



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 12:19 PM GMT

PDB ID : 3ALX  
Title : Crystal structure of the measles virus hemagglutinin bound to its cellular receptor SLAM (MV-H(L482R)-SLAM(N102H/R108Y)fusion)  
Authors : Hashiguchi, T.; Ose, T.; Kubota, M.; Maita, N.; Kamishikiryo, J.; Maenaka, K.; Yanagi, Y.  
Deposited on : 2010-08-09  
Resolution : 3.15 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

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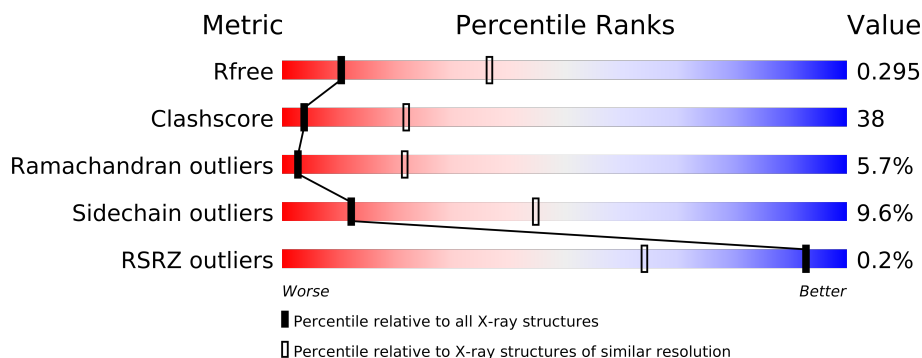
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.15 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))
$R_{free}$	66092	1360 (3.22-3.10)
Clashscore	79885	1681 (3.22-3.10)
Ramachandran outliers	78287	1639 (3.22-3.10)
Sidechain outliers	78261	1638 (3.22-3.10)
RSRZ outliers	66119	1361 (3.22-3.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	559	
1	B	559	
1	C	559	
1	D	559	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NAG	B	801	-	X
2	NAG	C	801	-	X
2	NAG	C	901	-	X
2	NAG	D	901	-	X

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16313 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Hemagglutinin, CDw150.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	0	0	0
			4053	2598	677	750	28			
1	B	526	Total	C	N	O	S	0	0	0
			4141	2651	695	767	28			
1	C	514	Total	C	N	O	S	0	0	0
			4051	2599	676	748	28			
1	D	504	Total	C	N	O	S	0	0	0
			3984	2562	663	732	27			

There are 60 discrepancies between the modelled and reference sequences:

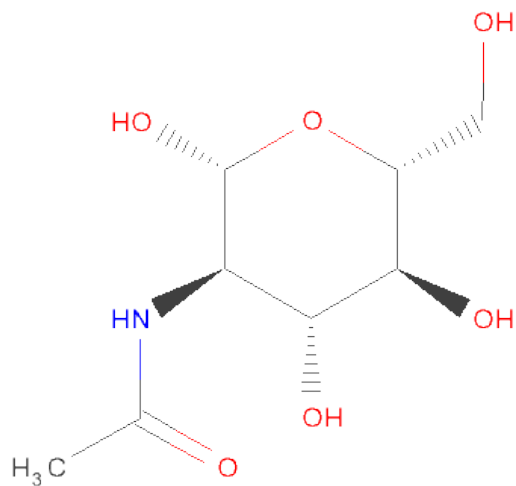
Chain	Residue	Modelled	Actual	Comment	Reference
A	181	GLU	-	EXPRESSION TAG	UNP E2RZS2
A	182	THR	-	EXPRESSION TAG	UNP E2RZS2
A	183	GLY	-	EXPRESSION TAG	UNP E2RZS2
A	482	ARG	LEU	ENGINEERED MUTATION	UNP E2RZS2
A	102	HIS	ASN	ENGINEERED MUTATION	UNP Q9GJT3
A	108	TYR	ARG	ENGINEERED MUTATION	UNP Q9GJT3
A	141	GLY	-	EXPRESSION TAG	UNP Q9GJT3
A	142	THR	-	EXPRESSION TAG	UNP Q9GJT3
A	143	LYS	-	EXPRESSION TAG	UNP Q9GJT3
A	144	HIS	-	EXPRESSION TAG	UNP Q9GJT3
A	145	HIS	-	EXPRESSION TAG	UNP Q9GJT3
A	146	HIS	-	EXPRESSION TAG	UNP Q9GJT3
A	147	HIS	-	EXPRESSION TAG	UNP Q9GJT3
A	148	HIS	-	EXPRESSION TAG	UNP Q9GJT3
A	149	HIS	-	EXPRESSION TAG	UNP Q9GJT3
B	181	GLU	-	EXPRESSION TAG	UNP E2RZS2
B	182	THR	-	EXPRESSION TAG	UNP E2RZS2
B	183	GLY	-	EXPRESSION TAG	UNP E2RZS2
B	482	ARG	LEU	ENGINEERED MUTATION	UNP E2RZS2
B	102	HIS	ASN	ENGINEERED MUTATION	UNP Q9GJT3
B	108	TYR	ARG	ENGINEERED MUTATION	UNP Q9GJT3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	141	GLY	-	EXPRESSION TAG	UNP Q9GJT3
B	142	THR	-	EXPRESSION TAG	UNP Q9GJT3
B	143	LYS	-	EXPRESSION TAG	UNP Q9GJT3
B	144	HIS	-	EXPRESSION TAG	UNP Q9GJT3
B	145	HIS	-	EXPRESSION TAG	UNP Q9GJT3
B	146	HIS	-	EXPRESSION TAG	UNP Q9GJT3
B	147	HIS	-	EXPRESSION TAG	UNP Q9GJT3
B	148	HIS	-	EXPRESSION TAG	UNP Q9GJT3
B	149	HIS	-	EXPRESSION TAG	UNP Q9GJT3
C	181	GLU	-	EXPRESSION TAG	UNP E2RZS2
C	182	THR	-	EXPRESSION TAG	UNP E2RZS2
C	183	GLY	-	EXPRESSION TAG	UNP E2RZS2
C	482	ARG	LEU	ENGINEERED MUTATION	UNP E2RZS2
C	102	HIS	ASN	ENGINEERED MUTATION	UNP Q9GJT3
C	108	TYR	ARG	ENGINEERED MUTATION	UNP Q9GJT3
C	141	GLY	-	EXPRESSION TAG	UNP Q9GJT3
C	142	THR	-	EXPRESSION TAG	UNP Q9GJT3
C	143	LYS	-	EXPRESSION TAG	UNP Q9GJT3
C	144	HIS	-	EXPRESSION TAG	UNP Q9GJT3
C	145	HIS	-	EXPRESSION TAG	UNP Q9GJT3
C	146	HIS	-	EXPRESSION TAG	UNP Q9GJT3
C	147	HIS	-	EXPRESSION TAG	UNP Q9GJT3
C	148	HIS	-	EXPRESSION TAG	UNP Q9GJT3
C	149	HIS	-	EXPRESSION TAG	UNP Q9GJT3
D	181	GLU	-	EXPRESSION TAG	UNP E2RZS2
D	182	THR	-	EXPRESSION TAG	UNP E2RZS2
D	183	GLY	-	EXPRESSION TAG	UNP E2RZS2
D	482	ARG	LEU	ENGINEERED MUTATION	UNP E2RZS2
D	102	HIS	ASN	ENGINEERED MUTATION	UNP Q9GJT3
D	108	TYR	ARG	ENGINEERED MUTATION	UNP Q9GJT3
D	141	GLY	-	EXPRESSION TAG	UNP Q9GJT3
D	142	THR	-	EXPRESSION TAG	UNP Q9GJT3
D	143	LYS	-	EXPRESSION TAG	UNP Q9GJT3
D	144	HIS	-	EXPRESSION TAG	UNP Q9GJT3
D	145	HIS	-	EXPRESSION TAG	UNP Q9GJT3
D	146	HIS	-	EXPRESSION TAG	UNP Q9GJT3
D	147	HIS	-	EXPRESSION TAG	UNP Q9GJT3
D	148	HIS	-	EXPRESSION TAG	UNP Q9GJT3
D	149	HIS	-	EXPRESSION TAG	UNP Q9GJT3

