



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:31 PM UTC

PDB ID : 5XJ5 / pdb_00005xj5
Title : Crystal structure of PlsY (YgiH), an integral membrane glycerol 3-phosphate acyltransferase - the monoacylglycerol form
Authors : Li, Z.; Li, D.
Deposited on : 2017-04-30
Resolution : 1.48 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

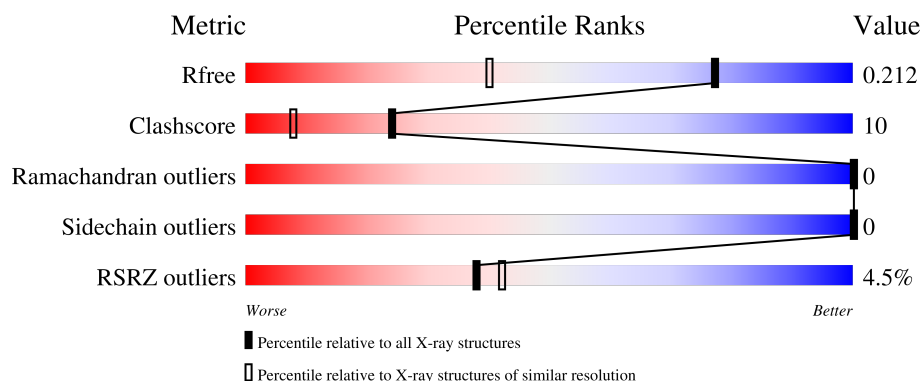
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.48 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	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (1.50-1.46)

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	201	

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
3	78M	A	315	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GLY	A	324	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2012 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 Glycerol-3-phosphate acyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	5	0
			1559	1052	251	253	3			

There are 11 discrepancies between the modelled and reference sequences:

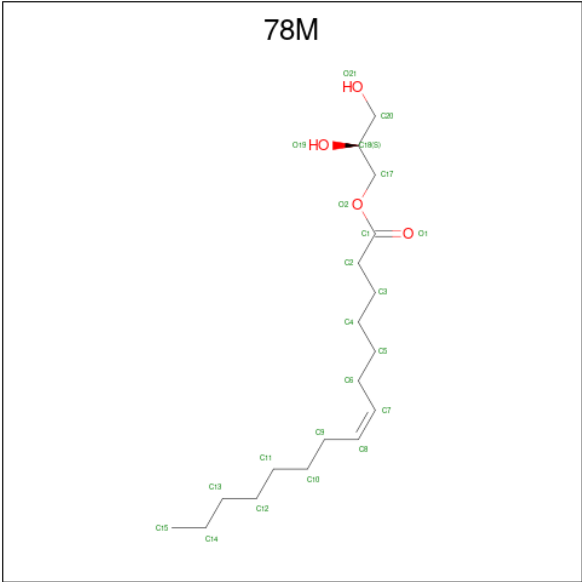
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	FME	-	expression tag	UNP O66905
A	1	GLY	-	expression tag	UNP O66905
A	2	SER	-	expression tag	UNP O66905
A	193	GLY	-	expression tag	UNP O66905
A	194	THR	-	expression tag	UNP O66905
A	195	LEU	-	expression tag	UNP O66905
A	196	GLU	-	expression tag	UNP O66905
A	197	VAL	-	expression tag	UNP O66905
A	198	LEU	-	expression tag	UNP O66905
A	199	PHE	-	expression tag	UNP O66905
A	200	GLN	-	expression tag	UNP O66905

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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



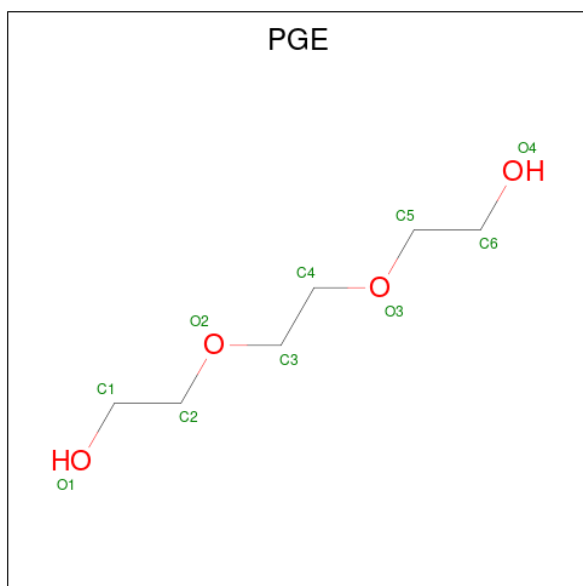
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			22	18	4		
3	A	1	Total	C	O	0	0
			22	18	4		
3	A	1	Total	C	O	0	0
			22	18	4		
3	A	1	Total	C	O	0	0
			22	18	4		
3	A	1	Total	C	O	0	0
			22	18	4		
3	A	1	Total	C	O	0	0
			22	18	4		
3	A	1	Total	C	O	0	0
			22	18	4		
3	A	1	Total	C	O	0	0
			22	18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

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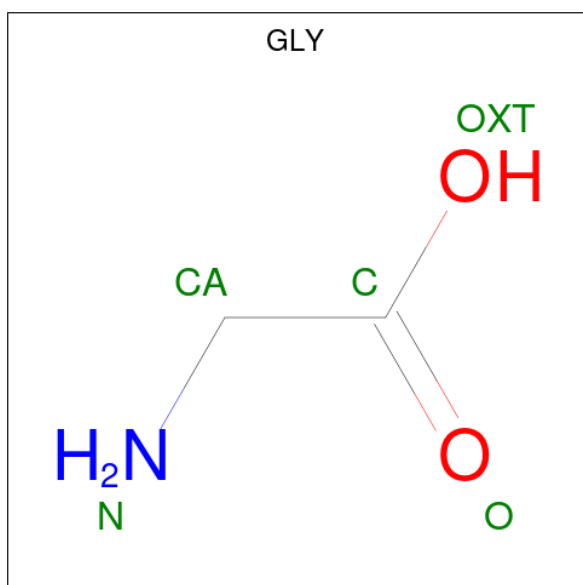
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			22	18	4		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 5 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			5	2	1	2		

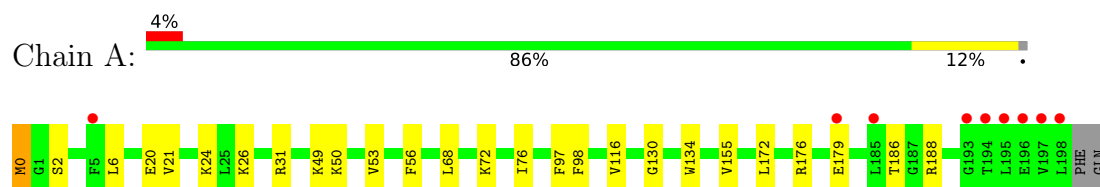
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	73	Total	O	0	0
			73	73		

3 Residue-property plots

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: Glycerol-3-phosphate acyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	57.67Å 83.44Å 107.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.58 – 1.48 35.58 – 1.48	Depositor EDS
% Data completeness (in resolution range)	98.1 (35.58-1.48) 98.1 (35.58-1.48)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 1.48Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.188 , 0.213 0.188 , 0.212	Depositor DCC
R_{free} test set	2112 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.9	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	0.96	EDS
Total number of atoms	2012	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.16% 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: PGE, 78M, SO4, FME

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	0.26	0/1603	0.46	0/2173

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	1559	0	1645	30	0
2	A	35	0	0	1	0
3	A	330	0	510	29	0
4	A	10	0	14	3	0
5	A	5	0	2	0	0
6	A	73	0	0	0	0
All	All	2012	0	2171	41	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 10.

