



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:04 AM UTC

PDB ID : 3Q3E / pdb_00003q3e
Title : Crystal structure of the Actinobacillus pleuropneumoniae HMW1C glycosyl-transferase
Authors : Kawai, F.; Yeo, H.J.
Deposited on : 2010-12-21
Resolution : 2.10 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
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

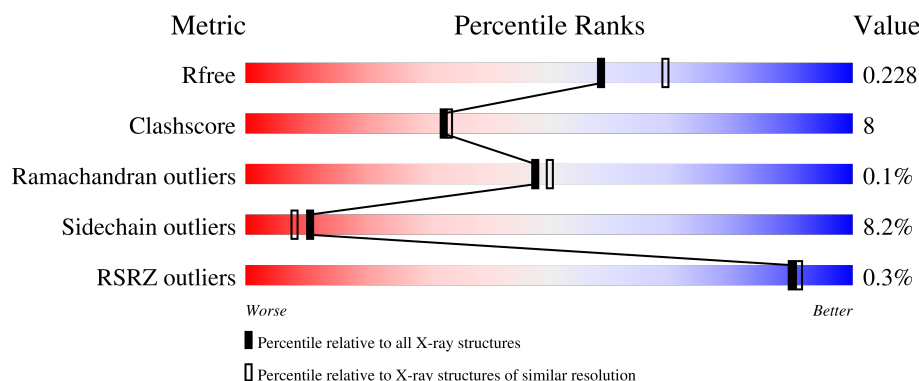
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	631	 78% 16% • •
1	B	631	 77% 14% • 6%

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
2	GOL	A	621	-	-	X	-
2	GOL	A	622	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10244 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	596	Total	C	N	O	S	0	0	0
			4775	3055	816	880	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 GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is water.

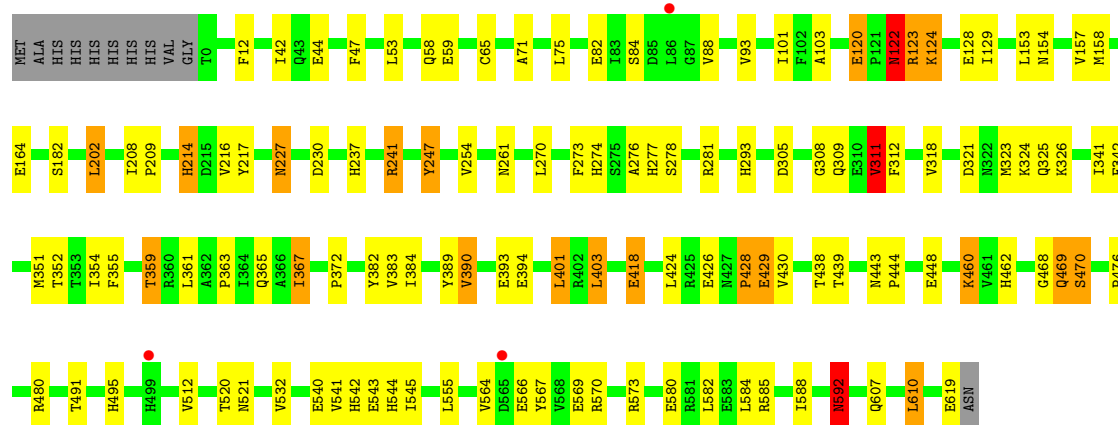
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	217	Total	O	0	0
			217	217		
3	B	267	Total	O	0	0
			267	267		

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.

