

Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 12:03 PM EDT

PDB ID	:	8FUA
Title	:	Crystal structure of mouse Importin alpha in complex with Hendra virus ma-
		trix protein NLS1
Authors	:	Donnelly, C.M.; Basler, C.F.; Scott, C.; Forwood, J.K.
Deposited on		
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

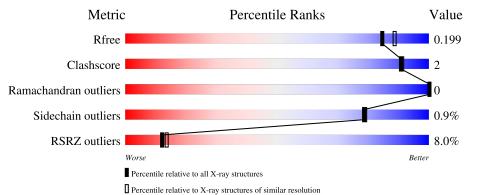
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.90 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	А	510	6%	79%		•	17%
2	В	20	20%		80%		
2	С	20		45%	55%		



8FUA

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6751 atoms, of which 3259 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 Importin subunit alpha-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	A	423	Total 6269	C 2009	Н 3135	N 529	O 586	S 10	0	0	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	20	MET	-	expression tag	UNP P52293
А	21	HIS	-	expression tag	UNP P52293
А	22	HIS	-	expression tag	UNP P52293
А	23	HIS	-	expression tag	UNP P52293
А	24	HIS	-	expression tag	UNP P52293
А	25	HIS	-	expression tag	UNP P52293
А	26	HIS	-	expression tag	UNP P52293
А	27	SER	-	expression tag	UNP P52293
А	28	SER	-	expression tag	UNP P52293
А	29	GLY	-	expression tag	UNP P52293
А	30	LEU	-	expression tag	UNP P52293
A	31	VAL	-	expression tag	UNP P52293
А	32	PRO	-	expression tag	UNP P52293
А	33	ARG	-	expression tag	UNP P52293
А	34	GLY	-	expression tag	UNP P52293
А	35	SER	-	expression tag	UNP P52293
A	36	GLY	-	expression tag	UNP P52293
A	37	MET	-	expression tag	UNP P52293
А	38	LEU	-	expression tag	UNP P52293
А	39	GLU	-	expression tag	UNP P52293
А	40	THR	-	expression tag	UNP P52293
А	41	ALA	-	expression tag	UNP P52293
А	42	ALA	-	expression tag	UNP P52293
А	43	ALA	-	expression tag	UNP P52293
A	44	LEU	-	expression tag	UNP P52293
А	45	PHE	-	expression tag	UNP P52293
А	46	GLU	-	expression tag	UNP P52293

There are 50 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
А	47	ARG	-	expression tag	UNP P52293
А	48	ASN	-	expression tag	UNP P52293
А	49	HIS	-	expression tag	UNP P52293
А	50	MET	-	expression tag	UNP P52293
А	51	ASP	-	expression tag	UNP P52293
А	52	SER	-	expression tag	UNP P52293
А	53	PRO	-	expression tag	UNP P52293
А	54	ASP	-	expression tag	UNP P52293
А	55	LEU	-	expression tag	UNP P52293
А	56	GLY	-	expression tag	UNP P52293
А	57	THR	-	expression tag	UNP P52293
А	58	ASP	-	expression tag	UNP P52293
А	59	ASP	-	expression tag	UNP P52293
А	60	ASP	-	expression tag	UNP P52293
А	61	ASP	-	expression tag	UNP P52293
А	62	LEU	-	expression tag	UNP P52293
A	63	ALA	-	expression tag	UNP P52293
А	64	MET	-	expression tag	UNP P52293
А	65	ALA	-	expression tag	UNP P52293
А	66	ASP	-	expression tag	UNP P52293
А	67	ILE	-	expression tag	UNP P52293
А	68	GLY	-	expression tag	UNP P52293
А	69	SER	-	expression tag	UNP P52293

Continued from previous page...

• Molecule 2 is a protein called Matrix protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
9	В	4	Total	С	Η	Ν	0	0	0	0
			74	20	41	9	4	0		
0	C	0	Total	С	Η	Ν	0	0	0	0
	C	9	155	44	83	17	11	0		

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	243	Total O 243 243	0	0
3	В	1	Total O 1 1	0	0
3	С	9	Total O 9 9	0	0





3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 (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.

Chain A:	<mark>%</mark> 79%	• 17%
MET HIS HIS HIS HIS HIS SER SER	GLAN CLEU LEU LEU LEU CLY CLU CLY CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	ALA ALA ALS ALS CLY SER SER ASW CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY
1136 1141 1142 1143 1144	A85 A85 L186 D207 D207 D207 D207 D207 D207 D207 D207	1425 1434 1440 1440 1448 4449 1448 1448 1448 8458 8458 8458 8458 8458
8461 1462 E466 C467 G468 A475	R4 78 R4 79 F4 80 F4 80 F4 80 F4 80 F4 80 F4 90 G1U G1U G1U G1U G1U G1U G1U G1U G1U G1U	GLM ASP GLY GLY CLY THR PRO CLY THR PHE PHE PHE
• Molecule	2: Matrix protein	
Chain B:	20% 80%	
SER G81 K82 K84 K84 LYS ILE ARG ARG	TLLA ALA TYR PRO LLEU GLY CLY CLY SER SER	
• Molecule	2: Matrix protein	
Chain C:	45% 55%	
S80 T88 ALA ALA ALA PR0 FR0	GLY GLY LYS SER	

