Full wwPDB X-ray Structure Validation Report ⓘ

Jul 3, 2023 – 10:19 pm BST

PDB ID	:	8AQ3
Title	:	In surfo structure of the membrane integral lipoprotein N-acyltransferase Lnt from E. coli in complex with PE
Authors	:	Huang, C.-Y.; Weichert, D.; Boland, C.; Smithers, L.; Olieric, V.; Wang, M.; Caffrey, M.
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:

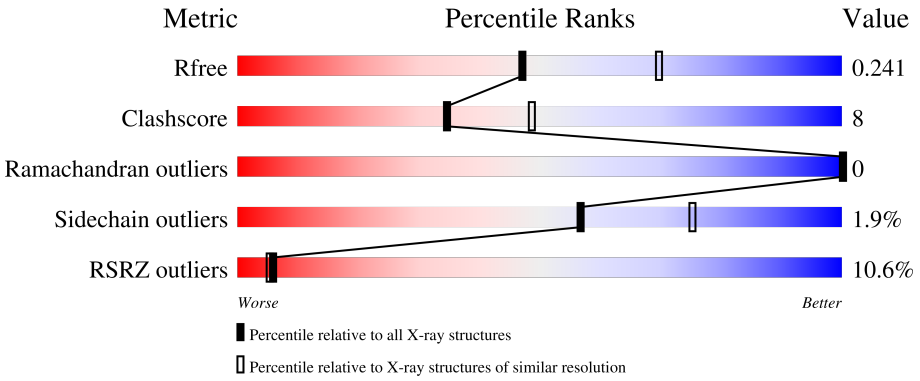
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	10% 80% 15% • 5%

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
2	6OU	A	602	-	-	-	X
8	LMT	A	613	-	-	-	X
8	LMT	A	619	-	-	-	X

2 Entry composition (i)

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.

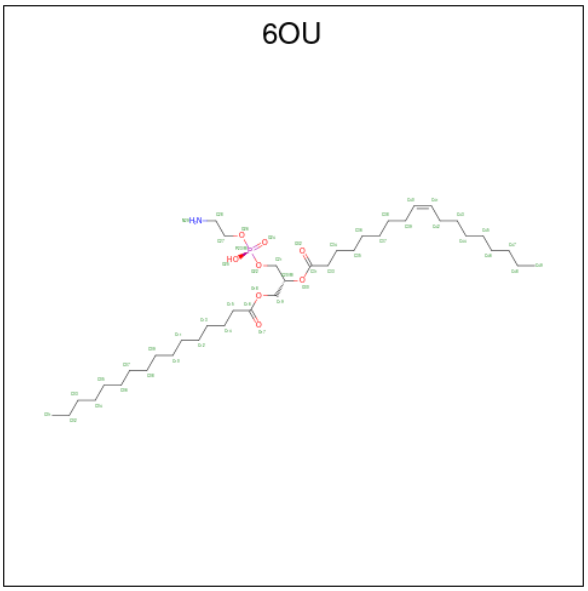
- Molecule 1 is a protein called Apolipoprotein N-acyltransferase.

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:

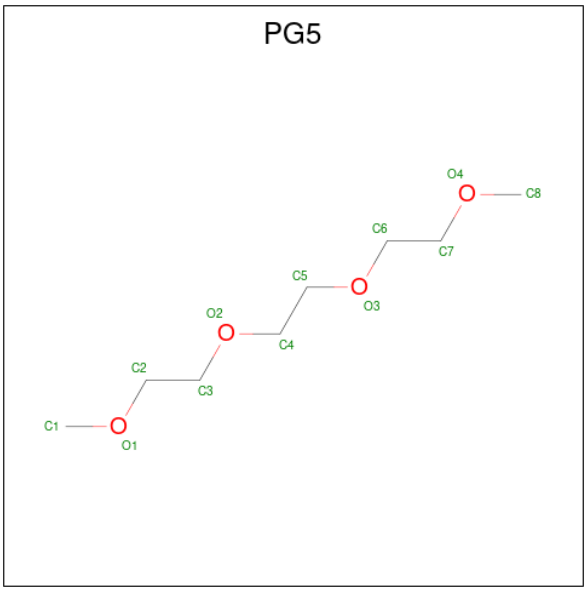
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P23930
A	-18	GLY	-	expression tag	UNP P23930
A	-17	SER	-	expression tag	UNP P23930
A	-16	SER	-	expression tag	UNP P23930
A	-15	HIS	-	expression tag	UNP P23930
A	-14	HIS	-	expression tag	UNP P23930
A	-13	HIS	-	expression 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-propan-2-yl] ({Z})-octadec-9-enoate (three-letter code: 6OU) (formula: $C_{39}H_{76}NO_8P$) (labeled as "Ligand of Interest" by depositor).



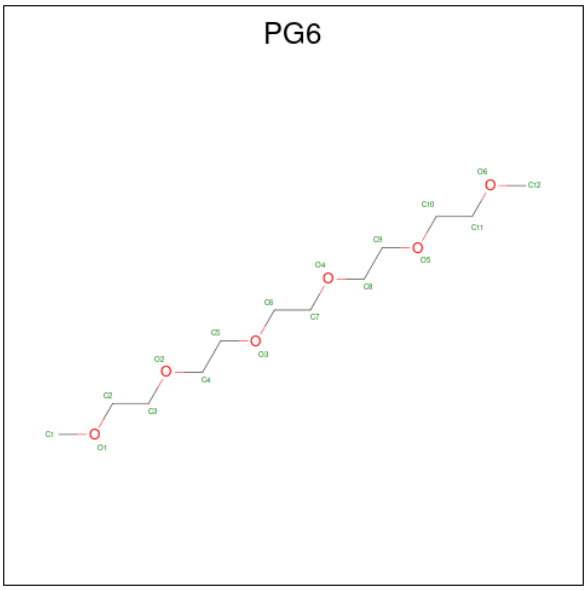
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
2	A	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

- Molecule 3 is 1-METHOXY-2-[2-(2-METHOXY-ETHOXY]-ETHANE (three-letter code: PG5) (formula: $C_8H_{18}O_4$).



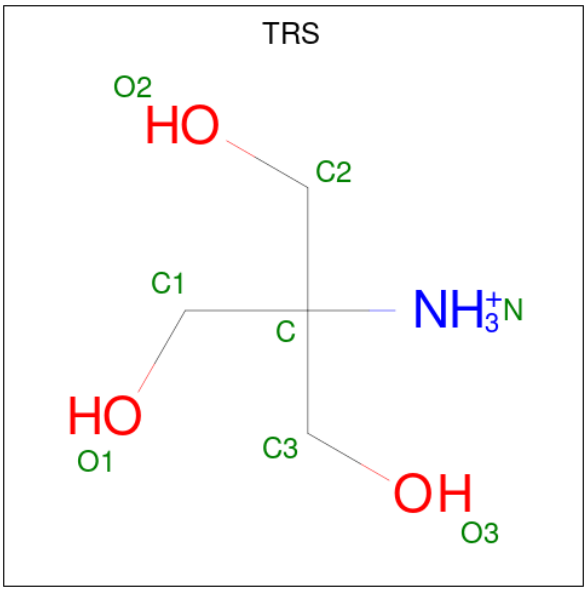
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 6 4	0	0
3	A	1	Total C O 11 7 4	0	0
3	A	1	Total C O 8 5 3	0	0
3	A	1	Total C O 10 6 4	0	0

- Molecule 4 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY]-ETHOXY}-ETHANE (three-letter code: PG6) (formula: $C_{12}H_{26}O_6$).



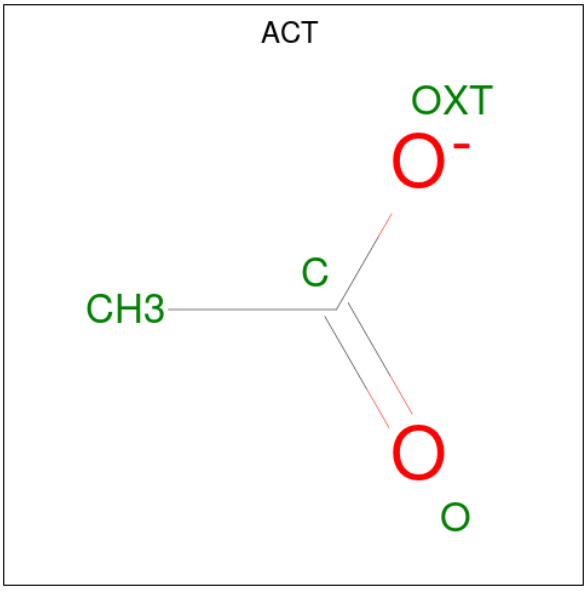
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 9 4	0	0

