



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 06:19 PM BST

PDB ID : 5GS6  
Title : Full-length NS1 structure of Zika virus from 2015 Brazil strain  
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Deposited on : 2016-08-14  
Resolution : 2.85 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

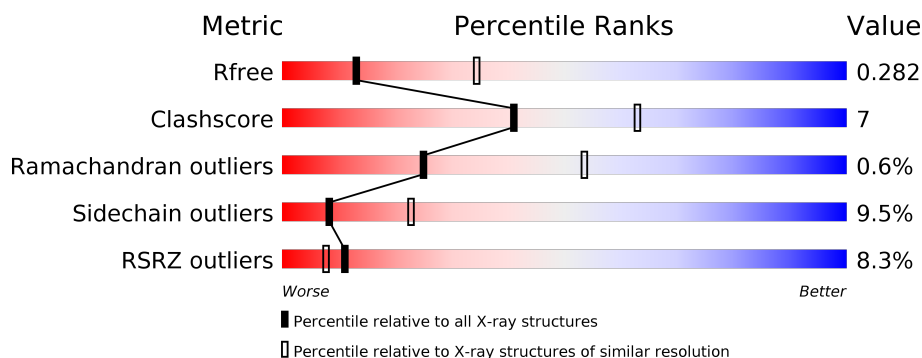
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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))
$R_{free}$	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 respectively. 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	357	<div> <div>%</div> <div> <div>78%</div> <div>18%</div> <div>..</div> </div> </div>
1	B	357	<div> <div>15%</div> <div>78%</div> <div>17%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5623 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 NS1 of Zika virus from 2015 Brazil strain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2812	1771	503	518	20			
1	B	349	Total	C	N	O	S	0	0	0
			2783	1746	505	512	20			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

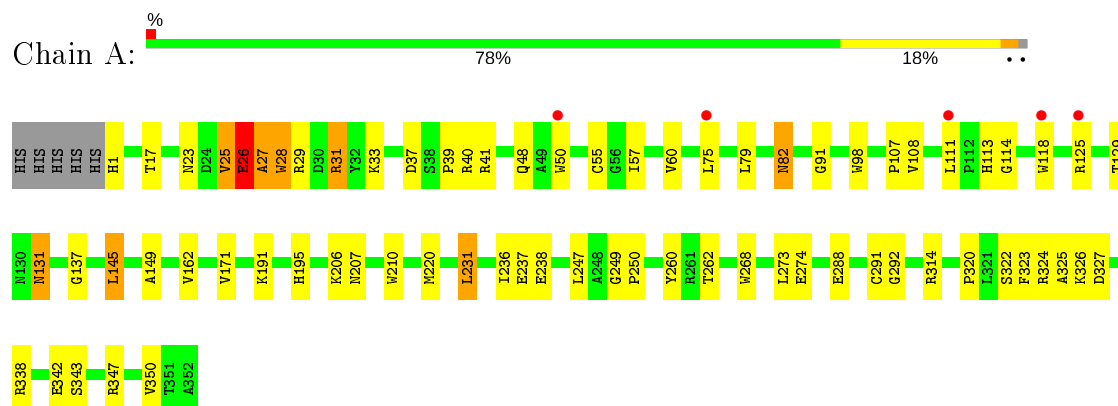


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

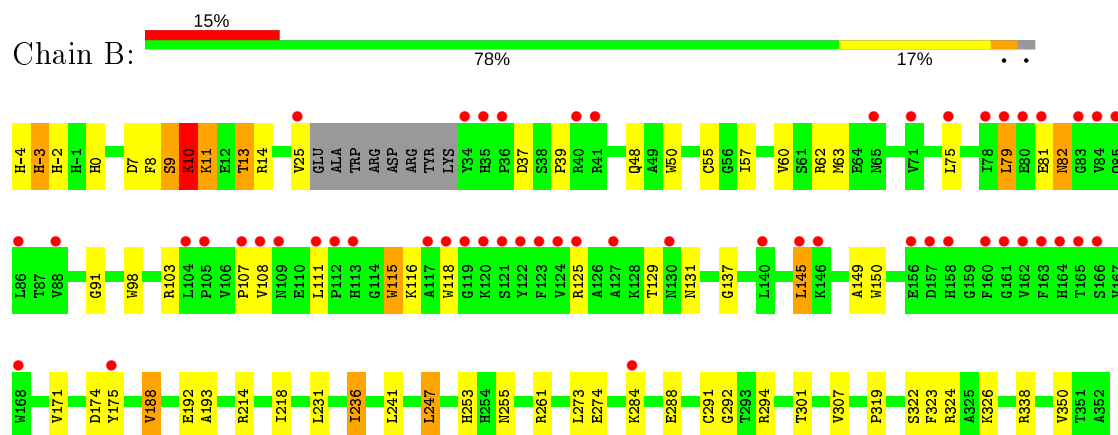
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: NS1 of Zika virus from 2015 Brazil strain



