Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 04:04 PM EST

PDB ID	:	3Q3H
Title	:	Crystal structure of the Actinobacillus pleuropneumoniae HMW1C glycosyl-transferase in complex with UDP-GLC
Authors	:	Kawai, F.; Yeo, H.J.
Deposited on	:	2010-12-21
Resolution	:	2.25 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36
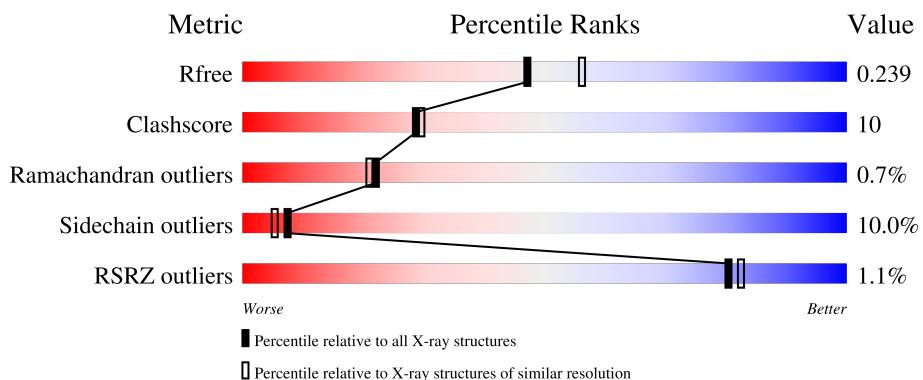
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*
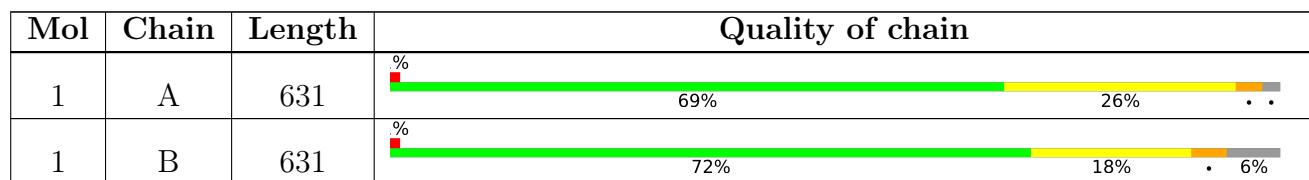
The reported resolution of this entry is 2.25 Å.

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	Percentile Ranks	Value
Rfree		0.239
Clashscore		10
Ramachandran outliers		0.7%
Sidechain outliers		10.0%
RSRZ outliers		1.1%

Worse *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	631	69% 26% · ·
1	B	631	72% 18% · 6%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 10078 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.
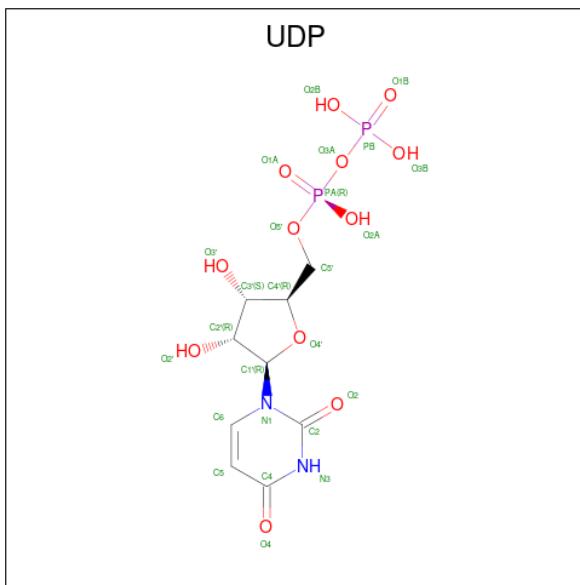
- Molecule 1 is a protein called HMW1C-like glycosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	620	Total	C	N	O	S	0	0	0
			4967	3170	852	920	25			
1	B	595	Total	C	N	O	S	0	0	0
			4769	3052	815	878	24			

There are 24 discrepancies between the modelled and reference sequences:
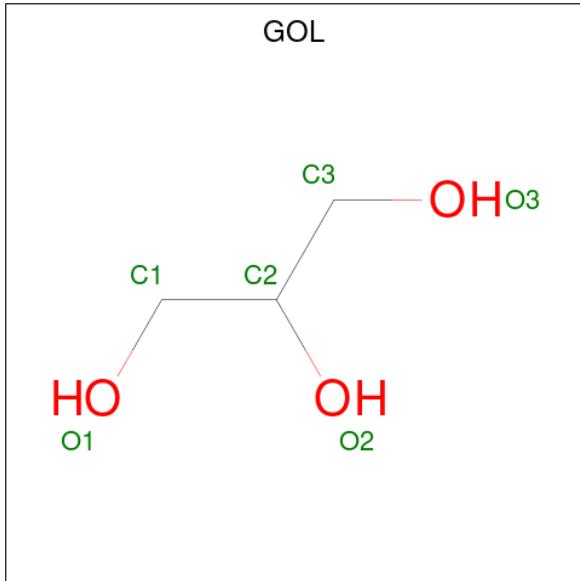
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP E0EAD4
A	-9	ALA	-	expression tag	UNP E0EAD4
A	-8	HIS	-	expression tag	UNP E0EAD4
A	-7	HIS	-	expression tag	UNP E0EAD4
A	-6	HIS	-	expression tag	UNP E0EAD4
A	-5	HIS	-	expression tag	UNP E0EAD4
A	-4	HIS	-	expression tag	UNP E0EAD4
A	-3	HIS	-	expression tag	UNP E0EAD4
A	-2	VAL	-	expression tag	UNP E0EAD4
A	-1	GLY	-	expression tag	UNP E0EAD4
A	0	THR	-	expression tag	UNP E0EAD4
A	428	PRO	SER	SEE REMARK 999	UNP E0EAD4
B	-10	MET	-	expression tag	UNP E0EAD4
B	-9	ALA	-	expression tag	UNP E0EAD4
B	-8	HIS	-	expression tag	UNP E0EAD4
B	-7	HIS	-	expression tag	UNP E0EAD4
B	-6	HIS	-	expression tag	UNP E0EAD4
B	-5	HIS	-	expression tag	UNP E0EAD4
B	-4	HIS	-	expression tag	UNP E0EAD4
B	-3	HIS	-	expression tag	UNP E0EAD4
B	-2	VAL	-	expression tag	UNP E0EAD4
B	-1	GLY	-	expression tag	UNP E0EAD4
B	0	THR	-	expression tag	UNP E0EAD4
B	428	PRO	SER	SEE REMARK 999	UNP E0EAD4

