



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 11:40 PM GMT

PDB ID : 4F15
Title : Molecular basis of infectivity of 2009 pandemic H1N1 influenza A viruses
Authors : Kim, K.H.; Cho, K.J.; Lee, J.H.; Park, Y.H.; Khan, T.G.; Lee, J.Y.; Kang, S.H.; Alam, I.
Deposited on : 2012-05-06
Resolution : 2.81 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>

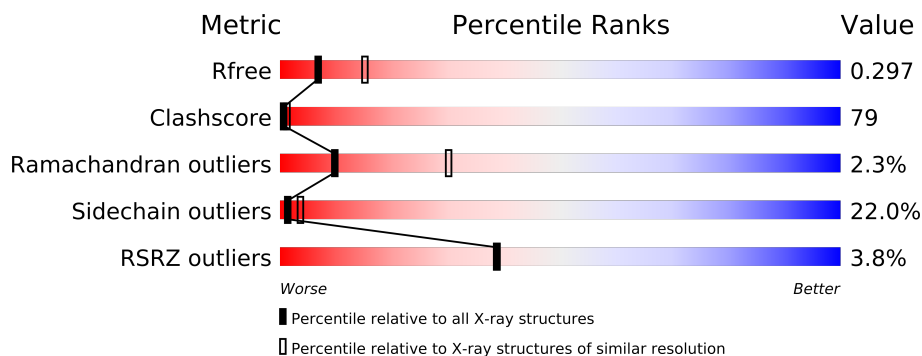
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
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 2.81 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}	66092	1963 (2.84-2.80)
Clashscore	79885	2478 (2.84-2.80)
Ramachandran outliers	78287	2429 (2.84-2.80)
Sidechain outliers	78261	2431 (2.84-2.80)
RSRZ outliers	66119	1966 (2.84-2.80)

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.

