



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:24 AM GMT

PDB ID : 2WW0  
Title : Structure of the Family GH92 Inverting Mannosidase BT3990 from Bacteroides  
          thetaiotaomicron VPI-5482  
Authors : Suits, M.D.L.; Thompson, A.; Zhu, Y.; Gilbert, H.J.; Davies, G.J.  
Deposited on : 2009-10-21  
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

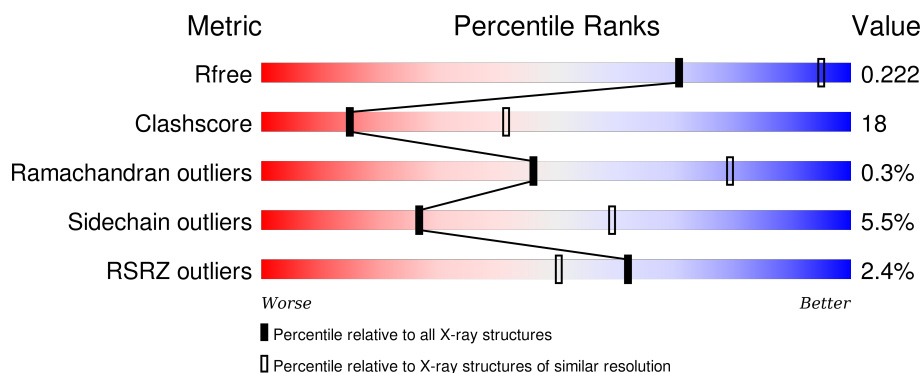
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	744	<div> <div></div> <div>71%25%..</div> </div>
1	B	744	<div> <div></div> <div>71%25%..</div> </div>
1	C	744	<div> <div></div> <div>72%23%..</div> </div>
1	D	744	<div> <div></div> <div>70%26%..</div> </div>
1	E	744	<div> <div>%</div> <div>72%24%..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	744	
1	G	744	
1	H	744	

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	GOL	A	802	-	-	-	X
4	GOL	A	803	-	-	-	X
4	GOL	A	804	-	-	-	X
4	GOL	A	806	-	-	-	X
4	GOL	B	802	-	-	-	X
4	GOL	B	804	-	-	X	X
4	GOL	C	803	-	-	X	X
4	GOL	C	804	-	-	-	X
4	GOL	D	802	-	-	-	X
4	GOL	D	803	-	-	-	X
4	GOL	D	804	-	-	-	X
4	GOL	E	803	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 48426 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 PUTATIVE ALPHA-1,2-MANNOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	736	Total	C	N	O	S	0	3	0
			5977	3834	984	1125	34			
1	B	736	Total	C	N	O	S	0	5	0
			5997	3847	984	1131	35			
1	C	737	Total	C	N	O	S	0	2	0
			5979	3835	984	1126	34			
1	D	738	Total	C	N	O	S	0	2	0
			5984	3837	984	1129	34			
1	E	736	Total	C	N	O	S	0	2	0
			5956	3820	983	1120	33			
1	F	736	Total	C	N	O	S	0	1	0
			5954	3818	981	1121	34			
1	G	736	Total	C	N	O	S	0	0	0
			5932	3802	975	1123	32			
1	H	736	Total	C	N	O	S	0	0	0
			5899	3779	968	1120	32			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

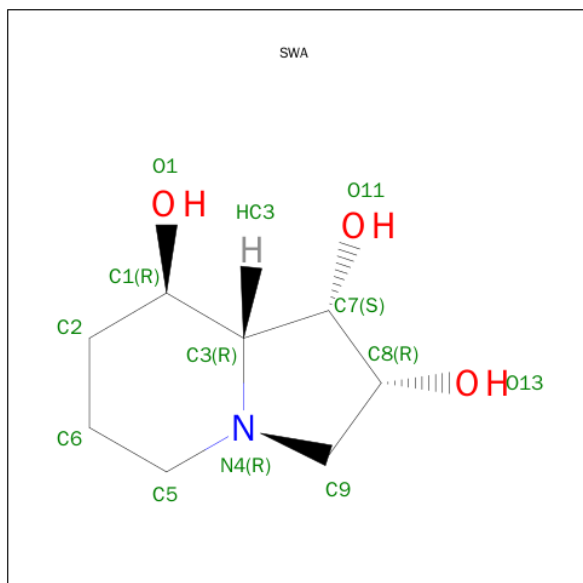
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	E	1	Total	Ca	0	0
			1	1		
2	H	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	F	1	Total	Ca	0	0
			1	1		

