



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 11:33 am BST

PDB ID : 2AHD
Title : The Apo structure of Methanococcus jannaschii phosphodiesterase MJ0936
Authors : Chen, S.; Kim, R.; Kim, S.-H.; Berkeley Structural Genomics Center (BSGC)
Deposited on : 2005-07-27
Resolution : 3.00 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

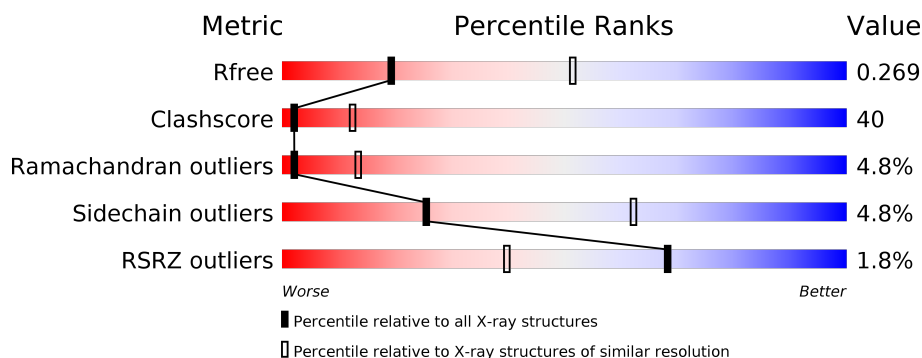
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 ≥ 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	165	<div> <div>%</div> <div> <div></div> <div>44%</div> <div>48%</div> <div>8%</div> </div> </div>
1	B	165	<div> <div>2%</div> <div> <div></div> <div>44%</div> <div>47%</div> <div>8%</div> </div> </div>
1	C	165	<div> <div>3%</div> <div> <div></div> <div>44%</div> <div>48%</div> <div>8%</div> </div> </div>
1	D	165	<div> <div>%</div> <div> <div></div> <div>42%</div> <div>49%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5469 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 Phosphodiesterase MJ0936.

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

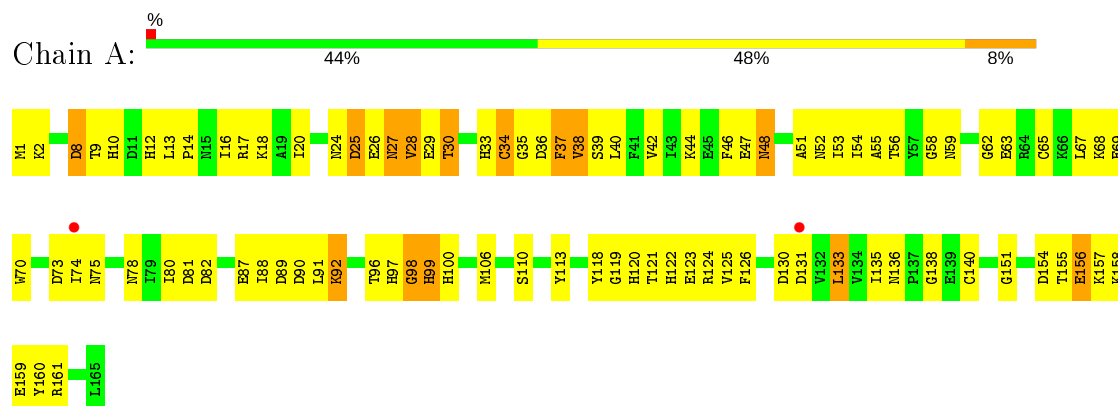
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	40	Total	O	0	0
			40	40		
2	B	30	Total	O	0	0
			30	30		
2	C	36	Total	O	0	0
			36	36		
2	D	43	Total	O	0	0
			43	43		

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 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: Phosphodiesterase MJ0936



K158
E159
Y160
R161
L165

● Molecule 1: Phosphodiesterase MJ0936



K201
K202
D208
T209
H210
K211
H212
L213
F214
N215
I216
R217
K218
A219
I220
E221
I222
F223
N224
D225
E226
N227
Y228
E229
T230
H233
C234
Q235
D236
F237
Y238
S239
L240
F241
Y242
I243
K244
E245
F246
E247
N248
A251
N252
I253
I254
A255
T256
Y257
G258
N259
E263
K264
C265
F266
I267
K268

