Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2023 – 04:46 PM EDT

PDB ID : 8FUC

Title : Crystal structure of mouse Importin alpha in complex with Hendra virus matrix protein minor site NLS2

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Deposited on : 2023-01-17

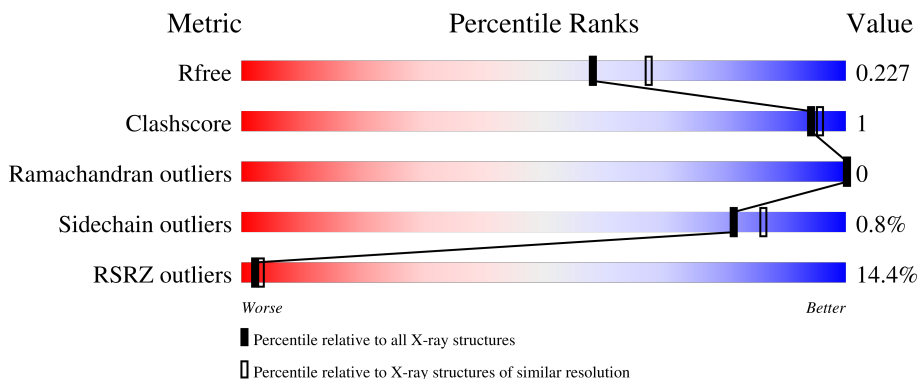Resolution : 2.10 Å(reported)

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 2.10 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	Percentile Ranks	Value
Rfree		0.227
Clashscore		1
Ramachandran outliers		0
Sidechain outliers		0.8%
RSRZ outliers		14.4%

Worse ... *Better*

▊ Percentile relative to all X-ray structures

▊ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	A	18	11% / 28% / 72%
2	B	510	12% / 80% / · / 16%
3	F	6	17% / 67% / 33%

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2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 7099 atoms, of which 3494 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 Matrix protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	5	Total	C	H	N	O	S	0	0	0
			98	27	55	10	5	1			

- Molecule 2 is a protein called Importin subunit alpha-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	426	Total	C	H	N	O	S	0	8	0
			6657	2090	3379	553	625	10			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	20	MET	-	expression tag	UNP P52293
B	21	HIS	-	expression tag	UNP P52293
B	22	HIS	-	expression tag	UNP P52293
B	23	HIS	-	expression tag	UNP P52293
B	24	HIS	-	expression tag	UNP P52293
B	25	HIS	-	expression tag	UNP P52293
B	26	HIS	-	expression tag	UNP P52293
B	27	SER	-	expression tag	UNP P52293
B	28	SER	-	expression tag	UNP P52293
B	29	GLY	-	expression tag	UNP P52293
B	30	LEU	-	expression tag	UNP P52293
B	31	VAL	-	expression tag	UNP P52293
B	32	PRO	-	expression tag	UNP P52293
B	33	ARG	-	expression tag	UNP P52293
B	34	GLY	-	expression tag	UNP P52293
B	35	SER	-	expression tag	UNP P52293
B	36	GLY	-	expression tag	UNP P52293
B	37	MET	-	expression tag	UNP P52293
B	38	LEU	-	expression tag	UNP P52293
B	39	GLU	-	expression tag	UNP P52293

