



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:43 AM GMT

PDB ID : 3FKU
Title : Crystal structure of influenza hemagglutinin (H5) in complex with a broadly neutralizing antibody F10
Authors : Hwang, W.C.; Santelli, E.; Stec, B.; Wei, G.; Cadwell, G.; Bankston, L.A.; Sui, J.; Perez, S.; Aird, D.; Chen, L.M.; Ali, M.; Murakami, A.; Yammanuru, A.; Han, T.; Cox, N.; Donis, R.O.; Liddington, R.C.; Marasco, W.A.
Deposited on : 2008-12-17
Resolution : 3.20 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (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

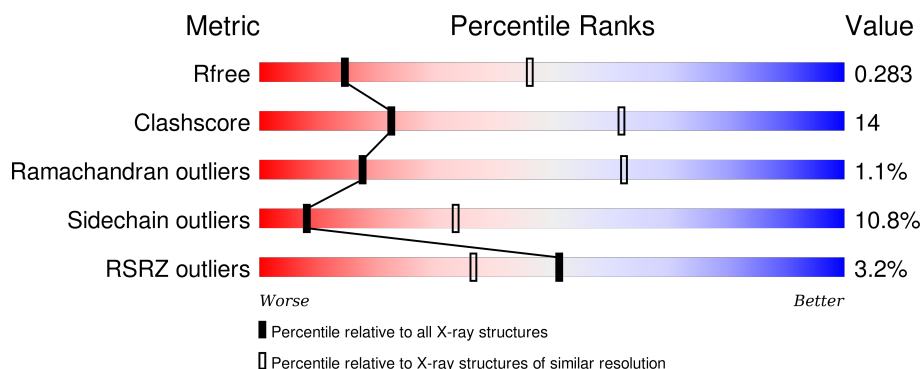
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 ≥ 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	338	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>28%</div> <div>.</div> <div>.</div> </div> </div>
1	C	338	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>30%</div> <div>.</div> <div>.</div> </div> </div>
1	E	338	<div> <div></div> <div> <div></div> <div>63%</div> <div>29%</div> <div>.</div> <div>.</div> </div> </div>
1	G	338	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>25%</div> <div>.</div> <div>.</div> </div> </div>
1	I	338	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>27%</div> <div>.</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	K	338	
2	B	182	
2	D	182	
2	F	182	
2	H	182	
2	J	182	
2	L	182	
3	S	280	
3	T	280	
3	U	280	
3	X	280	
3	Y	280	
3	Z	280	

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
5	NAG	G	601	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 34975 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	323	Total	C	N	O	S	0	0	0
			2567	1621	443	488	15			
1	C	323	Total	C	N	O	S	0	0	0
			2567	1621	443	488	15			
1	E	323	Total	C	N	O	S	0	0	0
			2567	1621	443	488	15			
1	G	323	Total	C	N	O	S	0	0	0
			2567	1621	443	488	15			
1	I	323	Total	C	N	O	S	0	0	0
			2567	1621	443	488	15			
1	K	323	Total	C	N	O	S	0	0	0
			2567	1621	443	488	15			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	EXPRESSION TAG	UNP Q6DQ33
A	-2	ASP	-	EXPRESSION TAG	UNP Q6DQ33
A	-1	PRO	-	EXPRESSION TAG	UNP Q6DQ33
A	0	GLY	-	EXPRESSION TAG	UNP Q6DQ33
A	1	TYR	-	EXPRESSION TAG	UNP Q6DQ33
A	2	LEU	-	EXPRESSION TAG	UNP Q6DQ33
A	3	LEU	-	EXPRESSION TAG	UNP Q6DQ33
A	4	GLU	-	EXPRESSION TAG	UNP Q6DQ33
C	-3	ALA	-	EXPRESSION TAG	UNP Q6DQ33
C	-2	ASP	-	EXPRESSION TAG	UNP Q6DQ33
C	-1	PRO	-	EXPRESSION TAG	UNP Q6DQ33
C	0	GLY	-	EXPRESSION TAG	UNP Q6DQ33
C	1	TYR	-	EXPRESSION TAG	UNP Q6DQ33
C	2	LEU	-	EXPRESSION TAG	UNP Q6DQ33
C	3	LEU	-	EXPRESSION TAG	UNP Q6DQ33
C	4	GLU	-	EXPRESSION TAG	UNP Q6DQ33
E	-3	ALA	-	EXPRESSION TAG	UNP Q6DQ33

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	ASP	-	EXPRESSION TAG	UNP Q6DQ33
E	-1	PRO	-	EXPRESSION TAG	UNP Q6DQ33
E	0	GLY	-	EXPRESSION TAG	UNP Q6DQ33
E	1	TYR	-	EXPRESSION TAG	UNP Q6DQ33
E	2	LEU	-	EXPRESSION TAG	UNP Q6DQ33
E	3	LEU	-	EXPRESSION TAG	UNP Q6DQ33
E	4	GLU	-	EXPRESSION TAG	UNP Q6DQ33
G	-3	ALA	-	EXPRESSION TAG	UNP Q6DQ33
G	-2	ASP	-	EXPRESSION TAG	UNP Q6DQ33
G	-1	PRO	-	EXPRESSION TAG	UNP Q6DQ33
G	0	GLY	-	EXPRESSION TAG	UNP Q6DQ33
G	1	TYR	-	EXPRESSION TAG	UNP Q6DQ33
G	2	LEU	-	EXPRESSION TAG	UNP Q6DQ33
G	3	LEU	-	EXPRESSION TAG	UNP Q6DQ33
G	4	GLU	-	EXPRESSION TAG	UNP Q6DQ33
I	-3	ALA	-	EXPRESSION TAG	UNP Q6DQ33
I	-2	ASP	-	EXPRESSION TAG	UNP Q6DQ33
I	-1	PRO	-	EXPRESSION TAG	UNP Q6DQ33
I	0	GLY	-	EXPRESSION TAG	UNP Q6DQ33
I	1	TYR	-	EXPRESSION TAG	UNP Q6DQ33
I	2	LEU	-	EXPRESSION TAG	UNP Q6DQ33
I	3	LEU	-	EXPRESSION TAG	UNP Q6DQ33
I	4	GLU	-	EXPRESSION TAG	UNP Q6DQ33
K	-3	ALA	-	EXPRESSION TAG	UNP Q6DQ33
K	-2	ASP	-	EXPRESSION TAG	UNP Q6DQ33
K	-1	PRO	-	EXPRESSION TAG	UNP Q6DQ33
K	0	GLY	-	EXPRESSION TAG	UNP Q6DQ33
K	1	TYR	-	EXPRESSION TAG	UNP Q6DQ33
K	2	LEU	-	EXPRESSION TAG	UNP Q6DQ33
K	3	LEU	-	EXPRESSION TAG	UNP Q6DQ33
K	4	GLU	-	EXPRESSION TAG	UNP Q6DQ33

