



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 12:30 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 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/ValidationPDFNotes.html>

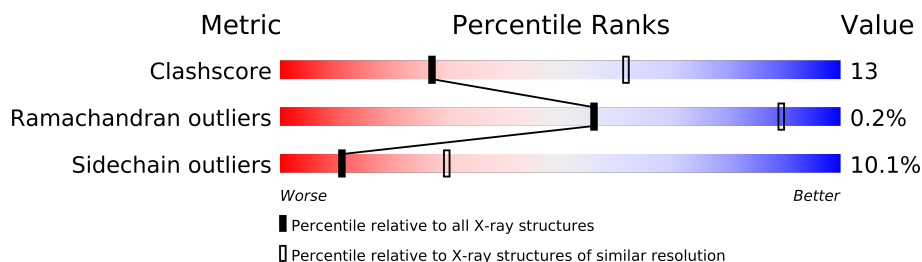
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	FAILED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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))
Clashscore	79885	1696 (2.90-2.86)
Ramachandran outliers	78287	1647 (2.90-2.86)
Sidechain outliers	78261	1650 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	333	
1	C	333	
1	E	333	
1	G	333	
1	I	333	
1	K	333	
2	B	181	
2	D	181	
2	F	181	
2	H	181	
2	J	181	
2	L	181	

2 Entry composition

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

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		

There are 30 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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
E	3	LEU	-	EXPRESSION TAG	UNP C3W5S1
E	4	GLY	-	EXPRESSION TAG	UNP C3W5S1
E	5	SER	-	EXPRESSION TAG	UNP C3W5S1
E	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

- 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		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

- 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		

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

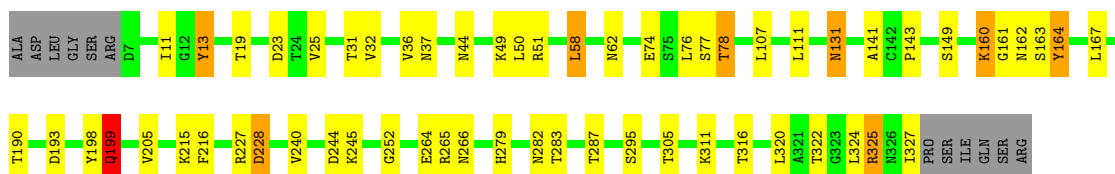
3 Residue-property plots

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.

Note EDS failed to run properly.

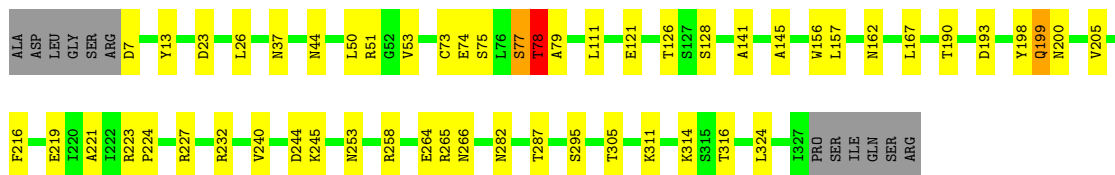
• Molecule 1: Hemagglutinin

Chain A: 



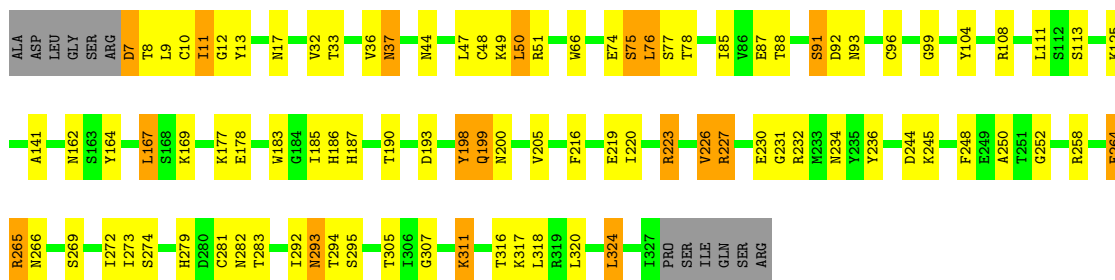
• Molecule 1: Hemagglutinin

Chain C: 