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Chain	Residue	Modelled	Actual	Comment	Reference
B	40	THR	-	expression tag	UNP P52293
B	41	ALA	-	expression tag	UNP P52293
B	42	ALA	-	expression tag	UNP P52293
B	43	ALA	-	expression tag	UNP P52293
B	44	LEU	-	expression tag	UNP P52293
B	45	PHE	-	expression tag	UNP P52293
B	46	GLU	-	expression tag	UNP P52293
B	47	ARG	-	expression tag	UNP P52293
B	48	ASN	-	expression tag	UNP P52293
B	49	HIS	-	expression tag	UNP P52293
B	50	MET	-	expression tag	UNP P52293
B	51	ASP	-	expression tag	UNP P52293
B	52	SER	-	expression tag	UNP P52293
B	53	PRO	-	expression tag	UNP P52293
B	54	ASP	-	expression tag	UNP P52293
B	55	LEU	-	expression tag	UNP P52293
B	56	GLY	-	expression tag	UNP P52293
B	57	THR	-	expression tag	UNP P52293
B	58	ASP	-	expression tag	UNP P52293
B	59	ASP	-	expression tag	UNP P52293
B	60	ASP	-	expression tag	UNP P52293
B	61	ASP	-	expression tag	UNP P52293
B	62	LEU	-	expression tag	UNP P52293
B	63	ALA	-	expression tag	UNP P52293
B	64	MET	-	expression tag	UNP P52293
B	65	ALA	-	expression tag	UNP P52293
B	66	ASP	-	expression tag	UNP P52293
B	67	ILE	-	expression tag	UNP P52293
B	68	GLY	-	expression tag	UNP P52293
B	69	SER	-	expression tag	UNP P52293

- Molecule 3 is a protein called Contaminant peptide KKLARE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
3	F	6	111	32	60	11	8	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	232	232	232	0	0

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

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.

• Molecule 1: Matrix protein

Chain A:
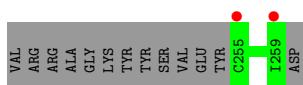
• Molecule 2: Importin subunit alpha-1

Chain B:
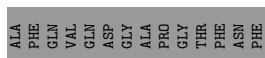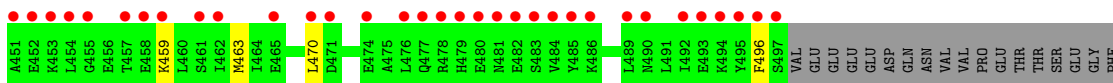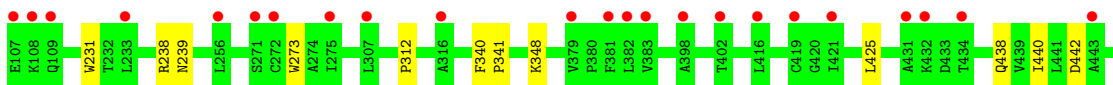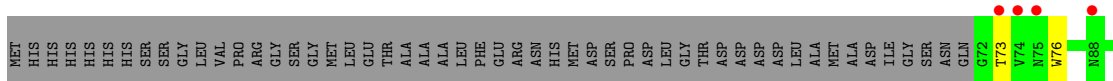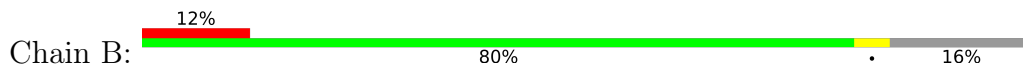
• Molecule 3: Contaminant peptide KKLARE

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.55Å 90.18Å 98.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.62 – 2.10 29.62 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.62-2.10) 99.8 (29.62-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.10Å)	Xtriage
Refinement program	REFMAC 1.19.2_4158	Depositor
R, R_{free}	0.175 , 0.217 0.190 , 0.227	Depositor DCC
R_{free} test set	2037 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 59.0	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7099	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.32	0/42	0.68	0/52
2	B	0.28	0/3363	0.47	0/4581
3	F	0.37	0/50	0.69	0/63
All	All	0.28	0/3455	0.48	0/4696

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	43	55	54	0	0
2	B	3278	3379	3379	9	0
3	F	51	60	60	2	0
4	B	232	0	0	0	1
4	F	1	0	0	0	0
All	All	3605	3494	3493	9	1

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 1.

