Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 01:13 AM EDT

PDB ID	:	5W5H
Title	:	Human IFIT1 dimer with m7Gppp-AAAA
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Deposited on	:	2017-06-15
Resolution	:	2.79 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 (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 (i)) were used in the production of this report:

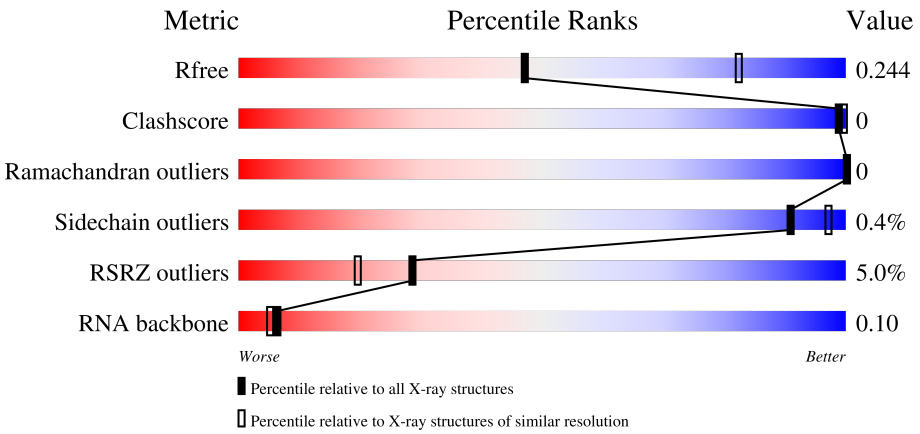
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.79 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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	479	3% 94% 6%
1	C	479	6% 91% • 7%
2	B	4	100%
2	D	4	100%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15229 atoms, of which 7543 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 Interferon-induced protein with tetratricopeptide repeats 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	451	7387	2343	3704	640	680	20	0	0	0
1	C	446	7311	2321	3667	630	673	20	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P09914
C	0	SER	-	expression tag	UNP P09914

- Molecule 2 is a RNA chain called RNA (5'-D(*(GTA))-R(P*AP*AP*A)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
2	B	4	254	72	86	35	52	9	0	1	0
2	D	4	254	72	86	35	52	9	0	1	0

- Molecule 3 is water.

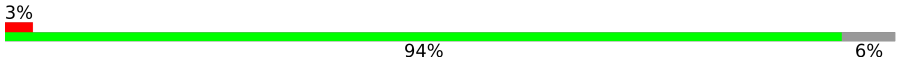
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	10	10	10	0	0
3	B	3	3	3	0	0
3	C	5	5	5	0	0
3	D	5	5	5	0	0

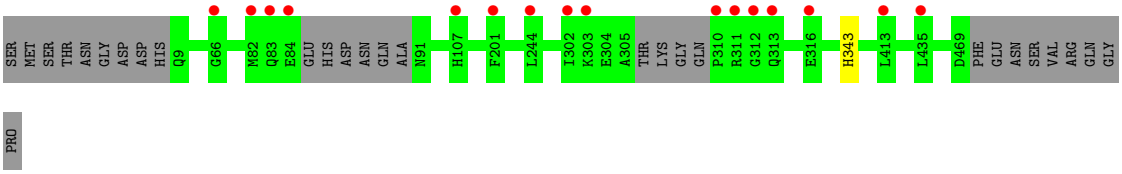
3 Residue-property plots (i)

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: Interferon-induced protein with tetratricopeptide repeats 1

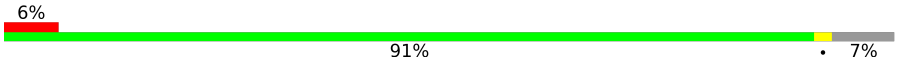
Chain A:

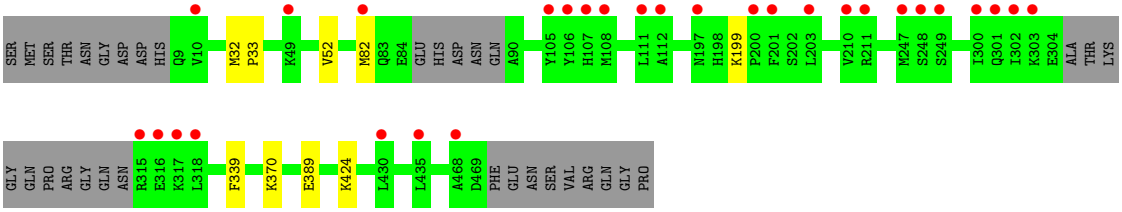




• Molecule 1: Interferon-induced protein with tetratricopeptide repeats 1

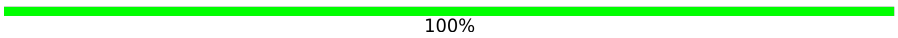
Chain C:





• Molecule 2: RNA (5'-D(*(GTA))-R(P*AP*AP*A)-3')

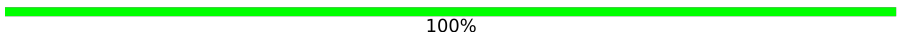
Chain B:



There are no outlier residues recorded for this chain.

