6,6,6	0.46	0
4	EPE	A	506	-	15,15,15	0.87	0	19,20,20	1.10	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	78N	A	508	-	-	8/21/21/21	-
5	78N	A	518	-	-	13/21/21/21	-
5	78N	A	525	-	-	7/21/21/21	-
6	78M	A	509	-	-	9/21/21/21	-
5	78N	A	513	-	-	8/21/21/21	-
6	78M	A	523	-	-	11/21/21/21	-
3	PG4	A	505	-	-	6/10/10/10	-
5	78N	A	524	-	-	9/21/21/21	-
5	78N	A	522	-	-	6/21/21/21	-
5	78N	A	515	-	-	7/21/21/21	-
6	78M	A	512	-	-	8/21/21/21	-
6	78M	A	521	-	-	11/21/21/21	-
5	78N	A	519	-	-	14/21/21/21	-
5	78N	A	514	-	-	10/21/21/21	-
5	78N	A	517	-	-	8/21/21/21	-
4	EPE	A	507	-	-	4/9/19/19	0/1/1/1
6	78M	A	520	-	-	13/21/21/21	-
5	78N	A	510	-	-	7/21/21/21	-
5	78N	A	516	-	-	10/21/21/21	-
5	78N	A	511	-	-	10/21/21/21	-
4	EPE	A	506	-	-	2/9/19/19	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	523	78M	O2-C1	3.38	1.43	1.33
6	A	521	78M	O2-C1	3.36	1.43	1.33
6	A	520	78M	O2-C1	3.31	1.43	1.33
6	A	509	78M	O2-C1	3.28	1.42	1.33
6	A	512	78M	O2-C1	3.26	1.42	1.33
5	A	524	78N	O16-C8	3.02	1.42	1.33
5	A	517	78N	O16-C8	3.01	1.42	1.33
5	A	510	78N	O16-C8	3.00	1.42	1.33
5	A	518	78N	O16-C8	3.00	1.42	1.33
5	A	514	78N	O16-C8	3.00	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	515	78N	O16-C8	3.00	1.42	1.33
5	A	525	78N	O16-C8	2.98	1.42	1.33
5	A	519	78N	O16-C8	2.97	1.42	1.33
5	A	511	78N	O16-C8	2.96	1.42	1.33
5	A	513	78N	O16-C8	2.95	1.42	1.33
5	A	508	78N	O16-C8	2.93	1.41	1.33
5	A	522	78N	O16-C8	2.93	1.41	1.33
5	A	516	78N	O16-C8	2.90	1.41	1.33
4	A	507	EPE	C6-N1	2.12	1.52	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	519	78N	O16-C8-C7	3.09	121.27	111.83
5	A	515	78N	O16-C8-C7	2.87	120.60	111.83
6	A	523	78M	O2-C1-C2	2.85	120.53	111.83
5	A	518	78N	O16-C8-C7	2.83	120.47	111.83
5	A	511	78N	O16-C8-C7	2.81	120.39	111.83
5	A	513	78N	O16-C8-C7	2.80	120.37	111.83
5	A	516	78N	O16-C8-C7	2.76	120.25	111.83
5	A	522	78N	O16-C8-C7	2.75	120.22	111.83
6	A	520	78M	O2-C1-C2	2.74	120.19	111.83
5	A	517	78N	O16-C8-C7	2.71	120.11	111.83
6	A	512	78M	O2-C1-C2	2.70	120.08	111.83
6	A	509	78M	O2-C1-C2	2.69	120.03	111.83
6	A	521	78M	O2-C1-C2	2.69	120.03	111.83
5	A	525	78N	O16-C8-C7	2.67	119.97	111.83
5	A	524	78N	O16-C8-C7	2.65	119.93	111.83
5	A	514	78N	O16-C8-C7	2.59	119.74	111.83
5	A	508	78N	O16-C8-C7	2.59	119.73	111.83
5	A	510	78N	O16-C8-C7	2.58	119.69	111.83
4	A	507	EPE	O1S-S-C10	-2.37	103.14	106.73
4	A	507	EPE	C9-N1-C6	-2.17	105.45	111.24
4	A	506	EPE	C9-N1-C6	-2.13	105.57	111.24

There are no chirality outliers.

All (181) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	506	EPE	C10-C9-N1-C2
4	A	507	EPE	C9-C10-S-O1S
5	A	508	78N	O16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
5	A	510	78N	O16-C17-C18-C19
5	A	510	78N	O16-C17-C18-O20
5	A	511	78N	C17-C18-C19-O22
5	A	514	78N	O20-C18-C19-O22
5	A	514	78N	C17-C18-C19-O22
5	A	515	78N	C17-C18-C19-O22
5	A	517	78N	C17-C18-C19-O22
5	A	518	78N	O20-C18-C19-O22
5	A	518	78N	C17-C18-C19-O22
5	A	519	78N	O16-C17-C18-O20
5	A	524	78N	C17-C18-C19-O22
6	A	509	78M	C17-C18-C20-O21
6	A	509	78M	O2-C17-C18-C20
6	A	509	78M	O2-C17-C18-O19
6	A	512	78M	C17-C18-C20-O21
6	A	520	78M	C17-C18-C20-O21
6	A	520	78M	O2-C17-C18-O19
6	A	521	78M	C17-C18-C20-O21
6	A	523	78M	O2-C17-C18-O19
6	A	523	78M	O1-C1-O2-C17
6	A	523	78M	C2-C1-O2-C17
5	A	519	78N	O15-C8-O16-C17
5	A	524	78N	O15-C8-O16-C17
4	A	507	EPE	N4-C7-C8-O8
5	A	519	78N	C7-C8-O16-C17
5	A	524	78N	C7-C8-O16-C17
5	A	508	78N	O16-C17-C18-O20
5	A	516	78N	O16-C17-C18-O20
5	A	515	78N	O16-C17-C18-C19
5	A	518	78N	O16-C17-C18-C19
6	A	523	78M	O2-C17-C18-C20
5	A	508	78N	C7-C8-O16-C17
6	A	521	78M	C1-C2-C3-C4
5	A	524	78N	C5-C6-C7-C8
4	A	507	EPE	C9-C10-S-O3S
5	A	525	78N	C5-C6-C7-C8
5	A	515	78N	O16-C17-C18-O20
5	A	518	78N	O16-C17-C18-O20
5	A	508	78N	O15-C8-O16-C17
3	A	505	PG4	O1-C1-C2-O2
5	A	516	78N	C5-C6-C7-C8
5	A	519	78N	O16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
6	A	520	78M	O2-C17-C18-C20
5	A	513	78N	O16-C17-C18-O20
5	A	508	78N	C17-C18-C19-O22
5	A	519	78N	C17-C18-C19-O22
5	A	522	78N	C17-C18-C19-O22
6	A	523	78M	C17-C18-C20-O21
5	A	518	78N	C10-C11-C12-C13
5	A	525	78N	C3-C4-C5-C6
5	A	524	78N	C9-C10-C11-C12
5	A	511	78N	O20-C18-C19-O22
5	A	515	78N	O20-C18-C19-O22
5	A	524	78N	O20-C18-C19-O22
6	A	520	78M	O19-C18-C20-O21
6	A	521	78M	O19-C18-C20-O21
5	A	517	78N	C9-C10-C11-C12
6	A	512	78M	C1-C2-C3-C4
6	A	512	78M	C3-C4-C5-C6
6	A	523	78M	C1-C2-C3-C4
5	A	515	78N	C4-C5-C6-C7
5	A	525	78N	C4-C5-C6-C7
5	A	518	78N	C9-C10-C11-C12
5	A	513	78N	O16-C17-C18-C19
5	A	516	78N	O16-C17-C18-C19
5	A	513	78N	C11-C10-C9-C1
5	A	511	78N	C4-C5-C6-C7
5	A	513	78N	C5-C6-C7-C8
5	A	513	78N	C4-C5-C6-C7
5	A	514	78N	C11-C10-C9-C1
5	A	511	78N	C3-C4-C5-C6
5	A	525	78N	C10-C11-C12-C13
5	A	513	78N	C10-C11-C12-C13
5	A	519	78N	C4-C5-C6-C7
5	A	517	78N	O20-C18-C19-O22
6	A	509	78M	O19-C18-C20-O21
6	A	512	78M	O19-C18-C20-O21
5	A	519	78N	C11-C12-C13-C14
5	A	524	78N	C2-C3-C4-C5
6	A	523	78M	C4-C5-C6-C7
5	A	518	78N	C3-C4-C5-C6
5	A	518	78N	C11-C12-C13-C14
5	A	514	78N	C7-C8-O16-C17
4	A	506	EPE	C10-C9-N1-C6