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 6	C 3	O 3	0	0
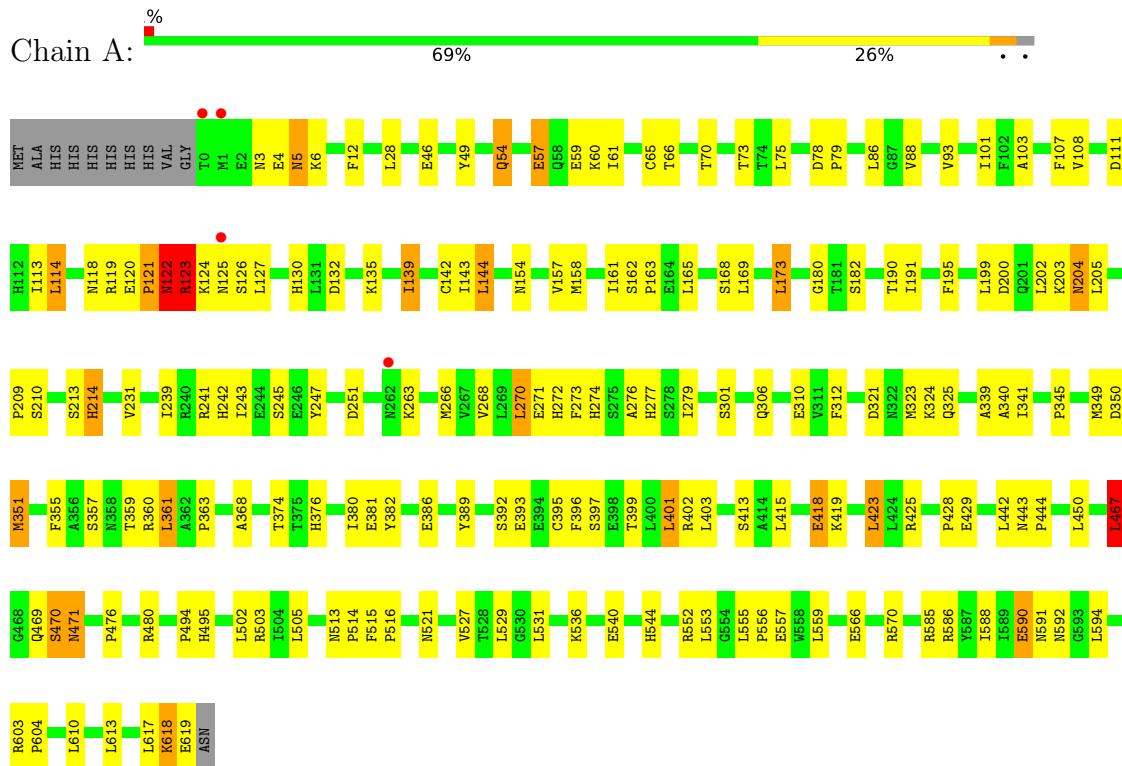
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	116	Total 116	O 116	0	0
4	B	164	Total 164	O 164	0	0
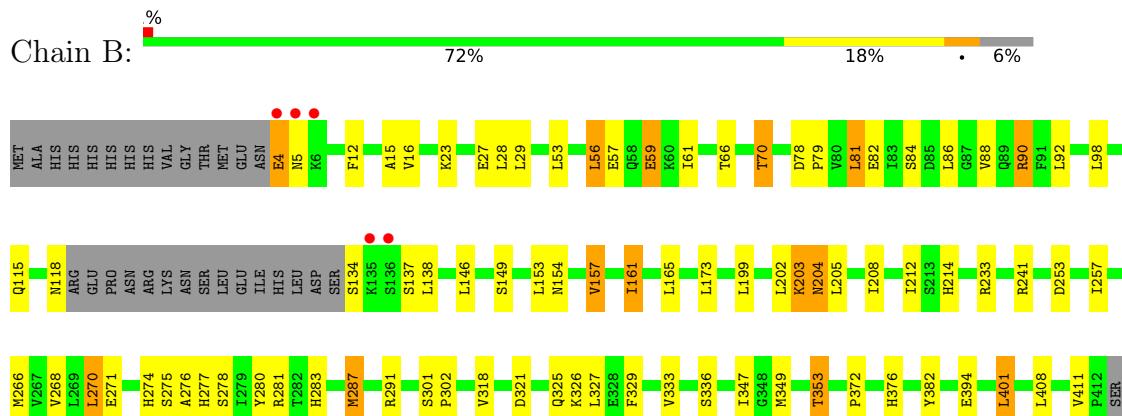
3 Residue-property plots ⓘ
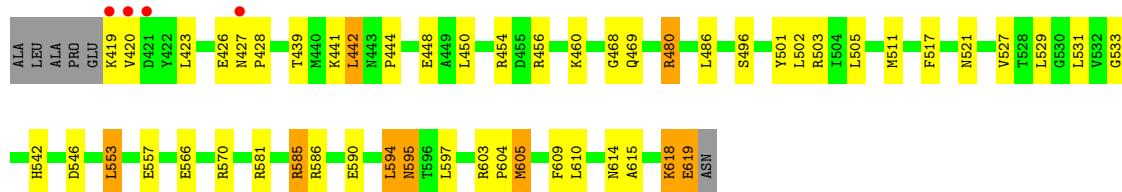
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: HMW1C-like glycosyltransferase

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4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.25Å 94.90Å 176.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.81 – 2.25 41.81 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.81-2.25) 93.3 (41.81-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.16 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.186 , 0.244 0.183 , 0.239	Depositor DCC
R_{free} test set	3065 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 37.2	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.47, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10078	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.91	4/5088 (0.1%)	0.88	6/6908 (0.1%)
1	B	0.93	0/4885	0.88	5/6630 (0.1%)
All	All	0.92	4/9973 (0.0%)	0.88	11/13538 (0.1%)

