Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 06:12 PM EDT

PDB ID	:	3TPO
Title	:	Crystal structure of D192A/E396A mutant of mouse importin alpha2
Authors	:	Hirano, H.; Matsuura, Y.
Deposited on	:	2011-09-08
Resolution	:	2.10 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:

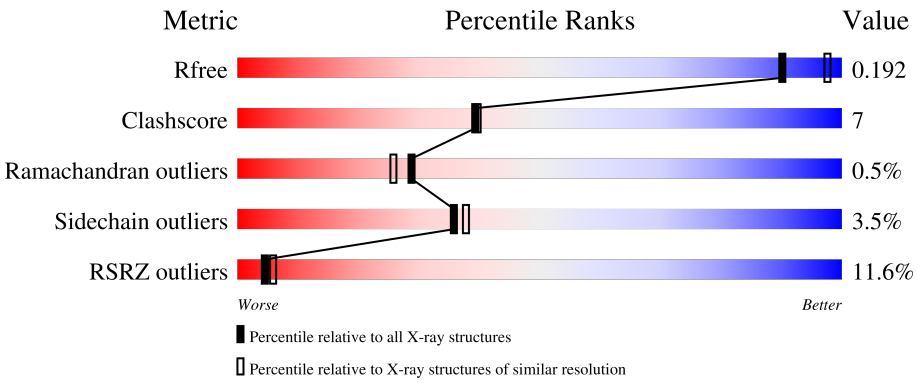
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.10 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	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	529	10% 67% 14% • 17%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3650 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-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	438	3342	2124	573	634	11	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	ALA	ASP	engineered mutation	UNP P52293
A	396	ALA	GLU	engineered mutation	UNP P52293

- Molecule 2 is water.

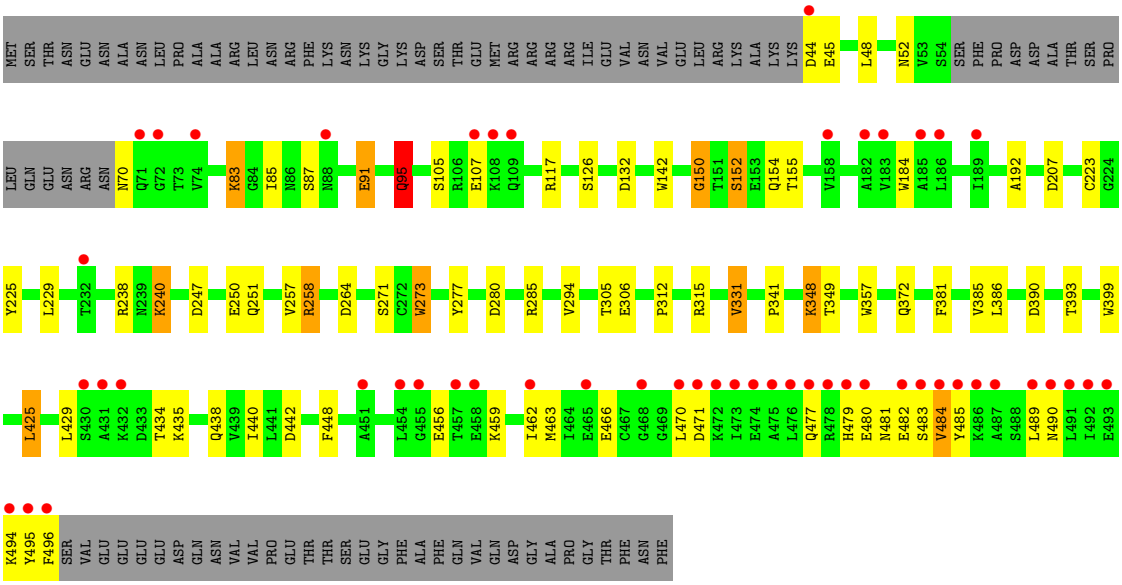
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	308	308	308	0	0

