



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:09 PM UTC

PDB ID : 9GEE / pdb_00009gee
Title : Entamoeba histolytica Gal/GalNAc lectin heavy chain residues 808-992 in the presence of galactose
Authors : Gerard, S.F.; Higgins, M.K.
Deposited on : 2024-08-07
Resolution : 1.82 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

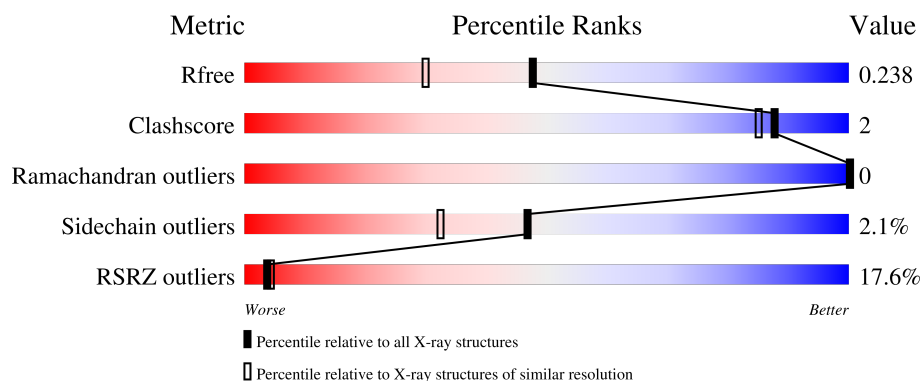
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	189	<div> <div>21%</div> <div>88%</div> <div>9%</div> <div>..</div> </div>
1	B	189	<div> <div>16%</div> <div>86%</div> <div>7%</div> <div>5%</div> </div>
1	C	189	<div> <div>14%</div> <div>90%</div> <div>5%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4878 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 Galactose/N-acetyl-D-galactosamine lectin heavy subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1491	933	241	302	15			
1	B	180	Total	C	N	O	S	0	0	0
			1457	914	235	293	15			
1	C	179	Total	C	N	O	S	0	0	0
			1450	909	234	292	15			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	811	SER	CYS	conflict	UNP P32022
A	972	SER	CYS	conflict	UNP P32022
A	993	GLY	THR	conflict	UNP P32022
B	811	SER	CYS	conflict	UNP P32022
B	972	SER	CYS	conflict	UNP P32022
B	993	GLY	THR	conflict	UNP P32022
C	811	SER	CYS	conflict	UNP P32022
C	972	SER	CYS	conflict	UNP P32022
C	993	GLY	THR	conflict	UNP P32022

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

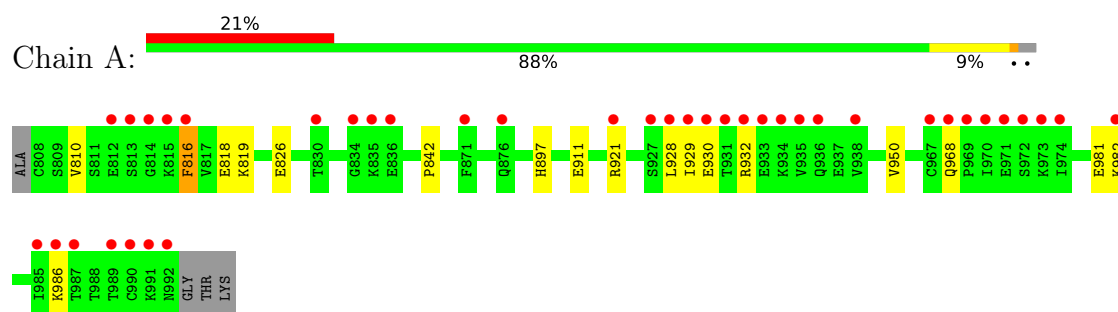
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	138	Total	O	0	0
			138	138		
3	B	164	Total	O	0	0
			164	164		
3	C	136	Total	O	0	0
			136	136		

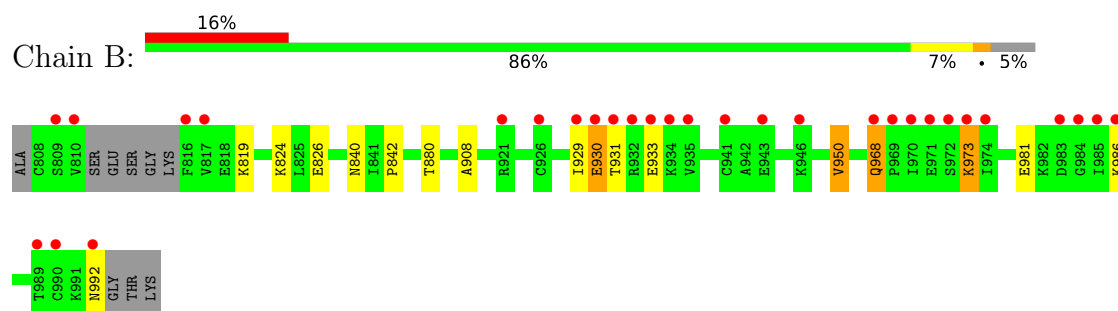
3 Residue-property plots [i](#)

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.

