



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:14 AM GMT

PDB ID : 2WDB  
Title : A FAMILY 32 CARBOHYDRATE-BINDING MODULE, FROM THE MU  
TOXIN PRODUCED BY CLOSTRIDIUM PERFRINGENS, IN COMPLEX  
WITH BETA-D-GLCNAC-BETA(1,2)MANNOSE  
Authors : Ficko-Blean, E.; Boraston, A.B.  
Deposited on : 2009-03-23  
Resolution : 2.03 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](mailto: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.

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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

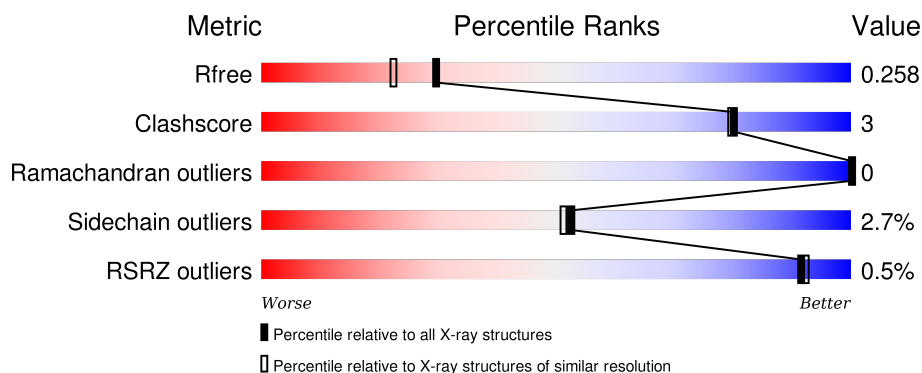
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.03 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	7858 (2.04-2.00)
Clashscore	102246	9060 (2.04-2.00)
Ramachandran outliers	100387	8952 (2.04-2.00)
Sidechain outliers	100360	8951 (2.04-2.00)
RSRZ outliers	91569	7873 (2.04-2.00)

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  $\geq 3$ , 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	192	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 66%, yellow 5%, orange 2%, grey 28%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>%</span> <span>66%</span> <span>5% ••</span> <span>28%</span> </div> </div>
1	B	192	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 69%, yellow 6%, orange 2%, grey 24%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>%</span> <span>69%</span> <span>6% ••</span> <span>24%</span> </div> </div>
1	C	192	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 66%, yellow 7%, orange 1%, grey 27%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>%</span> <span>66%</span> <span>7% •</span> <span>27%</span> </div> </div>
1	D	192	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 69%, yellow 5%, orange 1%, grey 26%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>%</span> <span>69%</span> <span>5% •</span> <span>26%</span> </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	MAN	A	1947	X	-	-	-
2	MAN	B	1951	X	-	-	-
2	MAN	C	1949	X	-	-	-
2	MAN	D	1949	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5090 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 HYALURONOGLUCOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	17	0	0
			1100	699	177	223	1			
1	B	146	Total	C	N	O	S	7	1	0
			1161	734	186	239	2			
1	C	141	Total	C	N	O	S	7	0	0
			1117	708	179	229	1			
1	D	143	Total	C	N	O	S	0	0	0
			1128	714	181	232	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	944	VAL	ILE	CONFLICT	UNP P26831
B	944	VAL	ILE	CONFLICT	UNP P26831
C	944	VAL	ILE	CONFLICT	UNP P26831
D	944	VAL	ILE	CONFLICT	UNP P26831

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			26	14	1	11		
2	B	2	Total	C	N	O	0	0
			26	14	1	11		
2	C	2	Total	C	N	O	0	0
			26	14	1	11		
2	D	2	Total	C	N	O	0	0
			26	14	1	11		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

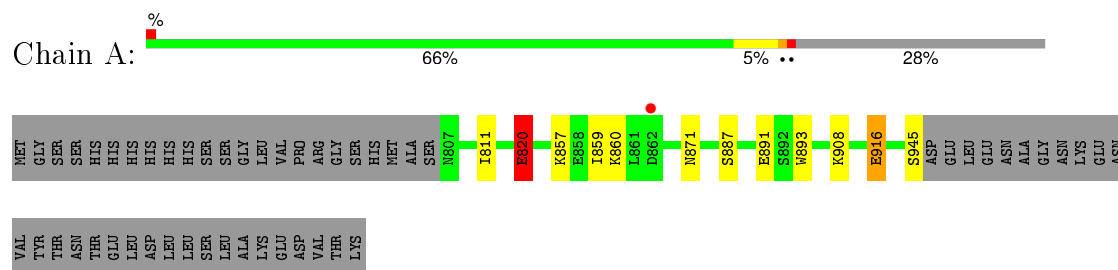
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	106	Total	O	0	0
			106	106		
4	B	131	Total	O	0	0
			131	131		
4	C	131	Total	O	0	0
			131	131		
4	D	108	Total	O	0	0
			108	108		

