



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 15, 2017 – 05:06 AM EST

PDB ID : 5T6S  
Title : Crystal structure of the A/Shanghai/2/2013 (H7N9) influenza virus hemagglutinin in complex with the antiviral drug arbidol  
Authors : Kadam, R.U.; Wilson, I.A.  
Deposited on : 2016-09-01  
Resolution : 2.36 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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-20028442

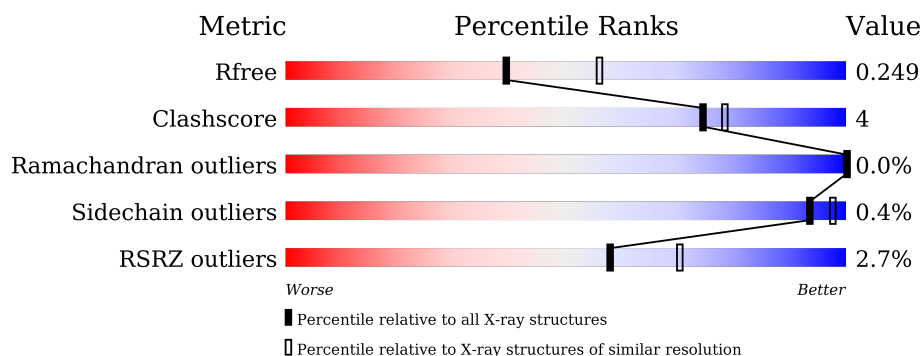
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.36 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))
$R_{free}$	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	321	<div> <div></div> <div>90% 9% .</div> </div>
1	C	321	<div> <div></div> <div>89% 9% .</div> </div>
1	E	321	<div> <div>%</div> <div>88% 10% .</div> </div>
1	G	321	<div> <div>8%</div> <div>83% 15% .</div> </div>
1	I	321	<div> <div>2%</div> <div>84% 14% .</div> </div>
1	K	321	<div> <div>4%</div> <div>88% 10% .</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	183	
2	D	183	
2	F	183	
2	H	183	
2	J	183	
2	L	183	

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	203	-	-	-	X
3	NAG	D	201	-	-	-	X
3	NAG	H	202	-	-	-	X
3	NAG	L	202	-	-	-	X
4	75U	B	202	-	-	-	X
4	75U	F	201	-	-	-	X
4	75U	H	201	-	-	-	X
4	75U	J	201	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24445 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 HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2411	1498	436	463	14			
1	C	316	Total	C	N	O	S	0	0	0
			2411	1498	436	463	14			
1	E	316	Total	C	N	O	S	0	0	0
			2411	1498	436	463	14			
1	G	316	Total	C	N	O	S	0	0	0
			2411	1498	436	463	14			
1	I	316	Total	C	N	O	S	0	0	0
			2411	1498	436	463	14			
1	K	316	Total	C	N	O	S	0	0	0
			2411	1498	436	463	14			

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	S	0	1	0
			1396	862	243	284	7			
2	D	171	Total	C	N	O	S	0	0	0
			1387	857	242	281	7			
2	F	171	Total	C	N	O	S	0	1	0
			1393	861	242	283	7			
2	H	171	Total	C	N	O	S	0	1	0
			1396	862	243	284	7			
2	J	171	Total	C	N	O	S	0	0	0
			1387	857	242	281	7			
2	L	171	Total	C	N	O	S	0	1	0
			1396	862	243	284	7			

There are 42 discrepancies between the modelled and reference sequences:

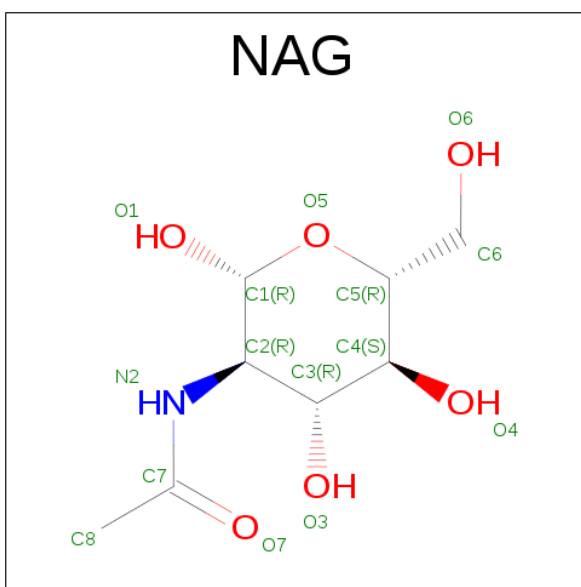
Chain	Residue	Modelled	Actual	Comment	Reference
B	177	SER	-	expression tag	UNP R4NN21