All (41) 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)
3:A:310:78M:H22C	3:A:316:78M:H201	1.52	0.91
3:A:315:78M:H31C	3:A:317:78M:H171	1.58	0.85
3:A:315:78M:H171	3:A:317:78M:H201	1.68	0.74
3:A:313:78M:H132	3:A:317:78M:H141	1.72	0.72
1:A:134:TRP:HA	3:A:308:78M:H22C	1.76	0.67
1:A:2:SER:HB2	3:A:312:78M:H42C	1.77	0.67
1:A:155:VAL:HA	3:A:318:78M:H171	1.82	0.62
1:A:49:LYS:NZ	4:A:323:PGE:O1	2.28	0.62
1:A:130:GLY:HA3	3:A:308:78M:H122	1.83	0.60
1:A:0:FME:HA	3:A:313:78M:H18	1.84	0.59
1:A:53:VAL:HA	4:A:323:PGE:H1	1.85	0.59
1:A:98:PHE:HD1	3:A:315:78M:H22C	1.69	0.57
1:A:20[B]:GLU:OE1	1:A:31:ARG:NH2	2.38	0.56
3:A:321:78M:H7	3:A:322:78M:H122	1.92	0.52
1:A:98:PHE:CD1	3:A:315:78M:H22C	2.44	0.51
1:A:97:PHE:HB3	3:A:315:78M:H92C	1.92	0.50
1:A:179:GLU:H	1:A:179:GLU:CD	2.19	0.50
3:A:315:78M:H31C	3:A:317:78M:C17	2.38	0.50
1:A:24:LYS:NZ	3:A:315:78M:H21C	2.27	0.48
1:A:186:THR:OG1	1:A:188:ARG:NE	2.49	0.45
2:A:304:SO4:O4	3:A:316:78M:O21	2.28	0.45
3:A:313:78M:H112	3:A:313:78M:H8	1.83	0.44
1:A:0:FME:HE1	3:A:312:78M:H201	1.98	0.44
1:A:26:LYS:HB3	1:A:26:LYS:HE3	1.77	0.44
1:A:0:FME:H	1:A:0:FME:HG3	1.33	0.43
3:A:314:78M:H51C	3:A:315:78M:H111	2.01	0.43
1:A:172:LEU:O	1:A:176:ARG:HG2	2.19	0.43
3:A:321:78M:H42C	4:A:323:PGE:H12	2.00	0.43
1:A:68:LEU:HD23	3:A:320:78M:H22C	2.00	0.42
1:A:68:LEU:HD11	1:A:72:LYS:HE2	2.01	0.42
1:A:21:VAL:HG13	3:A:314:78M:H42C	2.01	0.42
1:A:24:LYS:CE	3:A:315:78M:H21C	2.50	0.42
1:A:2:SER:CB	3:A:312:78M:H42C	2.49	0.41
3:A:321:78M:H8	3:A:322:78M:H142	2.01	0.41
1:A:0:FME:HE2	1:A:0:FME:HB2	1.92	0.41
1:A:6:LEU:HD13	3:A:312:78M:H91C	2.02	0.41
1:A:76:ILE:HD11	1:A:116:VAL:HG13	2.02	0.41
1:A:56:PHE:CD1	3:A:321:78M:H61C	2.56	0.41
1:A:50:LYS:HZ3	1:A:50:LYS:HG2	1.71	0.40
1:A:97:PHE:HD1	3:A:317:78M:H52C	1.87	0.40
1:A:72:LYS:HG3	3:A:320:78M:H171	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	202/201 (100%)	202 (100%)	0	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	162/159 (102%)	162 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
1	FME	A	0	1	8,9,10	2.03	3 (37%)	8,9,11	1.19	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
1	FME	A	0	1	-	5/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	0	FME	CN-N	3.81	1.45	1.33
1	A	0	FME	CE-SD	2.74	1.95	1.78
1	A	0	FME	CG-SD	2.72	1.95	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	0	FME	N-CA-CB-CG
1	A	0	FME	C-CA-CB-CG
1	A	0	FME	CB-CG-SD-CE
1	A	0	FME	CA-CB-CG-SD
1	A	0	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	0	FME	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 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	78M	A	308	-	21,21,21	0.17	0	22,22,22	0.28	0
3	78M	A	310	-	21,21,21	0.25	0	22,22,22	0.55	0
3	78M	A	309	-	21,21,21	0.17	0	22,22,22	0.18	0
3	78M	A	311	-	21,21,21	0.24	0	22,22,22	0.38	0
3	78M	A	316	-	21,21,21	0.21	0	22,22,22	0.36	0
3	78M	A	312	-	21,21,21	0.17	0	22,22,22	0.19	0
3	78M	A	319	-	21,21,21	0.20	0	22,22,22	0.26	0
3	78M	A	317	-	21,21,21	0.18	0	22,22,22	0.32	0
5	GLY	A	324	-	4,4,4	1.92	2 (50%)	3,4,4	2.23	2 (66%)
3	78M	A	320	-	21,21,21	0.19	0	22,22,22	0.31	0
2	SO4	A	305	-	4,4,4	0.22	0	6,6,6	0.13	0
3	78M	A	318	-	21,21,21	0.31	0	22,22,22	0.59	0
3	78M	A	314	-	21,21,21	0.18	0	22,22,22	0.20	0
4	PGE	A	323	-	9,9,9	0.05	0	8,8,8	0.15	0
2	SO4	A	306	-	4,4,4	0.22	0	6,6,6	0.07	0
3	78M	A	313	-	21,21,21	0.19	0	22,22,22	0.21	0
2	SO4	A	307	-	4,4,4	0.19	0	6,6,6	0.30	0
3	78M	A	315	-	21,21,21	0.19	0	22,22,22	0.29	0
2	SO4	A	303	-	4,4,4	0.27	0	6,6,6	0.40	0
2	SO4	A	304	-	4,4,4	0.24	0	6,6,6	0.14	0
2	SO4	A	302	-	4,4,4	0.22	0	6,6,6	0.13	0
3	78M	A	321	-	21,21,21	0.27	0	22,22,22	0.36	0
3	78M	A	322	-	21,21,21	0.20	0	22,22,22	0.26	0
2	SO4	A	301	-	4,4,4	0.31	0	6,6,6	0.14	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
3	78M	A	308	-	-	4/21/21/21	-
3	78M	A	310	-	-	10/21/21/21	-
3	78M	A	313	-	-	3/21/21/21	-
5	GLY	A	324	-	-	0/2/2/2	-
3	78M	A	320	-	-	11/21/21/21	-
3	78M	A	321	-	-	9/21/21/21	-
3	78M	A	322	-	-	4/21/21/21	-
3	78M	A	309	-	-	1/21/21/21	-
3	78M	A	311	-	-	4/21/21/21	-
3	78M	A	316	-	-	8/21/21/21	-
3	78M	A	315	-	-	2/21/21/21	-
3	78M	A	318	-	-	6/21/21/21	-
3	78M	A	312	-	-	3/21/21/21	-
4	PGE	A	323	-	-	2/7/7/7	-
3	78M	A	319	-	-	7/21/21/21	-
3	78M	A	314	-	-	5/21/21/21	-
3	78M	A	317	-	-	4/21/21/21	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	324	GLY	O-C	2.73	1.31	1.22
5	A	324	GLY	OXT-C	-2.68	1.22	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	324	GLY	OXT-C-CA	2.88	124.84	113.38
5	A	324	GLY	O-C-CA	-2.56	111.61	122.37

