



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:11 PM UTC

PDB ID : 3TPO / pdb_00003tpo
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 ⓘ 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

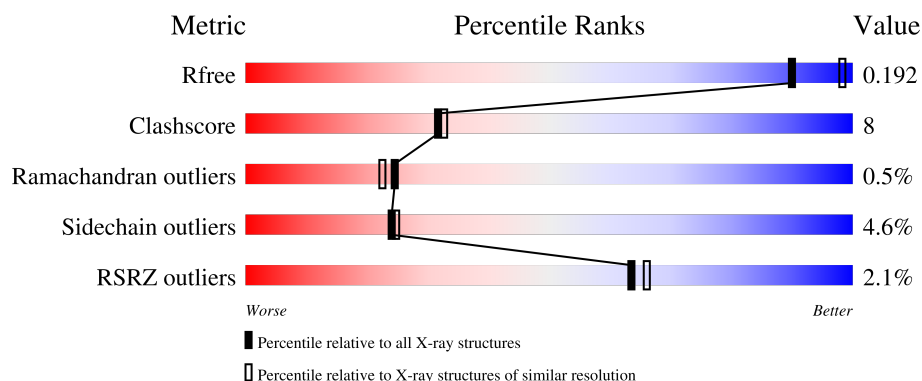
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

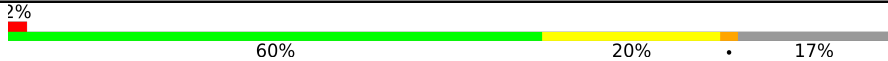
The reported resolution of this entry is 2.10 Å.

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 $\leq 5\%$. 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	

2 Entry composition

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
2	A	308	Total	O	0	0
			308	308		

- Molecule 1: Importin subunit alpha-2



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 , 56.3	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	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.*

¹Intensities estimated from amplitudes.

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.

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	1.68	40/3399 (1.2%)	1.51	37/4627 (0.8%)

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	VAL	N-CA	-8.50	1.37	1.46
1	A	223	CYS	N-CA	-7.89	1.36	1.46
1	A	169	SER	C-O	-7.86	1.14	1.24
1	A	241	ASN	N-CA	7.29	1.55	1.46
1	A	258	ARG	CD-NE	-7.02	1.36	1.46
1	A	95	GLN	CD-OE1	7.01	1.36	1.23
1	A	203	HIS	CG-CD2	6.70	1.43	1.35
1	A	111	PRO	CA-C	6.48	1.58	1.52
1	A	418	HIS	CG-CD2	6.44	1.43	1.35
1	A	207	ASP	N-CA	6.32	1.51	1.46
1	A	125	VAL	CA-CB	6.24	1.62	1.54
1	A	132	ASP	CB-CG	6.20	1.67	1.52
1	A	302	LEU	N-CA	6.19	1.54	1.46
1	A	349	THR	CB-OG1	-6.17	1.33	1.43
1	A	169	SER	N-CA	6.12	1.54	1.46
1	A	258	ARG	CZ-NH1	6.04	1.41	1.32
1	A	211	ALA	C-O	-5.93	1.16	1.24
1	A	150	GLY	N-CA	5.88	1.53	1.45
1	A	94	LEU	C-O	5.85	1.30	1.24
1	A	357	TRP	CG-CD2	5.84	1.54	1.43
1	A	295	VAL	C-O	-5.82	1.19	1.24
1	A	164	ILE	CA-CB	5.79	1.61	1.54
1	A	390	ASP	CA-C	5.74	1.59	1.52
1	A	187	GLY	N-CA	5.73	1.53	1.45
1	A	199	LEU	CA-C	5.73	1.60	1.52
1	A	53	VAL	C-O	-5.65	1.15	1.23
1	A	202	LYS	CA-C	5.65	1.60	1.52
1	A	423	GLU	CA-C	5.52	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	HIS	ND1-CE1	5.40	1.38	1.32
1	A	177	HIS	CG-CD2	5.36	1.41	1.35
1	A	418	HIS	CE1-NE2	5.36	1.38	1.32
1	A	296	PRO	CA-CB	5.31	1.61	1.53
1	A	153	GLU	CA-C	5.27	1.59	1.52
1	A	240	LYS	CA-C	-5.20	1.46	1.52
1	A	265	PRO	CA-C	5.19	1.59	1.52
1	A	315	ARG	CA-C	5.18	1.59	1.52
1	A	152	SER	CB-OG	-5.13	1.31	1.42
1	A	53	VAL	CA-C	5.09	1.59	1.52
1	A	290	VAL	CA-CB	5.05	1.60	1.54
1	A	399	TRP	CD2-CE2	5.02	1.49	1.41

