



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:52 am GMT

PDB ID : 3AL4
Title : Crystal structure of the swine-origin A (H1N1)-2009 influenza A virus hemagglutinin (HA) reveals similar antigenicity to that of the 1918 pandemic virus
Authors : Zhang, W.; Qi, J.X.; Shi, Y.; Li, Q.; Yan, J.H.; Gao, G.F.
Deposited on : 2010-07-22
Resolution : 2.87 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

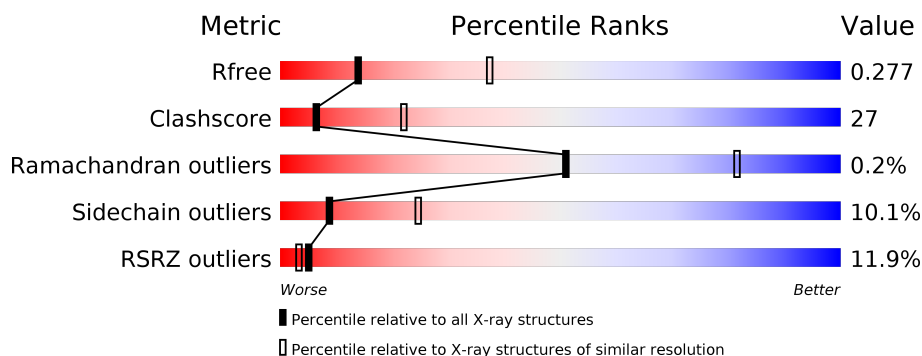
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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}	100719	2135 (2.90-2.86)
Clashscore	112137	2400 (2.90-2.86)
Ramachandran outliers	110173	2346 (2.90-2.86)
Sidechain outliers	110143	2349 (2.90-2.86)
RSRZ outliers	101464	2149 (2.90-2.86)

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	333	<div> <div>9%</div> <div>54% 36% 6% .</div> </div>
1	C	333	<div> <div>8%</div> <div>52% 41% . .</div> </div>
1	E	333	<div> <div>14%</div> <div>41% 47% 8% .</div> </div>
1	G	333	<div> <div>11%</div> <div>54% 37% 6% .</div> </div>
1	I	333	<div> <div>7%</div> <div>56% 35% 6% .</div> </div>
1	K	333	<div> <div>8%</div> <div>49% 40% 7% .</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	181	
2	D	181	
2	F	181	
2	H	181	
2	J	181	
2	L	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	607	-	-	-	X
3	NAG	L	601	-	-	X	X
4	NAG	A	602	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23626 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2505	1584	433	477	11			
1	C	321	Total	C	N	O	S	0	0	0
			2509	1586	433	479	11			
1	E	321	Total	C	N	O	S	0	0	0
			2509	1586	433	479	11			
1	G	321	Total	C	N	O	S	0	0	0
			2505	1584	433	477	11			
1	I	321	Total	C	N	O	S	0	0	0
			2509	1586	433	479	11			
1	K	321	Total	C	N	O	S	0	0	0
			2511	1588	433	479	11			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	EXPRESSION TAG	UNP C3W5S1
A	2	ASP	-	EXPRESSION TAG	UNP C3W5S1
A	3	LEU	-	EXPRESSION TAG	UNP C3W5S1
A	4	GLY	-	EXPRESSION TAG	UNP C3W5S1
A	5	SER	-	EXPRESSION TAG	UNP C3W5S1
A	6	ARG	-	EXPRESSION TAG	UNP C3W5S1
C	1	ALA	-	EXPRESSION TAG	UNP C3W5S1
C	2	ASP	-	EXPRESSION TAG	UNP C3W5S1
C	3	LEU	-	EXPRESSION TAG	UNP C3W5S1
C	4	GLY	-	EXPRESSION TAG	UNP C3W5S1
C	5	SER	-	EXPRESSION TAG	UNP C3W5S1
C	6	ARG	-	EXPRESSION TAG	UNP C3W5S1
E	1	ALA	-	EXPRESSION TAG	UNP C3W5S1
E	2	ASP	-	EXPRESSION TAG	UNP C3W5S1
E	3	LEU	-	EXPRESSION TAG	UNP C3W5S1
E	4	GLY	-	EXPRESSION TAG	UNP C3W5S1
E	5	SER	-	EXPRESSION TAG	UNP C3W5S1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	6	ARG	-	EXPRESSION TAG	UNP C3W5S1
G	1	ALA	-	EXPRESSION TAG	UNP C3W5S1
G	2	ASP	-	EXPRESSION TAG	UNP C3W5S1
G	3	LEU	-	EXPRESSION TAG	UNP C3W5S1
G	4	GLY	-	EXPRESSION TAG	UNP C3W5S1
G	5	SER	-	EXPRESSION TAG	UNP C3W5S1
G	6	ARG	-	EXPRESSION TAG	UNP C3W5S1
I	1	ALA	-	EXPRESSION TAG	UNP C3W5S1
I	2	ASP	-	EXPRESSION TAG	UNP C3W5S1
I	3	LEU	-	EXPRESSION TAG	UNP C3W5S1
I	4	GLY	-	EXPRESSION TAG	UNP C3W5S1
I	5	SER	-	EXPRESSION TAG	UNP C3W5S1
I	6	ARG	-	EXPRESSION TAG	UNP C3W5S1
K	1	ALA	-	EXPRESSION TAG	UNP C3W5S1
K	2	ASP	-	EXPRESSION TAG	UNP C3W5S1
K	3	LEU	-	EXPRESSION TAG	UNP C3W5S1
K	4	GLY	-	EXPRESSION TAG	UNP C3W5S1
K	5	SER	-	EXPRESSION TAG	UNP C3W5S1
K	6	ARG	-	EXPRESSION TAG	UNP C3W5S1