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	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	GLU	CG-CD	8.51	1.64	1.51
1	A	395	CYS	CB-SG	-6.15	1.71	1.82
1	A	57	GLU	CG-CD	5.36	1.59	1.51
1	A	59	GLU	CB-CG	5.29	1.62	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	LEU	CA-CB-CG	6.33	129.86	115.30
1	A	555	LEU	CA-CB-CG	5.92	128.92	115.30
1	B	241	ARG	NE-CZ-NH2	5.71	123.16	120.30
1	B	585	ARG	NE-CZ-NH1	-5.47	117.56	120.30
1	A	585	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	471	ASN	N-CA-CB	-5.27	101.12	110.60
1	A	503	ARG	NE-CZ-NH1	5.22	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	291	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	467	LEU	CA-CB-CG	5.08	126.98	115.30
1	B	594	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	585	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	470	SER	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	4967	0	4883	106	0
1	B	4769	0	4687	83	0
2	A	25	0	11	4	0
2	B	25	0	11	0	0
3	B	12	0	16	3	0
4	A	116	0	0	3	0
4	B	164	0	0	4	0
All	All	10078	0	9608	189	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 10.

All (189) 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:605:MET:HE2	1:B:609:PHE:HD2	1.06	1.19
1:B:605:MET:HE2	1:B:609:PHE:CD2	1.82	1.15
1:A:357:SER:HB2	1:A:380:ILE:HD11	1.31	1.07
1:B:278:SER:H	3:B:623:GOL:H31	1.21	1.05
1:B:605:MET:CE	1:B:609:PHE:HD2	1.73	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:SER:HB2	1:A:380:ILE:CD1	1.97	0.93
1:B:605:MET:CE	1:B:609:PHE:CD2	2.49	0.91
1:B:90:ARG:HG2	1:B:90:ARG:HH11	1.35	0.90
1:B:347:ILE:HG13	1:B:353:THR:HG23	1.54	0.88
1:A:521:ASN:HB2	2:A:621:UDP:O3B	1.73	0.88
1:A:382:TYR:HB3	1:A:401:LEU:HD22	1.59	0.84
1:B:281:ARG:HH21	1:B:521:ASN:ND2	1.75	0.82
1:B:233:ARG:HH22	1:B:376:HIS:CD2	1.99	0.81
1:B:278:SER:N	3:B:623:GOL:H31	1.99	0.77
1:A:124:LYS:O	1:A:124:LYS:HG2	1.83	0.77
1:A:4:GLU:HG3	1:A:5:ASN:ND2	2.00	0.76
1:B:233:ARG:NH2	1:B:376:HIS:CD2	2.53	0.76
1:B:382:TYR:HB3	1:B:401:LEU:HD22	1.68	0.74
1:A:376:HIS:HD2	1:A:397:SER:HB3	1.51	0.74
1:A:124:LYS:O	1:A:124:LYS:CG	2.37	0.73
1:B:566:GLU:O	1:B:570:ARG:HG3	1.89	0.72
1:A:359:THR:OG1	1:A:361:LEU:HD22	1.91	0.70
1:A:93:VAL:HG23	1:A:209:PRO:HB3	1.72	0.70
1:A:592:ASN:OD1	1:A:594:LEU:HB2	1.92	0.69
1:B:90:ARG:HG2	1:B:90:ARG:NH1	2.03	0.69
1:B:4:GLU:OE2	1:B:5:ASN:ND2	2.25	0.69
1:B:281:ARG:HH21	1:B:521:ASN:HD21	1.38	0.68
1:B:274:HIS:HD2	1:B:276:ALA:H	1.40	0.68
1:A:210:SER:O	1:A:351:MET:HE3	1.93	0.67
1:B:138:LEU:HD12	1:B:165:LEU:HD23	1.75	0.67
1:A:274:HIS:CD2	1:A:276:ALA:H	2.11	0.67
1:A:122:ASN:HB3	1:A:124:LYS:HE2	1.78	0.66
1:A:321:ASP:H	1:A:325:GLN:NE2	1.93	0.66
1:B:347:ILE:HA	1:B:353:THR:HG21	1.78	0.66
1:B:347:ILE:HG13	1:B:353:THR:CG2	2.25	0.66
1:B:271:GLU:OE1	1:B:353:THR:HG21	1.97	0.65
1:A:418:GLU:HG2	1:A:419:LYS:HG3	1.79	0.65
1:B:84:SER:O	1:B:88:VAL:HG23	1.96	0.65
1:A:4:GLU:HG3	1:A:5:ASN:HD22	1.62	0.64
1:B:426:GLU:O	1:B:428:PRO:HD3	1.97	0.64
1:B:66:THR:O	1:B:70:THR:HG23	1.98	0.64
1:A:274:HIS:HD2	1:A:276:ALA:H	1.46	0.63
1:B:283:HIS:O	1:B:287:MET:HE2	1.98	0.63
1:A:376:HIS:CD2	1:A:397:SER:HB3	2.34	0.61
1:B:301:SER:HB2	1:B:302:PRO:HD2	1.83	0.59
