wwPDB X-ray Structure Validation Summary Report (i)

Mar 1, 2026 – 05:09 AM UTC

PDB ID	:	3JYM / pdb_00003jym
Title	:	Crystal Structure of the 3 FKBP domains of wheat FKBP73
Authors	:	Dym, O.; Breiman, A.; Israel Structural Proteomics Center (ISPC)
Deposited on	:	2009-09-22
Resolution	:	2.28 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

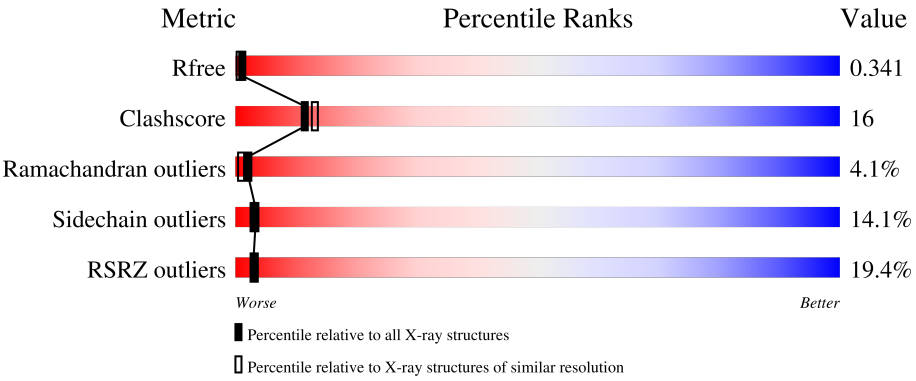
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	377	16% 33% 33% 11% · 20%
1	B	377	15% 41% 29% 8% · 18%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4726 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 FK506-binding protein (FKBP) from wheat.

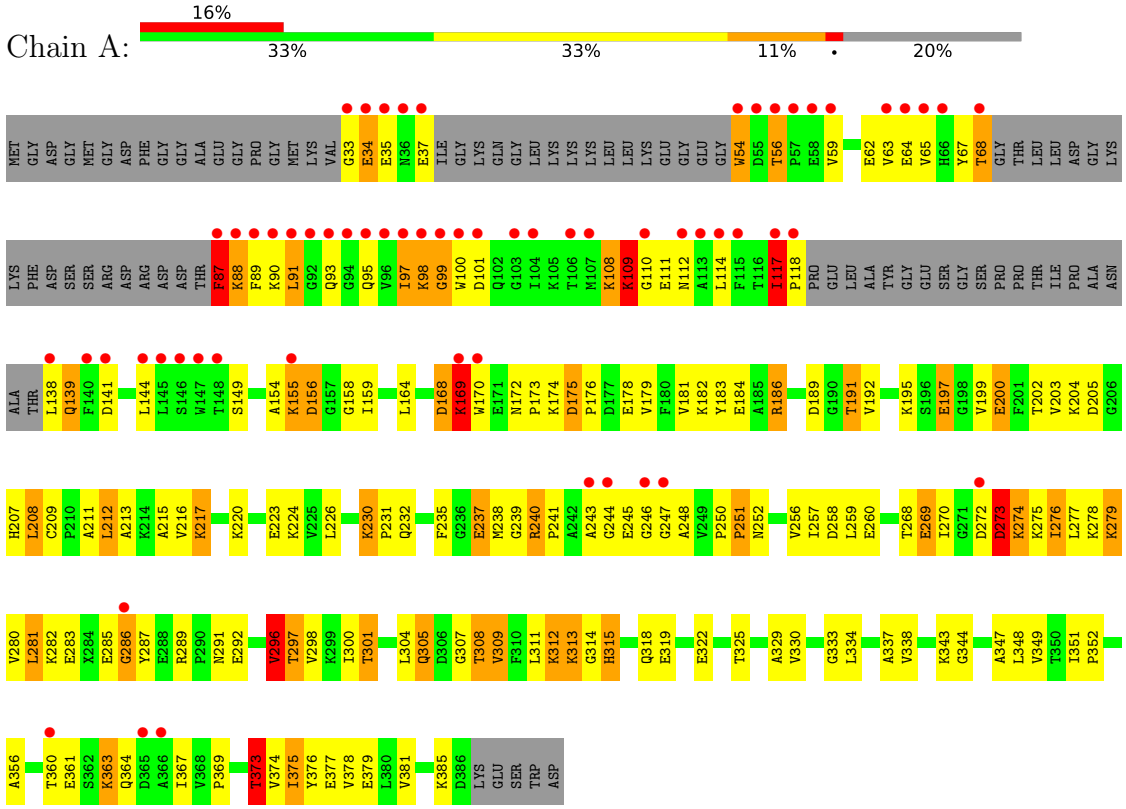
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2344	1501	378	460	5			
1	B	308	Total	C	N	O	S	0	0	0
			2382	1523	385	469	5			