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	0	0	0
			1455	905	254	288	8			
2	D	180	Total	C	N	O	S	0	0	0
			1455	905	254	288	8			
2	F	180	Total	C	N	O	S	0	0	0
			1455	905	254	288	8			
2	H	174	Total	C	N	O	S	0	0	0
			1412	878	245	281	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	174	Total	C	N	O	S	0	0	0
			1412	878	245	281	8			
2	L	174	Total	C	N	O	S	0	0	0
			1412	878	245	281	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	ARG	-	EXPRESSION TAG	UNP Q2F4V2
B	178	SER	-	EXPRESSION TAG	UNP Q2F4V2
B	179	LEU	-	EXPRESSION TAG	UNP Q2F4V2
B	180	VAL	-	EXPRESSION TAG	UNP Q2F4V2
B	181	PRO	-	EXPRESSION TAG	UNP Q2F4V2
B	182	ARG	-	EXPRESSION TAG	UNP Q2F4V2
D	177	ARG	-	EXPRESSION TAG	UNP Q2F4V2
D	178	SER	-	EXPRESSION TAG	UNP Q2F4V2
D	179	LEU	-	EXPRESSION TAG	UNP Q2F4V2
D	180	VAL	-	EXPRESSION TAG	UNP Q2F4V2
D	181	PRO	-	EXPRESSION TAG	UNP Q2F4V2
D	182	ARG	-	EXPRESSION TAG	UNP Q2F4V2
F	177	ARG	-	EXPRESSION TAG	UNP Q2F4V2
F	178	SER	-	EXPRESSION TAG	UNP Q2F4V2
F	179	LEU	-	EXPRESSION TAG	UNP Q2F4V2
F	180	VAL	-	EXPRESSION TAG	UNP Q2F4V2
F	181	PRO	-	EXPRESSION TAG	UNP Q2F4V2
F	182	ARG	-	EXPRESSION TAG	UNP Q2F4V2
H	177	ARG	-	EXPRESSION TAG	UNP Q2F4V2
H	178	SER	-	EXPRESSION TAG	UNP Q2F4V2
H	179	LEU	-	EXPRESSION TAG	UNP Q2F4V2
H	180	VAL	-	EXPRESSION TAG	UNP Q2F4V2
H	181	PRO	-	EXPRESSION TAG	UNP Q2F4V2
H	182	ARG	-	EXPRESSION TAG	UNP Q2F4V2
J	177	ARG	-	EXPRESSION TAG	UNP Q2F4V2
J	178	SER	-	EXPRESSION TAG	UNP Q2F4V2
J	179	LEU	-	EXPRESSION TAG	UNP Q2F4V2
J	180	VAL	-	EXPRESSION TAG	UNP Q2F4V2
J	181	PRO	-	EXPRESSION TAG	UNP Q2F4V2
J	182	ARG	-	EXPRESSION TAG	UNP Q2F4V2
L	177	ARG	-	EXPRESSION TAG	UNP Q2F4V2
L	178	SER	-	EXPRESSION TAG	UNP Q2F4V2
L	179	LEU	-	EXPRESSION TAG	UNP Q2F4V2
L	180	VAL	-	EXPRESSION TAG	UNP Q2F4V2

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Chain	Residue	Modelled	Actual	Comment	Reference
L	181	PRO	-	EXPRESSION TAG	UNP Q2F4V2
L	182	ARG	-	EXPRESSION TAG	UNP Q2F4V2

- Molecule 3 is a protein called Neutralizing antibody F10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	235	Total	C	N	O	S	0	0	0
			1765	1094	311	352	8			
3	Y	235	Total	C	N	O	S	0	0	0
			1765	1094	311	352	8			
3	Z	236	Total	C	N	O	S	0	0	0
			1769	1096	312	353	8			
3	S	233	Total	C	N	O	S	0	0	0
			1753	1088	309	348	8			
3	T	234	Total	C	N	O	S	0	0	0
			1759	1091	310	350	8			
3	U	234	Total	C	N	O	S	0	0	0
			1759	1091	310	350	8			

- 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	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	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	K	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