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	162	Total	C	N	O	S	0	0	0
			1305	822	220	257	6			
2	D	162	Total	C	N	O	S	0	0	0
			1300	818	219	257	6			
2	F	161	Total	C	N	O	S	0	0	0
			1302	821	219	256	6			
2	H	162	Total	C	N	O	S	0	0	0
			1305	822	220	257	6			
2	J	162	Total	C	N	O	S	0	0	0
			1305	822	220	257	6			
2	L	161	Total	C	N	O	S	0	0	0
			1302	821	219	256	6			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	ARG	-	EXPRESSION TAG	UNP C3W5S1
B	178	LEU	-	EXPRESSION TAG	UNP C3W5S1
B	179	VAL	-	EXPRESSION TAG	UNP C3W5S1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	180	PRO	-	EXPRESSION TAG	UNP C3W5S1
B	181	ARG	-	EXPRESSION TAG	UNP C3W5S1
D	177	ARG	-	EXPRESSION TAG	UNP C3W5S1
D	178	LEU	-	EXPRESSION TAG	UNP C3W5S1
D	179	VAL	-	EXPRESSION TAG	UNP C3W5S1
D	180	PRO	-	EXPRESSION TAG	UNP C3W5S1
D	181	ARG	-	EXPRESSION TAG	UNP C3W5S1
F	177	ARG	-	EXPRESSION TAG	UNP C3W5S1
F	178	LEU	-	EXPRESSION TAG	UNP C3W5S1
F	179	VAL	-	EXPRESSION TAG	UNP C3W5S1
F	180	PRO	-	EXPRESSION TAG	UNP C3W5S1
F	181	ARG	-	EXPRESSION TAG	UNP C3W5S1
H	177	ARG	-	EXPRESSION TAG	UNP C3W5S1
H	178	LEU	-	EXPRESSION TAG	UNP C3W5S1
H	179	VAL	-	EXPRESSION TAG	UNP C3W5S1
H	180	PRO	-	EXPRESSION TAG	UNP C3W5S1
H	181	ARG	-	EXPRESSION TAG	UNP C3W5S1
J	177	ARG	-	EXPRESSION TAG	UNP C3W5S1
J	178	LEU	-	EXPRESSION TAG	UNP C3W5S1
J	179	VAL	-	EXPRESSION TAG	UNP C3W5S1
J	180	PRO	-	EXPRESSION TAG	UNP C3W5S1
J	181	ARG	-	EXPRESSION TAG	UNP C3W5S1
L	177	ARG	-	EXPRESSION TAG	UNP C3W5S1
L	178	LEU	-	EXPRESSION TAG	UNP C3W5S1
L	179	VAL	-	EXPRESSION TAG	UNP C3W5S1
L	180	PRO	-	EXPRESSION TAG	UNP C3W5S1
L	181	ARG	-	EXPRESSION TAG	UNP C3W5S1

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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

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

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	36	Total	O	0	0
			36	36		
6	B	17	Total	O	0	0
			17	17		
6	C	38	Total	O	0	0
			38	38		
6	D	10	Total	O	0	0
			10	10		
6	E	31	Total	O	0	0
			31	31		
6	F	13	Total	O	0	0
			13	13		

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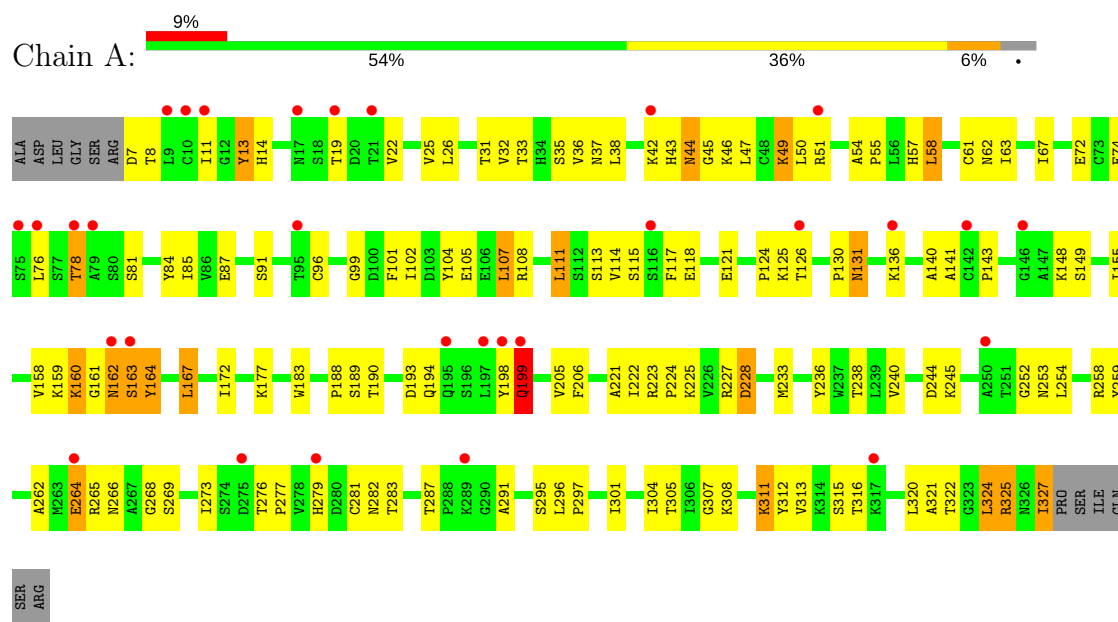
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	45	Total 45	O 45	0	0
6	H	23	Total 23	O 23	0	0
6	I	37	Total 37	O 37	0	0
6	J	21	Total 21	O 21	0	0
6	K	35	Total 35	O 35	0	0
6	L	11	Total 11	O 11	0	0

