



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 11, 2026 – 10:09 am BST

PDB ID : 29OM / pdb_000029om
Title : Crystal structure of the staphylococcal efflux pump QacA in the outward open state
Authors : Jodaitis, L.; Hutchin, A.; Govaerts, C.
Deposited on : 2026-03-26
Resolution : 2.83 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	:	1.8.4, CSD as541be (2020)
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

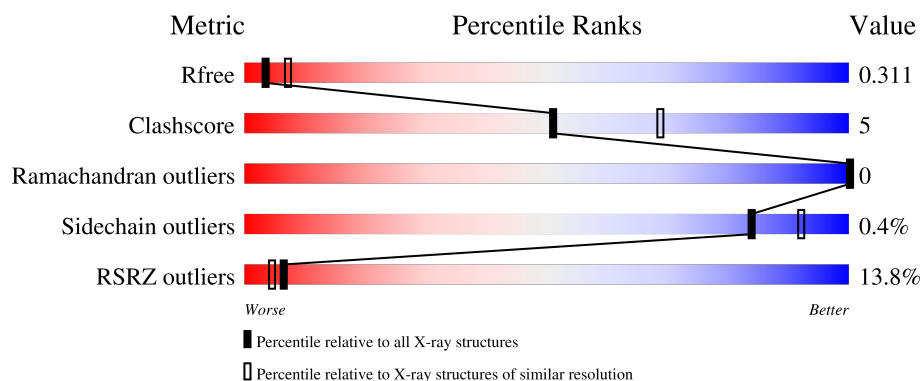
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	520	<div> <div>9%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
1	B	520	<div> <div>18%</div> <div>84%</div> <div>13%</div> <div>.</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8248 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 Antiseptic resistance protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	0	0	0
			3803	2521	591	668	23			
1	B	504	Total	C	N	O	S	0	0	0
			3728	2473	578	656	21			

There are 12 discrepancies between the modelled and reference sequences:

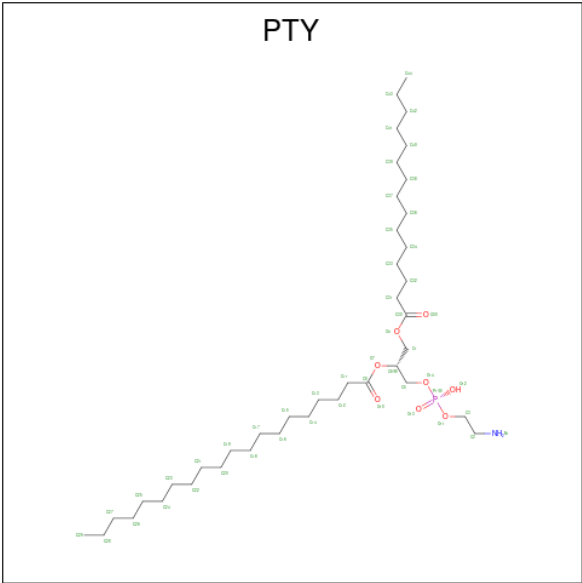
Chain	Residue	Modelled	Actual	Comment	Reference
A	515	LEU	-	expression tag	UNP P0A0J9
A	516	GLU	-	expression tag	UNP P0A0J9
A	517	VAL	-	expression tag	UNP P0A0J9
A	518	LEU	-	expression tag	UNP P0A0J9
A	519	PHE	-	expression tag	UNP P0A0J9
A	520	GLN	-	expression tag	UNP P0A0J9
B	515	LEU	-	expression tag	UNP P0A0J9
B	516	GLU	-	expression tag	UNP P0A0J9
B	517	VAL	-	expression tag	UNP P0A0J9
B	518	LEU	-	expression tag	UNP P0A0J9
B	519	PHE	-	expression tag	UNP P0A0J9
B	520	GLN	-	expression tag	UNP P0A0J9

- Molecule 2 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).

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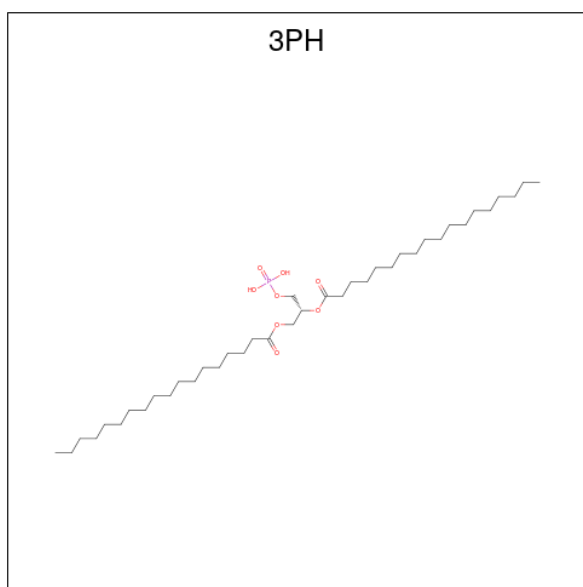
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			27	16	11		
3	A	1	Total	C	O	0	0
			27	16	11		
3	A	1	Total	C	O	0	0
			30	19	11		
3	A	1	Total	C	O	0	0
			29	18	11		
3	A	1	Total	C	O	0	0
			26	15	11		
3	B	1	Total	C	O	0	0
			33	22	11		
3	B	1	Total	C	O	0	0
			31	20	11		
3	B	1	Total	C	O	0	0
			27	16	11		

- Molecule 4 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



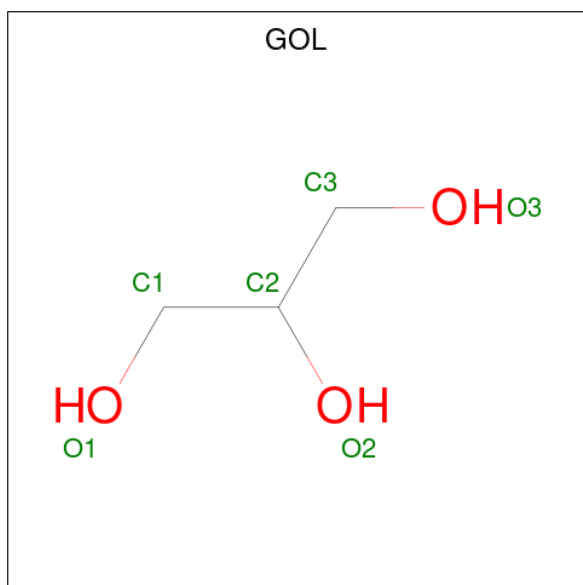
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	21	1	8	1		
4	A	1	Total	C	N	O	P	0	0
			28	18	1	8	1		

- Molecule 5 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: C₃₉H₇₇O₈P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			43	34	8	1		
5	A	1	Total	C	O	P	0	0
			44	35	8	1		
5	A	1	Total	C	O	P	0	0
			48	39	8	1		
5	A	1	Total	C	O	P	0	0
			41	32	8	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Na 1 1	0	0

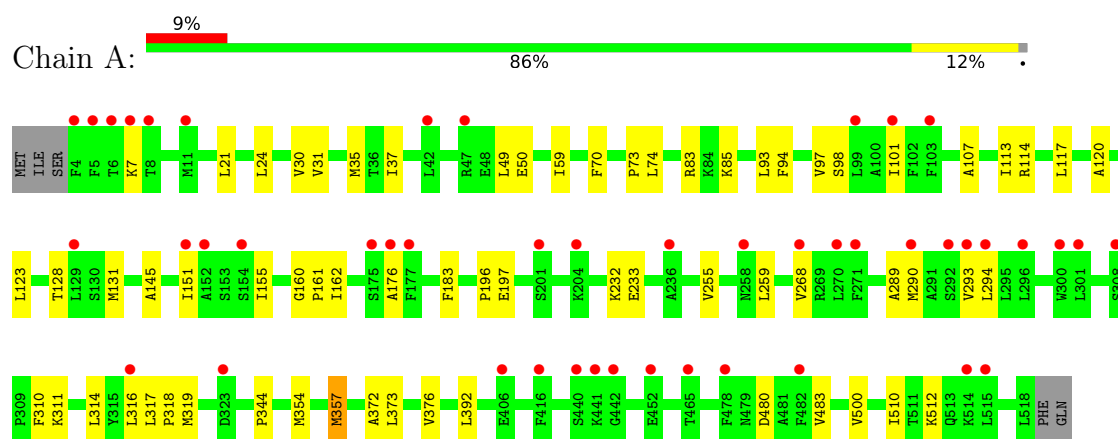
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	48	Total O 48 48	0	0
8	B	20	Total O 20 20	0	0

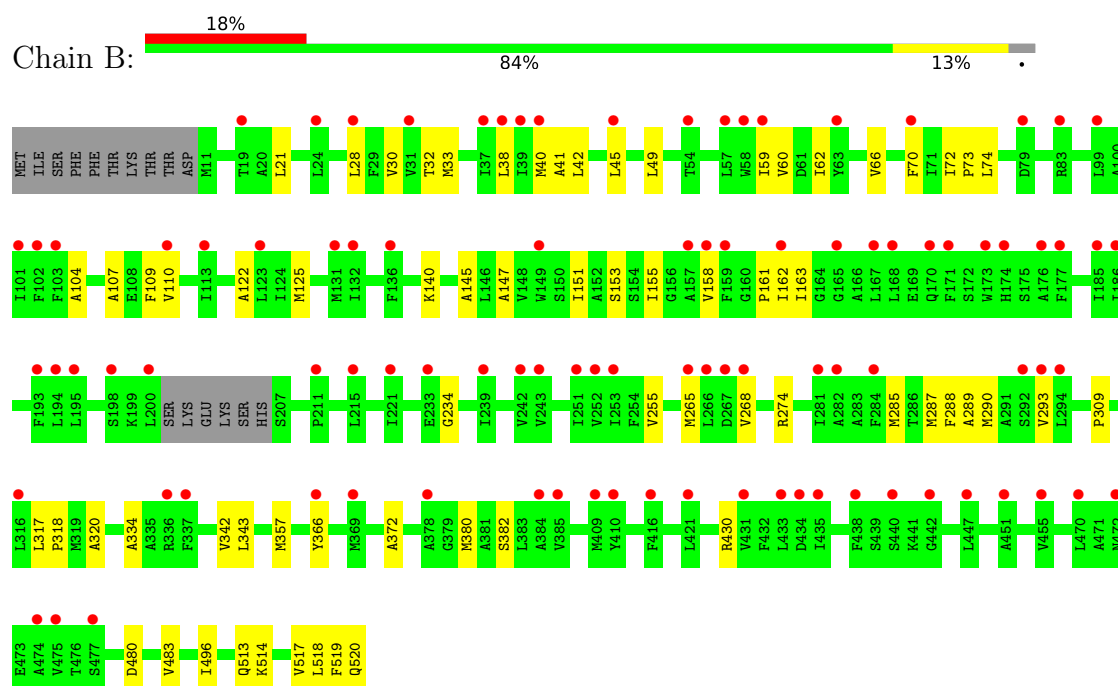
3 Residue-property plots [i](#)

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: Antiseptic resistance protein



- Molecule 1: Antiseptic resistance protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.70Å 74.21Å 279.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.51 – 2.83 46.51 – 2.83	Depositor EDS
% Data completeness (in resolution range)	85.4 (46.51-2.83) 85.3 (46.51-2.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.4 (17-JUL-2025)	Depositor
R, R_{free}	0.310 , 0.328 0.296 , 0.311	Depositor DCC
R_{free} test set	1240 reflections (3.93%)	wwPDB-VP
Wilson B-factor (Å ²)	86.1	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 75.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8248	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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: PGT, NA, 3PH, PTY, LMU, 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	0.83	0/3883	1.23	0/5291
1	B	0.81	0/3803	1.25	0/5180
All	All	0.82	0/7686	1.24	0/10471

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 [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	3803	0	3948	38	0
1	B	3728	0	3893	43	0
2	A	86	0	112	2	0
3	A	200	0	211	1	0
3	B	91	0	101	4	0
4	A	59	0	64	0	0
5	A	176	0	256	2	0
6	A	6	0	8	0	0
6	B	30	0	40	1	0
7	A	1	0	0	0	0
8	A	48	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	20	0	0	0	0
All	All	8248	0	8633	87	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 5.

