



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:59 PM UTC

PDB ID : 3C4V / pdb_00003c4v
Title : Structure of the retaining glycosyltransferase MshA: The first step in mycothiol biosynthesis. Organism: Corynebacterium glutamicum : Complex with UDP and 1L-INS-1-P.
Authors : Vetting, M.W.; Frantom, P.A.; Blanchard, J.S.
Deposited on : 2008-01-30
Resolution : 2.60 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

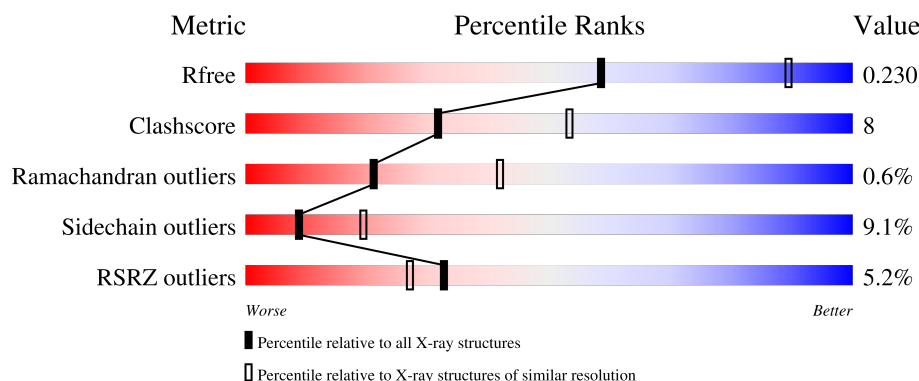
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	426	4% 74% 12% 5% 8%
1	B	426	5% 77% 11% • 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	LIP	B	601	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6189 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 Predicted glycosyltransferases.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			3026	1896	540	578	12			
1	B	393	Total	C	N	O	S	0	0	0
			3025	1895	540	578	12			

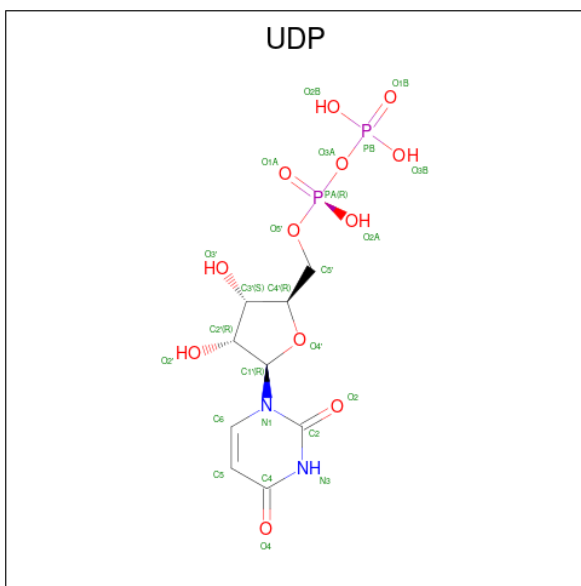
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	LEU	-	expression tag	UNP Q8NTA6
A	420	GLU	-	expression tag	UNP Q8NTA6
A	421	HIS	-	expression tag	UNP Q8NTA6
A	422	HIS	-	expression tag	UNP Q8NTA6
A	423	HIS	-	expression tag	UNP Q8NTA6
A	424	HIS	-	expression tag	UNP Q8NTA6
A	425	HIS	-	expression tag	UNP Q8NTA6
A	426	HIS	-	expression tag	UNP Q8NTA6
B	419	LEU	-	expression tag	UNP Q8NTA6
B	420	GLU	-	expression tag	UNP Q8NTA6
B	421	HIS	-	expression tag	UNP Q8NTA6
B	422	HIS	-	expression tag	UNP Q8NTA6
B	423	HIS	-	expression tag	UNP Q8NTA6
B	424	HIS	-	expression tag	UNP Q8NTA6
B	425	HIS	-	expression tag	UNP Q8NTA6
B	426	HIS	-	expression tag	UNP Q8NTA6

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

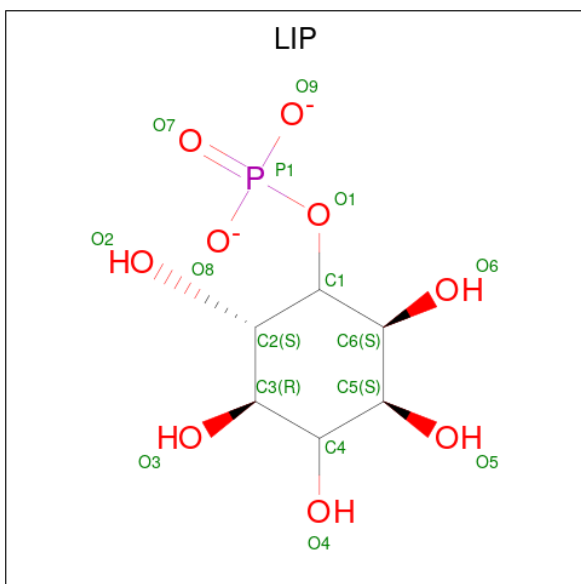
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 4 is L-MYO-INOSITOL-1-PHOSPHATE (CCD ID: LIP) (formula: $C_6H_{11}O_9P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	P	0	0
			16	6	9	1		

