



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:47 PM GMT

PDB ID : 4FQM  
Title : Structure of B/Brisbane/60/2008 Influenza Hemagglutinin  
Authors : Dreyfus, C.; Laursen, N.S.; Wilson, I.A.  
Deposited on : 2012-06-25  
Resolution : 3.45 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

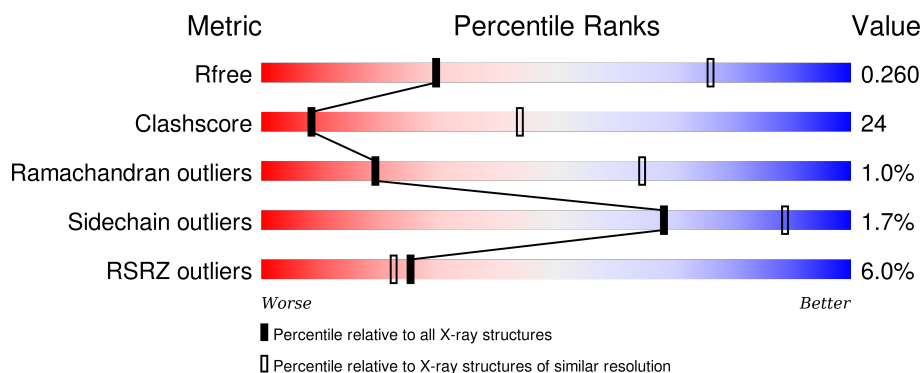
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.45 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	1000 (3.56-3.36)
Clashscore	102246	1090 (3.56-3.36)
Ramachandran outliers	100387	1057 (3.56-3.36)
Sidechain outliers	100360	1058 (3.56-3.36)
RSRZ outliers	91569	1005 (3.56-3.36)

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	347	<div> <div>5%</div> <div>61%</div> <div>36%</div> <div>..</div> </div>
1	C	347	<div> <div>3%</div> <div>61%</div> <div>36%</div> <div>..</div> </div>
1	E	347	<div> <div>3%</div> <div>65%</div> <div>32%</div> <div>..</div> </div>
1	G	347	<div> <div>3%</div> <div>64%</div> <div>32%</div> <div>..</div> </div>
1	I	347	<div> <div>3%</div> <div>66%</div> <div>31%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	347	
2	B	179	
2	D	179	
2	F	179	
2	H	179	
2	J	179	
2	L	179	

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	C	411	-	-	X	-
3	NAG	E	412	-	-	X	-
4	NAG	G	405	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24446 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	341	Total	C	N	O	S	0	0	0
			2588	1624	462	487	15			
1	C	341	Total	C	N	O	S	0	0	0
			2588	1624	462	487	15			
1	E	341	Total	C	N	O	S	0	0	0
			2588	1624	462	487	15			
1	G	341	Total	C	N	O	S	0	0	0
			2588	1624	462	487	15			
1	I	341	Total	C	N	O	S	0	0	0
			2588	1624	462	487	15			
1	K	341	Total	C	N	O	S	0	0	0
			2588	1624	462	487	15			

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	169	Total	C	N	O	S	0	0	0
			1282	801	218	257	6			
2	D	169	Total	C	N	O	S	0	0	0
			1282	801	218	257	6			
2	F	169	Total	C	N	O	S	0	0	0
			1282	801	218	257	6			
2	H	169	Total	C	N	O	S	0	0	0
			1282	801	218	257	6			
2	J	169	Total	C	N	O	S	0	0	0
			1282	801	218	257	6			
2	L	169	Total	C	N	O	S	0	0	0
			1282	801	218	257	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	524	SER	-	LINKER	UNP C0LT38

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Chain	Residue	Modelled	Actual	Comment	Reference
B	525	GLY	-	LINKER	UNP C0LT38
B	526	ARG	-	LINKER	UNP C0LT38
D	524	SER	-	LINKER	UNP C0LT38
D	525	GLY	-	LINKER	UNP C0LT38
D	526	ARG	-	LINKER	UNP C0LT38
F	524	SER	-	LINKER	UNP C0LT38
F	525	GLY	-	LINKER	UNP C0LT38
F	526	ARG	-	LINKER	UNP C0LT38
H	524	SER	-	LINKER	UNP C0LT38
H	525	GLY	-	LINKER	UNP C0LT38
H	526	ARG	-	LINKER	UNP C0LT38
J	524	SER	-	LINKER	UNP C0LT38
J	525	GLY	-	LINKER	UNP C0LT38
J	526	ARG	-	LINKER	UNP C0LT38
L	524	SER	-	LINKER	UNP C0LT38
L	525	GLY	-	LINKER	UNP C0LT38
L	526	ARG	-	LINKER	UNP C0LT38

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			39	22	2	15		
3	A	3	Total	C	N	O	0	0
			39	22	2	15		
3	A	3	Total	C	N	O	0	0
			39	22	2	15		
3	C	3	Total	C	N	O	0	0
			39	22	2	15		
3	C	3	Total	C	N	O	0	0
			39	22	2	15		
3	C	3	Total	C	N	O	0	0
			39	22	2	15		
3	E	3	Total	C	N	O	0	0
			39	22	2	15		
3	E	3	Total	C	N	O	0	0
			39	22	2	15		
3	E	3	Total	C	N	O	0	0
			39	22	2	15		
3	G	3	Total	C	N	O	0	0
			39	22	2	15		
3	G	3	Total	C	N	O	0	0
			39	22	2	15		

