



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:38 PM UTC

PDB ID : 8AQ3 / pdb_00008aq3
Title : In surfo structure of the membrane integral lipoprotein N-acyltransferase Lnt from E. coli in complex with PE
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Deposited on : 2022-08-11
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

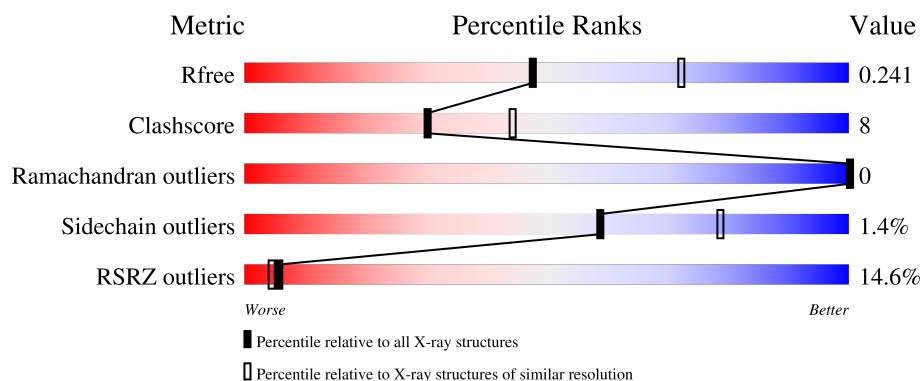
1 Overall quality at a glance

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	532	

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
8	LMT	A	617	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 4398 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.

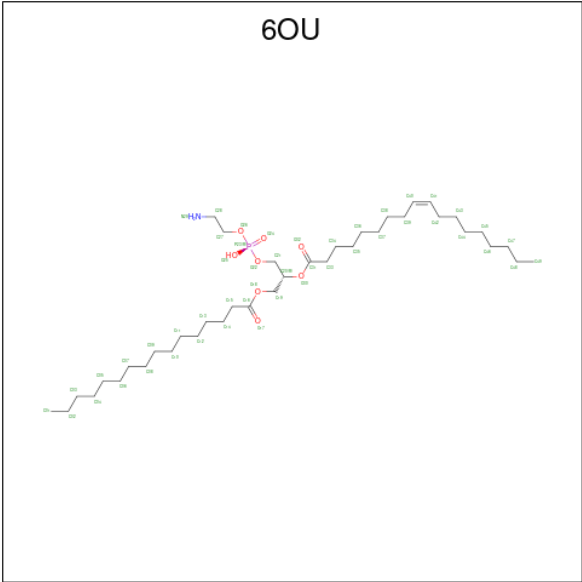
- Molecule 1 is a protein called Apolipoprotein N-acyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	508	Total	C	N	O	S	0	0	0
			3991	2626	660	690	15			

There are 21 discrepancies between the modelled and reference sequences:

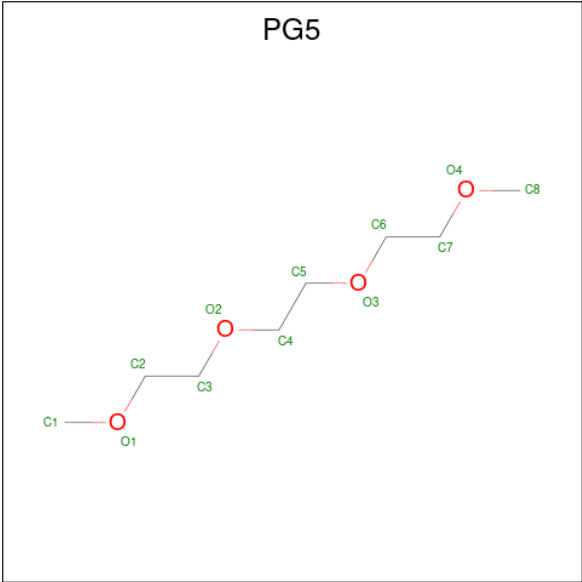
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P23930
A	-18	GLY	-	expression tag	UNP P23930
A	-17	SER	-	expression tag	UNP P23930
A	-16	SER	-	expression tag	UNP P23930
A	-15	HIS	-	expression tag	UNP P23930
A	-14	HIS	-	expression tag	UNP P23930
A	-13	HIS	-	expression tag	UNP P23930
A	-12	HIS	-	expression tag	UNP P23930
A	-11	HIS	-	expression tag	UNP P23930
A	-10	HIS	-	expression tag	UNP P23930
A	-9	SER	-	expression tag	UNP P23930
A	-8	SER	-	expression tag	UNP P23930
A	-7	GLY	-	expression tag	UNP P23930
A	-6	LEU	-	expression tag	UNP P23930
A	-5	VAL	-	expression tag	UNP P23930
A	-4	PRO	-	expression tag	UNP P23930
A	-3	ARG	-	expression tag	UNP P23930
A	-2	GLY	-	expression tag	UNP P23930
A	-1	SER	-	expression tag	UNP P23930
A	0	HIS	-	expression tag	UNP P23930
A	387	ALA	CYS	engineered mutation	UNP P23930

- Molecule 2 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-p ropan-2-yl] ({Z})-octadec-9-enoate (CCD ID: 6OU) (formula: C₃₉H₇₆NO₈P) (labeled as "Ligand of Interest" by depositor).



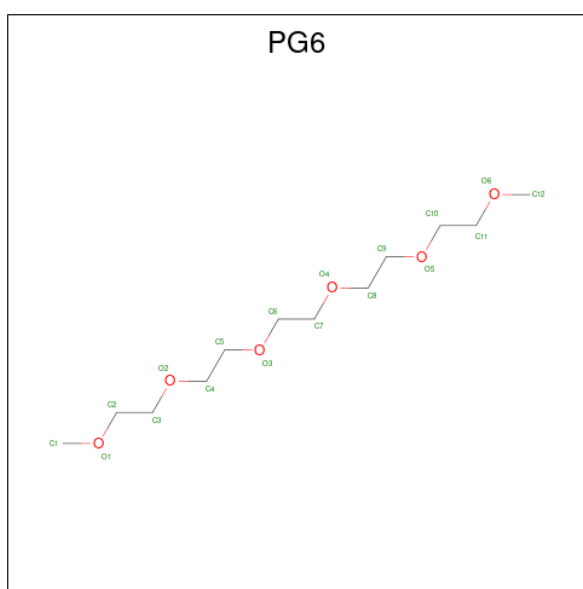
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

- Molecule 3 is 1-METHOXY-2-[2-(2-METHOXY-ETHOXY)-ETHANE] (CCD ID: PG5) (formula: C₈H₁₈O₄).



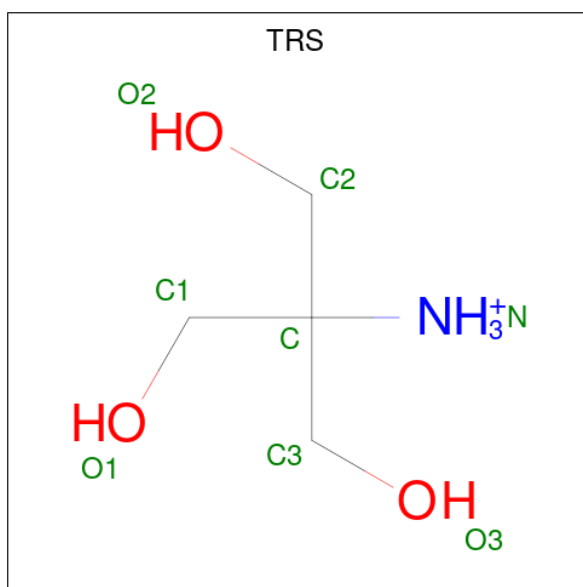
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			11	7	4		
3	A	1	Total	C	O	0	0
			8	5	3		
3	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANE (CCD ID: PG6) (formula: C₁₂H₂₆O₆).



