



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:26 PM UTC

PDB ID : 1AUE / pdb_00001aue
Title : FKBP-RAPAMYCIN BINDING DOMAIN (FRB) OF THE FKBP-RAPAMYCIN ASSOCIATED PROTEIN
Authors : Odagaki, Y.; Clardy, J.
Deposited on : 1997-08-25
Resolution : 2.33 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

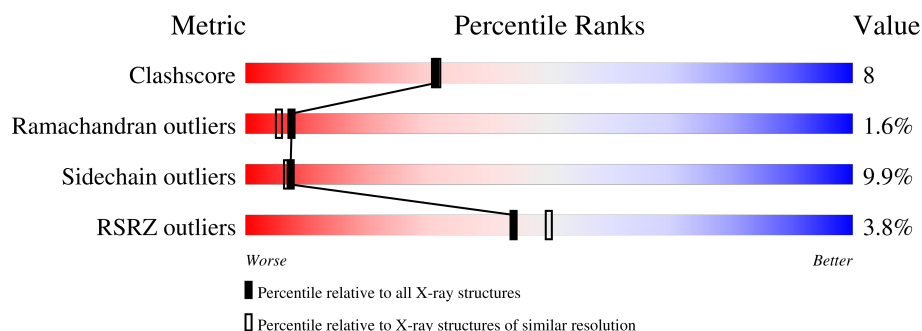
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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))
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	100	
1	B	100	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2139 atoms, of which 496 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 FKBP-RAPAMYCIN ASSOCIATED PROTEIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	92	Total	C	H	N	O	S	0	0	0
			961	497	180	138	139	7			
1	B	94	Total	C	H	N	O	S	0	0	0
			980	505	184	141	143	7			

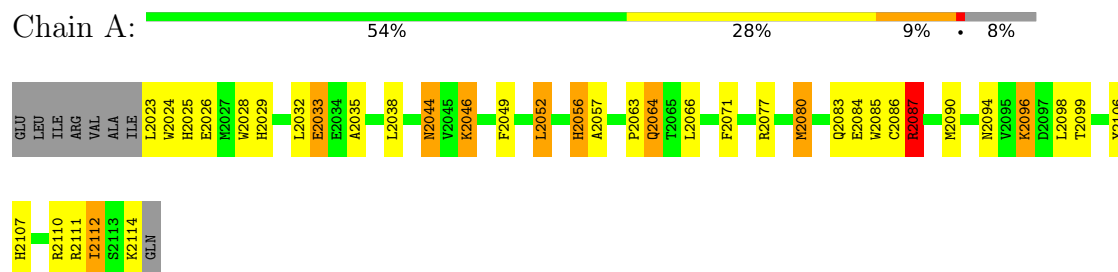
- Molecule 2 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	48	Total	H	O	0	0
			144	96	48		
2	B	18	Total	H	O	0	0
			54	36	18		

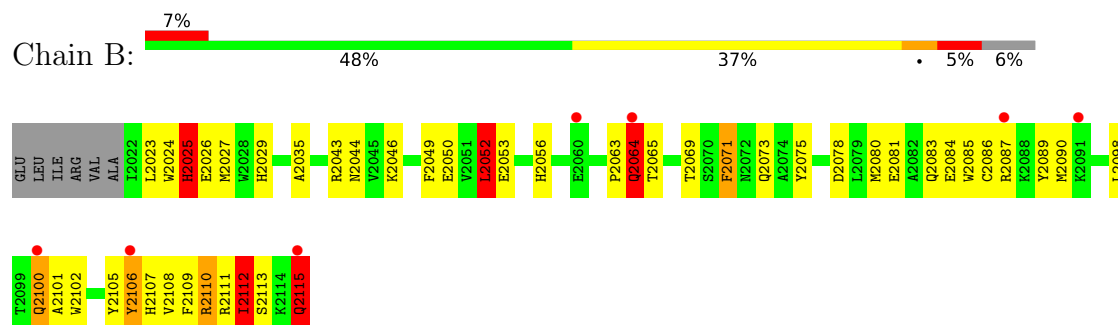
3 Residue-property plots [i](#)

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: FKBP-RAPAMYCIN ASSOCIATED PROTEIN



