



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:42 AM UTC

PDB ID : 3BUB / pdb\_00003bub  
Title : Golgi alpha-mannosidase II with an empty active site  
Authors : Kuntz, D.A.; Rose, D.R.  
Deposited on : 2008-01-02  
Resolution : 1.38 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](mailto: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>.

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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

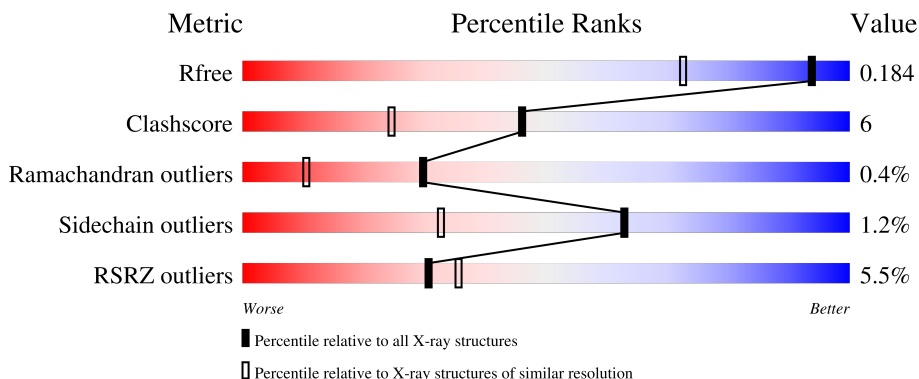
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.38 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	4403 (1.40-1.36)
Clashscore	190562	4528 (1.40-1.36)
Ramachandran outliers	187476	4459 (1.40-1.36)
Sidechain outliers	187428	4458 (1.40-1.36)
RSRZ outliers	180081	4399 (1.40-1.36)

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  $\geq 3$ , 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	1045	

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	NAG	A	1046	X	-	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10102 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 Alpha-mannosidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1016	8570	5456	1504	1565	45	0	52	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ARG	-	expression tag	UNP Q24451
A	2	SER	-	expression tag	UNP Q24451
A	3	SER	-	expression tag	UNP Q24451
A	4	HIS	-	expression tag	UNP Q24451
A	5	HIS	-	expression tag	UNP Q24451
A	6	HIS	-	expression tag	UNP Q24451
A	7	HIS	-	expression tag	UNP Q24451
A	8	HIS	-	expression tag	UNP Q24451
A	9	HIS	-	expression tag	UNP Q24451
A	10	GLY	-	expression tag	UNP Q24451
A	11	GLU	-	expression tag	UNP Q24451
A	12	PHE	-	expression tag	UNP Q24451
A	907	LYS	GLU	SEE REMARK 999	UNP Q24451

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).

