



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 22, 2019 – 12:39 PM EST

PDB ID : 6C6C  
Title : Structure of glycolipid aGSA[20,6P] in complex with mouse CD1d  
Authors : Zajonc, D.M.; Wang, J.  
Deposited on : 2018-01-18  
Resolution : 2.08 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.

---

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 : rb-20031633  
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) : rb-20031633

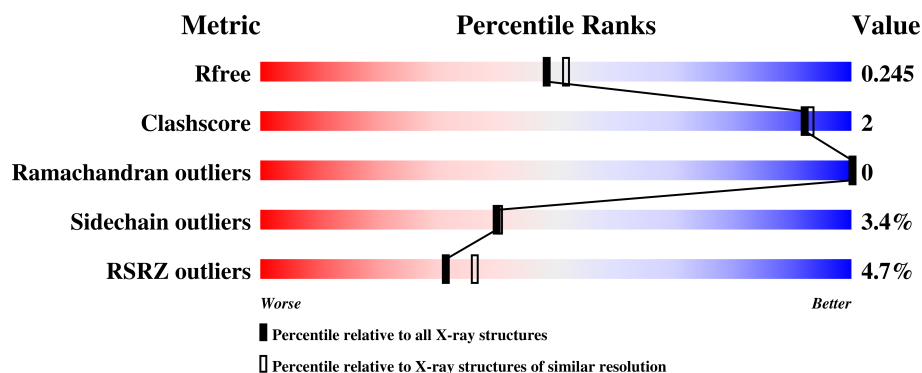
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.08 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	5409 (2.10-2.06)
Clashscore	122126	5943 (2.10-2.06)
Ramachandran outliers	120053	5886 (2.10-2.06)
Sidechain outliers	120020	5887 (2.10-2.06)
RSRZ outliers	108989	5279 (2.10-2.06)

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	285	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>7%</div> <div>7%</div> </div> </div>
2	B	99	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>6%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 3220 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 Antigen-presenting glycoprotein CD1d1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2134	1362	366	393	13			

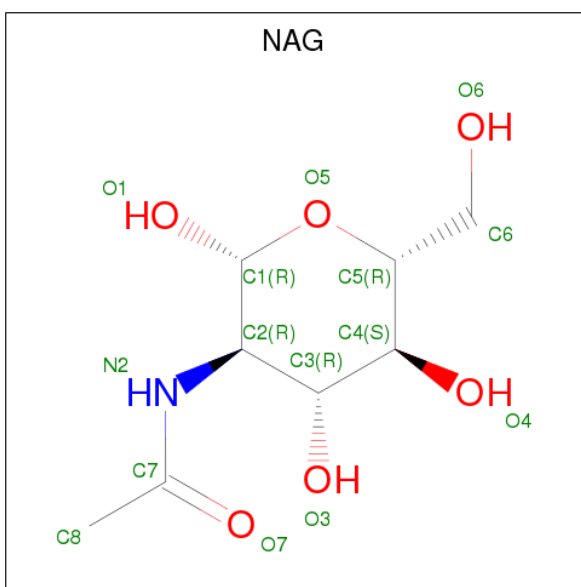
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	HIS	-	expression tag	UNP A0A0R4J090
A	281	HIS	-	expression tag	UNP A0A0R4J090
A	282	HIS	-	expression tag	UNP A0A0R4J090
A	283	HIS	-	expression tag	UNP A0A0R4J090
A	284	HIS	-	expression tag	UNP A0A0R4J090
A	285	HIS	-	expression tag	UNP A0A0R4J090

- Molecule 2 is a protein called Beta-2-microglobulin.

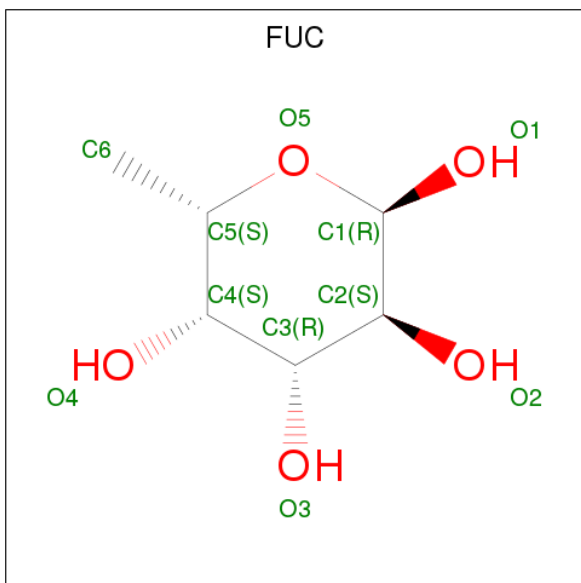
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			810	517	137	149	7			