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

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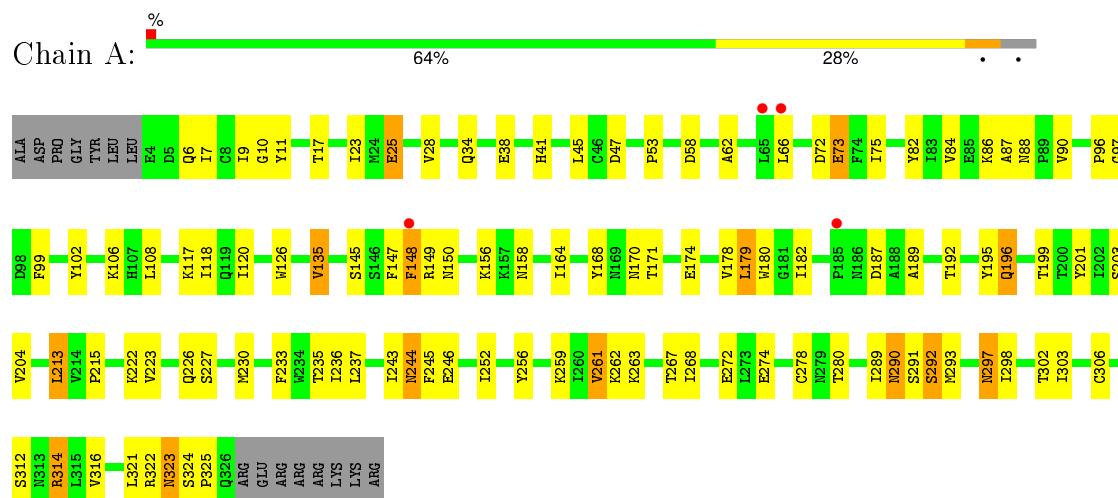
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	3	Total	C	N	O	0	0
			39	22	2	15		
5	G	3	Total	C	N	O	0	0
			39	22	2	15		
5	I	3	Total	C	N	O	0	0
			39	22	2	15		
5	K	3	Total	C	N	O	0	0
			39	22	2	15		

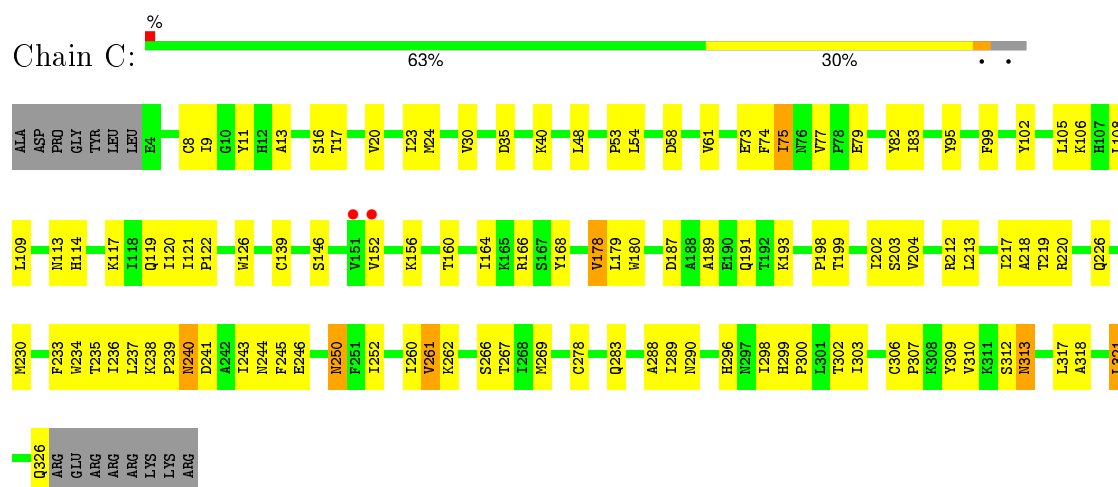
3 Residue-property plots

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.

