



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:46 PM GMT

PDB ID : 4FZQ  
Title : Crystal structure of HP0197-G5  
Authors : Yuan, Z.; Yan, X.  
Deposited on : 2012-07-07  
Resolution : 2.50 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

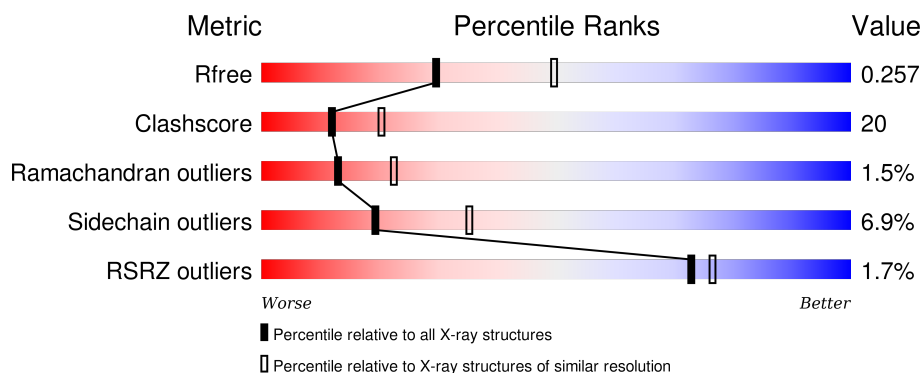
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	79	<div> <div>5%</div> <div>62% 34% .</div> </div>
1	B	79	<div> <div>71% 24% . .</div> </div>
1	C	79	<div> <div>73% 25% .</div> </div>
1	D	79	<div> <div>61% 28% 8% .</div> </div>
1	E	79	<div> <div>5% 57% 30% 8% . .</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	79	<div><div></div><div>4%</div><div>65%</div><div>29%</div><div></div><div></div></div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3943 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 Uncharacterized protein conserved in bacteria.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	79	Total	C	N	O	S	0	0	0
			616	389	102	124	1			
1	B	78	Total	C	N	O	S	0	0	0
			606	384	101	120	1			
1	C	79	Total	C	N	O	S	0	0	0
			616	389	102	124	1			
1	D	76	Total	C	N	O	S	0	0	0
			592	375	99	117	1			
1	E	76	Total	C	N	O	S	0	0	0
			592	375	99	117	1			
1	F	76	Total	C	N	O	S	0	0	0
			592	375	99	117	1			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	415	SER	-	EXPRESSION TAG	UNP A4VZ16
A	416	GLU	-	EXPRESSION TAG	UNP A4VZ16
A	470	MET	VAL	ENGINEERED MUTATION	UNP A4VZ16
B	415	SER	-	EXPRESSION TAG	UNP A4VZ16
B	416	GLU	-	EXPRESSION TAG	UNP A4VZ16
B	470	MET	VAL	ENGINEERED MUTATION	UNP A4VZ16
C	415	SER	-	EXPRESSION TAG	UNP A4VZ16
C	416	GLU	-	EXPRESSION TAG	UNP A4VZ16
C	470	MET	VAL	ENGINEERED MUTATION	UNP A4VZ16
D	415	SER	-	EXPRESSION TAG	UNP A4VZ16
D	416	GLU	-	EXPRESSION TAG	UNP A4VZ16
D	470	MET	VAL	ENGINEERED MUTATION	UNP A4VZ16
E	415	SER	-	EXPRESSION TAG	UNP A4VZ16
E	416	GLU	-	EXPRESSION TAG	UNP A4VZ16
E	470	MET	VAL	ENGINEERED MUTATION	UNP A4VZ16
F	416	SER	-	EXPRESSION TAG	UNP A4VZ16
F	417	GLU	-	EXPRESSION TAG	UNP A4VZ16

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Chain	Residue	Modelled	Actual	Comment	Reference
F	471	MET	VAL	ENGINEERED MUTATION	UNP A4VZ16

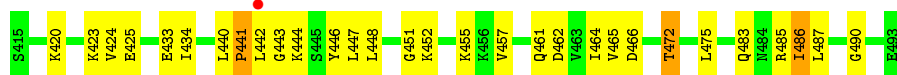
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	66	Total O 66 66	0	0
2	B	58	Total O 58 58	0	0
2	C	25	Total O 25 25	0	0
2	D	53	Total O 53 53	0	0
2	E	51	Total O 51 51	0	0
2	F	76	Total O 76 76	0	0

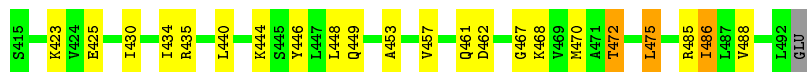
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

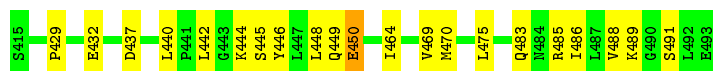
- Molecule 1: Uncharacterized protein conserved in bacteria



