wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 07:07 PM GMT

PDB ID	:	4N5Z
Title	:	Crystal structure of aerosol transmissible influenza H5 hemagglutinin mutant (N158D, N224K, Q226L and T318I) from the influenza virus A/Viet Nam/1203/2004 (H5N1)
Authors	:	Zhu, X.; Wilson, I.A.
Deposited on	:	2013-10-10
Resolution	:	2.95 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

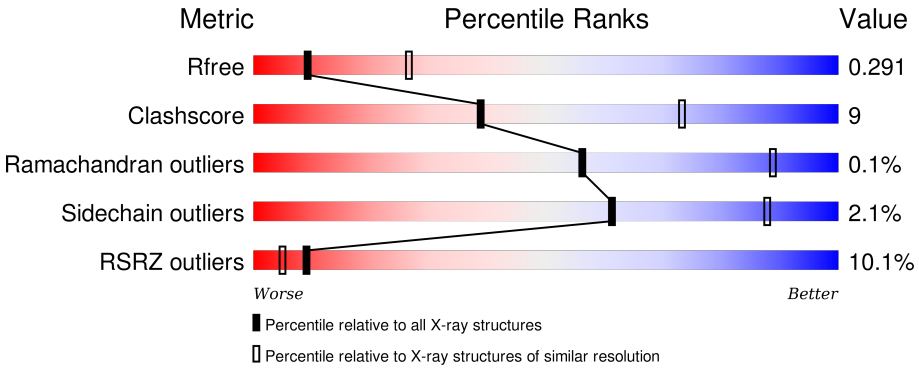
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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 <=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	334	2% 62% 33%
1	C	334	3% 63% 32%
1	E	334	2% 72% 23%
1	G	334	% 76% 20%
1	I	334	% 69% 26%

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Mol	Chain	Length	Quality of chain
1	K	334	2% 74% 22%
1	M	334	4% 71% 25%
1	O	334	3% 77% 19%
1	Q	334	2% 72% 22%
1	S	334	3% 72% 24%
1	U	334	4% 76% 19%
1	W	334	5% 72% 25%
1	Y	334	8% 76% 20%
1	a	334	10% 95%
1	c	334	12% 96%
2	B	181	4% 60% 36%
2	D	181	17% 64% 34%
2	F	181	17% 80% 18%
2	H	181	4% 71% 25%
2	J	181	8% 75% 23%
2	L	181	15% 77% 20%
2	N	181	18% 74% 24%
2	P	181	15% 78% 19%
2	R	181	22% 81% 17%
2	T	181	17% 77% 21%
2	V	181	14% 80% 18%
2	X	181	17% 75% 23%
2	Z	181	43% 68% 29%
2	b	181	47% 97%
2	d	181	43% 96%

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	M	2001	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 60979 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	C	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	E	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	G	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	I	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	K	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	M	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	O	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	Q	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	S	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	U	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	W	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	Y	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	a	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	c	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
A	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
A	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
A	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
A	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
A	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
A	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
A	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
C	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
C	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
C	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
C	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
C	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
C	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
C	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
C	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
E	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
E	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
E	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
E	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
E	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
E	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
E	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
E	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
G	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
G	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
G	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
G	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
G	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
G	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
G	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
G	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
I	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
I	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
I	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
I	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
I	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
I	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
I	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
I	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
K	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
K	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
K	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33

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Chain	Residue	Modelled	Actual	Comment	Reference
K	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
K	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
K	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
K	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
K	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
M	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
M	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
M	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
M	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
M	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
M	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
M	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
M	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
O	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
O	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
O	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
O	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
O	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
O	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
O	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
O	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
Q	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
Q	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
Q	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
Q	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
Q	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
Q	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
Q	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
Q	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
S	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
S	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
S	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
S	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
S	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
S	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
S	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
S	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
U	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
U	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
U	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
U	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
U	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33

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Chain	Residue	Modelled	Actual	Comment	Reference
U	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
U	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
U	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
W	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
W	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
W	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
W	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
W	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
W	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
W	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
W	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
Y	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
Y	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
Y	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
Y	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
Y	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
Y	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
Y	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
Y	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
a	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
a	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
a	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
a	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
a	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
a	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
a	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
a	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
c	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
c	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
c	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
c	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
c	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
c	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
c	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
c	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	D	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	H	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	J	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	L	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	N	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	P	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	R	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	T	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	V	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	X	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	Z	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	b	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	d	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
B	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
B	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
B	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
B	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
B	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
B	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
D	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
D	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
D	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
D	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
D	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
D	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33

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Chain	Residue	Modelled	Actual	Comment	Reference
D	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
F	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
F	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
F	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
F	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
F	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
F	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
F	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
H	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
H	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
H	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
H	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
H	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
H	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
H	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
J	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
J	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
J	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
J	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
J	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
J	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
J	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
L	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
L	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
L	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
L	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
L	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
L	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
L	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
N	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
N	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
N	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
N	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
N	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
N	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
N	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
P	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
P	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
P	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
P	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
P	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
P	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33

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Chain	Residue	Modelled	Actual	Comment	Reference
P	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
R	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
R	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
R	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
R	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
R	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
R	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
R	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
T	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
T	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
T	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
T	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
T	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
T	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
T	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
V	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
V	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
V	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
V	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
V	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
V	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
V	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
X	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
X	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
X	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
X	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
X	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
X	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
X	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
Z	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
Z	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
Z	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
Z	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
Z	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
Z	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
Z	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
b	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
b	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
b	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
b	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
b	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
b	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33

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Chain	Residue	Modelled	Actual	Comment	Reference
b	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
d	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
d	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
d	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
d	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
d	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
d	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
d	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33

- 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	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	G	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	M	3	Total	C	N	O	0	0
			39	22	2	15		
3	O	3	Total	C	N	O	0	0
			39	22	2	15		
3	Q	3	Total	C	N	O	0	0
			39	22	2	15		
3	S	3	Total	C	N	O	0	0
			39	22	2	15		
3	U	3	Total	C	N	O	0	0
			39	22	2	15		
3	W	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		

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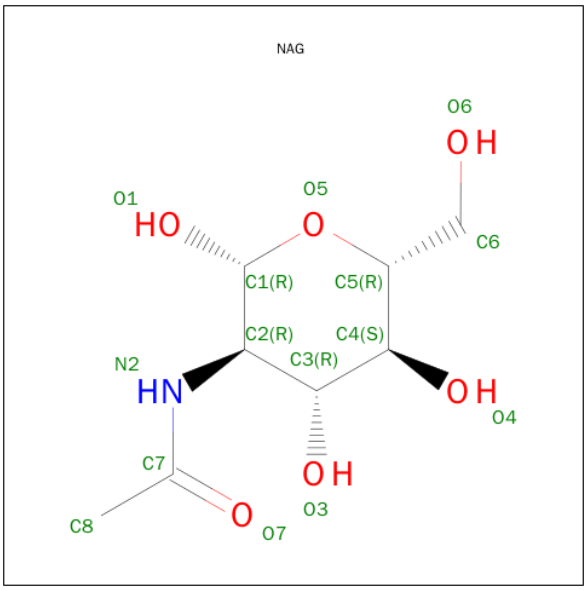
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	2	Total C N O 28 16 2 10	0	0
4	G	2	Total C N O 28 16 2 10	0	0
4	I	2	Total C N O 28 16 2 10	0	0
4	O	2	Total C N O 28 16 2 10	0	0
4	Q	2	Total C N O 28 16 2 10	0	0
4	S	2	Total C N O 28 16 2 10	0	0
4	U	2	Total C N O 28 16 2 10	0	0
4	W	2	Total C N O 28 16 2 10	0	0
4	Y	2	Total C N O 28 16 2 10	0	0
4	c	2	Total C N O 28 16 2 10	0	0

- 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	C	1	Total C N O 14 8 1 5	0	0

Continued on next page...

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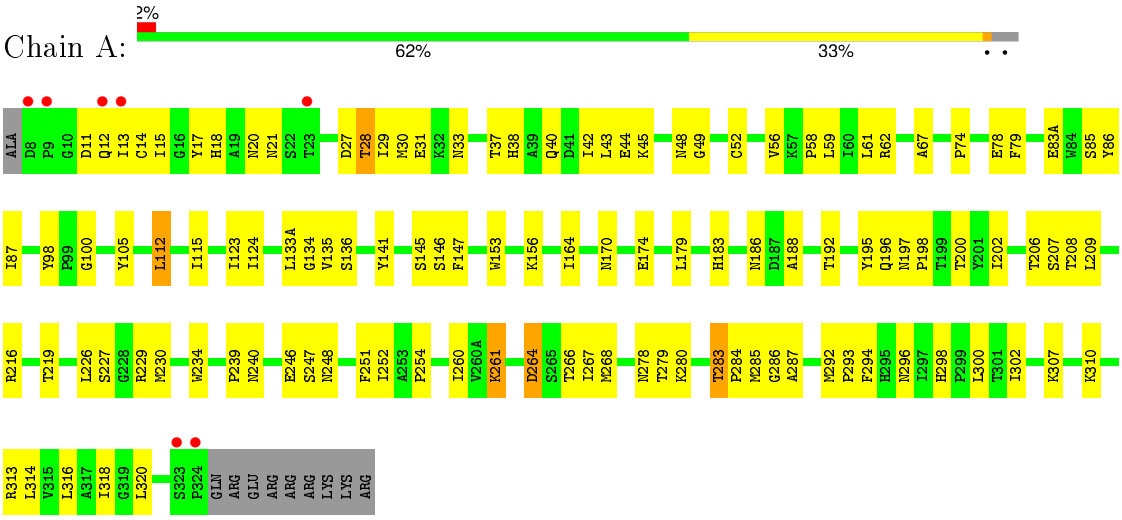
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	K	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	O	1	Total	C	N	O	0	0
			14	8	1	5		
5	Y	1	Total	C	N	O	0	0
			14	8	1	5		
5	a	1	Total	C	N	O	0	0
			14	8	1	5		
5	c	1	Total	C	N	O	0	0
			14	8	1	5		

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.

