



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:45 PM GMT

PDB ID : 4MHI
Title : Crystal structure of a H5N1 influenza virus hemagglutinin from A/goose/Guangdong/1/96
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2013-08-29
Resolution : 2.60 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

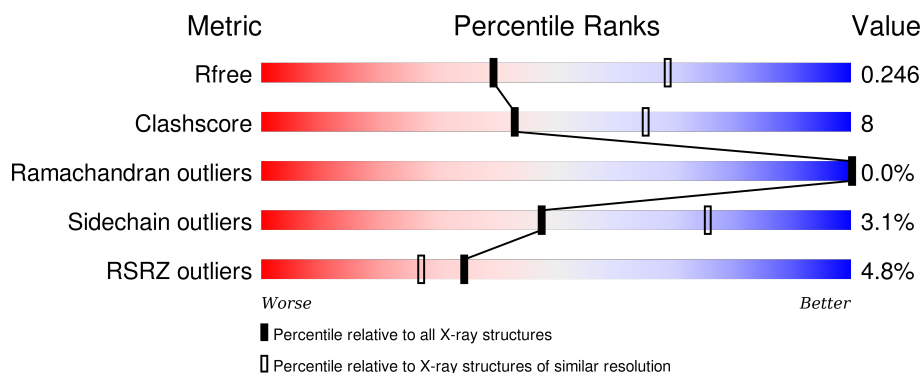
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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>2%</div> <div>77%</div> <div>19%</div> <div>• •</div> </div>
1	C	334	<div> <div>8%</div> <div>74%</div> <div>19%</div> <div>• •</div> </div>
1	E	334	<div> <div>6%</div> <div>72%</div> <div>22%</div> <div>• •</div> </div>
1	G	334	<div> <div>2%</div> <div>75%</div> <div>20%</div> <div>• •</div> </div>
1	I	334	<div> <div>0%</div> <div>78%</div> <div>18%</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	
2	B	182	
2	D	182	
2	F	182	
2	H	182	
2	J	182	
2	L	182	
2	N	182	
2	P	182	
2	R	182	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36134 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	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			
1	C	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			
1	E	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			
1	G	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			
1	I	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			
1	K	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			
1	M	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			
1	O	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			
1	Q	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	EXPRESSION TAG	UNP Q9Q0U6
A	8	ASP	-	EXPRESSION TAG	UNP Q9Q0U6
A	9	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
A	10	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
C	7	ALA	-	EXPRESSION TAG	UNP Q9Q0U6
C	8	ASP	-	EXPRESSION TAG	UNP Q9Q0U6
C	9	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
C	10	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
E	7	ALA	-	EXPRESSION TAG	UNP Q9Q0U6
E	8	ASP	-	EXPRESSION TAG	UNP Q9Q0U6
E	9	PRO	-	EXPRESSION TAG	UNP Q9Q0U6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	10	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
G	7	ALA	-	EXPRESSION TAG	UNP Q9Q0U6
G	8	ASP	-	EXPRESSION TAG	UNP Q9Q0U6
G	9	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
G	10	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
I	7	ALA	-	EXPRESSION TAG	UNP Q9Q0U6
I	8	ASP	-	EXPRESSION TAG	UNP Q9Q0U6
I	9	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
I	10	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
K	7	ALA	-	EXPRESSION TAG	UNP Q9Q0U6
K	8	ASP	-	EXPRESSION TAG	UNP Q9Q0U6
K	9	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
K	10	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
M	7	ALA	-	EXPRESSION TAG	UNP Q9Q0U6
M	8	ASP	-	EXPRESSION TAG	UNP Q9Q0U6
M	9	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
M	10	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
O	7	ALA	-	EXPRESSION TAG	UNP Q9Q0U6
O	8	ASP	-	EXPRESSION TAG	UNP Q9Q0U6
O	9	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
O	10	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
Q	7	ALA	-	EXPRESSION TAG	UNP Q9Q0U6
Q	8	ASP	-	EXPRESSION TAG	UNP Q9Q0U6
Q	9	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
Q	10	GLY	-	EXPRESSION TAG	UNP Q9Q0U6

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			
2	D	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			
2	F	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			
2	H	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			
2	J	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			
2	L	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			
2	N	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			
2	R	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	176	SER	-	EXPRESSION TAG	UNP Q9Q0U6
B	177	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
B	178	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
B	179	LEU	-	EXPRESSION TAG	UNP Q9Q0U6
B	180	VAL	-	EXPRESSION TAG	UNP Q9Q0U6
B	181	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
B	182	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
D	176	SER	-	EXPRESSION TAG	UNP Q9Q0U6
D	177	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
D	178	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
D	179	LEU	-	EXPRESSION TAG	UNP Q9Q0U6
D	180	VAL	-	EXPRESSION TAG	UNP Q9Q0U6
D	181	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
D	182	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
F	176	SER	-	EXPRESSION TAG	UNP Q9Q0U6
F	177	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
F	178	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
F	179	LEU	-	EXPRESSION TAG	UNP Q9Q0U6
F	180	VAL	-	EXPRESSION TAG	UNP Q9Q0U6
F	181	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
F	182	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
H	176	SER	-	EXPRESSION TAG	UNP Q9Q0U6
H	177	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
H	178	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
H	179	LEU	-	EXPRESSION TAG	UNP Q9Q0U6
H	180	VAL	-	EXPRESSION TAG	UNP Q9Q0U6
H	181	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
H	182	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
J	176	SER	-	EXPRESSION TAG	UNP Q9Q0U6
J	177	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
J	178	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
J	179	LEU	-	EXPRESSION TAG	UNP Q9Q0U6
J	180	VAL	-	EXPRESSION TAG	UNP Q9Q0U6
J	181	PRO	-	EXPRESSION TAG	UNP Q9Q0U6

