



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 11, 2026 – 10:06 am BST

PDB ID : 29ON / pdb_000029on
Title : Crystal structure of the staphylococcal efflux pump QacA in the inward open state in complex with nanobody 89
Authors : Jodaitis, L.; Hutchin, A.; Govaerts, C.
Deposited on : 2026-03-26
Resolution : 3.32 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

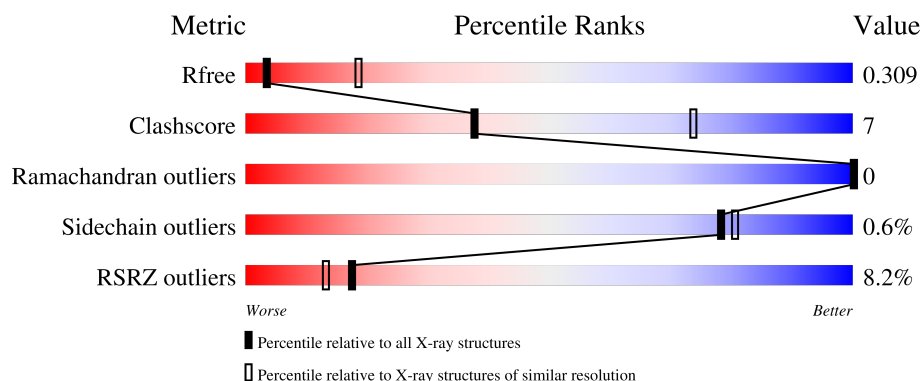
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.32 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	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

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>5%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>5%</div> </div> </div>
1	B	520	<div> <div>8%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>5%</div> </div> </div>
2	C	148	<div> <div>9%</div> <div> <div></div> <div>66%</div> <div>15%</div> <div>19%</div> </div> </div>
2	D	148	<div> <div>12%</div> <div> <div></div> <div>72%</div> <div>11%</div> <div>18%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9333 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	496	Total	C	N	O	S	0	0	0
			3650	2425	559	645	21			
1	B	495	Total	C	N	O	S	0	0	0
			3646	2418	564	643	21			

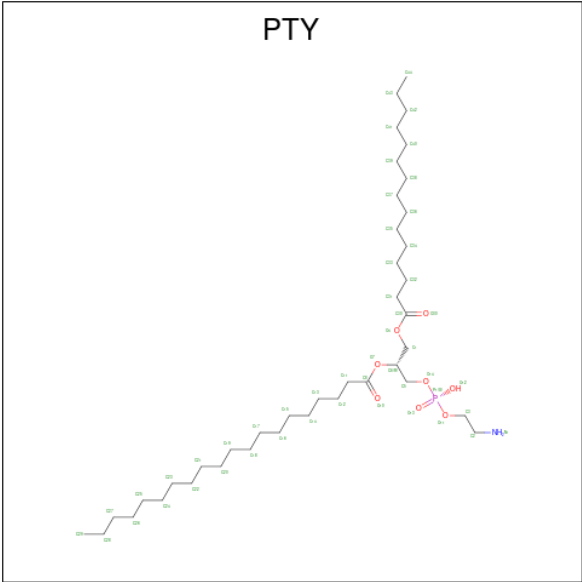
There are 12 discrepancies between the modelled and reference sequences:

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 a protein called Nanobody 89.

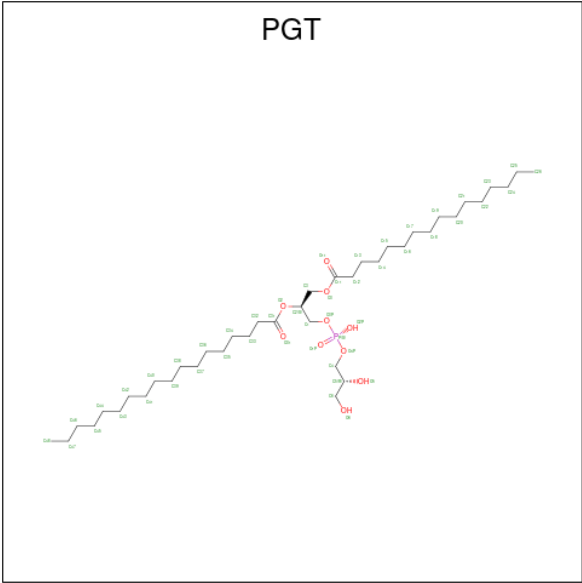
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	120	Total	C	N	O	S	0	0	0
			884	550	154	176	4			
2	D	122	Total	C	N	O	S	0	0	0
			899	561	155	179	4			

- Molecule 3 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			20	10	1	8	1		

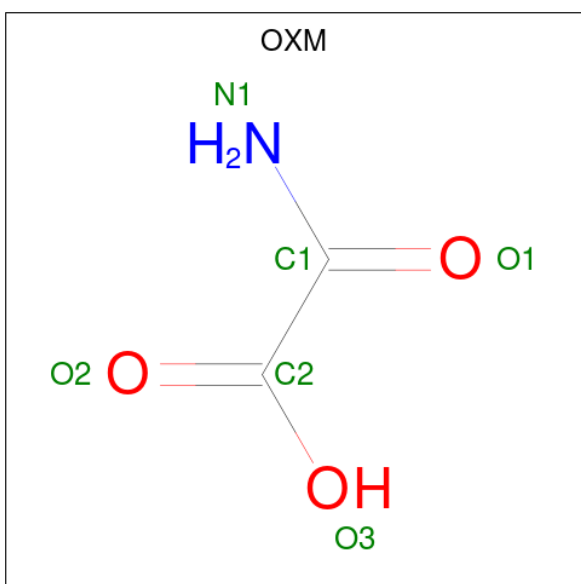
- Molecule 4 is (1S)-2-{[[(2R)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(palmitoyloxy)methyl]ethyl stearate (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).



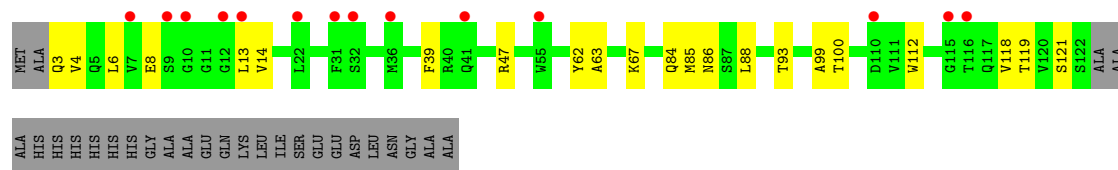
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			41	30	10	1		
4	B	1	Total	C	O	P	0	0
			47	36	10	1		

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- The image displays a complex chemical structure, likely a glycoside or a steroid derivative, featuring multiple sugar units and a long alkyl chain. The structure is labeled with atom numbers (C1-C12, O1-O12) and includes stereochemical indicators (wedges, dashes). The molecule consists of a central core with several sugar units attached via glycosidic bonds. A long alkyl chain is attached to one of the sugar units. The structure is highly detailed, showing the connectivity and stereochemistry of all atoms.

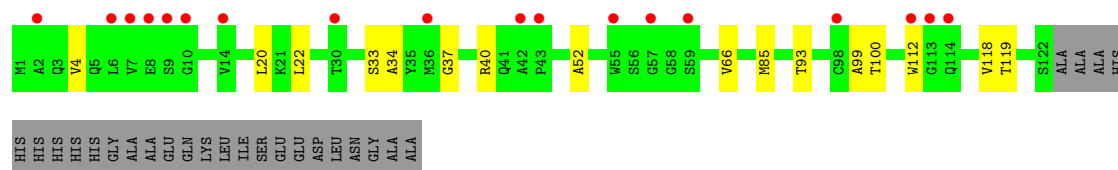
- Molecule 6 is OXAMIC ACID (CCD ID: OXM) (formula: $\text{C}_2\text{H}_3\text{NO}_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			6	2	1	3		



- Molecule 2: Nanobody 89



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	188.30Å 94.33Å 98.31Å 90.00° 97.47° 90.00°	Depositor
Resolution (Å)	31.53 – 3.32 31.53 – 3.32	Depositor EDS
% Data completeness (in resolution range)	66.8 (31.53-3.32) 66.8 (31.53-3.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.31Å)	Xtriage
Refinement program	BUSTER 2.10.4 (17-JUL-2025)	Depositor
R, R_{free}	0.297 , 0.327 0.283 , 0.309	Depositor DCC
R_{free} test set	838 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	81.0	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	9333	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.05% 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: LMU, PGT, PTY, OXM

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	0.84	0/3729	1.28	0/5089
1	B	0.83	0/3725	1.26	1/5081 (0.0%)
2	C	0.83	0/901	1.20	0/1219
2	D	0.89	0/919	1.27	0/1248
All	All	0.84	0/9274	1.27	1/12637 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	316	LEU	N-CA-C	-5.11	107.10	113.38

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	3650	0	3772	50	0
1	B	3646	0	3760	54	0
2	C	884	0	837	12	0
2	D	899	0	828	14	0
3	A	20	0	13	0	0
4	A	41	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	47	0	67	3	0
5	A	140	0	184	3	0
6	B	6	0	2	0	0
All	All	9333	0	9515	132	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 7.