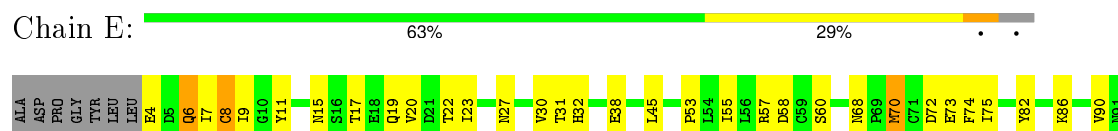
• Molecule 1: Hemagglutinin

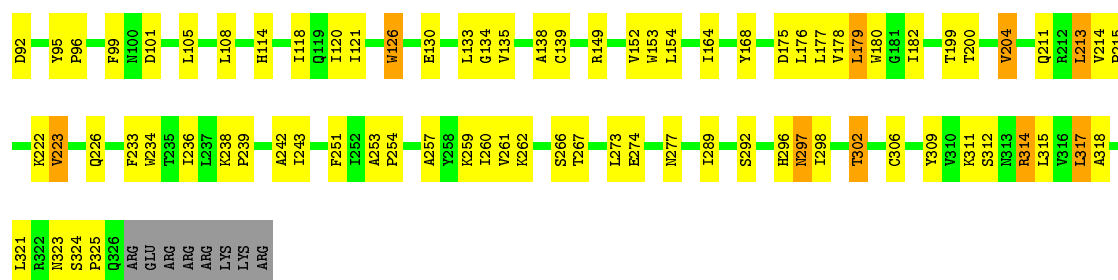


• Molecule 1: Hemagglutinin

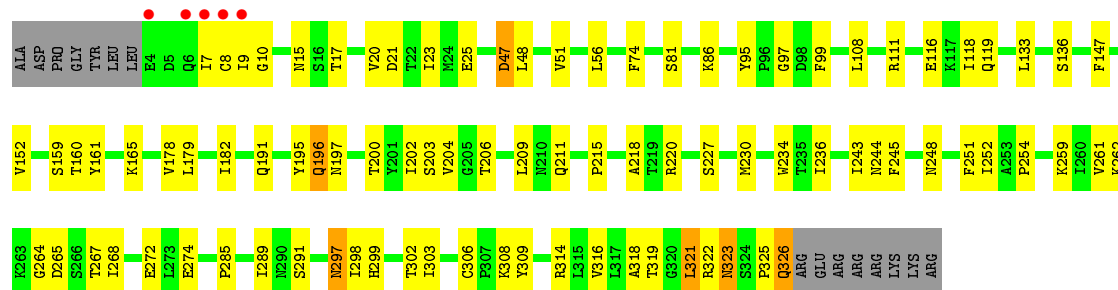


• Molecule 1: Hemagglutinin

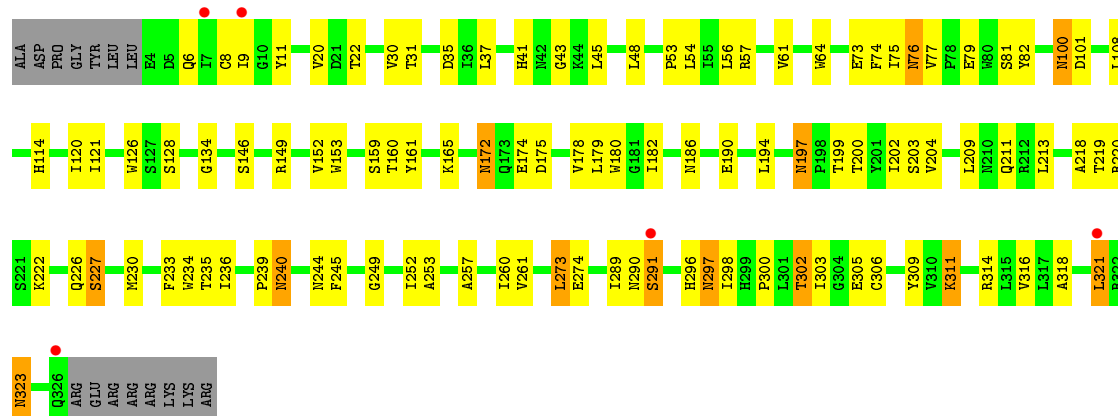




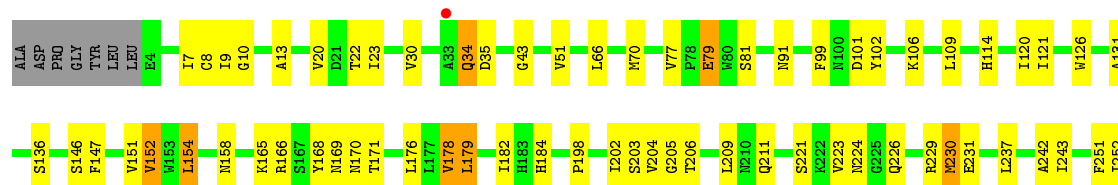
• Molecule 1: Hemagglutinin

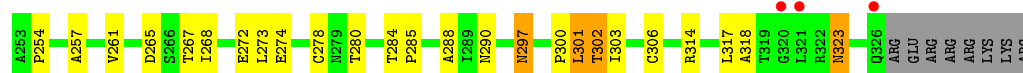


• Molecule 1: Hemagglutinin

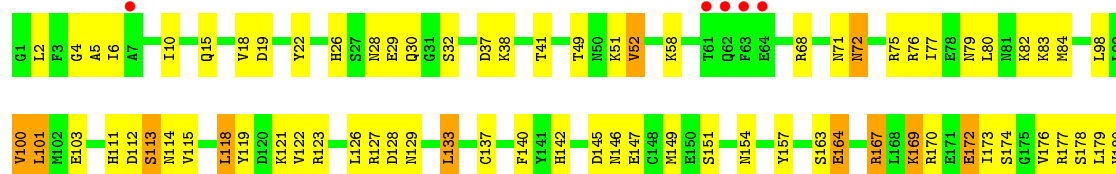


• Molecule 1: Hemagglutinin



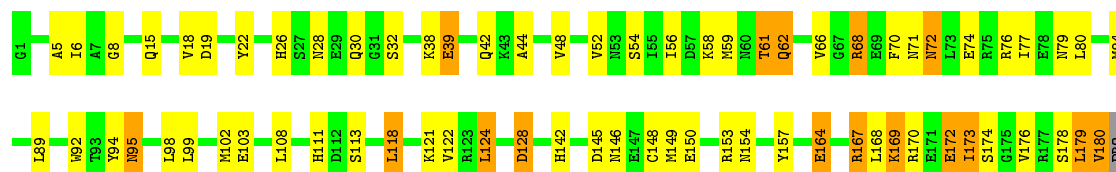


• Molecule 2: Hemagglutinin



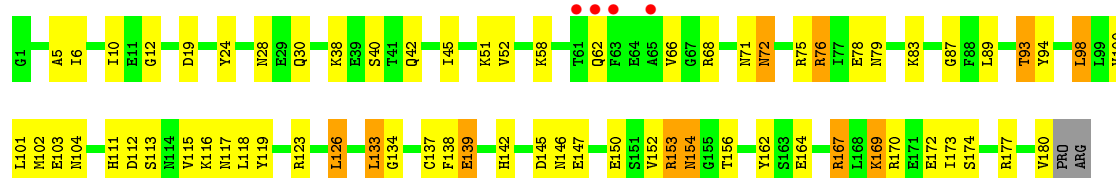
PRO
