



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:21 PM UTC

PDB ID : 3TPM / pdb_00003tpm
Title : Crystal structure of MAL RPEL domain in complex with importin-alpha
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

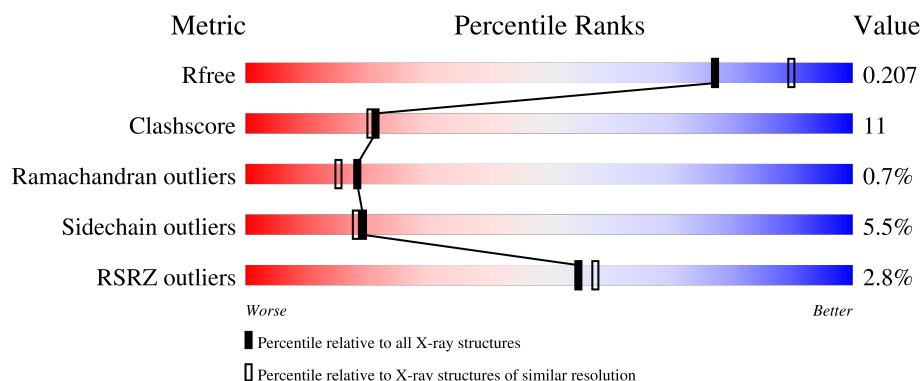
1 Overall quality at a glance

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	422	
2	B	120	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3618 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
1	A	422	Total	C	N	O	S	0	0	0
			3220	2052	546	612	10			

- Molecule 2 is a protein called MAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	0	0	0
			119	76	27	16			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	265	Total	O	0	0
			265	265		
3	B	14	Total	O	0	0
			14	14		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.66Å 90.12Å 98.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.00 – 2.10 41.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (41.00-2.10) 98.7 (41.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.166 , 0.208 0.165 , 0.207	Depositor DCC
R_{free} test set	2097 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3618	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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	1.46	14/3278 (0.4%)	1.36	23/4467 (0.5%)
2	B	1.40	0/117	1.44	2/149 (1.3%)
All	All	1.45	14/3395 (0.4%)	1.36	25/4616 (0.5%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	418	HIS	CG-CD2	8.52	1.45	1.35
1	A	418	HIS	CE1-NE2	8.31	1.40	1.32
1	A	379	VAL	CA-CB	6.61	1.57	1.54
1	A	295	VAL	CA-C	6.20	1.57	1.52
1	A	200	VAL	N-CA	6.09	1.53	1.46
1	A	258	ARG	CZ-NH1	5.95	1.41	1.32
1	A	261	HIS	CE1-NE2	5.88	1.38	1.32
1	A	188	ASN	N-CA	5.75	1.53	1.46
1	A	335	GLY	N-CA	5.57	1.52	1.45
1	A	177	HIS	CG-CD2	5.56	1.42	1.35
1	A	261	HIS	CG-CD2	5.55	1.42	1.35
1	A	418	HIS	ND1-CE1	5.29	1.37	1.32
1	A	135	PRO	CA-C	5.25	1.59	1.52
1	A	376	HIS	ND1-CE1	5.23	1.37	1.32

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	LYS	CA-C-N	-14.16	105.74	123.16
1	A	240	LYS	C-N-CA	-14.16	105.74	123.16
1	A	258	ARG	NE-CZ-NH2	-8.20	111.82	119.20
1	A	87	SER	CA-C-N	-7.51	108.04	122.61
1	A	87	SER	C-N-CA	-7.51	108.04	122.61
1	A	255	THR	N-CA-C	-6.85	103.27	111.69
1	A	342	SER	CB-CA-C	-6.50	100.63	110.90
1	A	271	SER	CB-CA-C	-6.24	100.43	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	447	ILE	N-CA-C	-6.08	104.38	111.00
1	A	134	SER	CA-C-N	-5.93	112.47	119.05
1	A	134	SER	C-N-CA	-5.93	112.47	119.05
1	A	258	ARG	NE-CZ-NH1	5.80	127.30	121.50
1	A	105	SER	N-CA-C	5.76	119.93	113.02
1	A	194	SER	CA-CB-OG	-5.57	99.96	111.10
1	A	272	CYS	CB-CA-C	-5.56	101.56	110.79
1	A	164	ILE	CA-C-N	-5.54	113.32	119.19
1	A	164	ILE	C-N-CA	-5.54	113.32	119.19
1	A	402	THR	CB-CA-C	5.52	121.27	110.67
1	A	414	VAL	CB-CA-C	-5.41	105.05	111.97
1	A	366	ARG	CB-CG-CD	-5.37	98.96	111.30
2	B	159	ALA	CA-C-N	5.35	131.33	121.70
2	B	159	ALA	C-N-CA	5.35	131.33	121.70
1	A	372	GLN	CA-CB-CG	-5.33	103.45	114.10
1	A	95	GLN	CB-CA-C	-5.21	102.14	110.79
1	A	349	THR	N-CA-C	5.19	116.93	111.28

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	3220	0	3296	66	1
2	B	119	0	147	11	0
3	A	265	0	0	10	1
3	B	14	0	0	2	0
All	All	3618	0	3443	74	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 11.