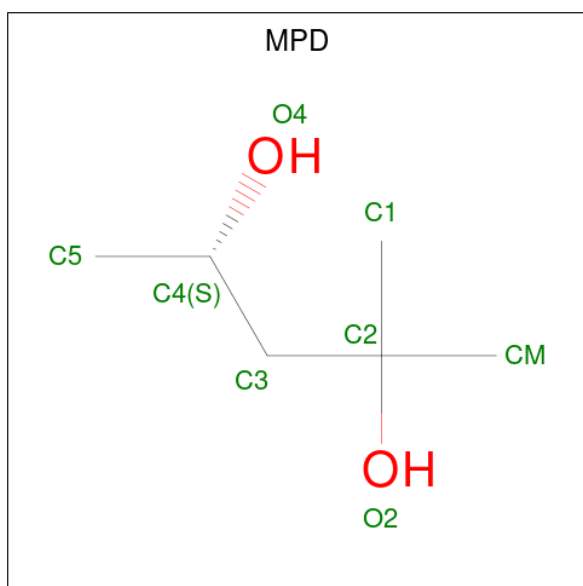


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0

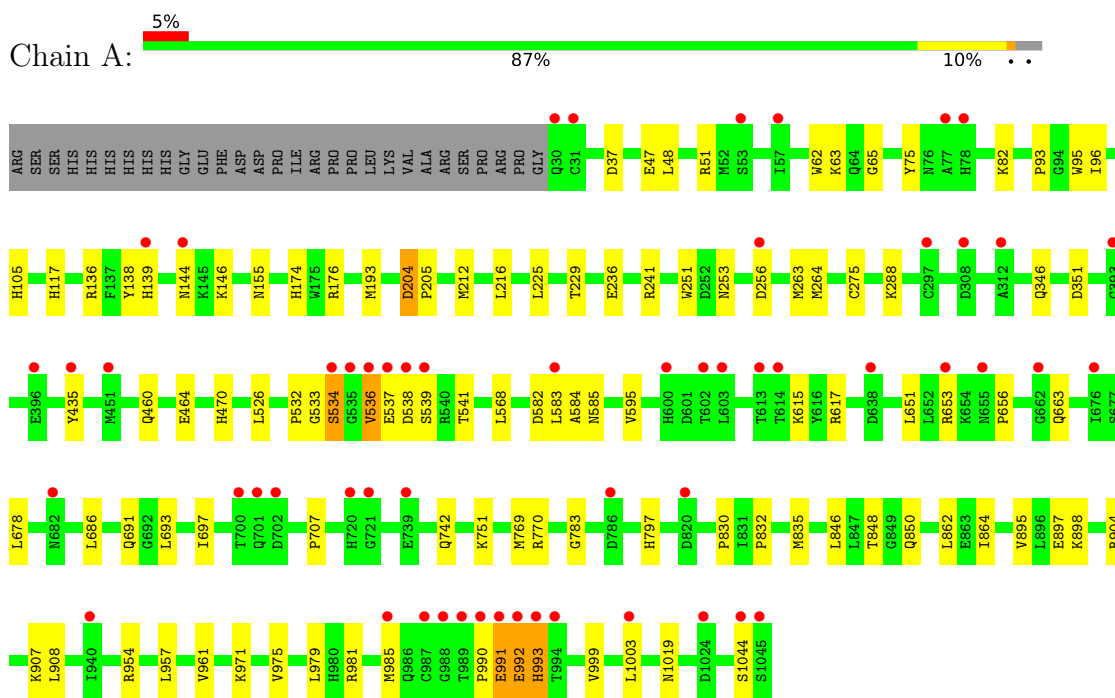
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1470	Total O 1493 1493	0	23

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Alpha-mannosidase 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.77Å 109.62Å 138.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.81 – 1.38 19.81 – 1.38	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.81-1.38) 97.9 (19.81-1.38)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 1.38Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.180 , 0.204 0.179 , 0.184	Depositor DCC
$R_{free}$ test set	3168 reflections (1.48%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.4	Xtrriage
Anisotropy	0.069	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 42.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10102	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.333 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: MPD, NAG, ZN

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	0.72	1/8884 (0.0%)	0.86	4/12051 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	992	GLU	CA-C	6.31	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	992	GLU	N-CA-C	7.29	119.71	108.12
1	A	534	SER	N-CA-C	-5.43	102.01	110.10
1	A	582	ASP	CA-C-N	-5.02	114.32	122.65
1	A	582	ASP	C-N-CA	-5.02	114.32	122.65

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	8570	0	8395	98	0
2	A	14	0	13	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	24	0	42	1	0
5	A	1493	0	0	37	0
All	All	10102	0	8450	100	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 6.

