



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:00 PM GMT

PDB ID : 4N5Y
Title : Crystal structure of H5 hemagglutinin mutant (N158D, N224K and Q226L)
from the influenza virus A/Viet Nam/1203/2004 (H5N1)
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2013-10-10
Resolution : 3.16 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

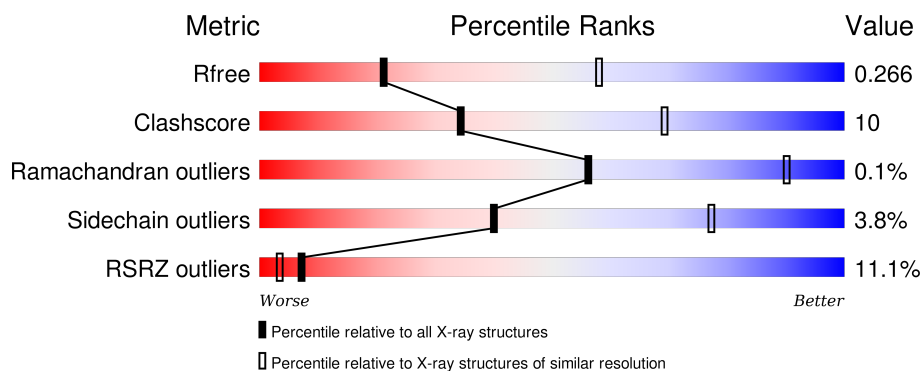
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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	334	<div> <div>%</div> <div> <div></div> <div>57%</div> <div>36%</div> <div>• •</div> </div> </div>
1	C	334	<div> <div>3%</div> <div> <div></div> <div>60%</div> <div>35%</div> <div>• •</div> </div> </div>
1	E	334	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>25%</div> <div>• •</div> </div> </div>
1	G	334	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>30%</div> <div>• •</div> </div> </div>
1	I	334	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	K	334	
1	M	334	
1	O	334	
1	Q	334	
1	S	334	
1	U	334	
1	W	334	
1	Y	334	
1	a	334	
1	c	334	
2	B	181	
2	D	181	
2	F	181	
2	H	181	
2	J	181	
2	L	181	
2	N	181	
2	P	181	
2	R	181	
2	T	181	
2	V	181	
2	X	181	
2	Z	181	
2	b	181	
2	d	181	

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	2001	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 60964 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
			2573	1628	442	488	15			
1	C	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	E	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	G	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	I	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	K	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	M	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	O	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	Q	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	S	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	U	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	W	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	Y	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	a	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	c	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			

There are 105 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
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
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
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
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
K	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
K	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
K	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
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
M	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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
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
U	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
U	226	LEU	GLN	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
Y	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

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			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	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		
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	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	W	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		
4	a	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	K	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	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		

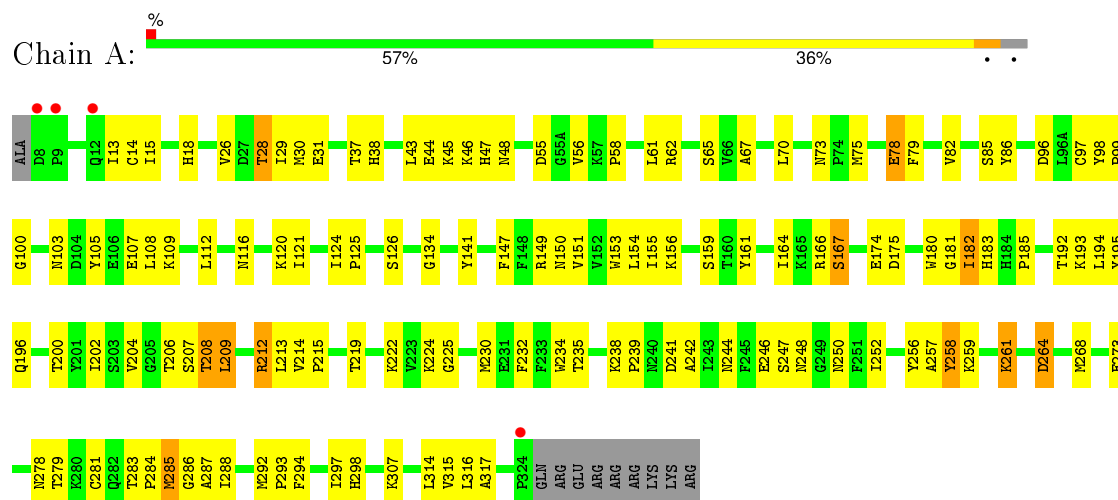
- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	Q	4	Total	C	N	O	0	0
			50	28	2	20		