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



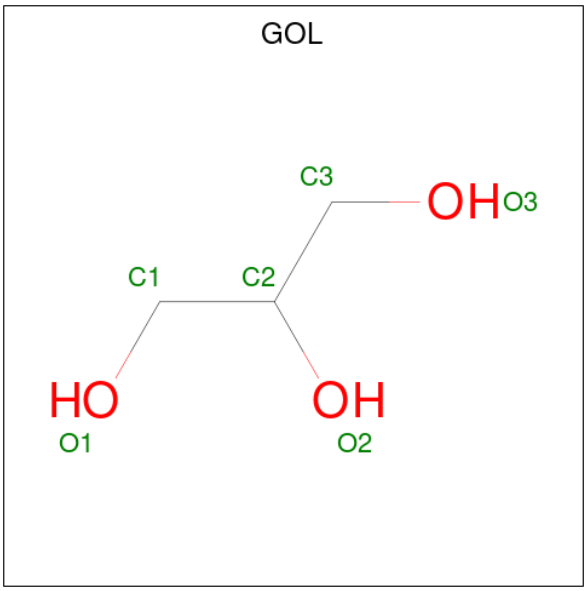
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 8 4 1 3	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



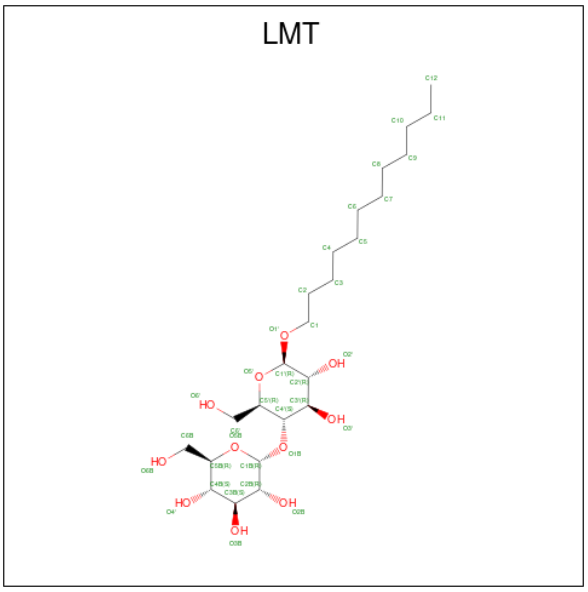
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



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 (three-letter code: CL) (formula: Cl).

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

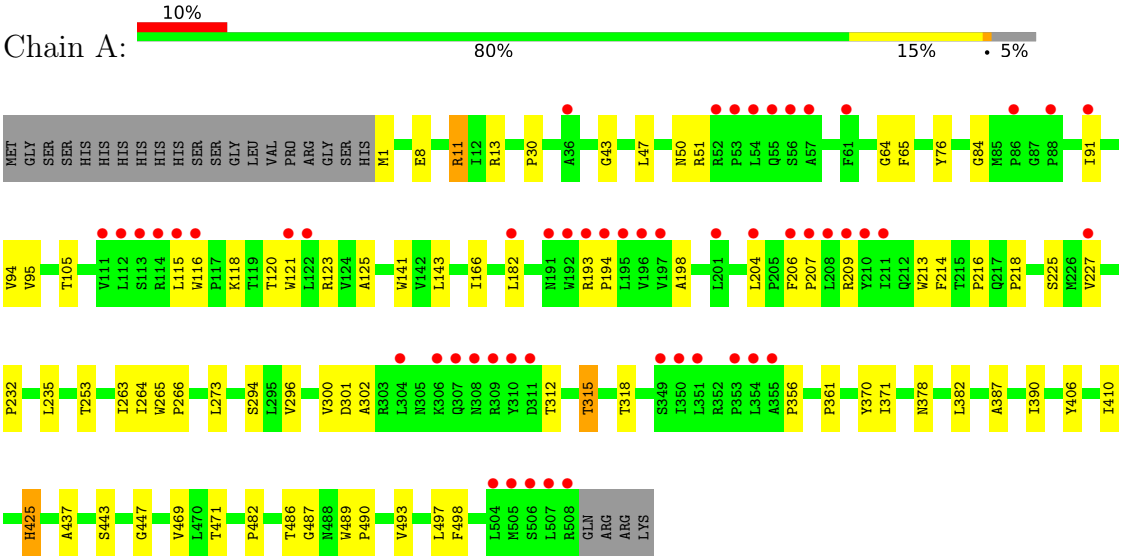
- Molecule 10 is water.

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 (i)

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 46.47 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.38-2.40) 87.2 (46.47-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.41 (at 2.39Å)	Xtriage
Refinement program	PHENIX dev_3494	Depositor
R, R_{free}	0.225 , 0.240 0.228 , 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)	0.30 , 58.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PG6, 6OU, CL, ACT, LMT, TRS, 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	0.39	0/4106	0.55	0/5611

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	3991	0	4057	60	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
10	A	57	0	0	1	0
All	All	4398	0	4340	72	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 (72) 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	0.76
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
1:A:486:THR:OG1	1:A:489:TRP:NE1	2.53	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	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%)	413 (98%)	8 (2%)	57 75

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	11	ARG
1	A	121	TRP
1	A	123	ARG
1	A	294	SER
1	A	315	THR
1	A	378	ASN
1	A	425	HIS

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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	619	-	11,11,36	0.90	0	10,10,47	0.59	0
4	PG6	A	607	-	12,12,17	0.59	0	11,11,16	0.42	0
8	LMT	A	617	-	11,11,36	0.78	0	10,10,47	0.72	0
2	6OU	A	602	-	48,48,48	1.02	4 (8%)	51,53,53	0.88	2 (3%)
8	LMT	A	618	-	11,11,36	0.95	0	10,10,47	0.57	0
6	ACT	A	609	-	3,3,3	1.43	1 (33%)	3,3,3	1.48	0
8	LMT	A	613	-	36,36,36	1.24	2 (5%)	47,47,47	1.27	4 (8%)
7	GOL	A	615	-	5,5,5	0.10	0	5,5,5	0.30	0
2	6OU	A	620	-	48,48,48	1.02	4 (8%)	51,53,53	0.87	2 (3%)
2	6OU	A	601	-	48,48,48	1.02	4 (8%)	51,53,53	0.90	2 (3%)
7	GOL	A	616	-	5,5,5	0.63	0	5,5,5	0.92	0
8	LMT	A	612	-	36,36,36	1.28	3 (8%)	47,47,47	0.79	1 (2%)
7	GOL	A	614	-	5,5,5	0.89	0	5,5,5	1.06	0
3	PG5	A	605	-	7,7,11	0.58	0	6,6,10	0.37	0
7	GOL	A	610	-	5,5,5	0.96	0	5,5,5	0.96	0
3	PG5	A	604	-	10,10,11	0.55	0	9,9,10	0.18	0
3	PG5	A	606	-	9,9,11	0.58	0	8,8,10	0.51	0
3	PG5	A	603	-	9,9,11	0.53	0	8,8,10	0.30	0
7	GOL	A	611	-	5,5,5	0.11	0	5,5,5	0.35	0
5	TRS	A	608	-	7,7,7	0.14	0	9,9,9	0.20	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	619	-	-	2/9/9/61	-
4	PG6	A	607	-	-	6/10/10/15	-
8	LMT	A	617	-	-	2/9/9/61	-
2	6OU	A	602	-	-	22/52/52/52	-
8	LMT	A	618	-	-	1/9/9/61	-
8	LMT	A	613	-	-	15/21/61/61	0/2/2/2
7	GOL	A	615	-	-	1/4/4/4	-
2	6OU	A	620	-	-	29/52/52/52	-
2	6OU	A	601	-	-	37/52/52/52	-
7	GOL	A	616	-	-	1/4/4/4	-
8	LMT	A	612	-	-	13/21/61/61	0/2/2/2
7	GOL	A	614	-	-	0/4/4/4	-
3	PG5	A	605	-	-	3/5/5/9	-
7	GOL	A	610	-	-	1/4/4/4	-
3	PG5	A	604	-	-	6/8/8/9	-
3	PG5	A	606	-	-	3/7/7/9	-
3	PG5	A	603	-	-	6/7/7/9	-
7	GOL	A	611	-	-	4/4/4/4	-
5	TRS	A	608	-	-	7/9/9/9	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	612	LMT	O5'-C1'	4.15	1.52	1.41
8	A	612	LMT	O5B-C1B	3.45	1.50	1.41
8	A	613	LMT	O5'-C1'	3.45	1.50	1.41
2	A	620	6OU	O18-C16	3.21	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	-2.72	1.39	1.46
8	A	613	LMT	O5B-C1B	2.70	1.48	1.41
2	A	620	6OU	O30-C20	-2.68	1.39	1.46
2	A	601	6OU	O30-C20	-2.53	1.40	1.46
2	A	620	6OU	O30-C31	2.31	1.40	1.34
2	A	602	6OU	O30-C31	2.30	1.40	1.34
2	A	601	6OU	O30-C31	2.27	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	612	LMT	O5'-C5'	2.17	1.49	1.44
2	A	601	6OU	P23-O22	2.13	1.67	1.59
2	A	602	6OU	P23-O22	2.12	1.67	1.59
2	A	620	6OU	P23-O22	2.11	1.67	1.59
6	A	609	ACT	CH3-C	2.09	1.57	1.49