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Mol	Chain	Res	Type	Atoms
5	A	519	78N	C10-C11-C12-C13
5	A	511	78N	C7-C8-O16-C17
5	A	519	78N	C3-C4-C5-C6
5	A	517	78N	C11-C12-C13-C14
5	A	516	78N	C12-C13-C14-C15
5	A	522	78N	C12-C13-C14-C15
5	A	511	78N	C12-C13-C14-C15
3	A	505	PG4	O4-C7-C8-O5
6	A	521	78M	C10-C11-C12-C13
6	A	523	78M	O19-C18-C20-O21
5	A	522	78N	O16-C17-C18-C19
5	A	518	78N	C7-C8-O16-C17
5	A	511	78N	C9-C10-C11-C12
5	A	522	78N	C9-C10-C11-C12
5	A	514	78N	O15-C8-O16-C17
6	A	521	78M	C3-C4-C5-C6
5	A	517	78N	C3-C4-C5-C6
5	A	525	78N	C12-C13-C14-C15
6	A	523	78M	C11-C12-C13-C14
5	A	515	78N	C5-C6-C7-C8
5	A	524	78N	C11-C10-C9-C1
5	A	522	78N	O16-C17-C18-O20
6	A	521	78M	C2-C3-C4-C5
6	A	520	78M	C11-C12-C13-C14
5	A	511	78N	O15-C8-O16-C17
4	A	507	EPE	C9-C10-S-O2S
5	A	518	78N	O15-C8-O16-C17
5	A	508	78N	C2-C3-C4-C5
5	A	514	78N	C4-C5-C6-C7
6	A	512	78M	C9-C10-C11-C12
3	A	505	PG4	C3-C4-O3-C5
5	A	514	78N	C9-C10-C11-C12
5	A	516	78N	C10-C11-C12-C13
6	A	520	78M	C11-C10-C9-C8
6	A	520	78M	C2-C3-C4-C5
5	A	508	78N	O20-C18-C19-O22
5	A	519	78N	O20-C18-C19-O22
5	A	510	78N	C11-C10-C9-C1
5	A	519	78N	C12-C13-C14-C15
5	A	511	78N	C2-C1-C9-C10
6	A	521	78M	C2-C1-O2-C17
5	A	524	78N	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
6	A	521	78M	O1-C1-O2-C17
5	A	525	78N	C9-C10-C11-C12
5	A	518	78N	C1-C2-C3-C4
3	A	505	PG4	C6-C5-O3-C4
6	A	509	78M	C4-C5-C6-C7
5	A	519	78N	C9-C10-C11-C12
6	A	520	78M	C4-C5-C6-C7
5	A	510	78N	C10-C11-C12-C13
5	A	514	78N	C3-C4-C5-C6
3	A	505	PG4	O2-C3-C4-O3
5	A	519	78N	C1-C2-C3-C4
6	A	520	78M	C3-C4-C5-C6
5	A	514	78N	C2-C3-C4-C5
5	A	514	78N	C1-C2-C3-C4
6	A	509	78M	C10-C11-C12-C13
5	A	510	78N	C1-C2-C3-C4
5	A	516	78N	C2-C1-C9-C10
5	A	511	78N	C11-C10-C9-C1
5	A	517	78N	C12-C13-C14-C15
5	A	513	78N	C1-C2-C3-C4
5	A	510	78N	C11-C12-C13-C14
5	A	517	78N	C4-C5-C6-C7
6	A	521	78M	C7-C8-C9-C10
6	A	523	78M	C7-C8-C9-C10
5	A	516	78N	O15-C8-O16-C17
5	A	516	78N	C7-C8-O16-C17
5	A	515	78N	C1-C2-C3-C4
5	A	516	78N	C1-C2-C3-C4
5	A	518	78N	C2-C1-C9-C10
6	A	509	78M	C7-C8-C9-C10
6	A	512	78M	C11-C10-C9-C8
5	A	525	78N	C1-C2-C3-C4
6	A	520	78M	C5-C6-C7-C8
5	A	516	78N	C2-C3-C4-C5
5	A	517	78N	C2-C1-C9-C10
6	A	520	78M	C7-C8-C9-C10
5	A	508	78N	C2-C1-C9-C10
6	A	509	78M	C5-C6-C7-C8
6	A	512	78M	C7-C8-C9-C10
5	A	519	78N	C2-C1-C9-C10
6	A	509	78M	C2-C3-C4-C5
6	A	520	78M	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	A	521	78M	C9-C10-C11-C12
3	A	505	PG4	C8-C7-O4-C6
6	A	521	78M	C11-C10-C9-C8
5	A	522	78N	C1-C2-C3-C4
5	A	510	78N	C3-C4-C5-C6
6	A	512	78M	C12-C13-C14-C15
5	A	518	78N	C11-C10-C9-C1
6	A	523	78M	C10-C11-C12-C13
5	A	513	78N	C11-C12-C13-C14
6	A	520	78M	O1-C1-C2-C3