All (100) 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:533:GLY:O	1:A:536:VAL:HG23	1.36	1.22
1:A:532:PRO:O	1:A:536:VAL:HG21	1.51	1.08
1:A:75[B]:TYR:HD2	5:A:1643:HOH:O	1.47	0.98
1:A:533:GLY:C	1:A:536:VAL:HG23	1.92	0.94
1:A:82[B]:LYS:HE3	5:A:1690:HOH:O	1.75	0.86
1:A:138[B]:TYR:CE1	1:A:146[B]:LYS:HE3	2.14	0.83
1:A:47[A]:GLU:HG3	5:A:1423:HOH:O	1.83	0.78
1:A:537:GLU:HB2	5:A:1887:HOH:O	1.83	0.78
4:A:1050:MPD:H12	5:A:2182:HOH:O	1.84	0.77
1:A:96[A]:ILE:HG22	5:A:1544:HOH:O	1.83	0.77
1:A:346[A]:GLN:NE2	5:A:1618:HOH:O	2.23	0.71
1:A:288:LYS:NZ	5:A:1621:HOH:O	2.23	0.71
1:A:136:ARG:HD3	5:A:1938[B]:HOH:O	1.93	0.69
1:A:532:PRO:O	1:A:536:VAL:CG2	2.38	0.68
1:A:533:GLY:O	1:A:536:VAL:CG2	2.30	0.68
1:A:783:GLY:HA3	5:A:2006:HOH:O	1.93	0.68
1:A:37:ASP:HB2	1:A:253[B]:ASN:ND2	2.10	0.67
1:A:971[B]:LYS:NZ	5:A:1791:HOH:O	2.24	0.66
1:A:663:GLN:HG3	5:A:2442:HOH:O	1.95	0.65
1:A:846:LEU:HD23	1:A:864[B]:ILE:CD1	2.27	0.64
1:A:96[A]:ILE:CG2	5:A:1544:HOH:O	2.40	0.64
1:A:75[B]:TYR:CD2	5:A:1643:HOH:O	2.32	0.64
1:A:1019:ASN:HB3	5:A:2329:HOH:O	2.00	0.61
1:A:617:ARG:HD2	5:A:1151:HOH:O	2.01	0.60
1:A:138[A]:TYR:CE1	1:A:193[A]:MET:CE	2.84	0.60
1:A:138[B]:TYR:CE1	1:A:146[B]:LYS:CE	2.85	0.59
1:A:954[A]:ARG:HH21	1:A:981[A]:ARG:NE	2.00	0.59
1:A:174:HIS:CE1	1:A:176:ARG:HD3	2.38	0.59
1:A:678:LEU:HD12	1:A:769[B]:MET:HE1	1.84	0.58
1:A:693:LEU:HD13	5:A:2403:HOH:O	2.04	0.57
1:A:848[B]:THR:HG22	1:A:850:GLN:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82[A]:LYS:NZ	5:A:1699:HOH:O	2.31	0.57
1:A:105[B]:HIS:ND1	5:A:2101:HOH:O	2.32	0.57
1:A:904:ARG:HA	1:A:985[B]:MET:HE1	1.87	0.56
1:A:957:LEU:HD11	1:A:979[B]:LEU:HG	1.89	0.55
1:A:678:LEU:CD1	1:A:769[B]:MET:HE1	2.37	0.55
1:A:256:ASP:HB2	5:A:1383:HOH:O	2.06	0.55
1:A:908:LEU:HD22	5:A:1419:HOH:O	2.08	0.54
1:A:538:ASP:HA	5:A:1164:HOH:O	2.08	0.54
1:A:904:ARG:HG2	1:A:985[A]:MET:SD	2.48	0.54
1:A:961:VAL:HG22	5:A:1915[B]:HOH:O	2.09	0.53
1:A:846:LEU:HD23	1:A:864[B]:ILE:HD11	1.91	0.52
1:A:82[B]:LYS:NZ	5:A:1700:HOH:O	2.41	0.52
1:A:686:LEU:HD22	1:A:697:ILE:HG12	1.92	0.52
1:A:846:LEU:CD2	1:A:864[B]:ILE:HD12	2.39	0.52
2:A:1046:NAG:H4	5:A:2328:HOH:O	2.09	0.51
1:A:653:ARG:HD3	1:A:656:PRO:HA	1.93	0.51
1:A:51[A]:ARG:NH2	5:A:1411:HOH:O	2.39	0.51
1:A:568:LEU:HD12	1:A:770:ARG:HD3	1.93	0.51
1:A:993:HIS:O	1:A:993:HIS:ND1	2.45	0.50
1:A:47[B]:GLU:OE2	1:A:51[B]:ARG:HD3	2.12	0.49