- Molecule 1: Uncharacterized protein conserved in bacteria



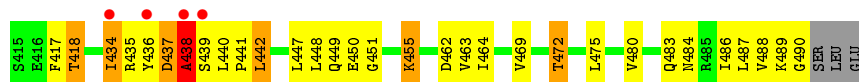
- Molecule 1: Uncharacterized protein conserved in bacteria



- Molecule 1: Uncharacterized protein conserved in bacteria

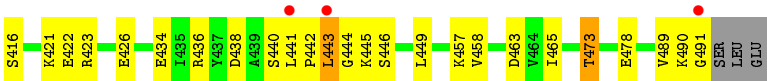


- Molecule 1: Uncharacterized protein conserved in bacteria



- Molecule 1: Uncharacterized protein conserved in bacteria





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.59Å 114.59Å 128.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.88 – 2.50 34.88 – 2.49	Depositor EDS
% Data completeness (in resolution range)	97.7 (34.88-2.50) 97.5 (34.88-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 2.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.255 , 0.278 0.256 , 0.257	Depositor DCC
$R_{free}$ test set	1491 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.8	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 48.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 29939 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3943	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.40	0/621	0.69	0/832
1	B	0.40	0/611	0.68	0/820
1	C	0.38	0/621	0.66	0/832
1	D	0.37	0/597	0.69	1/801 (0.1%)
1	E	0.34	0/597	0.79	3/801 (0.4%)
1	F	0.36	0/597	0.66	0/801
All	All	0.37	0/3644	0.70	4/4887 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	438	ALA	N-CA-C	-6.76	92.74	111.00
1	E	437	ASP	N-CA-C	5.21	125.06	111.00
1	E	436	TYR	N-CA-C	5.16	124.94	111.00
1	D	481	GLU	N-CA-C	5.09	124.74	111.00

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	616	0	642	25	0
1	B	606	0	636	21	0
1	C	616	0	642	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	592	0	620	29	0
1	E	592	0	620	38	0
1	F	592	0	620	20	0
2	A	66	0	0	2	0
2	B	58	0	0	0	0
2	C	25	0	0	1	0
2	D	53	0	0	0	0
2	E	51	0	0	2	0
2	F	76	0	0	1	0
All	All	3943	0	3780	148	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 20.

The worst 5 of 148 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:433:GLU:HB3	1:A:486:ILE:HD12	1.42	1.01
1:B:449:GLN:HB3	1:B:486:ILE:HD13	1.46	0.95
1:A:425:GLU:HG2	1:A:457:VAL:HG22	1.49	0.95
1:D:473:ASN:HD21	1:E:417:PHE:H	1.20	0.90
1:D:430:ILE:H	1:D:430:ILE:HD13	1.36	0.89

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	77/79 (98%)	73 (95%)	2 (3%)	2 (3%)	7	10
1	B	76/79 (96%)	76 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	77/79 (98%)	73 (95%)	4 (5%)	0	100	100
1	D	74/79 (94%)	72 (97%)	1 (1%)	1 (1%)	14	24
1	E	74/79 (94%)	66 (89%)	5 (7%)	3 (4%)	3	4
1	F	74/79 (94%)	70 (95%)	3 (4%)	1 (1%)	14	24
All	All	452/474 (95%)	430 (95%)	15 (3%)	7 (2%)	13	22

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	438	ALA
1	E	441	PRO
1	D	481	GLU
1	F	444	GLY
1	A	441	PRO

### 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	69/69 (100%)	65 (94%)	4 (6%)	25	45
1	B	68/69 (99%)	63 (93%)	5 (7%)	17	31
1	C	69/69 (100%)	67 (97%)	2 (3%)	50	77
1	D	66/69 (96%)	60 (91%)	6 (9%)	12	22
1	E	66/69 (96%)	59 (89%)	7 (11%)	8	16
1	F	66/69 (96%)	62 (94%)	4 (6%)	23	42
All	All	404/414 (98%)	376 (93%)	28 (7%)	19	35

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	426	GLU
1	D	472	THR

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Mol	Chain	Res	Type
1	F	422	GLU
1	D	430	ILE
1	D	432	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	461	GLN
1	E	483	GLN
1	C	483	GLN
1	A	461	GLN
1	D	473	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 carbohydrates 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, 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	79/79 (100%)	-0.08	1 (1%) 79 82	21, 34, 62, 90	0
1	B	78/79 (98%)	-0.15	0 100 100	18, 34, 55, 60	0
1	C	79/79 (100%)	-0.10	0 100 100	19, 40, 75, 99	0
1	D	76/79 (96%)	-0.13	0 100 100	18, 39, 70, 76	0
1	E	76/79 (96%)	0.35	4 (5%) 30 34	29, 49, 90, 104	0
1	F	76/79 (96%)	0.04	3 (3%) 43 48	17, 37, 75, 113	0
All	All	464/474 (97%)	-0.01	8 (1%) 73 76	17, 39, 72, 113	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	436	TYR	3.5
1	F	443	LEU	2.9
1	F	491	GLY	2.7
1	F	441	LEU	2.7
1	E	438	ALA	2.6

### 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 carbohydrates 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.