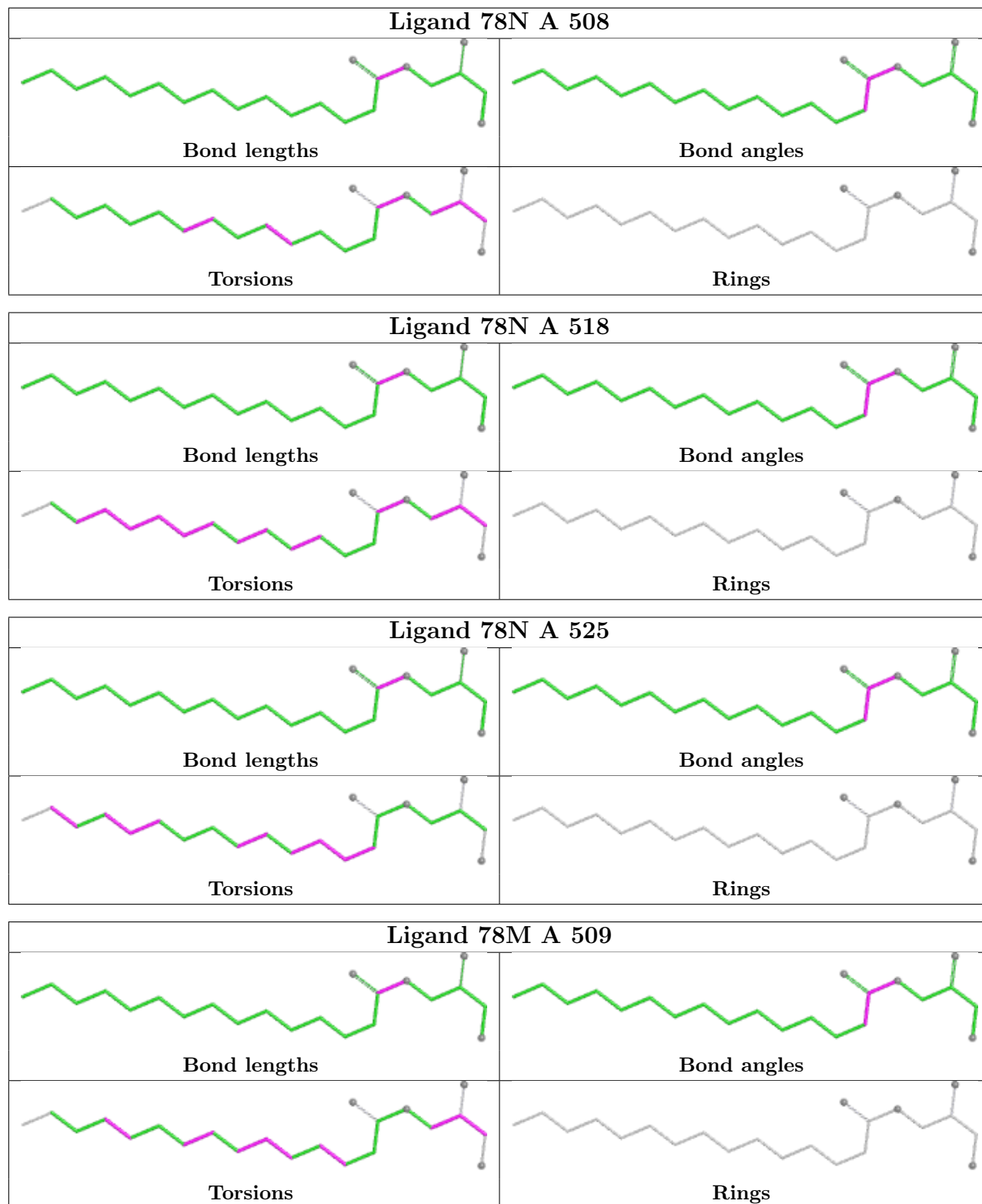
There are no ring outliers.

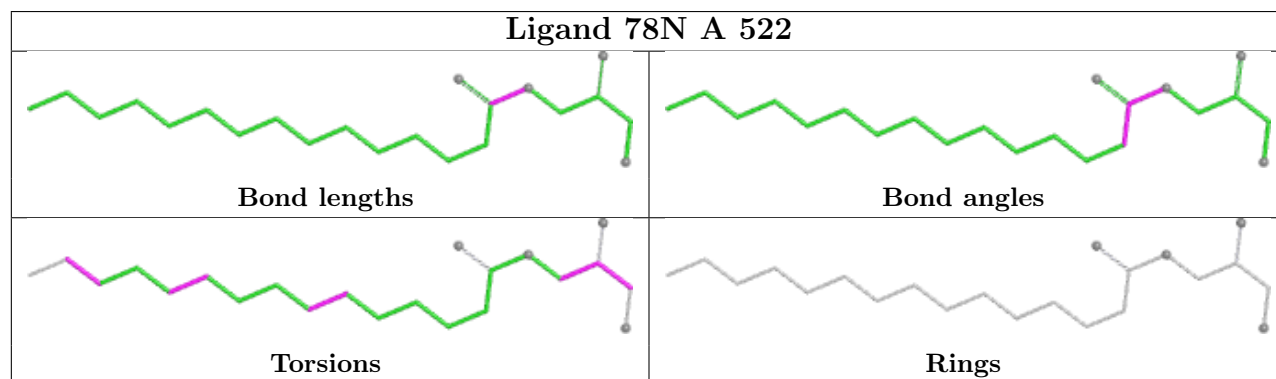
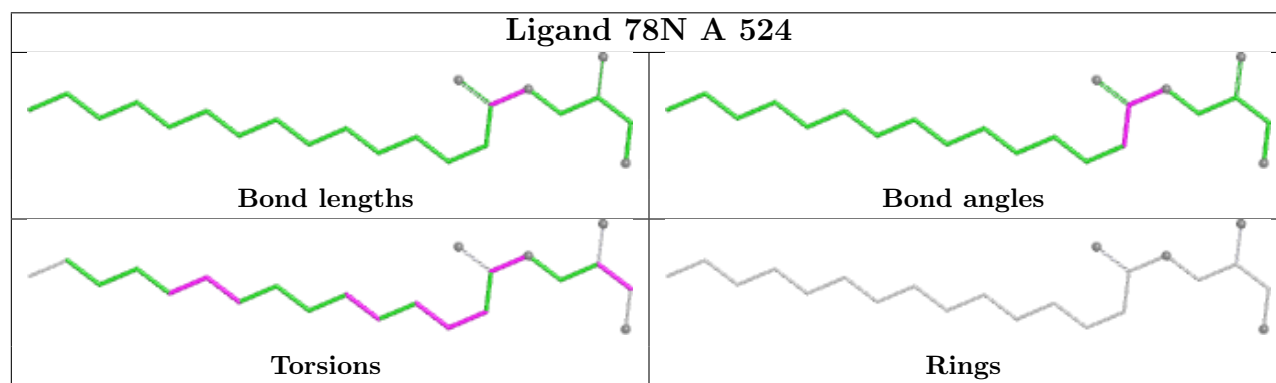
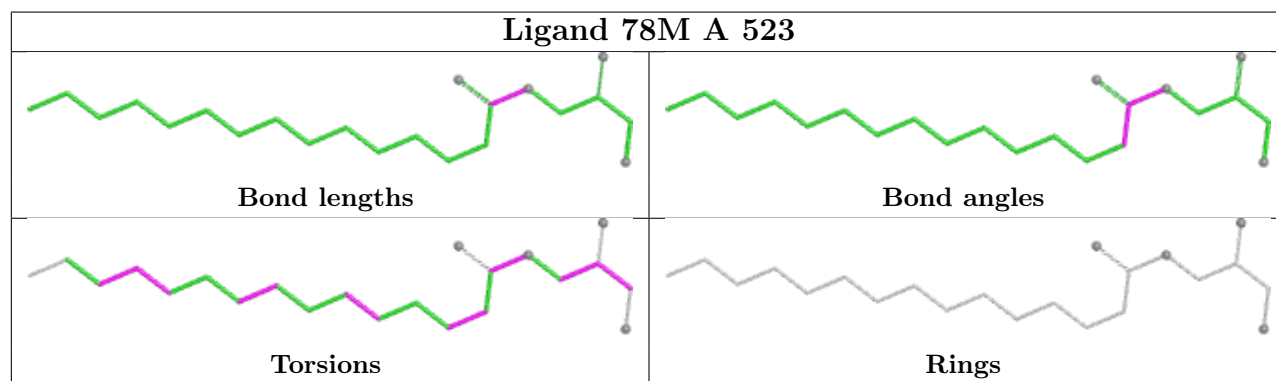
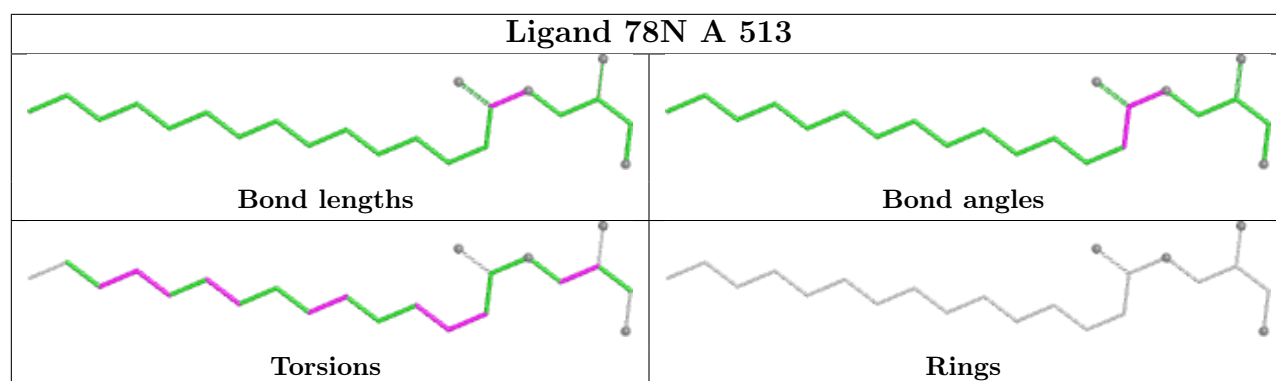
15 monomers are involved in 18 short contacts:

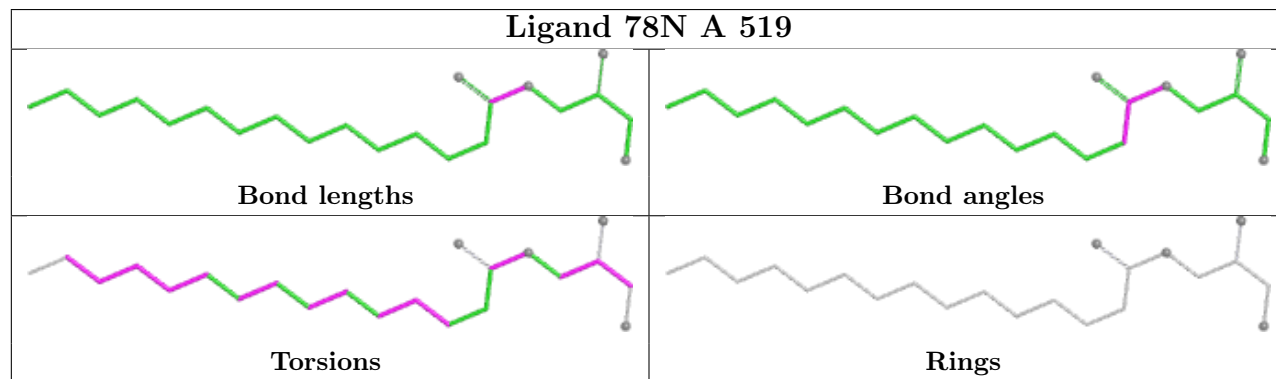
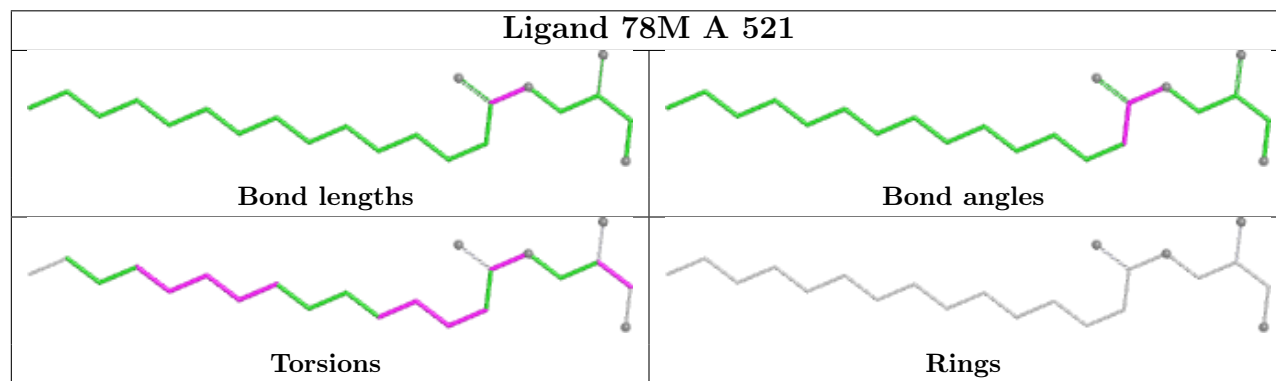
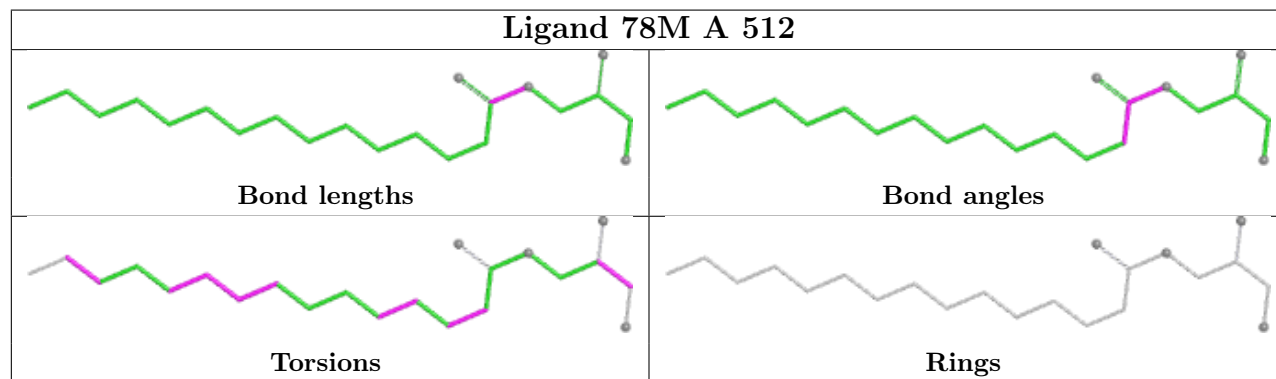
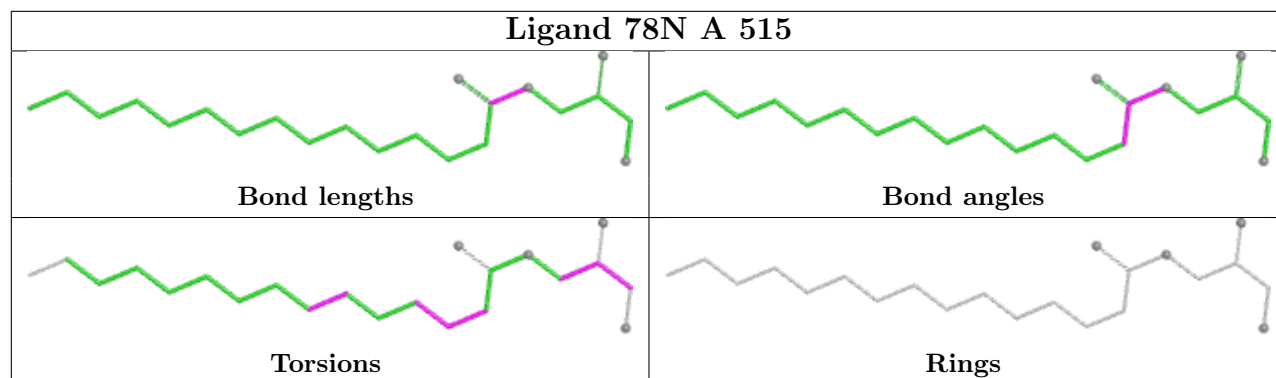
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	508	78N	2	0
5	A	518	78N	1	0
6	A	509	78M	2	0
3	A	505	PG4	2	0
5	A	522	78N	1	0
5	A	515	78N	1	0
6	A	512	78M	4	0
6	A	521	78M	2	0
5	A	514	78N	2	0
5	A	517	78N	1	0
6	A	520	78M	1	0
5	A	510	78N	1	0
5	A	516	78N	2	0
5	A	511	78N	1	0
4	A	506	EPE	1	0

