



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:29 PM UTC

PDB ID : 3K4P / pdb_00003k4p
Title : Aspergillus niger Phytase
Authors : Oakley, A.J.
Deposited on : 2009-10-06
Resolution : 2.40 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

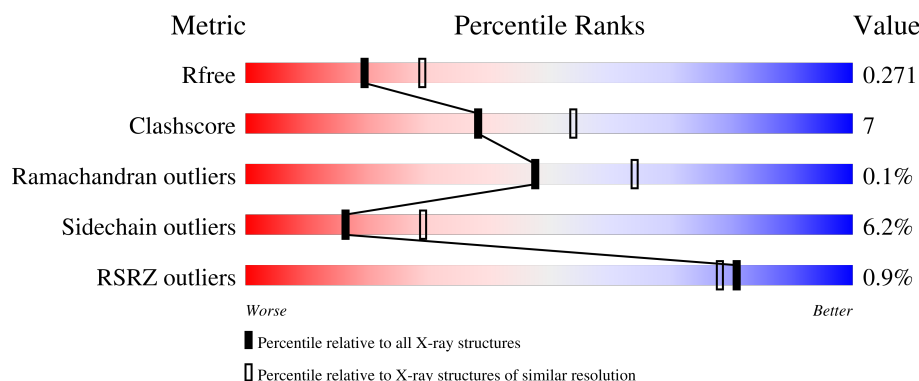
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 of 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	444	% 76% 21% ..
1	B	444	% 80% 17% ..

2 Entry composition [i](#)

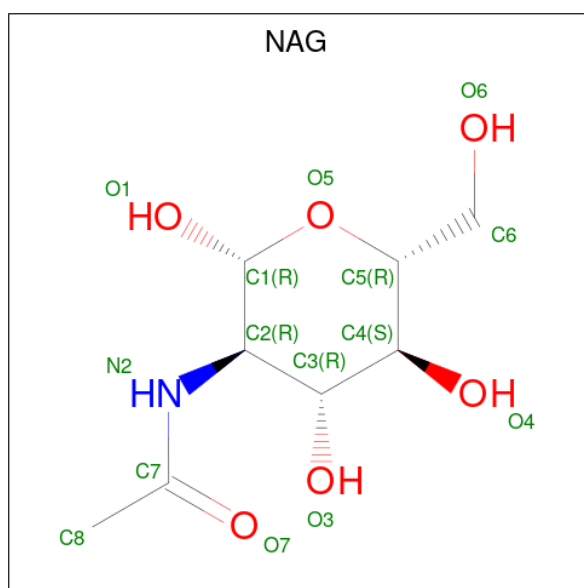
There are 3 unique types of molecules in this entry. The entry contains 7195 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-phytase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	1	0
			3396	2137	566	679	14			
1	B	438	Total	C	N	O	S	0	2	0
			3399	2138	565	682	14			

- 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
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	169	Total	O	0	0
			169	169		
3	B	147	Total	O	0	0
			147	147		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.07Å 87.46Å 82.19Å 90.00° 110.98° 90.00°	Depositor
Resolution (Å)	66.36 – 2.40 66.36 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.5 (66.36-2.40) 96.5 (66.36-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.215 , 0.275 0.214 , 0.271	Depositor DCC
R_{free} test set	1770 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7195	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.48% 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

5.1 Standard geometry

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	0.97	1/3480 (0.0%)	1.11	8/4736 (0.2%)
1	B	0.97	0/3486	1.14	6/4746 (0.1%)
All	All	0.97	1/6966 (0.0%)	1.12	14/9482 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	408	VAL	CA-CB	5.96	1.59	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	330	SER	N-CA-C	-10.46	97.22	110.19
1	A	330	SER	N-CA-C	-9.46	97.29	110.35
1	B	114	VAL	N-CA-C	-8.74	102.31	110.53
1	A	114	VAL	N-CA-C	-6.36	104.55	110.53
1	A	135	ILE	N-CA-C	5.91	116.38	107.75
1	B	415	VAL	CB-CA-C	-5.84	102.50	111.08
1	B	251	VAL	CB-CA-C	-5.53	102.22	111.29
1	A	8	CYS	N-CA-C	-5.49	106.25	113.17
1	A	216	ILE	N-CA-C	-5.32	105.66	110.82
1	B	143	VAL	CA-C-N	5.28	127.41	120.60
1	B	143	VAL	C-N-CA	5.28	127.41	120.60
1	A	70	LYS	N-CA-C	-5.22	104.66	111.02
1	A	143	VAL	CA-C-N	5.12	127.21	120.60
1	A	143	VAL	C-N-CA	5.12	127.21	120.60

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	3396	0	3230	50	0
1	B	3399	0	3226	43	0
2	A	42	0	39	1	0
2	B	42	0	39	0	0
3	A	169	0	0	6	0
3	B	147	0	0	2	0
All	All	7195	0	6534	93	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 7.

