



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:28 am BST

PDB ID : 3Q3I
Title : Crystal structure of the Actinobacillus pleuropneumoniae HMW1C glycosyl-transferase in the presence of peptide N1131
Authors : Kawai, F.; Yeo, H.J.
Deposited on : 2010-12-21
Resolution : 2.45 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 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 : 2.11
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) : 2.11

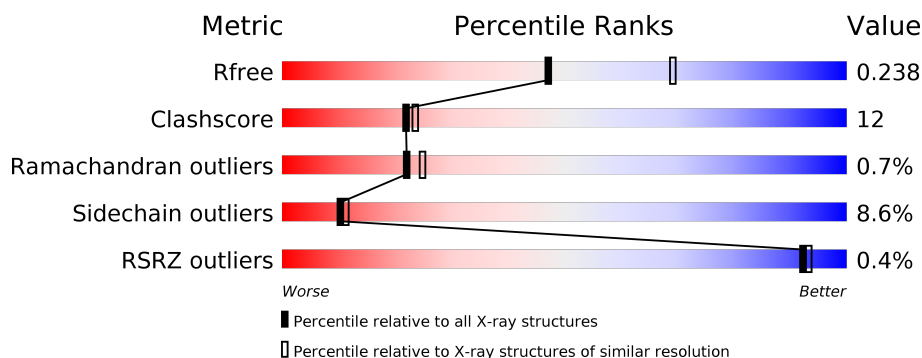
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 on 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	<div> <div style="width: 69%; background-color: green;"></div> <div style="width: 26%; background-color: yellow;"></div> <div style="width: 5%; background-color: orange;"></div> <div style="width: 0%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <p>69% 26% . .</p>
1	B	631	<div> <div style="width: 69%; background-color: green;"></div> <div style="width: 20%; background-color: yellow;"></div> <div style="width: 5%; background-color: orange;"></div> <div style="width: 6%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <p>% 69% 20% 5% 6%</p>

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	622	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9908 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	593	Total	C	N	O	S	0	0	0
			4754	3043	814	873	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 (three-letter code: 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		
2	B	1	Total	C	O	0	0
			6	3	3		

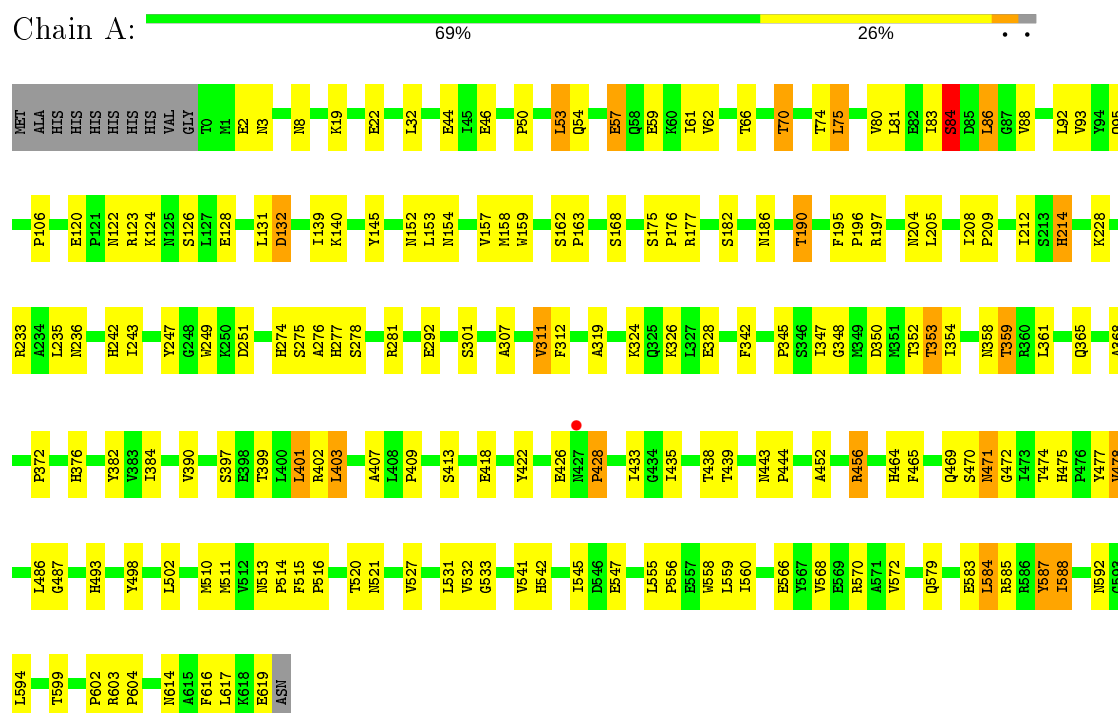
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	74	Total	O	0	0
			74	74		
3	B	89	Total	O	0	0
			89	89		