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Chain	Residue	Modelled	Actual	Comment	Reference
B	178	GLY	-	expression tag	UNP R4NN21
B	179	ARG	-	expression tag	UNP R4NN21
B	180	LEU	-	expression tag	UNP R4NN21
B	181	VAL	-	expression tag	UNP R4NN21
B	182	PRO	-	expression tag	UNP R4NN21
B	183	ARG	-	expression tag	UNP R4NN21
D	177	SER	-	expression tag	UNP R4NN21
D	178	GLY	-	expression tag	UNP R4NN21
D	179	ARG	-	expression tag	UNP R4NN21
D	180	LEU	-	expression tag	UNP R4NN21
D	181	VAL	-	expression tag	UNP R4NN21
D	182	PRO	-	expression tag	UNP R4NN21
D	183	ARG	-	expression tag	UNP R4NN21
F	177	SER	-	expression tag	UNP R4NN21
F	178	GLY	-	expression tag	UNP R4NN21
F	179	ARG	-	expression tag	UNP R4NN21
F	180	LEU	-	expression tag	UNP R4NN21
F	181	VAL	-	expression tag	UNP R4NN21
F	182	PRO	-	expression tag	UNP R4NN21
F	183	ARG	-	expression tag	UNP R4NN21
H	177	SER	-	expression tag	UNP R4NN21
H	178	GLY	-	expression tag	UNP R4NN21
H	179	ARG	-	expression tag	UNP R4NN21
H	180	LEU	-	expression tag	UNP R4NN21
H	181	VAL	-	expression tag	UNP R4NN21
H	182	PRO	-	expression tag	UNP R4NN21
H	183	ARG	-	expression tag	UNP R4NN21
J	177	SER	-	expression tag	UNP R4NN21
J	178	GLY	-	expression tag	UNP R4NN21
J	179	ARG	-	expression tag	UNP R4NN21
J	180	LEU	-	expression tag	UNP R4NN21
J	181	VAL	-	expression tag	UNP R4NN21
J	182	PRO	-	expression tag	UNP R4NN21
J	183	ARG	-	expression tag	UNP R4NN21
L	177	SER	-	expression tag	UNP R4NN21
L	178	GLY	-	expression tag	UNP R4NN21
L	179	ARG	-	expression tag	UNP R4NN21
L	180	LEU	-	expression tag	UNP R4NN21
L	181	VAL	-	expression tag	UNP R4NN21
L	182	PRO	-	expression tag	UNP R4NN21
L	183	ARG	-	expression tag	UNP R4NN21

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



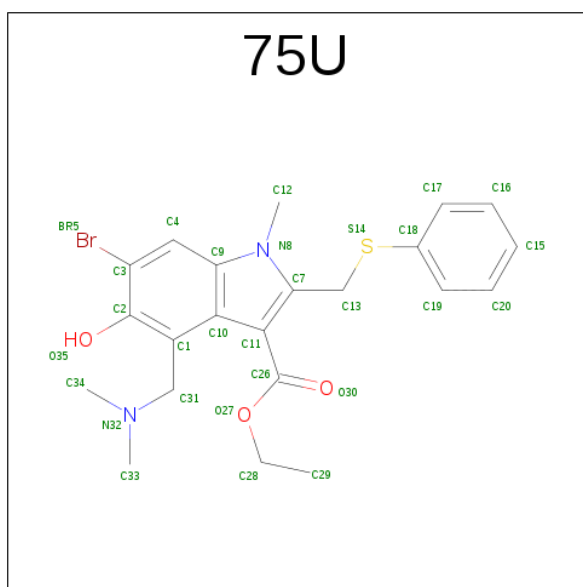
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	J	1	Total	C	N	O	0	0
			14	8	1	5		
3	J	1	Total	C	N	O	0	0
			14	8	1	5		
3	K	1	Total	C	N	O	0	0
			14	8	1	5		
3	K	1	Total	C	N	O	0	0
			14	8	1	5		
3	K	1	Total	C	N	O	0	0
			14	8	1	5		
3	L	1	Total	C	N	O	0	0
			14	8	1	5		
3	L	1	Total	C	N	O	0	0
			14	8	1	5		
3	L	1	Total	C	N	O	0	0
			14	8	1	5		

