



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:43 PM GMT

PDB ID : 4MJK  
Title : Crystal structure of a CRISPR protein from *Archaeoglobus fulgidus*  
Authors : Huang, Q.Q.  
Deposited on : 2013-09-03  
Resolution : 1.95 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](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

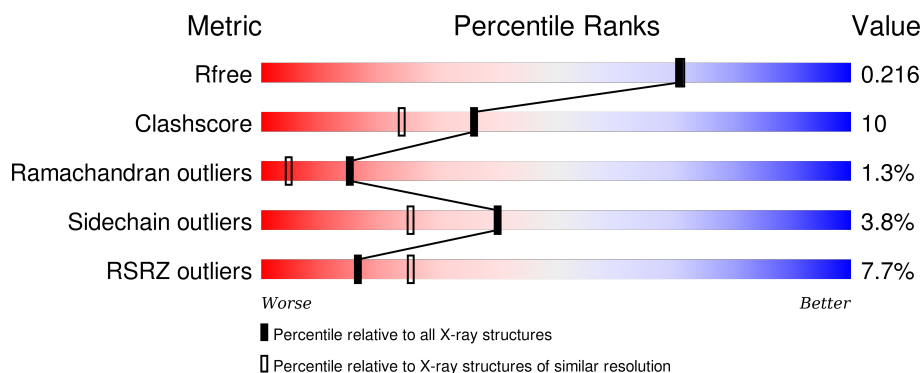
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	265	 8% 74% 13% • 10%
1	B	265	 5% 74% 14% 11%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3953 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 CRISPR protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	Se	0	0	0
			1871	1216	306	343	3	3			
1	B	235	Total	C	N	O	S	Se	0	0	0
			1850	1199	306	340	3	2			

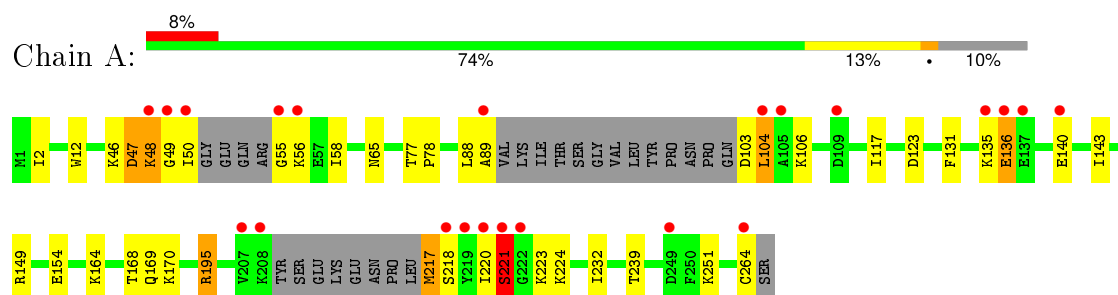
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	112	Total	O	0	0
			112	112		
2	B	120	Total	O	0	0
			120	120		

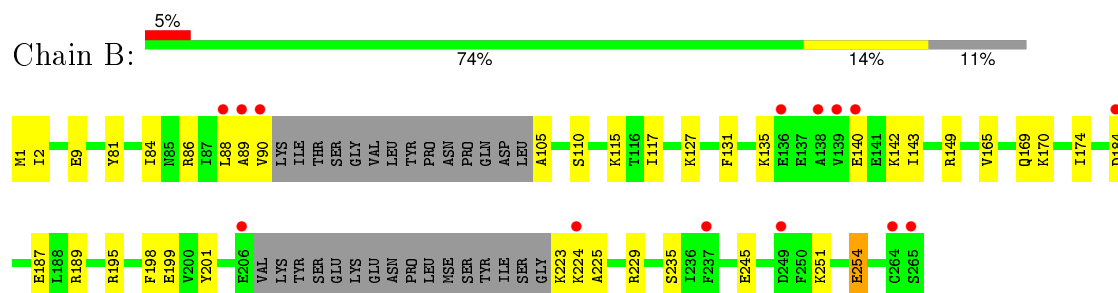
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: CRISPR protein



#### • Molecule 1: CRISPR protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.25Å 87.52Å 140.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.47 – 1.95 43.76 – 1.95	Depositor EDS
% Data completeness (in resolution range)	94.1 (33.47-1.95) 93.3 (43.76-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.48 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.195 , 0.216 0.194 , 0.216	Depositor DCC
$R_{free}$ test set	2000 reflections (5.76%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.2	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 63.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 38133 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3953	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.01% 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

### 5.1 Standard geometry

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	0.41	0/1909	0.55	0/2576
1	B	0.40	0/1888	0.53	0/2548
All	All	0.41	0/3797	0.54	0/5124

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

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	1871	0	1900	36	0
1	B	1850	0	1882	38	0
2	A	112	0	0	5	0
2	B	120	0	0	8	0
All	All	3953	0	3782	72	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 10.

