



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 01:41 PM BST

PDB ID : 6IUW  
Title : Crystal structure of influenza A virus H5 hemagglutinin globular head in complex with the Fab of antibody 3C11  
Authors : Wang, P.; Zuo, Y.; Sun, J.; Zhang, L.; Wang, X.  
Deposited on : 2018-11-30  
Resolution : 2.33 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

<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

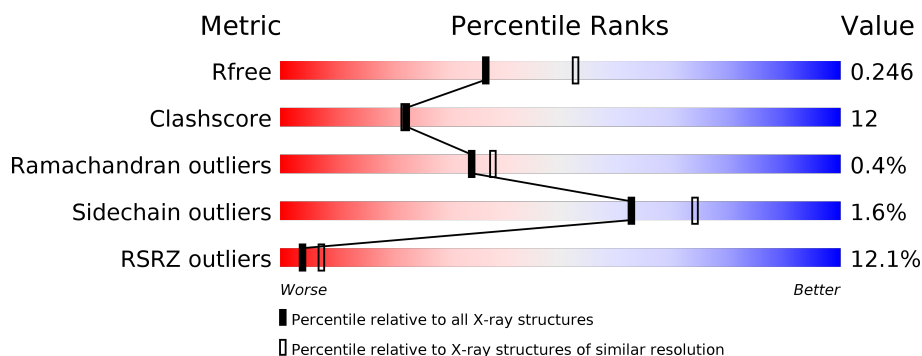
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.33 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.



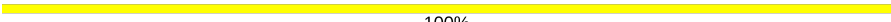

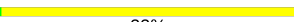
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	224	<div> <div>7%</div> <div>79%</div> <div>16%</div> <div>5%</div> </div>
1	B	224	<div> <div>13%</div> <div>73%</div> <div>21%</div> <div>5%</div> </div>
2	D	218	<div> <div>18%</div> <div>75%</div> <div>23%</div> <div>.</div> </div>
2	L	218	<div> <div>89%</div> <div>9%</div> <div>.</div> </div>
3	C	229	<div> <div>30%</div> <div>62%</div> <div>34%</div> <div>..</div> </div>
3	H	229	<div> <div>2%</div> <div>88%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
4	E	3	 100%
4	F	3	 67%  33%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10833 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1712	1095	292	319	6			
1	B	212	Total	C	N	O	S	0	0	0
			1704	1091	291	316	6			

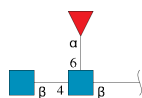
- Molecule 2 is a protein called 3C11 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	215	Total	C	N	O	S	0	0	0
			1656	1038	280	332	6			
2	D	215	Total	C	N	O	S	0	0	0
			1656	1038	280	332	6			

- Molecule 3 is a protein called 3C11 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	228	Total	C	N	O	S	0	0	0
			1723	1084	286	344	9			
3	C	224	Total	C	N	O	S	0	0	0
			1695	1067	281	339	8			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	3	Total	C	N	O	0	0	0
			38	22	2	14			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	3	Total	C	N	O	0	0	0
			38	22	2	14			


- Molecule 5 is water.

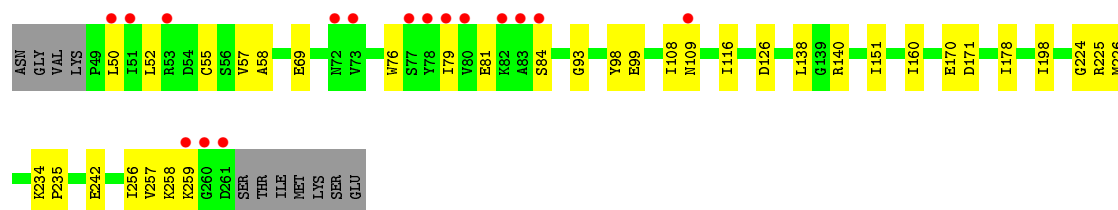
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	147	Total	O	0	0
			147	147		
5	L	172	Total	O	0	0
			172	172		
5	H	167	Total	O	0	0
			167	167		
5	B	34	Total	O	0	0
			34	34		
5	D	57	Total	O	0	0
			57	57		
5	C	34	Total	O	0	0
			34	34		