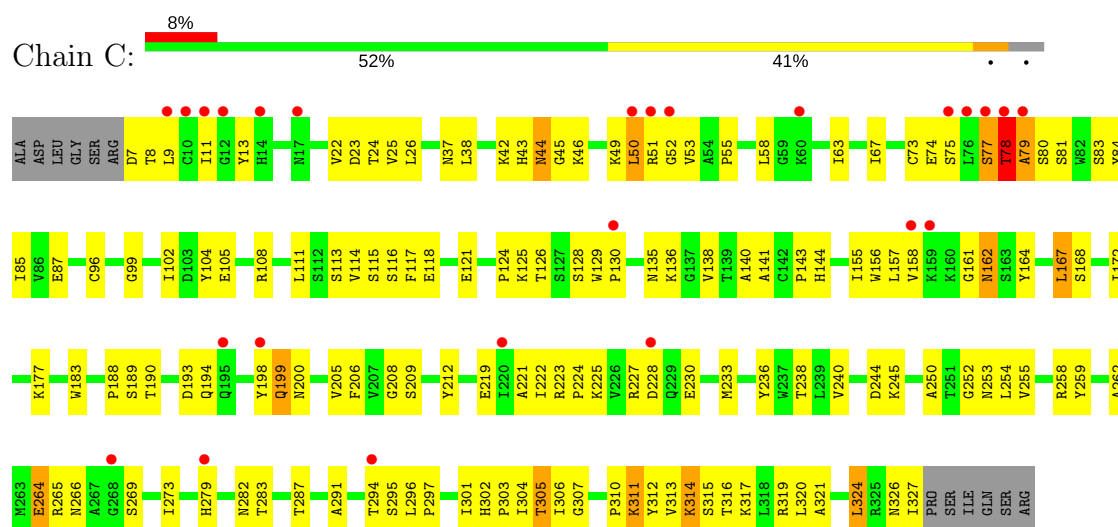
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

