



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 26, 2017 – 02:18 PM EDT

PDB ID : 4DAG  
Title : Structure of the Human Metapneumovirus Fusion Protein with Neutralizing Antibody Identifies a Pneumovirus Antigenic Site  
Authors : Jardetzky, T.S.; Wen, X.  
Deposited on : unknown  
Resolution : 3.39 Å(reported)

This is a wwPDB X-ray Structure 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/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20029824

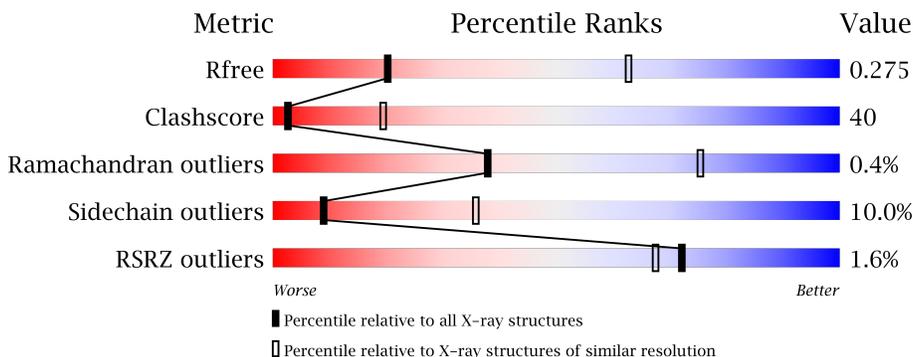
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.39 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))
$R_{free}$	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

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	415	
2	H	220	
3	L	213	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6064 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	383	2740	1707	473	540	20	0	0	0

- Molecule 2 is a protein called Neutralizing Antibody DS7 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	220	1621	1021	272	319	9	0	0	0

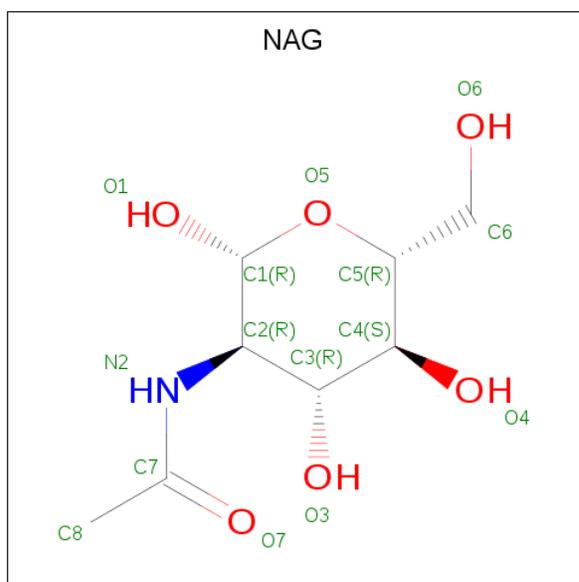
- Molecule 3 is a protein called Neutralizing Antibody DS7 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	213	1581	985	259	330	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

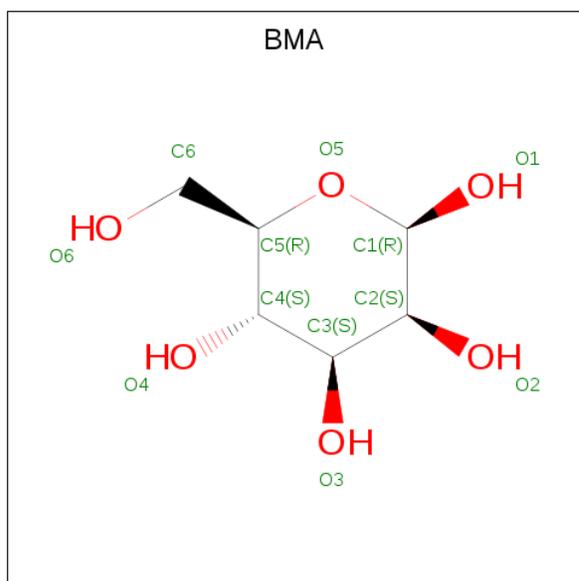
Chain	Residue	Modelled	Actual	Comment	Reference
L	233	MET	-	EXPRESSION TAG	UNP Q8N5F4