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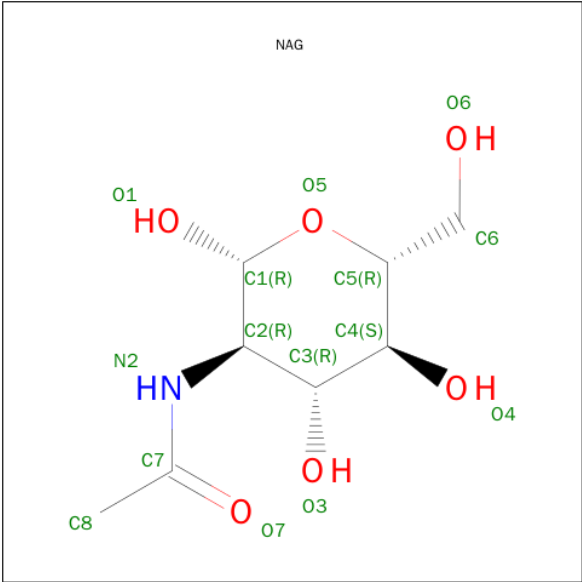
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	I	3	Total	C	N	O	0	0
			39	22	2	15		
3	I	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	C	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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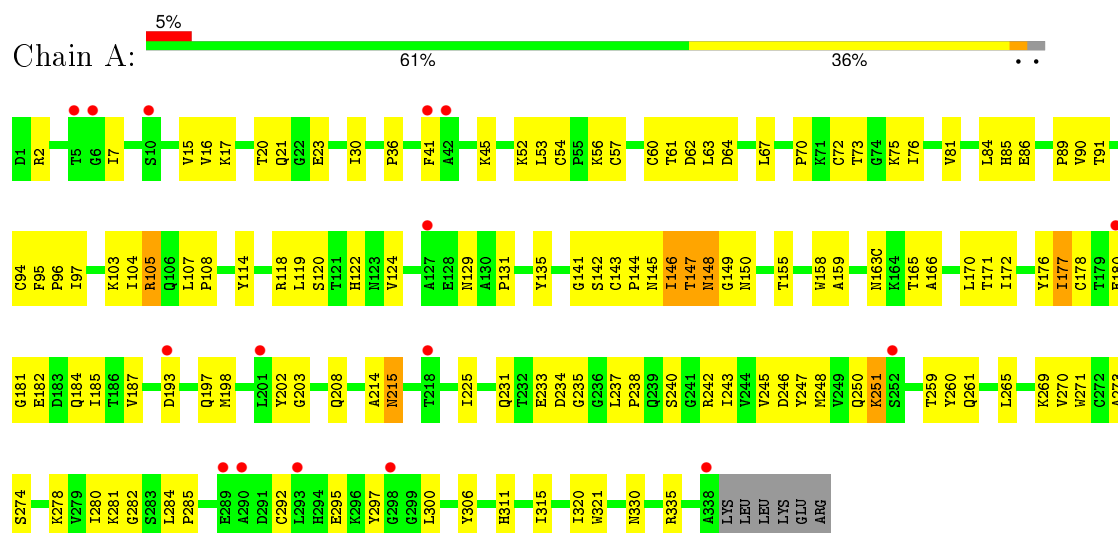
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1	Total	C	N	O	0	0
			14	8	1	5		



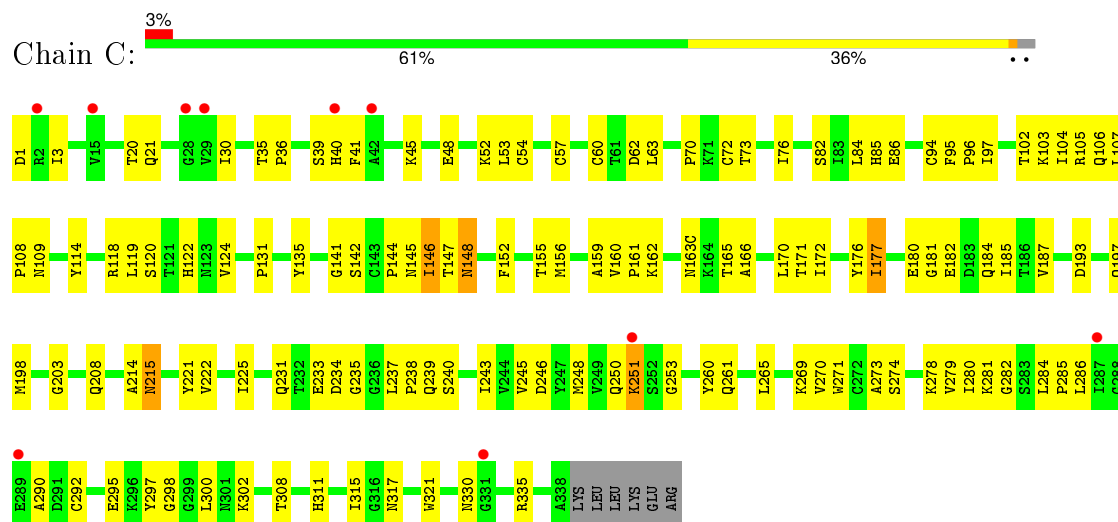
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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