### 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.

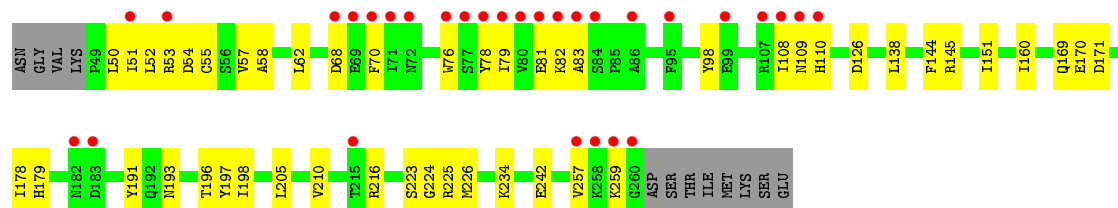
#### • Molecule 1: Hemagglutinin

Chain A: 



#### • Molecule 1: Hemagglutinin

Chain B: 




#### • Molecule 2: 3C11 Light Chain

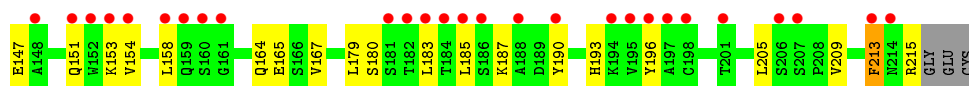
Chain L: 



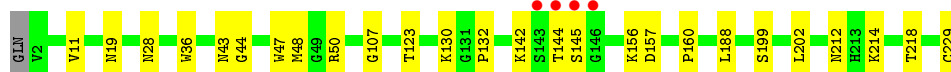
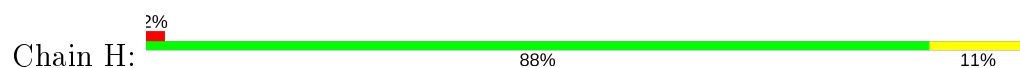
#### • Molecule 2: 3C11 Light Chain

Chain D: 

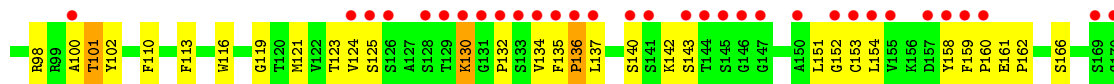




• Molecule 3: 3C11 Heavy Chain



• Molecule 3: 3C11 Heavy Chain



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.78 Å   62.24 Å   127.83 Å 90.00°   117.21°   90.00°	Depositor
Resolution (Å)	43.24 – 2.33 45.38 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.4 (43.24-2.33) 99.5 (45.38-2.33)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.94 (at 2.34 Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.207 , 0.246 0.208 , 0.246	Depositor DCC
$R_{free}$ test set	3637 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.1	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10833	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.45% 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, FUC

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	0.48	0/1761	0.62	0/2397
1	B	0.40	0/1753	0.61	0/2386
2	D	0.42	0/1693	0.64	0/2301
2	L	0.51	0/1693	0.65	0/2301
3	C	0.45	0/1739	0.71	0/2370
3	H	0.52	0/1768	0.66	0/2409
All	All	0.46	0/10407	0.65	0/14164

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
3	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	161	GLU	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	1712	0	1659	21	0
1	B	1704	0	1655	37	0
2	D	1656	0	1614	80	0
2	L	1656	0	1614	18	0
3	C	1695	0	1626	93	0
3	H	1723	0	1656	18	0
4	E	38	0	34	0	0
4	F	38	0	34	0	0
5	A	147	0	0	2	3
5	B	34	0	0	4	0
5	C	34	0	0	4	0
5	D	57	0	0	10	0
5	H	167	0	0	7	2
5	L	172	0	0	9	1
All	All	10833	0	9892	233	4

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 12.

The worst 5 of 233 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)
2:D:128:GLN:HG3	3:C:135:PHE:CZ	1.13	1.63
2:D:128:GLN:HG3	3:C:135:PHE:CE1	1.37	1.56
2:D:128:GLN:CG	3:C:135:PHE:CZ	1.96	1.46
2:D:128:GLN:HG3	3:C:135:PHE:CE2	1.68	1.29
2:D:128:GLN:CG	3:C:135:PHE:CE1	2.13	1.21

All (4) 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)
5:A:544:HOH:O	5:A:545:HOH:O[2_9410]	1.91	0.29
5:A:487:HOH:O	5:H:376:HOH:O[2_9510]	2.04	0.16
5:A:441:HOH:O	5:A:473:HOH:O[2_9510]	2.06	0.14
5:L:363:HOH:O	5:H:424:HOH:O[2_10410]	2.19	0.01

