WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jul 6, 2017 – 11:18 PM EDT

PDB ID : 2YL9

Title : INHIBITION OF THE PNEUMOCOCCAL VIRULENCE FACTOR STRH AND MOLECULAR INSIGHTS INTO N-GLYCAN RECOGNITION AND HYDROLYSIS

Authors : Pluvinage, B.; Higgins, M.A.; Abbott, D.W.; Robb, C.; Dalia, A.B.; Deng, L.; Weiser, J.N.; Parsons, T.B.; Fairbanks, A.J.; Vocadlo, D.J.; Boraston, A.B.

Deposited on : unknown
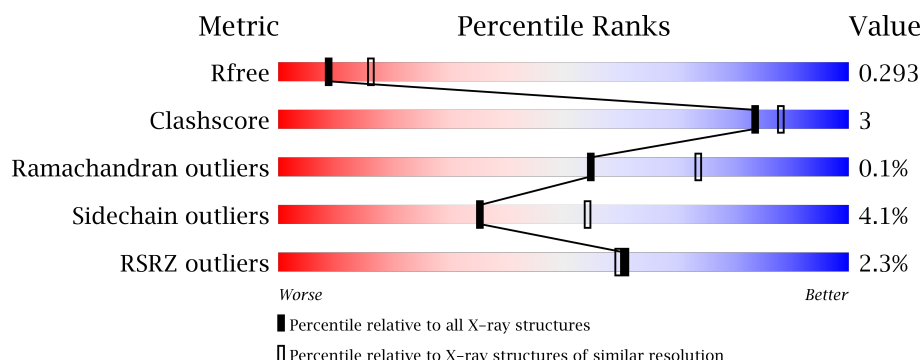
Resolution : 2.65 Å(reported)

---

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 2.65 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	Percentile Ranks	Value
Rfree		0.293
Clashscore		3
Ramachandran outliers		0.1%
Sidechain outliers		4.1%
RSRZ outliers		2.3%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	100719	3491 (2.70-2.62)
Clashscore	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)
RSRZ outliers	101464	3511 (2.70-2.62)

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	457	.% 80% 9% · 10%
1	B	457	2% 79% 9% · 11%
1	C	457	2% 79% 9% · 10%
1	D	457	4% 82% 6% · 10%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	1104	-	-	-	X
2	NAG	B	1101	-	-	-	X
2	NAG	B	1104	-	-	-	X
2	NAG	C	1104	-	-	-	X
2	NAG	D	1105	-	-	-	X
4	MAN	A	1103	-	-	-	X
4	MAN	B	1103	-	-	-	X
4	MAN	C	1103	-	-	-	X
4	MAN	D	1104	-	-	-	X
5	EDO	A	1108	-	-	-	X
5	EDO	A	1109	-	-	-	X
5	EDO	A	1110	-	-	-	X
5	EDO	A	1111	-	-	-	X
5	EDO	A	1113	-	-	-	X
5	EDO	A	1116	-	-	-	X
5	EDO	A	1118	-	-	-	X
5	EDO	B	1105	-	-	-	X
5	EDO	B	1107	-	-	-	X
5	EDO	C	1105	-	-	-	X
5	EDO	C	1106	-	-	-	X
5	EDO	C	1107	-	-	-	X
5	EDO	C	1110	-	-	-	X
5	EDO	D	1106	-	-	-	X
5	EDO	D	1107	-	-	-	X
5	EDO	D	1109	-	-	-	X
5	EDO	D	1110	-	-	-	X
5	EDO	D	1116	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14260 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-N-ACETYLHEXOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total 3269	C 2096	N 532	O 629	S 12	8	0	0
1	B	409	Total 3258	C 2089	N 530	O 627	S 12	17	0	0
1	C	410	Total 3271	C 2097	N 533	O 629	S 12	19	1	0
1	D	411	Total 3269	C 2096	N 532	O 629	S 12	36	0	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	606	MET	-	expression tag	UNP P49610
A	607	GLY	-	expression tag	UNP P49610
A	608	SER	-	expression tag	UNP P49610
A	609	SER	-	expression tag	UNP P49610
A	610	HIS	-	expression tag	UNP P49610
A	611	HIS	-	expression tag	UNP P49610
A	612	HIS	-	expression tag	UNP P49610
A	613	HIS	-	expression tag	UNP P49610
A	614	HIS	-	expression tag	UNP P49610
A	615	HIS	-	expression tag	UNP P49610
A	616	SER	-	expression tag	UNP P49610
A	617	SER	-	expression tag	UNP P49610
A	618	GLY	-	expression tag	UNP P49610
A	619	LEU	-	expression tag	UNP P49610
A	620	VAL	-	expression tag	UNP P49610
A	621	PRO	-	expression tag	UNP P49610
A	622	ARG	-	expression tag	UNP P49610
A	623	GLY	-	expression tag	UNP P49610
A	624	SER	-	expression tag	UNP P49610
A	625	HIS	-	expression tag	UNP P49610
A	626	MET	-	expression tag	UNP P49610