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Chain	Residue	Modelled	Actual	Comment	Reference
J	182	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
L	176	SER	-	EXPRESSION TAG	UNP Q9Q0U6
L	177	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
L	178	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
L	179	LEU	-	EXPRESSION TAG	UNP Q9Q0U6
L	180	VAL	-	EXPRESSION TAG	UNP Q9Q0U6
L	181	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
L	182	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
N	176	SER	-	EXPRESSION TAG	UNP Q9Q0U6
N	177	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
N	178	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
N	179	LEU	-	EXPRESSION TAG	UNP Q9Q0U6
N	180	VAL	-	EXPRESSION TAG	UNP Q9Q0U6
N	181	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
N	182	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
P	176	SER	-	EXPRESSION TAG	UNP Q9Q0U6
P	177	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
P	178	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
P	179	LEU	-	EXPRESSION TAG	UNP Q9Q0U6
P	180	VAL	-	EXPRESSION TAG	UNP Q9Q0U6
P	181	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
P	182	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
R	176	SER	-	EXPRESSION TAG	UNP Q9Q0U6
R	177	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
R	178	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
R	179	LEU	-	EXPRESSION TAG	UNP Q9Q0U6
R	180	VAL	-	EXPRESSION TAG	UNP Q9Q0U6
R	181	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
R	182	ARG	-	EXPRESSION TAG	UNP Q9Q0U6

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

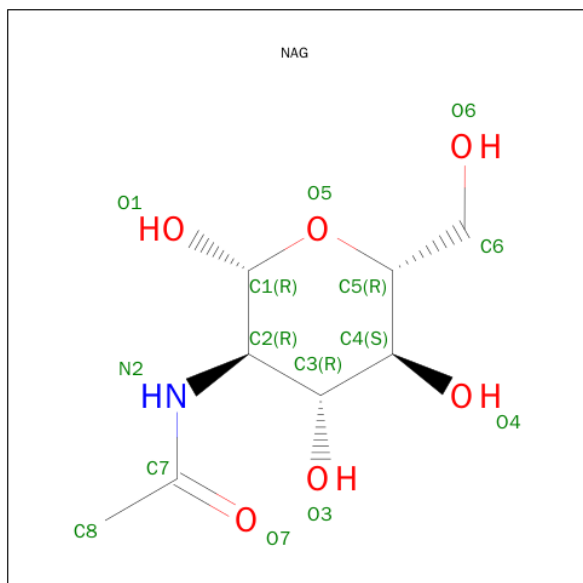
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	I	1	Total	C	N	O	0	0
			14	8	1	5		
4	K	1	Total	C	N	O	0	0
			14	8	1	5		
4	K	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	M	1	Total	C	N	O	0	0
			14	8	1	5		
4	M	1	Total	C	N	O	0	0
			14	8	1	5		
4	O	1	Total	C	N	O	0	0
			14	8	1	5		
4	O	1	Total	C	N	O	0	0
			14	8	1	5		
4	Q	1	Total	C	N	O	0	0
			14	8	1	5		

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total	O	0	0
			7	7		
6	B	5	Total	O	0	0
			5	5		
6	C	6	Total	O	0	0
			6	6		
6	D	8	Total	O	0	0
			8	8		
6	E	6	Total	O	0	0
			6	6		
6	F	2	Total	O	0	0
			2	2		
6	G	14	Total	O	0	0
			14	14		
6	H	4	Total	O	0	0
			4	4		
6	I	9	Total	O	0	0
			9	9		
6	J	12	Total	O	0	0
			12	12		
6	K	10	Total	O	0	0
			10	10		

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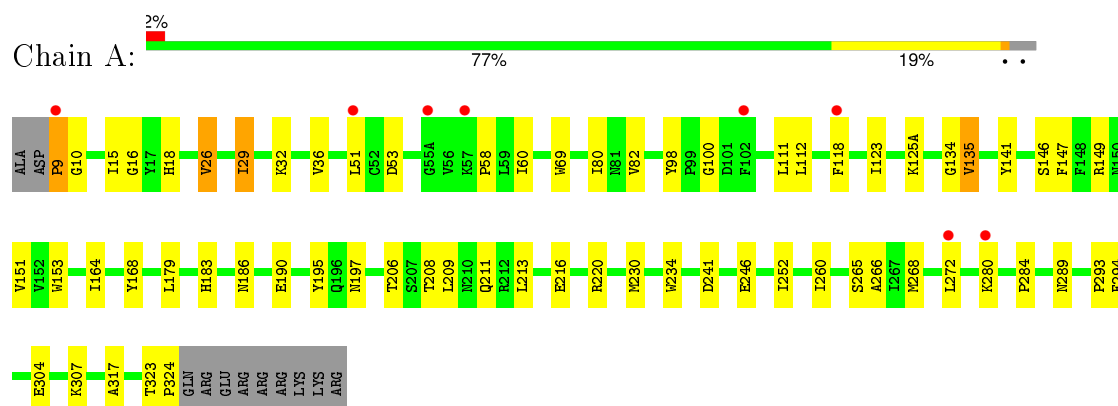
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	2	Total 2	O 2	0	0
6	M	5	Total 5	O 5	0	0
6	N	1	Total 1	O 1	0	0
6	O	8	Total 8	O 8	0	0
6	P	2	Total 2	O 2	0	0
6	Q	8	Total 8	O 8	0	0
6	R	8	Total 8	O 8	0	0

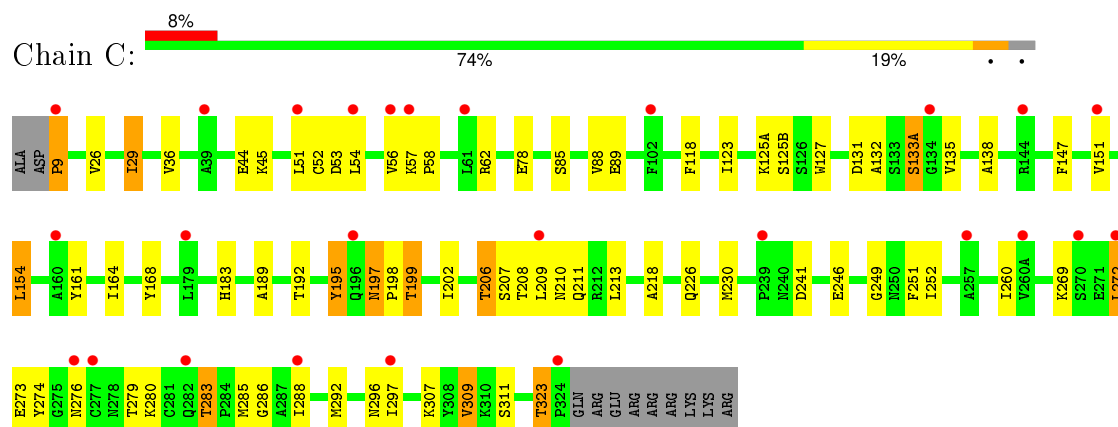
3 Residue-property plots

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.

