



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:59 PM GMT

PDB ID : 4GVF
Title : Crystal structure of Salmonella typhimurium family 3 glycoside hydrolase (NagZ) bound to GlcNAc
Authors : Bacik, J.P.; Mark, B.L.
Deposited on : 2012-08-30
Resolution : 1.35 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
<http://wwpdb.org/validation/2016/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 : 1.7 (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

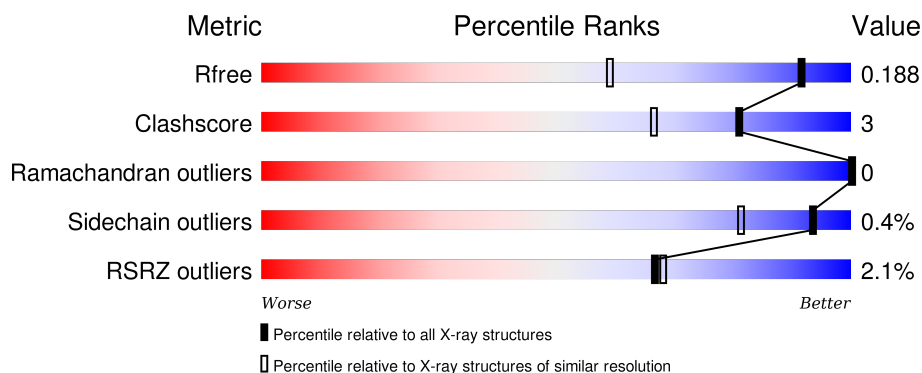
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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	2199 (1.40-1.32)
Clashscore	102246	2337 (1.40-1.32)
Ramachandran outliers	100387	2280 (1.40-1.32)
Sidechain outliers	100360	2279 (1.40-1.32)
RSRZ outliers	91569	2199 (1.40-1.32)

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 $\leq 5\%$. 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	349	 3% 91% 7% .
1	B	349	 1% 88% 6% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6264 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.

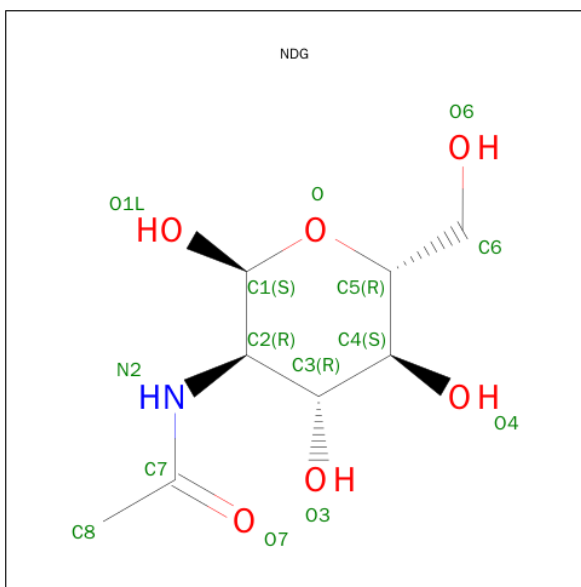
- Molecule 1 is a protein called Beta-hexosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	8	0
			2644	1650	477	497	20			
1	B	328	Total	C	N	O	S	0	7	0
			2560	1601	463	479	17			

There are 16 discrepancies between the modelled and reference sequences:

