Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 08:11 PM JST

PDB ID	:	5H43
Title	:	Structural and mechanistical studies of the nuclear import by Importin-alpha
Authors	:	Wang, R.; Li, Y.
Deposited on	:	2016-10-28
Resolution	:	2.30 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:

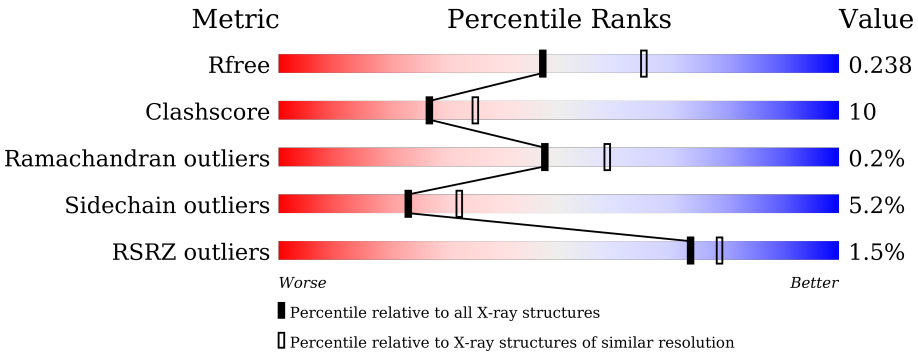
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	429	2% 85% 12%
2	B	10	40% 60%
3	C	15	67% 27% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3614 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 Importin subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3251	2070	547	623	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	SER	-	expression tag	UNP P52292

- Molecule 2 is a protein called Histone acetyltransferase KAT8.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	10	Total	C	N	O	0	0	0
			92	54	22	16			

- Molecule 3 is a protein called Histone acetyltransferase KAT8.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	15	Total	C	N	O	0	0	0
			125	74	25	26			

- Molecule 4 is water.

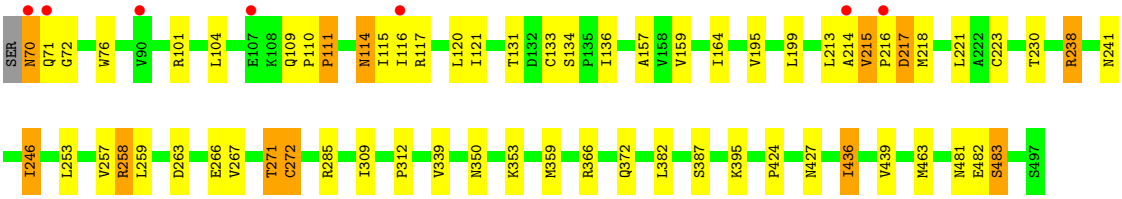
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	129	Total	O	0	0
			129	129		
4	B	7	Total	O	0	0
			7	7		
4	C	10	Total	O	0	0
			10	10		

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: Importin subunit alpha-1

Chain A:



• Molecule 2: Histone acetyltransferase KAT8

Chain B:

• Molecule 3: Histone acetyltransferase KAT8

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	82.22Å 82.22Å 169.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.90 – 2.30 46.48 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.90-2.30) 99.8 (46.48-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.53 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.211 , 0.243 0.216 , 0.238	Depositor DCC
R_{free} test set	1301 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	58.4	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3614	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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	0.77	1/3309 (0.0%)	0.87	6/4516 (0.1%)
2	B	0.81	0/92	1.23	2/119 (1.7%)
3	C	0.85	0/125	1.34	2/166 (1.2%)
All	All	0.77	1/3526 (0.0%)	0.90	10/4801 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	217	ASP	CG-OD1	6.06	1.39	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	217	ASP	CB-CA-C	-11.11	88.18	110.40
1	A	217	ASP	CB-CG-OD2	-7.34	111.69	118.30
2	B	144	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	A	217	ASP	N-CA-C	5.83	126.74	111.00
1	A	238	ARG	N-CA-C	5.75	126.53	111.00
1	A	258	ARG	NE-CZ-NH2	-5.69	117.45	120.30
2	B	144	ARG	NE-CZ-NH1	5.57	123.08	120.30
3	C	129	GLU	N-CA-C	5.43	125.67	111.00
1	A	366	ARG	NE-CZ-NH1	5.30	122.95	120.30
3	C	129	GLU	CB-CA-C	-5.20	100.00	110.40

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	3251	0	3313	65	1
2	B	92	0	93	5	0
3	C	125	0	124	7	0
4	A	129	0	0	15	1
4	B	7	0	0	0	1
4	C	10	0	0	1	0
All	All	3614	0	3530	71	3

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 10.