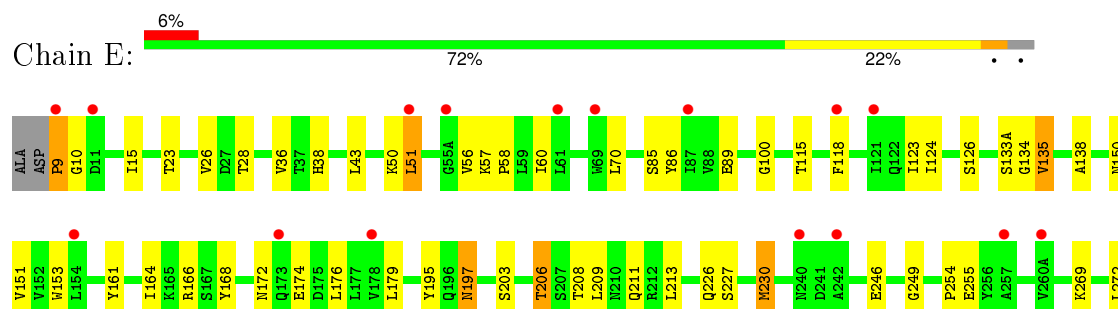
• Molecule 1: Hemagglutinin HA1 chain



• Molecule 1: Hemagglutinin HA1 chain

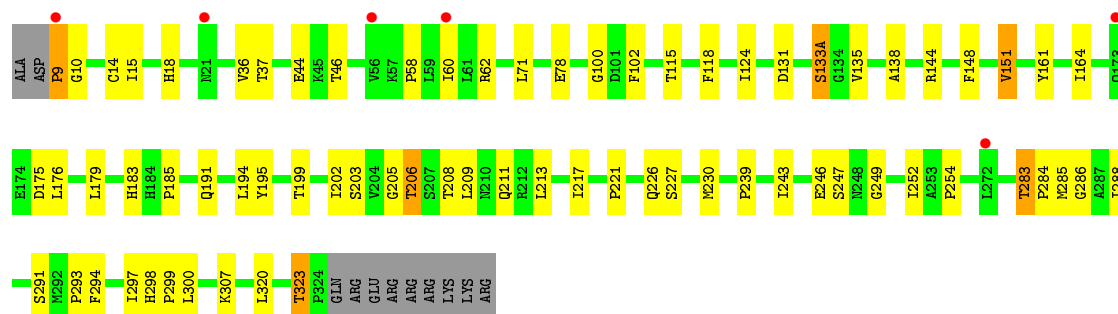
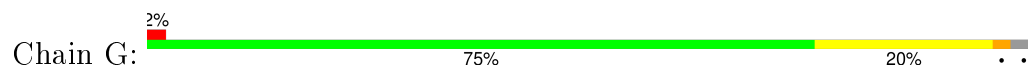


• Molecule 1: Hemagglutinin HA1 chain

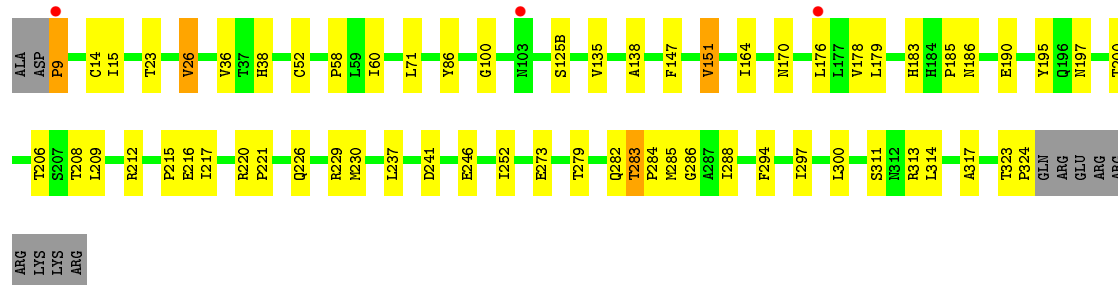
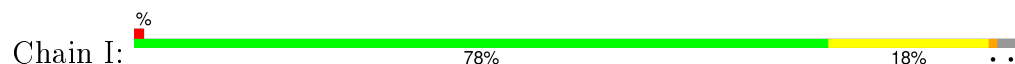




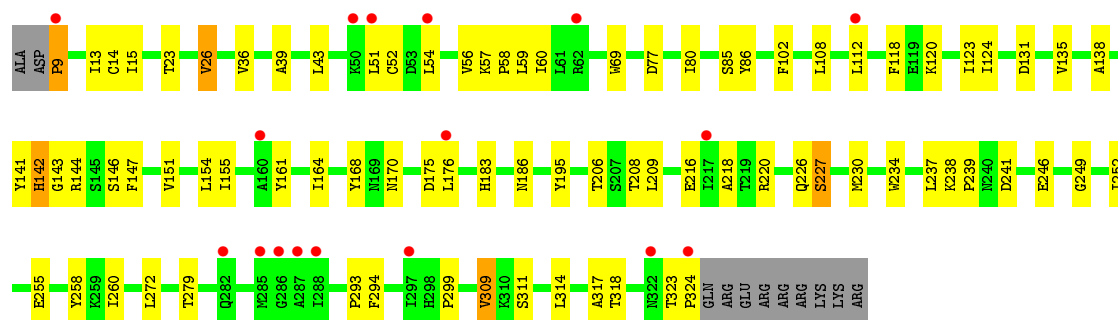
• Molecule 1: Hemagglutinin HA1 chain



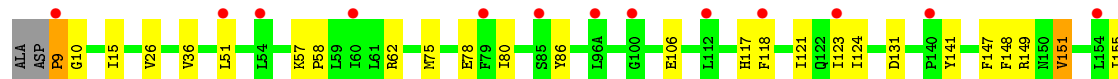
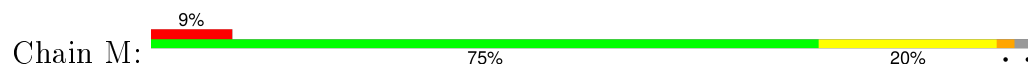
• Molecule 1: Hemagglutinin HA1 chain