ARG

• Molecule 2: Hemagglutinin

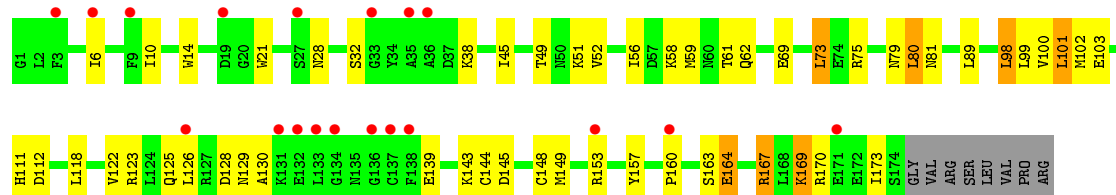


ARG

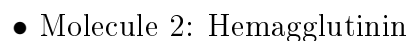
• Molecule 2: Hemagglutinin



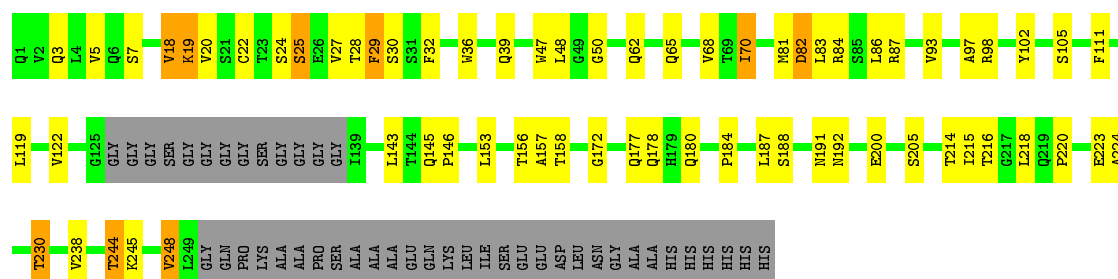
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin

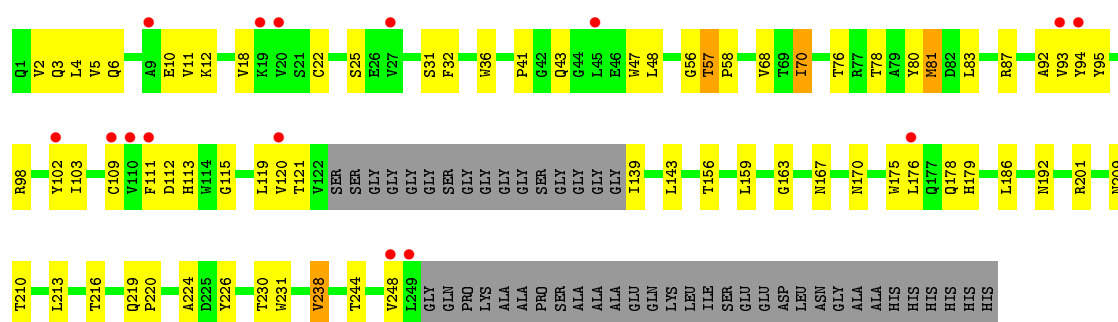


Chain Z: 



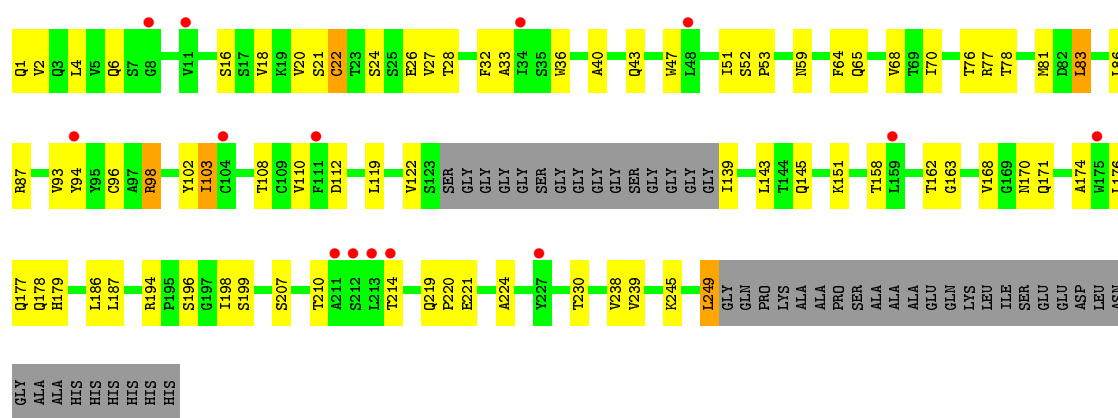
• Molecule 3: Neutralizing antibody F10

Chain S: 



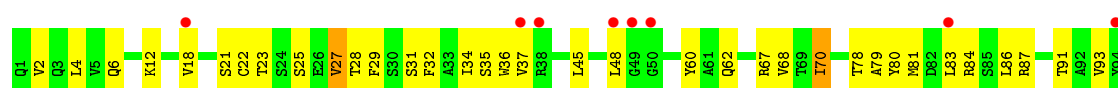
• Molecule 3: Neutralizing antibody F10

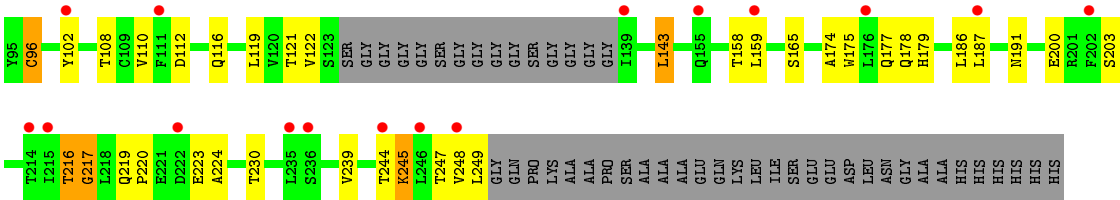
Chain T: 



• Molecule 3: Neutralizing antibody F10

Chain U: 