- Molecule 3 is 1S-8AB-OCTAHYDRO-INDOLIZIDINE-1A,2A,8B-TRIOL (three-letter code: SWA) (formula:  $C_8H_{15}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	8	1	3		
3	B	1	Total	C	N	O	0	0
			12	8	1	3		
3	C	1	Total	C	N	O	0	0
			12	8	1	3		
3	D	1	Total	C	N	O	0	0
			12	8	1	3		
3	E	1	Total	C	N	O	0	0
			12	8	1	3		
3	F	1	Total	C	N	O	0	0
			12	8	1	3		
3	G	1	Total	C	N	O	0	0
			12	8	1	3		
3	H	1	Total	C	N	O	0	0
			12	8	1	3		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

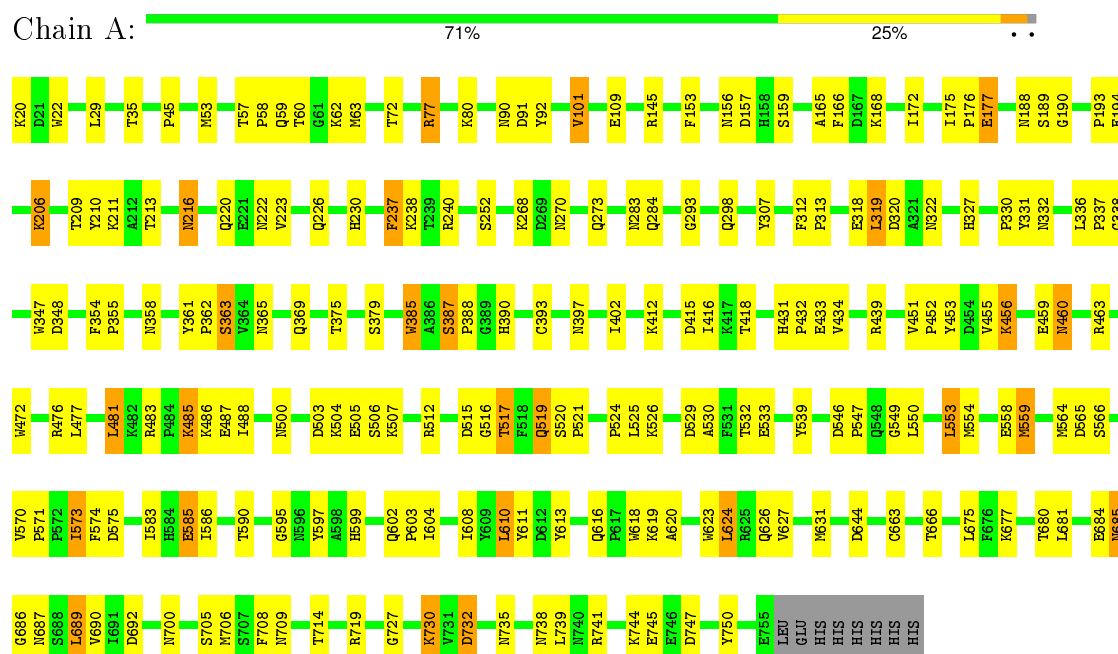
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	117	Total	O	0	0
			117	117		
5	B	105	Total	O	0	0
			105	105		
5	C	80	Total	O	0	0
			80	80		
5	D	110	Total	O	0	0
			110	110		
5	E	77	Total	O	0	0
			77	77		
5	F	42	Total	O	0	0
			42	42		
5	G	6	Total	O	0	0
			6	6		
5	H	5	Total	O	0	0
			5	5		