All (132) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:40:ARG:NH2	2:D:66:VAL:HG11	1.76	1.00
2:D:40:ARG:NH2	2:D:66:VAL:CG1	2.44	0.80
2:C:84:GLN:HG3	2:C:86:ASN:HD21	1.45	0.79
2:D:40:ARG:HH22	2:D:66:VAL:HG11	1.49	0.78
2:D:40:ARG:HH22	2:D:66:VAL:CG1	2.02	0.69
1:B:307:LEU:HD13	1:B:315:TYR:HD2	1.61	0.65
2:D:40:ARG:HH21	2:D:66:VAL:HG11	1.62	0.65
2:D:40:ARG:O	2:D:40:ARG:HG3	1.95	0.65
1:B:290:MET:HE3	1:B:294:LEU:HD12	1.80	0.64
1:A:36:THR:HG21	1:A:157:ALA:HA	1.80	0.64
1:B:30:VAL:HG21	1:B:183:PHE:CD1	2.32	0.64
1:A:354:MET:HE1	1:A:493:MET:HG3	1.80	0.62
1:B:462:ALA:CB	1:B:471:ALA:HB2	2.30	0.62
2:D:4:VAL:HG11	2:D:100:THR:HG21	1.83	0.61
1:B:30:VAL:HG21	1:B:183:PHE:CG	2.37	0.60
2:D:93:THR:HG23	2:D:119:THR:HA	1.85	0.58
1:A:85:LYS:HD2	5:A:603:LMU:H3'	1.85	0.58
1:B:354:MET:HE1	1:B:493:MET:HG3	1.86	0.58
2:C:85:MET:HE1	2:C:118:VAL:HG11	1.86	0.57
1:A:63:TYR:CZ	1:A:67:LEU:HD11	2.40	0.56
1:A:270:LEU:HD22	1:A:394:THR:HG22	1.88	0.56
1:A:317:LEU:O	1:A:318:PRO:C	2.49	0.56
1:A:361:GLY:HA2	1:A:364:LEU:HA	1.89	0.55
1:B:465:THR:OG1	1:B:467:ILE:HG22	2.07	0.54
1:B:349:ILE:HA	1:B:352:ILE:HD12	1.89	0.54
1:A:447:LEU:HD11	2:C:63:ALA:HA	1.89	0.53
2:D:37:GLY:HA2	2:D:52:ALA:HA	1.90	0.53
1:A:343:LEU:HD23	1:A:504:ILE:HD11	1.90	0.53
1:A:353:GLY:HA2	1:A:375:LEU:HD13	1.89	0.53
1:B:285:MET:HG3	1:B:496:ILE:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ALA:HA	1:A:109:PHE:HD2	1.73	0.52
1:B:337:PHE:HB2	1:B:342:VAL:HG23	1.92	0.52
1:A:350:ALA:HB2	1:A:379:GLY:HA3	1.92	0.52
1:B:108:GLU:HA	1:B:111:ILE:HD12	1.91	0.52
2:C:99:ALA:HB2	2:C:112:TRP:CE3	2.45	0.52
1:A:364:LEU:HD21	1:A:369:MET:HB3	1.93	0.51
1:B:462:ALA:HB3	1:B:471:ALA:HB2	1.93	0.51
1:A:275:SER:HB2	1:A:393:GLU:HG2	1.92	0.51
1:A:283:ALA:HB1	1:A:410:TYR:CE1	2.45	0.51
1:B:238:ILE:O	1:B:239:ILE:C	2.54	0.51
1:B:307:LEU:HD22	1:B:315:TYR:HE2	1.75	0.51
1:B:283:ALA:HB1	1:B:410:TYR:CE1	2.46	0.51
1:B:317:LEU:O	1:B:318:PRO:C	2.54	0.50
1:B:307:LEU:HD13	1:B:315:TYR:CD2	2.44	0.50
2:D:85:MET:HE1	2:D:118:VAL:HG11	1.92	0.50
1:B:264:PRO:O	1:B:265:MET:C	2.55	0.50
2:C:84:GLN:HG3	2:C:86:ASN:ND2	2.21	0.49
1:A:358:TYR:HA	1:A:483:VAL:HB	1.95	0.48
1:B:356:ILE:HG22	1:B:360:PHE:HE2	1.79	0.48
1:B:317:LEU:N	1:B:318:PRO:HD2	2.28	0.48
1:A:287:MET:HE1	1:A:290:MET:SD	2.54	0.47
1:B:358:TYR:HA	1:B:483:VAL:HB	1.96	0.47
1:A:337:PHE:HB2	1:A:342:VAL:HG23	1.95	0.47
2:C:13:LEU:HD11	2:C:121:SER:HB3	1.95	0.47
1:B:65:LEU:HD13	1:B:415:VAL:HG11	1.96	0.47
1:A:74:LEU:HD22	1:A:123:LEU:HD13	1.97	0.47
1:B:74:LEU:HD22	1:B:123:LEU:HD13	1.96	0.47
1:B:287:MET:HE3	1:B:383:LEU:HD11	1.97	0.46
1:A:35:MET:HE3	1:A:63:TYR:HD2	1.80	0.46
1:A:500:VAL:HA	1:A:503:LEU:HD12	1.96	0.46
1:A:46:VAL:HA	1:A:51:PRO:HD2	1.98	0.46
1:A:54:THR:HG23	1:A:228:LYS:HB3	1.98	0.46
1:A:416:PHE:HA	1:A:419:ALA:HB3	1.97	0.46
1:B:65:LEU:HD11	1:B:220:MET:HB3	1.96	0.46
1:A:131:MET:HG2	1:A:195:LEU:HD22	1.96	0.46
1:B:215:LEU:HD23	1:B:250:MET:HG2	1.97	0.46
1:A:104:ALA:HA	1:A:109:PHE:CD2	2.51	0.45
1:A:161:PRO:HG2	1:A:316:LEU:HD22	1.98	0.45
1:B:40:MET:CG	1:B:161:PRO:HA	2.47	0.45
2:C:14:VAL:HG11	2:C:88:LEU:HD12	1.98	0.45
1:A:333:LEU:C	1:A:342:VAL:HG21	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:SER:O	1:A:263:ASP:C	2.60	0.45
1:B:54:THR:HG23	1:B:228:LYS:HB3	1.99	0.45
1:B:270:LEU:HD22	1:B:394:THR:CG2	2.47	0.45
1:B:36:THR:HG21	1:B:161:PRO:HG3	1.98	0.44
1:B:270:LEU:HD22	1:B:394:THR:HG22	1.99	0.44
1:A:327:ALA:O	1:A:328:PRO:C	2.59	0.44
4:B:601:PGT:H211	4:B:601:PGT:H181	1.42	0.44
1:B:502:LEU:O	1:B:503:LEU:C	2.60	0.44
4:B:601:PGT:H412	4:B:601:PGT:H382	1.51	0.44
1:B:494:ILE:HD13	1:B:494:ILE:HA	1.91	0.44
1:B:435:ILE:HD11	1:B:470:LEU:HD11	2.00	0.44
2:C:93:THR:HG23	2:C:119:THR:HA	1.99	0.43
2:C:39:PHE:HB3	2:C:47:ARG:HD2	2.00	0.43
1:A:317:LEU:N	1:A:318:PRO:HD2	2.33	0.43
1:B:148:VAL:HA	1:B:151:ILE:HD12	1.99	0.43
1:B:156:GLY:O	1:B:160:GLY:N	2.52	0.43
1:B:239:ILE:N	1:B:240:PRO:HD2	2.34	0.43
1:B:327:ALA:N	1:B:328:PRO:HD2	2.33	0.43
1:A:85:LYS:CD	5:A:603:LMU:H3'	2.48	0.43
1:A:150:SER:O	1:A:151:ILE:C	2.62	0.43
1:B:130:SER:HA	1:B:133:ARG:HE	1.83	0.43
1:A:499:VAL:O	1:A:503:LEU:HG	2.18	0.43
1:B:263:ASP:O	1:B:264:PRO:C	2.61	0.43
1:B:287:MET:HE2	1:B:287:MET:HA	2.00	0.43
1:A:283:ALA:HB1	1:A:410:TYR:HE1	1.84	0.42
1:A:307:LEU:HD23	1:A:312:ALA:HA	2.00	0.42
1:B:356:ILE:HG22	1:B:360:PHE:CE2	2.54	0.42
4:B:601:PGT:H252	4:B:601:PGT:H221	1.69	0.42
2:C:6:LEU:HD11	2:C:100:THR:HG22	2.01	0.42
2:D:22:LEU:HD21	2:D:85:MET:HE2	2.02	0.42
1:A:138:ASN:O	1:A:139:PRO:C	2.60	0.42
1:A:285:MET:HG3	1:A:496:ILE:HG21	2.02	0.42
1:B:326:PHE:CD1	1:B:329:ILE:HD11	2.54	0.42
1:A:503:LEU:O	1:A:504:ILE:C	2.63	0.42
1:A:165:GLY:HA3	1:A:310:PHE:HA	2.02	0.42
1:A:300:TRP:CE3	1:A:369:MET:SD	3.13	0.42
1:B:289:ALA:O	1:B:293:VAL:HG23	2.19	0.42
1:A:105:GLU:HG2	1:A:106:SER:N	2.35	0.41
1:B:255:VAL:HG12	1:B:259:LEU:HD12	2.02	0.41
1:A:321:ILE:O	1:A:322:GLY:C	2.62	0.41
2:D:20:LEU:HD12	2:D:118:VAL:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:33:SER:O	2:D:34:ALA:C	2.63	0.41
1:A:36:THR:OG1	1:A:160:GLY:HA3	2.21	0.41
1:A:89:THR:HG23	5:A:603:LMU:H81	2.02	0.41
1:B:271:PHE:HZ	1:B:409:MET:HE3	1.85	0.41
1:B:426:SER:HB3	1:B:430:ARG:HH12	1.85	0.41
2:C:62:TYR:HB2	2:C:67:LYS:HD2	2.01	0.41
1:B:31:VAL:HG12	1:B:125:MET:HE2	2.02	0.41
1:B:467:ILE:HG23	1:B:470:LEU:HB3	2.03	0.41
1:A:64:SER:HA	1:A:67:LEU:HB2	2.02	0.41
1:B:290:MET:HE2	1:B:291:ALA:N	2.36	0.41
2:C:3:GLN:HG2	2:C:4:VAL:HG23	2.02	0.41
1:A:35:MET:HE1	1:A:64:SER:HB3	2.03	0.41
2:D:99:ALA:HB2	2:D:112:TRP:CD2	2.56	0.41
1:B:317:LEU:O	1:B:320:ALA:N	2.54	0.41
1:B:295:LEU:HD22	1:B:418:VAL:HG13	2.04	0.40
1:B:343:LEU:HD11	1:B:386:ALA:HB2	2.03	0.40
1:A:13:THR:O	1:A:14:SER:C	2.62	0.40
1:A:13:THR:HG22	1:A:14:SER:N	2.37	0.40
1:A:317:LEU:O	1:A:320:ALA:N	2.55	0.40
1:B:249:THR:O	1:B:253:ILE:HG13	2.21	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	494/520 (95%)	456 (92%)	38 (8%)	0	100	100
1	B	493/520 (95%)	461 (94%)	32 (6%)	0	100	100
2	C	118/148 (80%)	103 (87%)	15 (13%)	0	100	100
2	D	120/148 (81%)	101 (84%)	19 (16%)	0	100	100
All	All	1225/1336 (92%)	1121 (92%)	104 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	380/421 (90%)	378 (100%)	2 (0%)	81	82
1	B	378/421 (90%)	375 (99%)	3 (1%)	73	78
2	C	90/113 (80%)	89 (99%)	1 (1%)	65	74
2	D	89/113 (79%)	89 (100%)	0	100	100
All	All	937/1068 (88%)	931 (99%)	6 (1%)	78	80

