



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 05:05 pm GMT

PDB ID : 4C7L  
Title : Crystal structure of Mouse Hepatitis virus strain S Hemagglutinin- esterase  
Authors : Zeng, Q.H.; Huizinga, E.G.  
Deposited on : 2013-09-23  
Resolution : 2.10 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

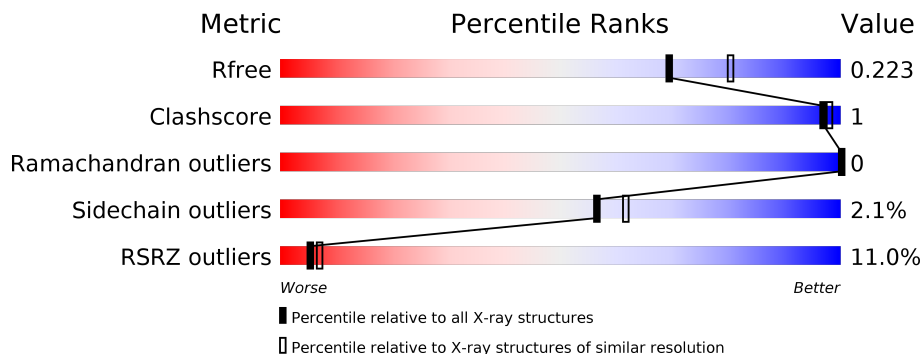
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	111664	4608 (2.10-2.10)
Clashscore	122126	5109 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)
RSRZ outliers	108989	4497 (2.10-2.10)

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. 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	386	
1	B	386	

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
3	NAG	B	1415	-	-	-	X
4	BMA	B	1421	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6388 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 HEMAGGLUTININ-ESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	4	0
			2714	1736	446	513	19			
1	B	368	Total	C	N	O	S	0	5	0
			2962	1885	488	569	20			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	ALA	SER	engineered mutation	UNP P28845
B	45	ALA	SER	engineered mutation	UNP P28845
A	404	SER	-	expression tag	UNP O55252
A	405	ASP	-	expression tag	UNP O55252
A	406	PRO	-	expression tag	UNP O55252
A	407	LEU	-	expression tag	UNP O55252
A	408	VAL	-	expression tag	UNP O55252
A	409	PRO	-	expression tag	UNP O55252
A	410	ARG	-	expression tag	UNP O55252
B	404	SER	-	expression tag	UNP O55252
B	405	ASP	-	expression tag	UNP O55252
B	406	PRO	-	expression tag	UNP O55252
B	407	LEU	-	expression tag	UNP O55252
B	408	VAL	-	expression tag	UNP O55252
B	409	PRO	-	expression tag	UNP O55252
B	410	ARG	-	expression tag	UNP O55252

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	K	0	0
			1	1		
2	A	1	Total	K	0	0
			1	1		

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



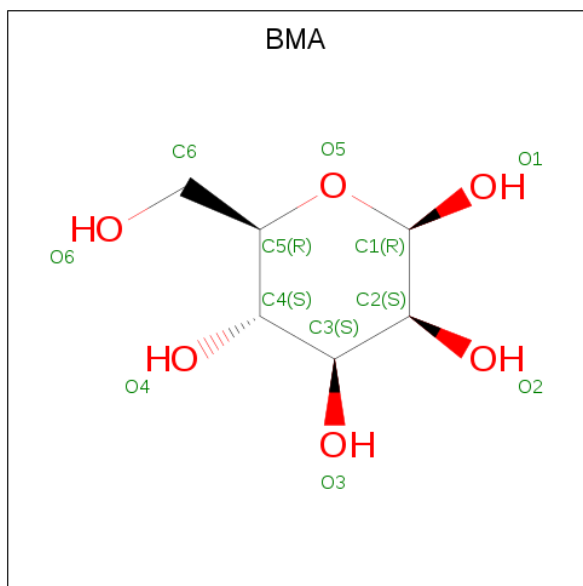
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1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

