



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:38 AM UTC

PDB ID : 6EI3 / pdb_00006ei3
Title : Crystal structure of auto inhibited POT family peptide transporter
Authors : Newstead, S.; Brinth, A.; Vogeley, L.; Caffrey, M.
Deposited on : 2017-09-17
Resolution : 2.10 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

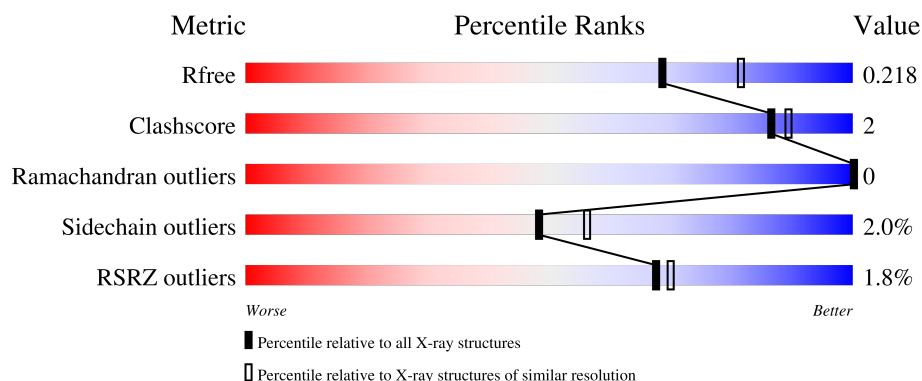
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

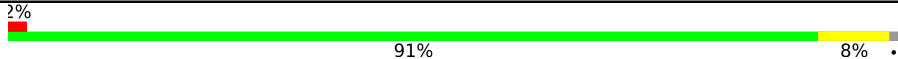
The reported resolution of this entry is 2.10 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	514	

2 Entry composition [i](#)

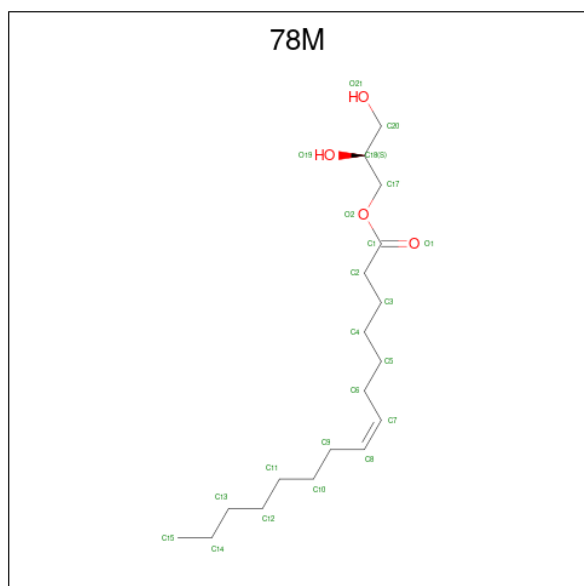
There are 3 unique types of molecules in this entry. The entry contains 4641 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Proton-dependent oligopeptide transporter family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	511	Total	C	N	O	S	0	4	0
			4007	2664	666	655	22			

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



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 22 18 4	0	0
2	A	1	Total C O 22 18 4	0	0
2	A	1	Total C O 22 18 4	0	0
2	A	1	Total C O 22 18 4	0	0
2	A	1	Total C O 22 18 4	0	0
2	A	1	Total C O 22 18 4	0	0
2	A	1	Total C O 22 18 4	0	0
2	A	1	Total C O 22 18 4	0	0
2	A	1	Total C O 22 18 4	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C O 22 18 4	0	0

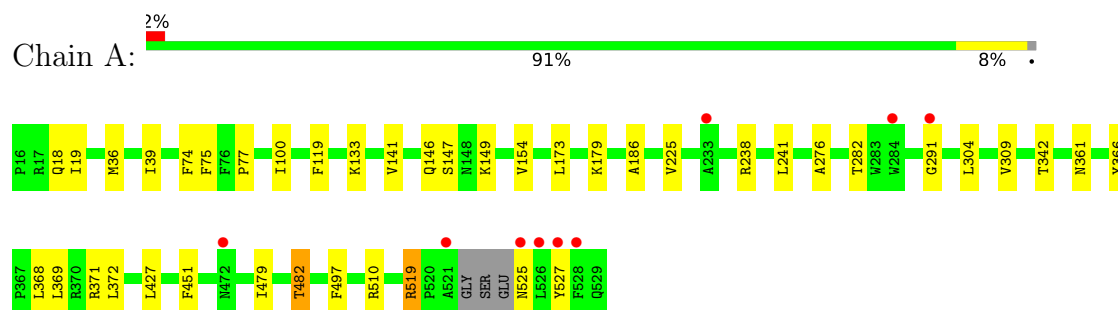
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	288	Total O 288 288	0	0

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: Proton-dependent oligopeptide transporter family protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.06Å 65.23Å 70.34Å 90.00° 96.84° 90.00°	Depositor
Resolution (Å)	24.65 – 2.10 24.65 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.65-2.10) 99.9 (24.65-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.179 , 0.213 0.179 , 0.218	Depositor DCC
R_{free} test set	1816 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 67.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4641	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.33% 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: 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	0.88	1/4134 (0.0%)	1.29	14/5625 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	ILE	CA-C	6.94	1.58	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	GLN	CA-C-N	6.22	124.16	120.24
1	A	18	GLN	C-N-CA	6.22	124.16	120.24
1	A	451	PHE	CA-CB-CG	5.67	119.47	113.80
1	A	100	ILE	CA-C-N	5.46	127.54	120.44
1	A	100	ILE	C-N-CA	5.46	127.54	120.44
1	A	173	LEU	CA-C-N	5.36	123.61	120.24
1	A	173	LEU	C-N-CA	5.36	123.61	120.24
1	A	368	LEU	CA-C-N	5.28	127.61	120.38
1	A	368	LEU	C-N-CA	5.28	127.61	120.38
1	A	427	LEU	CA-C-N	-5.25	117.78	123.08
1	A	427	LEU	C-N-CA	-5.25	117.78	123.08
1	A	291	GLY	CA-C-N	5.06	127.56	120.28
1	A	291	GLY	C-N-CA	5.06	127.56	120.28
1	A	497	PHE	CA-CB-CG	5.04	118.84	113.80

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	4007	0	4087	13	4
2	A	346	0	540	10	2
3	A	288	0	0	3	0
All	All	4641	0	4627	19	4

