



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:19 PM UTC

PDB ID : 5D6K / pdb_00005d6k
Title : PepT - CIM
Authors : Ma, P.; Caffrey, M.
Deposited on : 2015-08-12
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 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

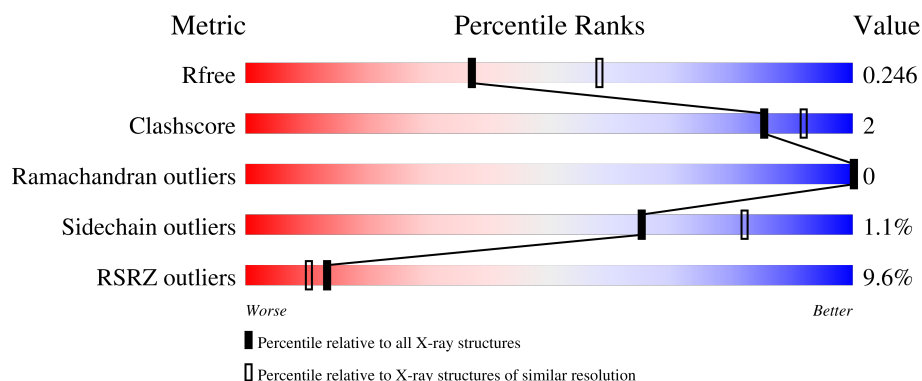
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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	483	9% 86% 6% 7%

2 Entry composition [i](#)

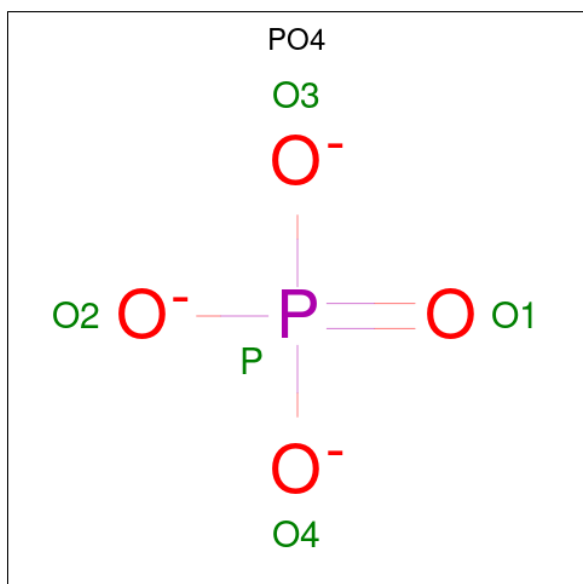
There are 5 unique types of molecules in this entry. The entry contains 3742 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

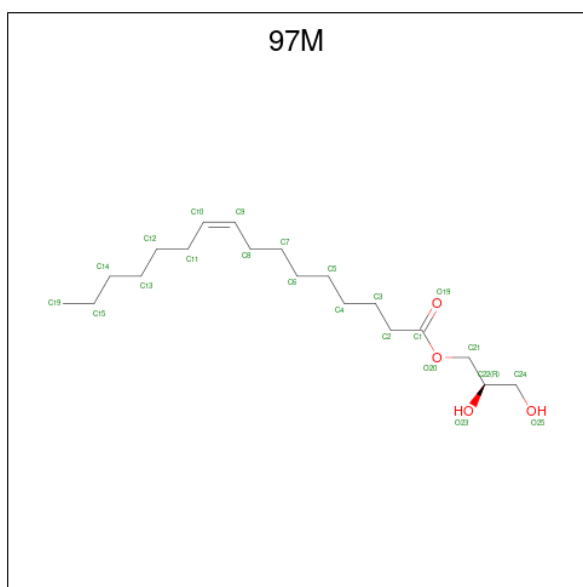
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	448	3488	2350	537	584	17	0	3	0

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



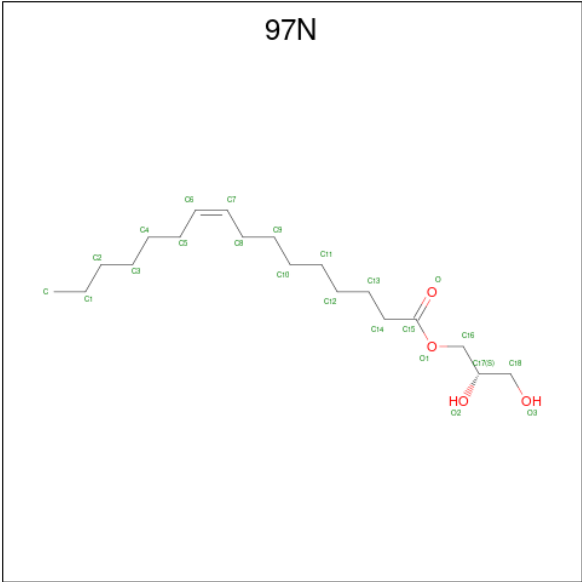
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0

- Molecule 3 is (2R)-2,3-dihydroxypropyl (9Z)-hexadec-9-enoate (CCD ID: 97M) (formula: C₁₉H₃₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	19	4		
3	A	1	Total	C	O	0	0
			23	19	4		
3	A	1	Total	C	O	0	0
			23	19	4		
3	A	1	Total	C	O	0	0
			23	19	4		
3	A	1	Total	C	O	0	0
			23	19	4		
3	A	1	Total	C	O	0	0
			23	19	4		
3	A	1	Total	C	O	0	0
			23	19	4		

- Molecule 4 is (2S)-2,3-dihydroxypropyl (9Z)-hexadec-9-enoate (CCD ID: 97N) (formula: C₁₉H₃₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			23	19	4		
4	A	1	Total	C	O	0	0
			23	19	4		

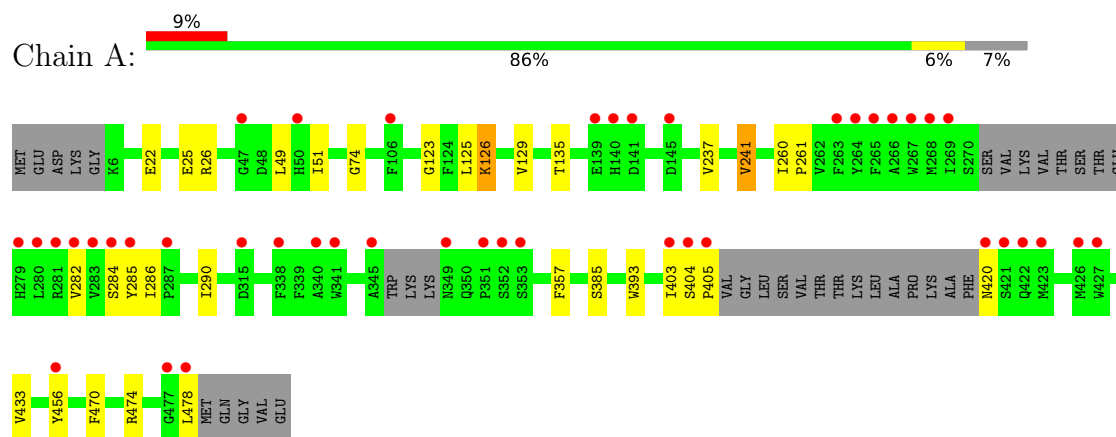
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	19	Total	O	0	0
			19	19		