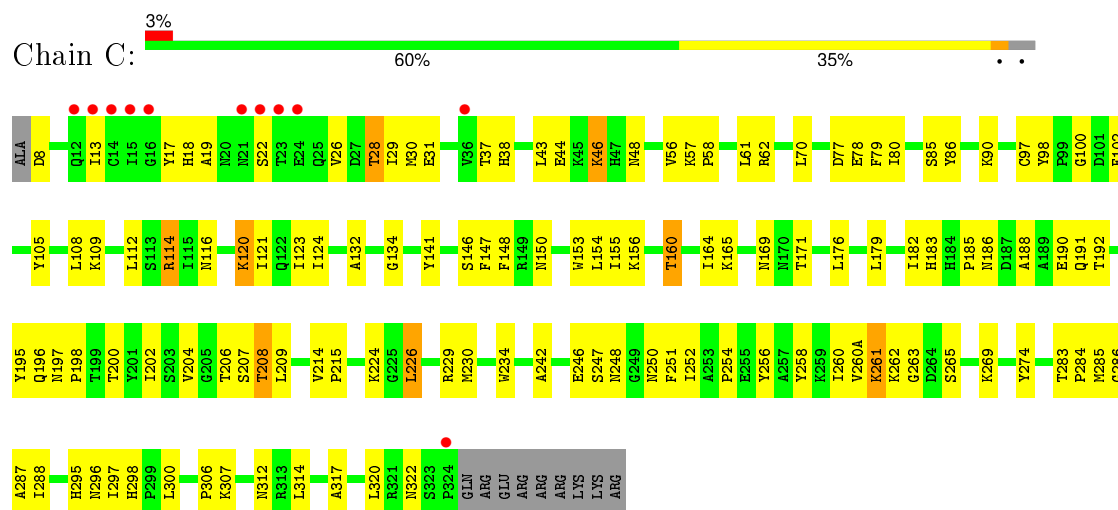
3 Residue-property plots

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 chain

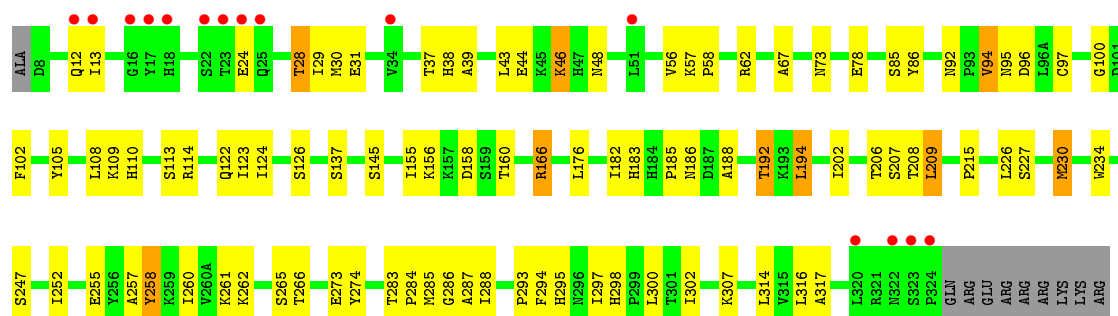


• Molecule 1: Hemagglutinin HA1 chain

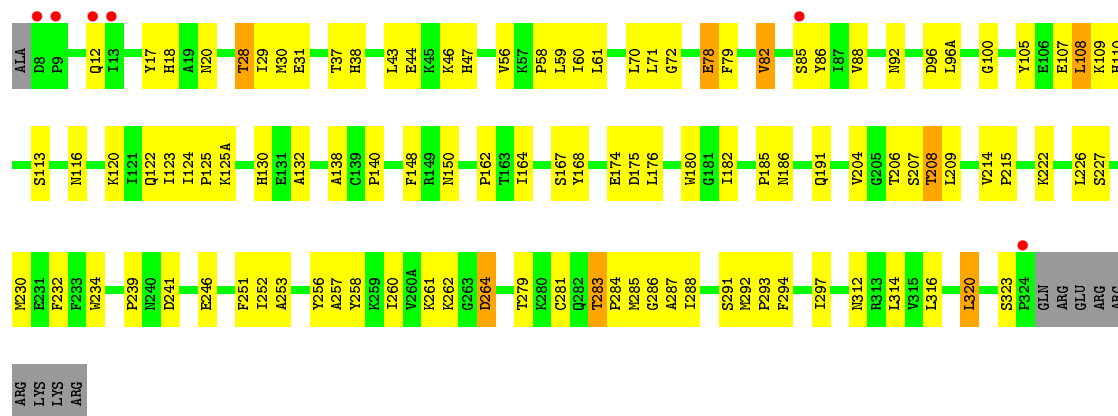


• Molecule 1: Hemagglutinin HA1 chain

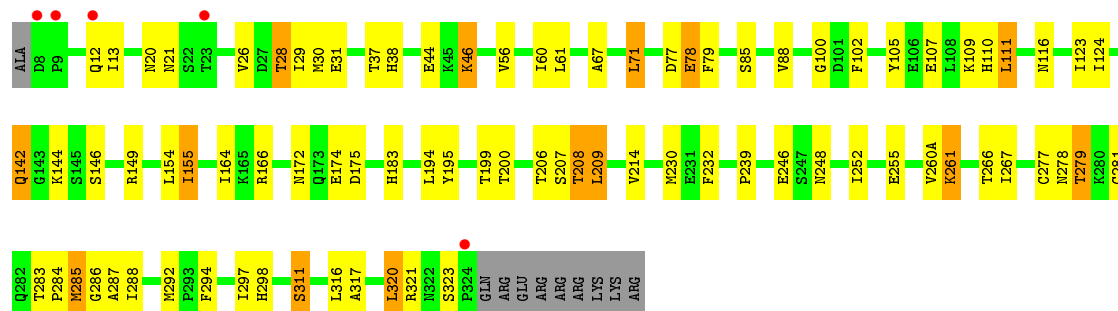




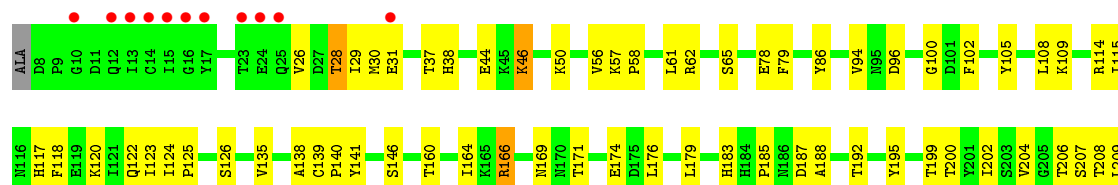
• Molecule 1: Hemagglutinin HA1 chain

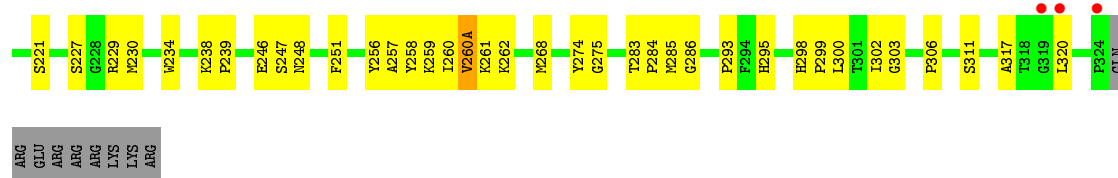


• Molecule 1: Hemagglutinin HA1 chain

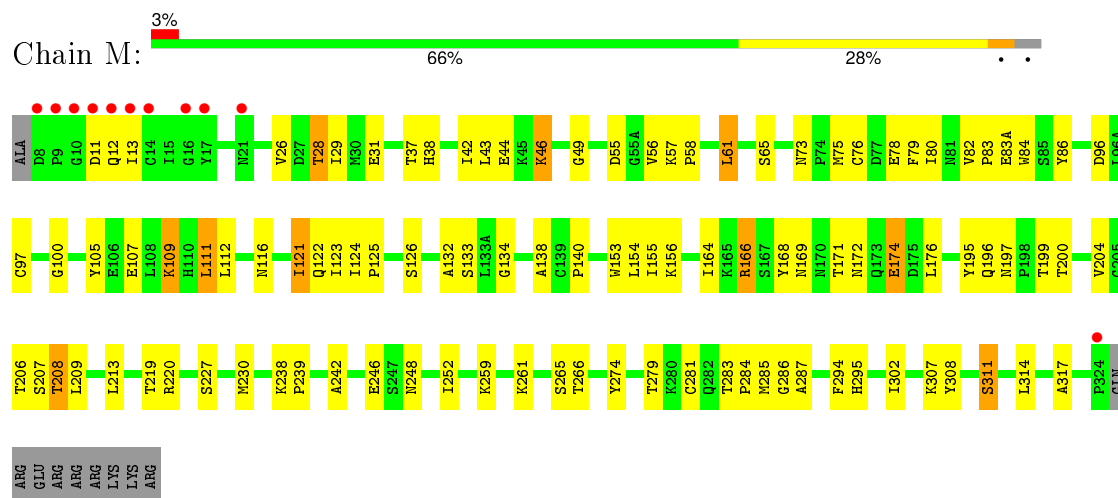


• Molecule 1: Hemagglutinin HA1 chain

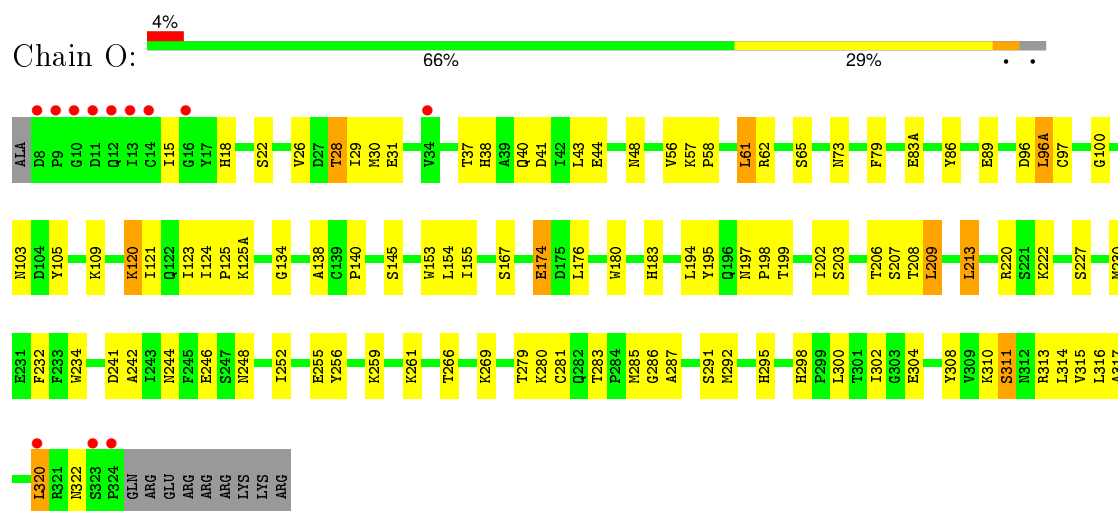




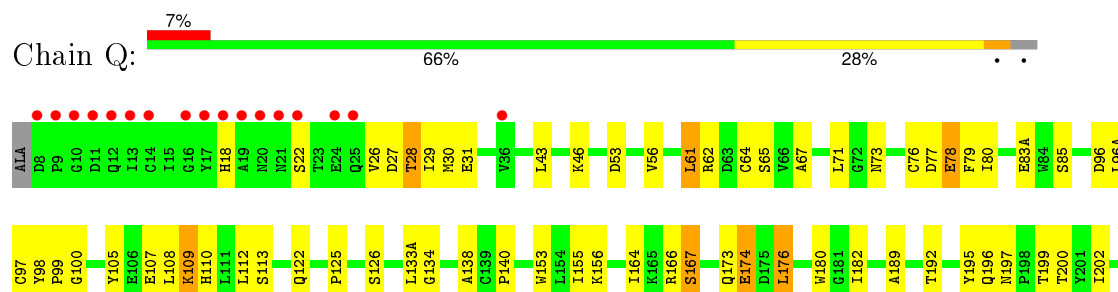
• Molecule 1: Hemagglutinin HA1 chain



• Molecule 1: Hemagglutinin HA1 chain

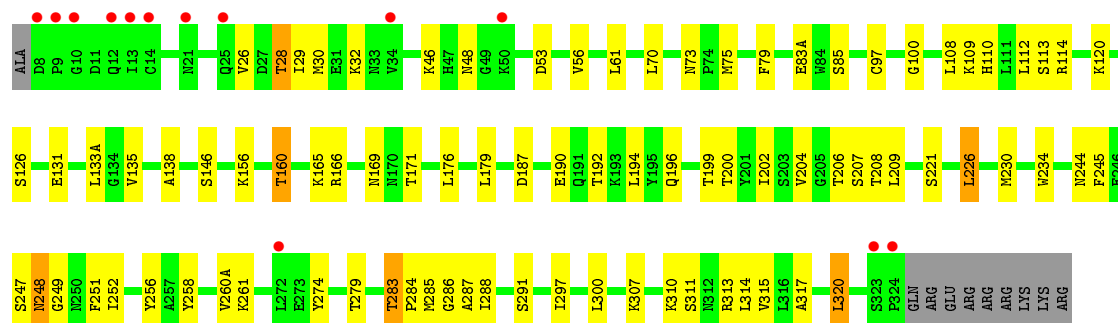


• Molecule 1: Hemagglutinin HA1 chain