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 (19) 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)
2:A:608:78M:O19	3:A:701:HOH:O	2.14	0.65
1:A:141:VAL:HG12	1:A:149:LYS:HE3	1.89	0.54
1:A:309:VAL:HG21	2:A:614:78M:H18	1.94	0.50
1:A:74:PHE:CE2	1:A:133:LYS:HE2	2.46	0.49
1:A:179:LYS:HD2	1:A:342:THR:HB	1.95	0.49
2:A:608:78M:H21C	2:A:611:78M:H51C	1.98	0.46
2:A:608:78M:C17	3:A:701:HOH:O	2.64	0.46
1:A:479:ILE:O	1:A:482:THR:HG22	2.16	0.46
1:A:39:ILE:HD13	1:A:186:ALA:HB1	1.99	0.44
1:A:510:ARG:HA	2:A:609:78M:H171	1.99	0.44
1:A:119:PHE:HB2	2:A:617:78M:H142	2.00	0.43
1:A:525:ASN:C	1:A:527:TYR:H	2.27	0.42
2:A:606:78M:H202	2:A:607:78M:H31C	2.01	0.42
2:A:608:78M:H171	3:A:701:HOH:O	2.20	0.42
1:A:75:PHE:C	1:A:77:PRO:HD2	2.45	0.42
1:A:225:VAL:HG22	1:A:282:THR:HG21	2.01	0.41
1:A:361:ASN:HB3	1:A:366:TYR:CZ	2.56	0.41
2:A:603:78M:H131	2:A:611:78M:H153	2.01	0.41
1:A:276:ALA:HA	2:A:614:78M:H52C	2.02	0.41

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:SER:OG	1:A:510:ARG:NH1[4_749]	1.84	0.36
1:A:154:VAL:CG1	2:A:611:78M:O19[2_759]	2.01	0.19
1:A:371:ARG:O	1:A:519:ARG:NH2[4_759]	2.11	0.09
1:A:146:GLN:N	2:A:609:78M:O21[4_749]	2.15	0.05

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	511/514 (99%)	501 (98%)	10 (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	409/407 (100%)	401 (98%)	8 (2%)	48	56

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	MET
1	A	238	ARG
1	A	241	LEU
1	A	304	LEU
1	A	369	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	372	LEU
1	A	482	THR
1	A	519	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	164	ASN
1	A	472	ASN
1	A	525	ASN
1	A	529	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	78M	A	608	-	21,21,21	0.21	0	22,22,22	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	78M	A	615	-	7,7,21	0.18	0	6,6,22	0.13	0
2	78M	A	606	-	21,21,21	0.19	0	22,22,22	0.24	0
2	78M	A	603	-	21,21,21	0.20	0	22,22,22	0.30	0
2	78M	A	613	-	21,21,21	0.23	0	22,22,22	0.23	0
2	78M	A	604	-	21,21,21	0.26	0	22,22,22	0.28	0
2	78M	A	602	-	21,21,21	0.22	0	22,22,22	0.22	0
2	78M	A	609	-	21,21,21	0.23	0	22,22,22	0.25	0
2	78M	A	607	-	21,21,21	0.20	0	22,22,22	0.24	0
2	78M	A	616	-	7,7,21	0.19	0	6,6,22	0.10	0
2	78M	A	610	-	21,21,21	0.23	0	22,22,22	0.29	0
2	78M	A	611	-	21,21,21	0.26	0	22,22,22	0.32	0
2	78M	A	612	-	21,21,21	0.24	0	22,22,22	0.26	0
2	78M	A	617	-	21,21,21	0.18	0	22,22,22	0.36	0
2	78M	A	605	-	21,21,21	0.21	0	22,22,22	0.30	0
2	78M	A	614	-	21,21,21	0.20	0	22,22,22	0.18	0
2	78M	A	601	-	21,21,21	0.24	0	22,22,22	0.23	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
2	78M	A	608	-	-	5/21/21/21	-
2	78M	A	615	-	-	0/5/5/21	-
2	78M	A	606	-	-	4/21/21/21	-
2	78M	A	603	-	-	5/21/21/21	-
2	78M	A	613	-	-	3/21/21/21	-
2	78M	A	604	-	-	2/21/21/21	-
2	78M	A	602	-	-	2/21/21/21	-
2	78M	A	609	-	-	1/21/21/21	-
2	78M	A	607	-	-	4/21/21/21	-
2	78M	A	616	-	-	0/5/5/21	-
2	78M	A	610	-	-	4/21/21/21	-
2	78M	A	611	-	-	6/21/21/21	-
2	78M	A	612	-	-	7/21/21/21	-
2	78M	A	617	-	-	6/21/21/21	-
2	78M	A	605	-	-	5/21/21/21	-
2	78M	A	614	-	-	7/21/21/21	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	78M	A	601	-	-	2/21/21/21	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	606	78M	O2-C17-C18-C20
2	A	606	78M	O2-C17-C18-O19
2	A	605	78M	C1-C2-C3-C4
2	A	617	78M	C1-C2-C3-C4
2	A	614	78M	C1-C2-C3-C4
2	A	611	78M	O2-C17-C18-O19
2	A	614	78M	C2-C3-C4-C5
2	A	608	78M	C10-C11-C12-C13
2	A	602	78M	C2-C3-C4-C5
2	A	605	78M	C2-C3-C4-C5
2	A	605	78M	C4-C5-C6-C7
2	A	611	78M	C3-C4-C5-C6
2	A	608	78M	C2-C3-C4-C5
2	A	606	78M	C1-C2-C3-C4
2	A	608	78M	C11-C12-C13-C14
2	A	603	78M	C11-C10-C9-C8
2	A	608	78M	C4-C5-C6-C7
2	A	612	78M	C1-C2-C3-C4
2	A	611	78M	C11-C10-C9-C8
2	A	614	78M	C11-C10-C9-C8
2	A	614	78M	C4-C5-C6-C7
2	A	611	78M	O2-C17-C18-C20
2	A	612	78M	O2-C17-C18-O19
2	A	611	78M	C2-C3-C4-C5
2	A	603	78M	O19-C18-C20-O21
2	A	610	78M	C11-C10-C9-C8
2	A	607	78M	C11-C12-C13-C14
2	A	607	78M	C1-C2-C3-C4
2	A	604	78M	C2-C3-C4-C5
2	A	604	78M	C9-C10-C11-C12
2	A	617	78M	C9-C10-C11-C12
2	A	605	78M	C9-C10-C11-C12
2	A	614	78M	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	606	78M	C5-C6-C7-C8
2	A	612	78M	C11-C10-C9-C8
2	A	612	78M	C10-C11-C12-C13
2	A	601	78M	C12-C13-C14-C15
2	A	601	78M	C7-C8-C9-C10
2	A	612	78M	C2-C3-C4-C5
2	A	603	78M	C12-C13-C14-C15
2	A	605	78M	C7-C8-C9-C10
2	A	610	78M	C2-C3-C4-C5
2	A	610	78M	C9-C10-C11-C12
2	A	611	78M	C7-C8-C9-C10
2	A	612	78M	O2-C17-C18-C20
2	A	617	78M	C3-C4-C5-C6
2	A	607	78M	C7-C8-C9-C10
2	A	608	78M	C7-C8-C9-C10
2	A	610	78M	C5-C6-C7-C8
2	A	602	78M	C10-C11-C12-C13
2	A	609	78M	C9-C10-C11-C12
2	A	612	78M	C5-C6-C7-C8
2	A	613	78M	O2-C1-C2-C3
2	A	607	78M	C5-C6-C7-C8
2	A	614	78M	C11-C12-C13-C14
2	A	614	78M	C3-C4-C5-C6
2	A	603	78M	O2-C1-C2-C3
2	A	613	78M	C11-C12-C13-C14
2	A	613	78M	O1-C1-C2-C3
2	A	603	78M	O1-C1-C2-C3
2	A	617	78M	C7-C8-C9-C10
2	A	617	78M	O2-C1-C2-C3
2	A	617	78M	O1-C1-C2-C3