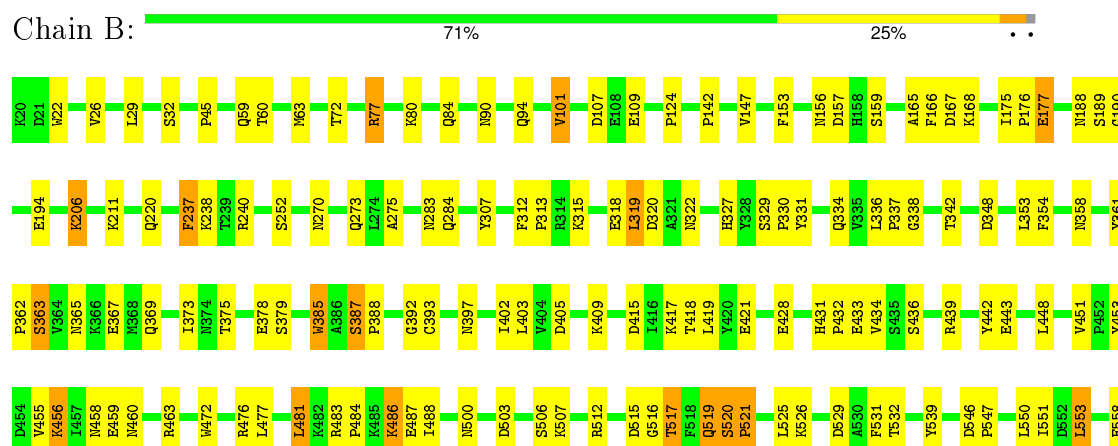
### 3 Residue-property plots

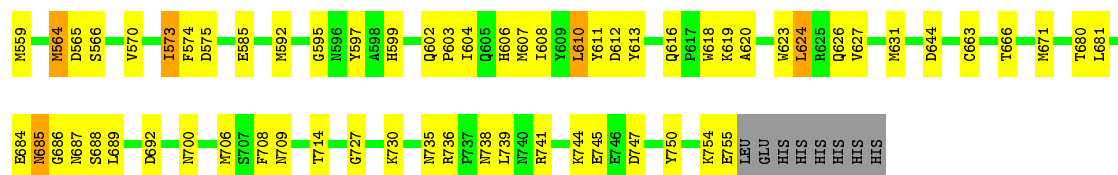
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: PUTATIVE ALPHA-1,2-MANNOSIDASE



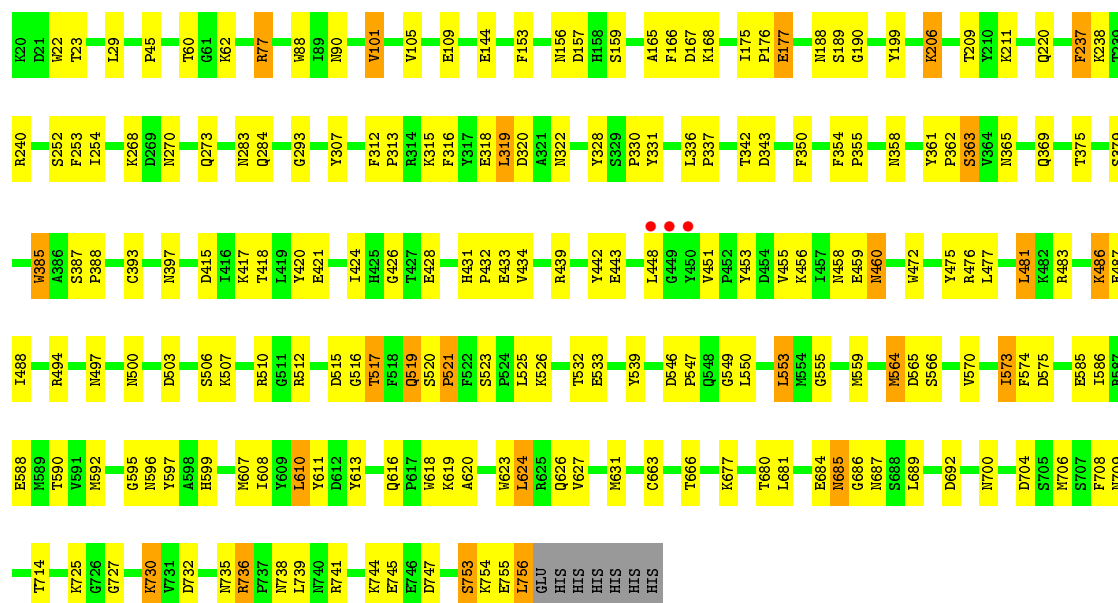
#### • Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE





