W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2017 – 03:00 AM EDT

PDB ID	:	3CZN
Title	:	Golgi alpha-mannosidase II (D204A nucleophile mutant) in complex with Gn-Man5Gn
Authors	:	Shah, N.; Rose, D.R.
Deposited on	:	unknown
Resolution	:	1.40 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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.
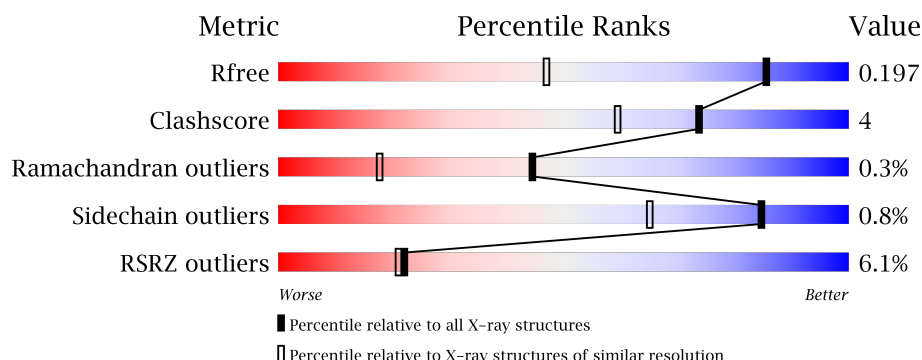
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1307 (1.40-1.40)
Clashscore	112137	1411 (1.40-1.40)
Ramachandran outliers	110173	1373 (1.40-1.40)
Sidechain outliers	110143	1372 (1.40-1.40)
RSRZ outliers	101464	1315 (1.40-1.40)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1045	6% ... 89% ... 8% .

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9691 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	1014	8434	5363	1484	1547	40	0	35	0

There are 14 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	204	ALA	ASP	ENGINEERED	UNP Q24451
A	907	LYS	GLU	SEE REMARK 999	UNP Q24451

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
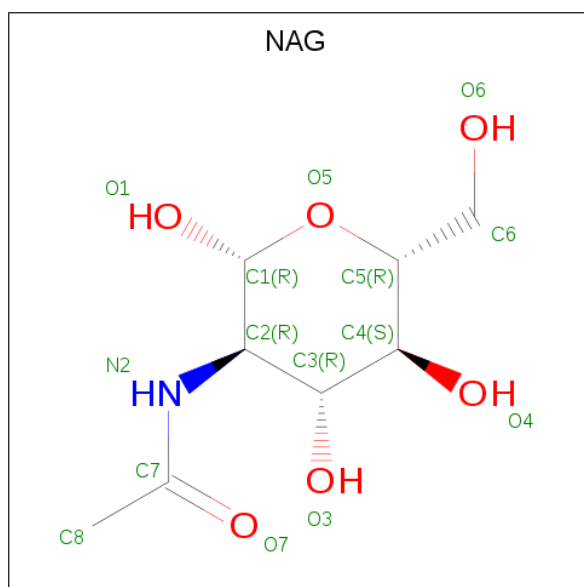
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is 2-(acetylamino)-2-deoxy-beta-D-glucopyranosyl-(1->2)-alpha-D-mannopyranosyl-(1->3)-[alpha-D-mannopyranosyl-(1->3)-[alpha-D-mannopyranosyl-(1->6)]-alpha-D-mannopyranosyl-(1->6)]-beta-D-mannopyranosyl-(1->4)-2-(acetylamino)-2-deoxy-alpha-D-glucopyranose (three-letter code: M5G) (formula: $C_{46}H_{78}N_2O_{36}$).
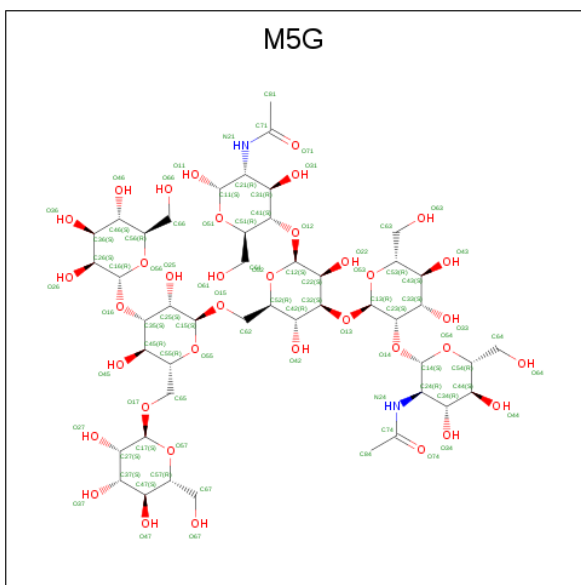
| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	84	46	2	36	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	1158	1158	1158	0	0