All (93) 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:185:ASN:HD22	1:A:185:ASN:C	1.84	0.84
1:A:97:ASN:ND2	3:A:521:HOH:O	2.11	0.81
1:B:185:ASN:C	1:B:185:ASN:HD22	1.88	0.79
1:B:246:ILE:HA	1:B:251:VAL:HG13	1.69	0.75
1:A:248:THR:OG1	1:A:249:SER:N	2.20	0.73
1:B:248:THR:OG1	1:B:249:SER:N	2.23	0.71
1:B:185:ASN:ND2	1:B:187:LEU:H	1.91	0.69
1:B:141:SER:HB2	3:B:452:HOH:O	1.92	0.68
1:B:280:TYR:O	1:B:286:ASN:HB2	1.94	0.67
1:A:52:PHE:HB3	1:A:388:MET:HB3	1.77	0.66
1:A:185:ASN:C	1:A:185:ASN:ND2	2.56	0.60
1:B:24:LEU:HB3	1:B:271:ASP:HB2	1.84	0.59
1:B:52:PHE:HB3	1:B:388:MET:HB3	1.85	0.58
1:A:410:LEU:HD13	1:A:426:PHE:CD1	2.39	0.58
1:A:136:ARG:HB2	1:A:335:ASP:OD1	2.03	0.58
1:B:313:THR:OG1	1:B:314:SER:N	2.36	0.58
1:B:185:ASN:HD22	1:B:187:LEU:H	1.52	0.58
1:B:118:ILE:O	1:B:122:GLN:HG3	2.04	0.56
1:B:9:ASP:HB3	1:B:252:ASP:OD1	2.05	0.56
1:A:429:GLY:HA3	3:A:485:HOH:O	2.06	0.56
1:A:185:ASN:ND2	1:A:187:LEU:H	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ASP:OD1	1:A:340:ASN:N	2.41	0.54
1:A:280:TYR:O	1:A:286:ASN:HB2	2.07	0.54
1:B:410:LEU:HD13	1:B:426:PHE:CD1	2.42	0.54
1:B:66:ASP:O	1:B:70:LYS:HG2	2.07	0.54
1:B:119:LYS:NZ	1:B:405:ASP:OD2	2.41	0.53
1:A:15:TYR:CD2	1:A:30:PRO:HG2	2.44	0.53
1:A:185:ASN:HD21	1:A:187:LEU:HB2	1.74	0.53
1:B:9:ASP:CB	1:B:252:ASP:OD1	2.58	0.52
1:A:9:ASP:HB3	1:A:252:ASP:OD1	2.09	0.52
1:B:185:ASN:HD22	1:B:186:THR:N	2.06	0.52
1:A:185:ASN:HD22	1:A:186:THR:N	2.09	0.51
1:A:119:LYS:NZ	1:A:405:ASP:OD2	2.43	0.50
1:B:15:TYR:CD2	1:B:30:PRO:HG2	2.47	0.50
1:B:339:ASP:OD1	1:B:340:ASN:N	2.44	0.50
1:A:406:ARG:NH1	1:A:408:VAL:HG22	2.27	0.50
1:B:113:LEU:O	1:B:150:PHE:HA	2.11	0.50
1:B:387:GLU:OE2	1:B:400:ARG:NE	2.40	0.50
1:A:118:ILE:O	1:A:122:GLN:HG3	2.11	0.50
1:B:342:ILE:O	1:B:346:LEU:HG	2.11	0.50
1:A:185:ASN:HD22	1:A:187:LEU:H	1.60	0.50
1:A:24:LEU:HB3	1:A:271:ASP:HB2	1.94	0.49
1:A:140:SER:O	1:A:141:SER:C	2.54	0.49
1:A:379:PRO:HG3	3:A:541:HOH:O	2.11	0.49
1:A:317:HIS:CE1	3:A:592:HOH:O	2.65	0.49
1:A:313:THR:HB	1:A:439:TRP:CD2	2.48	0.49
1:B:358:LEU:HD22	1:B:369:THR:HG22	1.95	0.48
1:B:136:ARG:HB2	1:B:335:ASP:OD1	2.13	0.48
