



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:15 AM UTC

PDB ID : 4AFK / pdb_00004afk
Title : In meso structure of alginate transporter, AlgE, from *Pseudomonas aeruginosa*, PAO1
Authors : Tan, J.; Pye, V.E.; Aragao, D.; Caffrey, M.
Deposited on : 2012-01-19
Resolution : 1.90 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

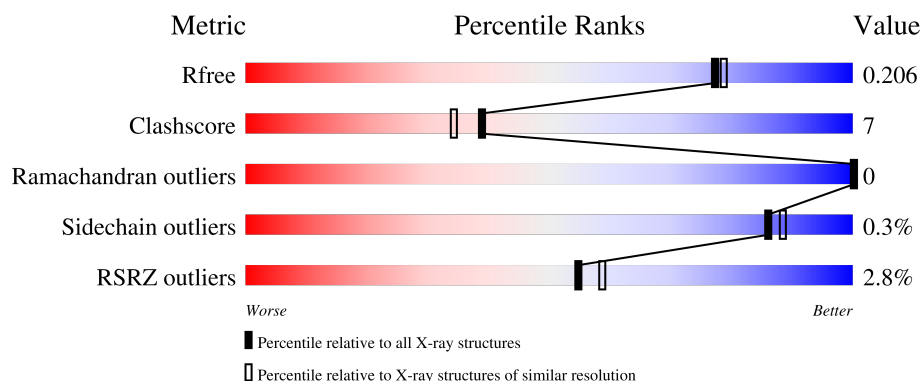
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

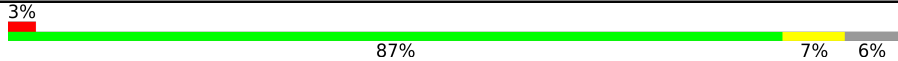
The reported resolution of this entry is 1.90 Å.

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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	458	

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
4	LDA	A	1494	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	78M	A	1515	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 4073 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.

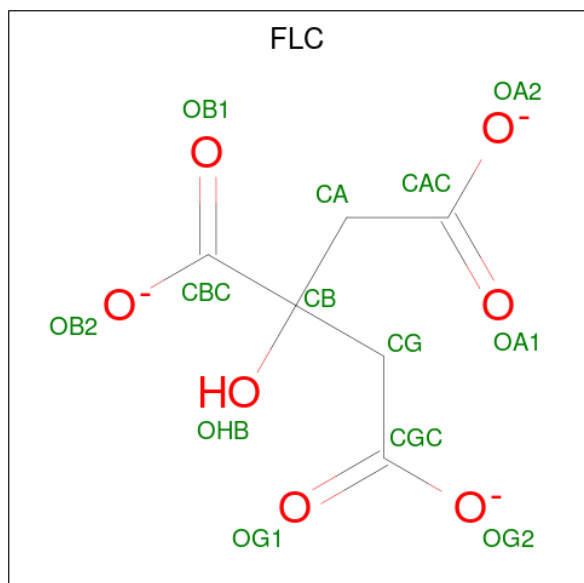
- Molecule 1 is a protein called ALGINATE PRODUCTION PROTEIN ALGE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	9	0
			3489	2181	620	685	3			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

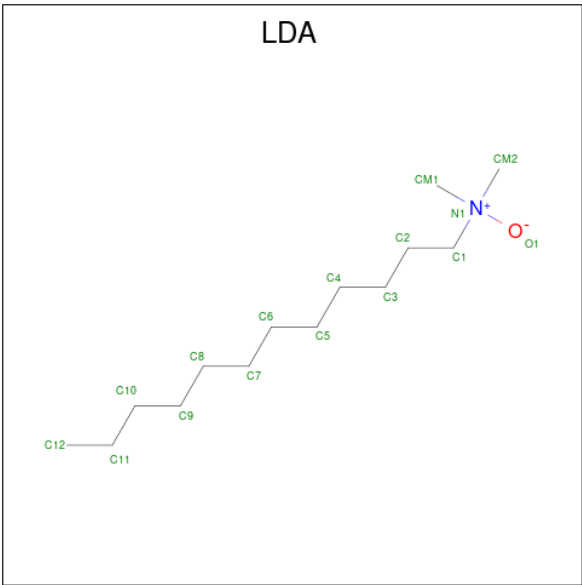
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is CITRATE ANION (CCD ID: FLC) (formula: C₆H₅O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			11	9	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			13	11	1	1		
4	A	1	Total	C			0	0
			9	9				
4	A	1	Total	C			0	0
			10	10				
4	A	1	Total	C			0	0
			12	12				
4	A	1	Total	C			0	0
			8	8				
4	A	1	Total	C			0	0
			7	7				
4	A	1	Total	C			0	0
			9	9				
4	A	1	Total	C			0	0
			9	9				
4	A	1	Total	C			0	0
			8	8				

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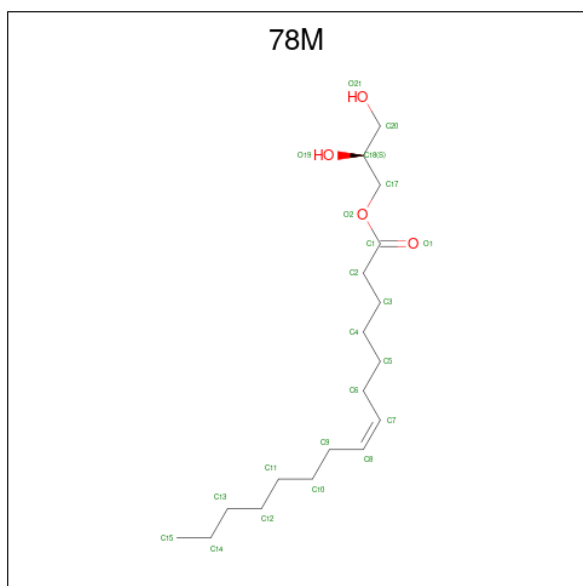
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	0
			11	11		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

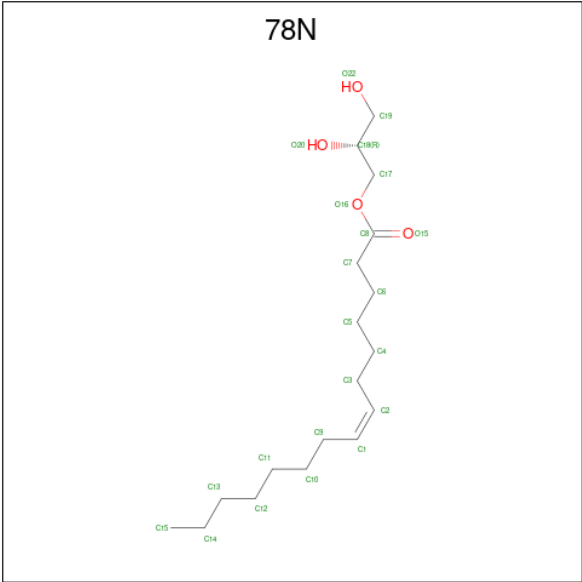
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Na	0	0
			2	2		