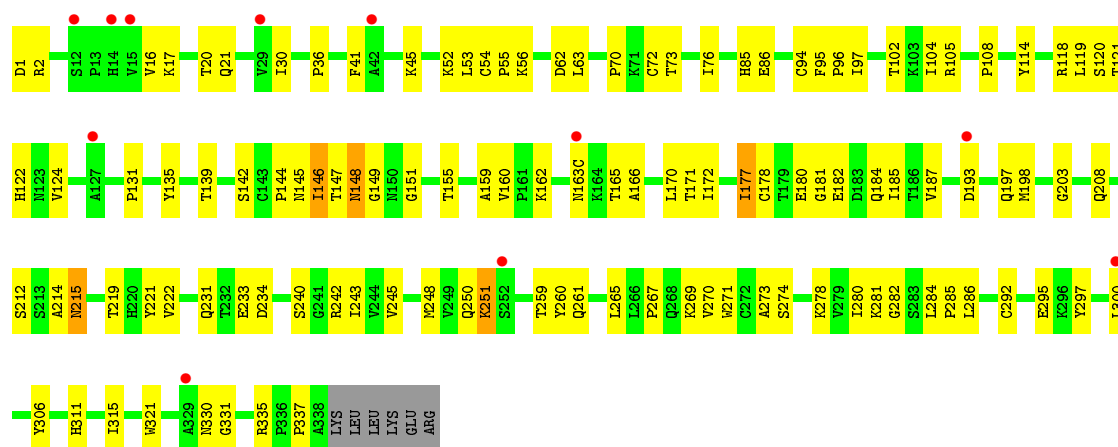


#### • Molecule 1: Hemagglutinin HA1

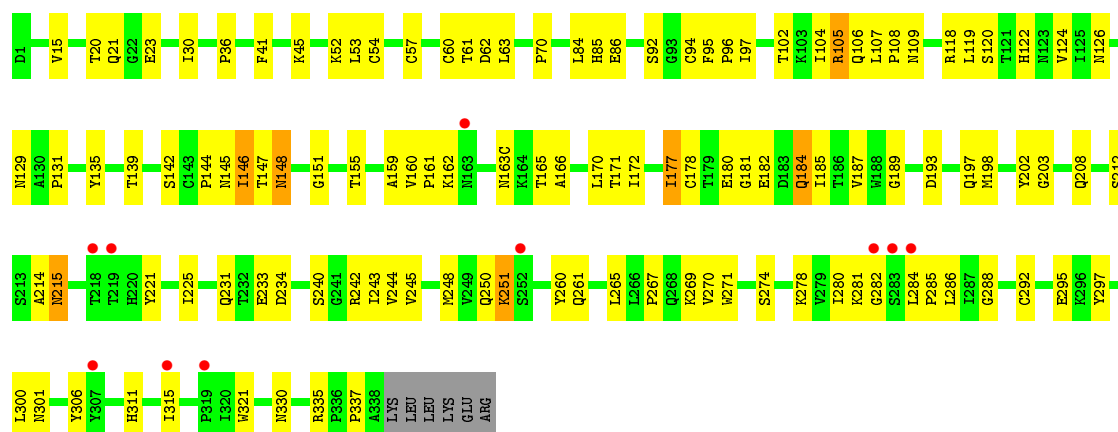


#### • Molecule 1: Hemagglutinin HA1

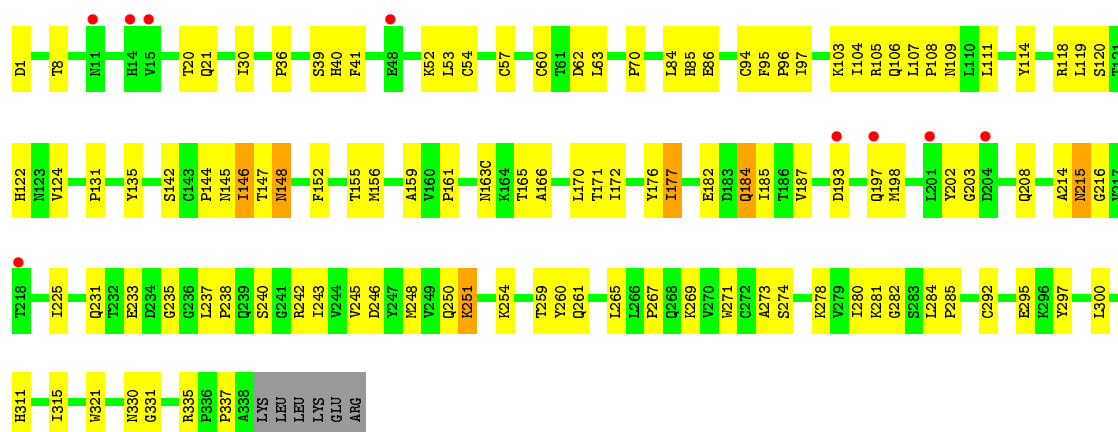




• Molecule 1: Hemagglutinin HA1

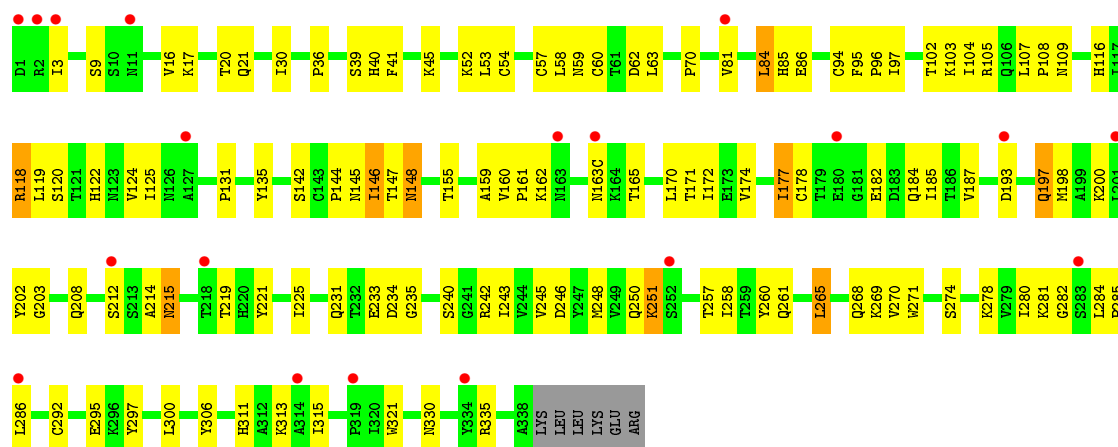


• Molecule 1: Hemagglutinin HA1



• Molecule 1: Hemagglutinin HA1





• Molecule 2: Hemagglutinin HA2



• Molecule 2: Hemagglutinin HA2

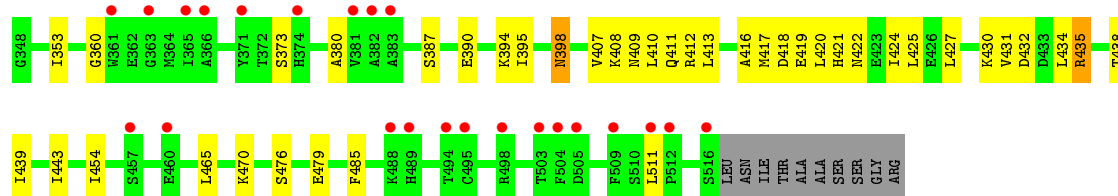


• Molecule 2: Hemagglutinin HA2

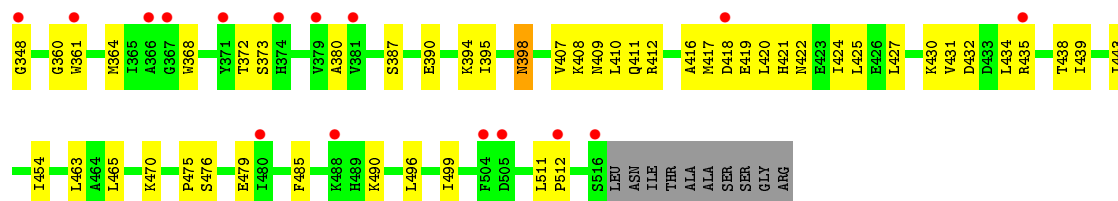


• Molecule 2: Hemagglutinin HA2

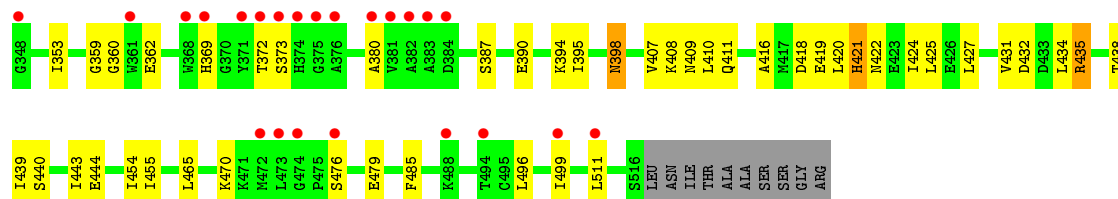




• Molecule 2: Hemagglutinin HA2



• Molecule 2: Hemagglutinin HA2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.69Å 242.54Å 135.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.07 – 3.45 49.07 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.07-3.45) 99.7 (49.07-3.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.23 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.257 , 0.268 0.249 , 0.260	Depositor DCC
$R_{free}$ test set	1922 reflections (3.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	82.4	Xtriage
Anisotropy	1.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 46.6	EDS
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 60738 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	24446	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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, 0.375 respectively for untwinned datasets, and 0.333, 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

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	0.64	0/2648	0.93	2/3598 (0.1%)
1	C	0.60	0/2648	0.79	0/3598
1	E	0.58	1/2648 (0.0%)	0.77	0/3598
1	G	0.55	0/2648	0.78	0/3598
1	I	0.56	1/2648 (0.0%)	0.75	0/3598
1	K	0.53	0/2648	0.75	1/3598 (0.0%)
2	B	0.43	0/1301	0.67	0/1753
2	D	0.44	0/1301	0.69	0/1753
2	F	0.44	0/1301	0.69	1/1753 (0.1%)
2	H	0.41	0/1301	0.66	1/1753 (0.1%)
2	J	0.40	0/1301	0.66	0/1753
2	L	0.40	0/1301	0.66	0/1753
All	All	0.53	2/23694 (0.0%)	0.76	5/32106 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	184	GLN	CD-NE2	-5.86	1.18	1.32