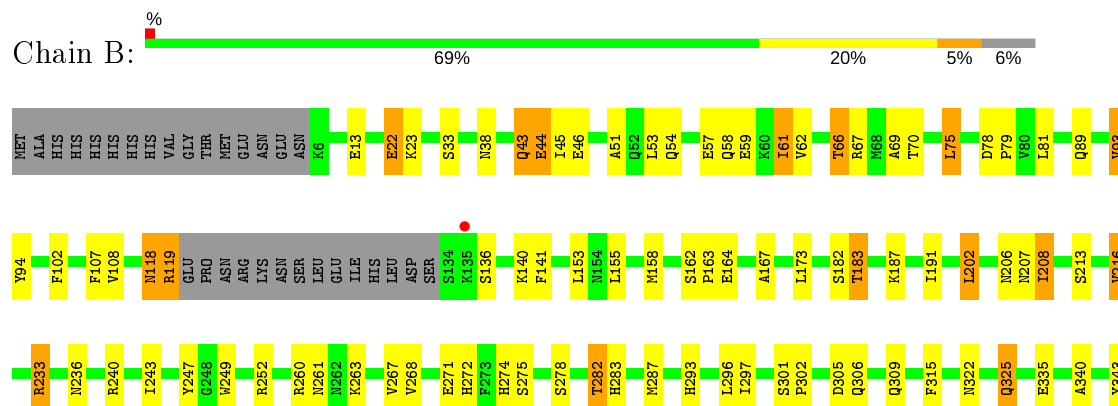
3 Residue-property plots

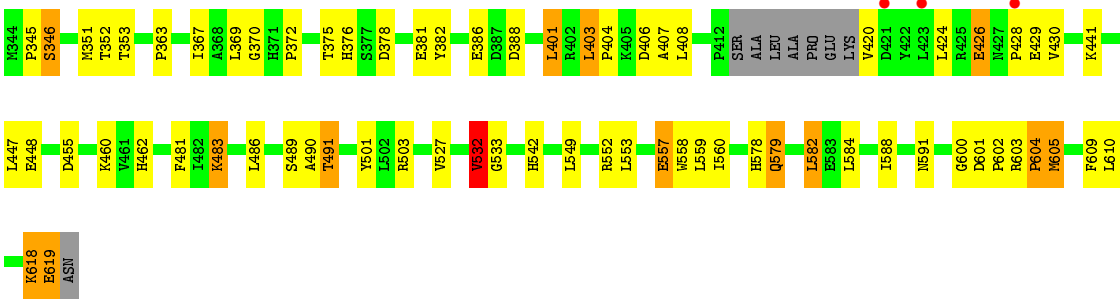
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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



- Molecule 1: HMW1C-like glycosyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.70 Å 93.26 Å 176.71 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.97 – 2.45 49.97 – 2.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.97-2.45) 93.9 (49.97-2.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.45 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.178 , 0.243 0.175 , 0.238	Depositor DCC
R_{free} test set	2329 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9908	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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: 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	0.99	5/5088 (0.1%)	0.92	4/6908 (0.1%)
1	B	1.02	4/4870 (0.1%)	0.96	7/6610 (0.1%)
All	All	1.00	9/9958 (0.1%)	0.94	11/13518 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	386	GLU	CD-OE1	7.31	1.33	1.25
1	A	22	GLU	CG-CD	6.82	1.62	1.51
1	A	477	TYR	CD1-CE1	6.23	1.48	1.39
1	B	532	VAL	CB-CG2	-6.14	1.40	1.52
1	A	422	TYR	CD2-CE2	-5.72	1.30	1.39
1	B	44	GLU	CB-CG	5.69	1.62	1.52
1	A	57	GLU	CG-CD	5.68	1.60	1.51
1	A	59	GLU	CG-CD	5.44	1.60	1.51
1	B	22	GLU	CG-CD	5.09	1.59	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	406	ASP	CB-CG-OD1	7.09	124.68	118.30
1	B	296	LEU	CB-CG-CD2	-6.33	100.23	111.00
1	A	402	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	B	552	ARG	NE-CZ-NH1	-6.05	117.28	120.30
1	B	233	ARG	CG-CD-NE	-5.81	99.60	111.80
1	B	406	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	B	455	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	378	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	86	LEU	CA-CB-CG	5.41	127.73	115.30
1	A	32	LEU	CB-CG-CD1	-5.32	101.95	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	177	ARG	NE-CZ-NH2	5.10	122.85	120.30

