



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:20 PM UTC

PDB ID : 3VMT / pdb_00003vmt
Title : Crystal structure of Staphylococcus aureus membrane-bound transglycosylase in complex with a Lipid II analog
Authors : Huang, C.Y.; Shih, H.W.; Lin, L.Y.; Tien, Y.W.; Cheng, T.J.R.; Cheng, W.C.; Wong, C.H.; Ma, C.
Deposited on : 2011-12-15
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

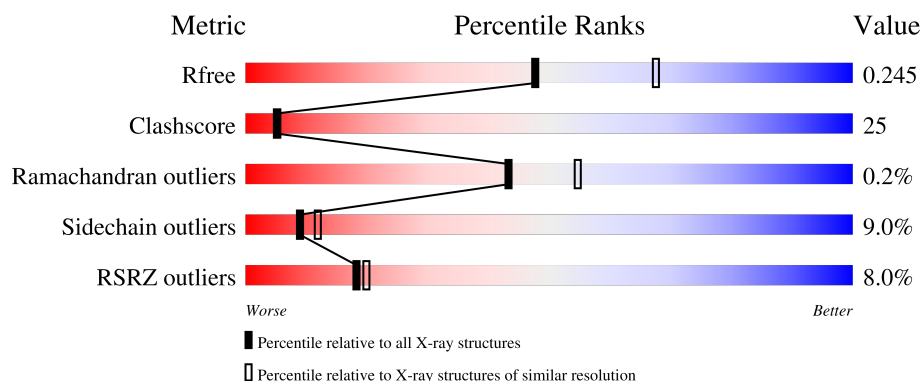
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	263	5% 49% 33% • 16%
1	B	263	8% 48% 29% 6% 17%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3695 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 Monofunctional glycosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1813	1151	311	344	7			
1	B	218	Total	C	N	O	S	0	0	0
			1785	1133	307	338	7			

There are 42 discrepancies between the modelled and reference sequences:

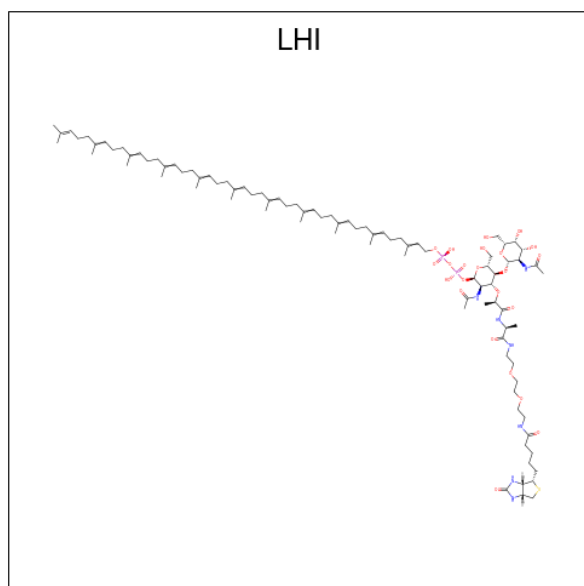
Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	expression tag	UNP Q99T05
A	8	GLY	-	expression tag	UNP Q99T05
A	9	SER	-	expression tag	UNP Q99T05
A	10	SER	-	expression tag	UNP Q99T05
A	11	HIS	-	expression tag	UNP Q99T05
A	12	HIS	-	expression tag	UNP Q99T05
A	13	HIS	-	expression tag	UNP Q99T05
A	14	HIS	-	expression tag	UNP Q99T05
A	15	HIS	-	expression tag	UNP Q99T05
A	16	HIS	-	expression tag	UNP Q99T05
A	17	SER	-	expression tag	UNP Q99T05
A	18	SER	-	expression tag	UNP Q99T05
A	19	GLY	-	expression tag	UNP Q99T05
A	20	LEU	-	expression tag	UNP Q99T05
A	21	VAL	-	expression tag	UNP Q99T05
A	22	PRO	-	expression tag	UNP Q99T05
A	23	ARG	-	expression tag	UNP Q99T05
A	24	GLY	-	expression tag	UNP Q99T05
A	25	SER	-	expression tag	UNP Q99T05
A	26	HIS	-	expression tag	UNP Q99T05
A	27	MET	-	expression tag	UNP Q99T05
B	7	MET	-	expression tag	UNP Q99T05
B	8	GLY	-	expression tag	UNP Q99T05
B	9	SER	-	expression tag	UNP Q99T05
B	10	SER	-	expression tag	UNP Q99T05