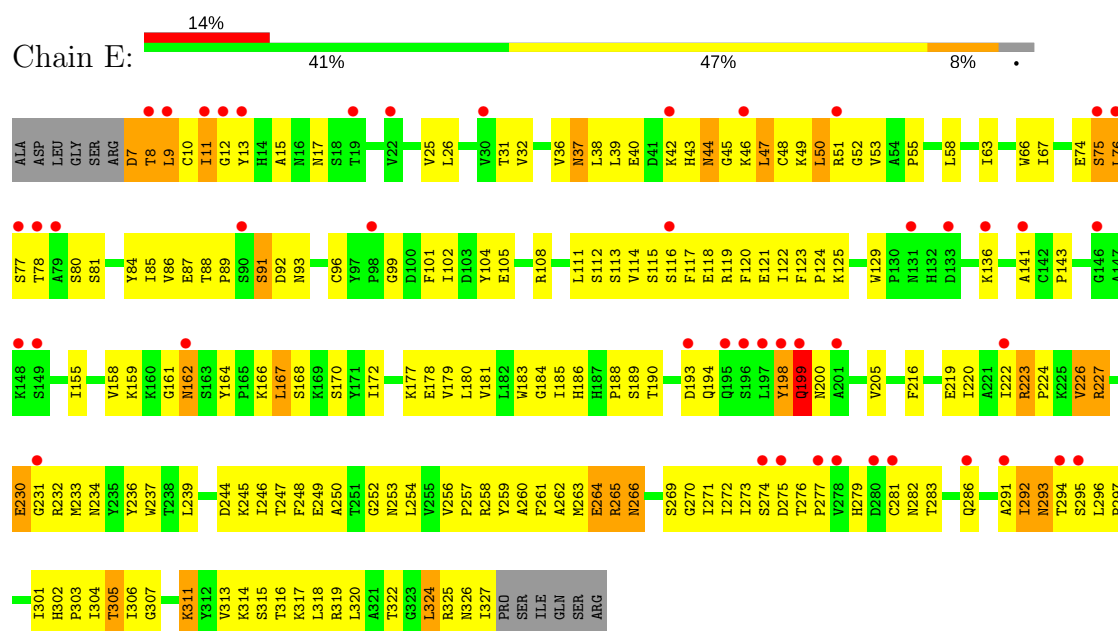
• Molecule 1: Hemagglutinin



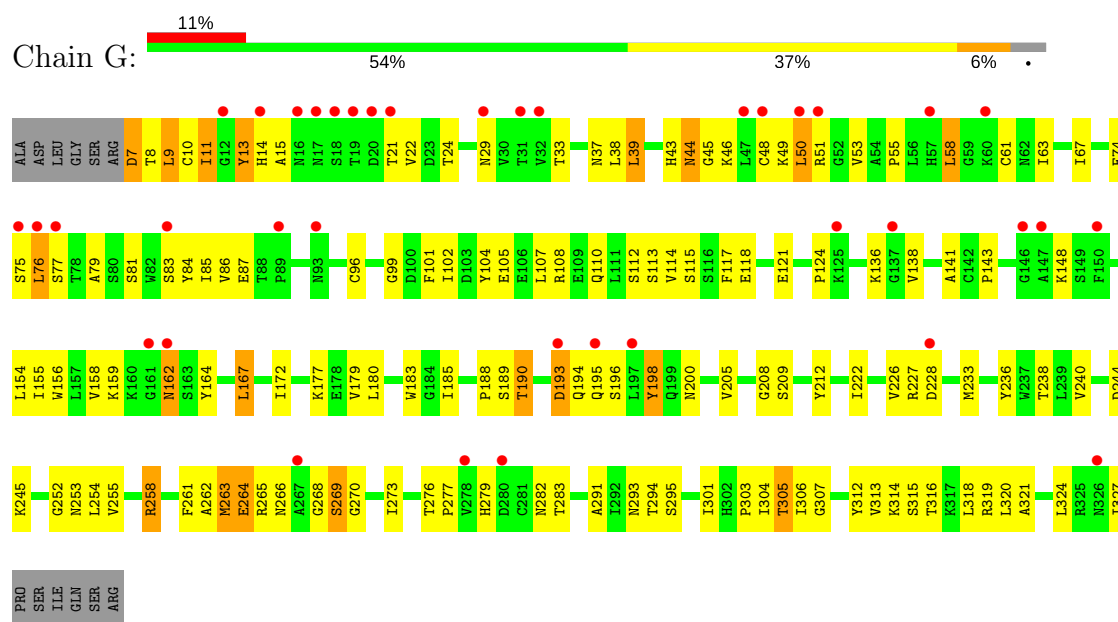
• Molecule 1: Hemagglutinin



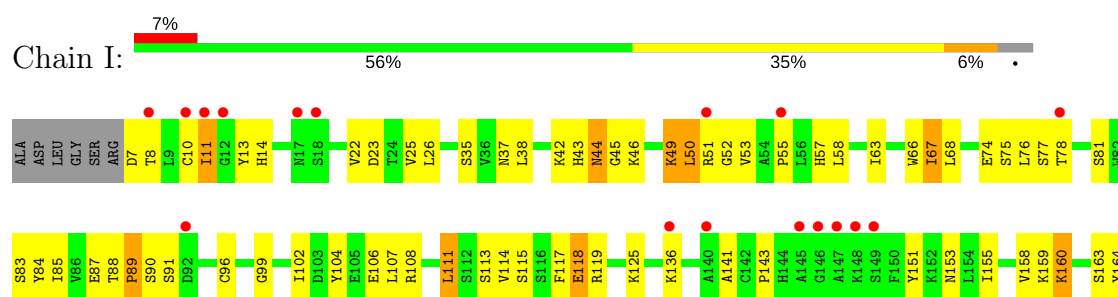
• Molecule 1: Hemagglutinin

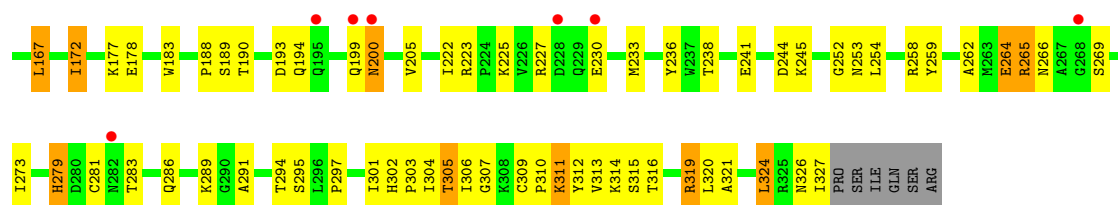


• Molecule 1: Hemagglutinin

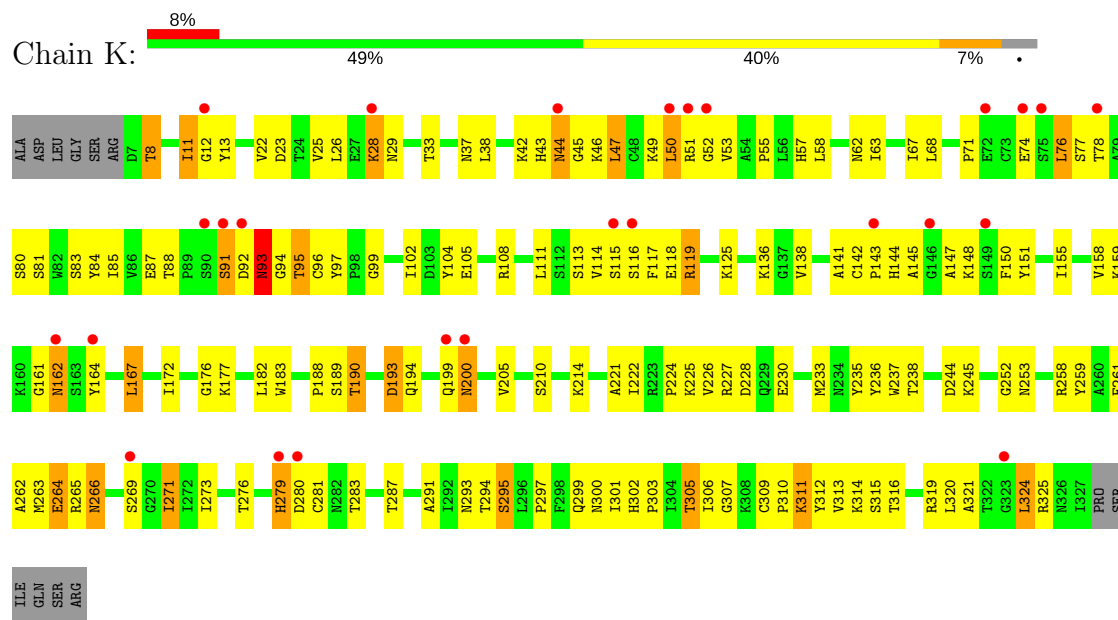


• Molecule 1: Hemagglutinin

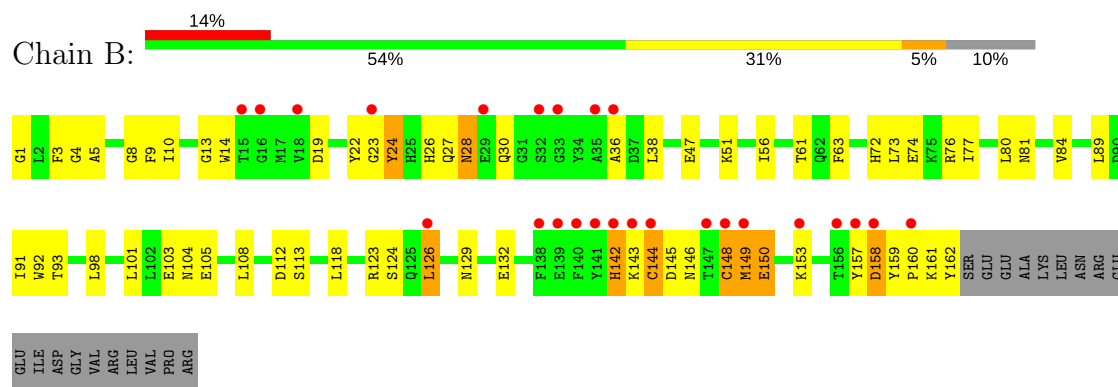




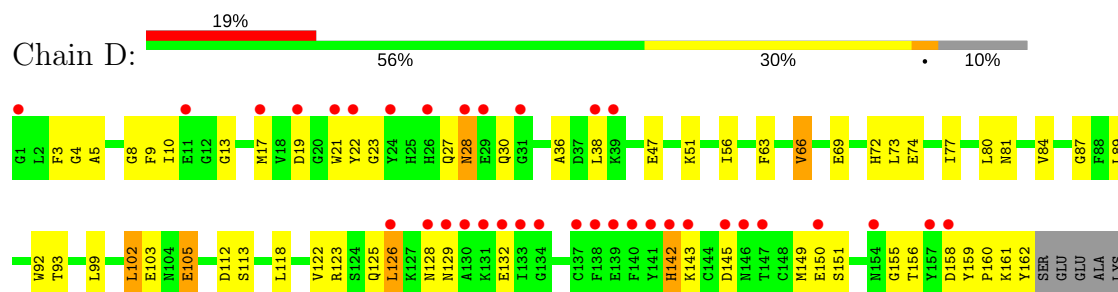