All (72) 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:56:LYS:HA	1:A:58:ILE:H	1.32	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:ARG:HG2	1:B:245:GLU:HG3	1.51	0.93
1:B:142:LYS:HG3	1:B:143:ILE:HD12	1.61	0.82
1:A:217:MSE:N	1:A:217:MSE:HE2	1.97	0.79
1:A:264:CYS:O	2:A:401:HOH:O	2.00	0.79
1:A:140:GLU:HB2	1:A:143:ILE:HG12	1.64	0.79
1:A:56:LYS:HA	1:A:58:ILE:N	1.99	0.78
1:A:104:LEU:HD12	1:A:106:LYS:HG3	1.67	0.76
1:B:187:GLU:HG2	2:B:356:HOH:O	1.86	0.76
1:B:86:ARG:NH1	2:B:402:HOH:O	2.16	0.76
1:B:198:PHE:CE1	1:B:229:ARG:HD3	2.21	0.75
1:A:117:ILE:HD13	1:B:117:ILE:HD12	1.70	0.73
1:A:103:ASP:N	2:A:358:HOH:O	2.23	0.71
1:B:140:GLU:HB2	1:B:143:ILE:HD13	1.74	0.69
1:A:88:LEU:O	1:A:89:ALA:HB2	1.93	0.69
1:B:169:GLN:HE21	1:B:251:LYS:HG3	1.58	0.68
1:B:170:LYS:NZ	1:B:254:GLU:HB3	2.08	0.67
1:B:187:GLU:OE2	2:B:414:HOH:O	2.12	0.67
1:A:195:ARG:HB3	1:A:232:ILE:HB	1.76	0.67
1:B:90:VAL:HA	2:B:403:HOH:O	1.95	0.66
1:A:117:ILE:CD1	1:B:117:ILE:HD12	2.26	0.66
1:B:105:ALA:N	2:B:324:HOH:O	2.29	0.65
1:A:12:TRP:HZ2	1:A:154:GLU:HG3	1.63	0.63
1:B:169:GLN:NE2	1:B:251:LYS:HG3	2.14	0.62
1:B:9:GLU:HG2	1:B:127:LYS:HG2	1.82	0.60
1:A:195:ARG:NH1	2:A:330:HOH:O	2.33	0.60
1:B:201:TYR:O	1:B:225:ALA:HA	2.02	0.60
1:B:170:LYS:HZ3	1:B:254:GLU:HB3	1.67	0.59
1:A:2:ILE:HD11	1:A:164:LYS:HG2	1.85	0.59
1:A:56:LYS:CA	1:A:58:ILE:H	2.09	0.59
1:A:224:LYS:HD2	1:A:224:LYS:N	2.20	0.56
1:A:49:GLY:O	1:A:50:ILE:HG22	2.05	0.56
1:A:12:TRP:CZ2	1:A:154:GLU:HG3	2.41	0.55
1:B:224:LYS:O	1:B:225:ALA:HB3	2.06	0.55
1:A:46:LYS:C	1:A:48:LYS:H	2.09	0.54
1:B:224:LYS:NZ	2:B:379:HOH:O	2.40	0.53
1:B:81:TYR:CD1	1:B:115:LYS:HG2	2.44	0.53
1:A:88:LEU:O	1:A:89:ALA:CB	2.57	0.53
1:A:168:THR:HG21	1:A:170:LYS:HE3	1.90	0.52
1:B:189:ARG:HD3	1:B:245:GLU:CD	2.30	0.52
1:B:198:PHE:CZ	1:B:229:ARG:HD3	2.45	0.50
1:B:174:ILE:HD12	1:B:174:ILE:C	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:VAL:HG12	2:B:363:HOH:O	2.12	0.49
1:B:1:MSE:HB3	1:B:135:LYS:O	2.14	0.48
1:A:55:GLY:HA2	1:A:56:LYS:O	2.13	0.48
1:A:65:ASN:ND2	1:A:136:GLU:OE2	2.47	0.48
1:B:189:ARG:HD2	1:B:189:ARG:HA	1.67	0.47
1:B:170:LYS:NZ	1:B:254:GLU:CB	2.76	0.47
1:A:195:ARG:HB2	1:A:232:ILE:O	2.16	0.46
1:A:47:ASP:O	1:A:48:LYS:HG3	2.15	0.46
1:B:224:LYS:HD2	1:B:224:LYS:HA	1.87	0.44
1:A:55:GLY:HA2	1:A:56:LYS:C	2.38	0.44
1:A:169:GLN:OE1	1:A:251:LYS:HG3	2.18	0.44
1:B:2:ILE:HD12	1:B:165:VAL:O	2.18	0.44
1:A:220:ILE:O	1:A:221:SER:C	2.56	0.43
1:A:218:SER:HA	1:A:221:SER:OG	2.18	0.43
1:B:88:LEU:C	1:B:90:VAL:H	2.21	0.43
1:B:84:ILE:O	1:B:88:LEU:HG	2.20	0.42
1:B:88:LEU:O	1:B:90:VAL:N	2.52	0.42
1:A:135:LYS:HE3	1:A:135:LYS:HB2	1.74	0.42
1:A:168:THR:CG2	1:A:170:LYS:HE3	2.50	0.42
1:B:81:TYR:HE1	1:B:117:ILE:HD11	1.84	0.41
1:B:88:LEU:C	1:B:90:VAL:N	2.73	0.41
1:B:195:ARG:NH2	2:B:384:HOH:O	2.54	0.41
1:B:199:GLU:HG2	1:B:201:TYR:CE2	2.55	0.41
1:A:46:LYS:O	1:A:48:LYS:N	2.52	0.41
1:A:77:THR:HA	1:A:78:PRO:HD3	1.94	0.41
1:A:103:ASP:HB2	2:A:358:HOH:O	2.20	0.41
1:B:189:ARG:HG2	1:B:245:GLU:CG	2.36	0.40
1:A:217:MSE:SE	2:A:337:HOH:O	2.89	0.40
1:B:229:ARG:HA	1:B:229:ARG:HD2	1.80	0.40
1:A:46:LYS:C	1:A:48:LYS:N	2.75	0.40