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



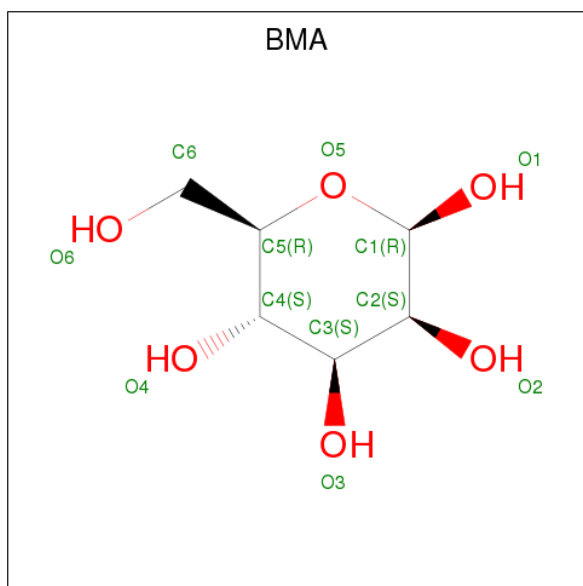
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula:  $C_6H_{12}O_5$ ).



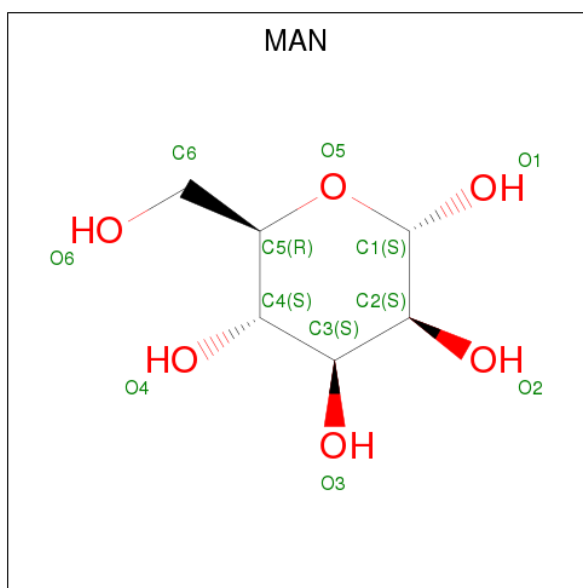
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		

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



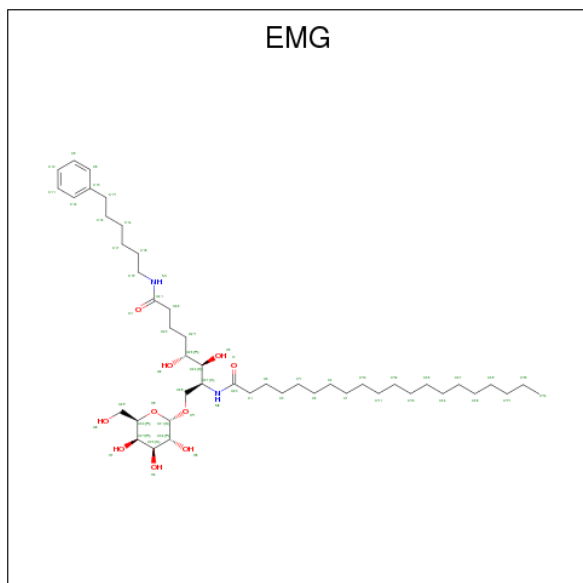
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



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		

- Molecule 7 is N-[(2S,3S,4R)-3,4-dihydroxy-8-oxo-8-[(6-phenylhexyl)amino]-1-{[(2S,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-2-yl]oxy}octan-2-yl]icosanamide (three-letter code: EMG) (formula: C<sub>46</sub>H<sub>82</sub>N<sub>2</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			58	46	2	10		

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Na	0	0
			1	1		
8	A	1	Total	Na	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	84	Total	O	0	0
			84	84		