• Molecule 1: Hemagglutinin



• Molecule 2: Hemagglutinin

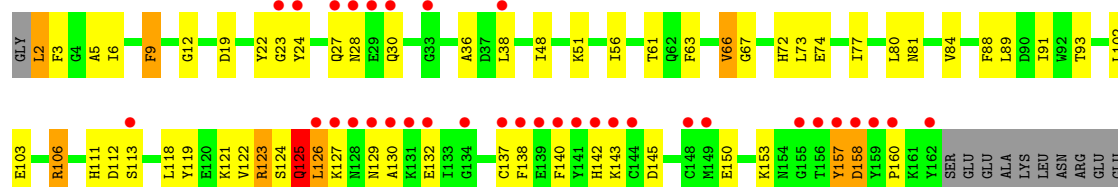


• Molecule 2: Hemagglutinin



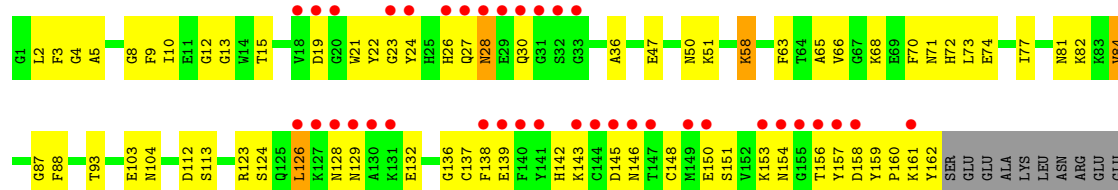
LEU
ASN
ARG
GLU
GLU
ILE
ASP
VAL
VAL
LEU
LEU
VAL
PRO
ARG

• Molecule 2: Hemagglutinin



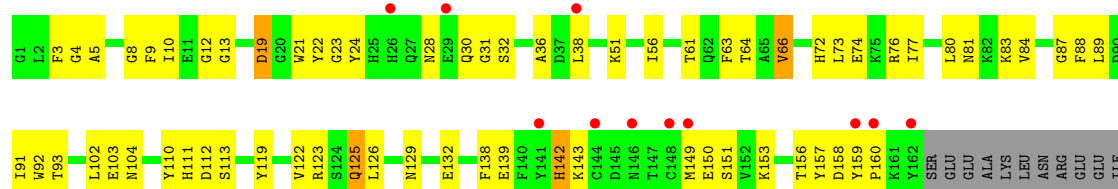
ILE
ASP
GLY
VAL
ARG
LEU
VAL
PRO
ARG

• Molecule 2: Hemagglutinin



ILE
ASP
GLY
VAL
ARG
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VAL
PRO
ARG