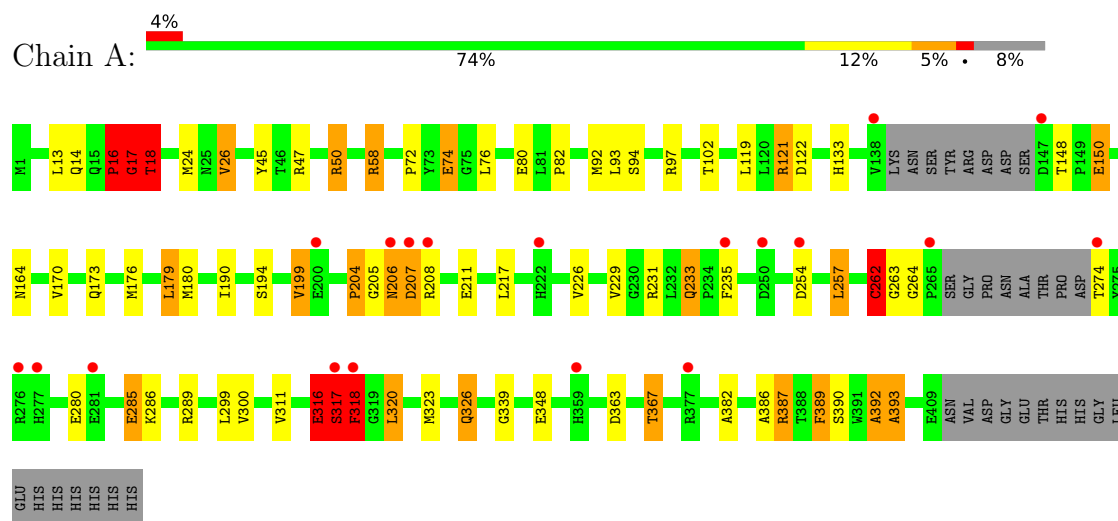
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	38	Total 38	O 38	0	0
5	B	32	Total 32	O 32	0	0

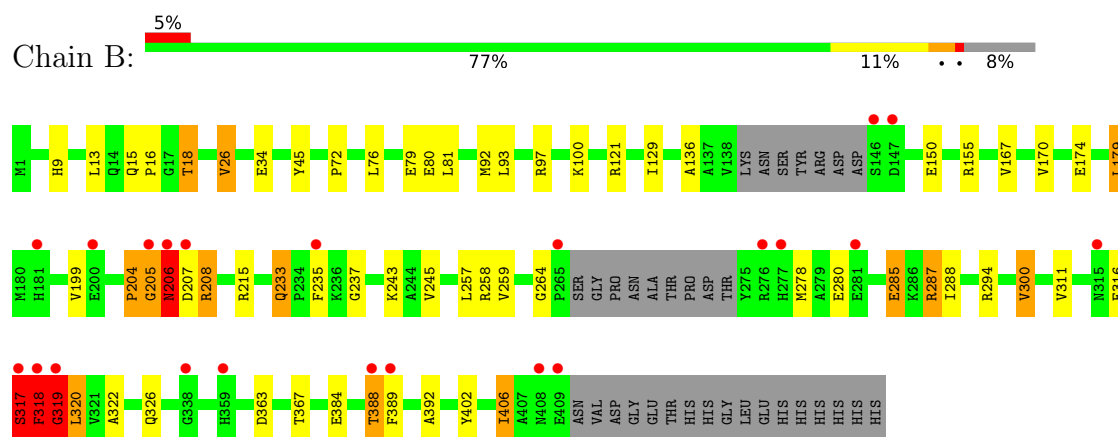
3 Residue-property plots [i](#)

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: Predicted glycosyltransferases



• Molecule 1: Predicted glycosyltransferases



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	223.94Å 223.94Å 125.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.18 – 2.60 79.18 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.4 (79.18-2.60) 99.4 (79.18-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.190 , 0.213 0.211 , 0.230	Depositor DCC
R_{free} test set	2463 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 26.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6189	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: LIP, MG, UDP

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	0.78	3/3086 (0.1%)	1.07	15/4199 (0.4%)
1	B	0.95	7/3085 (0.2%)	1.02	12/4197 (0.3%)
All	All	0.87	10/6171 (0.2%)	1.04	27/8396 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	4
All	All	0	12

