

wwPDB X-ray Structure Validation Summary Report (i)

Jan 24, 2023 - 01:26 PM EST

PDB ID : 3LOT

Title : Crystal structure of PROTEIN OF UNKNOWN FUNCTION (NP_070038.1)

from ARCHAEOGLOBUS FULGIDUS at 1.89 A resolution

Authors : Joint Center for Structural Genomics (JCSG)

Deposited on : 2010-02-04

Resolution : 1.89 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*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 (1)) 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 : 2.31.2

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

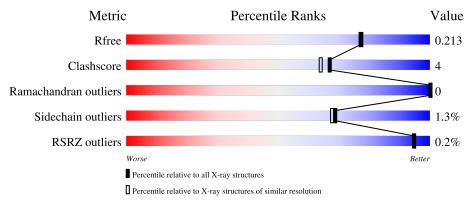
Validation Pipeline (wwPDB-VP) : 2.31.2

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 1.89 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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	314	94%	5% •
1	В	314	92%	6% ••
1	С	314	92%	6% •
1	D	314	90%	9% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard



residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UNL	A	502	-	-	X	-
3	UNL	A	503	-	-	X	-
3	UNL	A	504	-	-	X	-
3	UNL	В	502	-	-	X	-
3	UNL	В	503	-	-	X	-
3	UNL	С	502	-	-	X	-
3	UNL	С	503	-	-	X	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11503 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.

Mol	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace
1	Λ	310	Total	С	N	О	S	Se	0	7	0
1	A	310	2478	1582	424	457	3	12	0	1	
1	В	311	Total	С	N	О	S	Se	0	11	0
1	Ъ	911	2516	1608	425	468	3	12		11	
1	С	310	Total	С	N	О	S	Se	0	0	0
1		310	2487	1589	421	463	3	11		9	
1	D	313	Total	С	N	О	S	Se	0	0	0
1		313	2521	1609	434	464	3	11		Э	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	${f Comment}$	Reference
A	0	GLY	-	expression tag	UNP O29058
В	0	GLY	-	expression tag	UNP O29058
С	0	GLY	-	expression tag	UNP O29058
D	0	GLY	-	expression tag	UNP O29058

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

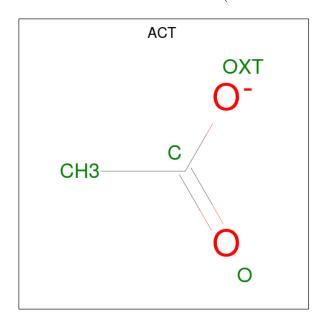
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	В	1	Total Zn 1 1	0	0
2	С	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

• Molecule 3 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total O 12 12	0	0
3	В	2	Total O 8 8	0	0
3	С	2	Total O 9 9	0	0
3	D	1	Total O 2 2	0	0

 \bullet Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $\mathrm{C_2H_3O_2}).$



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	С	1	Total C 4 2	O 2	0	0

• Molecule 5 is water.

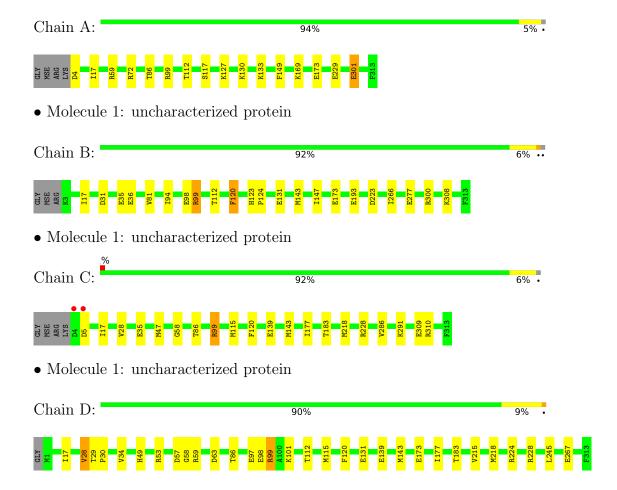
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	374	Total O 374 374	0	0
5	В	370	Total O 370 370	0	0
5	С	371	Total O 371 371	0	0
5	D	347	Total O 347 347	0	0



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: uncharacterized protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	75.79Å 103.08Å 156.55Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.97 - 1.89	Depositor
rtesolution (A)	48.95 - 1.89	EDS
% Data completeness	99.2 (48.97-1.89)	Depositor
(in resolution range)	99.3 (48.95-1.89)	EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.13 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0053, PHENIX	Depositor
D D.	0.156 , 0.206	Depositor
R, R_{free}	0.166 , 0.213	DCC
R_{free} test set	4891 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 44.1	EDS
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11503	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.78% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: UNL, ZN, ACT

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).