Mol	Chain	Length	Quality of chain
1	A	518	
1	D	518	
1	G	518	
1	J	518	
2	B	219	
2	E	219	
2	H	219	
2	K	219	
3	C	218	
3	F	218	
3	I	218	
3	L	218	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19900 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	234	Total	C	N	O	S	0	0	0
			1813	1152	311	344	6			
1	D	246	Total	C	N	O	S	0	0	0
			1872	1187	323	356	6			
1	G	227	Total	C	N	O	S	0	0	0
			1778	1131	304	337	6			
1	J	255	Total	C	N	O	S	0	0	0
			1918	1215	332	365	6			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ALA	-	EXPRESSION TAG	UNP C5MQE6
A	-7	ASP	-	EXPRESSION TAG	UNP C5MQE6
A	-6	PRO	-	EXPRESSION TAG	UNP C5MQE6
A	-5	GLY	-	EXPRESSION TAG	UNP C5MQE6
A	-4	TYR	-	EXPRESSION TAG	UNP C5MQE6
A	-3	LEU	-	EXPRESSION TAG	UNP C5MQE6
A	-2	LEU	-	EXPRESSION TAG	UNP C5MQE6
A	-1	GLU	-	EXPRESSION TAG	UNP C5MQE6
A	0	PHE	-	EXPRESSION TAG	UNP C5MQE6
A	507	ARG	-	EXPRESSION TAG	UNP C5MQE6
A	508	SER	-	EXPRESSION TAG	UNP C5MQE6
A	509	LEU	-	EXPRESSION TAG	UNP C5MQE6
A	510	VAL	-	EXPRESSION TAG	UNP C5MQE6
A	511	PRO	-	EXPRESSION TAG	UNP C5MQE6
A	512	ARG	-	EXPRESSION TAG	UNP C5MQE6
D	-8	ALA	-	EXPRESSION TAG	UNP C5MQE6
D	-7	ASP	-	EXPRESSION TAG	UNP C5MQE6
D	-6	PRO	-	EXPRESSION TAG	UNP C5MQE6
D	-5	GLY	-	EXPRESSION TAG	UNP C5MQE6
D	-4	TYR	-	EXPRESSION TAG	UNP C5MQE6
D	-3	LEU	-	EXPRESSION TAG	UNP C5MQE6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	LEU	-	EXPRESSION TAG	UNP C5MQE6
D	-1	GLU	-	EXPRESSION TAG	UNP C5MQE6
D	0	PHE	-	EXPRESSION TAG	UNP C5MQE6
D	507	ARG	-	EXPRESSION TAG	UNP C5MQE6
D	508	SER	-	EXPRESSION TAG	UNP C5MQE6
D	509	LEU	-	EXPRESSION TAG	UNP C5MQE6
