



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 01:01 PM BST

PDB ID : 4HJX  
Title : Crystal structure of F2YRS complexed with F2Y  
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Deposited on : 2012-10-14  
Resolution : 2.91 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](mailto: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.

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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 : 2.13.1  
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) : 2.13.1

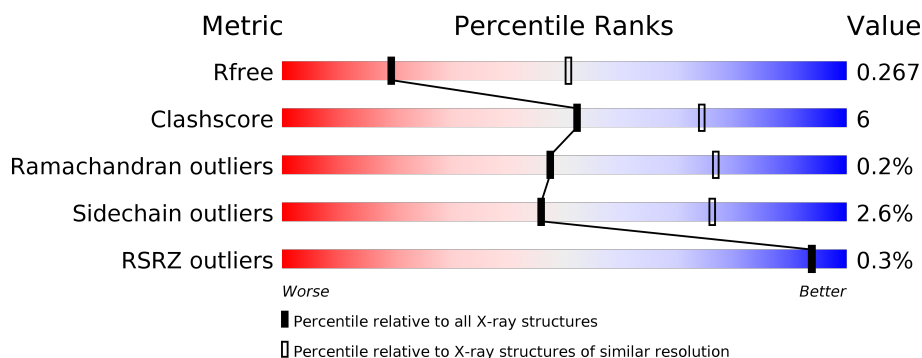
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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  $\geq 3$ , 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	314	
1	B	314	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4977 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 Tyrosine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2443	1556	415	458	14			
1	B	306	Total	C	N	O	S	0	0	0
			2440	1555	414	457	14			

There are 30 discrepancies between the modelled and reference sequences:

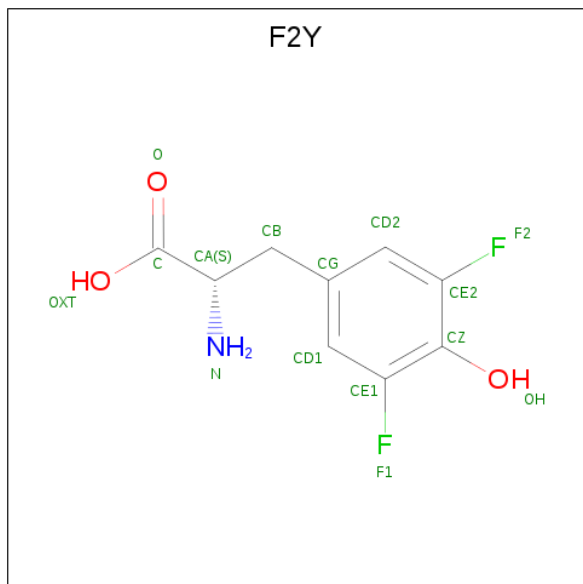
Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ARG	TYR	ENGINEERED MUTATION	UNP Q57834
A	65	TYR	LEU	ENGINEERED MUTATION	UNP Q57834
A	70	GLY	HIS	ENGINEERED MUTATION	UNP Q57834
A	108	ASN	PHE	ENGINEERED MUTATION	UNP Q57834
A	109	CYS	GLN	ENGINEERED MUTATION	UNP Q57834
A	158	ASN	ASP	ENGINEERED MUTATION	UNP Q57834
A	162	SER	LEU	ENGINEERED MUTATION	UNP Q57834
A	307	LEU	-	EXPRESSION TAG	UNP Q57834
A	308	GLU	-	EXPRESSION TAG	UNP Q57834
A	309	HIS	-	EXPRESSION TAG	UNP Q57834
A	310	HIS	-	EXPRESSION TAG	UNP Q57834
A	311	HIS	-	EXPRESSION TAG	UNP Q57834
A	312	HIS	-	EXPRESSION TAG	UNP Q57834
A	313	HIS	-	EXPRESSION TAG	UNP Q57834
A	314	HIS	-	EXPRESSION TAG	UNP Q57834
B	32	ARG	TYR	ENGINEERED MUTATION	UNP Q57834
B	65	TYR	LEU	ENGINEERED MUTATION	UNP Q57834
B	70	GLY	HIS	ENGINEERED MUTATION	UNP Q57834
B	108	ASN	PHE	ENGINEERED MUTATION	UNP Q57834
B	109	CYS	GLN	ENGINEERED MUTATION	UNP Q57834
B	158	ASN	ASP	ENGINEERED MUTATION	UNP Q57834
B	162	SER	LEU	ENGINEERED MUTATION	UNP Q57834
B	307	LEU	-	EXPRESSION TAG	UNP Q57834
B	308	GLU	-	EXPRESSION TAG	UNP Q57834
B	309	HIS	-	EXPRESSION TAG	UNP Q57834