All (71) 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:382:LEU:HD21	4:A:608:HOH:O	1.79	0.82
1:A:214:ALA:O	1:A:215:VAL:HG13	1.81	0.80
1:A:114:ASN:H	1:A:114:ASN:ND2	1.87	0.72
1:A:266:GLU:HG3	3:C:130:LEU:HD21	1.71	0.71
1:A:272:CYS:HB3	1:A:312:PRO:HB2	1.74	0.68
1:A:359:MET:HE2	4:A:608:HOH:O	1.94	0.68
3:C:128:SER:HA	3:C:129:GLU:CG	2.26	0.66
1:A:71:GLN:CG	1:A:76:TRP:HE1	2.11	0.63
1:A:215:VAL:HB	1:A:217:ASP:H	1.63	0.63
1:A:246:ILE:HG13	1:A:285:ARG:NH1	2.15	0.61
3:C:128:SER:HA	3:C:129:GLU:CB	2.31	0.61
1:A:267:VAL:O	1:A:271:THR:HG23	2.01	0.61
1:A:215:VAL:HG23	1:A:218:MET:HB2	1.83	0.60
1:A:214:ALA:HB2	4:A:502:HOH:O	2.01	0.60
1:A:111:PRO:O	1:A:115:ILE:HG12	2.02	0.59
1:A:353:LYS:NZ	2:B:149:ILE:CG2	2.66	0.59
1:A:71:GLN:HG3	1:A:76:TRP:HE1	1.68	0.58
1:A:71:GLN:HG3	1:A:72:GLY:N	2.17	0.58
1:A:238:ARG:NH1	4:A:501:HOH:O	2.19	0.57
1:A:217:ASP:OD1	1:A:218:MET:N	2.39	0.56
1:A:217:ASP:OD1	1:A:217:ASP:C	2.44	0.56
1:A:109:GLN:O	1:A:111:PRO:HD3	2.07	0.55
1:A:353:LYS:HZ1	2:B:149:ILE:CG2	2.21	0.54
1:A:114:ASN:H	1:A:114:ASN:HD22	1.54	0.53
1:A:114:ASN:HA	1:A:117:ARG:HD2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:VAL:HG23	4:A:530:HOH:O	2.08	0.52
1:A:115:ILE:HG23	1:A:120:LEU:HD12	1.93	0.51
1:A:116:ILE:HD13	1:A:157:ALA:CB	2.40	0.51
1:A:121:ILE:HG13	4:A:509:HOH:O	2.11	0.51
1:A:213:LEU:C	1:A:215:VAL:HG22	2.32	0.50
1:A:71:GLN:HG3	1:A:72:GLY:H	1.76	0.49
1:A:214:ALA:C	1:A:215:VAL:HG22	2.33	0.49
1:A:121:ILE:N	4:A:509:HOH:O	2.46	0.48
1:A:215:VAL:HG12	1:A:216:PRO:HD2	1.95	0.48
1:A:213:LEU:O	1:A:215:VAL:HG22	2.14	0.47
1:A:230:THR:HG23	1:A:271:THR:HG22	1.96	0.47
2:B:145:LYS:O	2:B:148:GLU:HB2	2.15	0.47
4:A:503:HOH:O	3:C:134:PRO:HG2	2.15	0.47
1:A:266:GLU:HG3	3:C:130:LEU:CD2	2.41	0.47
1:A:215:VAL:HG11	1:A:217:ASP:OD1	2.14	0.46
1:A:258:ARG:NH1	4:A:512:HOH:O	2.48	0.46
1:A:382:LEU:CG	4:A:608:HOH:O	2.62	0.46
1:A:104:LEU:HA	1:A:110:PRO:HB3	1.98	0.46
1:A:71:GLN:HG2	1:A:76:TRP:HE1	1.78	0.46
1:A:350:ASN:HB2	4:A:573:HOH:O	2.16	0.45
1:A:133:CYS:O	1:A:136:ILE:HG22	2.16	0.45
1:A:382:LEU:HD13	4:A:560:HOH:O	2.16	0.45
1:A:382:LEU:CD2	4:A:608:HOH:O	2.51	0.44
3:C:130:LEU:HD23	3:C:130:LEU:HA	1.92	0.44
1:A:214:ALA:O	1:A:215:VAL:CG1	2.60	0.44
1:A:241:ASN:HD22	1:A:241:ASN:N	2.14	0.44
1:A:353:LYS:HZ1	2:B:149:ILE:HG22	1.82	0.44
1:A:159:VAL:HG13	1:A:164:ILE:HD12	2.00	0.44
1:A:259:LEU:HB3	1:A:271:THR:HG21	2.00	0.44
1:A:481:ASN:OD1	1:A:483:SER:HB2	2.18	0.43
1:A:199:LEU:HD12	1:A:199:LEU:HA	1.95	0.43
1:A:71:GLN:CG	1:A:72:GLY:N	2.81	0.43
1:A:353:LYS:HZ2	2:B:149:ILE:CG2	2.32	0.42
1:A:218:MET:O	1:A:221:LEU:HB2	2.20	0.42
1:A:213:LEU:O	1:A:258:ARG:NH2	2.52	0.42
1:A:116:ILE:HD13	1:A:157:ALA:HB3	2.02	0.42
3:C:129:GLU:HB2	4:C:207:HOH:O	2.20	0.42
1:A:359:MET:CE	4:A:608:HOH:O	2.62	0.41
1:A:253:LEU:O	1:A:257:VAL:HG23	2.20	0.41
1:A:395:LYS:HG2	1:A:436:ILE:CD1	2.49	0.41
1:A:71:GLN:CG	1:A:72:GLY:H	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:LEU:HB2	4:A:509:HOH:O	2.21	0.41
1:A:339:VAL:O	1:A:339:VAL:HG12	2.21	0.41
1:A:101:ARG:HD2	1:A:101:ARG:C	2.41	0.41
1:A:424:PRO:HA	1:A:427:ASN:HD22	1.85	0.41
1:A:436:ILE:HA	1:A:439:VAL:HG22	2.03	0.40

