wwPDB X-ray Structure Validation Summary Report (i)

Feb 5, 2024 – 12:15 AM EST

PDB ID	:	1S3M
Title	:	Structural and Functional Characterization of a Novel Archaeal Phosphodiesterase
Authors	:	Chen, S.; Busso, D.; Yakunin, A.F.; Kuznetsova, E.; Proudfoot, M.; Jancrick, J.; Kim, R.; Kim, S.-H.; Berkeley Structural Genomics Center (BSGC)
Deposited on	:	2004-01-13
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*
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:

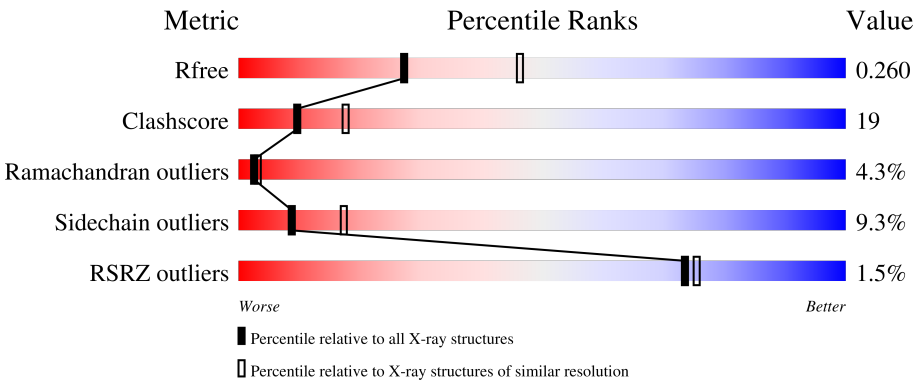
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 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	190	2% 54% 27% 5% • 13%
1	B	190	% 54% 27% 5% • 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2733 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 MJ0936.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	165	1330	847	216	260	7	0	0	0
1	B	165	1330	847	216	260	7	0	0	0

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	expression tag	UNP Q58346
A	-23	GLY	-	expression tag	UNP Q58346
A	-22	SER	-	expression tag	UNP Q58346
A	-21	SER	-	expression tag	UNP Q58346
A	-20	HIS	-	expression tag	UNP Q58346
A	-19	HIS	-	expression tag	UNP Q58346
A	-18	HIS	-	expression tag	UNP Q58346
A	-17	HIS	-	expression tag	UNP Q58346
A	-16	HIS	-	expression tag	UNP Q58346
A	-15	HIS	-	expression tag	UNP Q58346
A	-14	ASP	-	expression tag	UNP Q58346
A	-13	TYR	-	expression tag	UNP Q58346
A	-12	ASP	-	expression tag	UNP Q58346
A	-11	ILE	-	expression tag	UNP Q58346
A	-10	PRO	-	expression tag	UNP Q58346
A	-9	THR	-	expression tag	UNP Q58346
A	-8	THR	-	expression tag	UNP Q58346
A	-7	GLU	-	expression tag	UNP Q58346
A	-6	ASN	-	expression tag	UNP Q58346
A	-5	LEU	-	expression tag	UNP Q58346
A	-4	TYR	-	expression tag	UNP Q58346
A	-3	PHE	-	expression tag	UNP Q58346
A	-2	GLN	-	expression tag	UNP Q58346
A	-1	GLY	-	expression tag	UNP Q58346
A	0	HIS	-	expression tag	UNP Q58346

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	176	MET	-	expression tag	UNP Q58346
B	177	GLY	-	expression tag	UNP Q58346
B	178	SER	-	expression tag	UNP Q58346
B	179	SER	-	expression tag	UNP Q58346
B	180	HIS	-	expression tag	UNP Q58346
B	181	HIS	-	expression tag	UNP Q58346
B	182	HIS	-	expression tag	UNP Q58346
B	183	HIS	-	expression tag	UNP Q58346
B	184	HIS	-	expression tag	UNP Q58346
B	185	HIS	-	expression tag	UNP Q58346
B	186	ASP	-	expression tag	UNP Q58346
B	187	TYR	-	expression tag	UNP Q58346
B	188	ASP	-	expression tag	UNP Q58346
B	189	ILE	-	expression tag	UNP Q58346
B	190	PRO	-	expression tag	UNP Q58346
B	191	THR	-	expression tag	UNP Q58346
B	192	THR	-	expression tag	UNP Q58346
B	193	GLU	-	expression tag	UNP Q58346
B	194	ASN	-	expression tag	UNP Q58346
B	195	LEU	-	expression tag	UNP Q58346
B	196	TYR	-	expression tag	UNP Q58346
B	197	PHE	-	expression tag	UNP Q58346
B	198	GLN	-	expression tag	UNP Q58346
B	199	GLY	-	expression tag	UNP Q58346
B	200	HIS	-	expression tag	UNP Q58346

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
2	A	2	2	2	0	0
			Total	Ni		
2	B	2	2	2	0	0

- Molecule 3 is water.