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

Mol	Chain	Res	Type
1	A	352	ILE
1	A	375	LEU
1	B	28	LEU
1	B	37	ILE
1	B	272	LYS
2	C	8	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	A	258	ASN
1	B	180	ASN
1	B	299	GLN
1	B	469	GLN
2	C	64	HIS
2	C	84	GLN
2	C	86	ASN
2	C	105	ASN
2	D	3	GLN
2	D	41	GLN

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Mol	Chain	Res	Type
2	D	76	ASN

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 ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	LMU	A	605	-	36,36,36	0.26	0	47,47,47	0.61	1 (2%)
6	OXM	B	602	-	5,5,5	2.11	2 (40%)	4,6,6	1.64	1 (25%)
4	PGT	B	601	-	46,46,50	0.28	0	49,52,56	0.33	0
5	LMU	A	603	-	36,36,36	0.13	0	47,47,47	0.26	0
4	PGT	A	602	-	40,40,50	0.33	0	43,46,56	0.35	0
5	LMU	A	604	-	36,36,36	0.17	0	47,47,47	0.41	0
5	LMU	A	606	-	36,36,36	0.20	0	47,47,47	0.54	0
3	PTY	A	601	-	19,19,49	0.35	0	22,24,54	0.48	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
5	LMU	A	605	-	-	11/21/61/61	0/2/2/2
6	OXM	B	602	-	-	0/3/4/4	-
4	PGT	B	601	-	-	32/51/51/55	-
5	LMU	A	603	-	-	10/21/61/61	0/2/2/2
4	PGT	A	602	-	-	17/45/45/55	-
5	LMU	A	604	-	-	13/21/61/61	0/2/2/2
5	LMU	A	606	-	-	18/21/61/61	0/2/2/2
3	PTY	A	601	-	-	8/22/22/53	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	602	OXM	C1-C2	-3.99	1.50	1.55
6	B	602	OXM	O3-C2	-2.44	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	602	OXM	O2-C2-C1	-2.58	116.33	122.06
5	A	605	LMU	C3'-C4'-C5'	2.20	115.96	110.93

There are no chirality outliers.