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	310	78M	O19-C18-C20-O21
3	A	310	78M	C17-C18-C20-O21

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Mol	Chain	Res	Type	Atoms
3	A	314	78M	O2-C17-C18-O19
3	A	316	78M	O2-C17-C18-C20
3	A	316	78M	O2-C17-C18-O19
3	A	318	78M	O2-C17-C18-O19
3	A	319	78M	O19-C18-C20-O21
3	A	319	78M	C17-C18-C20-O21
3	A	321	78M	O2-C17-C18-O19
3	A	313	78M	O2-C17-C18-O19
3	A	310	78M	C2-C1-O2-C17
3	A	312	78M	O2-C17-C18-C20
3	A	318	78M	O2-C17-C18-C20
3	A	312	78M	O2-C17-C18-O19
3	A	317	78M	C1-C2-C3-C4
3	A	310	78M	O1-C1-O2-C17
3	A	310	78M	C1-C2-C3-C4
3	A	319	78M	C3-C4-C5-C6
3	A	322	78M	C10-C11-C12-C13
3	A	316	78M	C1-C2-C3-C4
3	A	320	78M	C10-C11-C12-C13
3	A	322	78M	C11-C12-C13-C14
3	A	321	78M	O2-C17-C18-C20
3	A	316	78M	C2-C3-C4-C5
3	A	316	78M	C9-C10-C11-C12
3	A	320	78M	C7-C8-C9-C10
3	A	317	78M	C3-C4-C5-C6
3	A	308	78M	C3-C4-C5-C6
3	A	308	78M	C4-C5-C6-C7
3	A	320	78M	C4-C5-C6-C7
3	A	316	78M	C10-C11-C12-C13
3	A	321	78M	C4-C5-C6-C7
3	A	318	78M	C2-C1-O2-C17
3	A	310	78M	C11-C12-C13-C14
3	A	320	78M	O19-C18-C20-O21
3	A	322	78M	C9-C10-C11-C12
3	A	320	78M	C9-C10-C11-C12
3	A	318	78M	O1-C1-O2-C17
3	A	315	78M	C11-C10-C9-C8
3	A	318	78M	C11-C10-C9-C8
3	A	320	78M	C11-C12-C13-C14
3	A	320	78M	C2-C3-C4-C5
3	A	308	78M	C12-C13-C14-C15
3	A	311	78M	C4-C5-C6-C7

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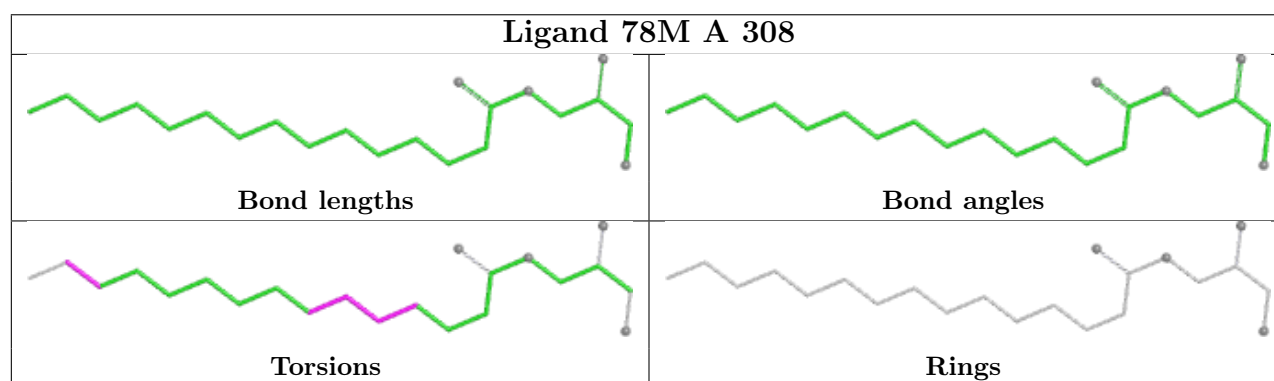
Mol	Chain	Res	Type	Atoms
3	A	320	78M	C3-C4-C5-C6
3	A	310	78M	C10-C11-C12-C13
3	A	315	78M	O19-C18-C20-O21
3	A	317	78M	C4-C5-C6-C7
3	A	311	78M	O2-C1-C2-C3
3	A	318	78M	C9-C10-C11-C12
3	A	322	78M	O2-C17-C18-C20
3	A	312	78M	C4-C5-C6-C7
3	A	310	78M	C7-C8-C9-C10
3	A	311	78M	C3-C4-C5-C6
3	A	320	78M	C17-C18-C20-O21
3	A	319	78M	C11-C10-C9-C8
3	A	311	78M	C12-C13-C14-C15
3	A	309	78M	C7-C8-C9-C10
3	A	314	78M	O2-C17-C18-C20
3	A	321	78M	C10-C11-C12-C13
3	A	314	78M	C7-C8-C9-C10
3	A	321	78M	C7-C8-C9-C10
3	A	321	78M	C5-C6-C7-C8
3	A	313	78M	C7-C8-C9-C10
4	A	323	PGE	C1-C2-O2-C3
3	A	308	78M	C5-C6-C7-C8
3	A	319	78M	O2-C1-C2-C3
4	A	323	PGE	C3-C4-O3-C5
3	A	321	78M	O2-C1-C2-C3
3	A	316	78M	O2-C1-C2-C3
3	A	320	78M	O2-C1-C2-C3
3	A	321	78M	C2-C3-C4-C5
3	A	317	78M	C2-C1-O2-C17
3	A	319	78M	O1-C1-C2-C3
3	A	321	78M	O1-C1-C2-C3
3	A	313	78M	C10-C11-C12-C13
3	A	320	78M	O1-C1-C2-C3
3	A	314	78M	C9-C10-C11-C12
3	A	316	78M	O1-C1-C2-C3
3	A	314	78M	O2-C1-C2-C3
3	A	310	78M	O1-C1-C2-C3
3	A	319	78M	C7-C8-C9-C10
3	A	310	78M	O2-C1-C2-C3