There are no ring outliers.

8 monomers are involved in 12 short contacts:

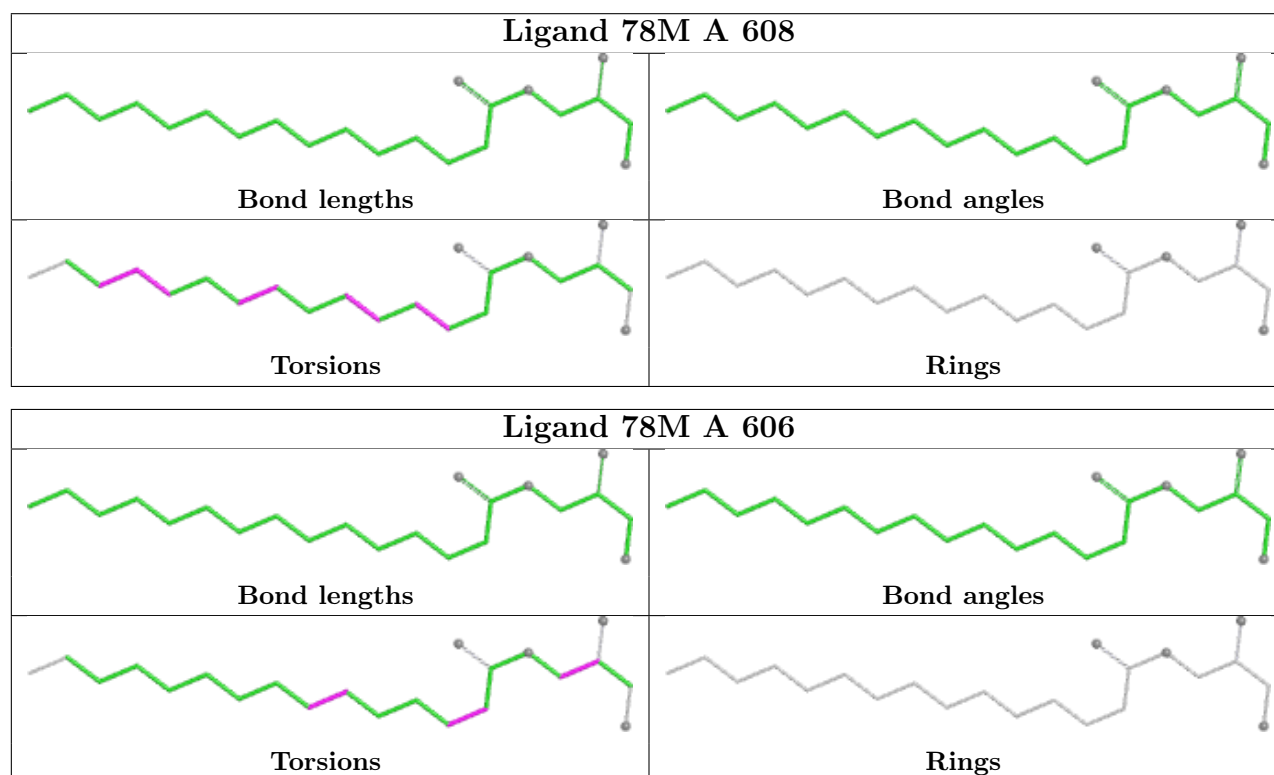
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	608	78M	4	0
2	A	606	78M	1	0
2	A	603	78M	1	0
2	A	609	78M	1	1
2	A	607	78M	1	0
2	A	611	78M	2	1
2	A	617	78M	1	0