All (74) 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	3:A:661:HOH:O	1.61	1.00
1:A:477:GLN:HA	1:A:485:TYR:HB2	1.52	0.91
1:A:75:ASN:N	3:A:511:HOH:O	2.05	0.88
1:A:346:ASN:HD22	1:A:348:LYS:H	1.21	0.87
1:A:426:MET:HE1	1:A:444:ILE:HD12	1.57	0.85
1:A:477:GLN:NE2	1:A:489:LEU:HA	1.92	0.84
2:B:159:ALA:HA	2:B:160:ASP:HB2	1.59	0.81
2:B:151:LEU:HD12	2:B:151:LEU:O	1.80	0.81
1:A:477:GLN:HE21	1:A:489:LEU:HA	1.43	0.80
2:B:152:LYS:HE3	3:B:192:HOH:O	1.83	0.78
2:B:151:LEU:O	2:B:152:LYS:HB3	1.85	0.75
1:A:477:GLN:HE21	1:A:489:LEU:CA	1.99	0.74
1:A:346:ASN:ND2	1:A:348:LYS:H	1.90	0.70
1:A:426:MET:HE1	1:A:444:ILE:CD1	2.21	0.70
1:A:477:GLN:O	1:A:485:TYR:HD1	1.76	0.69
1:A:434:THR:HG21	3:A:576:HOH:O	1.92	0.69
1:A:493:GLU:O	1:A:495:TYR:N	2.28	0.67
1:A:386:LEU:HD21	1:A:425:LEU:HD13	1.77	0.65
1:A:472:LYS:O	1:A:476:LEU:HG	1.96	0.65
1:A:470:LEU:HD13	1:A:496:PHE:CD1	2.33	0.63
1:A:272:CYS:HB3	1:A:312:PRO:HB2	1.81	0.63
1:A:477:GLN:O	1:A:485:TYR:CD1	2.52	0.63
1:A:307:LEU:HB3	1:A:308:PRO:HD3	1.82	0.62
1:A:292:LYS:NZ	3:A:653:HOH:O	2.33	0.61
1:A:348:LYS:HE3	1:A:350:ASN:HB3	1.82	0.60
1:A:285:ARG:HA	1:A:288:MET:HE3	1.83	0.60
1:A:75:ASN:N	3:A:525:HOH:O	2.35	0.59
1:A:477:GLN:HA	1:A:485:TYR:CB	2.28	0.59
1:A:402:THR:HB	1:A:443:ALA:HB2	1.84	0.59
1:A:426:MET:CE	1:A:444:ILE:HD12	2.32	0.57
1:A:132:ASP:HB2	3:A:54:HOH:O	2.03	0.57
1:A:402:THR:HG21	1:A:439:VAL:O	2.05	0.56
1:A:426:MET:HE3	1:A:464:ILE:HG12	1.88	0.54
2:B:151:LEU:O	2:B:151:LEU:CD1	2.54	0.54
1:A:485:TYR:HA	1:A:488:SER:OG	2.07	0.54
1:A:276:SER:HB2	1:A:315:ARG:HG3	1.91	0.52
1:A:322:THR:HB	2:B:121:LYS:HG2	1.91	0.52
1:A:457:THR:O	1:A:461:SER:HB2	2.12	0.49
1:A:292:LYS:HE2	3:A:21:HOH:O	2.11	0.49
1:A:440:ILE:O	1:A:444:ILE:HG12	2.12	0.48
1:A:418:HIS:HB2	3:A:48:HOH:O	2.12	0.48
1:A:285:ARG:HD2	3:A:52:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LYS:HE3	1:A:350:ASN:H	1.79	0.47
1:A:402:THR:CG2	1:A:439:VAL:CG1	2.93	0.47
1:A:368:ASP:O	1:A:372:GLN:HG3	2.15	0.47
1:A:109:GLN:HA	1:A:110:PRO:HD2	1.67	0.46
1:A:426:MET:CE	1:A:444:ILE:CD1	2.91	0.46
1:A:350:ASN:HB2	3:A:683:HOH:O	2.15	0.46
1:A:257:VAL:HG22	1:A:294:VAL:CG1	2.46	0.45
1:A:285:ARG:HD3	1:A:288:MET:CE	2.46	0.45
1:A:91:GLU:O	1:A:95:GLN:HG2	2.16	0.44
1:A:307:LEU:N	1:A:308:PRO:CD	2.81	0.44
2:B:151:LEU:O	2:B:152:LYS:CB	2.55	0.44
1:A:283:ASN:OD1	1:A:323:GLY:HA2	2.18	0.43
1:A:490:ASN:O	1:A:494:LYS:HB2	2.17	0.43
1:A:273:TRP:CD1	2:B:151:LEU:HD22	2.53	0.43
1:A:402:THR:HG21	1:A:439:VAL:CG1	2.50	0.42
1:A:207:ASP:OD1	1:A:251:GLN:NE2	2.52	0.42
1:A:402:THR:CG2	1:A:439:VAL:HG13	2.50	0.42
1:A:225:TYR:CE2	1:A:229:LEU:HD11	2.55	0.42
1:A:366:ARG:HD2	1:A:368:ASP:OD1	2.20	0.42
1:A:322:THR:HG21	2:B:121:LYS:HA	2.01	0.42
1:A:476:LEU:O	1:A:485:TYR:HB3	2.19	0.41
1:A:101:ARG:HD2	1:A:101:ARG:C	2.45	0.41
1:A:360:SER:HA	1:A:400:ALA:HA	2.02	0.41
1:A:433:ASP:HB3	1:A:436:ILE:HG22	2.01	0.41
1:A:180:GLU:HB2	1:A:225:TYR:CD1	2.55	0.41
1:A:285:ARG:HD3	1:A:288:MET:HE1	2.01	0.41
1:A:402:THR:CG2	1:A:439:VAL:HG12	2.51	0.41
1:A:301:LEU:HD23	1:A:301:LEU:HA	1.86	0.41
1:A:477:GLN:HG3	1:A:488:SER:HB2	2.02	0.41
2:B:152:LYS:HG2	2:B:155:ARG:HG3	2.03	0.41
2:B:152:LYS:CE	3:B:192:HOH:O	2.57	0.40
1:A:116:ILE:HG12	1:A:121:ILE:HD11	2.03	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)
1:A:95:GLN:OE1	3:A:679:HOH:O[3_554]	2.00	0.20