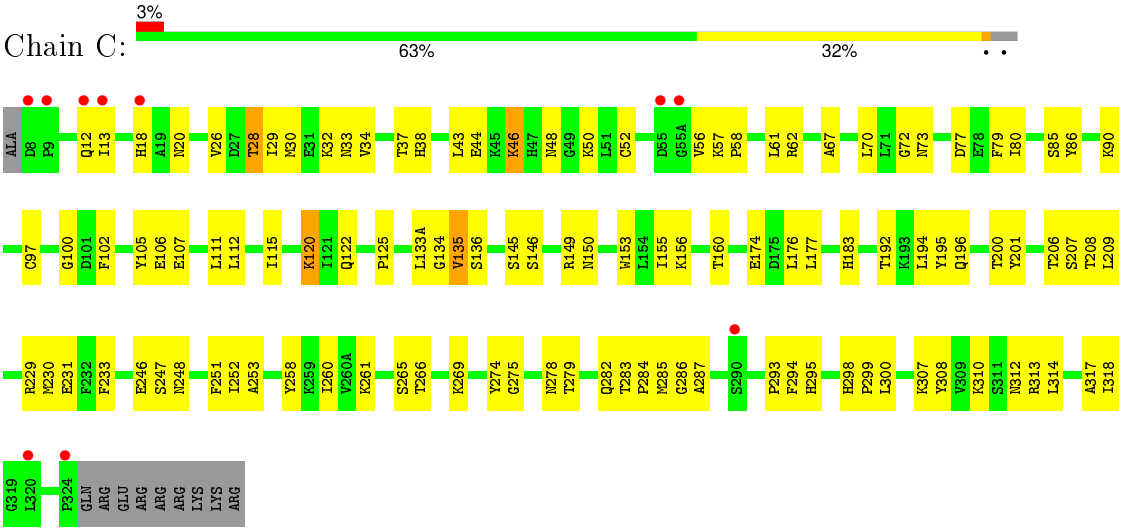
- Molecule 1: Hemagglutinin HA1 chain

Chain A:



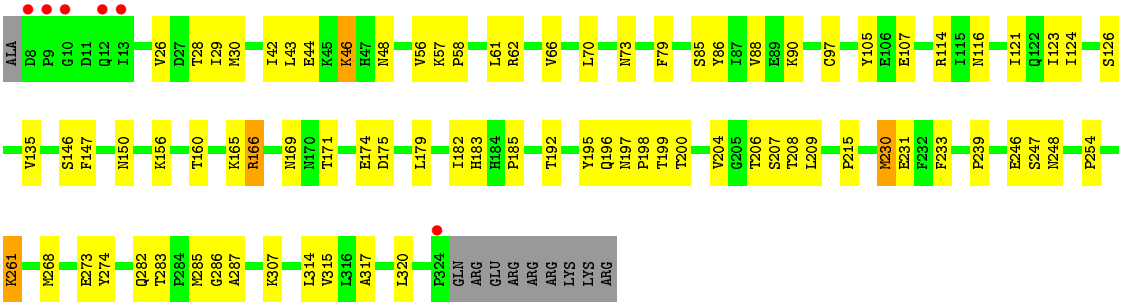
- Molecule 1: Hemagglutinin HA1 chain

Chain C:



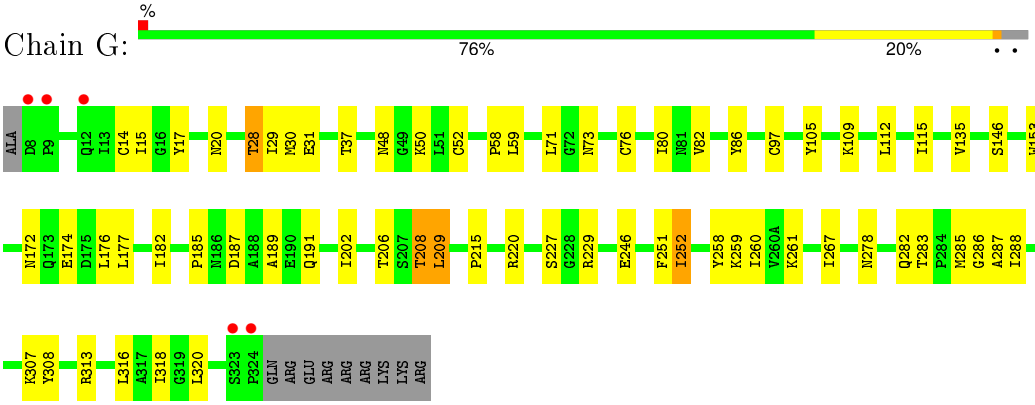
- Molecule 1: Hemagglutinin HA1 chain

Chain E:



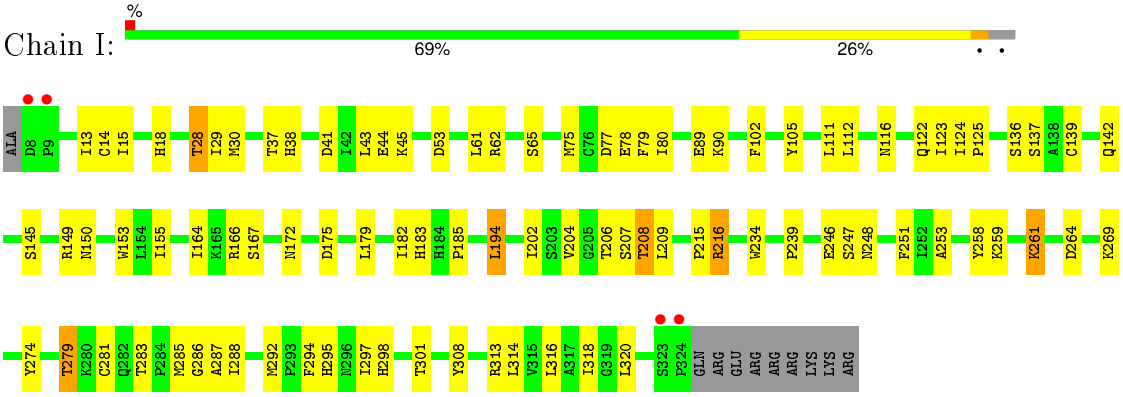
• Molecule 1: Hemagglutinin HA1 chain

Chain G:



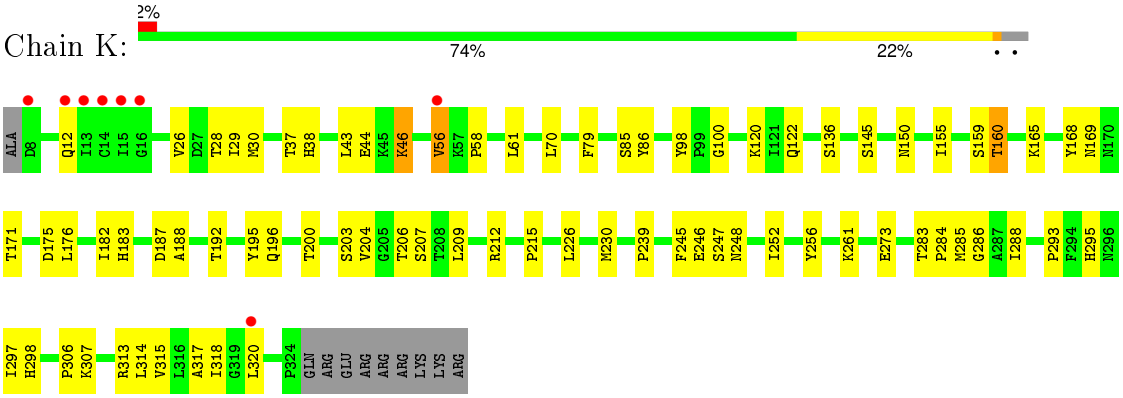
• Molecule 1: Hemagglutinin HA1 chain

Chain I:



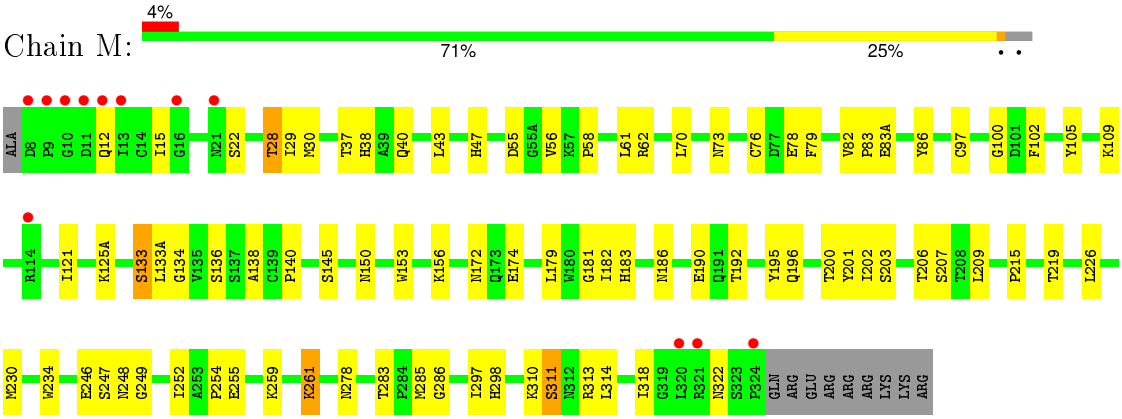
• Molecule 1: Hemagglutinin HA1 chain

Chain K:



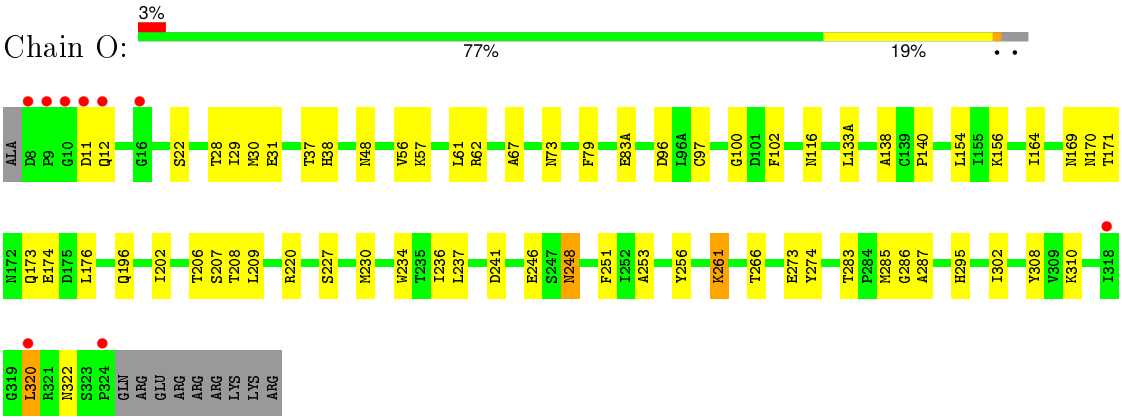
• Molecule 1: Hemagglutinin HA1 chain

Chain M:



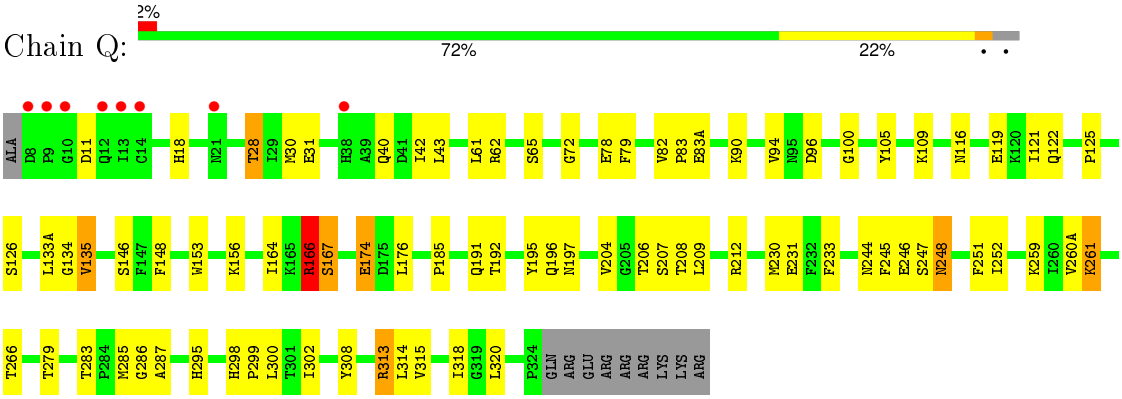
• Molecule 1: Hemagglutinin HA1 chain

Chain O:



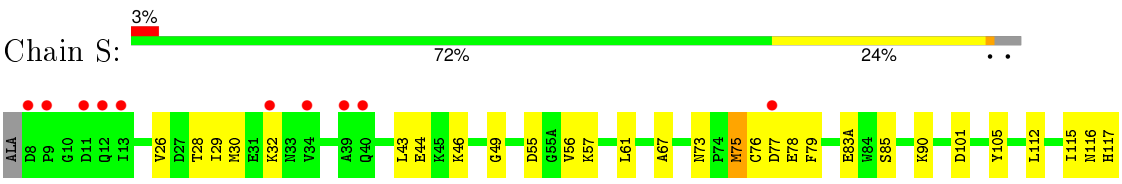
• Molecule 1: Hemagglutinin HA1 chain

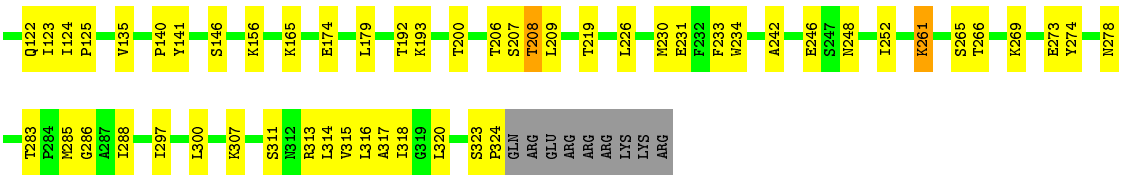
Chain Q:



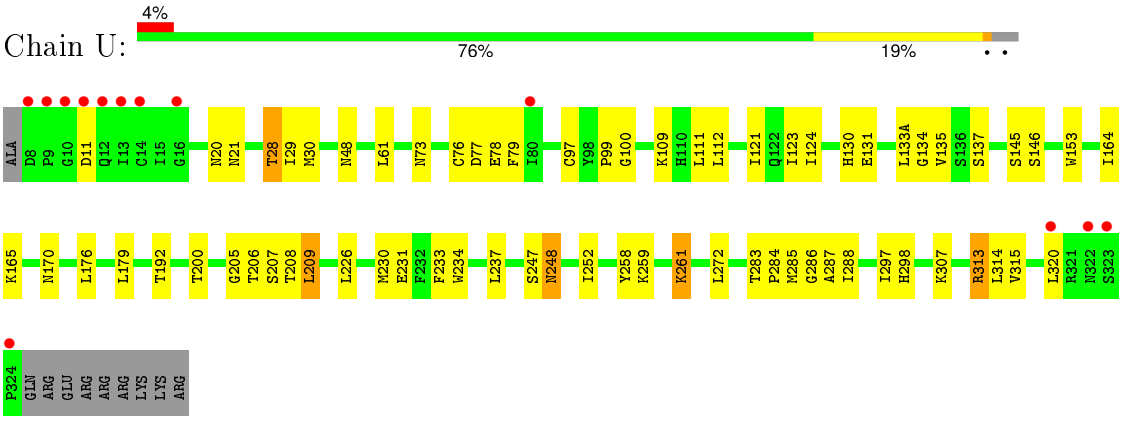
• Molecule 1: Hemagglutinin HA1 chain

Chain S:

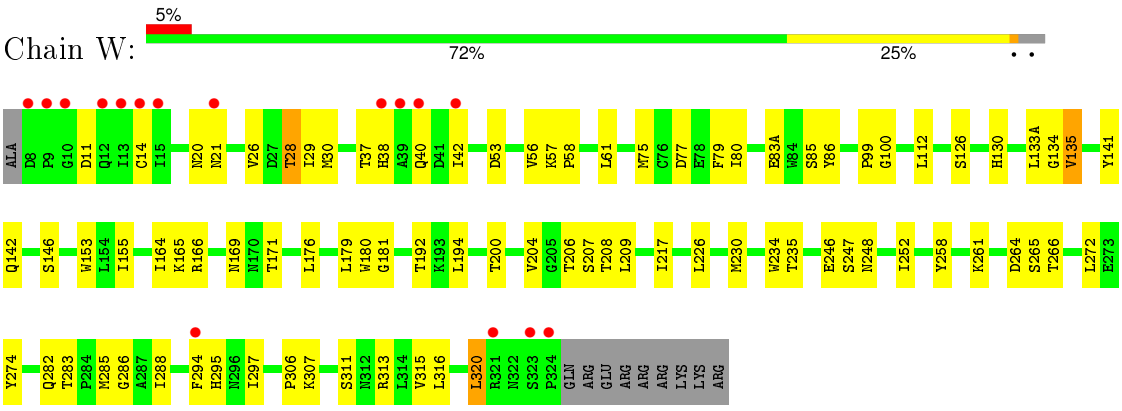




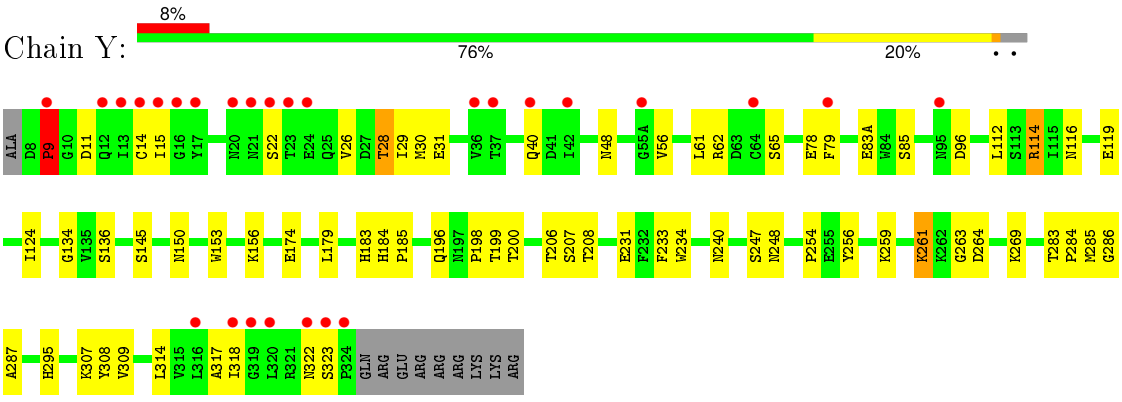
• Molecule 1: Hemagglutinin HA1 chain



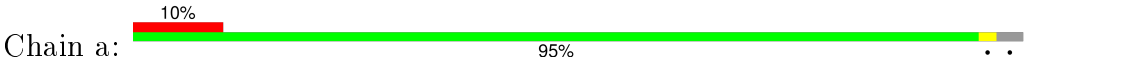
• Molecule 1: Hemagglutinin HA1 chain

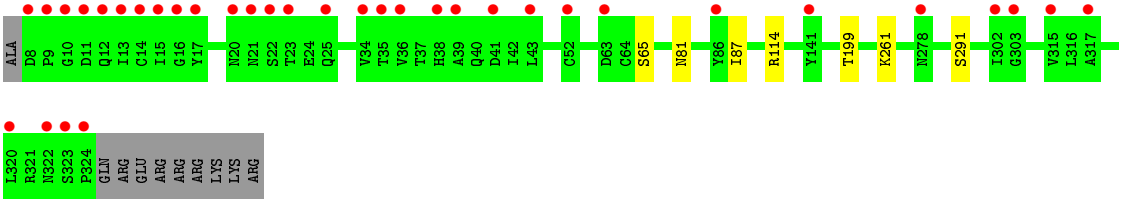


• Molecule 1: Hemagglutinin HA1 chain

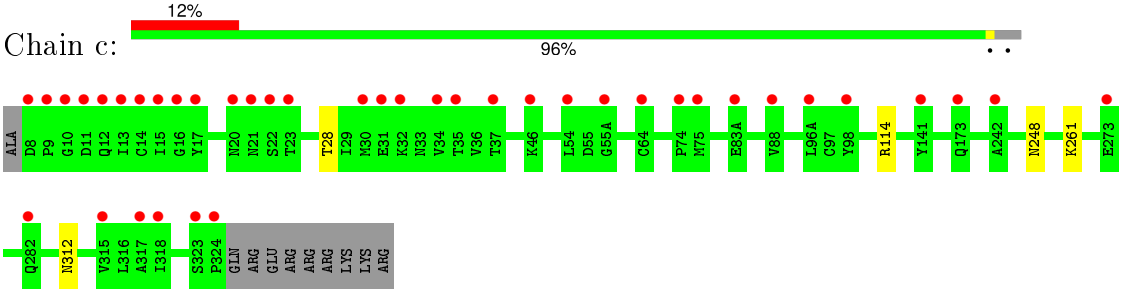


• Molecule 1: Hemagglutinin HA1 chain

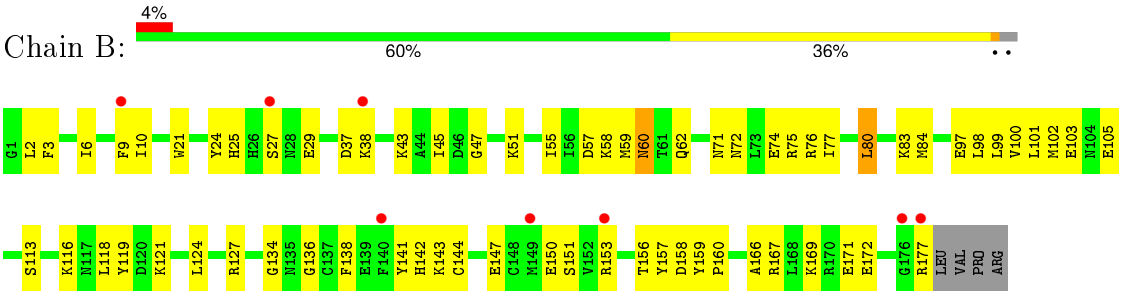




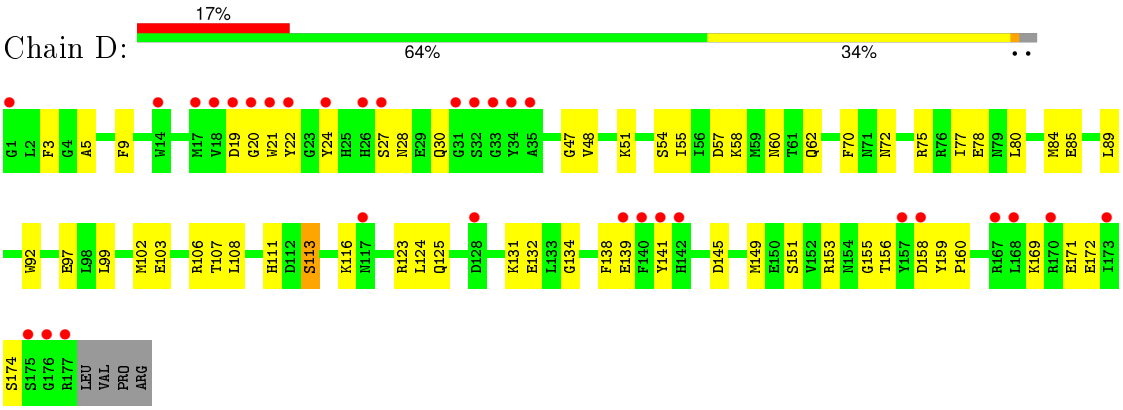
- Molecule 1: Hemagglutinin HA1 chain



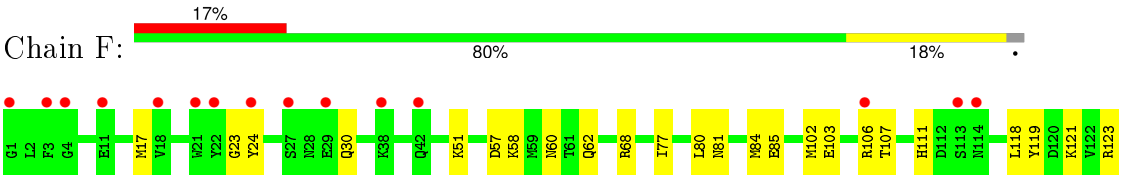
- Molecule 2: Hemagglutinin

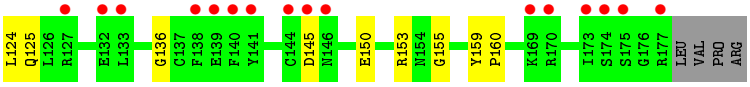


- Molecule 2: Hemagglutinin



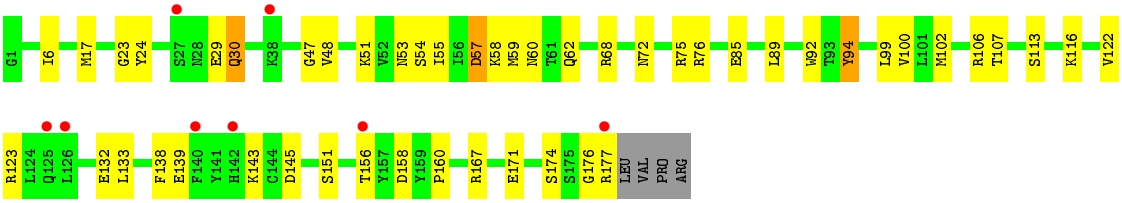
- Molecule 2: Hemagglutinin





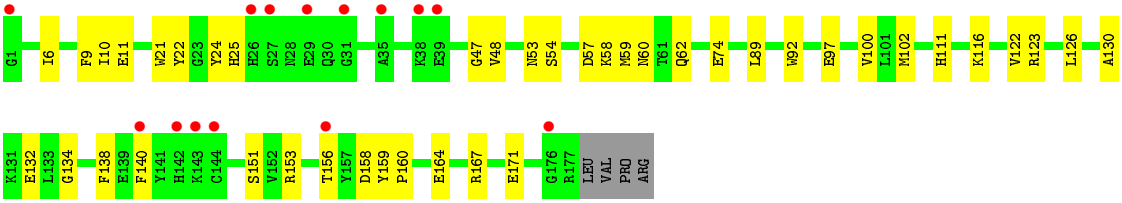
• Molecule 2: Hemagglutinin

Chain H:



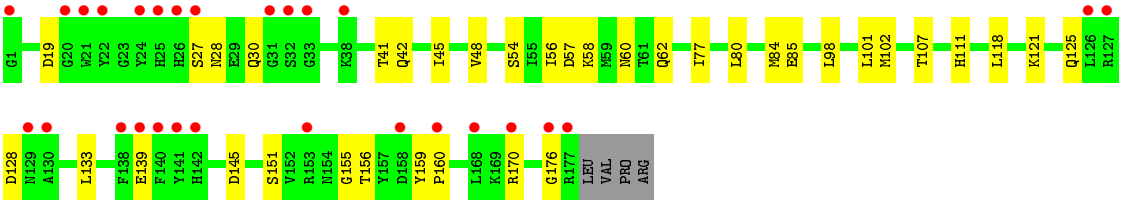
• Molecule 2: Hemagglutinin

Chain J:



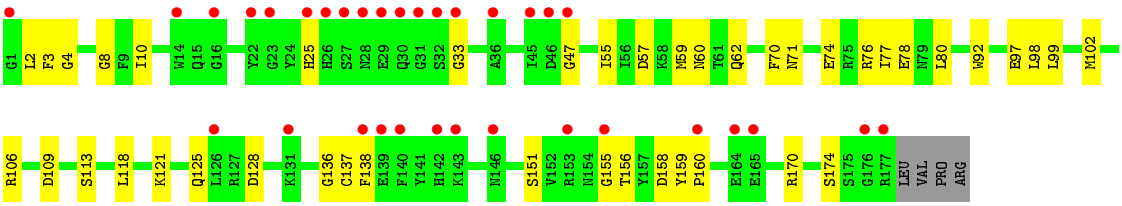
• Molecule 2: Hemagglutinin

Chain L:



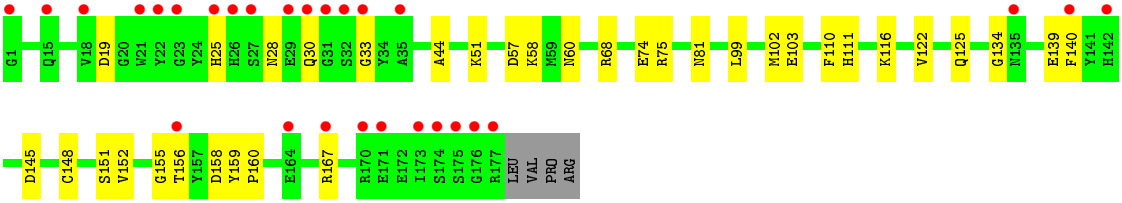
• Molecule 2: Hemagglutinin

Chain N:

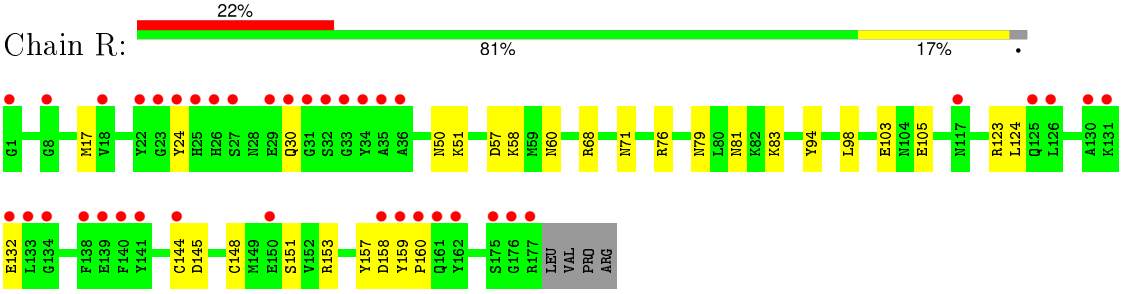


• Molecule 2: Hemagglutinin

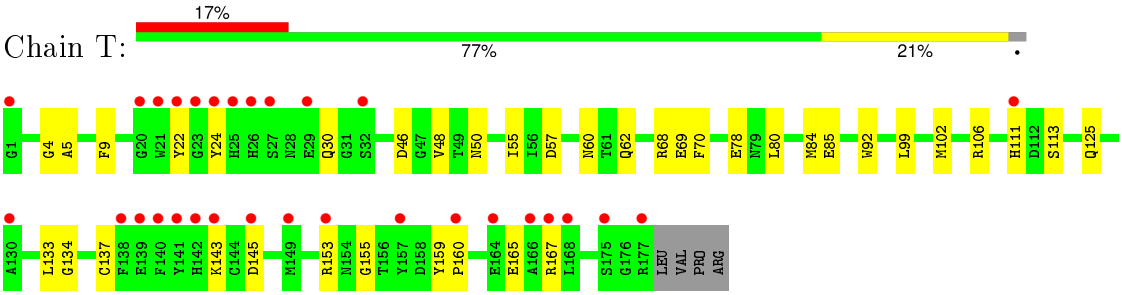
Chain P:



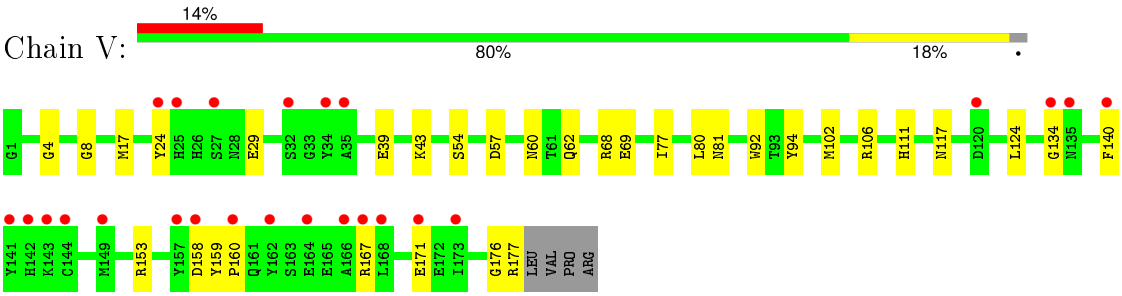
• Molecule 2: Hemagglutinin



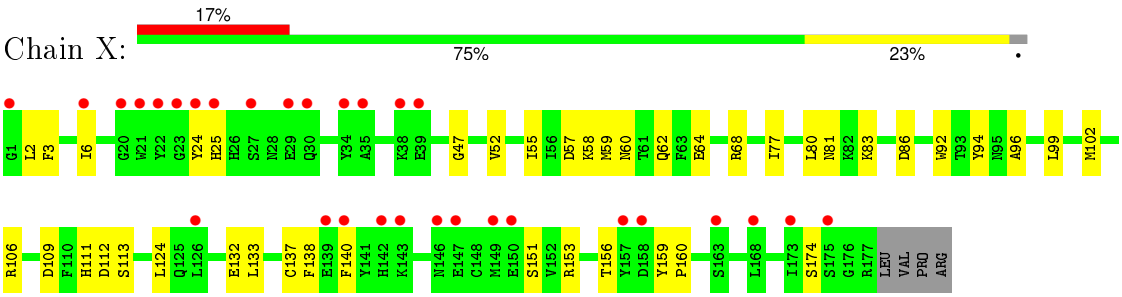
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin

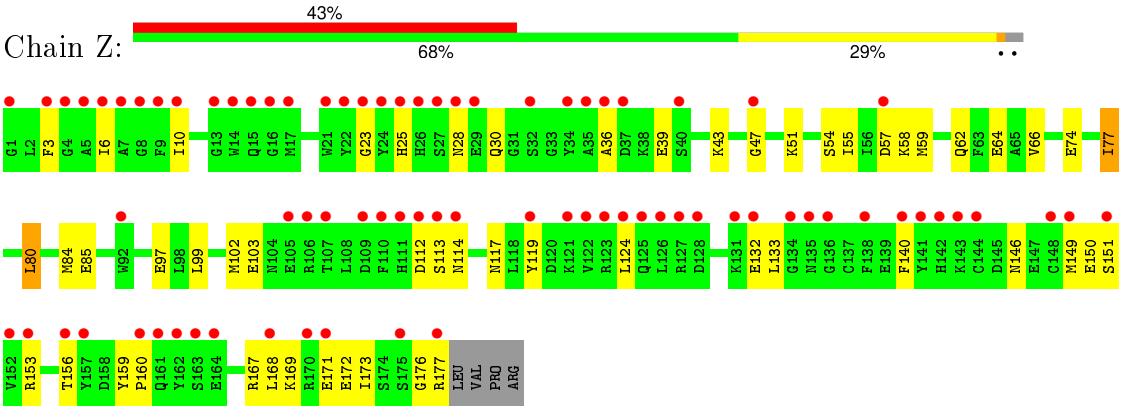


• Molecule 2: Hemagglutinin



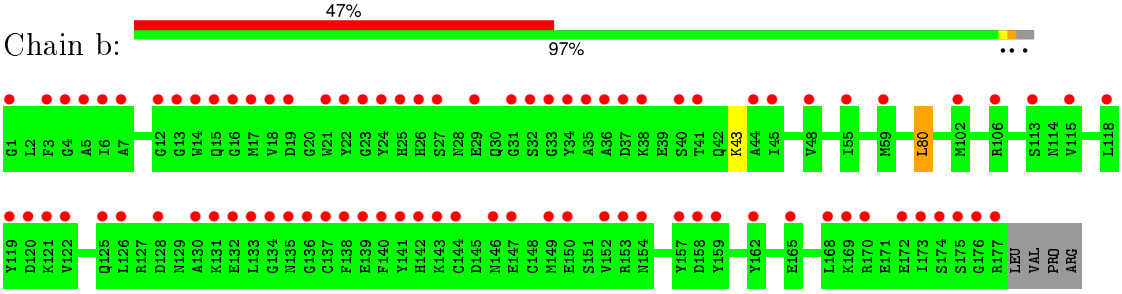
• Molecule 2: Hemagglutinin

Chain Z:



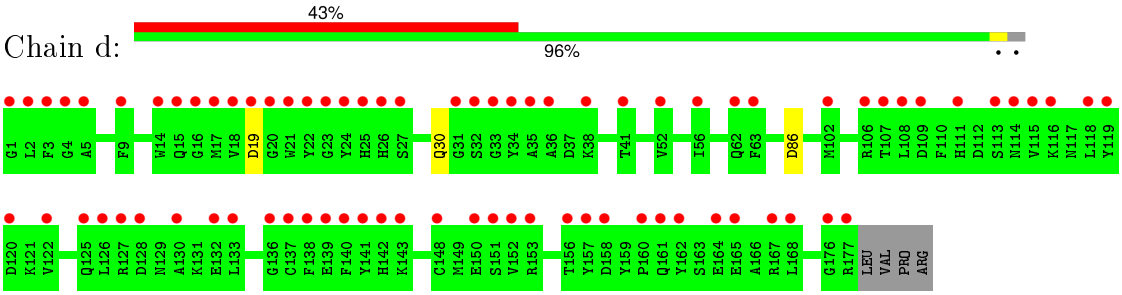
- Molecule 2: Hemagglutinin

Chain b:



- Molecule 2: Hemagglutinin

Chain d:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	117.24Å 118.94Å 273.41Å 88.43° 89.68° 60.26°	Depositor
Resolution (Å)	47.75 – 2.95 48.12 – 2.95	Depositor EDS
% Data completeness (in resolution range)	87.7 (47.75-2.95) 87.4 (48.12-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.233 , 0.281 0.245 , 0.291	Depositor DCC
R_{free} test set	11870 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	63.6	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 51.6	EDS
Estimated twinning fraction	0.013 for k,-h+k,l 0.013 for h-k,h,l 0.055 for -h+k,-h,l 0.055 for -k,h-k,l 0.067 for h,h-k,-l 0.027 for -k,-h,-l 0.012 for -h,-k,l 0.026 for -h+k,k,-l 0.017 for h-k,-k,-l 0.011 for -h,-h+k,-l 0.010 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 236037 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	60979	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.66	0/2640	0.83	0/3585
1	C	0.56	0/2640	0.75	1/3585 (0.0%)
1	E	0.59	0/2640	0.76	0/3585
1	G	0.68	1/2640 (0.0%)	0.86	6/3585 (0.2%)
1	I	0.69	1/2640 (0.0%)	0.87	2/3585 (0.1%)
1	K	0.61	0/2640	0.75	1/3585 (0.0%)
1	M	0.66	0/2640	0.80	0/3585
1	O	0.64	0/2640	0.79	1/3585 (0.0%)
1	Q	0.64	0/2640	0.82	1/3585 (0.0%)
1	S	0.57	0/2640	0.75	0/3585
1	U	0.57	0/2640	0.74	1/3585 (0.0%)
1	W	0.58	1/2640 (0.0%)	0.74	0/3585
1	Y	0.46	0/2640	0.65	1/3585 (0.0%)
1	a	0.44	0/2640	0.64	0/3585
1	c	0.44	0/2640	0.63	0/3585
2	B	0.50	0/1460	0.69	1/1961 (0.1%)
2	D	0.41	0/1460	0.56	0/1961
2	F	0.40	0/1460	0.56	0/1961
2	H	0.49	0/1460	0.64	0/1961
2	J	0.50	0/1460	0.67	0/1961
2	L	0.42	0/1460	0.54	0/1961
2	N	0.42	0/1460	0.61	0/1961
2	P	0.44	0/1460	0.60	0/1961
2	R	0.44	0/1460	0.57	0/1961
2	T	0.39	0/1460	0.57	0/1961
2	V	0.42	0/1460	0.58	0/1961
2	X	0.40	0/1460	0.59	0/1961
2	Z	0.35	0/1460	0.60	1/1961 (0.1%)
2	b	0.33	0/1460	0.56	1/1961 (0.1%)
2	d	0.36	0/1460	0.55	0/1961
All	All	0.54	3/61500 (0.0%)	0.71	17/83190 (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	Y	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	135	VAL	CB-CG2	-5.53	1.41	1.52
1	I	139	CYS	CB-SG	-5.52	1.72	1.81
1	G	153	TRP	CB-CG	5.50	1.60	1.50