1	E	178	CYS	CB-SG	-5.04	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	LEU	CB-CG-CD2	-5.77	101.19	111.00
1	A	67	LEU	CB-CG-CD2	-5.74	101.25	111.00
2	H	413	LEU	CA-CB-CG	5.73	128.47	115.30
1	K	84	LEU	CA-CB-CG	5.63	128.25	115.30
2	F	413	LEU	CA-CB-CG	5.42	127.76	115.30

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	2588	0	2589	168	0
1	C	2588	0	2589	159	0
1	E	2588	0	2589	141	0
1	G	2588	0	2589	145	0
1	I	2588	0	2589	151	0
1	K	2588	0	2590	138	0
2	B	1282	0	1248	65	0
2	D	1282	0	1248	74	0
2	F	1282	0	1248	63	0
2	H	1282	0	1248	65	0
2	J	1282	0	1248	93	0
2	L	1282	0	1249	78	0
3	A	117	0	102	7	0
3	C	117	0	102	7	0
3	E	117	0	102	9	0
3	G	78	0	68	0	0
3	I	78	0	68	6	0
3	K	117	0	102	6	0
4	A	56	0	50	0	0
4	C	28	0	25	0	0
4	E	56	0	50	0	0
4	G	84	0	75	13	0
4	I	84	0	75	0	0
4	K	56	0	50	0	0
5	A	28	0	26	0	0
5	B	14	0	13	0	0
5	C	42	0	39	0	0
5	D	14	0	13	0	0
5	E	28	0	26	0	0
5	F	14	0	13	0	0
5	G	28	0	26	0	0
5	H	14	0	13	0	0
5	I	28	0	26	0	0
5	J	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	14	0	13	0	0
All	All	24446	0	24114	1165	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 24.

The worst 5 of 1165 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:C:214:ALA:HB2	1:C:248:MET:CE	1.32	1.54
2:J:435:ARG:NH1	2:L:434:LEU:HD21	1.22	1.49
1:E:214:ALA:HB2	1:E:248:MET:CE	1.49	1.40
1:G:214:ALA:HB2	1:G:248:MET:CE	1.59	1.32
1:I:214:ALA:HB2	1:I:248:MET:CE	1.60	1.29

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	339/347 (98%)	311 (92%)	22 (6%)	6 (2%)	11	51
1	C	339/347 (98%)	314 (93%)	20 (6%)	5 (2%)	13	54
1	E	339/347 (98%)	314 (93%)	20 (6%)	5 (2%)	13	54
1	G	339/347 (98%)	314 (93%)	20 (6%)	5 (2%)	13	54
1	I	339/347 (98%)	314 (93%)	21 (6%)	4 (1%)	16	60
1	K	339/347 (98%)	316 (93%)	18 (5%)	5 (2%)	13	54
2	B	167/179 (93%)	162 (97%)	5 (3%)	0	100	100
2	D	167/179 (93%)	162 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	167/179 (93%)	162 (97%)	4 (2%)	1 (1%)	30	74
2	H	167/179 (93%)	162 (97%)	5 (3%)	0	100	100
2	J	167/179 (93%)	162 (97%)	5 (3%)	0	100	100
2	L	167/179 (93%)	162 (97%)	5 (3%)	0	100	100
All	All	3036/3156 (96%)	2855 (94%)	150 (5%)	31 (1%)	19	64

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	ILE
1	A	251	LYS
1	C	177	ILE
1	C	251	LYS
1	E	177	ILE