1:A:66:ASP:O	1:A:70:LYS:HG2	2.13	0.48
1:A:313:THR:OG1	1:A:314:SER:N	2.47	0.48
1:B:185:ASN:C	1:B:185:ASN:ND2	2.60	0.48
1:B:295:GLY:HA3	1:B:314:SER:OG	2.14	0.47
1:A:9:ASP:CB	1:A:252:ASP:OD1	2.62	0.47
1:B:95:THR:O	1:B:96:TYR:C	2.58	0.47
1:B:313:THR:HB	1:B:439:TRP:CD2	2.50	0.47
1:B:329:ASN:C	1:B:330:SER:O	2.55	0.47
1:A:136:ARG:HG2	1:A:175:VAL:HB	1.96	0.46
1:A:53:ALA:O	1:A:332:LEU:HA	2.16	0.46
1:A:61:ALA:HA	1:A:380:PHE:CD1	2.51	0.46
1:A:148:LYS:HE3	1:A:173:ILE:HD12	1.98	0.46
1:A:205:GLU:O	1:A:209:THR:HG23	2.15	0.46
1:A:358:LEU:HD22	1:A:369:THR:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:PRO:HA	3:B:525:HOH:O	2.15	0.45
1:A:356:LYS:O	1:A:357:PRO:C	2.60	0.45
1:A:113:LEU:O	1:A:150:PHE:HA	2.17	0.45
1:A:402:LEU:N	1:A:402:LEU:HD12	2.31	0.44
1:B:106:THR:O	1:B:107:PRO:C	2.58	0.44
1:A:83:ALA:HB2	1:A:227:VAL:HG23	1.98	0.44
1:B:45:PRO:O	1:B:48:CYS:HB2	2.17	0.44
1:B:140:SER:O	1:B:141:SER:C	2.60	0.44
1:A:126:SER:HA	1:A:129:ARG:HD3	1.99	0.44
1:A:11:VAL:HG22	1:A:115:ASN:CG	2.43	0.43
1:A:106:THR:O	1:A:107:PRO:C	2.58	0.43
1:A:78:GLU:HB3	2:A:1001:NAG:H82	1.99	0.43
1:B:185:ASN:HD21	1:B:187:LEU:HB2	1.83	0.42
1:A:107:PRO:O	1:A:110:GLU:HB2	2.18	0.42
1:B:108:PHE:CD1	1:B:251:VAL:HG11	2.54	0.42
1:A:20:GLU:HA	3:A:596:HOH:O	2.20	0.42
1:A:260:ASP:HB2	3:A:456:HOH:O	2.18	0.42
1:B:205:GLU:HG3	1:B:273:LEU:HD11	2.01	0.42
1:B:30:PRO:O	1:B:31:PHE:C	2.63	0.42
1:A:205:GLU:HG3	1:A:273:LEU:HD11	2.02	0.42
1:A:95:THR:O	1:A:96:TYR:C	2.63	0.42
1:B:356:LYS:O	1:B:357:PRO:C	2.63	0.42
1:B:53:ALA:O	1:B:332:LEU:HA	2.20	0.41
1:A:194:VAL:HG23	1:A:442:CYS:O	2.20	0.41
1:A:387:GLU:OE2	1:A:400:ARG:NE	2.46	0.41
1:A:342:ILE:O	1:A:346:LEU:HG	2.21	0.41
1:B:250:THR:O	1:B:251:VAL:C	2.62	0.41
1:B:136:ARG:HG2	1:B:175:VAL:HB	2.03	0.41
1:B:402:LEU:HD12	1:B:402:LEU:N	2.36	0.41
1:A:45:PRO:O	1:A:48:CYS:HB2	2.21	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	437/444 (98%)	413 (94%)	23 (5%)	1 (0%)	43	58
1	B	438/444 (99%)	415 (95%)	23 (5%)	0	100	100
All	All	875/888 (98%)	828 (95%)	46 (5%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	LEU