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	Interatomic distance (Å)	Clash overlap (Å)
4:B:207:HOH:O	4:B:207:HOH:O[7_557]	1.24	0.96
4:A:551:HOH:O	4:A:576:HOH:O[7_557]	1.71	0.49
1:A:70:ASN:ND2	1:A:263:ASP:OD2[3_745]	2.13	0.07

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	426/429 (99%)	413 (97%)	12 (3%)	1 (0%)	47 58
2	B	8/10 (80%)	7 (88%)	1 (12%)	0	100 100
3	C	13/15 (87%)	12 (92%)	1 (8%)	0	100 100
All	All	447/454 (98%)	432 (97%)	14 (3%)	1 (0%)	47 58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	PRO

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	360/362 (99%)	344 (96%)	16 (4%)	28 39
2	B	10/10 (100%)	8 (80%)	2 (20%)	1 1
3	C	14/14 (100%)	12 (86%)	2 (14%)	3 3
All	All	384/386 (100%)	364 (95%)	20 (5%)	23 32

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	114	ASN
1	A	131	THR
1	A	134	SER
1	A	215	VAL
1	A	223	CYS
1	A	246	ILE
1	A	271	THR
1	A	272	CYS
1	A	309	ILE
1	A	372	GLN
1	A	387	SER
1	A	436	ILE
1	A	463	MET
1	A	482	GLU
1	A	483	SER
2	B	140	ARG
2	B	147	ASP
3	C	129	GLU
3	C	142	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	241	ASN
1	A	427	ASN
3	C	141	ASN
3	C	142	GLN

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	428/429 (99%)	-0.18	7 (1%) 72 77	46, 63, 98, 129	0
2	B	10/10 (100%)	0.01	0 100 100	66, 78, 100, 101	0
3	C	15/15 (100%)	0.05	0 100 100	55, 82, 102, 103	0
All	All	453/454 (99%)	-0.17	7 (1%) 73 79	46, 64, 101, 129	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	71	GLN	2.9
1	A	216	PRO	2.9
1	A	90	VAL	2.6
1	A	116	ILE	2.3
1	A	107	GLU	2.2
1	A	214	ALA	2.1
1	A	70	ASN	2.1

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 (i)

There are no such residues in this entry.