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

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



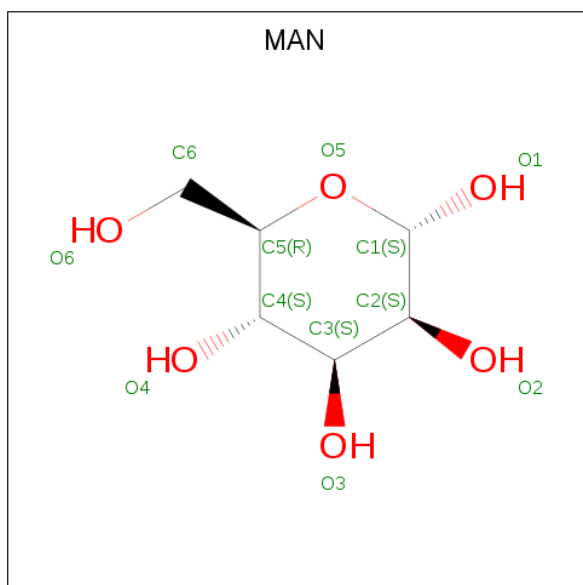
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 7 is water.

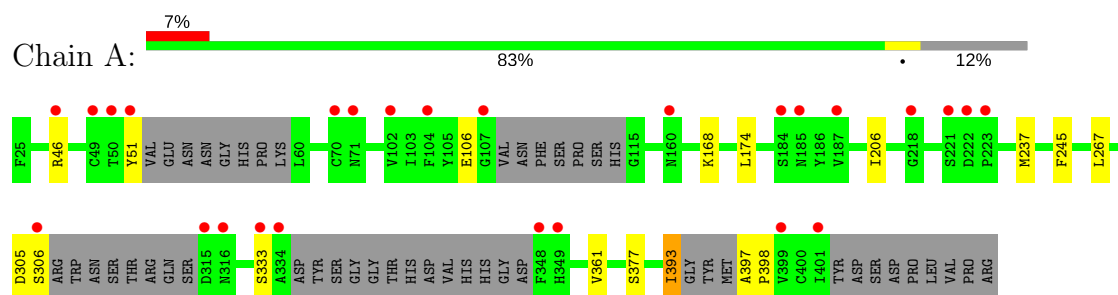
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	169	Total	O	0	0
			169	169		
7	B	122	Total	O	0	0
			122	122		



### 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 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: HEMAGGLUTININ-ESTERASE



#### • Molecule 1: HEMAGGLUTININ-ESTERASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.83Å 108.76Å 125.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.76 – 2.10 29.76 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.76-2.10) 99.6 (29.76-2.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.186 , 0.219 0.193 , 0.223	Depositor DCC
$R_{free}$ test set	3707 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 53.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6388	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL, K, BMA, 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	0.53	0/2785	0.62	0/3773
1	B	0.49	0/3045	0.58	0/4134
All	All	0.51	0/5830	0.60	0/7907

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2714	0	2548	7	0
1	B	2962	0	2754	4	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	126	0	112	0	0
3	B	182	0	162	1	0
4	A	22	0	19	0	0
4	B	22	0	18	0	0
5	A	11	0	10	0	0
5	B	44	0	38	0	0
6	B	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	169	0	0	1	0
7	B	122	0	0	0	0
All	All	6388	0	5677	12	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 1.

All (12) 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:397:ALA:N	1:A:398:PRO:HD2	1.90	0.86
1:B:309:ASN:OD1	1:B:311:THR:HG22	1.94	0.66
1:A:397:ALA:N	1:A:398:PRO:CD	2.57	0.66
1:B:74:ARG:O	1:B:75:ILE:HD13	2.13	0.49
1:A:305:ASP:O	1:A:306:SER:HB2	2.17	0.45
1:A:393:ILE:HG22	1:A:393:ILE:O	2.17	0.45
1:A:237:MET:HE1	7:A:2093:HOH:O	2.19	0.43
1:B:60:LEU:N	1:B:60:LEU:HD12	2.34	0.42
1:A:206:ILE:HA	1:A:267:LEU:O	2.19	0.42
1:B:41:LEU:HD23	1:B:75:ILE:HD12	2.01	0.42
3:B:1424:NAG:HO3	3:B:1425:NAG:C1	2.34	0.41
1:A:106:GLU:O	1:A:306:SER:N	2.50	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	330/386 (86%)	319 (97%)	11 (3%)	0	100	100
1	B	367/386 (95%)	355 (97%)	12 (3%)	0	100	100
All	All	697/772 (90%)	674 (97%)	23 (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	297/336 (88%)	288 (97%)	9 (3%)	44	47
1	B	327/336 (97%)	323 (99%)	4 (1%)	74	80
All	All	624/672 (93%)	611 (98%)	13 (2%)	56	62

