Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2023 – 10:35 AM EDT

PDB ID	:	7UMI
Title	:	Importin a1 bound to Cp183-CTD
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Deposited on	:	2022-04-07
Resolution	:	1.99 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 ⓘ 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 ⓘ) were used in the production of this report:

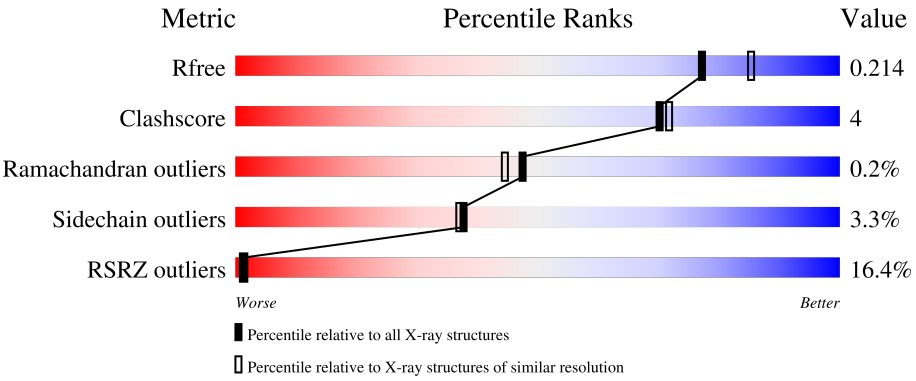
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	10	50% 70% 30%
2	E	467	14% 82% 9% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3587 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 HBV-NLS.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	10	95	53	27	15	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	424	3218	2048	546	614	10	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	63	HIS	-	expression tag	UNP P52293
E	64	HIS	-	expression tag	UNP P52293
E	65	HIS	-	expression tag	UNP P52293
E	66	HIS	-	expression tag	UNP P52293
E	67	HIS	-	expression tag	UNP P52293
E	68	HIS	-	expression tag	UNP P52293
E	69	MET	-	expression tag	UNP P52293

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	3	3	3	0	0
			Total	O		
3	E	271	271	271	0	0

3 Residue-property plots (i)

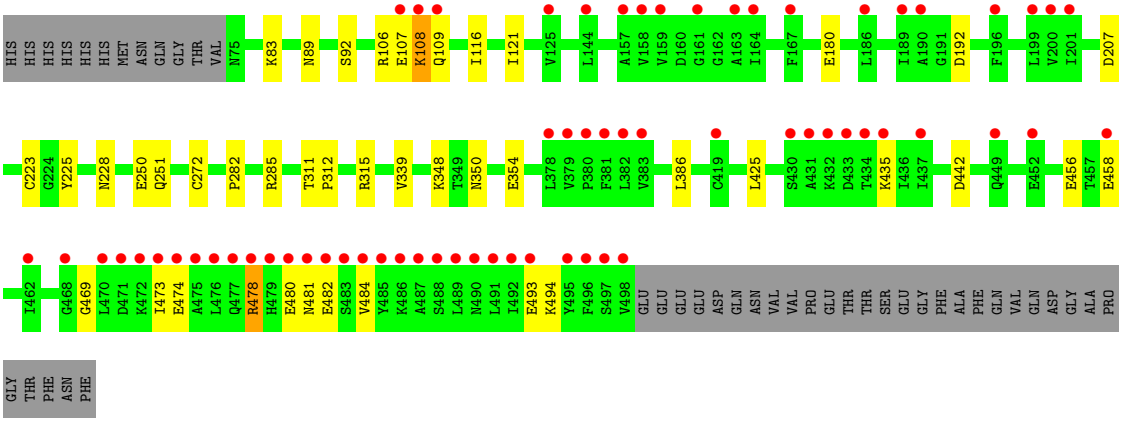
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

• Molecule 1: HBV-NLS

Chain A:

• Molecule 2: Importin subunit alpha-1

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.44Å 90.69Å 97.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.09 – 1.99 41.09 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.3 (41.09-1.99) 98.3 (41.09-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.184 , 0.215 0.183 , 0.214	Depositor DCC
R_{free} test set	2019 reflections (4.25%)	wwPDB-VP
Wilson B-factor (Å^2)	34.2	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3587	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.55	0/98	1.00	0/127
2	E	0.41	0/3275	0.58	0/4466
All	All	0.42	0/3373	0.60	0/4593

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	95	0	102	3	0
2	E	3218	0	3281	24	0
3	A	3	0	0	0	0
3	E	271	0	0	1	0
All	All	3587	0	3383	24	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 4.

