



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 02:15 AM GMT

PDB ID : 4JFI
Title : Increasing the Efficiency of Ligands for the FK506-Binding Protein 51 by Conformational Control: Complex of FKBP51 with compound 1-[(9S,13R,13aR)-1,3-dimethoxy-8-oxo-5,8,9,10,11,12,13,13a-octahydro-6H-9,13-epiminoazocino[2,1-a]isoquinolin-14-yl]-2-(3,4,5-trimethoxyphenyl)ethane-1,2-dione
Authors : Wang, Y.; Kirschner, A.; Fabian, A.; Gopalakrishnan, R.; Kress, C.; Hoogeland, B.; Koch, U.; Kozany, C.; Bracher, A.; Hausch, F.
Deposited on : 2013-02-28
Resolution : 1.05 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

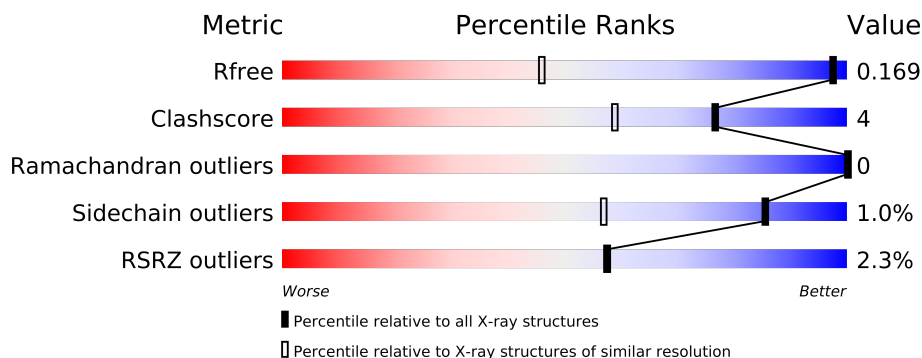
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.05 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}	66092	1012 (1.14-0.98)
Clashscore	79885	1122 (1.14-0.98)
Ramachandran outliers	78287	1057 (1.14-0.98)
Sidechain outliers	78261	1055 (1.14-0.98)
RSRZ outliers	66119	1012 (1.14-0.98)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	127	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	1KT	A	201	-	X
3	DMS	A	202[A]	-	X
3	DMS	A	202[B]	-	X
4	GOL	A	203	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 1273 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

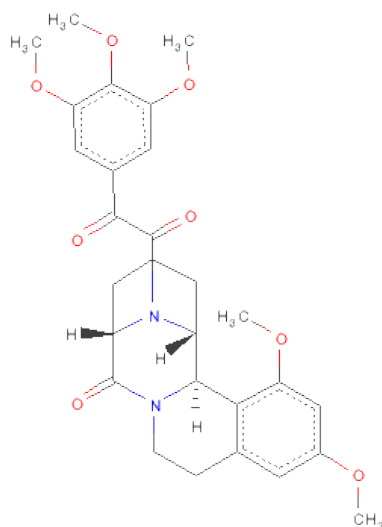
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	127	1014	645	170	195	4	0	7	0

There are 4 discrepancies between the modelled and reference sequences:

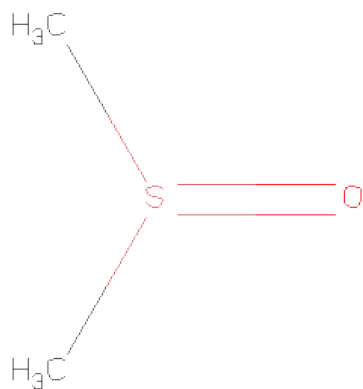
Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	-	EXPRESSION TAG	UNP Q13451
A	14	ALA	-	EXPRESSION TAG	UNP Q13451
A	15	PRO	-	EXPRESSION TAG	UNP Q13451
A	19	THR	ALA	ENGINEERED MUTATION	UNP Q13451

- Molecule 2 is 1-[(9S,13R,13AR)-1,3-DIMETHOXY-8-OXO-5,8,9,10,11,12,13,13A-OCTAHYDRO-6H-9,13-EPIMINOAZOCINO[2,1-A]ISOQUINOLIN-14-YL]-2-(3,4,5-TRIMETHOXYPHENYL)ETHANE-1,2-DIONE (three-letter code: 1KT) (formula: C₂₈H₃₂N₂O₈).