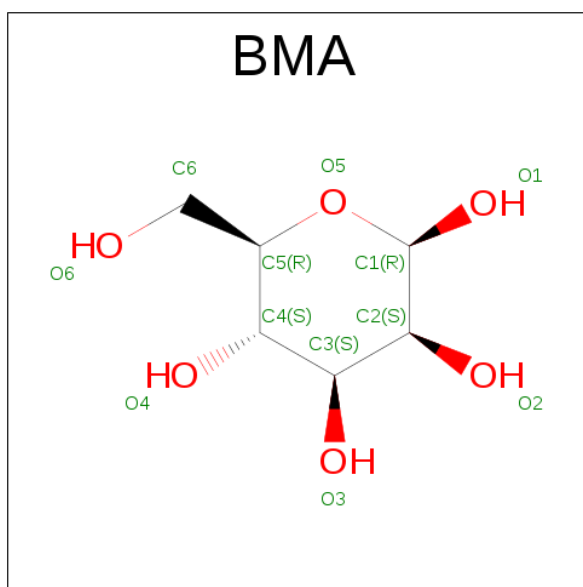
- Molecule 4 is ethyl 6-bromo-4-[(dimethylamino)methyl]-5-hydroxy-1-methyl-2-[(phenylsulfonyl)methyl]-1H-indole-3-carboxylate (three-letter code: 75U) (formula: C<sub>22</sub>H<sub>25</sub>BrN<sub>2</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	Br	C	N	O	S	0	0
			29	1	22	2	3	1		
4	B	1	Total	Br	C	N	O	S	0	0
			29	1	22	2	3	1		
4	F	1	Total	Br	C	N	O	S	0	0
			29	1	22	2	3	1		
4	H	1	Total	Br	C	N	O	S	0	0
			29	1	22	2	3	1		
4	J	1	Total	Br	C	N	O	S	0	0
			29	1	22	2	3	1		
4	L	1	Total	Br	C	N	O	S	0	0
			29	1	22	2	3	1		

- Molecule 5 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
5	C	1	Total	C	O	0	0
			11	6	5		
5	E	1	Total	C	O	0	0
			11	6	5		
5	I	1	Total	C	O	0	0
			11	6	5		
5	K	1	Total	C	O	0	0
			11	6	5		
5	L	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	1	Total	Na	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	116	Total	O	0	0
			116	116		
7	B	86	Total	O	0	0
			86	86		
7	C	142	Total	O	0	0
			142	142		

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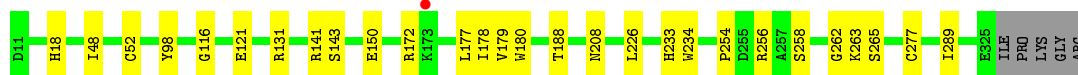
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	81	Total 81	O 81	0	0
7	E	143	Total 143	O 143	0	0
7	F	80	Total 80	O 80	0	0
7	G	33	Total 33	O 33	0	0
7	H	34	Total 34	O 34	0	0
7	I	90	Total 90	O 90	0	0
7	J	53	Total 53	O 53	0	0
7	K	59	Total 59	O 59	0	0
7	L	71	Total 71	O 71	0	0

### 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 errors 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.

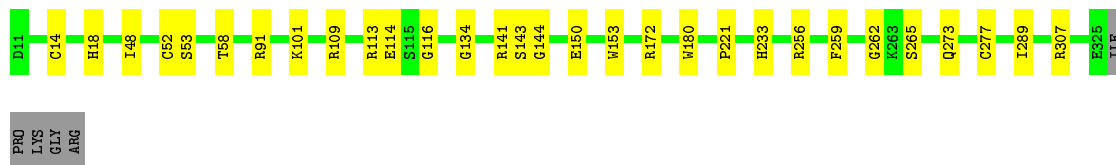
#### • Molecule 1: Hemagglutinin HA1

Chain A:  90% 9% .




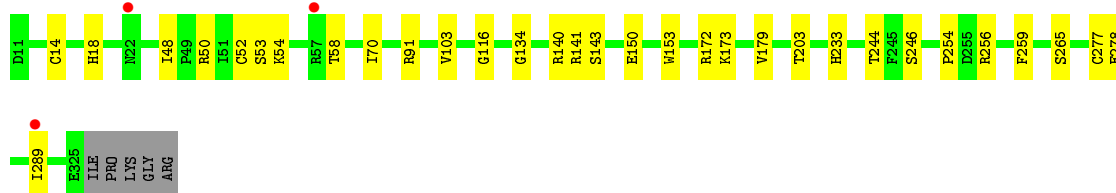
#### • Molecule 1: Hemagglutinin HA1

Chain C:  89% 9% .




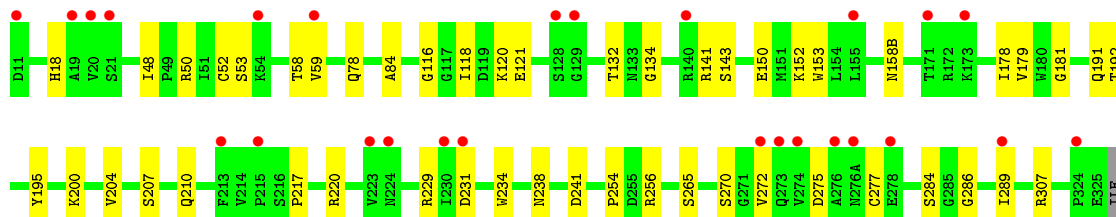
#### • Molecule 1: Hemagglutinin HA1

Chain E:  88% 10% .