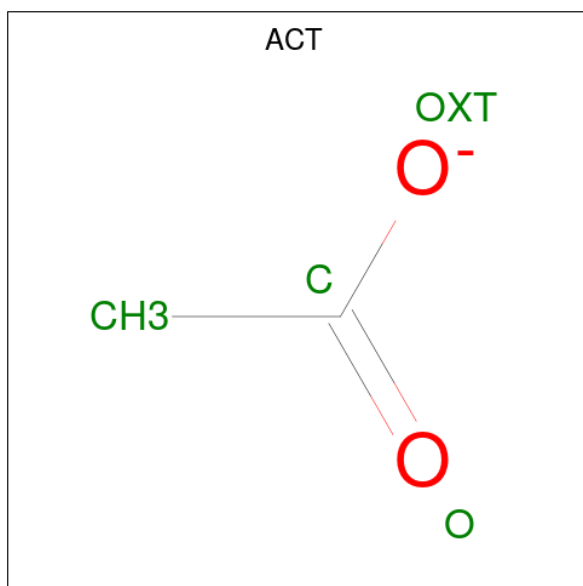
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	9	4		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



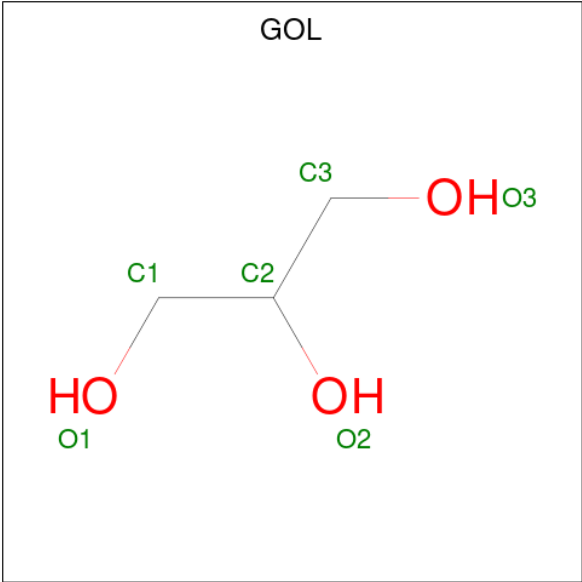
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



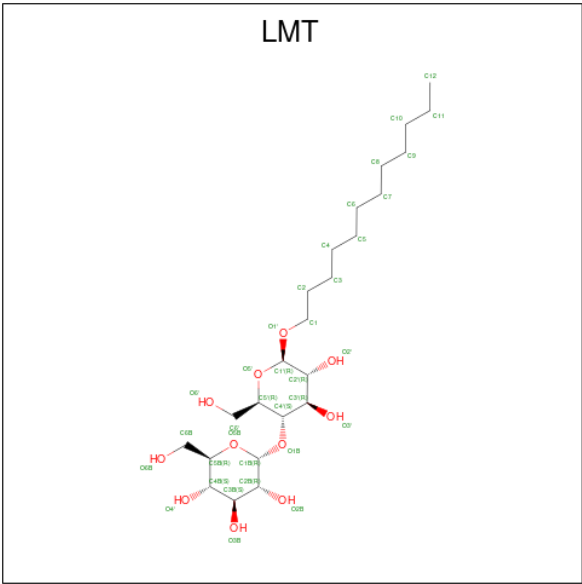
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 35 24 11	0	0
8	A	1	Total C O 35 24 11	0	0
8	A	1	Total C 12 12	0	0
8	A	1	Total C 12 12	0	0
8	A	1	Total C 12 12	0	0

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	3	Total Cl 3 3	0	0

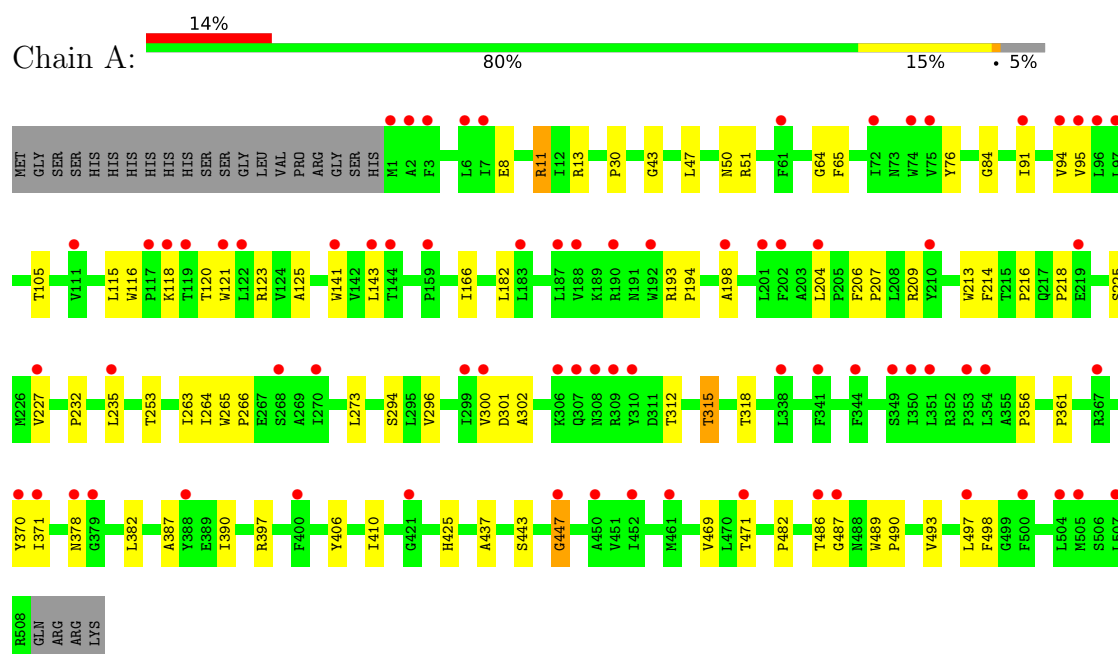
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	57	Total O 57 57	0	0

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: Apolipoprotein N-acyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.99Å 160.99Å 91.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.38 – 2.40 43.38 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.38-2.40) 87.1 (43.38-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.41 (at 2.39Å)	Xtriage
Refinement program	PHENIX dev_3494	Depositor
R, R_{free}	0.225 , 0.240 0.229 , 0.241	Depositor DCC
R_{free} test set	2004 reflections (3.72%)	wwPDB-VP
Wilson B-factor (Å ²)	53.0	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4398	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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: ACT, 6OU, TRS, PG6, CL, LMT, PG5, GOL

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	0.33	0/4106	0.56	2/5611 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	447	GLY	CA-C-N	-5.71	113.90	122.01
1	A	447	GLY	C-N-CA	-5.71	113.90	122.01

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	3991	0	4057	61	0
2	A	147	0	0	8	0
3	A	39	0	50	3	0
4	A	13	0	17	4	0
5	A	8	0	12	0	0
6	A	4	0	3	0	0
7	A	30	0	40	2	0
8	A	106	0	161	9	0
9	A	3	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	57	0	0	1	0
All	All	4398	0	4340	73	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 8.