### 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	288/294 (98%)	283 (98%)	5 (2%)	68	89
1	C	288/294 (98%)	285 (99%)	3 (1%)	82	93
1	E	288/294 (98%)	285 (99%)	3 (1%)	82	93
1	G	288/294 (98%)	280 (97%)	8 (3%)	51	82
1	I	288/294 (98%)	284 (99%)	4 (1%)	74	90
1	K	288/294 (98%)	282 (98%)	6 (2%)	61	86
2	B	136/143 (95%)	134 (98%)	2 (2%)	72	90
2	D	136/143 (95%)	134 (98%)	2 (2%)	72	90
2	F	136/143 (95%)	133 (98%)	3 (2%)	60	86
2	H	136/143 (95%)	134 (98%)	2 (2%)	72	90
2	J	136/143 (95%)	135 (99%)	1 (1%)	88	95
2	L	136/143 (95%)	133 (98%)	3 (2%)	60	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2544/2622 (97%)	2502 (98%)	42 (2%)	68 89

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	54	CYS
1	G	212	SER
1	K	265	LEU
1	G	105	ARG
1	G	184	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	126	ASN
1	G	129	ASN
1	I	184	GLN
1	C	231	GLN
1	E	268	GLN

### 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 ⓘ

74 carbohydrates 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
3	NAG	A	401	1,3	14,14,15	0.51	0	15,19,21	1.06	1 (6%)
3	NAG	A	402	3	14,14,15	0.47	0	15,19,21	0.85	1 (6%)
3	BMA	A	403	3	11,11,12	0.56	0	14,15,17	0.90	1 (7%)
4	NAG	A	404	1,4	14,14,15	0.38	0	15,19,21	1.86	2 (13%)
4	NAG	A	405	4	14,14,15	0.43	0	15,19,21	1.24	2 (13%)
4	NAG	A	406	1,4	14,14,15	0.37	0	15,19,21	2.01	1 (6%)
4	NAG	A	407	4	14,14,15	0.50	0	15,19,21	0.59	0
3	NAG	A	408	1,3	14,14,15	0.50	0	15,19,21	1.06	1 (6%)
3	NAG	A	409	3	14,14,15	0.46	0	15,19,21	0.84	1 (6%)
3	BMA	A	410	3	11,11,12	0.56	0	14,15,17	0.90	1 (7%)
3	NAG	A	412	1,3	14,14,15	0.50	0	15,19,21	1.53	3 (20%)
3	NAG	A	413	3	14,14,15	0.49	0	15,19,21	1.17	2 (13%)
3	BMA	A	414	3	11,11,12	0.62	0	14,15,17	1.45	3 (21%)
3	NAG	C	401	1,3	14,14,15	0.50	0	15,19,21	1.06	1 (6%)
3	NAG	C	402	3	14,14,15	0.47	0	15,19,21	0.84	1 (6%)
3	BMA	C	403	3	11,11,12	0.56	0	14,15,17	0.91	1 (7%)
4	NAG	C	405	1,4	14,14,15	0.36	0	15,19,21	2.02	1 (6%)
4	NAG	C	406	4	14,14,15	0.50	0	15,19,21	0.59	0
3	NAG	C	407	1,3	14,14,15	0.49	0	15,19,21	1.06	1 (6%)
3	NAG	C	408	3	14,14,15	0.47	0	15,19,21	0.84	1 (6%)
3	BMA	C	409	3	11,11,12	0.56	0	14,15,17	0.90	1 (7%)
3	NAG	C	411	1,3	14,14,15	0.49	0	15,19,21	1.53	4 (26%)
3	NAG	C	412	3	14,14,15	0.48	0	15,19,21	1.17	2 (13%)
3	BMA	C	413	3	11,11,12	0.61	0	14,15,17	1.45	3 (21%)
3	NAG	E	401	1,3	14,14,15	0.50	0	15,19,21	1.06	1 (6%)
3	NAG	E	402	3	14,14,15	0.45	0	15,19,21	0.84	1 (6%)
3	BMA	E	403	3	11,11,12	0.58	0	14,15,17	0.91	1 (7%)
4	NAG	E	404	1,4	14,14,15	0.38	0	15,19,21	1.85	2 (13%)
4	NAG	E	405	4	14,14,15	0.45	0	15,19,21	1.23	2 (13%)
4	NAG	E	406	1,4	14,14,15	0.37	0	15,19,21	2.02	1 (6%)
4	NAG	E	407	4	14,14,15	0.50	0	15,19,21	0.60	0
3	NAG	E	408	1,3	14,14,15	0.49	0	15,19,21	1.06	1 (6%)
3	NAG	E	409	3	14,14,15	0.45	0	15,19,21	0.84	1 (6%)
3	BMA	E	410	3	11,11,12	0.55	0	14,15,17	0.90	1 (7%)
3	NAG	E	412	1,3	14,14,15	0.51	0	15,19,21	1.53	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	E	413	3	14,14,15	0.48	0	15,19,21	1.17	2 (13%)
3	BMA	E	414	3	11,11,12	0.62	0	14,15,17	1.45	3 (21%)
3	NAG	G	401	1,3	14,14,15	0.50	0	15,19,21	1.06	1 (6%)
3	NAG	G	402	3	14,14,15	0.48	0	15,19,21	0.84	1 (6%)
3	BMA	G	403	3	11,11,12	0.55	0	14,15,17	0.90	1 (7%)
4	NAG	G	404	1,4	14,14,15	0.50	0	15,19,21	1.54	3 (20%)
4	NAG	G	405	4	14,14,15	0.49	0	15,19,21	1.18	2 (13%)
4	NAG	G	406	1,4	14,14,15	0.36	0	15,19,21	2.01	1 (6%)
4	NAG	G	407	4	14,14,15	0.50	0	15,19,21	0.59	0
3	NAG	G	408	1,3	14,14,15	0.49	0	15,19,21	1.07	1 (6%)
3	NAG	G	409	3	14,14,15	0.47	0	15,19,21	0.84	1 (6%)
3	BMA	G	410	3	11,11,12	0.57	0	14,15,17	0.90	1 (7%)
4	NAG	G	412	1,4	14,14,15	0.50	0	15,19,21	1.54	3 (20%)
4	NAG	G	413	4	14,14,15	0.49	0	15,19,21	1.17	2 (13%)
4	NAG	I	401	1,4	14,14,15	0.52	0	15,19,21	1.07	1 (6%)
4	NAG	I	402	4	14,14,15	0.47	0	15,19,21	0.85	1 (6%)
4	NAG	I	403	1,4	14,14,15	0.39	0	15,19,21	1.86	2 (13%)
4	NAG	I	404	4	14,14,15	0.44	0	15,19,21	1.23	2 (13%)
4	NAG	I	405	1,4	14,14,15	0.36	0	15,19,21	2.02	1 (6%)
4	NAG	I	406	4	14,14,15	0.50	0	15,19,21	0.59	0
3	NAG	I	407	1,3	14,14,15	0.49	0	15,19,21	1.06	1 (6%)
3	NAG	I	408	3	14,14,15	0.45	0	15,19,21	0.84	1 (6%)
3	BMA	I	409	3	11,11,12	0.56	0	14,15,17	0.90	1 (7%)
3	NAG	I	411	1,3	14,14,15	0.50	0	15,19,21	1.53	3 (20%)
3	NAG	I	412	3	14,14,15	0.49	0	15,19,21	1.18	2 (13%)
3	BMA	I	413	3	11,11,12	0.62	0	14,15,17	1.46	3 (21%)
3	NAG	K	401	1,3	14,14,15	0.50	0	15,19,21	1.06	1 (6%)
3	NAG	K	402	3	14,14,15	0.47	0	15,19,21	0.86	1 (6%)
3	BMA	K	403	3	11,11,12	0.56	0	14,15,17	0.90	1 (7%)
4	NAG	K	404	1,4	14,14,15	0.39	0	15,19,21	1.86	2 (13%)
4	NAG	K	405	4	14,14,15	0.45	0	15,19,21	1.24	2 (13%)
4	NAG	K	406	1,4	14,14,15	0.36	0	15,19,21	2.01	1 (6%)
4	NAG	K	407	4	14,14,15	0.51	0	15,19,21	0.59	0
3	NAG	K	408	1,3	14,14,15	0.51	0	15,19,21	1.06	1 (6%)
3	NAG	K	409	3	14,14,15	0.47	0	15,19,21	0.83	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BMA	K	410	3	11,11,12	0.56	0	14,15,17	0.90	1 (7%)
3	NAG	K	411	1,3	14,14,15	0.50	0	15,19,21	1.53	3 (20%)
3	NAG	K	412	3	14,14,15	0.48	0	15,19,21	1.17	2 (13%)
3	BMA	K	413	3	11,11,12	0.62	0	14,15,17	1.45	3 (21%)