3 Residue-property plots (i)

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: Alpha-mannosidase 2
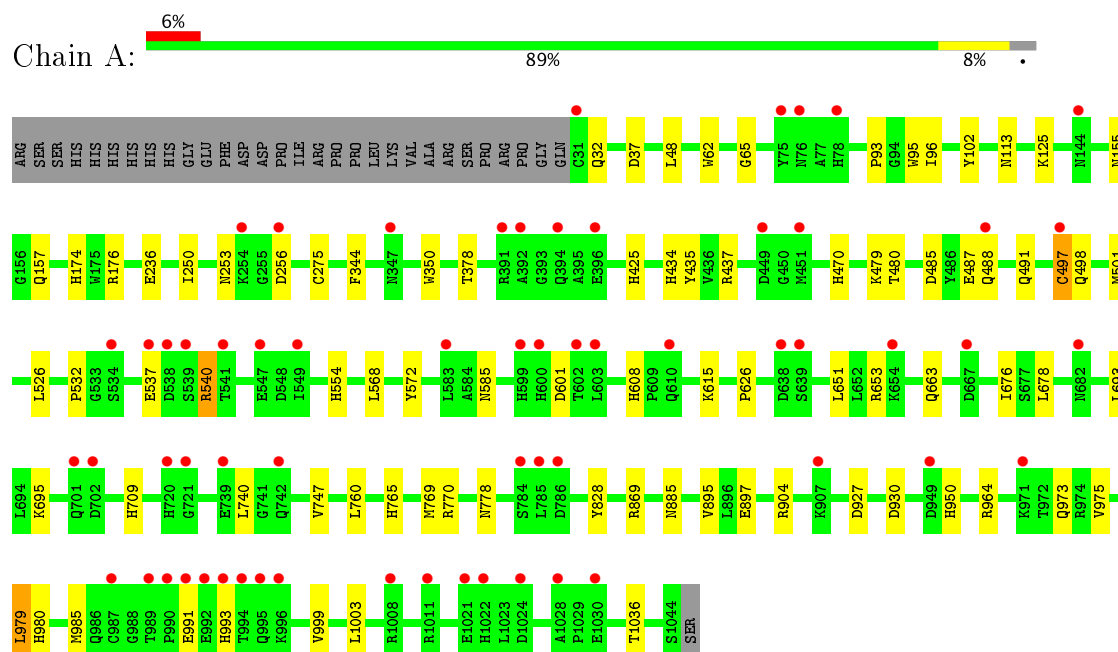
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.93Å 109.58Å 138.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.54 – 1.40 10.54 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (10.54-1.40) 99.9 (10.54-1.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	4.24 (at 1.40Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.177 , 0.197 0.176 , 0.197	Depositor DCC
R_{free} test set	10286 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	13.8	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 56.1	EDS
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9691	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: M5G, ZN, NAG

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	0.40	0/8696	0.60	0/11803

There are no bond length outliers.

There are no bond angle outliers.

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	8434	0	8249	64	0
2	A	14	0	13	0	0
3	A	1	0	0	0	0
4	A	84	0	77	1	0
5	A	1158	0	0	18	0
All	All	9691	0	8339	65	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 4.

