



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:22 pm BST

PDB ID : 1AUE
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 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 : 2.11
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) : 2.11

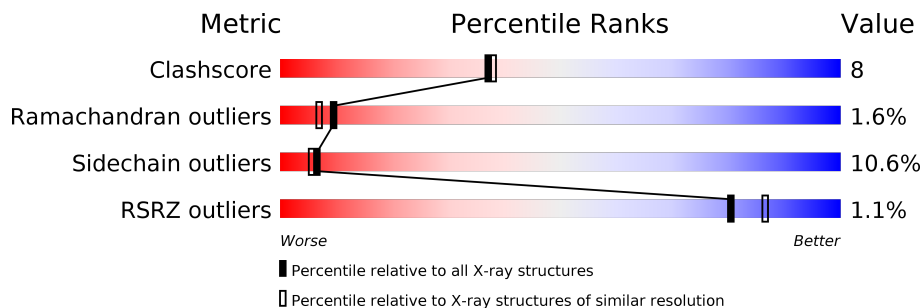
1 Overall quality at a glance

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	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (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 on 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	 59% 27% 5% • 8%
1	B	100	 2% 58% 29% 6% • 6%

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	
			Total	C	H	N	O				S
1	A	92	961	497	180	138	139	7	0	0	0
1	B	94	980	505	184	141	143	7	0	0	0

- Molecule 2 is water.

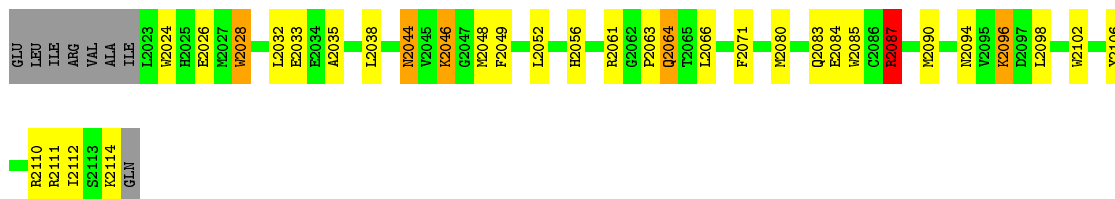
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
2	A	48	144	96	48	0	0
2	B	18	54	36	18	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

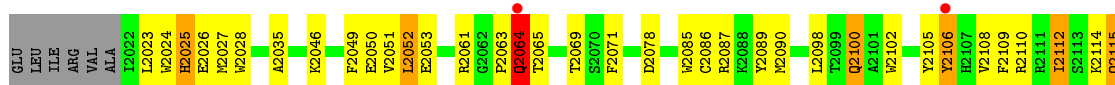
- Molecule 1: FKBP-RAPAMYCIN ASSOCIATED PROTEIN

Chain A: 



- Molecule 1: FKBP-RAPAMYCIN ASSOCIATED PROTEIN

Chain B: 



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 61.77 – 2.28	Depositor EDS
% Data completeness (in resolution range)	72.1 (20.00-2.33) 68.4 (61.77-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.16 (at 2.29Å)	Xtrriage
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	Xtrriage
Anisotropy	0.645	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 78.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 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	1.08	1/803 (0.1%)	1.81	24/1078 (2.2%)
1	B	1.19	0/818	1.93	29/1097 (2.6%)
All	All	1.14	1/1621 (0.1%)	1.87	53/2175 (2.4%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2033	GLU	CG-CD	6.27	1.61	1.51