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	205.30Å 118.50Å 338.90Å 90.00° 99.60° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 93.77 – 3.20	Depositor EDS
% Data completeness (in resolution range)	85.0 (50.00-3.20) 85.0 (93.77-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.232 , 0.286 0.231 , 0.283	Depositor DCC
R_{free} test set	5676 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	70.8	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 84.0	EDS
Estimated twinning fraction	0.116 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.107 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h- 1/2*k-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	1 of 112570 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	34975	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.50	0/2629	0.66	0/3570
1	C	0.51	0/2629	0.68	0/3570
1	E	0.49	1/2629 (0.0%)	0.65	0/3570
1	G	0.48	0/2629	0.63	0/3570
1	I	0.46	0/2629	0.64	0/3570
1	K	0.48	0/2629	0.63	0/3570
2	B	0.64	0/1482	0.78	0/1992
2	D	0.62	0/1482	0.76	0/1992
2	F	0.63	0/1482	0.75	1/1992 (0.1%)
2	H	0.47	0/1439	0.61	0/1934
2	J	0.46	0/1439	0.60	0/1934
2	L	0.47	0/1439	0.60	0/1934
3	S	0.39	0/1791	0.57	0/2436
3	T	0.39	0/1797	0.57	0/2444
3	U	0.41	0/1797	0.59	0/2444
3	X	0.49	0/1803	0.65	0/2452
3	Y	0.52	0/1803	0.68	0/2452
3	Z	0.55	0/1807	0.72	0/2457
All	All	0.50	1/35335 (0.0%)	0.65	1/47883 (0.0%)

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
1	A	0	2
1	E	0	3
1	G	0	1
1	I	0	1
1	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	Y	0	1
5	G	1	0
All	All	1	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	8	CYS	CB-SG	-5.67	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	76	ARG	NE-CZ-NH2	-5.45	117.57	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	601	NAG	C1

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	TRP	Peptide
1	A	290	ASN	Peptide
1	E	126	TRP	Peptide
1	E	323	ASN	Peptide
1	E	324	SER	Peptide

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	2567	0	2507	81	0
1	C	2567	0	2507	73	0
1	E	2567	0	2507	70	0
1	G	2567	0	2505	61	0
1	I	2567	0	2507	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	2567	0	2507	69	0
2	B	1455	0	1369	60	0
2	D	1455	0	1369	69	0
2	F	1455	0	1369	74	0
2	H	1412	0	1320	59	0
2	J	1412	0	1319	42	0
2	L	1412	0	1319	33	0
3	S	1753	0	1693	61	0
3	T	1759	0	1698	53	0
3	U	1759	0	1698	46	0
3	X	1765	0	1703	57	0
3	Y	1765	0	1703	39	0
3	Z	1769	0	1706	39	0
4	A	28	0	25	0	0
4	C	28	0	25	2	0
4	E	28	0	25	1	0
4	G	28	0	23	0	0
4	I	28	0	25	0	0
4	K	28	0	25	1	0
5	A	39	0	34	0	0
5	C	39	0	34	0	0
5	E	39	0	34	0	0
5	G	39	0	34	2	0
5	I	39	0	34	0	0
5	K	39	0	34	0	0
All	All	34975	0	33658	938	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 14.

The worst 5 of 938 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:302:THR:HG21	1:C:306:CYS:SG	1.63	1.36
3:Y:158:THR:HG22	3:Y:214:THR:HG23	1.21	1.15
2:B:169:LYS:NZ	2:B:173:ILE:HG21	1.62	1.14
2:H:98:LEU:HD21	2:H:102:MET:HE1	1.27	1.14
1:C:302:THR:CG2	1:C:306:CYS:SG	2.37	1.13

There are no symmetry-related clashes.

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	321/338 (95%)	278 (87%)	37 (12%)	6 (2%)	10	50
1	C	321/338 (95%)	282 (88%)	36 (11%)	3 (1%)	21	67
1	E	321/338 (95%)	271 (84%)	47 (15%)	3 (1%)	21	67
1	G	321/338 (95%)	280 (87%)	37 (12%)	4 (1%)	16	60
1	I	321/338 (95%)	282 (88%)	37 (12%)	2 (1%)	30	75
1	K	321/338 (95%)	287 (89%)	30 (9%)	4 (1%)	16	60
2	B	178/182 (98%)	159 (89%)	16 (9%)	3 (2%)	11	52
2	D	178/182 (98%)	155 (87%)	20 (11%)	3 (2%)	11	52
2	F	178/182 (98%)	153 (86%)	24 (14%)	1 (1%)	30	75
2	H	172/182 (94%)	150 (87%)	19 (11%)	3 (2%)	11	52
2	J	172/182 (94%)	146 (85%)	23 (13%)	3 (2%)	11	52
2	L	172/182 (94%)	158 (92%)	13 (8%)	1 (1%)	30	75
3	S	229/280 (82%)	206 (90%)	21 (9%)	2 (1%)	21	67
3	T	230/280 (82%)	204 (89%)	25 (11%)	1 (0%)	39	80
3	U	230/280 (82%)	204 (89%)	25 (11%)	1 (0%)	39	80
3	X	231/280 (82%)	204 (88%)	25 (11%)	2 (1%)	21	67
3	Y	231/280 (82%)	203 (88%)	25 (11%)	3 (1%)	15	59
3	Z	232/280 (83%)	201 (87%)	29 (12%)	2 (1%)	21	67
All	All	4359/4800 (91%)	3823 (88%)	489 (11%)	47 (1%)	17	62

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	E	73	GLU
3	Y	43	GLN
2	B	128	ASP

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Mol	Chain	Res	Type
2	B	178	SER