1:A:345:PRO:HA	1:A:368:ALA:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LYS:NZ	4:A:690:HOH:O	2.28	0.59
1:B:605:MET:HE2	1:B:609:PHE:CE2	2.38	0.59
1:A:205:LEU:H	1:A:242:HIS:HD2	1.52	0.58
1:A:123:ARG:HA	1:A:124:LYS:CB	2.32	0.58
1:B:203:LYS:O	1:B:204:ASN:HB3	2.03	0.58
1:B:90:ARG:HH11	1:B:90:ARG:CG	2.15	0.57
1:A:357:SER:CB	1:A:380:ILE:HD11	2.21	0.57
1:B:274:HIS:CD2	1:B:276:ALA:H	2.21	0.57
1:A:272:HIS:HB2	1:A:349:MET:CE	2.35	0.57
1:B:154:ASN:OD1	1:B:157:VAL:HG12	2.04	0.57
1:A:270:LEU:HD21	1:A:312:PHE:CZ	2.39	0.56
1:B:257:ILE:HG13	1:B:257:ILE:O	2.04	0.56
1:B:372:PRO:HG2	1:B:542:HIS:HB3	1.86	0.56
1:B:138:LEU:CD1	1:B:165:LEU:HD23	2.36	0.56
1:A:93:VAL:CG2	1:A:209:PRO:HB3	2.36	0.56
1:B:281:ARG:NH2	1:B:521:ASN:ND2	2.51	0.56
1:B:480:ARG:NH2	4:B:783:HOH:O	2.38	0.56
1:B:281:ARG:HG3	1:B:411:VAL:HG22	1.86	0.55
1:A:389:TYR:O	1:A:544:HIS:HB3	2.06	0.55
1:A:556:PRO:HD2	1:A:559:LEU:HD12	1.88	0.55
1:B:511:MET:O	1:B:533:GLY:HA2	2.07	0.55
1:A:521:ASN:HB2	2:A:621:UDP:PB	2.46	0.55
1:B:615:ALA:O	1:B:619:GLU:HG2	2.06	0.55
1:A:210:SER:O	1:A:351:MET:CE	2.54	0.55
1:A:277:HIS:HB3	4:A:718:HOH:O	2.06	0.55
1:A:521:ASN:ND2	2:A:621:UDP:O3B	2.35	0.55
1:A:3:ASN:HD22	1:A:6:LYS:HD3	1.72	0.54
1:A:272:HIS:HB2	1:A:349:MET:HE3	1.90	0.54
1:A:66:THR:O	1:A:70:THR:HG23	2.08	0.53
1:A:323:MET:HG2	1:A:355:PHE:CD1	2.43	0.53
1:B:12:PHE:CE1	1:B:28:LEU:HB2	2.43	0.53
1:B:444:PRO:O	1:B:448:GLU:HB2	2.09	0.53
1:A:169:LEU:HG	1:A:173:LEU:HD22	1.91	0.52
1:B:503:ARG:NH2	4:B:734:HOH:O	2.41	0.52
1:A:515:PHE:HB2	1:A:516:PRO:HA	1.90	0.52
1:A:191:ILE:HG23	1:A:195:PHE:HB2	1.92	0.52
1:B:614:ASN:HB3	1:B:618:LYS:HE2	1.91	0.52
1:A:200:ASP:O	1:A:241:ARG:NH1	2.43	0.52
1:A:103:ALA:O	1:A:480:ARG:NH2	2.43	0.52
1:B:134:SER:HB3	1:B:137:SER:HB2	1.92	0.51
1:B:581:ARG:O	1:B:585:ARG:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:GLU:OE2	1:A:402:ARG:NH2	2.42	0.50
1:A:618:LYS:N	1:A:618:LYS:HD3	2.26	0.50
1:B:214:HIS:CD2	1:B:214:HIS:H	2.30	0.50
1:A:360:ARG:NH1	1:A:381:GLU:OE1	2.39	0.50
1:B:586:ARG:O	1:B:590:GLU:HG3	2.12	0.50
1:A:306:GLN:O	1:A:310:GLU:HG3	2.11	0.50
1:A:123:ARG:HA	1:A:124:LYS:HB3	1.93	0.50
1:B:527:VAL:HG21	1:B:553:LEU:HD23	1.93	0.50
1:A:154:ASN:OD1	1:A:157:VAL:HG12	2.11	0.49
1:B:605:MET:CE	1:B:609:PHE:CE2	2.94	0.49
1:A:204:ASN:HB2	1:A:242:HIS:HD2	1.77	0.49
1:A:247:TYR:CD1	1:A:324:LYS:HB2	2.47	0.49
1:A:266:MET:HG3	1:A:341:ILE:HB	1.94	0.49
1:A:386:GLU:HG2	1:A:552:ARG:HH22	1.78	0.49
1:B:12:PHE:O	1:B:16:VAL:HG23	2.12	0.49
1:A:243:ILE:O	1:A:247:TYR:HB2	2.12	0.49
1:A:527:VAL:HG21	1:A:553:LEU:HD13	1.96	0.48
1:A:340:ALA:HB1	1:A:613:LEU:HD13	1.95	0.48
1:B:205:LEU:HD23	1:B:208:ILE:HD11	1.96	0.48
1:B:199:LEU:HD12	1:B:202:LEU:HD12	1.95	0.48
1:B:439:THR:HA	1:B:442:LEU:HD22	1.94	0.48
1:A:603:ARG:N	1:A:604:PRO:HD2	2.28	0.47
1:A:205:LEU:H	1:A:242:HIS:CD2	2.32	0.47
1:A:476:PRO:O	1:A:480:ARG:HG3	2.13	0.47
1:A:180:GLY:O	1:A:444:PRO:HD3	2.14	0.47
1:B:480:ARG:CB	1:B:480:ARG:HH21	2.27	0.47
1:A:49:TYR:OH	1:A:54:GLN:NE2	2.48	0.47
1:B:15:ALA:HB2	1:B:23:LYS:HD2	1.97	0.47
1:A:73:THR:HA	1:A:113:ILE:HD11	1.97	0.47
1:A:339:ALA:O	1:A:363:PRO:HD2	2.15	0.46
1:B:268:VAL:HG12	1:B:270:LEU:CD1	2.45	0.46
1:A:107:PHE:O	1:A:108:VAL:HB	2.15	0.46
1:A:122:ASN:HB3	1:A:123:ARG:H	1.50	0.46