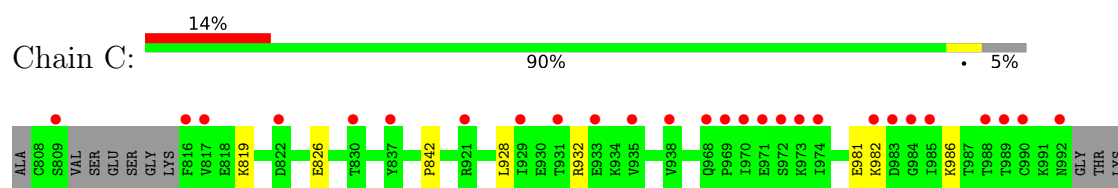
- Molecule 1: Galactose/N-acetyl-D-galactosamine lectin heavy subunit 1



- Molecule 1: Galactose/N-acetyl-D-galactosamine lectin heavy subunit 1



- Molecule 1: Galactose/N-acetyl-D-galactosamine lectin heavy subunit 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	83.24Å 146.31Å 85.33Å 90.00° 114.00° 90.00°	Depositor
Resolution (Å)	36.07 – 1.82 36.07 – 1.82	Depositor EDS
% Data completeness (in resolution range)	62.3 (36.07-1.82) 62.3 (36.07-1.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 1.82Å)	Xtriage
Refinement program	BUSTER 2.10.4 (26-JUL-2023)	Depositor
R, R_{free}	0.217 , 0.246 0.212 , 0.238	Depositor DCC
R_{free} test set	2527 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4878	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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 [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	0.76	0/1517	1.05	4/2045 (0.2%)
1	B	0.76	0/1482	1.03	6/1998 (0.3%)
1	C	0.74	0/1475	0.98	0/1988
All	All	0.75	0/4474	1.02	10/6031 (0.2%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	911	GLU	CB-CG-CD	8.24	126.61	112.60
1	A	816	PHE	CA-CB-CG	7.38	121.18	113.80
1	B	950	VAL	N-CA-CB	-6.17	105.04	111.64
1	A	930	GLU	CA-C-N	5.77	128.28	120.38
1	A	930	GLU	C-N-CA	5.77	128.28	120.38
1	B	950	VAL	CB-CA-C	5.61	114.83	109.33
1	B	930	GLU	CA-C-N	5.38	128.02	120.28
1	B	930	GLU	C-N-CA	5.38	128.02	120.28
1	B	908	ALA	N-CA-C	5.17	116.92	111.28
1	B	968	GLN	CB-CA-C	5.14	115.71	109.85

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	1491	0	1437	6	0
1	B	1457	0	1404	9	0
1	C	1450	0	1395	4	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
3	A	138	0	0	0	0
3	B	164	0	0	0	0
3	C	136	0	0	0	0
All	All	4878	0	4275	17	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 2.

All (17) 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:928:LEU:HD13	1:A:932:ARG:HE	1.52	0.74
1:A:981:GLU:HG2	1:A:986:LYS:HG2	1.77	0.66
1:C:981:GLU:HG2	1:C:986:LYS:HG2	1.78	0.65
1:B:981:GLU:HG2	1:B:986:LYS:HG2	1.79	0.64
1:B:929:ILE:HB	1:B:931:THR:HG22	1.86	0.57
1:B:973:LYS:NZ	1:B:992:ASN:HB3	2.30	0.47
1:C:928:LEU:HD13	1:C:932:ARG:HD2	1.96	0.47
1:B:931:THR:C	1:B:933:GLU:H	2.23	0.46
1:A:921:ARG:NH2	1:C:982:LYS:NZ	2.64	0.46
1:A:819:LYS:HD2	1:A:842:PRO:HB3	1.99	0.45
1:A:810:VAL:HG13	1:A:818:GLU:HB2	2.02	0.42
1:B:819:LYS:HD2	1:B:842:PRO:HB3	2.01	0.41
1:B:824:LYS:HD2	1:B:840:ASN:CG	2.46	0.41
1:C:819:LYS:HD2	1:C:842:PRO:HB3	2.01	0.41
1:B:929:ILE:HG22	1:B:930:GLU:H	1.86	0.41
1:B:973:LYS:HD2	1:B:973:LYS:HA	1.91	0.41
1:A:982:LYS:HG2	1:B:880:THR:HG23	2.03	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	183/189 (97%)	181 (99%)	2 (1%)	0	100	100
1	B	176/189 (93%)	172 (98%)	4 (2%)	0	100	100
1	C	175/189 (93%)	174 (99%)	1 (1%)	0	100	100
All	All	534/567 (94%)	527 (99%)	7 (1%)	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	174/176 (99%)	168 (97%)	6 (3%)	32	14
1	B	170/176 (97%)	166 (98%)	4 (2%)	43	27
1	C	169/176 (96%)	168 (99%)	1 (1%)	78	74
All	All	513/528 (97%)	502 (98%)	11 (2%)	47	32