All (87) 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:B:285:MET:HG3	1:B:496:ILE:HG21	1.72	0.71
1:B:40:MET:HE3	1:B:309:PRO:O	1.98	0.63
1:B:40:MET:HE2	1:B:161:PRO:HB3	1.81	0.61
1:B:30:VAL:HA	1:B:33:MET:HE2	1.82	0.60
1:B:38:LEU:HA	1:B:41:ALA:HB3	1.86	0.57
1:B:70:PHE:HA	1:B:73:PRO:HG2	1.92	0.52
5:A:611:3PH:H12	5:A:611:3PH:H2B2	1.91	0.51
1:A:59:ILE:HD11	1:A:107:ALA:HB1	1.92	0.51
1:B:287:MET:O	1:B:288:PHE:C	2.54	0.51
1:B:430:ARG:HH11	3:B:602:LMU:H2'	1.75	0.50
1:B:32:THR:HG22	1:B:125:MET:HE3	1.92	0.50
1:B:513:GLN:NE2	1:B:518:LEU:HD21	2.26	0.50
1:A:24:LEU:HD22	1:A:128:THR:HG23	1.94	0.49
1:B:42:LEU:HD22	1:B:60:VAL:CG2	2.42	0.49
1:A:344:PRO:HG3	1:A:500:VAL:HG12	1.95	0.49
1:B:151:ILE:HG22	1:B:155:ILE:HD13	1.95	0.49
1:B:59:ILE:HD11	1:B:107:ALA:HB1	1.95	0.49
5:A:611:3PH:H3B1	5:A:611:3PH:H3E2	1.56	0.48
1:B:74:LEU:HD12	1:B:122:ALA:HB3	1.95	0.48
1:B:49:LEU:HD11	1:B:110:VAL:HG21	1.96	0.48
1:A:311:LYS:HA	1:A:314:LEU:HD12	1.95	0.48
1:A:319:MET:HE3	1:A:373:LEU:HD23	1.95	0.48
2:A:604:PGT:H152	2:A:604:PGT:H182	1.41	0.48
1:B:317:LEU:N	1:B:318:PRO:CD	2.77	0.48
1:A:392:LEU:HD22	1:A:510:ILE:HD12	1.95	0.48
1:A:255:VAL:HG13	1:A:268:VAL:HG21	1.96	0.47
1:A:290:MET:HE1	1:A:376:VAL:HG12	1.95	0.47
1:A:83:ARG:HB2	1:A:131:MET:HE3	1.96	0.47
1:A:97:VAL:HG12	1:A:113:ILE:HG23	1.97	0.47
1:A:30:VAL:HG21	1:A:183:PHE:CD2	2.49	0.47
1:B:234:GLY:HA3	3:B:602:LMU:H72	1.97	0.46
1:B:357:MET:HE2	1:B:372:ALA:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LEU:HD23	1:A:120:ALA:HB2	1.97	0.46
1:A:151:ILE:O	1:A:155:ILE:HG12	2.15	0.46
1:B:45:LEU:HG	1:B:49:LEU:HD12	1.97	0.46
1:B:158:VAL:HG12	1:B:317:LEU:HD23	1.97	0.46
1:B:21:LEU:HD21	1:B:145:ALA:HA	1.98	0.46
1:B:290:MET:HB2	1:B:380:MET:SD	2.56	0.45
1:B:334:ALA:HA	1:B:342:VAL:HG21	1.97	0.45
1:A:480:ASP:HA	1:A:483:VAL:HG22	1.98	0.45
1:B:158:VAL:HG11	1:B:320:ALA:HB2	1.98	0.45
3:B:602:LMU:H62	3:B:602:LMU:H5'	1.98	0.45
1:A:162:ILE:CD1	1:A:317:LEU:HD21	2.47	0.45
1:A:49:LEU:O	1:A:50:GLU:C	2.60	0.45
1:B:162:ILE:HD12	1:B:163:ILE:HG13	1.98	0.44
1:A:70:PHE:HA	1:A:73:PRO:HG2	1.99	0.44
1:A:114:ARG:HD2	1:A:117:LEU:HD12	1.99	0.44
3:B:602:LMU:H2'	6:B:606:GOL:H12	1.98	0.44
1:B:62:ILE:O	1:B:66:VAL:HG23	2.17	0.44
1:A:293:VAL:HG22	1:A:354:MET:HE3	1.99	0.44
1:A:259:LEU:HG	1:A:268:VAL:CG2	2.47	0.44
1:A:317:LEU:N	1:A:318:PRO:CD	2.81	0.44
1:B:255:VAL:HG13	1:B:268:VAL:HG21	2.00	0.43
1:A:160:GLY:N	1:A:161:PRO:HD2	2.34	0.43
1:B:49:LEU:HD22	1:B:107:ALA:N	2.34	0.43
1:A:97:VAL:CG1	1:A:113:ILE:HG23	2.49	0.43
1:B:104:ALA:HA	1:B:109:PHE:CD1	2.55	0.42
1:A:21:LEU:HD21	1:A:145:ALA:HA	2.00	0.42
1:B:514:LYS:HB3	1:B:517:VAL:HG23	2.02	0.42
2:A:604:PGT:H201	2:A:604:PGT:H171	1.49	0.42
1:B:72:ILE:HG22	1:B:265:MET:HE3	2.01	0.42
1:A:70:PHE:HB3	1:A:74:LEU:HD12	2.01	0.42
1:A:289:ALA:O	1:A:290:MET:C	2.63	0.42
1:A:512:LYS:HD3	1:A:512:LYS:HA	1.74	0.42
1:A:294:LEU:HD23	1:A:316:LEU:HD22	2.02	0.42
1:B:366:TYR:O	1:B:366:TYR:CG	2.72	0.42
1:A:74:LEU:HD22	1:A:123:LEU:HD11	2.00	0.42
1:B:140:LYS:HB2	1:B:140:LYS:HE3	1.87	0.42
1:A:31:VAL:HG22	1:A:94:PHE:CE2	2.55	0.41
1:B:480:ASP:HA	1:B:483:VAL:HG22	2.02	0.41
1:A:232:LYS:HG3	1:A:233:GLU:HG2	2.02	0.41
1:B:42:LEU:HD12	1:B:45:LEU:HD23	2.02	0.41
1:B:343:LEU:HD12	1:B:382:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LYS:HB3	1:A:196:PRO:HA	2.02	0.41
1:A:37:ILE:CG2	1:A:176:ALA:HB1	2.51	0.41
1:A:85:LYS:HG3	1:A:197:GLU:OE2	2.21	0.41
1:A:294:LEU:HD11	1:A:319:MET:SD	2.61	0.41
1:A:310:PHE:CD2	3:A:608:LMU:H5B	2.56	0.41
1:A:357:MET:HE2	1:A:372:ALA:HB1	2.03	0.41
1:B:162:ILE:HG12	1:B:317:LEU:HD21	2.03	0.41
1:B:289:ALA:O	1:B:293:VAL:HG22	2.21	0.41
1:B:519:PHE:O	1:B:520:GLN:C	2.64	0.41
1:B:285:MET:HE3	1:B:285:MET:HB3	1.79	0.41
1:B:28:LEU:HD21	1:B:153:SER:OG	2.21	0.40
1:B:147:ALA:O	1:B:151:ILE:HG13	2.22	0.40
1:B:357:MET:HE2	1:B:372:ALA:HB3	2.02	0.40
1:A:98:SER:O	1:A:101:ILE:HG22	2.22	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	513/520 (99%)	502 (98%)	11 (2%)	0	100	100
1	B	500/520 (96%)	489 (98%)	11 (2%)	0	100	100
All	All	1013/1040 (97%)	991 (98%)	22 (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	397/421 (94%)	395 (100%)	2 (0%)	81	90
1	B	391/421 (93%)	390 (100%)	1 (0%)	86	94
All	All	788/842 (94%)	785 (100%)	3 (0%)	84	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	MET
1	A	357	MET
1	B	274	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	GLN
1	B	55	GLN
1	B	469	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 1 is monoatomic - leaving 24 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	$\# Z > 2$
3	LMU	B	603	-	28,28,36	0.26	0	39,39,47	0.61	0
5	3PH	A	611	-	47,47,47	0.30	0	51,52,52	0.31	0
3	LMU	A	615	-	27,27,36	0.20	0	37,38,47	0.30	0
5	3PH	A	609	-	42,42,47	0.34	0	46,47,52	0.36	0
6	GOL	B	606	-	5,5,5	0.10	0	5,5,5	0.23	0
3	LMU	A	602	-	32,32,36	0.31	0	43,43,47	0.34	0
6	GOL	B	607	-	5,5,5	0.04	0	5,5,5	0.22	0
3	LMU	A	607	-	28,28,36	0.31	0	39,39,47	0.86	2 (5%)
6	GOL	A	616	-	5,5,5	0.10	0	5,5,5	0.25	0
5	3PH	A	614	-	40,40,47	0.38	0	44,45,52	0.37	0
6	GOL	B	608	-	5,5,5	0.05	0	5,5,5	0.24	0
3	LMU	B	602	-	32,32,36	0.15	0	43,43,47	0.36	0
3	LMU	A	603	-	31,31,36	0.30	0	42,42,47	0.72	1 (2%)
6	GOL	B	605	-	5,5,5	0.08	0	5,5,5	0.27	0
3	LMU	A	608	-	31,31,36	0.20	0	42,42,47	0.95	2 (4%)
4	PTY	A	605	-	30,30,49	0.40	0	33,35,54	0.49	0
3	LMU	B	601	-	34,34,36	0.38	0	45,45,47	0.82	2 (4%)
6	GOL	B	604	-	5,5,5	0.05	0	5,5,5	0.24	0
2	PGT	A	604	-	38,38,50	0.31	0	41,44,56	0.34	0
5	3PH	A	610	-	43,43,47	0.38	0	47,48,52	0.35	0
3	LMU	A	612	-	30,30,36	0.25	0	41,41,47	0.41	0
4	PTY	A	613	-	27,27,49	0.35	0	30,32,54	0.49	0
2	PGT	A	601	-	46,46,50	0.26	0	49,52,56	0.34	0
3	LMU	A	606	-	28,28,36	0.20	0	39,39,47	0.63	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMU	B	603	-	-	0/13/53/61	0/2/2/2
5	3PH	A	611	-	-	27/49/49/49	-
3	LMU	A	615	-	-	5/12/52/61	0/2/2/2
5	3PH	A	609	-	-	20/44/44/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	606	-	-	2/4/4/4	-
3	LMU	A	602	-	-	7/17/57/61	0/2/2/2
6	GOL	B	607	-	-	0/4/4/4	-
3	LMU	A	607	-	-	10/13/53/61	0/2/2/2
6	GOL	A	616	-	-	4/4/4/4	-
5	3PH	A	614	-	-	21/42/42/49	-
6	GOL	B	608	-	-	0/4/4/4	-
3	LMU	B	602	-	-	10/17/57/61	0/2/2/2
3	LMU	A	603	-	-	9/16/56/61	0/2/2/2
6	GOL	B	605	-	-	1/4/4/4	-
3	LMU	A	608	-	-	10/16/56/61	0/2/2/2
4	PTY	A	605	-	-	21/34/34/53	-
3	LMU	B	601	-	-	6/19/59/61	0/2/2/2
6	GOL	B	604	-	-	0/4/4/4	-
2	PGT	A	604	-	-	27/43/43/55	-
5	3PH	A	610	-	-	24/45/45/49	-
3	LMU	A	612	-	-	3/15/55/61	0/2/2/2
4	PTY	A	613	-	-	7/31/31/53	-
2	PGT	A	601	-	-	6/51/51/55	-
3	LMU	A	606	-	-	6/13/53/61	0/2/2/2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	608	LMU	C1B-O1B-C4'	3.59	126.86	117.96
3	A	607	LMU	C3B-C4B-C5B	3.17	115.89	110.24
3	B	601	LMU	O5'-C5'-C4'	2.71	115.46	109.75
3	B	601	LMU	C2'-C3'-C4'	2.65	115.72	109.68
3	A	608	LMU	O1B-C4'-C5'	2.58	116.52	109.45
3	A	603	LMU	C3B-C4B-C5B	2.35	114.43	110.24
3	A	607	LMU	O5B-C5B-C4B	2.12	113.55	109.69

There are no chirality outliers.

All (226) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	PGT	C4-O4P-P-O3P
2	A	601	PGT	C4-O4P-P-O1P
2	A	604	PGT	C1-O3P-P-O1P
2	A	604	PGT	C4-O4P-P-O2P
3	A	602	LMU	C2'-C1'-O1'-C1
3	A	602	LMU	O5'-C1'-O1'-C1
3	A	602	LMU	C2-C1-O1'-C1'
3	A	603	LMU	C2-C1-O1'-C1'
3	A	608	LMU	C2-C1-O1'-C1'
3	B	602	LMU	C2'-C1'-O1'-C1
3	B	602	LMU	O5'-C1'-O1'-C1
4	A	605	PTY	C2-C3-O11-P1
4	A	605	PTY	C11-C8-O7-C6
4	A	605	PTY	C3-O11-P1-O12
4	A	605	PTY	C5-O14-P1-O12
4	A	613	PTY	C5-O14-P1-O11
5	A	610	3PH	C1-O11-P-O13
5	A	611	3PH	C1-O11-P-O13
5	A	611	3PH	C1-O11-P-O12
5	A	614	3PH	C22-C21-O21-C2
6	A	616	GOL	O1-C1-C2-C3
6	A	616	GOL	C1-C2-C3-O3
6	B	606	GOL	C1-C2-C3-O3
3	A	608	LMU	O5B-C1B-O1B-C4'
3	B	602	LMU	O5B-C1B-O1B-C4'
3	A	603	LMU	O5B-C1B-O1B-C4'
3	A	606	LMU	C3'-C4'-O1B-C1B
4	A	605	PTY	O10-C8-O7-C6
5	A	614	3PH	O22-C21-O21-C2
3	A	603	LMU	C2B-C1B-O1B-C4'
5	A	614	3PH	O32-C31-O31-C3
5	A	614	3PH	C32-C31-O31-C3
3	A	607	LMU	C5'-C4'-O1B-C1B
5	A	611	3PH	C2E-C2F-C2G-C2H
3	A	608	LMU	C1-C2-C3-C4
2	A	604	PGT	C15-C16-C17-C18
3	A	606	LMU	O5'-C5'-C6'-O6'
2	A	604	PGT	C33-C34-C35-C36
3	A	608	LMU	C5'-C4'-O1B-C1B
3	A	603	LMU	O5B-C5B-C6B-O6B
3	A	615	LMU	O5'-C5'-C6'-O6'
5	A	609	3PH	C22-C21-O21-C2
2	A	604	PGT	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
5	A	609	3PH	C32-C31-O31-C3
5	A	611	3PH	C3B-C3C-C3D-C3E
5	A	609	3PH	C36-C37-C38-C39
3	A	615	LMU	C4'-C5'-C6'-O6'
3	A	603	LMU	C4B-C5B-C6B-O6B
5	A	614	3PH	C31-C32-C33-C34
5	A	609	3PH	O32-C31-O31-C3
3	B	602	LMU	O5'-C5'-C6'-O6'
4	A	605	PTY	C30-C31-C32-C33
3	A	607	LMU	O5B-C5B-C6B-O6B
3	A	603	LMU	O5'-C1'-O1'-C1
5	A	609	3PH	O22-C21-O21-C2
5	A	611	3PH	C33-C34-C35-C36
2	A	604	PGT	C4-O4P-P-O3P
4	A	605	PTY	C3-O11-P1-O14
4	A	605	PTY	C5-O14-P1-O11
2	A	604	PGT	C31-C32-C33-C34
3	B	601	LMU	C3-C4-C5-C6
5	A	609	3PH	C3C-C3D-C3E-C3F
5	A	614	3PH	C2D-C2E-C2F-C2G
4	A	605	PTY	C12-C13-C14-C15
5	A	611	3PH	C24-C25-C26-C27
5	A	614	3PH	C22-C23-C24-C25
3	B	601	LMU	C4-C5-C6-C7
5	A	610	3PH	C2C-C2D-C2E-C2F
5	A	611	3PH	C2D-C2E-C2F-C2G
3	A	608	LMU	O1'-C1-C2-C3
5	A	614	3PH	C35-C36-C37-C38
5	A	611	3PH	C31-C32-C33-C34
2	A	604	PGT	C13-C14-C15-C16
3	A	607	LMU	O1'-C1-C2-C3
3	B	601	LMU	C2-C3-C4-C5
5	A	610	3PH	C26-C27-C28-C29
5	A	611	3PH	C21-C22-C23-C24
5	A	611	3PH	C37-C38-C39-C3A
5	A	614	3PH	C28-C29-C2A-C2B
3	B	602	LMU	O1'-C1-C2-C3
5	A	611	3PH	C25-C26-C27-C28
5	A	610	3PH	C37-C38-C39-C3A
4	A	605	PTY	N1-C2-C3-O11
5	A	609	3PH	C34-C35-C36-C37
5	A	610	3PH	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
2	A	604	PGT	C14-C15-C16-C17
5	A	610	3PH	C32-C33-C34-C35
6	A	616	GOL	O1-C1-C2-O2
6	A	616	GOL	O2-C2-C3-O3
6	B	606	GOL	O2-C2-C3-O3
4	A	605	PTY	C34-C35-C36-C37
3	A	607	LMU	C4'-C5'-C6'-O6'
3	A	608	LMU	O5B-C5B-C6B-O6B
2	A	604	PGT	C32-C31-O2-C2
5	A	614	3PH	C32-C33-C34-C35
5	A	610	3PH	C22-C23-C24-C25
5	A	611	3PH	C3F-C3G-C3H-C3I
2	A	604	PGT	C16-C17-C18-C19
3	B	602	LMU	C4-C5-C6-C7
2	A	604	PGT	C18-C19-C20-C21
3	A	602	LMU	C1-C2-C3-C4
3	A	615	LMU	O1'-C1-C2-C3
5	A	611	3PH	C2B-C2C-C2D-C2E
5	A	610	3PH	C22-C21-O21-C2
5	A	610	3PH	C32-C31-O31-C3
3	A	607	LMU	C1-C2-C3-C4
3	A	602	LMU	O5'-C5'-C6'-O6'
5	A	611	3PH	C2C-C2D-C2E-C2F
3	A	603	LMU	C1-C2-C3-C4
2	A	604	PGT	O31-C31-O2-C2
2	A	604	PGT	C1-O3P-P-O4P
5	A	611	3PH	C23-C24-C25-C26
4	A	605	PTY	C32-C33-C34-C35
5	A	609	3PH	C3A-C3B-C3C-C3D
5	A	609	3PH	C3E-C3F-C3G-C3H
5	A	610	3PH	O32-C31-O31-C3
3	A	606	LMU	C4'-C5'-C6'-O6'
5	A	611	3PH	C28-C29-C2A-C2B
4	A	605	PTY	C35-C36-C37-C38
4	A	605	PTY	C8-C11-C12-C13
2	A	604	PGT	C34-C35-C36-C37
3	B	602	LMU	C3-C4-C5-C6
3	A	612	LMU	O5'-C5'-C6'-O6'
3	B	602	LMU	O5B-C5B-C6B-O6B
5	A	610	3PH	C35-C36-C37-C38
5	A	610	3PH	O22-C21-O21-C2
3	A	603	LMU	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
5	A	611	3PH	C39-C3A-C3B-C3C
2	A	601	PGT	O3P-C1-C2-O2
5	A	609	3PH	C21-C22-C23-C24
5	A	610	3PH	C21-C22-C23-C24
3	A	608	LMU	C3'-C4'-O1B-C1B
4	A	605	PTY	C31-C30-O4-C1
2	A	604	PGT	O4P-C4-C5-C6
3	B	602	LMU	C4'-C5'-C6'-O6'
3	A	607	LMU	C3'-C4'-O1B-C1B
5	A	611	3PH	C22-C23-C24-C25
2	A	604	PGT	C5-C4-O4P-P
3	A	607	LMU	O5'-C5'-C6'-O6'
3	A	606	LMU	C2-C1-O1'-C1'
3	A	607	LMU	C2-C1-O1'-C1'
3	A	612	LMU	C2-C1-O1'-C1'
3	A	615	LMU	C4B-C5B-C6B-O6B
2	A	604	PGT	C1-C2-C3-O3
4	A	605	PTY	O4-C1-C6-C5
5	A	614	3PH	C1-C2-C3-O31
3	A	607	LMU	O5B-C1B-O1B-C4'
3	A	612	LMU	C3-C4-C5-C6
2	A	604	PGT	C35-C36-C37-C38
4	A	605	PTY	O30-C30-O4-C1
3	A	602	LMU	O1'-C1-C2-C3
2	A	604	PGT	O2-C2-C3-O3
4	A	613	PTY	O4-C1-C6-O7
5	A	610	3PH	O21-C2-C3-O31
5	A	611	3PH	C3A-C3B-C3C-C3D
2	A	604	PGT	C2-C1-O3P-P
5	A	609	3PH	C39-C3A-C3B-C3C
3	B	601	LMU	C5'-C4'-O1B-C1B
5	A	610	3PH	C1-O11-P-O14
5	A	609	3PH	C32-C33-C34-C35
5	A	614	3PH	C3-C2-O21-C21
4	A	613	PTY	O14-C5-C6-O7
5	A	614	3PH	C2F-C2G-C2H-C2I
5	A	611	3PH	C32-C33-C34-C35
4	A	605	PTY	O4-C1-C6-O7
5	A	614	3PH	O21-C2-C3-O31
3	A	608	LMU	C4-C5-C6-C7
3	A	608	LMU	C4'-C5'-C6'-O6'
5	A	610	3PH	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
3	B	601	LMU	C3'-C4'-O1B-C1B
3	A	607	LMU	C2B-C1B-O1B-C4'
5	A	610	3PH	C2-C1-O11-P
2	A	604	PGT	C1-O3P-P-O2P
4	A	605	PTY	C5-O14-P1-O13
4	A	613	PTY	C5-O14-P1-O12
5	A	609	3PH	C3B-C3C-C3D-C3E
3	A	603	LMU	C4-C5-C6-C7
4	A	605	PTY	C6-C5-O14-P1
2	A	604	PGT	C21-C22-C23-C24
5	A	611	3PH	C2A-C2B-C2C-C2D
5	A	614	3PH	C36-C37-C38-C39
3	A	615	LMU	O5B-C5B-C6B-O6B
3	A	602	LMU	C2-C3-C4-C5
2	A	601	PGT	O3P-C1-C2-C3
5	A	609	3PH	C24-C25-C26-C27
4	A	613	PTY	C3-O11-P1-O14
3	A	606	LMU	O1'-C1-C2-C3
4	A	605	PTY	C33-C34-C35-C36
2	A	601	PGT	O4P-C4-C5-O5
5	A	610	3PH	C34-C35-C36-C37
5	A	609	3PH	C23-C24-C25-C26
5	A	614	3PH	C2E-C2F-C2G-C2H
5	A	611	3PH	C3D-C3E-C3F-C3G
2	A	604	PGT	C19-C20-C21-C22
5	A	611	3PH	C3E-C3F-C3G-C3H
5	A	609	3PH	C37-C38-C39-C3A
3	A	608	LMU	O5'-C5'-C6'-O6'
4	A	613	PTY	O14-C5-C6-C1
3	B	601	LMU	C6-C7-C8-C9
5	A	611	3PH	C1-O11-P-O14
5	A	614	3PH	C1-O11-P-O13
3	A	606	LMU	C5'-C4'-O1B-C1B
2	A	604	PGT	O3-C11-C12-C13
5	A	609	3PH	C1-C2-O21-C21
5	A	610	3PH	C2E-C2F-C2G-C2H
5	A	614	3PH	O31-C31-C32-C33
2	A	601	PGT	C15-C16-C17-C18
5	A	614	3PH	C33-C34-C35-C36
5	A	610	3PH	C1-C2-C3-O31
5	A	611	3PH	O31-C31-C32-C33
2	A	604	PGT	O4P-C4-C5-O5