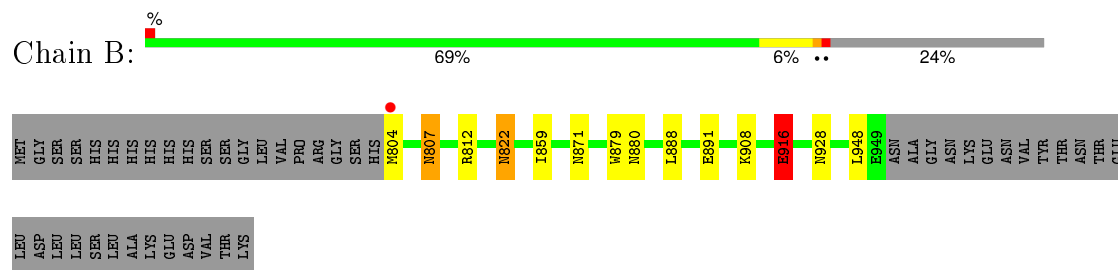
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

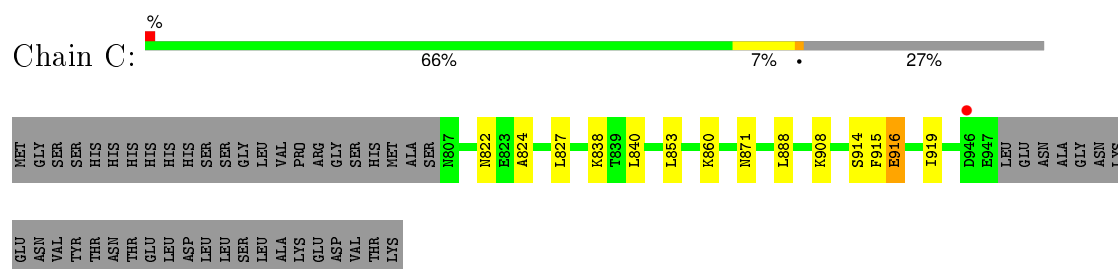
#### • Molecule 1: HYALURONOGLUCOSAMINIDASE



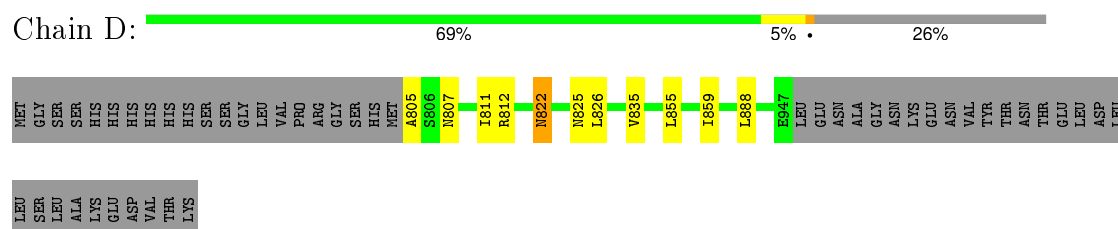
#### • Molecule 1: HYALURONOGLUCOSAMINIDASE