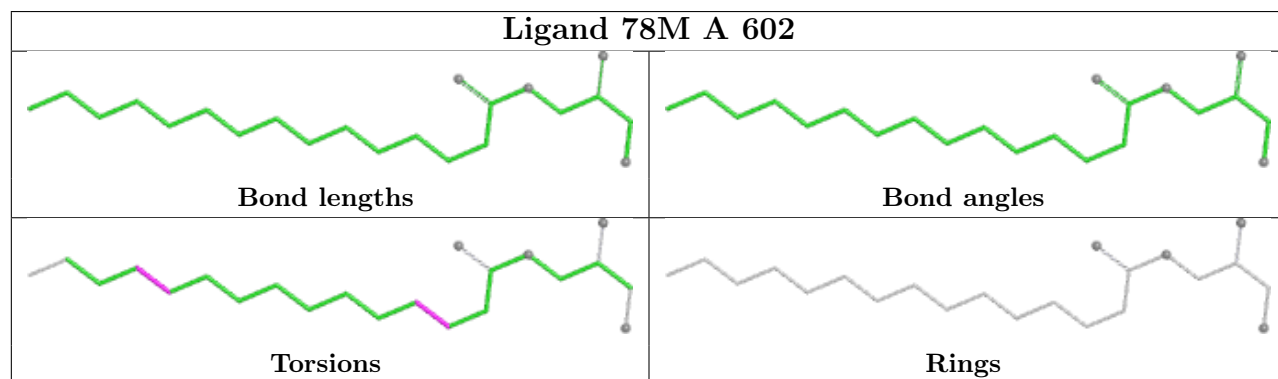
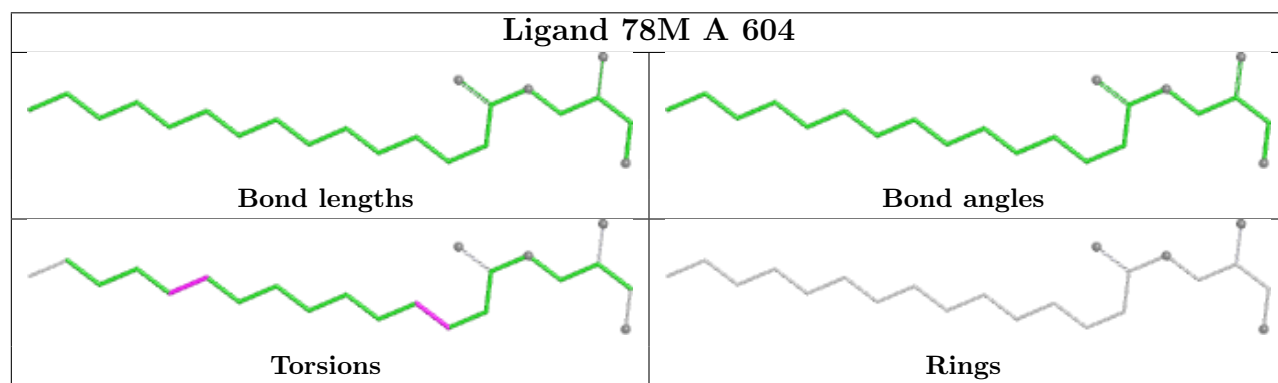
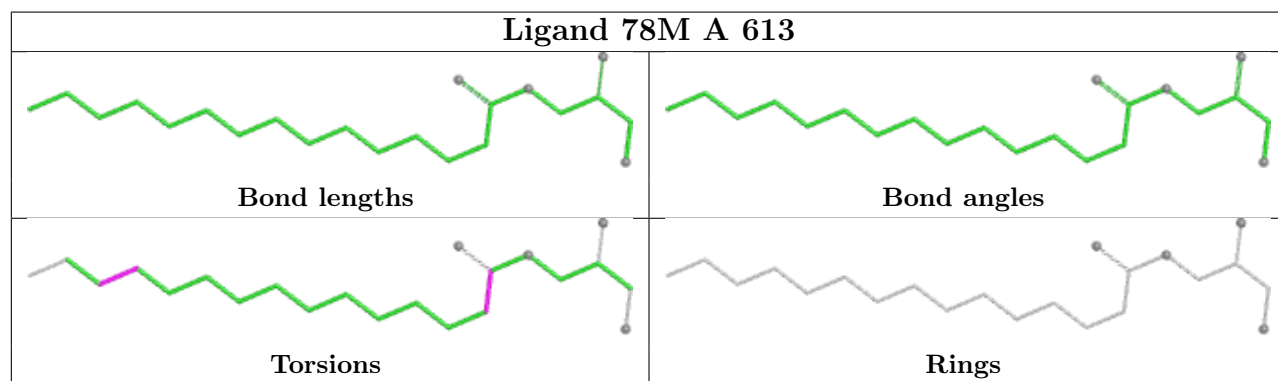
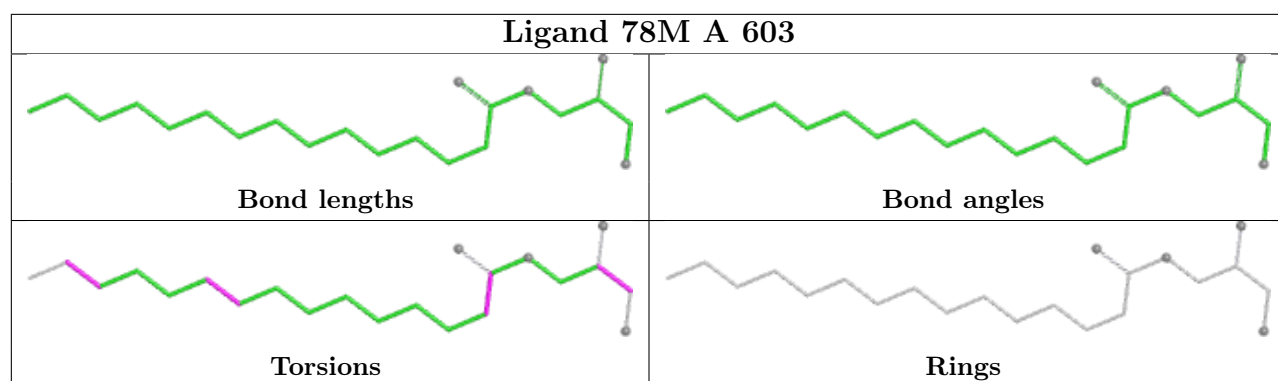
Continued on next page...