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	319	GLY	N-CA	30.04	1.89	1.45
1	A	317	SER	CB-OG	13.19	1.68	1.42
1	B	318	PHE	N-CA	12.88	1.62	1.46
1	B	318	PHE	C-N	11.01	1.49	1.33
1	B	319	GLY	C-O	8.64	1.35	1.23
1	A	17	GLY	CA-C	6.45	1.60	1.51
1	B	205	GLY	N-CA	6.15	1.54	1.45
1	A	263	GLY	N-CA	5.94	1.53	1.45
1	B	318	PHE	CA-C	5.91	1.60	1.52
1	B	319	GLY	CA-C	5.83	1.60	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	320	LEU	N-CA-C	-17.82	91.33	114.31
1	A	318	PHE	N-CA-C	15.55	129.99	111.02
1	A	18	THR	N-CA-C	12.46	128.66	110.59
1	B	319	GLY	N-CA-C	-11.19	86.66	113.18
1	A	17	GLY	N-CA-C	-9.82	89.91	113.18
1	B	318	PHE	N-CA-CB	8.55	124.94	110.49
1	B	205	GLY	N-CA-C	-8.06	94.08	113.18
1	B	318	PHE	CA-C-N	-7.83	106.06	121.41
1	B	318	PHE	C-N-CA	-7.83	106.06	121.41
1	A	317	SER	CA-C-N	7.27	130.89	120.79
1	A	317	SER	C-N-CA	7.27	130.89	120.79
1	A	18	THR	CB-CA-C	-7.12	97.05	110.51
1	B	300	VAL	CB-CA-C	-7.12	102.71	112.04
1	B	318	PHE	CA-CB-CG	-6.91	106.89	113.80
1	A	392	ALA	N-CA-C	6.91	120.19	111.69
1	A	317	SER	CA-CB-OG	-6.57	97.96	111.10
1	A	389	PHE	CB-CA-C	-6.45	97.91	109.71
1	A	74	GLU	N-CA-C	6.10	118.06	108.96
1	B	319	GLY	O-C-N	-5.92	115.01	122.70
1	B	204	PRO	N-CA-C	5.83	124.49	112.47
1	A	50	ARG	CA-C-N	5.68	125.53	119.28
1	A	50	ARG	C-N-CA	5.68	125.53	119.28
1	A	262	CYS	N-CA-C	5.56	117.29	107.61
1	B	237	GLY	N-CA-C	5.29	123.14	112.34
1	A	393	ALA	N-CA-C	5.14	121.74	110.80
1	B	318	PHE	N-CA-C	-5.13	99.87	110.80
1	A	16	PRO	CB-CA-C	5.03	118.25	111.71