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

Mol	Chain	Res	Type
1	A	46	ARG
1	A	51	TYR
1	A	168	LYS
1	A	174	LEU
1	A	245	PHE
1	A	333	SER
1	A	361	VAL
1	A	377	SER
1	A	393	ILE
1	B	81	ASN
1	B	245	PHE
1	B	312	ARG
1	B	351	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN

### 5.3.3 RNA ⓘ

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 35 ligands modelled in this entry, 2 are monoatomic - leaving 33 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	$\# Z  > 2$
3	NAG	A	1403	1	14,14,15	0.50	0	17,19,21	0.84	0
3	NAG	A	1404	1	14,14,15	0.61	0	17,19,21	1.02	1 (5%)
3	NAG	A	1405	1	14,14,15	0.53	0	17,19,21	0.95	0
3	NAG	A	1406	1,3	14,14,15	0.47	0	17,19,21	1.16	1 (5%)
3	NAG	A	1407	3,4	14,14,15	0.61	0	17,19,21	0.90	1 (5%)
4	BMA	A	1408	3	11,11,12	0.49	0	15,15,17	0.98	1 (6%)
3	NAG	A	1409	1,3	14,14,15	0.46	0	17,19,21	1.26	1 (5%)
3	NAG	A	1410	3	14,14,15	0.54	0	17,19,21	0.98	1 (5%)
3	NAG	A	1411	1,3	14,14,15	0.63	0	17,19,21	1.11	1 (5%)
3	NAG	A	1412	3,4	14,14,15	0.51	0	17,19,21	0.81	0
4	BMA	A	1413	3,5	11,11,12	0.55	0	15,15,17	1.42	3 (20%)
5	MAN	A	1414	4	11,11,12	0.59	0	15,15,17	0.97	2 (13%)
6	GOL	B	1412	-	5,5,5	0.35	0	5,5,5	0.57	0
6	GOL	B	1413	-	5,5,5	0.40	0	5,5,5	0.17	0
3	NAG	B	1414	1,3	14,14,15	0.51	0	17,19,21	0.98	1 (5%)
3	NAG	B	1415	3	14,14,15	0.51	0	17,19,21	0.80	1 (5%)
3	NAG	B	1416	1,3	14,14,15	0.46	0	17,19,21	0.66	0
3	NAG	B	1417	3	14,14,15	0.50	0	17,19,21	1.10	1 (5%)
3	NAG	B	1418	1	14,14,15	0.44	0	17,19,21	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	B	1419	1,3	14,14,15	0.39	0	17,19,21	1.09	1 (5%)
3	NAG	B	1420	3,4	14,14,15	0.61	0	17,19,21	1.12	1 (5%)
4	BMA	B	1421	3	11,11,12	0.49	0	15,15,17	0.77	0
3	NAG	B	1422	1	14,14,15	0.44	0	17,19,21	1.30	1 (5%)
3	NAG	B	1423	1	14,14,15	0.41	0	17,19,21	0.94	0
3	NAG	B	1424	1,3	14,14,15	0.73	0	17,19,21	1.10	1 (5%)
3	NAG	B	1425	3	14,14,15	0.54	0	17,19,21	0.84	0
3	NAG	B	1426	1,3	14,14,15	0.62	0	17,19,21	1.10	1 (5%)
3	NAG	B	1427	3,4	14,14,15	0.52	0	17,19,21	0.90	0
4	BMA	B	1428	3,5	11,11,12	0.42	0	15,15,17	0.83	0
5	MAN	B	1429	4	11,11,12	0.67	0	15,15,17	0.88	1 (6%)
5	MAN	B	1430	5,4	11,11,12	0.62	0	15,15,17	0.67	0
5	MAN	B	1431	5	11,11,12	0.69	0	15,15,17	1.25	2 (13%)
5	MAN	B	1432	5	11,11,12	0.66	0	15,15,17	1.43	2 (13%)