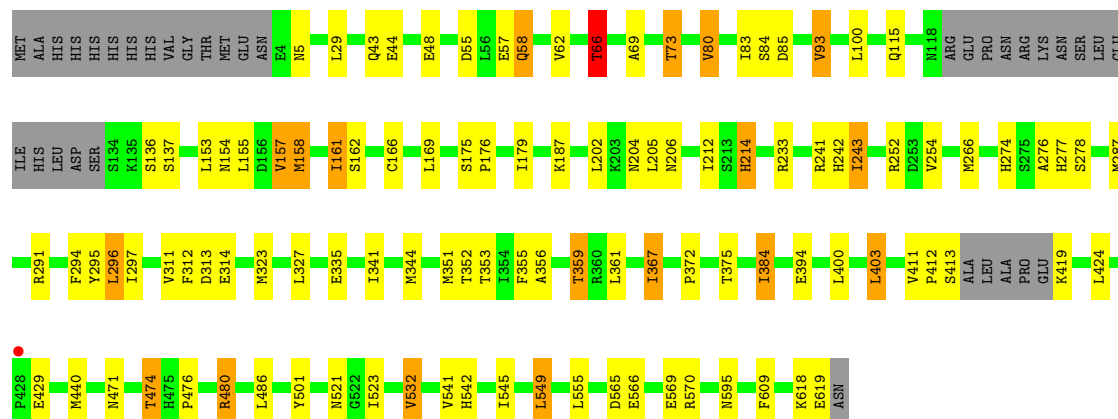
• Molecule 1: HMW1C-like glycosyltransferase

Chain A: 



• Molecule 1: HMW1C-like glycosyltransferase

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.37Å 94.68Å 176.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.10) 93.0 (50.00-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.184 , 0.226 0.185 , 0.228	Depositor DCC
R_{free} test set	3720 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10244	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.91	2/5088 (0.0%)	1.03	7/6908 (0.1%)
1	B	0.94	2/4891 (0.0%)	1.01	2/6638 (0.0%)
All	All	0.92	4/9979 (0.0%)	1.02	9/13546 (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	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	ASN	CA-C	9.28	1.58	1.52
1	B	93	VAL	CA-CB	5.82	1.63	1.54
1	A	311	VAL	CA-CB	5.07	1.60	1.54
1	B	80	VAL	CA-CB	5.07	1.61	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	ASN	N-CA-C	6.32	118.90	108.48
1	A	429	GLU	N-CA-C	-5.96	104.48	110.97
1	A	247	TYR	N-CA-C	-5.81	101.86	110.46
1	B	66	THR	CB-CA-C	5.77	121.25	110.70
1	A	592	ASN	N-CA-C	5.54	117.77	108.73
1	B	206	ASN	N-CA-C	5.28	116.84	111.14
1	A	59	GLU	N-CA-C	-5.23	105.66	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	470	SER	N-CA-C	5.20	117.22	108.96
1	A	390	VAL	N-CA-C	5.05	116.08	109.21