1:A:374:THR:HB	1:A:396:PHE:HA	1.98	0.46
1:A:12:PHE:CE1	1:A:28:LEU:HB2	2.51	0.46
1:B:161:ILE:HD13	4:B:701:HOH:O	2.16	0.46
1:B:318:VAL:HG12	1:B:326:LYS:HG2	1.98	0.46
1:B:146:LEU:O	1:B:149:SER:HB3	2.17	0.45
1:B:603:ARG:N	1:B:604:PRO:CD	2.80	0.45
1:A:65:CYS:HB3	1:A:101:ILE:O	2.16	0.45
1:B:23:LYS:O	1:B:27:GLU:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:ASN:N	1:B:595:ASN:HD22	2.14	0.45
1:A:566:GLU:O	1:A:570:ARG:HG2	2.17	0.45
1:A:214:HIS:H	1:A:214:HIS:CD2	2.35	0.44
1:A:251:ASP:HB3	1:A:360:ARG:HB3	1.98	0.44
1:B:56:LEU:HB3	1:B:59:GLU:HB2	1.98	0.44
1:A:57:GLU:O	1:A:61:ILE:HD12	2.17	0.44
1:A:190:THR:O	1:A:191:ILE:C	2.55	0.44
1:A:118:ASN:HD22	1:A:130:HIS:H	1.64	0.44
1:A:239:ILE:O	1:A:243:ILE:HG23	2.17	0.44
1:A:513:ASN:HA	1:A:514:PRO:HD3	1.91	0.44
1:A:78:ASP:HA	1:A:79:PRO:HD3	1.87	0.44
1:A:540:GLU:HB3	4:A:670:HOH:O	2.17	0.44
1:A:123:ARG:HH21	1:A:123:ARG:HB2	1.82	0.44
1:A:139:ILE:O	1:A:142:CYS:N	2.48	0.44
1:A:521:ASN:CB	2:A:621:UDP:O3B	2.57	0.44
1:A:123:ARG:HG2	1:A:125:ASN:O	2.17	0.43
1:A:162:SER:HA	1:A:163:PRO:HD2	1.81	0.43
1:A:123:ARG:CA	1:A:124:LYS:HB3	2.49	0.43
1:A:443:ASN:HB2	1:A:444:PRO:HD2	2.01	0.43
1:A:359:THR:OG1	1:A:361:LEU:CD2	2.63	0.43
1:B:78:ASP:C	1:B:78:ASP:OD2	2.57	0.43
1:B:287:MET:HE3	1:B:287:MET:HB2	1.83	0.43
1:B:266:MET:CE	1:B:605:MET:CE	2.96	0.43
1:B:441:LYS:HE2	1:B:517:PHE:CD2	2.54	0.43
1:B:347:ILE:HA	1:B:353:THR:CG2	2.48	0.43
1:A:467:LEU:HB3	1:A:470:SER:HB2	2.01	0.43
1:B:275:SER:HA	1:B:280:TYR:CD2	2.54	0.43
1:B:78:ASP:HA	1:B:79:PRO:HD3	1.90	0.42
1:A:143:ILE:HG22	1:A:144:LEU:HD13	2.01	0.42
1:B:57:GLU:O	1:B:61:ILE:HG13	2.19	0.42
1:A:603:ARG:N	1:A:604:PRO:CD	2.82	0.42
1:B:275:SER:HA	1:B:280:TYR:CG	2.55	0.42
1:A:268:VAL:HG12	1:A:270:LEU:HD13	2.00	0.42
1:B:266:MET:HE2	1:B:605:MET:HE3	2.01	0.42
1:A:588:ILE:HD13	1:A:588:ILE:HA	1.91	0.42
1:A:213:SER:HB2	1:A:351:MET:HE3	2.02	0.42
1:A:586:ARG:O	1:A:590:GLU:HB2	2.20	0.42
1:B:161:ILE:HD12	1:B:161:ILE:HA	1.85	0.42
1:B:266:MET:HE1	1:B:605:MET:HE1	2.02	0.42
1:B:605:MET:HE3	1:B:609:PHE:CD2	2.45	0.42
1:A:154:ASN:CG	1:A:157:VAL:HG12	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:ILE:HD12	1:A:588:ILE:HG23	1.82	0.41
1:A:423:LEU:HD11	1:A:425:ARG:NH2	2.35	0.41
1:A:119:ARG:O	1:A:121:PRO:HD3	2.20	0.41
1:B:277:HIS:CB	3:B:623:GOL:O1	2.68	0.41
1:B:456:ARG:NH2	4:B:654:HOH:O	2.52	0.41
1:A:111:ASP:HA	1:A:114:LEU:HB2	2.03	0.41
1:A:273:PHE:O	1:A:273:PHE:CG	2.74	0.41
1:B:329:PHE:O	1:B:333:VAL:HG23	2.21	0.41
1:A:168:SER:HA	1:A:209:PRO:HD3	2.03	0.40
1:B:266:MET:CE	1:B:605:MET:HE3	2.52	0.40
1:A:469:GLN:O	1:A:471:ASN:HB2	2.21	0.40
1:A:494:PRO:O	1:A:495:HIS:C	2.59	0.40
1:B:468:GLY:O	1:B:469:GLN:HB2	2.21	0.40
1:A:199:LEU:O	1:A:202:LEU:HB2	2.21	0.40
1:A:350:ASP:OD2	1:A:351:MET:N	2.55	0.40
1:A:88:VAL:HG21	1:A:139:ILE:HD13	2.04	0.40
1:B:321:ASP:H	1:B:325:GLN:NE2	2.20	0.40
1:A:247:TYR:CE1	1:A:324:LYS:HB2	2.56	0.40
1:A:271:GLU:O	1:A:272:HIS:C	2.60	0.40
1:B:271:GLU:OE1	1:B:353:THR:CG2	2.67	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	618/631 (98%)	586 (95%)	24 (4%)	8 (1%)	12	8
1	B	589/631 (93%)	563 (96%)	25 (4%)	1 (0%)	47	55
All	All	1207/1262 (96%)	1149 (95%)	49 (4%)	9 (1%)	22	21