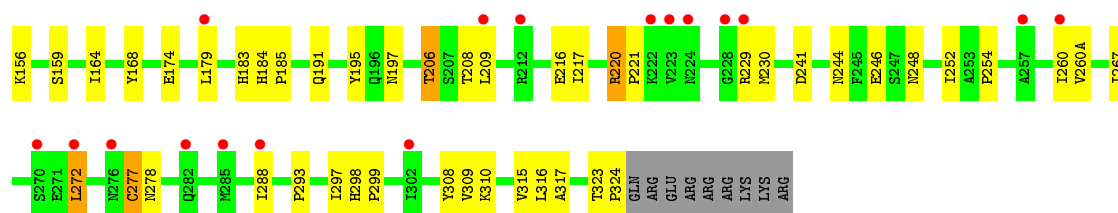


• Molecule 1: Hemagglutinin HA1 chain

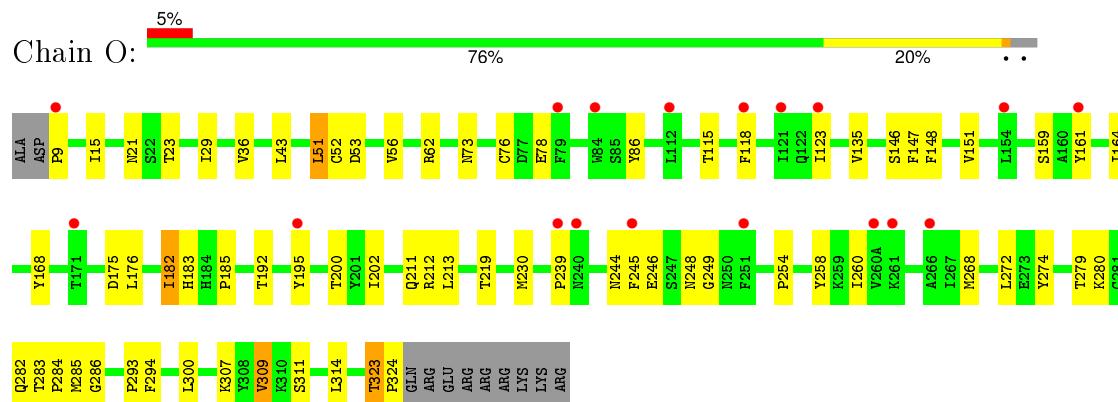


• Molecule 1: Hemagglutinin HA1 chain

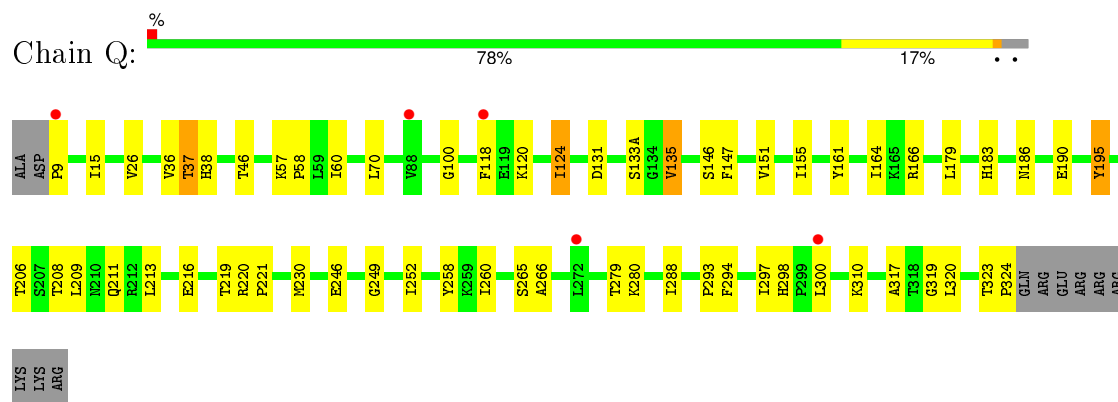




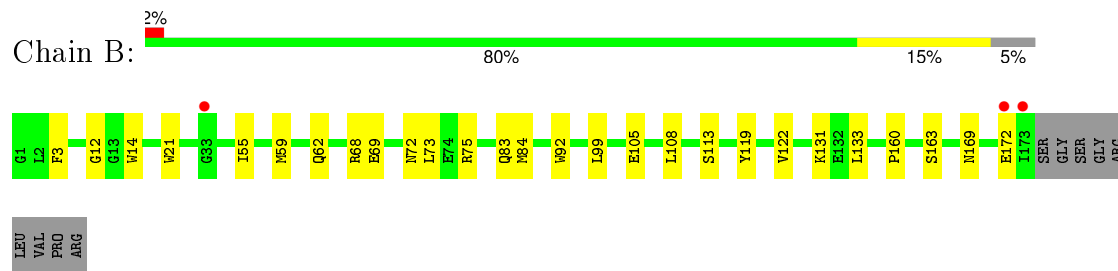
• Molecule 1: Hemagglutinin HA1 chain



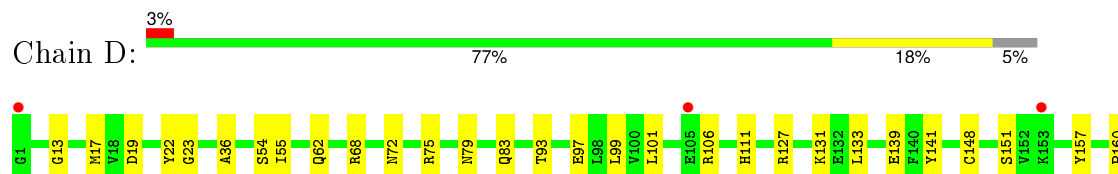
• Molecule 1: Hemagglutinin HA1 chain

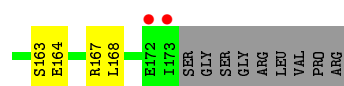


• Molecule 2: Hemagglutinin HA2 chain

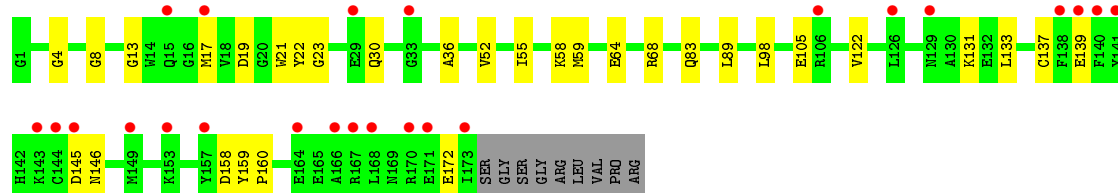
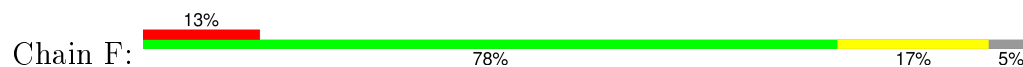