#### • Molecule 1: HYALURONOGLUCOSAMINIDASE



#### • Molecule 1: HYALURONOGLUCOSAMINIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.28Å 91.28Å 132.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	79.06 – 2.03 39.52 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.7 (79.06-2.03) 99.7 (39.52-2.03)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.70 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.194 , 0.260 0.199 , 0.258	Depositor DCC
$R_{free}$ test set	2110 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.9	EDS
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 41787 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5090	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	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 21.12 % 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 7.5052e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> 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: CA, 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	3.90	8/1123 (0.7%)	1.52	9/1518 (0.6%)
1	B	0.90	2/1184 (0.2%)	0.71	2/1600 (0.1%)
1	C	0.92	2/1140 (0.2%)	0.68	1/1541 (0.1%)
1	D	0.49	0/1151	0.61	0/1556
All	All	2.05	12/4598 (0.3%)	0.95	12/6215 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
2	A	1	0
2	B	1	0
2	C	1	0
2	D	1	0
All	All	4	3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	916	GLU	CD-OE1	93.48	2.28	1.25
1	A	916	GLU	CD-OE2	69.19	2.01	1.25
1	A	820	GLU	CG-CD	55.50	2.35	1.51
1	B	916	GLU	CD-OE2	23.05	1.51	1.25
1	C	916	GLU	CB-CG	-21.96	1.10	1.52
1	C	860	LYS	CG-CD	-13.48	1.06	1.52
1	A	860	LYS	CD-CE	-11.91	1.21	1.51
1	B	916	GLU	CD-OE1	-10.67	1.14	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	859	ILE	CB-CG2	-5.50	1.35	1.52
1	A	916	GLU	CA-CB	-5.49	1.41	1.53
1	A	820	GLU	CA-CB	-5.27	1.42	1.53
1	A	857	LYS	CA-CB	-5.06	1.42	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	820	GLU	CG-CD-OE2	-36.00	46.29	118.30
1	A	891	GLU	OE1-CD-OE2	-23.67	94.90	123.30
1	A	916	GLU	OE1-CD-OE2	-19.46	99.95	123.30
1	A	820	GLU	CG-CD-OE1	-14.23	89.83	118.30
1	A	860	LYS	CD-CE-NZ	-13.58	80.47	111.70
1	A	891	GLU	CG-CD-OE2	11.63	141.56	118.30
1	C	860	LYS	CB-CG-CD	9.62	136.60	111.60
1	B	916	GLU	OE1-CD-OE2	-8.48	113.13	123.30
1	B	916	GLU	CG-CD-OE1	7.61	133.51	118.30
1	A	859	ILE	CB-CG1-CD1	6.52	132.15	113.90
1	A	916	GLU	CG-CD-OE1	6.44	131.17	118.30
1	A	859	ILE	CG1-CB-CG2	-5.77	98.70	111.40

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1947	MAN	C1
2	B	1951	MAN	C1
2	C	1949	MAN	C1
2	D	1949	MAN	C1

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	820	GLU	Sidechain
1	A	916	GLU	Sidechain
1	B	916	GLU	Sidechain

## 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	1100	0	1057	4	0
1	B	1161	0	1108	13	0
1	C	1117	0	1067	7	0
1	D	1128	0	1077	11	0
2	A	26	0	23	0	0
2	B	26	0	23	0	0
2	C	26	0	20	0	0
2	D	26	0	23	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	106	0	0	2	0
4	B	131	0	0	1	1
4	C	131	0	0	0	1
4	D	108	0	0	1	0
All	All	5090	0	4398	30	1

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 (30) 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:D:805:ALA:N	4:D:2001:HOH:O	2.10	0.82
1:B:807:ASN:ND2	1:D:812:ARG:H	1.82	0.77
1:B:871:ASN:HD21	1:B:908:LYS:HE2	1.53	0.74
1:A:811:ILE:HD12	4:A:2060:HOH:O	1.89	0.72
1:C:822:ASN:HD22	1:C:824:ALA:H	1.36	0.71
1:B:871:ASN:ND2	1:B:908:LYS:HE2	2.05	0.71
1:D:822:ASN:HD22	1:D:822:ASN:C	1.97	0.68
1:A:871:ASN:ND2	1:A:908:LYS:NZ	2.47	0.63
1:C:871:ASN:ND2	1:C:908:LYS:H	1.95	0.62
1:D:826:LEU:HD21	1:D:835:VAL:HG12	1.83	0.60
1:B:859:ILE:HD13	1:B:948:LEU:HD11	1.85	0.59
1:B:812:ARG:H	1:D:807:ASN:ND2	2.00	0.59
1:B:807:ASN:H	1:B:807:ASN:HD22	1.52	0.58
1:C:827:LEU:HD21	1:C:853:LEU:HD21	1.87	0.57
1:A:887:SER:HB2	1:A:893:TRP:CE3	2.41	0.56
1:B:807:ASN:HD21	1:D:812:ARG:H	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:871:ASN:HD21	1:B:908:LYS:CE	2.18	0.54
1:B:807:ASN:HD21	1:D:811:ILE:HA	1.73	0.53
1:A:871:ASN:ND2	1:A:908:LYS:HZ1	2.07	0.53
1:B:880:ASN:ND2	4:B:2077:HOH:O	2.42	0.53
1:C:871:ASN:HD21	1:C:908:LYS:H	1.60	0.49
1:D:822:ASN:ND2	1:D:825:ASN:H	2.12	0.48
1:B:812:ARG:H	1:D:807:ASN:HD21	1.62	0.47
1:C:838:LYS:HE2	1:C:840:LEU:HD23	1.98	0.46
4:A:2015:HOH:O	1:B:822:ASN:HB2	2.16	0.45
1:D:855:LEU:HD13	1:D:859:ILE:HD12	1.99	0.44
1:C:822:ASN:ND2	1:C:824:ALA:H	2.08	0.43
1:D:822:ASN:C	1:D:822:ASN:ND2	2.69	0.43
1:C:915:PHE:CD1	1:C:919:ILE:HD12	2.54	0.42
1:B:879:TRP:CE2	1:B:928:ASN:HB2	2.56	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2082:HOH:O	4:C:2075:HOH:O[2_655]	2.03	0.17