Mal	Chain	Bo	nd lengths	Bond angles		
Mol		RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	0.84	0/2516	0.78	0/3382	
1	В	0.86	$2/2555 \ (0.1\%)$	0.82	4/3435 (0.1%)	
1	С	0.82	0/2526	0.76	2/3397 (0.1%)	
1	D	0.80	1/2560 (0.0%)	0.82	5/3442 (0.1%)	
All	All	0.83	3/10157 (0.0%)	0.80	11/13656 (0.1%)	

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	В	36	GLU	CD-OE1	5.87	1.32	1.25
1	В	81	VAL	CB-CG1	5.39	1.64	1.52
1	D	28	VAL	CA-CB	-5.15	1.44	1.54

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
1	В	99	ARG	NE-CZ-NH2	-10.38	115.11	120.30
1	В	99	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	D	99	ARG	NE-CZ-NH1	8.65	124.63	120.30
1	D	99	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	С	99	ARG	NE-CZ-NH1	-6.64	116.98	120.30

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	2478	0	2487	9	0
1	В	2516	0	2521	11	0
1	С	2487	0	2493	14	0
1	D	2521	0	2543	21	0
2	A	1	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
3	A	12	0	0	8	0
3	В	8	0	0	8	0
3	С	9	0	0	7	0
3	D	2	0	0	1	0
4	С	4	0	3	0	0
5	A	374	0	0	6	0
5	В	370	0	0	4	0
5	С	371	0	0	7	0
5	D	347	0	0	5	0
All	All	11503	0	10047	79	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 4.

The worst 5 of 79 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
3:A:503:UNL:O2	3:A:503:UNL:O4	1.59	1.18
3:C:503:UNL:O1	3:C:503:UNL:O5	1.64	1.16
3:A:502:UNL:O2	3:A:502:UNL:O4	1.66	1.12
3:B:503:UNL:O2	3:B:503:UNL:O3	1.71	1.07
3:A:503:UNL:O2	3:A:503:UNL:O3	1.74	1.04

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	315/314 (100%)	306 (97%)	9 (3%)	0	100	100
1	В	320/314 (102%)	312 (98%)	8 (2%)	0	100	100
1	С	317/314 (101%)	309 (98%)	8 (2%)	0	100	100
1	D	320/314 (102%)	309 (97%)	11 (3%)	0	100	100
All	All	1272/1256 (101%)	1236 (97%)	36 (3%)	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	Rotameric Outliers		Percentiles		
1	A	$262/254\ (103\%)$	257 (98%)	5 (2%)	57	53		
1	В	$267/254\ (105\%)$	264 (99%)	3 (1%)	73	73		
1	С	$264/254 \ (104\%)$	262 (99%)	2 (1%)	81	82		
1	D	$268/254 \ (106\%)$	265 (99%)	3 (1%)	73	73		
All	All	1061/1016 (104%)	1048 (99%)	13 (1%)	69	70		

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	308	LYS
1	С	17	ILE
1	D	131	GLU
1	D	17	ILE
1	D	120	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:



Mol	Chain	Res	Type
1	D	242	GLN
1	D	230	ASN
1	В	188	HIS
1	В	119	ASN
1	С	188	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 4 are monoatomic and 8 are unknown - leaving 1 for Mogul analysis.

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	Dec	Link	Bond lengths			Bond angles		
Mol	Type	Chain	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACT	С	314	-	3,3,3	0.80	0	3,3,3	1.92	1 (33%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
4	С	314	ACT	OXT-C-O	-2.71	112.07	122.05



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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^{th} 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>	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	A	300/314 (95%)	-0.38	0 100 100	9, 13, 23, 31	0
1	В	301/314 (95%)	-0.44	0 100 100	10, 13, 22, 37	0
1	С	300/314 (95%)	-0.46	2 (0%) 87 88	10, 13, 21, 30	0
1	D	302/314~(96%)	-0.43	0 100 100	10, 14, 26, 33	0
All	All	1203/1256 (95%)	-0.43	2 (0%) 95 95	9, 14, 24, 37	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	4	ASP	6.6
1	С	5[A]	ASP	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 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^{th} 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	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
3	UNL	С	503	5/-	0.90	0.12	20,33,35,47	0
3	UNL	В	503	3/-	0.92	0.13	22,22,25,30	0
3	UNL	A	504	3/-	0.92	0.10	19,19,32,38	0
3	UNL	A	503	4/-	0.94	0.12	29,30,31,38	0
3	UNL	С	502	4/-	0.96	0.10	11,14,21,34	0
3	UNL	В	502	5/-	0.96	0.10	10,14,39,48	0
3	UNL	D	502	2/-	0.97	0.14	16,16,16,19	0
3	UNL	A	502	5/-	0.98	0.14	11,14,26,42	0
2	ZN	С	501	1/1	0.99	0.05	36,36,36,36	0
2	ZN	D	501	1/1	0.99	0.07	43,43,43,43	0
4	ACT	С	314	4/4	0.99	0.07	14,14,15,16	0
2	ZN	В	501	1/1	1.00	0.07	34,34,34,34	0
2	ZN	A	501	1/1	1.00	0.04	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.