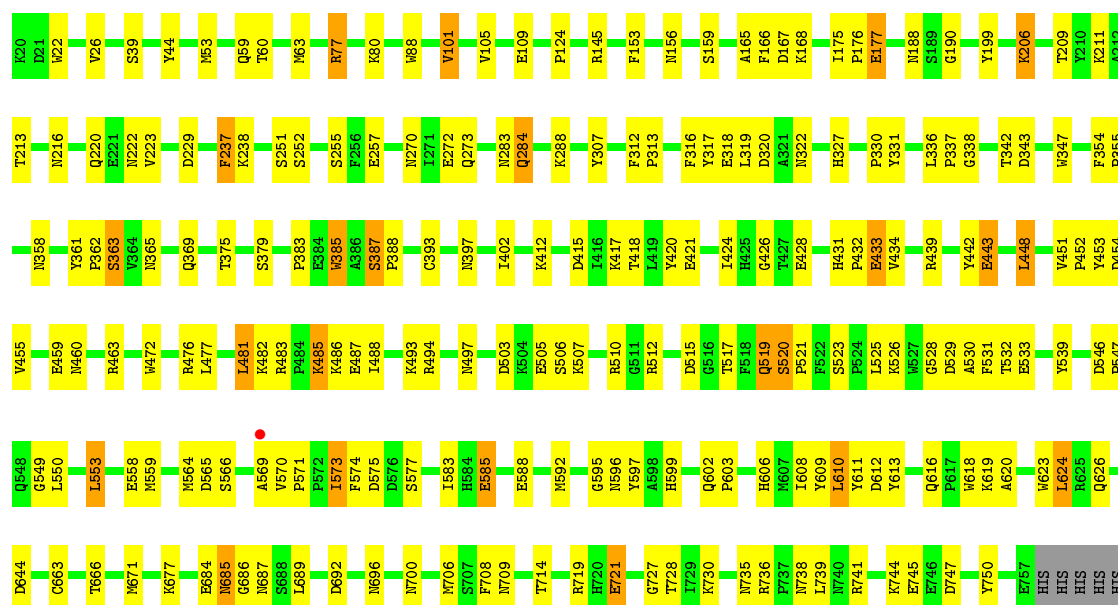
• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE

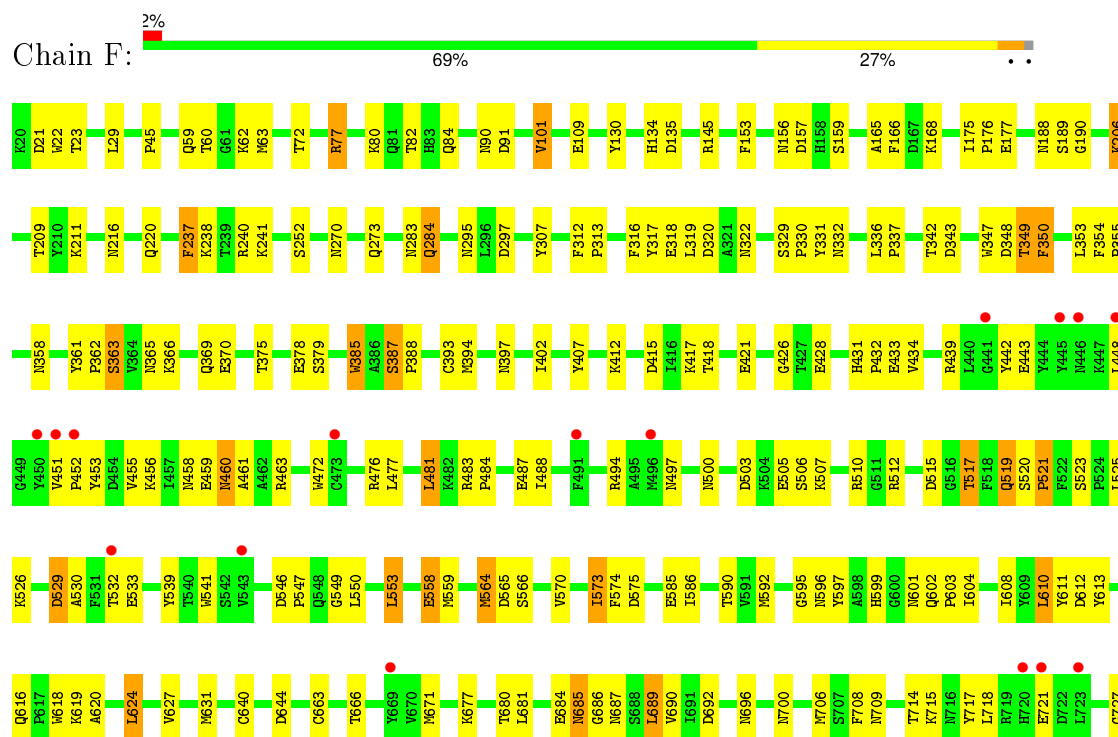
Chain C: 72% 23%

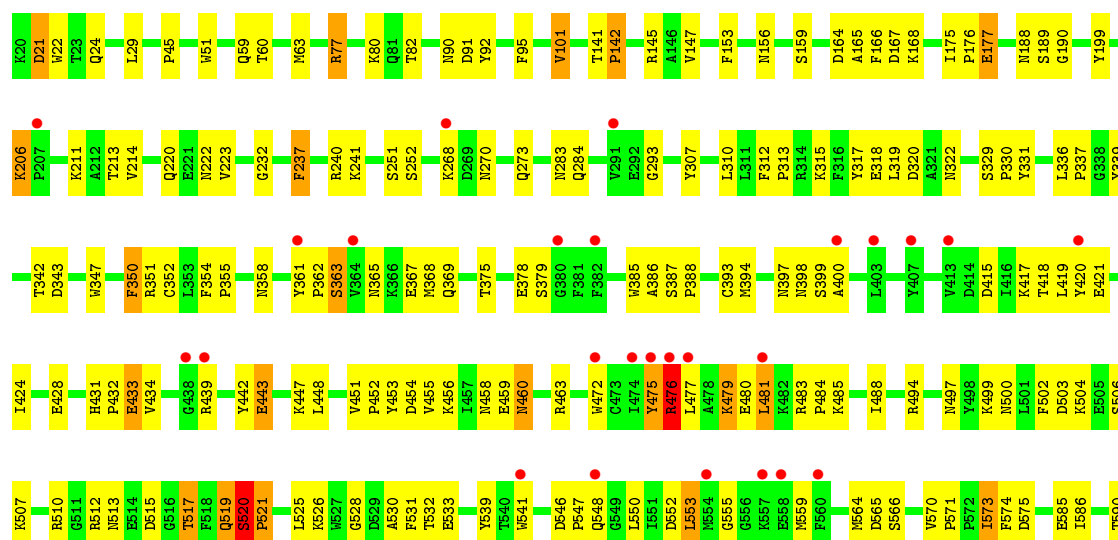


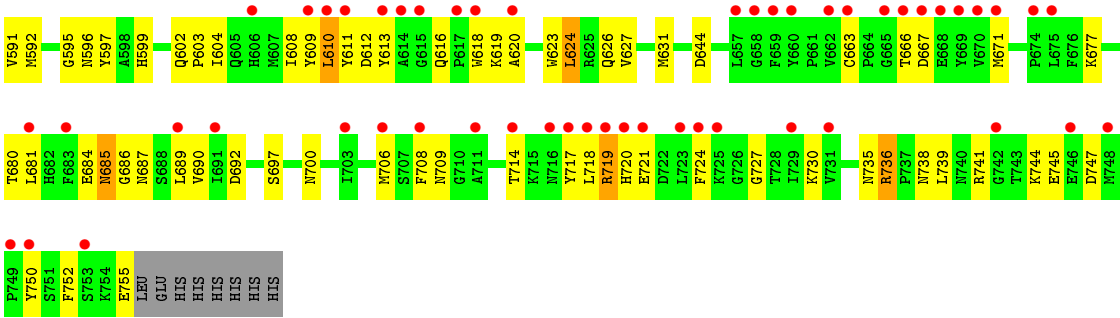
• Molecule 1: PUTATIVE ALPHA-1,2-MANNOSIDASE

Chain D: 70% 26%









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.81Å 151.96Å 218.62Å 90.00° 93.43° 90.00°	Depositor
Resolution (Å)	218.23 – 2.80 65.61 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.9 (218.23-2.80) 97.9 (65.61-2.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, $R_{free}$	0.184 , 0.212 0.195 , 0.222	Depositor DCC
$R_{free}$ test set	8504 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.0	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 38.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 169339 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	48426	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.64 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.7470e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: SWA, GOL, CA

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	0.58	0/6167	0.64	2/8365 (0.0%)
1	B	0.60	0/6193	0.63	2/8398 (0.0%)
1	C	0.57	0/6166	0.63	2/8365 (0.0%)
1	D	0.60	1/6171 (0.0%)	0.65	4/8373 (0.0%)
1	E	0.57	1/6143 (0.0%)	0.64	1/8337 (0.0%)
1	F	0.51	0/6138	0.61	3/8330 (0.0%)
1	G	0.46	0/6113	0.60	5/8303 (0.1%)
1	H	0.49	1/6079 (0.0%)	0.62	4/8265 (0.0%)
All	All	0.55	3/49170 (0.0%)	0.63	23/66736 (0.0%)

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	3
1	B	0	4
1	C	0	3
1	D	0	3
1	E	0	3
1	F	0	3
1	G	0	3
1	H	0	3
All	All	0	25

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	721	GLU	CG-CD	5.88	1.60	1.51
1	E	428	GLU	CG-CD	5.38	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	476	ARG	NE-CZ	5.28	1.40	1.33

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	448	LEU	CA-CB-CG	-7.07	99.05	115.30
1	G	145	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	B	211	LYS	CD-CE-NZ	6.31	126.20	111.70
1	E	643	GLU	CA-CB-CG	6.28	127.22	113.40
1	C	730	LYS	CB-CG-CD	6.27	127.91	111.60