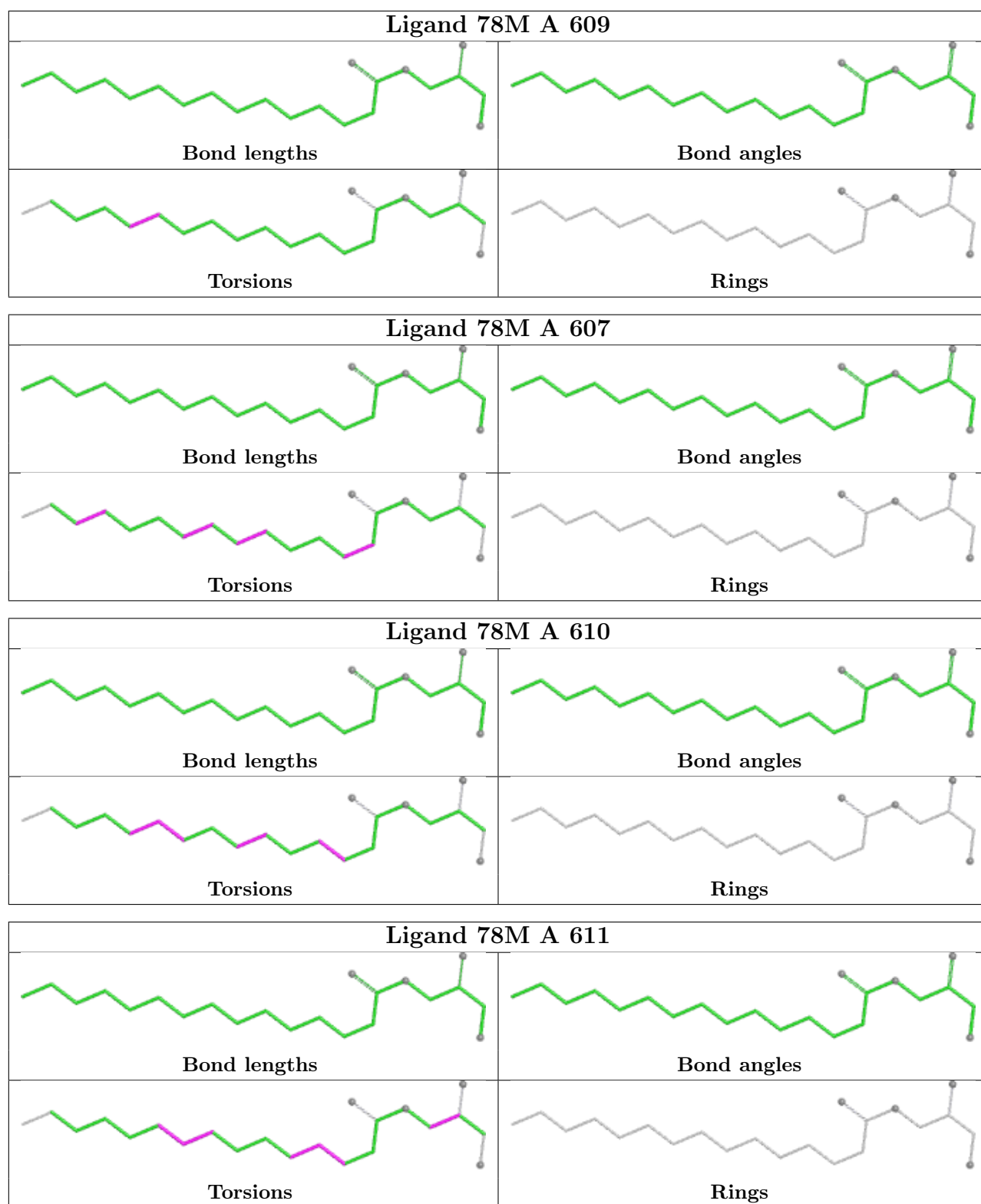
Continued from previous page...

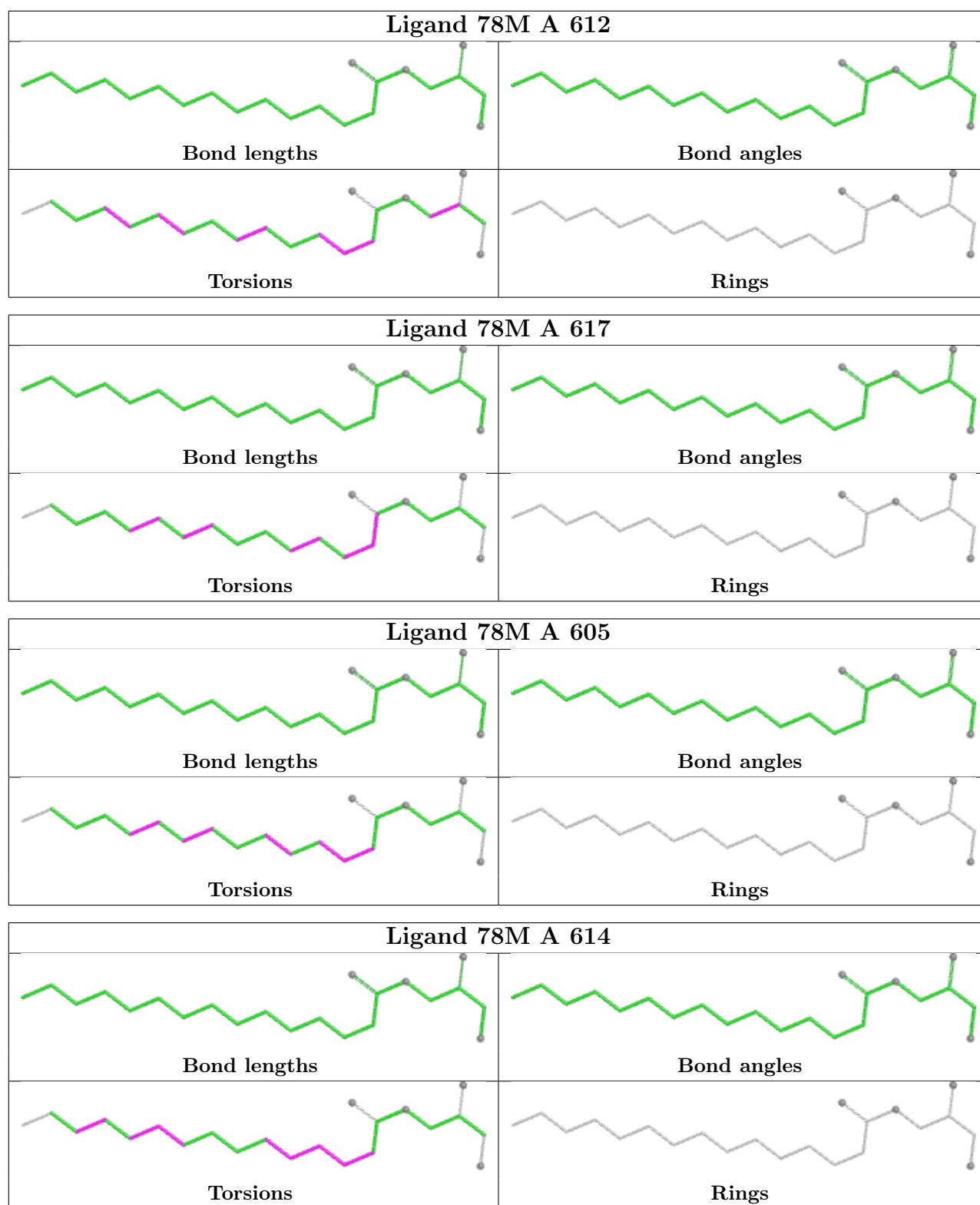
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	614	78M	2	0