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	166	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	Y	9	PRO	CA-N-CD	-7.79	100.59	111.50
1	G	229	ARG	NE-CZ-NH2	-7.40	116.60	120.30
2	Z	80	LEU	CA-CB-CG	7.16	131.78	115.30
1	G	229	ARG	NE-CZ-NH1	7.12	123.86	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Y	9	PRO	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2574	0	2525	96	0
1	C	2574	0	2525	90	0
1	E	2574	0	2525	58	0
1	G	2574	0	2525	46	0
1	I	2574	0	2525	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	2574	0	2525	55	0
1	M	2574	0	2525	56	0
1	O	2574	0	2524	45	0
1	Q	2574	0	2525	57	0
1	S	2574	0	2525	63	0
1	U	2574	0	2525	52	0
1	W	2574	0	2525	57	0
1	Y	2574	0	2525	47	0
1	a	2574	0	2526	0	0
1	c	2574	0	2525	0	0
2	B	1433	0	1340	65	0
2	D	1433	0	1340	60	0
2	F	1433	0	1340	23	0
2	H	1433	0	1340	39	0
2	J	1433	0	1340	37	0
2	L	1433	0	1340	28	0
2	N	1433	0	1340	34	0
2	P	1433	0	1340	24	0
2	R	1433	0	1340	22	0
2	T	1433	0	1340	32	0
2	V	1433	0	1340	26	0
2	X	1433	0	1340	29	0
2	Z	1433	0	1340	40	0
2	b	1433	0	1340	0	0
2	d	1433	0	1340	0	0
3	A	39	0	34	1	0
3	C	39	0	34	1	0
3	E	39	0	34	1	0
3	G	39	0	34	1	0
3	I	39	0	34	0	0
3	K	39	0	34	0	0
3	M	39	0	34	0	0
3	O	39	0	34	0	0
3	Q	39	0	34	0	0
3	S	39	0	34	1	0
3	U	39	0	34	0	0
3	W	39	0	34	0	0
4	A	28	0	25	0	0
4	E	28	0	25	0	0
4	G	28	0	25	1	0
4	I	28	0	25	1	0
4	O	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	28	0	25	1	0
4	S	28	0	25	1	0
4	U	28	0	25	0	0
4	W	28	0	25	1	0
4	Y	28	0	25	1	0
4	c	28	0	25	0	0
5	C	14	0	13	0	0
5	K	14	0	13	0	0
5	M	14	0	13	0	0
5	O	14	0	13	0	0
5	Y	14	0	13	1	0
5	a	14	0	13	0	0
5	c	14	0	13	0	0
All	All	60979	0	58749	1073	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 9.

The worst 5 of 1073 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:K:192:THR:HG21	1:S:192:THR:HG21	1.34	1.08
1:I:283:THR:HG22	1:I:285:MET:H	1.26	1.00
1:Q:283:THR:HG22	1:Q:285:MET:H	1.25	1.00
1:G:283:THR:HG22	1:G:285:MET:H	1.27	0.99
1:U:206:THR:HG22	1:U:208:THR:H	1.25	0.98

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	323/334 (97%)	301 (93%)	22 (7%)	0	100	100
1	C	323/334 (97%)	305 (94%)	18 (6%)	0	100	100
1	E	323/334 (97%)	302 (94%)	21 (6%)	0	100	100
1	G	323/334 (97%)	304 (94%)	19 (6%)	0	100	100
1	I	323/334 (97%)	301 (93%)	22 (7%)	0	100	100
1	K	323/334 (97%)	304 (94%)	19 (6%)	0	100	100
1	M	323/334 (97%)	301 (93%)	22 (7%)	0	100	100
1	O	323/334 (97%)	303 (94%)	19 (6%)	1 (0%)	46	81
1	Q	323/334 (97%)	300 (93%)	22 (7%)	1 (0%)	46	81
1	S	323/334 (97%)	299 (93%)	24 (7%)	0	100	100
1	U	323/334 (97%)	305 (94%)	16 (5%)	2 (1%)	30	70
1	W	323/334 (97%)	304 (94%)	19 (6%)	0	100	100
1	Y	323/334 (97%)	303 (94%)	20 (6%)	0	100	100
1	a	323/334 (97%)	299 (93%)	24 (7%)	0	100	100
1	c	323/334 (97%)	301 (93%)	21 (6%)	1 (0%)	46	81
2	B	175/181 (97%)	166 (95%)	8 (5%)	1 (1%)	30	70
2	D	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
2	F	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
2	H	175/181 (97%)	166 (95%)	9 (5%)	0	100	100
2	J	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
2	L	175/181 (97%)	164 (94%)	10 (6%)	1 (1%)	30	70
2	N	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
2	P	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
2	R	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
2	T	175/181 (97%)	166 (95%)	9 (5%)	0	100	100
2	V	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
2	X	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
2	Z	175/181 (97%)	164 (94%)	10 (6%)	1 (1%)	30	70
2	b	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
2	d	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
All	All	7470/7725 (97%)	7003 (94%)	459 (6%)	8 (0%)	56	89

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	77	ASP
1	O	248	ASN
1	Q	248	ASN
1	c	248	ASN
2	B	60	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	292/300 (97%)	282 (97%)	10 (3%)	44	79
1	C	292/300 (97%)	285 (98%)	7 (2%)	57	86
1	E	292/300 (97%)	284 (97%)	8 (3%)	52	84
1	G	292/300 (97%)	285 (98%)	7 (2%)	57	86
1	I	292/300 (97%)	277 (95%)	15 (5%)	29	67
1	K	292/300 (97%)	284 (97%)	8 (3%)	52	84
1	M	292/300 (97%)	284 (97%)	8 (3%)	52	84
1	O	292/300 (97%)	284 (97%)	8 (3%)	52	84
1	Q	292/300 (97%)	282 (97%)	10 (3%)	44	79
1	S	292/300 (97%)	285 (98%)	7 (2%)	57	86
1	U	292/300 (97%)	287 (98%)	5 (2%)	68	90
1	W	292/300 (97%)	284 (97%)	8 (3%)	52	84
1	Y	292/300 (97%)	286 (98%)	6 (2%)	61	88
1	a	292/300 (97%)	285 (98%)	7 (2%)	57	86
1	c	292/300 (97%)	288 (99%)	4 (1%)	74	92
2	B	151/155 (97%)	150 (99%)	1 (1%)	88	96
2	D	151/155 (97%)	150 (99%)	1 (1%)	88	96
2	F	151/155 (97%)	151 (100%)	0	100	100
2	H	151/155 (97%)	148 (98%)	3 (2%)	63	88
2	J	151/155 (97%)	150 (99%)	1 (1%)	88	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	L	151/155 (97%)	151 (100%)	0	100 100
2	N	151/155 (97%)	151 (100%)	0	100 100
2	P	151/155 (97%)	150 (99%)	1 (1%)	88 96
2	R	151/155 (97%)	149 (99%)	2 (1%)	76 92
2	T	151/155 (97%)	151 (100%)	0	100 100
2	V	151/155 (97%)	148 (98%)	3 (2%)	63 88
2	X	151/155 (97%)	149 (99%)	2 (1%)	76 92
2	Z	151/155 (97%)	146 (97%)	5 (3%)	45 80
2	b	151/155 (97%)	149 (99%)	2 (1%)	76 92
2	d	151/155 (97%)	148 (98%)	3 (2%)	63 88
All	All	6645/6825 (97%)	6503 (98%)	142 (2%)	61 88

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	176	LEU
1	Q	313	ARG
2	X	94	TYR
1	O	248	ASN
1	Q	94	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	322	ASN
1	Q	196	GLN
2	V	117	ASN
1	O	150	ASN
1	Q	117	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