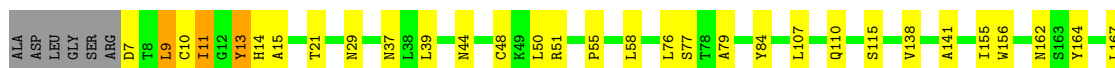
• Molecule 1: Hemagglutinin

Chain E: 



• Molecule 1: Hemagglutinin

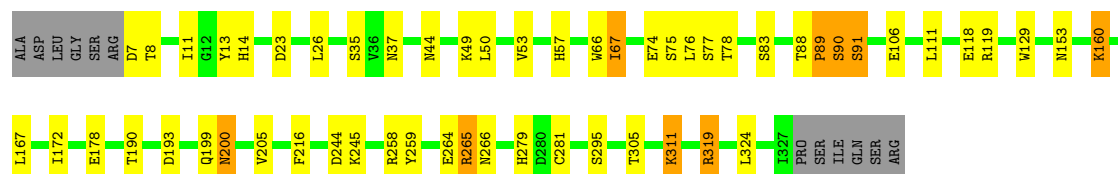
Chain G: 





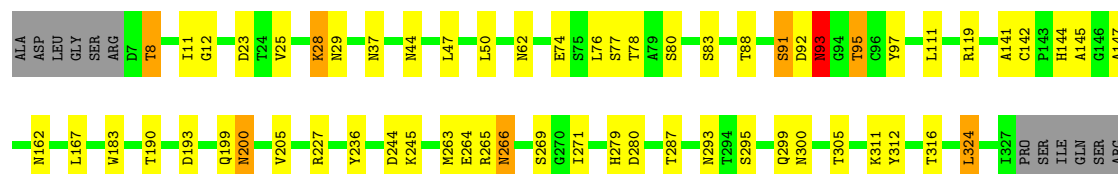
• Molecule 1: Hemagglutinin

Chain I:



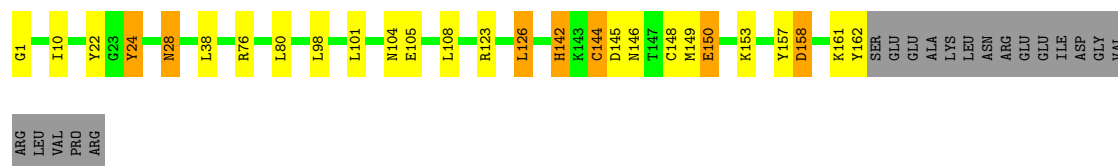
• Molecule 1: Hemagglutinin

Chain K:



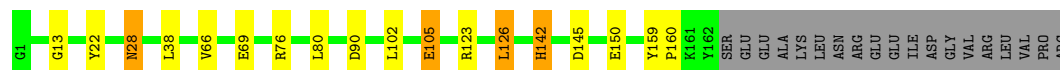
• Molecule 2: Hemagglutinin

Chain B:



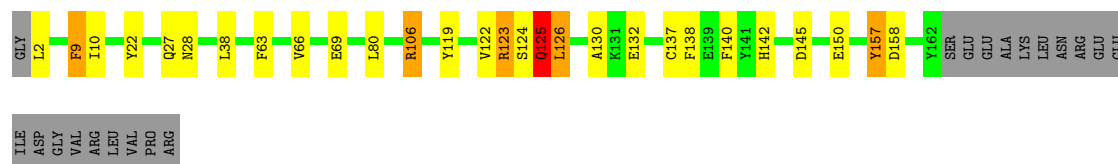
• Molecule 2: Hemagglutinin

Chain D:



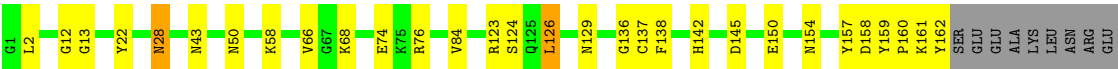
• Molecule 2: Hemagglutinin

Chain F:



• Molecule 2: Hemagglutinin

Chain H:



GLU
ILE
ASP
GLY
VAL
ARG
LEU
VAL
PRO
ARG

• Molecule 2: Hemagglutinin

Chain J:



ASP
GLY
VAL
ARG
LEU
VAL
PRO
ARG

• Molecule 2: Hemagglutinin

Chain L:



GLU
GLU
ILE
ASP
GLY
VAL
ARG
LEU
VAL
PRO
ARG

4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

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	Depositor
% Data completeness (in resolution range)	91.6 (24.19-2.87)	Depositor
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	Depositor
Wilson B-factor (Å ²)	61.4	Xtriage
Anisotropy	0.127	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 64768 reflections	Xtriage
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.