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	PRO	Peptide
1	A	17	GLY	Peptide
1	A	204	PRO	Peptide
1	A	262	CYS	Peptide
1	A	316	GLU	Peptide
1	A	317	SER	Peptide
1	A	389	PHE	Peptide
1	A	392	ALA	Peptide
1	B	204	PRO	Peptide
1	B	317	SER	Peptide
1	B	318	PHE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	319	GLY	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3026	0	2989	56	0
1	B	3025	0	2987	43	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	25	0	11	1	0
3	B	25	0	11	1	0
4	B	16	0	11	0	0
5	A	38	0	0	0	0
5	B	32	0	0	0	0
All	All	6189	0	6009	98	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (98) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:SER:OG	1:A:317:SER:CB	1.68	1.38
1:B:319:GLY:N	1:B:319:GLY:CA	1.88	1.35
1:A:316:GLU:HG3	1:A:317:SER:HB2	1.26	1.18
1:A:18:THR:CG2	1:A:264:GLY:HA3	2.01	0.91
1:A:18:THR:HG23	1:A:264:GLY:HA3	1.52	0.90
1:B:280:GLU:HB3	1:B:285:GLU:HG2	1.59	0.85
1:A:316:GLU:HG3	1:A:317:SER:CB	2.09	0.81
1:B:319:GLY:N	1:B:319:GLY:C	2.40	0.79
1:A:326:GLN:HG3	1:A:382:ALA:HB1	1.66	0.77
1:B:280:GLU:HA	1:B:285:GLU:CG	2.15	0.75
1:B:34:GLU:HG2	1:B:392:ALA:HA	1.69	0.74
1:A:316:GLU:CG	1:A:317:SER:HB2	2.13	0.73
1:B:318:PHE:CD2	1:B:319:GLY:N	2.57	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:PHE:CG	1:B:319:GLY:N	2.57	0.72
1:B:280:GLU:CB	1:B:285:GLU:HG2	2.18	0.72
1:A:318:PHE:H	1:A:318:PHE:HD1	1.37	0.71
1:B:280:GLU:HA	1:B:285:GLU:HG2	1.73	0.69
1:A:280:GLU:HA	1:A:285:GLU:HG3	1.74	0.68
1:A:17:GLY:HA2	1:A:231:ARG:HG3	1.74	0.68
1:A:26:VAL:HG22	1:A:320:LEU:HD21	1.75	0.68
1:B:316:GLU:HG3	1:B:318:PHE:H	1.59	0.67
1:A:17:GLY:HA2	1:A:231:ARG:CG	2.25	0.66
1:A:176:MET:HG2	1:A:180:MET:HE2	1.76	0.66
1:A:233:GLN:HG2	1:A:235:PHE:CE1	2.32	0.63
1:A:363:ASP:O	1:A:367:THR:HG23	1.98	0.63
1:A:317:SER:OG	1:A:317:SER:CA	2.47	0.63
1:A:205:GLY:O	1:A:206:ASN:CB	2.46	0.63
1:A:205:GLY:O	1:A:206:ASN:HB3	1.97	0.63
1:B:280:GLU:HA	1:B:285:GLU:HG3	1.79	0.62
1:A:121:ARG:NH2	1:A:164:ASN:O	2.33	0.62
1:B:318:PHE:C	1:B:319:GLY:CA	2.71	0.62
1:B:280:GLU:CA	1:B:285:GLU:HG2	2.29	0.62
1:A:280:GLU:HB3	1:A:285:GLU:HG2	1.83	0.60
1:A:18:THR:HG22	1:A:264:GLY:HA3	1.81	0.60
1:A:390:SER:HB3	1:A:393:ALA:HB3	1.84	0.60
1:A:280:GLU:CB	1:A:285:GLU:HG2	2.32	0.59
1:B:322:ALA:O	1:B:326:GLN:HG2	2.03	0.59
1:B:316:GLU:O	1:B:317:SER:C	2.46	0.59
1:A:199:VAL:HG11	1:A:387:ARG:HG3	1.84	0.58
1:B:205:GLY:O	1:B:206:ASN:HB3	2.03	0.57
1:B:205:GLY:O	1:B:206:ASN:CB	2.52	0.57
1:A:318:PHE:HB2	1:A:323:MET:HE3	1.86	0.56
1:B:72:PRO:HD2	1:B:76:LEU:HD22	1.88	0.56
1:A:317:SER:CB	1:A:317:SER:HG	2.12	0.56
1:A:280:GLU:HA	1:A:285:GLU:CG	2.37	0.53
1:B:318:PHE:HD2	1:B:320:LEU:HD23	1.74	0.52
1:A:74:GLU:OE1	1:B:294:ARG:NH1	2.37	0.52
1:B:402:TYR:O	1:B:406:ILE:HG12	2.09	0.52
1:B:388:THR:HG22	1:B:389:PHE:CD1	2.44	0.52
1:A:47:ARG:NH2	1:A:72:PRO:O	2.43	0.52
1:A:217:LEU:O	1:A:289:ARG:NH1	2.33	0.52
1:A:16:PRO:HB2	3:A:600:UDP:H1'	1.93	0.51
1:A:318:PHE:HB2	1:A:323:MET:CE	2.41	0.50
1:A:318:PHE:CD1	1:A:318:PHE:N	2.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PRO:HD2	1:A:76:LEU:HD22	1.93	0.50
1:B:18:THR:CG2	1:B:264:GLY:HA3	2.42	0.50
1:A:58:ARG:CG	1:A:58:ARG:HH11	2.26	0.49
1:B:207:ASP:OD2	1:B:208:ARG:HG2	2.13	0.49
1:A:317:SER:H	1:A:339:GLY:H	1.60	0.49
1:A:176:MET:HG3	1:A:190:ILE:HG21	1.95	0.48
1:A:316:GLU:HA	1:A:317:SER:OG	2.13	0.48
1:A:326:GLN:HB3	1:A:386:ALA:HB2	1.94	0.48
1:A:204:PRO:HB2	1:A:205:GLY:HA2	1.95	0.48
1:B:258:ARG:CZ	1:B:287:ARG:HH21	2.27	0.48
1:B:233:GLN:HB2	1:B:235:PHE:CE1	2.50	0.47
1:B:45:TYR:CG	1:B:92:MET:HE3	2.49	0.47
1:A:14:GLN:HE22	1:A:50:ARG:HE	1.62	0.47
1:A:24:MET:HG3	1:A:133:HIS:CG	2.50	0.47
1:A:318:PHE:HA	1:A:339:GLY:HA3	1.96	0.47
1:B:316:GLU:HG3	1:B:318:PHE:N	2.29	0.47
1:A:119:LEU:HD23	1:A:119:LEU:C	2.41	0.46
1:A:17:GLY:HA2	1:A:231:ARG:HG2	1.98	0.45
1:B:243:LYS:HG3	1:B:278:MET:CE	2.47	0.45
1:A:121:ARG:NH1	1:A:122:ASP:OD1	2.48	0.45
1:B:15:GLN:NE2	1:B:16:PRO:HD2	2.32	0.45
1:A:226:VAL:HG23	1:A:257:LEU:HD21	1.98	0.44
1:A:207:ASP:OD2	1:A:207:ASP:N	2.50	0.44
1:B:34:GLU:CG	1:B:392:ALA:HA	2.44	0.44
1:A:148:THR:OG1	1:A:150:GLU:HG2	2.17	0.43
1:A:317:SER:OG	1:A:317:SER:HA	2.19	0.43
1:A:45:TYR:CG	1:A:92:MET:HE3	2.52	0.43
1:B:206:ASN:ND2	1:B:207:ASP:H	2.17	0.43
1:A:58:ARG:NH1	1:A:58:ARG:HG2	2.33	0.43
1:B:129:ILE:HD12	1:B:167:VAL:HB	2.02	0.42
1:B:136:ALA:HB3	1:B:155:ARG:HB3	2.00	0.42
1:B:245:VAL:HG21	1:B:259:VAL:HG21	2.00	0.42
1:B:285:GLU:HG3	1:B:285:GLU:H	1.52	0.42
1:A:229:VAL:HA	1:A:262:CYS:O	2.19	0.42
1:B:170:VAL:HG11	1:B:179:LEU:HD22	2.01	0.42
1:A:80:GLU:C	1:A:82:PRO:HD2	2.45	0.41
1:B:206:ASN:ND2	1:B:207:ASP:N	2.68	0.41
1:A:170:VAL:HG11	1:A:179:LEU:HD22	2.03	0.41
1:A:170:VAL:CG1	1:A:179:LEU:HD22	2.50	0.41
1:B:363:ASP:O	1:B:367:THR:HG23	2.20	0.41
1:B:26:VAL:HG11	3:B:600:UDP:O3'	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:VAL:HB	1:B:288:ILE:HG12	2.03	0.41
1:B:9:HIS:HB2	1:B:81:LEU:HD12	2.03	0.40
1:B:243:LYS:HG3	1:B:278:MET:HE1	2.03	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	387/426 (91%)	369 (95%)	16 (4%)	2 (0%)	24	46
1	B	387/426 (91%)	373 (96%)	11 (3%)	3 (1%)	16	34
All	All	774/852 (91%)	742 (96%)	27 (4%)	5 (1%)	21	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ASN
1	B	206	ASN
1	B	317	SER
1	A	316	GLU
1	B	318	PHE