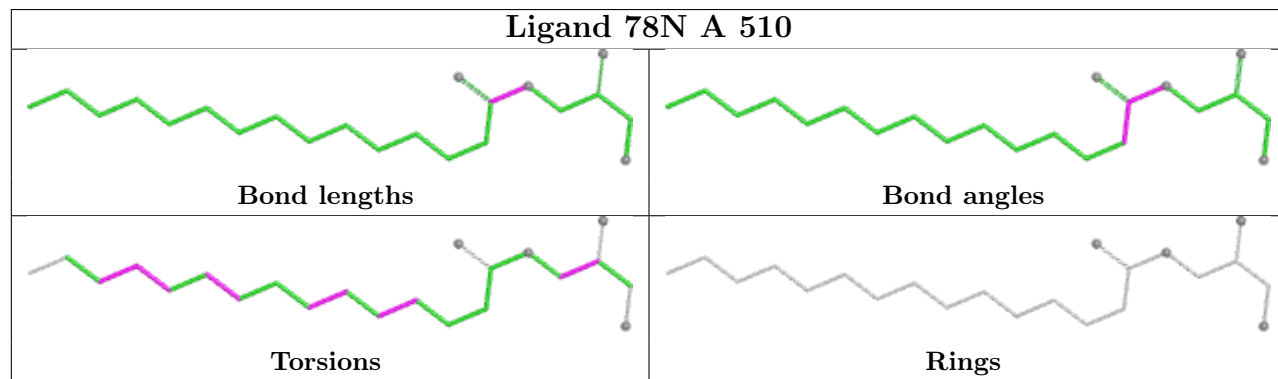
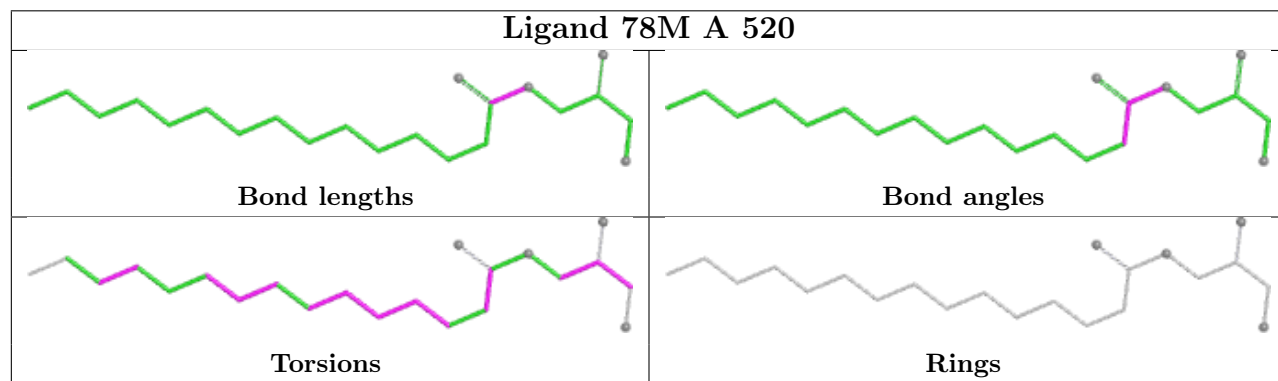
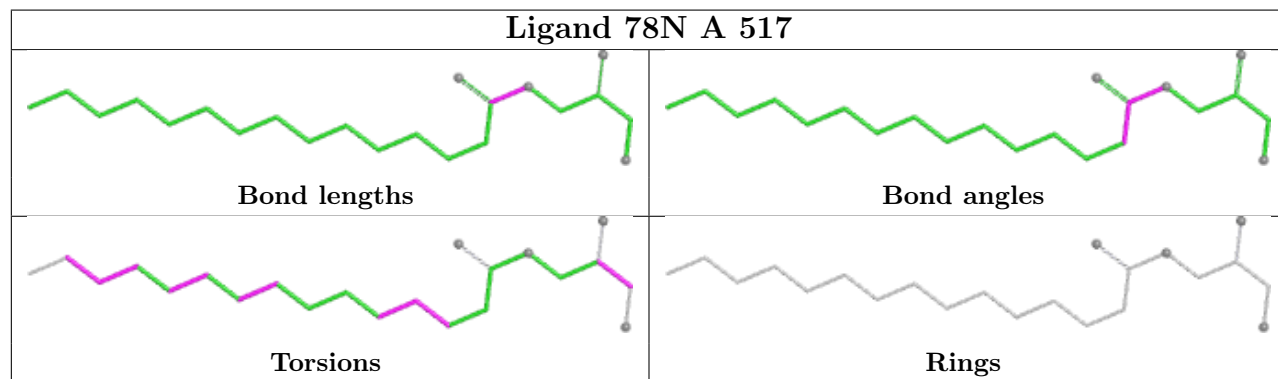
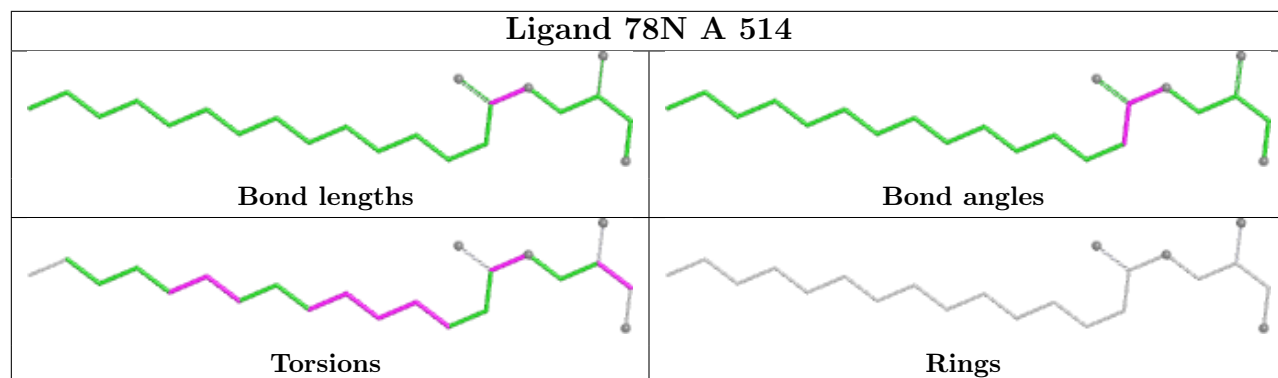
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