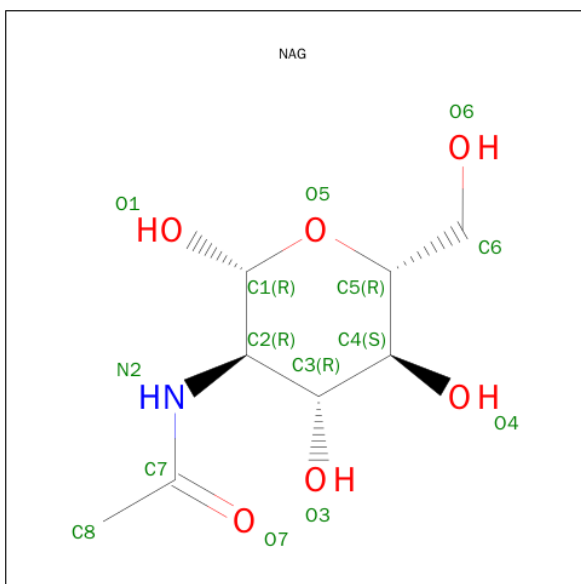
Chain	Residue	Modelled	Actual	Comment	Reference
A	342	GLY	-	EXPRESSION TAG	UNP Q8ZQ06
A	343	SER	-	EXPRESSION TAG	UNP Q8ZQ06
A	344	HIS	-	EXPRESSION TAG	UNP Q8ZQ06
A	345	HIS	-	EXPRESSION TAG	UNP Q8ZQ06
A	346	HIS	-	EXPRESSION TAG	UNP Q8ZQ06
A	347	HIS	-	EXPRESSION TAG	UNP Q8ZQ06
A	348	HIS	-	EXPRESSION TAG	UNP Q8ZQ06
A	349	HIS	-	EXPRESSION TAG	UNP Q8ZQ06
B	342	GLY	-	EXPRESSION TAG	UNP Q8ZQ06
B	343	SER	-	EXPRESSION TAG	UNP Q8ZQ06
B	344	HIS	-	EXPRESSION TAG	UNP Q8ZQ06
B	345	HIS	-	EXPRESSION TAG	UNP Q8ZQ06
B	346	HIS	-	EXPRESSION TAG	UNP Q8ZQ06
B	347	HIS	-	EXPRESSION TAG	UNP Q8ZQ06
B	348	HIS	-	EXPRESSION TAG	UNP Q8ZQ06
B	349	HIS	-	EXPRESSION TAG	UNP Q8ZQ06

- Molecule 2 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	1
			15	8	1	6		
2	B	1	Total	C	N	O	0	1
			15	8	1	6		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



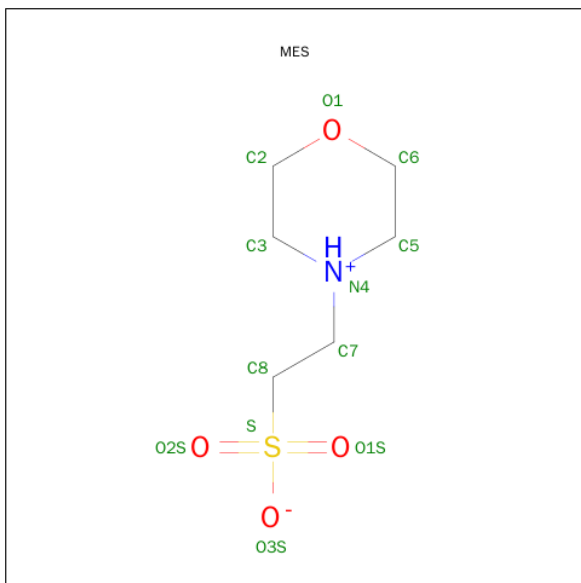
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			15	8	1	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	1
			15	8	1	6		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).

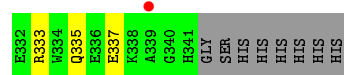


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	509	Total	O	0	0
			509	509		
5	B	479	Total	O	0	0
			479	479		

- Molecule 1: Beta-hexosaminidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.54Å 66.23Å 94.97Å 90.00° 99.32° 90.00°	Depositor
Resolution (Å)	48.89 – 1.35 48.89 – 1.35	Depositor EDS
% Data completeness (in resolution range)	96.9 (48.89-1.35) 96.8 (48.89-1.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.27 (at 1.35Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.4_486)	Depositor
R, R_{free}	0.167 , 0.190 0.164 , 0.188	Depositor DCC
R_{free} test set	3888 reflections (3.02%)	DCC
Wilson B-factor (Å ²)	7.9	Xtriage
Anisotropy	0.814	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 131642 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6264	wwPDB-VP
Average B, all atoms (Å ²)	13.0	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 52.51 % 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 4.8120e-05. 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, 0.375 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: NAG, NDG, MES