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	101.69Å 110.91Å 112.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.84 – 2.40 50.84 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.84-2.40) 99.8 (50.84-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.9_1690	Depositor
R, R_{free}	0.216 , 0.246 0.222 , 0.246	Depositor DCC
R_{free} test set	1216 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3742	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 5.06% 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: PO4, 97M, 97N

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	0/3601	0.74	2/4909 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	126	LYS	CA-C-N	-5.10	114.41	119.56
1	A	126	LYS	C-N-CA	-5.10	114.41	119.56

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	3488	0	3565	16	0
2	A	5	0	0	0	0
3	A	184	0	0	2	0
4	A	46	0	0	0	0
5	A	19	0	0	0	0
All	All	3742	0	3565	16	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 2.

All (16) 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:456:TYR:OH	3:A:510:97M:O23	2.26	0.54
1:A:282:VAL:HA	1:A:285[B]:TYR:HD2	1.73	0.53
1:A:49:LEU:HG	1:A:51:ILE:HG12	1.91	0.52
1:A:22:GLU:HG2	1:A:129:VAL:HG11	1.92	0.51
1:A:357:PHE:HA	1:A:403:ILE:HG12	1.95	0.48
1:A:25:GLU:HG3	1:A:125:LEU:HD22	1.96	0.47
1:A:404:SER:HB3	1:A:405:PRO:HD3	1.97	0.47
1:A:260:ILE:HB	1:A:261:PRO:HD3	1.99	0.45
1:A:385:SER:HB2	3:A:502:97M:C22	2.49	0.43
1:A:286:ILE:O	1:A:290:ILE:HG12	2.20	0.42
1:A:470:PHE:O	1:A:474:ARG:NH1	2.52	0.42
1:A:26:ARG:HH12	1:A:126:LYS:HZ2	1.67	0.42
1:A:237:VAL:O	1:A:241:VAL:HG23	2.20	0.42
1:A:74:GLY:HA3	1:A:123:GLY:O	2.20	0.41
1:A:284:SER:HB2	1:A:478:LEU:HD12	2.03	0.41
1:A:261:PRO:HG2	1:A:433:VAL:HG21	2.04	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	443/483 (92%)	436 (98%)	7 (2%)	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	364/391 (93%)	360 (99%)	4 (1%)	65 82

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	THR
1	A	241	VAL
1	A	393	TRP
1	A	420	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	156	ASN

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 ⓘ

11 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
3	97M	A	511	-	22,22,22	0.73	1 (4%)	23,23,23	0.75	1 (4%)
3	97M	A	505	-	22,22,22	0.73	1 (4%)	23,23,23	0.81	1 (4%)
3	97M	A	506	-	22,22,22	0.73	1 (4%)	23,23,23	0.73	1 (4%)
4	97N	A	504	-	22,22,22	0.72	1 (4%)	23,23,23	0.79	1 (4%)
3	97M	A	503	-	22,22,22	0.70	1 (4%)	23,23,23	0.84	1 (4%)
3	97M	A	502	-	22,22,22	0.72	1 (4%)	23,23,23	0.81	1 (4%)
4	97N	A	508	-	22,22,22	0.73	1 (4%)	23,23,23	0.81	1 (4%)
2	PO4	A	501	-	4,4,4	1.01	0	6,6,6	0.58	0
3	97M	A	509	-	22,22,22	0.72	1 (4%)	23,23,23	0.75	1 (4%)
3	97M	A	507	-	22,22,22	0.73	1 (4%)	23,23,23	0.84	1 (4%)
3	97M	A	510	-	22,22,22	0.74	1 (4%)	23,23,23	0.75	1 (4%)

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
3	97M	A	511	-	-	9/22/22/22	-
3	97M	A	505	-	-	8/22/22/22	-
3	97M	A	506	-	-	9/22/22/22	-
4	97N	A	504	-	-	11/22/22/22	-
3	97M	A	503	-	-	12/22/22/22	-
3	97M	A	502	-	-	11/22/22/22	-
4	97N	A	508	-	-	9/22/22/22	-
3	97M	A	509	-	-	6/22/22/22	-
3	97M	A	507	-	-	14/22/22/22	-
3	97M	A	510	-	-	10/22/22/22	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	510	97M	O20-C1	2.92	1.41	1.33
3	A	502	97M	O20-C1	2.70	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	504	97N	O1-C15	2.69	1.41	1.33
3	A	505	97M	O20-C1	2.69	1.41	1.33
3	A	509	97M	O20-C1	2.68	1.41	1.33
3	A	506	97M	O20-C1	2.68	1.41	1.33
4	A	508	97N	O1-C15	2.62	1.41	1.33
3	A	511	97M	O20-C1	2.61	1.40	1.33
3	A	503	97M	O20-C1	2.57	1.40	1.33
3	A	507	97M	O20-C1	2.57	1.40	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	505	97M	O20-C1-C2	2.89	120.64	111.83
3	A	503	97M	O20-C1-C2	2.84	120.51	111.83
4	A	508	97N	O1-C15-C14	2.84	120.48	111.83
3	A	502	97M	O20-C1-C2	2.83	120.45	111.83
4	A	504	97N	O1-C15-C14	2.81	120.39	111.83
3	A	507	97M	O20-C1-C2	2.75	120.23	111.83
3	A	510	97M	O20-C1-C2	2.68	120.01	111.83
3	A	506	97M	O20-C1-C2	2.60	119.76	111.83
3	A	511	97M	O20-C1-C2	2.56	119.65	111.83
3	A	509	97M	O20-C1-C2	2.50	119.47	111.83

There are no chirality outliers.