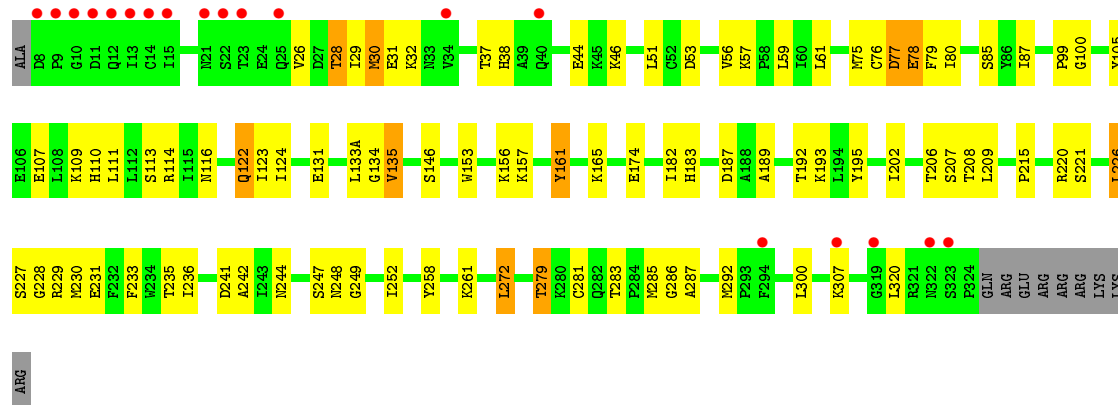




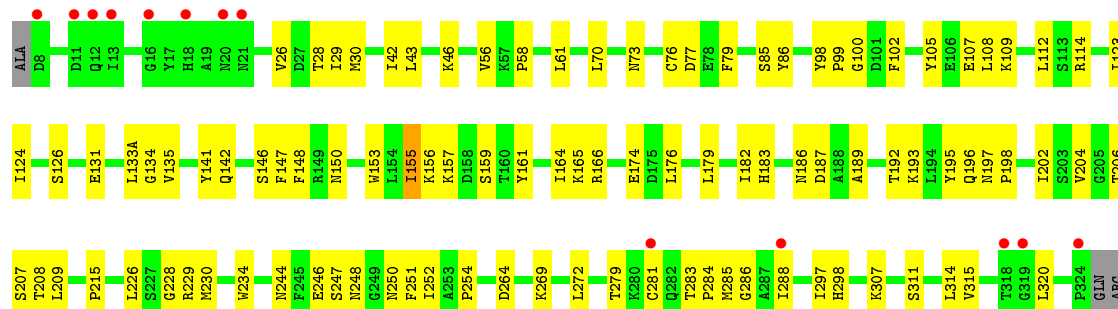
• Molecule 1: Hemagglutinin HA1 chain



• Molecule 1: Hemagglutinin HA1 chain

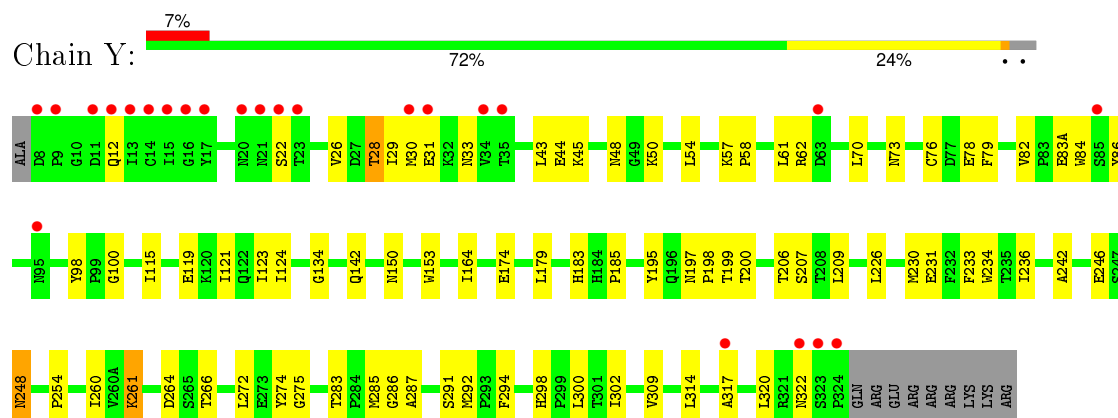


• Molecule 1: Hemagglutinin HA1 chain

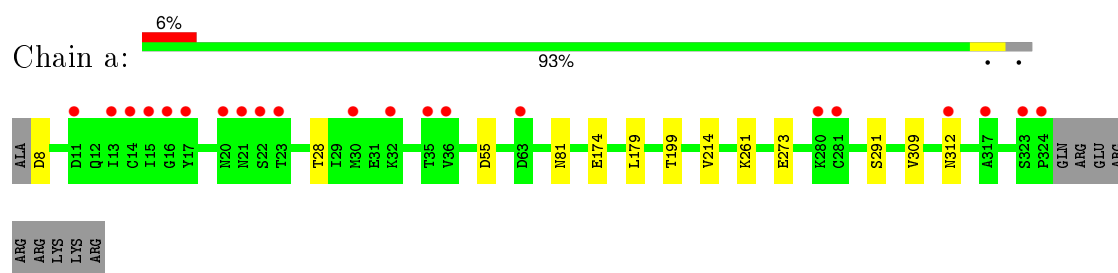


GLU
ARG
ARG
ARG
LYS
LYS
ARG

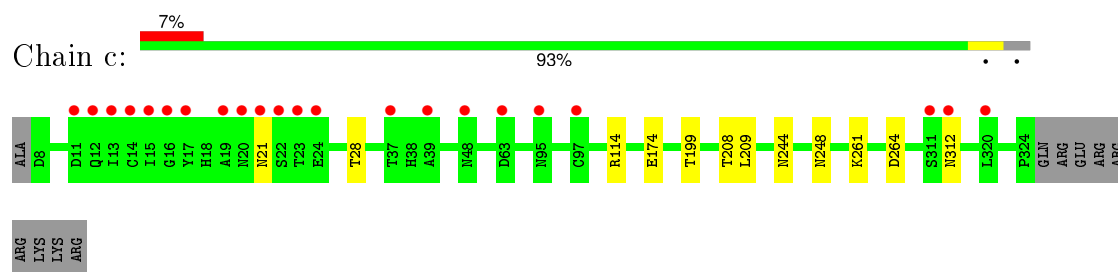
• Molecule 1: Hemagglutinin HA1 chain



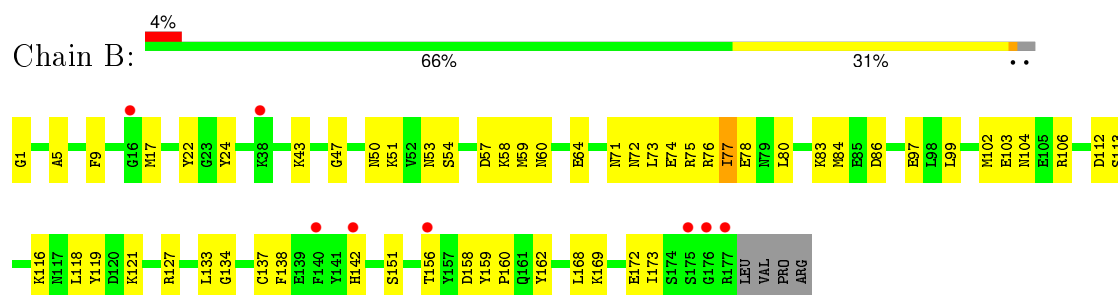
• Molecule 1: Hemagglutinin HA1 chain



• Molecule 1: Hemagglutinin HA1 chain

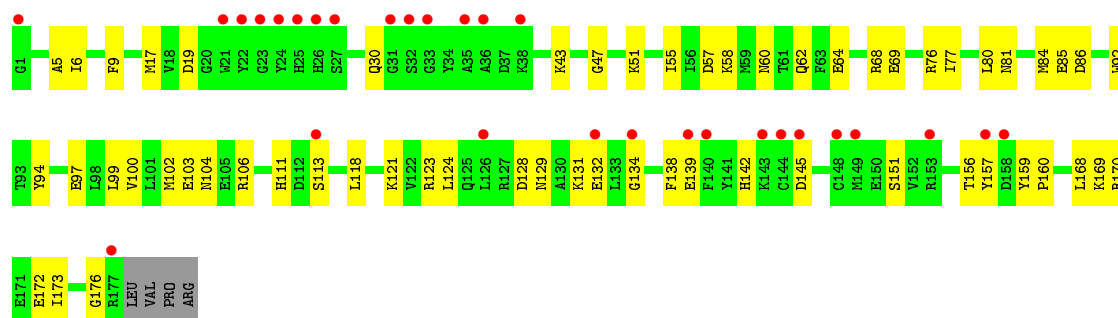


• Molecule 2: Hemagglutinin HA2 chain

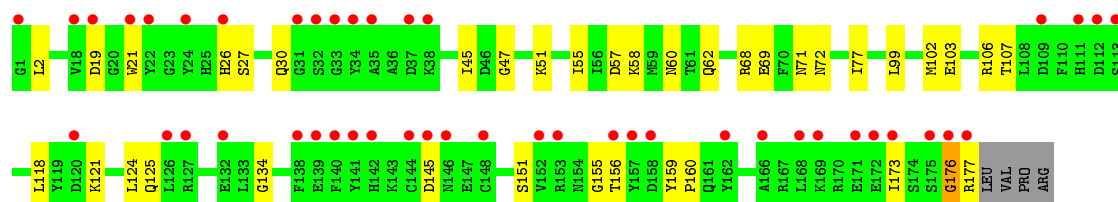
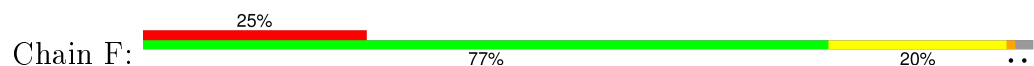


• Molecule 2: Hemagglutinin HA2 chain

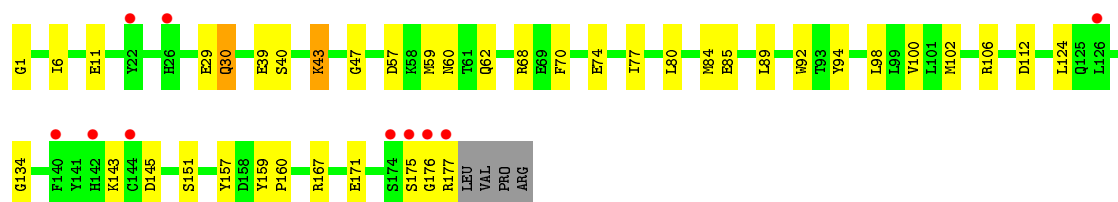
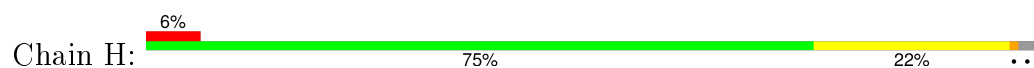




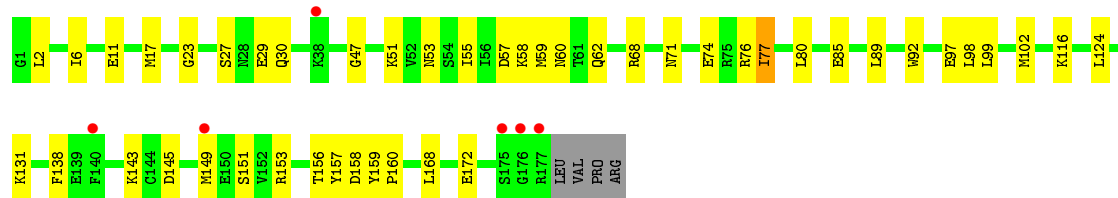