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	469	GLN	Peptide
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	83	0
1	B	4775	0	4692	70	0
2	A	12	0	16	11	0
2	B	6	0	8	1	0
3	A	217	0	0	2	0
3	B	267	0	0	4	0
All	All	10244	0	9599	153	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 (153) 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:123:ARG:H	1:A:124:LYS:HA	1.35	0.92
1:A:227:ASN:HD22	1:A:227:ASN:H	1.16	0.90
1:A:520:THR:H	2:A:622:GOL:H12	1.38	0.88
1:A:123:ARG:N	1:A:124:LYS:HA	1.92	0.84
1:B:243:ILE:HD11	1:B:355:PHE:CD1	2.14	0.83
1:B:243:ILE:HD11	1:B:355:PHE:HD1	1.42	0.82
1:B:480:ARG:HH21	1:B:480:ARG:HB2	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASN:HB2	1:A:123:ARG:HA	1.62	0.79
1:B:205:LEU:H	1:B:242:HIS:HD2	1.32	0.76
1:A:274:HIS:HD2	1:A:276:ALA:H	1.34	0.75
1:A:367:ILE:CD1	1:A:383:VAL:HG22	2.17	0.74
1:A:281:ARG:HH22	2:A:621:GOL:C1	2.01	0.73
1:A:122:ASN:CB	1:A:123:ARG:HA	2.18	0.73
1:B:205:LEU:H	1:B:242:HIS:CD2	2.08	0.71
1:A:462:HIS:HE1	1:A:491:THR:OG1	1.73	0.71
1:B:266:MET:HB3	1:B:296:LEU:HD22	1.72	0.71
1:B:204:ASN:HB2	1:B:242:HIS:HD2	1.56	0.71
1:B:274:HIS:HD2	1:B:276:ALA:H	1.39	0.71
1:B:480:ARG:HH21	1:B:480:ARG:CB	2.05	0.69
1:B:480:ARG:HB2	1:B:480:ARG:NH2	2.07	0.69
1:B:100:LEU:HD13	1:B:474:THR:HG22	1.74	0.69
1:B:323:MET:HE1	1:B:352:THR:HG23	1.74	0.69
1:B:158:MET:HE3	1:B:166:CYS:SG	2.34	0.68
1:A:521:ASN:HB2	2:A:622:GOL:H2	1.75	0.68
1:B:323:MET:HE2	1:B:327:LEU:HG	1.76	0.68
1:A:367:ILE:HD11	1:A:383:VAL:HG22	1.77	0.67
1:A:122:ASN:HD22	1:A:123:ARG:HA	1.59	0.67
1:A:323:MET:HG2	1:A:355:PHE:CD1	2.29	0.67
1:B:474:THR:HG21	3:B:873:HOH:O	1.94	0.67
1:A:274:HIS:CD2	1:A:276:ALA:H	2.14	0.66
1:A:321:ASP:H	1:A:325:GLN:NE2	1.94	0.66
1:B:204:ASN:HB2	1:B:242:HIS:CD2	2.31	0.65
1:B:359:THR:CG2	1:B:361:LEU:HG	2.26	0.65
1:A:426:GLU:O	1:A:428:PRO:HD3	1.96	0.65
1:A:584:LEU:O	1:A:588:ILE:HG13	1.96	0.65
1:B:69:ALA:O	1:B:73:THR:HG23	1.97	0.65
1:A:520:THR:HB	2:A:622:GOL:H31	1.78	0.65
1:A:592:ASN:HB2	3:A:674:HOH:O	1.97	0.64
1:B:521:ASN:H	2:B:621:GOL:H32	1.62	0.64
1:A:42:ILE:HD12	1:A:47:PHE:CE2	2.35	0.62
1:A:439:THR:HG23	1:A:469:GLN:HB2	1.82	0.62
1:A:58:GLN:HE22	1:A:476:PRO:HD3	1.65	0.61
1:A:438:THR:HB	1:A:469:GLN:HG2	1.81	0.61
1:A:247:TYR:HA	1:A:324:LYS:HE2	1.83	0.61
1:B:69:ALA:O	1:B:73:THR:CG2	2.49	0.61
1:B:252:ARG:HD2	1:B:335:GLU:OE1	2.00	0.61
1:B:62:VAL:O	1:B:66:THR:CG2	2.49	0.60
1:B:471:ASN:ND2	3:B:769:HOH:O	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:HIS:H	1:A:214:HIS:CD2	2.19	0.60
1:B:287:MET:HE3	1:B:312:PHE:CE1	2.36	0.60
1:A:541:VAL:O	1:A:545:ILE:HG13	2.01	0.59
1:B:58:GLN:HE21	1:B:476:PRO:HG3	1.67	0.59
1:B:480:ARG:HH21	1:B:480:ARG:CG	2.14	0.59
1:A:342:PHE:HB3	1:A:365:GLN:HG2	1.83	0.59
1:A:237:HIS:O	1:A:241:ARG:HG2	2.02	0.59
1:A:521:ASN:HD22	2:A:622:GOL:H2	1.68	0.58
1:B:541:VAL:O	1:B:545:ILE:HG12	2.03	0.58
1:B:277:HIS:CG	1:B:278:SER:H	2.21	0.58
1:A:281:ARG:HH22	2:A:621:GOL:H11	1.68	0.58
1:A:254:VAL:HB	1:A:363:PRO:HD3	1.85	0.58
1:B:341:ILE:HD13	1:B:609:PHE:HB3	1.86	0.58
1:B:287:MET:HE2	1:B:311:VAL:HG11	1.86	0.58
1:B:367:ILE:HD13	1:B:375:THR:HG21	1.86	0.58
1:A:42:ILE:HD12	1:A:47:PHE:HE2	1.68	0.58
1:A:573:ARG:NH2	1:A:580:GLU:OE2	2.34	0.57
1:A:123:ARG:H	1:A:124:LYS:CA	2.13	0.57
1:B:523:ILE:HB	1:B:549:LEU:HD13	1.86	0.57
1:B:566:GLU:O	1:B:570:ARG:HG2	2.04	0.57
1:B:62:VAL:O	1:B:66:THR:HG23	2.06	0.56
1:B:274:HIS:CD2	1:B:276:ALA:H	2.22	0.56
1:B:565:ASP:O	1:B:569:GLU:HG2	2.07	0.55
1:A:382:TYR:HB3	1:A:401:LEU:HD22	1.88	0.55
1:A:438:THR:HB	1:A:469:GLN:CG	2.37	0.55
1:A:564:VAL:HG11	3:A:838:HOH:O	2.05	0.55
1:B:297:ILE:HG12	1:B:314:GLU:HG2	1.90	0.54
1:B:356:ALA:O	1:B:359:THR:HB	2.08	0.54
1:A:227:ASN:H	1:A:227:ASN:ND2	1.98	0.53
1:B:243:ILE:CD1	1:B:355:PHE:CD1	2.89	0.53