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2087	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	B	2064	GLN	N-CA-C	9.07	135.49	111.00
1	B	2085	TRP	CD1-CG-CD2	8.69	113.25	106.30
1	A	2096	LYS	CA-CB-CG	7.97	130.93	113.40
1	A	2061	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	B	2028	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	B	2085	TRP	CE2-CD2-CG	-7.68	101.16	107.30
1	B	2105	TYR	CB-CG-CD2	-7.59	116.45	121.00
1	A	2111	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	B	2028	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	B	2110	ARG	CA-CB-CG	-7.31	97.31	113.40
1	A	2085	TRP	CD1-CG-CD2	7.10	111.98	106.30
1	B	2110	ARG	NE-CZ-NH2	-7.08	116.76	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2102	TRP	CE2-CD2-CG	-6.98	101.72	107.30
1	A	2028	TRP	CE2-CD2-CG	-6.96	101.73	107.30
1	B	2024	TRP	CE2-CD2-CG	-6.93	101.76	107.30
1	A	2085	TRP	CG-CD2-CE3	6.93	140.13	133.90
1	B	2102	TRP	CD1-CG-CD2	6.92	111.83	106.30
1	B	2064	GLN	CA-C-N	-6.75	102.35	117.20
1	A	2111	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	A	2085	TRP	CE2-CD2-CG	-6.70	101.94	107.30
1	A	2080	MET	CA-CB-CG	6.65	124.61	113.30
1	B	2102	TRP	CE2-CD2-CG	-6.59	102.03	107.30
1	A	2061	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	A	2024	TRP	CD1-CG-CD2	6.41	111.42	106.30
1	A	2102	TRP	CD1-CG-CD2	6.36	111.39	106.30
1	A	2028	TRP	CD1-CG-CD2	6.35	111.38	106.30
1	B	2065	THR	N-CA-C	-6.33	93.90	111.00
1	B	2024	TRP	CD1-CG-CD2	6.29	111.33	106.30
1	B	2110	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	B	2063	PRO	N-CA-C	6.24	128.31	112.10
1	A	2063	PRO	CA-C-N	6.19	130.82	117.20
1	A	2024	TRP	CE2-CD2-CG	-5.97	102.52	107.30
1	A	2046	LYS	CA-CB-CG	5.95	126.50	113.40
1	B	2102	TRP	CG-CD2-CE3	5.80	139.12	133.90
1	B	2027	MET	CA-CB-CG	-5.67	103.66	113.30
1	B	2061	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	2085	TRP	CB-CG-CD1	-5.62	119.69	127.00
1	B	2085	TRP	CG-CD1-NE1	-5.59	104.50	110.10
1	A	2064	GLN	N-CA-C	5.55	125.98	111.00
1	B	2051	VAL	CG1-CB-CG2	-5.50	102.09	110.90
1	B	2100	GLN	CG-CD-NE2	5.50	129.90	116.70
1	B	2087	ARG	CA-CB-CG	5.49	125.47	113.40
1	B	2028	TRP	CG-CD2-CE3	5.46	138.82	133.90
1	B	2106	TYR	CA-CB-CG	5.46	123.78	113.40
1	A	2064	GLN	O-C-N	-5.46	113.97	122.70
1	B	2085	TRP	CG-CD2-CE3	5.42	138.78	133.90
1	A	2024	TRP	N-CA-C	5.17	124.96	111.00
1	B	2102	TRP	CB-CG-CD1	-5.14	120.31	127.00
1	A	2114	LYS	CA-CB-CG	5.11	124.64	113.40
1	A	2064	GLN	CA-C-N	5.10	128.42	117.20
1	B	2106	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	B	2114	LYS	N-CA-C	-5.01	97.47	111.00

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	12	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	24	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 (24) 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:CD2	1:B:2025:HIS:H	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:HE21	1:B:2115:GLN:HA	1.75	0.52
1:B:2035:ALA:HB2	1:B:2052:LEU:HD13	1.91	0.52
1:A:2112:ILE:HG22	1:A:2112:ILE:O	2.11	0.51
1:B:2025:HIS:HD2	1:B:2025:HIS:H	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:N	1:B:2025:HIS:CD2	2.82	0.47
1:A:2044:ASN:HD21	1:A:2046:LYS:HE2	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	14	13
1	B	92/100 (92%)	84 (91%)	6 (6%)	2 (2%)	6	4
All	All	182/200 (91%)	169 (93%)	10 (6%)	3 (2%)	9	7

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%)	72 (90%)	8 (10%)	7	6
1	B	81/88 (92%)	72 (89%)	9 (11%)	6	5
All	All	161/176 (92%)	144 (89%)	17 (11%)	6	5

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

Mol	Chain	Res	Type
1	A	2026	GLU
1	A	2044	ASN
1	A	2048	MET
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	2053	GLU
1	B	2078	ASP
1	B	2100	GLN
1	B	2115	GLN

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

Mol	Chain	Res	Type
1	A	2044	ASN
1	A	2064	GLN
1	A	2072	ASN
1	A	2094	ASN
1	B	2029	HIS
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 carbohydrates 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%)	-0.24	0 100 100	3, 11, 26, 36	0
1	B	94/100 (94%)	0.05	2 (2%) 63 73	4, 16, 36, 44	0
All	All	186/200 (93%)	-0.10	2 (1%) 80 86	3, 13, 33, 44	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2106	TYR	3.1
1	B	2064	GLN	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 carbohydrates 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.