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



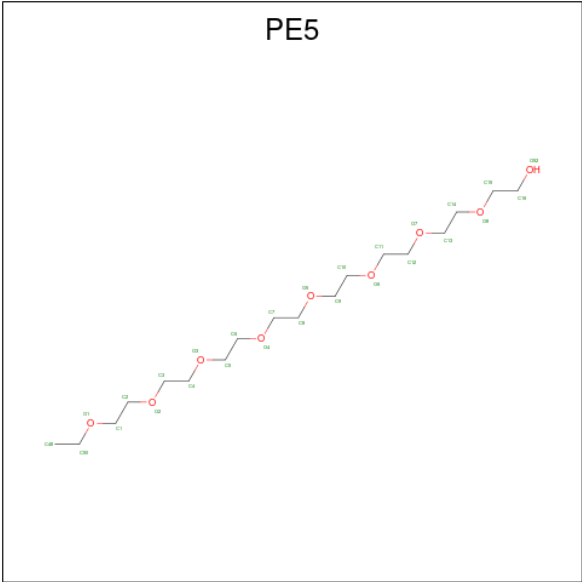
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			22	18	4		
6	A	1	Total	C	O	0	0
			22	18	4		
6	A	1	Total	C	O	0	0
			22	18	4		

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



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

- Molecule 8 is 3,6,9,12,15,18,21,24-OCTAOXAHEXACOSAN-1-OL (CCD ID: PE5) (formula: C₁₈H₃₈O₉).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			15	10	5		
8	A	1	Total	C	O	0	0
			8	5	3		

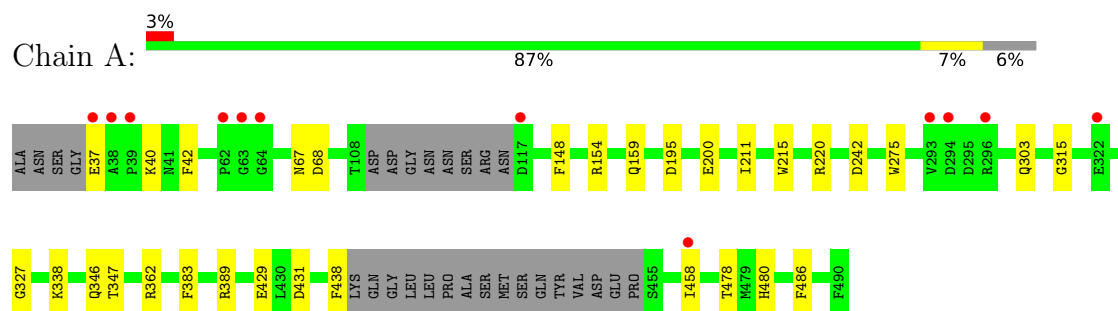
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	242	Total	O	0	0
			242	242		

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: ALGINATE PRODUCTION PROTEIN ALGE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	57.25Å 74.42Å 115.53Å 90.00° 101.56° 90.00°	Depositor
Resolution (Å)	19.77 – 1.90 19.77 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.5 (19.77-1.90) 97.6 (19.77-1.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 1.90Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.163 , 0.209 0.164 , 0.206	Depositor DCC
R_{free} test set	1846 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4073	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.94% 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: PE5, FLC, CA, 78N, 78M, LDA, 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	0.62	0/3581	0.82	1/4854 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	ARG	CB-CA-C	-6.29	109.31	116.54

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	3489	0	3243	36	1
2	A	1	0	0	0	0
3	A	13	0	5	0	0
4	A	171	0	297	24	0
5	A	2	0	0	0	0
6	A	66	0	102	12	0
7	A	66	0	102	2	0
8	A	23	0	26	4	0
9	A	242	0	0	3	0
All	All	4073	0	3775	52	1

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 7.