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	97M	O20-C21-C22-C24
3	A	505	97M	O20-C21-C22-C24
3	A	507	97M	C21-C22-C24-O25
3	A	507	97M	O23-C22-C24-O25
3	A	510	97M	O20-C21-C22-O23
3	A	511	97M	O20-C21-C22-C24
3	A	511	97M	O20-C21-C22-O23
4	A	504	97N	O1-C16-C17-C18
4	A	504	97N	C16-C17-C18-O3
3	A	511	97M	O19-C1-O20-C21
3	A	511	97M	C2-C1-O20-C21
3	A	507	97M	C2-C1-O20-C21
3	A	503	97M	O20-C21-C22-O23
4	A	504	97N	O1-C16-C17-O2
3	A	507	97M	O19-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
3	A	502	97M	C2-C1-O20-C21
3	A	505	97M	O20-C21-C22-O23
3	A	511	97M	C1-C2-C3-C4
3	A	507	97M	C1-C2-C3-C4
3	A	506	97M	C1-C2-C3-C4
3	A	502	97M	O19-C1-O20-C21
3	A	510	97M	O20-C21-C22-C24
4	A	508	97N	C16-C17-C18-O3
3	A	507	97M	C11-C12-C13-C14
4	A	504	97N	O2-C17-C18-O3
3	A	502	97M	C12-C13-C14-C15
3	A	509	97M	C1-C2-C3-C4
3	A	507	97M	C2-C3-C4-C5
4	A	504	97N	C11-C12-C13-C14
3	A	505	97M	C2-C3-C4-C5
3	A	507	97M	C3-C4-C5-C6
3	A	505	97M	C11-C12-C13-C14
3	A	509	97M	C12-C13-C14-C15
4	A	504	97N	C10-C11-C12-C13
3	A	505	97M	C5-C6-C7-C8
4	A	504	97N	C9-C10-C11-C12
4	A	504	97N	C2-C3-C4-C5
4	A	508	97N	C10-C11-C12-C13
4	A	508	97N	C12-C13-C14-C15
4	A	508	97N	C3-C4-C5-C6
3	A	502	97M	C4-C5-C6-C7
3	A	507	97M	C4-C5-C6-C7
3	A	503	97M	C10-C11-C12-C13
3	A	506	97M	C6-C7-C8-C9
3	A	502	97M	C5-C6-C7-C8
3	A	507	97M	C13-C14-C15-C19
4	A	508	97N	C14-C15-O1-C16
3	A	509	97M	C3-C4-C5-C6
3	A	506	97M	C3-C4-C5-C6
3	A	507	97M	C10-C11-C12-C13
4	A	504	97N	C1-C2-C3-C4
3	A	507	97M	C6-C7-C8-C9
3	A	510	97M	C3-C4-C5-C6
4	A	508	97N	C1-C2-C3-C4
4	A	508	97N	O2-C17-C18-O3
4	A	508	97N	O-C15-O1-C16
3	A	506	97M	C2-C1-O20-C21

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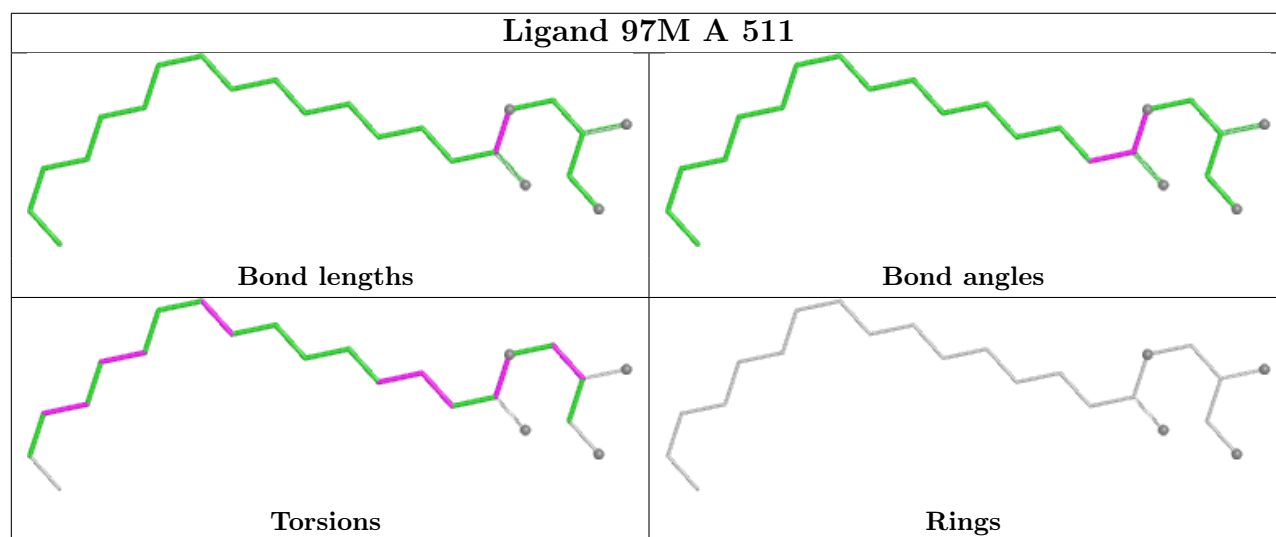
Mol	Chain	Res	Type	Atoms
3	A	506	97M	C12-C13-C14-C15
3	A	510	97M	C10-C11-C12-C13
3	A	503	97M	C13-C14-C15-C19
3	A	503	97M	C4-C5-C6-C7
3	A	505	97M	C12-C13-C14-C15
3	A	510	97M	C2-C3-C4-C5
3	A	510	97M	O23-C22-C24-O25
3	A	503	97M	O20-C1-C2-C3
3	A	506	97M	O19-C1-O20-C21
3	A	507	97M	C5-C6-C7-C8
3	A	502	97M	C3-C4-C5-C6
3	A	511	97M	C12-C13-C14-C15
3	A	509	97M	C13-C14-C15-C19
3	A	506	97M	C11-C12-C13-C14
3	A	503	97M	C7-C8-C9-C10
3	A	509	97M	C2-C3-C4-C5
3	A	506	97M	C9-C10-C11-C12
3	A	510	97M	C9-C10-C11-C12
3	A	511	97M	C2-C3-C4-C5
4	A	504	97N	C11-C10-C9-C8
3	A	511	97M	C7-C8-C9-C10
3	A	502	97M	C11-C12-C13-C14
3	A	506	97M	C4-C5-C6-C7
3	A	510	97M	C11-C12-C13-C14
3	A	502	97M	O20-C21-C22-C24
3	A	509	97M	O20-C1-C2-C3
3	A	510	97M	C7-C8-C9-C10
4	A	504	97N	C4-C5-C6-C7
3	A	502	97M	C21-C22-C24-O25
4	A	508	97N	C4-C5-C6-C7
3	A	503	97M	C6-C7-C8-C9
3	A	511	97M	C10-C11-C12-C13
3	A	510	97M	C12-C13-C14-C15
3	A	503	97M	O19-C1-C2-C3
3	A	503	97M	C1-C2-C3-C4
3	A	505	97M	C9-C10-C11-C12
3	A	507	97M	C9-C10-C11-C12
3	A	503	97M	C2-C3-C4-C5
3	A	505	97M	C7-C8-C9-C10
3	A	503	97M	C11-C12-C13-C14
3	A	502	97M	O20-C21-C22-O23
3	A	502	97M	O23-C22-C24-O25