All (65) 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:498[B]:GLN:HG2	1:A:526:LEU:HD12	1.26	1.17
1:A:434:HIS:HE1	1:A:930:ASP:OD1	1.61	0.82
1:A:651:LEU:HD11	1:A:653[B]:ARG:HE	1.46	0.81
1:A:435:TYR:HB3	1:A:497[A]:CYS:SG	2.22	0.79
1:A:497[A]:CYS:SG	1:A:501:MET:SD	2.81	0.78
1:A:964:ARG:HH11	1:A:973:GLN:HE21	1.34	0.76
1:A:709[A]:HIS:CD2	5:A:2137:HOH:O	2.44	0.70
1:A:155:ASN:HD21	1:A:157:GLN:HE21	1.42	0.67
1:A:498[A]:GLN:HE21	1:A:526:LEU:H	1.41	0.67
1:A:532[B]:PRO:CG	1:A:537:GLU:HB3	2.27	0.65
1:A:979:LEU:HD21	1:A:999:VAL:HG11	1.79	0.64
1:A:434:HIS:HD2	1:A:927:ASP:OD1	1.81	0.64
1:A:980:HIS:HE1	5:A:1217:HOH:O	1.81	0.62
1:A:765:HIS:HE1	5:A:1245:HOH:O	1.85	0.59
1:A:950:HIS:HE1	5:A:1495:HOH:O	1.87	0.58
1:A:980:HIS:HD2	1:A:1036:THR:OG1	1.88	0.57
1:A:434:HIS:CE1	1:A:930:ASP:OD1	2.51	0.57
1:A:174:HIS:CE1	1:A:176[A]:ARG:HD3	2.39	0.57
1:A:498[B]:GLN:HG2	1:A:526:LEU:CD1	2.18	0.56
1:A:626:PRO:O	1:A:950:HIS:HD2	1.89	0.56
1:A:532[B]:PRO:HG3	1:A:537:GLU:HB3	1.86	0.55
1:A:693:LEU:HD13	5:A:1586:HOH:O	2.07	0.55
1:A:572:TYR:CD2	1:A:615:LYS:HD3	2.42	0.55
1:A:532[B]:PRO:HG2	1:A:537:GLU:HB3	1.87	0.54
1:A:765:HIS:HD2	1:A:778:ASN:OD1	1.90	0.54
1:A:869:ARG:HH11	1:A:885:ASN:HD22	1.56	0.54
1:A:904:ARG:HG2	1:A:985:MET:SD	2.48	0.53
1:A:895:VAL:HG12	1:A:897:GLU:HG3	1.90	0.53
1:A:125[A]:LYS:HD3	1:A:157:GLN:HA	1.91	0.53
1:A:32:GLN:NE2	5:A:1903:HOH:O	2.41	0.52
1:A:256:ASP:HB2	5:A:1903:HOH:O	2.09	0.51
1:A:540:ARG:HG2	5:A:1841:HOH:O	2.10	0.51
1:A:62:TRP:CD2	1:A:65:GLY:HA3	2.46	0.51
1:A:491[B]:GLN:NE2	5:A:1562:HOH:O	2.44	0.49
1:A:975:VAL:HG21	1:A:1003:LEU:CD1	2.42	0.49
1:A:125[A]:LYS:HD2	1:A:378:THR:HG23	1.95	0.49
1:A:113:ASN:HB2	5:A:2229:HOH:O	2.13	0.49
1:A:176[B]:ARG:HH22	1:A:437:ARG:HB2	1.77	0.49
1:A:554:HIS:HD2	5:A:1499:HOH:O	1.95	0.49
1:A:663:GLN:HG3	5:A:1881:HOH:O	2.13	0.48
1:A:96:ILE:HA	1:A:479:LYS:HG3	1.95	0.48
1:A:96:ILE:HG13	1:A:102:TYR:OH	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ASP:HB3	1:A:253:ASN:ND2	2.29	0.47
1:A:540:ARG:HG3	1:A:572:TYR:CE2	2.48	0.47
1:A:498[A]:GLN:NE2	1:A:526:LEU:H	2.10	0.47
1:A:174:HIS:CE1	1:A:176[B]:ARG:HG3	2.49	0.46
1:A:709[A]:HIS:HD2	5:A:2137:HOH:O	1.86	0.46
1:A:425:HIS:HE1	1:A:487:GLU:OE1	1.99	0.45
1:A:601:ASP:HB2	1:A:608:HIS:CE1	2.52	0.45
1:A:653[B]:ARG:NH2	5:A:1734:HOH:O	2.44	0.45
1:A:93:PRO:HD2	1:A:470:HIS:CD2	2.52	0.45
4:A:1103:M5G:H61A	5:A:1875:HOH:O	2.17	0.44
1:A:488:GLN:NE2	5:A:2130:HOH:O	2.42	0.44
1:A:48:LEU:HD11	1:A:236:GLU:HG2	2.00	0.43
1:A:344:PHE:HB3	1:A:350:TRP:CE2	2.54	0.43
1:A:568:LEU:HD12	1:A:770:ARG:HD3	2.01	0.43
1:A:480:THR:HG23	5:A:1717:HOH:O	2.19	0.42
1:A:485:ASP:HA	1:A:488:GLN:HE21	1.84	0.42
1:A:250:ILE:HD11	5:A:1796:HOH:O	2.19	0.42
1:A:676:ILE:HD13	1:A:747:VAL:HG21	2.03	0.41
1:A:678:LEU:HD12	1:A:769:MET:HE1	2.01	0.41
1:A:975:VAL:HG21	1:A:1003:LEU:HD12	2.02	0.41
1:A:651:LEU:CD1	1:A:653[A]:ARG:HG2	2.50	0.41
1:A:885:ASN:ND2	1:A:885:ASN:H	2.19	0.40
1:A:740:LEU:HD22	1:A:760:LEU:HD22	2.03	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	1047/1045 (100%)	1020 (97%)	24 (2%)	3 (0%)	44	18

All (3) Ramachandran outliers are listed below:

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

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	935/928 (101%)	927 (99%)	8 (1%)	82	61

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	CYS
1	A	497[A]	CYS
1	A	497[B]	CYS
1	A	540	ARG
1	A	585	ASN
1	A	695	LYS
1	A	828	TYR
1	A	979	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	91	ASN
1	A	119	HIS
1	A	148	GLN
1	A	157	GLN
1	A	191	GLN
1	A	249	GLN
1	A	346	GLN
1	A	347	ASN
1	A	369	HIS
1	A	394	GLN