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	LYS	CA-C-N	-18.88	97.97	123.46
1	A	240	LYS	C-N-CA	-18.88	97.97	123.46
1	A	53	VAL	N-CA-C	-8.43	104.68	112.43
1	A	87	SER	CA-C-N	-8.17	106.76	122.61
1	A	87	SER	C-N-CA	-8.17	106.76	122.61
1	A	258	ARG	NE-CZ-NH2	-8.04	111.96	119.20
1	A	105	SER	CB-CA-C	-6.96	98.46	110.09
1	A	346	ASN	CA-C-N	6.82	126.52	119.56
1	A	346	ASN	C-N-CA	6.82	126.52	119.56
1	A	223	CYS	N-CA-CB	-6.74	100.19	110.16
1	A	194	SER	CA-CB-OG	-6.58	97.95	111.10
1	A	152	SER	CB-CA-C	-6.50	99.94	110.74
1	A	258	ARG	CB-CG-CD	-6.47	96.42	111.30
1	A	328	THR	N-CA-C	-6.27	104.44	111.28
1	A	342	SER	CB-CA-C	-6.08	101.29	110.90
1	A	169	SER	CA-CB-OG	-6.01	99.07	111.10
1	A	447	ILE	N-CA-C	-6.00	104.46	111.00
1	A	240	LYS	O-C-N	-5.87	115.70	122.09
1	A	272	CYS	CB-CA-C	-5.72	101.30	110.79
1	A	339	VAL	N-CA-C	-5.62	105.36	113.07
1	A	347	PRO	N-CA-C	-5.58	106.58	113.84
1	A	331	VAL	N-CA-C	5.36	116.14	110.72
1	A	364	ALA	N-CA-C	-5.36	106.59	113.02
1	A	255	THR	N-CA-C	-5.35	105.11	111.69
1	A	257	VAL	N-CA-C	-5.32	105.35	110.72
1	A	248	ALA	N-CA-C	-5.24	105.65	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	GLN	N-CA-C	-5.21	105.68	111.36
1	A	179	SER	N-CA-C	-5.20	105.73	111.71
1	A	340	PHE	CA-C-N	-5.20	113.39	119.32
1	A	340	PHE	C-N-CA	-5.20	113.39	119.32
1	A	342	SER	CA-CB-OG	-5.19	100.72	111.10
1	A	349	THR	CA-CB-CG2	5.13	119.22	110.50
1	A	219	SER	CA-CB-OG	-5.13	100.84	111.10
1	A	348	LYS	CB-CA-C	5.12	119.25	110.81
1	A	152	SER	CA-CB-OG	-5.09	100.92	111.10
1	A	193	GLY	CA-C-N	5.04	127.35	120.54
1	A	193	GLY	C-N-CA	5.04	127.35	120.54

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	3342	0	3425	55	0
2	A	308	0	0	12	0
All	All	3650	0	3425	55	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 8.

All (55) 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
1:A:83:LYS:HG3	2:A:692:HOH:O	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:47:MET:HE2	1:A:49:LYS:O	1.99	0.62
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:47:MET:HE1	2:A:632:HOH:O	2.15	0.47
1:A:426:MET:HE1	1:A:444:ILE:HG13	1.96	0.47
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:250:GLU:OE2	1:A:288:MET:HE3	2.17	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:102:LYS:NZ	2:A:707:HOH:O	2.53	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%)	24 22

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%)	350 (95%)	17 (5%)	24	25

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	LYS
1	A	85	ILE
1	A	88	ASN
1	A	95	GLN
1	A	152	SER
1	A	181	GLN
1	A	305	THR
1	A	331	VAL
1	A	348	LYS
1	A	349	THR
1	A	414	VAL
1	A	434	THR
1	A	442	ASP
1	A	459	LYS
1	A	480	GLU
1	A	486	LYS
1	A	492	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	70	ASN
1	A	86	ASN
1	A	95	GLN
1	A	98	GLN
1	A	177	HIS
1	A	261	HIS
1	A	283	ASN
1	A	367	GLN
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 oligosaccharides 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%)	-0.35	9 (2%) 63 66	21, 34, 84, 116	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	54	SER	4.1
1	A	107	GLU	2.7
1	A	72	GLY	2.7
1	A	489	LEU	2.5
1	A	53	VAL	2.3
1	A	485	TYR	2.3
1	A	476	LEU	2.3
1	A	74	VAL	2.2
1	A	496	PHE	2.1

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 oligosaccharides 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.