*Continued on next page...*

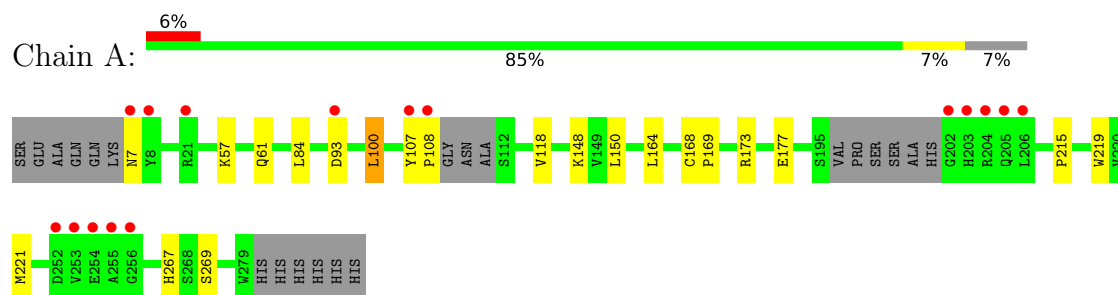
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	33	Total	O	0	0
			33	33		

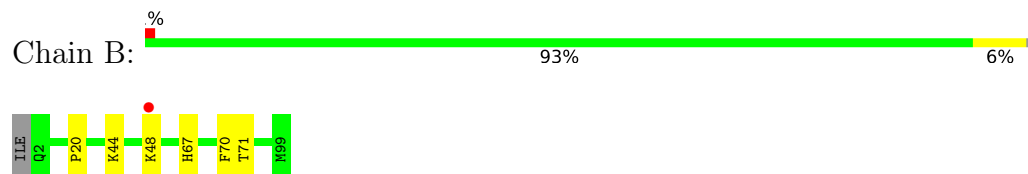
### 3 Residue-property plots

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: Antigen-presenting glycoprotein CD1d1



- Molecule 2: Beta-2-microglobulin





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.52Å 98.34Å 55.31Å 90.00° 106.25° 90.00°	Depositor
Resolution (Å)	36.10 – 2.08 36.08 – 2.08	Depositor EDS
% Data completeness (in resolution range)	94.0 (36.10-2.08) 94.1 (36.08-2.08)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.200 , 0.241 0.207 , 0.245	Depositor DCC
$R_{free}$ test set	929 reflections (3.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 37.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3220	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% 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: EMG, BMA, NAG, NA, FUC, 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	0.49	0/2195	0.66	0/2980
2	B	0.46	0/836	0.68	0/1133
All	All	0.48	0/3031	0.67	0/4113

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	2134	0	2040	8	0
2	B	810	0	783	2	0
3	A	56	0	49	0	0
4	A	10	0	10	0	0
5	A	11	0	8	0	0
6	A	22	0	20	0	0
7	A	58	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	84	0	0	1	0
9	B	33	0	0	1	0
All	All	3220	0	2910	10	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 2.

All (10) 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:168:CYS:HB3	1:A:169:PRO:HD3	1.89	0.54
1:A:57:LYS:NZ	1:A:177:GLU:OE2	2.37	0.53
1:A:215:PRO:O	1:A:267:HIS:HE1	1.94	0.50
1:A:100:LEU:HG	1:A:118:VAL:HG22	1.94	0.49
2:B:20:PRO:HA	2:B:71:THR:HG22	1.96	0.47
1:A:267:HIS:HD2	1:A:269:SER:OG	2.01	0.44
1:A:219:TRP:CZ2	1:A:221:MET:HG3	2.55	0.41
2:B:67:HIS:HD2	9:B:203:HOH:O	2.02	0.41
1:A:173:ARG:NH2	9:A:401:HOH:O	2.54	0.40
1:A:107:TYR:HB3	1:A:108:PRO:HD2	2.04	0.40

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	258/285 (90%)	254 (98%)	4 (2%)	0	100	100
2	B	96/99 (97%)	92 (96%)	4 (4%)	0	100	100
All	All	354/384 (92%)	346 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	232/249 (93%)	224 (97%)	8 (3%)	40	40
2	B	92/93 (99%)	89 (97%)	3 (3%)	41	42
All	All	324/342 (95%)	313 (97%)	11 (3%)	40	40

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	61	GLN
1	A	84	LEU
1	A	93	ASP
1	A	100	LEU
1	A	148	LYS
1	A	150	LEU
1	A	164	LEU
2	B	44	LYS
2	B	48	LYS
2	B	70	PHE

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	117	HIS
1	A	229	GLN
1	A	267	HIS
2	B	67	HIS

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	301	1	14,14,15	0.50	0	17,19,21	1.58	2 (11%)
3	NAG	A	302	1	14,14,15	0.34	0	17,19,21	1.19	1 (5%)
3	NAG	A	303	1,3,4	14,14,15	0.42	0	17,19,21	1.33	3 (17%)
3	NAG	A	304	3,5	14,14,15	0.39	0	17,19,21	1.08	1 (5%)
4	FUC	A	305	3	9,10,11	0.53	0	13,14,16	1.01	0
5	BMA	A	306	3,6	11,11,12	0.55	0	15,15,17	0.84	0
6	MAN	A	307	5	11,11,12	0.43	0	15,15,17	1.11	1 (6%)
6	MAN	A	308	5	11,11,12	0.36	0	15,15,17	1.05	1 (6%)
7	EMG	A	309	-	59,59,59	0.94	4 (6%)	66,71,71	1.46	10 (15%)