All (73) 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:227:VAL:HG12	1:A:469:VAL:CG2	1.73	1.18
1:A:227:VAL:HG12	1:A:469:VAL:HG22	1.16	1.10
1:A:227:VAL:CG1	1:A:469:VAL:HG22	2.01	0.91
8:A:613:LMT:H1B	8:A:613:LMT:C6'	2.04	0.87
1:A:8:GLU:CD	4:A:607:PG6:H71	2.06	0.81
1:A:227:VAL:HG12	1:A:469:VAL:HG21	1.68	0.72
1:A:30:PRO:HA	2:A:602:6OU:C06	2.20	0.71
8:A:613:LMT:H1B	8:A:613:LMT:O6'	1.89	0.71
3:A:606:PG5:H41	7:A:611:GOL:O2	1.93	0.69
8:A:613:LMT:H1B	8:A:613:LMT:H6E	1.75	0.68
3:A:606:PG5:H61	7:A:611:GOL:O2	1.95	0.66
1:A:193:ARG:NH1	9:A:622:CL:CL	2.59	0.64
1:A:273:LEU:HD23	1:A:300:VAL:HG12	1.78	0.64
1:A:296:VAL:HG12	1:A:318:THR:HG22	1.79	0.63
8:A:613:LMT:H22	8:A:613:LMT:O2'	1.98	0.62
1:A:361:PRO:O	2:A:601:6OU:N29	2.33	0.61
1:A:264:ILE:HG23	1:A:296:VAL:HG23	1.83	0.60
1:A:8:GLU:OE2	4:A:607:PG6:H71	2.02	0.60
1:A:387:ALA:HB1	2:A:601:6OU:C15	2.32	0.60
1:A:482:PRO:O	1:A:486:THR:HG22	2.02	0.59
1:A:447:GLY:N	10:A:705:HOH:O	2.33	0.58
1:A:76:TYR:HB2	1:A:94:VAL:HG21	1.85	0.57
1:A:141:TRP:CZ2	8:A:613:LMT:O3'	2.57	0.57
1:A:64:GLY:HA3	1:A:105:THR:HG21	1.86	0.56
1:A:204:LEU:O	1:A:207:PRO:HD2	2.08	0.54
1:A:115:LEU:HB2	1:A:116:TRP:CE3	2.43	0.54
1:A:387:ALA:HB1	2:A:601:6OU:C16	2.38	0.53
8:A:613:LMT:H4'	8:A:613:LMT:O2B	2.10	0.52
1:A:91:ILE:O	1:A:95:VAL:HG12	2.10	0.52
1:A:13:ARG:CZ	1:A:51:ARG:HD3	2.40	0.52
1:A:182:LEU:HB2	1:A:198:ALA:HB2	1.91	0.52
1:A:125:ALA:HB2	1:A:182:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:THR:HG23	1:A:487:GLY:O	2.10	0.51
2:A:620:6OU:C49	2:A:620:6OU:C03	2.89	0.51
1:A:302:ALA:HA	1:A:312:THR:HA	1.94	0.50
1:A:50:ASN:O	1:A:51:ARG:HD2	2.12	0.50
1:A:227:VAL:HG22	1:A:265:TRP:CD1	2.46	0.49
1:A:489:TRP:CG	1:A:490:PRO:HD3	2.48	0.49
1:A:84:GLY:HA3	1:A:356:PRO:HG2	1.93	0.48
1:A:206:PHE:O	1:A:209:ARG:HG2	2.13	0.48
1:A:387:ALA:CB	2:A:601:6OU:C16	2.92	0.48
1:A:166:ILE:HA	1:A:482:PRO:HB2	1.96	0.47
1:A:387:ALA:CB	2:A:601:6OU:O17	2.63	0.47
1:A:214:PHE:HB3	1:A:437:ALA:HB1	1.96	0.47
1:A:225:SER:OG	1:A:471:THR:HG22	2.16	0.46
1:A:490:PRO:O	1:A:493:VAL:HG22	2.16	0.46
1:A:387:ALA:HB1	2:A:601:6OU:O17	2.17	0.45
1:A:397:ARG:HD3	1:A:397:ARG:C	2.41	0.45
1:A:13:ARG:HH22	4:A:607:PG6:H62	1.81	0.44
1:A:193:ARG:HB3	1:A:194:PRO:HD3	2.00	0.44
1:A:410:ILE:HA	1:A:443:SER:O	2.18	0.44
1:A:65:PHE:CZ	1:A:95:VAL:HG23	2.53	0.44
1:A:118:LYS:O	1:A:120:THR:HG23	2.19	0.43
1:A:216:PRO:O	1:A:218:PRO:HD3	2.19	0.43
1:A:301:ASP:HB3	1:A:315:THR:HG21	1.99	0.43
4:A:607:PG6:H62	4:A:607:PG6:H42	1.51	0.42
3:A:604:PG5:C7	3:A:604:PG5:H42	2.49	0.42
1:A:11:ARG:HD3	9:A:623:CL:CL	2.56	0.42
1:A:13:ARG:NH1	1:A:51:ARG:HD3	2.34	0.42
1:A:43:GLY:O	1:A:47:LEU:HB2	2.19	0.42
1:A:213:TRP:CE3	1:A:482:PRO:HD3	2.54	0.42
1:A:227:VAL:CB	1:A:469:VAL:HG22	2.46	0.42
8:A:612:LMT:H1B	8:A:612:LMT:H5'	1.79	0.42
1:A:232:PRO:HG2	1:A:235:LEU:HD12	2.00	0.42
1:A:266:PRO:HA	1:A:410:ILE:HB	2.01	0.42
1:A:143:LEU:H	8:A:613:LMT:H1'	1.85	0.42
1:A:486:THR:OG1	1:A:489:TRP:NE1	2.53	0.42
8:A:613:LMT:C6'	8:A:613:LMT:C1B	2.85	0.41
1:A:382:LEU:HD23	1:A:406:TYR:HB2	2.02	0.41
1:A:253:THR:HG23	1:A:263:ILE:HD13	2.02	0.41
1:A:497:LEU:HD12	1:A:498:PHE:HD1	1.85	0.41
1:A:390:ILE:HG22	1:A:425:HIS:HE1	1.85	0.41
1:A:370:TYR:HD2	1:A:371:ILE:HG12	1.86	0.41

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	506/532 (95%)	488 (96%)	18 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	421/443 (95%)	415 (99%)	6 (1%)	59	79

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	121	TRP
1	A	123	ARG
1	A	294	SER
1	A	315	THR
1	A	378	ASN

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

Mol	Chain	Res	Type
1	A	50	ASN
1	A	228	GLN
1	A	278	GLN
1	A	308	ASN

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](#)

Of 23 ligands modelled in this entry, 3 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	LMT	A	613	-	36,36,36	1.25	2 (5%)	47,47,47	1.29	4 (8%)
5	TRS	A	608	-	7,7,7	0.14	0	9,9,9	0.25	0
3	PG5	A	603	-	9,9,11	0.54	0	8,8,10	0.29	0
2	6OU	A	601	-	48,48,48	1.04	4 (8%)	51,53,53	0.92	2 (3%)
7	GOL	A	614	-	5,5,5	0.92	0	5,5,5	1.14	0
3	PG5	A	605	-	7,7,11	0.59	0	6,6,10	0.36	0
7	GOL	A	616	-	5,5,5	0.66	0	5,5,5	0.99	0
2	6OU	A	602	-	48,48,48	1.04	4 (8%)	51,53,53	0.89	2 (3%)
8	LMT	A	618	-	11,11,36	1.05	0	10,10,47	0.57	0
7	GOL	A	610	-	5,5,5	1.00	0	5,5,5	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	LMT	A	612	-	36,36,36	1.29	3 (8%)	47,47,47	0.80	1 (2%)
3	PG5	A	604	-	10,10,11	0.56	0	9,9,10	0.18	0
6	ACT	A	609	-	3,3,3	1.52	1 (33%)	3,3,3	1.46	0
8	LMT	A	619	-	11,11,36	0.99	0	10,10,47	0.60	0
3	PG5	A	606	-	9,9,11	0.59	0	8,8,10	0.51	0
7	GOL	A	615	-	5,5,5	0.10	0	5,5,5	0.30	0
2	6OU	A	620	-	48,48,48	1.04	4 (8%)	51,53,53	0.89	2 (3%)
7	GOL	A	611	-	5,5,5	0.11	0	5,5,5	0.35	0
8	LMT	A	617	-	11,11,36	0.85	0	10,10,47	0.73	0
4	PG6	A	607	-	12,12,17	0.60	0	11,11,16	0.41	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
8	LMT	A	613	-	-	15/21/61/61	0/2/2/2
5	TRS	A	608	-	-	8/9/9/9	-
3	PG5	A	603	-	-	6/7/7/9	-
2	6OU	A	601	-	-	38/52/52/52	-
7	GOL	A	614	-	-	0/4/4/4	-
3	PG5	A	605	-	-	3/5/5/9	-
7	GOL	A	616	-	-	1/4/4/4	-
2	6OU	A	602	-	-	22/52/52/52	-
8	LMT	A	618	-	-	1/9/9/61	-
7	GOL	A	610	-	-	1/4/4/4	-
8	LMT	A	612	-	-	13/21/61/61	0/2/2/2
3	PG5	A	604	-	-	6/8/8/9	-
8	LMT	A	619	-	-	2/9/9/61	-
3	PG5	A	606	-	-	3/7/7/9	-
7	GOL	A	615	-	-	0/4/4/4	-
2	6OU	A	620	-	-	28/52/52/52	-
7	GOL	A	611	-	-	4/4/4/4	-
8	LMT	A	617	-	-	2/9/9/61	-
4	PG6	A	607	-	-	6/10/10/15	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	612	LMT	O5'-C1'	4.11	1.52	1.41
8	A	612	LMT	O5B-C1B	3.42	1.50	1.41
8	A	613	LMT	O5'-C1'	3.42	1.50	1.41
2	A	620	6OU	O18-C16	3.22	1.42	1.33
2	A	601	6OU	O18-C16	3.19	1.42	1.33
2	A	602	6OU	O18-C16	3.17	1.42	1.33
2	A	602	6OU	O30-C20	-2.90	1.39	1.46
2	A	620	6OU	O30-C20	-2.85	1.39	1.46
2	A	601	6OU	O30-C20	-2.69	1.40	1.46
8	A	613	LMT	O5B-C1B	2.67	1.48	1.41
2	A	620	6OU	O30-C31	2.32	1.40	1.34
2	A	602	6OU	O30-C31	2.30	1.40	1.34
2	A	601	6OU	O30-C31	2.28	1.40	1.34
6	A	609	ACT	CH3-C	2.23	1.57	1.49
2	A	601	6OU	P23-O22	2.17	1.67	1.59
2	A	602	6OU	P23-O22	2.17	1.67	1.59
2	A	620	6OU	P23-O22	2.15	1.67	1.59
8	A	612	LMT	O5'-C5'	2.14	1.49	1.44