There are no chirality outliers.

There are no planarity outliers.

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	119	0
1	B	4754	0	4675	109	0
2	A	12	0	16	6	0
2	B	12	0	16	1	0
3	A	74	0	0	1	0
3	B	89	0	0	3	0
All	All	9908	0	9590	228	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 12.

All (228) 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:462:HIS:HE1	1:B:491:THR:HG22	1.22	1.02
1:A:62:VAL:O	1:A:66:THR:HG23	1.60	1.01
1:B:462:HIS:HE1	1:B:491:THR:CG2	1.78	0.96
1:B:233:ARG:NH1	1:B:376:HIS:CD2	2.35	0.94
1:A:556:PRO:HD2	1:A:559:LEU:HD12	1.51	0.92
1:A:452:ALA:O	1:A:456:ARG:HG2	1.73	0.88
1:B:462:HIS:CE1	1:B:491:THR:HG22	2.08	0.88
1:A:439:THR:HG23	1:A:469:GLN:HB2	1.56	0.87
1:B:233:ARG:NH1	1:B:376:HIS:HD2	1.72	0.86
1:B:233:ARG:HH11	1:B:376:HIS:CD2	1.95	0.84
1:A:88:VAL:HG13	1:A:139:ILE:HG23	1.61	0.81
1:B:62:VAL:O	1:B:66:THR:CG2	2.30	0.80
1:A:520:THR:H	2:A:622:GOL:H31	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:SER:HB2	1:B:302:PRO:CD	2.12	0.80
1:A:66:THR:O	1:A:70:THR:HG23	1.82	0.78
1:A:426:GLU:O	1:A:428:PRO:HD3	1.83	0.78
1:B:153:LEU:HD11	1:B:158:MET:CE	2.18	0.74
1:A:464:HIS:HD2	1:A:493:HIS:HE1	1.32	0.73
1:A:568:VAL:O	1:A:572:VAL:HG23	1.89	0.73
1:A:92:LEU:HD13	1:A:168:SER:HB3	1.70	0.73
1:B:233:ARG:HH12	1:B:376:HIS:HD2	1.33	0.73
1:A:547:GLU:HG3	1:A:560:ILE:HG21	1.70	0.72
1:B:532:VAL:HG23	1:B:588:ILE:CD1	2.20	0.72
1:B:532:VAL:HG23	1:B:588:ILE:HD13	1.72	0.71
1:B:62:VAL:O	1:B:66:THR:HG22	1.90	0.70
1:B:301:SER:HB2	1:B:302:PRO:HD2	1.73	0.70
1:B:57:GLU:O	1:B:61:ILE:HG13	1.92	0.69
1:B:62:VAL:O	1:B:66:THR:HG23	1.92	0.68
1:A:464:HIS:HD2	1:A:493:HIS:CE1	2.11	0.68
1:A:274:HIS:HD2	1:A:276:ALA:H	1.41	0.67
1:B:53:LEU:HD22	1:B:59:GLU:HB3	1.77	0.67
1:A:88:VAL:CG1	1:A:139:ILE:HG23	2.25	0.67
1:B:462:HIS:CE1	1:B:491:THR:CG2	2.70	0.66
1:B:579:GLN:HA	1:B:579:GLN:HE21	1.61	0.66
1:B:283:HIS:O	1:B:287:MET:HE2	1.95	0.65
1:A:464:HIS:CD2	1:A:493:HIS:HE1	2.14	0.64
1:B:119:ARG:N	1:B:119:ARG:HD2	2.12	0.64
1:A:204:ASN:HB2	1:A:242:HIS:HD2	1.63	0.64
1:B:532:VAL:CG2	1:B:588:ILE:CD1	2.77	0.63