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	301	1	-	0/6/23/26	0/1/1/1
3	NAG	A	302	1	-	0/6/23/26	0/1/1/1
3	NAG	A	303	1,3,4	-	0/6/23/26	0/1/1/1
3	NAG	A	304	3,5	-	0/6/23/26	0/1/1/1
4	FUC	A	305	3	-	0/0/17/20	0/1/1/1
5	BMA	A	306	3,6	-	0/2/19/22	0/1/1/1
6	MAN	A	307	5	-	0/2/19/22	0/1/1/1
6	MAN	A	308	5	-	0/2/19/22	0/1/1/1
7	EMG	A	309	-	-	0/54/74/74	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	309	EMG	C34-C33	2.28	1.58	1.52
7	A	309	EMG	C27-N2	2.30	1.50	1.46
7	A	309	EMG	C1-C20	3.02	1.57	1.51
7	A	309	EMG	O4-C31	3.12	1.45	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	309	EMG	C23-C22-C21	-3.40	103.86	113.30
7	A	309	EMG	C16-C15-C14	-2.97	101.98	113.75
3	A	303	NAG	O5-C1-C2	-2.94	107.46	111.52
7	A	309	EMG	O8-C29-C30	-2.61	102.17	111.29
3	A	302	NAG	C3-C4-C5	-2.47	105.83	110.24
7	A	309	EMG	C24-C23-C22	-2.39	106.67	113.17
7	A	309	EMG	C23-C24-C25	-2.22	110.48	114.20
7	A	309	EMG	C18-C19-N1	-2.13	106.00	112.19
7	A	309	EMG	C2-C3-C4	-2.08	103.14	114.41
3	A	304	NAG	C3-C4-C5	2.01	113.83	110.24
3	A	303	NAG	C1-C2-N2	2.25	114.33	110.49
7	A	309	EMG	O9-C31-O4	2.36	115.54	109.96
3	A	303	NAG	O5-C5-C6	2.43	110.99	107.15
6	A	307	MAN	C1-O5-C5	2.68	115.87	112.19
6	A	308	MAN	C1-O5-C5	2.84	116.09	112.19
3	A	301	NAG	C1-O5-C5	3.17	116.56	112.19
7	A	309	EMG	C34-C33-C32	3.19	116.41	110.83
3	A	301	NAG	C4-C3-C2	4.11	117.04	111.02
7	A	309	EMG	C28-O4-C31	4.77	123.37	113.80

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	264/285 (92%)	0.24	16 (6%) 21 25	24, 36, 67, 100	0
2	B	98/99 (98%)	-0.06	1 (1%) 82 85	25, 36, 52, 58	0
All	All	362/384 (94%)	0.16	17 (4%) 31 36	24, 36, 61, 100	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	HIS	6.1
1	A	255	ALA	4.4
1	A	256	GLY	4.1
1	A	202	GLY	4.0
1	A	204	ARG	3.8
1	A	253	VAL	3.3
1	A	107	TYR	2.9
1	A	108	PRO	2.9
1	A	252	ASP	2.8
1	A	7	ASN	2.7
1	A	205	GLN	2.6
1	A	206	LEU	2.6
1	A	21	ARG	2.5
1	A	254	GLU	2.4
1	A	8	TYR	2.4
2	B	48	LYS	2.3
1	A	93	ASP	2.1

### 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
6	MAN	A	307	11/12	0.75	0.25	61,64,70,70	0
7	EMG	A	309	58/58	0.79	0.23	54,67,76,79	0
3	NAG	A	301	14/15	0.86	0.34	63,69,72,73	0
5	BMA	A	306	11/12	0.87	0.12	43,45,51,56	0
6	MAN	A	308	11/12	0.90	0.13	45,46,51,52	0
8	NA	B	101	1/1	0.91	0.09	46,46,46,46	0
3	NAG	A	302	14/15	0.92	0.11	40,42,47,49	0
4	FUC	A	305	10/11	0.93	0.10	35,36,37,38	0
3	NAG	A	303	14/15	0.95	0.09	29,30,33,35	0
3	NAG	A	304	14/15	0.95	0.09	33,37,40,41	0
8	NA	A	310	1/1	0.98	0.10	36,36,36,36	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.