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	613	LMT	C1B-O5B-C5B	-4.23	105.47	113.72
2	A	620	6OU	O30-C31-C33	3.93	119.99	111.48
2	A	601	6OU	O30-C31-C33	3.93	119.98	111.48
2	A	602	6OU	O30-C31-C33	3.92	119.95	111.48
8	A	613	LMT	O5'-C5'-C4'	3.55	117.06	109.72
8	A	613	LMT	C6'-C5'-C4'	-3.12	104.61	113.38
8	A	613	LMT	C1B-O1B-C4'	-3.04	110.76	117.98
2	A	601	6OU	O18-C16-C15	2.69	120.04	111.83
2	A	620	6OU	O18-C16-C15	2.68	120.02	111.83
2	A	602	6OU	O18-C16-C15	2.67	119.98	111.83
8	A	612	LMT	C1B-O1B-C4'	-2.41	112.27	117.98

There are no chirality outliers.

All (159) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	6OU	C15-C16-O18-C19
2	A	601	6OU	O30-C20-C21-O22
2	A	601	6OU	C21-O22-P23-O25
2	A	601	6OU	C27-O26-P23-O25

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Mol	Chain	Res	Type	Atoms
2	A	601	6OU	O26-C27-C28-N29
2	A	601	6OU	C33-C31-O30-C20
2	A	602	6OU	C27-O26-P23-O22
2	A	602	6OU	C27-O26-P23-O24
2	A	602	6OU	C27-O26-P23-O25
2	A	602	6OU	C33-C31-O30-C20
2	A	620	6OU	C21-O22-P23-O25
2	A	620	6OU	C21-O22-P23-O26
2	A	620	6OU	O26-C27-C28-N29
2	A	620	6OU	C33-C31-O30-C20
5	A	608	TRS	C2-C-C1-O1
5	A	608	TRS	C3-C-C1-O1
5	A	608	TRS	N-C-C1-O1
5	A	608	TRS	C1-C-C2-O2
5	A	608	TRS	C3-C-C2-O2
5	A	608	TRS	N-C-C2-O2
7	A	611	GOL	O1-C1-C2-C3
8	A	613	LMT	C2'-C1'-O1'-C1
8	A	613	LMT	O5'-C1'-O1'-C1
8	A	613	LMT	C2-C1-O1'-C1'
2	A	601	6OU	O17-C16-O18-C19
2	A	601	6OU	O32-C31-O30-C20
2	A	602	6OU	O32-C31-O30-C20
2	A	602	6OU	C15-C16-O18-C19
4	A	607	PG6	C4-C5-O3-C6
2	A	620	6OU	O32-C31-O30-C20
3	A	604	PG5	C4-C5-O3-C6
8	A	613	LMT	O5B-C5B-C6B-O6B
2	A	602	6OU	C33-C34-C35-C36
8	A	613	LMT	O5B-C1B-O1B-C4'
2	A	602	6OU	O17-C16-O18-C19
8	A	612	LMT	O5'-C1'-O1'-C1
4	A	607	PG6	O2-C4-C5-O3
8	A	613	LMT	C2B-C1B-O1B-C4'
2	A	601	6OU	C13-C14-C15-C16
8	A	613	LMT	O5'-C5'-C6'-O6'
3	A	603	PG5	O2-C4-C5-O3
8	A	613	LMT	C4'-C5'-C6'-O6'
8	A	612	LMT	O1'-C1-C2-C3
2	A	620	6OU	C15-C16-O18-C19
8	A	613	LMT	C7-C8-C9-C10
8	A	612	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
8	A	612	LMT	C4'-C5'-C6'-O6'
3	A	606	PG5	O2-C4-C5-O3
7	A	611	GOL	O1-C1-C2-O2
3	A	606	PG5	O1-C2-C3-O2
2	A	601	6OU	C31-C33-C34-C35
2	A	620	6OU	O17-C16-O18-C19
8	A	612	LMT	C5'-C4'-O1B-C1B
8	A	613	LMT	C4B-C5B-C6B-O6B
2	A	601	6OU	C37-C38-C39-C40
3	A	604	PG5	O2-C4-C5-O3
3	A	605	PG5	O3-C6-C7-O4
4	A	607	PG6	O1-C2-C3-O2
3	A	604	PG5	O3-C6-C7-O4
8	A	612	LMT	O5'-C5'-C6'-O6'
8	A	618	LMT	C11-C10-C9-C8
3	A	605	PG5	O2-C4-C5-O3
4	A	607	PG6	C9-C8-O4-C7
7	A	611	GOL	C1-C2-C3-O3
2	A	602	6OU	C06-C07-C08-C09
2	A	601	6OU	C02-C03-C04-C05
2	A	602	6OU	C35-C36-C37-C38
8	A	612	LMT	C4-C5-C6-C7
8	A	613	LMT	C2-C3-C4-C5
8	A	619	LMT	C3-C4-C5-C6
2	A	601	6OU	C03-C04-C05-C06
2	A	620	6OU	C08-C09-C10-C11
8	A	612	LMT	C3'-C4'-O1B-C1B
8	A	617	LMT	C6-C7-C8-C9
2	A	620	6OU	C09-C10-C11-C12
2	A	601	6OU	C10-C11-C12-C13
2	A	601	6OU	C05-C06-C07-C08
2	A	620	6OU	C07-C08-C09-C10
8	A	612	LMT	C7-C8-C9-C10
2	A	620	6OU	C37-C38-C39-C40
2	A	601	6OU	C43-C44-C45-C46
2	A	601	6OU	C45-C46-C47-C48
8	A	612	LMT	C1-C2-C3-C4
2	A	620	6OU	C35-C36-C37-C38
3	A	603	PG5	O1-C2-C3-O2
3	A	604	PG5	O1-C2-C3-O2
2	A	620	6OU	C43-C44-C45-C46
2	A	601	6OU	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
2	A	620	6OU	C13-C14-C15-C16
8	A	619	LMT	C5-C6-C7-C8
2	A	601	6OU	C41-C42-C43-C44
8	A	613	LMT	C6-C7-C8-C9
8	A	617	LMT	C7-C8-C9-C10
2	A	620	6OU	C34-C35-C36-C37
2	A	620	6OU	C05-C06-C07-C08
2	A	602	6OU	C01-C02-C03-C04
7	A	611	GOL	O2-C2-C3-O3
8	A	612	LMT	C2-C1-O1'-C1'
2	A	620	6OU	C36-C37-C38-C39
3	A	604	PG5	C2-C3-O2-C4
2	A	602	6OU	C43-C44-C45-C46
2	A	602	6OU	C34-C35-C36-C37
2	A	620	6OU	C12-C13-C14-C15
2	A	601	6OU	C09-C10-C11-C12
2	A	602	6OU	C44-C45-C46-C47
7	A	610	GOL	O1-C1-C2-O2
2	A	601	6OU	C19-C20-C21-O22
2	A	620	6OU	C19-C20-C21-O22
3	A	603	PG5	C5-C4-O2-C3
4	A	607	PG6	C6-C7-O4-C8
8	A	613	LMT	C5'-C4'-O1B-C1B
2	A	601	6OU	C19-C20-O30-C31
8	A	613	LMT	C3'-C4'-O1B-C1B
2	A	602	6OU	C10-C11-C12-C13
2	A	620	6OU	O30-C20-C21-O22
2	A	601	6OU	C07-C08-C09-C10
3	A	605	PG5	C7-C6-O3-C5
2	A	620	6OU	C06-C07-C08-C09
3	A	603	PG5	O3-C6-C7-O4
2	A	620	6OU	C33-C34-C35-C36
4	A	607	PG6	O3-C6-C7-O4
2	A	602	6OU	C45-C46-C47-C48
2	A	602	6OU	C03-C04-C05-C06
3	A	604	PG5	C7-C6-O3-C5
2	A	601	6OU	C21-O22-P23-O24
2	A	601	6OU	C21-O22-P23-O26
2	A	601	6OU	C27-O26-P23-O22
2	A	601	6OU	C27-O26-P23-O24
2	A	620	6OU	C27-O26-P23-O24
3	A	603	PG5	C2-C3-O2-C4