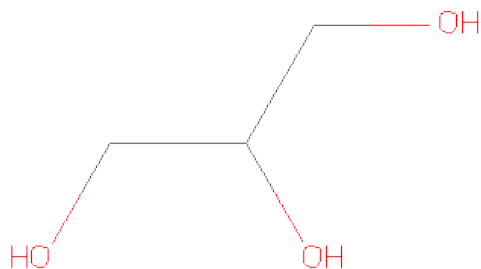
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			38	28	2	8		

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	1
			8	4	2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	198	Total	O	0	9
			207	207		

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- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP5

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	42.05Å 54.19Å 55.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.05 19.68 – 1.05	Depositor EDS
% Data completeness (in resolution range)	95.2 (20.00-1.05) 95.2 (19.68-1.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 1.05Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.137 , 0.158 0.146 , 0.169	Depositor DCC
R_{free} test set	2871 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	8.7	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 79.0	EDS
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 57435 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	1273	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, DMS, 1KT

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	1.11	3/1034 (0.3%)	1.02	3/1391 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	ARG	CG-CD	-5.95	1.37	1.51
1	A	138	LYS	C-O	-5.83	1.12	1.23
1	A	101	GLU	CD-OE2	-5.55	1.19	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	LEU	CB-CG-CD2	8.12	124.81	111.00
1	A	31	ARG	CG-CD-NE	6.42	125.29	111.80
1	A	31	ARG	CB-CG-CD	5.02	124.66	111.60

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1014	0	0	4	0
2	A	38	0	0	0	0
3	A	8	0	0	0	0
4	A	6	0	0	0	0
5	A	207	0	0	4	0
All	All	1273	0	0	4	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (4) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:88[A]:LYS:CD	5:A:490:HOH:O	1.83	1.25
1:A:136:ASP:OD1	5:A:471[A]:HOH:O	1.99	0.79
1:A:78:VAL:O	5:A:474:HOH:O	2.03	0.77
1:A:98[A]:LYS:NZ	5:A:486[A]:HOH:O	2.45	0.50

There are no symmetry-related clashes.

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	132/127 (104%)	130 (98%)	2 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	108/105 (103%)	107 (99%)	1 (1%)	87 61

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	1KT	A	201	-	42,42,42	1.54	4 (9%)	62,62,62	1.53	9 (14%)
3	DMS	A	202[A]	-	3,3,3	0.59	0	3,3,3	0.49	0
3	DMS	A	202[B]	-	3,3,3	2.39	1 (33%)	3,3,3	1.14	0
4	GOL	A	203	-	5,5,5	0.83	0	5,5,5	2.08	3 (60%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1KT	A	201	-	-	0/22/61/61	0/1/5/5
3	DMS	A	202[A]	-	-	0/0/0/0	0/0/0/0
3	DMS	A	202[B]	-	-	0/0/0/0	0/0/0/0
4	GOL	A	203	-	-	0/4/4/4	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	1KT	C12-C11	-5.69	1.41	1.51
2	A	201	1KT	C9-C8	4.79	1.60	1.51
3	A	202[B]	DMS	O-S	4.05	1.77	1.50
2	A	201	1KT	O4-C18	2.29	1.28	1.23
2	A	201	1KT	O1-C26	2.13	1.49	1.42

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	1KT	C8-C9-N10	-7.29	99.57	109.54
4	A	203	GOL	C3-C2-C1	2.75	123.39	111.26
2	A	201	1KT	O4-C18-N17	-2.62	120.28	124.34
2	A	201	1KT	C25-C20-C21	2.62	122.90	119.64
2	A	201	1KT	C20-C21-C22	-2.46	116.19	119.63
4	A	203	GOL	O3-C3-C2	-2.37	98.16	109.71
4	A	203	GOL	O1-C1-C2	2.33	121.10	109.71
2	A	201	1KT	C13-C12-C11	-2.30	110.30	112.47
2	A	201	1KT	O4-C18-C19	2.18	120.47	116.85
2	A	201	1KT	O8-C24-C23	2.14	119.04	115.31
2	A	201	1KT	C16-N17-C18	2.06	124.71	119.20
2	A	201	1KT	C9-N10-C11	2.03	121.79	119.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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	127/127 (100%)	-0.38	3 (2%) 56 55	6, 9, 19, 30	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	GLY	4.1
1	A	120	PRO	2.9
1	A	119	LEU	2.7

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 carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	DMS	A	202[A]	4/4	0.11	6.90	8,11,14,18	4
3	DMS	A	202[B]	4/4	0.11	6.90	12,15,20,21	4

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	GOL	A	203	6/6	0.20	5.01	19,31,35,46	0
2	1KT	A	201	38/38	0.14	2.00	11,17,31,44	0

6.5 Other polymers ⓘ

There are no such residues in this entry.