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	379/385 (98%)	356 (94%)	23 (6%)	17	30
1	B	380/385 (99%)	356 (94%)	24 (6%)	16	29
All	All	759/770 (99%)	712 (94%)	47 (6%)	16	29

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	43	GLU
1	A	67	SER
1	A	99	SER
1	A	105	LEU
1	A	113	LEU
1	A	170	SER
1	A	185	ASN
1	A	191	THR
1	A	222	ASN
1	A	227	VAL
1	A	228	THR

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Mol	Chain	Res	Type
1	A	248	THR
1	A	250	THR
1	A	291	THR
1	A	294	VAL
1	A	319	LEU
1	A	322	SER
1	A	331	THR
1	A	362	THR
1	A	387	GLU
1	A	390	GLN
1	A	415	VAL
1	B	12	ASP
1	B	43	GLU
1	B	49	ARG
1	B	67	SER
1	B	99	SER
1	B	105	LEU
1	B	113	LEU
1	B	185	ASN
1	B	191	THR
1	B	222	ASN
1	B	227	VAL
1	B	228	THR
1	B	248	THR
1	B	250	THR
1	B	251	VAL
1	B	291	THR
1	B	294	VAL
1	B	319	LEU
1	B	322	SER
1	B	325	THR
1	B	362	THR
1	B	387	GLU
1	B	390	GLN
1	B	415	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	ASN
1	A	317	HIS
1	A	390	GLN

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Mol	Chain	Res	Type
1	B	185	ASN
1	B	222	ASN
1	B	269	ASN
1	B	390	GLN
1	B	411	HIS

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](#)

6 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	A	1002	1	14,14,15	0.88	0	17,19,21	1.91	7 (41%)
2	NAG	A	1001	1	14,14,15	0.75	0	17,19,21	1.88	6 (35%)
2	NAG	B	1003	1	14,14,15	0.73	0	17,19,21	1.59	4 (23%)
2	NAG	B	1002	1	14,14,15	0.64	0	17,19,21	1.22	2 (11%)
2	NAG	B	1001	1	14,14,15	0.66	0	17,19,21	1.27	1 (5%)
2	NAG	A	1003	1	14,14,15	1.05	2 (14%)	17,19,21	1.26	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	A	1002	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1003	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1002	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1003	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1003	NAG	O5-C1	-2.37	1.39	1.43
2	A	1003	NAG	C2-N2	-2.18	1.42	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	NAG	C1-O5-C5	3.98	117.53	112.19
2	B	1003	NAG	C2-N2-C7	-3.88	117.70	122.90
2	A	1001	NAG	C3-C4-C5	-3.63	103.65	110.23
2	A	1002	NAG	O3-C3-C2	-3.51	102.10	109.40
2	A	1002	NAG	C2-N2-C7	-3.43	118.30	122.90
2	B	1002	NAG	O5-C1-C2	-3.19	106.35	111.29
2	A	1003	NAG	C1-C2-N2	-3.07	105.59	110.43
2	A	1001	NAG	C2-N2-C7	3.03	126.96	122.90
2	B	1003	NAG	O5-C5-C6	2.97	113.45	107.66
2	A	1002	NAG	O5-C1-C2	-2.79	106.97	111.29
2	A	1002	NAG	C1-C2-N2	2.77	114.79	110.43
2	B	1003	NAG	C1-O5-C5	2.62	115.70	112.19
2	A	1001	NAG	O5-C1-C2	-2.61	107.25	111.29
2	B	1002	NAG	C1-O5-C5	2.56	115.62	112.19
2	A	1002	NAG	O4-C4-C5	2.43	115.31	109.32
2	A	1002	NAG	C3-C4-C5	-2.39	105.89	110.23
2	B	1003	NAG	C6-C5-C4	-2.32	107.32	113.02
2	A	1001	NAG	O4-C4-C5	2.29	114.96	109.32
2	A	1001	NAG	C4-C3-C2	-2.02	108.06	111.02
2	A	1001	NAG	O5-C5-C4	-2.02	105.91	110.83
2	A	1002	NAG	C6-C5-C4	2.00	117.94	113.02

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1003	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	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	438/444 (98%)	0.07	4 (0%) 81 78	12, 25, 45, 55	1 (0%)
1	B	438/444 (98%)	0.05	4 (0%) 81 78	12, 25, 45, 55	2 (0%)
All	All	876/888 (98%)	0.06	8 (0%) 81 78	12, 25, 45, 55	3 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	393	ALA	2.7
1	B	444	ALA	2.7
1	A	444	ALA	2.7
1	A	392	GLN	2.7
1	B	392	GLN	2.7
1	B	7	SER	2.3
1	A	95	THR	2.2
1	B	393	ALA	2.1

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, 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($\text{\AA}^2$)	Q<0.9
2	NAG	B	1001	14/15	0.83	0.12	35,46,50,51	0
2	NAG	A	1002	14/15	0.85	0.12	36,40,42,43	0
2	NAG	B	1002	14/15	0.86	0.11	38,41,44,45	0
2	NAG	A	1003	14/15	0.90	0.09	24,29,30,32	0
2	NAG	A	1001	14/15	0.91	0.09	25,39,43,46	0
2	NAG	B	1003	14/15	0.94	0.07	23,26,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.