All (52) 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)
4:A:1494:LDA:H32	6:A:1515:78M:H32C	1.63	0.80
4:A:1496:LDA:H42	7:A:1511:78N:O15	1.83	0.78
1:A:438:PHE:HE2	1:A:458[A]:ILE:HG23	1.58	0.67
4:A:1494:LDA:CM1	6:A:1515:78M:H171	2.29	0.63
1:A:438:PHE:CE2	1:A:458[A]:ILE:HG23	2.32	0.63
1:A:362[B]:ARG:HG3	9:A:2201:HOH:O	1.98	0.63
4:A:1494:LDA:H51	6:A:1515:78M:H52C	1.82	0.62
1:A:458[A]:ILE:HG22	1:A:486:PHE:HD1	1.65	0.61
4:A:1494:LDA:H72	6:A:1515:78M:H52C	1.82	0.60
1:A:154:ARG:HE	1:A:362[B]:ARG:HH12	1.51	0.58
1:A:347:THR:HG23	8:A:1517:PE5:C5	2.32	0.58
4:A:1494:LDA:HM11	6:A:1515:78M:H171	1.88	0.56
1:A:275:TRP:CZ2	1:A:315:GLY:HA3	2.41	0.56
4:A:1494:LDA:H51	6:A:1515:78M:H32C	1.89	0.55
1:A:211[B]:ILE:HG13	4:A:1498:LDA:H41	1.88	0.55
4:A:1494:LDA:C3	6:A:1515:78M:H32C	2.35	0.54
1:A:480:HIS:CG	6:A:1515:78M:H31C	2.44	0.53
1:A:154:ARG:NE	1:A:362[B]:ARG:NH1	2.56	0.53
1:A:215:TRP:CZ2	4:A:1503:LDA:H62	2.44	0.52
4:A:1494:LDA:H51	6:A:1515:78M:C5	2.39	0.52
4:A:1494:LDA:C7	6:A:1515:78M:H52C	2.40	0.52
1:A:215:TRP:CD2	4:A:1503:LDA:H41	2.45	0.51
4:A:1499:LDA:H62	7:A:1514:78N:H61C	1.93	0.51
1:A:40:LYS:HE2	1:A:42:PHE:O	2.09	0.51
1:A:275:TRP:CE2	1:A:315:GLY:HA3	2.45	0.51
1:A:347:THR:H	8:A:1517:PE5:C5	2.24	0.50
1:A:67:ASN:O	4:A:1493:LDA:HM23	2.12	0.50
1:A:458[A]:ILE:CG2	1:A:486:PHE:HD1	2.25	0.50
1:A:346:GLN:HG2	8:A:1517:PE5:H42	1.93	0.50
1:A:438:PHE:HZ	1:A:458[A]:ILE:HD13	1.77	0.50
1:A:148:PHE:CE1	4:A:1506:LDA:H72	2.46	0.49
1:A:154:ARG:NH2	1:A:362[B]:ARG:NH1	2.60	0.48
1:A:220:ARG:HG2	9:A:2132:HOH:O	2.14	0.48
4:A:1494:LDA:HM12	6:A:1515:78M:H201	1.95	0.47
1:A:327:GLY:HA3	1:A:383:PHE:CZ	2.49	0.47
1:A:154:ARG:NE	1:A:362[B]:ARG:HH12	2.11	0.47
1:A:429:GLU:OE2	1:A:431:ASP:OD1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ARG:CZ	1:A:362[B]:ARG:NH1	2.78	0.46
4:A:1506:LDA:H51	4:A:1506:LDA:H22	1.67	0.45
1:A:154:ARG:HE	1:A:362[B]:ARG:NH1	2.15	0.44
4:A:1492:LDA:H22	4:A:1492:LDA:HM21	1.78	0.44
1:A:37[B]:GLU:N	1:A:37[B]:GLU:OE1	2.51	0.44
1:A:242:ASP:OD1	1:A:242:ASP:C	2.60	0.44
1:A:478:THR:HG22	6:A:1515:78M:H18	2.00	0.43
1:A:338:LYS:HE2	9:A:2188:HOH:O	2.18	0.43
4:A:1493:LDA:H32	4:A:1493:LDA:H62	1.49	0.43
1:A:159:GLN:O	8:A:1517:PE5:C5	2.68	0.41
1:A:195:ASP:HA	4:A:1496:LDA:HM13	2.02	0.41
1:A:215:TRP:CE3	4:A:1503:LDA:H21	2.56	0.41
1:A:68:ASP:HA	4:A:1493:LDA:H22	2.03	0.40
1:A:438:PHE:CZ	1:A:458[A]:ILE:HD13	2.55	0.40
4:A:1497:LDA:H32	4:A:1500:LDA:H22	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:GLN:NE2	1:A:303:GLN:NE2[2_655]	2.17	0.03

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	432/458 (94%)	417 (96%)	15 (4%)	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	356/370 (96%)	355 (100%)	1 (0%)	86	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	159	GLN
1	A	164	ASN
1	A	169	ASN
1	A	319	ASN
1	A	428	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 27 ligands modelled in this entry, 3 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LDA	A	1498	-	8,8,15	0.29	0	7,7,17	0.39	0
4	LDA	A	1505	-	7,7,15	0.35	0	6,6,17	0.40	0
4	LDA	A	1494	-	13,15,15	1.14	1 (7%)	14,17,17	0.49	0
4	LDA	A	1495	-	8,10,15	1.33	1 (12%)	9,12,17	0.31	0
6	78M	A	1512	-	21,21,21	1.04	1 (4%)	22,22,22	1.32	3 (13%)
7	78N	A	1511	-	21,21,21	1.01	1 (4%)	22,22,22	1.10	2 (9%)
6	78M	A	1515	-	21,21,21	1.03	1 (4%)	22,22,22	1.09	2 (9%)
4	LDA	A	1496	-	13,15,15	1.13	1 (7%)	14,17,17	0.45	0
4	LDA	A	1502	-	6,6,15	0.33	0	5,5,17	0.32	0
3	FLC	A	1491	-	12,12,12	2.05	4 (33%)	17,17,17	1.47	2 (11%)
8	PE5	A	1517	-	7,7,26	0.43	0	6,6,25	1.48	2 (33%)
4	LDA	A	1499	-	9,9,15	0.26	0	8,8,17	0.44	0
7	78N	A	1514	-	21,21,21	1.04	1 (4%)	22,22,22	0.91	2 (9%)
4	LDA	A	1501	-	7,7,15	0.26	0	6,6,17	0.49	0
4	LDA	A	1500	-	11,11,15	0.25	0	10,10,17	0.56	0
4	LDA	A	1493	-	13,15,15	1.09	1 (7%)	14,17,17	0.66	0
7	78N	A	1513	-	21,21,21	1.00	1 (4%)	22,22,22	1.13	2 (9%)
8	PE5	A	1516	-	14,14,26	0.42	0	13,13,25	1.24	0
4	LDA	A	1506	-	10,10,15	0.27	0	9,9,17	0.43	0
4	LDA	A	1504	-	8,8,15	0.24	0	7,7,17	0.55	0
4	LDA	A	1503	-	8,8,15	0.26	0	7,7,17	0.48	0
6	78M	A	1510	-	21,21,21	0.90	1 (4%)	22,22,22	0.99	2 (9%)
4	LDA	A	1492	-	13,15,15	1.12	1 (7%)	14,17,17	0.58	0
4	LDA	A	1497	-	10,12,15	1.30	1 (10%)	11,14,17	0.45	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
4	LDA	A	1498	-	-	2/6/6/13	-
4	LDA	A	1505	-	-	1/5/5/13	-
4	LDA	A	1494	-	-	9/13/13/13	-
4	LDA	A	1495	-	-	5/8/8/13	-
6	78M	A	1512	-	-	9/21/21/21	-
7	78N	A	1511	-	-	8/21/21/21	-
6	78M	A	1515	-	-	8/21/21/21	-
4	LDA	A	1496	-	-	6/13/13/13	-
4	LDA	A	1502	-	-	0/4/4/13	-
3	FLC	A	1491	-	-	0/16/16/16	-
8	PE5	A	1517	-	-	3/5/5/24	-
4	LDA	A	1499	-	-	2/7/7/13	-
7	78N	A	1514	-	-	8/21/21/21	-
4	LDA	A	1501	-	-	2/5/5/13	-
4	LDA	A	1500	-	-	2/9/9/13	-
4	LDA	A	1493	-	-	11/13/13/13	-
7	78N	A	1513	-	-	6/21/21/21	-
8	PE5	A	1516	-	-	5/12/12/24	-
4	LDA	A	1506	-	-	5/8/8/13	-
4	LDA	A	1504	-	-	4/6/6/13	-
4	LDA	A	1503	-	-	1/6/6/13	-
6	78M	A	1510	-	-	4/21/21/21	-
4	LDA	A	1492	-	-	6/13/13/13	-
4	LDA	A	1497	-	-	7/10/10/13	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1512	78M	O2-C1	4.55	1.46	1.33
7	A	1514	78N	O16-C8	4.49	1.46	1.33
6	A	1515	78M	O2-C1	4.41	1.46	1.33
7	A	1511	78N	O16-C8	4.35	1.46	1.33
7	A	1513	78N	O16-C8	4.33	1.46	1.33
3	A	1491	FLC	CB-CBC	-3.91	1.49	1.53
6	A	1510	78M	O2-C1	3.83	1.44	1.33
4	A	1497	LDA	C1-N1	-3.64	1.47	1.51
4	A	1496	LDA	C1-N1	-3.55	1.47	1.51
4	A	1492	LDA	C1-N1	-3.52	1.47	1.51
4	A	1494	LDA	C1-N1	-3.50	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1493	LDA	C1-N1	-3.49	1.47	1.51
3	A	1491	FLC	CG-CB	-3.48	1.49	1.54
4	A	1495	LDA	C1-N1	-3.12	1.48	1.51
3	A	1491	FLC	CA-CB	-2.88	1.50	1.54
3	A	1491	FLC	OHB-CB	-2.18	1.39	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1512	78M	O2-C1-C2	4.14	124.45	111.83
3	A	1491	FLC	OB2-CBC-CB	4.04	120.90	113.14
6	A	1515	78M	O2-C1-C2	3.47	122.41	111.83
7	A	1511	78N	O16-C8-C7	3.43	122.28	111.83
7	A	1513	78N	O16-C8-C7	3.20	121.58	111.83
7	A	1514	78N	O16-C8-C7	2.98	120.92	111.83
6	A	1510	78M	O2-C1-C2	2.61	119.79	111.83
7	A	1511	78N	O16-C8-O15	-2.42	117.57	123.63
6	A	1512	78M	O2-C1-O1	-2.39	117.66	123.63
8	A	1517	PE5	O2-C2-C1	2.36	120.50	110.11
6	A	1510	78M	O2-C1-O1	-2.29	117.89	123.63
6	A	1512	78M	C3-C2-C1	-2.27	105.39	113.69
6	A	1515	78M	O2-C1-O1	-2.12	118.33	123.63
7	A	1514	78N	O16-C8-O15	-2.11	118.34	123.63
3	A	1491	FLC	CB-CA-CAC	2.07	119.59	113.92
8	A	1517	PE5	O2-C3-C4	2.02	119.57	110.35
7	A	1513	78N	O16-C8-O15	-2.01	118.61	123.63