All (109) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	601	PGT	C1-O3P-P-O1P
4	B	601	PGT	O4P-C4-C5-O5
4	B	601	PGT	O4P-C4-C5-C6
5	A	603	LMU	O5'-C1'-O1'-C1
5	A	604	LMU	C2-C1-O1'-C1'
5	A	606	LMU	C2'-C1'-O1'-C1
5	A	606	LMU	O5'-C1'-O1'-C1
4	A	602	PGT	O11-C11-O3-C3
5	A	604	LMU	O5B-C1B-O1B-C4'
5	A	606	LMU	O5B-C1B-O1B-C4'
3	A	601	PTY	O30-C30-O4-C1
3	A	601	PTY	C31-C30-O4-C1
4	A	602	PGT	C12-C11-O3-C3
5	A	606	LMU	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
5	A	604	LMU	O5'-C5'-C6'-O6'
4	A	602	PGT	O4P-C4-C5-O5
4	B	601	PGT	C12-C11-O3-C3
4	B	601	PGT	C22-C23-C24-C25
4	B	601	PGT	O11-C11-O3-C3
5	A	606	LMU	O5'-C5'-C6'-O6'
4	B	601	PGT	C35-C36-C37-C38
4	B	601	PGT	C18-C19-C20-C21
5	A	603	LMU	C5-C6-C7-C8
5	A	606	LMU	C4B-C5B-C6B-O6B
5	A	604	LMU	C2B-C1B-O1B-C4'
5	A	604	LMU	C3-C4-C5-C6
4	B	601	PGT	C38-C39-C40-C41
5	A	603	LMU	C2'-C1'-O1'-C1
5	A	604	LMU	C4'-C5'-C6'-O6'
4	B	601	PGT	C11-C12-C13-C14
5	A	606	LMU	C4'-C5'-C6'-O6'
4	A	602	PGT	O4P-C4-C5-C6
4	B	601	PGT	C32-C31-O2-C2
4	B	601	PGT	C17-C18-C19-C20
5	A	606	LMU	C5-C6-C7-C8
4	A	602	PGT	C14-C15-C16-C17
5	A	606	LMU	O1'-C1-C2-C3
4	B	601	PGT	C34-C35-C36-C37
4	B	601	PGT	O31-C31-O2-C2
4	B	601	PGT	C31-C32-C33-C34
4	A	602	PGT	C34-C35-C36-C37
5	A	603	LMU	C4-C5-C6-C7
5	A	605	LMU	C3-C4-C5-C6
5	A	603	LMU	C2-C3-C4-C5
5	A	605	LMU	C2-C1-O1'-C1'
4	B	601	PGT	C12-C13-C14-C15
5	A	606	LMU	C1-C2-C3-C4
4	B	601	PGT	C37-C38-C39-C40
3	A	601	PTY	C11-C8-O7-C6
4	A	602	PGT	C38-C39-C40-C41
4	B	601	PGT	C16-C17-C18-C19
4	A	602	PGT	C18-C19-C20-C21
5	A	606	LMU	C3-C4-C5-C6
4	A	602	PGT	C32-C33-C34-C35
4	B	601	PGT	C40-C41-C42-C43
4	B	601	PGT	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
3	A	601	PTY	O10-C8-O7-C6
5	A	605	LMU	C11-C10-C9-C8
4	B	601	PGT	C15-C16-C17-C18
5	A	603	LMU	C11-C10-C9-C8
4	B	601	PGT	C1-O3P-P-O4P
4	B	601	PGT	C4-O4P-P-O3P
5	A	605	LMU	C4'-C5'-C6'-O6'
5	A	604	LMU	C2-C3-C4-C5
3	A	601	PTY	O4-C1-C6-C5
4	B	601	PGT	C20-C21-C22-C23
5	A	605	LMU	C9-C10-C11-C12
5	A	605	LMU	C7-C8-C9-C10
4	A	602	PGT	C35-C36-C37-C38
4	A	602	PGT	C40-C41-C42-C43
5	A	605	LMU	O1'-C1-C2-C3
5	A	603	LMU	C1-C2-C3-C4
5	A	604	LMU	C1-C2-C3-C4
5	A	604	LMU	O1'-C1-C2-C3
3	A	601	PTY	N1-C2-C3-O11
5	A	603	LMU	C3-C4-C5-C6
5	A	604	LMU	C7-C8-C9-C10
4	A	602	PGT	C11-C12-C13-C14
3	A	601	PTY	O4-C1-C6-O7
4	B	601	PGT	O2-C2-C3-O3
5	A	603	LMU	C7-C8-C9-C10
5	A	604	LMU	C11-C10-C9-C8
4	B	601	PGT	C1-O3P-P-O2P
5	A	606	LMU	C2-C1-O1'-C1'
5	A	605	LMU	C2-C3-C4-C5
4	B	601	PGT	C23-C24-C25-C26
5	A	606	LMU	C2B-C1B-O1B-C4'
4	B	601	PGT	C19-C20-C21-C22
4	B	601	PGT	O2-C31-C32-C33
4	B	601	PGT	C1-C2-C3-O3
5	A	605	LMU	O5'-C1'-O1'-C1
5	A	606	LMU	C3'-C4'-O1B-C1B
5	A	606	LMU	C5'-C4'-O1B-C1B
5	A	604	LMU	C9-C10-C11-C12
5	A	605	LMU	O5'-C5'-C6'-O6'
5	A	605	LMU	C1-C2-C3-C4
4	A	602	PGT	C36-C37-C38-C39
4	A	602	PGT	C4-C5-C6-O6

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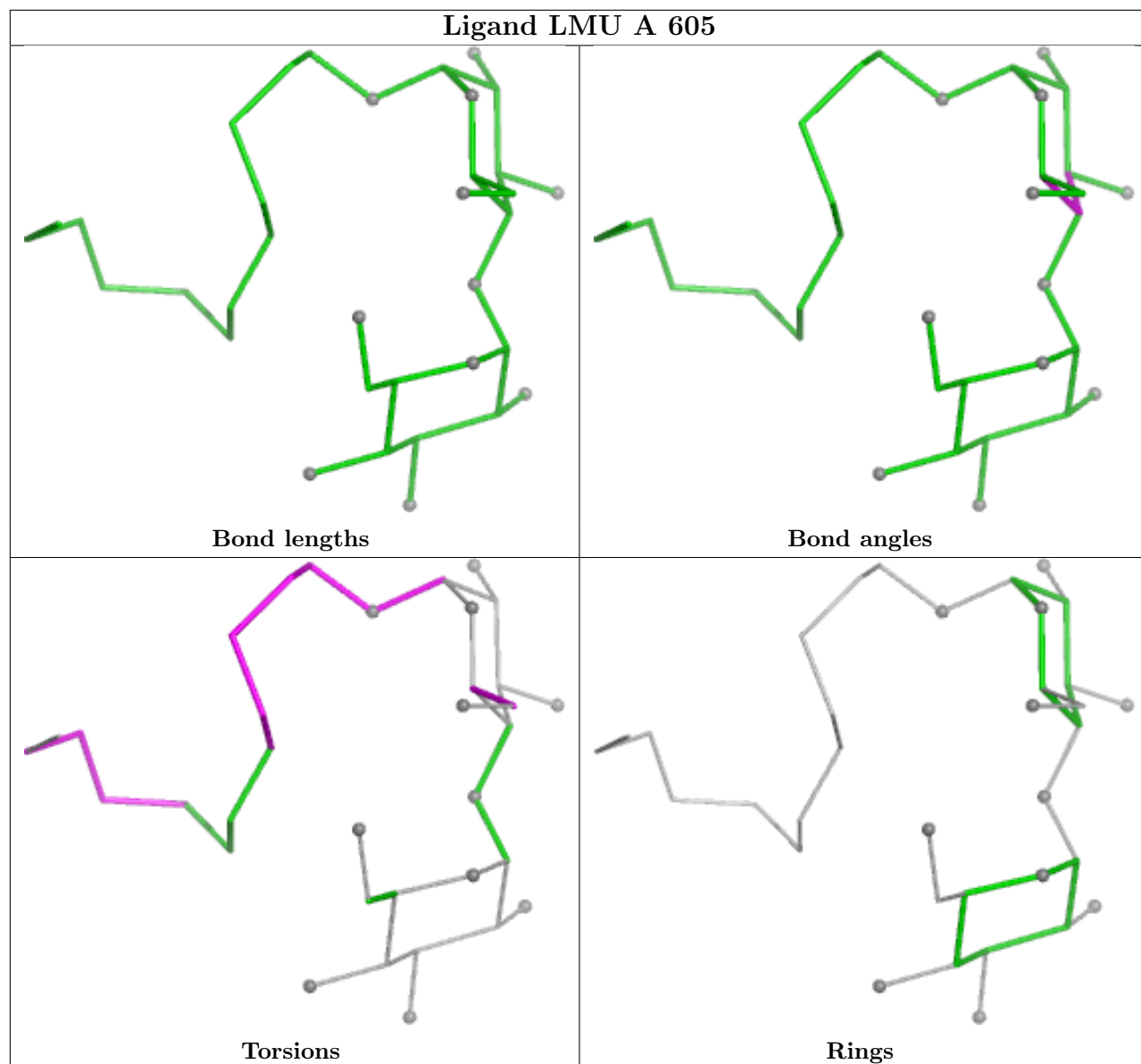
Mol	Chain	Res	Type	Atoms
4	A	602	PGT	C15-C16-C17-C18
5	A	606	LMU	C11-C10-C9-C8
5	A	603	LMU	C9-C10-C11-C12
4	A	602	PGT	O2-C31-C32-C33
4	B	601	PGT	C21-C22-C23-C24
4	B	601	PGT	C4-O4P-P-O1P
5	A	606	LMU	C2-C3-C4-C5
5	A	606	LMU	C7-C8-C9-C10
5	A	604	LMU	C6-C7-C8-C9
3	A	601	PTY	C12-C11-C8-O7
4	A	602	PGT	O31-C31-C32-C33