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



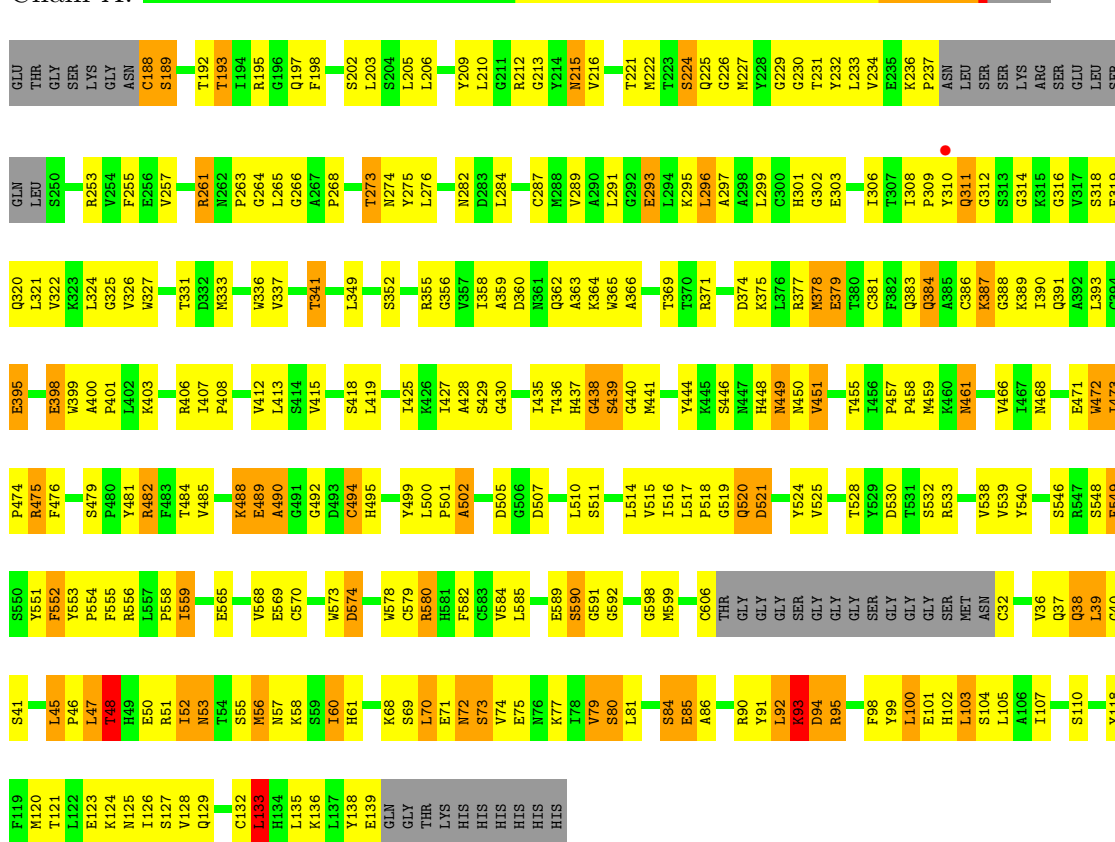
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

### 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 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.

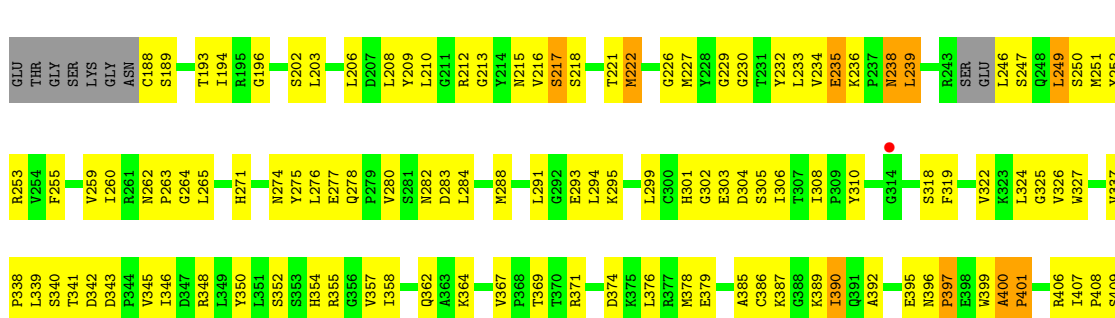
#### • Molecule 1: Hemagglutinin, CDw150

Chain A:



#### • Molecule 1: Hemagglutinin, CDw150

Chain B:









## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	187.71Å 170.07Å 110.68Å 90.00° 117.28° 90.00°	Depositor
Resolution (Å)	19.97 – 3.15 19.96 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.97-3.15) 99.2 (19.96-3.16)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 3.15Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.231 , 0.292 0.231 , 0.295	Depositor DCC
$R_{free}$ test set	2644 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.0	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 49.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 52452 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	16313	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.49	0/4155	0.74	2/5646 (0.0%)
1	B	0.44	0/4243	0.71	2/5763 (0.0%)
1	C	0.46	0/4151	0.71	1/5638 (0.0%)
1	D	0.41	0/4083	0.66	0/5545
All	All	0.45	0/16632	0.70	5/22592 (0.0%)

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	C	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	48	THR	N-CA-C	-6.29	94.02	111.00
1	C	132	CYS	CA-CB-SG	-6.03	103.15	114.00
1	A	48	THR	N-CA-C	-5.52	96.09	111.00
1	B	92	LEU	N-CA-C	-5.35	96.54	111.00
1	A	92	LEU	N-CA-C	-5.34	96.58	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	541	TYR	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4053	0	4023	288	0
1	B	4141	0	4119	297	0
1	C	4051	0	4024	313	0
1	D	3984	0	3964	350	0
2	A	14	0	13	0	0
2	B	28	0	26	0	0
2	C	28	0	26	1	0
2	D	14	0	13	1	0
All	All	16313	0	16208	1224	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 38.