• Molecule 1: FKBP-RAPAMYCIN ASSOCIATED PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	29.94Å 59.21Å 123.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.33 20.00 – 2.33	Depositor EDS
% Data completeness (in resolution range)	72.1 (20.00-2.33) 71.8 (20.00-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.16 (at 2.29Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.232 , 0.339 0.242 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.645	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	2139	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.46% 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	1.34	5/803 (0.6%)	2.04	21/1078 (1.9%)
1	B	1.43	5/818 (0.6%)	2.22	38/1097 (3.5%)
All	All	1.39	10/1621 (0.6%)	2.13	59/2175 (2.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2056	HIS	CD2-NE2	-7.82	1.29	1.37
1	A	2112	ILE	CA-CB	7.24	1.64	1.54
1	A	2029	HIS	CD2-NE2	-6.87	1.30	1.37
1	B	2107	HIS	CD2-NE2	-6.77	1.30	1.37
1	B	2029	HIS	CD2-NE2	-6.51	1.30	1.37
1	A	2056	HIS	CD2-NE2	-6.43	1.30	1.37
1	B	2025	HIS	CD2-NE2	-5.79	1.31	1.37
1	B	2112	ILE	CA-CB	5.71	1.62	1.54
1	A	2107	HIS	CD2-NE2	-5.60	1.31	1.37
1	A	2107	HIS	CG-ND1	-5.52	1.32	1.38

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2064	GLN	N-CA-C	11.59	135.49	110.80
1	B	2065	THR	N-CA-C	-9.88	93.90	109.50
1	A	2052	LEU	N-CA-C	9.44	121.65	111.36
1	B	2100	GLN	CG-CD-NE2	9.00	129.90	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2096	LYS	CA-CB-CG	8.41	130.93	114.10
1	B	2110	ARG	CA-CB-CG	-8.39	97.31	114.10
1	A	2024	TRP	N-CA-C	8.24	124.96	111.37
1	B	2053	GLU	O-C-N	-8.01	113.19	120.71
1	B	2100	GLN	OE1-CD-NE2	-7.96	114.64	122.60
1	B	2063	PRO	N-CA-C	7.69	128.31	112.47
1	B	2044	ASN	CA-CB-CG	7.49	120.09	112.60
1	A	2064	GLN	N-CA-C	7.13	125.98	110.80
1	B	2056	HIS	CB-CG-CD2	-7.08	122.00	131.20
1	A	2099	THR	N-CA-C	-7.08	103.61	111.82
1	B	2115	GLN	OE1-CD-NE2	-6.90	115.70	122.60
1	B	2073	GLN	OE1-CD-NE2	-6.51	116.09	122.60
1	A	2064	GLN	O-C-N	-6.48	113.97	122.59
1	A	2044	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	B	2029	HIS	CB-CG-CD2	-6.43	122.84	131.20
1	B	2064	GLN	CA-C-O	6.40	129.66	120.51
1	A	2033	GLU	CB-CG-CD	6.37	123.43	112.60
1	B	2071	PHE	N-CA-C	-6.25	104.56	111.82
1	A	2085	TRP	CG-CD2-CE3	6.24	140.13	133.90
1	A	2046	LYS	CA-CB-CG	6.20	126.50	114.10
1	B	2113	SER	N-CA-C	-6.06	107.11	114.75
1	B	2107	HIS	CA-CB-CG	6.04	119.84	113.80
1	B	2115	GLN	CG-CD-NE2	6.03	125.45	116.40
1	A	2056	HIS	CB-CG-CD2	-5.96	123.45	131.20
1	B	2084	GLU	CB-CG-CD	5.88	122.61	112.60
1	B	2075	TYR	CA-C-N	5.88	126.63	119.99
1	B	2075	TYR	C-N-CA	5.88	126.63	119.99
1	B	2080	MET	N-CA-C	-5.80	104.33	111.40
1	A	2087	ARG	CB-CG-CD	5.78	124.59	111.30
1	B	2087	ARG	CA-CB-CG	5.68	125.47	114.10
1	B	2111	ARG	O-C-N	-5.67	115.96	122.09
1	B	2087	ARG	CB-CG-CD	5.65	124.30	111.30
1	A	2057	ALA	CA-C-O	-5.60	114.94	120.82
1	B	2106	TYR	CA-CB-CG	5.49	123.78	113.90
1	B	2056	HIS	CB-CG-ND1	5.40	130.80	122.70
1	A	2025	HIS	CB-CG-CD2	-5.38	124.21	131.20
1	B	2043	ARG	O-C-N	-5.33	116.30	122.86
1	B	2083	GLN	O-C-N	-5.32	115.32	122.23
1	A	2114	LYS	CA-CB-CG	5.27	124.64	114.10
1	A	2080	MET	CA-CB-CG	5.25	124.61	114.10
1	B	2024	TRP	CA-C-O	5.25	126.30	120.63
1	B	2084	GLU	O-C-N	-5.24	116.18	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2101	ALA	O-C-N	-5.23	116.57	122.12
1	B	2027	MET	CA-CB-CG	-5.22	103.66	114.10
1	B	2102	TRP	CG-CD2-CE3	5.22	139.12	133.90
1	A	2023	LEU	CA-C-N	5.20	128.62	120.82
1	A	2023	LEU	C-N-CA	5.20	128.62	120.82
1	B	2025	HIS	N-CA-C	-5.14	105.76	111.36
1	A	2086	CYS	CA-C-O	5.12	125.98	120.55
1	A	2063	PRO	CA-C-O	-5.07	111.37	120.60
1	B	2081	GLU	CB-CG-CD	5.07	121.23	112.60
1	B	2085	TRP	CE2-CD2-CG	-5.04	101.16	107.20
1	B	2105	TYR	CA-C-O	-5.03	115.21	120.55
1	B	2052	LEU	N-CA-C	5.03	118.57	112.23
1	A	2111	ARG	CA-C-O	-5.01	115.11	120.42