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	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	402	3	-	0/6/23/26	0/1/1/1
3	BMA	A	403	3	-	0/2/19/22	0/1/1/1
4	NAG	A	404	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	405	4	-	0/6/23/26	0/1/1/1
4	NAG	A	406	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	407	4	-	0/6/23/26	0/1/1/1
3	NAG	A	408	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	409	3	-	0/6/23/26	0/1/1/1
3	BMA	A	410	3	-	0/2/19/22	0/1/1/1
3	NAG	A	412	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	413	3	-	0/6/23/26	0/1/1/1
3	BMA	A	414	3	-	0/2/19/22	0/1/1/1
3	NAG	C	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	402	3	-	0/6/23/26	0/1/1/1
3	BMA	C	403	3	-	0/2/19/22	0/1/1/1
4	NAG	C	405	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	406	4	-	0/6/23/26	0/1/1/1
3	NAG	C	407	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	408	3	-	0/6/23/26	0/1/1/1
3	BMA	C	409	3	-	0/2/19/22	0/1/1/1
3	NAG	C	411	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	412	3	-	0/6/23/26	0/1/1/1
3	BMA	C	413	3	-	0/2/19/22	0/1/1/1
3	NAG	E	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	402	3	-	0/6/23/26	0/1/1/1
3	BMA	E	403	3	-	0/2/19/22	0/1/1/1
4	NAG	E	404	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	405	4	-	0/6/23/26	0/1/1/1
4	NAG	E	406	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	407	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	408	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	409	3	-	0/6/23/26	0/1/1/1
3	BMA	E	410	3	-	0/2/19/22	0/1/1/1
3	NAG	E	412	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	413	3	-	0/6/23/26	0/1/1/1
3	BMA	E	414	3	-	0/2/19/22	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
3	BMA	G	403	3	-	0/2/19/22	0/1/1/1
4	NAG	G	404	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	405	4	-	0/6/23/26	0/1/1/1
4	NAG	G	406	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	407	4	-	0/6/23/26	0/1/1/1
3	NAG	G	408	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	409	3	-	0/6/23/26	0/1/1/1
3	BMA	G	410	3	-	0/2/19/22	0/1/1/1
4	NAG	G	412	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	413	4	-	0/6/23/26	0/1/1/1
4	NAG	I	401	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	402	4	-	0/6/23/26	0/1/1/1
4	NAG	I	403	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	404	4	-	0/6/23/26	0/1/1/1
4	NAG	I	405	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	406	4	-	0/6/23/26	0/1/1/1
3	NAG	I	407	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	408	3	-	0/6/23/26	0/1/1/1
3	BMA	I	409	3	-	0/2/19/22	0/1/1/1
3	NAG	I	411	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	412	3	-	0/6/23/26	0/1/1/1
3	BMA	I	413	3	-	0/2/19/22	0/1/1/1
3	NAG	K	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	402	3	-	0/6/23/26	0/1/1/1
3	BMA	K	403	3	-	0/2/19/22	0/1/1/1
4	NAG	K	404	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	405	4	-	0/6/23/26	0/1/1/1
4	NAG	K	406	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	407	4	-	0/6/23/26	0/1/1/1
3	NAG	K	408	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	409	3	-	0/6/23/26	0/1/1/1
3	BMA	K	410	3	-	0/2/19/22	0/1/1/1
3	NAG	K	411	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	412	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	K	413	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	404	NAG	O7-C7-C8	-2.88	116.78	122.06
4	K	405	NAG	C2-N2-C7	-2.85	119.37	123.04
3	E	412	NAG	O7-C7-C8	-2.85	116.83	122.06
4	A	405	NAG	C2-N2-C7	-2.85	119.38	123.04
4	G	412	NAG	O7-C7-C8	-2.83	116.86	122.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	NAG	1	0
3	A	412	NAG	6	0
3	C	411	NAG	7	0
3	E	401	NAG	2	0
3	E	412	NAG	7	0
4	G	404	NAG	1	0
4	G	405	NAG	7	0
4	G	412	NAG	5	0
3	I	411	NAG	6	0
3	K	403	BMA	3	0
3	K	411	NAG	3	0