D	510	VAL	-	EXPRESSION TAG	UNP C5MQE6
D	511	PRO	-	EXPRESSION TAG	UNP C5MQE6
D	512	ARG	-	EXPRESSION TAG	UNP C5MQE6
G	-8	ALA	-	EXPRESSION TAG	UNP C5MQE6
G	-7	ASP	-	EXPRESSION TAG	UNP C5MQE6
G	-6	PRO	-	EXPRESSION TAG	UNP C5MQE6
G	-5	GLY	-	EXPRESSION TAG	UNP C5MQE6
G	-4	TYR	-	EXPRESSION TAG	UNP C5MQE6
G	-3	LEU	-	EXPRESSION TAG	UNP C5MQE6
G	-2	LEU	-	EXPRESSION TAG	UNP C5MQE6
G	-1	GLU	-	EXPRESSION TAG	UNP C5MQE6
G	0	PHE	-	EXPRESSION TAG	UNP C5MQE6
G	507	ARG	-	EXPRESSION TAG	UNP C5MQE6
G	508	SER	-	EXPRESSION TAG	UNP C5MQE6
G	509	LEU	-	EXPRESSION TAG	UNP C5MQE6
G	510	VAL	-	EXPRESSION TAG	UNP C5MQE6
G	511	PRO	-	EXPRESSION TAG	UNP C5MQE6
G	512	ARG	-	EXPRESSION TAG	UNP C5MQE6
J	-8	ALA	-	EXPRESSION TAG	UNP C5MQE6
J	-7	ASP	-	EXPRESSION TAG	UNP C5MQE6
J	-6	PRO	-	EXPRESSION TAG	UNP C5MQE6
J	-5	GLY	-	EXPRESSION TAG	UNP C5MQE6
J	-4	TYR	-	EXPRESSION TAG	UNP C5MQE6
J	-3	LEU	-	EXPRESSION TAG	UNP C5MQE6
J	-2	LEU	-	EXPRESSION TAG	UNP C5MQE6
J	-1	GLU	-	EXPRESSION TAG	UNP C5MQE6
J	0	PHE	-	EXPRESSION TAG	UNP C5MQE6
J	507	ARG	-	EXPRESSION TAG	UNP C5MQE6
J	508	SER	-	EXPRESSION TAG	UNP C5MQE6
J	509	LEU	-	EXPRESSION TAG	UNP C5MQE6
J	510	VAL	-	EXPRESSION TAG	UNP C5MQE6
J	511	PRO	-	EXPRESSION TAG	UNP C5MQE6
J	512	ARG	-	EXPRESSION TAG	UNP C5MQE6

- Molecule 2 is a protein called Fab fragment, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	208	Total	C	N	O	S	0	0	0
			1544	962	268	307	7			
2	E	208	Total	C	N	O	S	0	0	0
			1544	962	268	307	7			
2	H	208	Total	C	N	O	S	0	0	0
			1544	962	268	307	7			
2	K	208	Total	C	N	O	S	0	0	0
			1544	962	268	307	7			