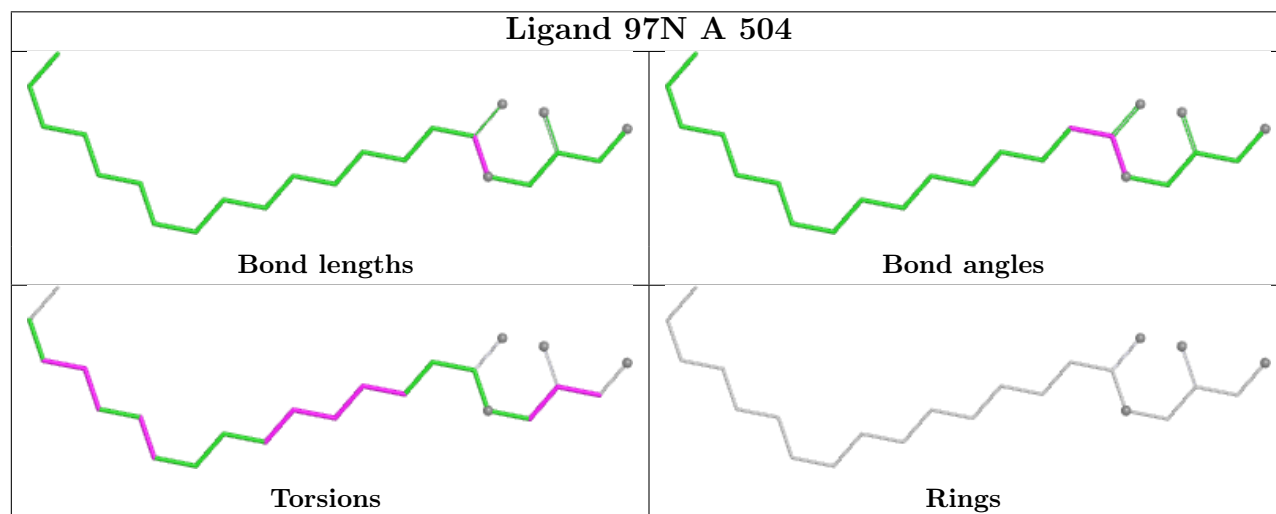
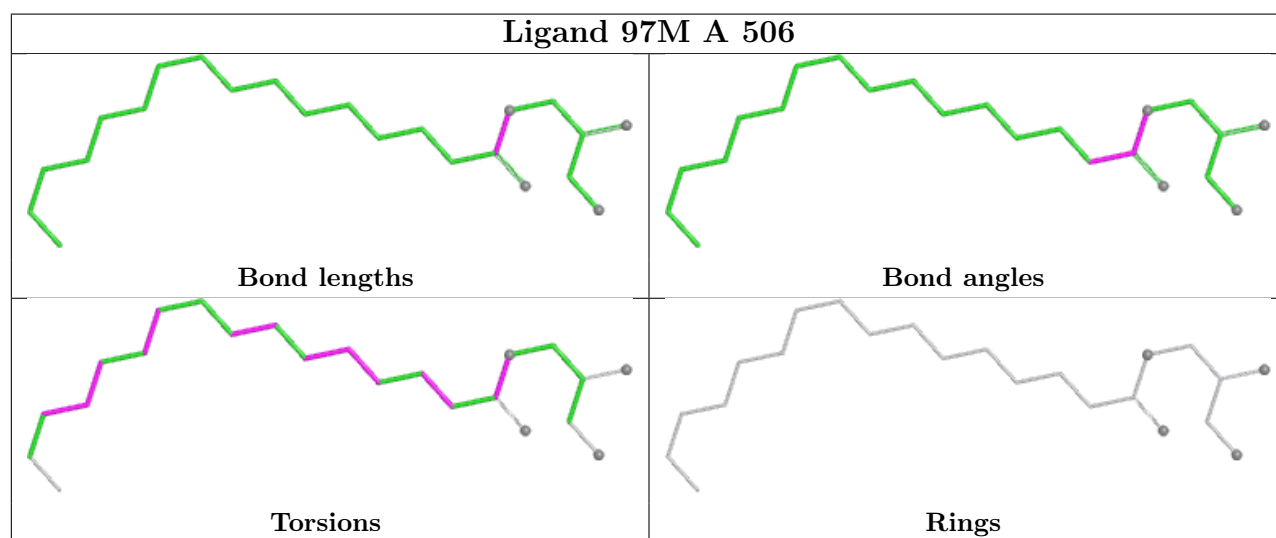
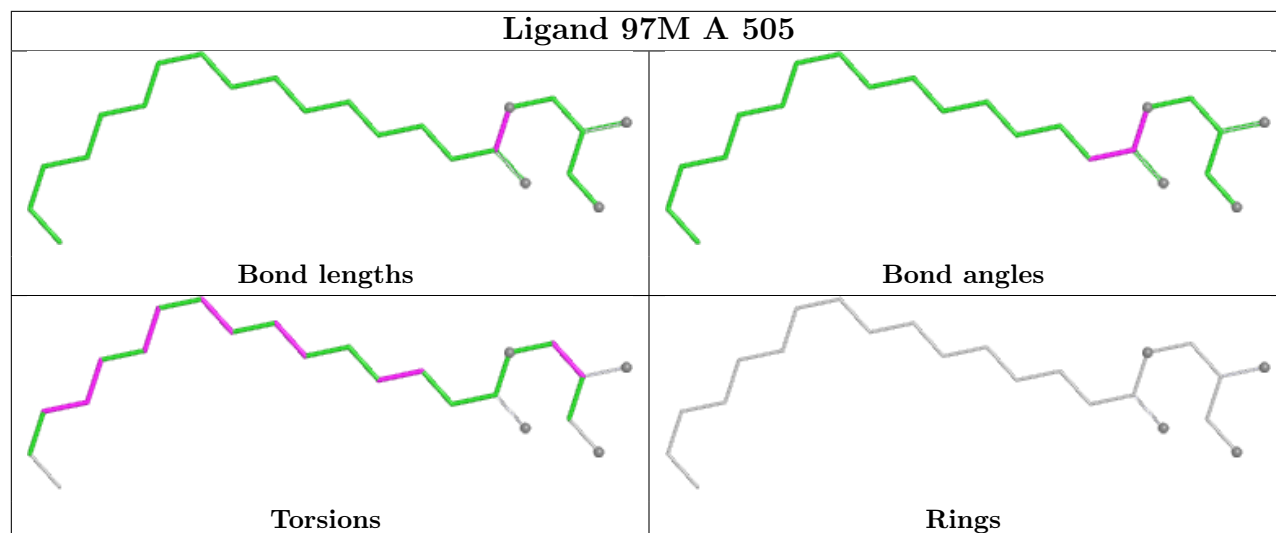
There are no ring outliers.