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	123	ARG
1	B	204	ASN
1	A	161	ILE
1	A	139	ILE
1	A	204	ASN
1	A	132	ASP
1	A	121	PRO
1	A	428	PRO

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	546/555 (98%)	495 (91%)	51 (9%)	9	6
1	B	523/555 (94%)	467 (89%)	56 (11%)	6	4
All	All	1069/1110 (96%)	962 (90%)	107 (10%)	7	5

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	46	GLU
1	A	54	GLN
1	A	75	LEU
1	A	86	LEU
1	A	114	LEU
1	A	120	GLU
1	A	122	ASN
1	A	123	ARG
1	A	126	SER
1	A	127	LEU
1	A	135	LYS
1	A	144	LEU
1	A	158	MET
1	A	165	LEU

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Mol	Chain	Res	Type
1	A	173	LEU
1	A	182	SER
1	A	203	LYS
1	A	214	HIS
1	A	231	VAL
1	A	245	SER
1	A	263	LYS
1	A	270	LEU
1	A	279	ILE
1	A	301	SER
1	A	351	MET
1	A	361	LEU
1	A	392	SER
1	A	399	THR
1	A	401	LEU
1	A	403	LEU
1	A	413	SER
1	A	415	LEU
1	A	418	GLU
1	A	423	LEU
1	A	429	GLU
1	A	442	LEU
1	A	450	LEU
1	A	467	LEU
1	A	502	LEU
1	A	505	LEU
1	A	529	LEU
1	A	531	LEU
1	A	536	LYS
1	A	557	GLU
1	A	590	GLU
1	A	591	ASN
1	A	610	LEU
1	A	617	LEU
1	A	618	LYS
1	A	619	GLU
1	B	4	GLU
1	B	29	LEU
1	B	53	LEU
1	B	56	LEU
1	B	59	GLU
1	B	70	THR

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Mol	Chain	Res	Type
1	B	81	LEU
1	B	82	GLU
1	B	86	LEU
1	B	90	ARG
1	B	92	LEU
1	B	98	LEU
1	B	115	GLN
1	B	118	ASN
1	B	153	LEU
1	B	157	VAL
1	B	161	ILE
1	B	173	LEU
1	B	203	LYS
1	B	212	ILE
1	B	253	ASP
1	B	270	LEU
1	B	287	MET
1	B	327	LEU
1	B	336	SER
1	B	349	MET
1	B	353	THR
1	B	394	GLU
1	B	401	LEU
1	B	408	LEU
1	B	419	LYS
1	B	420	VAL
1	B	423	LEU
1	B	427	ASN
1	B	442	LEU
1	B	450	LEU
1	B	454	ARG
1	B	460	LYS
1	B	480	ARG
1	B	486	LEU
1	B	496	SER
1	B	501	TYR
1	B	502	LEU
1	B	505	LEU
1	B	529	LEU
1	B	531	LEU
1	B	546	ASP
1	B	553	LEU

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Mol	Chain	Res	Type
1	B	557	GLU
1	B	594	LEU
1	B	595	ASN
1	B	597	LEU
1	B	605	MET
1	B	610	LEU
1	B	618	LYS
1	B	619	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	5	ASN
1	A	11	ASN
1	A	54	GLN
1	A	118	ASN
1	A	206	ASN
1	A	214	HIS
1	A	242	HIS
1	A	261	ASN
1	A	274	HIS
1	A	277	HIS
1	A	325	GLN
1	A	376	HIS
1	A	469	GLN
1	A	595	ASN
1	A	607	GLN
1	B	5	ASN
1	B	11	ASN
1	B	54	GLN
1	B	115	GLN
1	B	214	HIS
1	B	261	ASN
1	B	272	HIS
1	B	274	HIS
1	B	325	GLN
1	B	376	HIS
1	B	493	HIS
1	B	521	ASN
1	B	595	ASN
1	B	607	GLN

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Mol	Chain	Res	Type
1	B	614	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 monosaccharides in this entry.

5.6　Ligand geometry ⓘ

4 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	$\#|Z| > 2$
3	GOL	B	622	-	5,5,5	0.34	0	5,5,5	0.90	0
2	UDP	B	621	-	24,26,26	1.08	2 (8%)	37,40,40	1.57	7 (18%)
3	GOL	B	623	-	5,5,5	0.37	0	5,5,5	1.04	1 (20%)
2	UDP	A	621	-	24,26,26	1.01	1 (4%)	37,40,40	2.01	11 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	622	-	-	3/4/4/4	-
2	UDP	B	621	-	-	6/16/32/32	0/2/2/2
3	GOL	B	623	-	-	4/4/4/4	-
2	UDP	A	621	-	-	2/16/32/32	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	621	UDP	O4'-C4'	-2.27	1.39	1.45
2	A	621	UDP	C2-N1	2.14	1.41	1.38
2	B	621	UDP	C6-C5	2.13	1.40	1.35

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	621	UDP	C4-N3-C2	-5.23	119.68	126.58
2	A	621	UDP	C5-C4-N3	4.57	121.67	114.84
2	A	621	UDP	N3-C2-N1	3.96	120.15	114.89
2	B	621	UDP	O5'-C5'-C4'	-3.78	95.98	108.99
2	B	621	UDP	C4-N3-C2	-3.51	121.95	126.58
2	A	621	UDP	O2-C2-N3	-3.38	115.20	121.50
2	A	621	UDP	PA-O3A-PB	-3.26	121.62	132.83
2	A	621	UDP	C3'-C2'-C1'	3.02	107.16	101.43
2	B	621	UDP	C5-C6-N1	-2.87	117.00	121.81
2	B	621	UDP	C5-C4-N3	2.87	119.13	114.84
2	A	621	UDP	C1'-N1-C2	2.50	122.10	117.57
2	A	621	UDP	O3'-C3'-C2'	-2.48	103.81	111.82
2	A	621	UDP	O2B-PB-O3A	2.28	112.27	104.64
2	B	621	UDP	N3-C2-N1	2.24	117.86	114.89
2	A	621	UDP	O4'-C1'-N1	2.20	113.39	108.36
2	A	621	UDP	C2'-C1'-N1	-2.19	107.00	113.22
2	B	621	UDP	O4'-C4'-C3'	2.14	109.36	105.11
3	B	623	GOL	O3-C3-C2	2.09	120.21	110.20
2	B	621	UDP	C6-N1-C2	-2.03	118.39	120.99

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	621	UDP	C3'-C4'-C5'-O5'
2	B	621	UDP	O4'-C4'-C5'-O5'