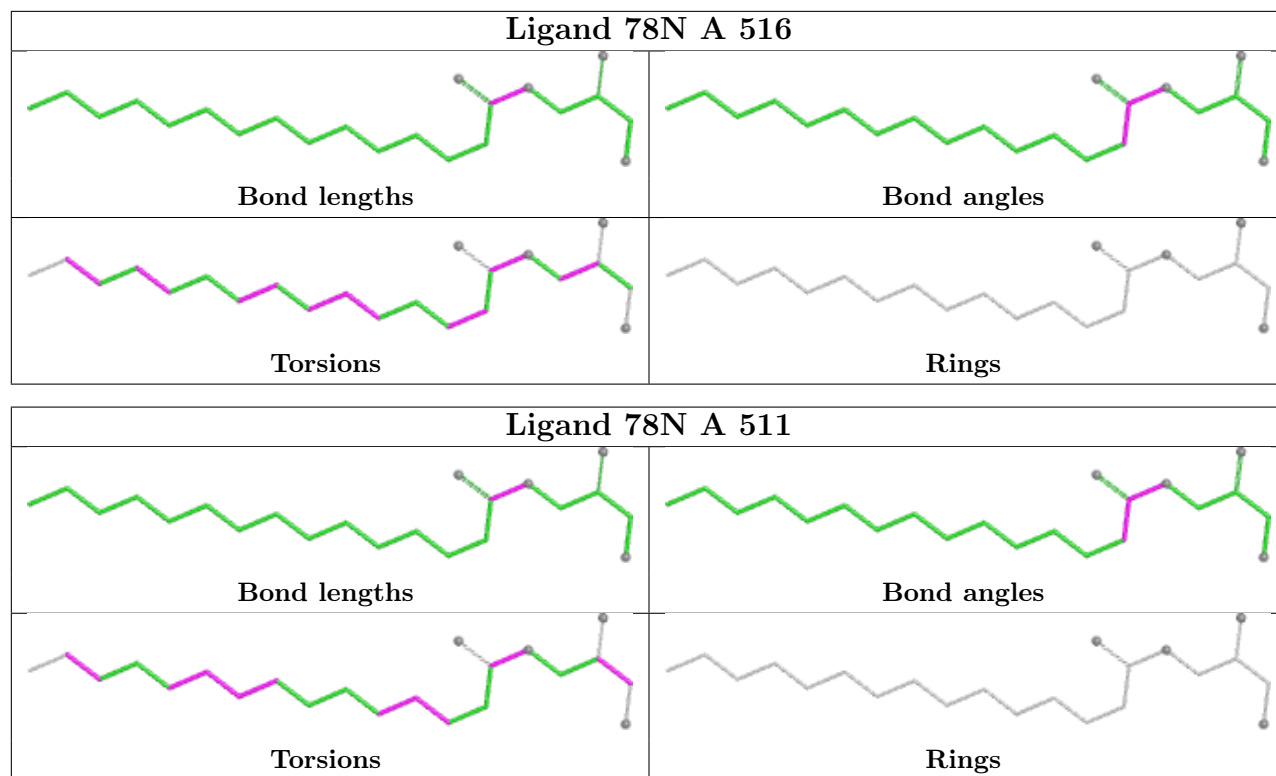
equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	464/490 (94%)	0.27	25 (5%)	31 30	22, 42, 92, 146	3 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	THR	4.1
1	A	269	ILE	4.0
1	A	268	MET	3.5
1	A	284	SER	3.5
1	A	412	THR	3.2
1	A	280	LEU	3.2
1	A	478	LEU	3.2
1	A	315	ASP	3.2
1	A	423	MET	3.1
1	A	414	LEU	3.1
1	A	264	TYR	3.1
1	A	265	PHE	3.0
1	A	420	ASN	2.9
1	A	279	HIS	2.6
1	A	422	GLN	2.5
1	A	476	GLN	2.5
1	A	346	TRP	2.4
1	A	316	SER	2.3
1	A	267	TRP	2.3
1	A	428	PHE	2.2
1	A	263	PHE	2.1
1	A	140	HIS	2.1
1	A	408	LEU	2.0
1	A	411	THR	2.0
1	A	5	GLY	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 oligosaccharides 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.

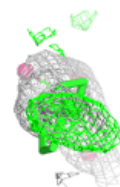
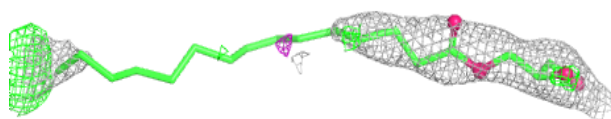
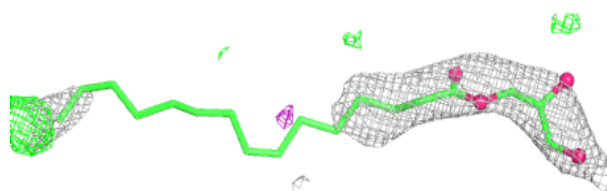
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	78N	A	513	22/22	0.71	0.23	87,95,109,111	0
4	EPE	A	507	15/15	0.76	0.21	115,117,120,121	0
4	EPE	A	506	15/15	0.77	0.17	63,68,96,96	0
5	78N	A	514	22/22	0.77	0.23	79,99,114,116	0
2	PO4	A	502	5/5	0.79	0.17	109,110,114,115	0
6	78M	A	521	22/22	0.79	0.21	65,92,106,117	0
6	78M	A	520	22/22	0.80	0.22	61,92,109,115	0
5	78N	A	510	22/22	0.80	0.23	91,102,105,108	0
5	78N	A	524	22/22	0.81	0.23	66,78,115,116	0
6	78M	A	509	22/22	0.81	0.20	77,87,106,110	0
5	78N	A	518	22/22	0.82	0.19	72,99,103,105	0
5	78N	A	519	22/22	0.82	0.21	59,83,88,90	0
2	PO4	A	503	5/5	0.82	0.15	113,115,117,119	0
3	PG4	A	505	13/13	0.84	0.20	81,84,87,87	0
5	78N	A	511	22/22	0.84	0.20	64,84,94,94	0
6	78M	A	523	22/22	0.85	0.21	64,77,91,93	0
5	78N	A	516	22/22	0.86	0.17	61,72,78,82	0
5	78N	A	522	22/22	0.87	0.17	45,61,87,88	0
5	78N	A	515	22/22	0.87	0.18	59,80,89,90	0
2	PO4	A	504	5/5	0.87	0.15	96,97,99,100	0
5	78N	A	517	22/22	0.89	0.23	65,91,97,100	0
6	78M	A	512	22/22	0.90	0.20	67,83,103,104	0
5	78N	A	508	22/22	0.90	0.16	47,65,77,81	0
5	78N	A	525	22/22	0.92	0.17	66,76,87,91	0
2	PO4	A	501	5/5	0.93	0.07	64,66,71,73	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.