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	613	LMT	C1B-O5B-C5B	-4.19	105.47	113.69
2	A	620	6OU	O30-C31-C33	3.94	119.99	111.50
2	A	601	6OU	O30-C31-C33	3.93	119.98	111.50
2	A	602	6OU	O30-C31-C33	3.92	119.95	111.50
8	A	613	LMT	O5'-C5'-C4'	3.46	117.06	109.75
8	A	613	LMT	C6'-C5'-C4'	-3.00	104.61	113.33
8	A	613	LMT	C1B-O1B-C4'	-2.91	110.76	117.96
2	A	601	6OU	O18-C16-C15	2.59	120.04	111.91
2	A	620	6OU	O18-C16-C15	2.58	120.02	111.91
2	A	602	6OU	O18-C16-C15	2.57	119.98	111.91
8	A	612	LMT	C1B-O1B-C4'	-2.30	112.27	117.96

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
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	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

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Mol	Chain	Res	Type	Atoms
5	A	608	TRS	N-C-C2-O2
7	A	611	GOL	O1-C1-C2-C3
8	A	612	LMT	C2'-C1'-O1'-C1
8	A	612	LMT	O5'-C1'-O1'-C1
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
4	A	607	PG6	C4-C5-O3-C6
2	A	602	6OU	C15-C16-O18-C19
2	A	620	6OU	O32-C31-O30-C20
3	A	604	PG5	C4-C5-O3-C6
8	A	613	LMT	O5B-C1B-O1B-C4'
2	A	602	6OU	C33-C34-C35-C36
8	A	613	LMT	C2B-C1B-O1B-C4'
8	A	613	LMT	C7-C8-C9-C10
8	A	613	LMT	O5B-C5B-C6B-O6B
8	A	613	LMT	O5'-C5'-C6'-O6'
4	A	607	PG6	O2-C4-C5-O3
2	A	602	6OU	O17-C16-O18-C19
3	A	603	PG5	O2-C4-C5-O3
2	A	601	6OU	C13-C14-C15-C16
8	A	612	LMT	O1'-C1-C2-C3
8	A	612	LMT	C4'-C5'-C6'-O6'
8	A	613	LMT	C4'-C5'-C6'-O6'
2	A	620	6OU	C15-C16-O18-C19
3	A	606	PG5	O2-C4-C5-O3
2	A	601	6OU	C31-C33-C34-C35
7	A	611	GOL	O1-C1-C2-O2
8	A	618	LMT	C11-C10-C9-C8
3	A	604	PG5	O2-C4-C5-O3
3	A	605	PG5	O3-C6-C7-O4
3	A	606	PG5	O1-C2-C3-O2
4	A	607	PG6	O1-C2-C3-O2
2	A	620	6OU	O17-C16-O18-C19
3	A	604	PG5	O3-C6-C7-O4
8	A	612	LMT	C5'-C4'-O1B-C1B
2	A	601	6OU	C37-C38-C39-C40
8	A	613	LMT	C4B-C5B-C6B-O6B
2	A	601	6OU	C27-O26-P23-O22

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Mol	Chain	Res	Type	Atoms
2	A	620	6OU	C21-O22-P23-O26
8	A	612	LMT	O5'-C5'-C6'-O6'
3	A	605	PG5	O2-C4-C5-O3
2	A	601	6OU	C02-C03-C04-C05
2	A	602	6OU	C06-C07-C08-C09
2	A	602	6OU	C35-C36-C37-C38
8	A	613	LMT	C2-C3-C4-C5
8	A	619	LMT	C3-C4-C5-C6
2	A	601	6OU	C03-C04-C05-C06
4	A	607	PG6	C9-C8-O4-C7
8	A	612	LMT	C4-C5-C6-C7
8	A	617	LMT	C6-C7-C8-C9
2	A	601	6OU	C10-C11-C12-C13
2	A	601	6OU	C05-C06-C07-C08
7	A	611	GOL	C1-C2-C3-O3
2	A	620	6OU	C37-C38-C39-C40
2	A	620	6OU	C07-C08-C09-C10
8	A	612	LMT	C7-C8-C9-C10
2	A	620	6OU	C08-C09-C10-C11
2	A	601	6OU	C45-C46-C47-C48
2	A	620	6OU	C35-C36-C37-C38
8	A	612	LMT	C2-C1-O1'-C1'
2	A	620	6OU	C09-C10-C11-C12
2	A	601	6OU	C43-C44-C45-C46
8	A	612	LMT	C3'-C4'-O1B-C1B
2	A	620	6OU	C13-C14-C15-C16
2	A	620	6OU	C43-C44-C45-C46
8	A	613	LMT	C6-C7-C8-C9
2	A	601	6OU	C42-C43-C44-C45
8	A	612	LMT	C1-C2-C3-C4
2	A	601	6OU	C21-O22-P23-O26
8	A	617	LMT	C7-C8-C9-C10
8	A	619	LMT	C5-C6-C7-C8
2	A	620	6OU	C34-C35-C36-C37
2	A	620	6OU	C05-C06-C07-C08
3	A	603	PG5	O1-C2-C3-O2
3	A	604	PG5	O1-C2-C3-O2
2	A	602	6OU	C01-C02-C03-C04
2	A	601	6OU	C41-C42-C43-C44
2	A	620	6OU	C36-C37-C38-C39
3	A	604	PG5	C2-C3-O2-C4
2	A	602	6OU	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
2	A	602	6OU	C34-C35-C36-C37
2	A	620	6OU	C12-C13-C14-C15
2	A	601	6OU	C09-C10-C11-C12
7	A	611	GOL	O2-C2-C3-O3
2	A	602	6OU	C44-C45-C46-C47
2	A	601	6OU	C19-C20-C21-O22
2	A	620	6OU	C19-C20-C21-O22
2	A	602	6OU	C10-C11-C12-C13
2	A	601	6OU	C07-C08-C09-C10
2	A	601	6OU	C19-C20-O30-C31
3	A	603	PG5	C5-C4-O2-C3
4	A	607	PG6	C6-C7-O4-C8
2	A	620	6OU	O30-C20-C21-O22
3	A	605	PG5	C7-C6-O3-C5
7	A	610	GOL	O1-C1-C2-O2
4	A	607	PG6	O3-C6-C7-O4
2	A	620	6OU	C06-C07-C08-C09
8	A	613	LMT	C3'-C4'-O1B-C1B
8	A	613	LMT	C5'-C4'-O1B-C1B
2	A	620	6OU	C33-C34-C35-C36
2	A	602	6OU	C45-C46-C47-C48
2	A	601	6OU	C21-O22-P23-O24
2	A	601	6OU	C27-O26-P23-O24
2	A	620	6OU	C21-O22-P23-O25
2	A	602	6OU	C03-C04-C05-C06
3	A	603	PG5	O3-C6-C7-O4
2	A	620	6OU	C42-C43-C44-C45
2	A	620	6OU	C20-C21-O22-P23
3	A	604	PG5	C7-C6-O3-C5
8	A	613	LMT	C5-C6-C7-C8
3	A	603	PG5	C2-C3-O2-C4
2	A	620	6OU	C27-O26-P23-O22
2	A	601	6OU	C44-C45-C46-C47
2	A	601	6OU	C40-C41-C42-C43
8	A	612	LMT	C5-C6-C7-C8
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
2	A	601	6OU	C06-C07-C08-C09
2	A	601	6OU	C20-C21-O22-P23
3	A	606	PG5	C7-C6-O3-C5

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Mol	Chain	Res	Type	Atoms
2	A	620	6OU	C31-C33-C34-C35
8	A	612	LMT	C6-C7-C8-C9
2	A	602	6OU	C02-C03-C04-C05
2	A	601	6OU	C46-C47-C48-C49
2	A	601	6OU	O18-C19-C20-O30
2	A	601	6OU	C38-C39-C40-C41
5	A	608	TRS	C2-C-C3-O3
2	A	601	6OU	C04-C05-C06-C07
2	A	602	6OU	C38-C39-C40-C41
7	A	615	GOL	O1-C1-C2-C3
2	A	601	6OU	C36-C37-C38-C39
2	A	620	6OU	C27-O26-P23-O24
2	A	620	6OU	O30-C31-C33-C34
2	A	620	6OU	C02-C03-C04-C05
7	A	616	GOL	O2-C2-C3-O3
2	A	602	6OU	C09-C10-C11-C12

There are no ring outliers.