The worst 5 of 1224 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:85:GLU:HG2	1:A:86:ALA:H	1.09	1.16
1:A:236:LYS:HB3	1:A:237:PRO:HD2	1.30	1.14
1:D:503:GLU:HB2	1:D:76:ASN:HD22	1.05	1.09
1:A:60:ILE:HG22	1:A:61:HIS:H	1.13	1.08
1:A:540:TYR:HE1	1:A:568:VAL:HG21	1.22	1.04

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	509/559 (91%)	416 (82%)	62 (12%)	31 (6%)	2	19
1	B	520/559 (93%)	412 (79%)	86 (16%)	22 (4%)	4	31
1	C	504/559 (90%)	407 (81%)	67 (13%)	30 (6%)	2	20
1	D	492/559 (88%)	389 (79%)	70 (14%)	33 (7%)	2	16
All	All	2025/2236 (91%)	1624 (80%)	285 (14%)	116 (6%)	3	22

5 of 116 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	GLN
1	A	389	LYS
1	A	439	SER
1	A	490	ALA
1	A	494	CYS

### 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	457/489 (94%)	403 (88%)	54 (12%)	8	32
1	B	468/489 (96%)	433 (92%)	35 (8%)	19	61
1	C	457/489 (94%)	400 (88%)	57 (12%)	7	29
1	D	449/489 (92%)	419 (93%)	30 (7%)	23	66
All	All	1831/1956 (94%)	1655 (90%)	176 (10%)	12	45

5 of 176 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	34	LYS
1	C	248	GLN
1	D	520	GLN
1	B	45	LEU
1	C	192	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	334	GLN
1	C	567	GLN
1	D	72	ASN
1	C	383	GLN
1	C	461	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	A	901	1	12,14,15	0.85	1 (8%)	15,19,21	1.29	3 (20%)
2	NAG	B	801	1	12,14,15	0.59	0	15,19,21	1.07	2 (13%)
2	NAG	B	901	1	12,14,15	0.55	0	15,19,21	0.79	1 (6%)
2	NAG	C	801	1	12,14,15	0.66	0	15,19,21	0.60	0
2	NAG	C	901	1	12,14,15	0.61	0	15,19,21	0.94	1 (6%)
2	NAG	D	901	1	12,14,15	0.76	0	15,19,21	0.81	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	901	1	-	0/6/23/26	0/1/1/1
2	NAG	B	801	1	-	1/6/23/26	0/1/1/1
2	NAG	B	901	1	-	0/6/23/26	0/1/1/1
2	NAG	C	801	1	-	0/6/23/26	0/1/1/1
2	NAG	C	901	1	-	0/6/23/26	0/1/1/1
2	NAG	D	901	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	NAG	C4-C5	2.07	1.57	1.53

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	NAG	C3-C4-C5	3.01	115.58	110.20
2	C	901	NAG	C3-C2-N2	-2.41	108.09	111.76
2	A	901	NAG	O5-C5-C4	2.41	113.72	110.65
2	A	901	NAG	C2-N2-C7	-2.20	119.39	123.09
2	B	801	NAG	C3-C2-N2	-2.10	108.56	111.76

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	NAG	O7-C7-N2-C2

There are no ring outliers.

## 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 ⓘ

### 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, 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	515/559 (92%)	-0.26	1 (0%) 93 64	33, 57, 97, 115	0
1	B	526/559 (94%)	-0.18	2 (0%) 90 49	38, 66, 109, 122	0
1	C	514/559 (91%)	-0.20	1 (0%) 93 64	39, 66, 101, 118	0
1	D	504/559 (90%)	-0.15	0 100 100	49, 75, 114, 130	0
All	All	2059/2236 (92%)	-0.20	4 (0%) 93 64	33, 67, 108, 130	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	589	GLU	2.8
1	B	314	GLY	2.4
1	A	310	TYR	2.3
1	C	314	GLY	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	D	901	14/15	0.43	13.97	95,98,103,105	0
2	NAG	C	801	14/15	0.48	7.38	90,94,98,98	0
2	NAG	B	801	14/15	0.43	5.55	89,91,93,93	0
2	NAG	C	901	14/15	0.33	4.76	94,97,99,99	0
2	NAG	B	901	14/15	0.27	0.94	100,102,104,104	0
2	NAG	A	901	14/15	0.27	0.72	88,90,91,91	0

## 6.5 Other polymers

There are no such residues in this entry.