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: Importin subunit alpha-2

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.34Å 89.76Å 99.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.94 – 2.10 38.94 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.94-2.10) 99.7 (38.94-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.160 , 0.192 0.159 , 0.192	Depositor DCC
R_{free} test set	2115 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 54.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	3650	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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 (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	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	1.31	19/3399 (0.6%)	1.20	17/4627 (0.4%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	152	SER	CB-OG	-7.98	1.31	1.42
1	A	132	ASP	CB-CG	7.52	1.67	1.51
1	A	271	SER	CB-OG	-7.52	1.32	1.42
1	A	91	GLU	CB-CG	-7.46	1.38	1.52
1	A	399	TRP	CD2-CE2	7.11	1.49	1.41
1	A	277	TYR	CG-CD1	6.85	1.48	1.39
1	A	273	TRP	CD2-CE2	6.61	1.49	1.41
1	A	105	SER	CB-OG	-6.52	1.33	1.42
1	A	258	ARG	CZ-NH1	6.28	1.41	1.33
1	A	357	TRP	CG-CD2	6.25	1.54	1.43
1	A	184	TRP	CD2-CE2	5.99	1.48	1.41
1	A	142	TRP	CD2-CE2	5.96	1.48	1.41
1	A	258	ARG	CD-NE	-5.90	1.36	1.46
1	A	95	GLN	CD-OE1	5.87	1.36	1.24
1	A	126	SER	CB-OG	-5.61	1.34	1.42
1	A	150	GLY	N-CA	5.23	1.53	1.46
1	A	250	GLU	CD-OE1	5.10	1.31	1.25
1	A	306	GLU	CD-OE1	5.05	1.31	1.25
1	A	357	TRP	CD2-CE2	5.02	1.47	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	258	ARG	NE-CZ-NH2	-16.68	111.96	120.30
1	A	258	ARG	NE-CZ-NH1	10.14	125.37	120.30
1	A	240	LYS	C-N-CA	-9.49	97.97	121.70
1	A	117	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	A	48	LEU	CA-CB-CG	7.12	131.68	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	48	LEU	CB-CG-CD1	6.31	121.73	111.00
1	A	238	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	105	SER	CB-CA-C	-6.12	98.46	110.10
1	A	87	SER	C-N-CA	-5.98	106.76	121.70
1	A	258	ARG	CB-CG-CD	-5.84	96.42	111.60
1	A	223	CYS	N-CA-CB	-5.78	100.19	110.60
1	A	331	VAL	CG1-CB-CG2	5.72	120.05	110.90
1	A	132	ASP	CB-CG-OD2	5.58	123.33	118.30
1	A	264	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	152	SER	CB-CA-C	-5.35	99.94	110.10
1	A	390	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	A	425	LEU	CA-CB-CG	5.06	126.93	115.30

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	A	3342	0	3425	50	0
2	A	308	0	0	10	0
All	All	3650	0	3425	50	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 7.

All (50) 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:247:ASP:HB3	2:A:736:HOH:O	1.45	1.15
1:A:44:ASP:OD1	1:A:45:GLU:HB3	1.58	1.03
1:A:44:ASP:HB2	1:A:315:ARG:HH22	1.23	1.01
1:A:107:GLU:HG2	2:A:601:HOH:O	1.63	0.97
1:A:477:GLN:HE21	1:A:489:LEU:HA	1.32	0.92
1:A:44:ASP:CB	1:A:315:ARG:HH22	1.86	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LYS:HG3	2:A:692:HOH:O	1.83	0.79
1:A:386:LEU:HD21	1:A:425:LEU:HD13	1.65	0.77
1:A:482:GLU:HG3	1:A:483:SER:N	2.01	0.74
1:A:477:GLN:NE2	1:A:489:LEU:HA	2.02	0.73
1:A:44:ASP:HB2	1:A:315:ARG:NH2	2.03	0.71
1:A:348:LYS:HD2	2:A:560:HOH:O	1.93	0.68
1:A:207:ASP:OD1	1:A:251:GLN:NE2	2.28	0.67
1:A:70:ASN:HB3	2:A:604:HOH:O	1.98	0.62
1:A:372:GLN:HG3	2:A:664:HOH:O	2.01	0.61
1:A:91:GLU:O	1:A:95:GLN:HG2	2.00	0.60
1:A:435:LYS:HD3	1:A:438:GLN:HE21	1.68	0.59
1:A:70:ASN:N	2:A:793:HOH:O	2.38	0.57
1:A:462:ILE:O	1:A:466:GLU:HG2	2.04	0.57
1:A:45:GLU:HB2	2:A:725:HOH:O	2.06	0.56
1:A:470:LEU:HD13	1:A:496:PHE:CD1	2.42	0.55
1:A:456:GLU:OE1	1:A:459:LYS:HE2	2.06	0.54
1:A:45:GLU:HG3	1:A:45:GLU:O	2.06	0.54
1:A:247:ASP:CB	2:A:736:HOH:O	2.23	0.53
1:A:385:VAL:CG1	1:A:393:THR:HG22	2.38	0.53
1:A:490:ASN:OD1	1:A:494:LYS:HD3	2.08	0.53
1:A:479:HIS:HD2	1:A:481:ASN:HB3	1.73	0.52
1:A:385:VAL:HG13	1:A:393:THR:HG22	1.92	0.51
1:A:481:ASN:OD1	1:A:484:VAL:HG23	2.10	0.51
1:A:477:GLN:HE21	1:A:489:LEU:CA	2.15	0.49
1:A:425:LEU:HG	1:A:440:ILE:HG23	1.96	0.48
1:A:285:ARG:HD2	2:A:593:HOH:O	2.15	0.46
1:A:273:TRP:CD2	1:A:312:PRO:HB3	2.52	0.45
1:A:463:MET:HA	1:A:466:GLU:HG3	1.99	0.45
1:A:448:PHE:HB3	1:A:495:TYR:CZ	2.53	0.44
1:A:482:GLU:CG	1:A:483:SER:N	2.78	0.44
1:A:95:GLN:HE21	1:A:95:GLN:HA	1.83	0.43
1:A:225:TYR:CE2	1:A:229:LEU:HD11	2.53	0.43
1:A:240:LYS:HD3	1:A:280:ASP:O	2.18	0.43
1:A:482:GLU:HA	1:A:485:TYR:CE2	2.54	0.43
1:A:386:LEU:HD21	1:A:425:LEU:CD1	2.41	0.43
1:A:44:ASP:HB3	1:A:273:TRP:CH2	2.54	0.42
1:A:225:TYR:HE2	1:A:229:LEU:HD11	1.85	0.42
1:A:429:LEU:HD23	1:A:429:LEU:HA	1.87	0.42
1:A:479:HIS:O	1:A:485:TYR:HD2	2.02	0.41
1:A:150:GLY:HA3	1:A:154:GLN:OE1	2.21	0.41
1:A:257:VAL:HG22	1:A:294:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:HIS:CD2	1:A:481:ASN:HB3	2.53	0.41
1:A:155:THR:HG21	1:A:192:ALA:HB2	2.03	0.40
1:A:341:PRO:HB3	1:A:381:PHE:CZ	2.56	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	434/529 (82%)	417 (96%)	15 (4%)	2 (0%)	29 26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	471	ASP
1	A	484	VAL