• Molecule 2: Hemagglutinin HA2 chain



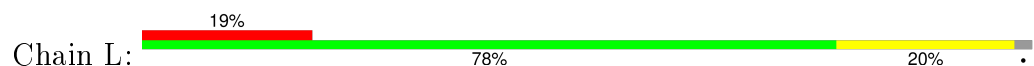
• Molecule 2: Hemagglutinin HA2 chain

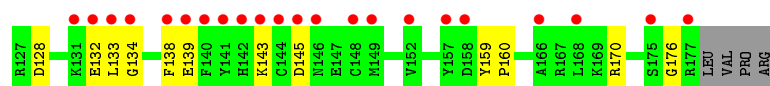


• Molecule 2: Hemagglutinin HA2 chain

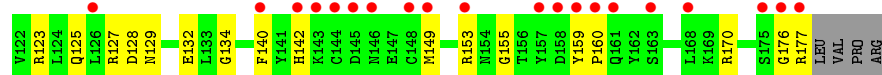
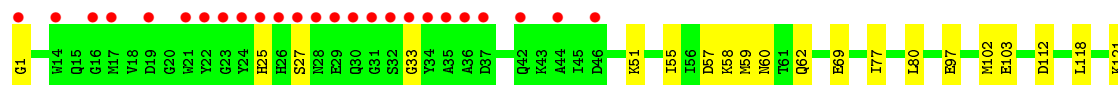
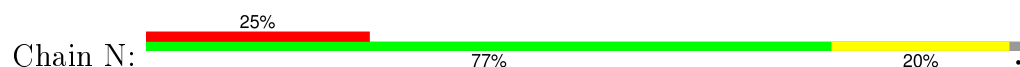


• Molecule 2: Hemagglutinin HA2 chain

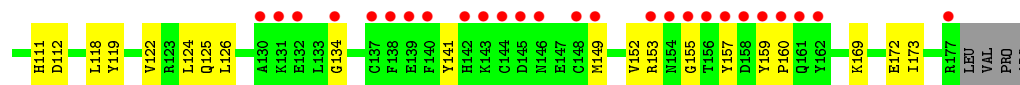
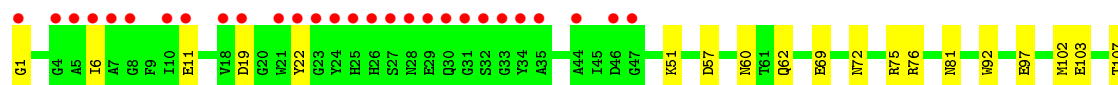
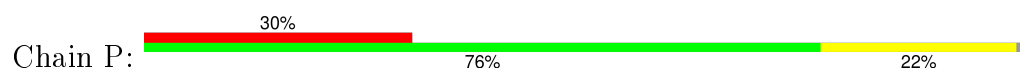




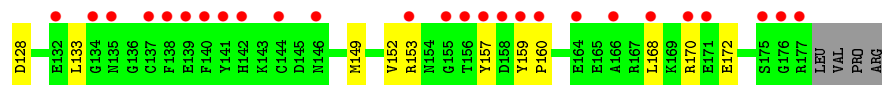
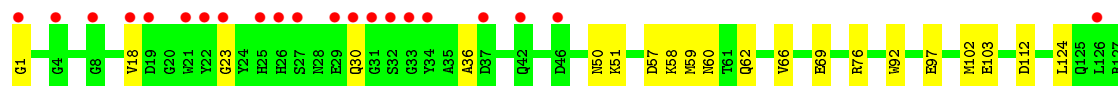
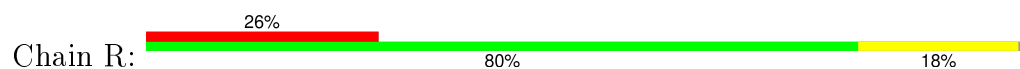
• Molecule 2: Hemagglutinin HA2 chain



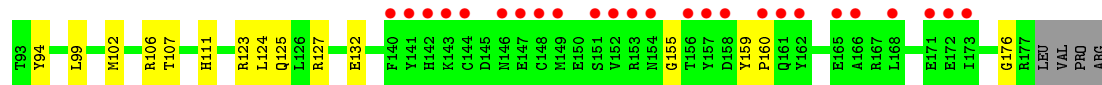
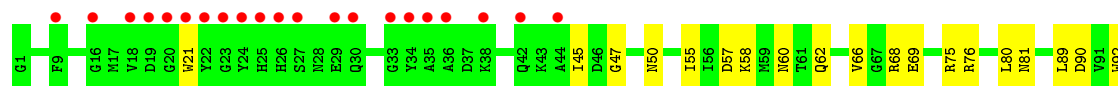
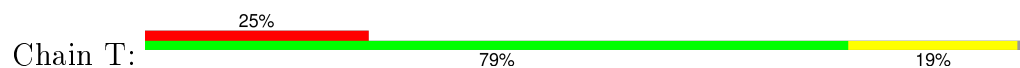
• Molecule 2: Hemagglutinin HA2 chain