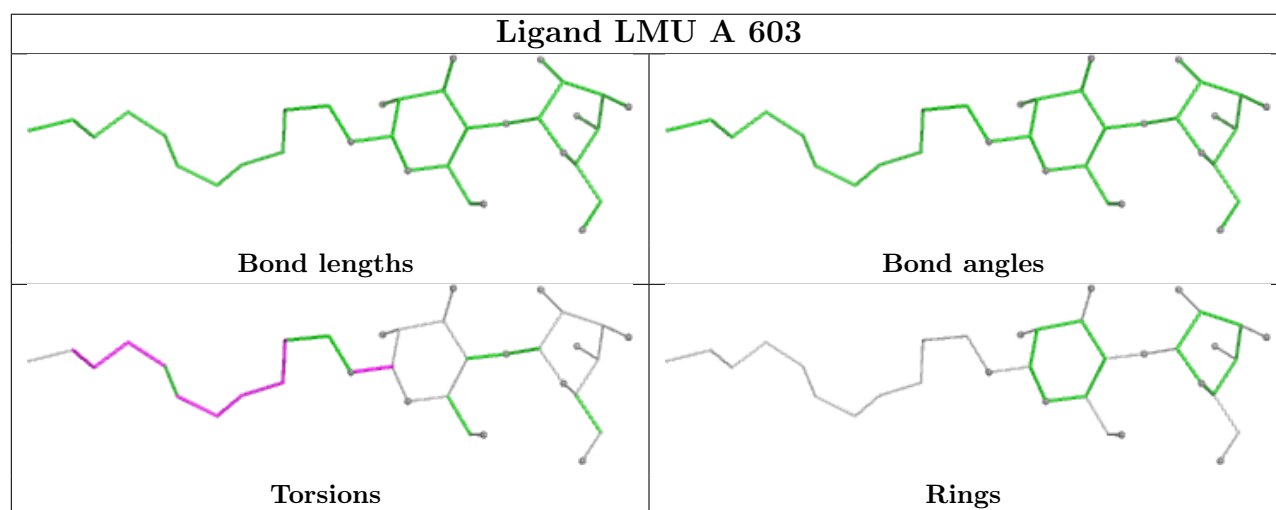
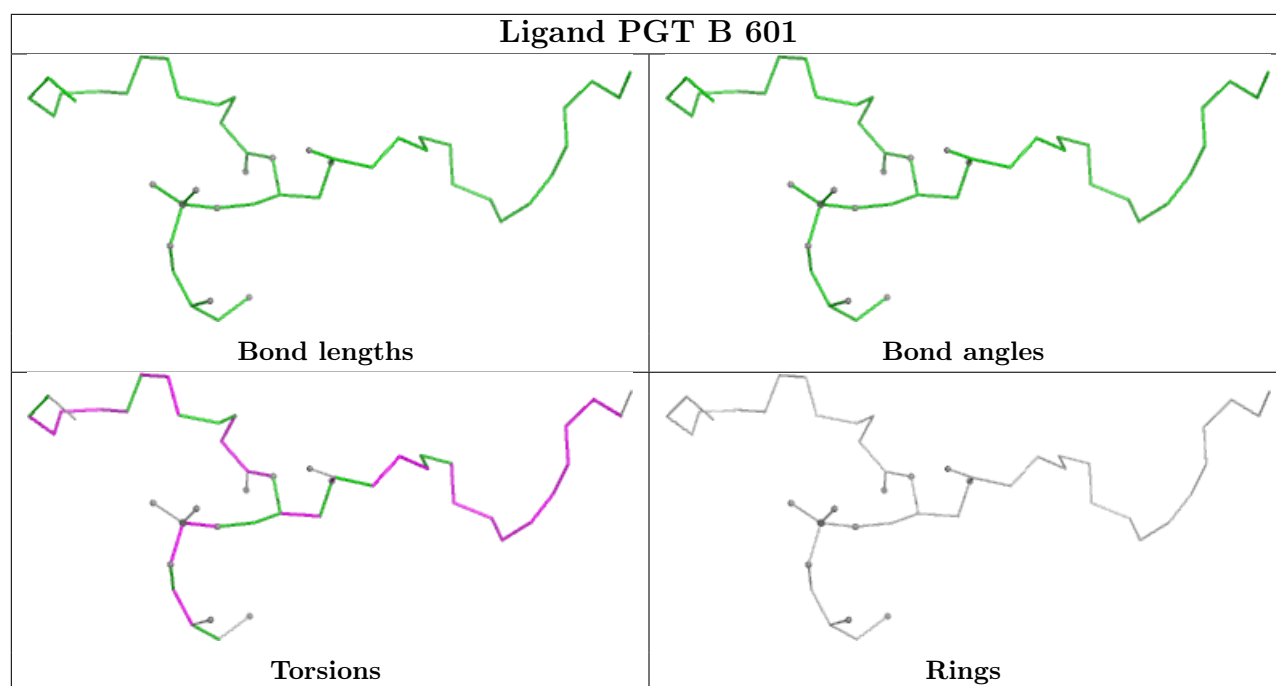
There are no ring outliers.

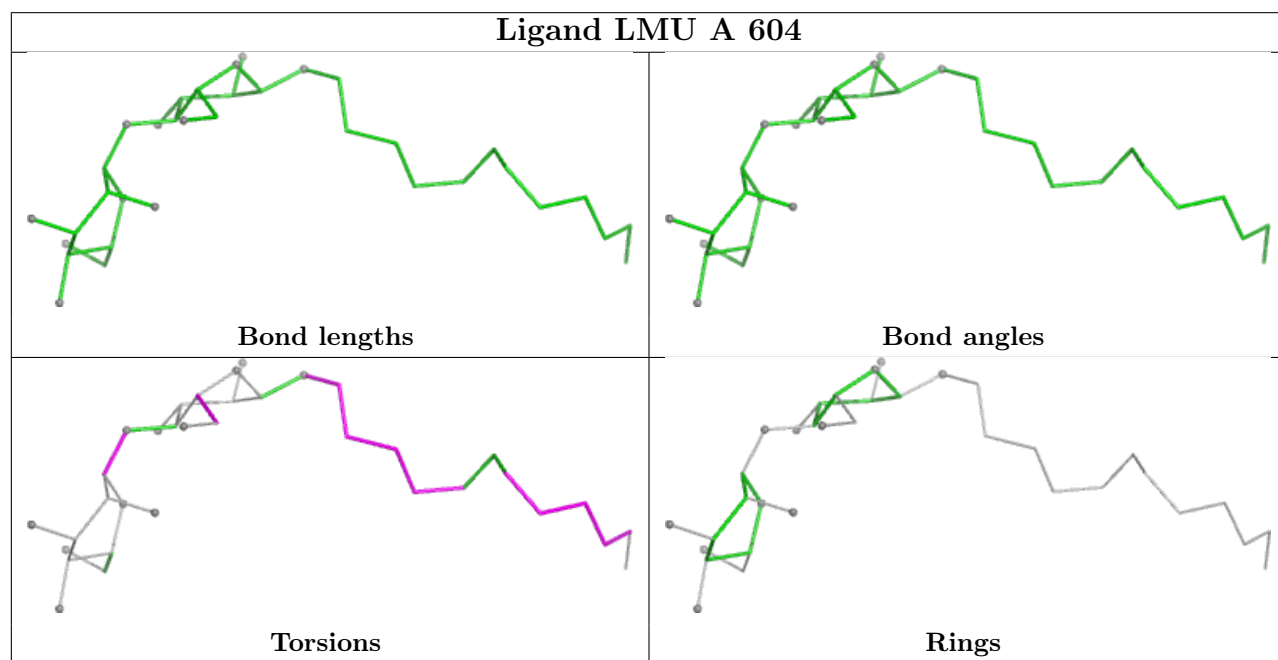
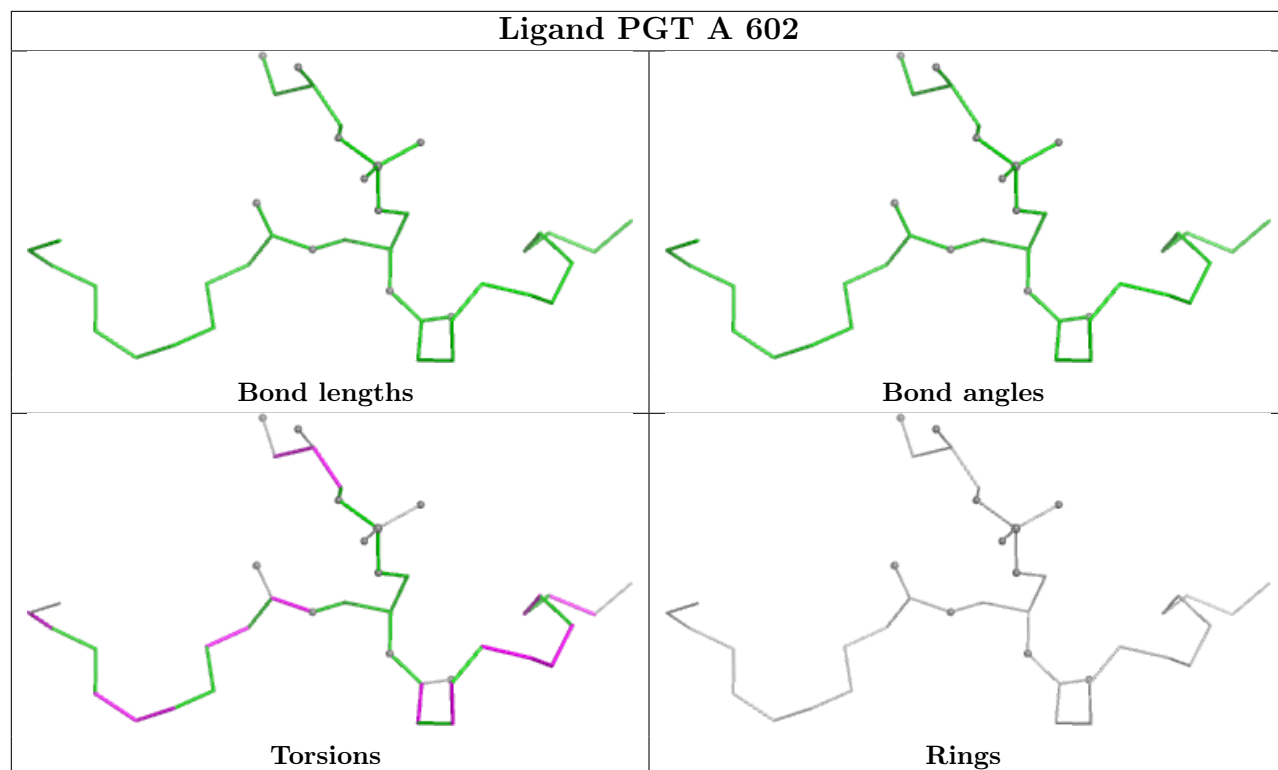
2 monomers are involved in 6 short contacts:

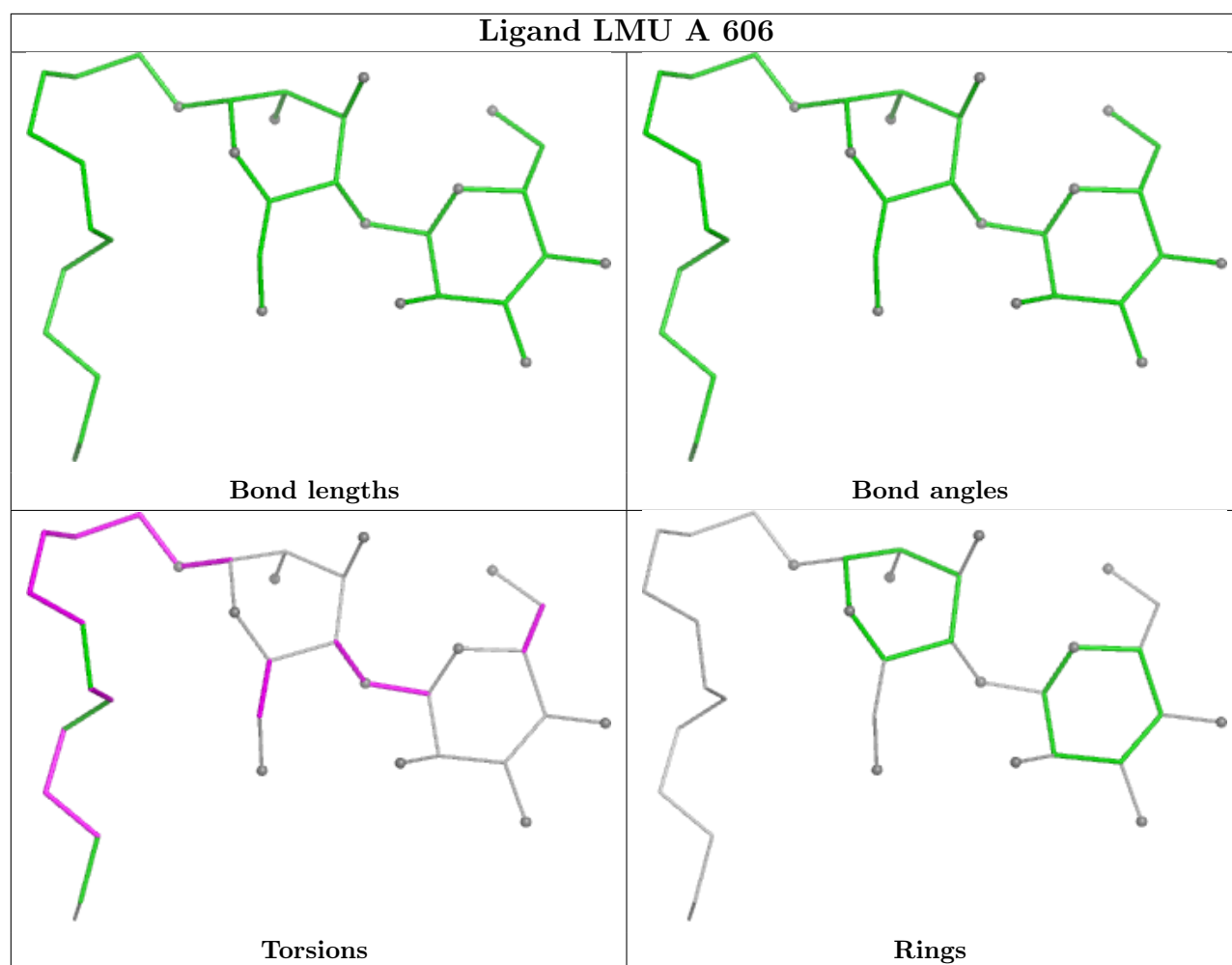
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	PGT	3	0
5	A	603	LMU	3	0