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	805	GLN	GLU	engineered mutation	UNP P49610
B	606	MET	-	expression tag	UNP P49610
B	607	GLY	-	expression tag	UNP P49610
B	608	SER	-	expression tag	UNP P49610
B	609	SER	-	expression tag	UNP P49610
B	610	HIS	-	expression tag	UNP P49610
B	611	HIS	-	expression tag	UNP P49610
B	612	HIS	-	expression tag	UNP P49610
B	613	HIS	-	expression tag	UNP P49610
B	614	HIS	-	expression tag	UNP P49610
B	615	HIS	-	expression tag	UNP P49610
B	616	SER	-	expression tag	UNP P49610
B	617	SER	-	expression tag	UNP P49610
B	618	GLY	-	expression tag	UNP P49610
B	619	LEU	-	expression tag	UNP P49610
B	620	VAL	-	expression tag	UNP P49610
B	621	PRO	-	expression tag	UNP P49610
B	622	ARG	-	expression tag	UNP P49610
B	623	GLY	-	expression tag	UNP P49610
B	624	SER	-	expression tag	UNP P49610
B	625	HIS	-	expression tag	UNP P49610
B	626	MET	-	expression tag	UNP P49610
B	805	GLN	GLU	engineered mutation	UNP P49610
C	606	MET	-	expression tag	UNP P49610
C	607	GLY	-	expression tag	UNP P49610
C	608	SER	-	expression tag	UNP P49610
C	609	SER	-	expression tag	UNP P49610
C	610	HIS	-	expression tag	UNP P49610
C	611	HIS	-	expression tag	UNP P49610
C	612	HIS	-	expression tag	UNP P49610
C	613	HIS	-	expression tag	UNP P49610
C	614	HIS	-	expression tag	UNP P49610
C	615	HIS	-	expression tag	UNP P49610
C	616	SER	-	expression tag	UNP P49610
C	617	SER	-	expression tag	UNP P49610
C	618	GLY	-	expression tag	UNP P49610
C	619	LEU	-	expression tag	UNP P49610
C	620	VAL	-	expression tag	UNP P49610
C	621	PRO	-	expression tag	UNP P49610
C	622	ARG	-	expression tag	UNP P49610
C	623	GLY	-	expression tag	UNP P49610
C	624	SER	-	expression tag	UNP P49610

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	625	HIS	-	expression tag	UNP P49610
C	626	MET	-	expression tag	UNP P49610
C	805	GLN	GLU	engineered mutation	UNP P49610
D	606	MET	-	expression tag	UNP P49610
D	607	GLY	-	expression tag	UNP P49610
D	608	SER	-	expression tag	UNP P49610
D	609	SER	-	expression tag	UNP P49610
D	610	HIS	-	expression tag	UNP P49610
D	611	HIS	-	expression tag	UNP P49610
D	612	HIS	-	expression tag	UNP P49610
D	613	HIS	-	expression tag	UNP P49610
D	614	HIS	-	expression tag	UNP P49610
D	615	HIS	-	expression tag	UNP P49610
D	616	SER	-	expression tag	UNP P49610
D	617	SER	-	expression tag	UNP P49610
D	618	GLY	-	expression tag	UNP P49610
D	619	LEU	-	expression tag	UNP P49610
D	620	VAL	-	expression tag	UNP P49610
D	621	PRO	-	expression tag	UNP P49610
D	622	ARG	-	expression tag	UNP P49610
D	623	GLY	-	expression tag	UNP P49610
D	624	SER	-	expression tag	UNP P49610
D	625	HIS	-	expression tag	UNP P49610
D	626	MET	-	expression tag	UNP P49610
D	805	GLN	GLU	engineered mutation	UNP P49610