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	319/348 (92%)	287 (90%)	32 (10%)	7	16
1	B	319/348 (92%)	293 (92%)	26 (8%)	10	24
All	All	638/696 (92%)	580 (91%)	58 (9%)	9	19

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	18	THR
1	A	26	VAL
1	A	58	ARG
1	A	93	LEU
1	A	94	SER
1	A	97	ARG
1	A	102	THR
1	A	121	ARG
1	A	150	GLU
1	A	173	GLN
1	A	179	LEU
1	A	194	SER
1	A	199	VAL
1	A	207	ASP
1	A	208	ARG
1	A	211	GLU
1	A	233	GLN
1	A	254	ASP
1	A	257	LEU
1	A	274	THR
1	A	285	GLU
1	A	286	LYS
1	A	299	LEU
1	A	300	VAL
1	A	311	VAL
1	A	318	PHE
1	A	320	LEU
1	A	326	GLN
1	A	348	GLU
1	A	367	THR
1	A	387	ARG
1	B	13	LEU
1	B	18	THR
1	B	26	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	79	GLU
1	B	80	GLU
1	B	93	LEU
1	B	97	ARG
1	B	100	LYS
1	B	121	ARG
1	B	150	GLU
1	B	174	GLU
1	B	179	LEU
1	B	199	VAL
1	B	206	ASN
1	B	208	ARG
1	B	215	ARG
1	B	233	GLN
1	B	257	LEU
1	B	285	GLU
1	B	287	ARG
1	B	300	VAL
1	B	311	VAL
1	B	317	SER
1	B	384	GLU
1	B	388	THR
1	B	406	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	15	GLN
1	A	84	GLN
1	A	177	GLN
1	A	256	ASN
1	A	326	GLN
1	A	385	HIS
1	A	397	GLN
1	B	15	GLN
1	B	62	ASN
1	B	84	GLN
1	B	173	GLN
1	B	177	GLN
1	B	182	HIS
1	B	326	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	403	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 ⓘ

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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$
4	LIP	B	601	-	16,16,16	1.72	3 (18%)	25,25,25	0.93	0
3	UDP	A	600	-	25,26,26	1.19	2 (8%)	38,40,40	1.58	7 (18%)
3	UDP	B	600	-	25,26,26	1.20	2 (8%)	38,40,40	1.90	8 (21%)

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
4	LIP	B	601	-	2/2/7/7	2/5/29/29	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UDP	A	600	-	-	3/16/32/32	0/2/2/2
3	UDP	B	600	-	-	4/16/32/32	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	LIP	P1-O7	4.39	1.64	1.50
3	B	600	UDP	PA-O3A	3.25	1.63	1.59
3	A	600	UDP	PA-O3A	2.91	1.62	1.59
4	B	601	LIP	P1-O1	2.68	1.64	1.59
4	B	601	LIP	P1-O9	2.65	1.64	1.54
3	B	600	UDP	C5-C4	-2.33	1.38	1.43
3	A	600	UDP	PB-O2B	-2.29	1.46	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	600	UDP	C4-N3-C2	-5.50	119.78	126.61
3	A	600	UDP	C4-N3-C2	-5.17	120.19	126.61
3	B	600	UDP	O2-C2-N1	-4.01	117.58	122.80
3	B	600	UDP	O4-C4-C5	-3.55	119.05	125.16
3	A	600	UDP	C5-C4-N3	3.54	119.75	114.80
3	A	600	UDP	N3-C2-N1	3.42	119.34	114.89
3	B	600	UDP	O3'-C3'-C4'	-3.40	101.33	111.08
3	B	600	UDP	N3-C2-N1	3.29	119.17	114.89
3	B	600	UDP	C5-C4-N3	3.14	119.19	114.80
3	B	600	UDP	O3B-PB-O3A	2.94	114.50	104.64
3	B	600	UDP	C5-C6-N1	-2.83	117.23	121.84
3	A	600	UDP	O2B-PB-O3A	2.73	113.79	104.64
3	A	600	UDP	C5-C6-N1	-2.51	117.77	121.84
3	A	600	UDP	O4-C4-C5	-2.39	121.04	125.16
3	A	600	UDP	O3A-PA-O1A	2.07	116.93	110.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	601	LIP	C3
4	B	601	LIP	C5

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	600	UDP	PA-O3A-PB-O3B
3	A	600	UDP	PA-O3A-PB-O2B
3	B	600	UDP	PB-O3A-PA-O1A
3	B	600	UDP	C5'-O5'-PA-O3A
4	B	601	LIP	C6-C1-O1-P1
4	B	601	LIP	C1-O1-P1-O8
3	B	600	UDP	PA-O3A-PB-O2B
3	B	600	UDP	O4'-C4'-C5'-O5'
3	A	600	UDP	PB-O3A-PA-O2A