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.

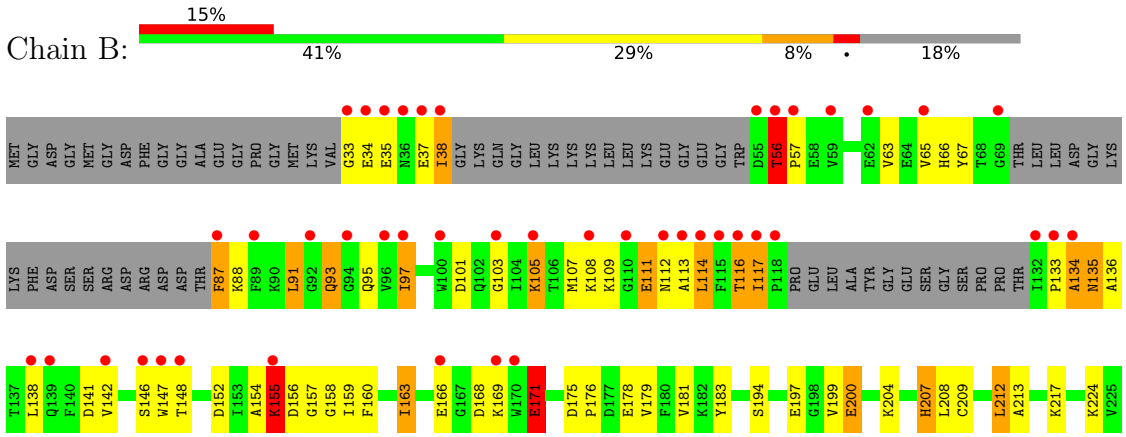
• Molecule 1: FK506-binding protein (FKBP) from wheat

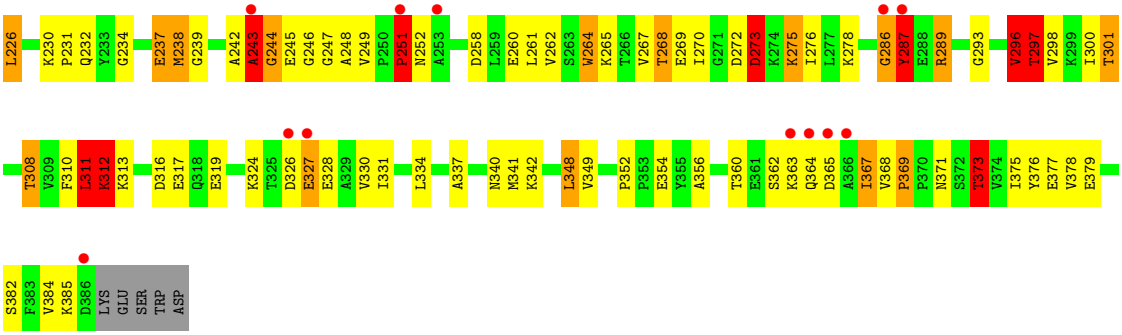
Chain A:



• Molecule 1: FK506-binding protein (FKBP) from wheat

Chain B:




L226 K230 P231 Q232 Y233 G234 E237 M238 G239 A242 A243 G244 E245 G246 G247 A248 V249 P250 P251 N252 A253 D258 L259 E260 L261 V262 S263 W264 K265 T266 V267 T268 E269 I270 G271 D272 D273 K274 K275 I276 L277 K278 G286 Y287 E288 R289 G293 V296 T297 V298 K299 I300 T301
T308 V309 F310 L311 K312 K313 D316 E317 Q318 E319 K324 T325 D326 E327 E328 A329 V330 I331 L334 A337 N340 M341 K342 L348 V349 P352 P353 E354 Y355 A356 T360 E361 S362 K363 Q364 D365 A366 I367 V368 P369 P370 N371 S372 T373 V374 I375 Y376 E377 V378 E379
S382 F383 V384 K385 D386 LYS GLU SER TRP ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	186.96Å 31.01Å 68.98Å 90.00° 93.59° 90.00°	Depositor
Resolution (Å)	46.63 – 2.28 46.63 – 2.28	Depositor EDS
% Data completeness (in resolution range)	98.6 (46.63-2.28) 98.6 (46.63-2.28)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	5.97 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.270 , 0.343 0.271 , 0.341	Depositor DCC
R_{free} test set	1834 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 32.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	4726	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% 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

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	2.08	83/2382 (3.5%)	1.65	49/3210 (1.5%)
1	B	1.89	52/2419 (2.1%)	1.61	34/3261 (1.0%)
All	All	1.99	135/4801 (2.8%)	1.63	83/6471 (1.3%)

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	A	1	1
1	B	0	4
All	All	1	5

The worst 5 of 135 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	369	PRO	CA-C	9.56	1.57	1.51
1	A	337	ALA	C-O	-9.48	1.13	1.24
1	A	312	LYS	C-O	-9.48	1.13	1.24
1	A	374	VAL	C-O	-9.24	1.14	1.24
1	A	174	LYS	CA-C	-8.72	1.41	1.52

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	247	GLY	N-CA-C	-10.67	92.80	111.46
1	B	230	LYS	CA-C-N	9.38	130.01	119.32
1	B	230	LYS	C-N-CA	9.38	130.01	119.32
1	A	230	LYS	CA-C-N	8.60	130.59	119.84
1	A	230	LYS	C-N-CA	8.60	130.59	119.84

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	268	THR	CB

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	245	GLU	Peptide
1	B	155	LYS	Peptide
1	B	243	ALA	Peptide
1	B	286	GLY	Peptide
1	B	87	PHE	Peptide

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	2344	0	2347	64	0
1	B	2382	0	2392	88	0
All	All	4726	0	4739	152	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 16.

The worst 5 of 152 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:273:ASP:OD1	1:A:275:LYS:HD2	1.27	1.33
1:B:273:ASP:OD1	1:B:275:LYS:CD	1.90	1.18
1:B:273:ASP:OD1	1:B:275:LYS:HD2	0.93	1.10
1:B:243:ALA:HB1	1:B:244:GLY:HA3	1.11	1.06
1:A:65:VAL:O	1:A:87:PHE:N	2.00	0.94

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	292/377 (78%)	261 (89%)	17 (6%)	14 (5%)	2 1
1	B	299/377 (79%)	266 (89%)	23 (8%)	10 (3%)	3 1
All	All	591/754 (78%)	527 (89%)	40 (7%)	24 (4%)	2 1

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	LYS
1	A	246	GLY
1	B	134	ALA
1	B	135	ASN
1	B	287	TYR

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	254/311 (82%)	221 (87%)	33 (13%)	4 4
1	B	258/311 (83%)	219 (85%)	39 (15%)	3 2
All	All	512/622 (82%)	440 (86%)	72 (14%)	3 3

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	268	THR

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Mol	Chain	Res	Type
1	B	385	LYS
1	B	296	VAL
1	B	328	GLU
1	A	296	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	232	GLN
1	B	207	HIS
1	A	315	HIS
1	A	232	GLN
1	B	172	ASN

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

6.1 Protein, DNA and RNA chains

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	300/377 (79%)	0.88	62 (20%)	2 3	8, 26, 67, 81	0
1	B	307/377 (81%)	0.91	56 (18%)	3 4	11, 30, 61, 80	0
All	All	607/754 (80%)	0.89	118 (19%)	3 3	8, 28, 63, 81	0

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	TRP	9.3
1	A	54	TRP	7.2
1	A	59	VAL	6.9
1	B	38	ILE	6.5
1	B	33	GLY	6.4

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.