• Molecule 2: RNA (5'-D(*(GTA))-R(P*AP*AP*A)-3')

Chain D:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	184.35Å 184.35Å 88.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.01 – 2.79 42.01 – 2.79	Depositor EDS
% Data completeness (in resolution range)	87.4 (42.01-2.79) 87.4 (42.01-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.24 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.10_2142: ???)	Depositor
R, R_{free}	0.219 , 0.241 0.219 , 0.244	Depositor DCC
R_{free} test set	1637 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	45.9	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 22.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	15229	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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 (i)

5.1 Standard geometry (i)

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

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	0.24	0/3751	0.37	0/5036
1	C	0.26	1/3711 (0.0%)	0.37	0/4983
2	B	0.21	0/74	0.63	0/113
2	D	0.21	0/74	0.66	0/113
All	All	0.25	1/7610 (0.0%)	0.38	0/10245

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	199	LYS	C-N	5.59	1.44	1.34

There are no bond angle outliers.

There are no chirality outliers.

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	3683	3704	3703	0	0
1	C	3644	3667	3665	6	0
2	B	168	86	86	0	0
2	D	168	86	86	0	0
3	A	10	0	0	0	0
3	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	5	0	0	0	0
3	D	5	0	0	0	0
All	All	7686	7543	7540	6	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 0.

All (6) 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:C:52:VAL:HG11	1:C:82:MET:HE1	1.82	0.62
1:C:52:VAL:HG21	1:C:82:MET:HE2	1.89	0.53
1:C:52:VAL:HG21	1:C:82:MET:CE	2.41	0.50
1:C:389:GLU:OE2	1:C:424:LYS:NZ	2.49	0.41
1:C:32:MET:HB2	1:C:33:PRO:HD3	2.03	0.41
1:C:52:VAL:CG2	1:C:82:MET:HE2	2.51	0.40

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	445/479 (93%)	441 (99%)	4 (1%)	0	100 100
1	C	440/479 (92%)	431 (98%)	9 (2%)	0	100 100
All	All	885/958 (92%)	872 (98%)	13 (2%)	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	394/418 (94%)	393 (100%)	1 (0%)	92	98
1	C	390/418 (93%)	388 (100%)	2 (0%)	88	96
All	All	784/836 (94%)	781 (100%)	3 (0%)	91	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	343	HIS
1	C	339	PHE
1	C	370	LYS

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

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	2/4 (50%)	0	0
2	D	2/4 (50%)	0	0
All	All	4/8 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 monosaccharides 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	451/479 (94%)	0.34	16 (3%) 44 34	17, 46, 77, 103	0
1	C	446/479 (93%)	0.46	29 (6%) 18 11	21, 55, 82, 112	0
2	B	3/4 (75%)	0.26	0 100 100	30, 30, 31, 42	0
2	D	3/4 (75%)	0.06	0 100 100	38, 38, 42, 52	0
All	All	903/966 (93%)	0.40	45 (4%) 28 19	17, 50, 81, 112	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	313	GLN	6.1
1	C	315	ARG	5.2
1	C	201	PHE	4.9
1	A	84	GLU	4.4
1	C	302	ILE	4.2
1	C	82	MET	3.9
1	C	303	LYS	3.8
1	A	311	ARG	3.7
1	C	435	LEU	3.6
1	C	210	VAL	3.6
1	A	66	GLY	3.5
1	C	111	LEU	3.5
1	A	302	ILE	3.4
1	A	310	PRO	3.3
1	A	303	LYS	3.3
1	C	249	SER	3.2
1	C	316	GLU	3.2
1	C	317	LYS	3.2
1	A	201	PHE	3.0
1	C	468	ALA	3.0
1	C	318	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	247	MET	3.0
1	C	248	SER	2.9
1	A	435	LEU	2.9
1	C	49	LYS	2.8
1	C	108	MET	2.7
1	A	316	GLU	2.7
1	C	107	HIS	2.6
1	A	312	GLY	2.5
1	C	197	ASN	2.5
1	A	413	LEU	2.4
1	C	200	PRO	2.4
1	A	82	MET	2.3
1	A	244	LEU	2.3
1	C	300	ILE	2.3
1	C	105	TYR	2.3
1	C	10	VAL	2.3
1	A	107	HIS	2.3
1	C	211	ARG	2.3
1	A	83	GLN	2.2
1	C	301	GLN	2.2
1	C	106	TYR	2.1
1	C	430	LEU	2.0
1	C	203	LEU	2.0
1	C	112	ALA	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 monosaccharides 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.