58 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	2001	1,3	14,14,15	1.06	1 (7%)	15,19,21	1.00	1 (6%)
3	NAG	A	2002	3	14,14,15	0.30	0	15,19,21	0.47	0
3	BMA	A	2003	3	11,11,12	1.65	3 (27%)	14,15,17	1.37	3 (21%)
4	NAG	A	2004	1,4	14,14,15	0.99	1 (7%)	15,19,21	1.22	2 (13%)
4	NAG	A	2005	4	14,14,15	1.44	2 (14%)	15,19,21	1.27	1 (6%)
3	NAG	C	2001	1,3	14,14,15	0.34	0	15,19,21	0.52	0
3	NAG	C	2002	3	14,14,15	0.58	0	15,19,21	0.58	0
3	BMA	C	2003	3	11,11,12	2.11	4 (36%)	14,15,17	1.63	4 (28%)
3	NAG	E	2001	1,3	14,14,15	0.65	1 (7%)	15,19,21	1.01	1 (6%)
3	NAG	E	2002	3	14,14,15	1.24	1 (7%)	15,19,21	1.27	2 (13%)
3	BMA	E	2003	3	11,11,12	1.55	1 (9%)	14,15,17	1.79	3 (21%)
4	NAG	E	2004	1,4	14,14,15	1.19	1 (7%)	15,19,21	1.42	3 (20%)
4	NAG	E	2005	4	14,14,15	0.67	1 (7%)	15,19,21	0.33	0
3	NAG	G	2001	1,3	14,14,15	1.62	1 (7%)	15,19,21	1.31	2 (13%)
3	NAG	G	2002	3	14,14,15	0.86	1 (7%)	15,19,21	0.68	0
3	BMA	G	2003	3	11,11,12	1.97	4 (36%)	14,15,17	1.22	1 (7%)
4	NAG	G	2004	1,4	14,14,15	1.25	1 (7%)	15,19,21	1.41	2 (13%)
4	NAG	G	2005	4	14,14,15	0.63	0	15,19,21	0.32	0
3	NAG	I	2001	1,3	14,14,15	1.39	1 (7%)	15,19,21	1.26	3 (20%)
3	NAG	I	2002	3	14,14,15	1.00	1 (7%)	15,19,21	0.83	1 (6%)
3	BMA	I	2003	3	11,11,12	2.37	5 (45%)	14,15,17	1.74	3 (21%)
4	NAG	I	2004	1,4	14,14,15	0.77	1 (7%)	15,19,21	1.14	2 (13%)
4	NAG	I	2005	4	14,14,15	1.60	2 (14%)	15,19,21	0.94	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	K	2001	1,3	14,14,15	0.63	1 (7%)	15,19,21	0.70	1 (6%)
3	NAG	K	2002	3	14,14,15	0.43	0	15,19,21	0.75	0
3	BMA	K	2003	3	11,11,12	2.18	4 (36%)	14,15,17	1.71	3 (21%)
3	NAG	M	2001	1,3	14,14,15	0.59	0	15,19,21	0.54	0
3	NAG	M	2002	3	14,14,15	0.92	1 (7%)	15,19,21	0.84	1 (6%)
3	BMA	M	2003	3	11,11,12	1.95	3 (27%)	14,15,17	1.60	3 (21%)
3	NAG	O	2001	1,3	14,14,15	0.35	0	15,19,21	0.94	1 (6%)
3	NAG	O	2002	3	14,14,15	0.64	1 (7%)	15,19,21	0.30	0
3	BMA	O	2003	3	11,11,12	1.60	3 (27%)	14,15,17	1.41	3 (21%)
4	NAG	O	2004	1,4	14,14,15	1.16	1 (7%)	15,19,21	1.09	2 (13%)
4	NAG	O	2005	4	14,14,15	0.43	0	15,19,21	0.70	1 (6%)
3	NAG	Q	2001	1,3	14,14,15	0.61	1 (7%)	15,19,21	0.74	1 (6%)
3	NAG	Q	2002	3	14,14,15	0.21	0	15,19,21	0.48	0
3	BMA	Q	2003	3	11,11,12	0.70	0	14,15,17	2.03	4 (28%)
4	NAG	Q	2004	1,4	14,14,15	1.12	1 (7%)	15,19,21	0.99	0
4	NAG	Q	2005	4	14,14,15	0.48	0	15,19,21	0.46	0
3	NAG	S	2001	1,3	14,14,15	0.29	0	15,19,21	0.72	1 (6%)
3	NAG	S	2002	3	14,14,15	0.48	0	15,19,21	0.73	0
3	BMA	S	2003	3	11,11,12	1.98	2 (18%)	14,15,17	2.03	5 (35%)
4	NAG	S	2004	1,4	14,14,15	0.53	0	15,19,21	0.68	0
4	NAG	S	2005	4	14,14,15	1.52	2 (14%)	15,19,21	1.13	1 (6%)
3	NAG	U	2001	1,3	14,14,15	0.42	0	15,19,21	0.51	0
3	NAG	U	2002	3	14,14,15	1.48	2 (14%)	15,19,21	0.91	1 (6%)
3	BMA	U	2003	3	11,11,12	1.14	0	14,15,17	1.86	2 (14%)
4	NAG	U	2004	1,4	14,14,15	0.45	0	15,19,21	0.47	0
4	NAG	U	2005	4	14,14,15	0.39	0	15,19,21	0.30	0
3	NAG	W	2001	1,3	14,14,15	0.59	0	15,19,21	1.06	2 (13%)
3	NAG	W	2002	3	14,14,15	0.57	0	15,19,21	0.88	0
3	BMA	W	2003	3	11,11,12	0.57	0	14,15,17	0.79	0
4	NAG	W	2004	1,4	14,14,15	1.31	1 (7%)	15,19,21	1.44	3 (20%)
4	NAG	W	2005	4	14,14,15	0.69	0	15,19,21	0.63	0
4	NAG	Y	2002	1,4	14,14,15	0.36	0	15,19,21	0.25	0
4	NAG	Y	2003	4	14,14,15	0.33	0	15,19,21	0.44	0
4	NAG	c	2002	1,4	14,14,15	0.59	0	15,19,21	0.98	1 (6%)
4	NAG	c	2003	4	14,14,15	0.42	0	15,19,21	0.35	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
3	NAG	A	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2002	3	-	0/6/23/26	0/1/1/1
3	BMA	A	2003	3	-	0/2/19/22	0/1/1/1
4	NAG	A	2004	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2005	4	-	0/6/23/26	0/1/1/1
3	NAG	C	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2002	3	-	0/6/23/26	0/1/1/1
3	BMA	C	2003	3	-	0/2/19/22	0/1/1/1
3	NAG	E	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2002	3	-	0/6/23/26	0/1/1/1
3	BMA	E	2003	3	-	0/2/19/22	0/1/1/1
4	NAG	E	2004	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2005	4	-	0/6/23/26	0/1/1/1
3	NAG	G	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2002	3	-	0/6/23/26	0/1/1/1
3	BMA	G	2003	3	-	0/2/19/22	0/1/1/1
4	NAG	G	2004	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2005	4	-	0/6/23/26	0/1/1/1
3	NAG	I	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2002	3	-	0/6/23/26	0/1/1/1
3	BMA	I	2003	3	-	0/2/19/22	0/1/1/1
4	NAG	I	2004	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2005	4	-	0/6/23/26	0/1/1/1
3	NAG	K	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2002	3	-	0/6/23/26	0/1/1/1
3	BMA	K	2003	3	-	0/2/19/22	0/1/1/1
3	NAG	M	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	2002	3	-	0/6/23/26	0/1/1/1
3	BMA	M	2003	3	-	0/2/19/22	0/1/1/1
3	NAG	O	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	O	2002	3	-	0/6/23/26	0/1/1/1
3	BMA	O	2003	3	-	0/2/19/22	0/1/1/1
4	NAG	O	2004	1,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2005	4	-	0/6/23/26	0/1/1/1
3	NAG	Q	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Q	2002	3	-	0/6/23/26	0/1/1/1
3	BMA	Q	2003	3	-	0/2/19/22	0/1/1/1
4	NAG	Q	2004	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	2005	4	-	0/6/23/26	0/1/1/1
3	NAG	S	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	S	2002	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	S	2003	3	-	0/2/19/22	0/1/1/1
4	NAG	S	2004	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	2005	4	-	0/6/23/26	0/1/1/1
3	NAG	U	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	U	2002	3	-	0/6/23/26	0/1/1/1
3	BMA	U	2003	3	-	0/2/19/22	0/1/1/1
4	NAG	U	2004	1,4	-	0/6/23/26	0/1/1/1
4	NAG	U	2005	4	-	0/6/23/26	0/1/1/1
3	NAG	W	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	W	2002	3	-	0/6/23/26	0/1/1/1
3	BMA	W	2003	3	-	0/2/19/22	0/1/1/1
4	NAG	W	2004	1,4	-	0/6/23/26	0/1/1/1
4	NAG	W	2005	4	-	0/6/23/26	0/1/1/1
4	NAG	Y	2002	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Y	2003	4	-	0/6/23/26	0/1/1/1
4	NAG	c	2002	1,4	-	0/6/23/26	0/1/1/1
4	NAG	c	2003	4	-	0/6/23/26	0/1/1/1

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2001	NAG	O5-C1	-5.56	1.34	1.43
3	U	2002	NAG	O5-C1	-4.81	1.35	1.43
4	S	2005	NAG	O5-C1	-4.74	1.35	1.43
3	I	2001	NAG	O5-C1	-4.71	1.35	1.43
4	W	2004	NAG	O5-C1	-4.58	1.36	1.43

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Q	2003	BMA	O5-C1-C2	-3.37	105.39	110.86
3	Q	2003	BMA	O3-C3-C4	-3.36	102.78	110.34
3	M	2002	NAG	C1-O5-C5	-2.73	108.78	112.25
3	E	2003	BMA	O2-C2-C3	-2.64	104.80	110.12
4	E	2004	NAG	C1-O5-C5	-2.60	108.94	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	NAG	1	0
3	C	2002	NAG	1	0
3	E	2001	NAG	1	0
3	E	2002	NAG	1	0
3	G	2001	NAG	1	0
4	G	2004	NAG	1	0
4	G	2005	NAG	1	0
4	I	2004	NAG	1	0
4	I	2005	NAG	1	0
4	Q	2004	NAG	1	0
4	Q	2005	NAG	1	0
3	S	2001	NAG	1	0
4	S	2004	NAG	1	0
4	S	2005	NAG	1	0
4	W	2004	NAG	1	0
4	W	2005	NAG	1	0
4	Y	2002	NAG	1	0
4	Y	2003	NAG	1	0