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1492	LDA	C2-C1-N1-O1
4	A	1492	LDA	C2-C1-N1-CM2
4	A	1493	LDA	C2-C1-N1-O1
4	A	1493	LDA	C2-C1-N1-CM2
4	A	1494	LDA	C2-C1-N1-CM1
4	A	1495	LDA	C2-C1-N1-O1
4	A	1495	LDA	C2-C1-N1-CM2
4	A	1496	LDA	C2-C1-N1-O1
4	A	1496	LDA	C2-C1-N1-CM1
4	A	1497	LDA	C2-C1-N1-O1
4	A	1497	LDA	C2-C1-N1-CM2

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Mol	Chain	Res	Type	Atoms
6	A	1510	78M	O2-C17-C18-C20
6	A	1515	78M	O1-C1-O2-C17
6	A	1515	78M	C2-C1-O2-C17
7	A	1513	78N	C17-C18-C19-O22
7	A	1514	78N	O15-C8-O16-C17
7	A	1514	78N	C7-C8-O16-C17
6	A	1512	78M	O1-C1-O2-C17
6	A	1512	78M	C2-C1-O2-C17
7	A	1513	78N	C7-C8-O16-C17
7	A	1513	78N	O15-C8-O16-C17
6	A	1510	78M	O2-C17-C18-O19
6	A	1512	78M	O2-C17-C18-O19
8	A	1516	PE5	O1-C1-C2-O2
7	A	1511	78N	C7-C8-O16-C17
8	A	1516	PE5	C10-C9-O5-C8
4	A	1493	LDA	C3-C4-C5-C6
8	A	1517	PE5	O1-C1-C2-O2
7	A	1511	78N	O15-C8-O16-C17
7	A	1511	78N	C17-C18-C19-O22
7	A	1514	78N	C17-C18-C19-O22
7	A	1514	78N	O20-C18-C19-O22
7	A	1514	78N	C10-C11-C12-C13
4	A	1504	LDA	C2-C3-C4-C5
4	A	1496	LDA	C5-C6-C7-C8
4	A	1499	LDA	C5-C6-C7-C8
4	A	1494	LDA	C4-C5-C6-C7
7	A	1514	78N	C11-C12-C13-C14
4	A	1504	LDA	C4-C5-C6-C7
4	A	1505	LDA	C2-C3-C4-C5
6	A	1512	78M	C3-C4-C5-C6
4	A	1495	LDA	C2-C3-C4-C5
4	A	1503	LDA	C3-C4-C5-C6
4	A	1506	LDA	C5-C6-C7-C8
7	A	1511	78N	O20-C18-C19-O22
4	A	1492	LDA	C7-C8-C9-C10
6	A	1512	78M	C2-C3-C4-C5
6	A	1515	78M	C11-C12-C13-C14
4	A	1506	LDA	C2-C3-C4-C5
4	A	1495	LDA	C1-C2-C3-C4
4	A	1501	LDA	C1-C2-C3-C4
4	A	1493	LDA	N1-C1-C2-C3
4	A	1494	LDA	N1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	1493	LDA	C6-C7-C8-C9
4	A	1493	LDA	C5-C6-C7-C8
4	A	1504	LDA	C3-C4-C5-C6
4	A	1492	LDA	C6-C7-C8-C9
7	A	1513	78N	O20-C18-C19-O22
4	A	1506	LDA	C3-C4-C5-C6
4	A	1493	LDA	C11-C10-C9-C8
4	A	1497	LDA	C1-C2-C3-C4
4	A	1492	LDA	C1-C2-C3-C4
7	A	1511	78N	C10-C11-C12-C13
4	A	1496	LDA	C6-C7-C8-C9
4	A	1506	LDA	C4-C5-C6-C7
4	A	1499	LDA	C2-C3-C4-C5
6	A	1515	78M	C9-C10-C11-C12
4	A	1496	LDA	C4-C5-C6-C7
4	A	1498	LDA	C5-C6-C7-C8
4	A	1494	LDA	C3-C4-C5-C6
6	A	1515	78M	C12-C13-C14-C15
4	A	1498	LDA	C1-C2-C3-C4
4	A	1492	LDA	C2-C1-N1-CM1
4	A	1493	LDA	C2-C1-N1-CM1
4	A	1494	LDA	C2-C1-N1-CM2
4	A	1495	LDA	C2-C1-N1-CM1
4	A	1496	LDA	C2-C1-N1-CM2
4	A	1497	LDA	C2-C1-N1-CM1
8	A	1516	PE5	O4-C7-C8-O5
7	A	1513	78N	O16-C17-C18-O20
8	A	1516	PE5	C1-C2-O2-C3
4	A	1494	LDA	C11-C10-C9-C8
4	A	1501	LDA	C4-C5-C6-C7
4	A	1497	LDA	C4-C5-C6-C7
4	A	1497	LDA	C5-C6-C7-C8
7	A	1513	78N	C2-C1-C9-C10
6	A	1515	78M	C11-C10-C9-C8
4	A	1500	LDA	C2-C3-C4-C5
4	A	1494	LDA	C2-C3-C4-C5
4	A	1493	LDA	C2-C3-C4-C5
6	A	1515	78M	C5-C6-C7-C8
7	A	1511	78N	C12-C13-C14-C15
7	A	1511	78N	C4-C5-C6-C7
6	A	1512	78M	C9-C10-C11-C12
4	A	1500	LDA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
6	A	1512	78M	O19-C18-C20-O21
4	A	1493	LDA	C7-C8-C9-C10
4	A	1497	LDA	C3-C4-C5-C6
6	A	1512	78M	O2-C17-C18-C20
6	A	1512	78M	C5-C6-C7-C8
7	A	1511	78N	C1-C2-C3-C4
7	A	1514	78N	C2-C1-C9-C10
6	A	1510	78M	O2-C1-C2-C3
8	A	1516	PE5	C4-C3-O2-C2
7	A	1514	78N	C1-C2-C3-C4
8	A	1517	PE5	C3-C4-O3-C5
4	A	1493	LDA	C9-C10-C11-C12
4	A	1494	LDA	C7-C8-C9-C10
4	A	1506	LDA	C7-C8-C9-C10
4	A	1494	LDA	C2-C1-N1-O1
6	A	1510	78M	C7-C8-C9-C10
6	A	1515	78M	O2-C1-C2-C3
8	A	1517	PE5	O2-C3-C4-O3
4	A	1504	LDA	C5-C6-C7-C8