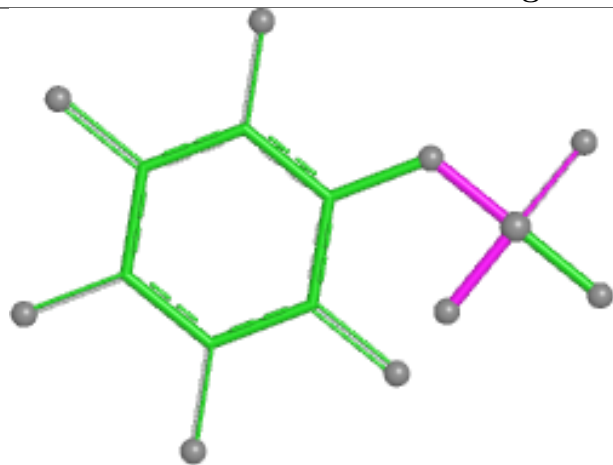
There are no ring outliers.

2 monomers are involved in 2 short contacts:

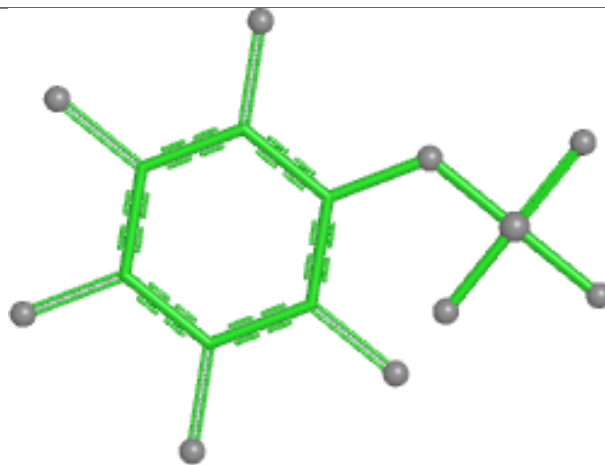
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	UDP	1	0
3	B	600	UDP	1	0

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.