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

Mol	Chain	Res	Type
1	A	816	PHE
1	A	826	GLU
1	A	897	HIS
1	A	929	ILE
1	A	950	VAL

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Mol	Chain	Res	Type
1	A	968	GLN
1	B	826	GLU
1	B	950	VAL
1	B	968	GLN
1	B	973	LYS
1	C	826	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	840	ASN
1	A	964	ASN
1	B	840	ASN
1	B	964	ASN
1	C	840	ASN
1	C	964	ASN

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](#)

3 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	0.27	0	17,19,21	0.58	0
2	NAG	C	1001	1	14,14,15	0.24	0	17,19,21	0.57	0
2	NAG	A	1001	1	14,14,15	0.32	0	17,19,21	0.79	0

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	-	0/6/23/26	0/1/1/1
2	NAG	C	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1001	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

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 [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

6.1 Protein, DNA and RNA chains

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	185/189 (97%)	1.16	39 (21%) 2 2	21, 43, 78, 96	0
1	B	180/189 (95%)	0.81	30 (16%) 4 5	23, 38, 68, 86	0
1	C	179/189 (94%)	0.89	27 (15%) 5 6	22, 43, 70, 85	0
All	All	544/567 (95%)	0.95	96 (17%) 4 4	21, 41, 74, 96	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	816	PHE	7.6
1	A	974	ILE	7.3
1	B	810	VAL	7.0
1	A	929	ILE	6.7
1	A	815	LYS	6.0
1	C	816	PHE	6.0
1	A	970	ILE	5.4
1	B	931	THR	5.3
1	B	974	ILE	5.2
1	A	816	PHE	5.1
1	A	931	THR	4.9
1	B	929	ILE	4.9
1	B	970	ILE	4.9
1	B	973	LYS	4.8
1	A	989	THR	4.8
1	B	972	SER	4.7
1	A	972	SER	4.6
1	C	970	ILE	4.5
1	A	814	GLY	4.3
1	C	972	SER	4.3
1	A	813	SER	4.1
1	B	935	VAL	4.1
1	A	812	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	968	GLN	3.9
1	C	974	ILE	3.9
1	A	932	ARG	3.8
1	A	973	LYS	3.8
1	B	809	SER	3.6
1	A	971	GLU	3.6
1	A	992	ASN	3.6
1	C	968	GLN	3.5
1	C	983	ASP	3.5
1	C	992	ASN	3.4
1	A	991	LYS	3.4
1	C	973	LYS	3.4
1	A	928	LEU	3.4
1	A	969	PRO	3.4
1	B	985	ILE	3.2
1	B	992	ASN	3.2
1	B	971	GLU	3.2
1	C	984	GLY	3.2
1	A	933	GLU	3.2
1	C	989	THR	3.1
1	A	985	ILE	3.1
1	A	930	GLU	3.1
1	B	817	VAL	3.0
1	A	921	ARG	3.0
1	B	930	GLU	3.0
1	A	982	LYS	3.0
1	B	926	CYS	3.0
1	C	817	VAL	2.9
1	B	934	LYS	2.9
1	A	935	VAL	2.9
1	A	934	LYS	2.9
1	A	936	GLN	2.9
1	C	990	CYS	2.8
1	A	990	CYS	2.8
1	A	938	VAL	2.8
1	C	830	THR	2.8
1	B	983	ASP	2.7
1	C	988	THR	2.7
1	B	990	CYS	2.6
1	C	931	THR	2.6
1	A	927	SER	2.6
1	C	982	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	968	GLN	2.6
1	B	969	PRO	2.6
1	C	971	GLU	2.5
1	C	938	VAL	2.5
1	A	830	THR	2.5
1	B	941	CYS	2.5
1	A	871	PHE	2.5
1	C	921	ARG	2.4
1	A	987	THR	2.3
1	C	985	ILE	2.3
1	A	835	LYS	2.3
1	A	986	LYS	2.3
1	B	932	ARG	2.2
1	B	933	GLU	2.2
1	C	809	SER	2.2
1	C	822	ASP	2.2
1	C	935	VAL	2.2
1	C	933	GLU	2.2
1	B	986	LYS	2.2
1	A	876	GLN	2.2
1	B	921	ARG	2.2
1	C	929	ILE	2.1
1	A	834	GLY	2.1
1	B	984	GLY	2.1
1	A	836	GLU	2.1
1	C	969	PRO	2.1
1	B	943	GLU	2.1
1	B	946	LYS	2.1
1	A	967	CYS	2.1
1	C	837	TYR	2.0
1	B	989	THR	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, 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	B	1001	14/15	0.88	0.12	43,46,49,51	0
2	NAG	A	1001	14/15	0.91	0.10	37,39,41,43	0
2	NAG	C	1001	14/15	0.92	0.09	30,34,37,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.