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Mol	Chain	Res	Type	Atoms
2	A	620	6OU	C42-C43-C44-C45
8	A	613	LMT	C5-C6-C7-C8
2	A	601	6OU	C40-C41-C42-C43
2	A	601	6OU	C44-C45-C46-C47
8	A	612	LMT	C5-C6-C7-C8
2	A	620	6OU	C20-C21-O22-P23
5	A	608	TRS	C2-C-C3-O3
2	A	602	6OU	C04-C05-C06-C07
2	A	601	6OU	C01-C02-C03-C04
2	A	602	6OU	C11-C12-C13-C14
3	A	603	PG5	C7-C6-O3-C5
3	A	606	PG5	C7-C6-O3-C5
2	A	601	6OU	C06-C07-C08-C09
2	A	602	6OU	C02-C03-C04-C05
8	A	612	LMT	C6-C7-C8-C9
2	A	601	6OU	O18-C19-C20-O30
2	A	601	6OU	C38-C39-C40-C41
2	A	601	6OU	C46-C47-C48-C49
2	A	620	6OU	C31-C33-C34-C35
2	A	601	6OU	C20-C21-O22-P23
7	A	616	GOL	O2-C2-C3-O3
2	A	602	6OU	C38-C39-C40-C41
2	A	601	6OU	C04-C05-C06-C07
2	A	620	6OU	C02-C03-C04-C05
2	A	601	6OU	C36-C37-C38-C39
2	A	602	6OU	C09-C10-C11-C12
5	A	608	TRS	N-C-C3-O3
2	A	601	6OU	O18-C19-C20-C21
2	A	620	6OU	O30-C31-C33-C34

There are no ring outliers.

9 monomers are involved in 24 short contacts:

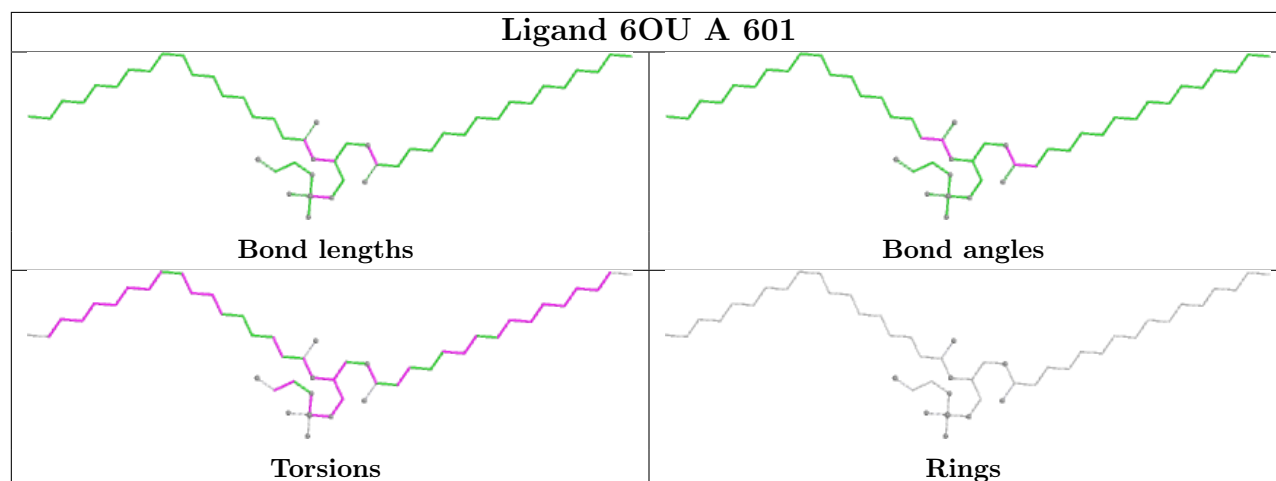
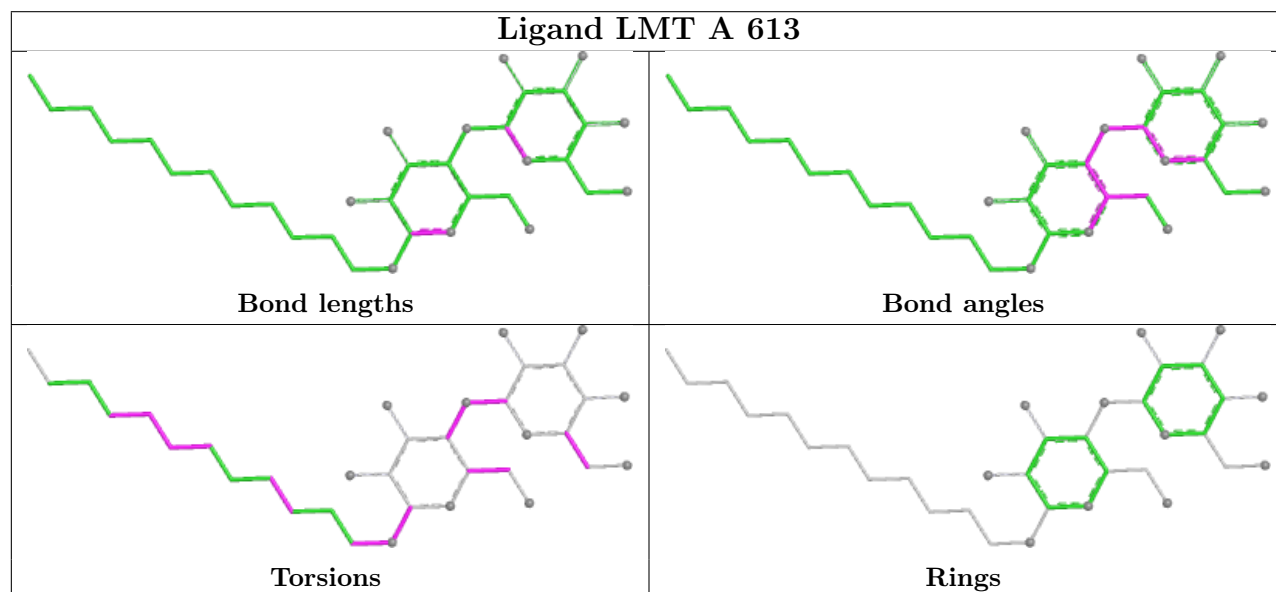
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	613	LMT	8	0
2	A	601	6OU	6	0
2	A	602	6OU	1	0
8	A	612	LMT	1	0
3	A	604	PG5	1	0
3	A	606	PG5	2	0
2	A	620	6OU	1	0
7	A	611	GOL	2	0