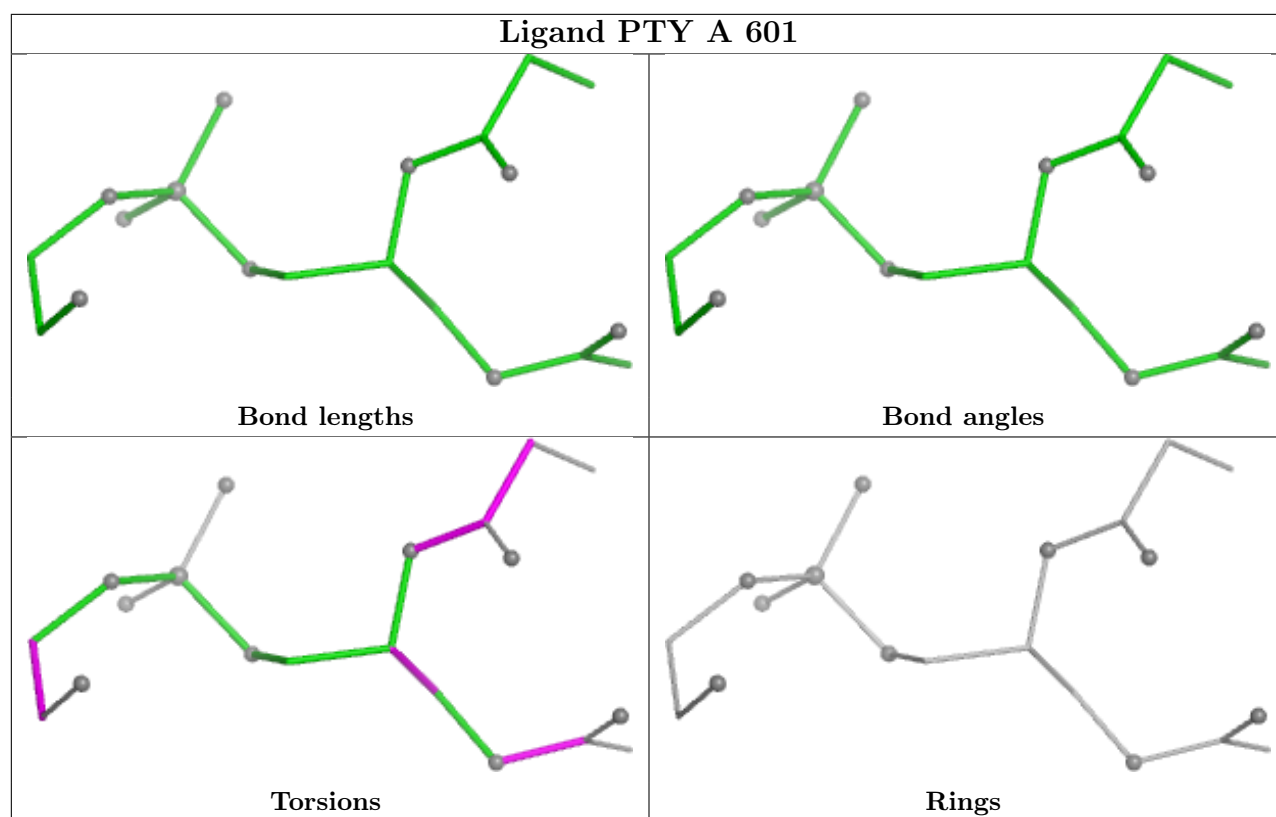
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	496/520 (95%)	0.55	25 (5%)	34	23	44, 72, 96, 109	0
1	B	495/520 (95%)	0.74	44 (8%)	15	12	59, 84, 102, 125	0
2	C	120/148 (81%)	0.96	14 (11%)	9	8	51, 93, 110, 115	0
2	D	122/148 (82%)	1.14	18 (14%)	5	5	57, 106, 119, 123	0
All	All	1233/1336 (92%)	0.72	101 (8%)	17	13	44, 82, 109, 125	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	46	VAL	4.4
1	A	374	ILE	4.4
1	B	275	SER	4.4
2	C	110	ASP	4.0
1	B	456	VAL	4.0
1	B	450	VAL	3.9
1	A	199	LYS	3.8
1	B	475	VAL	3.7
2	D	114	GLN	3.7
2	D	6	LEU	3.6
2	D	113	GLY	3.5
2	C	36	MET	3.5
2	D	7	VAL	3.5
2	C	116	THR	3.5
2	C	9	SER	3.4
1	B	457	GLY	3.4
2	D	55	TRP	3.4
1	B	149	TRP	3.3
1	A	275	SER	3.3
2	C	10	GLY	3.3
2	C	32	SER	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	30	THR	3.2
1	A	264	PRO	3.2
1	B	429	TYR	3.2
2	C	7	VAL	3.2
1	B	125	MET	3.1
2	D	57	GLY	3.1
2	C	115	GLY	3.1
2	D	8	GLU	3.1
1	B	70	PHE	3.1
1	B	455	VAL	3.1
2	C	31	PHE	3.1
1	A	145	ALA	3.1
2	D	42	ALA	3.1
1	A	410	TYR	3.1
2	D	9	SER	3.0
1	A	171	PHE	3.0
1	B	454	SER	2.9
1	A	277	SER	2.9
2	C	55	TRP	2.9
2	D	98	CYS	2.9
1	B	296	LEU	2.8
1	B	56	GLN	2.8
1	B	199	LYS	2.8
1	B	357	MET	2.7
1	A	450	VAL	2.7
2	D	14	VAL	2.6
2	C	22	LEU	2.6
1	B	402	ALA	2.6
2	C	12	GLY	2.6
1	B	171	PHE	2.5
1	A	128	THR	2.5
1	B	157	ALA	2.5
2	D	36	MET	2.5
1	A	68	ALA	2.5
1	B	453	GLU	2.5
1	B	158	VAL	2.5
1	B	426	SER	2.4
1	B	35	MET	2.4
1	A	266	LEU	2.4
1	B	353	GLY	2.4
1	B	387	SER	2.4
2	D	2	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	153	SER	2.4
1	A	152	ALA	2.3
1	B	487	LEU	2.3
1	A	258	ASN	2.3
1	B	34	ASP	2.3
2	D	112	TRP	2.3
1	A	18	TRP	2.3
1	B	174	HIS	2.3
1	B	172	SER	2.3
1	A	132	ILE	2.2
1	B	39	ILE	2.2
1	A	178	LEU	2.2
1	B	295	LEU	2.2
1	B	28	LEU	2.2
1	A	37	ILE	2.2
1	B	356	ILE	2.1
1	B	360	PHE	2.1
1	A	149	TRP	2.1
1	A	167	LEU	2.1
1	A	316	LEU	2.1
1	B	37	ILE	2.1
1	A	70	PHE	2.1
1	B	505	PRO	2.1
1	A	424	LEU	2.1
2	C	41	GLN	2.1
1	B	91	PHE	2.1
1	B	271	PHE	2.1
1	B	276	PHE	2.1
1	B	452	GLU	2.1
2	D	43	PRO	2.1
2	D	59	SER	2.0
1	A	505	PRO	2.0
1	B	217	ILE	2.0
1	B	479	ASN	2.0
1	A	144	THR	2.0
2	D	10	GLY	2.0
1	B	270	LEU	2.0
2	C	13	LEU	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

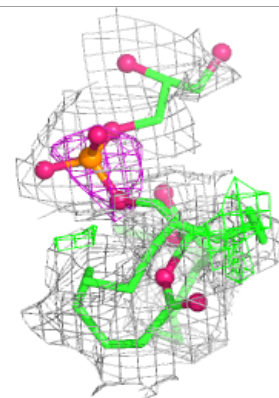
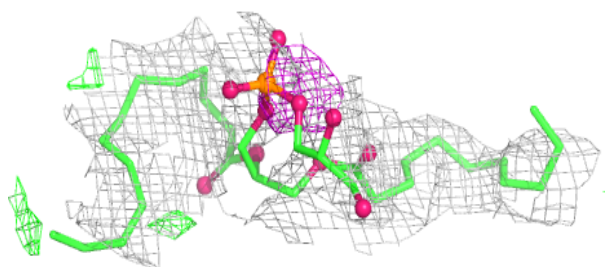
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PGT	A	602	41/51	0.50	0.22	130,132,135,136	0
5	LMU	A	604	35/35	0.52	0.22	20,20,20,20	35
3	PTY	A	601	20/50	0.58	0.19	146,146,147,147	0
4	PGT	B	601	47/51	0.61	0.22	131,135,136,136	0
5	LMU	A	606	35/35	0.61	0.26	20,20,20,20	35
5	LMU	A	605	35/35	0.64	0.25	20,20,20,20	35
6	OXM	B	602	6/6	0.65	0.16	130,130,130,130	0
5	LMU	A	603	35/35	0.69	0.20	20,20,20,20	35

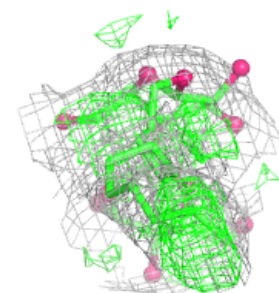
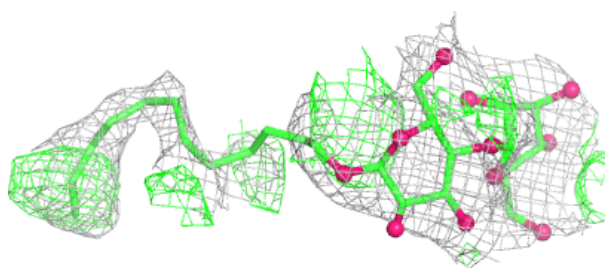
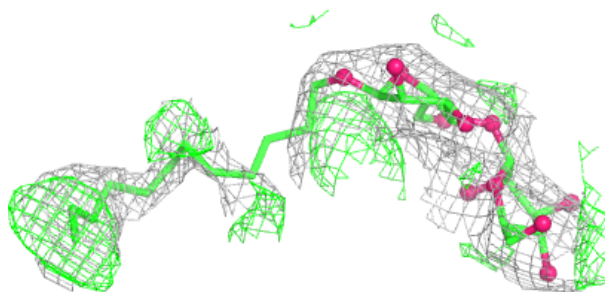
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PGT 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)

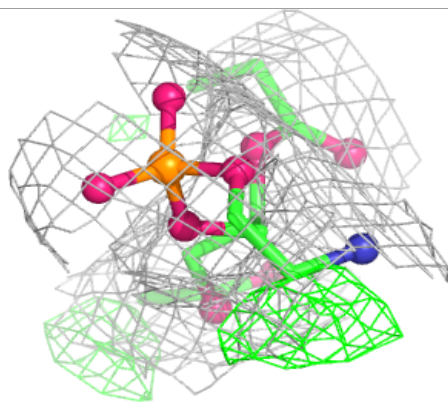
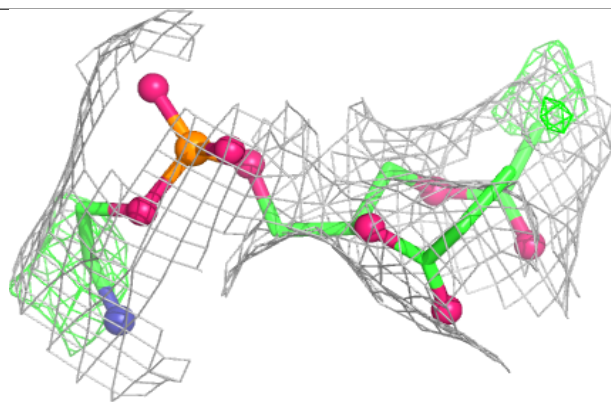
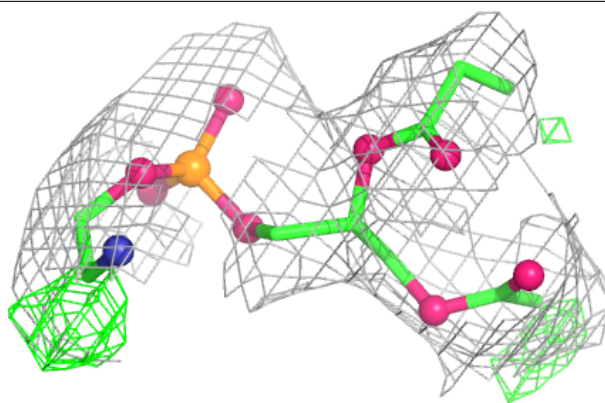
**Electron density around LMU A 604:**