• Molecule 2: Hemagglutinin HA2 chain

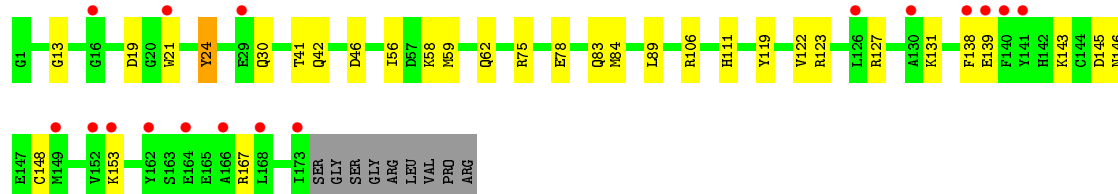
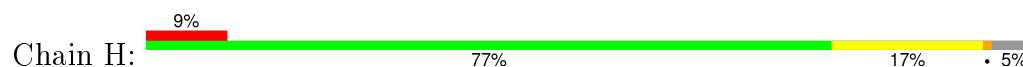




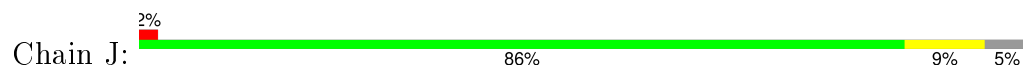
• Molecule 2: Hemagglutinin HA2 chain



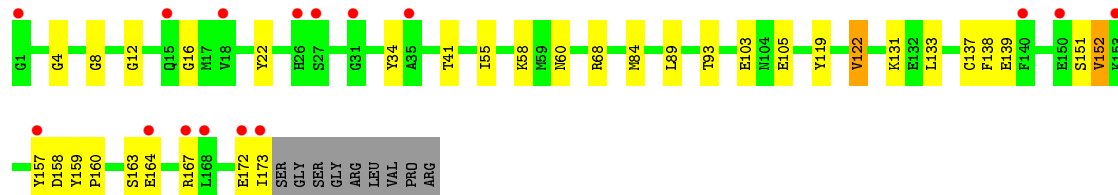
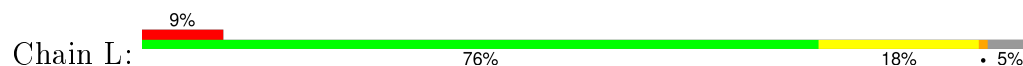
• Molecule 2: Hemagglutinin HA2 chain



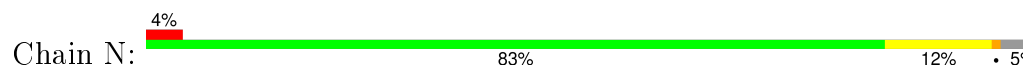
• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain

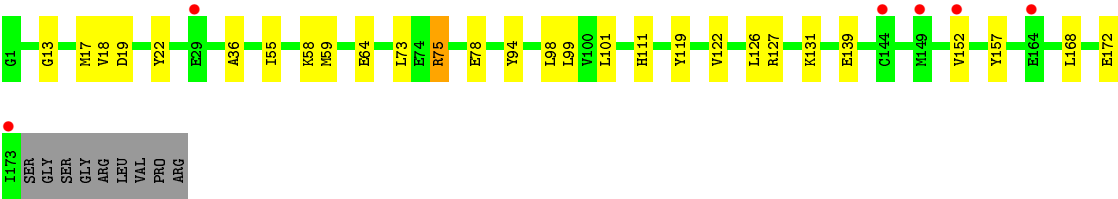
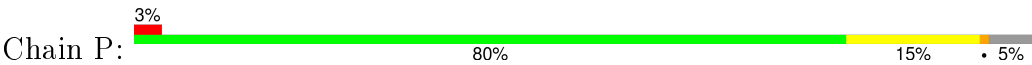