1:A:430:VAL:HG22	1:A:460:LYS:HG2	1.90	0.52
1:B:202:LEU:O	1:B:241:ARG:NH1	2.41	0.52
1:B:252:ARG:NH2	3:B:704:HOH:O	2.30	0.52
1:B:323:MET:HE3	1:B:323:MET:HA	1.90	0.52
1:A:120:GLU:HG2	1:A:122:ASN:HD21	1.75	0.52
1:A:278:SER:H	2:A:621:GOL:H32	1.75	0.52
1:A:566:GLU:O	1:A:570:ARG:HG2	2.09	0.51
1:A:359:THR:CG2	1:A:361:LEU:HG	2.41	0.50
1:A:521:ASN:HD22	2:A:622:GOL:C2	2.25	0.49
1:B:62:VAL:O	1:B:66:THR:HG22	2.13	0.49
1:A:308:GLY:O	1:A:311:VAL:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:HIS:CG	1:B:278:SER:N	2.80	0.49
1:B:287:MET:HE3	1:B:312:PHE:HE1	1.78	0.49
1:B:372:PRO:HG2	1:B:542:HIS:HB3	1.95	0.48
1:B:43:GLN:O	1:B:44:GLU:HB2	2.12	0.48
1:B:161:ILE:HG13	1:B:162:SER:N	2.27	0.48
1:A:122:ASN:ND2	1:A:123:ARG:HA	2.26	0.48
1:B:291:ARG:HG3	1:B:296:LEU:HG	1.94	0.48
1:A:154:ASN:O	1:A:157:VAL:HG12	2.14	0.48
1:B:341:ILE:CD1	1:B:609:PHE:HB3	2.44	0.48
1:A:123:ARG:N	1:A:124:LYS:CA	2.73	0.48
1:A:521:ASN:H	2:A:622:GOL:H31	1.78	0.47
1:B:595:ASN:HB2	3:B:666:HOH:O	2.15	0.47
1:B:480:ARG:CB	1:B:480:ARG:NH2	2.71	0.47
1:B:295:TYR:CE1	1:B:313:ASP:HB3	2.50	0.47
1:B:359:THR:HG22	1:B:361:LEU:HG	1.96	0.46
1:B:532:VAL:HG23	1:B:555:LEU:CD2	2.44	0.46
1:A:443:ASN:HB2	1:A:444:PRO:CD	2.45	0.46
1:B:214:HIS:CD2	1:B:214:HIS:H	2.33	0.46
1:A:84:SER:O	1:A:88:VAL:HG23	2.16	0.46
1:A:424:LEU:HD23	1:A:585:ARG:CZ	2.46	0.46
1:A:12:PHE:CE2	1:A:71:ALA:HB3	2.51	0.45
1:A:367:ILE:HD13	1:A:383:VAL:HG22	1.98	0.45
1:B:175:SER:N	1:B:176:PRO:HD3	2.32	0.45
1:A:202:LEU:HD12	1:A:208:ILE:HD13	1.98	0.45
1:A:372:PRO:HG2	1:A:542:HIS:HB3	1.98	0.45
1:B:367:ILE:CD1	1:B:375:THR:HG21	2.46	0.45
1:A:540:GLU:HB2	1:A:543:GLU:HG3	1.99	0.45
1:B:411:VAL:HA	1:B:412:PRO:HD3	1.82	0.45
1:A:227:ASN:HB2	1:A:230:ASP:OD2	2.17	0.45
1:A:93:VAL:HG12	1:A:209:PRO:HB3	1.97	0.45
1:B:367:ILE:HD13	1:B:375:THR:CG2	2.46	0.45
1:B:154:ASN:OD1	1:B:157:VAL:HG12	2.16	0.44
1:A:424:LEU:HB3	1:A:582:LEU:HD22	2.00	0.44
1:A:122:ASN:HD22	1:A:123:ARG:CA	2.29	0.44
1:A:227:ASN:HD22	1:A:227:ASN:N	1.90	0.44
1:B:175:SER:N	1:B:176:PRO:CD	2.81	0.44
1:A:277:HIS:HB3	2:A:621:GOL:H32	2.00	0.43
1:B:344:MET:O	1:B:367:ILE:HA	2.18	0.43
1:A:214:HIS:H	1:A:214:HIS:HD2	1.62	0.43
1:A:214:HIS:CD2	1:A:214:HIS:N	2.87	0.43
1:A:103:ALA:O	1:A:480:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:VAL:HB	1:A:567:TYR:OH	2.19	0.42
1:B:179:ILE:O	1:B:179:ILE:HG22	2.19	0.42
1:A:418:GLU:H	1:A:418:GLU:HG3	1.57	0.42
1:A:439:THR:H	1:A:469:GLN:HB2	1.84	0.42
1:A:311:VAL:HG22	1:A:312:PHE:CE2	2.55	0.41
1:B:175:SER:HB3	1:B:212:ILE:HD12	2.02	0.41
1:A:217:TYR:CG	1:A:354:ILE:HD13	2.55	0.41
1:A:584:LEU:HD23	1:A:584:LEU:HA	1.83	0.41
1:B:100:LEU:CD1	1:B:474:THR:HG22	2.46	0.41
1:A:389:TYR:O	1:A:544:HIS:HB3	2.20	0.41
1:A:521:ASN:ND2	2:A:622:GOL:H32	2.35	0.41
1:A:65:CYS:HB3	1:A:101:ILE:O	2.21	0.41
1:A:384:ILE:HG23	1:A:403:LEU:HD22	2.03	0.41
1:B:83:ILE:HG22	1:B:84:SER:O	2.21	0.41
1:A:227:ASN:ND2	1:A:227:ASN:N	2.63	0.41
1:A:532:VAL:HG23	1:A:555:LEU:CD2	2.51	0.41
1:B:294:PHE:CE1	1:B:341:ILE:HD12	2.56	0.41
1:B:158:MET:HE1	1:B:169:LEU:HD23	2.03	0.41
1:B:384:ILE:HG23	1:B:403:LEU:HD22	2.03	0.41
1:A:293:HIS:HB3	1:A:610:LEU:HG	2.03	0.40
1:A:468:GLY:O	1:A:495:HIS:ND1	2.53	0.40
1:A:270:LEU:HD22	1:A:273:PHE:CG	2.56	0.40
1:A:305:ASP:O	1:A:309:GLN:HG3	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	618/631 (98%)	587 (95%)	30 (5%)	1 (0%)	43 44
1	B	590/631 (94%)	572 (97%)	18 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1208/1262 (96%)	1159 (96%)	48 (4%)	1 (0%)	48 50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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%)	504 (92%)	42 (8%)	12 9
1	B	524/555 (94%)	478 (91%)	46 (9%)	9 7
All	All	1070/1110 (96%)	982 (92%)	88 (8%)	10 8