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	11	HIS	-	expression tag	UNP Q99T05
B	12	HIS	-	expression tag	UNP Q99T05
B	13	HIS	-	expression tag	UNP Q99T05
B	14	HIS	-	expression tag	UNP Q99T05
B	15	HIS	-	expression tag	UNP Q99T05
B	16	HIS	-	expression tag	UNP Q99T05
B	17	SER	-	expression tag	UNP Q99T05
B	18	SER	-	expression tag	UNP Q99T05
B	19	GLY	-	expression tag	UNP Q99T05
B	20	LEU	-	expression tag	UNP Q99T05
B	21	VAL	-	expression tag	UNP Q99T05
B	22	PRO	-	expression tag	UNP Q99T05
B	23	ARG	-	expression tag	UNP Q99T05
B	24	GLY	-	expression tag	UNP Q99T05
B	25	SER	-	expression tag	UNP Q99T05
B	26	HIS	-	expression tag	UNP Q99T05
B	27	MET	-	expression tag	UNP Q99T05

- Molecule 2 is [(2R,3R,4R,5S,6R)-4-[(2R)-1-[(2S)-1-[2-[2-[2-[5-[(3aS,4S,6aR)-2-oxidanylidene-1,3,3a,4,6,6a-hexahydrothieno[3,4-d]imidazol-4-yl]pentanoylamino]ethoxy]ethoxy]ethylamino]-1-oxidanylidene-propan-2-yl]amino]-1-oxidanylidene-propan-2-yl]oxy-3-acetamido-5-[(2S,3R,4R,5R,6R)-3-acetamido-6-(hydroxymethyl)-4,5-bis(oxidanyl)oxan-2-yl]oxy-6-(hydroxymethyl)oxan-2-yl] [oxidanyl(3,7,11,15,19,23,27,31,35,39,43-undecamethyltetraetraconta-2,6,10,14,18,22,26,30,34,38,42-undecaenoxy)phosphoryl] hydrogen phosphate (CCD ID: LHI) (formula: C₉₃H₁₅₅N₇O₂₃P₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			43	20	3	18	2		

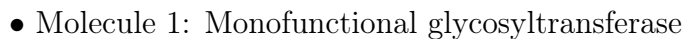
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total	O	0	0
			41	41		
4	B	11	Total	O	0	0
			11	11		

- Molecule 1: Monofunctional glycosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.49Å 67.43Å 152.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.08 – 2.30 28.08 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.4 (28.08-2.30) 98.0 (28.08-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.197 , 0.242 0.203 , 0.245	Depositor DCC
R_{free} test set	1547 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.967	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 75.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3695	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: MG, LHI

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	0.41	0/1845	0.76	0/2487
1	B	0.33	0/1816	0.73	2/2448 (0.1%)
All	All	0.37	0/3661	0.75	2/4935 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	ASN	N-CA-C	-7.20	103.75	112.54
1	B	144	TYR	N-CA-C	6.24	120.40	109.80

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	1813	0	1791	92	0
1	B	1785	0	1767	85	0
2	A	43	0	33	9	0
3	A	2	0	0	0	0
4	A	41	0	0	0	0
4	B	11	0	0	0	0
All	All	3695	0	3591	178	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 25.