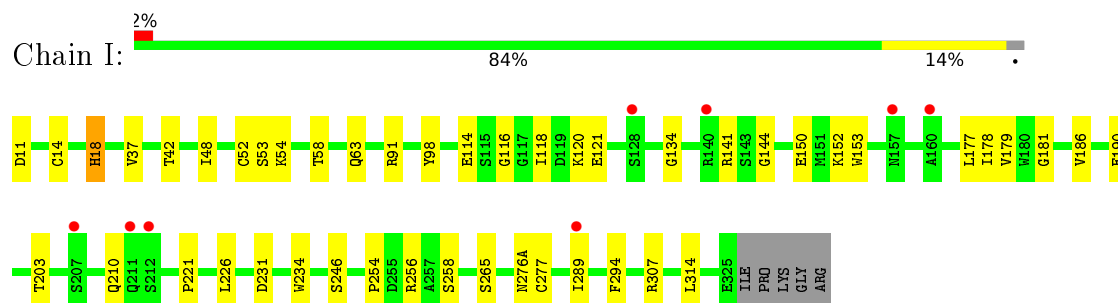
#### • Molecule 1: Hemagglutinin HA1

Chain G:  83% 15% .

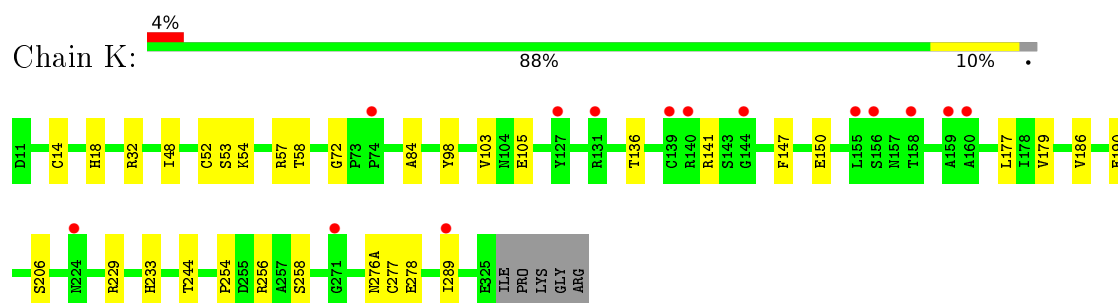


PRO  
LYS  
GLY  
ARG

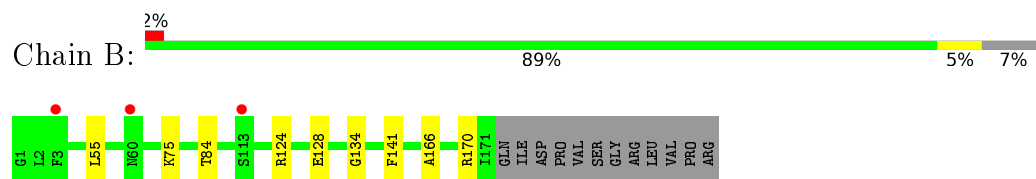
- Molecule 1: Hemagglutinin HA1



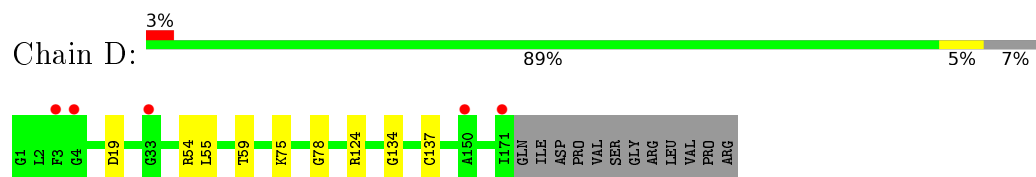
- Molecule 1: Hemagglutinin HA1



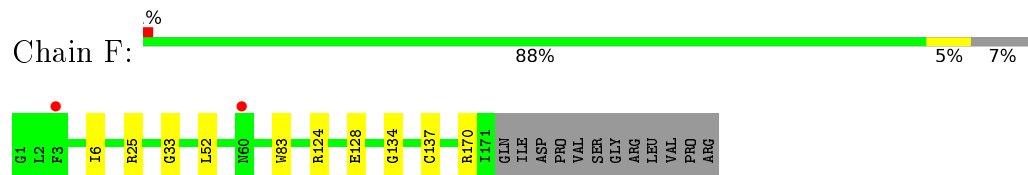
- Molecule 2: Hemagglutinin HA2



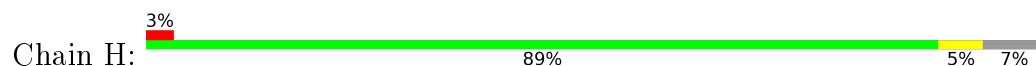
- Molecule 2: Hemagglutinin HA2

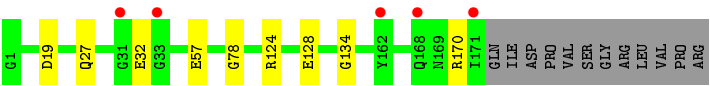


- Molecule 2: Hemagglutinin HA2

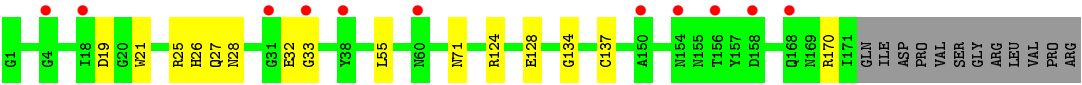
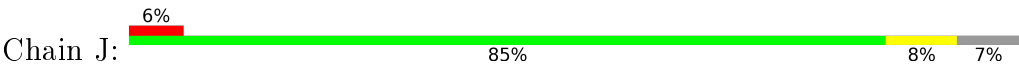


- Molecule 2: Hemagglutinin HA2

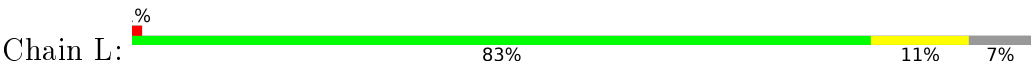




● Molecule 2: Hemagglutinin HA2



● Molecule 2: Hemagglutinin HA2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.42Å 231.49Å 127.85Å 90.00° 96.88° 90.00°	Depositor
Resolution (Å)	48.50 – 2.36 49.02 – 2.36	Depositor EDS
% Data completeness (in resolution range)	97.0 (48.50-2.36) 91.2 (49.02-2.36)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.37Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.204 , 0.250 0.201 , 0.249	Depositor DCC
$R_{free}$ test set	7159 reflections (4.94%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.9	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 33.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	24445	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.85% 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: NA, BMA, NAG, 75U

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	0.30	0/2457	0.53	0/3321
1	C	0.31	0/2457	0.54	0/3321
1	E	0.31	0/2457	0.53	0/3321