• Molecule 2: Hemagglutinin HA2 chain



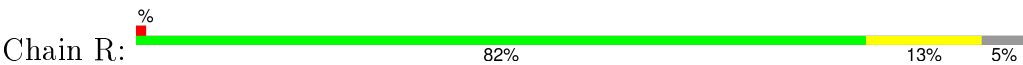
LEU
VAL
PRO
ARG

• Molecule 2: Hemagglutinin HA2 chain



I173
SER
GLY
SER
GLY
ARG
LEU
VAL
PRO
ARG

• Molecule 2: Hemagglutinin HA2 chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.48 Å 225.73 Å 211.63 Å 90.00° 98.97° 90.00°	Depositor
Resolution (Å)	49.66 – 2.60 49.66 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.8 (49.66-2.60) 95.1 (49.66-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.58 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.189 , 0.243 0.196 , 0.246	Depositor DCC
R_{free} test set	9835 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	65.9	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 63.0	EDS
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	6 of 196437 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	36134	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.26 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.7239e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.47	0/2616	0.67	1/3557 (0.0%)
1	C	0.44	0/2616	0.66	2/3557 (0.1%)
1	E	0.44	0/2616	0.65	2/3557 (0.1%)
1	G	0.46	0/2616	0.66	2/3557 (0.1%)
1	I	0.49	0/2616	0.70	1/3557 (0.0%)
1	K	0.44	0/2616	0.64	1/3557 (0.0%)
1	M	0.40	0/2616	0.62	2/3557 (0.1%)
1	O	0.42	0/2616	0.64	1/3557 (0.0%)
1	Q	0.46	0/2616	0.67	1/3557 (0.0%)
2	B	0.49	0/1430	0.65	0/1924
2	D	0.46	0/1430	0.58	0/1924
2	F	0.47	0/1430	0.60	0/1924
2	H	0.47	0/1430	0.60	0/1924
2	J	0.47	0/1430	0.61	0/1924
2	L	0.45	0/1430	0.55	0/1924
2	N	0.43	0/1430	0.59	0/1924
2	P	0.46	0/1430	0.60	0/1924
2	R	0.49	0/1430	0.62	0/1924
All	All	0.45	0/36414	0.64	13/49329 (0.0%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	9	PRO	CA-N-CD	-8.94	98.98	111.50
1	C	9	PRO	CA-N-CD	-8.81	99.17	111.50
1	O	9	PRO	CA-N-CD	-8.72	99.29	111.50
1	G	9	PRO	CA-N-CD	-8.66	99.38	111.50
1	K	9	PRO	CA-N-CD	-8.51	99.59	111.50

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	2551	0	2476	45	0
1	C	2551	0	2476	55	0
1	E	2551	0	2474	54	0
1	G	2551	0	2476	54	0
1	I	2551	0	2476	49	0
1	K	2551	0	2475	58	0
1	M	2551	0	2475	60	0
1	O	2551	0	2476	48	0
1	Q	2551	0	2476	43	0
2	B	1403	0	1302	22	0
2	D	1403	0	1302	24	0
2	F	1403	0	1302	24	0
2	H	1403	0	1302	31	0
2	J	1403	0	1302	13	0
2	L	1403	0	1302	24	0
2	N	1403	0	1302	21	0
2	P	1403	0	1302	22	0
2	R	1403	0	1301	23	0
3	A	28	0	25	0	0
3	C	28	0	25	0	0
3	E	28	0	25	3	0
3	I	28	0	25	1	0
3	K	28	0	25	1	0
3	M	28	0	25	1	0
3	R	28	0	25	0	0
4	A	14	0	13	0	0
4	C	14	0	13	0	0
4	E	28	0	26	0	0
4	G	28	0	26	0	0
4	I	14	0	13	0	0
4	K	28	0	26	3	0
4	M	28	0	26	0	0
4	O	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	14	0	13	0	0
5	Q	39	0	34	0	0
6	A	7	0	0	1	0
6	B	5	0	0	0	0
6	C	6	0	0	0	0
6	D	8	0	0	0	0
6	E	6	0	0	0	0
6	F	2	0	0	0	0
6	G	14	0	0	0	0
6	H	4	0	0	0	0
6	I	9	0	0	0	0
6	J	12	0	0	0	0
6	K	10	0	0	3	0
6	L	2	0	0	0	0
6	M	5	0	0	0	0
6	N	1	0	0	0	0
6	O	8	0	0	1	0
6	P	2	0	0	0	0
6	Q	8	0	0	0	0
6	R	8	0	0	0	0
All	All	36134	0	34388	578	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 8.

The worst 5 of 578 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:M:9:PRO:HD2	1:M:10:GLY:H	1.17	1.07
1:E:9:PRO:HD2	1:E:10:GLY:H	1.20	1.05
1:A:9:PRO:HD2	1:A:10:GLY:H	1.23	0.99
1:I:170:ASN:CG	1:I:176:LEU:HD23	1.85	0.97
1:I:170:ASN:ND2	1:I:176:LEU:HD23	1.81	0.96

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/334 (96%)	312 (97%)	9 (3%)	0	100	100
1	C	321/334 (96%)	309 (96%)	12 (4%)	0	100	100
1	E	321/334 (96%)	311 (97%)	10 (3%)	0	100	100
1	G	321/334 (96%)	311 (97%)	10 (3%)	0	100	100
1	I	321/334 (96%)	310 (97%)	11 (3%)	0	100	100
1	K	321/334 (96%)	311 (97%)	9 (3%)	1 (0%)	46	72
1	M	321/334 (96%)	309 (96%)	12 (4%)	0	100	100
1	O	321/334 (96%)	314 (98%)	7 (2%)	0	100	100
1	Q	321/334 (96%)	311 (97%)	10 (3%)	0	100	100
2	B	171/182 (94%)	167 (98%)	4 (2%)	0	100	100
2	D	171/182 (94%)	167 (98%)	4 (2%)	0	100	100
2	F	171/182 (94%)	166 (97%)	5 (3%)	0	100	100
2	H	171/182 (94%)	168 (98%)	3 (2%)	0	100	100
2	J	171/182 (94%)	168 (98%)	3 (2%)	0	100	100
2	L	171/182 (94%)	166 (97%)	5 (3%)	0	100	100
2	N	171/182 (94%)	167 (98%)	3 (2%)	1 (1%)	30	56
2	P	171/182 (94%)	167 (98%)	4 (2%)	0	100	100
2	R	171/182 (94%)	167 (98%)	4 (2%)	0	100	100
All	All	4428/4644 (95%)	4301 (97%)	125 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	142	HIS
2	N	12	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	287/297 (97%)	277 (96%)	10 (4%)	43	71
1	C	287/297 (97%)	273 (95%)	14 (5%)	31	57
1	E	287/297 (97%)	272 (95%)	15 (5%)	29	54
1	G	287/297 (97%)	274 (96%)	13 (4%)	34	62
1	I	287/297 (97%)	276 (96%)	11 (4%)	40	68
1	K	287/297 (97%)	277 (96%)	10 (4%)	43	71
1	M	287/297 (97%)	277 (96%)	10 (4%)	43	71
1	O	287/297 (97%)	276 (96%)	11 (4%)	40	68
1	Q	287/297 (97%)	278 (97%)	9 (3%)	47	76
2	B	148/155 (96%)	147 (99%)	1 (1%)	88	96
2	D	148/155 (96%)	147 (99%)	1 (1%)	88	96
2	F	148/155 (96%)	147 (99%)	1 (1%)	88	96
2	H	148/155 (96%)	146 (99%)	2 (1%)	74	90
2	J	148/155 (96%)	146 (99%)	2 (1%)	74	90
2	L	148/155 (96%)	141 (95%)	7 (5%)	32	59
2	N	148/155 (96%)	147 (99%)	1 (1%)	88	96
2	P	148/155 (96%)	145 (98%)	3 (2%)	63	85
2	R	148/155 (96%)	147 (99%)	1 (1%)	88	96
All	All	3915/4068 (96%)	3793 (97%)	122 (3%)	47	76