All (178) 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:41:ARG:HD2	1:B:44:LEU:HD11	1.50	0.93
1:B:66:THR:HA	1:B:67:ARG:HG3	1.53	0.89
1:B:202:ASN:HD22	1:B:204:ASN:H	1.19	0.87
1:B:67:ARG:HH22	1:B:70:VAL:HG22	1.42	0.84
1:A:61:MET:HE3	1:A:61:MET:HA	1.60	0.83
1:B:266:GLN:O	1:B:269:ARG:HB2	1.84	0.77
1:A:130:GLY:HA2	2:A:301:LHI:H20	1.66	0.77
1:B:67:ARG:HH21	1:B:162:ARG:HD2	1.52	0.74
1:B:217:ALA:HB2	1:B:249:MET:HE1	1.69	0.74
1:A:67:ARG:HB3	1:A:68:ASP:C	2.13	0.73
1:B:246:LEU:HA	1:B:249:MET:HE3	1.71	0.73
1:B:67:ARG:HH21	1:B:162:ARG:CD	2.02	0.73
1:A:42:ILE:HG23	1:A:43:LEU:HD12	1.72	0.72
1:A:114:GLY:HA2	1:A:117:ARG:NH2	2.04	0.72
1:B:151:THR:HG22	1:B:155:LYS:HE3	1.71	0.72
1:A:109:GLY:O	1:A:133:THR:HG21	1.90	0.71
1:B:44:LEU:HD12	1:B:45:LYS:HG2	1.72	0.70
1:B:141:ASN:ND2	1:B:180:ILE:HG22	2.07	0.70
1:B:202:ASN:ND2	1:B:204:ASN:H	1.89	0.69
1:A:66:THR:HG23	1:A:67:ARG:HG3	1.75	0.68
1:A:66:THR:HA	1:A:67:ARG:HG2	1.75	0.68
1:B:54:ILE:O	1:B:58:ILE:HG12	1.93	0.68
1:B:168:ASN:H	1:B:168:ASN:HD22	1.42	0.68
1:B:67:ARG:HG2	1:B:68:ASP:O	1.94	0.68
1:B:217:ALA:CB	1:B:249:MET:HE1	2.23	0.67
1:B:234:MET:HE2	1:B:239:THR:HG22	1.76	0.66
1:A:107:HIS:NE2	1:A:133:THR:OG1	2.29	0.66
1:A:202:ASN:HD21	1:A:204:ASN:HB2	1.60	0.65
1:B:181:TYR:CZ	1:B:183:GLY:HA2	2.32	0.65
1:B:150:PHE:O	1:B:154:VAL:HG23	1.98	0.64
1:A:155:LYS:O	1:A:159:VAL:HG23	1.98	0.64
1:B:67:ARG:NH2	1:B:70:VAL:HG22	2.12	0.63
1:A:56:LEU:O	1:A:60:ILE:HG13	1.99	0.63
1:B:159:VAL:O	1:B:163:VAL:HG23	1.98	0.63
1:A:225:ALA:HB1	1:A:229:TYR:CD2	2.34	0.62
1:A:130:GLY:N	2:A:301:LHI:HOA6	1.97	0.62
1:B:152:ARG:HA	1:B:155:LYS:HD3	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:SER:HB3	1:A:155:LYS:HB2	1.81	0.61
1:B:113:LYS:O	1:B:117:ARG:HD2	2.01	0.61
1:A:112:LEU:O	1:A:116:THR:HG23	2.01	0.60
1:A:130:GLY:CA	2:A:301:LHI:H20	2.31	0.60
1:B:52:ILE:HG13	1:B:53:ILE:N	2.17	0.60
1:B:212:THR:H	1:B:215:GLN:NE2	1.99	0.60
1:A:106:ASN:N	1:A:106:ASN:HD22	2.00	0.59
1:B:45:LYS:HZ2	1:B:48:LEU:HB2	1.66	0.59
1:A:133:THR:HG22	1:A:136:GLN:HG3	1.85	0.59
1:A:230:ASN:ND2	1:A:232:ASN:H	2.00	0.59
1:B:67:ARG:HG2	1:B:69:ASN:HA	1.85	0.58
1:A:118:ALA:HB2	1:A:131:GLY:HA3	1.86	0.58
1:A:144:TYR:C	1:A:146:ASN:H	2.11	0.58
1:A:46:ILE:HA	1:A:49:THR:HG22	1.84	0.57
1:B:110:PHE:CG	1:B:111:ASP:N	2.72	0.57
1:A:98:SER:HA	1:A:252:GLN:HE22	1.68	0.57
1:A:180:ILE:HG13	1:A:182:PHE:CE2	2.40	0.57
1:B:226:PRO:HB2	1:B:228:VAL:HG22	1.85	0.57
1:A:45:LYS:HD3	1:A:46:ILE:HG23	1.85	0.57
1:A:65:SER:O	1:A:68:ASP:HB2	2.05	0.56
1:A:66:THR:HA	1:A:67:ARG:CG	2.34	0.56
1:A:202:ASN:HD22	1:A:202:ASN:C	2.13	0.56
1:B:66:THR:HB	1:B:67:ARG:HD2	1.87	0.56