1	G	0.28	0/2457	0.50	0/3321
1	I	0.29	0/2457	0.51	0/3321
1	K	0.28	0/2457	0.49	0/3321
2	B	0.29	0/1420	0.49	0/1913
2	D	0.36	0/1411	0.50	0/1901
2	F	0.31	0/1420	0.49	0/1913
2	H	0.28	0/1420	0.46	0/1913
2	J	0.33	0/1411	0.48	0/1901
2	L	0.29	0/1420	0.48	0/1913
All	All	0.30	0/23244	0.51	0/31380

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 [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	2411	0	2368	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2411	0	2368	19	0
1	E	2411	0	2368	22	0
1	G	2411	0	2369	29	0
1	I	2411	0	2368	33	0
1	K	2411	0	2368	20	0
2	B	1396	0	1295	8	0
2	D	1387	0	1290	9	0
2	F	1393	0	1296	9	0
2	H	1396	0	1296	8	0
2	J	1387	0	1290	13	0
2	L	1396	0	1295	18	0
3	A	28	0	26	0	0
3	B	28	0	26	1	0
3	C	42	0	37	0	0
3	D	28	0	26	2	0
3	E	42	0	37	1	0
3	F	42	0	38	0	0
3	G	28	0	25	0	0
3	H	14	0	13	1	0
3	I	42	0	37	1	0
3	J	28	0	26	0	0
3	K	42	0	37	0	0
3	L	42	0	37	3	0
4	B	58	0	0	2	0
4	F	29	0	0	0	0
4	H	29	0	0	1	0
4	J	29	0	0	2	0
4	L	29	0	0	0	0
5	C	11	0	10	0	0
5	E	11	0	10	0	0
5	I	11	0	10	0	0
5	K	11	0	10	0	0
5	L	11	0	10	1	0
6	J	1	0	0	0	0
7	A	116	0	0	2	0
7	B	86	0	0	0	0
7	C	142	0	0	3	0
7	D	81	0	0	2	0
7	E	143	0	0	3	0
7	F	80	0	0	2	0
7	G	33	0	0	3	0
7	H	34	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	I	90	0	0	4	0
7	J	53	0	0	2	0
7	K	59	0	0	0	0
7	L	71	0	0	2	0
All	All	24445	0	22386	182	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 4.

The worst 5 of 182 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:F:6:ILE:O	7:F:301:HOH:O	2.03	0.76
1:G:231:ASP:OD1	1:I:210:GLN:NE2	2.19	0.74
2:D:134:GLY:HA2	2:F:124:ARG:HD3	1.70	0.71
2:D:19:ASP:OD2	7:D:301:HOH:O	2.14	0.65
2:L:128:GLU:HG3	2:L:170:ARG:HH12	1.63	0.62