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Mol	Chain	Res	Type
1	A	425	HIS
1	A	434	HIS
1	A	460	GLN
1	A	469	GLN
1	A	470	HIS
1	A	488	GLN
1	A	554	HIS
1	A	608	HIS
1	A	698	GLN
1	A	765	HIS
1	A	809	ASN
1	A	885	ASN
1	A	919	HIS
1	A	945	GLN
1	A	950	HIS
1	A	973	GLN
1	A	980	HIS
1	A	995	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)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	#$|Z| > 2$
2	NAG	A	1101	1	14,14,15	0.50	0	15,19,21	0.67	0
4	M5G	A	1103	3	90,90,90	1.01	2 (2%)	132,133,133	1.09	12 (9%)

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	NAG	A	1101	1	-	0/6/23/26	0/1/1/1
4	M5G	A	1103	3	-	0/44/184/184	0/7/7/7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1103	M5G	C81-C71	-8.39	1.32	1.50
4	A	1103	M5G	O17-C17	2.00	1.43	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1103	M5G	C13-O13-C32	-3.36	109.82	118.00
4	A	1103	M5G	C11-C21-N21	-3.29	106.91	110.73
4	A	1103	M5G	C44-C34-C24	-2.30	106.92	110.33
4	A	1103	M5G	C12-O12-C41	-2.17	112.71	118.00
4	A	1103	M5G	C14-C24-N24	-2.14	107.41	111.03
4	A	1103	M5G	O14-C14-O54	-2.00	105.83	110.70
4	A	1103	M5G	C17-C27-C37	2.03	113.76	109.98
4	A	1103	M5G	C31-C41-C51	2.10	115.33	110.88
4	A	1103	M5G	O13-C32-C42	2.10	112.25	107.19
4	A	1103	M5G	C11-O51-C51	2.84	118.52	113.39
4	A	1103	M5G	O51-C51-C41	2.93	115.75	109.75
4	A	1103	M5G	O17-C65-C55	3.54	114.87	108.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1103	M5G	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(Å²)	Q<0.9
1	A	1014/1045 (97%)	0.24	62 (6%)	22	21	9, 15, 26, 41	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	993	HIS	11.0
1	A	702	ASP	8.2
1	A	1024	ASP	6.6
1	A	990	PRO	6.4
1	A	701	GLN	6.4
1	A	992	GLU	6.3
1	A	78	HIS	6.1
1	A	583	LEU	5.5
1	A	784[A]	SER	5.3
1	A	538	ASP	4.9
1	A	638	ASP	4.8
1	A	600	HIS	4.8
1	A	991	GLU	4.6
1	A	987	CYS	4.5
1	A	451	MET	4.5
1	A	537	GLU	4.4
1	A	682	ASN	4.3
1	A	547	GLU	4.2
1	A	602	THR	4.0
1	A	31	CYS	3.9
1	A	721	GLY	3.8
1	A	603	LEU	3.8
1	A	396	GLU	3.7
1	A	534	SER	3.5
1	A	256	ASP	3.3
1	A	720[A]	HIS	3.3
1	A	654	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1008	ARG	3.1
1	A	497[A]	CYS	3.0
1	A	549	ILE	3.0
1	A	786[A]	ASP	3.0
1	A	996	LYS	2.9
1	A	739	GLU	2.9
1	A	392	ALA	2.8
1	A	1022	HIS	2.8
1	A	1021	GLU	2.7
1	A	449	ASP	2.7
1	A	599	HIS	2.7
1	A	391	ARG	2.6
1	A	907	LYS	2.6
1	A	994	THR	2.6
1	A	742	GLN	2.5
1	A	971	LYS	2.5
1	A	610	GLN	2.4
1	A	254	LYS	2.4
1	A	347	ASN	2.4
1	A	785	LEU	2.3
1	A	144	ASN	2.3
1	A	488	GLN	2.3
1	A	541	THR	2.2
1	A	1028	ALA	2.2
1	A	75	TYR	2.1
1	A	539	SER	2.1
1	A	667	ASP	2.1
1	A	989	THR	2.1
1	A	1030	GLU	2.1
1	A	949	ASP	2.1
1	A	76	ASN	2.1
1	A	639	SER	2.0
1	A	1011	ARG	2.0
1	A	394	GLN	2.0
1	A	995	GLN	2.0

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 (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. 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, 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	LLDF	B-factors($Å^2$)	Q<0.9
4	M5G	A	1103	84/84	0.90	0.11	0.59	11,17,32,35	0
3	ZN	A	1102	1/1	1.00	0.02	-5.20	12,12,12,12	0
2	NAG	A	1101	14/15	0.51	0.39	-	31,37,38,39	0

6.5 Other polymers (i)

There are no such residues in this entry.