1:A:211:ILE:HG13	1:A:215:GLN:HE21	1.70	0.56
1:A:61:MET:HE3	1:A:64:LEU:HD23	1.88	0.55
1:A:220:ALA:HB3	1:A:245:ASN:HD21	1.72	0.55
1:A:61:MET:HA	1:A:61:MET:CE	2.35	0.55
1:A:110:PHE:CE1	1:A:115:THR:HG21	2.42	0.54
1:A:149:SER:HB3	1:A:152:ARG:HG2	1.89	0.54
1:B:41:ARG:CD	1:B:44:LEU:HD11	2.32	0.54
1:B:60:ILE:O	1:B:64:LEU:HD23	2.07	0.54
1:B:135:THR:HG21	1:B:164:GLU:HG2	1.88	0.54
1:A:148:ARG:HA	1:A:148:ARG:HE	1.72	0.54
1:B:62:TYR:O	1:B:66:THR:HG23	2.08	0.54
1:B:47:LEU:O	1:B:51:LEU:HD13	2.08	0.53
1:B:225:ALA:HB1	1:B:229:TYR:CD2	2.43	0.53
1:A:114:GLY:HA3	2:A:301:LHI:HA1B	1.90	0.53
1:B:202:ASN:HD22	1:B:202:ASN:C	2.17	0.53
1:A:50:ILE:O	1:A:54:ILE:HG23	2.09	0.53
1:A:230:ASN:HD22	1:A:231:ILE:N	2.07	0.53
1:B:48:LEU:C	1:B:48:LEU:HD23	2.34	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ARG:NH2	1:B:162:ARG:HD2	2.23	0.52
1:A:110:PHE:HE2	1:A:112:LEU:HD23	1.75	0.51
1:A:133:THR:CG2	1:A:136:GLN:H	2.23	0.51
1:B:67:ARG:NH1	1:B:69:ASN:OD1	2.44	0.51
1:B:67:ARG:HG2	1:B:68:ASP:C	2.35	0.51
1:A:230:ASN:HD22	1:A:230:ASN:C	2.18	0.51
1:A:180:ILE:HD12	1:A:223:VAL:HG21	1.93	0.50
1:B:66:THR:HA	1:B:67:ARG:CG	2.35	0.50
1:B:53:ILE:O	1:B:57:PHE:N	2.42	0.50
1:A:190:GLU:OE1	1:A:201:VAL:HG22	2.11	0.50
1:A:131:GLY:HA2	2:A:301:LHI:HN7	1.77	0.49
1:A:168:ASN:OD1	1:A:171:GLU:HG3	2.12	0.49
1:B:67:ARG:HH22	1:B:70:VAL:CG2	2.21	0.49
1:A:47:LEU:O	1:A:51:LEU:HB2	2.12	0.49
1:A:50:ILE:O	1:A:53:ILE:HG22	2.13	0.49
1:B:99:MET:CE	1:B:248:LYS:HD2	2.42	0.49
1:A:130:GLY:N	2:A:301:LHI:H20	2.28	0.49
1:A:235:SER:O	1:A:239:THR:HG23	2.13	0.48
1:A:250:LYS:HD2	1:A:257:GLU:OE1	2.13	0.48
1:A:44:LEU:C	1:A:44:LEU:HD12	2.39	0.48
1:A:133:THR:HG22	1:A:136:GLN:CG	2.43	0.48
1:B:190:GLU:OE1	1:B:201:VAL:HG22	2.14	0.48
1:B:141:ASN:HD21	1:B:180:ILE:HG22	1.79	0.47
1:B:189:LEU:HG	1:B:201:VAL:HG11	1.96	0.47
1:A:114:GLY:O	1:A:118:ALA:HB2	2.14	0.47
1:A:86:ASP:N	1:A:170:ASN:HD21	2.13	0.47
1:A:152:ARG:HA	1:A:155:LYS:HE2	1.96	0.47
1:A:100:GLU:OE1	2:A:301:LHI:H17	2.15	0.47
1:B:180:ILE:HD12	1:B:223:VAL:HG21	1.96	0.47
1:A:131:GLY:O	2:A:301:LHI:HA1A	2.15	0.47
1:B:50:ILE:O	1:B:54:ILE:HD13	2.15	0.46
1:B:202:ASN:HD21	1:B:204:ASN:HB2	1.79	0.46
1:A:54:ILE:HG13	1:A:55:ALA:N	2.31	0.46
1:A:79:LYS:NZ	1:A:179:ASN:HD22	2.14	0.46
1:B:63:PHE:O	1:B:66:THR:O	2.33	0.46
1:B:199:THR:HA	1:B:209:SER:O	2.15	0.46
1:A:49:THR:HA	1:A:52:ILE:HG22	1.97	0.46
1:A:202:ASN:ND2	1:A:204:ASN:HB2	2.29	0.46
1:B:146:ASN:HD22	1:B:146:ASN:N	2.14	0.45
1:B:235:SER:O	1:B:239:THR:HG23	2.17	0.45
1:A:42:ILE:HG23	1:A:43:LEU:CD1	2.45	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:THR:CA	1:B:67:ARG:HG3	2.37	0.45
1:B:197:PHE:CD2	1:B:215:GLN:HG2	2.51	0.45