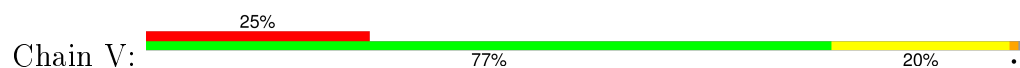
• Molecule 2: Hemagglutinin HA2 chain

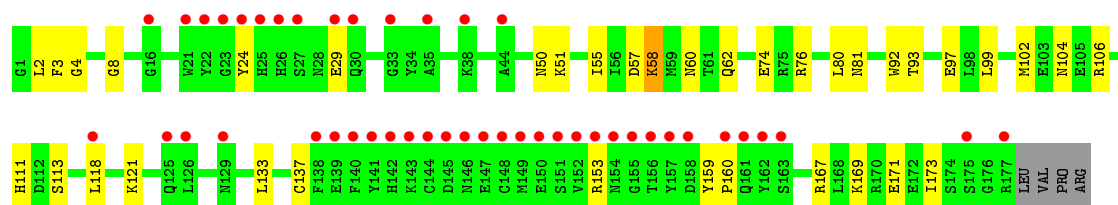


• Molecule 2: Hemagglutinin HA2 chain

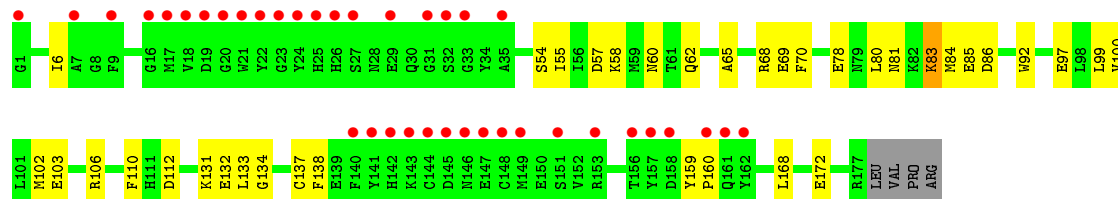
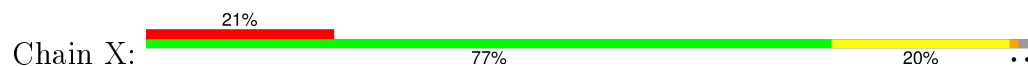


• Molecule 2: Hemagglutinin HA2 chain

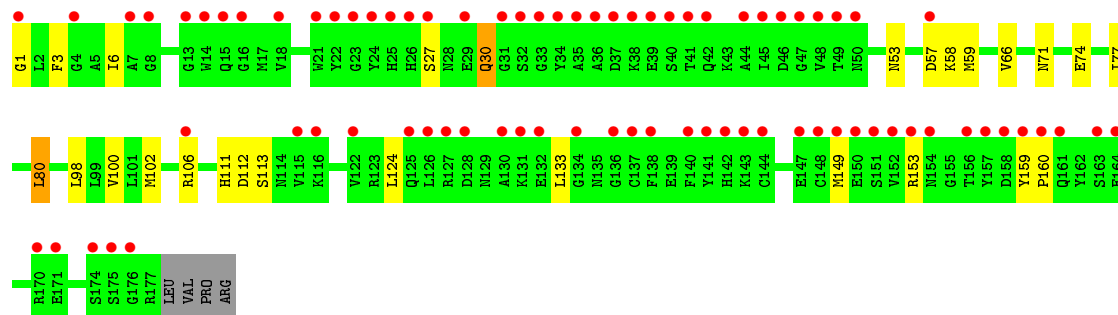
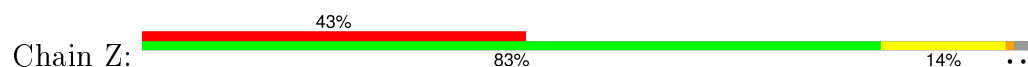




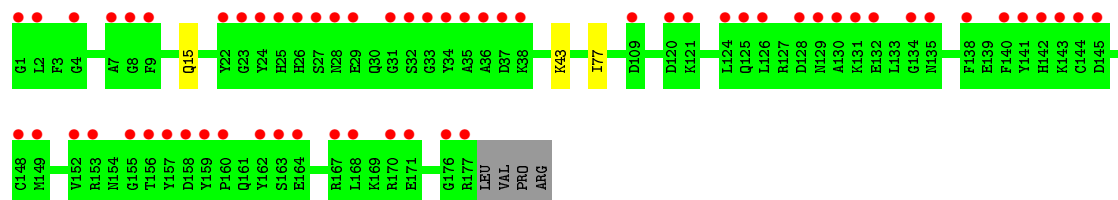
• Molecule 2: Hemagglutinin HA2 chain



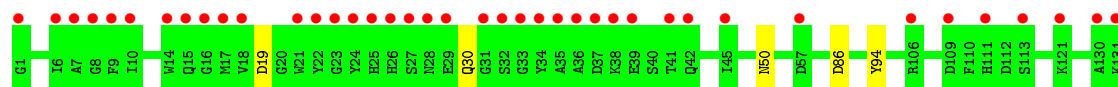
• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain



E132	E133	G134	N135	G136	G137	F138	E139	F140	Y141	H142	K143	G144	C148	M149	E150	S151	V152	R153	N154	G155	T156	Y157	D158	Y159	P160	Q161	Y162	S163	E164	E165	A166	R167	L168	K169	R170	E171	E172	I173	R177	LEU	VAL	PRO	ARG
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	117.92Å 118.11Å 273.80Å 91.50° 90.18° 119.87°	Depositor
Resolution (Å)	45.28 – 3.16 45.28 – 3.16	Depositor EDS
% Data completeness (in resolution range)	91.1 (45.28-3.16) 91.0 (45.28-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.213 , 0.262 0.219 , 0.266	Depositor DCC
R_{free} test set	9996 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	0.750	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 67.0	EDS
Estimated twinning fraction	0.004 for h+k,-h,l 0.004 for -k,h+k,l 0.057 for k,-h-k,l 0.057 for -h-k,h,l 0.024 for h,-h-k,-l 0.011 for -h-k,k,-l 0.000 for -h,-k,l 0.004 for k,h,-l 0.001 for -k,-h,-l 0.000 for -h,h+k,-l 0.000 for h+k,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 199723 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	60964	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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	0.71	0/2639	0.93	4/3584 (0.1%)
1	C	0.62	0/2639	0.82	2/3584 (0.1%)
1	E	0.61	0/2639	0.81	2/3584 (0.1%)
1	G	0.73	0/2639	0.91	1/3584 (0.0%)
1	I	0.72	0/2639	0.91	2/3584 (0.1%)
1	K	0.62	0/2639	0.81	1/3584 (0.0%)
1	M	0.70	0/2639	0.88	3/3584 (0.1%)
1	O	0.68	0/2639	0.87	7/3584 (0.2%)
1	Q	0.69	1/2639 (0.0%)	0.86	4/3584 (0.1%)
1	S	0.55	0/2639	0.77	0/3584
1	U	0.58	1/2639 (0.0%)	0.76	0/3584
1	W	0.59	0/2639	0.77	1/3584 (0.0%)
1	Y	0.43	0/2639	0.67	0/3584
1	a	0.44	0/2639	0.66	0/3584
1	c	0.43	0/2639	0.67	0/3584
2	B	0.47	0/1460	0.67	1/1961 (0.1%)
2	D	0.40	0/1460	0.58	0/1961
2	F	0.40	0/1460	0.59	1/1961 (0.1%)
2	H	0.50	0/1460	0.68	0/1961
2	J	0.50	0/1460	0.68	0/1961
2	L	0.43	0/1460	0.57	0/1961
2	N	0.44	0/1460	0.61	0/1961
2	P	0.44	0/1460	0.60	0/1961
2	R	0.45	0/1460	0.63	0/1961
2	T	0.37	0/1460	0.59	0/1961
2	V	0.38	0/1460	0.56	0/1961
2	X	0.37	0/1460	0.58	0/1961
2	Z	0.32	0/1460	0.56	1/1961 (0.1%)
2	b	0.33	0/1460	0.55	0/1961
2	d	0.33	0/1460	0.53	0/1961
All	All	0.55	2/61485 (0.0%)	0.74	30/83175 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	135	VAL	CB-CG2	-5.77	1.40	1.52
1	Q	180	TRP	CB-CG	5.20	1.59	1.50