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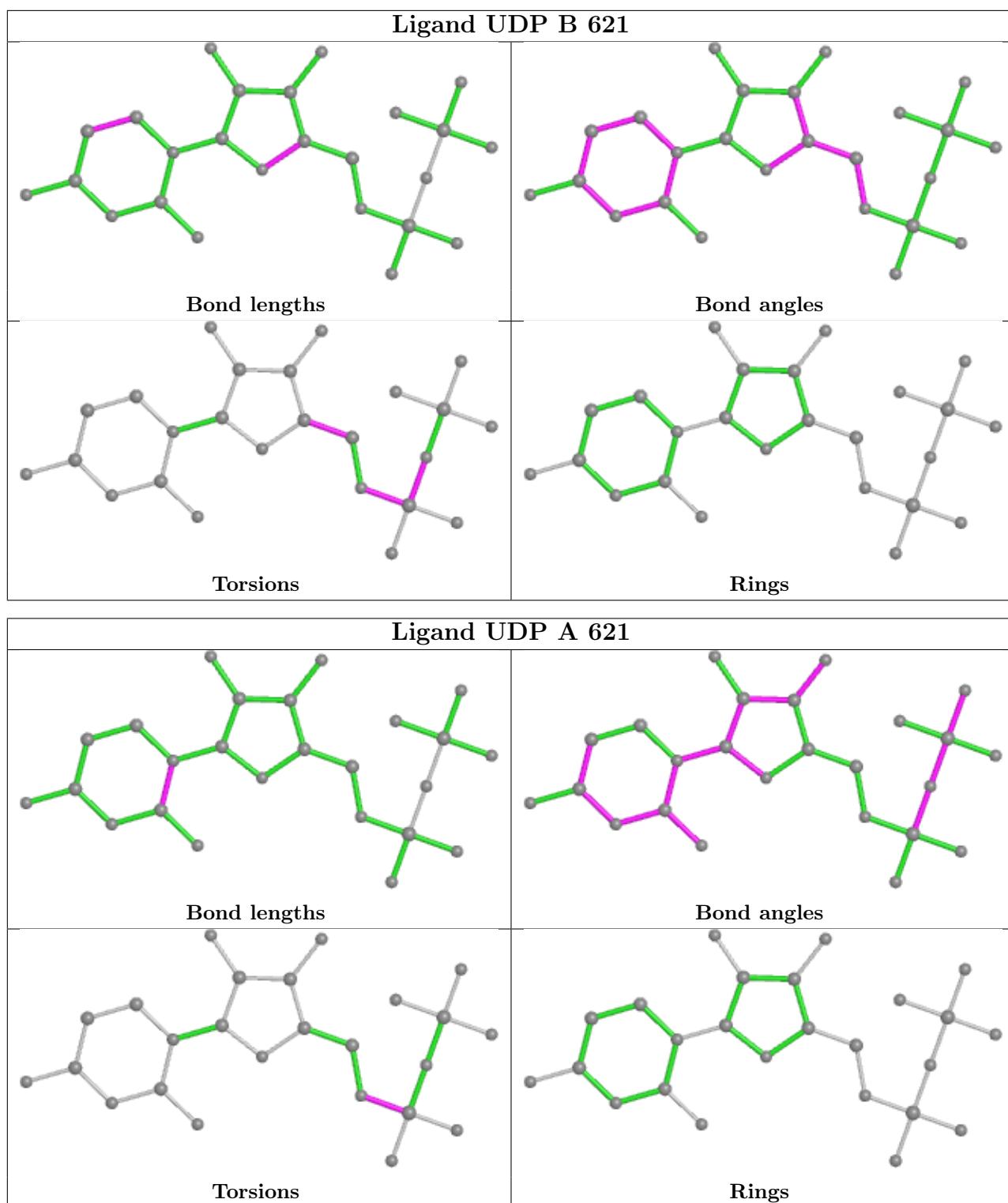
Mol	Chain	Res	Type	Atoms
2	B	621	UDP	C5'-O5'-PA-O1A
2	B	621	UDP	C5'-O5'-PA-O2A
3	B	622	GOL	C1-C2-C3-O3
3	B	622	GOL	O2-C2-C3-O3
3	B	623	GOL	O1-C1-C2-C3
3	B	623	GOL	C1-C2-C3-O3
3	B	623	GOL	O1-C1-C2-O2
3	B	623	GOL	O2-C2-C3-O3
2	B	621	UDP	PB-O3A-PA-O5'
2	A	621	UDP	C5'-O5'-PA-O3A
3	B	622	GOL	O1-C1-C2-O2
2	B	621	UDP	C5'-O5'-PA-O3A
2	A	621	UDP	C5'-O5'-PA-O1A

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	623	GOL	3	0
2	A	621	UDP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand UDP B 621

Bond lengths

Bond angles

Torsions

Rings

Ligand UDP A 621

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	620/631 (98%)	-0.34	4 (0%) 89	89	19, 36, 58, 73	0
1	B	595/631 (94%)	-0.48	9 (1%) 73	75	18, 31, 49, 88	0
All	All	1215/1262 (96%)	-0.41	13 (1%) 80	82	18, 33, 56, 88	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	GLU	4.9
1	A	1	MET	4.3
1	B	427	ASN	3.9
1	B	135	LYS	3.5
1	A	0	THR	3.4
1	B	5	ASN	3.3
1	B	419	LYS	3.0
1	B	421	ASP	2.9
1	B	136	SER	2.8
1	B	420	VAL	2.5
1	A	262	ASN	2.4
1	B	6	LYS	2.3
1	A	125	ASN	2.1