1:B:66:THR:HB	1:B:67:ARG:CD	2.47	0.45
1:A:133:THR:HG23	1:A:136:GLN:H	1.82	0.45
1:B:151:THR:O	1:B:155:LYS:HD2	2.17	0.45
1:A:181:TYR:CZ	1:A:183:GLY:HA2	2.51	0.44
1:A:150:PHE:O	1:A:154:VAL:HG23	2.16	0.44
1:B:140:LYS:HA	1:B:144:TYR:HB2	1.99	0.44
1:A:106:ASN:N	1:A:106:ASN:ND2	2.64	0.44
1:A:121:SER:O	1:A:122:THR:C	2.60	0.44
1:B:104:PHE:CD1	1:B:134:ILE:HB	2.51	0.44
1:A:41:ARG:HB2	1:A:41:ARG:NH1	2.33	0.44
1:A:60:ILE:O	1:A:64:LEU:HD22	2.17	0.44
1:A:56:LEU:HD12	1:A:56:LEU:HA	1.82	0.44
1:B:155:LYS:O	1:B:156:GLU:C	2.60	0.44
1:A:202:ASN:HD22	1:A:204:ASN:N	2.15	0.44
1:A:203:LYS:O	1:A:210:HIS:HE1	2.01	0.44
1:A:250:LYS:HD3	1:A:260:TYR:CG	2.53	0.44
1:B:146:ASN:N	1:B:146:ASN:ND2	2.65	0.43
1:A:130:GLY:HA2	1:A:131:GLY:HA2	1.54	0.43
1:B:96:PHE:CE2	1:B:220:ALA:HA	2.53	0.43
1:A:144:TYR:C	1:A:146:ASN:N	2.74	0.43
1:A:266:GLN:HA	1:A:269:ARG:HD3	1.99	0.43
1:B:168:ASN:HD21	1:B:171:GLU:HG3	1.84	0.43
1:A:45:LYS:HD3	1:A:46:ILE:N	2.34	0.43
1:A:149:SER:HB3	1:A:152:ARG:CG	2.47	0.43
1:B:70:VAL:O	1:B:73:LEU:HB2	2.19	0.43
1:B:180:ILE:O	1:B:187:TYR:HA	2.18	0.43
1:B:74:ARG:HH12	1:B:171:GLU:CD	2.27	0.43
1:B:165:LYS:O	1:B:165:LYS:HD3	2.19	0.43
2:A:301:LHI:H13	2:A:301:LHI:H19	2.01	0.42
1:B:144:TYR:HB3	1:B:145:ASP:H	1.55	0.42
1:B:147:ASP:OD2	1:B:147:ASP:C	2.61	0.42
1:A:230:ASN:ND2	1:A:230:ASN:C	2.77	0.42
1:A:69:ASN:C	1:A:69:ASN:HD22	2.26	0.42
1:B:99:MET:O	1:B:99:MET:HG3	2.19	0.42
1:B:229:TYR:OH	1:B:237:ASN:HB3	2.19	0.42
1:A:48:LEU:C	1:A:48:LEU:HD23	2.45	0.42
1:A:202:ASN:HD22	1:A:204:ASN:H	1.66	0.42
1:A:118:ALA:C	1:A:120:PHE:H	2.28	0.42
1:B:53:ILE:H	1:B:53:ILE:HG13	1.59	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:ARG:HD3	1:B:155:LYS:HD3	2.01	0.41
1:A:52:ILE:C	1:A:52:ILE:HD13	2.45	0.41
1:A:60:ILE:HG22	1:A:64:LEU:CD2	2.50	0.41
1:A:65:SER:O	1:A:67:ARG:HA	2.21	0.41
1:B:168:ASN:HD21	1:B:171:GLU:CG	2.34	0.41
1:B:45:LYS:HA	1:B:45:LYS:NZ	2.36	0.41
1:B:107:HIS:ND1	1:B:107:HIS:C	2.79	0.41
1:B:110:PHE:CD2	1:B:111:ASP:N	2.88	0.41
1:A:202:ASN:C	1:A:202:ASN:ND2	2.79	0.41
1:A:47:LEU:HD23	1:A:47:LEU:C	2.46	0.41
1:A:133:THR:HG23	1:A:135:THR:N	2.35	0.41
1:A:202:ASN:ND2	1:A:204:ASN:H	2.18	0.41
1:B:67:ARG:NH1	1:B:69:ASN:HA	2.36	0.41
1:B:117:ARG:HE	1:B:117:ARG:N	2.18	0.41
1:B:223:VAL:HG12	1:B:224:ASN:ND2	2.36	0.41
1:A:67:ARG:HA	1:A:68:ASP:HB2	2.02	0.40
1:B:144:TYR:C	1:B:146:ASN:H	2.29	0.40
1:B:49:THR:O	1:B:53:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	218/263 (83%)	205 (94%)	13 (6%)	0	100	100
1	B	214/263 (81%)	206 (96%)	7 (3%)	1 (0%)	24	31
All	All	432/526 (82%)	411 (95%)	20 (5%)	1 (0%)	43	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	145	ASP