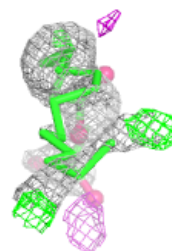
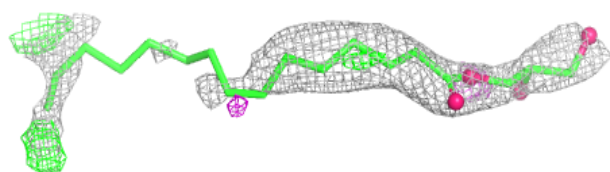
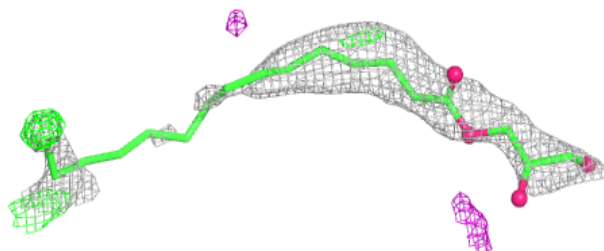
Electron density around 78N A 513:

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

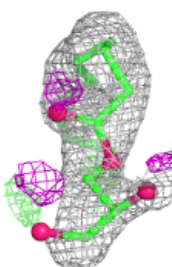
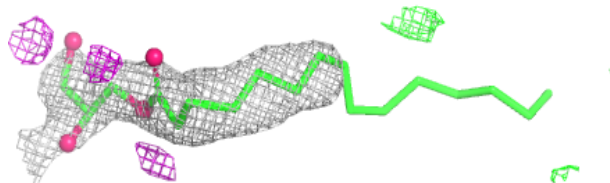
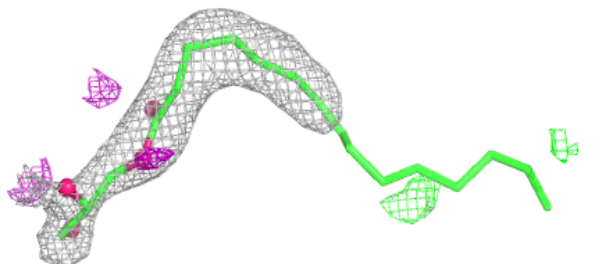


Electron density around 78N A 514:

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

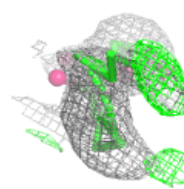
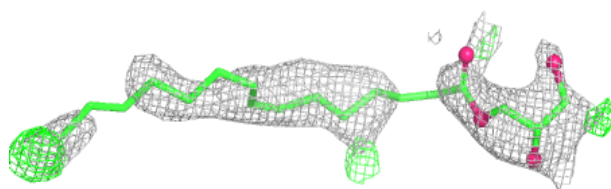
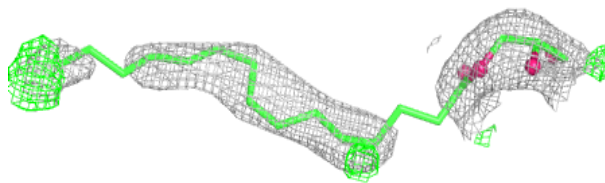
**Electron density around 78M A 521:**

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

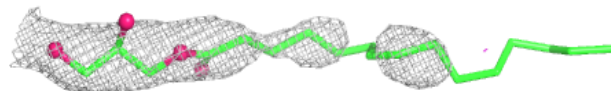
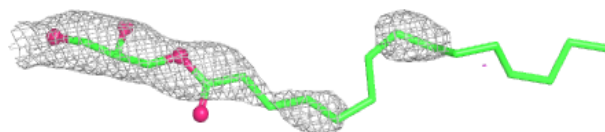


Electron density around 78M A 520:

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

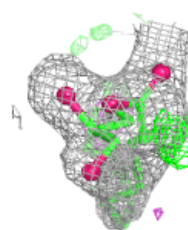
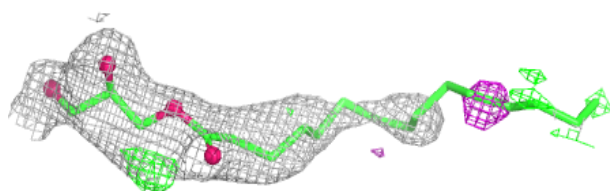
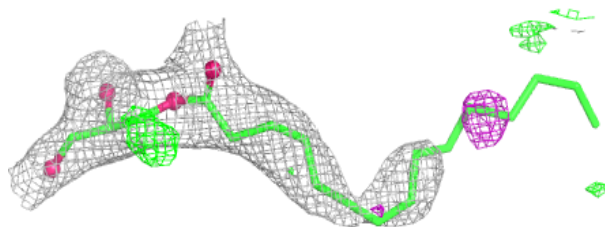
**Electron density around 78N A 510:**

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

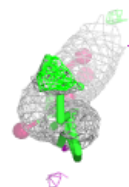
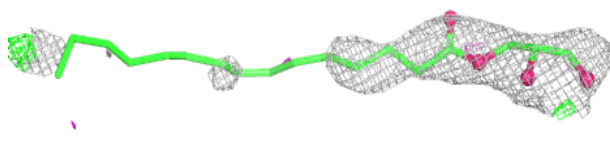
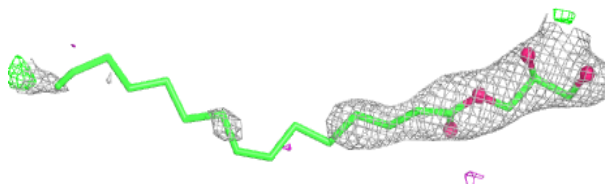


Electron density around 78N A 524:

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

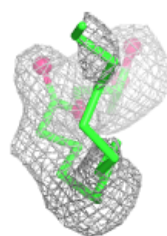
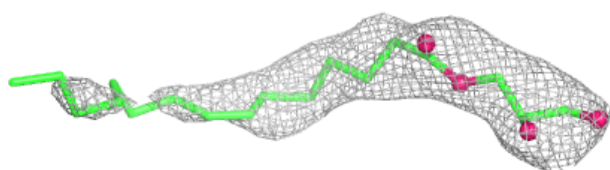
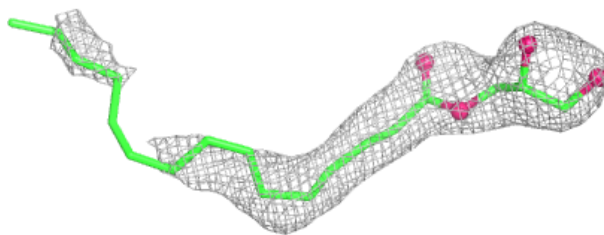
**Electron density around 78M A 509:**

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

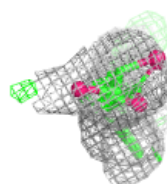
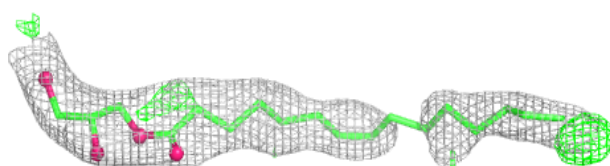
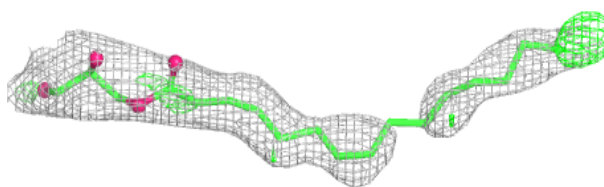


Electron density around 78N A 518:

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

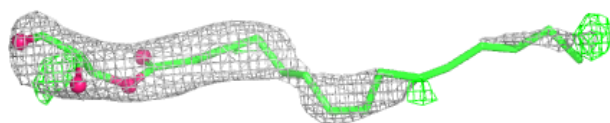
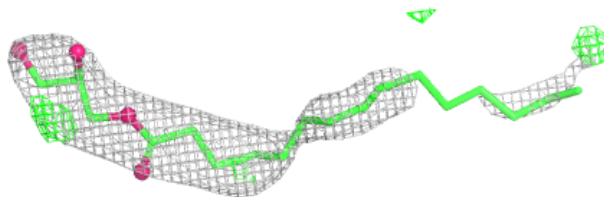
**Electron density around 78N A 519:**