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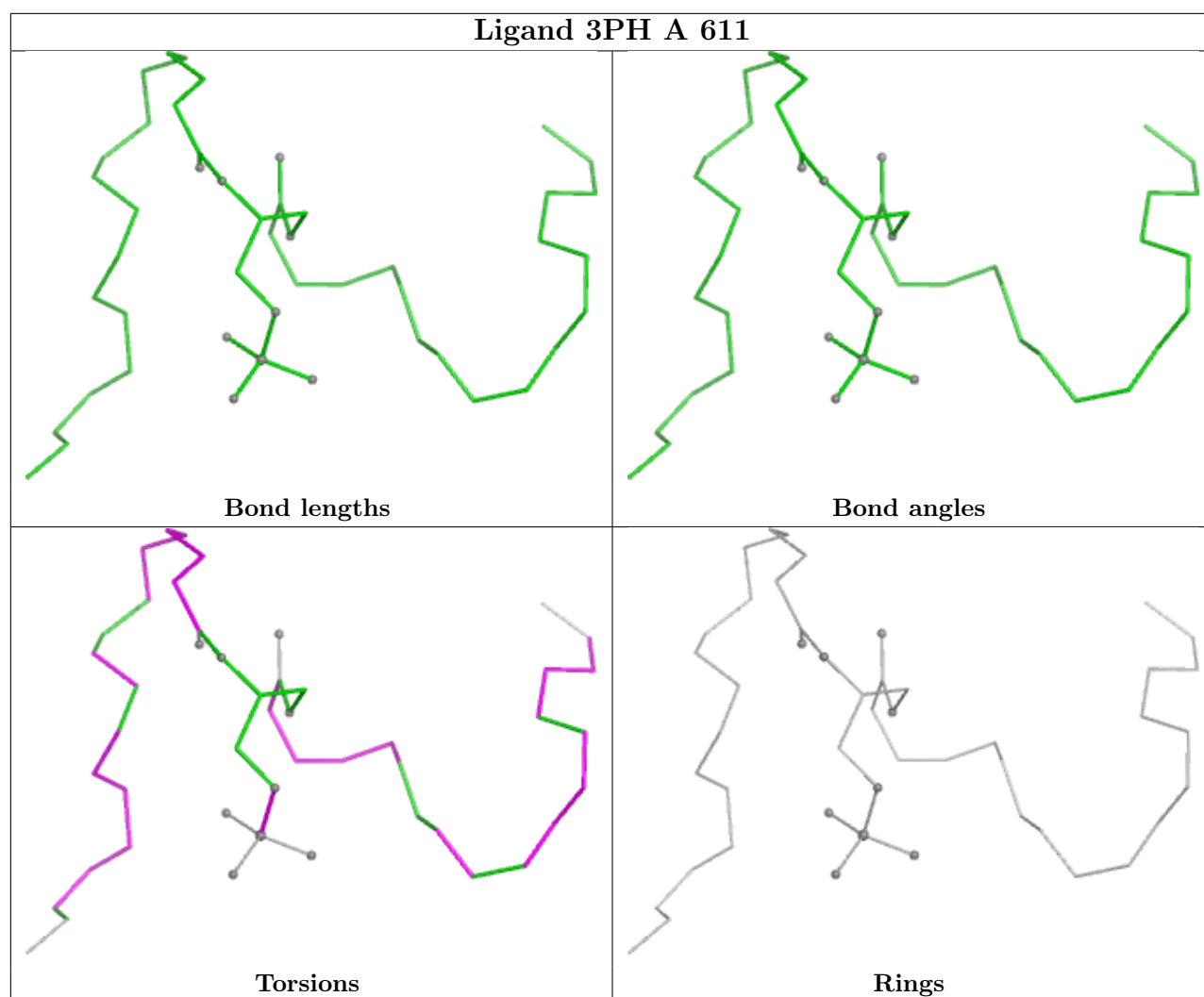
Mol	Chain	Res	Type	Atoms
5	A	610	3PH	C27-C28-C29-C2A
6	B	605	GOL	O2-C2-C3-O3
5	A	609	3PH	O21-C21-C22-C23
5	A	614	3PH	C2A-C2B-C2C-C2D
5	A	609	3PH	C2A-C2B-C2C-C2D
2	A	604	PGT	O11-C11-C12-C13
5	A	611	3PH	C34-C35-C36-C37
5	A	610	3PH	O21-C21-C22-C23
5	A	614	3PH	O32-C31-C32-C33
5	A	609	3PH	O22-C21-C22-C23
4	A	613	PTY	C2-C3-O11-P1
5	A	610	3PH	O31-C31-C32-C33
5	A	610	3PH	O22-C21-C22-C23
5	A	611	3PH	O21-C21-C22-C23
3	B	602	LMU	C1-C2-C3-C4

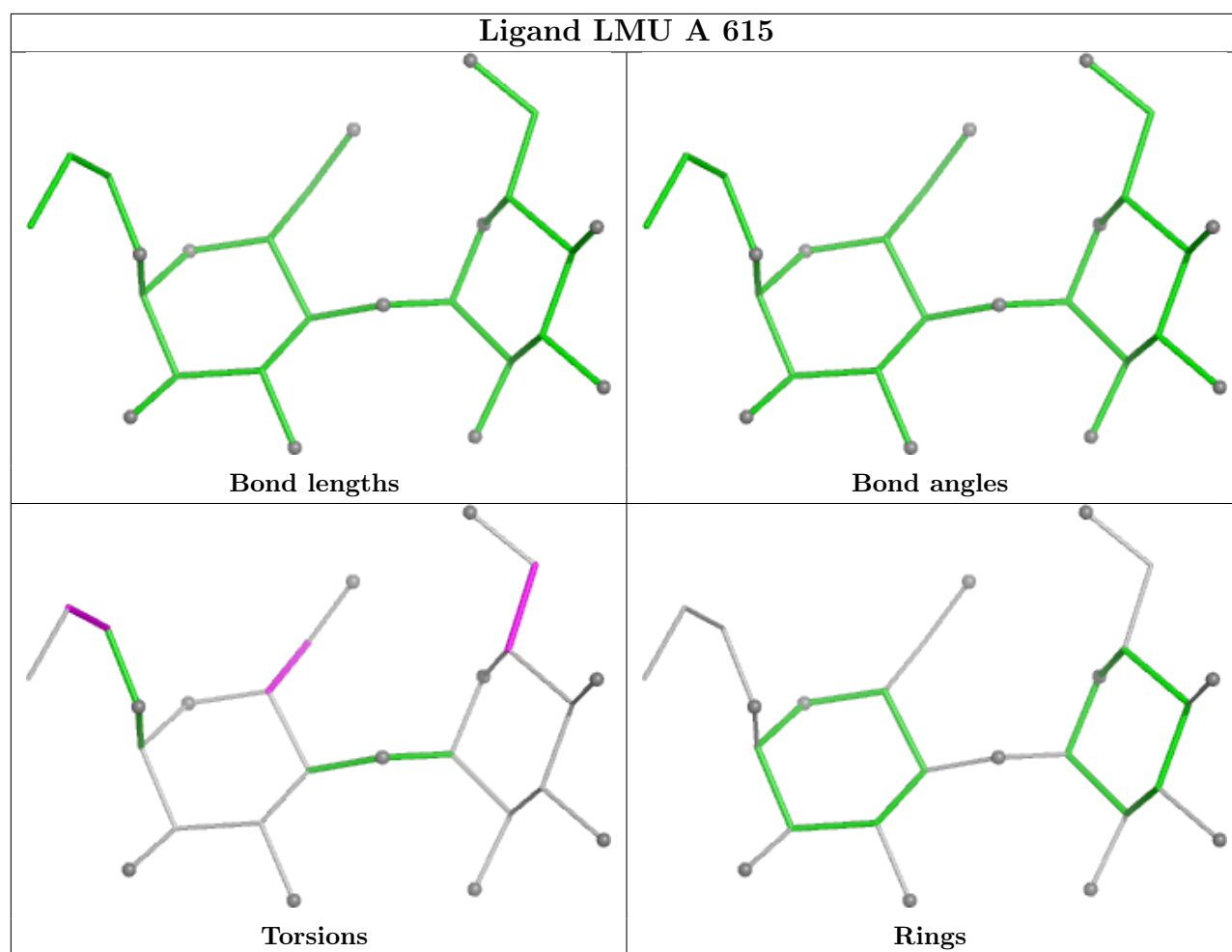
There are no ring outliers.