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

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2505	0	0	30	0
1	C	2509	0	0	22	3
1	E	2509	0	0	59	0
1	G	2505	0	0	43	0
1	I	2509	0	0	29	0
1	K	2511	0	0	28	3
2	B	1305	0	0	20	0
2	D	1300	0	0	10	0
2	F	1302	0	0	17	0
2	H	1305	0	0	28	0
2	J	1305	0	0	16	0
2	L	1302	0	0	26	0
3	A	28	0	0	1	0
3	C	28	0	0	3	0
3	E	42	0	0	1	0
3	F	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	42	0	0	2	0
3	K	56	0	0	3	0
3	L	14	0	0	2	0
4	A	56	0	0	5	0
4	C	28	0	0	1	0
4	E	28	0	0	2	0
4	I	28	0	0	1	0
5	C	39	0	0	1	0
5	I	39	0	0	2	0
6	A	36	0	0	12	0
6	B	17	0	0	8	0
6	C	38	0	0	8	0
6	D	10	0	0	1	0
6	E	31	0	0	6	0
6	F	13	0	0	1	0
6	G	45	0	0	20	0
6	H	23	0	0	9	0
6	I	37	0	0	11	0
6	J	21	0	0	4	0
6	K	35	0	0	6	0
6	L	11	0	0	3	0
All	All	23626	0	0	301	3

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

The worst 5 of 301 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:I:66:TRP:CE3	6:I:353:HOH:O	2.18	0.95
1:E:141:ALA:O	1:E:227:ARG:NH1	2.00	0.94
1:G:269:SER:OG	1:G:270:GLY:N	1.94	0.93

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	Distance(Å)	Clash(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

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	319/333 (96%)	286 (90%)	32 (10%)	1 (0%)	50	85
1	C	319/333 (96%)	296 (93%)	22 (7%)	1 (0%)	50	85
1	E	319/333 (96%)	291 (91%)	24 (8%)	4 (1%)	18	53
1	G	319/333 (96%)	299 (94%)	19 (6%)	1 (0%)	50	85
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%)	56	89

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 ⓘ

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%)	8	22
1	C	282/292 (97%)	255 (90%)	27 (10%)	12	33
1	E	282/292 (97%)	247 (88%)	35 (12%)	7	18
1	G	281/292 (96%)	252 (90%)	29 (10%)	10	28
1	I	282/292 (97%)	251 (89%)	31 (11%)	9	24
1	K	282/292 (97%)	249 (88%)	33 (12%)	8	20
2	B	139/156 (89%)	126 (91%)	13 (9%)	13	34
2	D	138/156 (88%)	128 (93%)	10 (7%)	21	50
2	F	139/156 (89%)	124 (89%)	15 (11%)	9	25
2	H	139/156 (89%)	132 (95%)	7 (5%)	34	72
2	J	139/156 (89%)	127 (91%)	12 (9%)	15	40
2	L	139/156 (89%)	127 (91%)	12 (9%)	15	40
All	All	2523/2688 (94%)	2267 (90%)	256 (10%)	11	30