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
3	NAG	A	1403	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1404	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1405	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1406	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1407	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	1408	3	-	0/2/19/22	0/1/1/1
3	NAG	A	1409	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1410	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1411	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1412	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	1413	3,5	-	0/2/19/22	0/1/1/1
5	MAN	A	1414	4	-	0/2/19/22	0/1/1/1
6	GOL	B	1412	-	-	0/4/4/4	0/0/0/0
6	GOL	B	1413	-	-	0/4/4/4	0/0/0/0
3	NAG	B	1414	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1415	3	-	0/6/23/26	0/1/1/1
3	NAG	B	1416	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1417	3	-	0/6/23/26	0/1/1/1
3	NAG	B	1418	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1419	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1420	3,4	-	0/6/23/26	0/1/1/1
4	BMA	B	1421	3	-	0/2/19/22	0/1/1/1
3	NAG	B	1422	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1423	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1424	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1425	3	-	0/6/23/26	0/1/1/1
3	NAG	B	1426	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1427	3,4	-	0/6/23/26	0/1/1/1
4	BMA	B	1428	3,5	-	0/2/19/22	0/1/1/1
5	MAN	B	1429	4	-	0/2/19/22	0/1/1/1
5	MAN	B	1430	5,4	-	0/2/19/22	0/1/1/1
5	MAN	B	1431	5	-	0/2/19/22	0/1/1/1
5	MAN	B	1432	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1420	NAG	O5-C1-C2	-3.47	106.73	111.52
3	B	1426	NAG	O5-C1-C2	-3.14	107.18	111.52
3	A	1407	NAG	O5-C1-C2	-2.34	108.30	111.52
4	A	1413	BMA	O5-C5-C4	-2.26	105.34	110.83
5	B	1429	MAN	C1-O5-C5	2.01	114.96	112.19
3	A	1410	NAG	C4-C3-C2	2.10	114.10	111.02
3	B	1415	NAG	C1-O5-C5	2.11	115.09	112.19
5	A	1414	MAN	C1-C2-C3	2.19	112.44	109.66
4	A	1413	BMA	C1-C2-C3	2.23	112.48	109.66
5	B	1431	MAN	O5-C5-C6	2.31	110.80	107.15
4	A	1408	BMA	C3-C4-C5	2.31	114.38	110.24
5	A	1414	MAN	C1-O5-C5	2.32	115.38	112.19
5	B	1431	MAN	C1-C2-C3	2.33	112.61	109.66
3	A	1404	NAG	C1-O5-C5	2.39	115.47	112.19
5	B	1432	MAN	O5-C5-C6	2.46	111.04	107.15
3	B	1414	NAG	C1-O5-C5	2.63	115.81	112.19
3	A	1411	NAG	O5-C5-C6	2.65	111.35	107.15
3	B	1417	NAG	C4-C3-C2	2.78	115.10	111.02
5	B	1432	MAN	C1-O5-C5	2.93	116.21	112.19
3	B	1424	NAG	C1-O5-C5	3.21	116.60	112.19
3	B	1419	NAG	C1-O5-C5	3.75	117.34	112.19
4	A	1413	BMA	O5-C5-C6	3.79	113.14	107.15
3	A	1406	NAG	C1-O5-C5	4.17	117.93	112.19
3	A	1409	NAG	C1-O5-C5	4.53	118.42	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1422	NAG	C1-O5-C5	4.60	118.51	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1424	NAG	1	0
3	B	1425	NAG	1	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