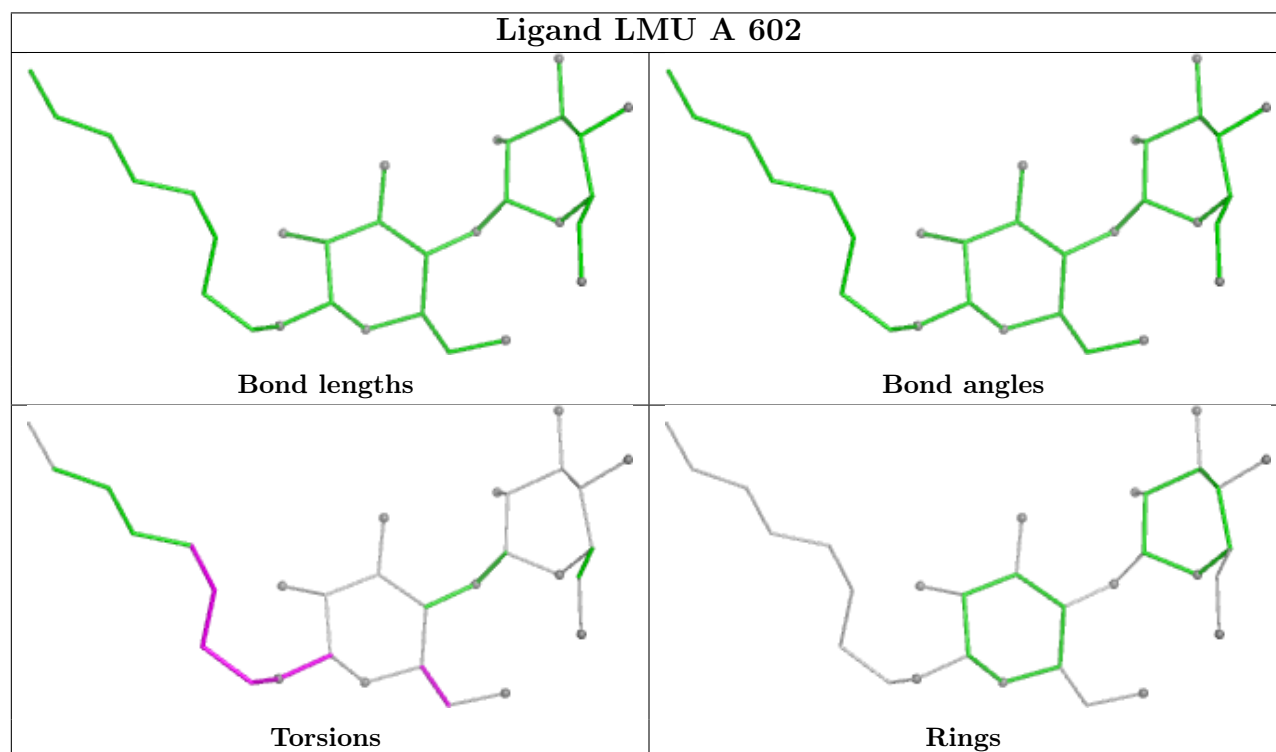
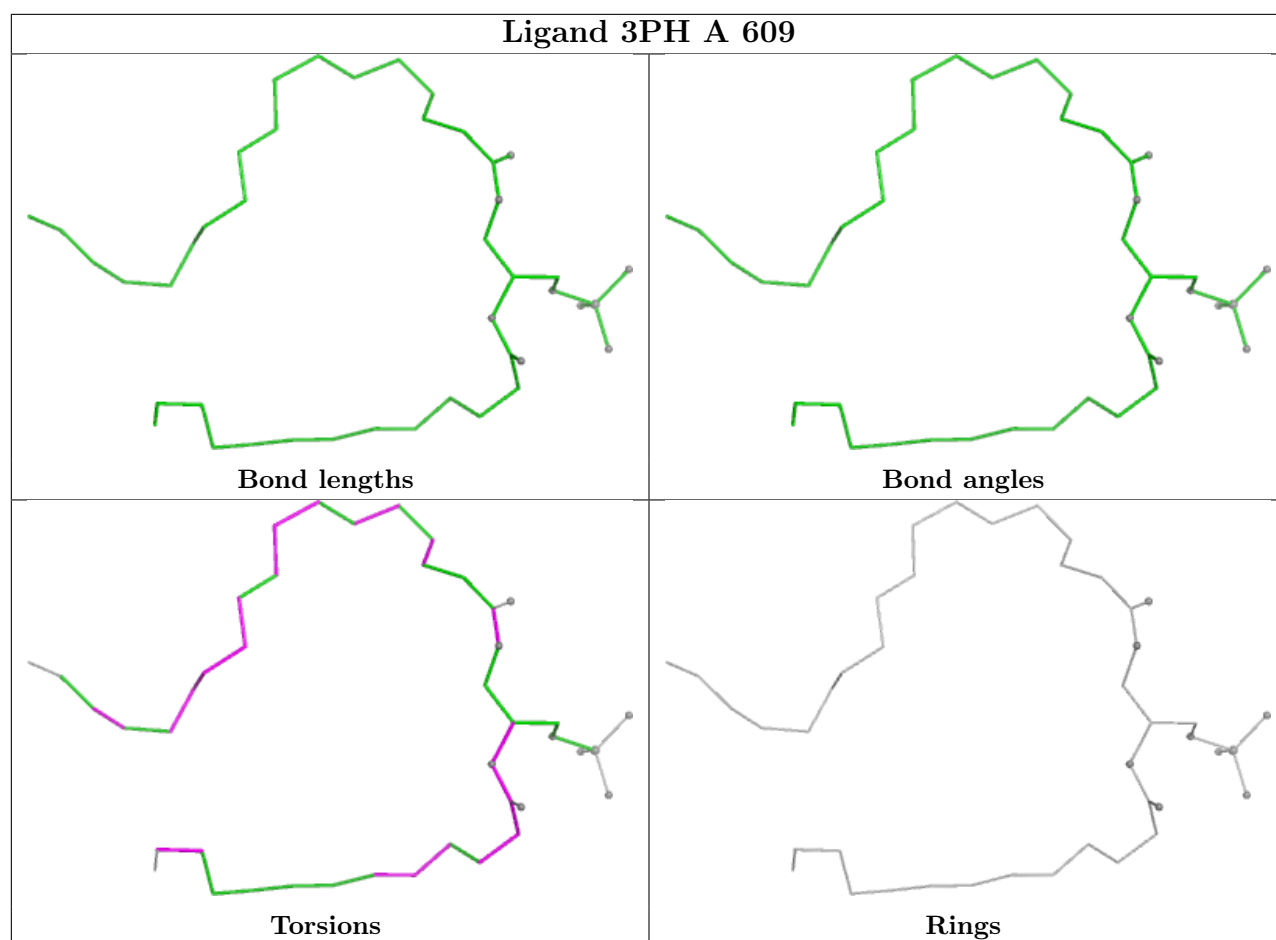
5 monomers are involved in 9 short contacts:

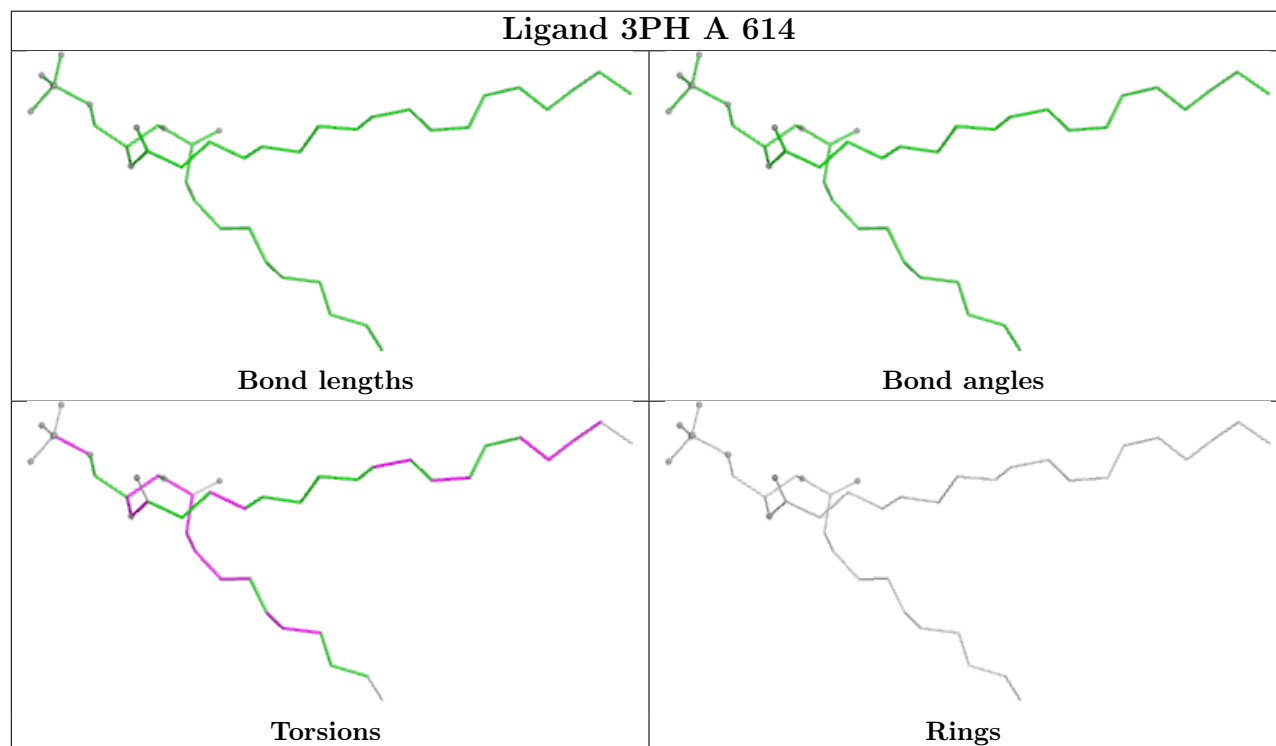
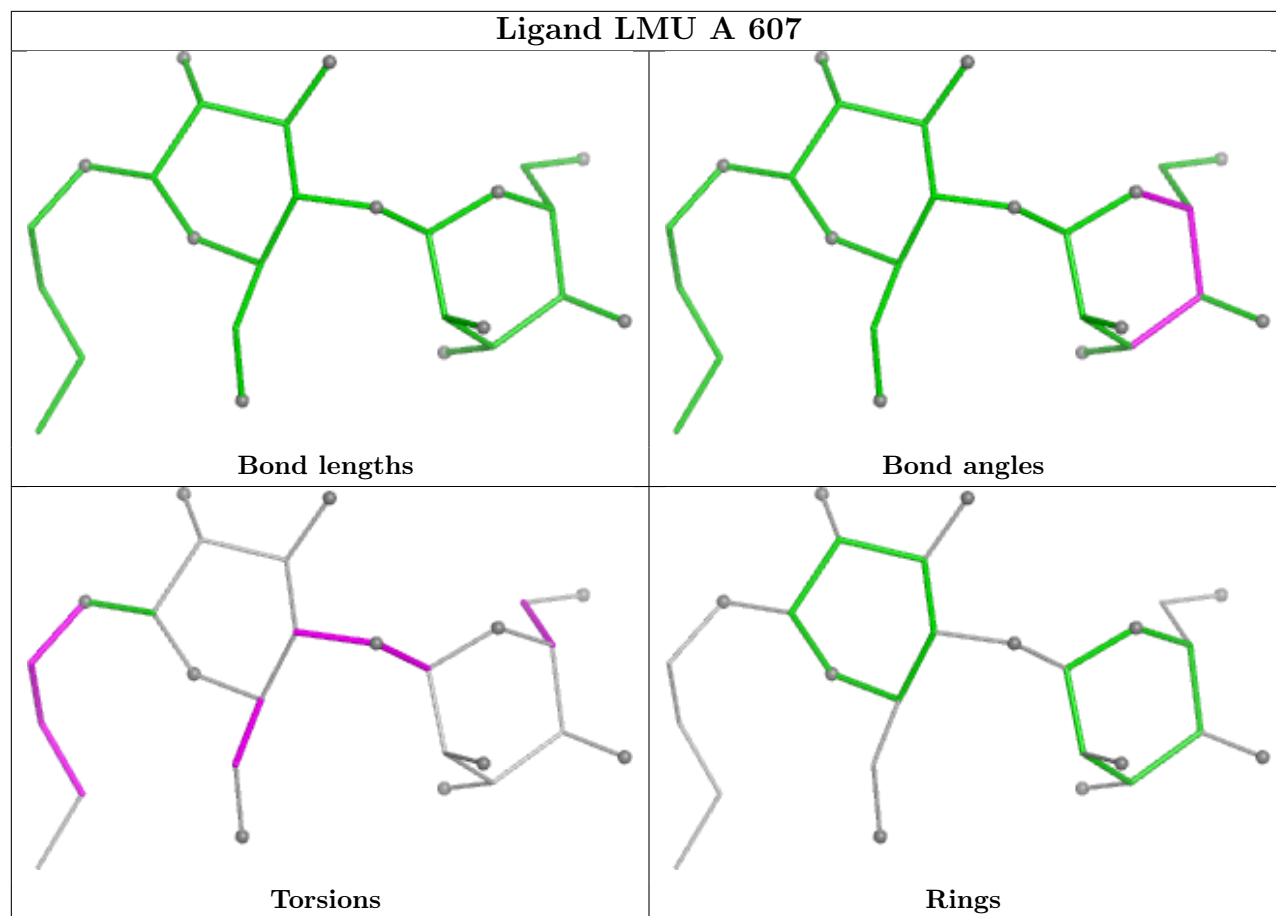
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	611	3PH	2	0
6	B	606	GOL	1	0
3	B	602	LMU	4	0
3	A	608	LMU	1	0
2	A	604	PGT	2	0

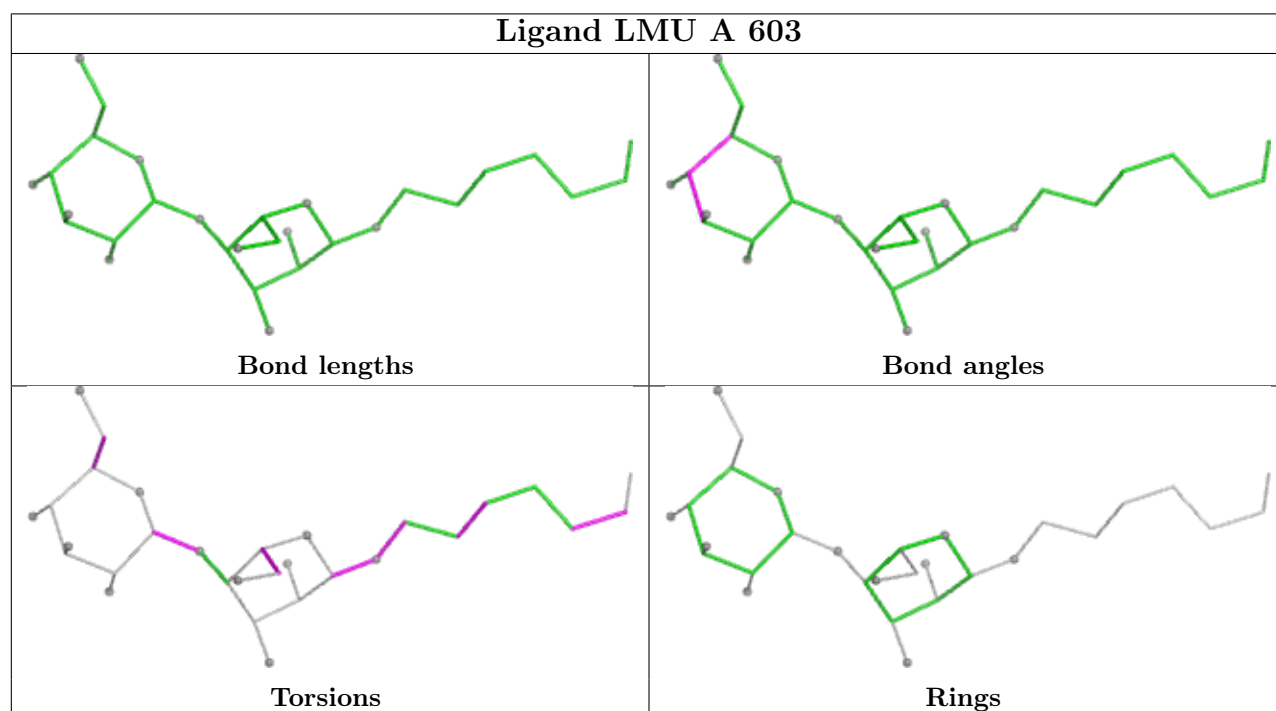
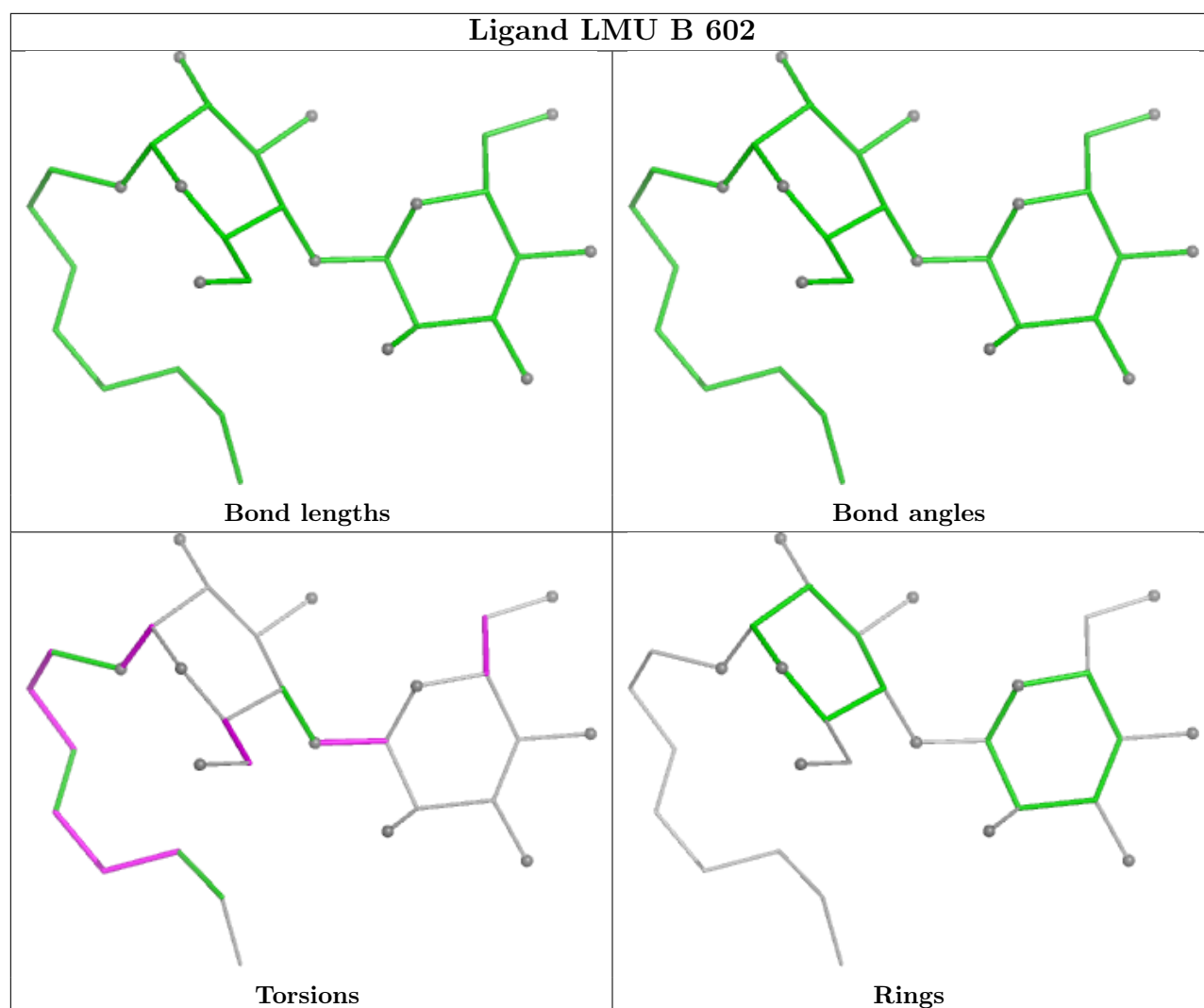
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