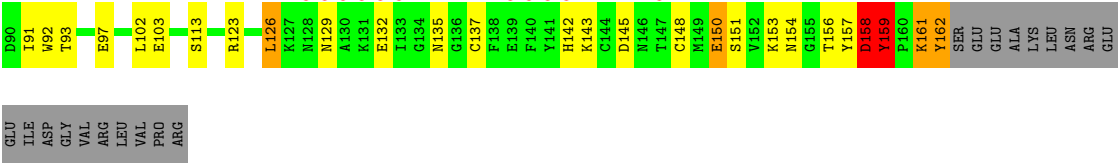
• Molecule 2: Hemagglutinin



ASP
GLY
VAL
ARG
LEU
VAL
PRO
ARG

• Molecule 2: Hemagglutinin





GLU
ILE
ASP
GLY
VAL
ARG
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	66.02Å 115.19Å 114.98Å 62.31° 77.94° 81.05°	Depositor
Resolution (Å)	24.19 – 2.87 35.21 – 2.87	Depositor EDS
% Data completeness (in resolution range)	91.6 (24.19-2.87) 82.7 (35.21-2.87)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.85Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.5_2)	Depositor
R, R_{free}	0.246 , 0.270 0.253 , 0.277	Depositor DCC
R_{free} test set	3292 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	61.4	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	23626	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/2568	0.56	5/3488 (0.1%)
1	C	0.26	0/2572	0.53	3/3493 (0.1%)
1	E	0.25	0/2572	0.62	7/3493 (0.2%)
1	G	0.26	0/2568	0.52	1/3488 (0.0%)
1	I	0.25	0/2572	0.51	3/3493 (0.1%)
1	K	0.28	0/2574	0.55	4/3497 (0.1%)
2	B	0.25	0/1333	0.43	0/1797
2	D	0.23	0/1328	0.38	0/1791
2	F	0.24	0/1330	0.45	1/1794 (0.1%)
2	H	0.25	0/1333	0.43	0/1797
2	J	0.25	0/1333	0.40	0/1797
2	L	0.28	0/1330	0.55	3/1794 (0.2%)
All	All	0.26	0/23413	0.52	27/31722 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
1	E	0	1
2	F	0	1
2	L	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	226	VAL	O-C-N	-14.34	99.75	122.70
1	A	199	GLN	N-CA-CB	-11.55	89.81	110.60
2	L	159	TYR	N-CA-CB	-11.34	90.19	110.60
1	E	76	LEU	N-CA-CB	-10.33	89.75	110.40
1	E	226	VAL	CA-C-N	9.25	137.55	117.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	73	CYS	Peptide
1	C	77	SER	Peptide
1	E	226	VAL	Mainchain
2	F	125	GLN	Peptide
2	L	159	TYR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2505	0	2442	156	0
1	C	2509	0	2447	133	3
1	E	2509	0	2449	213	0
1	G	2505	0	2443	141	0
1	I	2509	0	2450	136	0
1	K	2511	0	2454	164	3
2	B	1305	0	1228	71	0
2	D	1300	0	1216	54	0
2	F	1302	0	1224	70	0
2	H	1305	0	1228	92	0
2	J	1305	0	1228	77	0
2	L	1302	0	1225	73	0
3	A	28	0	26	0	0
3	C	28	0	26	3	0
3	E	42	0	39	2	0
3	F	14	0	13	0	0
3	G	42	0	39	3	0
3	K	56	0	52	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	14	0	13	10	0
4	A	56	0	50	13	0
4	C	28	0	25	2	0
4	E	28	0	25	3	0
4	I	28	0	25	5	0
5	C	39	0	34	3	0
5	I	39	0	34	3	0
6	A	36	0	0	19	0
6	B	17	0	0	11	0
6	C	38	0	0	15	0
6	D	10	0	0	2	0
6	E	31	0	0	10	0
6	F	13	0	0	4	0
6	G	45	0	0	25	0
6	H	23	0	0	13	0
6	I	37	0	0	21	0
6	J	21	0	0	7	0
6	K	35	0	0	15	0
6	L	11	0	0	2	0
All	All	23626	0	22435	1215	3

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 27.

The worst 5 of 1215 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:E:17:ASN:HD21	3:E:601:NAG:C1	1.30	1.42
1:E:7:ASP:HA	2:F:27:GLN:O	1.37	1.21
1:E:66:TRP:HE1	1:E:77:SER:HB2	1.08	1.14
4:A:603:NAG:O7	1:K:280:ASP:OD1	1.65	1.14
1:C:282:ASN:OD1	3:C:607:NAG:O7	1.67	1.13

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:GLU:OE1	1:K:144:HIS:NE2[1_455]	1.89	0.31
1:C:74:GLU:OE1	1:K:144:HIS:CD2[1_455]	2.04	0.16
1:C:74:GLU:OE2	1:K:144:HIS:ND1[1_455]	2.13	0.07

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	319/333 (96%)	286 (90%)	32 (10%)	1 (0%)	44	75
1	C	319/333 (96%)	296 (93%)	22 (7%)	1 (0%)	44	75
1	E	319/333 (96%)	291 (91%)	24 (8%)	4 (1%)	14	42
1	G	319/333 (96%)	299 (94%)	19 (6%)	1 (0%)	44	75
1	I	319/333 (96%)	294 (92%)	25 (8%)	0	100	100
1	K	319/333 (96%)	288 (90%)	31 (10%)	0	100	100
2	B	160/181 (88%)	143 (89%)	17 (11%)	0	100	100
2	D	160/181 (88%)	146 (91%)	14 (9%)	0	100	100
2	F	159/181 (88%)	147 (92%)	12 (8%)	0	100	100
2	H	160/181 (88%)	145 (91%)	15 (9%)	0	100	100
2	J	160/181 (88%)	148 (92%)	12 (8%)	0	100	100
2	L	159/181 (88%)	145 (91%)	14 (9%)	0	100	100
All	All	2872/3084 (93%)	2628 (92%)	237 (8%)	7 (0%)	51	81

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	92	ASP
1	E	199	GLN
1	A	199	GLN
1	E	75	SER
1	G	268	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	281/292 (96%)	249 (89%)	32 (11%)	7	18
1	C	282/292 (97%)	255 (90%)	27 (10%)	10	27
1	E	282/292 (97%)	247 (88%)	35 (12%)	5	15
1	G	281/292 (96%)	252 (90%)	29 (10%)	8	23
1	I	282/292 (97%)	251 (89%)	31 (11%)	7	20
1	K	282/292 (97%)	249 (88%)	33 (12%)	6	17
2	B	139/156 (89%)	126 (91%)	13 (9%)	10	28
2	D	138/156 (88%)	128 (93%)	10 (7%)	17	42
2	F	139/156 (89%)	124 (89%)	15 (11%)	7	21
2	H	139/156 (89%)	132 (95%)	7 (5%)	28	60
2	J	139/156 (89%)	127 (91%)	12 (9%)	12	33
2	L	139/156 (89%)	127 (91%)	12 (9%)	12	33
All	All	2523/2688 (94%)	2267 (90%)	256 (10%)	9	24

