



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 02:17 PM BST

PDB ID : 5D5D
Title : In meso in situ serial X-ray crystallography structure of AlgE at 100 K
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Deposited on : 2015-08-10
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
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) : 2.13

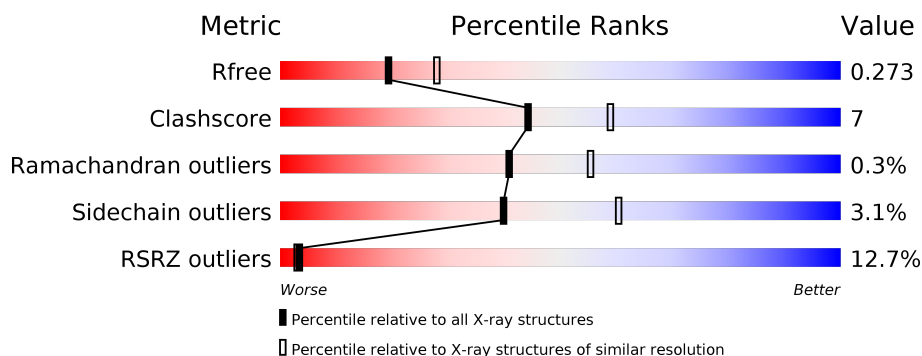
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	490	

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
6	78M	A	516	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3478 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	403	Total	C	N	O	S	0	1	0
			3222	2021	581	617	3			

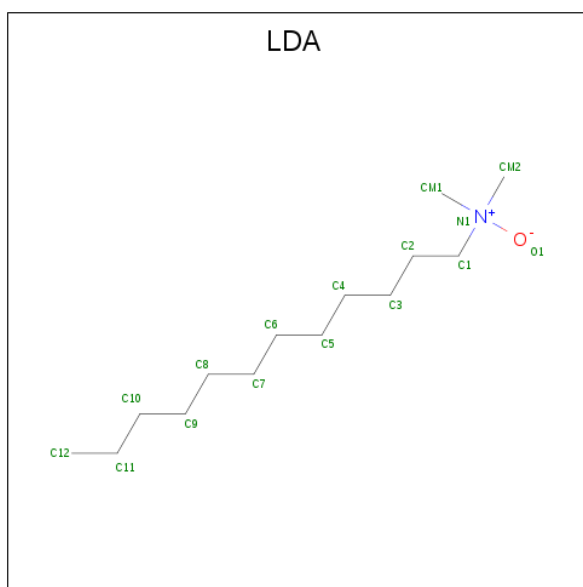
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

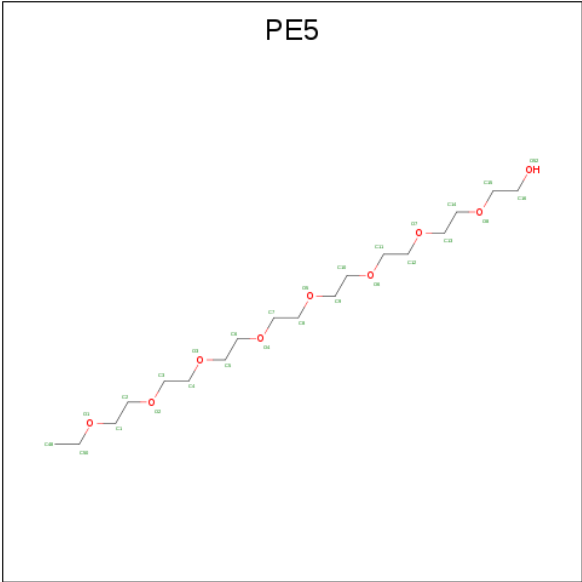
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).



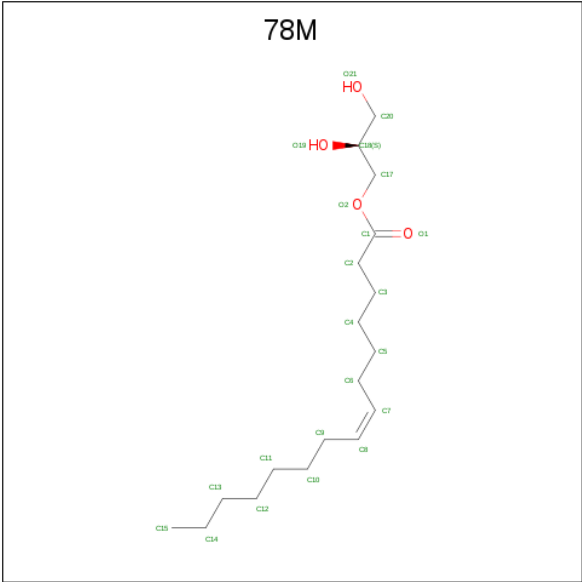
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			13	11	1	1		

- Molecule 5 is 3,6,9,12,15,18,21,24-OCTAOXAHEXACOSAN-1-OL (three-letter code: PE5) (formula: C₁₈H₃₈O₉).



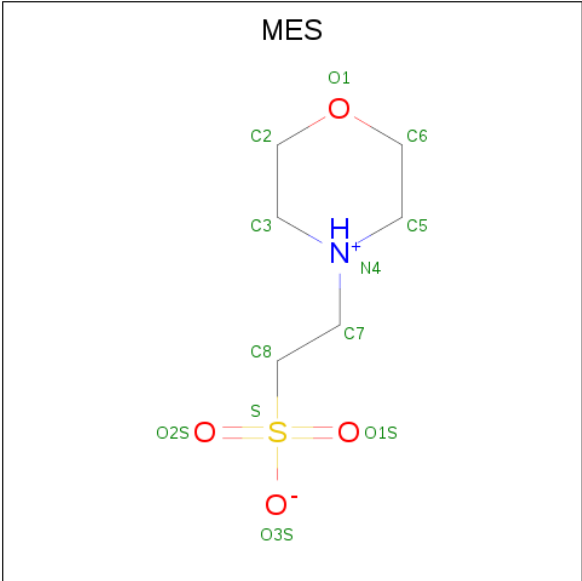
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	5	3		
5	A	1	Total	C	O	0	0
			12	8	4		
5	A	1	Total	C	O	0	0
			12	8	4		
5	A	1	Total	C	O	0	0
			9	6	3		
5	A	1	Total	C	O	0	0
			12	8	4		