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	312	PHE	Peptide
1	A	387	SER	Peptide
1	A	520	SER	Peptide
1	B	312	PHE	Peptide
1	B	387	SER	Mainchain

## 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	5977	0	5654	180	0
1	B	5997	0	5677	199	0
1	C	5979	0	5652	165	0
1	D	5984	0	5647	194	0
1	E	5956	0	5614	173	0
1	F	5954	0	5610	220	0
1	G	5932	0	5554	236	0
1	H	5899	0	5483	274	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	12	0	13	3	0
3	B	12	0	14	2	0
3	C	12	0	14	4	0
3	D	12	0	14	5	0
3	E	12	0	14	1	0
3	F	12	0	13	5	0
3	G	12	0	13	5	0
3	H	12	0	12	5	0
4	A	30	0	40	3	0
4	B	18	0	24	6	0
4	C	18	0	24	6	0
4	D	18	0	24	5	0
4	E	12	0	16	0	0
4	F	6	0	8	0	0
5	A	117	0	0	6	0
5	B	105	0	0	11	0
5	C	80	0	0	2	0
5	D	110	0	0	14	0
5	E	77	0	0	2	0
5	F	42	0	0	8	0
5	G	6	0	0	0	0
5	H	5	0	0	0	0
All	All	48426	0	45134	1638	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 18.

The worst 5 of 1638 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:592[B]:MET:CE	1:B:631:MET:HE1	1.22	1.60
1:C:592[B]:MET:CE	1:C:631:MET:HE1	1.27	1.59
1:B:592[B]:MET:HE2	1:B:631:MET:CE	1.20	1.58
1:H:472:TRP:CE2	1:H:476:ARG:HD3	1.02	1.54
1:H:472:TRP:CE2	1:H:476:ARG:CD	1.92	1.52

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	737/744 (99%)	713 (97%)	22 (3%)	2 (0%)	46	79
1	B	739/744 (99%)	711 (96%)	26 (4%)	2 (0%)	46	79
1	C	737/744 (99%)	712 (97%)	23 (3%)	2 (0%)	46	79
1	D	738/744 (99%)	710 (96%)	26 (4%)	2 (0%)	46	79
1	E	736/744 (99%)	711 (97%)	23 (3%)	2 (0%)	46	79
1	F	735/744 (99%)	709 (96%)	23 (3%)	3 (0%)	39	74
1	G	734/744 (99%)	707 (96%)	25 (3%)	2 (0%)	46	79
1	H	734/744 (99%)	707 (96%)	25 (3%)	2 (0%)	46	79
All	All	5890/5952 (99%)	5680 (96%)	193 (3%)	17 (0%)	46	79

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	521	PRO
1	C	521	PRO
1	F	521	PRO
1	G	521	PRO
1	A	521	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	636/643 (99%)	598 (94%)	38 (6%)	24	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	640/643 (100%)	609 (95%)	31 (5%)	31	66
1	C	636/643 (99%)	599 (94%)	37 (6%)	25	57
1	D	636/643 (99%)	602 (95%)	34 (5%)	28	61
1	E	631/643 (98%)	595 (94%)	36 (6%)	25	58
1	F	631/643 (98%)	595 (94%)	36 (6%)	25	58
1	G	626/643 (97%)	594 (95%)	32 (5%)	29	63
1	H	618/643 (96%)	581 (94%)	37 (6%)	24	56
All	All	5054/5144 (98%)	4773 (94%)	281 (6%)	27	59