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Chain	Residue	Modelled	Actual	Comment	Reference
B	310	HIS	-	EXPRESSION TAG	UNP Q57834
B	311	HIS	-	EXPRESSION TAG	UNP Q57834
B	312	HIS	-	EXPRESSION TAG	UNP Q57834
B	313	HIS	-	EXPRESSION TAG	UNP Q57834
B	314	HIS	-	EXPRESSION TAG	UNP Q57834

- Molecule 2 is 3,5-difluoro-L-tyrosine (three-letter code: F2Y) (formula: C<sub>9</sub>H<sub>9</sub>F<sub>2</sub>NO<sub>3</sub>).



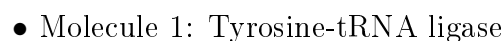
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			15	9	2	1	3		
2	B	1	Total	C	F	N	O	0	0
			15	9	2	1	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total	O	0	0
			36	36		
3	B	28	Total	O	0	0
			28	28		



- Molecule 1: Tyrosine-tRNA ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.31Å 101.31Å 71.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.59 – 2.91 26.16 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.59-2.91) 99.7 (26.16-2.91)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 2.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.211 , 0.268 0.214 , 0.267	Depositor DCC
$R_{free}$ test set	805 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.5	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 2.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.488 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4977	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: F2Y

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	0.20	0/2482	0.36	0/3332
1	B	0.20	0/2479	0.36	0/3328
All	All	0.20	0/4961	0.36	0/6660

There are no bond length outliers.

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	2443	0	2505	31	0
1	B	2440	0	2501	26	0
2	A	15	0	7	1	0
2	B	15	0	7	1	0
3	A	36	0	0	0	0
3	B	28	0	0	0	0
All	All	4977	0	5020	55	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 6.

The worst 5 of 55 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:B:104:TYR:HB2	1:B:107:GLU:HG2	1.77	0.66
1:A:265:LEU:HD21	1:A:276:LEU:HD13	1.82	0.62
1:B:129:ARG:NH2	1:B:182:GLU:OE1	2.34	0.61
1:A:129:ARG:NH2	1:A:182:GLU:OE1	2.34	0.60
1:B:265:LEU:HD21	1:B:276:LEU:HD13	1.83	0.59

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	304/314 (97%)	298 (98%)	5 (2%)	1 (0%)	41	70
1	B	304/314 (97%)	301 (99%)	3 (1%)	0	100	100
All	All	608/628 (97%)	599 (98%)	8 (1%)	1 (0%)	47	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	GLU

### 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	265/275 (96%)	257 (97%)	8 (3%)	41	73
1	B	264/275 (96%)	258 (98%)	6 (2%)	50	79
All	All	529/550 (96%)	515 (97%)	14 (3%)	46	76

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	295	LEU
1	A	303	ARG
1	B	237	GLU
1	A	287	LEU
1	B	129	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 molecules 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

2 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	F2Y	A	401	-	12,15,15	1.50	1 (8%)	16,21,21	3.18	5 (31%)
2	F2Y	B	401	-	12,15,15	1.51	1 (8%)	16,21,21	3.16	5 (31%)

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	F2Y	A	401	-	-	0/4/8/8	0/1/1/1
2	F2Y	B	401	-	-	0/4/8/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	F2Y	CB-CG	-4.91	1.39	1.51
2	A	401	F2Y	CB-CG	-4.90	1.39	1.51

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	F2Y	CD2-CE2-CZ	-6.76	118.49	123.79
2	B	401	F2Y	CD2-CE2-CZ	-6.72	118.53	123.79
2	B	401	F2Y	CD1-CE1-CZ	-6.53	118.68	123.79
2	A	401	F2Y	CD1-CE1-CZ	-6.50	118.70	123.79
2	B	401	F2Y	F2-CE2-CZ	5.01	120.85	117.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	F2Y	1	0
2	B	401	F2Y	1	0

## 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	306/314 (97%)	-0.21	1 (0%) 94 94	9, 24, 50, 69	0
1	B	306/314 (97%)	-0.23	1 (0%) 94 94	9, 24, 50, 67	0
All	All	612/628 (97%)	-0.22	2 (0%) 94 94	9, 24, 51, 69	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	237	GLU	2.5
1	A	1	MET	2.2

### 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](#)

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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	F2Y	B	401	15/15	0.96	0.16	9,12,15,16	0
2	F2Y	A	401	15/15	0.97	0.15	8,12,15,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.