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	202/239 (84%)	187 (93%)	15 (7%)	13	17
1	B	199/239 (83%)	178 (89%)	21 (11%)	6	8
All	All	401/478 (84%)	365 (91%)	36 (9%)	9	12

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	45	LYS
1	A	51	LEU
1	A	52	ILE
1	A	61	MET
1	A	64	LEU
1	A	73	LEU
1	A	74	ARG
1	A	119	LEU
1	A	163	VAL
1	A	177	LEU
1	A	180	ILE
1	A	202	ASN
1	A	228	VAL
1	A	242	VAL
1	B	43	LEU
1	B	45	LYS
1	B	46	ILE
1	B	52	ILE
1	B	53	ILE
1	B	56	LEU
1	B	64	LEU
1	B	66	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	73	LEU
1	B	99	MET
1	B	113	LYS
1	B	117	ARG
1	B	146	ASN
1	B	147	ASP
1	B	148	ARG
1	B	153	LYS
1	B	155	LYS
1	B	168	ASN
1	B	170	ASN
1	B	202	ASN
1	B	205	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	78	ASN
1	A	87	ASN
1	A	106	ASN
1	A	166	GLN
1	A	170	ASN
1	A	179	ASN
1	A	186	GLN
1	A	202	ASN
1	A	210	HIS
1	A	215	GLN
1	A	230	ASN
1	A	232	ASN
1	A	233	ASN
1	A	245	ASN
1	A	252	GLN
1	A	262	GLN
1	A	266	GLN
1	A	268	ASN
1	B	78	ASN
1	B	87	ASN
1	B	106	ASN
1	B	136	GLN
1	B	146	ASN
1	B	168	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	202	ASN
1	B	215	GLN
1	B	224	ASN
1	B	251	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z > 2$
2	LHI	A	301	3	42,44,129	4.61	17 (40%)	61,65,170	2.58	29 (47%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LHI	A	301	3	-	14/36/77/191	0/2/2/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	LHI	OC3-C97	12.84	1.52	1.23
2	A	301	LHI	C15-N2	12.00	1.50	1.33
2	A	301	LHI	OA4-C15	10.59	1.43	1.23
2	A	301	LHI	OC4-C99	10.38	1.46	1.23
2	A	301	LHI	C97-N6	7.03	1.57	1.34
2	A	301	LHI	C20-N7	6.99	1.56	1.45
2	A	301	LHI	C10-N6	6.53	1.56	1.45
2	A	301	LHI	C99-N7	5.67	1.52	1.34
2	A	301	LHI	C98-C97	5.64	1.62	1.50
2	A	301	LHI	C9-C10	5.33	1.61	1.53
2	A	301	LHI	OB3-C14	4.81	1.54	1.44
2	A	301	LHI	C19-C20	4.78	1.60	1.53
2	A	301	LHI	C11-C10	4.49	1.60	1.53
2	A	301	LHI	C14-C15	3.81	1.63	1.52
2	A	301	LHI	CA1-C99	3.51	1.57	1.50
2	A	301	LHI	C39-C14	3.05	1.61	1.51
2	A	301	LHI	C16-C20	2.63	1.58	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	LHI	OA5-C18-C17	6.64	121.67	109.70
2	A	301	LHI	OA4-C15-N2	-5.36	114.19	123.13
2	A	301	LHI	C16-C17-C18	5.25	119.75	110.23
2	A	301	LHI	C9-C10-N6	5.21	119.22	110.91
2	A	301	LHI	C16-C20-N7	4.96	119.76	110.62
2	A	301	LHI	C19-C20-N7	4.66	118.73	110.92
2	A	301	LHI	C11-OA2-C12	-4.54	104.86	113.72
2	A	301	LHI	C11-C10-N6	4.29	118.12	110.92
2	A	301	LHI	OB3-C14-C39	3.64	117.67	107.54
2	A	301	LHI	OA3-C11-C10	3.62	114.95	108.40
2	A	301	LHI	C19-OA5-C18	3.47	120.49	113.72
2	A	301	LHI	OB3-C9-C8	3.32	115.86	107.42
2	A	301	LHI	OA2-C11-OA3	-3.19	107.20	111.36
2	A	301	LHI	C9-C8-C12	3.12	116.97	110.58
2	A	301	LHI	OA7-C16-C20	2.99	115.54	109.58
2	A	301	LHI	OC4-C99-CA1	-2.98	116.74	122.05
2	A	301	LHI	C17-C16-C20	2.84	114.54	110.40
2	A	301	LHI	OC3-C97-C98	-2.76	117.14	122.05
2	A	301	LHI	OA5-C18-C21	2.73	113.22	106.44
2	A	301	LHI	C10-N6-C97	-2.70	116.78	123.11
2	A	301	LHI	OC3-C97-N6	-2.63	117.33	121.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	LHI	C8-C9-C10	2.50	115.21	110.55
2	A	301	LHI	CA1-C99-N7	2.31	119.96	116.12
2	A	301	LHI	OB2-C8-C9	2.29	113.23	107.42
2	A	301	LHI	OA5-C19-C20	2.27	114.89	110.59
2	A	301	LHI	C19-OB2-C8	-2.22	112.72	117.98
2	A	301	LHI	OA2-C12-C8	2.16	114.18	109.72
2	A	301	LHI	C39-C14-C15	2.13	116.41	111.11
2	A	301	LHI	OC2-PC6-OB6	2.12	111.73	104.64