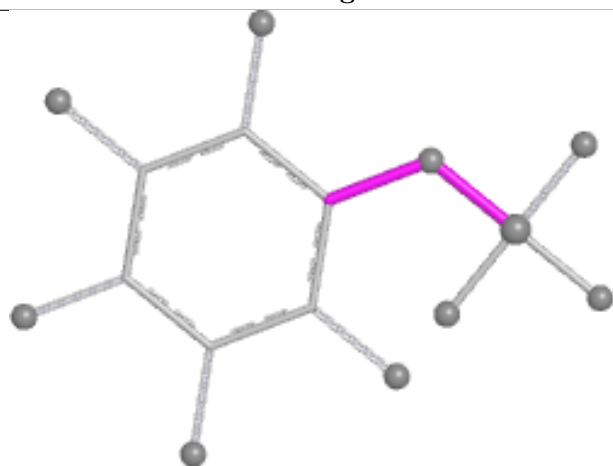
Ligand LIP B 601



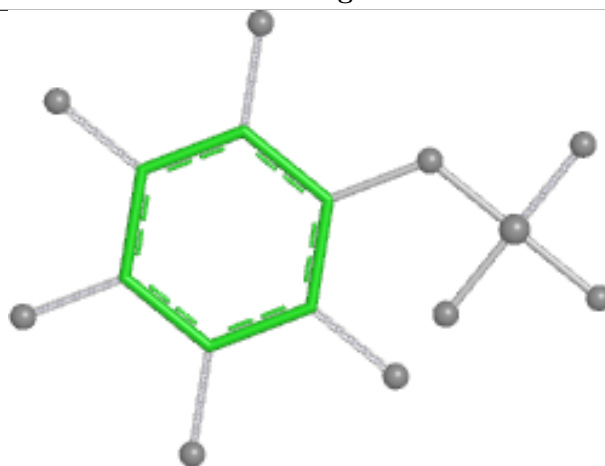
Bond lengths



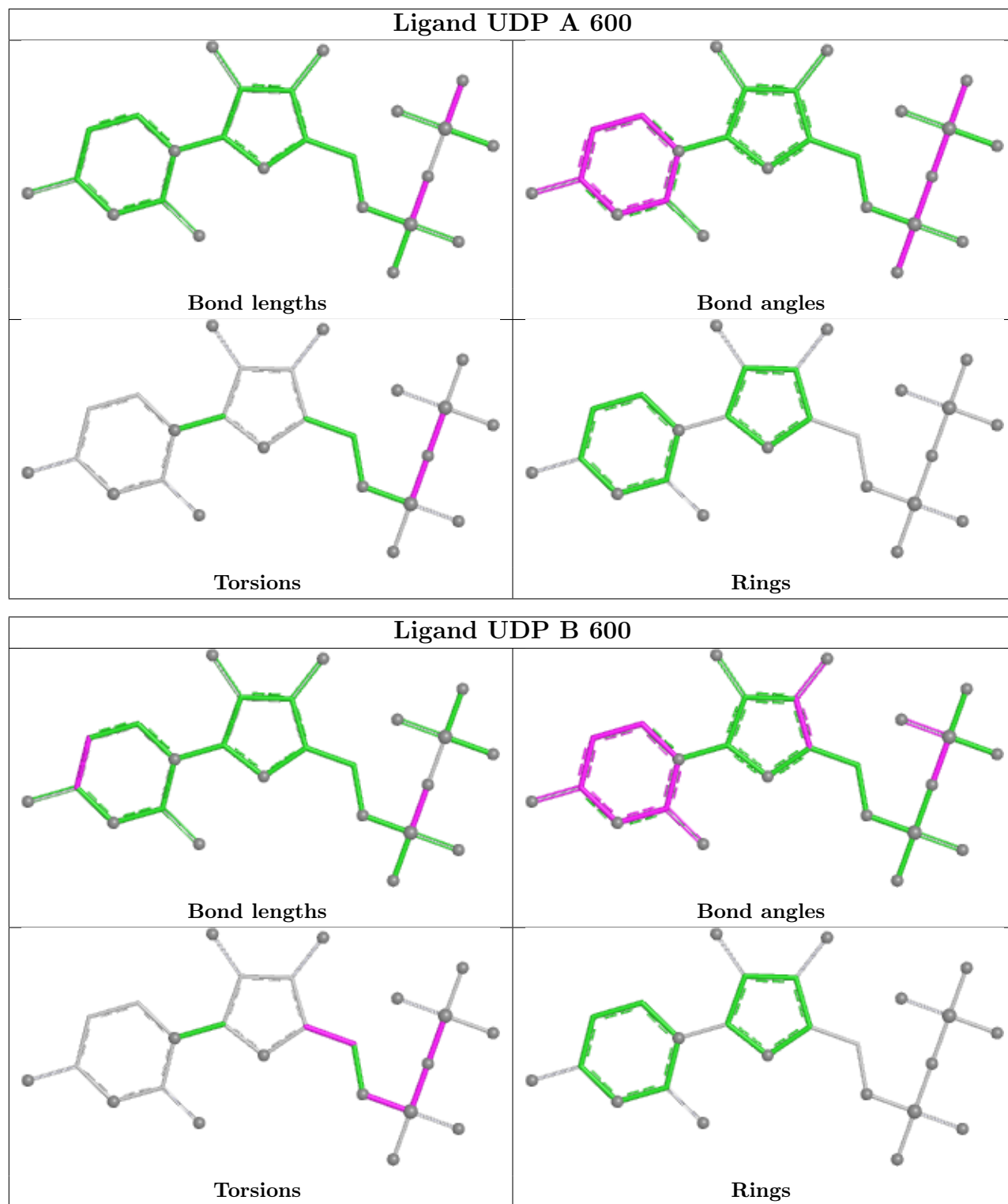
Bond angles



Torsions



Rings



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	393/426 (92%)	0.11	19 (4%) 35 30	25, 42, 56, 64	0
1	B	393/426 (92%)	0.45	22 (5%) 30 24	35, 46, 58, 71	0
All	All	786/852 (92%)	0.28	41 (5%) 33 27	25, 45, 57, 71	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	THR	5.0
1	B	207	ASP	4.9
1	B	319	GLY	4.7
1	A	317	SER	4.4
1	B	146	SER	4.4
1	B	318	PHE	4.3
1	B	317	SER	4.2
1	B	315	ASN	4.1
1	B	359	HIS	4.1
1	B	147	ASP	4.0
1	B	281	GLU	3.9
1	B	277	HIS	3.5
1	A	277	HIS	3.5
1	B	276	ARG	3.4
1	B	206	ASN	3.2
1	A	359	HIS	3.1
1	B	409	GLU	3.1
1	B	265	PRO	3.1
1	A	207	ASP	3.0
1	B	389	PHE	3.0
1	A	147	ASP	2.9
1	A	318	PHE	2.9
1	B	181	HIS	2.7
1	B	408	ASN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	235	PHE	2.6
1	A	206	ASN	2.4
1	A	377	ARG	2.4
1	A	235	PHE	2.4
1	B	200	GLU	2.4
1	A	276	ARG	2.4
1	A	250	ASP	2.3
1	A	222	HIS	2.2
1	A	200	GLU	2.2
1	A	265	PRO	2.1
1	B	205	GLY	2.1
1	A	138	VAL	2.1
1	B	338	GLY	2.1
1	A	254	ASP	2.1
1	A	281	GLU	2.0
1	B	388	THR	2.0
1	A	208	ARG	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 ⓘ