All (9) 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)
2:B:238:ARG:HH12	3:F:58:LYS:HE3	1.70	0.57
2:B:425:LEU:HG	2:B:440:ILE:HG23	1.91	0.52
2:B:459:LYS:HZ1	2:B:463:MET:HG2	1.78	0.48
2:B:470:LEU:HD13	2:B:496:PHE:CD2	2.51	0.46
2:B:340:PHE:N	2:B:341:PRO:CD	2.82	0.42
2:B:238:ARG:O	2:B:239:ASN:HB2	2.19	0.42
2:B:231:TRP:CZ2	3:F:60:LEU:HG	2.54	0.42
2:B:73:THR:HA	2:B:76:TRP:NE1	2.35	0.41
2:B:273:TRP:CD2	2:B:312:PRO:HB3	2.57	0.40

All (1) 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)
4:B:647:HOH:O	4:B:663:HOH:O[4_466]	1.99	0.21

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	3/18 (17%)	3 (100%)	0	0	100	100
2	B	433/510 (85%)	428 (99%)	5 (1%)	0	100	100
3	F	4/6 (67%)	4 (100%)	0	0	100	100
All	All	440/534 (82%)	435 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	5/16 (31%)	5 (100%)	0	100	100
2	B	366/426 (86%)	363 (99%)	3 (1%)	81	86
3	F	5/5 (100%)	5 (100%)	0	100	100
All	All	376/447 (84%)	373 (99%)	3 (1%)	81	86

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

Mol	Chain	Res	Type
2	B	348	LYS
2	B	438	GLN
2	B	442	ASP

Sometimes 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 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 ⓘ

There are no monosaccharides 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.

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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	5/18 (27%)	1.95	2 (40%)	0	0	64, 65, 80, 100	0
2	B	426/510 (83%)	0.76	60 (14%)	2	3	29, 43, 94, 129	0
3	F	6/6 (100%)	1.23	1 (16%)	1	2	59, 65, 87, 99	0
All	All	437/534 (81%)	0.78	63 (14%)	2	3	29, 43, 95, 129	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	485	TYR	7.5
2	B	497	SER	6.4
2	B	432	LYS	5.9
2	B	496	PHE	5.1
2	B	454	LEU	5.1
2	B	493	GLU	5.1
2	B	478	ARG	4.9
2	B	482	GLU	4.4
1	A	259	ILE	4.2
2	B	462	ILE	4.0
2	B	452	GLU	3.9
2	B	458	GLU	3.8
2	B	457	THR	3.8
2	B	480	GLU	3.7
2	B	109	GLN	3.7
2	B	492	ILE	3.7
2	B	455	GLY	3.7
2	B	73	THR	3.6
2	B	431	ALA	3.6
1	A	255	CYS	3.4
2	B	471	ASP	3.4
2	B	74	VAL	3.4
2	B	470	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	494	LYS	3.3
3	F	63	GLU	3.3
2	B	479	HIS	3.2
2	B	484	VAL	3.2
2	B	108	LYS	3.2
2	B	481	ASN	3.1
2	B	107	GLU	3.1
2	B	419	CYS	3.1
2	B	486	LYS	3.1
2	B	275	ILE	3.1
2	B	477	GLN	3.0
2	B	483	SER	3.0
2	B	88	ASN	3.0
2	B	443	ALA	3.0
2	B	382	LEU	2.9
2	B	256[A]	LEU	2.9
2	B	461	SER	2.9
2	B	383	VAL	2.8
2	B	416	LEU	2.8
2	B	421	ILE	2.7
2	B	75	ASN	2.7
2	B	459	LYS	2.7
2	B	398	ALA	2.7
2	B	476	LEU	2.7
2	B	495	TYR	2.7
2	B	271	SER	2.6
2	B	453	LYS	2.5
2	B	489	LEU	2.5
2	B	474	GLU	2.5
2	B	381	PHE	2.5
2	B	490	ASN	2.4
2	B	434	THR	2.4
2	B	379	VAL	2.4
2	B	316	ALA	2.3
2	B	233	LEU	2.1
2	B	451	ALA	2.1
2	B	402	THR	2.1
2	B	272	CYS	2.1
2	B	307	LEU	2.0
2	B	465	GLU	2.0

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 monosaccharides 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.