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	24	TYR
2	J	26	HIS
1	Q	36	VAL
2	H	41	THR
1	I	135	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	211	GLN
1	I	38	HIS
2	N	83	GLN
2	F	129	ASN
1	M	211	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 ⓘ

17 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	0.46	0	15,19,21	1.26	1 (6%)
3	NAG	A	2002	3	14,14,15	0.49	0	15,19,21	1.00	1 (6%)
3	NAG	C	2001	1,3	14,14,15	0.44	0	15,19,21	1.06	1 (6%)
3	NAG	C	2002	3	14,14,15	0.40	0	15,19,21	0.93	1 (6%)
3	NAG	E	2002	1,3	14,14,15	0.52	0	15,19,21	1.75	4 (26%)
3	NAG	E	2003	3	14,14,15	0.51	0	15,19,21	1.50	1 (6%)
3	NAG	I	2001	1,3	14,14,15	0.58	0	15,19,21	1.70	2 (13%)
3	NAG	I	2002	3	14,14,15	0.52	0	15,19,21	0.96	1 (6%)
3	NAG	K	2001	1,3	14,14,15	0.48	0	15,19,21	1.66	2 (13%)
3	NAG	K	2002	3	14,14,15	0.51	0	15,19,21	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	M	2001	1,3	14,14,15	0.52	0	15,19,21	1.79	3 (20%)
3	NAG	M	2002	3	14,14,15	0.54	0	15,19,21	1.25	1 (6%)
5	NAG	Q	2001	1,5	14,14,15	0.44	0	15,19,21	1.11	0
5	NAG	Q	2002	5	14,14,15	0.46	0	15,19,21	0.99	1 (6%)
5	MAN	Q	2003	5	11,11,12	0.50	0	14,15,17	1.62	2 (14%)
3	NAG	R	2001	3,2	14,14,15	0.60	0	15,19,21	1.59	2 (13%)
3	NAG	R	2002	3	14,14,15	0.50	0	15,19,21	1.67	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
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	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	NAG	E	2002	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2003	3	-	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	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	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
5	NAG	Q	2001	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Q	2002	5	-	0/6/23/26	0/1/1/1
5	MAN	Q	2003	5	-	0/2/19/22	0/1/1/1
3	NAG	R	2001	3,2	-	0/6/23/26	0/1/1/1
3	NAG	R	2002	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	2001	NAG	O4-C4-C3	-3.15	103.25	110.34
3	K	2001	NAG	C2-N2-C7	-2.95	119.25	123.04
3	I	2001	NAG	O4-C4-C3	-2.85	103.91	110.34
3	M	2001	NAG	C2-N2-C7	-2.72	119.55	123.04
5	Q	2002	NAG	C2-N2-C7	-2.54	119.78	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2002	NAG	3	0
3	E	2003	NAG	3	0
3	I	2001	NAG	1	0
3	K	2001	NAG	1	0
3	M	2001	NAG	1	0