5 of 256 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	316	THR
1	G	107	LEU
1	K	271	ILE
2	F	22	TYR
2	F	150	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	129	ASN
1	G	253	ASN
1	K	266	ASN
2	F	146	ASN
1	G	132	HIS

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 ⓘ

16 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	602	1,4	14,14,15	0.54	0	15,19,21	1.15	1 (6%)
4	NAG	A	603	4	14,14,15	0.56	0	15,19,21	1.68	3 (20%)
4	NAG	A	604	1,4	14,14,15	0.56	0	15,19,21	0.60	0
4	NAG	A	605	4	14,14,15	0.45	0	15,19,21	0.88	0
5	NAG	C	602	1,5	14,14,15	0.59	0	15,19,21	1.11	1 (6%)
5	NAG	C	603	5	14,14,15	0.53	0	15,19,21	0.99	0
5	BMA	C	604	5	11,11,12	0.26	0	13,15,17	0.54	0
4	NAG	C	605	1,4	14,14,15	0.54	0	15,19,21	0.80	0
4	NAG	C	606	4	14,14,15	0.43	0	15,19,21	2.07	4 (26%)
4	NAG	E	602	1,4	14,14,15	0.55	0	15,19,21	0.63	0
4	NAG	E	603	4	14,14,15	0.57	0	15,19,21	0.82	1 (6%)
5	NAG	I	601	1,5	14,14,15	0.51	0	15,19,21	1.80	3 (20%)
5	NAG	I	602	5	14,14,15	0.40	0	15,19,21	1.99	4 (26%)
5	BMA	I	603	5	11,11,12	0.26	0	13,15,17	0.54	0
4	NAG	I	604	1,4	14,14,15	0.53	0	15,19,21	1.90	3 (20%)
4	NAG	I	605	4	14,14,15	0.60	0	15,19,21	1.20	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
4	NAG	A	602	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	603	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	604	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	605	4	-	0/6/23/26	0/1/1/1
5	NAG	C	602	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	603	5	-	0/6/23/26	0/1/1/1
5	BMA	C	604	5	-	0/2/19/22	0/1/1/1
4	NAG	C	605	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	606	4	-	0/6/23/26	0/1/1/1
4	NAG	E	602	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	603	4	-	0/6/23/26	0/1/1/1
5	NAG	I	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	602	5	-	0/6/23/26	0/1/1/1
5	BMA	I	603	5	-	0/2/19/22	0/1/1/1
4	NAG	I	604	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	605	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	601	NAG	C2-N2-C7	-4.83	115.90	122.94
4	A	603	NAG	C2-N2-C7	-4.21	116.80	122.94
5	I	602	NAG	C4-C3-C2	-4.13	104.97	111.02
4	A	603	NAG	O5-C1-C2	-3.31	106.87	111.47
4	C	606	NAG	C2-N2-C7	-3.30	118.13	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	NAG	6	0
4	A	603	NAG	3	0
4	A	604	NAG	4	0
4	A	605	NAG	1	0
5	C	602	NAG	3	0
4	C	605	NAG	2	0
4	E	602	NAG	3	0
5	I	601	NAG	1	0
5	I	602	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	603	BMA	2	0
4	I	604	NAG	3	0
4	I	605	NAG	3	0