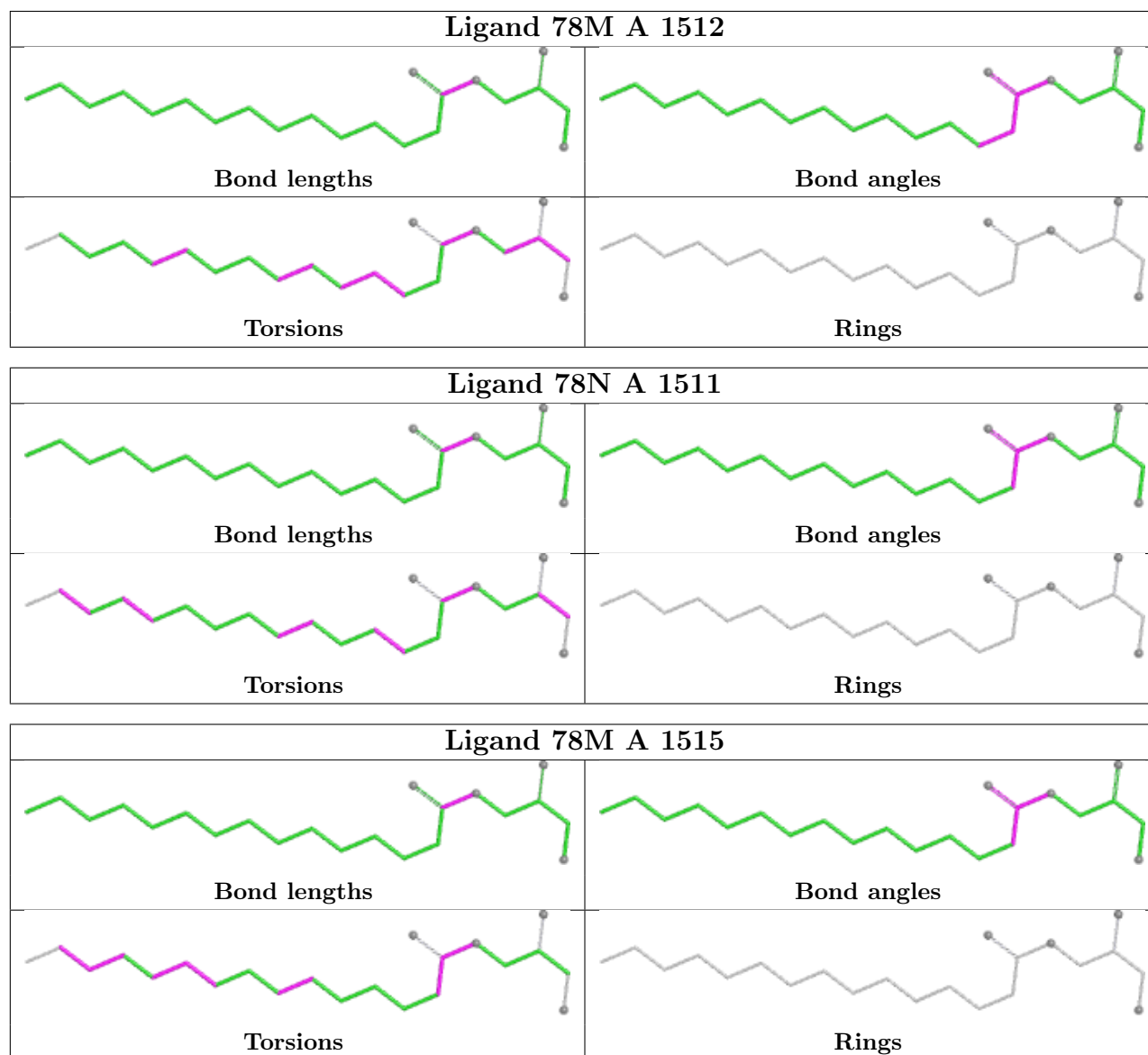
There are no ring outliers.