- Molecule 3 is a protein called Fab fragment, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	203	Total	C	N	O	S	0	0	0
			1557	975	263	313	6			
3	F	203	Total	C	N	O	S	0	0	0
			1557	975	263	313	6			
3	I	203	Total	C	N	O	S	0	0	0
			1557	975	263	313	6			
3	L	203	Total	C	N	O	S	0	0	0
			1557	975	263	313	6			

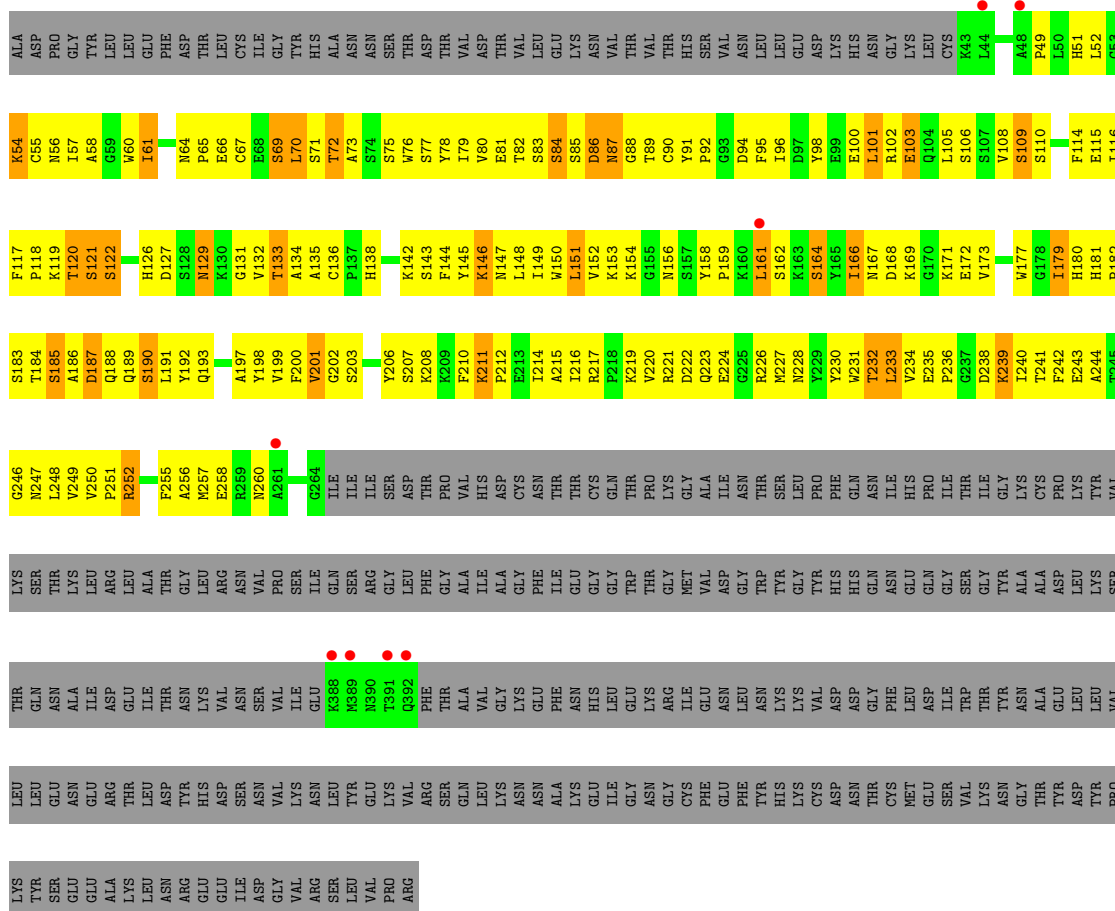
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total	O	0	0
			11	11		
4	B	8	Total	O	0	0
			8	8		
4	C	11	Total	O	0	0
			11	11		
4	D	7	Total	O	0	0
			7	7		
4	E	11	Total	O	0	0
			11	11		
4	F	9	Total	O	0	0
			9	9		
4	G	8	Total	O	0	0
			8	8		
4	H	10	Total	O	0	0
			10	10		
4	I	12	Total	O	0	0
			12	12		
4	J	7	Total	O	0	0
			7	7		