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
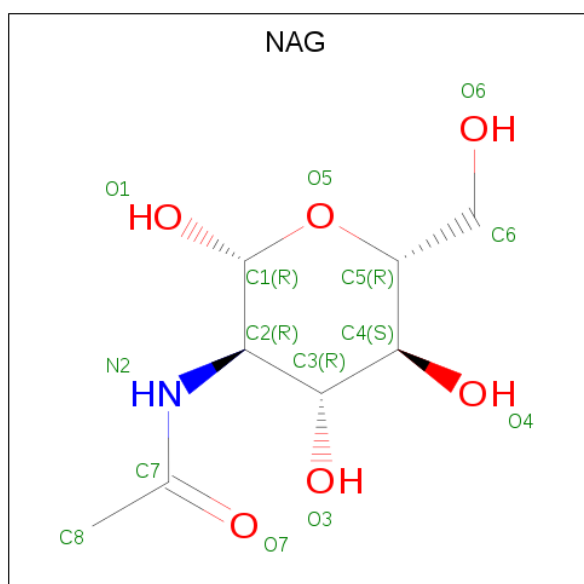
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 15	C 8	N 1	O 6	0	0
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 15	C 8	N 1	O 6	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	C	1	Total 15	C 8	N 1	O 6	0	0
2	C	1	Total 14	C 8	N 1	O 5	0	0
2	D	1	Total 15	C 8	N 1	O 6	0	0
2	D	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).
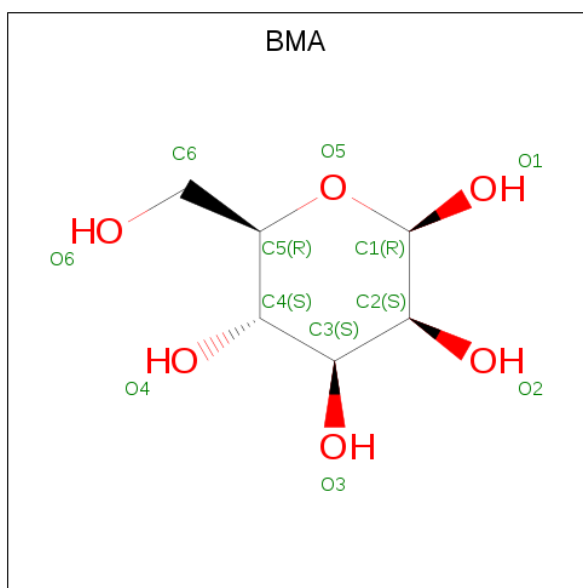
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 11	C 6	O 5	0	0
3	B	1	Total 11	C 6	O 5	0	0
3	C	1	Total 11	C 6	O 5	0	0
3	D	1	Total 11	C 6	O 5	0	0

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).
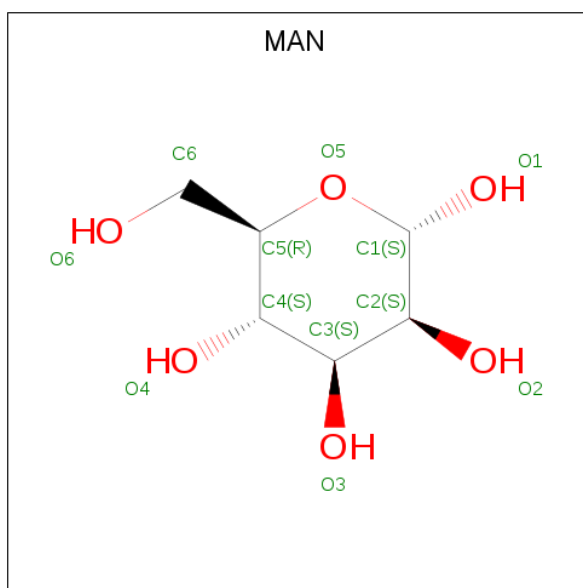
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
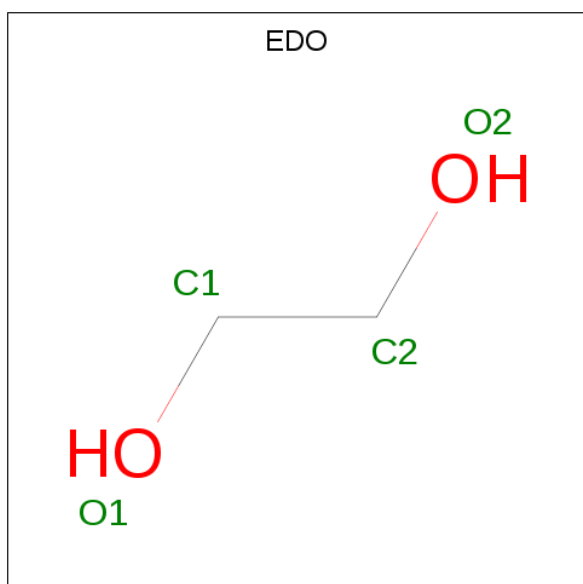
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 1		O 1	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	208	Total 214	O 214	0	6
6	B	196	Total 197	O 197	0	1
6	C	206	Total 207	O 207	0	1
6	D	187	Total 190	O 190	0	3