5.6 Ligand geometry [i](#)

16 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	$\# Z > 2$
3	NAG	A	601	1	14,14,15	0.55	0	15,19,21	0.63	0
3	NAG	A	606	1	14,14,15	0.54	0	15,19,21	0.86	0
3	NAG	C	601	1	14,14,15	0.56	0	15,19,21	0.63	0
3	NAG	C	607	1	14,14,15	0.54	0	15,19,21	0.63	0
3	NAG	E	601	1	14,14,15	0.55	0	15,19,21	0.62	0
3	NAG	E	604	1	14,14,15	0.53	0	15,19,21	0.69	0
3	NAG	E	605	1	14,14,15	0.54	0	15,19,21	1.34	3 (20%)
3	NAG	F	601	2	14,14,15	0.54	0	15,19,21	0.63	0
3	NAG	G	601	1	14,14,15	0.53	0	15,19,21	0.67	0
3	NAG	G	602	1	14,14,15	0.55	0	15,19,21	0.63	0
3	NAG	G	603	1	14,14,15	0.55	0	15,19,21	0.62	0
3	NAG	K	601	1	14,14,15	0.45	0	15,19,21	2.55	3 (20%)
3	NAG	K	602	1	14,14,15	0.55	0	15,19,21	0.63	0
3	NAG	K	603	1	14,14,15	0.56	0	15,19,21	0.62	0
3	NAG	K	604	1	14,14,15	0.55	0	15,19,21	0.63	0
3	NAG	L	601	2	14,14,15	0.56	0	15,19,21	0.62	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	601	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	606	1	-	0/6/23/26	0/1/1/1
3	NAG	C	601	1	-	0/6/23/26	0/1/1/1
3	NAG	C	607	1	-	0/6/23/26	0/1/1/1
3	NAG	E	601	1	-	0/6/23/26	0/1/1/1
3	NAG	E	604	1	-	0/6/23/26	0/1/1/1
3	NAG	E	605	1	-	0/6/23/26	0/1/1/1
3	NAG	F	601	2	-	0/6/23/26	0/1/1/1
3	NAG	G	601	1	-	0/6/23/26	0/1/1/1
3	NAG	G	602	1	-	0/6/23/26	0/1/1/1
3	NAG	G	603	1	-	0/6/23/26	0/1/1/1
3	NAG	K	601	1	-	0/6/23/26	0/1/1/1
3	NAG	K	602	1	-	0/6/23/26	0/1/1/1
3	NAG	K	603	1	-	0/6/23/26	0/1/1/1
3	NAG	K	604	1	-	0/6/23/26	0/1/1/1
3	NAG	L	601	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	605	NAG	O5-C1-C2	-3.18	107.05	111.47
3	E	605	NAG	C6-C5-C4	-2.43	107.32	113.00
3	K	601	NAG	C4-C3-C2	-2.07	107.98	111.02
3	E	605	NAG	C3-C4-C5	2.18	114.06	110.22
3	K	601	NAG	O5-C1-C2	3.40	116.20	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	607	NAG	3	0
3	E	601	NAG	2	0
3	G	602	NAG	2	0
3	G	603	NAG	1	0
3	K	602	NAG	4	0
3	K	603	NAG	3	0
3	K	604	NAG	2	0
3	L	601	NAG	10	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	321/333 (96%)	0.55	30 (9%) 9 6	39, 70, 122, 226	0
1	C	321/333 (96%)	0.41	25 (7%) 14 10	36, 67, 116, 196	0
1	E	321/333 (96%)	0.86	46 (14%) 3 2	41, 74, 130, 215	0
1	G	321/333 (96%)	0.71	38 (11%) 5 3	46, 76, 128, 232	0
1	I	321/333 (96%)	0.51	24 (7%) 15 11	37, 70, 120, 228	0
1	K	321/333 (96%)	0.40	26 (8%) 13 9	38, 70, 121, 195	0
2	B	162/181 (89%)	0.84	25 (15%) 2 2	32, 77, 167, 209	0
2	D	162/181 (89%)	1.02	35 (21%) 1 1	34, 72, 186, 246	0
2	F	161/181 (88%)	0.99	34 (21%) 1 1	34, 74, 178, 241	0
2	H	162/181 (89%)	1.17	37 (22%) 1 1	33, 80, 174, 289	0
2	J	162/181 (89%)	0.61	11 (6%) 18 14	32, 69, 165, 200	0
2	L	161/181 (88%)	0.58	14 (8%) 11 8	36, 73, 169, 199	0
All	All	2896/3084 (93%)	0.67	345 (11%) 5 3	32, 72, 157, 289	0

The worst 5 of 345 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	159	TYR	12.8
2	F	128	ASN	10.2
2	D	139	GLU	9.2
2	D	140	PHE	8.1
2	H	31	GLY	8.0

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
4	NAG	A	602	14/15	0.88	0.40	2.80	82,113,129,130	0
4	NAG	A	604	14/15	0.78	0.34	0.58	68,108,117,126	0
4	NAG	E	602	14/15	0.82	0.26	0.28	108,129,134,135	0
4	NAG	I	604	14/15	0.83	0.27	0.14	94,114,139,150	0
5	NAG	I	601	14/15	0.81	0.21	-0.80	72,82,95,97	0
5	BMA	C	604	11/12	0.74	0.28	-1.18	89,112,124,151	0
5	NAG	C	602	14/15	0.89	0.12	-1.69	61,76,95,102	0
4	NAG	C	605	14/15	0.90	0.19	-2.85	70,86,98,99	0
5	NAG	C	603	14/15	0.82	0.28	-	55,84,111,120	0
4	NAG	I	605	14/15	0.77	0.31	-	128,134,141,147	0
4	NAG	E	603	14/15	0.75	0.49	-	119,139,166,193	0
4	NAG	A	603	14/15	0.66	0.54	-	120,148,155,174	0
5	NAG	I	602	14/15	0.92	0.32	-	92,117,138,145	0
4	NAG	A	605	14/15	0.66	0.39	-	124,134,147,148	0
4	NAG	C	606	14/15	0.75	0.34	-	91,106,136,144	0
5	BMA	I	603	11/12	0.50	0.30	-	108,135,142,143	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(Å ²)	Q<0.9
3	NAG	L	601	14/15	0.33	0.55	2.58	132,161,178,187	0
3	NAG	A	601	14/15	0.63	0.34	0.46	53,78,94,104	0
3	NAG	C	607	14/15	0.71	0.40	0.30	95,116,142,146	0
3	NAG	G	601	14/15	0.72	0.32	-	141,158,176,181	0
3	NAG	K	602	14/15	0.62	0.35	-	68,115,138,139	0
3	NAG	E	605	14/15	0.57	0.58	-	134,171,193,199	0
3	NAG	K	604	14/15	0.76	0.49	-	108,133,146,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	E	604	14/15	0.72	0.53	-	26,28,30,30	0
3	NAG	K	603	14/15	0.72	0.51	-	84,126,147,153	0
3	NAG	C	601	14/15	0.66	0.49	-	157,180,192,198	0
3	NAG	F	601	14/15	0.62	0.45	-	154,173,188,194	0
3	NAG	E	601	14/15	0.55	0.53	-	117,156,185,194	0
3	NAG	K	601	14/15	0.54	0.35	-	88,113,140,142	0
3	NAG	A	606	14/15	0.53	0.51	-	103,126,141,143	0
3	NAG	G	602	14/15	0.70	0.49	-	171,186,198,202	0
3	NAG	G	603	14/15	0.73	0.43	-	139,163,185,199	0

6.5 Other polymers [i](#)

There are no such residues in this entry.