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	213	LEU	CA-CB-CG	8.43	134.69	115.30
1	M	213	LEU	CA-CB-CG	8.43	134.69	115.30
1	E	209	LEU	CA-CB-CG	7.10	131.62	115.30
1	A	212	ARG	NE-CZ-NH1	6.38	123.49	120.30
2	Z	80	LEU	CA-CB-CG	6.29	129.76	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	2573	0	2521	105	0
1	C	2573	0	2522	105	0
1	E	2573	0	2521	66	0
1	G	2573	0	2521	75	0
1	I	2573	0	2521	61	0
1	K	2573	0	2521	75	0
1	M	2573	0	2521	71	0
1	O	2573	0	2520	71	0
1	Q	2573	0	2521	67	0
1	S	2573	0	2521	61	0
1	U	2573	0	2521	64	0
1	W	2573	0	2521	70	0
1	Y	2573	0	2521	50	0
1	a	2573	0	2522	0	0
1	c	2573	0	2521	0	0
2	B	1433	0	1340	56	0
2	D	1433	0	1340	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1433	0	1340	28	0
2	H	1433	0	1340	28	0
2	J	1433	0	1340	37	0
2	L	1433	0	1340	26	0
2	N	1433	0	1340	27	0
2	P	1433	0	1340	27	0
2	R	1433	0	1340	21	0
2	T	1433	0	1340	33	0
2	V	1433	0	1340	36	0
2	X	1433	0	1340	36	0
2	Z	1433	0	1340	21	0
2	b	1433	0	1340	0	0
2	d	1433	0	1340	0	0
3	A	39	0	34	3	0
3	C	39	0	34	2	0
3	E	39	0	34	0	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	1	0
3	O	39	0	34	2	0
3	U	39	0	34	2	0
3	W	39	0	34	0	0
4	A	28	0	25	2	0
4	E	28	0	25	0	0
4	G	28	0	25	0	0
4	I	28	0	25	1	0
4	M	28	0	25	0	0
4	O	28	0	25	1	0
4	Q	28	0	25	0	0
4	S	56	0	50	0	0
4	U	28	0	25	0	0
4	W	28	0	25	1	0
4	Y	28	0	25	1	0
4	a	28	0	25	0	0
5	K	14	0	13	0	0
5	O	14	0	13	0	0
5	Y	14	0	13	1	0
5	c	28	0	26	0	0
6	Q	50	0	43	5	0
All	All	60964	0	58689	1190	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 10.

The worst 5 of 1190 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	1.28	1.14
6:Q:2003:BMA:H2	6:Q:2004:MAN:H5	1.11	1.09
1:I:283:THR:HG22	1:I:285:MET:H	1.24	1.03
1:O:283:THR:HG22	1:O:285:MET:H	1.27	0.98
1:A:283:THR:HG22	1:A:285:MET:H	1.27	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%)	295 (91%)	28 (9%)	0	100	100
1	C	323/334 (97%)	300 (93%)	23 (7%)	0	100	100
1	E	323/334 (97%)	301 (93%)	22 (7%)	0	100	100
1	G	323/334 (97%)	299 (93%)	24 (7%)	0	100	100
1	I	323/334 (97%)	300 (93%)	23 (7%)	0	100	100
1	K	323/334 (97%)	299 (93%)	24 (7%)	0	100	100
1	M	323/334 (97%)	298 (92%)	25 (8%)	0	100	100
1	O	323/334 (97%)	299 (93%)	24 (7%)	0	100	100
1	Q	323/334 (97%)	298 (92%)	25 (8%)	0	100	100
1	S	323/334 (97%)	302 (94%)	20 (6%)	1 (0%)	46	84
1	U	323/334 (97%)	298 (92%)	23 (7%)	2 (1%)	30	74
1	W	323/334 (97%)	299 (93%)	24 (7%)	0	100	100
1	Y	323/334 (97%)	297 (92%)	25 (8%)	1 (0%)	46	84

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	323/334 (97%)	297 (92%)	26 (8%)	0	100	100
1	c	323/334 (97%)	300 (93%)	22 (7%)	1 (0%)	46	84
2	B	175/181 (97%)	163 (93%)	12 (7%)	0	100	100
2	D	175/181 (97%)	162 (93%)	12 (7%)	1 (1%)	30	74
2	F	175/181 (97%)	163 (93%)	11 (6%)	1 (1%)	30	74
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%)	160 (91%)	14 (8%)	1 (1%)	30	74
2	N	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
2	P	175/181 (97%)	167 (95%)	8 (5%)	0	100	100
2	R	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
2	T	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
2	V	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
2	X	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
2	Z	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
2	b	175/181 (97%)	163 (93%)	12 (7%)	0	100	100
2	d	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
All	All	7470/7725 (97%)	6943 (93%)	519 (7%)	8 (0%)	56	90

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	77	ASP
1	Y	248	ASN
1	S	248	ASN
1	U	78	GLU
1	c	248	ASN

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	292/300 (97%)	273 (94%)	19 (6%)	21	60
1	C	292/300 (97%)	281 (96%)	11 (4%)	40	77
1	E	292/300 (97%)	279 (96%)	13 (4%)	34	73
1	G	292/300 (97%)	277 (95%)	15 (5%)	29	69
1	I	292/300 (97%)	272 (93%)	20 (7%)	20	57
1	K	292/300 (97%)	282 (97%)	10 (3%)	44	80
1	M	292/300 (97%)	274 (94%)	18 (6%)	23	62
1	O	292/300 (97%)	277 (95%)	15 (5%)	29	69
1	Q	292/300 (97%)	275 (94%)	17 (6%)	25	64
1	S	292/300 (97%)	278 (95%)	14 (5%)	31	71
1	U	292/300 (97%)	277 (95%)	15 (5%)	29	69
1	W	292/300 (97%)	285 (98%)	7 (2%)	57	86
1	Y	292/300 (97%)	281 (96%)	11 (4%)	40	77
1	a	292/300 (97%)	279 (96%)	13 (4%)	34	73
1	c	292/300 (97%)	280 (96%)	12 (4%)	37	75
2	B	151/155 (97%)	146 (97%)	5 (3%)	45	80
2	D	151/155 (97%)	149 (99%)	2 (1%)	76	92
2	F	151/155 (97%)	150 (99%)	1 (1%)	88	97
2	H	151/155 (97%)	147 (97%)	4 (3%)	54	85
2	J	151/155 (97%)	147 (97%)	4 (3%)	54	85
2	L	151/155 (97%)	151 (100%)	0	100	100
2	N	151/155 (97%)	150 (99%)	1 (1%)	88	97
2	P	151/155 (97%)	150 (99%)	1 (1%)	88	97
2	R	151/155 (97%)	149 (99%)	2 (1%)	76	92
2	T	151/155 (97%)	149 (99%)	2 (1%)	76	92
2	V	151/155 (97%)	148 (98%)	3 (2%)	63	88
2	X	151/155 (97%)	148 (98%)	3 (2%)	63	88
2	Z	151/155 (97%)	147 (97%)	4 (3%)	54	85
2	b	151/155 (97%)	148 (98%)	3 (2%)	63	88
2	d	151/155 (97%)	146 (97%)	5 (3%)	45	80
All	All	6645/6825 (97%)	6395 (96%)	250 (4%)	40	77

5 of 250 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	199	THR
1	S	46	LYS
2	T	66	VAL
1	O	248	ASN
1	Q	78	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	W	196	GLN
1	Y	197	ASN
2	b	62	GLN
1	Y	110	HIS
2	F	62	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 ⓘ