## 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	137/192 (71%)	130 (95%)	7 (5%)	0	100	100
1	B	145/192 (76%)	139 (96%)	6 (4%)	0	100	100
1	C	139/192 (72%)	135 (97%)	4 (3%)	0	100	100
1	D	141/192 (73%)	139 (99%)	2 (1%)	0	100	100
All	All	562/768 (73%)	543 (97%)	19 (3%)	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	119/165 (72%)	117 (98%)	2 (2%)	68	70
1	B	126/165 (76%)	120 (95%)	6 (5%)	31	25
1	C	121/165 (73%)	118 (98%)	3 (2%)	55	54
1	D	122/165 (74%)	120 (98%)	2 (2%)	70	72
All	All	488/660 (74%)	475 (97%)	13 (3%)	52	51

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	820	GLU
1	A	945	SER
1	B	804	MET
1	B	807	ASN
1	B	822	ASN
1	B	888	LEU
1	B	891	GLU
1	B	916	GLU
1	C	888	LEU
1	C	914	SER
1	C	916	GLU
1	D	822	ASN
1	D	888	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	871	ASN
1	B	807	ASN
1	B	871	ASN
1	B	880	ASN

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Mol	Chain	Res	Type
1	C	822	ASN
1	C	871	ASN
1	C	880	ASN
1	C	933	ASN
1	D	807	ASN
1	D	822	ASN
1	D	880	ASN

### 5.3.3 RNA ⓘ

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 ⓘ

8 carbohydrates 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	1946	2	14,14,15	0.45	0	15,19,21	0.68	0
2	MAN	A	1947	2	12,12,12	2.13	4 (33%)	17,17,17	2.54	6 (35%)
2	NAG	B	1950	2	14,14,15	0.82	1 (7%)	15,19,21	1.14	1 (6%)
2	MAN	B	1951	2	12,12,12	2.12	6 (50%)	17,17,17	2.44	4 (23%)
2	NAG	C	1948	2	14,14,15	0.52	0	15,19,21	0.97	1 (6%)
2	MAN	C	1949	2	12,12,12	2.43	4 (33%)	17,17,17	3.06	7 (41%)
2	NAG	D	1948	2	14,14,15	0.53	0	15,19,21	0.90	0
2	MAN	D	1949	2	12,12,12	1.91	3 (25%)	17,17,17	2.35	4 (23%)