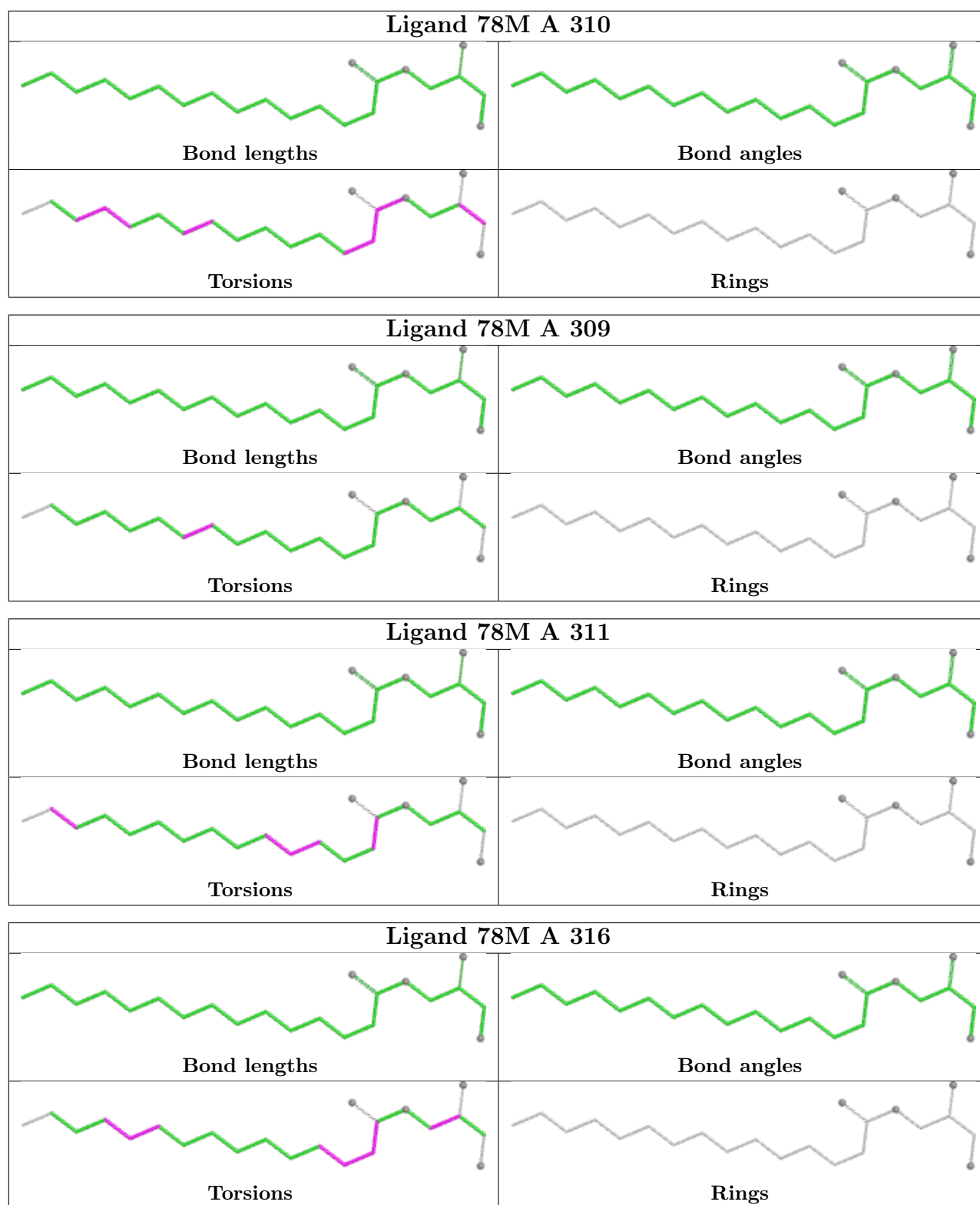
There are no ring outliers.

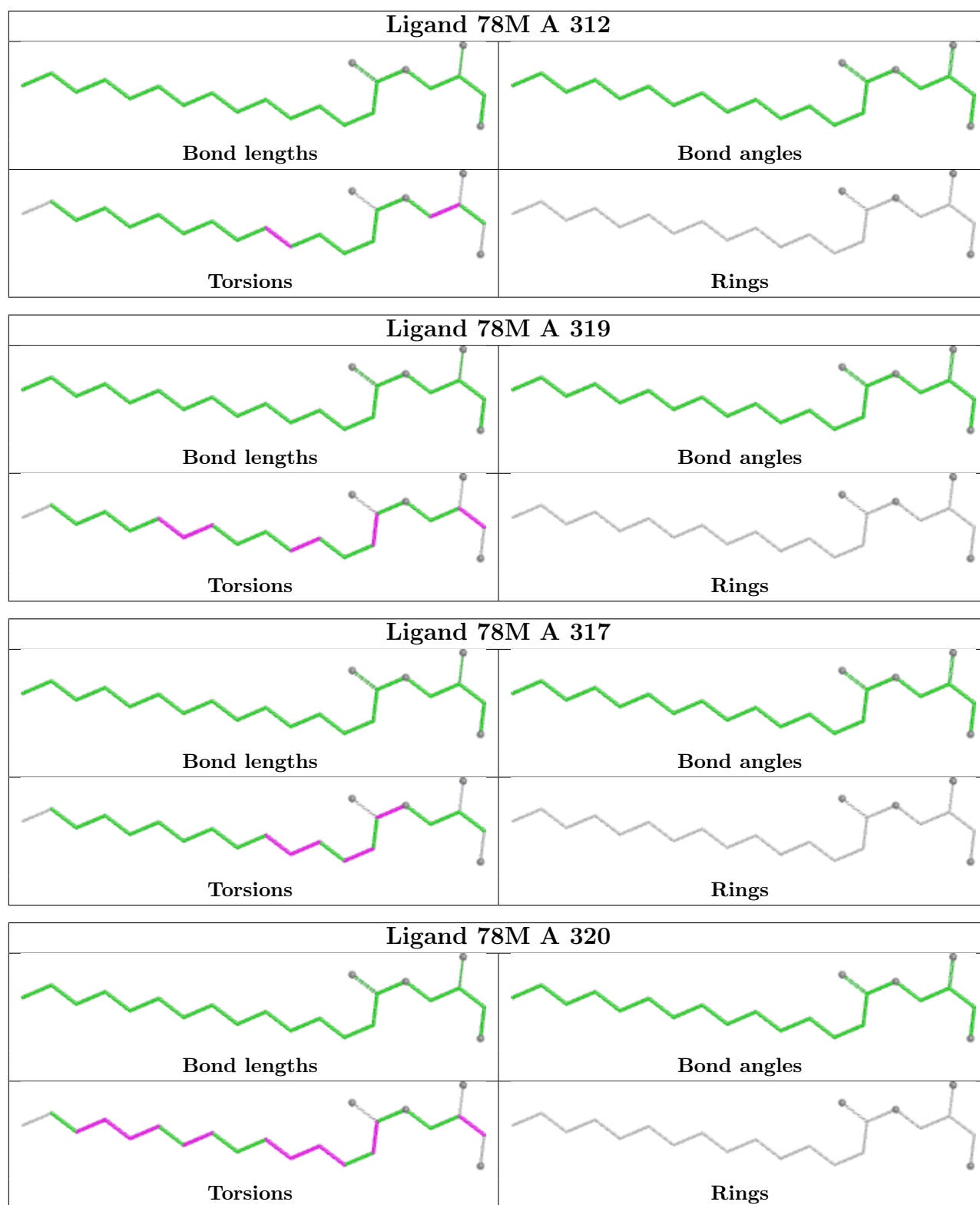
14 monomers are involved in 31 short contacts:

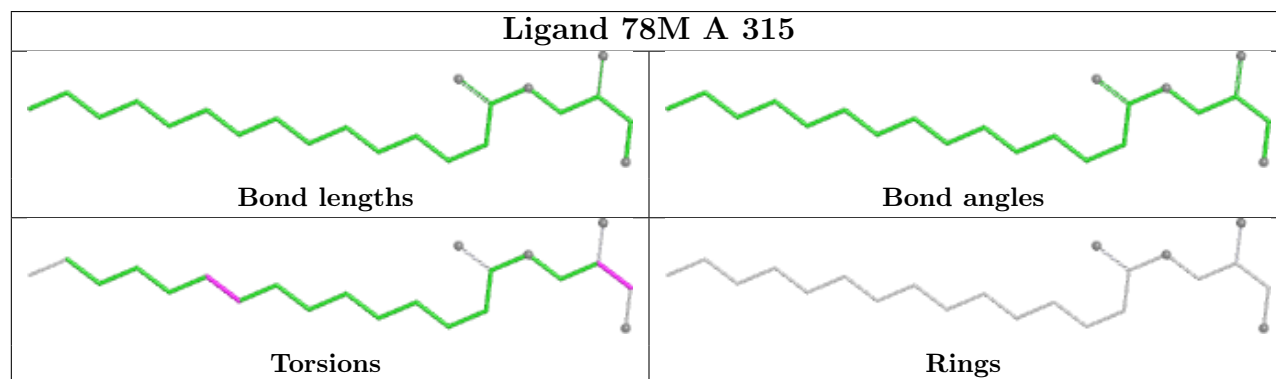
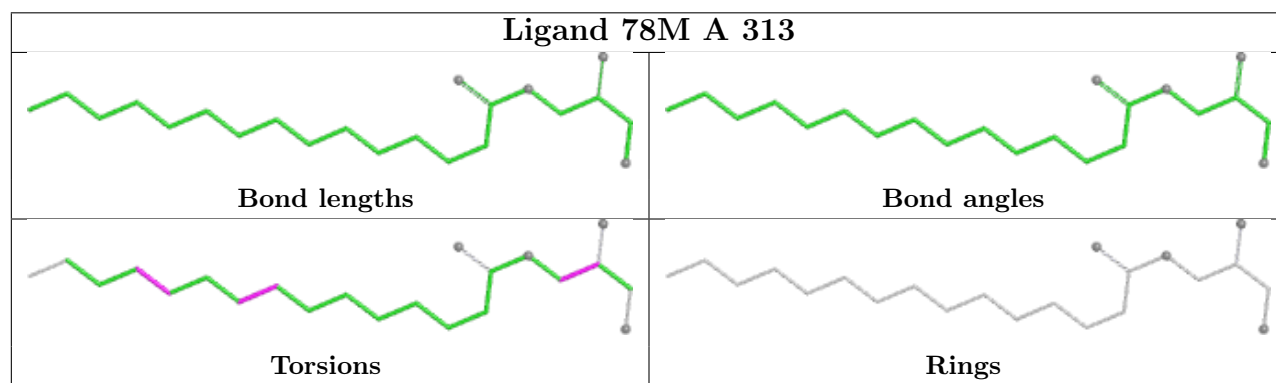
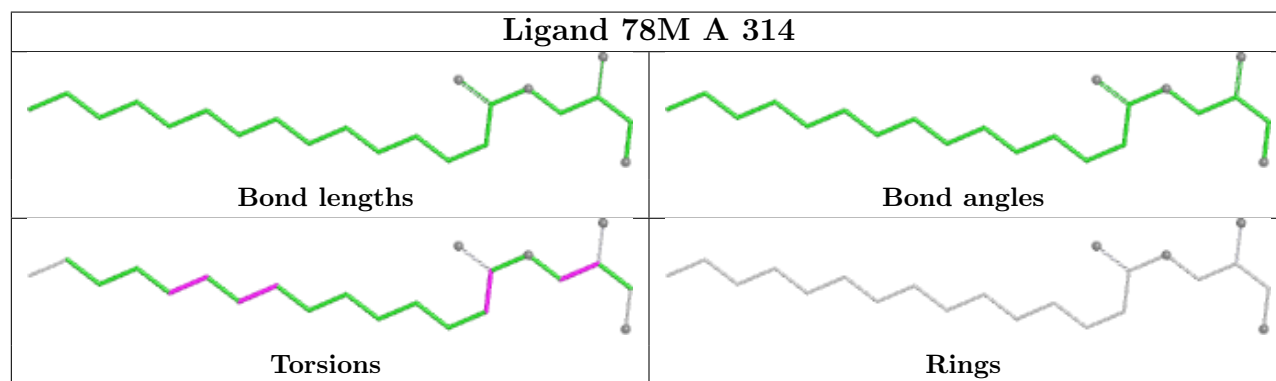
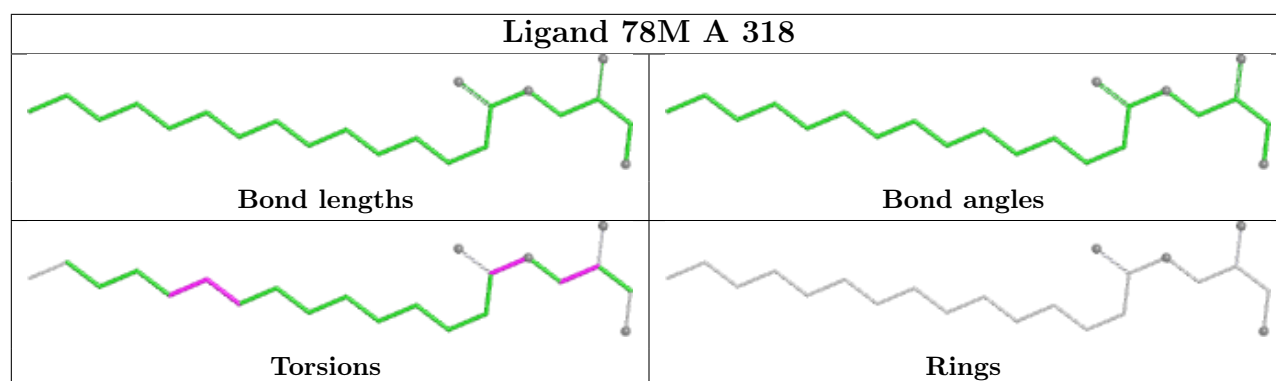
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	308	78M	2	0
3	A	310	78M	1	0
3	A	316	78M	2	0
3	A	312	78M	4	0
3	A	317	78M	5	0
3	A	320	78M	2	0
3	A	318	78M	1	0
3	A	314	78M	2	0
4	A	323	PGE	3	0
3	A	313	78M	3	0
3	A	315	78M	9	0
2	A	304	SO4	1	0
3	A	321	78M	4	0
3	A	322	78M	2	0