60 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	1.36	2 (14%)	15,19,21	1.13	1 (6%)
3	NAG	A	2002	3	14,14,15	0.49	0	15,19,21	0.44	0
3	BMA	A	2003	3	11,11,12	1.93	3 (27%)	14,15,17	1.95	5 (35%)
4	NAG	A	2004	1,4	14,14,15	1.01	1 (7%)	15,19,21	1.27	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	2005	4	14,14,15	1.79	2 (14%)	15,19,21	1.27	1 (6%)
3	NAG	C	2001	1,3	14,14,15	0.61	0	15,19,21	0.61	0
3	NAG	C	2002	3	14,14,15	0.63	0	15,19,21	0.79	0
3	BMA	C	2003	3	11,11,12	1.74	2 (18%)	14,15,17	2.86	5 (35%)
3	NAG	E	2001	1,3	14,14,15	0.79	1 (7%)	15,19,21	1.57	1 (6%)
3	NAG	E	2002	3	14,14,15	0.99	1 (7%)	15,19,21	1.43	3 (20%)
3	BMA	E	2003	3	11,11,12	2.46	7 (63%)	14,15,17	1.51	3 (21%)
4	NAG	E	2004	1,4	14,14,15	1.18	1 (7%)	15,19,21	1.33	3 (20%)
4	NAG	E	2005	4	14,14,15	0.58	1 (7%)	15,19,21	0.35	0
3	NAG	G	2001	1,3	14,14,15	1.70	1 (7%)	15,19,21	1.31	3 (20%)
3	NAG	G	2002	3	14,14,15	1.22	1 (7%)	15,19,21	1.18	3 (20%)
3	BMA	G	2003	3	11,11,12	2.24	5 (45%)	14,15,17	1.71	3 (21%)
4	NAG	G	2004	1,4	14,14,15	1.25	1 (7%)	15,19,21	1.38	2 (13%)
4	NAG	G	2005	4	14,14,15	1.77	3 (21%)	15,19,21	0.89	1 (6%)
3	NAG	I	2001	1,3	14,14,15	1.25	1 (7%)	15,19,21	1.42	2 (13%)
3	NAG	I	2002	3	14,14,15	0.71	1 (7%)	15,19,21	0.48	0
3	BMA	I	2003	3	11,11,12	1.93	3 (27%)	14,15,17	1.59	3 (21%)
4	NAG	I	2004	1,4	14,14,15	0.75	1 (7%)	15,19,21	1.17	1 (6%)
4	NAG	I	2005	4	14,14,15	1.52	2 (14%)	15,19,21	1.07	1 (6%)
3	NAG	K	2001	1,3	14,14,15	0.51	0	15,19,21	0.74	0
3	NAG	K	2002	3	14,14,15	0.90	1 (7%)	15,19,21	1.22	2 (13%)
3	BMA	K	2003	3	11,11,12	1.96	4 (36%)	14,15,17	1.69	3 (21%)
3	NAG	M	2001	1,3	14,14,15	0.66	1 (7%)	15,19,21	0.66	0
3	NAG	M	2002	3	14,14,15	0.83	1 (7%)	15,19,21	0.68	0
3	BMA	M	2003	3	11,11,12	1.89	5 (45%)	14,15,17	2.08	5 (35%)
4	NAG	M	2004	1,4	14,14,15	0.71	0	15,19,21	0.71	0
4	NAG	M	2005	4	14,14,15	1.45	1 (7%)	15,19,21	1.37	3 (20%)
3	NAG	O	2001	1,3	14,14,15	0.92	1 (7%)	15,19,21	0.55	0
3	NAG	O	2002	3	14,14,15	0.32	0	15,19,21	0.33	0
3	BMA	O	2003	3	11,11,12	1.51	2 (18%)	14,15,17	2.30	4 (28%)
4	NAG	O	2004	1,4	14,14,15	0.83	1 (7%)	15,19,21	0.94	1 (6%)
4	NAG	O	2005	4	14,14,15	0.30	0	15,19,21	0.64	1 (6%)
6	NAG	Q	2001	1,6	14,14,15	0.54	0	15,19,21	1.34	3 (20%)
6	NAG	Q	2002	6	14,14,15	0.44	0	15,19,21	1.01	0
6	BMA	Q	2003	6	11,11,12	0.70	0	14,15,17	2.03	4 (28%)
6	MAN	Q	2004	6	11,11,12	0.70	0	14,15,17	1.49	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	Q	2005	1,4	14,14,15	1.23	1 (7%)	15,19,21	1.28	3 (20%)
4	NAG	Q	2006	4	14,14,15	1.02	1 (7%)	15,19,21	0.94	1 (6%)
4	NAG	S	2001	1,4	14,14,15	0.26	0	15,19,21	0.34	0
4	NAG	S	2002	4	14,14,15	0.91	1 (7%)	15,19,21	0.84	0
4	NAG	S	2003	1,4	14,14,15	0.93	1 (7%)	15,19,21	0.98	2 (13%)
4	NAG	S	2004	4	14,14,15	1.23	2 (14%)	15,19,21	0.97	1 (6%)
3	NAG	U	2001	1,3	14,14,15	0.30	0	15,19,21	0.55	0
3	NAG	U	2002	3	14,14,15	1.89	1 (7%)	15,19,21	1.35	2 (13%)
3	BMA	U	2003	3	11,11,12	1.32	2 (18%)	14,15,17	1.46	3 (21%)
4	NAG	U	2004	1,4	14,14,15	1.13	1 (7%)	15,19,21	1.29	3 (20%)
4	NAG	U	2005	4	14,14,15	0.38	0	15,19,21	0.57	1 (6%)
3	NAG	W	2001	1,3	14,14,15	0.61	0	15,19,21	1.05	2 (13%)
3	NAG	W	2002	3	14,14,15	0.56	0	15,19,21	0.88	0
3	BMA	W	2003	3	11,11,12	0.56	0	14,15,17	0.78	0
4	NAG	W	2004	1,4	14,14,15	1.39	1 (7%)	15,19,21	1.33	3 (20%)
4	NAG	W	2005	4	14,14,15	0.91	1 (7%)	15,19,21	0.73	1 (6%)
4	NAG	Y	2001	1,4	14,14,15	0.37	0	15,19,21	0.40	0
4	NAG	Y	2002	4	14,14,15	0.29	0	15,19,21	0.52	0
4	NAG	a	2001	1,4	14,14,15	0.46	0	15,19,21	1.25	2 (13%)
4	NAG	a	2002	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
4	NAG	M	2004	1,4	-	0/6/23/26	0/1/1/1
4	NAG	M	2005	4	-	0/6/23/26	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
6	NAG	Q	2001	1,6	-	0/6/23/26	0/1/1/1
6	NAG	Q	2002	6	-	0/6/23/26	0/1/1/1
6	BMA	Q	2003	6	-	0/2/19/22	0/1/1/1
6	MAN	Q	2004	6	-	0/2/19/22	0/1/1/1
4	NAG	Q	2005	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	2006	4	-	0/6/23/26	0/1/1/1
4	NAG	S	2001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	2002	4	-	0/6/23/26	0/1/1/1
4	NAG	S	2003	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	2004	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	1/1/1/1
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	W	2005	4	-	0/6/23/26	0/1/1/1
4	NAG	Y	2001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Y	2002	4	-	0/6/23/26	0/1/1/1
4	NAG	a	2001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	a	2002	4	-	0/6/23/26	0/1/1/1

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	2002	NAG	O5-C1	-6.89	1.32	1.43
3	G	2001	NAG	O5-C1	-5.80	1.34	1.43
4	M	2005	NAG	O5-C1	-4.85	1.35	1.43
4	W	2004	NAG	O5-C1	-4.83	1.35	1.43
4	G	2004	NAG	O5-C1	-4.46	1.36	1.43

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	2001	NAG	C1-O5-C5	-3.47	107.84	112.25
6	Q	2003	BMA	O5-C1-C2	-3.39	105.36	110.86
6	Q	2003	BMA	O3-C3-C4	-3.34	102.81	110.34
4	M	2005	NAG	C1-O5-C5	-3.30	108.06	112.25
3	A	2003	BMA	C1-O5-C5	-3.15	108.25	112.25

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	U	2003	BMA	C1-C2-C3-C4-C5-O5

19 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	NAG	3	0
4	A	2004	NAG	2	0
4	A	2005	NAG	2	0
3	C	2001	NAG	2	0
3	G	2001	NAG	1	0
4	I	2004	NAG	1	0
4	I	2005	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	2001	NAG	1	0
3	O	2001	NAG	2	0
4	O	2004	NAG	1	0
4	O	2005	NAG	1	0
6	Q	2001	NAG	1	0
6	Q	2003	BMA	4	0
6	Q	2004	MAN	4	0
3	U	2001	NAG	2	0
3	U	2002	NAG	1	0
4	W	2004	NAG	1	0
4	W	2005	NAG	1	0
4	Y	2001	NAG	1	0

5.6 Ligand geometry [i](#)

5 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	K	2004	1	14,14,15	0.69	1 (7%)	15,19,21	0.44	0
5	NAG	O	2006	1	14,14,15	1.16	2 (14%)	15,19,21	1.02	2 (13%)
5	NAG	Y	2003	1	14,14,15	0.56	0	15,19,21	0.36	0
5	NAG	c	2001	1	14,14,15	0.54	0	15,19,21	0.38	0
5	NAG	c	2002	1	14,14,15	1.13	2 (14%)	15,19,21	1.19	2 (13%)

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	K	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	2003	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	c	2001	1	-	0/6/23/26	0/1/1/1
5	NAG	c	2002	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	c	2002	NAG	O5-C1	-3.37	1.38	1.43
5	O	2006	NAG	O5-C1	-2.98	1.38	1.43
5	K	2004	NAG	C1-C2	2.03	1.55	1.52
5	c	2002	NAG	C1-C2	2.14	1.55	1.52
5	O	2006	NAG	C1-C2	2.75	1.56	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	c	2002	NAG	C1-O5-C5	-2.18	109.49	112.25
5	O	2006	NAG	C3-C4-C5	2.27	114.15	110.20
5	O	2006	NAG	C4-C3-C2	2.45	115.04	111.23
5	c	2002	NAG	C4-C3-C2	3.03	115.95	111.23