- Molecule 6 is (2S)-2,3-DIHYDROXYPROPYL(7Z)-PENTADEC-7-ENOATE (three-letter code: 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		

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

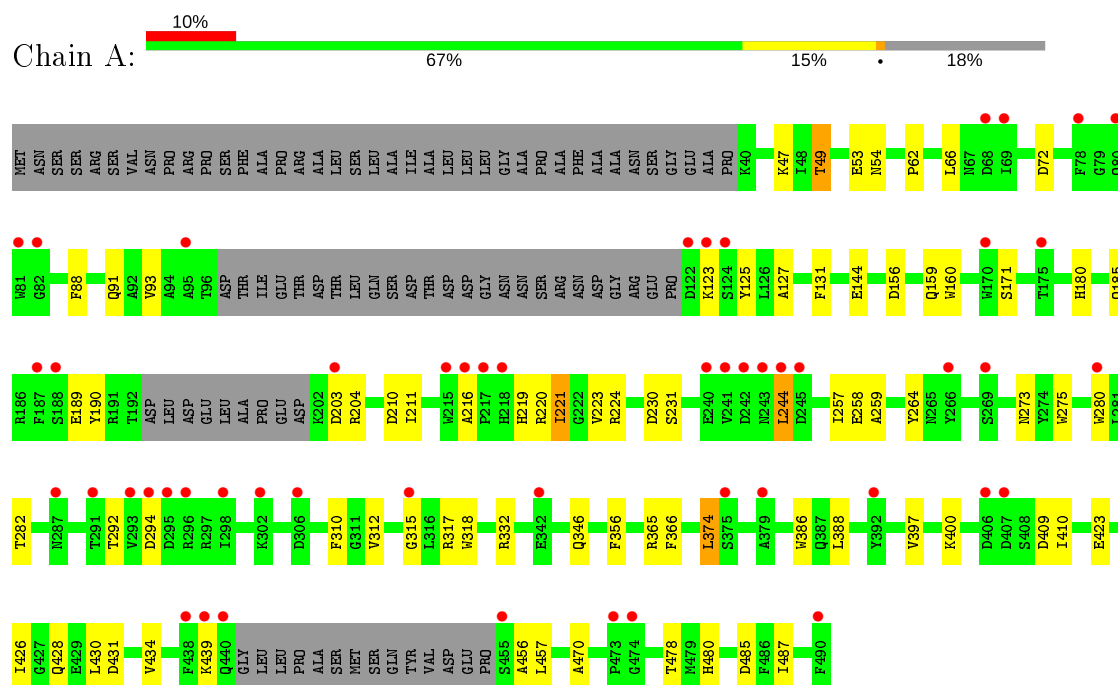
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	23	Total	O	0	0
			23	23		

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	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	46.33 Å 66.35 Å 176.84 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.22 – 2.40 24.53 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.8 (25.22-2.40) 92.8 (24.53-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.41 Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.219 , 0.260 0.228 , 0.273	Depositor DCC
R_{free} test set	999 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3478	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, NA, CA, MES, PE5, 78M

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.53	0/3308	0.79	0/4478

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

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	3222	0	3004	45	0
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	109	0	208	3	0
5	A	53	0	61	3	0
6	A	44	0	68	1	0
7	A	24	0	26	0	0
8	A	23	0	0	0	0
All	All	3478	0	3367	45	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 7.

All (45) 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:409:ASP:H	5:A:513:PE5:H72	1.49	0.77
1:A:457:LEU:HD11	1:A:487:ILE:HD12	1.70	0.73
1:A:47:LYS:HB3	1:A:72:ASP:HB3	1.84	0.60
1:A:88:PHE:HB2	4:A:508:LDA:H91	1.83	0.59
1:A:180:HIS:HB2	1:A:210:ASP:OD2	2.05	0.57
1:A:423:GLU:CB	1:A:470:ALA:HA	2.34	0.57
1:A:434:VAL:HG12	6:A:517:78M:H202	1.88	0.56
1:A:275:TRP:CE2	1:A:315:GLY:HA3	2.40	0.56
1:A:53:GLU:HB3	1:A:66:LEU:HB2	1.88	0.56
1:A:223:VAL:HG12	1:A:257:ILE:HG22	1.88	0.55
1:A:280:TRP:CZ3	1:A:310:PHE:HB2	2.41	0.55
1:A:423:GLU:HB2	1:A:470:ALA:HA	1.88	0.55
1:A:127:ALA:HA	1:A:190:TYR:O	2.11	0.51
1:A:275:TRP:CZ2	1:A:315:GLY:HA3	2.46	0.50
1:A:91:GLN:HG2	1:A:93:VAL:HG23	1.94	0.50
1:A:189:GLU:HG3	1:A:244:LEU:HD11	1.94	0.50
1:A:54:ASN:HB3	1:A:480:HIS:CE1	2.49	0.48
1:A:216:ALA:HB3	1:A:219:HIS:HB2	1.96	0.47
1:A:346:GLN:HA	5:A:511:PE5:H111	1.96	0.47
1:A:397:VAL:HB	1:A:431:ASP:HB2	1.97	0.47
1:A:410:ILE:HG21	1:A:426:ILE:HD11	1.97	0.46
1:A:430:LEU:HD23	4:A:509:LDA:HM21	1.96	0.46
1:A:318:TRP:CD1	4:A:505:LDA:H61	2.51	0.45
1:A:400:LYS:HG2	1:A:428:GLN:HG2	1.97	0.45
1:A:456:ALA:HA	1:A:487:ILE:O	2.16	0.45
1:A:160:TRP:CE2	1:A:224:ARG:HD2	2.52	0.45
1:A:159:GLN:HB3	5:A:511:PE5:H132	1.98	0.45
1:A:123:LYS:HE3	1:A:125:TYR:HE1	1.81	0.45
1:A:185:GLN:HG2	1:A:203:ASP:OD2	2.17	0.44
1:A:366:PHE:CZ	1:A:374:LEU:HD13	2.52	0.44
1:A:221:ILE:HD12	1:A:259:ALA:HB2	1.99	0.44
1:A:280:TRP:CD1	1:A:282:THR:HG23	2.53	0.44
1:A:386:TRP:CZ2	1:A:388:LEU:HB2	2.53	0.43
1:A:204:ARG:HG3	1:A:230:ASP:HB2	2.00	0.43
1:A:457:LEU:CD1	1:A:487:ILE:HD12	2.45	0.43
1:A:374:LEU:HD12	1:A:374:LEU:HA	1.90	0.42
1:A:49:THR:HG23	1:A:485:ASP:OD1	2.20	0.42
1:A:131:PHE:HZ	1:A:190:TYR:CZ	2.38	0.42
1:A:144:GLU:HA	1:A:171:SER:O	2.20	0.41
1:A:423:GLU:HB3	1:A:470:ALA:HA	2.01	0.41
1:A:273:ASN:HB2	1:A:317:ARG:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ASP:HB3	1:A:264:TYR:CD2	2.54	0.41
1:A:312:VAL:HG12	1:A:332:ARG:HB3	2.02	0.41
1:A:356:PHE:CE1	1:A:365:ARG:HA	2.55	0.41
1:A:62:PRO:HG2	1:A:294:ASP:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	396/490 (81%)	379 (96%)	16 (4%)	1 (0%)	41	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	LEU