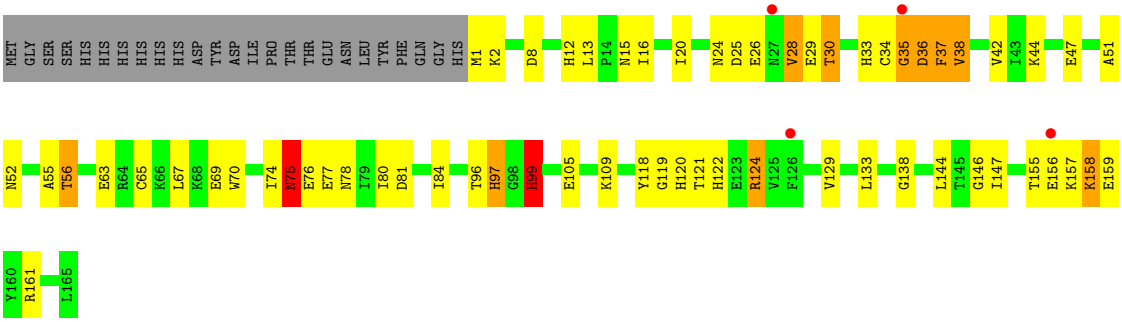
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	35	35	35	0	0
			Total	O		
3	B	34	34	34	0	0

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.

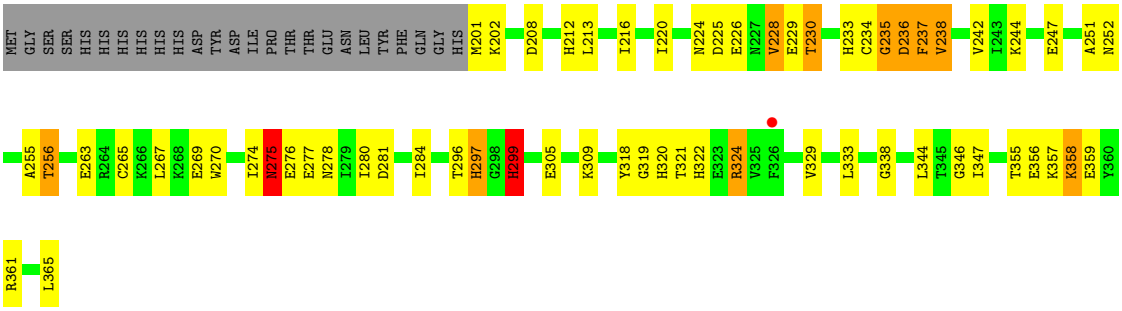
• Molecule 1: Hypothetical protein MJ0936

Chain A: 2% 54% 27% 5% • 13%



• Molecule 1: Hypothetical protein MJ0936

Chain B: % 54% 27% 5% • 13%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	70.11Å 70.11Å 196.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.05 – 2.50 35.05 – 2.50	Depositor EDS
% Data completeness (in resolution range)	84.3 (35.05-2.50) 93.3 (35.05-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.246 0.218 , 0.260	Depositor DCC
R_{free} test set	1594 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å^2)	47.1	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 30.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.487 for -h,k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2733	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical 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.

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: NI

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	0.66	0/1355	0.86	3/1832 (0.2%)
1	B	0.66	0/1355	0.86	3/1832 (0.2%)
All	All	0.66	0/2710	0.86	6/3664 (0.2%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	299	HIS	N-CA-CB	-5.43	100.82	110.60
1	B	237	PHE	N-CA-C	-5.42	96.38	111.00
1	A	99	HIS	N-CA-CB	-5.41	100.87	110.60
1	A	37	PHE	N-CA-C	-5.33	96.62	111.00
1	B	297	HIS	N-CA-C	-5.17	97.05	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	1330	0	1298	50	0
1	B	1330	0	1295	52	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	35	0	0	2	0
3	B	34	0	0	2	0
All	All	2733	0	2593	102	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 19.

The worst 5 of 102 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:208:ASP:H	1:B:235:GLY:HA3	1.14	1.12
1:A:8:ASP:H	1:A:35:GLY:HA3	1.14	1.09
1:A:1:MET:HA	1:A:29:GLU:OE2	1.84	0.77
1:A:30:THR:HB	1:A:52:ASN:OD1	1.85	0.75
1:A:8:ASP:N	1:A:35:GLY:HA3	1.98	0.74

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	163/190 (86%)	145 (89%)	11 (7%)	7 (4%)	2 3
1	B	163/190 (86%)	146 (90%)	10 (6%)	7 (4%)	2 3
All	All	326/380 (86%)	291 (89%)	21 (6%)	14 (4%)	2 3

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	HIS
1	B	299	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	25	ASP
1	A	28	VAL
1	A	35	GLY

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	150/173 (87%)	136 (91%)	14 (9%)	9 17
1	B	150/173 (87%)	136 (91%)	14 (9%)	9 17
All	All	300/346 (87%)	272 (91%)	28 (9%)	9 17

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

Mol	Chain	Res	Type
1	B	213	LEU
1	B	361	ARG
1	B	236	ASP
1	B	355	THR
1	B	234	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	212	HIS
1	B	275	ASN
1	B	301	GLN
1	A	75	ASN
1	A	12	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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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, 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	165/190 (86%)	0.19	4 (2%)	59	62	28, 51, 76, 88	0
1	B	165/190 (86%)	0.15	1 (0%)	89	90	29, 50, 76, 87	0
All	All	330/380 (86%)	0.17	5 (1%)	73	75	28, 51, 76, 88	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	GLY	3.2
1	B	326	PHE	2.5
1	A	27	ASN	2.4
1	A	126	PHE	2.2
1	A	156	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 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, 95th 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^2)	Q<0.9
2	NI	B	501	1/1	0.93	0.11	66,66,66,66	0
2	NI	A	503	1/1	0.95	0.17	65,65,65,65	0
2	NI	B	502	1/1	0.96	0.17	46,46,46,46	0
2	NI	A	504	1/1	0.98	0.10	46,46,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.