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



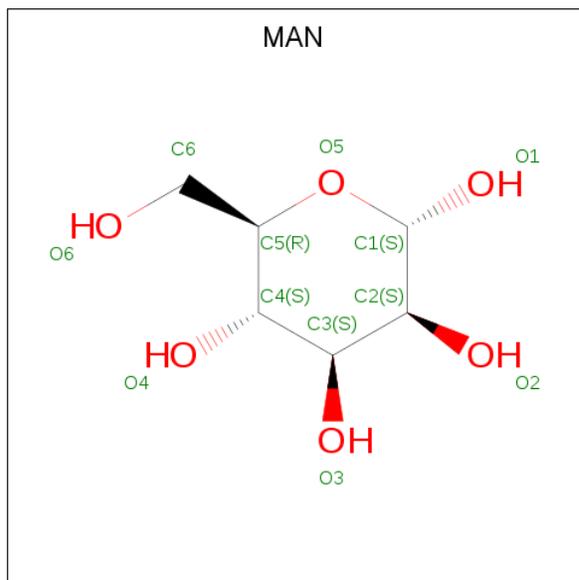
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

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

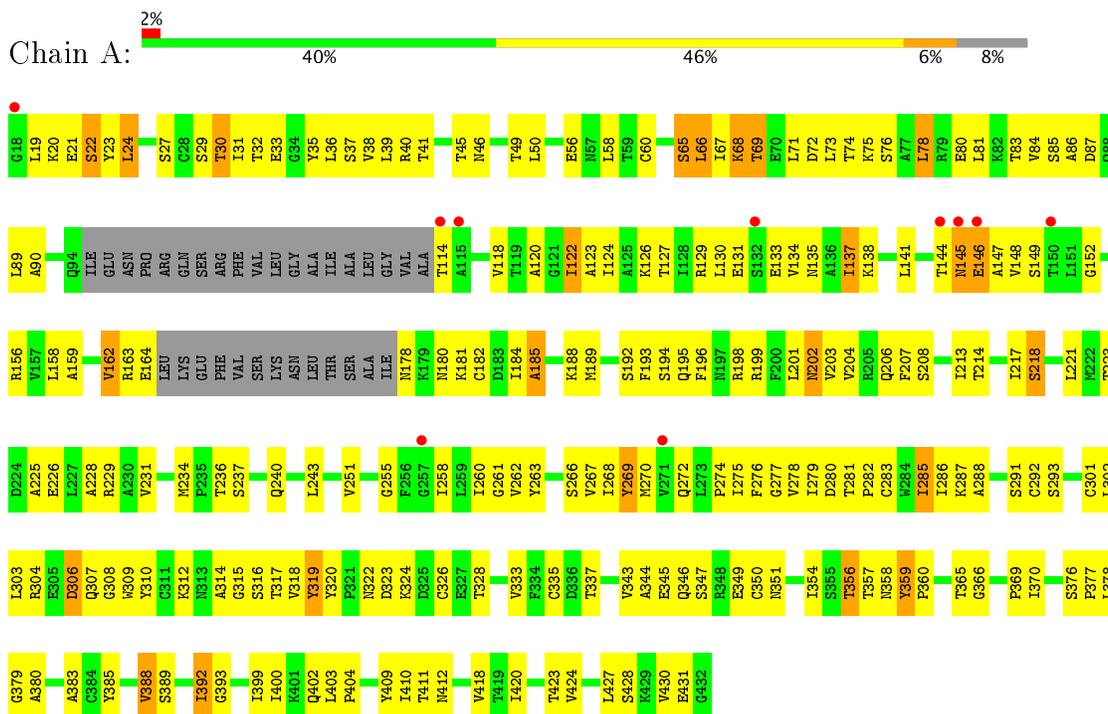


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		

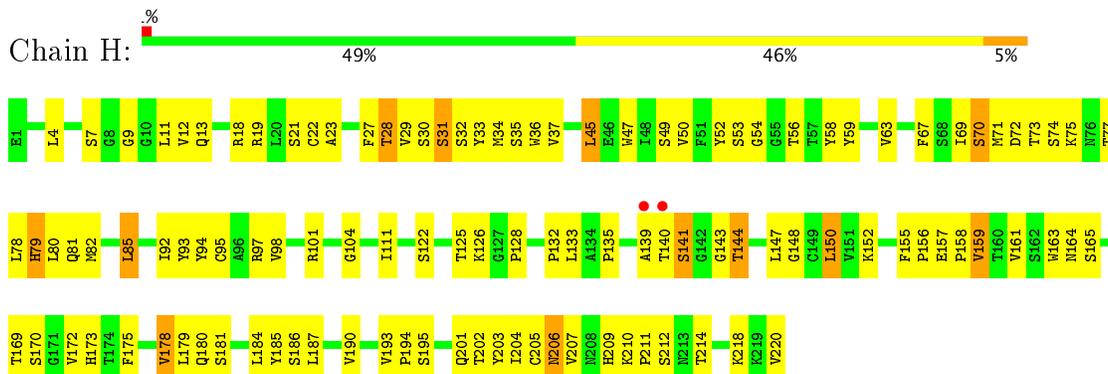
### 3 Residue-property plots [i](#)

