Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:16 pm BST

PDB ID	:	1OSY
Title	:	Crystal structure of FIP-Fve fungal immunomodulatory protein
Authors	:	Palasingam, P.; Joseph, J.S.; Seow, S.V.; Shai, V.; Robinson, H.; Chua, K.Y.; Kolatkar, P.R.
Deposited on	:	2003-03-20
Resolution	:	1.70 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:

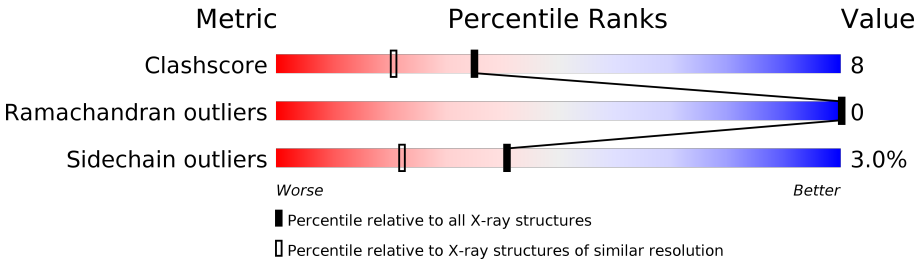
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.70 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	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	115	86% 12% •
1	B	115	89% 8% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BR	A	1001	-	-	X	-
2	BR	A	1010	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1940 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 IMMUNOMODULATORY PROTEIN FIP-FVE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	115	Total	C	N	O	0	0	0
			901	583	142	176			
1	B	113	Total	C	N	O	0	0	0
			887	574	139	174			

- Molecule 2 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	7	Total	Br	0	0
			7	7		
2	A	9	Total	Br	0	0
			9	9		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	61	Total	O	0	0
			61	61		
3	B	75	Total	O	0	0
			75	75		

3 Residue-property plots (i)

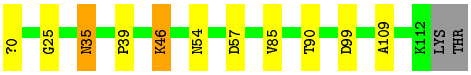
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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: IMMUNOMODULATORY PROTEIN FIP-FVE

Chain A:

- Molecule 1: IMMUNOMODULATORY PROTEIN FIP-FVE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	97.12Å 97.12Å 61.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.02 – 1.70 29.97 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.02-1.70) 98.8 (29.97-1.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	18.77 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.182 , 0.210 0.266 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	13.6	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	1940	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 4.94% 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

Bond lengths and bond angles in the following residue types are not validated in this section: BR, ACE

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	0.54	1/921 (0.1%)	0.85	4/1255 (0.3%)
1	B	0.53	0/907	0.83	3/1237 (0.2%)
All	All	0.53	1/1828 (0.1%)	0.84	7/2492 (0.3%)

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	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	0	ACE	C-N	6.13	1.48	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	0	ACE	O-C-N	-9.69	107.20	122.70
1	B	57	ASP	CB-CG-OD2	6.91	124.52	118.30
1	B	99	ASP	CB-CG-OD2	6.61	124.25	118.30
1	A	99	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	44	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	87	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	0	ACE	O-C-N	-5.38	114.09	122.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	43	THR	CB

There are no planarity outliers.

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	901	0	882	16	0
1	B	887	0	867	9	0
2	A	9	0	0	7	0
2	B	7	0	0	4	0
3	A	61	0	0	5	0
3	B	75	0	0	2	0
All	All	1940	0	1749	29	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 (29) 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:81:LYS:HE3	2:A:1001:BR:BR	1.80	1.35
1:A:81:LYS:CE	2:A:1001:BR:BR	2.37	1.26
1:A:81:LYS:HE2	2:A:1001:BR:BR	2.14	0.96
1:A:63:ASN:HB2	3:A:1069:HOH:O	1.68	0.93
2:B:1012:BR:BR	3:B:1056:HOH:O	2.49	0.84
2:A:1001:BR:BR	2:A:1007:BR:BR	3.09	0.80
1:B:46:LYS:HD3	1:B:46:LYS:N	1.98	0.79
1:A:12:LEU:HD22	3:A:1076:HOH:O	1.85	0.77
2:B:1014:BR:BR	3:B:1066:HOH:O	2.62	0.71
1:A:100:THR:O	1:A:103:SER:OG	2.14	0.65
1:A:63:ASN:HD21	1:A:78:GLN:NE2	1.95	0.64
2:A:1010:BR:BR	3:A:1031:HOH:O	2.71	0.62
1:B:46:LYS:CD	1:B:46:LYS:N	2.65	0.58
1:B:46:LYS:HD3	1:B:46:LYS:H	1.67	0.57
1:A:54:ASN:ND2	1:A:90:THR:H	2.05	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LYS:CD	1:B:46:LYS:H	2.22	0.53
1:B:54:ASN:ND2	1:B:90:THR:H	2.06	0.53
1:A:63:ASN:HD21	1:A:78:GLN:HE22	1.58	0.49
2:A:1010:BR:BR	1:B:109:ALA:HA	2.69	0.47
1:B:39:PRO:HG3	2:B:1009:BR:BR	2.69	0.47
1:B:25:GLY:HA3	1:B:35:ASN:HD21	1.81	0.46
1:A:81:LYS:HD2	3:A:1018:HOH:O	2.15	0.46
1:A:63:ASN:ND2	1:A:78:GLN:HE22	2.13	0.45
1:A:100:THR:CG2	1:A:104:GLU:H	2.31	0.44
1:A:26:ARG:HD2	2:A:1003:BR:BR	2.74	0.43
1:B:85:VAL:HA	2:B:1011:BR:BR	2.74	0.42
1:A:63:ASN:CB	3:A:1069:HOH:O	2.47	0.41
1:A:63:ASN:O	1:A:63:ASN:ND2	2.53	0.41
1:A:63:ASN:HD22	1:A:63:ASN:N	2.19	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	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
1	B	111/115 (96%)	107 (96%)	4 (4%)	0	100	100
All	All	224/230 (97%)	216 (96%)	8 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	99/100 (99%)	95 (96%)	4 (4%)	31 13
1	B	98/100 (98%)	96 (98%)	2 (2%)	55 38
All	All	197/200 (98%)	191 (97%)	6 (3%)	41 22

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	45	LYS
1	A	63	ASN
1	A	100	THR
1	B	35	ASN
1	B	46	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	63	ASN
1	A	72	GLN
1	A	80	ASN
1	A	92	GLN
1	B	35	ASN
1	B	54	ASN
1	B	72	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

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.