3 Residue-property plots ⓘ

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: BETA-N-ACETYLHEXOSAMINIDASE
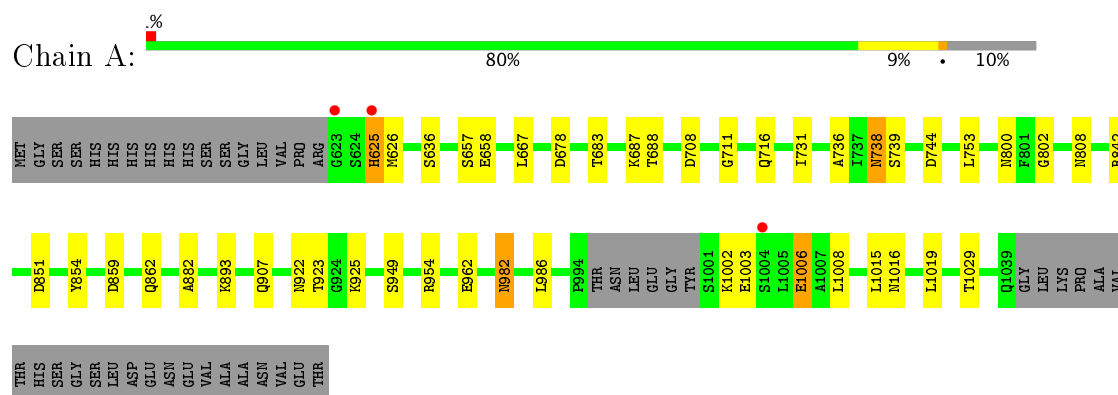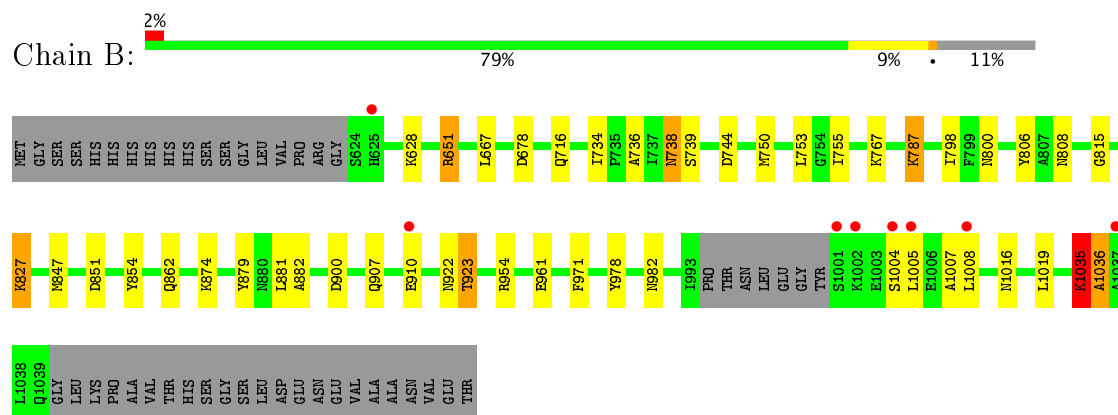
Chain A:

- Molecule 1: BETA-N-ACETYLHEXOSAMINIDASE

Chain B:

- Molecule 1: BETA-N-ACETYLHEXOSAMINIDASE

Chain C:
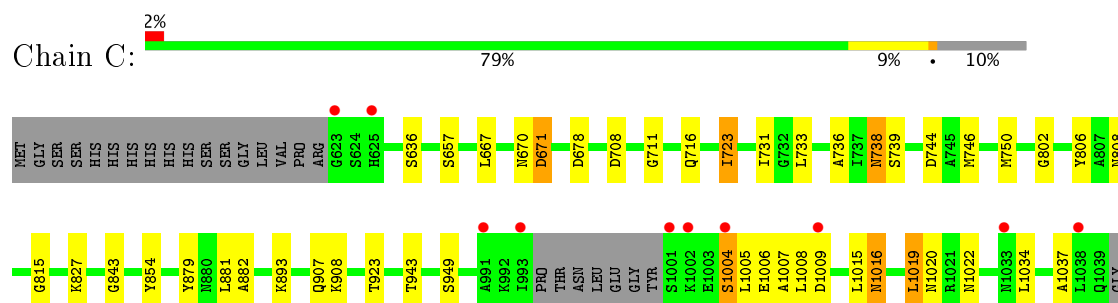
LEU LYS PRO ALA VAL THR HIS SER GLY SER LEU ASP GLU ASN GLU VAL ALA ALA ASN VAL GLU THR

● Molecule 1: BETA-N-ACETYLHEXOSAMINIDASE

Chain D:

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG G623 S624 S636 D678 Q716 N738 S739 D744 M750 L753 G754 I755 H761 K767 N808 D851 K858 W872 T897 D900 E910 N922 T923 S949

R954 E962 H974 L990 A991 K992 I993 P994 THR ASN LEU GLU GLY TYR S1001 K1002 E1003 S1004 L1005 E1006 A1007 L1008 D1009 A1010 A1011 A1014 L1015 N1016 Y1017 N1018 L1019 K1035 L1038 Q1039 GLY LEU LYS PRO ALA VAL THR HIS SER GLY SER LEU ASP GLU ASN GLU VAL ALA ALA ASN