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	1946	2	-	0/6/23/26	0/1/1/1
2	MAN	A	1947	2	1/1/5/5	0/2/22/22	0/1/1/1
2	NAG	B	1950	2	-	0/6/23/26	0/1/1/1
2	MAN	B	1951	2	1/1/5/5	0/2/22/22	0/1/1/1
2	NAG	C	1948	2	-	0/6/23/26	0/1/1/1
2	MAN	C	1949	2	1/1/5/5	0/2/22/22	0/1/1/1
2	NAG	D	1948	2	-	0/6/23/26	0/1/1/1
2	MAN	D	1949	2	1/1/5/5	0/2/22/22	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1947	MAN	O5-C5	-5.73	1.30	1.44
2	C	1949	MAN	O1-C1	-5.52	1.19	1.39
2	D	1949	MAN	O5-C5	-4.39	1.33	1.44
2	B	1951	MAN	O5-C5	-3.85	1.34	1.44
2	C	1949	MAN	O5-C1	-3.20	1.37	1.43
2	B	1951	MAN	O1-C1	-2.87	1.29	1.39
2	C	1949	MAN	O3-C3	-2.63	1.36	1.43
2	A	1947	MAN	O5-C1	-2.61	1.38	1.43
2	C	1949	MAN	O5-C5	-2.61	1.37	1.44
2	A	1947	MAN	C4-C3	-2.48	1.45	1.52
2	B	1951	MAN	O4-C4	-2.41	1.37	1.43
2	D	1949	MAN	C4-C5	-2.26	1.48	1.53
2	B	1950	NAG	O5-C1	-2.24	1.40	1.43
2	D	1949	MAN	O1-C1	-2.21	1.31	1.39
2	B	1951	MAN	O5-C1	-2.15	1.39	1.43
2	B	1951	MAN	C4-C5	-2.13	1.48	1.53
2	A	1947	MAN	O1-C1	-2.13	1.31	1.39
2	B	1951	MAN	O2-C2	2.94	1.50	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1949	MAN	C1-C2-C3	-7.92	98.65	110.43
2	B	1951	MAN	C1-C2-C3	-6.41	100.90	110.43
2	D	1949	MAN	C1-C2-C3	-6.06	101.42	110.43
2	A	1947	MAN	C1-C2-C3	-5.15	102.77	110.43
2	A	1947	MAN	O3-C3-C4	-2.69	104.28	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1948	NAG	C3-C4-C5	-2.12	106.51	110.20
2	D	1949	MAN	O5-C5-C6	2.07	111.58	106.36
2	C	1949	MAN	O5-C5-C4	2.17	113.75	109.68
2	A	1947	MAN	O4-C4-C5	2.53	115.94	109.24
2	B	1951	MAN	C1-O5-C5	2.56	118.20	113.47
2	C	1949	MAN	O5-C5-C6	2.56	112.83	106.36
2	D	1949	MAN	O5-C5-C4	2.62	114.61	109.68
2	B	1950	NAG	C1-O5-C5	2.97	116.01	112.25
2	A	1947	MAN	C1-O5-C5	3.12	119.25	113.47
2	A	1947	MAN	O5-C5-C4	3.39	116.05	109.68
2	B	1951	MAN	O5-C5-C6	3.64	115.55	106.36
2	C	1949	MAN	O2-C2-C3	3.89	119.09	110.34
2	C	1949	MAN	O1-C1-C2	4.19	120.44	109.21
2	C	1949	MAN	O1-C1-O5	4.26	121.90	110.25
2	C	1949	MAN	O5-C1-C2	4.69	117.28	109.80
2	B	1951	MAN	O1-C1-O5	5.33	124.81	110.25
2	D	1949	MAN	O1-C1-C2	5.42	123.75	109.21
2	A	1947	MAN	O1-C1-C2	6.10	125.56	109.21

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1951	MAN	C1
2	A	1947	MAN	C1
2	C	1949	MAN	C1
2	D	1949	MAN	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	139/192 (72%)	-0.18	1 (0%) 89 89	20, 31, 48, 54	7 (5%)
1	B	146/192 (76%)	-0.48	1 (0%) 89 89	16, 22, 36, 57	2 (1%)
1	C	141/192 (73%)	-0.47	1 (0%) 89 89	14, 22, 41, 54	2 (1%)
1	D	143/192 (74%)	-0.38	0 100 100	19, 27, 38, 53	0
All	All	569/768 (74%)	-0.38	3 (0%) 91 92	14, 25, 43, 57	11 (1%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	862	ASP	2.4
1	C	946	ASP	2.1
1	B	804	MET	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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	NAG	C	1948	14/15	0.95	0.08	-0.16	19,22,24,24	0
2	NAG	A	1946	14/15	0.90	0.10	-0.42	35,37,40,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	B	1950	14/15	0.96	0.08	-0.54	25,26,27,28	0
2	NAG	D	1948	14/15	0.97	0.08	-0.55	24,27,29,30	0
2	MAN	C	1949	12/12	0.90	0.11	-	27,29,31,33	0
2	MAN	A	1947	12/12	0.87	0.21	-	47,54,56,57	0
2	MAN	D	1949	12/12	0.88	0.13	-	35,43,45,46	0
2	MAN	B	1951	12/12	0.89	0.17	-	33,43,46,46	0

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	CA	C	1950	1/1	0.99	0.07	-0.83	19,19,19,19	0
3	CA	B	1952	1/1	0.99	0.06	-1.08	20,20,20,20	0
3	CA	A	1948	1/1	0.97	0.04	-3.26	31,31,31,31	0
3	CA	D	1950	1/1	0.99	0.04	-4.34	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.