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 ⓘ
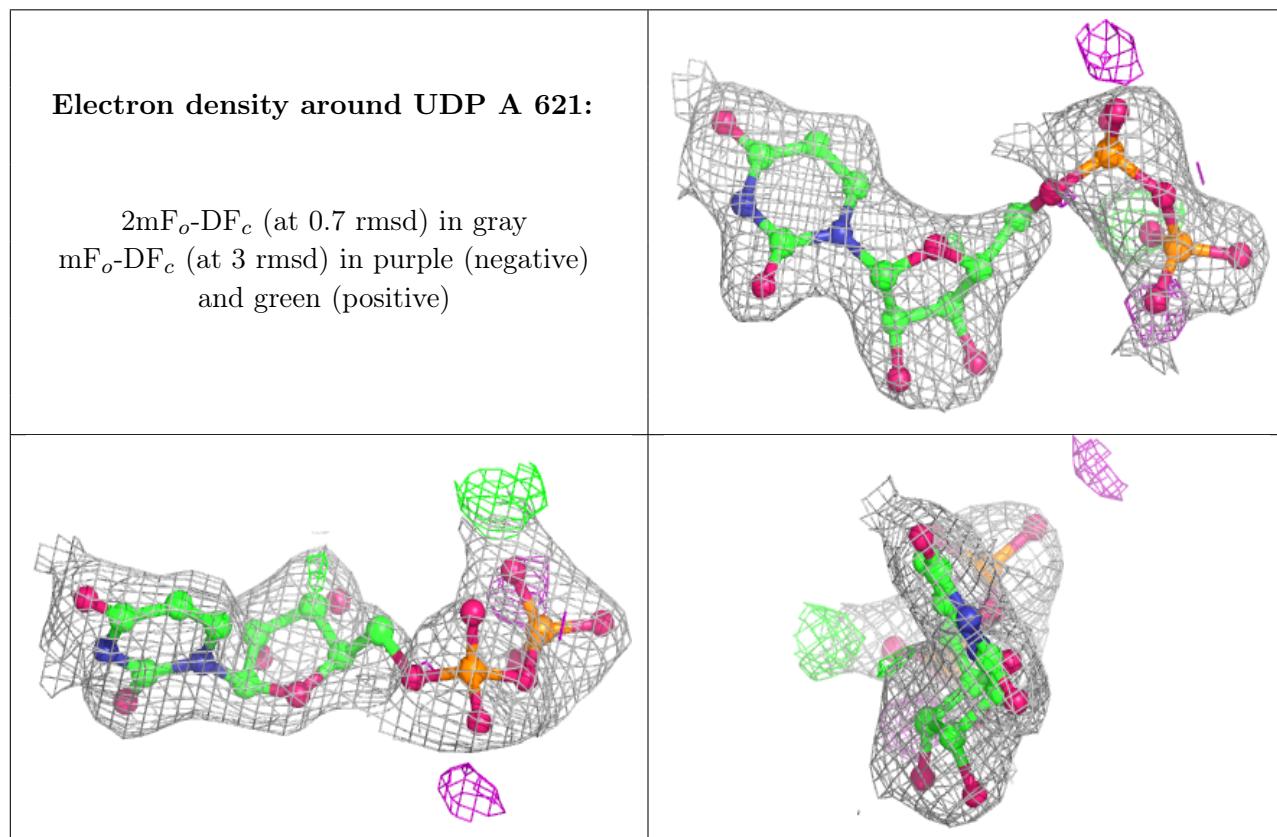
There are no monosaccharides in this entry.
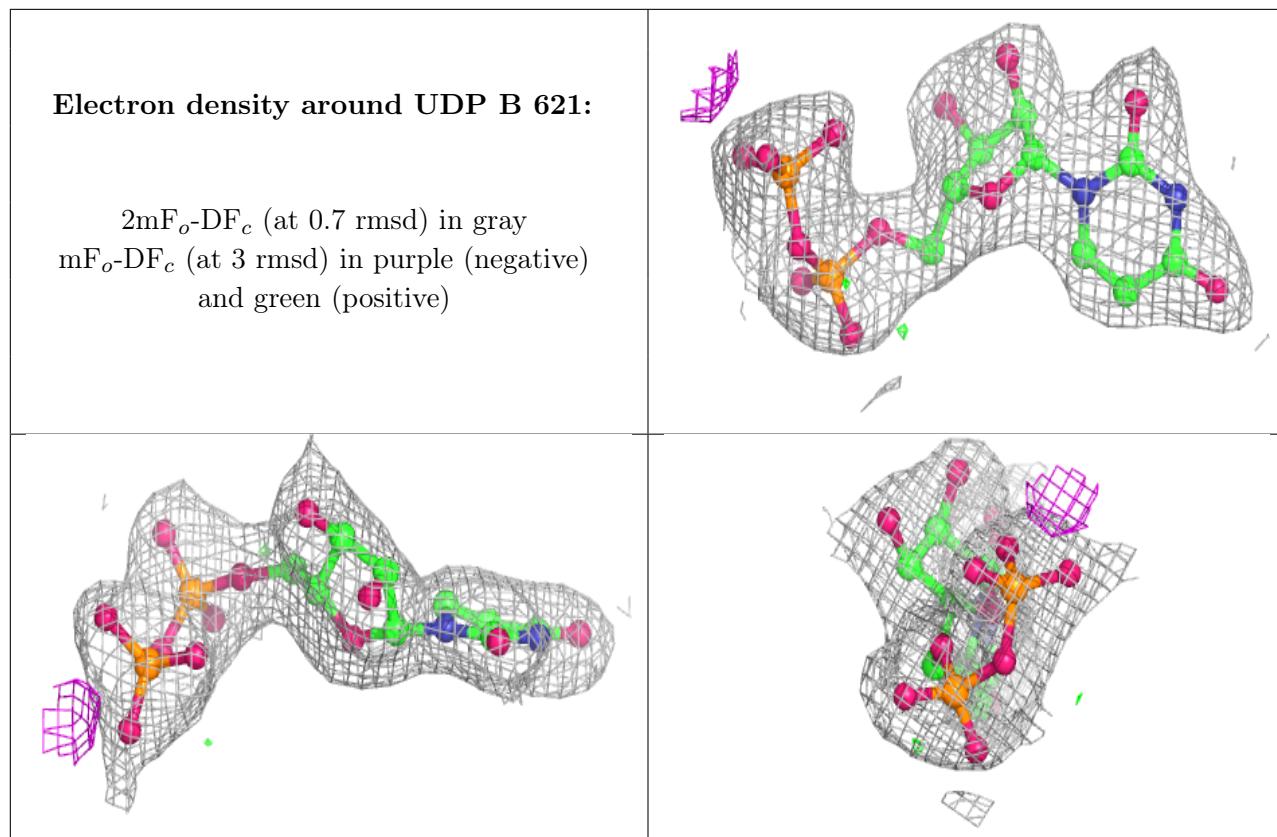
6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	GOL	B	622	6/6	0.86	0.12	49,51,53,53	0
2	UDP	A	621	25/25	0.90	0.12	40,57,74,75	0
3	GOL	B	623	6/6	0.91	0.16	48,52,53,57	0
2	UDP	B	621	25/25	0.95	0.10	36,43,55,56	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 UDP A 621:

$2mF_o$-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 621:

$2mF_o$-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 ⓘ

There are no such residues in this entry.