5.6 Ligand geometry

14 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	$\# Z > 2$
4	NAG	A	2003	1	14,14,15	0.57	0	15,19,21	1.63	3 (20%)
4	NAG	C	2003	1	14,14,15	0.55	0	15,19,21	1.58	3 (20%)
4	NAG	E	2001	1	14,14,15	0.45	0	15,19,21	1.08	1 (6%)
4	NAG	E	2004	1	14,14,15	0.37	0	15,19,21	0.72	0
4	NAG	G	2001	1	14,14,15	0.43	0	15,19,21	1.46	1 (6%)
4	NAG	G	2002	1	14,14,15	0.45	0	15,19,21	1.88	1 (6%)
4	NAG	I	2003	1	14,14,15	0.44	0	15,19,21	1.26	1 (6%)
4	NAG	K	2003	1	14,14,15	0.58	0	15,19,21	1.52	3 (20%)
4	NAG	K	2004	1	14,14,15	0.41	0	15,19,21	1.38	2 (13%)
4	NAG	M	2003	1	14,14,15	0.43	0	15,19,21	0.86	0
4	NAG	M	2004	1	14,14,15	0.50	0	15,19,21	0.80	0
4	NAG	O	2001	1	14,14,15	0.45	0	15,19,21	1.57	1 (6%)
4	NAG	O	2002	1	14,14,15	0.37	0	15,19,21	1.50	1 (6%)
4	NAG	Q	2004	1	14,14,15	0.52	0	15,19,21	1.33	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	2003	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2003	1	-	0/6/23/26	0/1/1/1
4	NAG	E	2001	1	-	0/6/23/26	0/1/1/1
4	NAG	E	2004	1	-	0/6/23/26	0/1/1/1
4	NAG	G	2001	1	-	0/6/23/26	0/1/1/1
4	NAG	G	2002	1	-	0/6/23/26	0/1/1/1
4	NAG	I	2003	1	-	0/6/23/26	0/1/1/1
4	NAG	K	2003	1	-	0/6/23/26	0/1/1/1
4	NAG	K	2004	1	-	0/6/23/26	0/1/1/1
4	NAG	M	2003	1	-	0/6/23/26	0/1/1/1
4	NAG	M	2004	1	-	0/6/23/26	0/1/1/1
4	NAG	O	2001	1	-	0/6/23/26	0/1/1/1
4	NAG	O	2002	1	-	0/6/23/26	0/1/1/1
4	NAG	Q	2004	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	2003	NAG	O4-C4-C5	-3.78	99.22	109.24
4	K	2004	NAG	C2-N2-C7	-3.09	119.07	123.04
4	A	2003	NAG	O3-C3-C2	-2.26	104.64	109.11
4	K	2003	NAG	O3-C3-C2	-2.18	104.80	109.11
4	C	2003	NAG	C4-C3-C2	2.38	114.93	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	2004	NAG	3	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	323/334 (96%)	0.21	8 (2%) 61 54	62, 86, 117, 157	0
1	C	323/334 (96%)	0.48	26 (8%) 15 10	69, 102, 130, 161	0
1	E	323/334 (96%)	0.33	19 (5%) 26 19	67, 94, 121, 167	0
1	G	323/334 (96%)	0.27	6 (1%) 70 64	63, 85, 112, 148	0
1	I	323/334 (96%)	0.13	3 (0%) 85 83	46, 80, 100, 138	0
1	K	323/334 (96%)	0.37	17 (5%) 30 23	52, 93, 121, 164	0
1	M	323/334 (96%)	0.57	30 (9%) 11 7	79, 112, 143, 176	0
1	O	323/334 (96%)	0.35	18 (5%) 28 21	65, 102, 130, 154	0
1	Q	323/334 (96%)	0.13	5 (1%) 76 71	61, 82, 107, 135	0
2	B	173/182 (95%)	0.33	3 (1%) 73 68	54, 83, 115, 159	0
2	D	173/182 (95%)	0.39	5 (2%) 55 48	62, 91, 124, 171	0
2	F	173/182 (95%)	1.00	24 (13%) 4 2	57, 104, 165, 216	0
2	H	173/182 (95%)	0.83	17 (9%) 10 6	62, 101, 155, 194	0
2	J	173/182 (95%)	0.26	3 (1%) 73 68	58, 84, 120, 167	0
2	L	173/182 (95%)	0.70	16 (9%) 11 7	64, 101, 153, 167	0
2	N	173/182 (95%)	0.53	8 (4%) 36 29	69, 97, 135, 155	0
2	P	173/182 (95%)	0.63	6 (3%) 48 40	63, 91, 126, 181	0
2	R	173/182 (95%)	0.26	1 (0%) 90 88	61, 79, 106, 147	0
All	All	4464/4644 (96%)	0.40	215 (4%) 34 27	46, 91, 134, 216	0

The worst 5 of 215 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	9	PRO	10.6
2	P	173	ILE	8.9
2	F	140	PHE	8.2

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Mol	Chain	Res	Type	RSRZ
1	E	9	PRO	7.3
2	H	173	ILE	7.0

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	A	2001	14/15	0.96	0.12	-0.52	85,105,126,131	0
5	NAG	Q	2001	14/15	0.95	0.12	-0.72	86,104,121,126	0
3	NAG	K	2001	14/15	0.96	0.08	-0.79	74,93,106,109	0
3	NAG	I	2001	14/15	0.93	0.12	-1.73	68,84,96,98	0
3	NAG	M	2001	14/15	0.93	0.10	-1.83	91,109,123,143	0
3	NAG	C	2001	14/15	0.92	0.12	-1.95	82,103,115,116	0
3	NAG	E	2003	14/15	0.80	0.35	-	135,145,154,158	0
3	NAG	R	2002	14/15	0.91	0.21	-	119,142,154,163	0
3	NAG	R	2001	14/15	0.88	0.31	-	96,115,120,135	0
3	NAG	I	2002	14/15	0.89	0.20	-	111,122,137,152	0
3	NAG	C	2002	14/15	0.87	0.24	-	109,132,145,152	0
3	NAG	M	2002	14/15	0.82	0.19	-	144,161,171,177	0
5	MAN	Q	2003	11/12	0.84	0.32	-	143,164,169,173	0
3	NAG	A	2002	14/15	0.81	0.24	-	121,139,156,167	0
5	NAG	Q	2002	14/15	0.87	0.20	-	122,141,155,162	0
3	NAG	K	2002	14/15	0.90	0.17	-	123,135,150,165	0
3	NAG	E	2002	14/15	0.86	0.16	-	92,126,137,139	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
4	NAG	E	2001	14/15	0.84	0.30	0.64	103,118,138,158	0
4	NAG	G	2001	14/15	0.91	0.14	0.14	86,106,114,116	0
4	NAG	O	2001	14/15	0.86	0.18	-0.58	75,105,120,122	0
4	NAG	I	2003	14/15	0.91	0.18	-	102,115,121,121	0
4	NAG	G	2002	14/15	0.91	0.14	-	107,124,130,133	0
4	NAG	K	2003	14/15	0.82	0.19	-	103,125,134,148	0
4	NAG	M	2003	14/15	0.90	0.16	-	112,129,135,138	0
4	NAG	M	2004	14/15	0.85	0.33	-	112,151,162,166	0
4	NAG	O	2002	14/15	0.91	0.13	-	92,112,118,125	0
4	NAG	C	2003	14/15	0.88	0.31	-	115,124,136,149	0
4	NAG	E	2004	14/15	0.81	0.22	-	119,136,150,151	0
4	NAG	Q	2004	14/15	0.85	0.20	-	115,127,133,135	0
4	NAG	K	2004	14/15	0.74	0.23	-	133,149,159,163	0
4	NAG	A	2003	14/15	0.86	0.20	-	102,127,143,157	0

6.5 Other polymers

There are no such residues in this entry.