5.6 Ligand geometry (i)

7 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	C	2004	1	14,14,15	0.86	1 (7%)	15,19,21	0.87	0
5	NAG	K	2004	1	14,14,15	0.63	0	15,19,21	0.46	0
5	NAG	M	2004	1	14,14,15	0.30	0	15,19,21	0.30	0
5	NAG	O	2006	1	14,14,15	0.98	1 (7%)	15,19,21	0.98	2 (13%)
5	NAG	Y	2001	1	14,14,15	0.35	0	15,19,21	1.01	1 (6%)
5	NAG	a	2001	1	14,14,15	0.58	0	15,19,21	0.66	1 (6%)
5	NAG	c	2001	1	14,14,15	0.62	1 (7%)	15,19,21	0.54	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
5	NAG	C	2004	1	-	0/6/23/26	0/1/1/1
5	NAG	K	2004	1	-	0/6/23/26	0/1/1/1
5	NAG	M	2004	1	-	0/6/23/26	0/1/1/1
5	NAG	O	2006	1	-	0/6/23/26	0/1/1/1
5	NAG	Y	2001	1	-	0/6/23/26	0/1/1/1
5	NAG	a	2001	1	-	0/6/23/26	0/1/1/1
5	NAG	c	2001	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	2006	NAG	O5-C1	-2.93	1.38	1.43
5	C	2004	NAG	O5-C1	-2.46	1.39	1.43
5	c	2001	NAG	O5-C1	-2.11	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	a	2001	NAG	C1-O5-C5	2.29	115.15	112.25
5	O	2006	NAG	C3-C4-C5	2.37	114.34	110.20
5	O	2006	NAG	C4-C3-C2	2.46	115.06	111.23
5	Y	2001	NAG	C1-O5-C5	3.64	116.86	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Y	2001	NAG	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^{th} 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	324/334 (97%)	-0.18	7 (2%) 65 44	32, 52, 87, 162	0
1	C	324/334 (97%)	0.04	10 (3%) 52 33	38, 63, 124, 185	0
1	E	324/334 (97%)	-0.03	6 (1%) 70 50	36, 58, 115, 196	0
1	G	324/334 (97%)	-0.15	5 (1%) 76 57	28, 51, 92, 170	0
1	I	324/334 (97%)	-0.12	4 (1%) 81 63	27, 49, 94, 166	0
1	K	324/334 (97%)	-0.04	8 (2%) 61 39	37, 59, 112, 178	0
1	M	324/334 (97%)	-0.16	12 (3%) 45 27	28, 54, 114, 206	0
1	O	324/334 (97%)	-0.07	9 (2%) 56 36	32, 54, 117, 190	0
1	Q	324/334 (97%)	-0.13	8 (2%) 61 39	34, 53, 117, 181	0
1	S	324/334 (97%)	-0.10	10 (3%) 52 33	37, 63, 128, 177	0
1	U	324/334 (97%)	0.05	13 (4%) 42 25	36, 66, 124, 186	0
1	W	324/334 (97%)	0.12	16 (4%) 33 19	41, 64, 125, 183	0
1	Y	324/334 (97%)	0.58	27 (8%) 14 7	57, 83, 178, 247	0
1	a	324/334 (97%)	0.59	35 (10%) 8 4	59, 86, 197, 263	0
1	c	324/334 (97%)	0.60	40 (12%) 5 2	55, 87, 184, 267	0
2	B	177/181 (97%)	0.27	8 (4%) 37 21	36, 94, 134, 165	0
2	D	177/181 (97%)	0.97	31 (17%) 2 1	42, 124, 175, 199	0
2	F	177/181 (97%)	0.88	31 (17%) 2 1	45, 123, 173, 182	0
2	H	177/181 (97%)	0.24	8 (4%) 37 21	35, 97, 139, 151	0
2	J	177/181 (97%)	0.45	14 (7%) 15 8	36, 95, 136, 152	0
2	L	177/181 (97%)	0.89	28 (15%) 3 1	42, 123, 163, 171	0
2	N	177/181 (97%)	0.94	33 (18%) 2 1	37, 123, 176, 197	0
2	P	177/181 (97%)	0.81	28 (15%) 3 1	31, 120, 174, 185	0
2	R	177/181 (97%)	1.10	39 (22%) 1 1	42, 122, 189, 220	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
2	T	177/181 (97%)	0.74	30 (16%)	2 1	48, 123, 166, 184	0
2	V	177/181 (97%)	0.76	25 (14%)	4 2	45, 123, 167, 180	0
2	X	177/181 (97%)	0.88	30 (16%)	2 1	47, 123, 171, 182	0
2	Z	177/181 (97%)	2.49	78 (44%)	0 0	68, 193, 265, 299	0
2	b	177/181 (97%)	2.89	85 (48%)	0 0	74, 189, 251, 272	0
2	d	177/181 (97%)	2.57	78 (44%)	0 0	68, 193, 239, 274	0
All	All	7515/7725 (97%)	0.44	756 (10%)	9 5	27, 75, 185, 299	0

The worst 5 of 756 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Y	16	GLY	35.5
2	b	16	GLY	29.2
2	Z	23	GLY	27.5
1	c	16	GLY	18.1
2	Z	24	TYR	16.1

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
3	NAG	M	2001	14/15	0.94	0.15	3.59	50,58,79,79	0
3	NAG	U	2001	14/15	0.88	0.22	1.79	59,71,87,99	0
3	NAG	E	2001	14/15	0.93	0.24	1.28	74,93,116,124	0
3	NAG	W	2001	14/15	0.85	0.16	0.81	64,71,80,92	0
3	NAG	O	2001	14/15	0.89	0.19	0.38	58,72,90,97	0
3	NAG	C	2001	14/15	0.90	0.23	0.20	70,89,102,112	0
3	NAG	S	2001	14/15	0.94	0.13	-0.07	57,81,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	G	2001	14/15	0.93	0.16	-0.18	57,65,73,85	0
3	NAG	Q	2001	14/15	0.94	0.14	-0.64	52,67,75,77	0
3	NAG	A	2001	14/15	0.92	0.13	-0.65	49,69,79,82	0
3	NAG	I	2001	14/15	0.93	0.13	-0.99	50,58,78,80	0
4	NAG	I	2004	14/15	0.91	0.17	-	89,94,103,109	0
3	BMA	U	2003	11/12	0.73	0.30	-	114,127,131,133	0
3	NAG	M	2002	14/15	0.83	0.24	-	76,91,113,128	0
4	NAG	U	2005	14/15	0.83	0.20	-	136,154,160,165	0
3	NAG	S	2002	14/15	0.81	0.18	-	87,110,127,135	0
3	BMA	O	2003	11/12	0.79	0.14	-	119,127,132,132	0
3	NAG	Q	2002	14/15	0.93	0.11	-	67,88,103,115	0
3	BMA	C	2003	11/12	0.82	0.24	-	48,70,90,94	0
4	NAG	A	2005	14/15	0.62	0.18	-	112,122,129,132	0
4	NAG	S	2005	14/15	0.81	0.18	-	150,164,166,166	0
3	NAG	I	2002	14/15	0.95	0.12	-	44,57,67,71	0
4	NAG	Q	2005	14/15	0.76	0.26	-	120,148,158,161	0
3	BMA	W	2003	11/12	0.74	0.17	-	113,124,130,135	0
4	NAG	O	2004	14/15	0.80	0.15	-	123,134,139,143	0
4	NAG	Y	2002	14/15	0.85	0.20	-	155,161,168,175	0
4	NAG	O	2005	14/15	0.68	0.20	-	117,139,146,146	0
3	NAG	U	2002	14/15	0.81	0.19	-	89,104,121,126	0
4	NAG	S	2004	14/15	0.78	0.18	-	128,150,163,163	0
3	NAG	C	2002	14/15	0.86	0.30	-	98,106,110,110	0
3	BMA	M	2003	11/12	0.65	0.22	-	105,121,134,135	0
3	NAG	K	2002	14/15	0.91	0.25	-	81,97,102,102	0
4	NAG	W	2005	14/15	0.83	0.19	-	122,134,141,141	0
3	BMA	A	2003	11/12	0.83	0.17	-	81,83,101,101	0
3	NAG	G	2002	14/15	0.92	0.13	-	49,63,83,84	0
4	NAG	E	2005	14/15	0.81	0.20	-	106,128,134,134	0
4	NAG	U	2004	14/15	0.74	0.17	-	130,142,151,153	0
4	NAG	Q	2004	14/15	0.84	0.14	-	101,118,133,146	0
4	NAG	G	2004	14/15	0.88	0.13	-	102,107,113,114	0
3	BMA	Q	2003	11/12	0.85	0.12	-	116,120,126,127	0
3	NAG	W	2002	14/15	0.80	0.23	-	77,96,107,119	0
3	NAG	K	2001	14/15	0.85	0.20	-	56,78,99,101	0
4	NAG	I	2005	14/15	0.85	0.13	-	111,117,124,133	0
4	NAG	E	2004	14/15	0.90	0.10	-	112,124,125,126	0
3	BMA	I	2003	11/12	0.80	0.20	-	56,83,91,91	0
3	NAG	O	2002	14/15	0.83	0.20	-	83,102,117,123	0
4	NAG	G	2005	14/15	0.85	0.15	-	106,120,127,128	0
3	BMA	G	2003	11/12	0.82	0.16	-	63,85,93,95	0
3	NAG	A	2002	14/15	0.92	0.14	-	59,82,94,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	c	2003	14/15	0.69	0.25	-	168,181,188,188	0
3	NAG	E	2002	14/15	0.81	0.33	-	103,121,127,128	0
3	BMA	E	2003	11/12	0.68	0.23	-	74,81,103,103	0
4	NAG	c	2002	14/15	0.87	0.21	-	159,180,187,188	0
4	NAG	W	2004	14/15	0.79	0.19	-	114,128,139,141	0
3	BMA	S	2003	11/12	0.62	0.24	-	110,125,137,139	0
4	NAG	Y	2003	14/15	0.64	0.23	-	159,180,187,187	0
4	NAG	A	2004	14/15	0.84	0.15	-	93,112,119,119	0
3	BMA	K	2003	11/12	0.77	0.21	-	67,77,85,86	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^{th} 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	Y	2001	14/15	0.84	0.20	0.65	75,93,108,120	0
5	NAG	a	2001	14/15	0.82	0.20	-0.09	92,112,119,128	0
5	NAG	c	2001	14/15	0.88	0.22	-0.21	91,102,120,122	0
5	NAG	C	2004	14/15	0.78	0.17	-	125,149,153,153	0
5	NAG	O	2006	14/15	0.88	0.24	-	96,105,117,126	0
5	NAG	K	2004	14/15	0.84	0.11	-	127,135,145,149	0
5	NAG	M	2004	14/15	0.88	0.11	-	119,135,154,161	0

6.5 Other polymers (i)

There are no such residues in this entry.