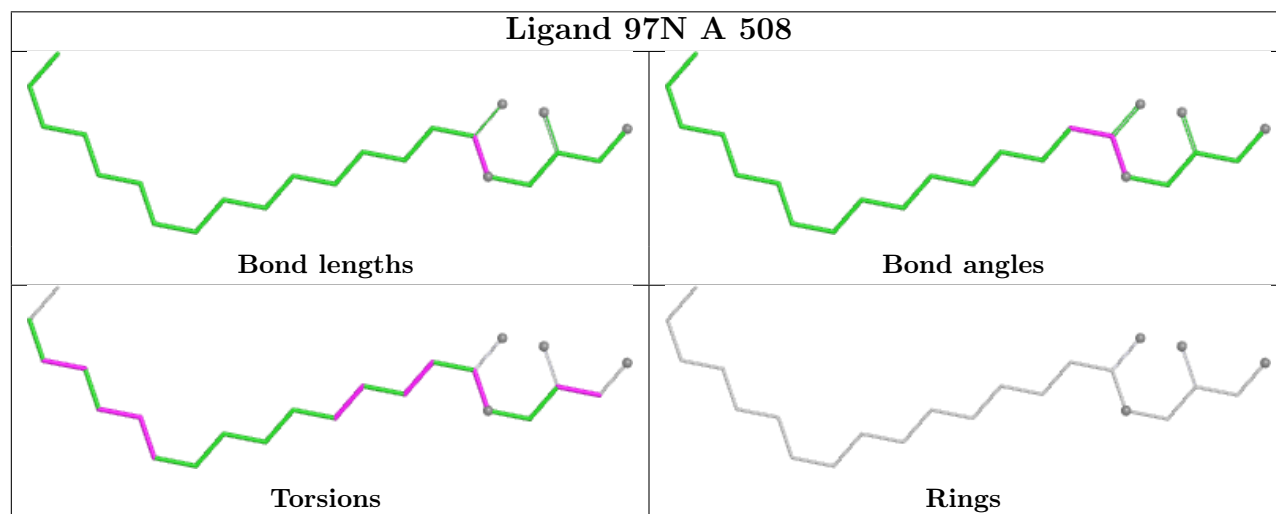
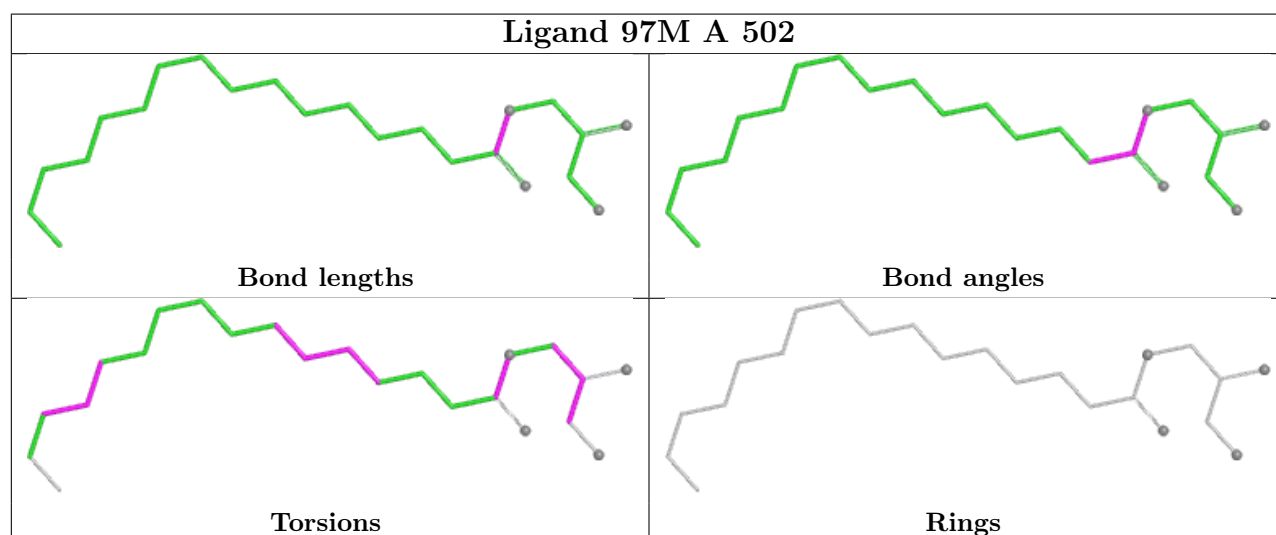
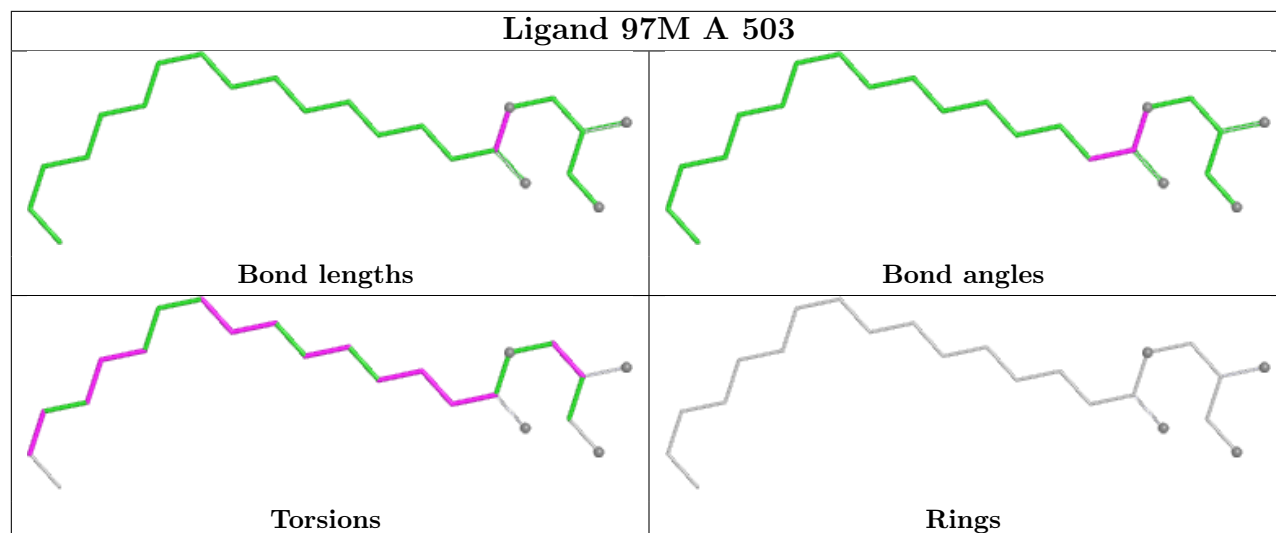
2 monomers are involved in 2 short contacts:

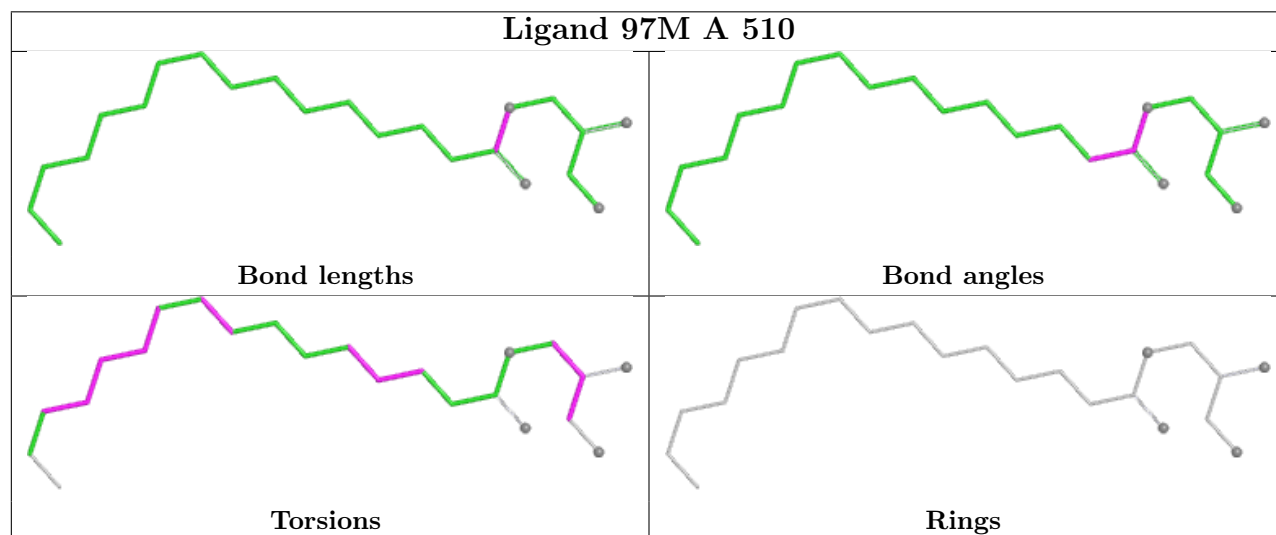
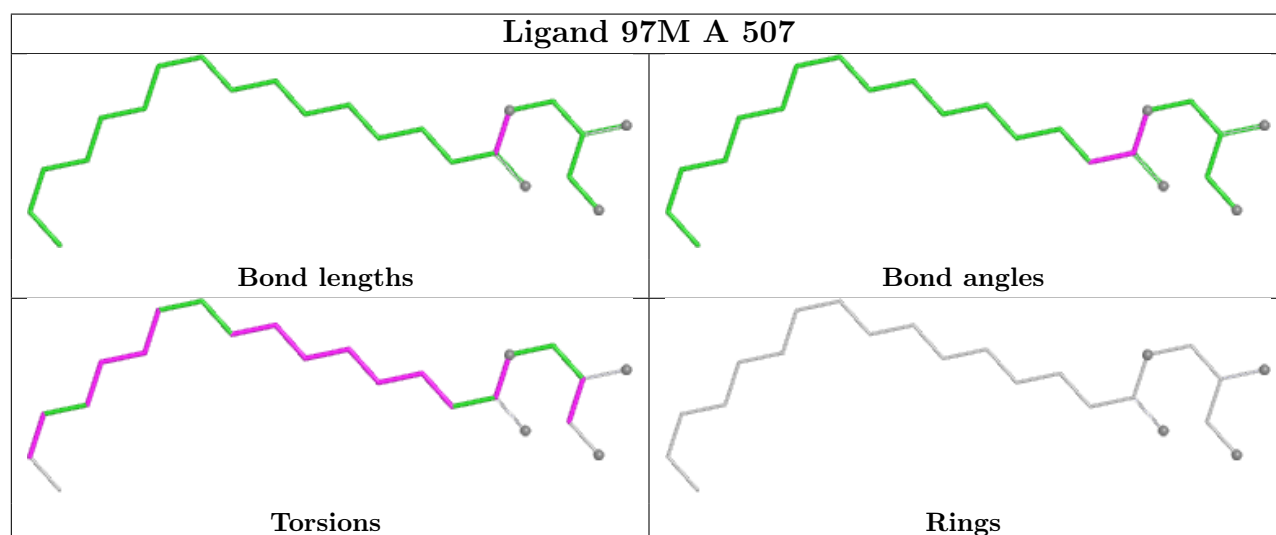
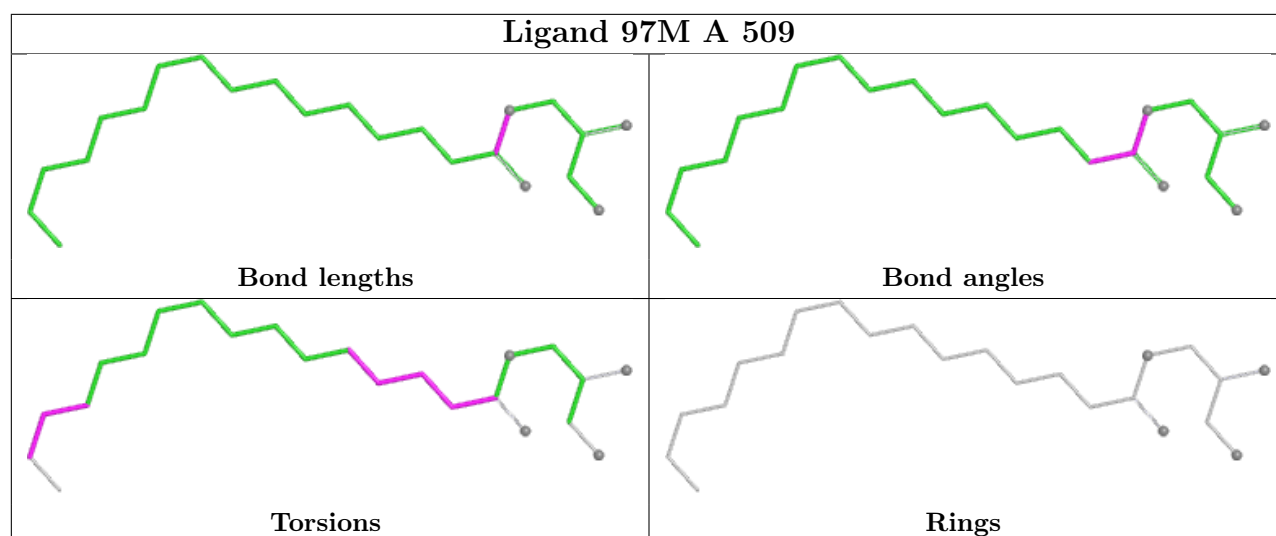
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	97M	1	0
3	A	510	97M	1	0