VAL GLU THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.27Å 115.89Å 132.35Å 90.00° 99.46° 90.00°	Depositor
Resolution (Å)	40.74 – 2.65 40.74 – 2.65	Depositor EDS
% Data completeness (in resolution range)	95.5 (40.74-2.65) 95.5 (40.74-2.65)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.51 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.229 , 0.298 0.228 , 0.293	Depositor DCC
R_{free} test set	2822 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	18.3	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 27.6	EDS
L-test for twinning[2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14260	wwPDB-VP
Average B, all atoms (Å^2)	15.0	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 52.84 % 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 4.5886e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

---

[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: BMA, EDO, NAG, MAN

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	0.70	2/3342 (0.1%)	0.58	3/4513 (0.1%)
1	B	0.77	5/3330 (0.2%)	0.76	10/4496 (0.2%)
1	C	0.62	6/3343 (0.2%)	0.72	12/4512 (0.3%)
1	D	1.07	10/3342 (0.3%)	1.19	10/4513 (0.2%)
All	All	0.81	23/13357 (0.2%)	0.85	35/18034 (0.2%)

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1002	LYS	CE-NZ	-33.42	0.65	1.49
1	D	1009	ASP	CG-OD1	32.43	2.00	1.25
1	D	1009	ASP	CG-OD2	-30.59	0.55	1.25
1	B	767	LYS	CE-NZ	-27.92	0.79	1.49
1	D	767	LYS	CE-NZ	-26.48	0.82	1.49

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1009	ASP	CB-CG-OD2	54.85	167.67	118.30
1	D	1009	ASP	CB-CG-OD1	-41.39	81.05	118.30
1	B	1007	ALA	N-CA-CB	24.16	143.92	110.10
1	B	787	LYS	CD-CE-NZ	-20.73	64.01	111.70
1	C	1005	LEU	N-CA-CB	17.23	144.87	110.40

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	3269	0	3197	20	0
1	B	3258	0	3187	22	0
1	C	3271	0	3202	18	0
1	D	3269	0	3197	17	0
2	A	29	0	27	0	0
2	B	29	0	27	0	0
2	C	29	0	27	0	0
2	D	29	0	27	1	0
3	A	11	0	9	0	0
3	B	11	0	9	0	0
3	C	11	0	9	0	0
3	D	11	0	9	0	0
4	A	11	0	9	0	0
4	B	11	0	9	0	0
4	C	11	0	9	0	0
4	D	11	0	9	0	0
5	A	61	0	90	1	0
5	B	32	0	48	0	0
5	C	28	0	42	0	0
5	D	60	0	90	2	0
6	A	214	0	0	0	0
6	B	197	0	0	0	0
6	C	207	0	0	1	0
6	D	190	0	0	0	0
All	All	14260	0	13233	75	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.

The worst 5 of 75 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:678:ASP:H	1:B:716:GLN:HE21	1.41	0.66
1:A:683:THR:HG23	1:A:688:THR:HG22	1.77	0.65
1:D:1016:ASN:HD22	1:D:1018:ASN:H	1.46	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:678:ASP:H	1:C:716:GLN:NE2	2.00	0.60
1:A:625:HIS:CD2	1:A:626:MET:HG3	2.37	0.58

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	407/457 (89%)	390 (96%)	17 (4%)	0	100	100
1	B	405/457 (89%)	391 (96%)	14 (4%)	0	100	100
1	C	407/457 (89%)	387 (95%)	19 (5%)	1 (0%)	51	69
1	D	407/457 (89%)	389 (96%)	17 (4%)	1 (0%)	51	69
All	All	1626/1828 (89%)	1557 (96%)	67 (4%)	2 (0%)	55	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	624	SER
1	C	671	ASP

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	338/376 (90%)	321 (95%)	17 (5%)	28	44
1	B	337/376 (90%)	322 (96%)	15 (4%)	32	50
1	C	338/376 (90%)	327 (97%)	11 (3%)	43	63
1	D	338/376 (90%)	325 (96%)	13 (4%)	38	57
All	All	1351/1504 (90%)	1295 (96%)	56 (4%)	35	54