- Molecule 1: NS1 of Zika virus from 2015 Brazil strain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.95Å 96.95Å 270.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.47 – 2.85 48.47 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.47-2.85) 95.5 (48.47-2.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.244 , 0.284 0.247 , 0.282	Depositor DCC
$R_{free}$ test set	1563 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.2	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 50.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5623	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: 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	0.25	0/2890	0.45	1/3919 (0.0%)
1	B	0.30	0/2861	0.55	2/3879 (0.1%)
All	All	0.27	0/5751	0.50	3/7798 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	10	LYS	N-CA-CB	-13.14	86.95	110.60
1	B	62	ARG	CB-CA-C	-6.96	96.48	110.40
1	A	31	ARG	N-CA-C	5.49	125.81	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	2812	0	2714	31	1
1	B	2783	0	2676	49	2
2	A	14	0	13	1	0
2	B	14	0	13	1	0
All	All	5623	0	5416	78	2

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 7.

All (78) 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:B:10:LYS:O	1:B:11:LYS:HG3	1.20	1.34
1:B:7:ASP:OD1	1:B:10:LYS:CE	1.85	1.24
1:B:10:LYS:O	1:B:11:LYS:CG	1.93	1.16
1:B:7:ASP:OD1	1:B:10:LYS:HE2	1.58	1.03
1:B:7:ASP:OD1	1:B:10:LYS:HE3	1.70	0.91
1:B:7:ASP:OD1	1:B:10:LYS:CD	2.32	0.77
1:B:10:LYS:C	1:B:11:LYS:CG	2.53	0.73
1:A:107:PRO:O	1:A:108:VAL:HG12	1.89	0.73
1:B:288:GLU:OE2	1:B:338:ARG:NH2	2.23	0.72
1:B:39:PRO:HD2	1:B:116:LYS:O	1.91	0.70
1:B:107:PRO:O	1:B:108:VAL:HG12	1.92	0.69
1:B:39:PRO:CD	1:B:116:LYS:O	2.41	0.69
1:B:98:TRP:HB3	1:B:145:LEU:HD11	1.78	0.65
1:B:322:SER:OG	1:B:324:ARG:NH1	2.33	0.61
1:B:81:GLU:OE1	1:B:115:TRP:HZ3	1.84	0.60
1:A:207:ASN:OD1	2:A:601:NAG:N2	2.34	0.59
1:A:98:TRP:HB3	1:A:145:LEU:HD11	1.83	0.59
1:A:342:GLU:O	1:A:347:ARG:NH2	2.34	0.59
1:B:57:ILE:HD13	1:B:149:ALA:HB3	1.84	0.59
1:A:129:THR:HG22	1:A:131:ASN:H	1.67	0.59
1:B:301:THR:HG22	1:B:307:VAL:HG22	1.85	0.58
1:A:91:GLY:HA3	1:A:137:GLY:HA3	1.83	0.57
1:B:91:GLY:HA3	1:B:137:GLY:HA3	1.87	0.57
1:A:57:ILE:HD13	1:A:149:ALA:HB3	1.88	0.56
1:B:188:VAL:HG13	1:B:193:ALA:HB2	1.87	0.56
1:B:103:ARG:HH11	1:B:175:TYR:HB2	1.69	0.56
1:A:195:HIS:CE1	1:A:231:LEU:HD12	2.41	0.55
1:B:108:VAL:HG13	1:B:108:VAL:O	2.04	0.55
1:B:103:ARG:HH21	1:B:150:TRP:HE3	1.55	0.54
1:B:7:ASP:OD1	1:B:10:LYS:HD2	2.08	0.54
1:A:82:ASN:HD21	1:A:113:HIS:H	1.56	0.53
1:B:81:GLU:OE2	1:B:115:TRP:CZ3	2.62	0.53
1:B:103:ARG:HD3	1:B:175:TYR:HB2	1.91	0.52