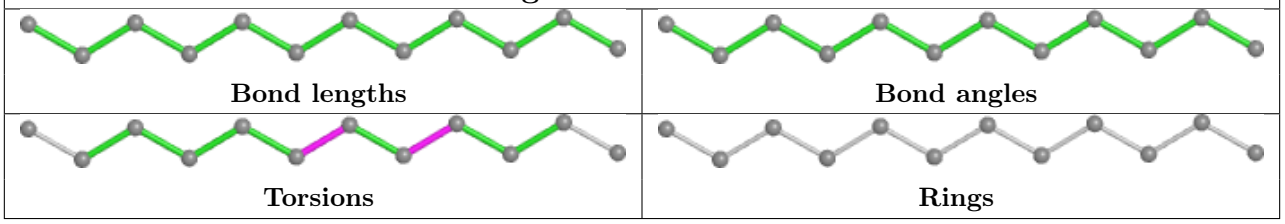
9 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	607	PG6	4	0
2	A	602	6OU	1	0
8	A	613	LMT	8	0
2	A	620	6OU	1	0
2	A	601	6OU	6	0
8	A	612	LMT	1	0
3	A	604	PG5	1	0
3	A	606	PG5	2	0
7	A	611	GOL	2	0

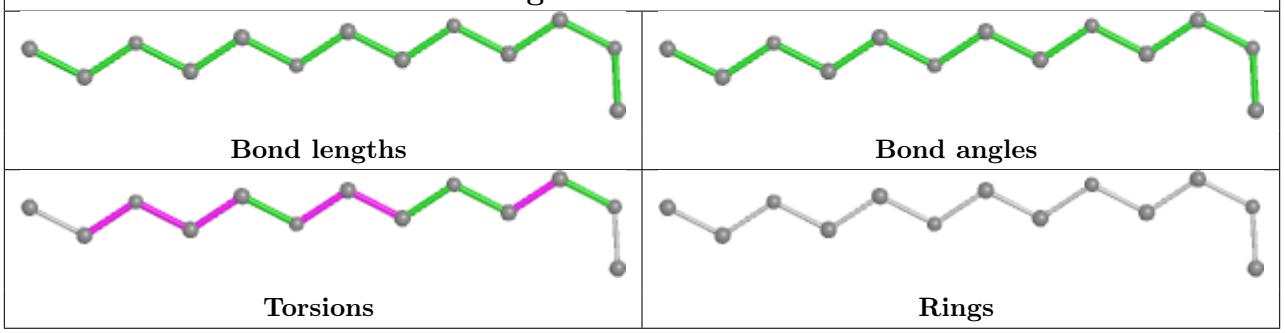
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

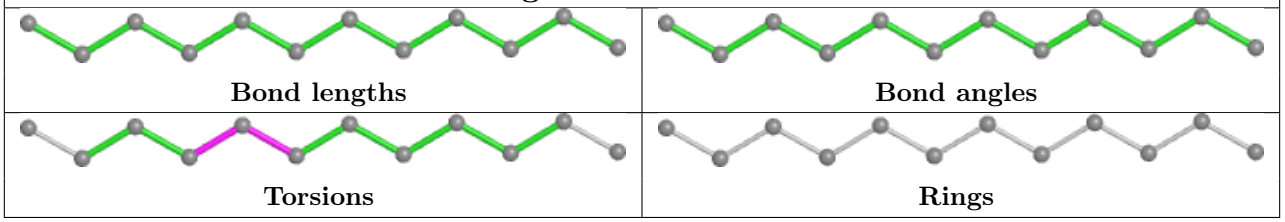
Ligand LMT A 619



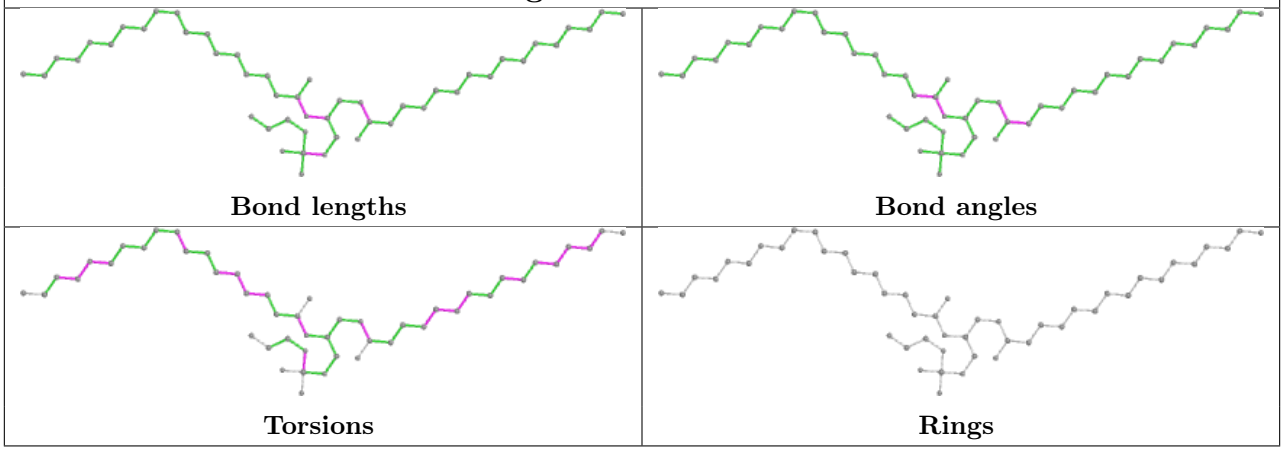
Ligand PG6 A 607



Ligand LMT A 617



Ligand 6OU A 602



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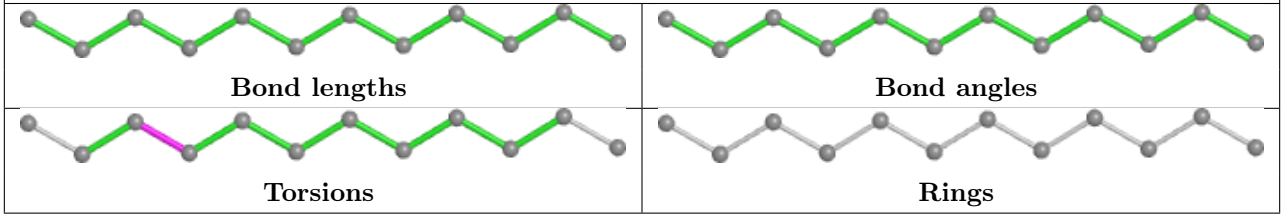

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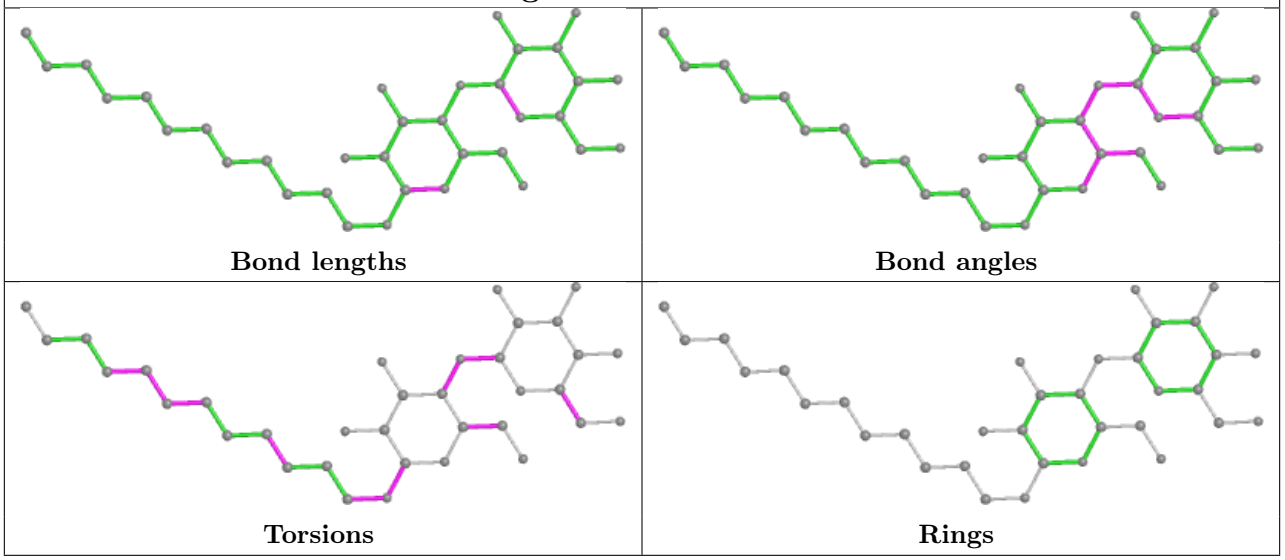