### 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	338/386 (87%)	0.25	26 (7%) 13 17	28, 43, 93, 158	6 (1%)
1	B	368/386 (95%)	0.56	52 (14%) 2 3	34, 52, 104, 169	0
All	All	706/772 (91%)	0.41	78 (11%) 5 7	28, 48, 100, 169	6 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	62	TRP	10.2
1	B	336	TYR	9.1
1	A	334	ALA	9.1
1	B	395	TYR	8.3
1	B	337	SER	8.1
1	B	60	LEU	7.5
1	B	348	PHE	7.5
1	B	61	ASP	7.3
1	B	220	SER	6.6
1	B	311	THR	6.5
1	A	401	ILE	6.2
1	B	310	SER	6.2
1	A	221	SER	5.9
1	B	335	ASP	5.4
1	A	51	TYR	5.4
1	B	334	ALA	5.4
1	B	397	ALA	5.3
1	B	219	SER	5.2
1	B	221	SER	5.2
1	B	314	SER	4.9
1	A	333	SER	4.8
1	A	187	VAL	4.7
1	B	313	GLN	4.6
1	A	49	CYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	71	ASN	4.5
1	B	170	LYS	4.3
1	B	312	ARG	4.2
1	A	50	THR	4.2
1	B	396	MET	4.1
1	B	114	HIS	4.0
1	B	393	ILE	4.0
1	A	348	PHE	3.6
1	B	398	PRO	3.6
1	B	71	ASN	3.5
1	B	225	ASN	3.5
1	B	333	SER	3.4
1	B	171	THR	3.4
1	B	394	GLY	3.3
1	B	187	VAL	3.3
1	B	309	ASN	3.3
1	B	224	ALA	3.1
1	B	353	LEU	3.1
1	B	347	ASP	3.0
1	B	351	ARG	3.0
1	A	223	PRO	3.0
1	B	222	ASP	3.0
1	B	105	TYR	2.9
1	A	315	ASP	2.9
1	B	83	LEU	2.8
1	B	308	TRP	2.8
1	B	223	PRO	2.8
1	B	209	LEU	2.7
1	A	107	GLY	2.7
1	A	222	ASP	2.7
1	A	184	SER	2.6
1	B	41	LEU	2.6
1	A	102	VAL	2.6
1	B	111	SER	2.5
1	A	160	ASN	2.5
1	B	113	SER	2.5
1	B	63	LEU	2.5
1	A	399	VAL	2.5
1	A	46	ARG	2.4
1	B	104	PHE	2.4
1	B	392	ASN	2.4
1	B	262	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	349	HIS	2.2
1	A	104	PHE	2.2
1	B	218	GLY	2.2
1	A	316	ASN	2.2
1	A	218	GLY	2.2
1	A	185	ASN	2.1
1	B	190	TYR	2.1
1	B	103	ILE	2.1
1	B	70	CYS	2.1
1	B	112	PRO	2.1
1	A	306	SER	2.1
1	A	70	CYS	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 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BMA	B	1421	11/12	0.71	0.41	81,84,84,85	0
3	NAG	B	1417	14/15	0.72	0.40	83,84,85,86	0
4	BMA	A	1408	11/12	0.75	0.34	82,84,86,87	0
6	GOL	B	1412	6/6	0.79	0.36	60,61,64,65	0
4	BMA	A	1413	11/12	0.80	0.21	79,81,81,82	0
3	NAG	B	1415	14/15	0.80	0.50	84,88,89,90	0
3	NAG	A	1410	14/15	0.82	0.42	73,77,80,83	0
3	NAG	B	1425	14/15	0.83	0.48	82,87,88,89	0
3	NAG	B	1423	14/15	0.83	0.33	60,69,71,72	0
3	NAG	A	1403	14/15	0.83	0.30	57,64,65,65	0
5	MAN	A	1414	11/12	0.84	0.29	83,84,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	1405	14/15	0.84	0.24	56,63,67,69	0
3	NAG	A	1407	14/15	0.85	0.23	60,66,72,77	0
3	NAG	B	1416	14/15	0.86	0.34	63,72,74,79	0
3	NAG	B	1420	14/15	0.87	0.25	62,66,72,77	0
3	NAG	A	1404	14/15	0.87	0.31	60,68,70,73	0
3	NAG	B	1424	14/15	0.89	0.15	56,65,69,76	0
6	GOL	B	1413	6/6	0.89	0.18	81,82,82,82	0
3	NAG	B	1414	14/15	0.89	0.30	62,70,73,79	0
3	NAG	A	1406	14/15	0.90	0.10	45,51,54,60	0
5	MAN	B	1431	11/12	0.90	0.14	46,51,53,55	0
3	NAG	B	1418	14/15	0.92	0.26	58,64,69,69	0
3	NAG	B	1422	14/15	0.92	0.38	61,69,72,73	0
3	NAG	B	1426	14/15	0.93	0.11	41,46,49,50	0
3	NAG	A	1409	14/15	0.94	0.10	44,50,59,66	0
5	MAN	B	1429	11/12	0.94	0.18	47,50,52,54	0
3	NAG	A	1412	14/15	0.94	0.23	68,70,74,77	0
3	NAG	B	1419	14/15	0.94	0.08	44,51,53,59	0
5	MAN	B	1432	11/12	0.94	0.15	56,60,63,66	0
3	NAG	B	1427	14/15	0.95	0.09	46,47,48,48	0
4	BMA	B	1428	11/12	0.96	0.06	40,41,44,45	0
3	NAG	A	1411	14/15	0.97	0.12	47,53,58,63	0
5	MAN	B	1430	11/12	0.97	0.09	39,43,47,53	0
2	K	B	1411	1/1	0.99	0.14	53,53,53,53	0
2	K	A	1402	1/1	0.99	0.15	49,49,49,49	0

## 6.5 Other polymers

There are no such residues in this entry.