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	0.30	0/2718	0.51	0/3674
1	B	0.30	0/2628	0.51	0/3550
All	All	0.30	0/5346	0.51	0/7224

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

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	2644	0	2578	18	0
1	B	2560	0	2513	16	0
2	A	15	0	15	0	0
2	B	15	0	15	0	0
3	A	15	0	15	0	0
3	B	15	0	15	0	0
4	B	12	0	12	0	0
5	A	509	0	0	6	0
5	B	479	0	0	7	0
All	All	6264	0	5163	34	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 3.

All (34) 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:302:ARG:HD2	5:A:1004:HOH:O	1.64	0.94
1:B:302:ARG:HD2	5:B:974:HOH:O	1.73	0.88
1:B:213:HIS:HE1	5:B:975:HOH:O	1.73	0.72
1:A:250:LEU:HD11	1:A:276:ILE:HG21	1.75	0.67
1:B:331:HIS:O	1:B:335:GLN:HG2	1.98	0.63
1:B:265:ALA:HB1	1:B:276:ILE:HD12	1.81	0.61
1:A:213:HIS:HE1	1:A:253:GLU:OE1	1.86	0.58
1:A:190:ARG:NH2	1:A:238:GLU:OE1	2.37	0.58
1:B:159:LYS:HD3	5:B:803:HOH:O	2.06	0.55
1:A:209:ILE:HD12	1:A:235:LEU:HD11	1.90	0.53
1:A:213:HIS:HD2	5:A:724:HOH:O	1.93	0.52
1:A:307:GLY:HA3	5:A:718:HOH:O	2.10	0.50
1:B:265:ALA:HB1	1:B:276:ILE:CD1	2.40	0.49
1:B:32:PHE:CD1	1:B:34[B]:ARG:NH1	2.80	0.49
1:B:213:HIS:HD2	5:B:977:HOH:O	1.95	0.49
1:A:16:GLU:HG2	5:A:944:HOH:O	2.13	0.49
1:A:163:LYS:HB3	1:A:210[B]:MET:HB3	1.95	0.48
1:A:185:PRO:HG2	1:A:188:ASP:OD2	2.14	0.48
1:A:72[B]:ARG:NH1	5:A:1003:HOH:O	2.47	0.48
1:B:47:ARG:HD2	5:B:893:HOH:O	2.15	0.47
1:A:126:ILE:HG12	5:A:640:HOH:O	2.13	0.47
1:A:190:ARG:HH22	1:A:238:GLU:CD	2.18	0.46
1:A:250:LEU:HD11	1:A:276:ILE:CG2	2.44	0.46
1:A:333:ARG:NH1	1:A:337:GLU:HB2	2.32	0.45
1:B:333:ARG:O	1:B:337:GLU:HG2	2.16	0.45
1:A:174:ASP:O	1:A:175:SER:HB3	2.18	0.44
1:B:16:GLU:HG2	5:B:778:HOH:O	2.18	0.44
1:B:211:PRO:HD2	1:B:246:PHE:O	2.17	0.44
1:B:159:LYS:HD2	1:B:207:ASP:CG	2.39	0.43
1:A:211:PRO:HD2	1:A:246:PHE:O	2.19	0.43
1:B:185:PRO:HG2	1:B:188:ASP:OD2	2.19	0.43
1:A:213:HIS:CE1	1:A:253:GLU:OE1	2.71	0.41
1:B:237:GLN:HG3	5:B:919:HOH:O	2.20	0.41
1:B:220:ASP:HA	1:B:221:PRO:HD3	1.93	0.41