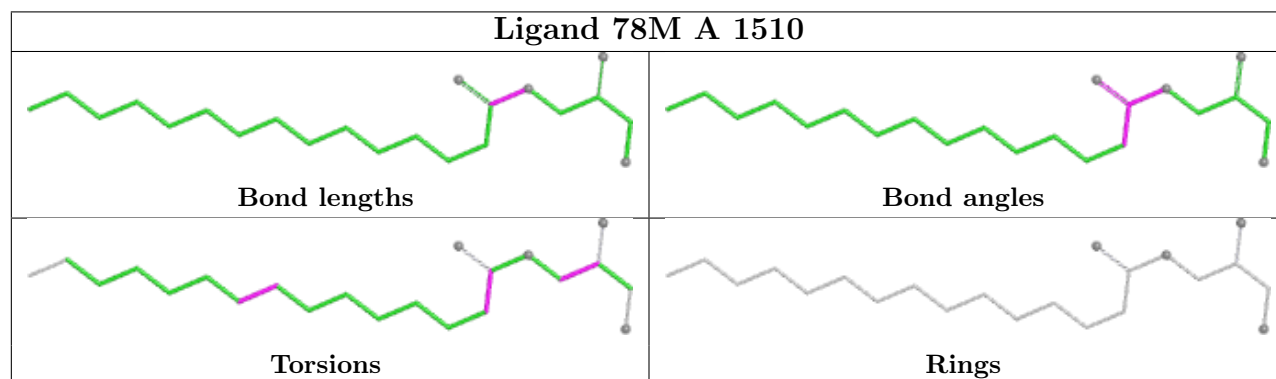
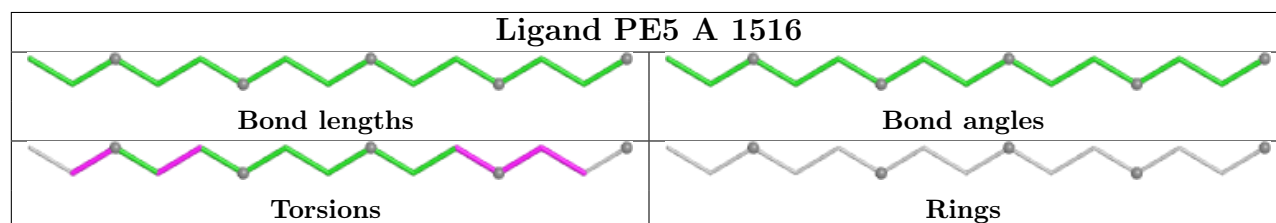
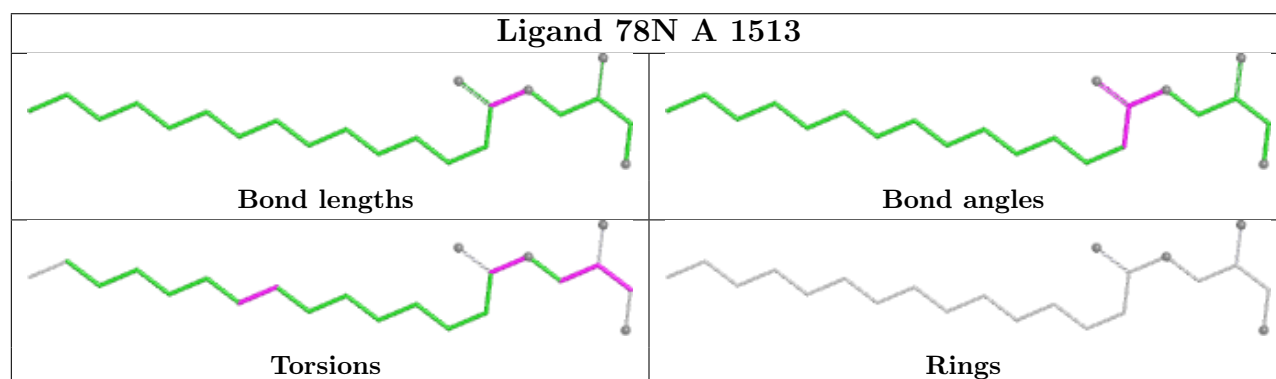
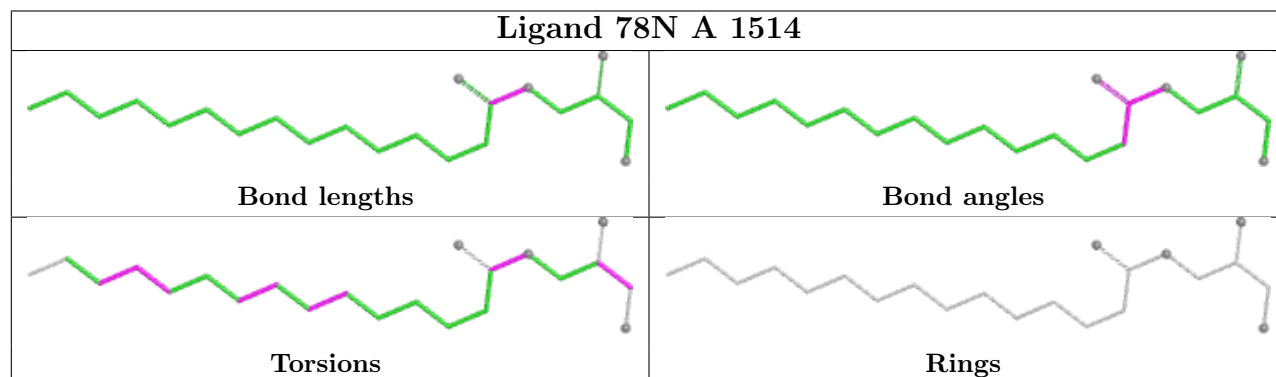
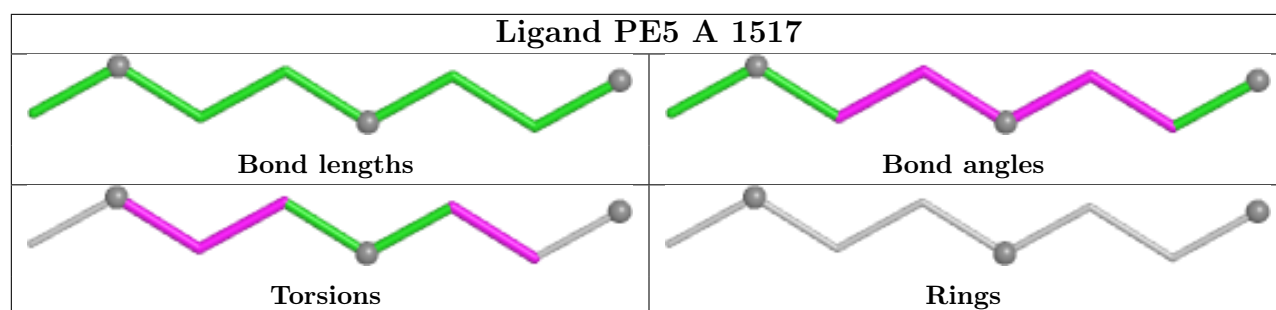
14 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1498	LDA	1	0
4	A	1494	LDA	10	0
7	A	1511	78N	1	0
6	A	1515	78M	12	0
4	A	1496	LDA	2	0
8	A	1517	PE5	4	0
4	A	1499	LDA	1	0
7	A	1514	78N	1	0
4	A	1500	LDA	1	0
4	A	1493	LDA	3	0
4	A	1506	LDA	2	0
4	A	1503	LDA	3	0
4	A	1492	LDA	1	0
4	A	1497	LDA	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	430/458 (93%)	-0.35	12 (2%) 55 59	5, 17, 44, 99	9 (2%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	63	GLY	4.3
1	A	458[A]	ILE	3.6
1	A	38	ALA	3.0
1	A	293	VAL	2.9
1	A	39	PRO	2.8
1	A	322	GLU	2.7
1	A	62	PRO	2.6
1	A	117	ASP	2.6
1	A	294	ASP	2.5
1	A	64	GLY	2.4
1	A	296	ARG	2.3
1	A	37[A]	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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,