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	862	GLN
1	B	1035	LYS
1	D	1002	LYS
1	B	910	GLU
1	B	982	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	929	ASN
1	C	632	ASN
1	D	975	ASN
1	B	982	ASN
1	C	670	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 62 ligands modelled in this entry, 1 is modelled with single atom - leaving 61 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	3	15,15,15	0.42	0	21,21,21	0.67	0
3	BMA	A	1102	2,4	11,11,12	0.70	0	13,15,17	0.97	1 (7%)
4	MAN	A	1103	3,2	11,11,12	0.61	0	13,15,17	0.86	0
2	NAG	A	1104	4	14,14,15	0.69	1 (7%)	15,19,21	2.30	5 (33%)
5	EDO	A	1105	-	3,3,3	0.47	0	2,2,2	0.34	0
5	EDO	A	1106	-	3,3,3	0.48	0	2,2,2	0.30	0
5	EDO	A	1107	-	3,3,3	0.44	0	2,2,2	0.40	0
5	EDO	A	1108	-	3,3,3	0.49	0	2,2,2	0.20	0
5	EDO	A	1109	-	3,3,3	0.50	0	2,2,2	0.10	0
5	EDO	A	1110	-	3,3,3	0.47	0	2,2,2	0.09	0
5	EDO	A	1111	-	3,3,3	0.47	0	2,2,2	0.30	0
5	EDO	A	1113	-	3,3,3	0.46	0	2,2,2	0.35	0
5	EDO	A	1114	-	3,3,3	0.47	0	2,2,2	0.32	0
5	EDO	A	1115	-	3,3,3	0.46	0	2,2,2	0.30	0
5	EDO	A	1116	-	3,3,3	0.48	0	2,2,2	0.33	0
5	EDO	A	1117	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	A	1118	-	3,3,3	0.47	0	2,2,2	0.29	0
5	EDO	A	1119	-	3,3,3	0.47	0	2,2,2	0.31	0
5	EDO	A	1120	-	3,3,3	0.47	0	2,2,2	0.36	0
2	NAG	B	1101	3	15,15,15	0.45	0	21,21,21	0.81	0
3	BMA	B	1102	2,4	11,11,12	0.68	0	13,15,17	0.86	1 (7%)
4	MAN	B	1103	3,2	11,11,12	0.63	0	13,15,17	0.92	1 (7%)
2	NAG	B	1104	4	14,14,15	0.68	1 (7%)	15,19,21	2.25	5 (33%)
5	EDO	B	1105	-	3,3,3	0.49	0	2,2,2	0.20	0
5	EDO	B	1106	-	3,3,3	0.48	0	2,2,2	0.35	0
5	EDO	B	1107	-	3,3,3	0.46	0	2,2,2	0.32	0
5	EDO	B	1108	-	3,3,3	0.44	0	2,2,2	0.36	0
5	EDO	B	1109	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	B	1110	-	3,3,3	0.46	0	2,2,2	0.35	0
5	EDO	B	1111	-	3,3,3	0.44	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	EDO	B	1112	-	3,3,3	0.47	0	2,2,2	0.32	0
2	NAG	C	1101	3	15,15,15	0.49	0	21,21,21	1.06	1 (4%)
3	BMA	C	1102	2,4	11,11,12	0.67	0	13,15,17	0.81	0
4	MAN	C	1103	3,2	11,11,12	0.57	0	13,15,17	1.12	1 (7%)
2	NAG	C	1104	4	14,14,15	0.69	1 (7%)	15,19,21	2.43	4 (26%)
5	EDO	C	1105	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	C	1106	-	3,3,3	0.49	0	2,2,2	0.25	0
5	EDO	C	1107	-	3,3,3	0.47	0	2,2,2	0.29	0
5	EDO	C	1108	-	3,3,3	0.47	0	2,2,2	0.33	0
5	EDO	C	1109	-	3,3,3	0.46	0	2,2,2	0.33	0
5	EDO	C	1110	-	3,3,3	0.48	0	2,2,2	0.26	0
5	EDO	C	1111	-	3,3,3	0.46	0	2,2,2	0.36	0
5	EDO	D	1101	-	3,3,3	0.46	0	2,2,2	0.36	0
2	NAG	D	1102	3	15,15,15	0.65	0	21,21,21	1.50	5 (23%)
3	BMA	D	1103	2,4	11,11,12	0.71	0	13,15,17	0.93	1 (7%)
4	MAN	D	1104	3,2	11,11,12	0.62	0	13,15,17	0.90	0
2	NAG	D	1105	4	14,14,15	0.50	0	15,19,21	1.70	2 (13%)
5	EDO	D	1106	-	3,3,3	0.48	0	2,2,2	0.30	0
5	EDO	D	1107	-	3,3,3	0.45	0	2,2,2	0.30	0
5	EDO	D	1108	-	3,3,3	0.47	0	2,2,2	0.29	0
5	EDO	D	1109	-	3,3,3	0.46	0	2,2,2	0.31	0
5	EDO	D	1110	-	3,3,3	0.45	0	2,2,2	0.40	0
5	EDO	D	1111	-	3,3,3	0.46	0	2,2,2	0.35	0
5	EDO	D	1112	-	3,3,3	0.48	0	2,2,2	0.30	0
5	EDO	D	1113	-	3,3,3	0.45	0	2,2,2	0.38	0
5	EDO	D	1114	-	3,3,3	0.47	0	2,2,2	0.33	0
5	EDO	D	1115	-	3,3,3	0.46	0	2,2,2	0.36	0
5	EDO	D	1116	-	3,3,3	0.44	0	2,2,2	0.37	0
5	EDO	D	1117	-	3,3,3	0.46	0	2,2,2	0.39	0
5	EDO	D	1118	-	3,3,3	0.46	0	2,2,2	0.35	0
5	EDO	D	1119	-	3,3,3	0.47	0	2,2,2	0.33	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	A	1101	3	-	0/6/26/26	0/1/1/1
3	BMA	A	1102	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1103	3,2	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1104	4	-	0/6/23/26	0/1/1/1