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2064	GLN	Peptide
1	B	2089	TYR	Sidechain

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	781	180	739	13	0
1	B	796	184	749	12	0
2	A	48	96	0	0	0
2	B	18	36	0	0	0
All	All	1643	496	1488	25	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 (25) 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:2094:ASN:ND2	1:A:2096:LYS:HB2	2.06	0.71
1:A:2049:PHE:HE2	1:A:2090:MET:SD	2.18	0.66
1:A:2094:ASN:HD21	1:A:2096:LYS:HB2	1.63	0.62
1:A:2028:TRP:O	1:A:2032:LEU:HB2	2.01	0.60
1:B:2025:HIS:H	1:B:2025:HIS:CD2	2.19	0.59
1:A:2056:HIS:CE1	1:A:2083:GLN:HB2	2.40	0.57
1:B:2049:PHE:HE1	1:B:2098:LEU:HD11	1.70	0.57
1:B:2086:CYS:O	1:B:2090:MET:HG3	2.07	0.54
1:B:2115:GLN:HA	1:B:2115:GLN:HE21	1.75	0.52
1:B:2035:ALA:HB2	1:B:2052:LEU:HD13	1.91	0.52
1:A:2112:ILE:O	1:A:2112:ILE:HG22	2.11	0.51
1:B:2025:HIS:H	1:B:2025:HIS:HD2	1.61	0.48
1:B:2064:GLN:HG2	1:B:2069:THR:OG1	2.14	0.47
1:B:2049:PHE:CE1	1:B:2098:LEU:HD11	2.50	0.47
1:B:2025:HIS:CD2	1:B:2025:HIS:N	2.82	0.47
1:A:2077:ARG:HA	1:A:2080:MET:HE3	1.96	0.47
1:A:2044:ASN:HD21	1:A:2046:LYS:HE2	1.80	0.47
1:B:2025:HIS:HA	1:B:2071:PHE:CE2	2.51	0.46
1:A:2028:TRP:CD1	1:A:2071:PHE:CZ	3.03	0.46
1:B:2106:TYR:HA	1:B:2109:PHE:HB3	1.99	0.44
1:A:2046:LYS:HE2	1:A:2046:LYS:HB3	1.51	0.44
1:A:2083:GLN:HG3	1:A:2087:ARG:HD3	2.01	0.43
1:B:2108:VAL:O	1:B:2112:ILE:HG12	2.18	0.43
1:A:2035:ALA:HA	1:A:2038:LEU:HD12	2.02	0.42
1:A:2106:TYR:O	1:A:2110:ARG:HG3	2.20	0.41

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	90/100 (90%)	85 (94%)	4 (4%)	1 (1%)	11 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	92/100 (92%)	84 (91%)	6 (6%)	2 (2%)	5	3
All	All	182/200 (91%)	169 (93%)	10 (6%)	3 (2%)	7	5

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2064	GLN
1	B	2023	LEU
1	B	2112	ILE

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	80/88 (91%)	73 (91%)	7 (9%)	9	9
1	B	81/88 (92%)	72 (89%)	9 (11%)	6	4
All	All	161/176 (92%)	145 (90%)	16 (10%)	7	7

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2026	GLU
1	A	2033	GLU
1	A	2052	LEU
1	A	2066	LEU
1	A	2084	GLU
1	A	2087	ARG
1	A	2098	LEU
1	B	2025	HIS
1	B	2026	GLU
1	B	2046	LYS
1	B	2050	GLU
1	B	2052	LEU
1	B	2078	ASP

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Mol	Chain	Res	Type
1	B	2100	GLN
1	B	2110	ARG
1	B	2115	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	2044	ASN
1	A	2064	GLN
1	B	2029	HIS
1	B	2083	GLN
1	B	2115	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 [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	92/100 (92%)	0.20	0	100	100	3, 9, 21, 25	0
1	B	94/100 (94%)	0.65	7 (7%)	20	25	3, 13, 26, 36	0
All	All	186/200 (93%)	0.43	7 (3%)	44	50	3, 11, 25, 36	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2091	LYS	3.2
1	B	2064	GLN	3.1
1	B	2115	GLN	2.8
1	B	2100	GLN	2.4
1	B	2106	TYR	2.3
1	B	2060	GLU	2.3
1	B	2087	ARG	2.2

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.