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	346/349 (99%)	333 (96%)	13 (4%)	0	100	100
1	B	329/349 (94%)	317 (96%)	12 (4%)	0	100	100
All	All	675/698 (97%)	650 (96%)	25 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	272/281 (97%)	271 (100%)	1 (0%)	93	81
1	B	267/281 (95%)	266 (100%)	1 (0%)	93	81
All	All	539/562 (96%)	537 (100%)	2 (0%)	93	81

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	ASP
1	B	193	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	HIS

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Mol	Chain	Res	Type
1	B	213	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 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	NDG	A	401[A]	-	15,15,15	1.63	3 (20%)	17,21,21	0.79	0
3	NAG	A	402[B]	-	15,15,15	1.63	3 (20%)	17,21,21	0.79	0
2	NDG	B	401[A]	-	15,15,15	1.55	3 (20%)	17,21,21	0.69	0
3	NAG	B	402[B]	-	15,15,15	1.55	3 (20%)	17,21,21	0.69	0
4	MES	B	403	-	11,12,12	0.59	0	14,16,16	2.92	4 (28%)

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	NDG	A	401[A]	-	-	0/6/26/26	0/1/1/1
3	NAG	A	402[B]	-	-	0/6/26/26	0/1/1/1
2	NDG	B	401[A]	-	-	0/6/26/26	0/1/1/1
3	NAG	B	402[B]	-	-	0/6/26/26	0/1/1/1
4	MES	B	403	-	-	0/6/14/14	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401[A]	NDG	C4-C3	-3.05	1.44	1.52
3	A	402[B]	NAG	C4-C3	-3.05	1.44	1.52
2	A	401[A]	NDG	C1-C2	-3.03	1.49	1.53
3	A	402[B]	NAG	C1-C2	-3.03	1.49	1.53
3	B	402[B]	NAG	C4-C3	-2.88	1.44	1.52
2	B	401[A]	NDG	C4-C3	-2.88	1.44	1.52
3	B	402[B]	NAG	C1-C2	-2.58	1.50	1.53
2	B	401[A]	NDG	C1-C2	-2.58	1.50	1.53
3	B	402[B]	NAG	C3-C2	-2.56	1.48	1.53
2	B	401[A]	NDG	C3-C2	-2.56	1.48	1.53
2	A	401[A]	NDG	C3-C2	-2.43	1.48	1.53
3	A	402[B]	NAG	C3-C2	-2.43	1.48	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	403	MES	O2S-S-C8	2.10	108.69	106.91
4	B	403	MES	C7-N4-C3	2.68	118.13	111.27
4	B	403	MES	C5-N4-C3	3.15	115.72	108.90
4	B	403	MES	O1S-S-C8	9.14	114.70	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

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, 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	340/349 (97%)	0.01	11 (3%) 51 52	4, 9, 23, 34	0
1	B	328/349 (93%)	-0.01	3 (0%) 85 86	4, 9, 24, 34	0
All	All	668/698 (95%)	0.00	14 (2%) 67 68	4, 9, 24, 34	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	309	PHE	4.0
1	A	255	ALA	3.9
1	A	175	SER	3.7
1	A	173	ALA	3.3
1	B	339	ALA	3.3
1	A	254	GLY	3.2
1	A	308	SER	3.2
1	A	276	ILE	3.1
1	A	252	MET	3.1
1	A	257	ILE	3.0
1	A	307	GLY	2.9
1	A	295	ILE	2.5
1	B	250	LEU	2.4
1	B	279	CYS	2.3

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 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	MES	B	403	12/12	0.96	0.12	1.40	11,19,23,26	3
3	NAG	B	402[B]	15/15	0.98	0.07	-0.37	4,6,7,14	15
2	NDG	B	401[A]	15/15	0.98	0.07	-0.56	4,6,7,8	15
3	NAG	A	402[B]	15/15	0.98	0.06	-0.69	5,6,9,14	15
2	NDG	A	401[A]	15/15	0.98	0.06	-0.91	5,6,9,9	15

6.5 Other polymers [i](#)

There are no such residues in this entry.