1:B:167:ALA:HB3	1:B:208:ILE:HD11	1.81	0.62
1:B:57:GLU:O	1:B:61:ILE:CG1	2.48	0.62
1:B:23:LYS:NZ	3:B:661:HOH:O	2.30	0.62
1:B:153:LEU:HD21	1:B:155:LEU:HD23	1.83	0.60
1:B:252:ARG:HD2	1:B:335:GLU:OE1	2.01	0.60
1:B:293:HIS:CD2	1:B:610:LEU:HD22	2.36	0.60
1:A:342:PHE:HB3	1:A:365:GLN:HG2	1.84	0.60
1:A:347:ILE:HG13	1:A:353:THR:HG23	1.83	0.60
1:B:66:THR:O	1:B:70:THR:HG23	2.01	0.60
1:B:309:GLN:HG2	1:B:315:PHE:CD2	2.37	0.60
1:A:205:LEU:H	1:A:242:HIS:HD2	1.47	0.60
1:B:532:VAL:CG2	1:B:588:ILE:HD11	2.32	0.60
1:A:274:HIS:CD2	1:A:276:ALA:H	2.18	0.60
1:A:205:LEU:H	1:A:242:HIS:CD2	2.21	0.59
1:A:588:ILE:O	1:A:592:ASN:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:GLU:O	1:A:3:ASN:HB2	2.04	0.57
1:B:271:GLU:O	1:B:272:HIS:C	2.43	0.57
1:A:214:HIS:H	1:A:214:HIS:CD2	2.20	0.57
1:B:301:SER:CB	1:B:302:PRO:CD	2.79	0.57
1:B:275:SER:HB3	1:B:305:ASP:OD1	2.05	0.57
1:A:93:VAL:HG22	1:A:209:PRO:HB3	1.87	0.56
1:A:205:LEU:HD23	1:A:208:ILE:HD11	1.87	0.56
1:A:439:THR:HG23	1:A:469:GLN:CB	2.33	0.56
1:A:243:ILE:HG22	1:A:247:TYR:CD2	2.40	0.56
1:A:204:ASN:HB2	1:A:242:HIS:CD2	2.40	0.56
1:B:441:LYS:HZ1	2:B:622:GOL:H31	1.71	0.55
1:A:311:VAL:HG22	1:A:312:PHE:CE2	2.41	0.55
1:A:515:PHE:HB2	1:A:516:PRO:HA	1.88	0.55
1:A:443:ASN:HB2	1:A:444:PRO:CD	2.36	0.55
1:A:443:ASN:HB2	1:A:444:PRO:HD2	1.89	0.55
1:B:605:MET:HE2	1:B:609:PHE:HD2	1.71	0.55
1:B:213:SER:HA	1:B:216:VAL:HG13	1.89	0.54
1:A:521:ASN:H	2:A:622:GOL:H31	1.71	0.54
1:B:584:LEU:O	1:B:588:ILE:HG13	2.07	0.54
1:B:301:SER:HB2	1:B:302:PRO:HD3	1.90	0.54
1:B:369:LEU:HB3	1:B:372:PRO:HA	1.90	0.53
1:B:426:GLU:O	1:B:428:PRO:HD3	2.08	0.53
1:A:145:TYR:CE2	1:A:153:LEU:HD22	2.43	0.53
1:B:268:VAL:HA	1:B:343:TYR:O	2.08	0.53
1:A:359:THR:CG2	1:A:361:LEU:HG	2.38	0.52
1:A:350:ASP:O	1:A:353:THR:HG22	2.09	0.52
1:B:340:ALA:HA	1:B:363:PRO:HD2	1.91	0.52
1:B:33:SER:HB3	1:B:94:TYR:OH	2.09	0.52
1:B:118:ASN:HD22	1:B:118:ASN:H	1.56	0.52
1:A:498:TYR:CE1	1:A:502:LEU:HD11	2.45	0.52
1:B:382:TYR:HB3	1:B:401:LEU:HD22	1.92	0.52
1:A:168:SER:HA	1:A:209:PRO:HD3	1.92	0.51
1:B:187:LYS:O	1:B:191:ILE:HG13	2.10	0.51
1:B:367:ILE:HD13	1:B:375:THR:HG23	1.92	0.51