1:A:848[B]:THR:CG2	1:A:850:GLN:NE2	2.75	0.49
1:A:895:VAL:HG12	1:A:897:GLU:HG3	1.94	0.49
1:A:533:GLY:C	1:A:536:VAL:CG2	2.78	0.49
1:A:742[A]:GLN:HG3	5:A:1991:HOH:O	2.13	0.49
1:A:904:ARG:HG2	1:A:985[B]:MET:SD	2.53	0.48
1:A:595:VAL:HG21	1:A:615:LYS:HG3	1.96	0.48
1:A:975:VAL:HG21	1:A:1003:LEU:HD22	1.95	0.48
1:A:979[A]:LEU:HD21	1:A:999:VAL:HG11	1.97	0.47
1:A:204:ASP:H	1:A:205:PRO:HD3	1.80	0.47
1:A:532:PRO:C	1:A:536:VAL:HG21	2.34	0.47
1:A:93:PRO:HD2	1:A:470:HIS:CE1	2.49	0.47
1:A:954[A]:ARG:NH2	1:A:981[A]:ARG:HD2	2.30	0.46
1:A:707:PRO:HG2	1:A:797[A]:HIS:CD2	2.50	0.46
1:A:75[B]:TYR:HE2	5:A:1642:HOH:O	1.97	0.46
1:A:835:MET:HE2	1:A:862:LEU:HD22	1.97	0.46
1:A:229:THR:HG21	1:A:263:MET:HE2	1.97	0.46
1:A:241[B]:ARG:CZ	5:A:2208:HOH:O	2.64	0.46
1:A:62:TRP:CD2	1:A:65:GLY:HA3	2.51	0.45
1:A:82[B]:LYS:CE	5:A:1690:HOH:O	2.50	0.45
1:A:144:ASN:HB3	5:A:2116:HOH:O	2.15	0.45
1:A:954[A]:ARG:HH21	1:A:981[A]:ARG:CD	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ASP:HB2	1:A:253[B]:ASN:HD21	1.82	0.44
1:A:251:TRP:CD1	1:A:251:TRP:C	2.95	0.44
1:A:990:PRO:O	1:A:991:GLU:C	2.61	0.44
1:A:993:HIS:O	1:A:993:HIS:CG	2.70	0.44
1:A:47[B]:GLU:HG2	5:A:1435:HOH:O	2.18	0.43
1:A:584:ALA:O	1:A:585[B]:ASN:HB2	2.17	0.43
1:A:117[B]:HIS:HE1	1:A:351:ASP:OD1	2.02	0.43
1:A:538:ASP:CG	5:A:1885:HOH:O	2.61	0.43
1:A:37:ASP:HB2	5:A:1388:HOH:O	2.19	0.43
1:A:954[A]:ARG:CZ	1:A:954[A]:ARG:HB3	2.50	0.42
1:A:848[B]:THR:HG23	1:A:850:GLN:NE2	2.34	0.42
1:A:435[A]:TYR:CE2	1:A:526:LEU:HD13	2.54	0.42
1:A:155:ASN:C	1:A:155:ASN:OD1	2.62	0.42
1:A:138[A]:TYR:CE1	1:A:193[A]:MET:HE1	2.54	0.42
1:A:532:PRO:HB2	1:A:536:VAL:HB	2.02	0.42
1:A:954[A]:ARG:HH21	1:A:981[A]:ARG:HD2	1.83	0.42
1:A:981[A]:ARG:NH2	5:A:1328:HOH:O	2.52	0.42
1:A:225:LEU:HD21	1:A:264[A]:MET:SD	2.60	0.42
1:A:990:PRO:O	1:A:992:GLU:HG3	2.20	0.42
1:A:138[B]:TYR:CD1	1:A:146[B]:LYS:HE3	2.55	0.41
1:A:63:LYS:HE2	5:A:1081:HOH:O	2.21	0.41
1:A:830:PRO:C	1:A:832:PRO:HD3	2.45	0.41
1:A:537:GLU:HG2	1:A:539:SER:HB3	2.02	0.41
1:A:48:LEU:HD11	1:A:236:GLU:HG2	2.01	0.41
1:A:460:GLN:O	1:A:464:GLU:HG2	2.21	0.40
1:A:139[B]:HIS:HB3	5:A:1930:HOH:O	2.20	0.40
1:A:212[B]:MET:HG3	1:A:216:LEU:CD1	2.52	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	1066/1045 (102%)	1042 (98%)	20 (2%)	4 (0%)	30 10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	TRP
1	A	991	GLU
1	A	993	HIS
1	A	204	ASP