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	448/483 (92%)	0.53	43 (9%) 13 10	28, 47, 86, 112	3 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	284	SER	6.2
1	A	280	LEU	4.4
1	A	338	PHE	4.3
1	A	264	TYR	4.3
1	A	283	VAL	3.9
1	A	269	ILE	3.9
1	A	349	ASN	3.8
1	A	267	TRP	3.7
1	A	285[A]	TYR	3.7
1	A	265	PHE	3.7
1	A	405	PRO	3.7
1	A	427	TRP	3.6
1	A	268	MET	3.6
1	A	345	ALA	3.4
1	A	421	SER	3.2
1	A	340	ALA	3.2
1	A	351	PRO	3.2
1	A	341	TRP	3.1
1	A	478	LEU	3.0
1	A	50	HIS	2.9
1	A	279	HIS	2.7
1	A	477	GLY	2.7
1	A	282	VAL	2.7
1	A	420	ASN	2.7
1	A	266	ALA	2.6
1	A	141	ASP	2.6
1	A	426	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	281	ARG	2.6
1	A	423	MET	2.5
1	A	404	SER	2.5
1	A	139	GLU	2.4
1	A	47	GLY	2.4
1	A	287	PRO	2.3
1	A	263	PHE	2.3
1	A	403	ILE	2.2
1	A	315	ASP	2.1
1	A	352	SER	2.1
1	A	456	TYR	2.1
1	A	353	SER	2.1
1	A	140	HIS	2.1
1	A	422	GLN	2.0
1	A	106	PHE	2.0
1	A	145	ASP	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(Å ²)	Q<0.9
3	97M	A	510	23/23	0.76	0.21	55,69,84,85	0
3	97M	A	506	23/23	0.79	0.17	64,70,77,87	0
3	97M	A	502	23/23	0.80	0.20	46,61,72,78	0
4	97N	A	504	23/23	0.81	0.18	62,69,77,85	0
3	97M	A	509	23/23	0.83	0.20	57,71,78,84	0
3	97M	A	511	23/23	0.84	0.17	54,60,68,80	0
3	97M	A	505	23/23	0.85	0.18	51,65,72,75	0

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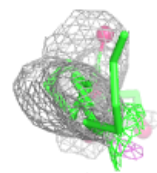
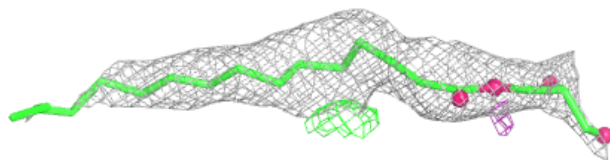
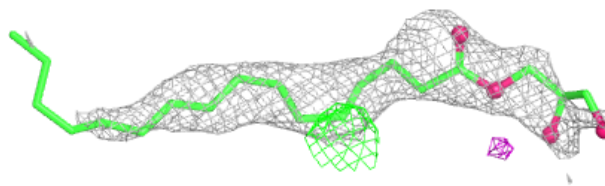
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	97M	A	507	23/23	0.85	0.18	58,69,78,82	0
3	97M	A	503	23/23	0.86	0.16	50,59,71,74	0
4	97N	A	508	23/23	0.86	0.18	53,67,77,84	0
2	PO4	A	501	5/5	0.93	0.10	65,66,72,76	0

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.

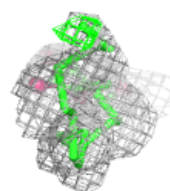
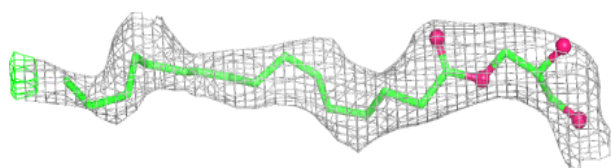
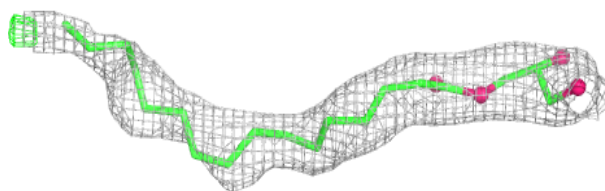
Electron density around 97M A 510:

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

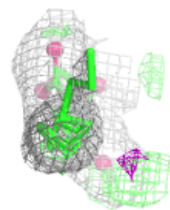
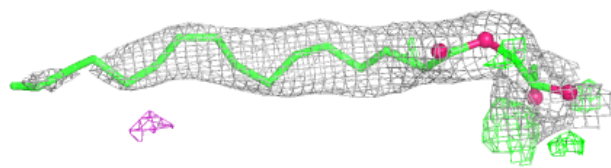
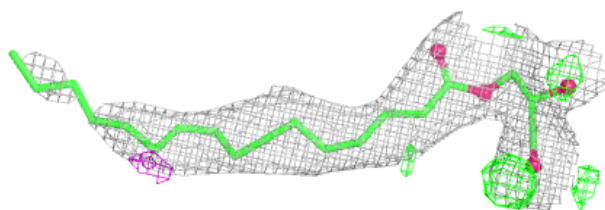


Electron density around 97M A 506:

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

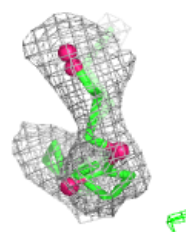
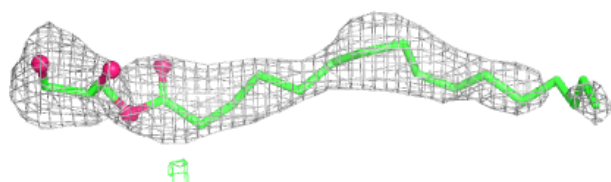
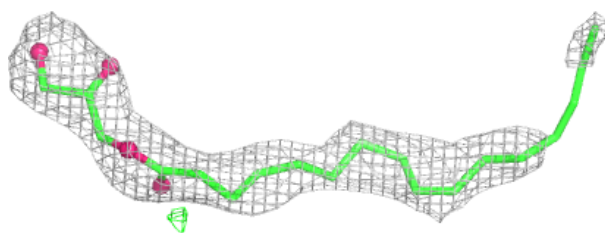
**Electron density around 97M A 502:**

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and green (positive)