## 5.6 Ligand geometry

17 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
5	NAG	A	411	1	14,14,15	0.51	0	15,19,21	0.74	0
5	NAG	A	415	1	14,14,15	0.46	0	15,19,21	1.02	1 (6%)
5	NAG	B	600	2	14,14,15	0.48	0	15,19,21	0.71	0
5	NAG	C	404	1	14,14,15	0.38	0	15,19,21	1.85	2 (13%)
5	NAG	C	410	1	14,14,15	0.49	0	15,19,21	1.53	3 (20%)
5	NAG	C	414	1	14,14,15	0.47	0	15,19,21	1.02	1 (6%)
5	NAG	D	600	2	14,14,15	0.48	0	15,19,21	0.71	0
5	NAG	E	411	1	14,14,15	0.52	0	15,19,21	0.74	0
5	NAG	E	415	1	14,14,15	0.46	0	15,19,21	1.02	1 (6%)
5	NAG	F	600	2	14,14,15	0.47	0	15,19,21	0.71	0
5	NAG	G	411	1	14,14,15	0.51	0	15,19,21	0.74	0
5	NAG	G	414	1	14,14,15	0.45	0	15,19,21	1.02	1 (6%)
5	NAG	H	600	2	14,14,15	0.49	0	15,19,21	0.71	0
5	NAG	I	410	1	14,14,15	0.52	0	15,19,21	0.74	0
5	NAG	I	414	1	14,14,15	0.46	0	15,19,21	1.01	1 (6%)
5	NAG	J	600	2	14,14,15	0.47	0	15,19,21	0.71	0
5	NAG	K	414	1	14,14,15	0.47	0	15,19,21	1.02	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
5	NAG	A	411	1	-	0/6/23/26	0/1/1/1
5	NAG	A	415	1	-	0/6/23/26	0/1/1/1
5	NAG	B	600	2	-	0/6/23/26	0/1/1/1
5	NAG	C	404	1	-	0/6/23/26	0/1/1/1
5	NAG	C	410	1	-	0/6/23/26	0/1/1/1
5	NAG	C	414	1	-	0/6/23/26	0/1/1/1
5	NAG	D	600	2	-	0/6/23/26	0/1/1/1
5	NAG	E	411	1	-	0/6/23/26	0/1/1/1
5	NAG	E	415	1	-	0/6/23/26	0/1/1/1
5	NAG	F	600	2	-	0/6/23/26	0/1/1/1
5	NAG	G	411	1	-	0/6/23/26	0/1/1/1
5	NAG	G	414	1	-	0/6/23/26	0/1/1/1
5	NAG	H	600	2	-	0/6/23/26	0/1/1/1
5	NAG	I	410	1	-	0/6/23/26	0/1/1/1
5	NAG	I	414	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	J	600	2	-	0/6/23/26	0/1/1/1
5	NAG	K	414	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	410	NAG	O7-C7-C8	-2.83	116.87	122.06
5	C	410	NAG	C4-C3-C2	-2.61	107.17	111.23
5	C	404	NAG	C3-C4-C5	2.30	114.22	110.20
5	C	410	NAG	C3-C2-N2	2.46	116.45	110.56
5	I	414	NAG	C1-O5-C5	2.55	115.48	112.25

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 [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	341/347 (98%)	0.26	16 (4%) 35 30	33, 64, 133, 208	0
1	C	341/347 (98%)	0.14	10 (2%) 55 48	30, 61, 135, 195	0
1	E	341/347 (98%)	0.17	11 (3%) 51 45	26, 63, 141, 237	0
1	G	341/347 (98%)	0.23	10 (2%) 55 48	35, 73, 151, 210	0
1	I	341/347 (98%)	0.17	9 (2%) 59 52	39, 71, 141, 193	0
1	K	341/347 (98%)	0.41	19 (5%) 28 25	45, 77, 157, 209	0
2	B	169/179 (94%)	0.49	13 (7%) 16 15	30, 142, 219, 275	0
2	D	169/179 (94%)	0.55	20 (11%) 6 7	30, 132, 212, 252	0
2	F	169/179 (94%)	0.40	15 (8%) 12 12	34, 130, 207, 274	0
2	H	169/179 (94%)	0.64	23 (13%) 4 5	42, 143, 202, 255	0
2	J	169/179 (94%)	0.52	16 (9%) 10 11	40, 138, 225, 266	0
2	L	169/179 (94%)	0.72	23 (13%) 4 5	43, 149, 223, 260	0
All	All	3060/3156 (96%)	0.34	185 (6%) 25 22	26, 77, 195, 275	0

The worst 5 of 185 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	383	ALA	8.3
2	B	516	SER	7.8
2	L	382	ALA	5.7
2	D	372	THR	5.4
2	H	382	ALA	5.3