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	324/394 (82%)	314 (97%)	10 (3%)	40	60

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	THR
1	A	211	ILE
1	A	220	ARG
1	A	221	ILE
1	A	231	SER
1	A	244	LEU
1	A	258	GLU
1	A	292	THR
1	A	439	LYS
1	A	478	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	159	GLN
1	A	243	ASN
1	A	378	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 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 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	504	-	12,15,15	2.41	1 (8%)	14,17,17	1.05	2 (14%)
4	LDA	A	505	-	12,15,15	2.50	1 (8%)	14,17,17	0.84	0
5	PE5	A	512	-	11,11,26	0.78	0	10,10,25	0.20	0
7	MES	A	519	-	12,12,12	0.67	0	14,16,16	0.37	0
7	MES	A	518	-	12,12,12	0.75	0	14,16,16	0.59	0
4	LDA	A	506	-	12,15,15	2.57	1 (8%)	14,17,17	0.83	1 (7%)
5	PE5	A	514	-	8,8,26	0.84	0	7,7,25	0.38	0
6	78M	A	516	-	21,21,21	0.79	1 (4%)	22,22,22	0.80	1 (4%)
4	LDA	A	508	-	12,15,15	2.50	1 (8%)	14,17,17	0.88	1 (7%)
4	LDA	A	510	-	9,12,15	2.96	1 (11%)	11,14,17	0.75	0
4	LDA	A	507	-	12,15,15	2.50	1 (8%)	14,17,17	0.88	2 (14%)
4	LDA	A	509	-	12,15,15	2.56	1 (8%)	14,17,17	0.72	0
5	PE5	A	515	-	11,11,26	0.85	0	10,10,25	0.51	0
6	78M	A	517	-	21,21,21	0.80	1 (4%)	22,22,22	0.83	1 (4%)
5	PE5	A	511	-	7,7,26	0.47	0	6,6,25	0.26	0
5	PE5	A	513	-	11,11,26	0.96	0	10,10,25	0.32	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	504	-	-	4/13/13/13	-
4	LDA	A	505	-	-	6/13/13/13	-
5	PE5	A	512	-	-	5/9/9/24	-
7	MES	A	519	-	-	5/6/14/14	0/1/1/1
7	MES	A	518	-	-	3/6/14/14	0/1/1/1
4	LDA	A	506	-	-	7/13/13/13	-
5	PE5	A	514	-	-	4/6/6/24	-
6	78M	A	516	-	-	14/21/21/21	-
4	LDA	A	508	-	-	10/13/13/13	-
4	LDA	A	510	-	-	5/10/10/13	-
4	LDA	A	507	-	-	9/13/13/13	-
4	LDA	A	509	-	-	7/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PE5	A	515	-	-	7/9/9/24	-
6	78M	A	517	-	-	6/21/21/21	-
5	PE5	A	511	-	-	2/5/5/24	-
5	PE5	A	513	-	-	6/9/9/24	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	510	LDA	O1-N1	-8.66	1.21	1.42
4	A	506	LDA	O1-N1	-8.57	1.22	1.42
4	A	509	LDA	O1-N1	-8.56	1.22	1.42
4	A	505	LDA	O1-N1	-8.41	1.22	1.42
4	A	507	LDA	O1-N1	-8.35	1.22	1.42
4	A	508	LDA	O1-N1	-8.28	1.22	1.42
4	A	504	LDA	O1-N1	-7.99	1.23	1.42
6	A	517	78M	O2-C1	3.02	1.42	1.33
6	A	516	78M	O2-C1	2.98	1.42	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	504	LDA	CM1-N1-C1	-2.59	104.79	110.23
6	A	517	78M	O2-C1-C2	2.54	119.89	111.91
4	A	504	LDA	O1-N1-C1	2.34	115.01	109.27
4	A	506	LDA	CM1-N1-C1	-2.30	105.40	110.23
4	A	508	LDA	O1-N1-C1	2.15	114.54	109.27
4	A	507	LDA	O1-N1-C1	2.13	114.50	109.27
4	A	507	LDA	CM1-N1-C1	-2.07	105.89	110.23
6	A	516	78M	O2-C1-C2	2.02	118.24	111.91

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	505	LDA	N1-C1-C2-C3
7	A	518	MES	C7-C8-S-O2S
4	A	506	LDA	N1-C1-C2-C3
7	A	519	MES	C8-C7-N4-C5
7	A	519	MES	C7-C8-S-O2S
7	A	519	MES	C7-C8-S-O3S