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	367/447 (82%)	354 (96%)	13 (4%)	36 38

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	83	LYS
1	A	85	ILE
1	A	95	GLN
1	A	152	SER
1	A	258	ARG
1	A	305	THR
1	A	331	VAL
1	A	348	LYS
1	A	349	THR
1	A	434	THR
1	A	442	ASP
1	A	480	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	86	ASN
1	A	95	GLN
1	A	177	HIS
1	A	261	HIS
1	A	283	ASN
1	A	438	GLN
1	A	477	GLN
1	A	479	HIS

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, 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	438/529 (82%)	0.54	51 (11%) 4 6	21, 34, 84, 116	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	489	LEU	8.3
1	A	485	TYR	8.1
1	A	478	ARG	5.4
1	A	474	GLU	5.4
1	A	496	PHE	5.3
1	A	475	ALA	5.3
1	A	480	GLU	5.1
1	A	476	LEU	4.9
1	A	493	GLU	4.6
1	A	490	ASN	4.6
1	A	482	GLU	4.4
1	A	492	ILE	4.4
1	A	71	GLN	4.0
1	A	486	LYS	4.0
1	A	484	VAL	4.0
1	A	455	GLY	3.9
1	A	432	LYS	3.9
1	A	477	GLN	3.9
1	A	470	LEU	3.8
1	A	44	ASP	3.7
1	A	487	ALA	3.7
1	A	454	LEU	3.7
1	A	431	ALA	3.7
1	A	479	HIS	3.6
1	A	495	TYR	3.3
1	A	491	LEU	3.3
1	A	483	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	458	GLU	3.2
1	A	107	GLU	3.0
1	A	457	THR	2.9
1	A	108	LYS	2.9
1	A	472	LYS	2.7
1	A	471	ASP	2.7
1	A	494	LYS	2.7
1	A	186	LEU	2.6
1	A	468	GLY	2.4
1	A	74	VAL	2.4
1	A	189	ILE	2.4
1	A	183	VAL	2.4
1	A	88	ASN	2.3
1	A	451	ALA	2.3
1	A	473	ILE	2.3
1	A	465	GLU	2.3
1	A	158	VAL	2.2
1	A	109	GLN	2.2
1	A	462	ILE	2.2
1	A	182	ALA	2.1
1	A	430	SER	2.0
1	A	232	THR	2.0
1	A	185	ALA	2.0
1	A	72	GLY	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.