1:B:462:HIS:HE1	1:B:491:THR:HG23	1.72	0.51
1:A:382:TYR:HB3	1:A:401:LEU:HD22	1.93	0.50
1:A:435:ILE:HD12	1:A:465:PHE:CZ	2.45	0.50
1:A:154:ASN:OD1	1:A:157:VAL:HG23	2.11	0.50
1:B:274:HIS:CE1	1:B:305:ASP:HB3	2.46	0.50
1:A:439:THR:H	1:A:469:GLN:HB2	1.76	0.50
1:A:80:VAL:HG12	1:A:80:VAL:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:THR:HG21	3:B:641:HOH:O	2.10	0.50
1:B:346:SER:HB2	1:B:370:GLY:HA3	1.93	0.50
1:B:579:GLN:HE21	1:B:579:GLN:CA	2.24	0.50
1:B:136:SER:O	1:B:140:LYS:HG3	2.12	0.49
1:B:153:LEU:HD23	1:B:153:LEU:C	2.32	0.49
1:A:603:ARG:N	1:A:604:PRO:HD2	2.26	0.49
1:B:236:ASN:ND2	1:B:375:THR:O	2.44	0.49
1:A:84:SER:O	1:A:88:VAL:CG2	2.60	0.49
1:B:532:VAL:HG21	1:B:588:ILE:HD11	1.93	0.49
1:B:272:HIS:N	1:B:272:HIS:CD2	2.80	0.49
1:B:89:GLN:O	1:B:93:VAL:HG13	2.13	0.49
1:A:521:ASN:N	2:A:622:GOL:H31	2.28	0.49
1:B:13:GLU:OE2	1:B:67:ARG:HD2	2.13	0.48
1:A:54:GLN:HA	1:A:54:GLN:HE21	1.78	0.48
1:A:54:GLN:HA	1:A:54:GLN:NE2	2.28	0.48
1:A:214:HIS:HD2	1:A:214:HIS:H	1.59	0.48
1:A:214:HIS:N	1:A:214:HIS:CD2	2.82	0.48
1:A:93:VAL:CG2	1:A:209:PRO:HB3	2.43	0.48
1:B:271:GLU:OE1	1:B:346:SER:OG	2.31	0.48
1:A:407:ALA:O	1:A:602:PRO:HA	2.14	0.47
1:A:587:TYR:HD2	1:A:588:ILE:HD12	1.78	0.47
1:A:435:ILE:HD12	1:A:465:PHE:CE1	2.49	0.47
1:A:579:GLN:O	1:A:583:GLU:HG3	2.14	0.47
1:B:164:GLU:OE2	1:B:207:ASN:HB2	2.15	0.47
1:B:345:PRO:HD2	3:B:687:HOH:O	2.13	0.47
1:A:527:VAL:CG1	1:A:594:LEU:HG	2.45	0.47
1:A:558:TRP:O	1:A:570:ARG:HD2	2.14	0.47
1:A:521:ASN:HB2	2:A:622:GOL:H2	1.97	0.47
1:B:388:ASP:N	1:B:388:ASP:OD1	2.44	0.47
1:B:430:VAL:HG22	1:B:460:LYS:HD3	1.95	0.47
1:B:527:VAL:HG21	1:B:553:LEU:HD13	1.97	0.47
1:B:619:GLU:OE1	1:B:619:GLU:HA	2.15	0.47
1:A:486:LEU:O	1:A:487:GLY:C	2.51	0.47
1:A:249:TRP:NE1	1:A:251:ASP:OD1	2.39	0.46
1:A:319:ALA:O	1:A:326:LYS:HA	2.15	0.46
1:B:372:PRO:HB2	1:B:542:HIS:HB3	1.97	0.46
1:A:587:TYR:CD2	1:A:588:ILE:HD12	2.50	0.46
1:A:8:ASN:ND2	1:A:46:GLU:HG2	2.31	0.46
1:B:118:ASN:N	1:B:118:ASN:HD22	2.13	0.46
1:A:348:GLY:H	1:A:353:THR:HG21	1.79	0.46
