



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 09:40 PM BST

PDB ID : 1WMR
Title : Crystal Structure of Isopullulanase from *Aspergillus niger* ATCC 9642
Authors : Mizuno, M.; Tonozone, T.; Miyasaka, Y.; Akeboshi, H.; Kamitori, S.;
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Deposited on : 2004-07-15
Resolution : 2.40 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

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	:	2.13.1
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)	:	2.13.1

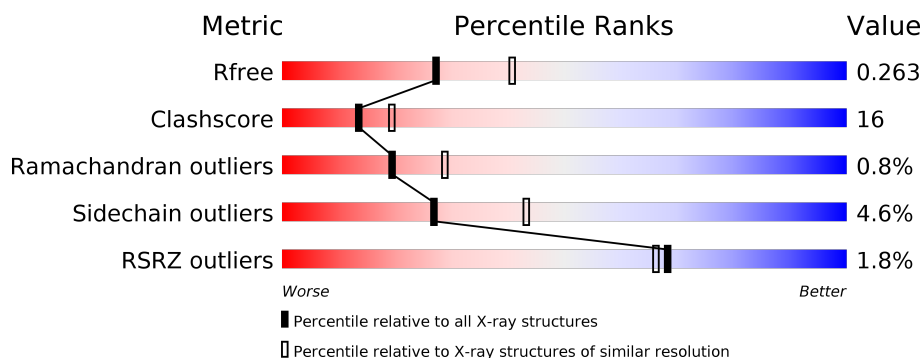
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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	549	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>29%</div> <div>.</div> </div> </div>
1	B	549	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>27%</div> <div>.</div> </div> </div>

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	B	1000	X	-	-	-
2	NAG	B	1005	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9361 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 Isopullulanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4242	2676	710	845	11			
1	B	549	Total	C	N	O	S	0	0	0
			4242	2676	710	845	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ARG	-	expression tag	UNP O00105
A	17	GLU	-	expression tag	UNP O00105
A	18	PHE	-	expression tag	UNP O00105
A	19	MET	-	expression tag	UNP O00105
B	16	ARG	-	expression tag	UNP O00105
B	17	GLU	-	expression tag	UNP O00105
B	18	PHE	-	expression tag	UNP O00105
B	19	MET	-	expression tag	UNP O00105

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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

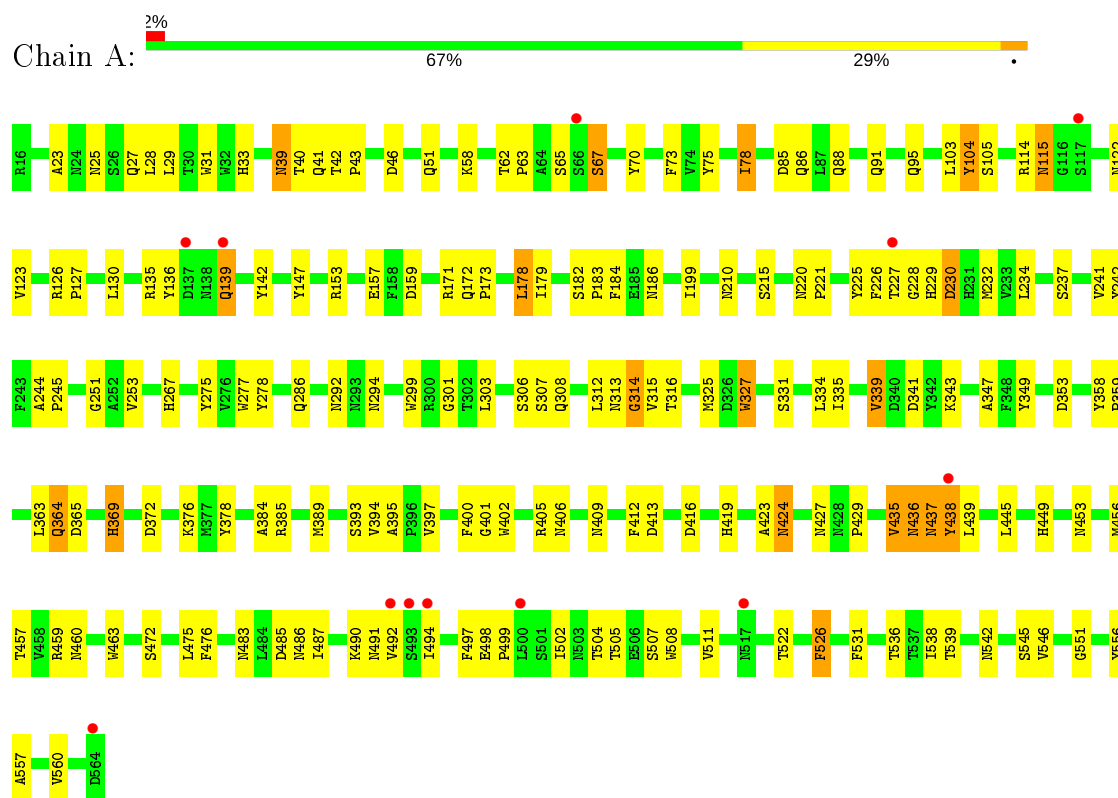
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	246	Total	O	0	0
			246	246		
3	B	351	Total	O	0	0
			351	351		

