



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2I5H / pdb_00002i5h
Title : Crystal structure of Af1531 from Archaeoglobus fulgidus, Pfam DUF655
Authors : Eswaramoorthy, S.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2006-08-24
Resolution : 1.74 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

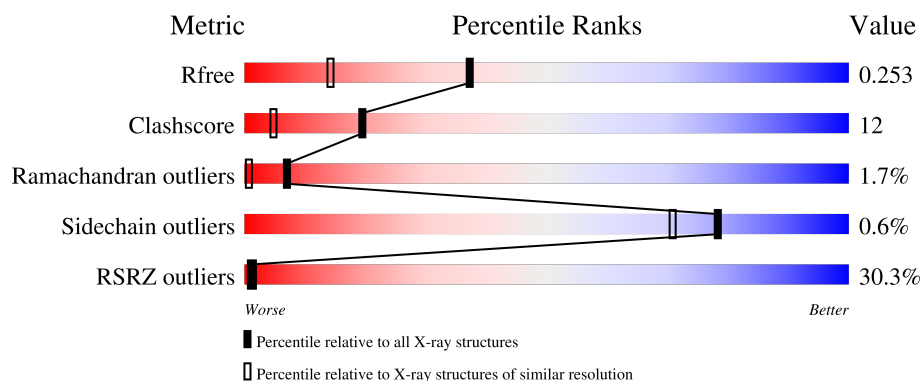
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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}	180053	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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 $\leq 5\%$. 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	205	26% 66% 20% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1589 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 Hypothetical protein AF1531.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1457	940	256	256	5			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	cloning artifact	UNP O28741
A	0	SER	-	cloning artifact	UNP O28741
A	1	LEU	-	cloning artifact	UNP O28741
A	196	GLU	-	expression tag	UNP O28741
A	197	GLY	-	expression tag	UNP O28741
A	198	HIS	-	expression tag	UNP O28741
A	199	HIS	-	expression tag	UNP O28741
A	200	HIS	-	expression tag	UNP O28741
A	201	HIS	-	expression tag	UNP O28741
A	202	HIS	-	expression tag	UNP O28741
A	203	HIS	-	expression tag	UNP O28741

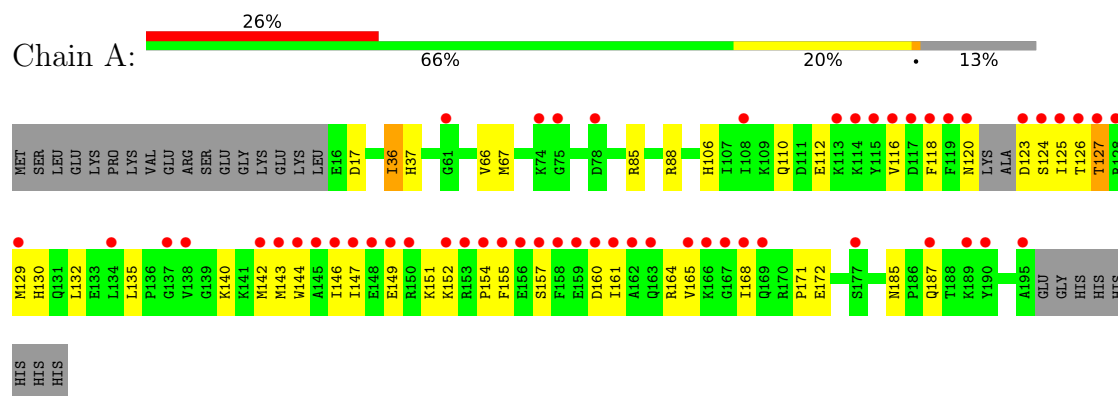
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	132	Total	O	0	0
			132	132		

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: Hypothetical protein AF1531



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	76.73Å 37.49Å 85.25Å 90.00° 95.60° 90.00°	Depositor
Resolution (Å)	31.80 – 1.74 31.80 – 1.74	Depositor EDS
% Data completeness (in resolution range)	90.8 (31.80-1.74) 90.9 (31.80-1.74)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 1.74Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.258 0.227 , 0.253	Depositor DCC
R_{free} test set	907 reflections (3.87%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	1589	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

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	0.33	0/1488	0.83	2/2004 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	ARG	N-CA-C	-5.86	101.79	110.46
1	A	36	ILE	N-CA-C	5.25	116.61	110.62

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	1457	0	1479	34	0
2	A	132	0	0	3	0
All	All	1589	0	1479	34	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 12.