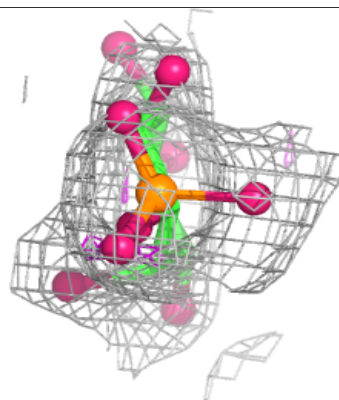
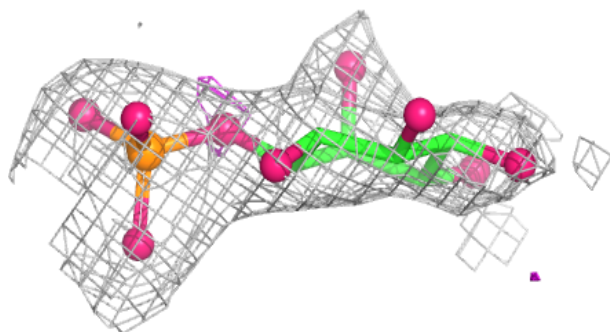
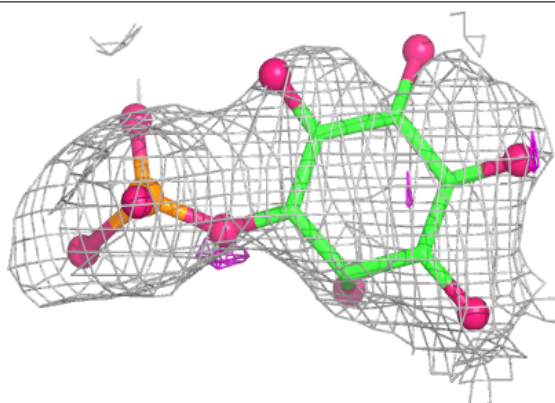
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	LIP	B	601	16/16	0.82	0.20	80,84,85,85	0
2	MG	B	602	1/1	0.87	0.13	46,46,46,46	0
3	UDP	A	600	25/25	0.92	0.10	29,34,55,57	0
3	UDP	B	600	25/25	0.93	0.08	24,33,48,50	0
2	MG	A	602	1/1	0.95	0.09	41,41,41,41	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.

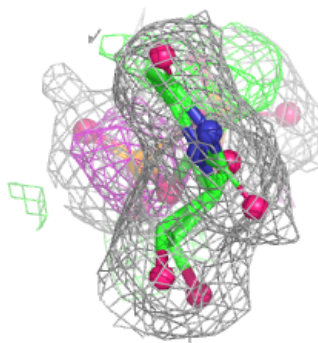
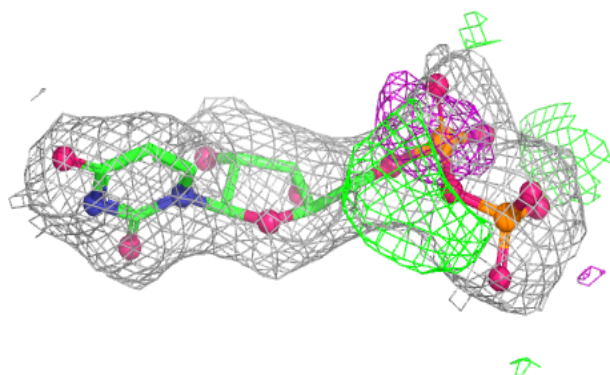
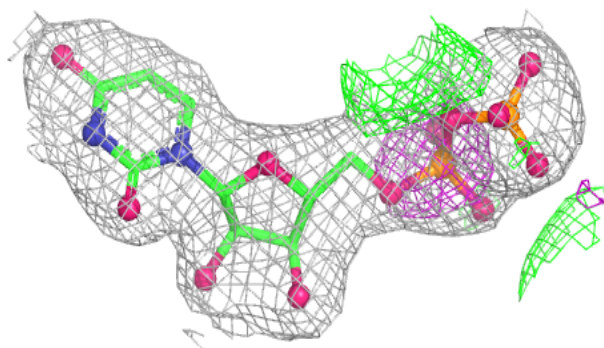
Electron density around LIP B 601:

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

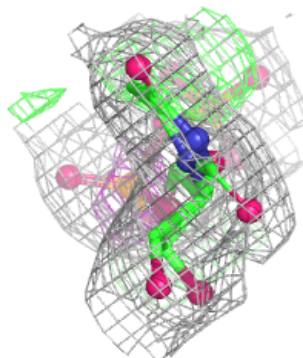
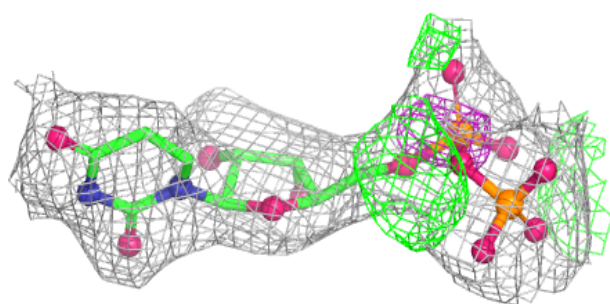
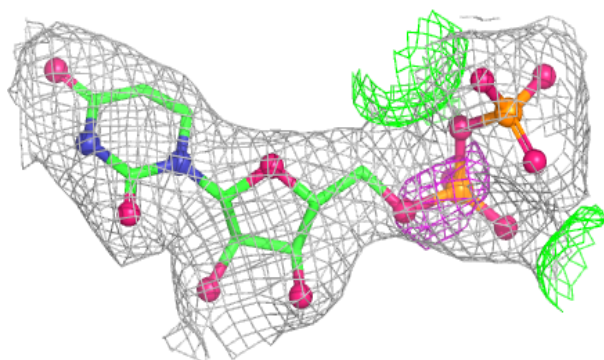


Electron density around UDP A 600:

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

**Electron density around UDP B 600:**

$2mF_o-DF_c$ (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.