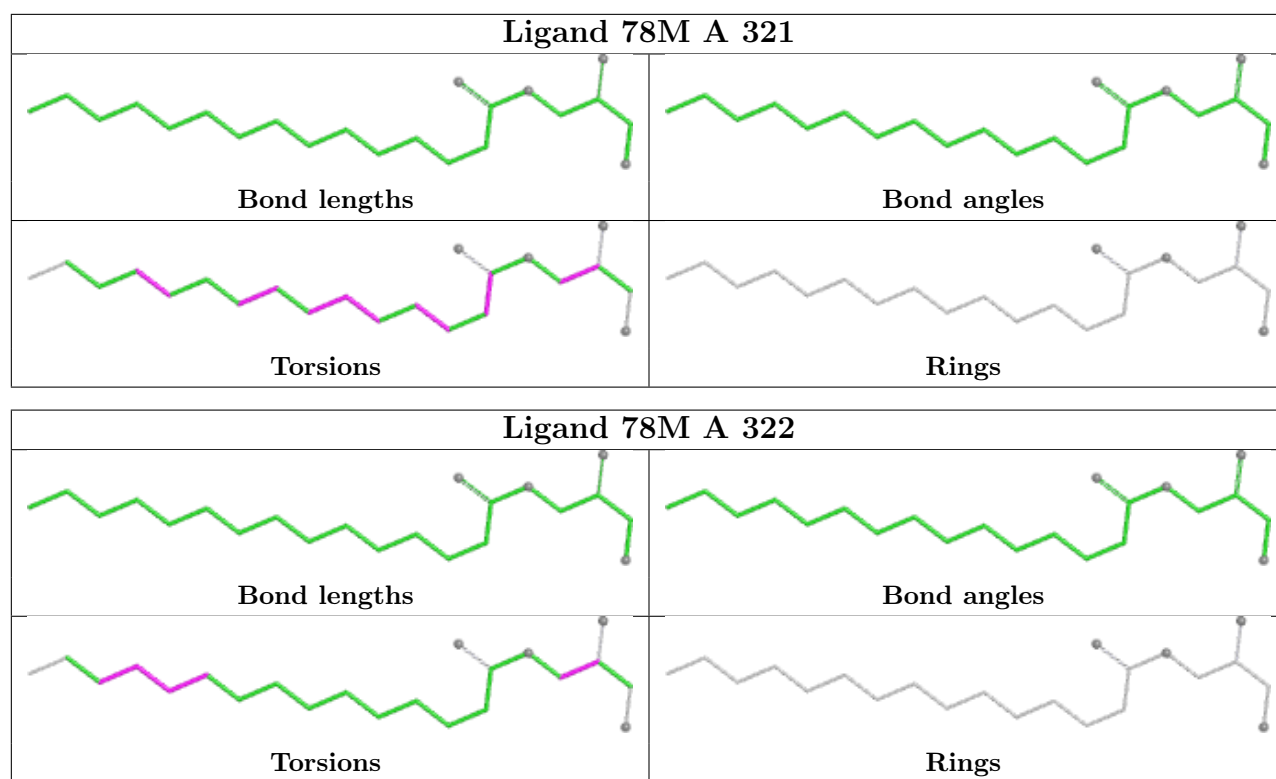
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [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	198/201 (98%)	0.31	9 (4%) 38 42	11, 20, 35, 61	5 (2%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	VAL	8.2
1	A	195	LEU	6.5
1	A	196	GLU	6.2
1	A	198	LEU	4.7
1	A	185	LEU	4.2
1	A	193	GLY	4.1
1	A	194	THR	3.4
1	A	5	PHE	3.0
1	A	179	GLU	2.7

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	FME	A	0	10/11	0.80	0.16	27,37,50,61	1

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

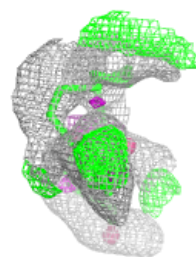
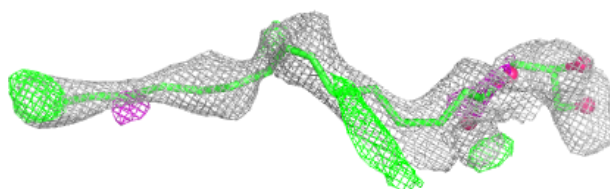
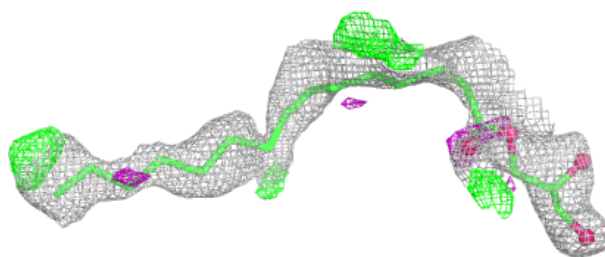
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	78M	A	318	22/22	0.50	0.21	36,47,59,61	0
3	78M	A	317	22/22	0.60	0.19	37,47,59,64	0
3	78M	A	312	22/22	0.61	0.18	38,48,62,69	0
3	78M	A	314	22/22	0.61	0.21	42,47,54,59	0
3	78M	A	315	22/22	0.62	0.18	41,47,58,60	0
3	78M	A	321	22/22	0.62	0.23	36,46,54,65	0
3	78M	A	316	22/22	0.68	0.19	32,42,50,59	0
3	78M	A	313	22/22	0.68	0.17	46,51,57,58	0
3	78M	A	319	22/22	0.70	0.19	36,48,63,67	0
3	78M	A	322	22/22	0.70	0.19	27,45,56,61	0
3	78M	A	308	22/22	0.72	0.20	29,35,58,73	0
5	GLY	A	324	5/5	0.72	0.14	46,47,51,58	0
3	78M	A	320	22/22	0.73	0.17	41,51,59,65	0
2	SO4	A	305	5/5	0.73	0.17	48,61,66,68	0
3	78M	A	310	22/22	0.74	0.19	28,38,48,54	0
2	SO4	A	307	5/5	0.76	0.13	31,33,56,61	0
3	78M	A	309	22/22	0.79	0.16	36,45,61,67	0
2	SO4	A	306	5/5	0.83	0.12	45,51,59,71	0
4	PGE	A	323	10/10	0.85	0.15	36,39,46,47	0
3	78M	A	311	22/22	0.86	0.13	20,25,32,38	0
2	SO4	A	304	5/5	0.94	0.08	40,42,45,56	0
2	SO4	A	302	5/5	0.95	0.09	39,40,43,50	0
2	SO4	A	301	5/5	0.98	0.06	24,24,27,28	0
2	SO4	A	303	5/5	0.99	0.04	15,16,17,18	0