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLU
1	A	53	LEU
1	A	75	LEU
1	A	82	GLU
1	A	120	GLU
1	A	122	ASN
1	A	123	ARG
1	A	124	LYS
1	A	128	GLU
1	A	129	ILE
1	A	153	LEU
1	A	158	MET
1	A	164	GLU
1	A	182	SER
1	A	202	LEU
1	A	214	HIS
1	A	216	VAL

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Mol	Chain	Res	Type
1	A	227	ASN
1	A	241	ARG
1	A	261	ASN
1	A	311	VAL
1	A	318	VAL
1	A	326	LYS
1	A	341	ILE
1	A	351	MET
1	A	352	THR
1	A	359	THR
1	A	367	ILE
1	A	390	VAL
1	A	393	GLU
1	A	394	GLU
1	A	401	LEU
1	A	403	LEU
1	A	418	GLU
1	A	429	GLU
1	A	448	GLU
1	A	460	LYS
1	A	569	GLU
1	A	592	ASN
1	A	607	GLN
1	A	610	LEU
1	A	619	GLU
1	B	5	ASN
1	B	29	LEU
1	B	48	GLU
1	B	55	ASP
1	B	57	GLU
1	B	58	GLN
1	B	66	THR
1	B	73	THR
1	B	80	VAL
1	B	85	ASP
1	B	93	VAL
1	B	115	GLN
1	B	136	SER
1	B	137	SER
1	B	153	LEU
1	B	155	LEU
1	B	157	VAL