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Mol	Chain	Res	Type	Atoms
4	A	508	LDA	C2-C1-N1-CM1
4	A	508	LDA	C2-C1-N1-CM2
4	A	507	LDA	C2-C1-N1-CM1
4	A	509	LDA	C2-C1-N1-CM1
4	A	509	LDA	C2-C1-N1-CM2
4	A	509	LDA	N1-C1-C2-C3
6	A	517	78M	O1-C1-O2-C17
6	A	517	78M	C2-C1-O2-C17
5	A	512	PE5	O2-C3-C4-O3
5	A	513	PE5	O3-C5-C6-O4
6	A	516	78M	O19-C18-C20-O21
6	A	516	78M	C1-C2-C3-C4
5	A	513	PE5	O6-C10-C9-O5
5	A	514	PE5	O2-C3-C4-O3
5	A	513	PE5	O4-C7-C8-O5
6	A	517	78M	C11-C12-C13-C14
4	A	506	LDA	C6-C7-C8-C9
4	A	507	LDA	C6-C7-C8-C9
4	A	506	LDA	C2-C3-C4-C5
4	A	504	LDA	C4-C5-C6-C7
4	A	508	LDA	C2-C3-C4-C5
4	A	510	LDA	C4-C5-C6-C7
6	A	516	78M	C17-C18-C20-O21
6	A	516	78M	C4-C5-C6-C7
4	A	509	LDA	C4-C5-C6-C7
4	A	505	LDA	C7-C8-C9-C10
4	A	508	LDA	C7-C8-C9-C10
4	A	505	LDA	C2-C3-C4-C5
6	A	516	78M	C9-C10-C11-C12
6	A	517	78M	C9-C10-C11-C12
6	A	516	78M	C11-C12-C13-C14
4	A	506	LDA	C7-C8-C9-C10
4	A	506	LDA	C3-C4-C5-C6
4	A	507	LDA	C1-C2-C3-C4
4	A	508	LDA	C11-C10-C9-C8
4	A	504	LDA	C7-C8-C9-C10
6	A	517	78M	C11-C10-C9-C8
4	A	505	LDA	C5-C6-C7-C8
6	A	516	78M	C10-C11-C12-C13
4	A	509	LDA	C6-C7-C8-C9
4	A	504	LDA	C2-C3-C4-C5
4	A	508	LDA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
4	A	507	LDA	C4-C5-C6-C7
4	A	506	LDA	C4-C5-C6-C7
4	A	507	LDA	C3-C4-C5-C6
5	A	514	PE5	C8-C7-O4-C6
4	A	508	LDA	C5-C6-C7-C8
4	A	507	LDA	N1-C1-C2-C3
4	A	506	LDA	C9-C10-C11-C12
4	A	507	LDA	C9-C10-C11-C12
7	A	519	MES	C8-C7-N4-C3
5	A	515	PE5	O4-C7-C8-O5
5	A	515	PE5	C10-C9-O5-C8
6	A	517	78M	C12-C13-C14-C15
7	A	518	MES	C7-C8-S-O3S
6	A	516	78M	C12-C13-C14-C15
5	A	515	PE5	C6-C5-O3-C4
5	A	512	PE5	C2-C1-O1-C50
5	A	514	PE5	C3-C4-O3-C5
4	A	507	LDA	C2-C1-N1-CM2
4	A	510	LDA	C2-C1-N1-CM1
4	A	510	LDA	C2-C1-N1-CM2
4	A	508	LDA	C4-C5-C6-C7
5	A	515	PE5	O2-C3-C4-O3
5	A	515	PE5	O3-C5-C6-O4
7	A	518	MES	C7-C8-S-O1S
7	A	519	MES	C7-C8-S-O1S
4	A	507	LDA	C2-C1-N1-O1
4	A	509	LDA	C2-C1-N1-O1
4	A	510	LDA	C2-C1-N1-O1
5	A	511	PE5	C11-C12-O7-C13
5	A	515	PE5	C7-C8-O5-C9
5	A	511	PE5	C14-C13-O7-C12
4	A	505	LDA	C11-C10-C9-C8
6	A	516	78M	O2-C17-C18-C20
6	A	516	78M	C3-C4-C5-C6
5	A	512	PE5	C6-C5-O3-C4
5	A	513	PE5	C7-C8-O5-C9
4	A	509	LDA	C1-C2-C3-C4
4	A	508	LDA	C3-C4-C5-C6
5	A	513	PE5	C5-C6-O4-C7
5	A	515	PE5	C3-C4-O3-C5
5	A	512	PE5	O3-C5-C6-O4
5	A	512	PE5	C4-C3-O2-C2