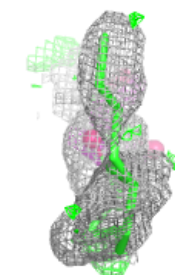
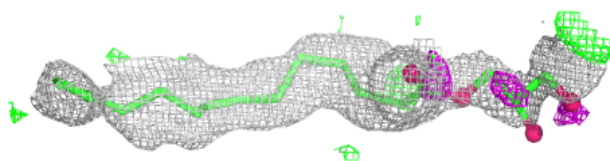
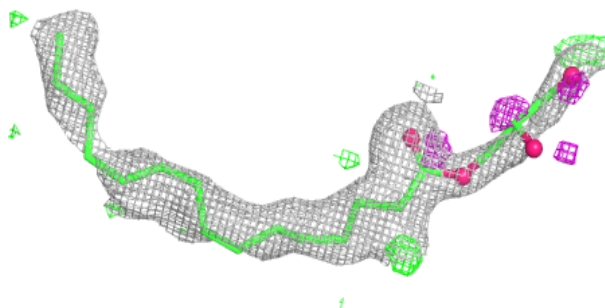
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 78M A 318:

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

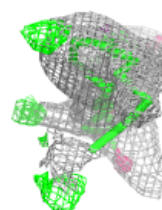
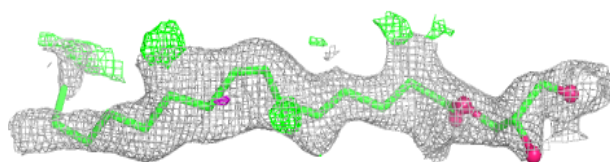
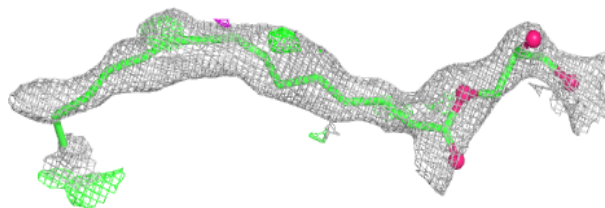
**Electron density around 78M A 317:**

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

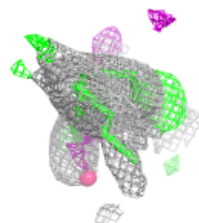
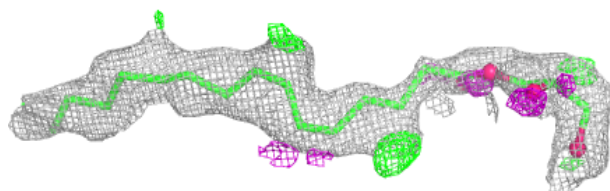
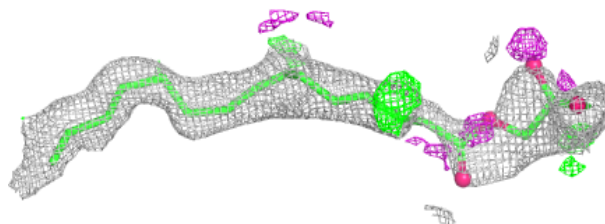


Electron density around 78M A 312:

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

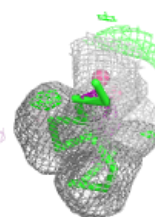
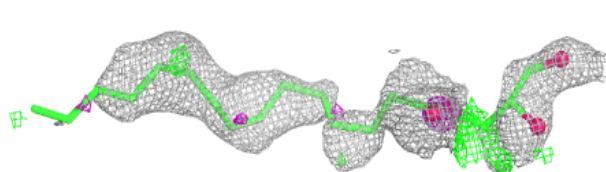
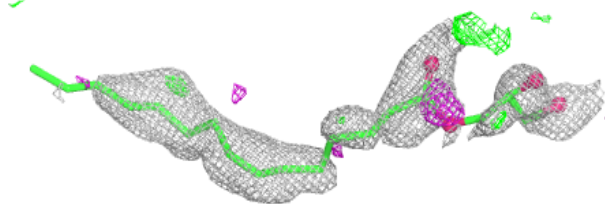
**Electron density around 78M A 314:**

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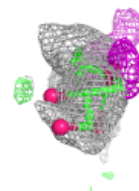
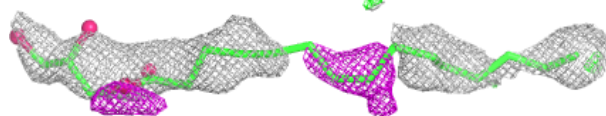
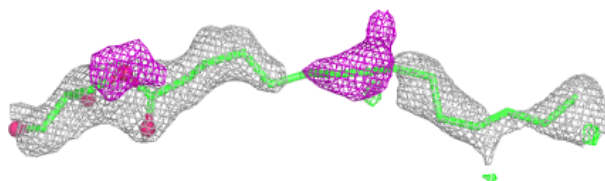


Electron density around 78M A 315:

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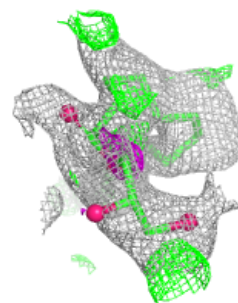
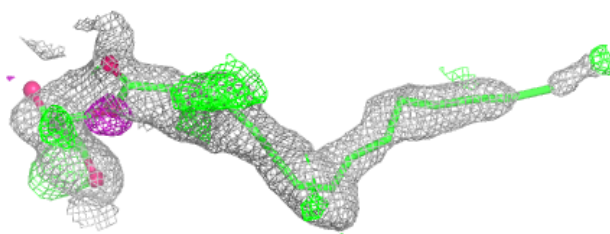
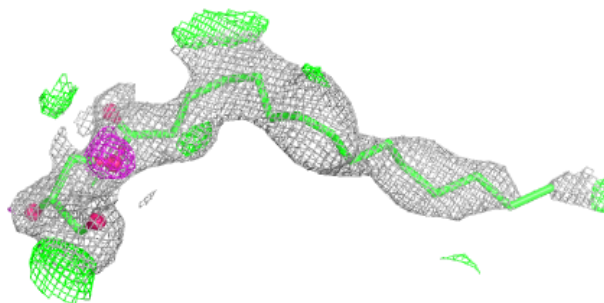
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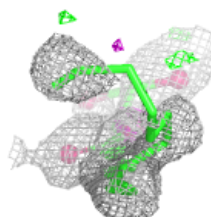
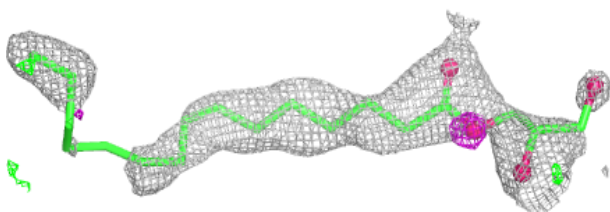
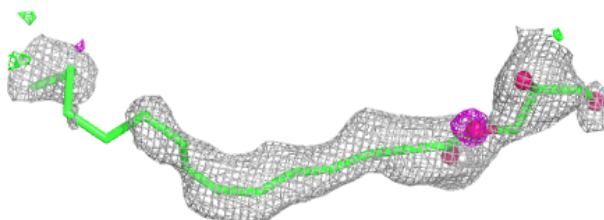


Electron density around 78M A 316:

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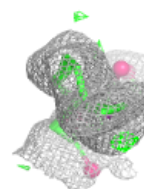
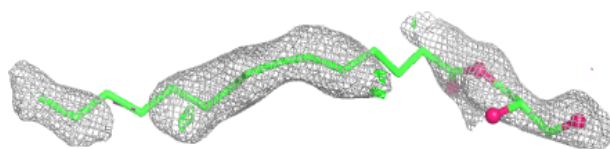
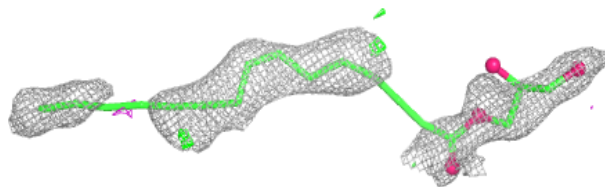
**Electron density around 78M A 313:**

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and green (positive)

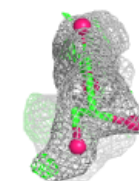
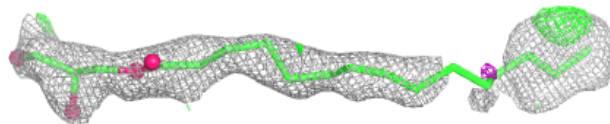
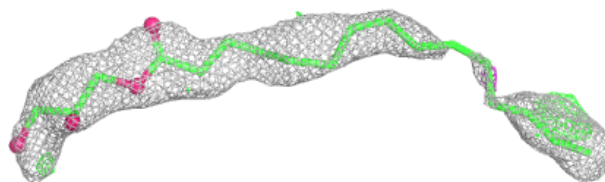


Electron density around 78M A 319:

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and green (positive)

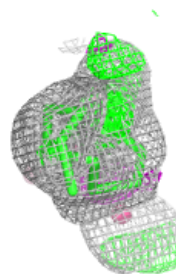
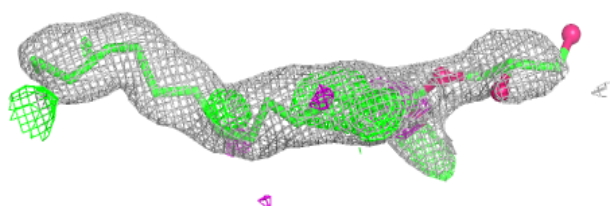
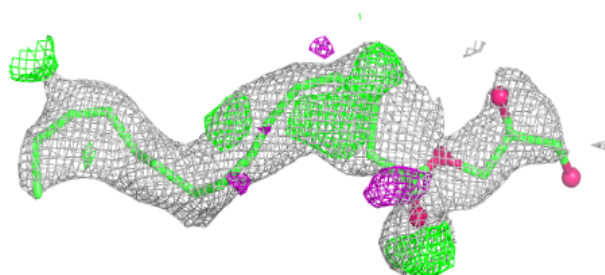
**Electron density around 78M A 322:**

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

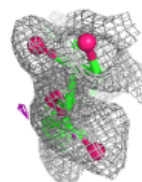
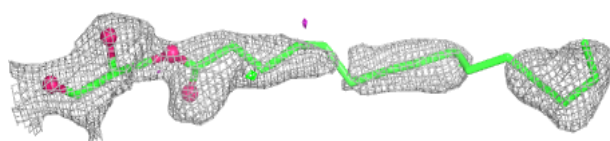
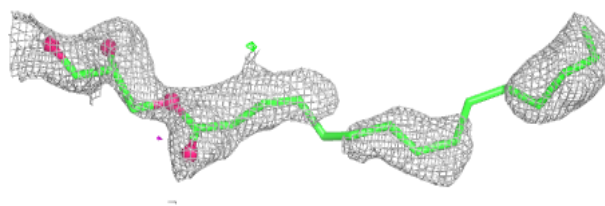


Electron density around 78M A 308:

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

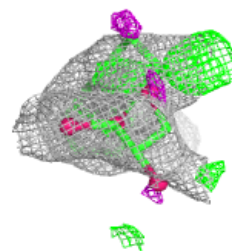
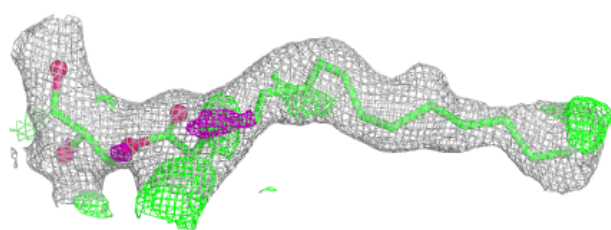
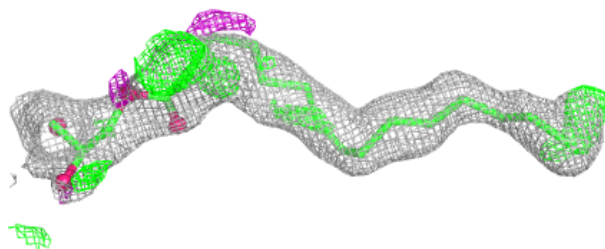
**Electron density around 78M A 320:**

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

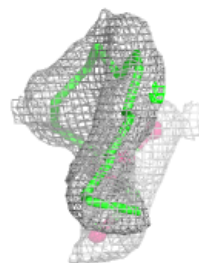
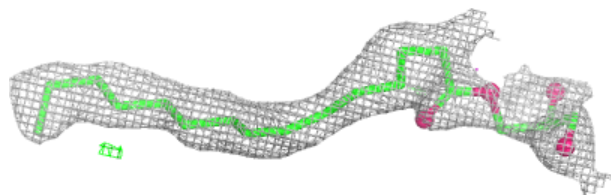
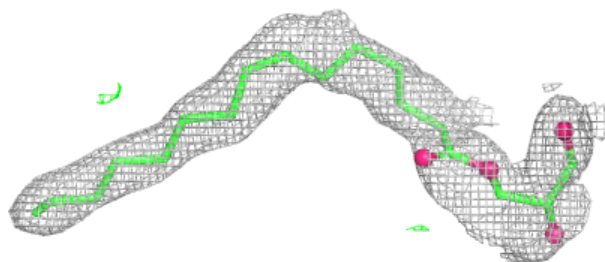


Electron density around 78M A 310:

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

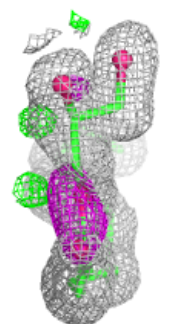
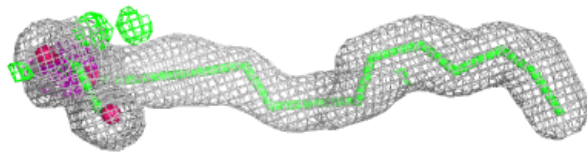
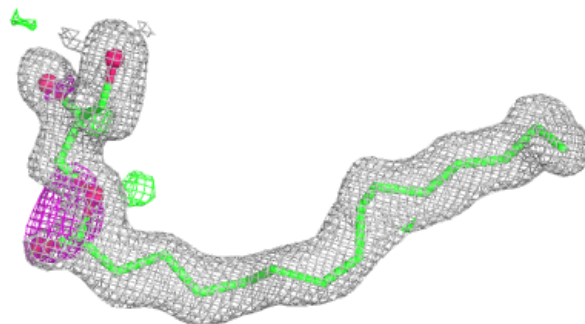
**Electron density around 78M A 309:**

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



Electron density around 78M A 311:

$2mF_o-DF_c$ (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.