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: Fusion glycoprotein F0

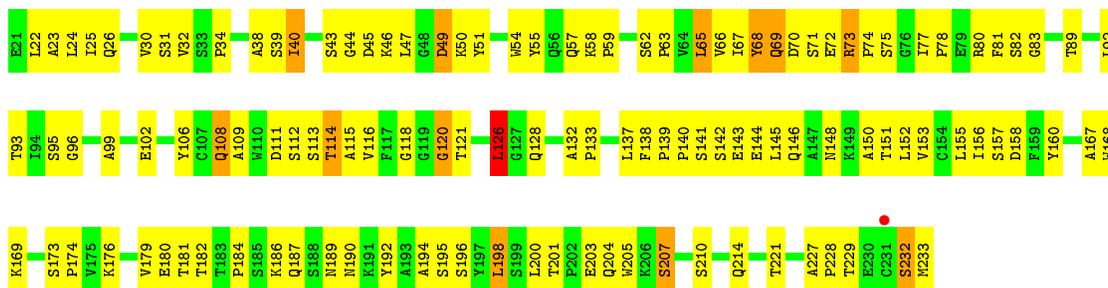


- Molecule 2: Neutralizing Antibody DS7 heavy chain



- Molecule 3: Neutralizing Antibody DS7 light chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	258.96Å 258.96Å 167.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.85 – 3.39 44.85 – 3.39	Depositor EDS
% Data completeness (in resolution range)	78.8 (44.85-3.39) 78.5 (44.85-3.39)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 3.40Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.260 , 0.289 0.236 , 0.275	Depositor DCC
$R_{free}$ test set	1852 reflections (5.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.4	Xtrriage
Anisotropy	0.027	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 52.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	6064	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.46	0/2776	0.74	1/3785 (0.0%)
2	H	0.58	0/1659	0.81	0/2260
3	L	0.47	0/1618	0.73	1/2211 (0.0%)
All	All	0.50	0/6053	0.76	2/8256 (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	A	0	8
3	L	0	4
All	All	0	12

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	118	GLY	N-CA-C	-6.46	96.96	113.10
1	A	316	SER	N-CA-C	-5.35	96.56	111.00

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ILE	Peptide
1	A	145	ASN	Peptide
1	A	185	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	A	66	LEU	Peptide
1	A	68	LYS	Peptide

## 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	2740	0	2604	236	0
2	H	1621	0	1596	124	0
3	L	1581	0	1519	127	0
4	A	56	0	48	4	0
5	A	22	0	16	4	0
6	A	44	0	38	2	0
All	All	6064	0	5821	470	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 40.

The worst 5 of 470 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:45:THR:HG22	1:A:272:GLN:HG2	1.38	1.06
2:H:34:MET:HE3	2:H:78:LEU:HD22	1.43	1.00
3:L:47:LEU:O	3:L:50:LYS:N	1.97	0.97
1:A:314:ALA:N	1:A:315:GLY:HA2	1.80	0.97
1:A:39:LEU:HB2	1:A:278:VAL:HG23	1.46	0.96

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	377/415 (91%)	327 (87%)	48 (13%)	2 (0%)	32	71
2	H	218/220 (99%)	204 (94%)	13 (6%)	1 (0%)	32	71
3	L	211/213 (99%)	197 (93%)	14 (7%)	0	100	100
All	All	806/848 (95%)	728 (90%)	75 (9%)	3 (0%)	38	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	MET
2	H	141	SER
1	A	162	VAL

### 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	279/347 (80%)	254 (91%)	25 (9%)	11	41
2	H	182/182 (100%)	162 (89%)	20 (11%)	7	31
3	L	178/178 (100%)	159 (89%)	19 (11%)	8	33
All	All	639/707 (90%)	575 (90%)	64 (10%)	9	36

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	45	LEU
2	H	125	THR
3	L	173	SER
2	H	53	SER
2	H	81	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	ASN
1	A	247	ASN
1	A	272	GLN
3	L	26	GLN