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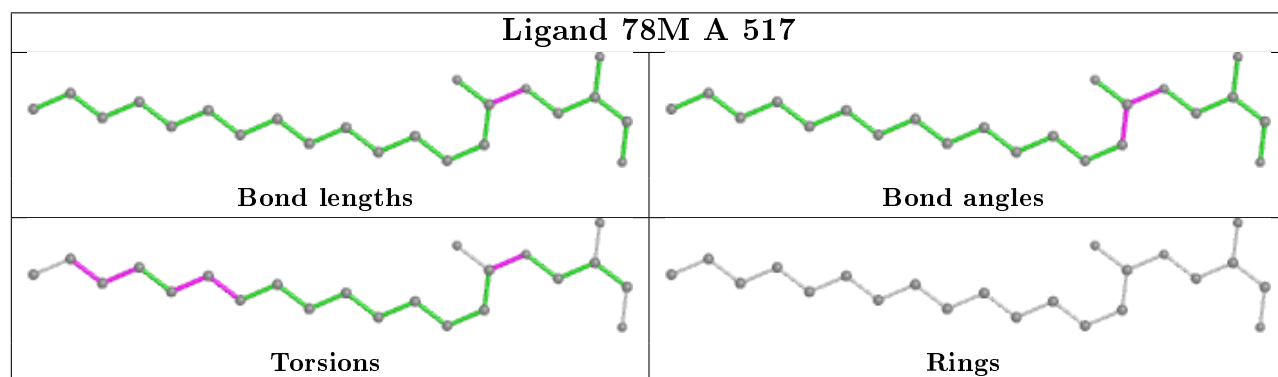
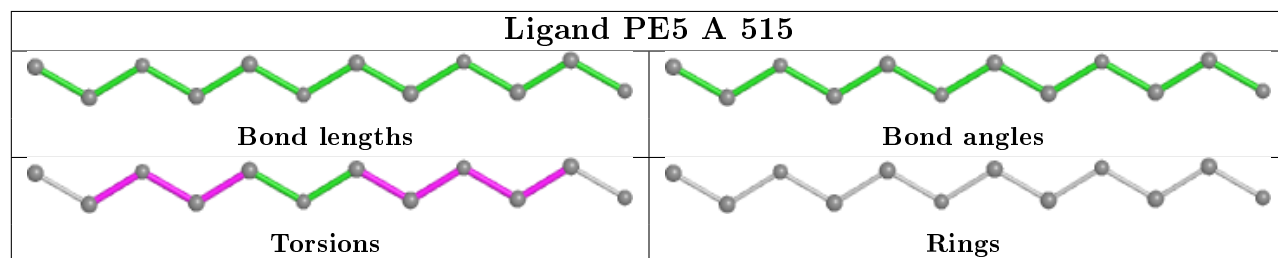
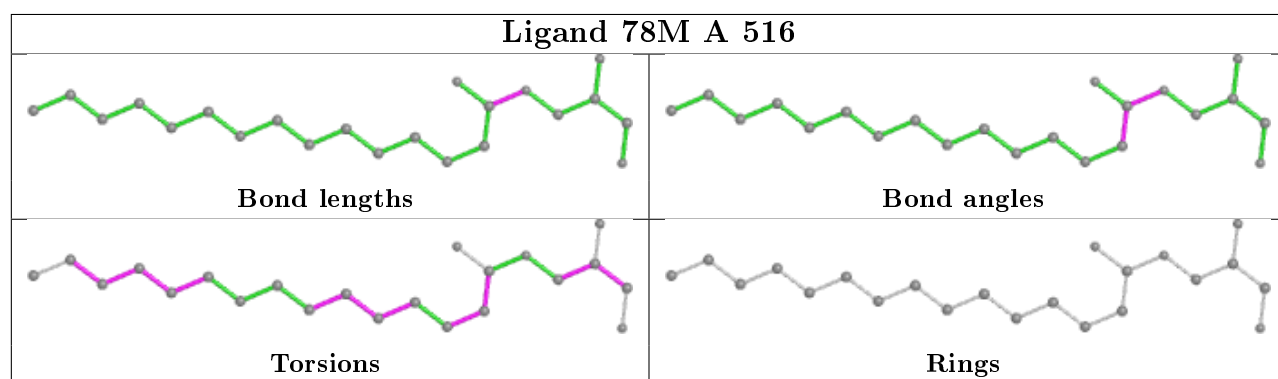
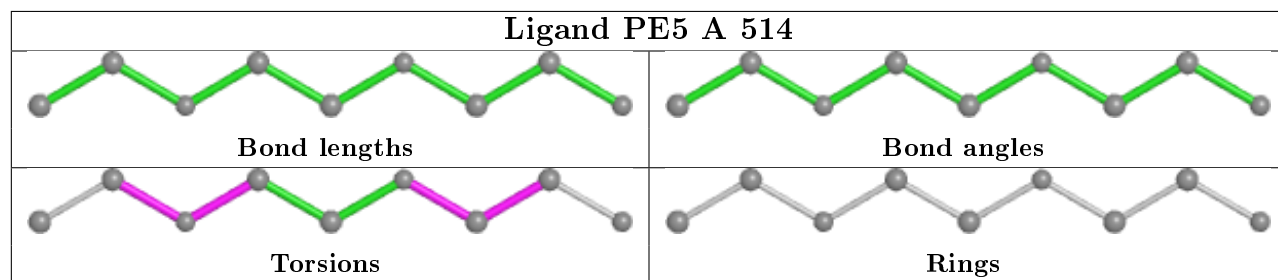
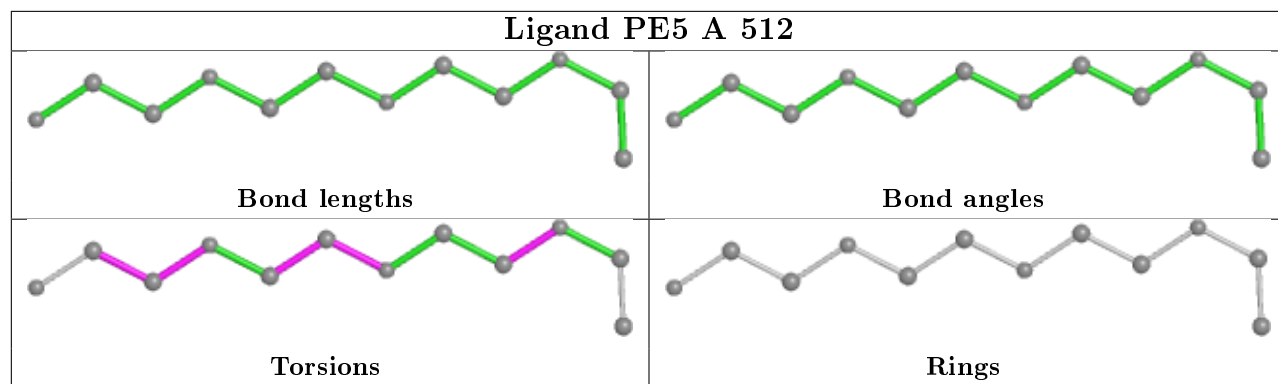
Mol	Chain	Res	Type	Atoms
4	A	504	LDA	C1-C2-C3-C4
6	A	516	78M	C5-C6-C7-C8
6	A	516	78M	O2-C1-C2-C3
4	A	510	LDA	C6-C7-C8-C9
6	A	516	78M	O2-C17-C18-O19
5	A	513	PE5	C9-C10-O6-C11
6	A	516	78M	O1-C1-C2-C3
4	A	508	LDA	C2-C1-N1-O1
4	A	505	LDA	C4-C5-C6-C7
5	A	514	PE5	C5-C6-O4-C7