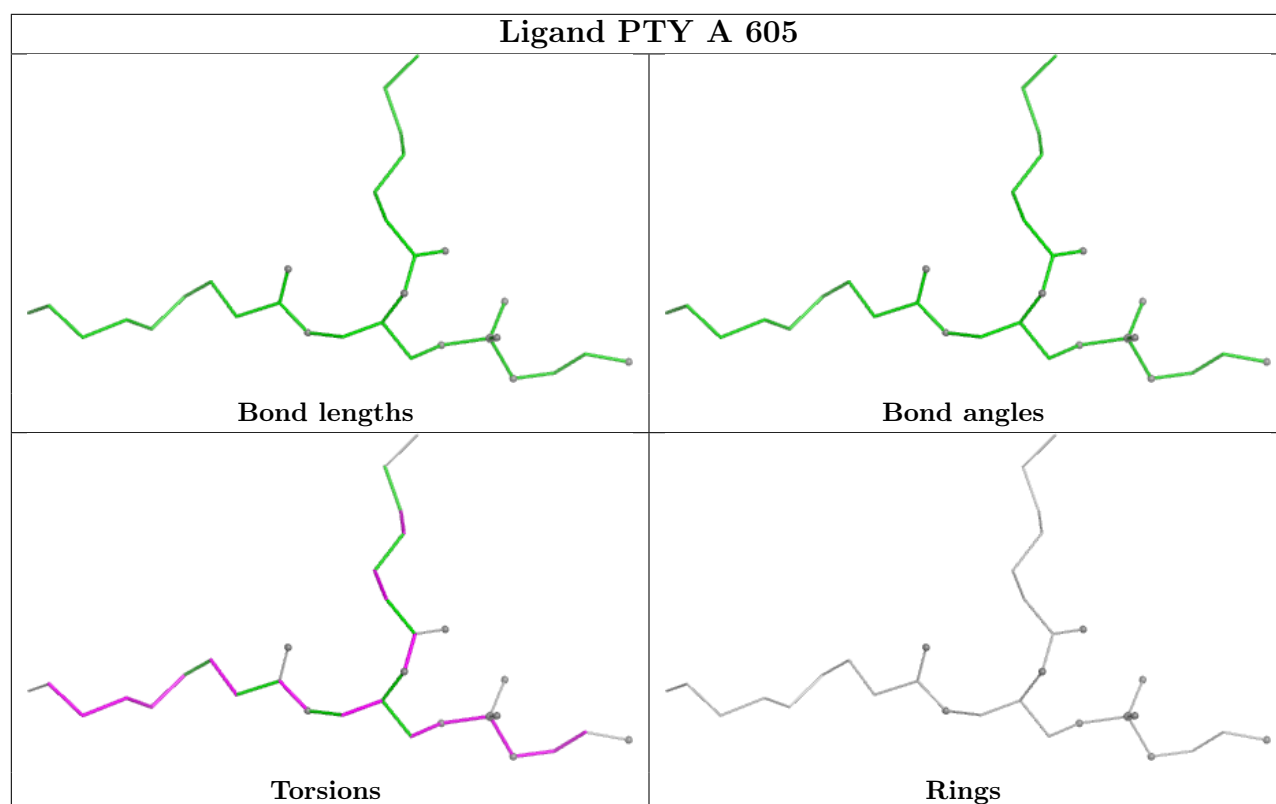
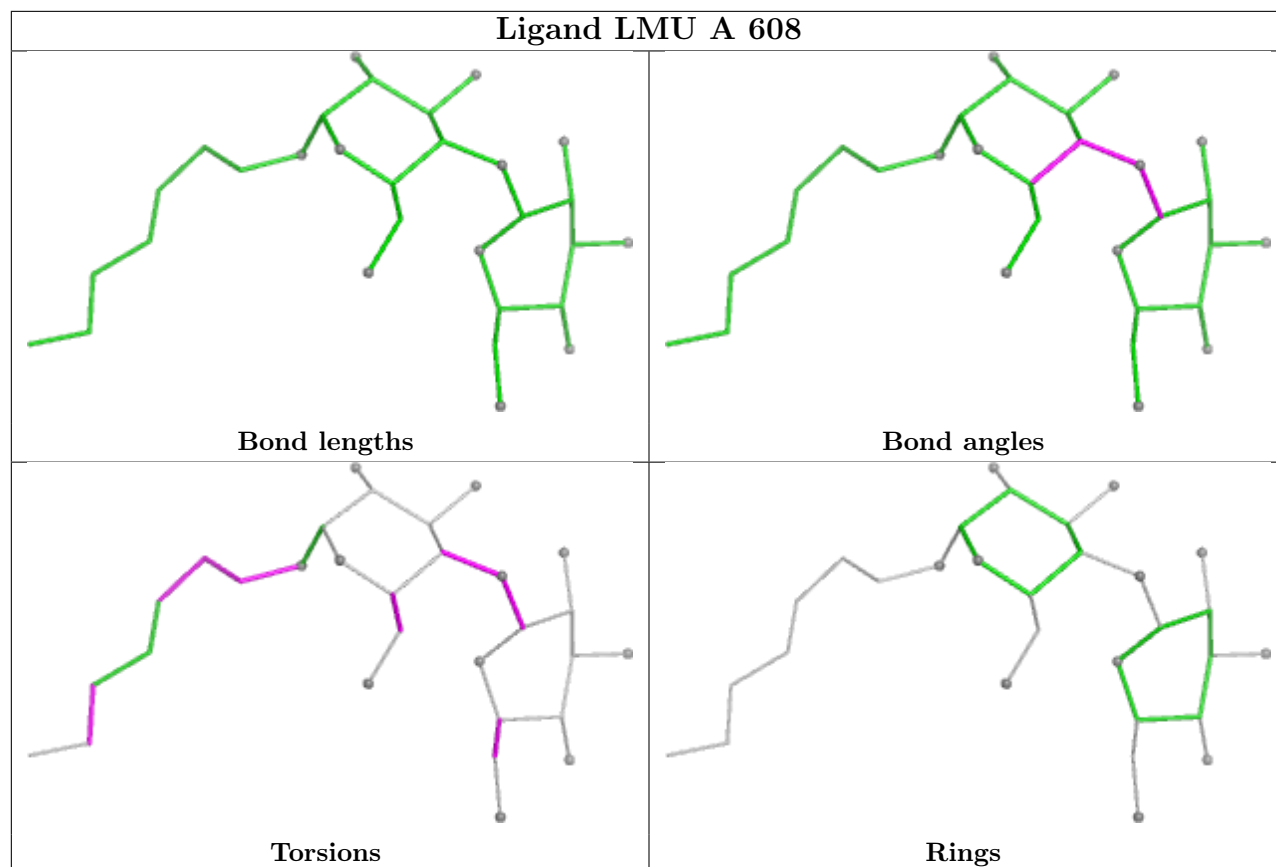


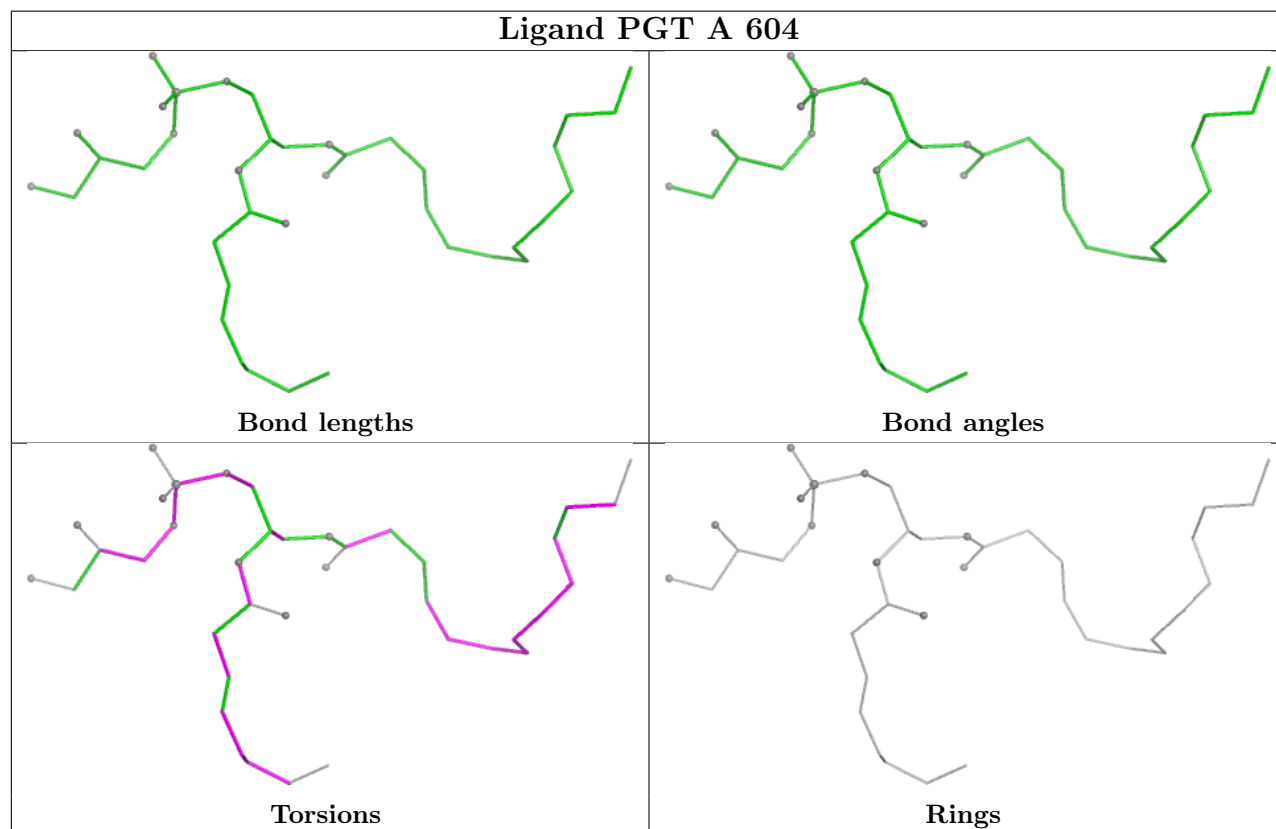
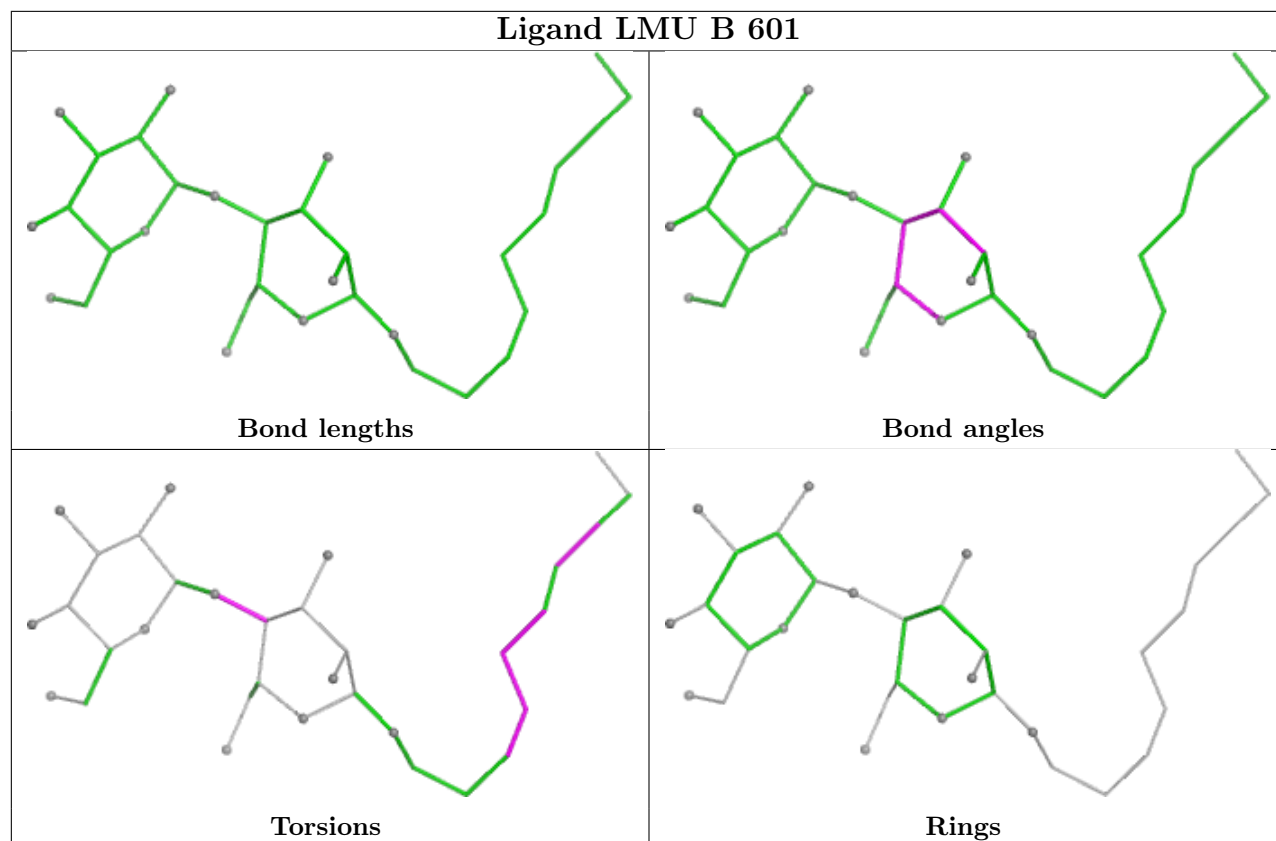