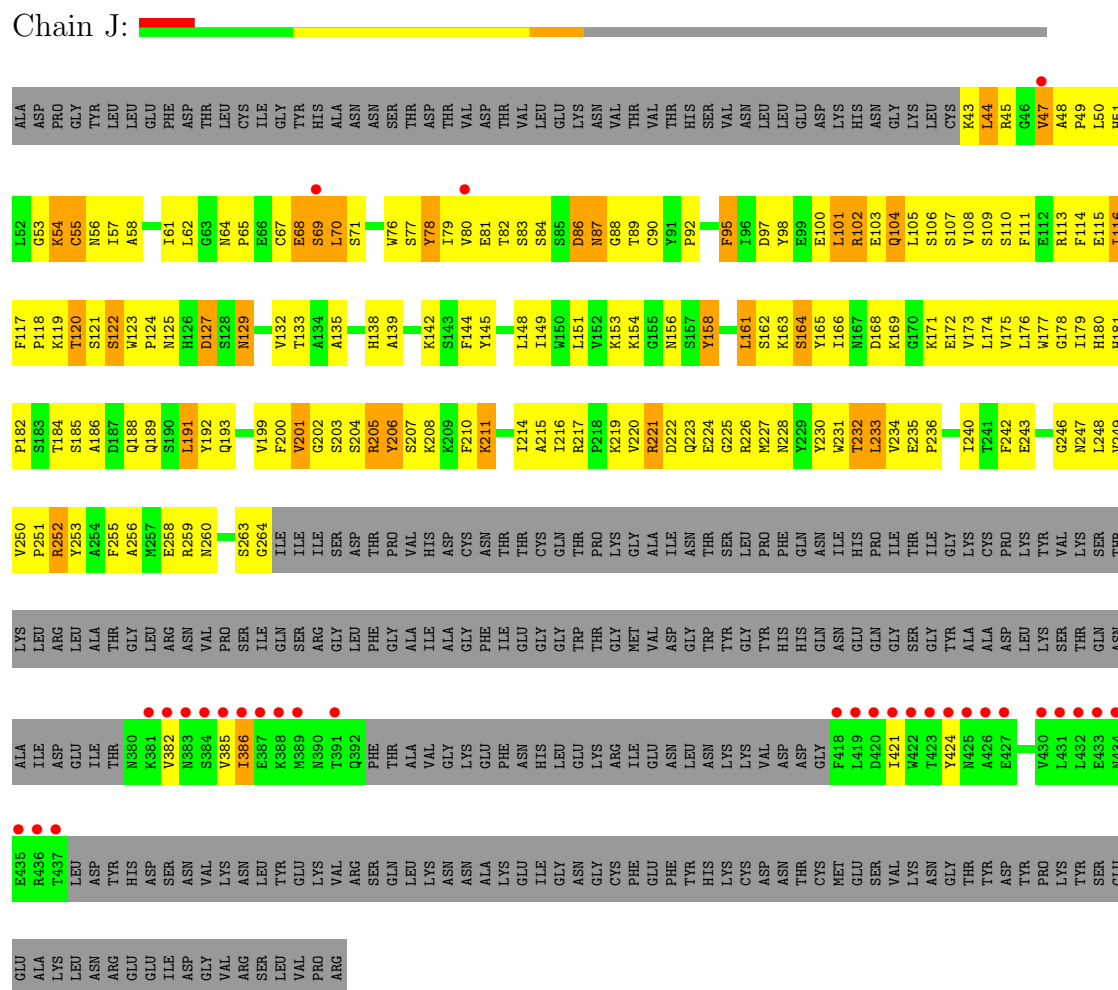
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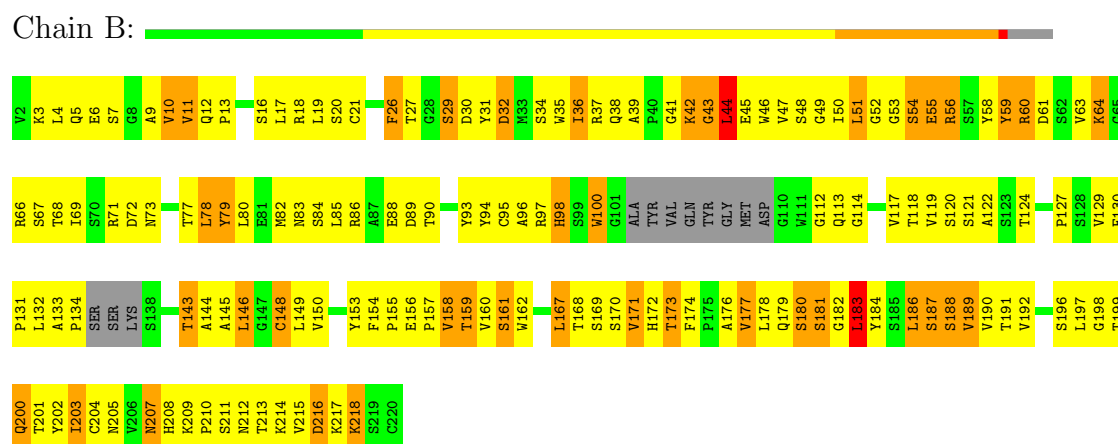
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	6	Total 6	O 6	0	0
4	L	15	Total 15	O 15	0	0