1:B:603:ARG:N	1:B:604:PRO:CD	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:SER:O	1:B:282:THR:HG23	2.15	0.46
1:B:141:PHE:CE2	1:B:153:LEU:HD12	2.51	0.46
1:A:407:ALA:C	1:A:409:PRO:HD3	2.35	0.46
1:B:588:ILE:H	1:B:588:ILE:HG13	1.58	0.46
1:B:240:ARG:O	1:B:243:ILE:HG12	2.16	0.46
1:B:428:PRO:HG2	1:B:578:HIS:ND1	2.31	0.46
1:A:382:TYR:CB	1:A:401:LEU:HD22	2.46	0.46
1:B:426:GLU:HA	1:B:582:LEU:HD11	1.98	0.46
1:A:469:GLN:OE1	1:A:469:GLN:HA	2.17	0.45
1:A:243:ILE:HG22	1:A:247:TYR:CE2	2.51	0.45
1:A:57:GLU:O	1:A:61:ILE:HG12	2.17	0.45
1:A:66:THR:CG2	1:A:106:PRO:HD3	2.47	0.45
1:A:372:PRO:HB2	1:A:542:HIS:HB3	1.97	0.45
1:B:483:LYS:NZ	1:B:490:ALA:O	2.46	0.45
1:A:438:THR:HB	1:A:469:GLN:HG2	1.98	0.45
1:B:162:SER:HA	1:B:163:PRO:HD3	1.67	0.45
1:B:403:LEU:HB3	1:B:407:ALA:HB3	1.97	0.45
1:A:75:LEU:HD22	1:A:81:LEU:HD22	1.98	0.45
1:A:566:GLU:O	1:A:570:ARG:HG2	2.17	0.45
1:B:322:ASN:OD1	1:B:325:GLN:HB2	2.17	0.45
1:A:236:ASN:HB3	1:A:358:ASN:OD1	2.16	0.45
1:A:54:GLN:CA	1:A:54:GLN:NE2	2.80	0.45
1:A:438:THR:HB	1:A:469:GLN:CG	2.48	0.44
1:B:153:LEU:HD11	1:B:158:MET:HE1	1.97	0.44
1:B:605:MET:CE	1:B:609:PHE:HD2	2.31	0.44
1:A:324:LYS:O	1:A:328:GLU:HG3	2.18	0.44
1:A:175:SER:N	1:A:176:PRO:CD	2.81	0.44
1:A:159:TRP:O	1:A:163:PRO:HG3	2.17	0.44
1:A:186:ASN:O	1:A:190:THR:HG23	2.18	0.43
1:A:511:MET:O	1:A:533:GLY:HA3	2.18	0.43
1:B:367:ILE:HD13	1:B:375:THR:CG2	2.49	0.43
1:B:202:LEU:HD12	1:B:202:LEU:HA	1.77	0.43
1:B:486:LEU:O	1:B:489:SER:HB2	2.17	0.43
1:A:531:LEU:HD23	1:A:585:ARG:CZ	2.49	0.43
1:B:582:LEU:HA	1:B:582:LEU:HD22	1.84	0.43
1:A:195:PHE:N	1:A:196:PRO:CD	2.81	0.43
1:B:153:LEU:CD2	1:B:155:LEU:HD23	2.49	0.43
1:B:38:ASN:ND2	1:B:43:GLN:O	2.52	0.43
1:A:131:LEU:C	1:A:132:ASP:O	2.54	0.43
1:A:175:SER:HB3	1:A:212:ILE:HD12	2.01	0.43
1:A:345:PRO:HA	1:A:368:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:ASN:HA	1:A:514:PRO:HD3	1.89	0.43
1:A:527:VAL:HG11	1:A:594:LEU:HG	2.01	0.43
1:A:84:SER:O	1:A:88:VAL:HG23	2.18	0.43
1:B:532:VAL:HG21	1:B:584:LEU:HG	2.01	0.43
1:A:603:ARG:N	1:A:604:PRO:CD	2.82	0.43
1:B:267:VAL:HG22	1:B:297:ILE:HB	2.01	0.43
1:B:301:SER:CB	1:B:302:PRO:HD2	2.44	0.43