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	314/321 (98%)	305 (97%)	9 (3%)	0	100	100
1	C	314/321 (98%)	305 (97%)	8 (2%)	1 (0%)	46	55
1	E	314/321 (98%)	305 (97%)	9 (3%)	0	100	100
1	G	314/321 (98%)	303 (96%)	11 (4%)	0	100	100
1	I	314/321 (98%)	305 (97%)	9 (3%)	0	100	100
1	K	314/321 (98%)	306 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	170/183 (93%)	164 (96%)	6 (4%)	0	100	100
2	D	169/183 (92%)	165 (98%)	4 (2%)	0	100	100
2	F	170/183 (93%)	165 (97%)	5 (3%)	0	100	100
2	H	170/183 (93%)	166 (98%)	4 (2%)	0	100	100
2	J	169/183 (92%)	165 (98%)	4 (2%)	0	100	100
2	L	170/183 (93%)	165 (97%)	5 (3%)	0	100	100
All	All	2902/3024 (96%)	2819 (97%)	82 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	262	GLY

### 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	264/269 (98%)	262 (99%)	2 (1%)	86	94
1	C	264/269 (98%)	263 (100%)	1 (0%)	93	97
1	E	264/269 (98%)	263 (100%)	1 (0%)	93	97
1	G	264/269 (98%)	262 (99%)	2 (1%)	86	94
1	I	264/269 (98%)	262 (99%)	2 (1%)	86	94
1	K	264/269 (98%)	263 (100%)	1 (0%)	93	97
2	B	147/157 (94%)	147 (100%)	0	100	100
2	D	146/157 (93%)	145 (99%)	1 (1%)	88	95
2	F	147/157 (94%)	146 (99%)	1 (1%)	88	95
2	H	147/157 (94%)	147 (100%)	0	100	100
2	J	146/157 (93%)	146 (100%)	0	100	100
2	L	147/157 (94%)	147 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2464/2556 (96%)	2453 (100%)	11 (0%)	93 97

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	18	HIS
2	F	52	LEU
1	I	18	HIS
2	D	59	THR
1	G	121	GLU

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

Mol	Chain	Res	Type
1	I	18	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 41 ligands modelled in this entry, 1 is monoatomic - leaving 40 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	401	1	14,14,15	0.20	0	15,19,21	0.39	0
3	NAG	A	402	1	14,14,15	0.34	0	15,19,21	0.33	0
4	75U	B	201	-	29,31,31	3.90	8 (27%)	30,44,44	1.80	8 (26%)
4	75U	B	202	-	29,31,31	3.57	8 (27%)	30,44,44	1.83	6 (20%)
3	NAG	B	203	2	14,14,15	0.55	0	15,19,21	0.47	0
3	NAG	B	204	2	14,14,15	0.29	0	15,19,21	0.36	0
3	NAG	C	401	1,3	14,14,15	0.27	0	15,19,21	0.58	1 (6%)
3	NAG	C	402	3,5	14,14,15	0.21	0	15,19,21	0.38	0
5	BMA	C	403	3	11,11,12	0.74	0	15,15,17	0.74	0
3	NAG	C	404	1	14,14,15	0.22	0	15,19,21	0.26	0
3	NAG	D	201	2	14,14,15	0.62	1 (7%)	15,19,21	0.58	0
3	NAG	D	202	2	14,14,15	0.16	0	15,19,21	0.32	0
3	NAG	E	401	1,3	14,14,15	0.25	0	15,19,21	0.36	0
3	NAG	E	402	3,5	14,14,15	0.24	0	15,19,21	0.46	0
5	BMA	E	403	3	11,11,12	0.81	0	15,15,17	0.73	0
3	NAG	E	404	1	14,14,15	0.28	0	15,19,21	0.36	0
4	75U	F	201	-	29,31,31	3.75	8 (27%)	30,44,44	1.57	6 (20%)
3	NAG	F	202	2	14,14,15	0.43	0	15,19,21	0.65	1 (6%)
3	NAG	F	203	3,2	14,14,15	0.20	0	15,19,21	0.29	0
3	NAG	F	204	3	14,14,15	0.15	0	15,19,21	0.31	0
3	NAG	G	401	1,3	14,14,15	0.27	0	15,19,21	0.38	0
3	NAG	G	402	3	14,14,15	0.26	0	15,19,21	0.42	0
4	75U	H	201	-	29,31,31	3.74	8 (27%)	30,44,44	1.85	6 (20%)
3	NAG	H	202	2	14,14,15	0.49	0	15,19,21	0.59	1 (6%)
3	NAG	I	401	1,3	14,14,15	0.48	0	15,19,21	0.36	0
3	NAG	I	402	3,5	14,14,15	0.27	0	15,19,21	0.45	0
5	BMA	I	403	3	11,11,12	0.69	0	15,15,17	0.74	0
3	NAG	I	404	1	14,14,15	0.14	0	15,19,21	0.47	0
4	75U	J	201	-	29,31,31	3.55	8 (27%)	30,44,44	1.68	7 (23%)
3	NAG	J	202	2	14,14,15	0.36	0	15,19,21	0.54	0
3	NAG	J	203	2	14,14,15	0.18	0	15,19,21	0.33	0
3	NAG	K	401	1,3	14,14,15	0.16	0	15,19,21	0.51	0
3	NAG	K	402	3,5	14,14,15	0.24	0	15,19,21	0.49	0
5	BMA	K	403	3	11,11,12	0.82	0	15,15,17	0.73	0
3	NAG	K	404	1	14,14,15	0.24	0	15,19,21	0.42	0
4	75U	L	201	-	29,31,31	3.78	8 (27%)	30,44,44	1.72	6 (20%)
3	NAG	L	202	2	14,14,15	0.51	0	15,19,21	0.70	1 (6%)
3	NAG	L	203	3,2	14,14,15	0.23	0	15,19,21	0.46	0
3	NAG	L	204	3,5	14,14,15	0.60	0	15,19,21	0.82	0
5	BMA	L	205	3	11,11,12	0.57	0	15,15,17	1.29	1 (6%)