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

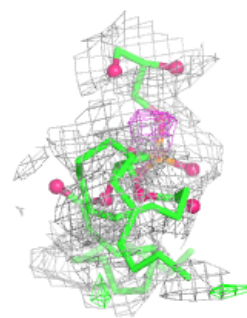
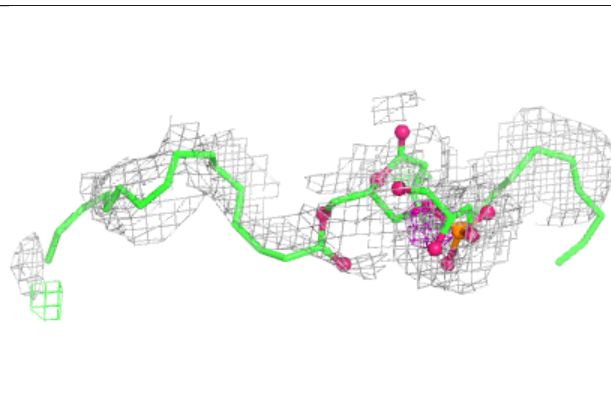
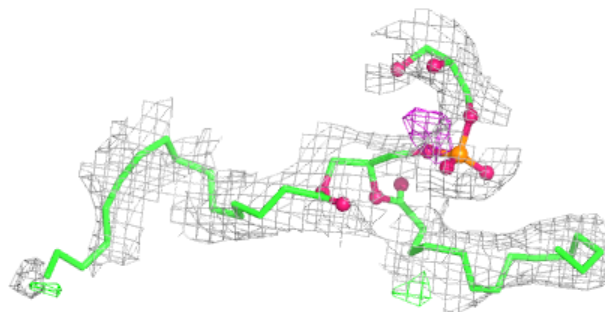


Electron density around PTY A 601:

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

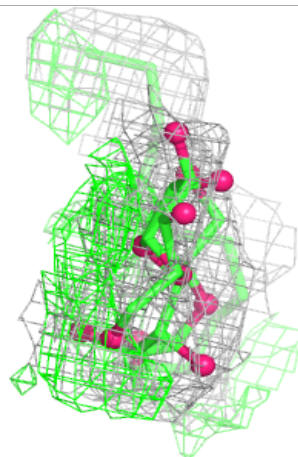
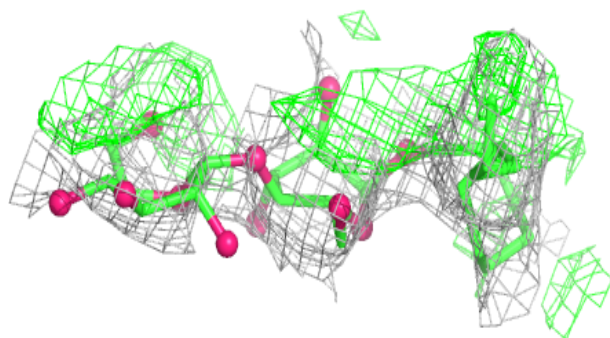
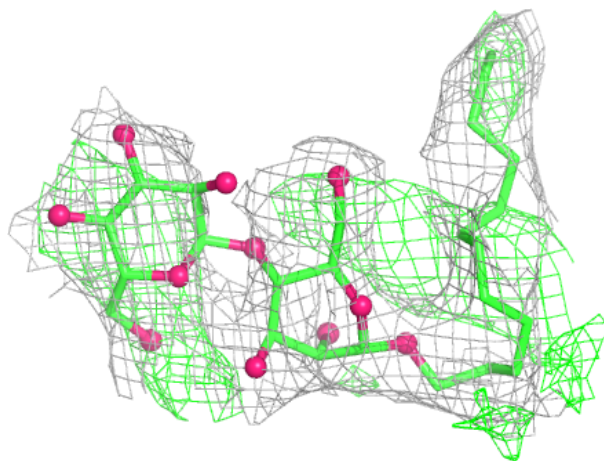
**Electron density around PGT B 601:**

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



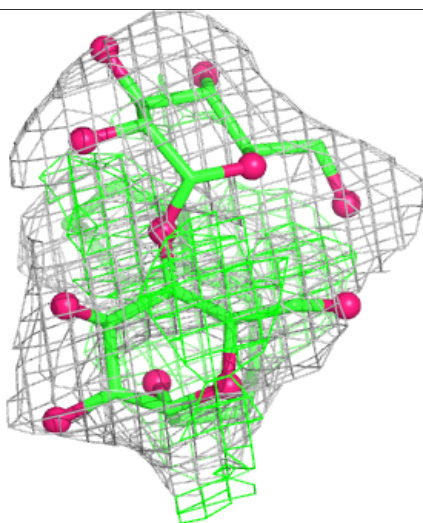
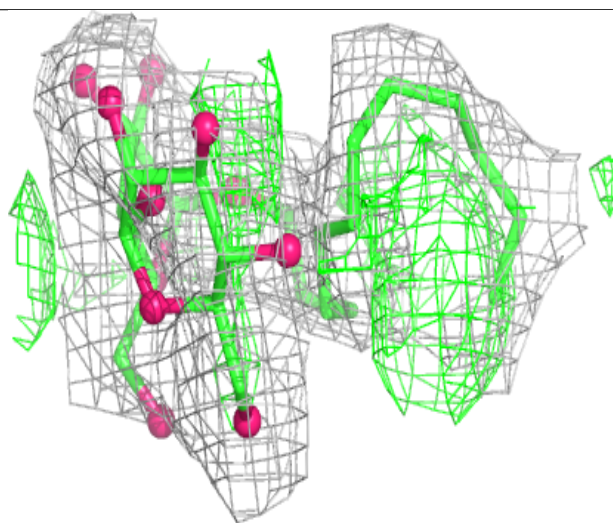
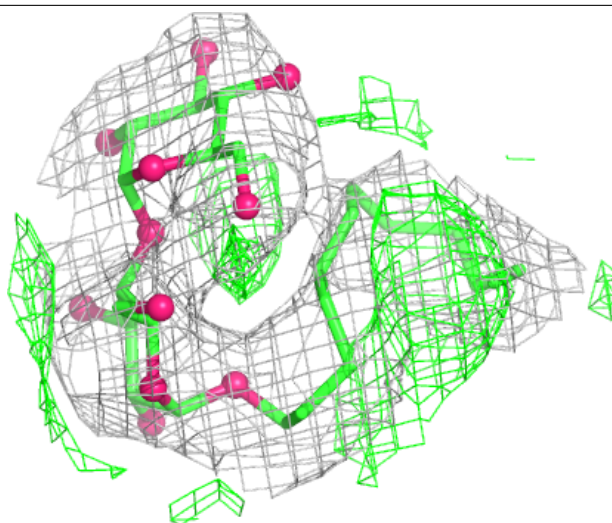
Electron density around LMU A 606:

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



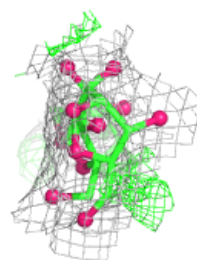
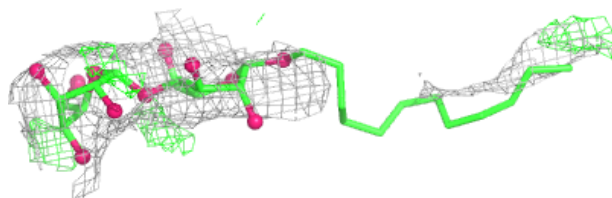
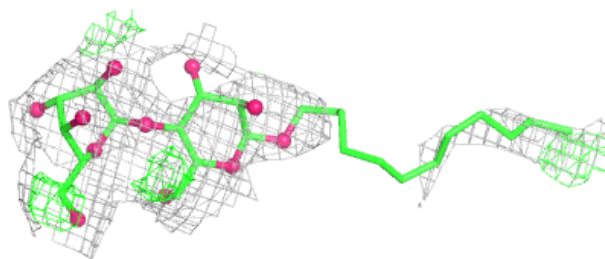
Electron density around LMU A 605:

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.