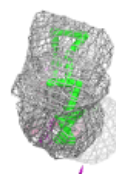
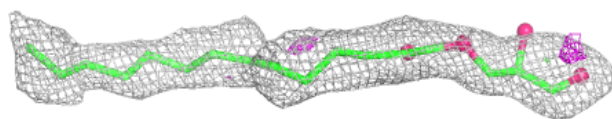
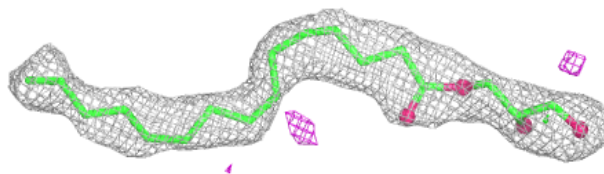
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	LDA	A	1499	10/16	0.74	0.17	49,51,53,54	0
4	LDA	A	1501	8/16	0.75	0.14	39,45,53,54	0
4	LDA	A	1502	7/16	0.75	0.14	43,44,47,48	0
4	LDA	A	1494	16/16	0.76	0.15	40,49,61,62	0
4	LDA	A	1505	8/16	0.77	0.15	42,46,47,49	0
4	LDA	A	1498	9/16	0.78	0.14	34,41,46,47	0
4	LDA	A	1497	13/16	0.79	0.13	37,46,59,59	0
4	LDA	A	1493	16/16	0.79	0.16	34,49,70,71	0
6	78M	A	1512	22/22	0.79	0.14	44,49,58,61	0
4	LDA	A	1500	12/16	0.80	0.13	32,47,59,59	0
7	78N	A	1513	22/22	0.80	0.14	41,52,60,65	0
7	78N	A	1514	22/22	0.81	0.13	36,46,53,56	0
4	LDA	A	1503	9/16	0.82	0.12	44,46,54,56	0
7	78N	A	1511	22/22	0.82	0.13	39,44,60,63	0
6	78M	A	1515	22/22	0.83	0.13	38,47,53,55	0
4	LDA	A	1495	11/16	0.83	0.13	35,46,63,63	0
4	LDA	A	1506	11/16	0.85	0.12	28,34,36,37	0
4	LDA	A	1504	9/16	0.85	0.12	36,39,41,41	0
4	LDA	A	1492	16/16	0.85	0.15	21,35,62,65	0
3	FLC	A	1491	13/13	0.87	0.10	22,34,55,55	0
4	LDA	A	1496	16/16	0.89	0.12	21,45,52,57	0
8	PE5	A	1517	8/27	0.90	0.11	0,25,32,35	0
2	CA	A	1509	1/1	0.93	0.18	62,62,62,62	0
8	PE5	A	1516	15/27	0.93	0.08	20,27,43,47	0
6	78M	A	1510	22/22	0.93	0.08	18,25,32,39	0
5	NA	A	1508	1/1	0.94	0.14	32,32,32,32	0
5	NA	A	1507	1/1	0.98	0.04	21,21,21,21	0

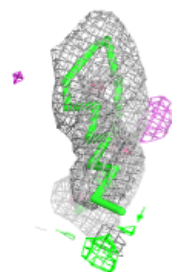
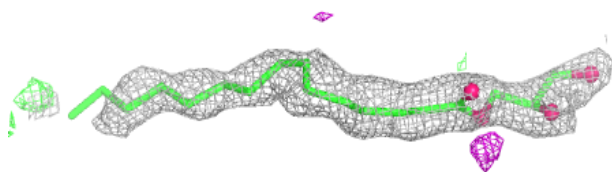
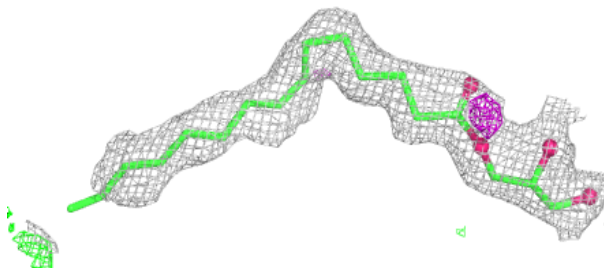
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 78M A 1512:

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

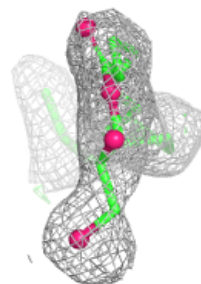
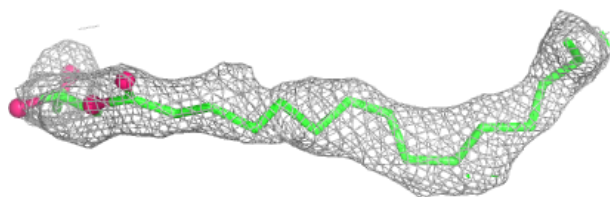
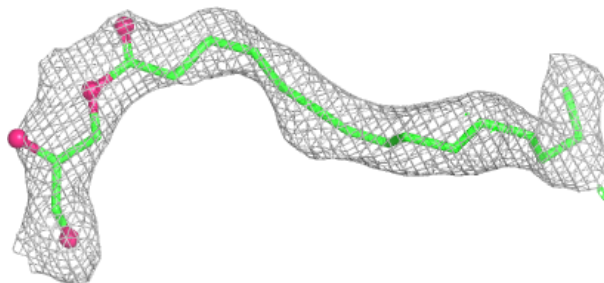
**Electron density around 78N A 1513:**