### 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](#)

10 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
4	NAG	A	501	1,4	14,14,15	2.26	6 (42%)	15,19,21	1.34	3 (20%)
4	NAG	A	502	5,4	14,14,15	2.26	6 (42%)	15,19,21	1.28	2 (13%)
5	BMA	A	503	4,6	11,11,12	2.54	4 (36%)	13,15,17	1.51	3 (23%)
6	MAN	A	504	5	11,11,12	2.57	6 (54%)	13,15,17	1.20	0
6	MAN	A	505	5	11,11,12	2.47	5 (45%)	13,15,17	1.19	1 (7%)
4	NAG	A	506	1,4	14,14,15	2.16	5 (35%)	15,19,21	1.74	4 (26%)
4	NAG	A	507	5,4	14,14,15	2.31	6 (42%)	15,19,21	1.63	3 (20%)
5	BMA	A	508	4,6	11,11,12	2.68	6 (54%)	13,15,17	2.32	5 (38%)
6	MAN	A	509	5	11,11,12	2.30	3 (27%)	13,15,17	2.48	7 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	MAN	A	510	5	11,11,12	2.19	4 (36%)	13,15,17	1.13	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
4	NAG	A	501	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	502	5,4	-	0/6/23/26	0/1/1/1
5	BMA	A	503	4,6	-	0/2/19/22	0/1/1/1
6	MAN	A	504	5	-	0/2/19/22	1/1/1/1
6	MAN	A	505	5	-	0/2/19/22	1/1/1/1
4	NAG	A	506	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	507	5,4	-	0/6/23/26	0/1/1/1
5	BMA	A	508	4,6	-	0/2/19/22	0/1/1/1
6	MAN	A	509	5	-	0/2/19/22	0/1/1/1
6	MAN	A	510	5	-	0/2/19/22	1/1/1/1

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	508	BMA	C2-C3	-5.12	1.45	1.52
5	A	508	BMA	C4-C3	-4.99	1.39	1.52
5	A	503	BMA	C4-C3	-4.84	1.40	1.52
4	A	502	NAG	C1-C2	-4.40	1.46	1.52
4	A	506	NAG	C1-C2	-4.12	1.46	1.52

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	508	BMA	C1-C2-C3	-6.08	101.95	109.65
4	A	506	NAG	C2-N2-C7	-3.73	117.51	122.94
5	A	508	BMA	O4-C4-C3	-3.27	103.25	110.36
4	A	507	NAG	O7-C7-C8	-2.94	116.70	122.06
5	A	503	BMA	O4-C4-C3	-2.89	104.07	110.36

There are no chirality outliers.

There are no torsion outliers.

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	510	MAN	C1-C2-C3-C4-C5-O5
6	A	504	MAN	C1-C2-C3-C4-C5-O5
6	A	505	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	503	BMA	1	0
6	A	505	MAN	1	0
4	A	506	NAG	2	0
4	A	507	NAG	3	0
5	A	508	BMA	3	0
6	A	509	MAN	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 [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	383/415 (92%)	-0.11	10 (2%) 56 52	55, 111, 158, 178	0
2	H	220/220 (100%)	-0.23	2 (0%) 84 80	44, 69, 135, 193	0
3	L	213/213 (100%)	-0.22	1 (0%) 90 88	45, 86, 125, 181	0
All	All	816/848 (96%)	-0.17	13 (1%) 72 67	44, 91, 152, 193	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	SER	6.2
1	A	145	ASN	3.8
1	A	115	ALA	3.4
1	A	114	THR	3.4
1	A	144	THR	3.4

### 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, 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
4	NAG	A	506	14/15	0.83	0.19	0.54	40,48,70,91	0
6	MAN	A	505	11/12	0.55	0.50	-	138,167,189,189	0
4	NAG	A	502	14/15	0.83	0.49	-	138,164,173,178	0
6	MAN	A	509	11/12	0.56	0.29	-	124,151,190,240	0
5	BMA	A	508	11/12	0.80	0.25	-	143,148,164,185	0
4	NAG	A	501	14/15	0.90	0.41	-	127,144,158,169	0
6	MAN	A	504	11/12	0.86	0.44	-	144,162,175,175	0
5	BMA	A	503	11/12	0.57	0.43	-	175,182,187,190	0
6	MAN	A	510	11/12	0.91	0.22	-	105,158,187,207	0
4	NAG	A	507	14/15	0.91	0.26	-	97,123,150,163	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.