All (34) 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:123:ASP:OD1	1:A:132:LEU:HG	1.80	0.81
1:A:106:HIS:O	1:A:110:GLN:HG2	1.92	0.69
1:A:185:ASN:HA	1:A:187:GLN:HE22	1.60	0.66
1:A:126:THR:HG22	1:A:127:THR:HG22	1.78	0.64
1:A:143:MET:HG3	1:A:144:TRP:N	2.15	0.62
1:A:118:PHE:O	1:A:123:ASP:HB2	2.01	0.60
1:A:66:VAL:O	1:A:67:MET:HB2	2.03	0.58
1:A:187:GLN:H	1:A:187:GLN:CD	2.12	0.57
1:A:112:GLU:O	1:A:116:VAL:HG22	2.04	0.57
1:A:127:THR:C	1:A:129:MET:H	2.10	0.57
1:A:118:PHE:HE2	1:A:135:LEU:HD11	1.70	0.57
1:A:187:GLN:HB3	2:A:260:HOH:O	2.04	0.57
1:A:165:VAL:O	1:A:168:ILE:HG22	2.07	0.55
1:A:36:ILE:HG13	1:A:37:HIS:N	2.22	0.54
1:A:120:ASN:HB3	1:A:155:PHE:HD1	1.73	0.54
1:A:143:MET:O	1:A:147:ILE:HG13	2.09	0.53
1:A:127:THR:C	1:A:129:MET:N	2.67	0.53
1:A:36:ILE:HG23	2:A:280:HOH:O	2.08	0.52
1:A:85:ARG:CZ	2:A:277:HOH:O	2.58	0.52
1:A:125:ILE:HG12	1:A:126:THR:N	2.24	0.52
1:A:127:THR:HG23	1:A:127:THR:O	2.11	0.51
1:A:126:THR:HB	1:A:129:MET:O	2.13	0.48
1:A:142:MET:O	1:A:146:ILE:HG13	2.15	0.47
1:A:147:ILE:O	1:A:151:LYS:HG2	2.15	0.46
1:A:185:ASN:HA	1:A:187:GLN:NE2	2.29	0.46
1:A:157:SER:O	1:A:161:ILE:HG13	2.16	0.45
1:A:155:PHE:HA	1:A:160:ASP:OD2	2.16	0.45
1:A:110:GLN:NE2	1:A:110:GLN:HA	2.33	0.43
1:A:140:LYS:O	1:A:143:MET:HG2	2.17	0.43
1:A:123:ASP:OD1	1:A:130:HIS:HE1	2.00	0.43
1:A:120:ASN:HD22	1:A:154:PRO:HB2	1.84	0.43
1:A:125:ILE:CG1	1:A:126:THR:N	2.83	0.41
1:A:149:GLU:O	1:A:164:ARG:NH2	2.55	0.40
1:A:171:PRO:HG2	1:A:172:GLU:OE1	2.22	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	174/205 (85%)	164 (94%)	7 (4%)	3 (2%)	7 1

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	SER
1	A	127	THR
1	A	152	LYS

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	154/187 (82%)	153 (99%)	1 (1%)	78 71

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	106	HIS

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Mol	Chain	Res	Type
1	A	110	GLN
1	A	187	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 oligosaccharides 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 ⓘ

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, 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	178/205 (86%)	1.29	54 (30%) ⓘ ⓘ	12, 28, 50, 53	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	124	SER	5.5
1	A	125	ILE	5.4
1	A	165	VAL	5.1
1	A	127	THR	4.7
1	A	123	ASP	4.6
1	A	168	ILE	4.6
1	A	169	GLN	4.5
1	A	158	PHE	4.3
1	A	116	VAL	4.0
1	A	195	ALA	3.9
1	A	120	ASN	3.7
1	A	153	ARG	3.5
1	A	152	LYS	3.5
1	A	155	PHE	3.5
1	A	161	ILE	3.4
1	A	129	MET	3.3
1	A	114	LYS	3.2
1	A	143	MET	3.2
1	A	146	ILE	3.2
1	A	75	GLY	3.1
1	A	74	LYS	3.0
1	A	128	ARG	3.0
1	A	126	THR	3.0
1	A	190	TYR	3.0
1	A	154	PRO	3.0
1	A	108	ILE	2.9
1	A	147	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	150	ARG	2.9
1	A	138	VAL	2.8
1	A	113	LYS	2.8
1	A	118	PHE	2.7
1	A	144	TRP	2.7
1	A	119	PHE	2.7
1	A	163	GLN	2.7
1	A	115	TYR	2.7
1	A	142	MET	2.7
1	A	187	GLN	2.6
1	A	167	GLY	2.6
1	A	159	GLU	2.5
1	A	162	ALA	2.5
1	A	137	GLY	2.5
1	A	157	SER	2.4
1	A	117	ASP	2.4
1	A	149	GLU	2.3
1	A	78	ASP	2.3
1	A	134	LEU	2.3
1	A	166	LYS	2.3
1	A	160	ASP	2.3
1	A	156	GLU	2.2
1	A	177	SER	2.2
1	A	189	LYS	2.2
1	A	61	GLY	2.1
1	A	148	GLU	2.1
1	A	145	ALA	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 oligosaccharides 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.