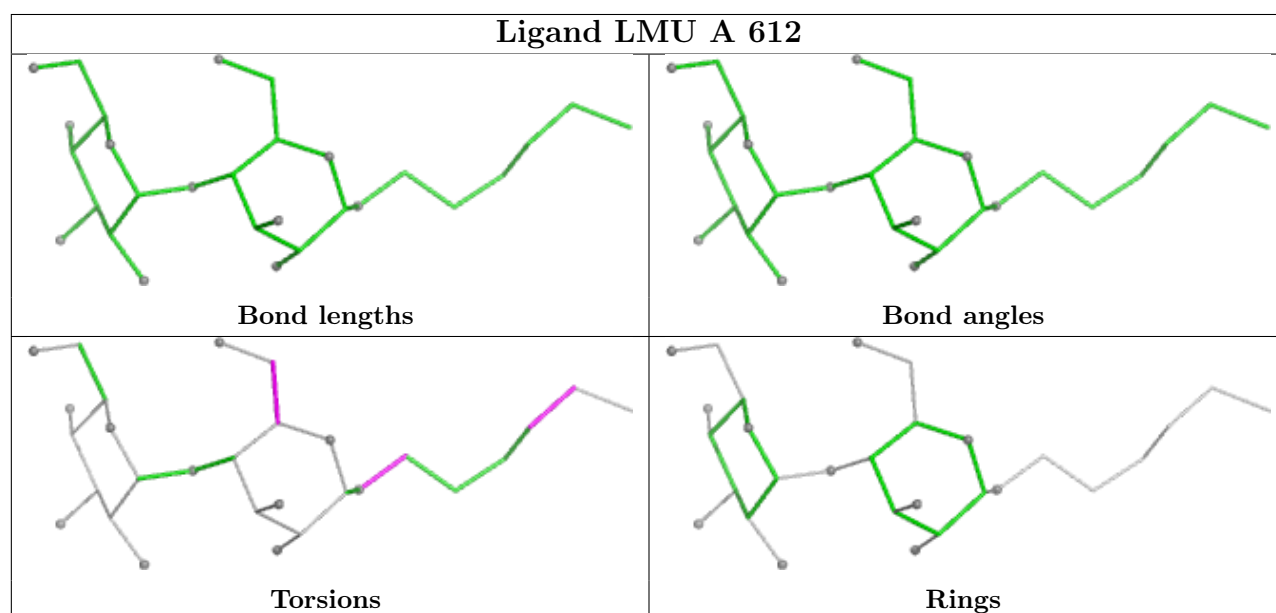
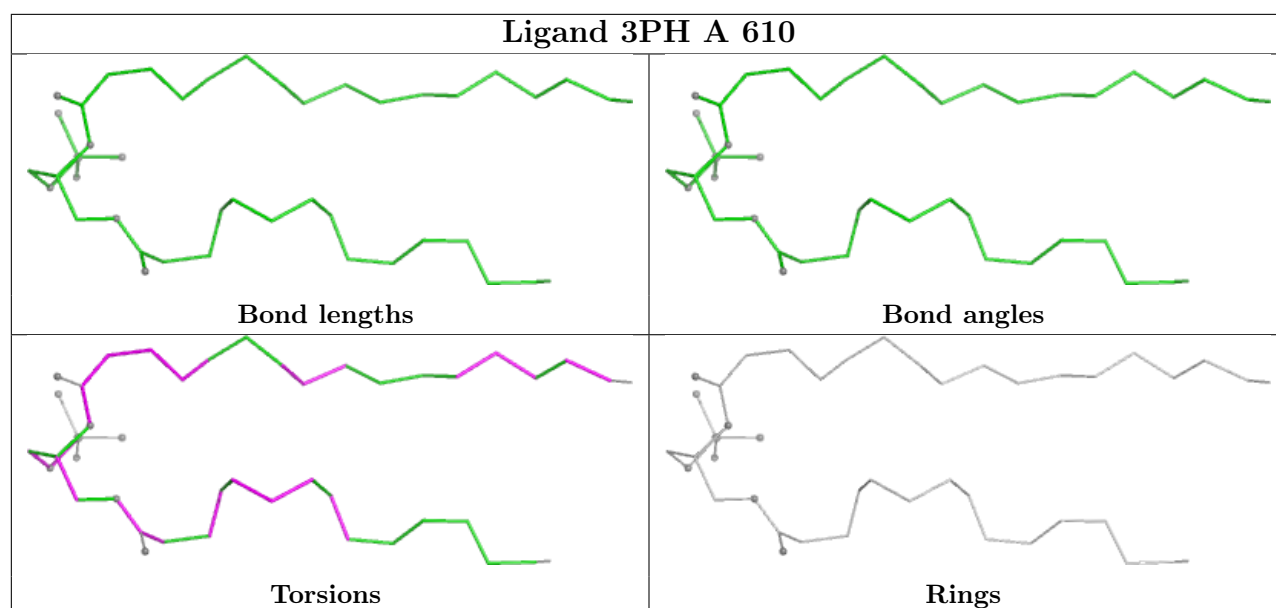


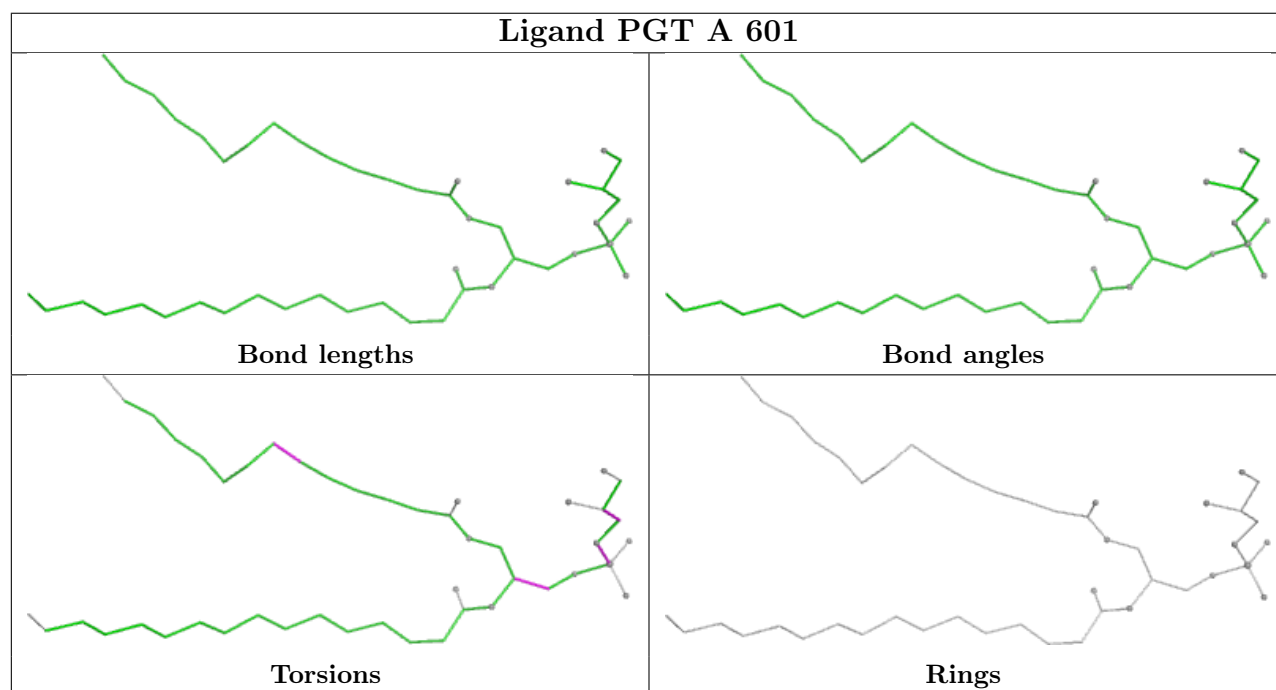
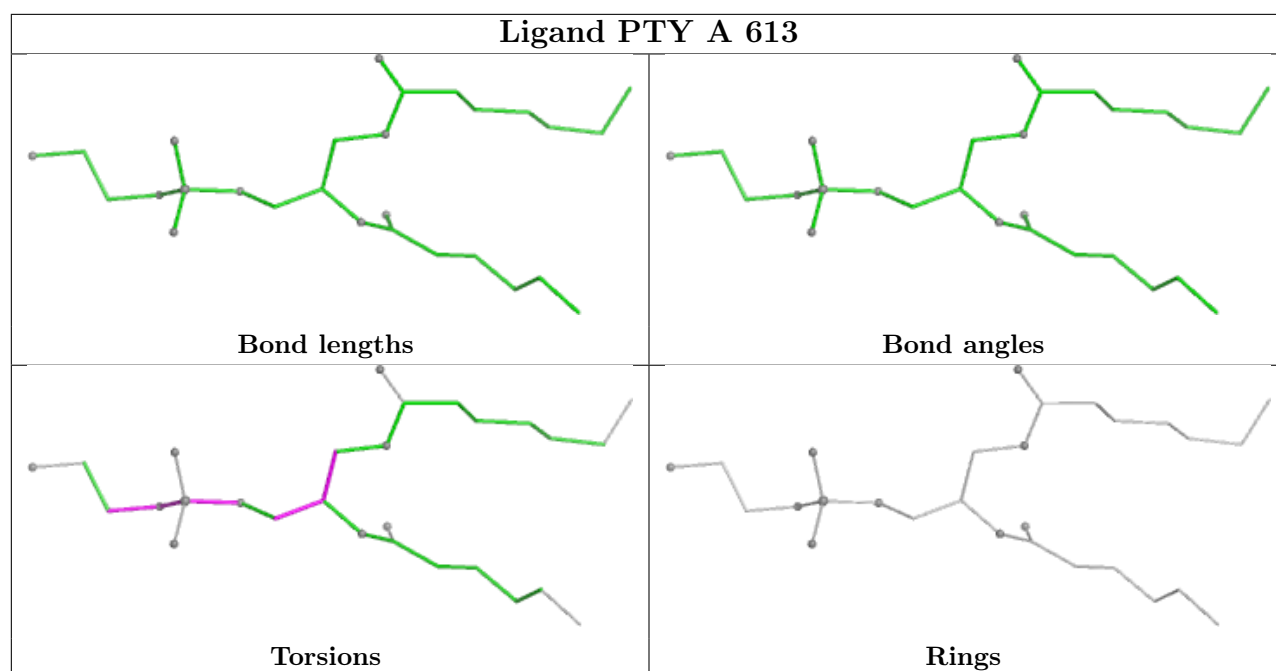


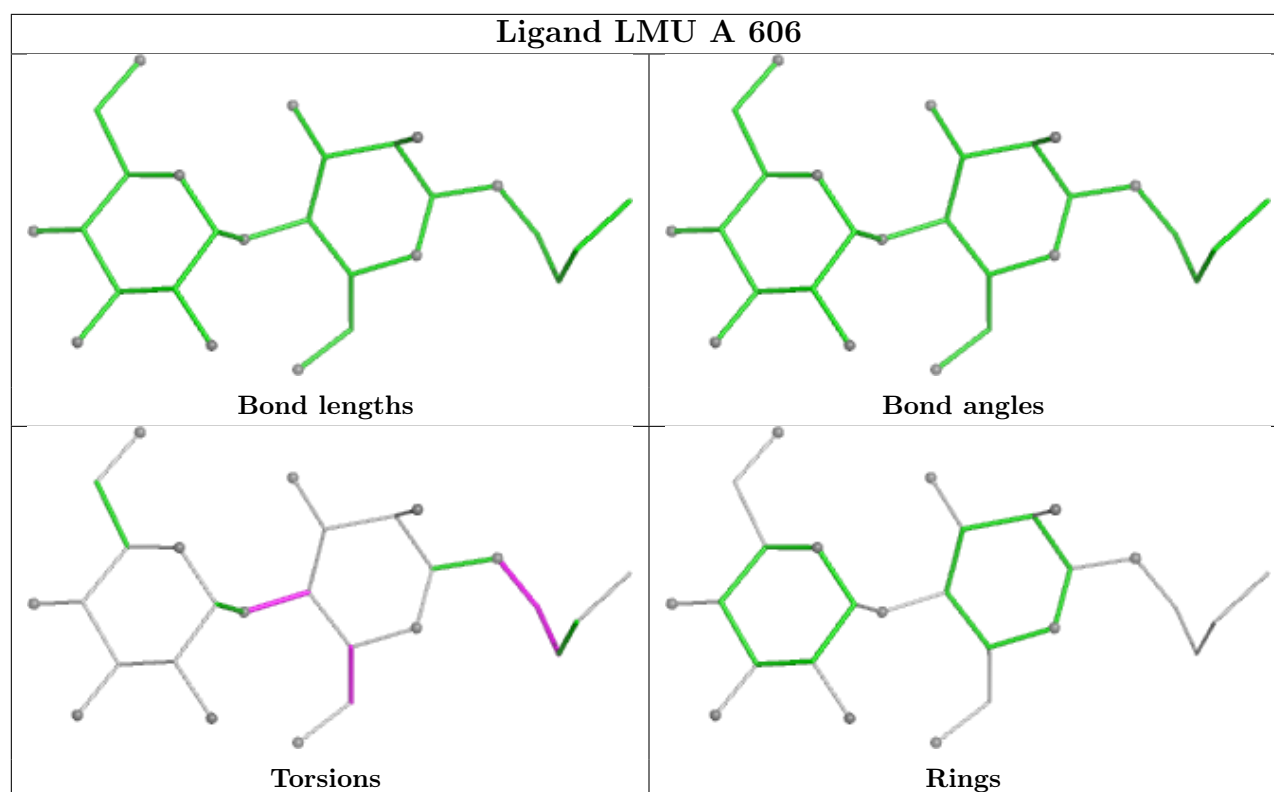












5.7 Other polymers [i](#)

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

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	515/520 (99%)	0.86	46 (8%) 15 12	30, 66, 97, 113	0
1	B	504/520 (96%)	1.26	95 (18%) 3 2	51, 96, 139, 172	0
All	All	1019/1040 (97%)	1.06	141 (13%) 6 4	30, 81, 127, 172	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	102	PHE	5.0
1	B	173	TRP	4.8
1	A	515	LEU	4.7
1	B	19	THR	4.7
1	B	265	MET	4.6
1	B	54	THR	4.4
1	B	194	LEU	4.4
1	A	440	SER	4.4
1	B	266	LEU	4.4
1	B	435	ILE	4.3
1	B	252	VAL	4.1
1	B	384	ALA	3.9
1	A	5	PHE	3.9
1	B	99	LEU	3.6
1	B	251	ILE	3.5
1	B	198	SER	3.4
1	B	171	PHE	3.4
1	B	442	GLY	3.4
1	B	472	ASN	3.3
1	B	57	LEU	3.2
1	A	293	VAL	3.2
1	B	409	MET	3.1
1	B	293	VAL	3.1
1	B	239	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	8	THR	3.1
1	B	103	PHE	3.1
1	B	281	ILE	3.1
1	B	195	LEU	3.0
1	B	242	VAL	3.0
1	A	201	SER	3.0
1	A	204	LYS	3.0
1	B	39	ILE	3.0
1	B	215	LEU	3.0
1	A	176	ALA	3.0
1	B	174	HIS	3.0
1	B	176	ALA	3.0
1	B	45	LEU	3.0
1	B	455	VAL	3.0
1	A	441	LYS	2.9
1	B	167	LEU	2.9
1	B	162	ILE	2.9
1	B	170	GLN	2.9
1	B	40	MET	2.9
1	B	268	VAL	2.9
1	A	452	GLU	2.8
1	B	447	LEU	2.8
1	B	337	PHE	2.8
1	B	316	LEU	2.8
1	B	58	TRP	2.7
1	A	478	PHE	2.7
1	B	470	LEU	2.7
1	B	336	ARG	2.7
1	B	431	VAL	2.7
1	A	290	MET	2.7
1	B	440	SER	2.7
1	B	177	PHE	2.7
1	B	451	ALA	2.7
1	A	11	MET	2.7
1	B	433	LEU	2.7
1	B	157	ALA	2.6
1	B	410	TYR	2.6
1	A	416	PHE	2.6
1	A	308	SER	2.6
1	A	268	VAL	2.6
1	A	465	THR	2.6
1	B	110	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	385	VAL	2.6
1	B	123	LEU	2.5
1	A	177	PHE	2.5
1	B	267	ASP	2.5
1	B	211	PRO	2.5
1	B	132	ILE	2.5
1	A	482	PHE	2.5
1	A	7	LYS	2.5
1	B	37	ILE	2.5
1	A	152	ALA	2.5
1	B	369	MET	2.5
1	A	47	ARG	2.5
1	A	151	ILE	2.4
1	A	442	GLY	2.4
1	A	294	LEU	2.4
1	A	296	LEU	2.4
1	A	292	SER	2.4
1	B	63	TYR	2.4
1	B	131	MET	2.3
1	A	316	LEU	2.3
1	B	83	ARG	2.3
1	B	475	VAL	2.3
1	A	4	PHE	2.3
1	B	136	PHE	2.3
1	B	31	VAL	2.3
1	B	438	PHE	2.3
1	B	253	ILE	2.3
1	A	6	THR	2.3
1	B	70	PHE	2.3
1	B	28	LEU	2.3
1	B	294	LEU	2.3
1	B	434	ASP	2.3
1	A	236	ALA	2.2
1	A	323	ASP	2.2
1	B	101	ILE	2.2
1	B	185	ILE	2.2
1	A	175	SER	2.2
1	B	284	PHE	2.2
1	B	292	SER	2.2
1	B	477	SER	2.2
1	A	271	PHE	2.2
1	B	168	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	421	LEU	2.2
1	B	378	ALA	2.2
1	B	59	ILE	2.2
1	B	221	ILE	2.2
1	A	514	LYS	2.2
1	A	154	SER	2.2
1	A	270	LEU	2.2
1	B	113	ILE	2.1
1	B	149	TRP	2.1
1	A	406	GLU	2.1
1	A	101	ILE	2.1
1	A	99	LEU	2.1
1	A	103	PHE	2.1
1	B	24	LEU	2.1
1	A	300	TRP	2.1
1	B	282	ALA	2.1
1	B	186	ILE	2.1
1	B	38	LEU	2.1
1	B	200	LEU	2.1
1	B	243	VAL	2.1
1	A	301	LEU	2.1
1	B	159	PHE	2.1
1	B	416	PHE	2.1
1	A	42	LEU	2.0
1	A	129	LEU	2.0
1	B	165	GLY	2.0
1	B	193	PHE	2.0
1	B	79	ASP	2.0
1	B	233	GLU	2.0
1	B	366	TYR	2.0
1	B	158	VAL	2.0
1	A	258	ASN	2.0
1	B	474	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