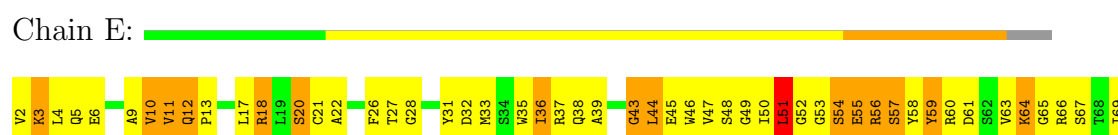
- Molecule 1: Hemagglutinin

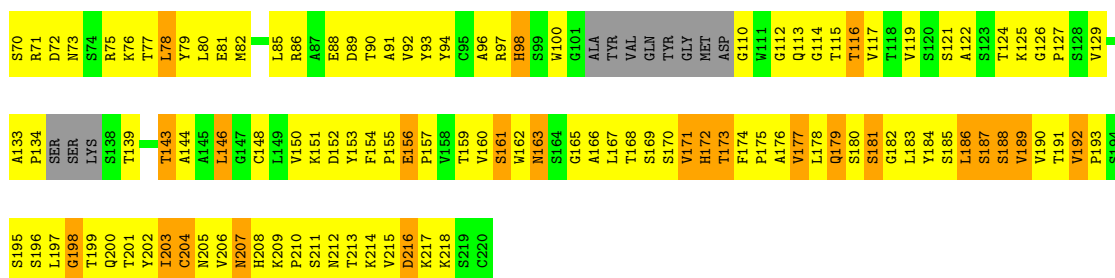


- Molecule 2: Fab fragment, heavy chain



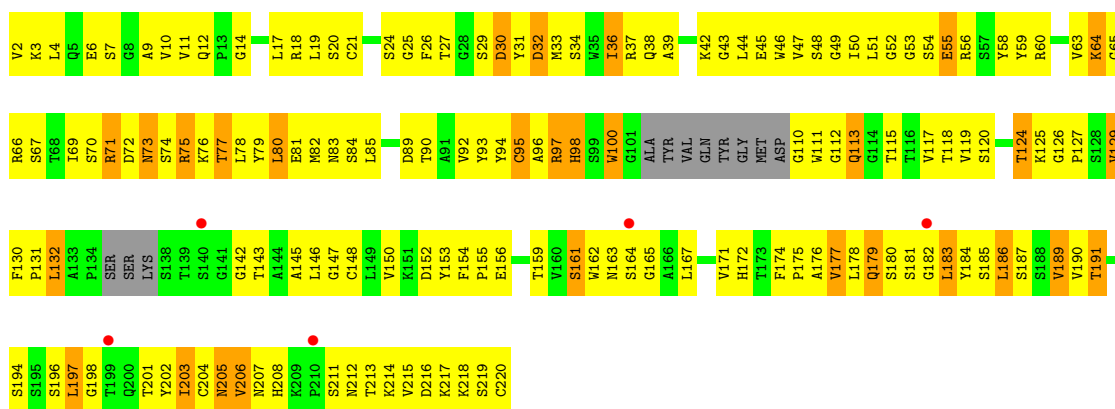
- Molecule 2: Fab fragment, heavy chain





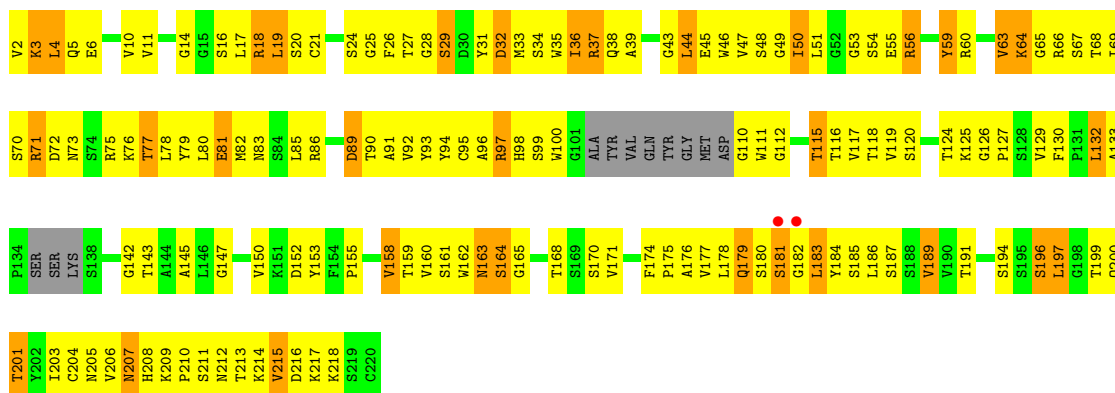
• Molecule 2: Fab fragment, heavy chain

Chain H:



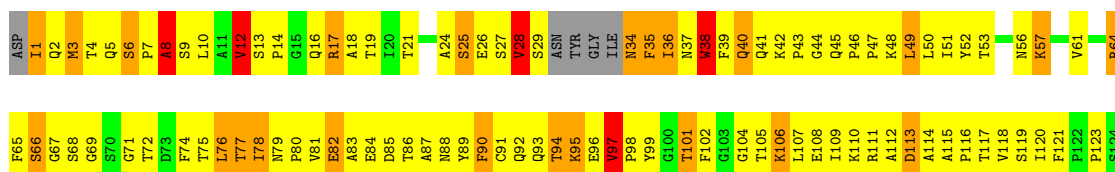
• Molecule 2: Fab fragment, heavy chain

Chain K:



• Molecule 3: Fab fragment, light chain

Chain C:



Y189	E190	R191	H192	N193	S194	Y195	T196	C197	E198	A199	T200	H201	K202	T203	S204	T205	S206	P207	T208	V209	K210	S211	F212	N213	ARG	ASN	GLU	CYS
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.70Å 90.13Å 238.18Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	49.68 – 2.81 49.68 – 2.81	Depositor EDS
% Data completeness (in resolution range)	87.5 (49.68-2.81) 84.4 (49.68-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.233 , 0.289 0.236 , 0.297	Depositor DCC
R_{free} test set	3266 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 20.9	EDS
Estimated twinning fraction	0.492 for h,-k,-l 0.457 for h,-k,-l	Xtriage
Reported twinning fraction	0.492 for h,-k,-l	Depositor
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	2 of 66880 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19900	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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 50.53 % 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 6.3850e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.39	0/1861	0.63	0/2523
1	D	0.41	0/1919	0.67	0/2602
1	G	0.42	0/1826	0.69	0/2474
1	J	0.41	0/1965	0.67	1/2667 (0.0%)
2	B	0.45	0/1577	0.76	3/2141 (0.1%)
2	E	0.42	0/1577	0.74	3/2141 (0.1%)
2	H	0.43	0/1577	0.73	0/2141
2	K	0.43	0/1577	0.72	0/2141
3	C	0.50	0/1590	0.86	4/2157 (0.2%)
3	F	0.51	0/1590	0.79	1/2157 (0.0%)
3	I	0.78	1/1591 (0.1%)	0.85	5/2160 (0.2%)
3	L	0.84	1/1591 (0.1%)	0.90	7/2160 (0.3%)
All	All	0.52	2/20241 (0.0%)	0.75	24/27464 (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	A	0	2
1	D	0	3
1	G	0	3
1	J	0	2
2	B	0	1
2	E	0	1
2	H	0	1
2	K	0	1
3	C	0	8
3	F	0	13
3	I	0	6
3	L	0	2
All	All	0	43

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	145	LYS	C-N	27.80	1.98	1.34
3	I	145	LYS	C-N	24.11	1.89	1.34

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	145	LYS	O-C-N	-12.89	102.07	122.70
3	L	145	LYS	C-N-CA	9.08	144.39	121.70
2	E	43	GLY	N-CA-C	-6.80	96.09	113.10
2	B	43	GLY	N-CA-C	-6.76	96.19	113.10
3	C	94	THR	N-CA-C	-6.63	93.11	111.00

There are no chirality outliers.

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	ASN	Peptide
1	A	74	SER	Peptide
2	B	44	LEU	Peptide
3	C	28	VAL	Peptide
3	C	8	ALA	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	1813	0	1716	191	0
1	D	1872	0	1743	214	0
1	G	1778	0	1702	239	0
1	J	1918	0	1760	219	0
2	B	1544	0	1505	262	0
2	E	1544	0	1505	254	0
2	H	1544	0	1505	274	0
2	K	1544	0	1505	247	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1557	0	1503	343	0
3	F	1557	0	1503	355	0
3	I	1557	0	1503	317	0
3	L	1557	0	1503	332	0
4	A	11	0	0	2	0
4	B	8	0	0	3	0
4	C	11	0	0	3	0
4	D	7	0	0	1	0
4	E	11	0	0	3	0
4	F	9	0	0	5	0
4	G	8	0	0	2	0
4	H	10	0	0	3	0
4	I	12	0	0	2	0
4	J	7	0	0	3	0
4	K	6	0	0	4	0
4	L	15	0	0	8	0
All	All	19900	0	18953	3059	0

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 79.

The worst 5 of 3059 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:145:LYS:C	3:I:147:ILE:N	1.89	1.25
3:C:38:TRP:CD2	3:C:39:PHE:HA	1.74	1.21
2:B:171:VAL:HG21	3:C:176:TYR:CE1	1.76	1.19
3:L:145:LYS:C	3:L:147:ILE:N	1.98	1.16
2:E:32:ASP:HB3	2:E:51:LEU:HA	1.27	1.15