1:A:19:LYS:HD2	3:A:657:HOH:O	2.19	0.42
1:B:407:ALA:HA	1:B:601:ASP:O	2.19	0.42
1:B:75:LEU:HD22	1:B:81:LEU:HD22	2.02	0.42
1:A:83:ILE:HD12	1:A:140:LYS:HG2	2.00	0.42
1:A:278:SER:HB3	1:A:281:ARG:NH2	2.35	0.42
1:A:275:SER:HB3	1:A:307:ALA:HB3	2.01	0.42
1:B:13:GLU:OE2	1:B:67:ARG:CD	2.67	0.42
1:A:470:SER:HB3	1:A:475:HIS:ND1	2.34	0.42
1:A:50:PRO:HD2	1:A:53:LEU:HD22	2.01	0.42
1:B:533:GLY:O	1:B:559:LEU:HD13	2.19	0.42
1:B:57:GLU:O	1:B:61:ILE:HG12	2.19	0.42
1:B:605:MET:HE3	1:B:609:PHE:CE2	2.54	0.42
1:B:69:ALA:HB1	1:B:102:PHE:CE1	2.54	0.42
1:A:92:LEU:CD1	1:A:168:SER:HB3	2.47	0.42
1:A:584:LEU:HD13	1:A:584:LEU:HA	1.90	0.42
1:A:474:THR:O	1:A:478:VAL:HG12	2.19	0.41
1:A:555:LEU:HA	1:A:555:LEU:HD23	1.77	0.41
1:B:107:PHE:O	1:B:108:VAL:HB	2.19	0.41
1:B:420:VAL:HG22	1:B:420:VAL:O	2.20	0.41
1:B:605:MET:CE	1:B:609:PHE:CD2	3.04	0.41
1:A:384:ILE:HG23	1:A:403:LEU:HD22	2.01	0.41
1:A:541:VAL:O	1:A:545:ILE:HG13	2.20	0.41
1:B:600:GLY:O	1:B:602:PRO:HD3	2.20	0.41
1:A:587:TYR:C	1:A:587:TYR:CD2	2.94	0.41
1:B:78:ASP:HA	1:B:79:PRO:HD3	1.92	0.41
1:A:614:ASN:HA	1:A:617:LEU:HD12	2.03	0.41
1:B:153:LEU:HD11	1:B:158:MET:HE3	2.00	0.41
1:B:260:ARG:O	1:B:263:LYS:N	2.41	0.41
1:B:447:LEU:HG	1:B:481:PHE:CZ	2.56	0.41
1:A:66:THR:HG21	1:A:106:PRO:HD3	2.03	0.41
1:A:162:SER:HA	1:A:163:PRO:HD3	1.93	0.41
1:A:354:ILE:HG22	1:A:354:ILE:O	2.20	0.41
1:A:153:LEU:HD11	1:A:158:MET:CE	2.51	0.41
1:A:520:THR:H	2:A:622:GOL:C3	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:THR:H	1:A:469:GLN:CG	2.34	0.40
1:B:557:GLU:HA	1:B:560:ILE:HD12	2.03	0.40
1:A:376:HIS:HD2	1:A:397:SER:HB3	1.86	0.40
1:A:433:ILE:HA	1:A:510:MET:O	2.22	0.40
1:A:277:HIS:ND1	2:A:621:GOL:H31	2.36	0.40
1:A:471:ASN:O	1:A:472:GLY:C	2.59	0.40
1:A:475:HIS:HA	1:A:478:VAL:HG13	2.04	0.40
1:B:173:LEU:HD12	1:B:191:ILE:HD11	2.03	0.40
1:B:558:TRP:CZ3	1:B:559:LEU:HD23	2.57	0.40
1:A:359:THR:HG22	1:A:361:LEU:HG	2.03	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%)	575 (93%)	39 (6%)	4 (1%)	25	29
1	B	587/631 (93%)	553 (94%)	29 (5%)	5 (1%)	17	19
All	All	1205/1262 (96%)	1128 (94%)	68 (6%)	9 (1%)	22	25