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Mol	Chain	Res	Type
1	B	158	MET
1	B	161	ILE
1	B	187	LYS
1	B	214	HIS
1	B	233	ARG
1	B	243	ILE
1	B	254	VAL
1	B	296	LEU
1	B	351	MET
1	B	353	THR
1	B	359	THR
1	B	367	ILE
1	B	384	ILE
1	B	394	GLU
1	B	400	LEU
1	B	403	LEU
1	B	413	SER
1	B	419	LYS
1	B	424	LEU
1	B	429	GLU
1	B	440	MET
1	B	474	THR
1	B	480	ARG
1	B	486	LEU
1	B	501	TYR
1	B	532	VAL
1	B	549	LEU
1	B	618	LYS
1	B	619	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	5	ASN
1	A	54	GLN
1	A	58	GLN
1	A	89	GLN
1	A	122	ASN
1	A	125	ASN
1	A	193	GLN
1	A	201	GLN

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Mol	Chain	Res	Type
1	A	214	HIS
1	A	227	ASN
1	A	274	HIS
1	A	293	HIS
1	A	462	HIS
1	A	521	ASN
1	A	562	ASN
1	A	591	ASN
1	A	592	ASN
1	B	11	ASN
1	B	34	GLN
1	B	38	ASN
1	B	54	GLN
1	B	58	GLN
1	B	89	GLN
1	B	214	HIS
1	B	242	HIS
1	B	274	HIS
1	B	309	GLN
1	B	427	ASN
1	B	521	ASN
1	B	562	ASN
1	B	591	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 ⓘ

3 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	$\# Z > 2$
2	GOL	A	621	-	5,5,5	0.56	0	5,5,5	0.65	0
2	GOL	A	622	-	5,5,5	0.53	0	5,5,5	0.81	0
2	GOL	B	621	-	5,5,5	0.37	0	5,5,5	0.55	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
2	GOL	A	621	-	-	4/4/4/4	-
2	GOL	A	622	-	-	1/4/4/4	-
2	GOL	B	621	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	621	GOL	C1-C2-C3-O3
2	B	621	GOL	C1-C2-C3-O3
2	A	621	GOL	O1-C1-C2-C3
2	A	621	GOL	O2-C2-C3-O3
2	B	621	GOL	O2-C2-C3-O3
2	A	621	GOL	O1-C1-C2-O2
2	A	622	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	621	GOL	4	0
2	A	622	GOL	7	0
2	B	621	GOL	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.23	3 (0%) 87 88	12, 26, 44, 61	0
1	B	596/631 (94%)	-0.48	1 (0%) 91 92	10, 21, 37, 61	0
All	All	1216/1262 (96%)	-0.35	4 (0%) 90 91	10, 23, 43, 61	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	428	PRO	4.2
1	A	86	LEU	3.2
1	A	499	HIS	2.5
1	A	565	ASP	2.2

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
2	GOL	A	622	6/6	0.78	0.15	41,43,44,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	A	621	6/6	0.84	0.12	42,43,45,46	0
2	GOL	B	621	6/6	0.89	0.12	35,41,43,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.