1:B:129:THR:HG22	1:B:131:ASN:H	1.73	0.52
1:A:322:SER:OG	1:A:324:ARG:NH1	2.42	0.51
1:A:288:GLU:OE2	1:A:338:ARG:NH2	2.43	0.51
1:B:39:PRO:HA	1:B:118:TRP:CZ2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:LYS:C	1:B:11:LYS:HG2	2.31	0.50
1:B:174:ASP:N	1:B:174:ASP:OD1	2.43	0.50
1:B:291:CYS:SG	1:B:292:GLY:N	2.85	0.50
1:B:319:PRO:HD2	2:B:601:NAG:H81	1.94	0.50
1:A:206:LYS:HD3	1:A:210:TRP:CD1	2.49	0.48
1:B:81:GLU:CD	1:B:115:TRP:HZ3	2.16	0.48
1:A:39:PRO:HA	1:A:118:TRP:CZ2	2.50	0.47
1:B:115:TRP:N	1:B:115:TRP:CE3	2.83	0.47
1:A:273:LEU:HD23	1:A:325:ALA:HB2	1.98	0.46
1:B:115:TRP:CD2	1:B:115:TRP:N	2.83	0.46
1:A:37:ASP:OD2	1:A:171:VAL:N	2.47	0.46
1:A:27:ALA:O	1:A:29:ARG:N	2.49	0.46
1:A:291:CYS:SG	1:A:292:GLY:N	2.89	0.45
1:B:82:ASN:N	1:B:82:ASN:OD1	2.50	0.45
1:A:260:TYR:OH	1:A:320:PRO:HA	2.17	0.45
1:B:273:LEU:HD22	1:B:323:PHE:HB3	1.97	0.45
1:B:241:LEU:HD22	1:B:255:ASN:HB3	1.98	0.44
1:A:191:LYS:HB3	1:A:206:LYS:HB3	2.00	0.44
1:B:247:LEU:HD22	1:B:247:LEU:HA	1.82	0.44
1:A:40:ARG:HD3	1:A:114:GLY:O	2.17	0.43
1:B:10:LYS:O	1:B:11:LYS:HG2	2.04	0.43
1:B:79:LEU:HD12	1:B:79:LEU:HA	1.87	0.43
1:B:103:ARG:HD3	1:B:175:TYR:CB	2.47	0.43
1:A:231:LEU:HG	1:B:231:LEU:HD23	2.00	0.42
1:A:273:LEU:HD22	1:A:323:PHE:HB3	2.00	0.42
1:B:236:ILE:HG12	1:B:253:HIS:CD2	2.54	0.42
1:A:162:VAL:HG11	1:B:14:ARG:NE	2.35	0.42
1:B:81:GLU:CD	1:B:115:TRP:CZ3	2.93	0.42
1:B:236:ILE:HG12	1:B:253:HIS:NE2	2.36	0.41
1:A:26:GLU:O	1:A:28:TRP:N	2.53	0.41
1:B:37:ASP:OD2	1:B:171:VAL:N	2.53	0.41
1:B:37:ASP:O	1:B:118:TRP:NE1	2.45	0.41
1:B:103:ARG:NH1	1:B:175:TYR:HB2	2.35	0.41
1:A:291:CYS:O	1:A:314:ARG:HD3	2.21	0.41
1:A:82:ASN:OD1	1:A:82:ASN:N	2.54	0.41
1:A:249:GLY:HA2	1:A:250:PRO:HD3	1.90	0.40
1:A:23:ASN:OD1	1:A:25:VAL:HB	2.22	0.40
1:A:274:GLU:HB3	1:A:324:ARG:HB2	2.03	0.40
1:A:220:MET:HE2	1:A:268:TRP:HE3	1.86	0.40
1:A:37:ASP:OD1	1:A:41:ARG:HD2	2.22	0.40
1:B:284:LYS:HB2	1:B:284:LYS:HE3	1.91	0.40



All (2) 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)
1:A:237:GLU:CB	1:B:261:ARG:NH2[5_1055]	1.97	0.23
1:B:-3:HIS:NE2	1:B:13:THR:CG2[8_885]	2.18	0.02

## 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	350/357 (98%)	315 (90%)	32 (9%)	3 (1%)	17	43
1	B	345/357 (97%)	316 (92%)	28 (8%)	1 (0%)	41	68
All	All	695/714 (97%)	631 (91%)	60 (9%)	4 (1%)	25	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	TRP
1	A	27	ALA
1	B	9	SER
1	A	26	GLU

### 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	305/312 (98%)	279 (92%)	26 (8%)	10	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	304/312 (97%)	272 (90%)	32 (10%)	7	18
All	All	609/624 (98%)	551 (90%)	58 (10%)	8	23