• Molecule 1: Importin subunit alpha-1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	78.49Å 89.86Å 99.83Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.42 - 1.90	Depositor
Resolution (A)	24.42 - 1.90	EDS
% Data completeness	99.9 (24.42-1.90)	Depositor
(in resolution range)	95.3 (24.42-1.90)	EDS
R _{merge}	0.09	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.24 (at 1.90 \text{\AA})$	Xtriage
Refinement program	REFMAC 1.14_3260	Depositor
D D.	0.173 , 0.190	Depositor
R, R_{free}	0.186 , 0.199	DCC
R_{free} test set	2864 reflections $(5.09%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	32.6	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.42 , 47.6	EDS
L-test for twinning ²	$ \langle L \rangle = 0.48, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6751	wwPDB-VP
Average B, all atoms $(Å^2)$	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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		Bo	nd lengths	Bond angles		
	Ullalli	RMSZ $\# Z > 5$		RMSZ	# Z > 5	
1	А	0.70	2/3189~(0.1%)	0.69	1/4358~(0.0%)	
2	В	0.61	0/32	0.65	0/38	
2	С	0.69	0/71	0.83	0/90	
All	All	0.70	2/3292~(0.1%)	0.70	1/4486~(0.0%)	

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	237	CYS	CB-SG	-5.30	1.73	1.81
1	А	373	VAL	CB-CG2	5.30	1.64	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
1	А	197	ARG	NE-CZ-NH2	-5.30	117.65	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	А	3134	3135	3135	11	0
2	В	33	41	41	0	0
2	С	72	83	83	0	0
3	А	243	0	0	2	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 2.

All (11) 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:A:95:GLN:NE2	3:A:601:HOH:O	1.86	1.09
1:A:136:ILE:CG1	1:A:136:ILE:CA	2.61	0.79
1:A:136:ILE:CA	1:A:136:ILE:CG2	2.70	0.69
1:A:136:ILE:CG1	1:A:136:ILE:CG2	2.71	0.68
1:A:207:ASP:OD1	1:A:251:GLN:NE2	2.40	0.54
1:A:386:LEU:HD21	1:A:425:LEU:HD13	1.92	0.51
1:A:425:LEU:HG	1:A:440:ILE:HG23	1.94	0.48
1:A:273:TRP:CD2	1:A:312:PRO:HB3	2.50	0.47
1:A:448:PHE:CD1	1:A:460:LEU:HD23	2.53	0.43
1:A:285:ARG:HD2	3:A:677:HOH:O	2.20	0.42
1:A:284:GLU:O	1:A:288:MET:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	421/510 (82%)	415 (99%)	6 (1%)	0	100	100
2	В	2/20~(10%)	2 (100%)	0	0	100	100
2	С	7/20~(35%)	7 (100%)	0	0	100	100



Chain Non-H H(model) H(added) Clashes Symm-Clashes Mol 3 В 0 0 0 0 1 3 $\overline{\mathrm{C}}$ 9 0 0 0 0 All All 3492 3259 3259 11 0

Continued from previous page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	430/550~(78%)	424 (99%)	6 (1%)	0	100 100

There are no Ramachandran outliers to report.

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	325/426~(76%)	322~(99%)	3~(1%)	78 79
2	В	3/15~(20%)	3~(100%)	0	100 100
2	С	7/15 (47%)	7~(100%)	0	100 100
All	All	335/456~(74%)	332~(99%)	3 (1%)	78 79

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	483	SER
1	А	488	SER
1	А	492	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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



5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9
1	А	423/510~(82%)	0.36	33 (7%) 13 14	26, 37, 82, 104	0
2	В	4/20~(20%)	2.30	2 (50%) 0 0	56, 58, 58, 68	0
2	С	9/20~(45%)	0.28	0 100 100	32, 37, 53, 59	0
All	All	436/550~(79%)	0.38	35 (8%) 12 13	26, 38, 82, 104	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	74	VAL	4.9
1	А	493	GLU	4.7
1	А	454	LEU	4.3
1	А	481	ASN	4.1
1	А	455	GLY	4.0
2	В	81	GLY	4.0
1	А	144	LEU	3.9
1	А	458	GLU	3.9
1	А	479	HIS	3.2
1	А	186	LEU	3.2
1	А	462	ILE	3.0
1	А	185	ALA	3.0
1	А	425	LEU	3.0
1	А	467	CYS	3.0
1	А	107	GLU	3.0
1	А	143	ALA	3.0
1	А	182	ALA	2.9
1	А	478	ARG	2.9
1	А	167	PHE	2.8
1	А	136	ILE	2.6
1	А	466	GLU	2.5
1	А	434	THR	2.3
2	В	83	ARG	2.3



Mol	Chain	Res	Type	RSRZ
1	А	317	ILE	2.2
1	А	232	THR	2.2
1	А	256	LEU	2.2
1	А	141	ALA	2.2
1	А	274	ALA	2.2
1	А	475	ALA	2.2
1	А	106	ARG	2.1
1	А	340	PHE	2.1
1	А	482	GLU	2.0
1	А	440	ILE	2.0
1	А	449	GLN	2.0
1	А	468	GLY	2.0

Continued from previous page...

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)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