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	420/422 (100%)	400 (95%)	18 (4%)	2 (0%)	24	22
2	B	10/120 (8%)	9 (90%)	0	1 (10%)	0	0
All	All	430/542 (79%)	409 (95%)	18 (4%)	3 (1%)	18	15

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	494	LYS
1	A	484	VAL
2	B	152	LYS

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	354/354 (100%)	335 (95%)	19 (5%)	20	18
2	B	12/109 (11%)	11 (92%)	1 (8%)	10	8
All	All	366/463 (79%)	346 (94%)	20 (6%)	19	18

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

Mol	Chain	Res	Type
1	A	83	LYS
1	A	88	ASN
1	A	91	GLU

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Mol	Chain	Res	Type
1	A	95	GLN
1	A	108	LYS
1	A	152	SER
1	A	258	ARG
1	A	291	LYS
1	A	331	VAL
1	A	348	LYS
1	A	349	THR
1	A	402	THR
1	A	425	LEU
1	A	438	GLN
1	A	459	LYS
1	A	480	GLU
1	A	482	GLU
1	A	485	TYR
1	A	488	SER
2	B	118	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	95	GLN
1	A	261	HIS
1	A	346	ASN
1	A	367	GLN
1	A	477	GLN

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

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 [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	422/422 (100%)	-0.24	7 (1%) 69 71	26, 40, 91, 117	0
2	B	14/120 (11%)	1.15	5 (35%) 1 1	36, 73, 88, 88	0
All	All	436/542 (80%)	-0.19	12 (2%) 55 57	26, 40, 91, 117	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	151	LEU	3.4
2	B	118	LEU	2.8
1	A	485	TYR	2.6
2	B	121	LYS	2.6
2	B	160	ASP	2.6
1	A	88	ASN	2.6
1	A	496	PHE	2.5
1	A	476	LEU	2.5
1	A	491	LEU	2.4
2	B	119	LYS	2.4
1	A	495	TYR	2.3
1	A	107	GLU	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.