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	LHI	OA4-C15-N2-C22
2	A	301	LHI	OA2-C11-OA3-PC5
2	A	301	LHI	C39-C14-OB3-C9
2	A	301	LHI	PC5-OB6-PC6-OC2
2	A	301	LHI	C17-C18-C21-OA8
2	A	301	LHI	OA5-C18-C21-OA8
2	A	301	LHI	C8-C12-C13-OA9
2	A	301	LHI	OC3-C97-N6-C10
2	A	301	LHI	OB3-C14-C15-OA4
2	A	301	LHI	C16-C20-N7-C99
2	A	301	LHI	PC5-OB6-PC6-OB5
2	A	301	LHI	OA2-C12-C13-OA9
2	A	301	LHI	OA5-C19-OB2-C8
2	A	301	LHI	C11-OA3-PC5-O23

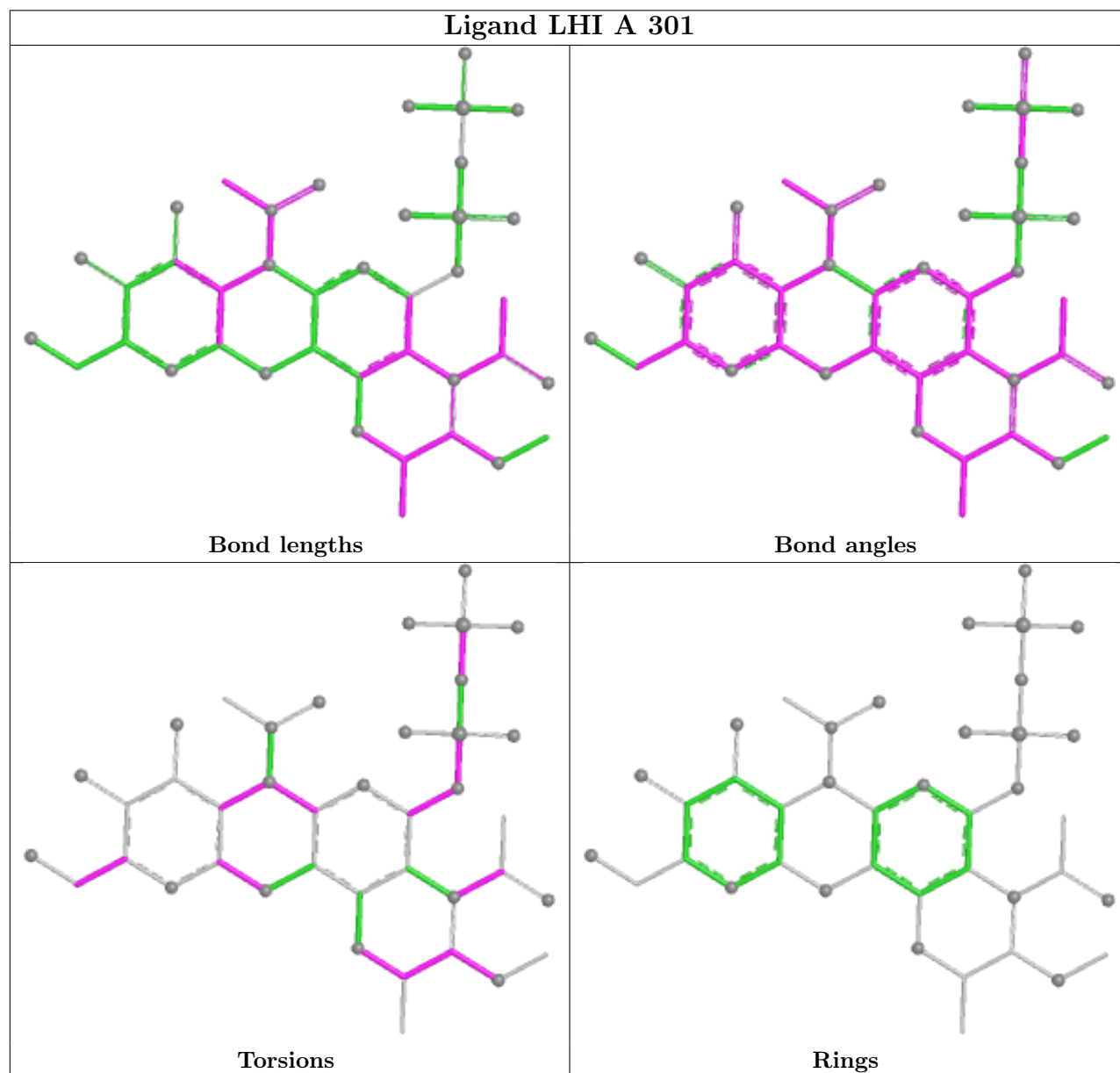
There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	LHI	9	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	222/263 (84%)	0.55	14 (6%) 26 28	40, 60, 153, 206	0
1	B	218/263 (82%)	0.81	21 (9%) 13 15	49, 91, 170, 209	0
All	All	440/526 (83%)	0.68	35 (7%) 18 20	40, 74, 161, 209	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	118	ALA	6.3
1	A	42	ILE	4.4
1	B	44	LEU	4.0
1	B	163	VAL	3.8
1	B	114	GLY	3.6
1	B	119	LEU	3.6
1	B	61	MET	3.5
1	B	46	ILE	3.5
1	A	55	ALA	3.4
1	A	66	THR	3.0
1	A	59	GLY	3.0
1	A	149	SER	2.9
1	B	42	ILE	2.9
1	B	43	LEU	2.9
1	A	46	ILE	2.8
1	B	149	SER	2.7
1	B	47	LEU	2.7
1	A	130	GLY	2.7
1	B	158	PHE	2.6
1	B	50	ILE	2.6
1	B	145	ASP	2.5
1	B	144	TYR	2.5
1	A	43	LEU	2.4
1	B	132	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	225	ALA	2.3
1	A	113	LYS	2.3
1	A	268	ASN	2.3
1	A	122	THR	2.3
1	A	120	PHE	2.2
1	B	48	LEU	2.2
1	B	63	PHE	2.2
1	A	53	ILE	2.1
1	B	110	PHE	2.1
1	B	51	LEU	2.1
1	B	228	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