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	955/929 (103%)	944 (99%)	11 (1%)	63 33

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	CYS
1	A	534	SER
1	A	536	VAL
1	A	541	THR
1	A	583	LEU
1	A	651	LEU
1	A	691	GLN
1	A	751	LYS
1	A	898	LYS
1	A	907	LYS
1	A	1044	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MPD	A	1048	-	7,7,7	0.34	0	9,10,10	1.23	1 (11%)
4	MPD	A	1050	-	7,7,7	0.33	0	9,10,10	0.43	0
4	MPD	A	1049	-	7,7,7	0.30	0	9,10,10	0.48	0
2	NAG	A	1046	1	14,14,15	1.09	2 (14%)	17,19,21	2.08	4 (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
4	MPD	A	1048	-	-	4/5/5/5	-
4	MPD	A	1050	-	-	2/5/5/5	-
4	MPD	A	1049	-	-	1/5/5/5	-
2	NAG	A	1046	1	1/1/5/7	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1046	NAG	O5-C5	2.37	1.48	1.43
2	A	1046	NAG	O5-C1	-2.29	1.39	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1046	NAG	O5-C1-C2	-5.98	102.03	111.29
2	A	1046	NAG	C4-C3-C2	-4.12	104.98	111.02
2	A	1046	NAG	O5-C5-C4	3.05	118.24	110.83
2	A	1046	NAG	C2-N2-C7	-2.46	119.60	122.90
4	A	1048	MPD	O2-C2-C3	-2.09	101.45	109.27

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1046	NAG	C5

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1048	MPD	C2-C3-C4-C5
2	A	1046	NAG	C8-C7-N2-C2
2	A	1046	NAG	O7-C7-N2-C2
4	A	1049	MPD	O2-C2-C3-C4
4	A	1048	MPD	O2-C2-C3-C4
4	A	1050	MPD	O2-C2-C3-C4
4	A	1048	MPD	C2-C3-C4-O4
4	A	1048	MPD	CM-C2-C3-C4
4	A	1050	MPD	C1-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1050	MPD	1	0
2	A	1046	NAG	1	0

## 5.7 Other polymers [i](#)

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 [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, 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	1016/1045 (97%)	0.24	56 (5%) <span style="border: 1px solid red; padding: 2px;">30</span> <span style="border: 1px solid red; padding: 2px;">35</span>	3, 10, 23, 44	52 (5%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	534	SER	8.7
1	A	536	VAL	8.5
1	A	538	ASP	5.9
1	A	539	SER	5.8
1	A	537	GLU	4.8
1	A	993	HIS	4.7
1	A	535	GLY	4.4
1	A	583	LEU	4.4
1	A	1045	SER	4.1
1	A	655	ASN	3.8
1	A	603	LEU	3.6
1	A	987	CYS	3.6
1	A	31	CYS	3.5
1	A	720	HIS	3.5
1	A	435[A]	TYR	3.5
1	A	721	GLY	3.4
1	A	78	HIS	3.3
1	A	702	ASP	3.2
1	A	701	GLN	3.1
1	A	53	SER	3.1
1	A	991	GLU	3.0
1	A	602	THR	3.0
1	A	614	THR	2.9
1	A	989	THR	2.9
1	A	990	PRO	2.9
1	A	451	MET	2.8
1	A	1024	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	682	ASN	2.8
1	A	739	GLU	2.8
1	A	985[A]	MET	2.7
1	A	613	THR	2.7
1	A	638	ASP	2.7
1	A	144	ASN	2.6
1	A	396	GLU	2.6
1	A	1003	LEU	2.5
1	A	139[A]	HIS	2.5
1	A	992	GLU	2.5
1	A	600	HIS	2.5
1	A	57	ILE	2.5
1	A	308	ASP	2.4
1	A	653	ARG	2.4
1	A	256	ASP	2.4
1	A	30	GLN	2.3
1	A	77	ALA	2.3
1	A	786	ASP	2.3
1	A	662	GLY	2.3
1	A	700	THR	2.2
1	A	676	ILE	2.2
1	A	297	CYS	2.2
1	A	994	THR	2.2
1	A	988	GLY	2.2
1	A	940	ILE	2.1
1	A	820	ASP	2.1
1	A	312	ALA	2.0
1	A	1044	SER	2.0
1	A	393	GLY	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 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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	1046	14/15	0.57	0.20	26,46,66,71	0
4	MPD	A	1049	8/8	0.76	0.16	36,38,38,39	0
4	MPD	A	1050	8/8	0.76	0.16	30,33,35,36	0
4	MPD	A	1048	8/8	0.89	0.12	12,18,20,22	0
3	ZN	A	1047	1/1	0.99	0.02	8,8,8,8	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.