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	ASP
1	B	51	ALA
1	B	618	LYS
1	A	84	SER
1	A	428	PRO
1	B	249	TRP
1	B	261	ASN
1	A	228	LYS

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Mol	Chain	Res	Type
1	B	404	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%)	503 (92%)	43 (8%)	12	14
1	B	521/555 (94%)	472 (91%)	49 (9%)	8	9
All	All	1067/1110 (96%)	975 (91%)	92 (9%)	10	11

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLU
1	A	53	LEU
1	A	70	THR
1	A	74	THR
1	A	75	LEU
1	A	84	SER
1	A	86	LEU
1	A	95	GLN
1	A	120	GLU
1	A	122	ASN
1	A	123	ARG
1	A	124	LYS
1	A	126	SER
1	A	128	GLU
1	A	152	ASN
1	A	182	SER
1	A	190	THR
1	A	197	ARG
1	A	214	HIS
1	A	233	ARG
1	A	235	LEU
1	A	292	GLU

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Mol	Chain	Res	Type
1	A	301	SER
1	A	311	VAL
1	A	352	THR
1	A	353	THR
1	A	359	THR
1	A	390	VAL
1	A	399	THR
1	A	401	LEU
1	A	403	LEU
1	A	413	SER
1	A	418	GLU
1	A	456	ARG
1	A	471	ASN
1	A	478	VAL
1	A	532	VAL
1	A	584	LEU
1	A	587	TYR
1	A	588	ILE
1	A	599	THR
1	A	616	PHE
1	A	619	GLU
1	B	22	GLU
1	B	43	GLN
1	B	44	GLU
1	B	45	ILE
1	B	46	GLU
1	B	54	GLN
1	B	58	GLN
1	B	61	ILE
1	B	66	THR
1	B	75	LEU
1	B	93	VAL
1	B	118	ASN
1	B	119	ARG
1	B	182	SER
1	B	183	THR
1	B	202	LEU
1	B	206	ASN
1	B	208	ILE
1	B	216	VAL
1	B	247	TYR
1	B	282	THR

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Mol	Chain	Res	Type
1	B	306	GLN
1	B	325	GLN
1	B	346	SER
1	B	351	MET
1	B	352	THR
1	B	353	THR
1	B	381	GLU
1	B	401	LEU
1	B	403	LEU
1	B	408	LEU
1	B	424	LEU
1	B	426	GLU
1	B	429	GLU
1	B	448	GLU
1	B	483	LYS
1	B	491	THR
1	B	501	TYR
1	B	503	ARG
1	B	532	VAL
1	B	549	LEU
1	B	557	GLU
1	B	579	GLN
1	B	582	LEU
1	B	591	ASN
1	B	604	PRO
1	B	605	MET
1	B	618	LYS
1	B	619	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	58	GLN
1	A	214	HIS
1	A	242	HIS
1	A	274	HIS
1	A	376	HIS
1	A	464	HIS
1	A	471	ASN
1	A	493	HIS
1	A	579	GLN

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Mol	Chain	Res	Type
1	A	614	ASN
1	B	34	GLN
1	B	38	ASN
1	B	115	GLN
1	B	118	ASN
1	B	206	ASN
1	B	214	HIS
1	B	261	ASN
1	B	272	HIS
1	B	274	HIS
1	B	293	HIS
1	B	376	HIS
1	B	462	HIS
1	B	499	HIS
1	B	579	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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
2	GOL	A	622	-	5,5,5	0.29	0	5,5,5	0.53	0
2	GOL	B	622	-	5,5,5	0.74	0	5,5,5	1.19	1 (20%)
2	GOL	B	621	-	5,5,5	0.47	0	5,5,5	0.61	0
2	GOL	A	621	-	5,5,5	0.69	0	5,5,5	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	622	-	-	2/4/4/4	-
2	GOL	B	622	-	-	2/4/4/4	-
2	GOL	B	621	-	-	3/4/4/4	-
2	GOL	A	621	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	622	GOL	O3-C3-C2	-2.13	99.99	110.20

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	622	GOL	5	0
2	B	622	GOL	1	0
2	A	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%)	-0.52	1 (0%) 95 95	22, 36, 57, 76	0
1	B	593/631 (93%)	-0.58	4 (0%) 87 88	21, 34, 54, 97	0
All	All	1213/1262 (96%)	-0.55	5 (0%) 92 93	21, 35, 57, 97	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	421	ASP	4.1
1	B	423	LEU	3.0
1	B	428	PRO	2.8
1	A	427	ASN	2.2
1	B	135	LYS	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 carbohydrates 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(\AA^2)	Q<0.9
2	GOL	B	621	6/6	0.90	0.11	39,45,51,53	0
2	GOL	A	622	6/6	0.93	0.14	44,47,48,49	0
2	GOL	A	621	6/6	0.96	0.14	44,47,52,56	0
2	GOL	B	622	6/6	0.97	0.15	43,44,46,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.