5	EDO	A	1105	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1106	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1107	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1108	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1109	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1110	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1111	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1113	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1114	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1115	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1116	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1117	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1118	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1119	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1120	-	-	0/1/1/1	0/0/0/0
2	NAG	B	1101	3	-	0/6/26/26	0/1/1/1
3	BMA	B	1102	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1103	3,2	-	0/2/19/22	0/1/1/1
2	NAG	B	1104	4	-	0/6/23/26	0/1/1/1
5	EDO	B	1105	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1106	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1107	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1108	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1109	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1110	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1111	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1112	-	-	0/1/1/1	0/0/0/0
2	NAG	C	1101	3	-	0/6/26/26	0/1/1/1
3	BMA	C	1102	2,4	-	0/2/19/22	0/1/1/1
4	MAN	C	1103	3,2	-	0/2/19/22	0/1/1/1
2	NAG	C	1104	4	-	0/6/23/26	0/1/1/1
5	EDO	C	1105	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1106	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1107	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1108	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1109	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1110	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1111	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1101	-	-	0/1/1/1	0/0/0/0
2	NAG	D	1102	3	-	0/6/26/26	0/1/1/1
3	BMA	D	1103	2,4	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	D	1104	3,2	-	0/2/19/22	0/1/1/1
2	NAG	D	1105	4	-	0/6/23/26	0/1/1/1
5	EDO	D	1106	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1107	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1108	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1109	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1110	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1111	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1112	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1113	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1114	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1115	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1116	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1117	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1118	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1119	-	-	0/1/1/1	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1104	NAG	C1-C2	2.17	1.55	1.52
2	B	1104	NAG	C1-C2	2.18	1.55	1.52
2	C	1104	NAG	C1-C2	2.21	1.55	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1102	NAG	O7-C7-C8	-2.44	117.61	122.06
2	A	1104	NAG	C3-C4-C5	-2.39	106.00	110.22
2	B	1104	NAG	C3-C4-C5	-2.16	106.41	110.22
4	B	1103	MAN	C1-O5-C5	2.05	114.98	112.17
3	B	1102	BMA	C1-C2-C3	2.06	112.26	109.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1108	EDO	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1102	NAG	1	0
5	D	1107	EDO	2	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	411/457 (89%)	-0.22	3 (0%)	87	88	5, 14, 33, 46	11 (2%)
1	B	409/457 (89%)	-0.21	8 (1%)	65	64	3, 13, 37, 55	16 (3%)
1	C	410/457 (89%)	-0.21	10 (2%)	59	58	4, 12, 37, 51	16 (3%)
1	D	411/457 (89%)	-0.15	16 (3%)	40	38	4, 14, 42, 55	18 (4%)
All	All	1641/1828 (89%)	-0.20	37 (2%)	61	59	3, 13, 37, 55	61 (3%)