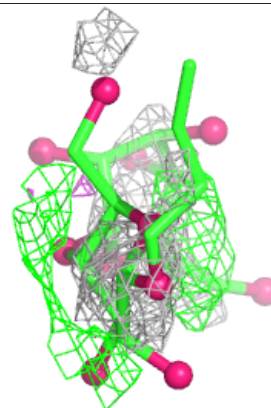
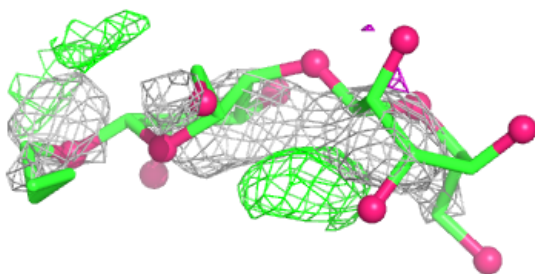
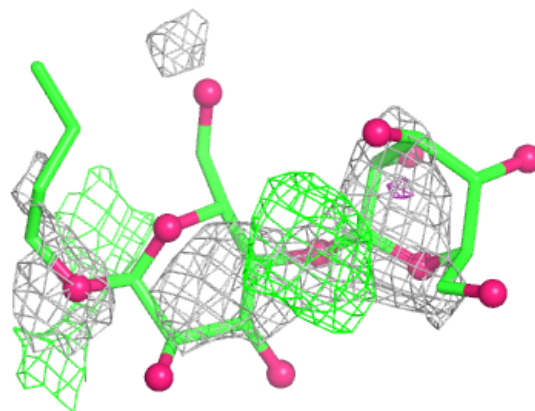
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	LMU	A	607	27/35	0.44	0.18	20,20,20,20	27
3	LMU	A	615	26/35	0.47	0.17	120,122,122,123	0
3	LMU	B	602	31/35	0.49	0.22	146,148,148,148	0
2	PGT	A	604	39/51	0.53	0.24	151,155,157,157	0
5	3PH	A	611	48/48	0.57	0.26	107,112,119,119	0
3	LMU	A	603	30/35	0.61	0.22	95,102,106,106	0
3	LMU	A	612	29/35	0.62	0.18	102,104,105,105	0
3	LMU	A	606	27/35	0.62	0.15	20,20,20,20	0
3	LMU	A	602	31/35	0.62	0.21	100,105,106,107	0
3	LMU	A	608	30/35	0.62	0.15	20,20,20,20	0
5	3PH	A	609	43/48	0.63	0.26	97,102,113,113	0
6	GOL	B	604	6/6	0.63	0.17	122,122,122,122	0
5	3PH	A	610	44/48	0.65	0.29	95,104,118,118	0
6	GOL	B	607	6/6	0.67	0.20	106,106,106,106	0
4	PTY	A	605	31/50	0.70	0.20	95,98,100,100	0
5	3PH	A	614	41/48	0.71	0.27	89,102,109,109	0
2	PGT	A	601	47/51	0.73	0.22	101,106,114,115	0
6	GOL	B	605	6/6	0.76	0.20	125,125,125,125	0
3	LMU	B	601	33/35	0.78	0.23	133,138,139,139	0
6	GOL	B	608	6/6	0.78	0.15	115,116,116,116	0
4	PTY	A	613	28/50	0.80	0.22	126,129,132,132	0
6	GOL	B	606	6/6	0.81	0.17	142,142,142,142	0
6	GOL	A	616	6/6	0.87	0.16	94,94,94,94	0
3	LMU	B	603	27/35	0.88	0.13	74,75,79,80	0
7	NA	A	617	1/1	0.95	0.06	30,30,30,30	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.

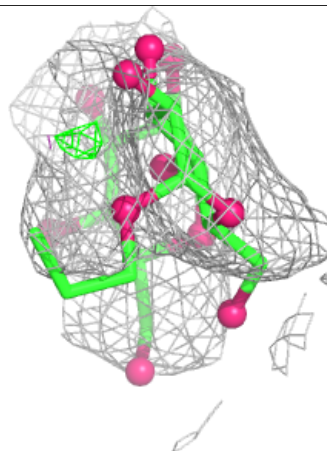
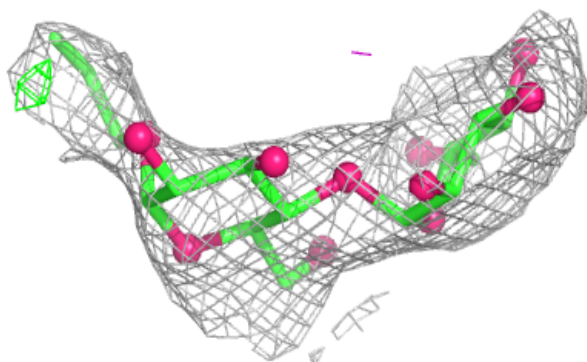
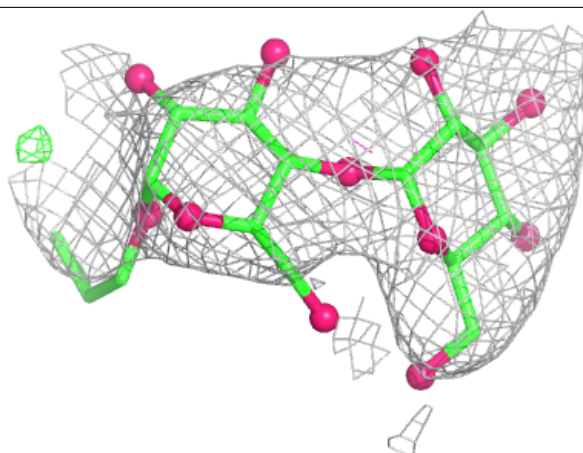
Electron density around LMU A 607:

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



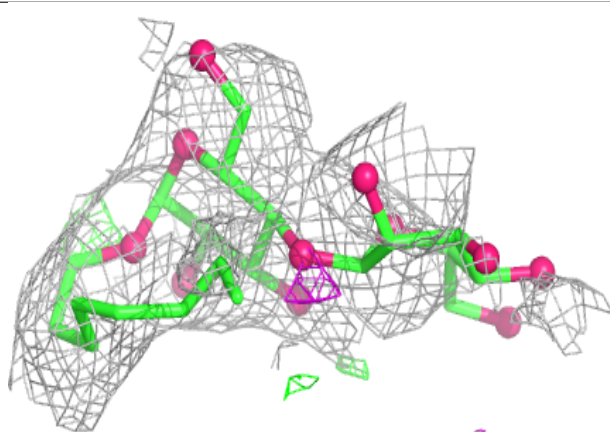
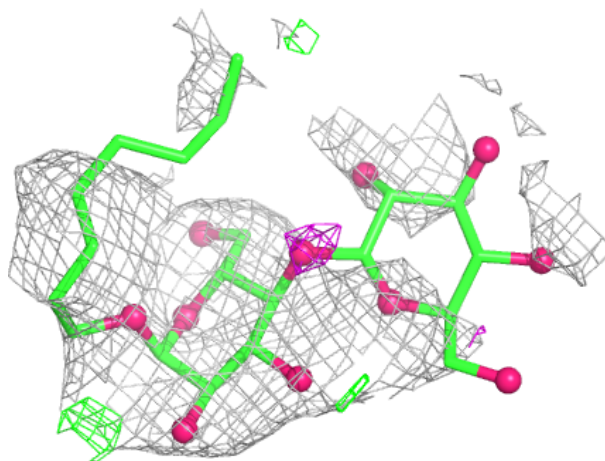
Electron density around LMU A 615:

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



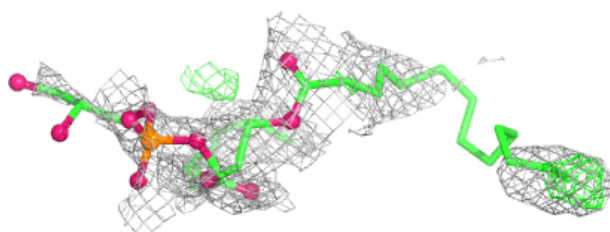
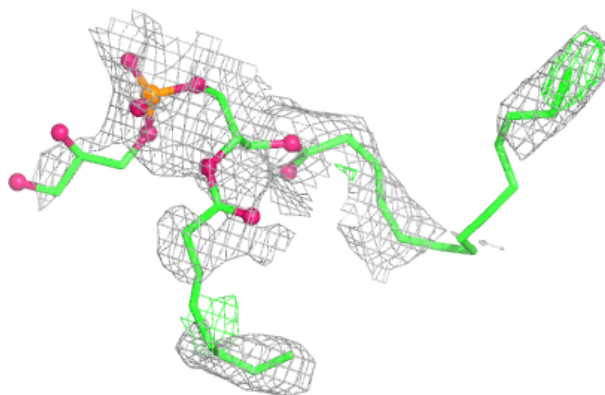
Electron density around LMU B 602:

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



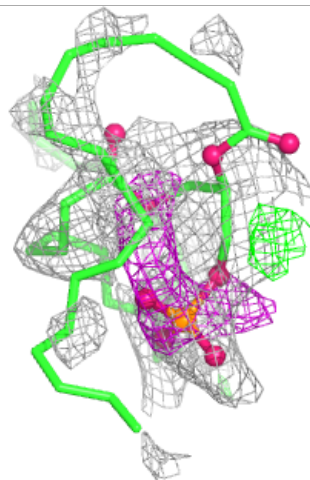
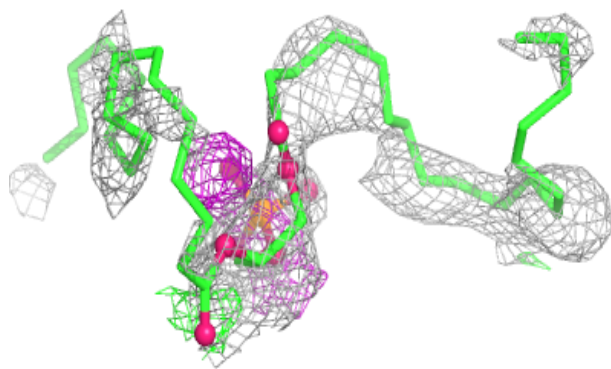
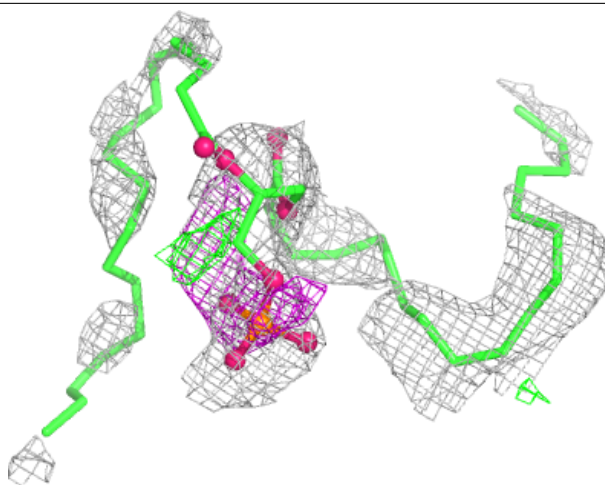
Electron density around PGT A 604:

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



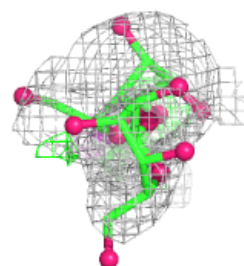
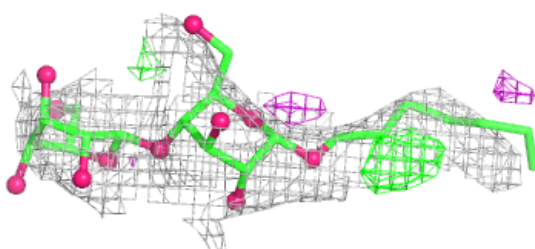
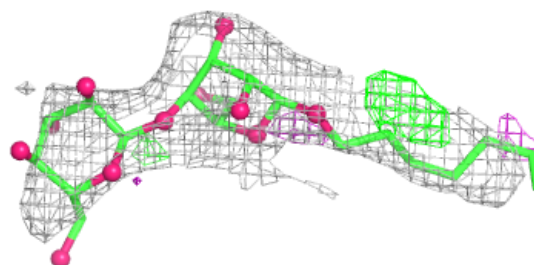
Electron density around 3PH A 611:

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

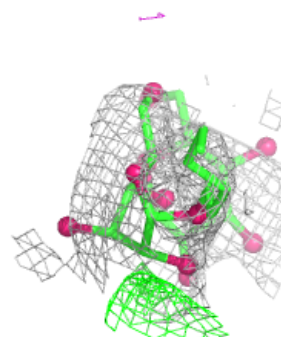
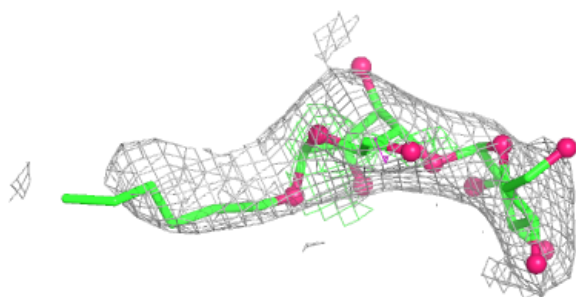
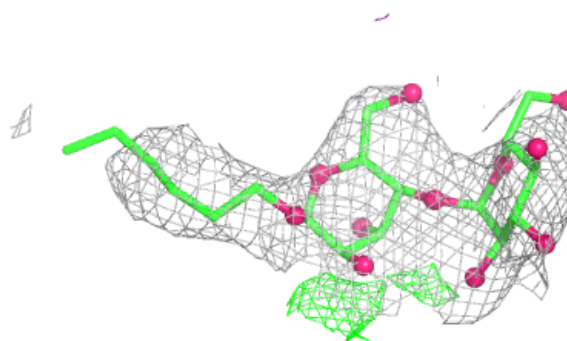