5 of 281 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	577	SER
1	E	519	GLN
1	H	443	GLU
1	D	610	LEU
1	E	177	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 176 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	497	ASN
1	E	446	ASN
1	H	374	ASN
1	D	519	GLN
1	E	59	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 33 ligands modelled in this entry, 8 are monoatomic - leaving 25 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$
3	SWA	A	801	2	13,13,13	0.63	0	13,19,19	3.48	2 (15%)
4	GOL	A	802	-	5,5,5	0.31	0	5,5,5	0.16	0
4	GOL	A	803	-	5,5,5	0.42	0	5,5,5	1.19	0
4	GOL	A	804	-	5,5,5	0.51	0	5,5,5	1.26	0
4	GOL	A	805	-	5,5,5	0.31	0	5,5,5	0.61	0
4	GOL	A	806	-	5,5,5	0.38	0	5,5,5	0.32	0
3	SWA	B	801	2	13,13,13	1.08	1 (7%)	13,19,19	2.32	2 (15%)
4	GOL	B	802	-	5,5,5	0.34	0	5,5,5	0.64	0
4	GOL	B	803	-	5,5,5	0.43	0	5,5,5	0.50	0
4	GOL	B	804	-	5,5,5	0.47	0	5,5,5	0.98	0
3	SWA	C	801	2	13,13,13	0.94	1 (7%)	13,19,19	2.34	3 (23%)
4	GOL	C	802	-	5,5,5	0.38	0	5,5,5	0.24	0
4	GOL	C	803	-	5,5,5	0.42	0	5,5,5	0.59	0
4	GOL	C	804	-	5,5,5	0.42	0	5,5,5	1.14	1 (20%)
3	SWA	D	801	2	13,13,13	1.42	2 (15%)	13,19,19	2.83	2 (15%)
4	GOL	D	802	-	5,5,5	0.39	0	5,5,5	0.25	0
4	GOL	D	803	-	5,5,5	0.40	0	5,5,5	0.84	0
4	GOL	D	804	-	5,5,5	0.34	0	5,5,5	0.59	0
3	SWA	E	801	2	13,13,13	0.85	0	13,19,19	2.49	2 (15%)
4	GOL	E	802	-	5,5,5	0.33	0	5,5,5	0.84	0
4	GOL	E	803	-	5,5,5	0.37	0	5,5,5	0.42	0
3	SWA	F	801	2	13,13,13	0.78	0	13,19,19	0.92	1 (7%)
4	GOL	F	802	-	5,5,5	0.37	0	5,5,5	0.44	0
3	SWA	G	801	2	13,13,13	1.41	2 (15%)	13,19,19	2.09	2 (15%)
3	SWA	H	801	2	13,13,13	1.26	1 (7%)	13,19,19	3.00	3 (23%)

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	SWA	A	801	2	-	0/0/26/26	0/2/2/2
4	GOL	A	802	-	-	0/4/4/4	0/0/0/0
4	GOL	A	803	-	-	0/4/4/4	0/0/0/0
4	GOL	A	804	-	-	0/4/4/4	0/0/0/0
4	GOL	A	805	-	-	0/4/4/4	0/0/0/0
4	GOL	A	806	-	-	0/4/4/4	0/0/0/0
3	SWA	B	801	2	-	0/0/26/26	0/2/2/2
4	GOL	B	802	-	-	0/4/4/4	0/0/0/0
4	GOL	B	803	-	-	0/4/4/4	0/0/0/0
4	GOL	B	804	-	-	0/4/4/4	0/0/0/0
3	SWA	C	801	2	-	0/0/26/26	0/2/2/2
4	GOL	C	802	-	-	0/4/4/4	0/0/0/0
4	GOL	C	803	-	-	0/4/4/4	0/0/0/0
4	GOL	C	804	-	-	0/4/4/4	0/0/0/0
3	SWA	D	801	2	-	0/0/26/26	0/2/2/2
4	GOL	D	802	-	-	0/4/4/4	0/0/0/0
4	GOL	D	803	-	-	0/4/4/4	0/0/0/0
4	GOL	D	804	-	-	0/4/4/4	0/0/0/0
3	SWA	E	801	2	-	0/0/26/26	0/2/2/2
4	GOL	E	802	-	-	0/4/4/4	0/0/0/0
4	GOL	E	803	-	-	0/4/4/4	0/0/0/0
3	SWA	F	801	2	-	0/0/26/26	0/2/2/2
4	GOL	F	802	-	-	0/4/4/4	0/0/0/0
3	SWA	G	801	2	-	0/0/26/26	1/2/2/2
3	SWA	H	801	2	-	0/0/26/26	0/2/2/2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	SWA	C8-C7	-2.54	1.49	1.53
3	G	801	SWA	C8-C7	2.01	1.56	1.53
3	C	801	SWA	C2-C1	2.11	1.55	1.52
3	D	801	SWA	C1-C3	2.50	1.56	1.53
3	H	801	SWA	C7-C3	2.71	1.57	1.53

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	801	SWA	C5-N4-C3	-5.48	107.75	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	801	SWA	C5-N4-C9	-4.09	104.48	115.29
3	G	801	SWA	C5-N4-C9	-3.46	106.14	115.29
3	H	801	SWA	C9-N4-C3	-2.96	99.07	104.94
3	E	801	SWA	O11-C7-C8	-2.73	105.19	111.68