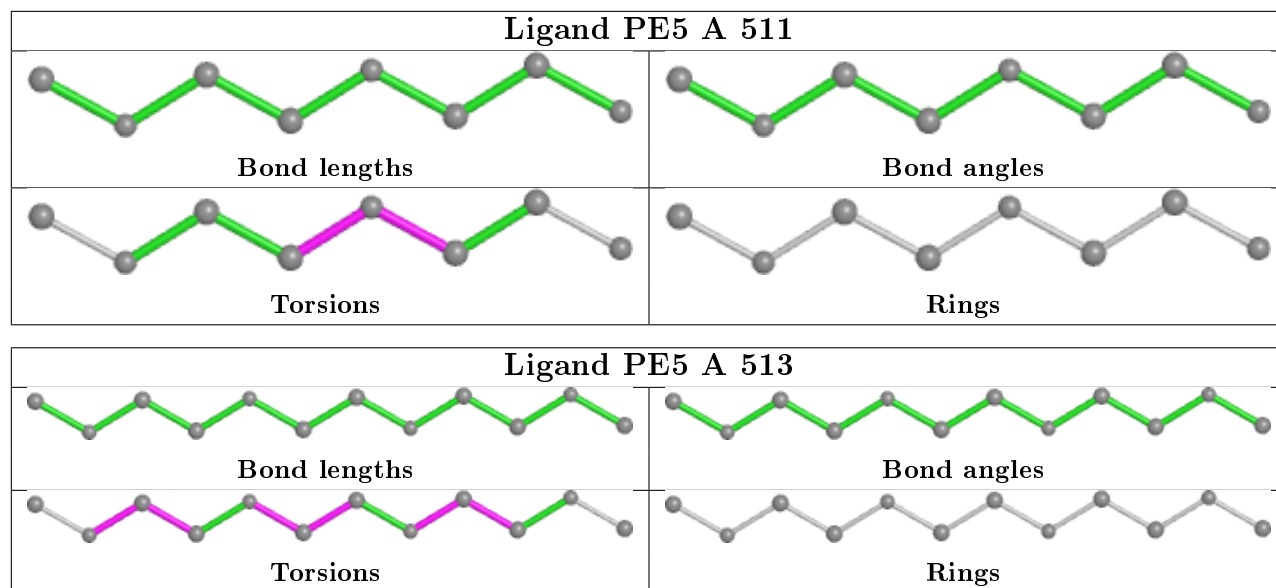
There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	505	LDA	1	0
4	A	508	LDA	1	0
4	A	509	LDA	1	0
6	A	517	78M	1	0
5	A	511	PE5	2	0
5	A	513	PE5	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	403/490 (82%)	0.61	51 (12%) 3 3	29, 46, 72, 96	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	293	VAL	7.2
1	A	81	TRP	6.2
1	A	244	LEU	5.8
1	A	122	ASP	5.8
1	A	294	ASP	4.9
1	A	295	ASP	4.9
1	A	407	ASP	4.8
1	A	124	SER	4.6
1	A	216	ALA	4.4
1	A	218	HIS	4.4
1	A	69	ILE	4.3
1	A	242	ASP	4.1
1	A	269	SER	4.0
1	A	392	TYR	3.8
1	A	215	TRP	3.7
1	A	296	ARG	3.6
1	A	473	PRO	3.5
1	A	266	TYR	3.5
1	A	280	TRP	3.4
1	A	440	GLN	3.3
1	A	406	ASP	3.3
1	A	123	LYS	3.3
1	A	80	GLN	3.2
1	A	78	PHE	3.1
1	A	302	LYS	3.0
1	A	439	LYS	2.9
1	A	240	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	243	ASN	2.8
1	A	298	ILE	2.8
1	A	379	ALA	2.8
1	A	474	GLY	2.8
1	A	188	SER	2.7
1	A	287	ASN	2.7
1	A	241	VAL	2.6
1	A	490	PHE	2.6
1	A	455	SER	2.5
1	A	315	GLY	2.5
1	A	95	ALA	2.4
1	A	217	PRO	2.4
1	A	203	ASP	2.4
1	A	306	ASP	2.3
1	A	245	ASP	2.3
1	A	82	GLY	2.3
1	A	68	ASP	2.2
1	A	438	PHE	2.2
1	A	375	SER	2.1
1	A	175	THR	2.1
1	A	170	TRP	2.1
1	A	342	GLU	2.1
1	A	187	PHE	2.0
1	A	291	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

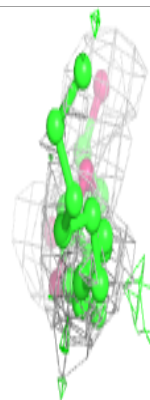
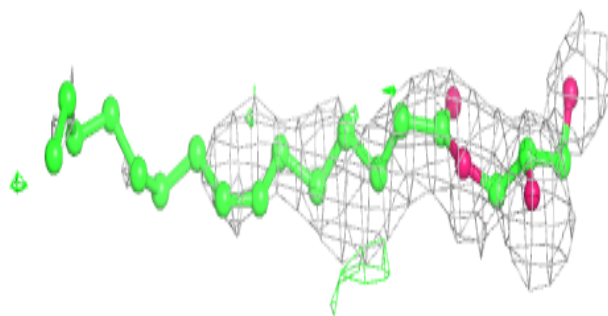
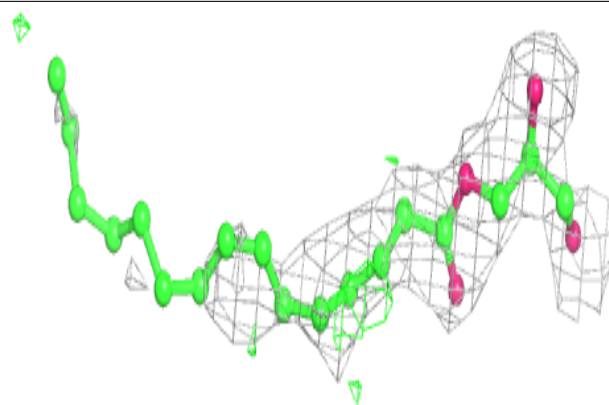
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	LDA	A	507	16/16	0.52	0.36	65,74,92,93	0
4	LDA	A	505	16/16	0.62	0.31	52,58,91,91	0
6	78M	A	516	22/22	0.63	0.42	87,93,95,95	0
4	LDA	A	508	16/16	0.67	0.32	56,72,85,87	0
4	LDA	A	509	16/16	0.70	0.29	57,67,71,71	0
5	PE5	A	513	12/27	0.75	0.30	55,60,75,77	0
5	PE5	A	515	12/27	0.76	0.29	57,69,71,72	0
4	LDA	A	506	16/16	0.80	0.23	60,75,84,84	0
5	PE5	A	514	9/27	0.81	0.64	64,66,68,68	0
5	PE5	A	512	12/27	0.81	0.23	59,64,67,68	0
4	LDA	A	510	13/16	0.82	0.21	58,66,71,72	0
4	LDA	A	504	16/16	0.84	0.29	44,52,64,65	0
6	78M	A	517	22/22	0.87	0.16	57,72,74,75	0
7	MES	A	519	12/12	0.90	0.16	61,65,66,68	0
2	NA	A	502	1/1	0.90	0.21	67,67,67,67	0
3	CA	A	503	1/1	0.92	0.21	48,48,48,48	0
7	MES	A	518	12/12	0.95	0.18	50,54,57,58	0
2	NA	A	501	1/1	0.95	0.10	25,25,25,25	0
5	PE5	A	511	8/27	0.96	0.29	38,40,54,55	0