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1004	SER	5.3
1	D	1004	SER	5.2
1	D	991	ALA	4.8
1	D	994	PRO	3.6
1	D	623	GLY	3.6

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(Å²)	Q<0.9
4	MAN	B	1103	11/12	0.80	0.40	21.67	49,51,52,52	0
5	EDO	C	1105	4/4	0.75	0.29	18.19	51,52,52,52	0
2	NAG	B	1104	14/15	0.87	0.31	11.03	45,46,46,47	0
5	EDO	C	1110	4/4	0.79	0.36	10.51	27,28,28,28	0
5	EDO	A	1109	4/4	0.61	0.47	10.33	38,39,39,39	0
4	MAN	C	1103	11/12	0.85	0.31	10.25	57,59,60,60	0
4	MAN	D	1104	11/12	0.77	0.45	9.10	55,57,57,57	0
5	EDO	B	1105	4/4	0.74	0.35	8.71	23,24,24,24	0
5	EDO	A	1118	4/4	0.72	0.34	7.80	56,57,57,57	0
2	NAG	D	1105	14/15	0.80	0.26	7.56	52,53,53,54	0
2	NAG	B	1101	15/15	0.60	0.52	7.02	56,58,58,58	0
5	EDO	C	1107	4/4	0.80	0.32	6.86	30,30,30,31	0
5	EDO	B	1107	4/4	0.86	0.23	6.83	39,39,39,39	0
5	EDO	A	1110	4/4	0.75	0.33	6.79	34,34,34,34	0
5	EDO	A	1111	4/4	0.77	0.31	6.26	50,50,50,50	0
5	EDO	D	1109	4/4	0.80	0.33	5.95	38,38,38,39	0
2	NAG	A	1104	14/15	0.82	0.28	5.93	55,56,56,57	0
5	EDO	A	1108	4/4	0.79	0.31	5.92	26,27,27,27	0
5	EDO	D	1106	4/4	0.78	0.37	5.87	31,32,32,32	0
5	EDO	A	1116	4/4	0.86	0.24	5.63	37,38,38,38	0
4	MAN	A	1103	11/12	0.84	0.27	5.51	58,59,60,60	0
2	NAG	C	1104	14/15	0.89	0.24	5.07	53,54,55,55	0
5	EDO	A	1113	4/4	0.83	0.35	4.86	47,47,47,47	0
5	EDO	D	1107	4/4	0.77	0.27	4.57	27,27,27,27	0
5	EDO	D	1116	4/4	0.81	0.32	4.34	31,31,31,31	0
5	EDO	C	1106	4/4	0.81	0.26	3.20	21,22,22,22	0
5	EDO	D	1110	4/4	0.91	0.20	2.40	24,25,25,25	0
5	EDO	B	1106	4/4	0.90	0.24	1.86	15,15,15,15	0
5	EDO	B	1108	4/4	0.87	0.18	0.46	25,25,25,25	0
5	EDO	D	1112	4/4	0.95	0.15	-0.42	20,20,20,20	0
2	NAG	A	1101	15/15	0.54	0.43	-	62,63,63,63	0
5	EDO	A	1120	4/4	0.80	0.26	-	32,32,32,32	0
5	EDO	D	1113	4/4	0.86	0.22	-	41,42,42,42	0
5	EDO	A	1114	4/4	0.79	0.24	-	55,55,55,55	0
2	NAG	D	1102	15/15	0.51	0.56	-	61,63,63,63	0
5	EDO	C	1108	4/4	0.86	0.21	-	27,27,28,28	0
5	EDO	D	1117	4/4	0.92	0.15	-	34,34,34,34	0
5	EDO	B	1111	4/4	0.91	0.22	-	40,40,40,41	0
3	BMA	A	1102	11/12	0.75	0.32	-	60,61,62,62	0
5	EDO	B	1109	4/4	0.85	0.33	-	52,53,53,53	0

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
5	EDO	D	1115	4/4	0.91	0.19	-	49,49,49,49	0
5	EDO	C	1111	4/4	0.80	0.29	-	47,47,47,47	0
5	EDO	A	1115	4/4	0.86	0.14	-	32,32,32,32	0
5	EDO	D	1118	4/4	0.86	0.25	-	38,38,38,38	0
3	BMA	D	1103	11/12	0.76	0.32	-	58,60,60,60	0
5	EDO	A	1119	4/4	0.86	0.17	-	41,41,41,41	0
5	EDO	C	1109	4/4	0.70	0.21	-	51,52,52,52	0
5	EDO	A	1112	1/4	0.86	0.24	-	22,22,22,22	0
5	EDO	D	1114	4/4	0.83	0.32	-	44,45,45,45	0
5	EDO	D	1111	4/4	0.83	0.22	-	31,31,31,31	0
5	EDO	A	1117	4/4	0.88	0.27	-	43,43,43,43	0
3	BMA	C	1102	11/12	0.75	0.37	-	61,64,64,64	0
5	EDO	D	1108	4/4	0.78	0.33	-	31,31,32,32	0
5	EDO	B	1110	4/4	0.92	0.23	-	25,26,26,26	0
5	EDO	A	1106	4/4	0.86	0.26	-	29,30,30,30	0
5	EDO	B	1112	4/4	0.85	0.15	-	41,42,42,42	0
3	BMA	B	1102	11/12	0.80	0.24	-	53,55,55,55	0
5	EDO	A	1107	4/4	0.89	0.20	-	24,24,24,24	0
5	EDO	A	1105	4/4	0.87	0.24	-	31,31,31,31	0
5	EDO	D	1101	4/4	0.79	0.22	-	50,50,50,50	0
5	EDO	D	1119	4/4	0.75	0.30	-	45,46,46,46	0
2	NAG	C	1101	15/15	0.51	0.61	-	65,67,68,68	0

6.5 Other polymers (i)

There are no such residues in this entry.