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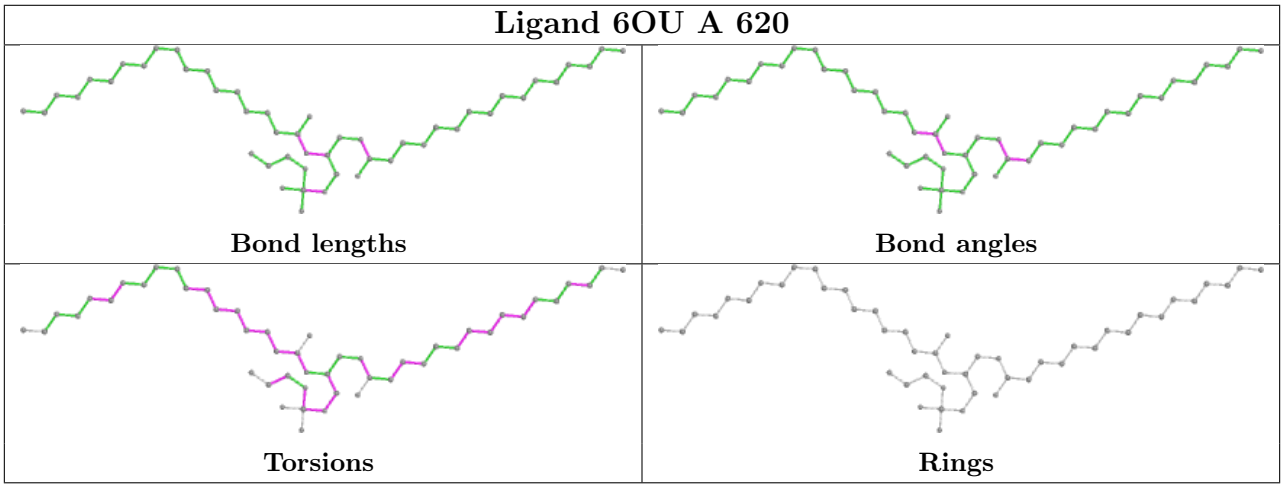
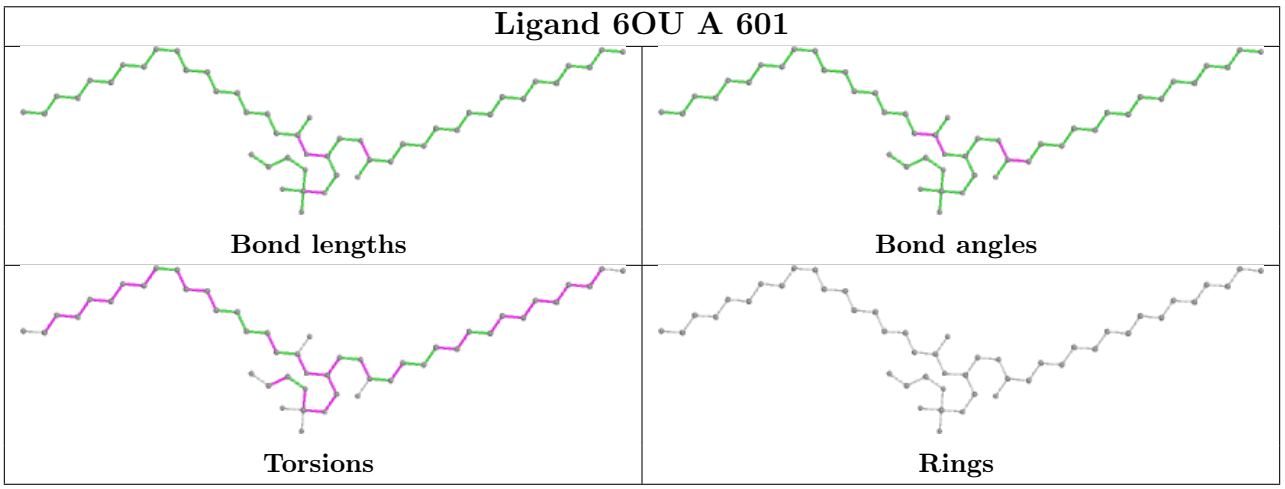


Ligand 6OU A 601



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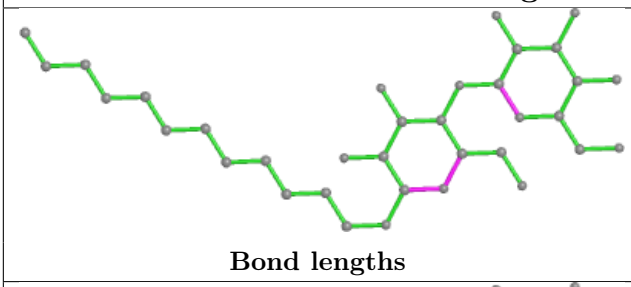
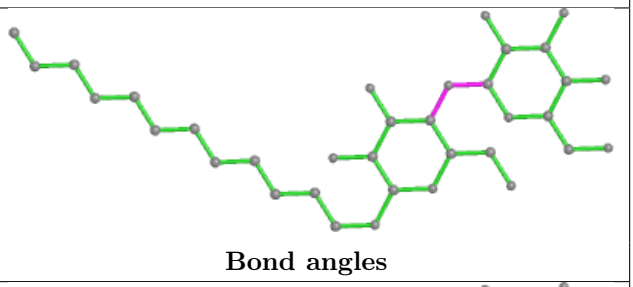
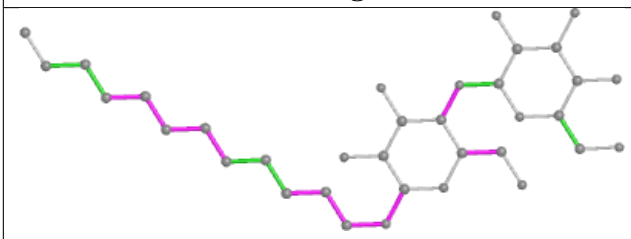


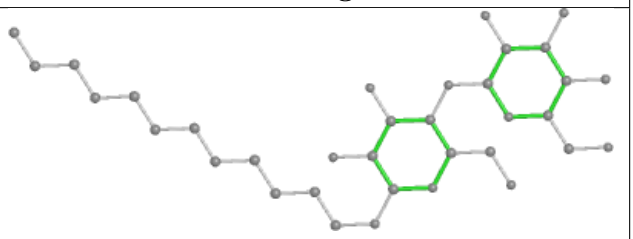
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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%)	0.56	54 (10%) 6 5	48, 70, 105, 128	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308	ASN	6.7
1	A	192	TRP	6.7
1	A	309	ARG	6.0
1	A	354	LEU	6.0
1	A	121	TRP	5.6
1	A	210	TYR	5.2
1	A	310	TYR	4.4
1	A	306	LYS	4.2
1	A	505	MET	4.2
1	A	53	PRO	4.2
1	A	506	SER	3.8
1	A	52	ARG	3.8
1	A	307	GLN	3.8
1	A	193	ARG	3.7
1	A	56	SER	3.7
1	A	88	PRO	3.6
1	A	350	ILE	3.6
1	A	196	VAL	3.5
1	A	507	LEU	3.5
1	A	353	PRO	3.4
1	A	115	LEU	3.4
1	A	54	LEU	3.3
1	A	351	LEU	3.3
1	A	113	SER	3.3
1	A	111	VAL	3.2
1	A	55	GLN	3.1
1	A	191	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	211	ILE	3.0
1	A	201	LEU	3.0
1	A	197	VAL	2.9
1	A	204	LEU	2.9
1	A	504	LEU	2.8
1	A	122	LEU	2.7
1	A	116	TRP	2.7
1	A	207	PRO	2.7
1	A	508	ARG	2.6
1	A	304	LEU	2.5
1	A	86	PRO	2.5
1	A	206	PHE	2.4
1	A	227	VAL	2.4
1	A	194	PRO	2.3
1	A	355	ALA	2.3
1	A	114	ARG	2.3
1	A	209	ARG	2.3
1	A	91	ILE	2.3
1	A	112	LEU	2.2
1	A	182	LEU	2.2
1	A	311	ASP	2.2
1	A	208	LEU	2.2
1	A	349	SER	2.2
1	A	57	ALA	2.1
1	A	195	LEU	2.1
1	A	36	ALA	2.1
1	A	61	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