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	401	1	-	0/6/23/26	0/1/1/1
3	NAG	A	402	1	-	0/6/23/26	0/1/1/1
4	75U	B	201	-	-	0/16/16/16	0/3/3/3
4	75U	B	202	-	-	0/16/16/16	0/3/3/3
3	NAG	B	203	2	-	0/6/23/26	0/1/1/1
3	NAG	B	204	2	-	0/6/23/26	0/1/1/1
3	NAG	C	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	402	3,5	-	0/6/23/26	0/1/1/1
5	BMA	C	403	3	-	0/2/19/22	0/1/1/1
3	NAG	C	404	1	-	0/6/23/26	0/1/1/1
3	NAG	D	201	2	-	0/6/23/26	0/1/1/1
3	NAG	D	202	2	-	0/6/23/26	0/1/1/1
3	NAG	E	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	402	3,5	-	0/6/23/26	0/1/1/1
5	BMA	E	403	3	-	0/2/19/22	0/1/1/1
3	NAG	E	404	1	-	0/6/23/26	0/1/1/1
4	75U	F	201	-	-	0/16/16/16	0/3/3/3
3	NAG	F	202	2	-	0/6/23/26	0/1/1/1
3	NAG	F	203	3,2	-	0/6/23/26	0/1/1/1
3	NAG	F	204	3	-	0/6/23/26	0/1/1/1
3	NAG	G	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	402	3	-	0/6/23/26	0/1/1/1
4	75U	H	201	-	-	0/16/16/16	0/3/3/3
3	NAG	H	202	2	-	0/6/23/26	0/1/1/1
3	NAG	I	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	402	3,5	-	0/6/23/26	0/1/1/1
5	BMA	I	403	3	-	0/2/19/22	0/1/1/1
3	NAG	I	404	1	-	0/6/23/26	0/1/1/1
4	75U	J	201	-	-	0/16/16/16	0/3/3/3
3	NAG	J	202	2	-	0/6/23/26	0/1/1/1
3	NAG	J	203	2	-	0/6/23/26	0/1/1/1
3	NAG	K	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	402	3,5	-	0/6/23/26	0/1/1/1
5	BMA	K	403	3	-	0/2/19/22	0/1/1/1
3	NAG	K	404	1	-	0/6/23/26	0/1/1/1
4	75U	L	201	-	-	0/16/16/16	0/3/3/3
3	NAG	L	202	2	-	0/6/23/26	0/1/1/1
3	NAG	L	203	3,2	-	0/6/23/26	0/1/1/1
3	NAG	L	204	3,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	L	205	3	-	0/2/19/22	0/1/1/1

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	201	75U	C31-C1	-17.03	1.39	1.51
4	L	201	75U	C31-C1	-16.10	1.39	1.51
4	H	201	75U	C31-C1	-15.91	1.40	1.51
4	F	201	75U	C31-C1	-15.80	1.40	1.51
4	B	202	75U	C31-C1	-14.90	1.40	1.51