Electron density around LMU A 603:

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

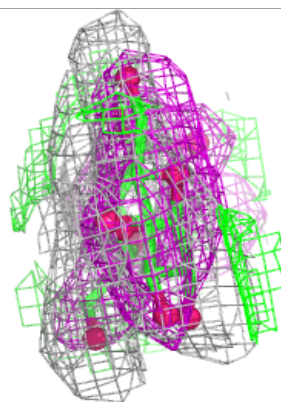
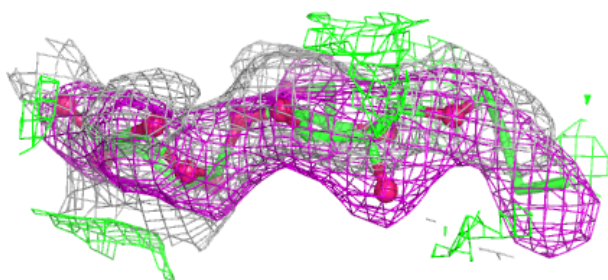
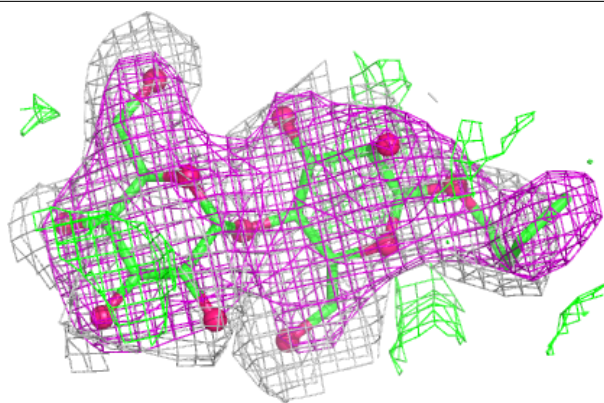
**Electron density around LMU A 612:**

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

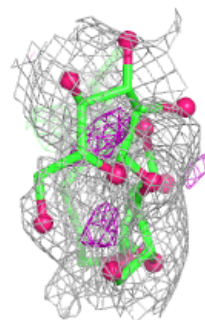
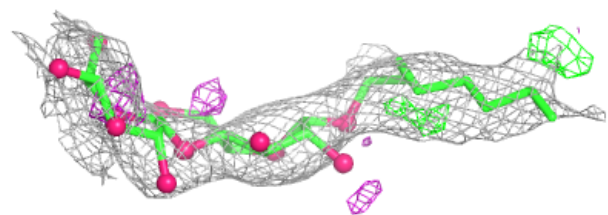
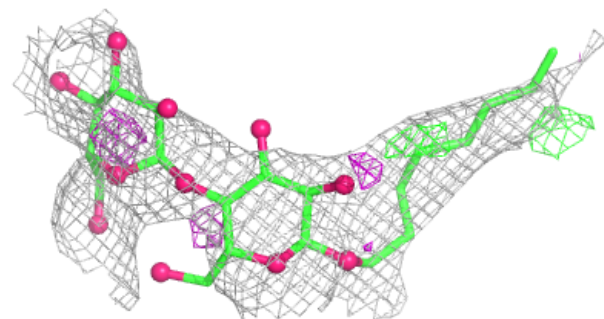


Electron density around LMU A 606:

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

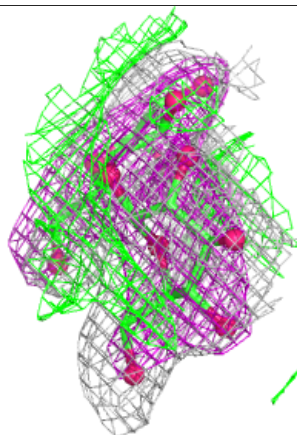
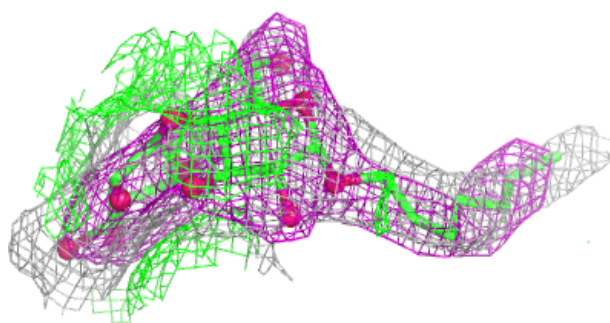
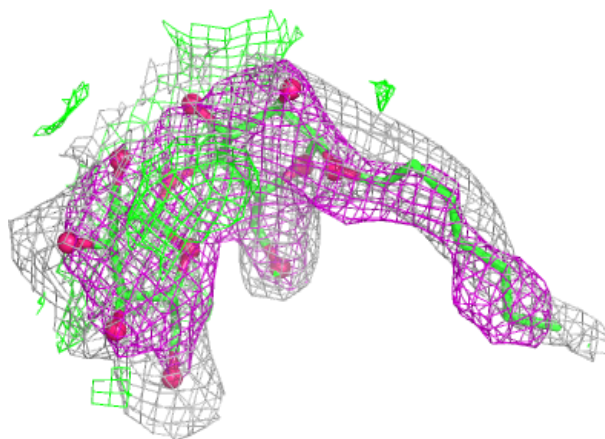
**Electron density around LMU A 602:**

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



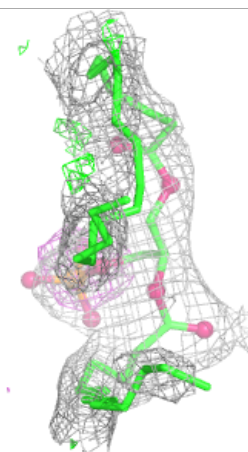
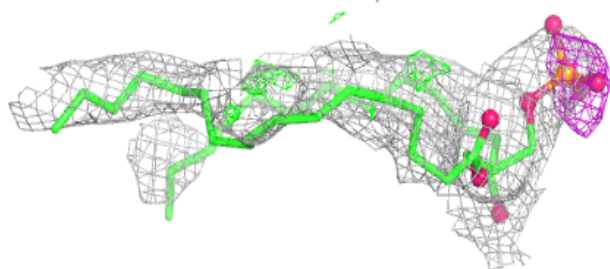
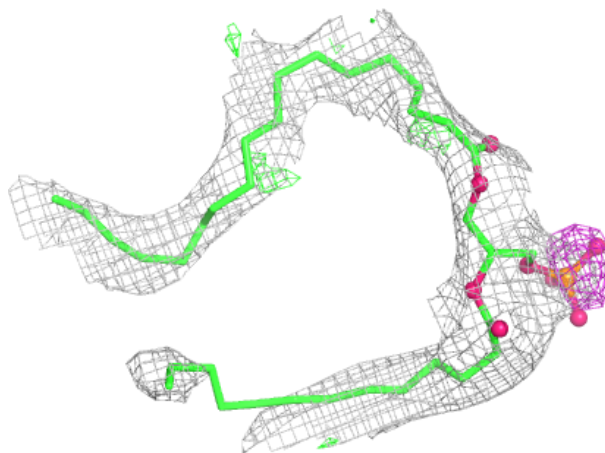
Electron density around LMU A 608:

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



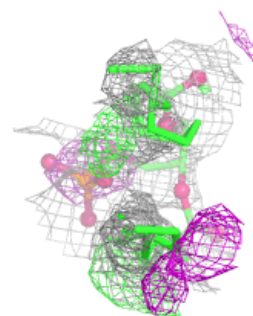
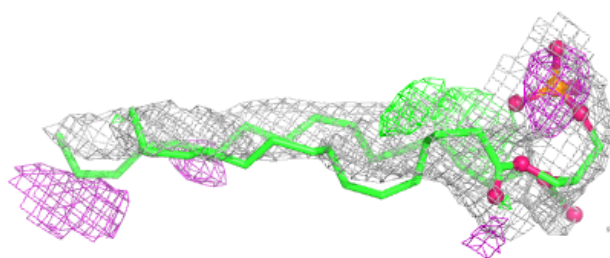
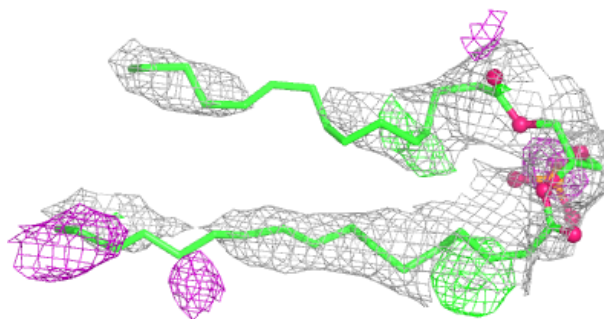
Electron density around 3PH A 609:

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

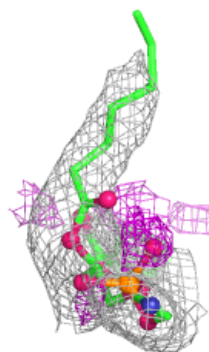
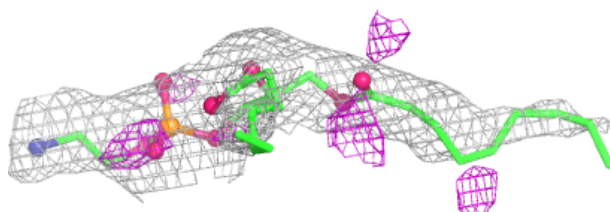
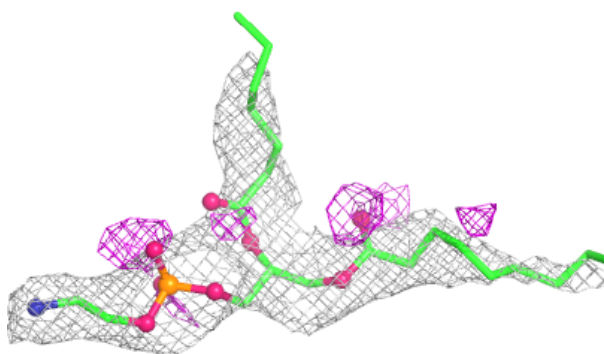


Electron density around 3PH A 610:

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

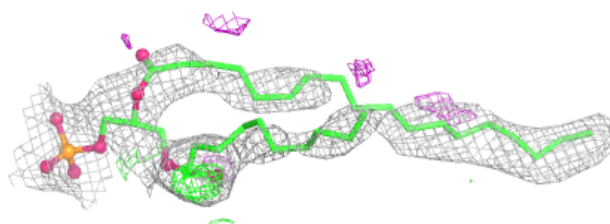
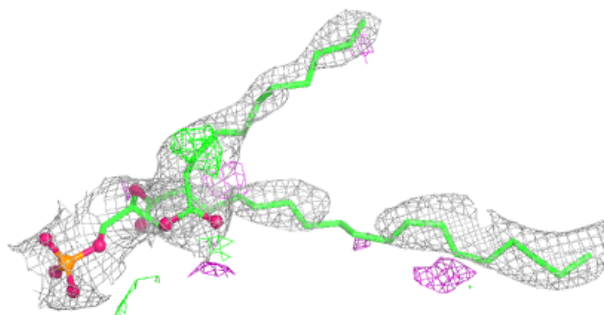
**Electron density around PTY A 605:**

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

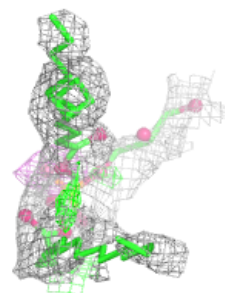
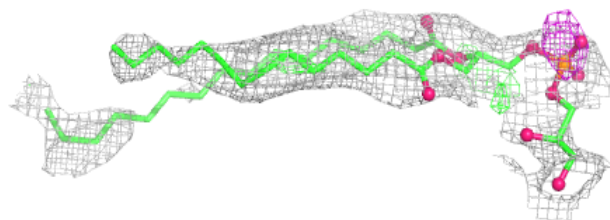
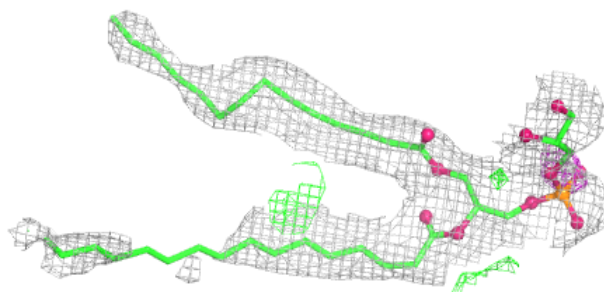


Electron density around 3PH A 614:

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

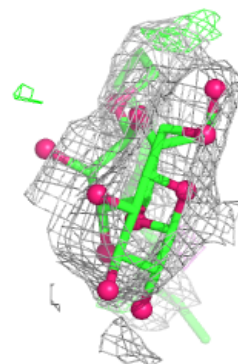
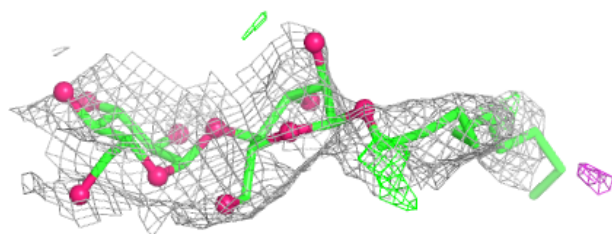
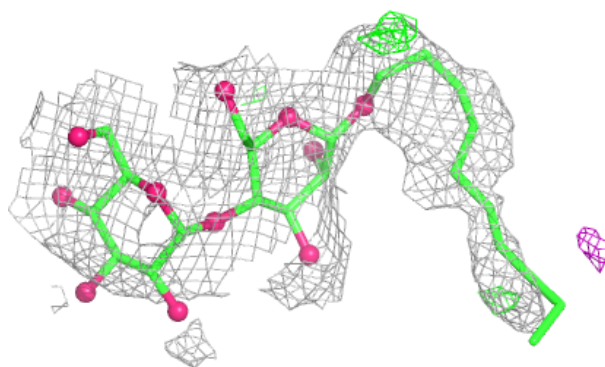
**Electron density around PGT A 601:**

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

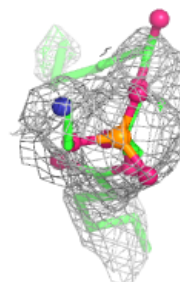
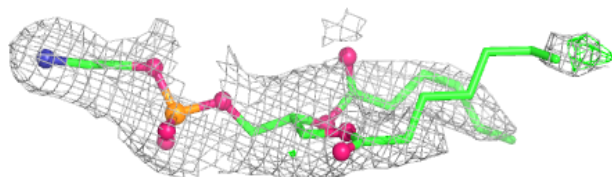
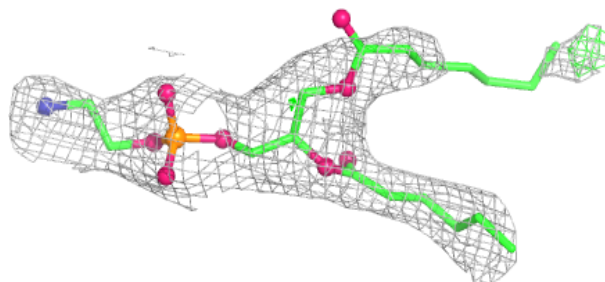


Electron density around LMU B 601:

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

**Electron density around PTY 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.