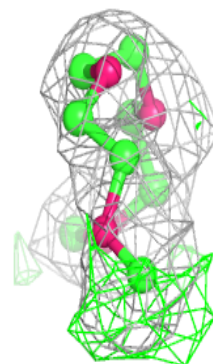
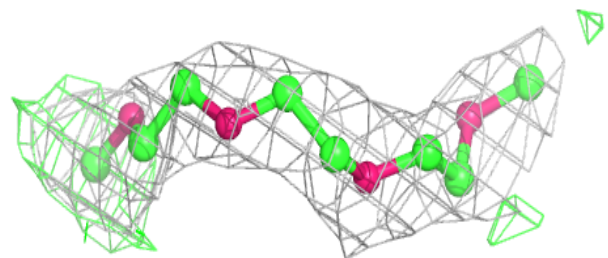
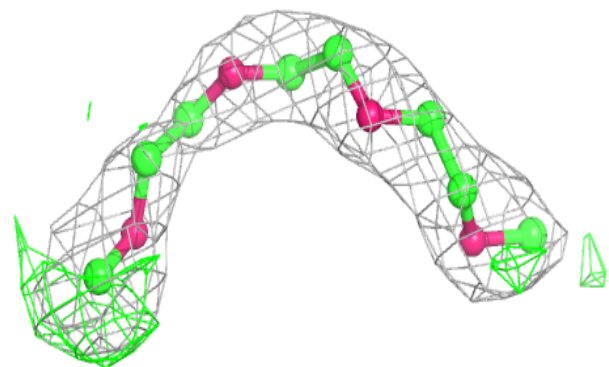
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 78M A 516:

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

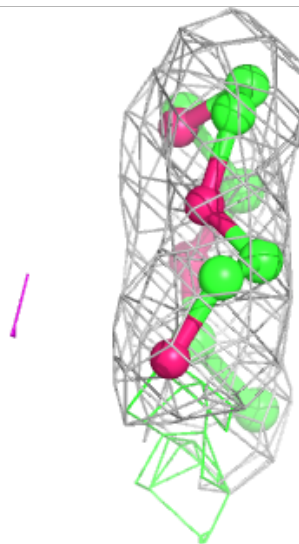
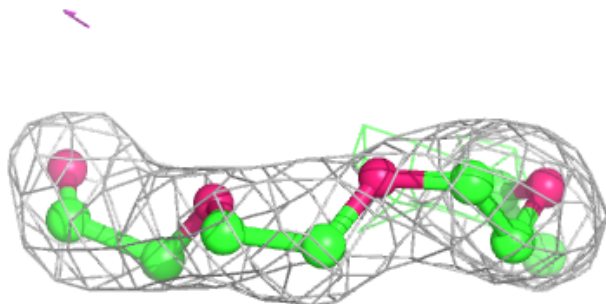
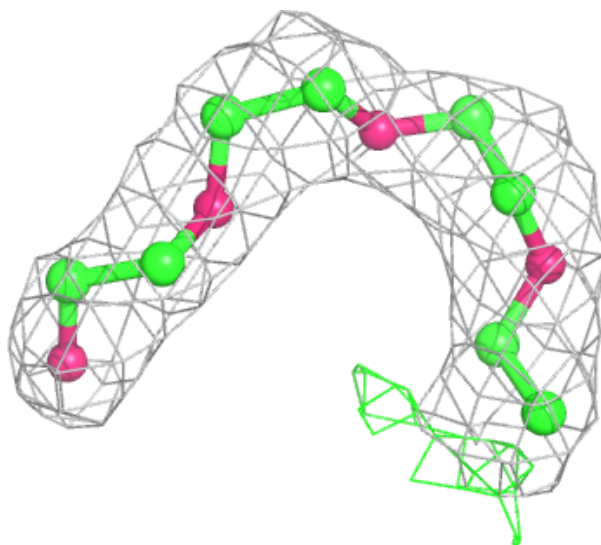
**Electron density around PE5 A 513:**

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



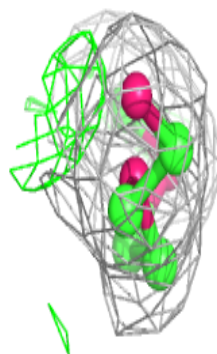
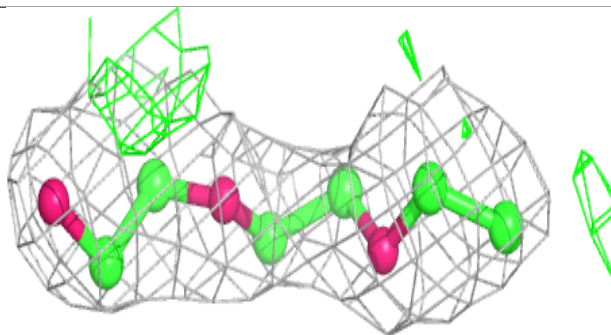
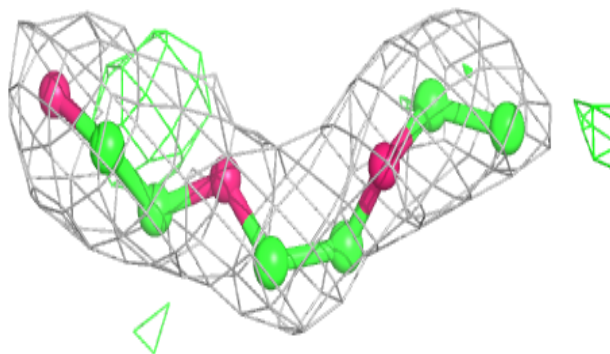
Electron density around PE5 A 515:

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

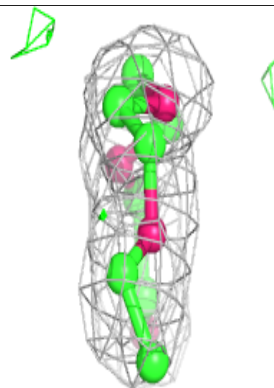
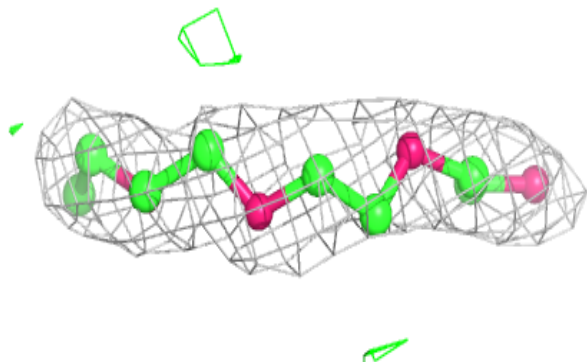
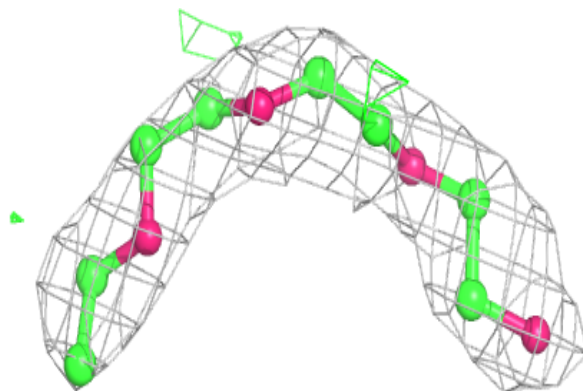


Electron density around PE5 A 514:

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

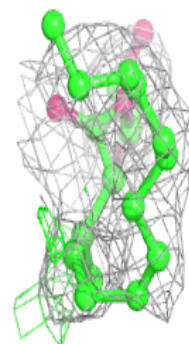
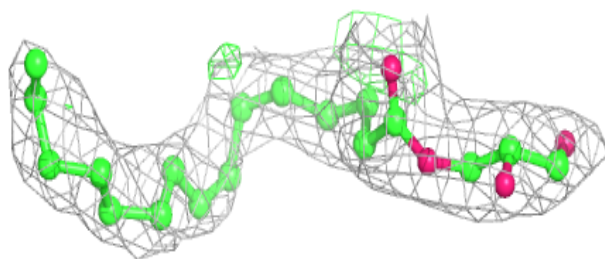
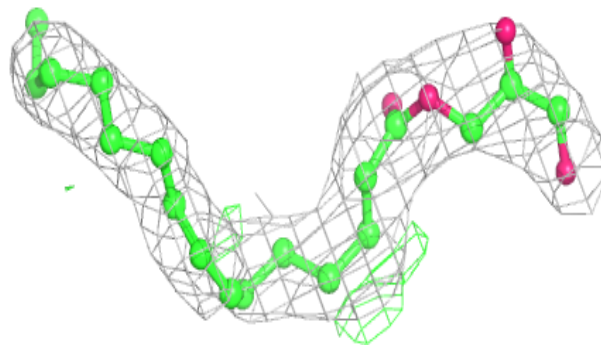
**Electron density around PE5 A 512:**

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

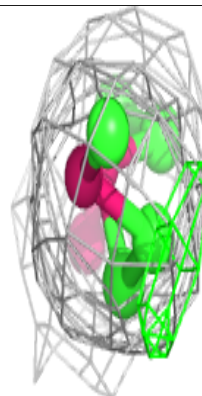
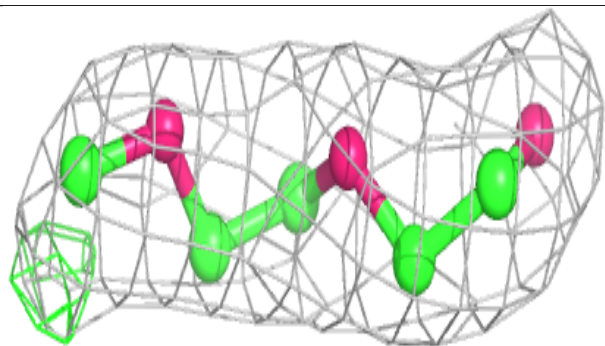
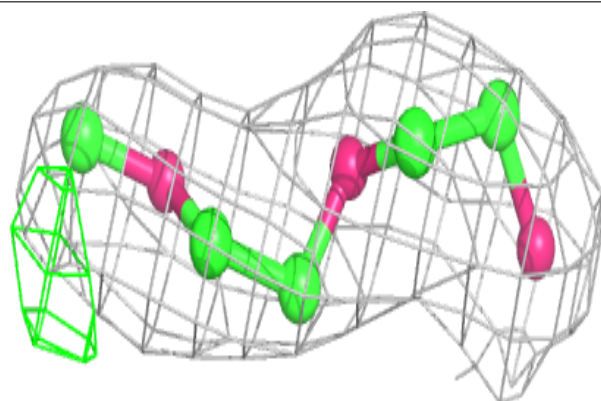


Electron density around 78M A 517:

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

**Electron density around PE5 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.