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	801	SWA	C1-C2-C3-C5-C6-N4

15 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	SWA	3	0
4	A	803	GOL	2	0
4	A	804	GOL	1	0
3	B	801	SWA	2	0
4	B	803	GOL	2	0
4	B	804	GOL	4	0
3	C	801	SWA	4	0
4	C	803	GOL	6	0
3	D	801	SWA	5	0
4	D	802	GOL	2	0
4	D	804	GOL	3	0
3	E	801	SWA	1	0
3	F	801	SWA	5	0
3	G	801	SWA	5	0
3	H	801	SWA	5	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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	736/744 (98%)	-0.30	0	100 100	7, 12, 20, 24	0
1	B	736/744 (98%)	-0.28	0	100 100	7, 12, 20, 25	0
1	C	737/744 (99%)	-0.23	3 (0%)	93 90	7, 12, 20, 29	0
1	D	738/744 (99%)	-0.31	1 (0%)	95 95	7, 12, 20, 36	0
1	E	736/744 (98%)	-0.13	7 (0%)	84 77	7, 12, 19, 26	0
1	F	736/744 (98%)	0.00	16 (2%)	65 54	7, 12, 19, 24	0
1	G	736/744 (98%)	0.29	39 (5%)	30 20	7, 12, 19, 24	0
1	H	736/744 (98%)	0.56	77 (10%)	8 4	7, 12, 19, 24	0
All	All	5891/5952 (98%)	-0.05	143 (2%)	62 50	7, 12, 19, 36	0

The worst 5 of 143 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	717	TYR	5.9
1	H	723	LEU	5.7
1	H	708	PHE	5.6
1	H	613	TYR	4.8
1	H	681	LEU	4.7

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	D	802	6/6	0.93	0.34	14.89	30,33,34,36	0
4	GOL	B	802	6/6	0.93	0.29	7.29	29,30,30,31	0
4	GOL	C	804	6/6	0.83	0.34	5.72	32,33,33,35	0
4	GOL	A	804	6/6	0.87	0.25	5.03	19,19,21,22	0
4	GOL	D	804	6/6	0.89	0.30	4.68	29,30,31,34	0
4	GOL	A	802	6/6	0.94	0.24	4.47	42,43,44,45	0
4	GOL	E	803	6/6	0.88	0.21	3.67	38,39,39,39	0
4	GOL	A	806	6/6	0.91	0.18	3.02	42,43,44,45	0
4	GOL	D	803	6/6	0.95	0.29	2.61	32,33,35,35	0
4	GOL	B	804	6/6	0.89	0.19	2.57	22,26,26,28	0
4	GOL	C	803	6/6	0.81	0.27	2.51	32,33,34,34	0
4	GOL	A	803	6/6	0.95	0.21	2.37	32,35,35,36	0
3	SWA	C	801	12/12	0.97	0.23	1.25	18,21,22,24	0
4	GOL	F	802	6/6	0.95	0.18	1.23	30,32,33,33	0
4	GOL	B	803	6/6	0.95	0.18	0.98	45,45,46,47	0
3	SWA	A	801	12/12	0.95	0.18	0.91	37,39,40,41	0
4	GOL	A	805	6/6	0.94	0.19	0.85	31,33,34,34	0
3	SWA	H	801	12/12	0.79	0.23	0.52	25,27,30,33	0
3	SWA	G	801	12/12	0.88	0.23	0.39	39,40,42,45	0
3	SWA	F	801	12/12	0.96	0.21	0.33	22,24,24,25	0
4	GOL	E	802	6/6	0.95	0.16	-0.48	30,31,31,31	0
3	SWA	D	801	12/12	0.95	0.14	-1.20	17,18,20,21	0
3	SWA	B	801	12/12	0.98	0.13	-1.32	9,14,15,17	0
2	CA	G	800	1/1	0.98	0.14	-1.47	39,39,39,39	0
3	SWA	E	801	12/12	0.96	0.12	-1.74	8,11,13,14	0
2	CA	H	800	1/1	0.88	0.10	-3.22	43,43,43,43	0
2	CA	D	800	1/1	0.95	0.05	-3.56	30,30,30,30	0
2	CA	E	800	1/1	0.93	0.06	-3.64	33,33,33,33	0
2	CA	F	800	1/1	0.94	0.07	-3.72	22,22,22,22	0
2	CA	A	800	1/1	0.96	0.07	-4.79	28,28,28,28	0
2	CA	B	800	1/1	0.99	0.07	-4.92	11,11,11,11	0
2	CA	C	800	1/1	0.96	0.06	-5.14	23,23,23,23	0
4	GOL	C	802	6/6	0.66	0.34	-	59,60,60,61	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.