### 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 ⓘ

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	E	401	14/15	0.79	0.25	1.32	84,93,101,102	0
4	NAG	I	401	14/15	0.72	0.28	0.66	94,99,102,105	0
4	NAG	G	406	14/15	0.81	0.20	-0.01	126,139,148,148	0
3	NAG	A	401	14/15	0.86	0.20	-0.19	79,85,89,90	0
4	NAG	K	406	14/15	0.79	0.24	-0.76	125,137,147,147	0
4	NAG	I	405	14/15	0.74	0.27	-0.81	102,115,124,125	0
4	NAG	C	405	14/15	0.83	0.17	-1.03	96,109,118,118	0
3	NAG	K	401	14/15	0.89	0.18	-1.07	95,101,105,106	0
4	NAG	E	406	14/15	0.82	0.23	-1.13	108,122,133,133	0
4	NAG	A	406	14/15	0.93	0.11	-1.33	123,135,144,144	0
3	NAG	G	408	14/15	0.82	0.29	-	116,128,139,139	0
4	NAG	G	407	14/15	0.82	0.16	-	133,143,154,156	0
4	NAG	A	407	14/15	0.87	0.14	-	131,141,153,155	0
3	NAG	C	408	14/15	0.74	0.36	-	131,144,152,153	0
3	BMA	I	409	11/12	0.70	0.26	-	157,161,173,174	0
4	NAG	K	405	14/15	0.71	0.38	-	134,138,145,150	0
3	NAG	K	408	14/15	0.88	0.26	-	116,128,138,138	0
4	NAG	I	402	14/15	0.71	0.43	-	96,101,106,107	0
3	BMA	A	414	11/12	0.47	0.35	-	161,166,172,174	0
3	NAG	K	402	14/15	0.80	0.26	-	95,100,108,108	0
3	BMA	E	403	11/12	0.61	0.28	-	107,111,121,124	0
3	BMA	C	403	11/12	0.69	0.23	-	100,104,110,110	0
3	BMA	C	409	11/12	0.50	0.24	-	157,160,173,174	0
3	NAG	I	408	14/15	0.79	0.24	-	149,162,170,171	0
3	NAG	C	412	14/15	0.73	0.41	-	134,138,141,142	0
3	BMA	C	413	11/12	0.55	0.43	-	156,159,163,164	0
3	NAG	C	411	14/15	0.80	0.28	-	92,101,107,107	0
4	NAG	K	404	14/15	0.91	0.26	-	100,110,121,123	0
3	NAG	G	402	14/15	0.76	0.46	-	83,88,97,98	0
3	NAG	A	408	14/15	0.88	0.23	-	133,145,154,154	0
4	NAG	G	413	14/15	0.64	0.54	-	152,155,158,159	0
3	NAG	A	409	14/15	0.84	0.19	-	138,151,159,160	0
3	NAG	E	413	14/15	0.70	0.47	-	153,158,161,163	0
3	BMA	E	414	11/12	0.47	0.40	-	179,186,190,193	0
4	NAG	E	404	14/15	0.90	0.27	-	80,91,102,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BMA	K	410	11/12	0.51	0.24	-	184,188,200,201	0
3	BMA	A	403	11/12	0.61	0.29	-	100,104,110,111	0
3	BMA	G	410	11/12	0.57	0.20	-	171,174,187,188	0
3	NAG	G	401	14/15	0.88	0.24	-	85,91,95,95	0
3	NAG	I	411	14/15	0.66	0.26	-	98,105,109,110	0
3	NAG	E	409	14/15	0.82	0.37	-	135,150,159,160	0
3	NAG	K	411	14/15	0.66	0.30	-	127,132,137,139	0
3	NAG	C	401	14/15	0.85	0.23	-	78,83,86,88	0
3	NAG	A	402	14/15	0.82	0.33	-	79,85,92,93	0
3	BMA	G	403	11/12	0.64	0.36	-	101,105,111,113	0
3	NAG	I	412	14/15	0.66	0.30	-	139,142,144,145	0
3	NAG	K	409	14/15	0.82	0.22	-	145,159,167,167	0
4	NAG	I	403	14/15	0.87	0.22	-	76,87,99,101	0
3	NAG	E	408	14/15	0.78	0.34	-	112,127,138,139	0
4	NAG	A	405	14/15	0.79	0.36	-	106,110,116,120	0
4	NAG	E	407	14/15	0.85	0.27	-	117,129,142,144	0
4	NAG	A	404	14/15	0.90	0.43	-	92,101,112,113	0
3	NAG	C	407	14/15	0.79	0.32	-	107,119,128,128	0
3	NAG	A	413	14/15	0.64	0.45	-	136,141,145,146	0
3	NAG	K	412	14/15	0.66	0.41	-	156,159,163,165	0
4	NAG	I	406	14/15	0.72	0.22	-	115,125,137,138	0
3	NAG	A	412	14/15	0.79	0.31	-	96,104,110,111	0
3	BMA	K	413	11/12	0.68	0.32	-	136,141,144,147	0
3	BMA	E	410	11/12	0.64	0.23	-	167,171,185,186	0
3	NAG	I	407	14/15	0.86	0.25	-	106,118,127,127	0
4	NAG	G	405	14/15	0.62	0.34	-	134,141,145,146	0
3	NAG	E	402	14/15	0.76	0.26	-	85,94,106,107	0
4	NAG	C	406	14/15	0.72	0.25	-	135,144,156,157	0
3	NAG	E	412	14/15	0.67	0.32	-	99,110,115,116	0
3	NAG	C	402	14/15	0.89	0.19	-	80,84,89,90	0
4	NAG	I	404	14/15	0.73	0.32	-	127,132,138,141	0
4	NAG	K	407	14/15	0.74	0.22	-	131,142,155,157	0
4	NAG	G	412	14/15	0.79	0.23	-	104,111,114,115	0
3	NAG	G	409	14/15	0.82	0.23	-	147,160,168,169	0
4	NAG	G	404	14/15	0.79	0.30	-	100,105,109,109	0
4	NAG	E	405	14/15	0.70	0.28	-	98,104,113,119	0
3	BMA	K	403	11/12	0.48	0.28	-	114,118,124,126	0
3	BMA	I	413	11/12	0.47	0.40	-	166,170,173,175	0
3	BMA	A	410	11/12	0.64	0.20	-	182,186,198,199	0

## 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(Å <sup>2</sup> )	Q<0.9
5	NAG	C	404	14/15	0.74	0.29	-0.17	85,96,107,109	0
5	NAG	J	600	14/15	0.58	0.38	-	197,206,213,214	0
5	NAG	E	411	14/15	0.57	0.56	-	126,134,139,142	0
5	NAG	A	415	14/15	0.90	0.16	-	117,130,138,139	0
5	NAG	B	600	14/15	0.74	0.26	-	194,202,209,210	0
5	NAG	G	411	14/15	0.84	0.36	-	130,138,142,145	0
5	NAG	D	600	14/15	0.41	0.44	-	200,206,211,213	0
5	NAG	A	411	14/15	0.81	0.35	-	80,87,91,93	0
5	NAG	I	410	14/15	0.64	0.42	-	119,125,127,129	0
5	NAG	G	414	14/15	0.55	0.37	-	106,119,127,128	0
5	NAG	C	410	14/15	0.76	0.27	-	103,107,111,111	0
5	NAG	F	600	14/15	0.58	0.26	-	186,193,200,200	0
5	NAG	K	414	14/15	0.74	0.23	-	106,117,125,126	0
5	NAG	I	414	14/15	0.46	0.54	-	150,161,168,169	0
5	NAG	C	414	14/15	0.56	0.51	-	111,122,129,129	0
5	NAG	E	415	14/15	0.80	0.22	-	109,119,127,129	0
5	NAG	H	600	14/15	0.64	0.27	-	203,207,210,211	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.