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	231/265 (87%)	215 (93%)	11 (5%)	5 (2%)	8	2
1	B	229/265 (86%)	220 (96%)	8 (4%)	1 (0%)	39	27
All	All	460/530 (87%)	435 (95%)	19 (4%)	6 (1%)	15	4

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	SER
1	B	89	ALA
1	A	47	ASP
1	A	48	LYS
1	A	195	ARG
1	A	104	LEU

### 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	200/223 (90%)	192 (96%)	8 (4%)	38	23
1	B	198/223 (89%)	191 (96%)	7 (4%)	43	29
All	All	398/446 (89%)	383 (96%)	15 (4%)	40	25

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	ASP
1	A	131	PHE
1	A	136	GLU
1	A	149	ARG
1	A	217	MSE
1	A	221	SER
1	A	223	LYS

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Mol	Chain	Res	Type
1	A	239	THR
1	B	110	SER
1	B	131	PHE
1	B	149	ARG
1	B	184	ASP
1	B	223	LYS
1	B	235	SER
1	B	254	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	B	53	GLN
1	B	169	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 [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 ⓘ

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, 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	236/265 (89%)	0.48	22 (9%) 11 17	9, 20, 45, 64	0
1	B	233/265 (87%)	0.30	14 (6%) 25 35	9, 22, 40, 51	0
All	All	469/530 (88%)	0.39	36 (7%) 16 25	9, 21, 43, 64	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	50	ILE	8.0
1	A	55	GLY	6.1
1	A	104	LEU	6.0
1	B	90	VAL	5.3
1	B	264	CYS	4.5
1	A	208	LYS	4.4
1	A	221	SER	4.3
1	A	207	VAL	4.0
1	A	137	GLU	3.8
1	A	219	TYR	3.7
1	A	264	CYS	3.7
1	A	49	GLY	3.7
1	A	220	ILE	3.6
1	A	218	SER	3.5
1	B	265	SER	3.5
1	B	206	GLU	3.4
1	A	222	GLY	2.9
1	A	56	LYS	2.7
1	B	136	GLU	2.6
1	B	138	ALA	2.6
1	B	224	LYS	2.6
1	B	249	ASP	2.5
1	B	184	ASP	2.5
1	B	237	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	135	LYS	2.5
1	A	109	ASP	2.5
1	A	48	LYS	2.3
1	A	105	ALA	2.3
1	B	139	VAL	2.2
1	B	89	ALA	2.2
1	A	136	GLU	2.2
1	B	88	LEU	2.2
1	A	140	GLU	2.2
1	A	89	ALA	2.1
1	A	249	ASP	2.1
1	B	140	GLU	2.1

## 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.