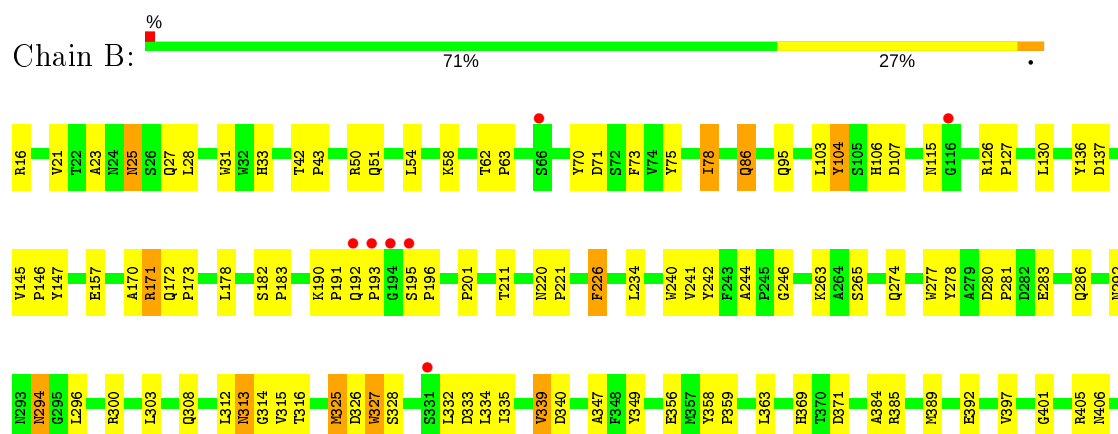
3 Residue-property plots

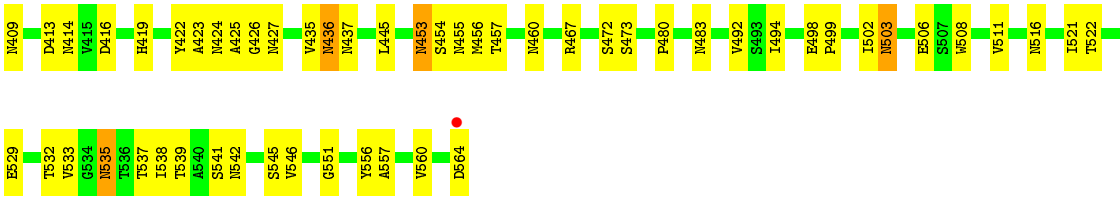
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Isopullulanase