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	HIS
1	A	17	THR
1	A	25	VAL
1	A	26	GLU
1	A	31	ARG
1	A	33	LYS
1	A	48	GLN
1	A	50	TRP
1	A	55	CYS
1	A	60	VAL
1	A	75	LEU
1	A	79	LEU
1	A	82	ASN
1	A	111	LEU
1	A	125	ARG
1	A	131	ASN
1	A	145	LEU
1	A	231	LEU
1	A	236	ILE
1	A	238	GLU
1	A	247	LEU
1	A	262	THR
1	A	326	LYS
1	A	327	ASP
1	A	343	SER
1	A	350	VAL
1	B	-4	HIS
1	B	-3	HIS
1	B	-2	HIS
1	B	0	HIS
1	B	8	PHE
1	B	9	SER
1	B	10	LYS
1	B	11	LYS
1	B	13	THR
1	B	25	VAL

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Mol	Chain	Res	Type
1	B	48	GLN
1	B	50	TRP
1	B	55	CYS
1	B	60	VAL
1	B	63	MET
1	B	75	LEU
1	B	79	LEU
1	B	82	ASN
1	B	111	LEU
1	B	115	TRP
1	B	125	ARG
1	B	145	LEU
1	B	188	VAL
1	B	192	GLU
1	B	214	ARG
1	B	218	ILE
1	B	236	ILE
1	B	247	LEU
1	B	274	GLU
1	B	294	ARG
1	B	326	LYS
1	B	350	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

2 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	601	1	14,14,15	0.49	0	17,19,21	0.50	0
2	NAG	B	601	1	14,14,15	0.31	0	17,19,21	0.29	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	601	1	-	2/6/23/26	0/1/1/1
2	NAG	B	601	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	NAG	O5-C5-C6-O6
2	B	601	NAG	C4-C5-C6-O6
2	A	601	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAG	1	0
2	B	601	NAG	1	0

## 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	352/357 (98%)	0.28	5 (1%) 75 74	46, 72, 115, 162	0
1	B	349/357 (97%)	1.03	53 (15%) 2 1	48, 78, 187, 268	0
All	All	701/714 (98%)	0.66	58 (8%) 11 8	46, 74, 162, 268	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	161	GLY	18.3
1	B	157	ASP	18.3
1	B	119	GLY	18.3
1	B	162	VAL	12.6
1	B	160	PHE	10.7
1	B	118	TRP	8.1
1	B	109	ASN	7.0
1	B	120	LYS	6.9
1	B	158	HIS	6.3
1	B	163	PHE	5.8
1	B	156	GLU	5.6
1	B	124	VAL	5.4
1	B	166	SER	5.4
1	B	130	ASN	5.2
1	B	75	LEU	5.0
1	B	164	HIS	4.8
1	B	108	VAL	4.7
1	B	122	TYR	4.7
1	B	175	TYR	4.4
1	B	111	LEU	4.4
1	B	88	VAL	4.3
1	B	168	TRP	4.2
1	B	35	HIS	4.2
1	B	79	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	117	ALA	4.0
1	B	112	PRO	3.9
1	B	113	HIS	3.9
1	B	85	GLN	3.9
1	B	121	SER	3.6
1	B	84	VAL	3.6
1	B	165	THR	3.6
1	A	111	LEU	3.4
1	A	125	ARG	3.4
1	A	75	LEU	3.1
1	B	123	PHE	3.0
1	B	36	PRO	3.0
1	B	71	VAL	3.0
1	B	41	ARG	2.9
1	B	125	ARG	2.8
1	B	140	LEU	2.8
1	B	105	PRO	2.7
1	B	107	PRO	2.7
1	B	25	VAL	2.6
1	B	34	TYR	2.6
1	B	284	LYS	2.5
1	B	40	ARG	2.4
1	B	146	LYS	2.3
1	B	86	LEU	2.2
1	B	145	LEU	2.2
1	B	83	GLY	2.2
1	B	80	GLU	2.2
1	B	104	LEU	2.1
1	A	50	TRP	2.1
1	A	118	TRP	2.1
1	B	78	ILE	2.1
1	B	127	ALA	2.1
1	B	81	GLU	2.1
1	B	65	ASN	2.0

## 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 [i](#)

There are no monosaccharides 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
2	NAG	B	601	14/15	0.83	0.29	112,123,140,141	0
2	NAG	A	601	14/15	0.84	0.17	121,133,136,136	0

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

There are no such residues in this entry.