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. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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	12,14,15	0.73	0	15,19,21	1.09	0
4	NAG	A	603	4	12,14,15	0.69	0	15,19,21	1.31	1 (6%)
4	NAG	A	604	1,4	12,14,15	0.73	1 (8%)	15,19,21	0.87	1 (6%)
4	NAG	A	605	4	12,14,15	0.63	0	15,19,21	1.31	1 (6%)
5	NAG	C	602	1,5	12,14,15	0.74	1 (8%)	15,19,21	1.45	4 (26%)
5	NAG	C	603	5	12,14,15	0.70	0	15,19,21	1.40	1 (6%)
5	BMA	C	604	5	10,11,12	0.52	0	11,15,17	0.87	1 (9%)
4	NAG	C	605	1,4	12,14,15	0.67	0	15,19,21	1.17	1 (6%)
4	NAG	C	606	4	12,14,15	0.52	0	15,19,21	1.44	4 (26%)
4	NAG	E	602	1,4	12,14,15	0.72	1 (8%)	15,19,21	0.86	1 (6%)
4	NAG	E	603	4	12,14,15	0.71	1 (8%)	15,19,21	0.90	1 (6%)
5	NAG	I	601	1,5	12,14,15	0.65	0	15,19,21	1.53	2 (13%)
5	NAG	I	602	5	12,14,15	0.52	0	15,19,21	1.17	1 (6%)
5	BMA	I	603	5	10,11,12	0.51	0	11,15,17	0.91	1 (9%)
4	NAG	I	604	1,4	12,14,15	0.70	1 (8%)	15,19,21	1.91	4 (26%)
4	NAG	I	605	4	12,14,15	0.73	1 (8%)	15,19,21	1.12	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	605	NAG	O5-C5	-2.24	1.41	1.45
4	A	604	NAG	O5-C5	-2.16	1.41	1.45
4	I	604	NAG	O5-C5	-2.16	1.41	1.45
5	C	602	NAG	O5-C5	-2.15	1.41	1.45
4	E	602	NAG	O5-C5	-2.14	1.41	1.45

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	604	NAG	O4-C4-C3	5.11	121.81	110.35
4	A	605	NAG	O5-C5-C6	4.30	111.50	106.98
5	I	601	NAG	C2-N2-C7	-4.28	115.90	123.09
5	C	603	NAG	O5-C5-C6	4.22	111.41	106.98
4	A	603	NAG	C2-N2-C7	-3.75	116.80	123.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

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	12,14,15	0.72	1 (8%)	15,19,21	0.86	1 (6%)
3	NAG	A	606	1	12,14,15	0.70	1 (8%)	15,19,21	1.15	2 (13%)
3	NAG	C	601	1	12,14,15	0.72	1 (8%)	15,19,21	0.87	1 (6%)
3	NAG	C	607	1	12,14,15	0.71	1 (8%)	15,19,21	0.86	1 (6%)
3	NAG	E	601	1	12,14,15	0.70	1 (8%)	15,19,21	0.86	1 (6%)
3	NAG	E	604	1	12,14,15	0.67	1 (8%)	15,19,21	0.89	1 (6%)
3	NAG	E	605	1	12,14,15	0.77	0	15,19,21	1.55	4 (26%)
3	NAG	F	601	2	12,14,15	0.71	1 (8%)	15,19,21	0.86	1 (6%)
3	NAG	G	601	1	12,14,15	0.69	1 (8%)	15,19,21	1.14	1 (6%)
3	NAG	G	602	1	12,14,15	0.71	1 (8%)	15,19,21	0.86	1 (6%)
3	NAG	G	603	1	12,14,15	0.71	1 (8%)	15,19,21	0.86	1 (6%)
3	NAG	K	601	1	12,14,15	0.57	0	15,19,21	1.48	2 (13%)
3	NAG	K	602	1	12,14,15	0.71	1 (8%)	15,19,21	0.88	1 (6%)
3	NAG	K	603	1	12,14,15	0.71	1 (8%)	15,19,21	0.86	1 (6%)
3	NAG	K	604	1	12,14,15	0.71	1 (8%)	15,19,21	0.88	1 (6%)
3	NAG	L	601	2	12,14,15	0.72	1 (8%)	15,19,21	0.86	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
3	NAG	A	601	1	-	0/6/23/26	0/1/1/1
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	604	NAG	O5-C5	-2.15	1.41	1.45
3	L	601	NAG	O5-C5	-2.14	1.41	1.45
3	A	601	NAG	O5-C5	-2.14	1.41	1.45
3	F	601	NAG	O5-C5	-2.14	1.41	1.45
3	C	601	NAG	O5-C5	-2.14	1.41	1.45

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	601	NAG	O5-C5-C4	4.34	116.16	110.65
3	G	601	NAG	O5-C5-C6	3.57	110.72	106.98
3	E	605	NAG	O5-C5-C6	3.56	110.72	106.98
3	A	606	NAG	O5-C5-C6	2.94	110.07	106.98
3	A	606	NAG	C3-C2-N2	-2.44	108.04	111.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

EDS failed to run properly - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.