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	201	75U	C28-O27-C26	-5.28	104.91	116.46
4	L	201	75U	C28-O27-C26	-4.56	106.50	116.46
4	B	202	75U	C28-O27-C26	-4.55	106.52	116.46
4	F	201	75U	C28-O27-C26	-4.49	106.64	116.46
4	B	201	75U	C28-O27-C26	-4.30	107.06	116.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	201	75U	1	0
4	B	202	75U	1	0
3	B	203	NAG	1	0
3	D	201	NAG	2	0
3	E	401	NAG	1	0
3	E	402	NAG	1	0
4	H	201	75U	1	0
3	H	202	NAG	1	0
3	I	401	NAG	1	0
3	I	402	NAG	1	0
4	J	201	75U	2	0
3	L	202	NAG	2	0
3	L	204	NAG	1	0
5	L	205	BMA	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	316/321 (98%)	-0.17	1 (0%) 94 97	24, 39, 53, 73	0
1	C	316/321 (98%)	-0.17	0 100 100	24, 36, 57, 74	1 (0%)
1	E	316/321 (98%)	-0.03	3 (0%) 85 92	24, 38, 58, 73	1 (0%)
1	G	316/321 (98%)	0.56	26 (8%) 14 23	34, 58, 83, 103	0
1	I	316/321 (98%)	0.16	8 (2%) 61 73	29, 46, 75, 107	0
1	K	316/321 (98%)	0.21	14 (4%) 38 52	31, 51, 74, 118	0
2	B	171/183 (93%)	0.14	3 (1%) 71 81	25, 40, 58, 117	0
2	D	171/183 (93%)	0.27	5 (2%) 55 67	23, 39, 57, 73	0
2	F	171/183 (93%)	0.23	2 (1%) 81 89	25, 36, 58, 93	0
2	H	171/183 (93%)	0.40	5 (2%) 55 67	31, 53, 79, 104	0
2	J	171/183 (93%)	0.38	11 (6%) 23 34	28, 49, 74, 103	0
2	L	171/183 (93%)	0.18	2 (1%) 81 89	29, 40, 62, 87	0
All	All	2922/3024 (96%)	0.15	80 (2%) 58 70	23, 43, 72, 118	2 (0%)

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	224	ASN	4.3
1	K	289	ILE	4.1
1	G	140	ARG	4.0
1	G	155	LEU	3.9
1	G	289	ILE	3.7

### 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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(Å <sup>2</sup> )	Q<0.9
3	NAG	L	202	14/15	0.75	0.32	5.53	57,67,69,71	0
3	NAG	B	203	14/15	0.80	0.21	4.15	58,62,65,68	0
3	NAG	H	202	14/15	0.81	0.24	3.05	46,63,73,77	0
4	75U	J	201	29/29	0.80	0.24	3.03	54,73,88,105	0
4	75U	H	201	29/29	0.78	0.26	2.77	58,74,84,109	0
3	NAG	D	201	14/15	0.79	0.24	2.54	50,57,63,65	0
4	75U	B	202	29/29	0.82	0.25	2.38	51,61,75,98	0
4	75U	F	201	29/29	0.81	0.23	2.12	44,60,77,99	0
4	75U	L	201	29/29	0.84	0.23	1.92	48,61,75,94	0
3	NAG	J	202	14/15	0.81	0.20	1.59	59,66,69,70	0
4	75U	B	201	29/29	0.86	0.19	0.79	48,58,73,90	0
3	NAG	F	202	14/15	0.87	0.18	0.57	46,53,65,68	0
3	NAG	F	204	14/15	0.67	0.49	-	114,122,126,126	0
3	NAG	K	401	14/15	0.78	0.32	-	67,76,86,87	0
3	NAG	C	401	14/15	0.63	0.27	-	79,85,93,98	0
3	NAG	E	404	14/15	0.72	0.27	-	94,98,104,105	0
5	BMA	E	403	11/12	0.62	0.43	-	119,126,128,128	0
3	NAG	E	402	14/15	0.80	0.30	-	71,84,92,106	0
3	NAG	J	203	14/15	0.67	0.45	-	96,108,113,116	0
3	NAG	L	204	14/15	0.76	0.35	-	103,107,112,112	0
3	NAG	I	402	14/15	0.57	0.39	-	102,112,117,125	0
3	NAG	A	401	14/15	0.45	0.40	-	100,112,118,118	0
5	BMA	L	205	11/12	0.68	0.45	-	108,114,116,118	0
3	NAG	K	404	14/15	0.68	0.33	-	100,105,108,108	0
3	NAG	I	401	14/15	0.80	0.26	-	77,81,92,99	0
3	NAG	F	203	14/15	0.73	0.32	-	73,78,90,102	0
5	BMA	I	403	11/12	0.57	0.36	-	130,133,134,134	0
3	NAG	C	404	14/15	0.86	0.41	-	94,97,102,105	0
3	NAG	L	203	14/15	0.74	0.32	-	72,79,85,94	0
3	NAG	A	402	14/15	0.87	0.38	-	66,74,81,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	B	204	14/15	0.73	0.28	-	90,98,101,102	0
3	NAG	G	402	14/15	0.67	0.58	-	105,113,116,117	0
3	NAG	K	402	14/15	0.80	0.40	-	74,93,106,122	0
5	BMA	C	403	11/12	0.63	0.46	-	121,122,125,125	0
3	NAG	D	202	14/15	0.55	0.40	-	101,106,111,114	0
3	NAG	E	401	14/15	0.84	0.24	-	61,67,77,77	0
3	NAG	G	401	14/15	0.80	0.26	-	100,106,110,113	0
3	NAG	I	404	14/15	0.58	0.34	-	97,100,102,105	0
5	BMA	K	403	11/12	0.40	0.54	-	141,146,148,148	0
3	NAG	C	402	14/15	0.81	0.36	-	95,105,111,116	0
6	NA	J	204	1/1	0.94	0.56	-	56,56,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.