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

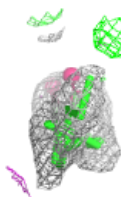
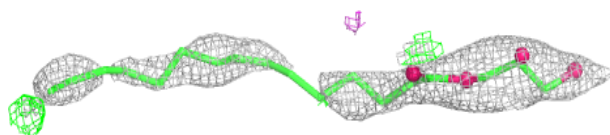
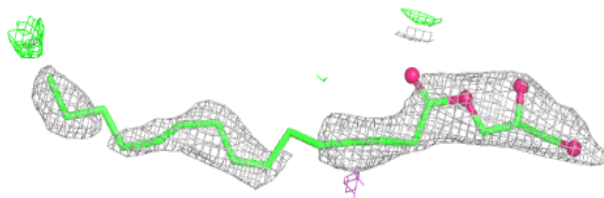


Electron density around 78N A 511:

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

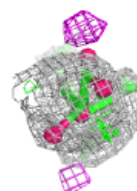
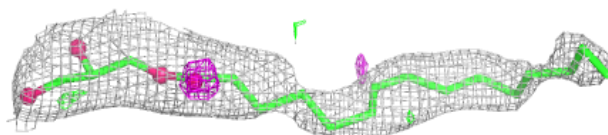
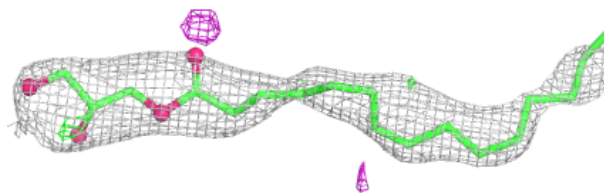
**Electron density around 78M A 523:**

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

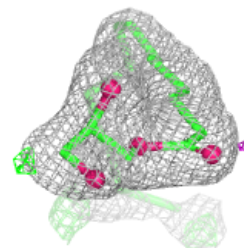
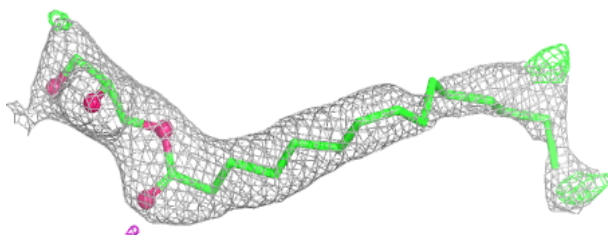
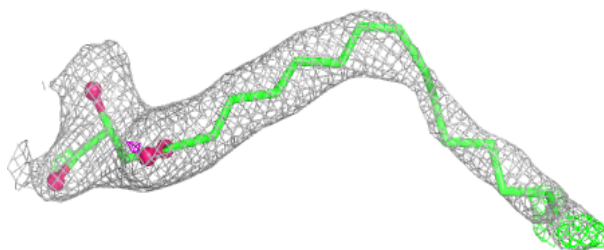


Electron density around 78N A 516:

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

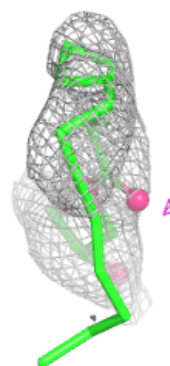
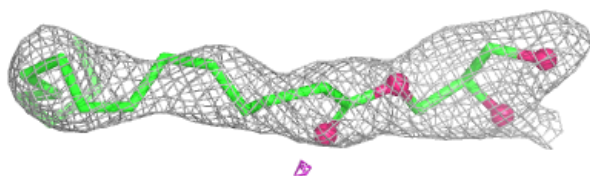
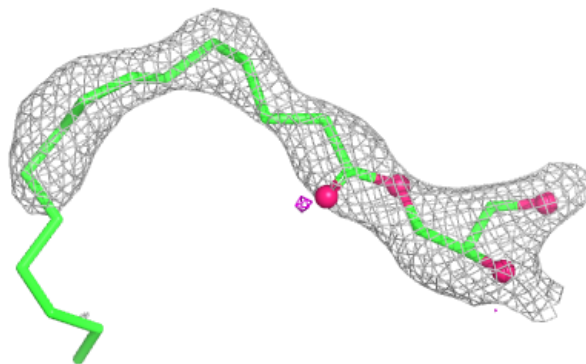
**Electron density around 78N A 522:**

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

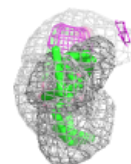
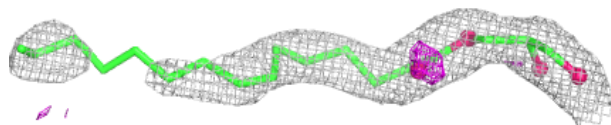
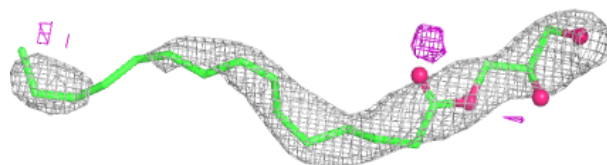


Electron density around 78N A 515:

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

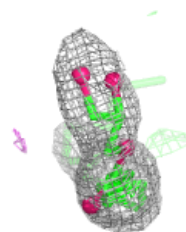
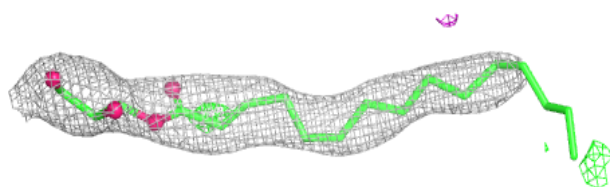
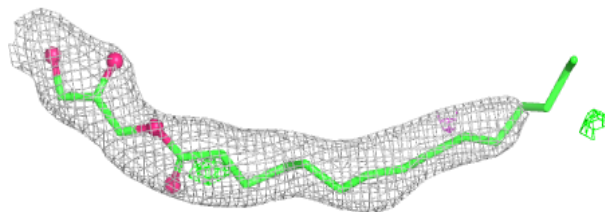
**Electron density around 78N A 517:**

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

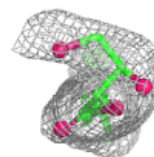
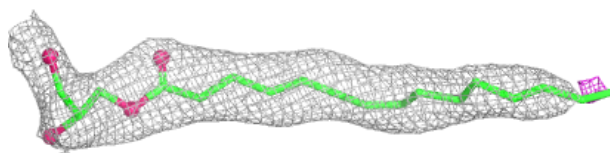
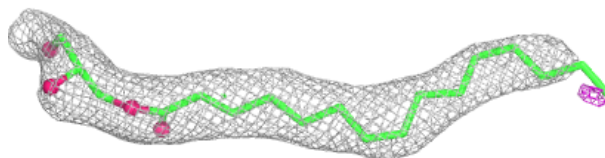


Electron density around 78M A 512:

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

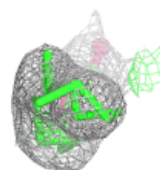
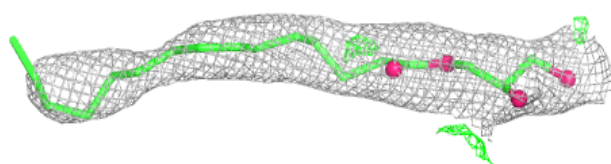
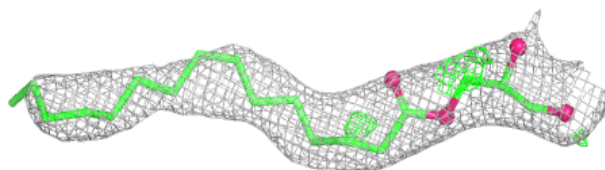
**Electron density around 78N A 508:**

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



Electron density around 78N A 525:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.