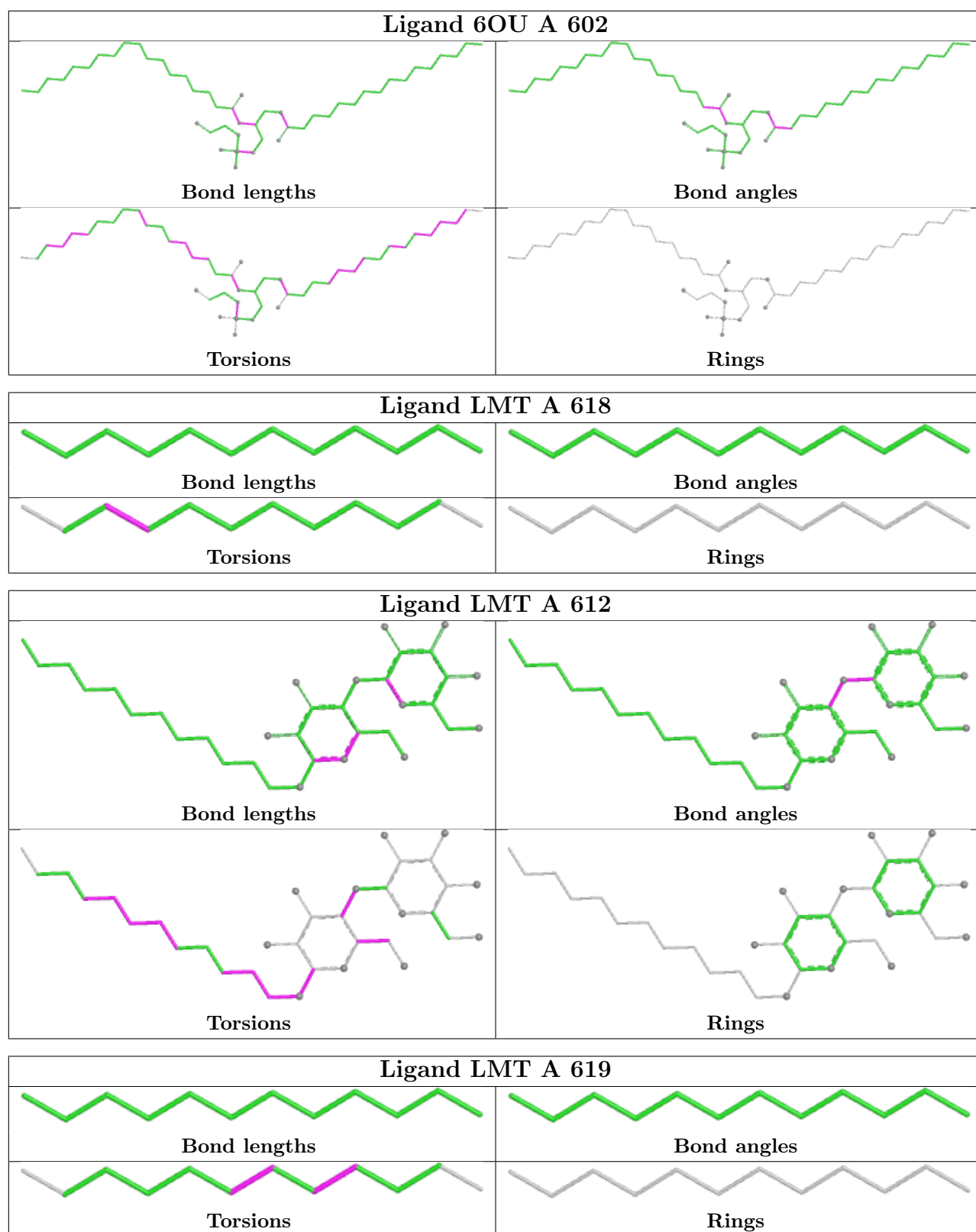
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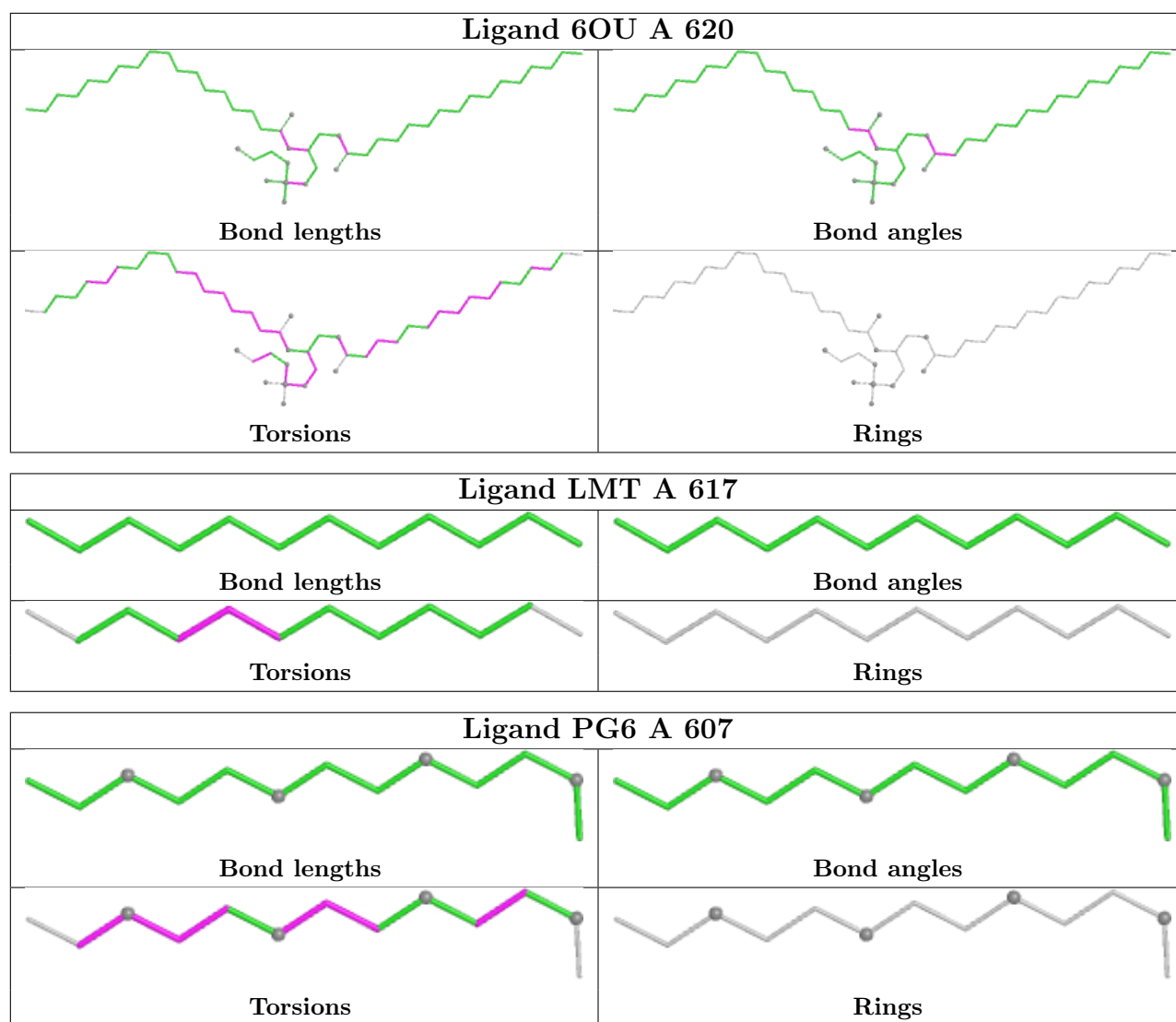
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	607	PG6	4	0

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	508/532 (95%)	0.91	74 (14%) 6 4	48, 70, 105, 128	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	354	LEU	6.2
1	A	370	TYR	5.6
1	A	74	TRP	5.4
1	A	219	GLU	5.3
1	A	379	GLY	5.2
1	A	1	MET	5.0
1	A	378	ASN	4.5
1	A	7	ILE	4.1
1	A	350	ILE	4.0
1	A	75	VAL	3.9
1	A	111	VAL	3.8
1	A	3	PHE	3.6
1	A	121	TRP	3.6
1	A	504	LEU	3.5
1	A	400	PHE	3.3
1	A	388	TYR	3.3
1	A	500	PHE	3.3
1	A	210	TYR	3.3
1	A	353	PRO	3.2
1	A	72	ILE	3.2
1	A	300	VAL	3.2
1	A	141	TRP	3.1
1	A	95	VAL	3.0
1	A	447	GLY	3.0
1	A	201	LEU	3.0
1	A	97	LEU	2.9
1	A	227	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	306	LYS	2.8
1	A	507	LEU	2.8
1	A	187	LEU	2.8
1	A	450	ALA	2.8
1	A	299	ILE	2.7
1	A	2	ALA	2.7
1	A	344	PHE	2.7
1	A	144	THR	2.6
1	A	307	GLN	2.6
1	A	122	LEU	2.6
1	A	118	LYS	2.5
1	A	421	GLY	2.5
1	A	349	SER	2.5
1	A	308	ASN	2.5
1	A	119	THR	2.5
1	A	204	LEU	2.5
1	A	497	LEU	2.5
1	A	188	VAL	2.4
1	A	270	ILE	2.4
1	A	341	PHE	2.4
1	A	461	MET	2.4
1	A	96	LEU	2.4
1	A	91	ILE	2.3
1	A	371	ILE	2.3
1	A	351	LEU	2.2
1	A	309	ARG	2.2
1	A	143	LEU	2.2
1	A	235	LEU	2.2
1	A	367	ARG	2.2
1	A	183	LEU	2.2
1	A	61	PHE	2.2
1	A	487	GLY	2.2
1	A	486	THR	2.2
1	A	198	ALA	2.1
1	A	190	ARG	2.1
1	A	310	TYR	2.1
1	A	117	PRO	2.1
1	A	159	PRO	2.1
1	A	338	LEU	2.1
1	A	192	TRP	2.1
1	A	268	SER	2.0
1	A	505	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	452	ILE	2.0
1	A	94	VAL	2.0
1	A	202	PHE	2.0
1	A	471	THR	2.0
1	A	6	LEU	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.