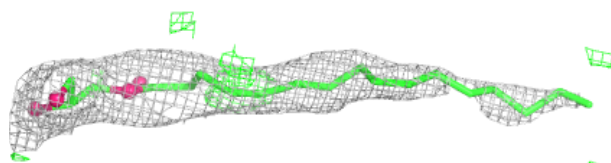
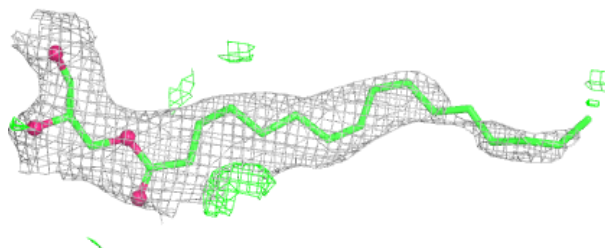


Electron density around 97N A 504:

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and green (positive)

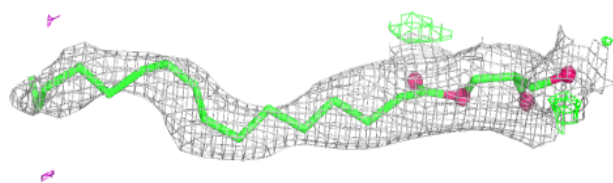
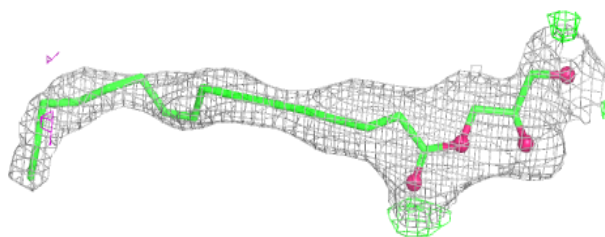
**Electron density around 97M A 509:**

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and green (positive)

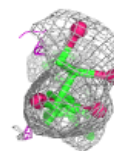
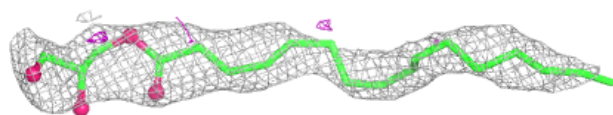
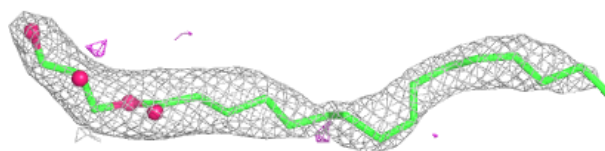


Electron density around 97M A 511:

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and green (positive)

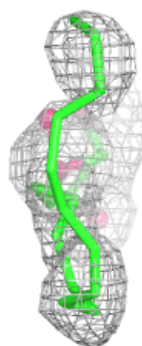
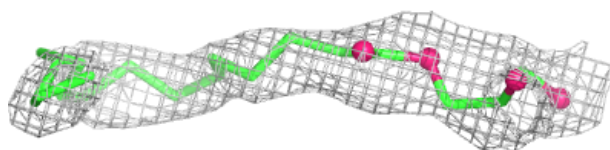
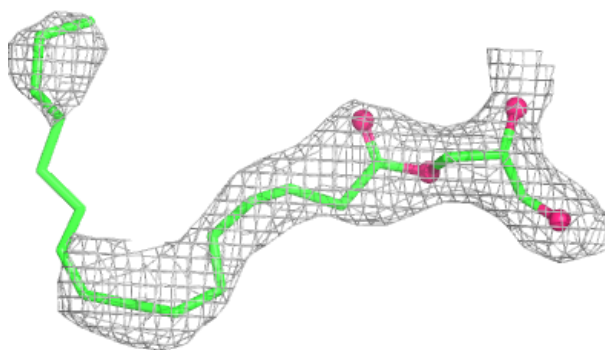
**Electron density around 97M A 505:**

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and green (positive)

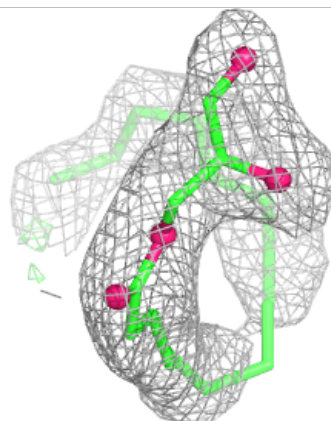
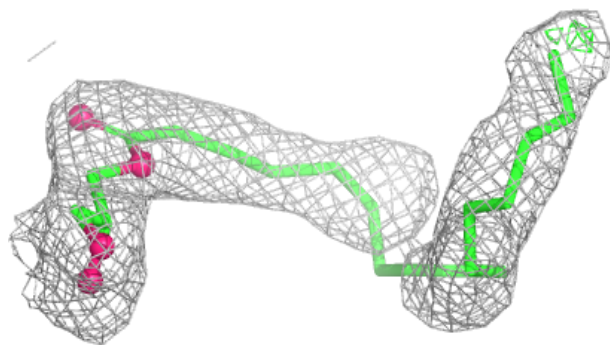
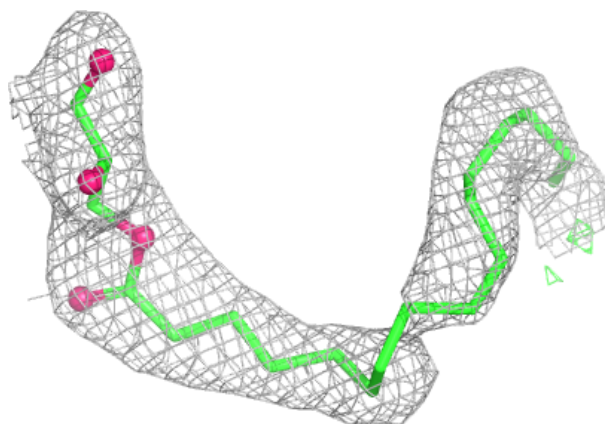


Electron density around 97M A 507:

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and green (positive)

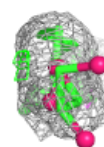
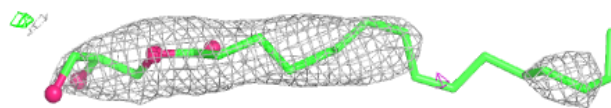
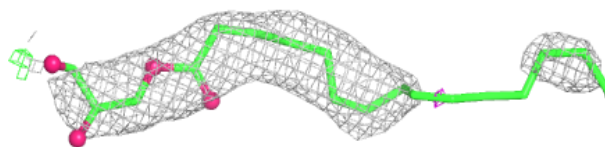
**Electron density around 97M A 503:**

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and green (positive)



Electron density around 97N 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.