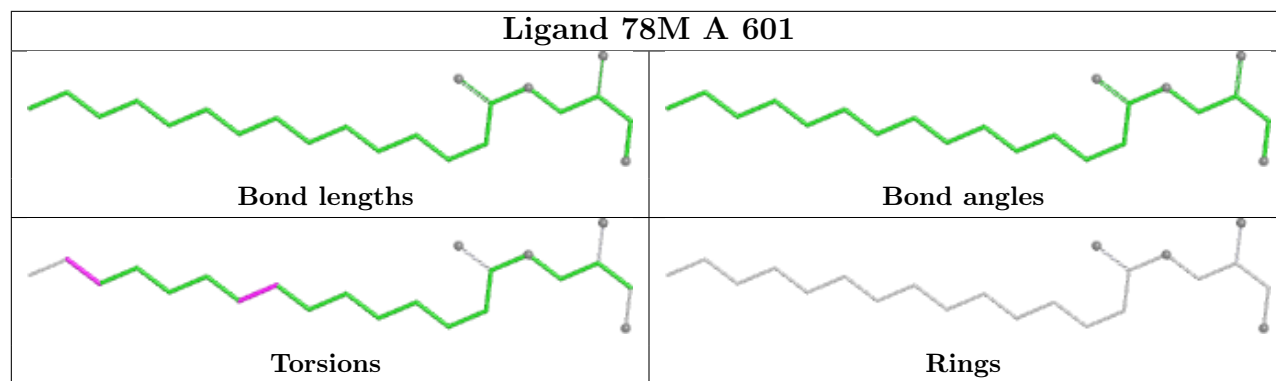
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	511/514 (99%)	-0.01	9 (1%) 67 70	18, 36, 72, 108	7 (1%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	284	TRP	3.3
1	A	526	LEU	2.8
1	A	525	ASN	2.7
1	A	291	GLY	2.3
1	A	521	ALA	2.2
1	A	233	ALA	2.2
1	A	527	TYR	2.2
1	A	528	PHE	2.1
1	A	472	ASN	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

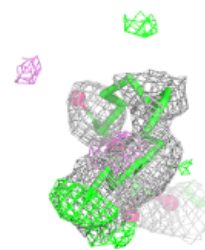
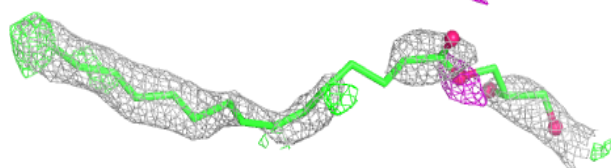
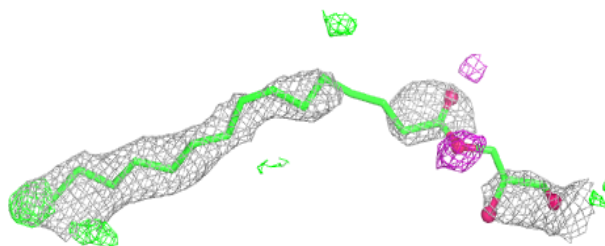
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	78M	A	617	22/22	0.64	0.20	74,87,94,95	0
2	78M	A	615	8/22	0.67	0.29	81,82,82,83	0
2	78M	A	613	22/22	0.69	0.18	83,102,117,118	0
2	78M	A	607	22/22	0.70	0.21	80,101,108,109	0
2	78M	A	604	22/22	0.72	0.20	74,83,94,96	0
2	78M	A	614	22/22	0.72	0.22	77,86,89,89	0
2	78M	A	601	22/22	0.72	0.19	72,79,85,88	0
2	78M	A	611	22/22	0.72	0.22	67,75,96,98	0
2	78M	A	610	22/22	0.73	0.22	62,74,83,85	0
2	78M	A	612	22/22	0.73	0.17	73,75,91,93	0
2	78M	A	602	22/22	0.77	0.18	65,73,97,99	0
2	78M	A	608	22/22	0.79	0.17	63,71,94,96	0
2	78M	A	609	22/22	0.79	0.17	66,74,92,94	0
2	78M	A	603	22/22	0.79	0.20	64,70,76,77	0
2	78M	A	605	22/22	0.83	0.16	66,73,89,91	0
2	78M	A	606	22/22	0.83	0.16	55,59,73,74	0
2	78M	A	616	8/22	0.84	0.17	71,75,79,80	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.

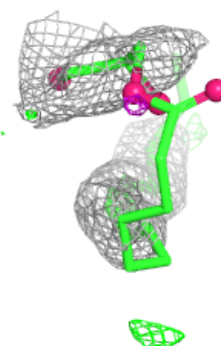
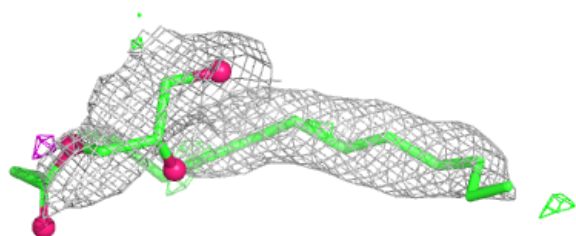
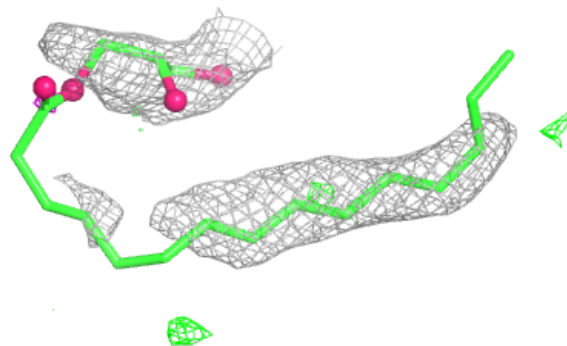
Electron density around 78M A 617:

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

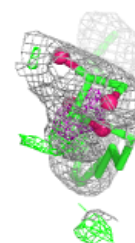
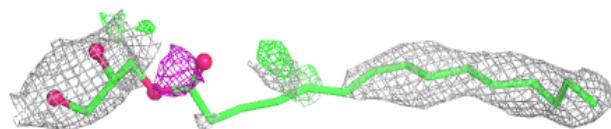
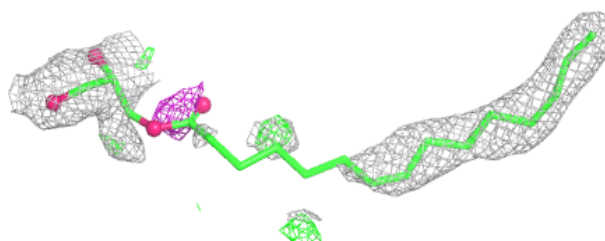


Electron density around 78M A 613:

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

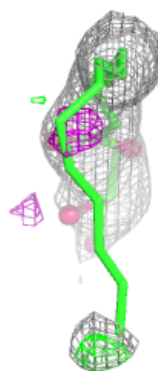
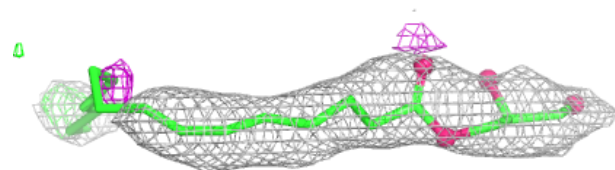
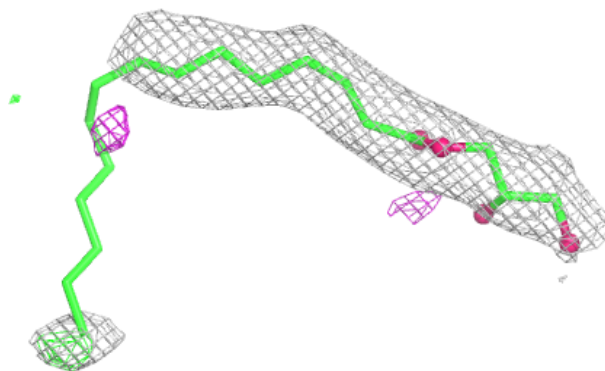
**Electron density around 78M A 607:**

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

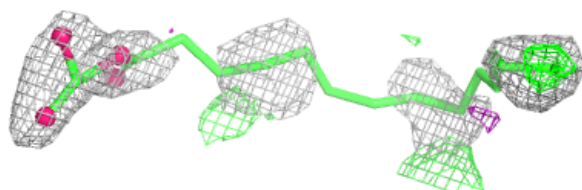
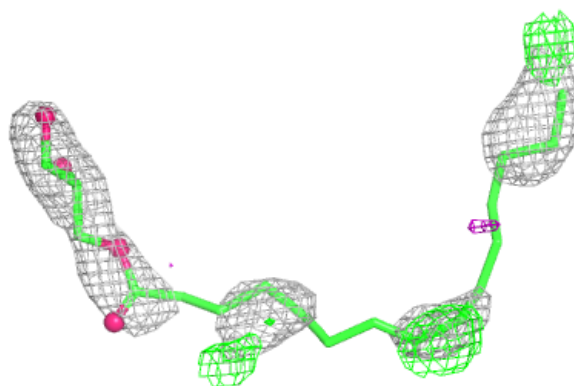


Electron density around 78M A 604:

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

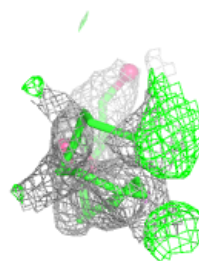
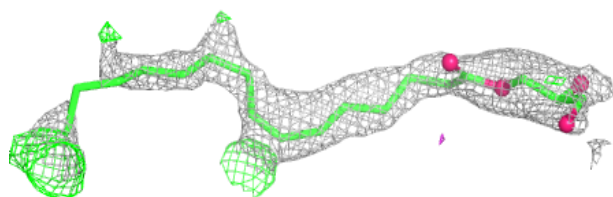
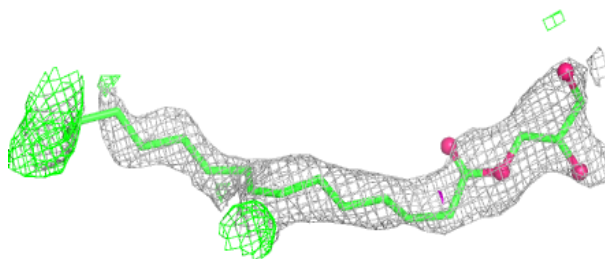
**Electron density around 78M A 614:**

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

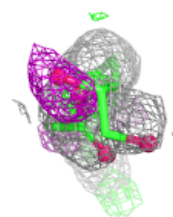
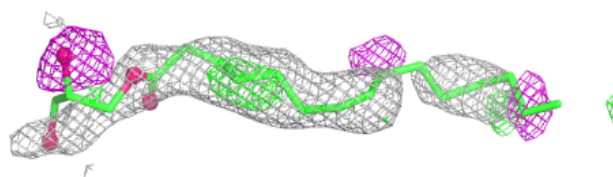
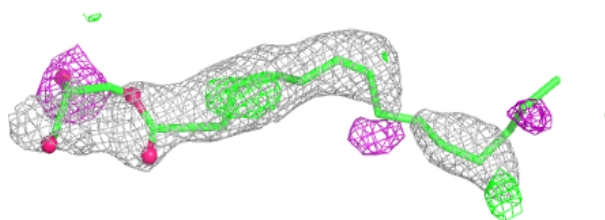


Electron density around 78M A 601:

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

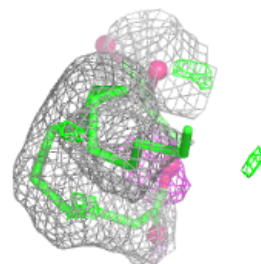
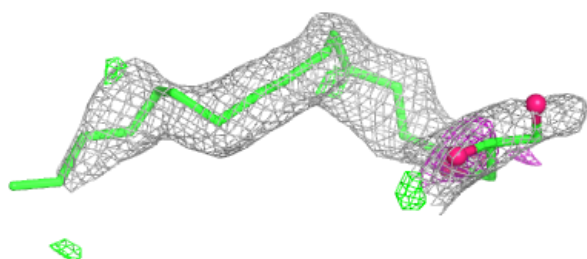
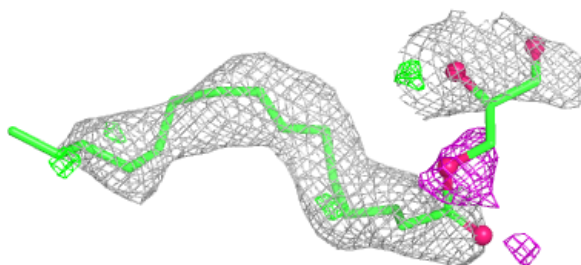
**Electron density around 78M A 611:**

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

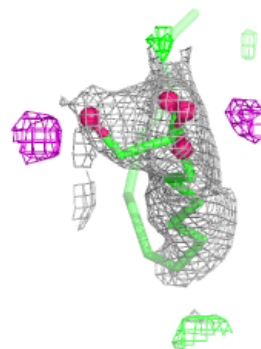
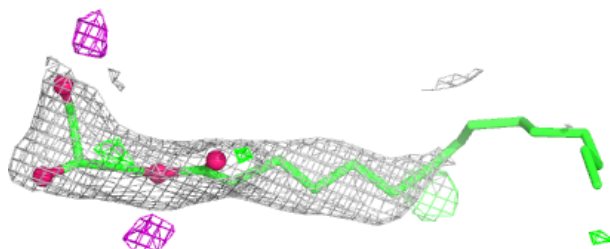
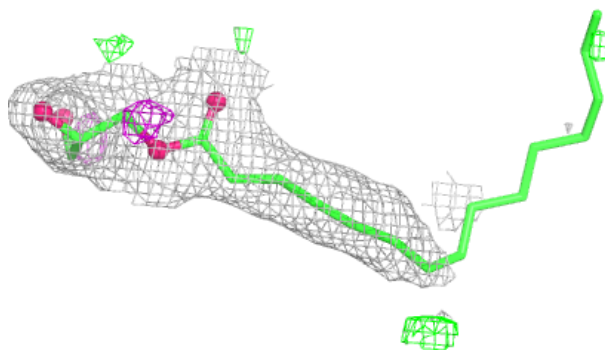