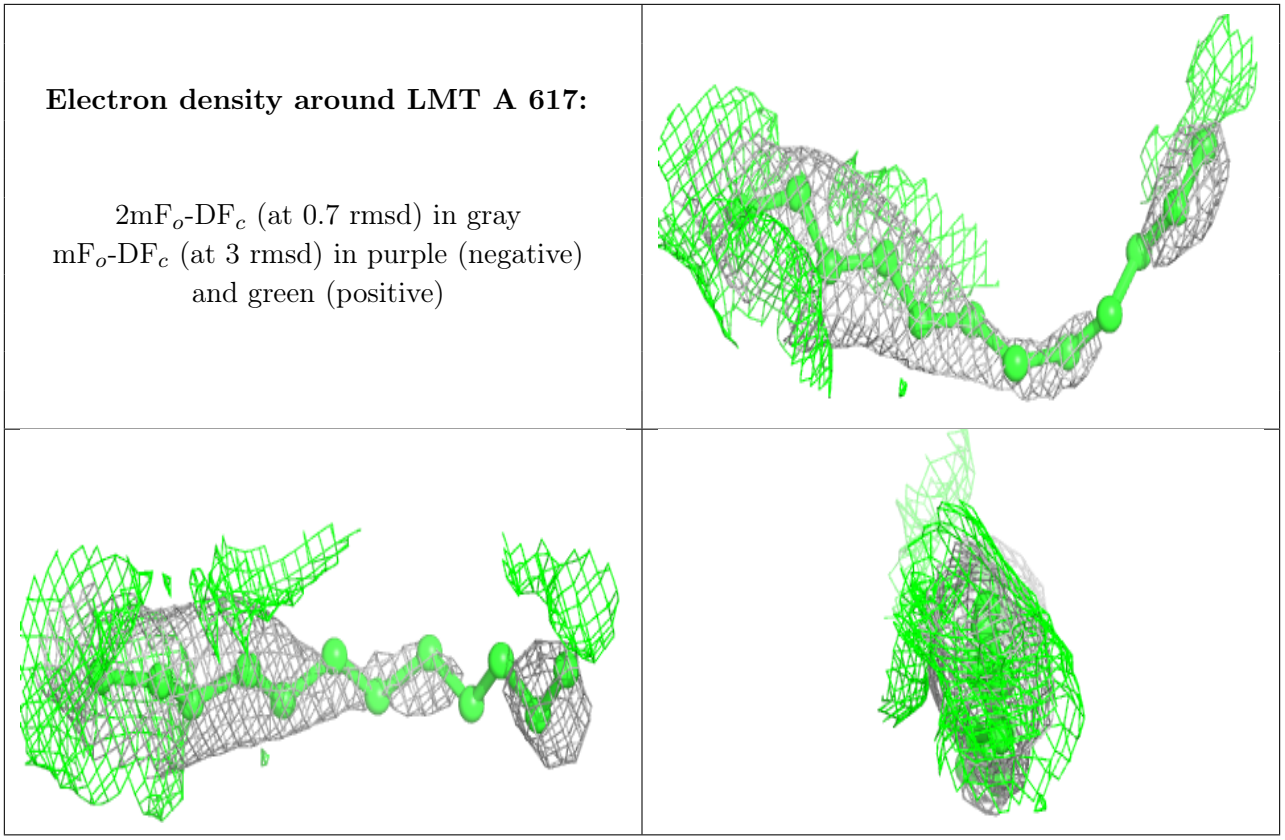
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	CL	A	623	1/1	0.46	0.17	150,150,150,150	0
8	LMT	A	617	12/35	0.50	0.40	86,90,93,96	0
8	LMT	A	619	12/35	0.52	0.48	79,93,102,102	0
8	LMT	A	612	35/35	0.52	0.37	91,139,159,162	0
2	6OU	A	602	49/49	0.53	0.42	70,95,142,237	0
7	GOL	A	611	6/6	0.59	0.20	94,116,117,118	0
8	LMT	A	618	12/35	0.59	0.31	75,89,93,94	0
3	PG5	A	604	11/12	0.65	0.18	95,112,117,118	0
2	6OU	A	620	49/49	0.67	0.29	88,96,136,190	0
7	GOL	A	615	6/6	0.68	0.22	115,120,124,126	0
7	GOL	A	610	6/6	0.69	0.24	114,115,118,124	0
3	PG5	A	603	10/12	0.70	0.40	100,117,125,126	0
5	TRS	A	608	8/8	0.73	0.23	84,90,102,109	0
4	PG6	A	607	13/18	0.74	0.14	87,102,113,115	0
3	PG5	A	606	10/12	0.74	0.19	104,112,120,123	0
8	LMT	A	613	35/35	0.75	0.41	89,125,146,148	0
9	CL	A	622	1/1	0.77	0.34	118,118,118,118	0
7	GOL	A	616	6/6	0.77	0.28	110,110,116,116	0
7	GOL	A	614	6/6	0.83	0.65	104,112,114,118	0
3	PG5	A	605	8/12	0.86	0.57	76,94,112,115	0
6	ACT	A	609	4/4	0.86	0.35	92,100,101,104	0
2	6OU	A	601	49/49	0.93	0.22	68,79,88,110	0
9	CL	A	621	1/1	0.94	0.07	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.

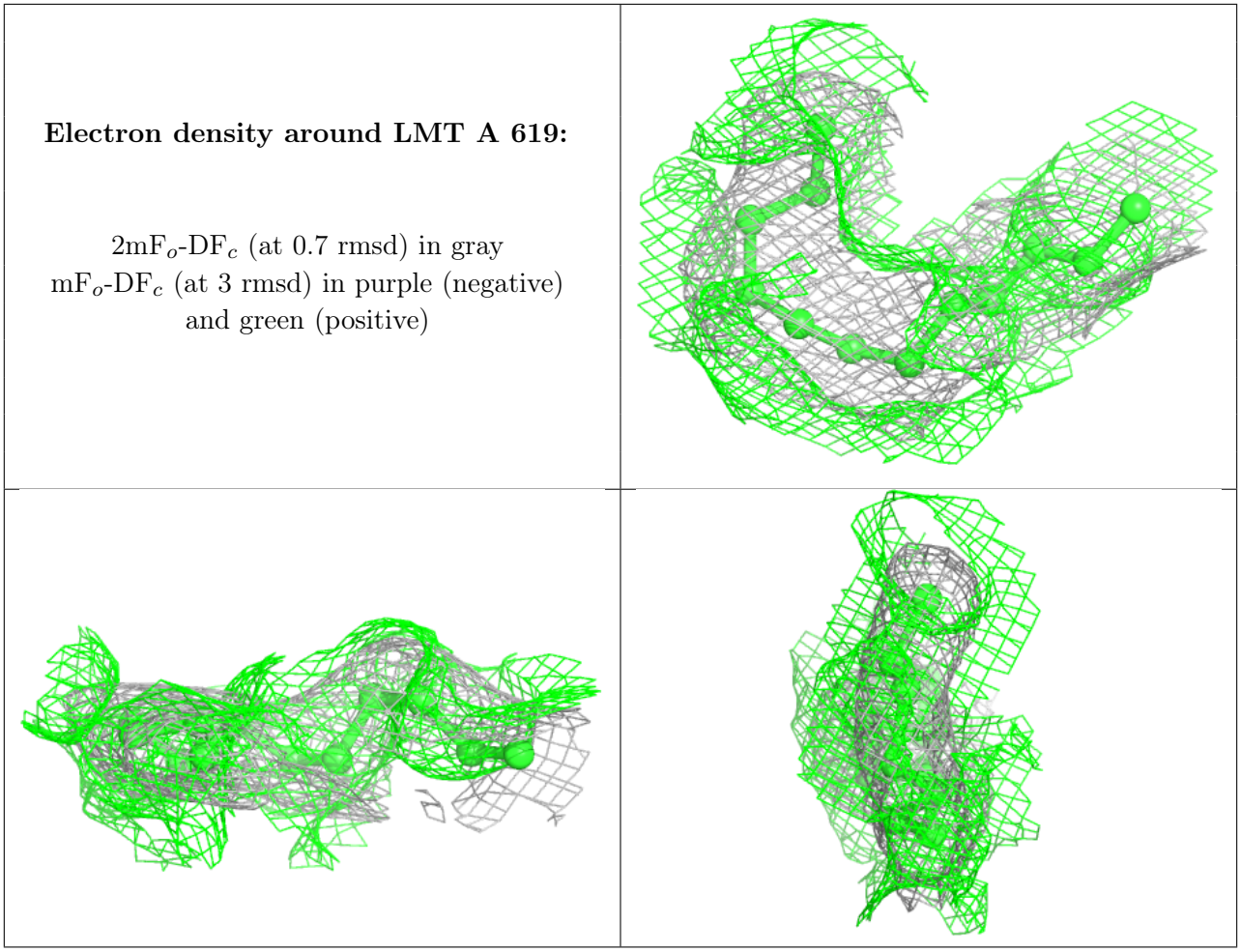
Electron density around LMT A 617:

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



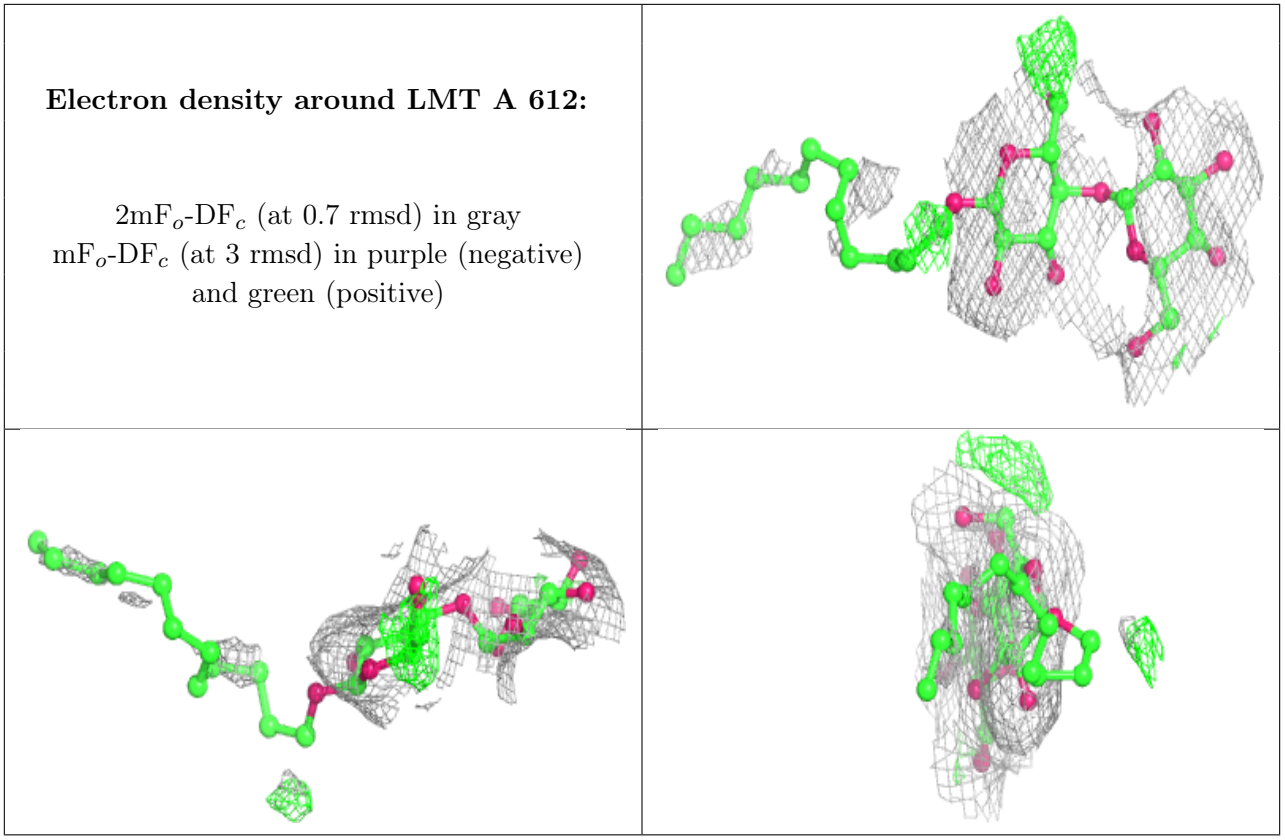
Electron density around LMT A 619:

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



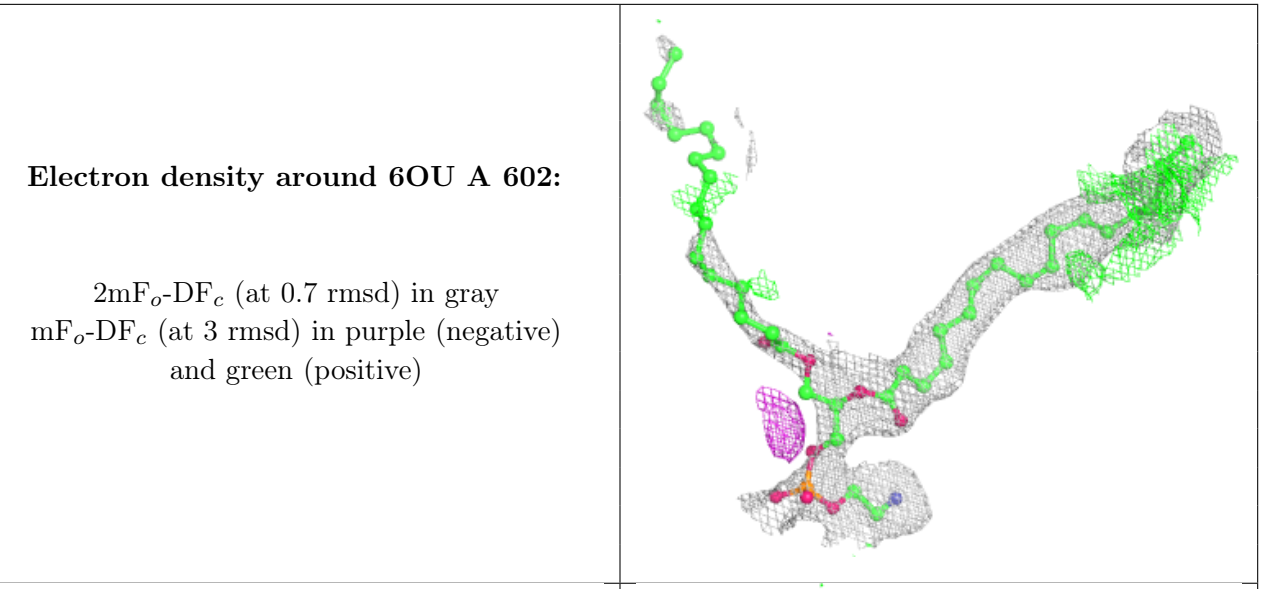
Electron density around LMT A 612:

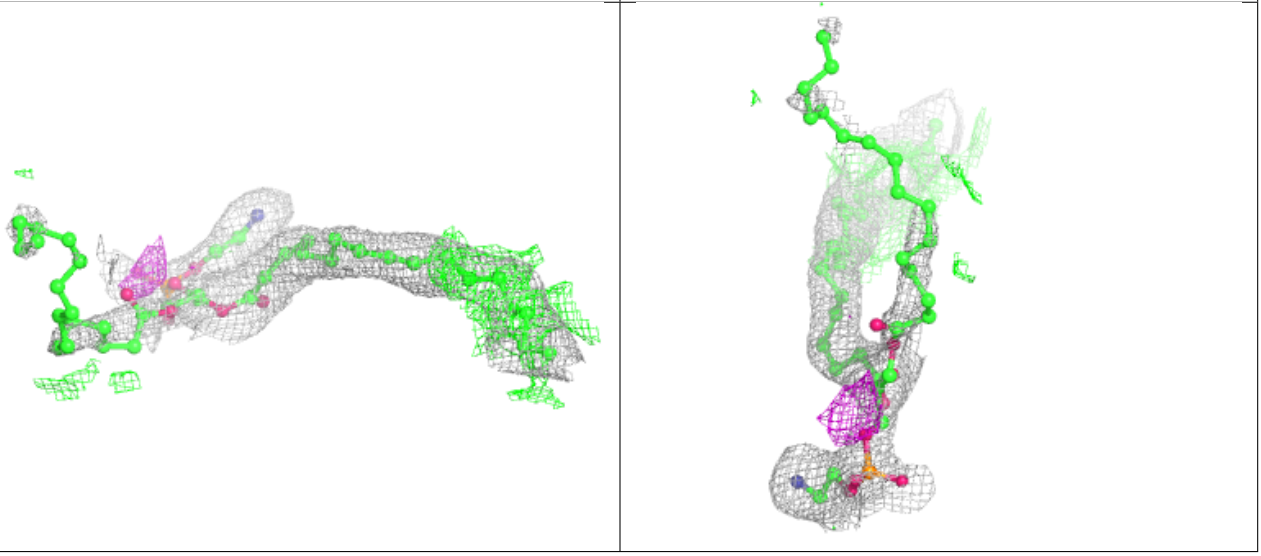
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 6OU A 602:

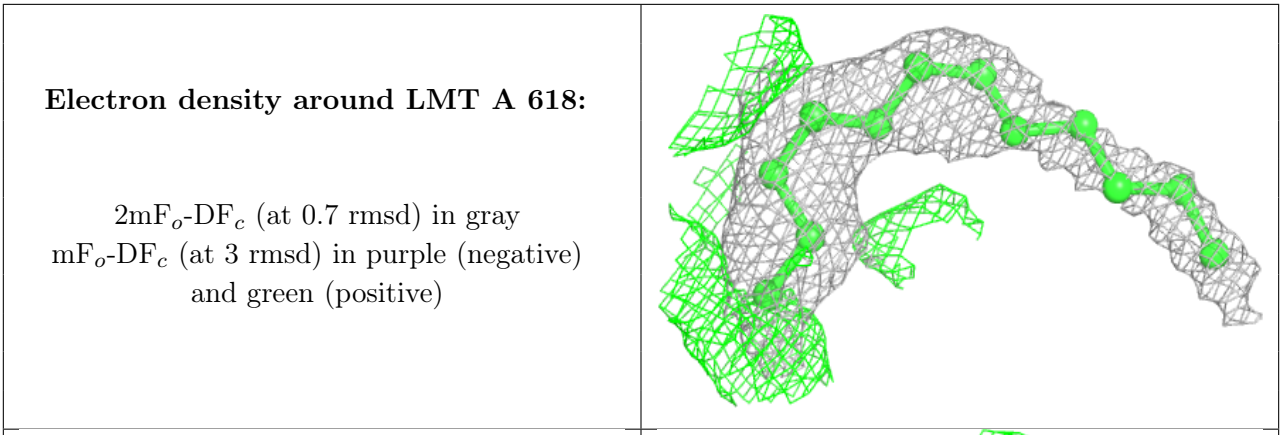
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