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	230/518 (44%)	198 (86%)	29 (13%)	3 (1%)	18	50
1	D	240/518 (46%)	199 (83%)	35 (15%)	6 (2%)	9	27
1	G	223/518 (43%)	193 (86%)	27 (12%)	3 (1%)	18	50
1	J	249/518 (48%)	211 (85%)	35 (14%)	3 (1%)	19	53
2	B	202/219 (92%)	175 (87%)	25 (12%)	2 (1%)	22	59
2	E	202/219 (92%)	172 (85%)	29 (14%)	1 (0%)	38	75
2	H	202/219 (92%)	174 (86%)	26 (13%)	2 (1%)	22	59
2	K	202/219 (92%)	177 (88%)	21 (10%)	4 (2%)	11	34
3	C	193/218 (88%)	150 (78%)	37 (19%)	6 (3%)	7	20
3	F	193/218 (88%)	142 (74%)	38 (20%)	13 (7%)	2	5
3	I	195/218 (89%)	141 (72%)	45 (23%)	9 (5%)	4	11
3	L	195/218 (89%)	145 (74%)	44 (23%)	6 (3%)	7	20
All	All	2526/3820 (66%)	2077 (82%)	391 (16%)	58 (2%)	10	30

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	8	ALA
3	F	173	ASP
3	L	144	PRO
3	L	147	ILE
1	A	120	THR

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	190/451 (42%)	161 (85%)	29 (15%)	4	11
1	D	190/451 (42%)	154 (81%)	36 (19%)	2	6
1	G	190/451 (42%)	157 (83%)	33 (17%)	3	8
1	J	190/451 (42%)	156 (82%)	34 (18%)	2	7
2	B	173/182 (95%)	130 (75%)	43 (25%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	173/182 (95%)	129 (75%)	44 (25%)	1	2
2	H	173/182 (95%)	140 (81%)	33 (19%)	2	6
2	K	173/182 (95%)	139 (80%)	34 (20%)	2	5
3	C	177/190 (93%)	128 (72%)	49 (28%)	0	1
3	F	177/190 (93%)	135 (76%)	42 (24%)	1	3
3	I	177/190 (93%)	130 (73%)	47 (27%)	1	2
3	L	177/190 (93%)	125 (71%)	52 (29%)	0	1
All	All	2160/3292 (66%)	1684 (78%)	476 (22%)	1	3

5 of 476 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	82	GLU
1	G	187	ASP
3	L	75	THR
3	F	118	VAL
3	F	198	GLU

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

Mol	Chain	Res	Type
3	F	141	ASN
1	G	129	ASN
3	L	92	GLN
3	F	193	ASN
1	G	193	GLN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	234/518 (45%)	0.11	15 (6%) 19 17	19, 35, 59, 76	8 (3%)
1	D	246/518 (47%)	0.34	26 (10%) 7 6	18, 32, 58, 95	21 (8%)
1	G	227/518 (43%)	-0.22	8 (3%) 42 42	18, 32, 57, 70	2 (0%)
1	J	255/518 (49%)	0.40	31 (12%) 5 4	21, 33, 57, 71	30 (11%)
2	B	208/219 (94%)	-0.32	0 100 100	13, 29, 44, 58	0
2	E	208/219 (94%)	-0.39	0 100 100	19, 30, 42, 62	0
2	H	208/219 (94%)	-0.36	5 (2%) 56 57	20, 29, 43, 53	0
2	K	208/219 (94%)	-0.30	2 (0%) 79 80	21, 29, 41, 48	0
3	C	203/218 (93%)	-0.23	2 (0%) 79 80	13, 28, 50, 68	0
3	F	203/218 (93%)	-0.19	3 (1%) 70 71	20, 29, 49, 58	0
3	I	203/218 (93%)	-0.17	4 (1%) 62 63	20, 30, 53, 71	0
3	L	203/218 (93%)	-0.16	4 (1%) 62 63	18, 30, 57, 75	0
All	All	2606/3820 (68%)	-0.11	100 (3%) 38 39	13, 31, 54, 95	61 (2%)

The worst 5 of 100 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	388	LYS	14.7
1	A	389	MET	13.4
1	J	387	GLU	12.3
1	D	389	MET	12.3
1	D	419	LEU	11.7

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.