• Molecule 1: Isopullulanase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.51Å 135.70Å 83.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.76 – 2.40 49.76 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.76-2.40) 99.9 (49.76-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.76 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.203 , 0.253 0.215 , 0.263	Depositor DCC
R_{free} test set	4553 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9361	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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 30.91 % 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 1.2081e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: 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	0.34	0/4357	0.63	2/5962 (0.0%)
1	B	0.36	0/4357	0.65	1/5962 (0.0%)
All	All	0.35	0/8714	0.64	3/11924 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	PHE	N-CA-C	-6.99	92.12	111.00
1	A	226	PHE	N-CA-C	-6.57	93.26	111.00
1	A	369	HIS	N-CA-C	-5.18	97.01	111.00

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	4242	0	3979	152	0
1	B	4242	0	3977	119	0
2	A	126	0	117	4	0
2	B	154	0	143	4	0
3	A	246	0	0	7	0
3	B	351	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9361	0	8216	272	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 16.

The worst 5 of 272 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:25:ASN:HD22	1:B:27:GLN:H	1.16	0.92
1:A:25:ASN:HD22	1:A:27:GLN:H	1.15	0.92
1:B:192:GLN:HG2	1:B:193:PRO:HD2	1.54	0.90
1:A:347:ALA:H	1:A:369:HIS:HD2	1.24	0.85
1:B:424:ASN:H	1:B:427:ASN:ND2	1.72	0.85

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	547/549 (100%)	503 (92%)	36 (7%)	8 (2%)	10	14
1	B	547/549 (100%)	509 (93%)	37 (7%)	1 (0%)	47	62
All	All	1094/1098 (100%)	1012 (92%)	73 (7%)	9 (1%)	19	29

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	SER
1	A	115	ASN
1	B	115	ASN
1	A	491	ASN

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Mol	Chain	Res	Type
1	A	545	SER

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	466/466 (100%)	446 (96%)	20 (4%)	29	46
1	B	466/466 (100%)	443 (95%)	23 (5%)	25	40
All	All	932/932 (100%)	889 (95%)	43 (5%)	27	43

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	526	PHE
1	B	104	TYR
1	B	436	ASN
1	B	16	ARG
1	B	25	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	427	ASN
1	A	520	GLN
1	B	436	ASN
1	A	436	ASN
1	A	449	HIS

5.3.3 RNA [i](#)

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

20 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	NAG	B	1001	1	14,14,15	0.45	0	17,19,21	0.66	0
2	NAG	A	1007	1	14,14,15	0.47	0	17,19,21	0.55	0
2	NAG	A	1000	1	14,14,15	0.67	0	17,19,21	0.68	0
2	NAG	B	1005	1	14,14,15	0.68	0	17,19,21	0.67	0
2	NAG	B	1002	1	14,14,15	0.49	0	17,19,21	0.62	0
2	NAG	A	1002	1	14,14,15	0.54	0	17,19,21	0.70	1 (5%)
2	NAG	A	1008	1	14,14,15	0.59	0	17,19,21	0.64	0
2	NAG	B	1006	1	14,14,15	0.54	0	17,19,21	0.66	1 (5%)
2	NAG	A	1006	1	14,14,15	0.54	0	17,19,21	0.60	0
2	NAG	B	1008	1	14,14,15	0.56	0	17,19,21	0.66	0
2	NAG	B	1007	1	14,14,15	0.49	0	17,19,21	0.67	0
2	NAG	A	1001	1	14,14,15	0.53	0	17,19,21	0.75	1 (5%)
2	NAG	A	1005	1	14,14,15	0.52	0	17,19,21	0.65	0
2	NAG	B	1000	1	14,14,15	0.83	1 (7%)	17,19,21	1.10	1 (5%)
2	NAG	A	1004	1	14,14,15	0.51	0	17,19,21	0.65	0
2	NAG	B	1009	1	14,14,15	0.50	0	17,19,21	0.59	0
2	NAG	B	1004	1	14,14,15	0.44	0	17,19,21	0.83	1 (5%)
2	NAG	B	1003	1	14,14,15	0.55	0	17,19,21	0.70	0
2	NAG	B	1010	1	14,14,15	0.57	0	17,19,21	0.69	1 (5%)
2	NAG	A	1003	1	14,14,15	0.54	0	17,19,21	0.76	1 (5%)