## 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	211/224 (94%)	201 (95%)	10 (5%)	0	100	100
1	B	210/224 (94%)	201 (96%)	9 (4%)	0	100	100
2	D	213/218 (98%)	208 (98%)	5 (2%)	0	100	100
2	L	213/218 (98%)	207 (97%)	6 (3%)	0	100	100
3	C	222/229 (97%)	212 (96%)	7 (3%)	3 (1%)	11	8
3	H	226/229 (99%)	217 (96%)	7 (3%)	2 (1%)	17	17
All	All	1295/1342 (96%)	1246 (96%)	44 (3%)	5 (0%)	34	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	144	THR
3	C	162	PRO
3	H	145	SER
3	C	85	SER
3	C	101	THR

### 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	190/200 (95%)	188 (99%)	2 (1%)	73	83
1	B	189/200 (94%)	187 (99%)	2 (1%)	73	83
2	D	189/191 (99%)	187 (99%)	2 (1%)	73	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	189/191 (99%)	186 (98%)	3 (2%)	62	74
3	C	191/196 (97%)	185 (97%)	6 (3%)	40	49
3	H	195/196 (100%)	192 (98%)	3 (2%)	65	76
All	All	1143/1174 (97%)	1125 (98%)	18 (2%)	62	74

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	55	CYS
1	B	205	LEU
3	C	130	LYS
3	H	142	LYS
3	H	199	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
2	L	203	GLN
2	D	151	GLN
3	C	28	ASN
3	C	213	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 ⓘ

6 monosaccharides 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	E	1	1,4	14,14,15	0.84	1 (7%)	17,19,21	0.64	0
4	NAG	E	2	4	14,14,15	1.03	1 (7%)	17,19,21	0.75	1 (5%)
4	FUC	E	3	4	10,10,11	0.87	0	14,14,16	1.49	2 (14%)
4	NAG	F	1	1,4	14,14,15	0.28	0	17,19,21	0.57	0
4	NAG	F	2	4	14,14,15	0.43	0	17,19,21	0.35	0
4	FUC	F	3	4	10,10,11	1.05	1 (10%)	14,14,16	1.04	1 (7%)

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	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	FUC	E	3	4	-	-	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	4/6/23/26	0/1/1/1
4	FUC	F	3	4	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2	NAG	O5-C1	-3.75	1.37	1.43
4	E	1	NAG	O5-C1	-3.05	1.38	1.43
4	F	3	FUC	C1-C2	2.56	1.58	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	3	FUC	C1-O5-C5	3.38	120.44	112.78
4	E	3	FUC	O5-C5-C4	3.04	114.97	109.52
4	E	2	NAG	C1-O5-C5	2.42	115.47	112.19
4	F	3	FUC	C1-C2-C3	2.27	112.46	109.67

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	2	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	F	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	213/224 (95%)	0.32	16 (7%) 14 21	18, 27, 65, 112	0
1	B	212/224 (94%)	0.60	30 (14%) 2 4	29, 46, 78, 101	0
2	D	215/218 (98%)	0.78	40 (18%) 1 2	28, 45, 107, 116	0
2	L	215/218 (98%)	-0.13	0 100 100	18, 27, 36, 44	0
3	C	224/229 (97%)	1.71	68 (30%) 0 0	30, 65, 107, 114	0
3	H	228/229 (99%)	-0.08	4 (1%) 68 76	17, 25, 43, 69	0
All	All	1307/1342 (97%)	0.53	158 (12%) 4 7	17, 36, 96, 116	0

The worst 5 of 158 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	146	GLY	11.3
3	C	145	SER	10.9
1	A	261	ASP	10.8
3	C	204	THR	9.0
3	C	220	VAL	9.0

### 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](#)

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	NAG	E	2	14/15	0.82	0.17	62,75,80,86	0
4	NAG	F	2	14/15	0.82	0.17	68,75,83,89	0
4	NAG	F	1	14/15	0.89	0.12	45,58,66,70	0
4	NAG	E	1	14/15	0.92	0.18	34,51,62,67	0
4	FUC	E	3	10/11	0.93	0.19	52,62,74,74	0
4	FUC	F	3	10/11	0.93	0.15	54,63,68,74	0

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.