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

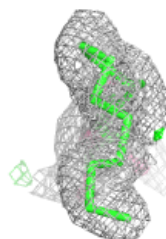
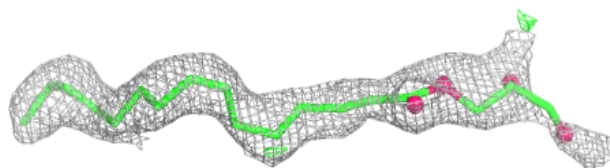
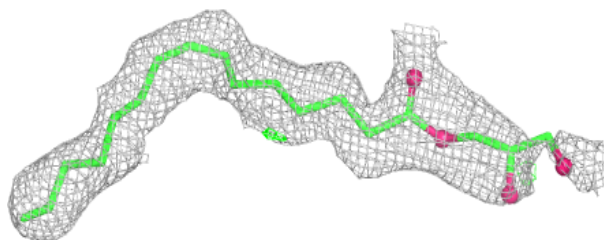


Electron density around 78N A 1514:

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

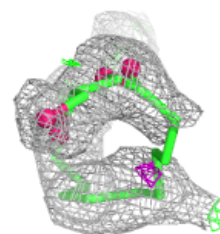
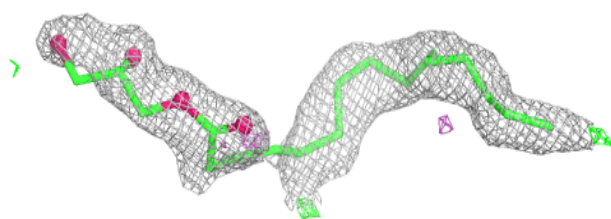
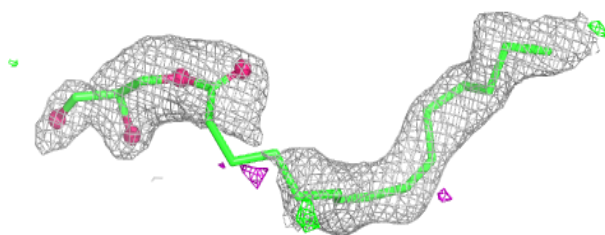
**Electron density around 78N A 1511:**

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

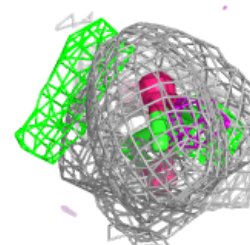
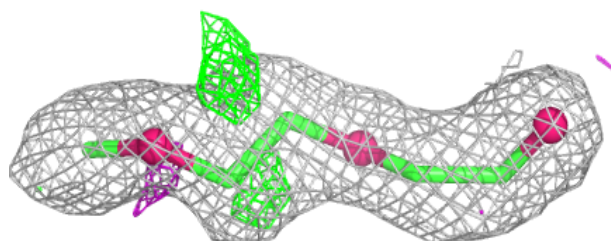
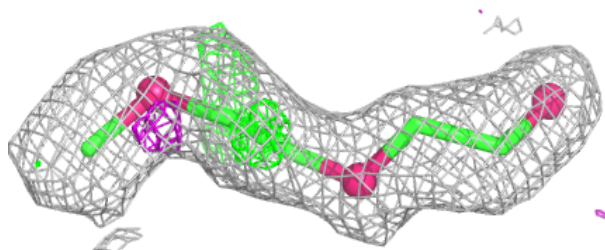


Electron density around 78M A 1515:

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

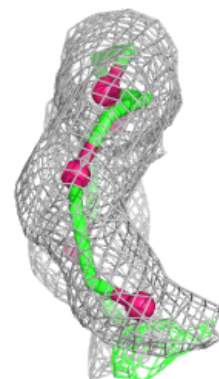
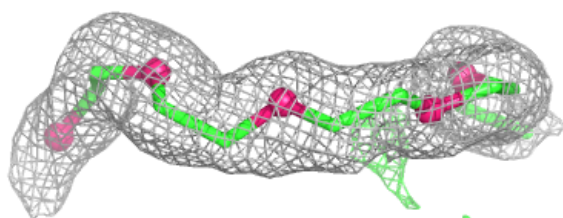
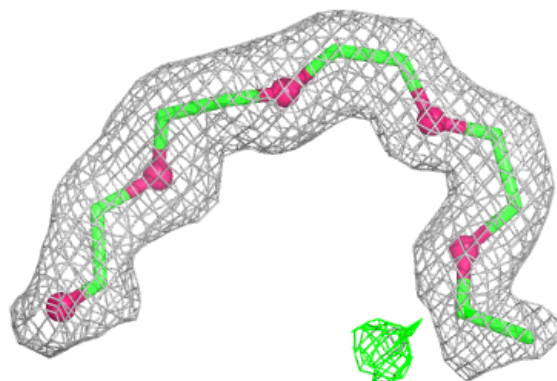
**Electron density around PE5 A 1517:**

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

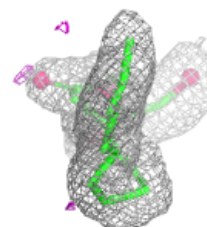
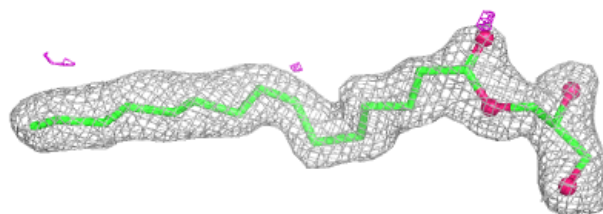
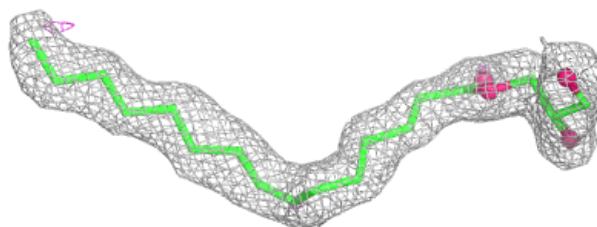


Electron density around PE5 A 1516:

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

**Electron density around 78M A 1510:**

$2mF_o-DF_c$ (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.