Electron density around 78M A 610:

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

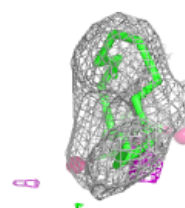
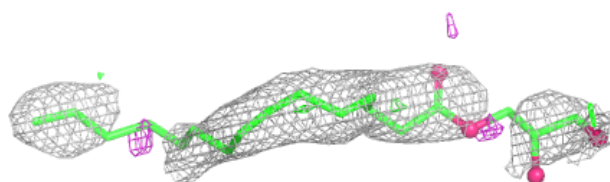
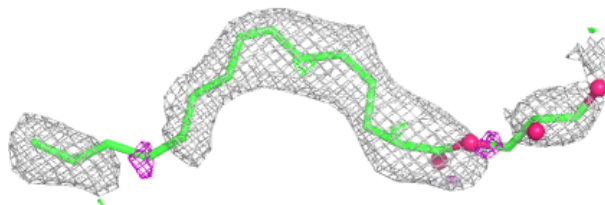
**Electron density around 78M A 612:**

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

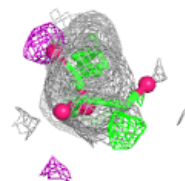
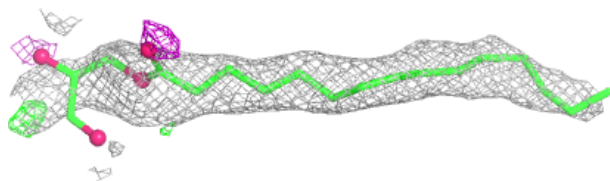
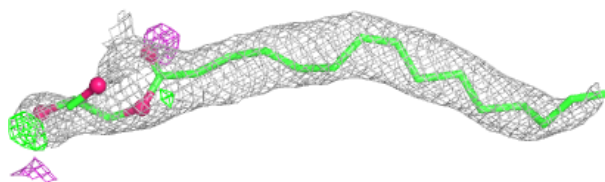


Electron density around 78M A 602:

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

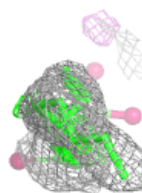
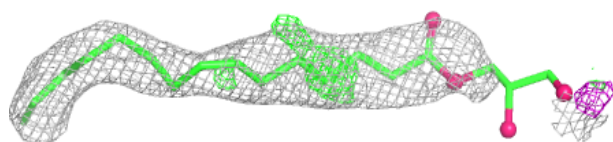
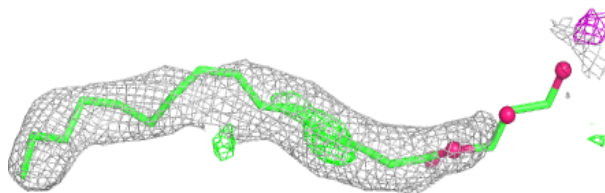
**Electron density around 78M A 608:**

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

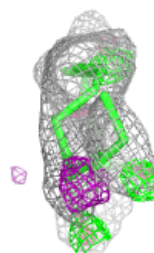
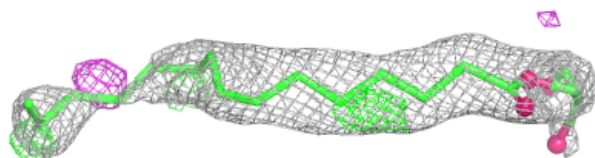
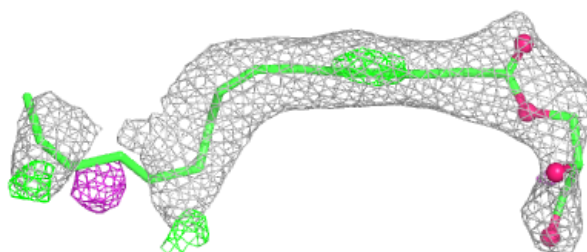


Electron density around 78M A 609:

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

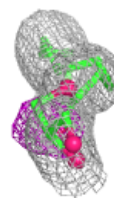
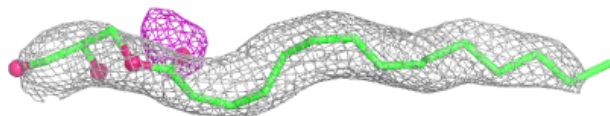
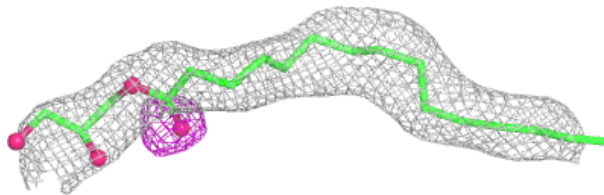
**Electron density around 78M A 603:**

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

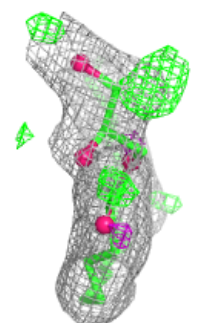
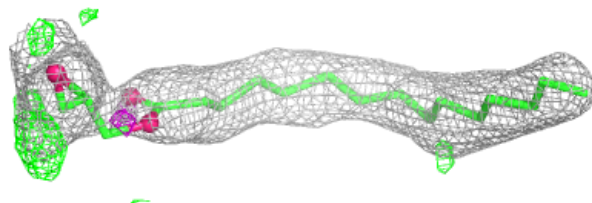
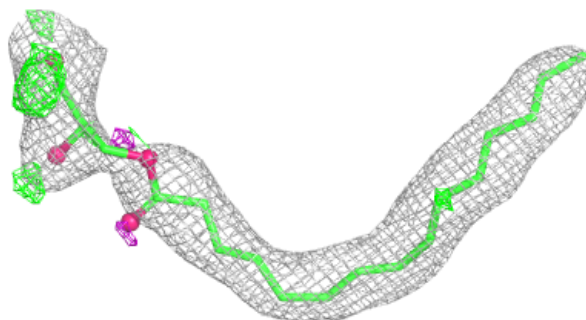


Electron density around 78M A 605:

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

**Electron density around 78M A 606:**

$2mF_o-DF_c$ (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.