All (24) 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:E:348:LYS:HE3	2:E:350:ASN:H	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:473:ILE:HD12	2:E:473:ILE:H	1.67	0.59
1:A:40[B]:ARG:NH2	2:E:228:ASN:OD1	2.33	0.58
2:E:116:ILE:HG12	2:E:121:ILE:HD11	1.86	0.58
2:E:272:CYS:HB3	2:E:312:PRO:HB2	1.88	0.55
2:E:282:PRO:HD2	2:E:285:ARG:HG3	1.87	0.55
2:E:348:LYS:CE	2:E:350:ASN:H	2.20	0.54
2:E:469:GLY:O	2:E:473:ILE:HD12	2.09	0.53
2:E:386:LEU:HD21	2:E:425:LEU:HD13	1.92	0.49
2:E:207:ASP:OD1	2:E:251:GLN:NE2	2.44	0.49
2:E:481:ASN:HB3	2:E:484:VAL:HB	1.96	0.47
1:A:41:ARG:HH22	2:E:107:GLU:HA	1.78	0.46
2:E:89:ASN:HB3	2:E:92:SER:HB2	1.98	0.46
2:E:315:ARG:HD2	2:E:354:GLU:OE1	2.17	0.45
2:E:348:LYS:HE3	2:E:350:ASN:HB2	1.97	0.45
2:E:311:THR:O	2:E:315:ARG:HG2	2.18	0.44
2:E:106:ARG:HD2	2:E:108:LYS:HE3	2.00	0.43
2:E:180:GLU:HB2	2:E:225:TYR:CD1	2.55	0.41
2:E:348:LYS:HE3	2:E:350:ASN:N	2.27	0.41
2:E:494:LYS:HB2	2:E:494:LYS:HE2	1.90	0.41
2:E:250:GLU:HB2	3:E:815:HOH:O	2.20	0.41
2:E:474:GLU:OE2	2:E:478:ARG:NH2	2.53	0.40
1:A:39:ARG:NH2	2:E:192:ASP:OD1	2.53	0.40
2:E:478:ARG:H	2:E:478:ARG:HG2	1.71	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	Percentiles
1	A	9/10 (90%)	8 (89%)	1 (11%)	0	100 100
2	E	422/467 (90%)	416 (99%)	5 (1%)	1 (0%)	47 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	431/477 (90%)	424 (98%)	6 (1%)	1 (0%)	47 44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	109	GLN

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	11/10 (110%)	11 (100%)	0	100 100
2	E	353/393 (90%)	341 (97%)	12 (3%)	37 36
All	All	364/403 (90%)	352 (97%)	12 (3%)	38 37

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	83	LYS
2	E	108	LYS
2	E	223	CYS
2	E	339	VAL
2	E	435	LYS
2	E	442	ASP
2	E	456	GLU
2	E	458	GLU
2	E	478	ARG
2	E	480	GLU
2	E	482	GLU
2	E	493	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	88	ASN

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.

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, 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	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	10/10 (100%)	2.10	5 (50%)	0	0	38, 49, 66, 67	0
2	E	424/467 (90%)	0.78	66 (15%)	2	1	24, 35, 80, 95	0
All	All	434/477 (90%)	0.81	71 (16%)	1	1	24, 36, 80, 95	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	496	PHE	8.2
2	E	476	LEU	7.1
2	E	489	LEU	6.6
2	E	473	ILE	6.1
2	E	478	ARG	6.0
2	E	491	LEU	6.0
2	E	479	HIS	6.0
2	E	497	SER	5.3
2	E	431	ALA	5.0
2	E	492	ILE	5.0
2	E	477	GLN	5.0
2	E	484	VAL	4.8
1	A	44	GLN	4.6
1	A	36	GLN	4.5
2	E	482	GLU	4.4
2	E	483	SER	4.4
2	E	480	GLU	4.4
2	E	498	VAL	4.4
1	A	37	SER	4.4
1	A	35	SER	4.3
2	E	485	TYR	4.1
2	E	474	GLU	4.0
2	E	493	GLU	4.0
2	E	481	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
2	E	159	VAL	3.9
2	E	108	LYS	3.8
2	E	452	GLU	3.7
2	E	199	LEU	3.6
2	E	437	ILE	3.6
2	E	434	THR	3.6
2	E	495	TYR	3.5
2	E	158	VAL	3.5
2	E	107	GLU	3.3
2	E	419	CYS	3.2
2	E	475	ALA	3.2
2	E	471	ASP	3.2
2	E	472	LYS	3.2
2	E	487	ALA	3.1
2	E	430	SER	3.0
2	E	458	GLU	2.9
2	E	125	VAL	2.9
2	E	200	VAL	2.9
2	E	189	ILE	2.9
2	E	470	LEU	2.8
2	E	164	ILE	2.7
2	E	490	ASN	2.7
2	E	383	VAL	2.6
2	E	435	LYS	2.6
2	E	449	GLN	2.6
2	E	144	LEU	2.5
2	E	109	GLN	2.5
2	E	462	ILE	2.5
2	E	163	ALA	2.5
2	E	381	PHE	2.5
2	E	488	SER	2.5
2	E	380	PRO	2.4
2	E	201	ILE	2.4
2	E	432	LYS	2.4
2	E	433	ASP	2.4
2	E	486	LYS	2.3
2	E	157	ALA	2.3
2	E	196	PHE	2.3
2	E	378	LEU	2.3
2	E	379	VAL	2.3
2	E	382	LEU	2.2
2	E	167	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	468	GLY	2.1
2	E	186	LEU	2.1
2	E	190	ALA	2.1
2	E	161	GLY	2.1
1	A	43	SER	2.0

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)

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.