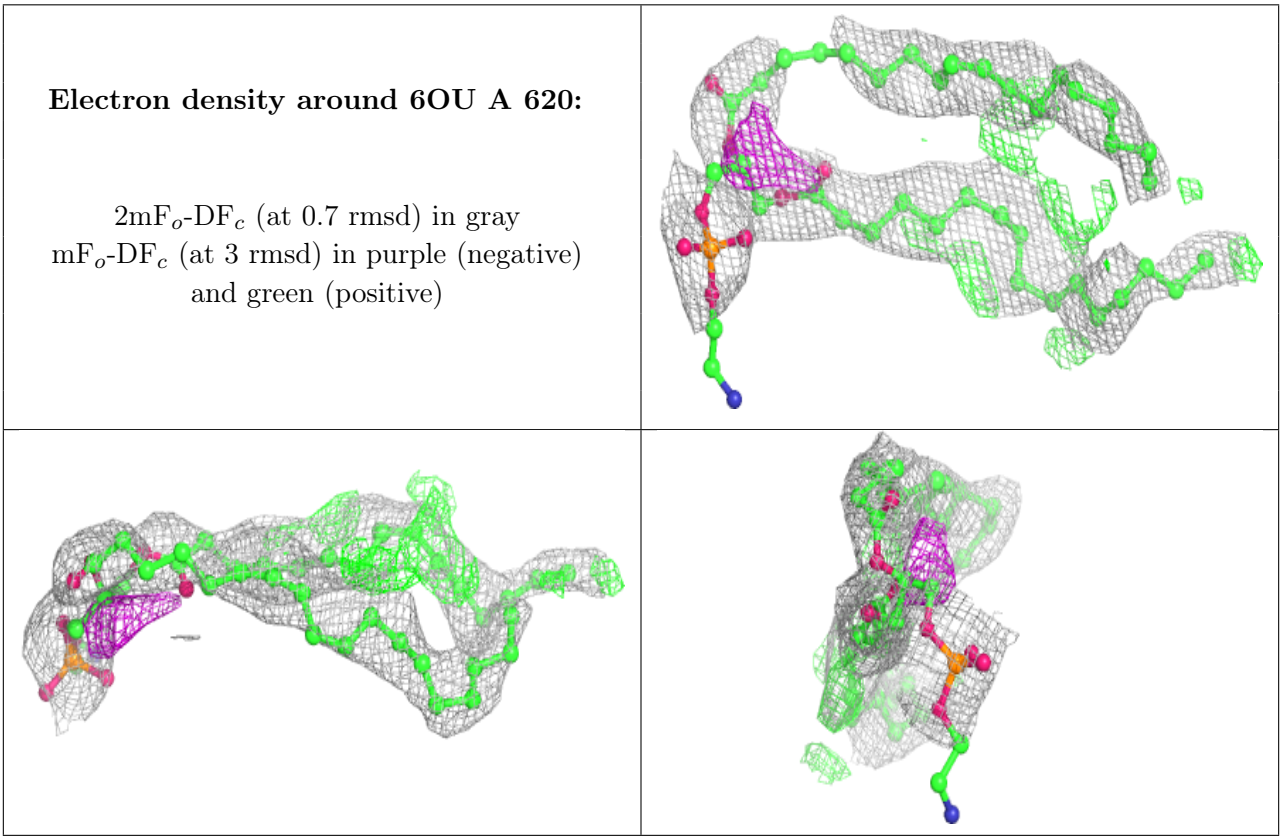
Electron density around LMT A 618:

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



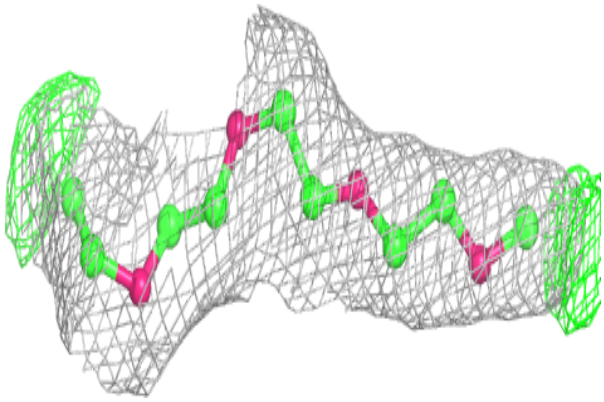
Electron density around 6OU A 620:

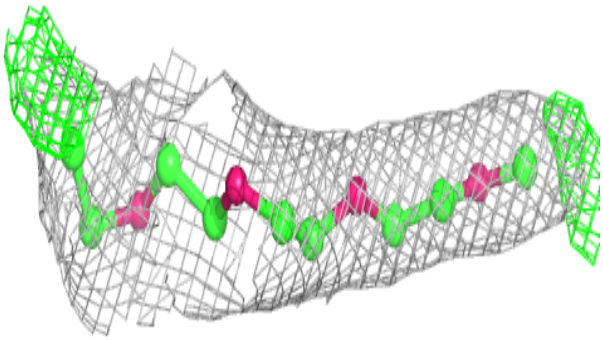
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

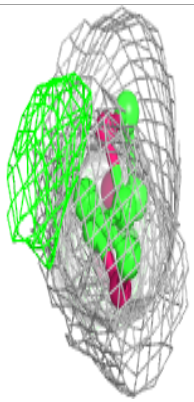


Electron density around PG6 A 607:

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

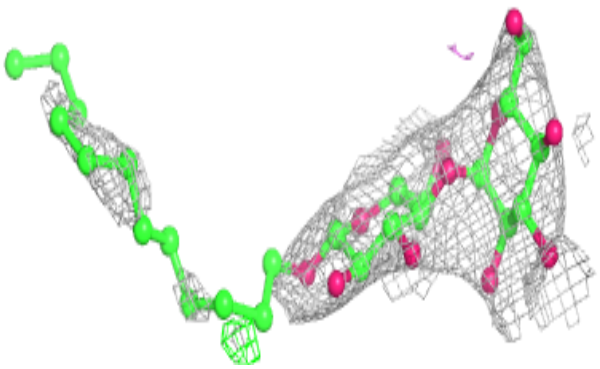


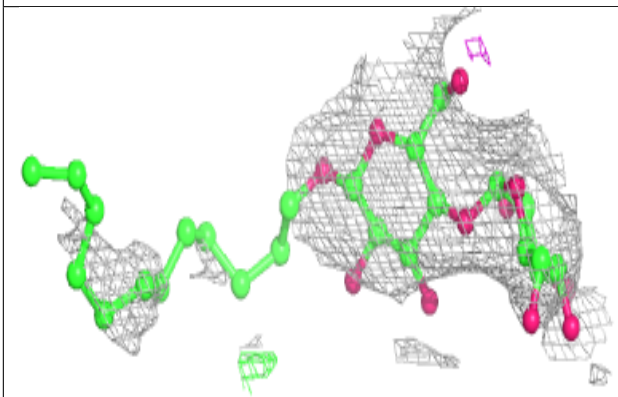


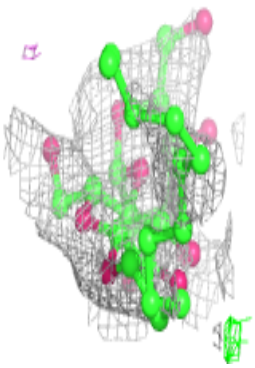


Electron density around LMT A 613:

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

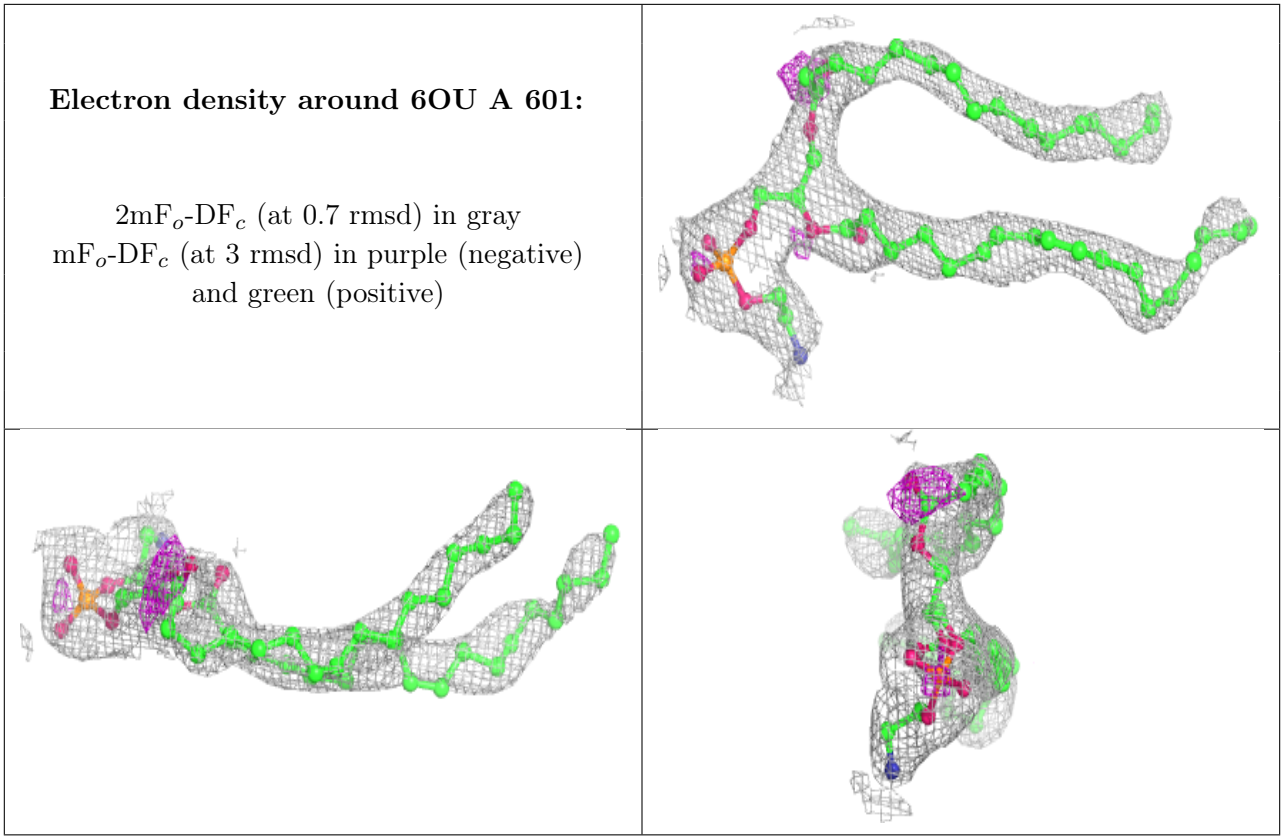






Electron density around 6OU A 601:

$2mF_o$-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.