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	2003	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, 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	324/334 (97%)	-0.23	4 (1%) 81 69	22, 45, 101, 176	0
1	C	324/334 (97%)	-0.07	11 (3%) 49 32	30, 56, 143, 199	0
1	E	324/334 (97%)	-0.06	15 (4%) 36 21	30, 56, 144, 203	0
1	G	324/334 (97%)	-0.25	6 (1%) 70 54	19, 46, 102, 183	0
1	I	324/334 (97%)	-0.31	5 (1%) 76 62	24, 44, 100, 186	0
1	K	324/334 (97%)	0.00	14 (4%) 39 23	33, 57, 143, 218	0
1	M	324/334 (97%)	-0.14	11 (3%) 49 32	26, 50, 152, 220	0
1	O	324/334 (97%)	-0.08	12 (3%) 45 28	25, 50, 140, 226	0
1	Q	324/334 (97%)	-0.06	23 (7%) 19 10	25, 49, 151, 212	0
1	S	324/334 (97%)	-0.03	13 (4%) 42 26	35, 64, 158, 195	0
1	U	324/334 (97%)	-0.01	19 (5%) 26 13	31, 64, 158, 214	0
1	W	324/334 (97%)	-0.06	13 (4%) 42 26	35, 64, 148, 211	0
1	Y	324/334 (97%)	0.31	24 (7%) 17 9	55, 91, 189, 248	0
1	a	324/334 (97%)	0.30	21 (6%) 22 11	55, 87, 184, 263	0
1	c	324/334 (97%)	0.36	22 (6%) 20 10	59, 90, 185, 253	0
2	B	177/181 (97%)	0.39	8 (4%) 37 21	26, 113, 153, 173	0
2	D	177/181 (97%)	0.85	29 (16%) 2 1	41, 155, 195, 210	0
2	F	177/181 (97%)	1.16	46 (25%) 1 0	42, 154, 196, 206	0
2	H	177/181 (97%)	0.34	10 (5%) 28 14	23, 113, 154, 174	0
2	J	177/181 (97%)	0.20	6 (3%) 49 32	27, 113, 153, 166	0
2	L	177/181 (97%)	1.11	35 (19%) 1 1	42, 148, 195, 206	0
2	N	177/181 (97%)	1.28	45 (25%) 1 0	38, 158, 213, 231	0
2	P	177/181 (97%)	1.44	54 (30%) 1 0	38, 163, 213, 231	0
2	R	177/181 (97%)	1.31	47 (26%) 1 0	34, 163, 210, 222	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
2	T	177/181 (97%)	1.13	46 (25%)	1	0	45, 153, 201, 209	0
2	V	177/181 (97%)	1.27	45 (25%)	1	0	49, 153, 213, 228	0
2	X	177/181 (97%)	1.11	38 (21%)	1	1	50, 155, 204, 220	0
2	Z	177/181 (97%)	2.11	78 (44%)	0	0	74, 191, 237, 256	0
2	b	177/181 (97%)	1.91	61 (34%)	0	0	73, 187, 239, 254	0
2	d	177/181 (97%)	2.15	73 (41%)	0	0	78, 194, 247, 269	0
All	All	7515/7725 (97%)	0.40	834 (11%)	7	3	19, 79, 201, 269	0

The worst 5 of 834 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	c	16	GLY	18.4
2	d	23	GLY	15.8
1	O	13	ILE	15.4
2	b	141	TYR	14.8
1	U	12	GLN	14.3

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	C	2001	14/15	0.84	0.32	2.96	56,75,85,89	0
3	NAG	O	2001	14/15	0.95	0.28	1.60	39,57,67,74	0
3	NAG	A	2001	14/15	0.93	0.22	1.14	61,66,70,73	0
3	NAG	I	2001	14/15	0.93	0.22	0.89	50,59,64,64	0
3	NAG	E	2001	14/15	0.89	0.22	0.51	54,72,97,102	0
3	NAG	U	2001	14/15	0.91	0.20	0.47	54,66,81,92	0
4	NAG	a	2001	14/15	0.88	0.28	0.16	86,95,107,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	W	2001	14/15	0.87	0.17	0.04	64,71,80,92	0
3	NAG	G	2001	14/15	0.95	0.18	-0.18	54,63,66,66	0
3	BMA	K	2003	11/12	0.78	0.21	-0.19	32,49,59,61	0
4	NAG	S	2001	14/15	0.90	0.18	-0.19	50,69,87,102	0
4	NAG	Y	2001	14/15	0.90	0.19	-1.36	95,100,108,119	0
4	NAG	Y	2002	14/15	0.79	0.24	-	115,131,144,145	0
4	NAG	A	2005	14/15	0.67	0.26	-	119,129,135,136	0
3	NAG	W	2002	14/15	0.86	0.29	-	77,96,107,119	0
3	NAG	I	2002	14/15	0.92	0.27	-	65,75,86,89	0
3	BMA	W	2003	11/12	0.47	0.44	-	113,124,130,135	0
3	NAG	O	2002	14/15	0.88	0.26	-	61,90,101,113	0
3	BMA	U	2003	11/12	0.76	0.23	-	114,122,125,127	0
4	NAG	E	2004	14/15	0.90	0.20	-	126,134,144,151	0
3	NAG	K	2001	14/15	0.87	0.28	-	59,73,92,93	0
3	BMA	M	2003	11/12	0.65	0.21	-	102,115,128,131	0
4	NAG	a	2002	14/15	0.89	0.31	-	96,118,126,129	0
4	NAG	M	2004	14/15	0.85	0.12	-	128,145,151,160	0
4	NAG	S	2003	14/15	0.77	0.19	-	133,146,152,153	0
4	NAG	O	2004	14/15	0.84	0.18	-	142,148,151,153	0
3	BMA	C	2003	11/12	0.84	0.17	-	35,55,68,70	0
4	NAG	A	2004	14/15	0.82	0.20	-	104,114,123,124	0
4	NAG	U	2005	14/15	0.78	0.20	-	156,166,172,172	0
3	NAG	G	2002	14/15	0.90	0.24	-	53,70,85,96	0
4	NAG	G	2004	14/15	0.83	0.20	-	87,103,110,112	0
4	NAG	Q	2006	14/15	0.81	0.23	-	124,153,157,160	0
4	NAG	W	2005	14/15	0.86	0.21	-	139,152,158,160	0
6	NAG	Q	2002	14/15	0.91	0.21	-	94,99,105,115	0
6	MAN	Q	2004	11/12	0.70	0.29	-	111,129,131,135	0
6	BMA	Q	2003	11/12	0.79	0.18	-	116,120,126,127	0
4	NAG	O	2005	14/15	0.81	0.20	-	138,149,152,152	0
4	NAG	M	2005	14/15	0.75	0.26	-	137,162,176,177	0
3	BMA	I	2003	11/12	0.81	0.39	-	83,95,103,110	0
3	NAG	E	2002	14/15	0.71	0.26	-	79,102,115,117	0
3	NAG	A	2002	14/15	0.96	0.19	-	52,75,87,93	0
3	NAG	M	2001	14/15	0.94	0.16	-	42,57,74,81	0
3	NAG	C	2002	14/15	0.91	0.24	-	69,81,86,90	0
3	NAG	U	2002	14/15	0.82	0.22	-	95,102,117,127	0
4	NAG	W	2004	14/15	0.81	0.23	-	145,151,158,159	0
6	NAG	Q	2001	14/15	0.82	0.23	-	68,80,90,103	0
4	NAG	S	2002	14/15	0.70	0.25	-	96,108,125,129	0
4	NAG	Q	2005	14/15	0.90	0.13	-	122,138,141,145	0
3	NAG	M	2002	14/15	0.84	0.23	-	64,91,98,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	BMA	O	2003	11/12	0.78	0.14	-	102,115,125,130	0
4	NAG	S	2004	14/15	0.79	0.17	-	116,143,150,154	0
3	BMA	G	2003	11/12	0.75	0.30	-	80,97,103,107	0
3	NAG	K	2002	14/15	0.91	0.21	-	61,76,88,94	0
4	NAG	I	2005	14/15	0.83	0.14	-	109,125,128,129	0
4	NAG	G	2005	14/15	0.89	0.13	-	106,115,120,122	0
4	NAG	I	2004	14/15	0.82	0.20	-	94,108,117,122	0
4	NAG	E	2005	14/15	0.68	0.36	-	129,148,157,159	0
3	BMA	E	2003	11/12	0.74	0.20	-	43,57,80,88	0
4	NAG	U	2004	14/15	0.82	0.15	-	141,148,158,159	0
3	BMA	A	2003	11/12	0.83	0.23	-	65,90,98,98	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, 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(\AA^2)	Q<0.9
5	NAG	c	2001	14/15	0.80	0.28	-0.31	94,106,117,123	0
5	NAG	c	2002	14/15	0.67	0.19	-	143,162,169,170	0
5	NAG	K	2004	14/15	0.88	0.10	-	127,140,146,149	0
5	NAG	Y	2003	14/15	0.65	0.27	-	149,160,166,170	0
5	NAG	O	2006	14/15	0.87	0.24	-	87,95,100,102	0

6.5 Other polymers [i](#)

There are no such residues in this entry.