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	291/304 (96%)	264 (91%)	27 (9%)	11	41
1	C	291/304 (96%)	263 (90%)	28 (10%)	10	39
1	E	291/304 (96%)	264 (91%)	27 (9%)	11	41
1	G	291/304 (96%)	266 (91%)	25 (9%)	13	46
1	I	291/304 (96%)	261 (90%)	30 (10%)	9	36
1	K	291/304 (96%)	265 (91%)	26 (9%)	12	44
2	B	154/156 (99%)	126 (82%)	28 (18%)	2	10
2	D	154/156 (99%)	126 (82%)	28 (18%)	2	10
2	F	154/156 (99%)	133 (86%)	21 (14%)	5	22
2	H	149/156 (96%)	134 (90%)	15 (10%)	9	36
2	J	149/156 (96%)	127 (85%)	22 (15%)	4	18
2	L	149/156 (96%)	127 (85%)	22 (15%)	4	18
3	S	194/220 (88%)	185 (95%)	9 (5%)	33	74
3	T	195/220 (89%)	180 (92%)	15 (8%)	16	54
3	U	195/220 (89%)	173 (89%)	22 (11%)	7	31
3	X	196/220 (89%)	178 (91%)	18 (9%)	11	41
3	Y	196/220 (89%)	166 (85%)	30 (15%)	3	17
3	Z	196/220 (89%)	176 (90%)	20 (10%)	9	36
All	All	3827/4080 (94%)	3414 (89%)	413 (11%)	8	33

5 of 413 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	59	MET

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Mol	Chain	Res	Type
2	J	38	LYS
3	T	98	ARG
2	H	100	VAL
1	I	172	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 123 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	114	HIS
2	H	129	ASN
3	Z	191	ASN
1	G	224	ASN
2	H	53	ASN

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 ⓘ

30 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	$\# Z > 2$
4	NAG	A	501	1,4	14,14,15	0.57	0	15,19,21	0.75	0
4	NAG	A	502	4	14,14,15	0.53	0	15,19,21	1.50	1 (6%)
5	NAG	A	601	1,5	14,14,15	0.67	0	15,19,21	1.23	1 (6%)
5	NAG	A	602	5	14,14,15	0.39	0	15,19,21	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	A	603	5	11,11,12	0.52	0	14,15,17	1.39	1 (7%)
4	NAG	C	501	1,4	14,14,15	0.50	0	15,19,21	1.51	1 (6%)
4	NAG	C	502	4	14,14,15	0.67	1 (7%)	15,19,21	1.15	1 (6%)
5	NAG	C	601	1,5	14,14,15	0.52	0	15,19,21	0.62	0
5	NAG	C	602	5	14,14,15	0.48	0	15,19,21	0.88	0
5	BMA	C	603	5	11,11,12	0.35	0	14,15,17	0.98	1 (7%)
4	NAG	E	501	1,4	14,14,15	0.55	0	15,19,21	1.65	4 (26%)
4	NAG	E	502	4	14,14,15	0.78	0	15,19,21	1.26	2 (13%)
5	NAG	E	601	1,5	14,14,15	0.56	0	15,19,21	0.69	0
5	NAG	E	602	5	14,14,15	0.43	0	15,19,21	0.78	0
5	BMA	E	603	5	11,11,12	0.48	0	14,15,17	0.93	1 (7%)
4	NAG	G	501	1,4	14,14,15	0.59	0	15,19,21	1.10	2 (13%)
4	NAG	G	502	4	14,14,15	0.66	0	15,19,21	1.24	1 (6%)
5	NAG	G	601	1,5	14,14,15	0.67	0	15,19,21	1.04	1 (6%)
5	NAG	G	602	5	14,14,15	0.64	0	15,19,21	0.99	0
5	BMA	G	603	5	11,11,12	0.70	0	14,15,17	1.69	3 (21%)
4	NAG	I	501	1,4	14,14,15	0.47	0	15,19,21	1.80	3 (20%)
4	NAG	I	502	4	14,14,15	0.77	0	15,19,21	1.07	0
5	NAG	I	601	1,5	14,14,15	0.58	0	15,19,21	0.96	1 (6%)
5	NAG	I	602	5	14,14,15	0.59	0	15,19,21	1.02	1 (6%)
5	BMA	I	603	5	11,11,12	0.63	0	14,15,17	1.33	1 (7%)
4	NAG	K	501	1,4	14,14,15	0.38	0	15,19,21	1.83	2 (13%)
4	NAG	K	502	4	14,14,15	0.76	1 (7%)	15,19,21	1.47	2 (13%)
5	NAG	K	601	1,5	14,14,15	0.57	0	15,19,21	0.99	1 (6%)
5	NAG	K	602	5	14,14,15	0.62	0	15,19,21	1.14	1 (6%)
5	BMA	K	603	5	11,11,12	0.54	0	14,15,17	0.86	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
4	NAG	A	501	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	502	4	-	0/6/23/26	0/1/1/1
5	NAG	A	601	1,5	-	1/6/23/26	0/1/1/1
5	NAG	A	602	5	-	0/6/23/26	0/1/1/1
5	BMA	A	603	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	501	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	502	4	-	0/6/23/26	0/1/1/1
5	NAG	C	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	602	5	-	0/6/23/26	0/1/1/1
5	BMA	C	603	5	-	0/2/19/22	0/1/1/1
4	NAG	E	501	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	502	4	-	1/6/23/26	0/1/1/1
5	NAG	E	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	602	5	-	0/6/23/26	0/1/1/1
5	BMA	E	603	5	-	0/2/19/22	0/1/1/1
4	NAG	G	501	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	502	4	-	0/6/23/26	0/1/1/1
5	NAG	G	601	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	G	602	5	-	0/6/23/26	0/1/1/1
5	BMA	G	603	5	-	0/2/19/22	0/1/1/1
4	NAG	I	501	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	502	4	-	0/6/23/26	0/1/1/1
5	NAG	I	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	602	5	-	0/6/23/26	0/1/1/1
5	BMA	I	603	5	-	0/2/19/22	0/1/1/1
4	NAG	K	501	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	502	4	-	0/6/23/26	0/1/1/1
5	NAG	K	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	K	602	5	-	0/6/23/26	0/1/1/1
5	BMA	K	603	5	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	502	NAG	C1-C2	2.08	1.55	1.52
4	C	502	NAG	C1-C2	2.12	1.55	1.52

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	NAG	C4-C3-C2	-4.24	104.64	111.23
4	I	501	NAG	C4-C3-C2	-3.98	105.04	111.23
4	E	501	NAG	C4-C3-C2	-3.71	105.46	111.23
4	K	501	NAG	C4-C3-C2	-3.43	105.90	111.23
4	I	501	NAG	O4-C4-C3	2.02	114.89	110.34

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	601	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	502	NAG	O7-C7-N2-C2
5	A	601	NAG	C8-C7-N2-C2

There are no ring outliers.