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	B	1001	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1007	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1000	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1005	1	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	B	1002	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1002	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1008	1	-	4/6/23/26	0/1/1/1
2	NAG	B	1006	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1006	1	-	4/6/23/26	0/1/1/1
2	NAG	B	1008	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1007	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1001	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1005	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1000	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	1004	1	-	4/6/23/26	0/1/1/1
2	NAG	B	1009	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1004	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1003	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1010	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1003	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	NAG	C1-C2	2.39	1.55	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1004	NAG	C2-N2-C7	-2.61	119.18	122.90
2	A	1003	NAG	C2-N2-C7	-2.38	119.51	122.90
2	A	1001	NAG	C2-N2-C7	-2.32	119.59	122.90
2	B	1000	NAG	O5-C1-C2	2.30	114.91	111.29
2	A	1002	NAG	C2-N2-C7	-2.19	119.78	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1005	NAG	C1
2	B	1000	NAG	C1

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	NAG	C8-C7-N2-C2
2	A	1000	NAG	O7-C7-N2-C2
2	B	1005	NAG	C8-C7-N2-C2
2	B	1005	NAG	O7-C7-N2-C2
2	A	1002	NAG	C8-C7-N2-C2

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	NAG	1	0
2	B	1005	NAG	1	0
2	B	1002	NAG	1	0
2	A	1002	NAG	2	0
2	B	1008	NAG	1	0
2	A	1005	NAG	1	0
2	B	1009	NAG	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	549/549 (100%)	-0.07	12 (2%) 62 60	6, 19, 39, 56	0
1	B	549/549 (100%)	-0.34	8 (1%) 73 72	6, 13, 31, 53	0
All	All	1098/1098 (100%)	-0.21	20 (1%) 68 66	6, 16, 37, 56	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	193	PRO	5.0
1	B	564	ASP	4.1
1	A	66	SER	3.9
1	A	564	ASP	3.7
1	A	227	THR	3.5

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 monosaccharides 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	NAG	A	1008	14/15	0.64	0.40	40,40,41,43	0
2	NAG	B	1000	14/15	0.68	0.24	41,44,50,51	0
2	NAG	B	1005	14/15	0.72	0.31	50,53,56,57	0
2	NAG	B	1006	14/15	0.75	0.25	34,39,43,44	0
2	NAG	A	1000	14/15	0.76	0.23	47,49,51,51	0
2	NAG	B	1009	14/15	0.80	0.32	58,59,61,62	0
2	NAG	A	1006	14/15	0.82	0.21	34,39,41,41	0
2	NAG	A	1001	14/15	0.82	0.19	34,36,40,40	0
2	NAG	B	1008	14/15	0.84	0.19	34,37,38,38	0
2	NAG	A	1005	14/15	0.84	0.29	42,44,47,49	0
2	NAG	B	1010	14/15	0.84	0.19	37,39,40,42	0
2	NAG	A	1002	14/15	0.87	0.20	29,32,38,38	0
2	NAG	A	1004	14/15	0.89	0.15	32,34,37,38	0
2	NAG	B	1003	14/15	0.90	0.14	24,26,29,33	0
2	NAG	A	1007	14/15	0.90	0.19	30,31,35,35	0
2	NAG	A	1003	14/15	0.90	0.13	24,28,31,37	0
2	NAG	B	1007	14/15	0.92	0.19	21,24,28,33	0
2	NAG	B	1004	14/15	0.93	0.13	22,26,33,34	0
2	NAG	B	1002	14/15	0.96	0.15	17,20,23,23	0
2	NAG	B	1001	14/15	0.96	0.12	16,18,21,21	0

6.5 Other polymers

There are no such residues in this entry.