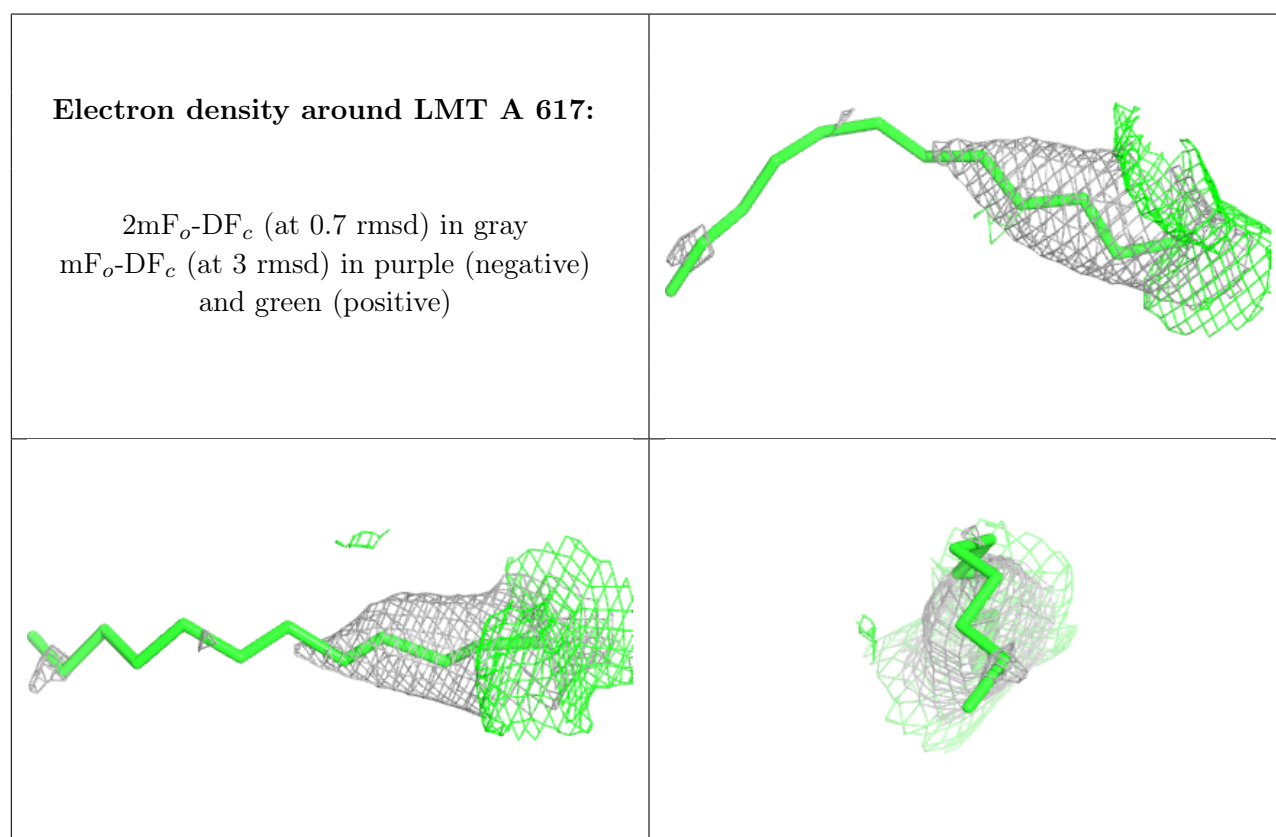
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	A	610	6/6	0.38	0.32	114,115,118,124	0
7	GOL	A	615	6/6	0.44	0.24	115,120,124,126	0
9	CL	A	623	1/1	0.58	0.19	150,150,150,150	0
6	ACT	A	609	4/4	0.62	0.16	92,100,101,104	0
8	LMT	A	617	12/35	0.63	0.53	86,90,93,96	0
3	PG5	A	606	10/12	0.68	0.26	104,112,120,123	0
8	LMT	A	613	35/35	0.68	0.24	89,125,146,148	0
3	PG5	A	604	11/12	0.69	0.24	95,112,117,118	0
8	LMT	A	612	35/35	0.70	0.30	91,139,159,162	0
7	GOL	A	616	6/6	0.75	0.20	110,110,116,116	0
2	6OU	A	620	49/49	0.76	0.32	88,96,136,190	0
3	PG5	A	603	10/12	0.76	0.22	100,117,125,126	0
2	6OU	A	602	49/49	0.76	0.34	70,95,142,237	0
4	PG6	A	607	13/18	0.77	0.26	87,102,113,115	0
3	PG5	A	605	8/12	0.78	0.28	76,94,112,115	0
7	GOL	A	614	6/6	0.78	0.22	104,112,114,118	0
8	LMT	A	618	12/35	0.82	0.37	75,89,93,94	0
7	GOL	A	611	6/6	0.82	0.21	94,116,117,118	0

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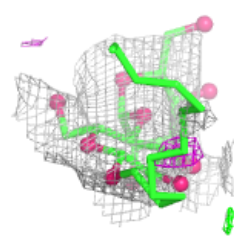
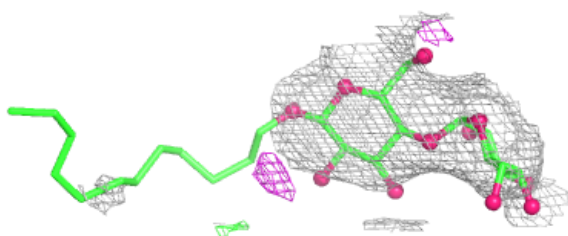
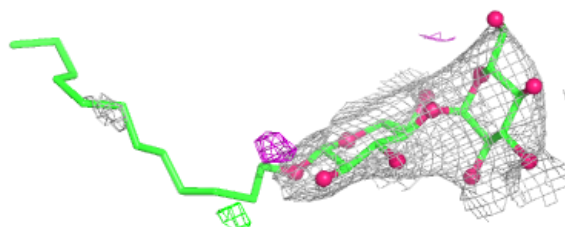
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	TRS	A	608	8/8	0.84	0.22	84,90,102,109	0
9	CL	A	622	1/1	0.85	0.12	118,118,118,118	0
8	LMT	A	619	12/35	0.86	0.36	79,93,102,102	0
2	6OU	A	601	49/49	0.92	0.18	68,79,88,110	0
9	CL	A	621	1/1	0.94	0.13	89,89,89,89	0

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.

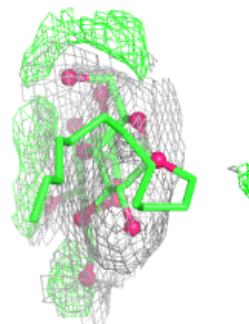
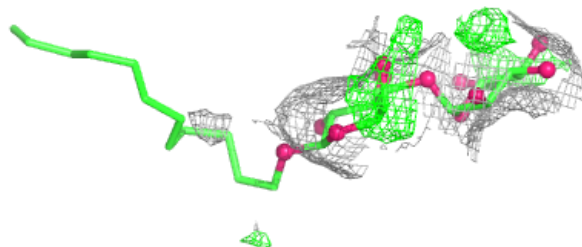
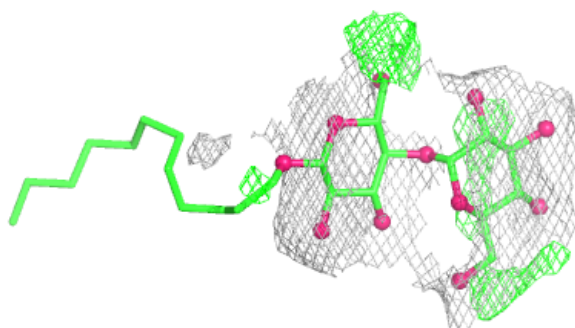


Electron density around LMT A 613:

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

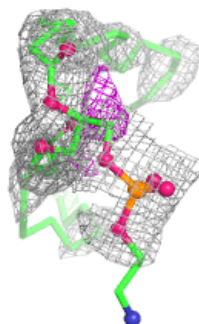
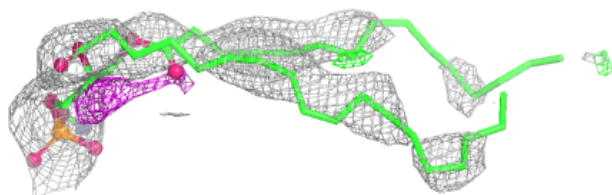
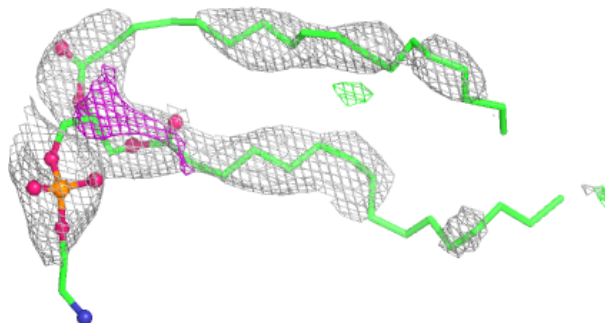
**Electron density around LMT A 612:**

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



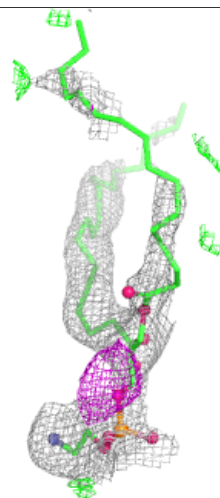
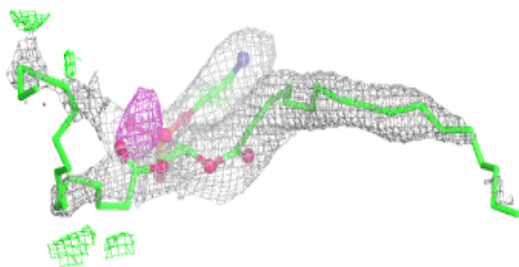
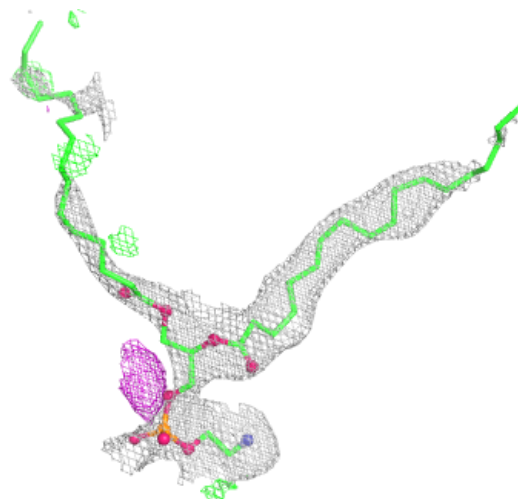
Electron density around 6OU A 620:

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



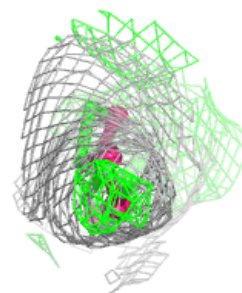
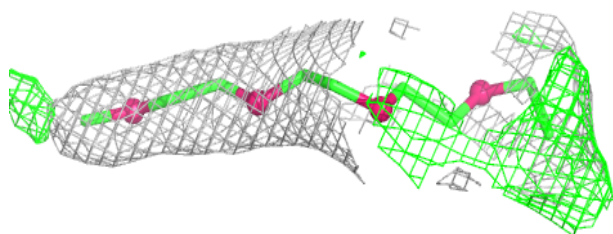
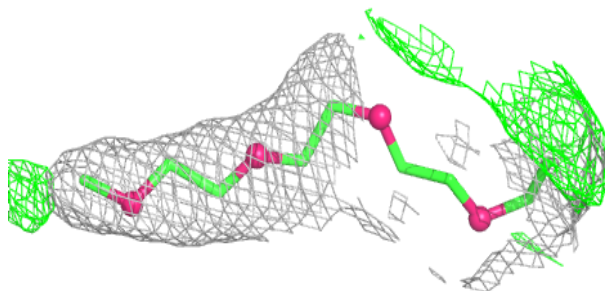
Electron density around 6OU A 602:

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

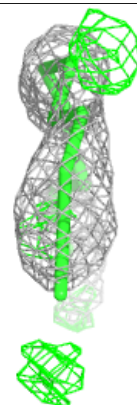
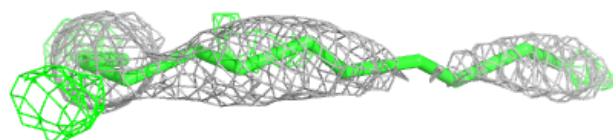
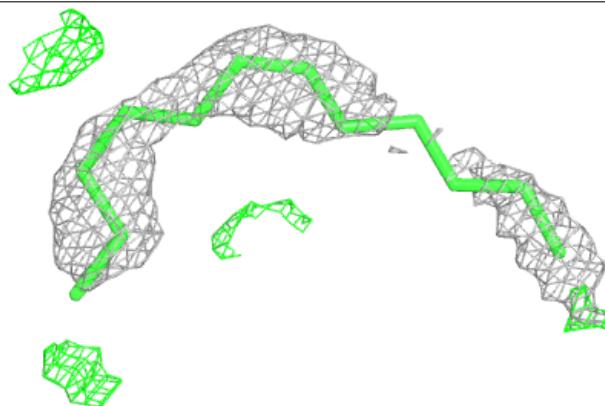


Electron density around PG6 A 607:

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

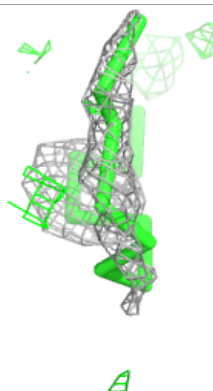
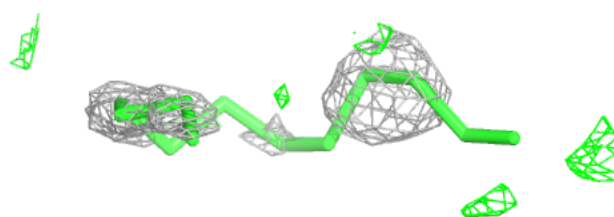
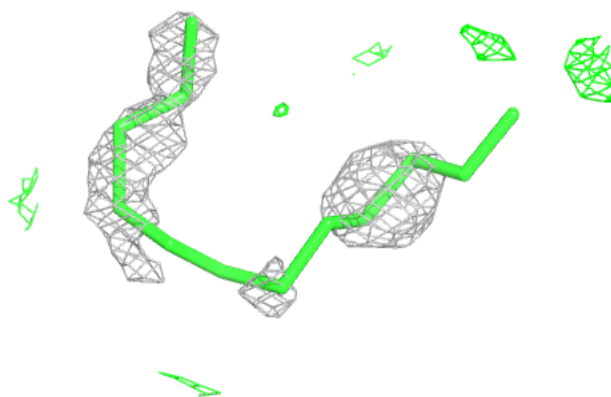
**Electron density around LMT A 618:**

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

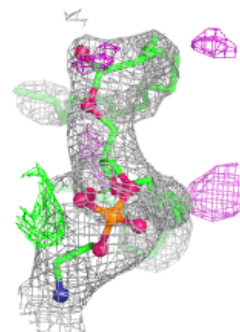
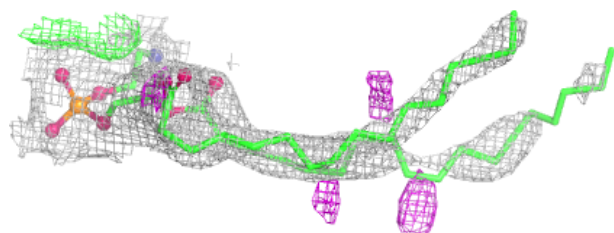
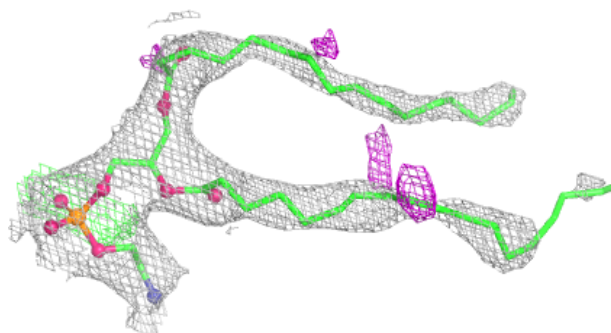


Electron density around LMT A 619:

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

**Electron density around 6OU 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.