7 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	501	NAG	2	0
4	C	502	NAG	2	0
4	E	502	NAG	1	0
5	G	601	NAG	2	0
5	G	602	NAG	2	0
4	K	501	NAG	1	0
4	K	502	NAG	1	0

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 ⓘ

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, 95th 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 ²)	Q<0.9
1	A	323/338 (95%)	0.24	4 (1%) 81 69	64, 86, 103, 127	0
1	C	323/338 (95%)	0.07	2 (0%) 90 84	60, 85, 101, 122	0
1	E	323/338 (95%)	0.02	0 100 100	54, 86, 102, 135	0
1	G	323/338 (95%)	0.04	5 (1%) 76 63	66, 86, 101, 106	0
1	I	323/338 (95%)	0.02	5 (1%) 76 63	64, 84, 99, 113	0
1	K	323/338 (95%)	0.21	4 (1%) 81 69	64, 85, 98, 120	0
2	B	180/182 (98%)	0.42	5 (2%) 56 42	62, 82, 125, 138	0
2	D	180/182 (98%)	0.11	0 100 100	62, 82, 111, 141	0
2	F	180/182 (98%)	0.23	4 (2%) 65 50	61, 81, 121, 141	0
2	H	174/182 (95%)	0.50	19 (10%) 7 4	61, 92, 118, 147	0
2	J	174/182 (95%)	0.54	17 (9%) 10 5	65, 89, 118, 130	0
2	L	174/182 (95%)	0.59	20 (11%) 6 4	64, 90, 117, 132	0
3	S	233/280 (83%)	0.27	15 (6%) 23 13	86, 117, 134, 143	0
3	T	234/280 (83%)	0.36	14 (5%) 25 14	82, 113, 136, 147	0
3	U	234/280 (83%)	0.48	24 (10%) 9 5	88, 117, 134, 142	0
3	X	235/280 (83%)	-0.02	0 100 100	45, 64, 87, 94	0
3	Y	235/280 (83%)	0.10	1 (0%) 93 90	42, 61, 84, 100	0
3	Z	236/280 (84%)	0.02	0 100 100	43, 62, 88, 115	0
All	All	4407/4800 (91%)	0.20	139 (3%) 51 36	42, 86, 125, 147	0

The worst 5 of 139 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	6	GLN	8.2
2	B	63	PHE	5.2
2	H	134	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
2	F	63	PHE	4.8
2	H	132	GLU	4.5

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. 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, 95th 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 ²)	Q<0.9
5	NAG	C	601	14/15	0.94	0.14	-1.23	101,110,119,120	0
5	NAG	E	601	14/15	0.95	0.13	-1.60	93,105,110,114	0
5	NAG	I	601	14/15	0.96	0.12	-2.09	100,107,127,132	0
5	NAG	A	601	14/15	0.95	0.11	-3.01	100,109,112,119	0
4	NAG	E	501	14/15	0.91	0.11	-	93,112,126,138	0
5	NAG	G	602	14/15	0.87	0.14	-	110,123,130,139	0
5	NAG	I	602	14/15	0.80	0.17	-	142,147,153,161	0
5	BMA	I	603	11/12	0.69	0.20	-	161,168,170,172	0
5	NAG	K	601	14/15	0.94	0.14	-	76,84,97,110	0
4	NAG	G	501	14/15	0.86	0.17	-	120,133,141,143	0
4	NAG	I	501	14/15	0.86	0.16	-	109,123,133,140	0
5	NAG	A	602	14/15	0.94	0.12	-	99,110,116,124	0
5	BMA	C	603	11/12	0.83	0.14	-	142,144,147,151	0
4	NAG	A	501	14/15	0.91	0.12	-	89,107,123,135	0
4	NAG	C	501	14/15	0.91	0.14	-	85,102,113,126	0
5	BMA	A	603	11/12	0.86	0.16	-	118,130,133,139	0
5	BMA	E	603	11/12	0.83	0.14	-	125,131,135,138	0
5	NAG	C	602	14/15	0.88	0.23	-	111,122,132,139	0
5	NAG	E	602	14/15	0.91	0.16	-	96,110,123,131	0
5	NAG	G	601	14/15	0.95	0.13	-	76,98,109,116	0
5	NAG	K	602	14/15	0.86	0.18	-	111,125,129,133	0
4	NAG	I	502	14/15	0.85	0.20	-	139,149,154,154	0
4	NAG	G	502	14/15	0.76	0.27	-	143,147,157,159	0
4	NAG	C	502	14/15	0.84	0.15	-	121,134,139,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	A	502	14/15	0.91	0.13	-	130,143,150,152	0
5	BMA	K	603	11/12	0.78	0.16	-	130,132,134,135	0
4	NAG	K	502	14/15	0.76	0.19	-	140,152,156,157	0
4	NAG	E	502	14/15	0.82	0.30	-	150,157,163,163	0
5	BMA	G	603	11/12	0.86	0.16	-	135,143,146,147	0
4	NAG	K	501	14/15	0.90	0.13	-	108,125,132,136	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.