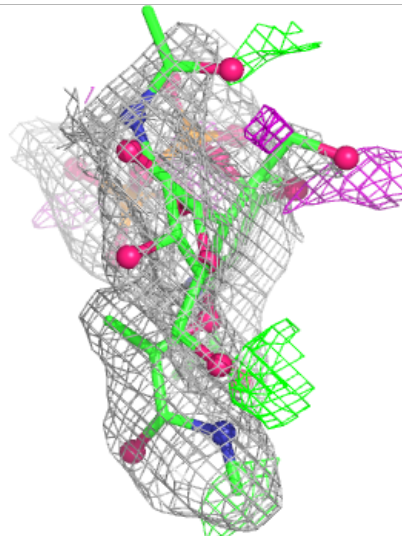
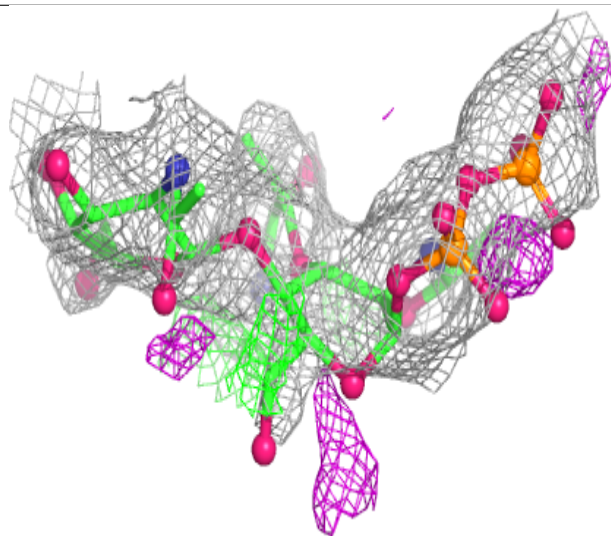
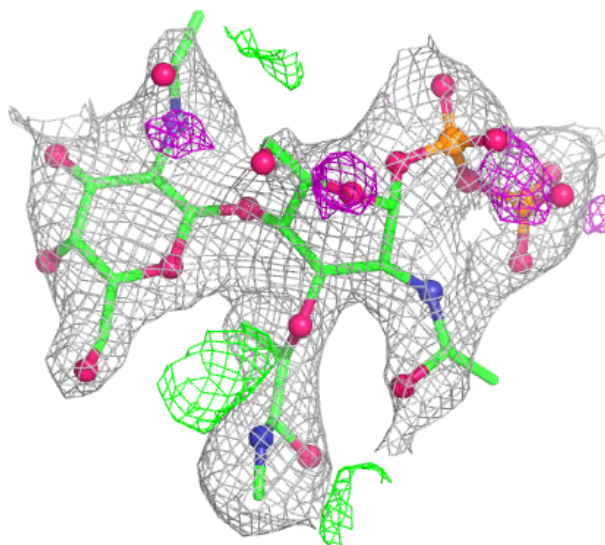
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	A	302	1/1	0.83	0.25	90,90,90,90	0
2	LHI	A	301	43/126	0.88	0.12	59,98,136,226	0
3	MG	A	303	1/1	0.89	0.14	88,88,88,88	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 LHI A 301:

$2mF_o-DF_c$ (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.