E269
W270
D273
I274
N275
N278
I279
I280
D281
D282
E287
I288
D289
D290
L291
K292
T296
H297
G298
H299
H300
Q301
S302
K306
Y313
Y318
G319
H320
T321
H322
E323
R324
Y325
F326
D330
D331
V332
L333
V334
I335
N336
P337
G338
E339
C340
L344
G351
D354
T355

E356
K357
K358
E359
Y360
L365

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	209.87Å 71.34Å 62.97Å 90.00° 98.13° 90.00°	Depositor
Resolution (Å)	44.78 – 3.00 44.77 – 2.99	Depositor EDS
% Data completeness (in resolution range)	93.5 (44.78-3.00) 93.2 (44.77-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.69 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.275 0.234 , 0.269	Depositor DCC
R_{free} test set	1831 reflections (9.77%)	wwPDB-VP
Wilson B-factor (Å ²)	72.7	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 79.2	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	0.93	EDS
Total number of atoms	5469	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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

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	0.43	0/1355	0.67	1/1832 (0.1%)
1	B	0.42	0/1355	0.68	1/1832 (0.1%)
1	C	0.42	0/1355	0.68	1/1832 (0.1%)
1	D	0.44	0/1355	0.67	1/1832 (0.1%)
All	All	0.43	0/5420	0.67	4/7328 (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	D	237	PHE	N-CA-C	-6.65	93.06	111.00
1	B	237	PHE	N-CA-C	-6.64	93.07	111.00
1	A	37	PHE	N-CA-C	-6.56	93.29	111.00
1	C	37	PHE	N-CA-C	-6.39	93.75	111.00

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	1330	0	1298	107	0
1	B	1330	0	1295	109	0
1	C	1330	0	1298	112	0
1	D	1330	0	1295	102	0
2	A	40	0	0	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	30	0	0	12	0
2	C	36	0	0	19	0
2	D	43	0	0	11	0
All	All	5469	0	5186	418	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 40.

The worst 5 of 418 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:247:GLU:HB3	1:B:274:ILE:HD12	1.44	0.99
1:A:47:GLU:HB3	1:A:74:ILE:HD12	1.44	0.99
1:D:247:GLU:HB3	1:D:274:ILE:HD12	1.45	0.98
1:C:47:GLU:HB3	1:C:74:ILE:HD12	1.45	0.97
1:D:306:MET:HG2	2:D:667:HOH:O	1.67	0.94

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	163/165 (99%)	133 (82%)	22 (14%)	8 (5%)	2	13
1	B	163/165 (99%)	133 (82%)	22 (14%)	8 (5%)	2	13
1	C	163/165 (99%)	133 (82%)	23 (14%)	7 (4%)	2	15
1	D	163/165 (99%)	133 (82%)	22 (14%)	8 (5%)	2	13
All	All	652/660 (99%)	532 (82%)	89 (14%)	31 (5%)	2	13

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	98	GLY
1	B	227	ASN
1	B	298	GLY
1	C	27	ASN

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	150/150 (100%)	143 (95%)	7 (5%)	26	63
1	B	150/150 (100%)	143 (95%)	7 (5%)	26	63
1	C	150/150 (100%)	142 (95%)	8 (5%)	22	58
1	D	150/150 (100%)	143 (95%)	7 (5%)	26	63
All	All	600/600 (100%)	571 (95%)	29 (5%)	25	62

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	333	LEU
1	C	34	CYS
1	D	292	LYS
1	C	29	GLU
1	C	73	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	320	HIS
1	C	12	HIS
1	D	212	HIS
1	B	300	HIS
1	D	248	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, 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	165/165 (100%)	-0.18	2 (1%) 79 54	50, 76, 100, 107	0
1	B	165/165 (100%)	-0.01	3 (1%) 68 40	55, 79, 102, 107	0
1	C	165/165 (100%)	0.07	5 (3%) 50 22	53, 79, 102, 108	0
1	D	165/165 (100%)	-0.08	2 (1%) 79 54	48, 77, 101, 108	0
All	All	660/660 (100%)	-0.05	12 (1%) 68 40	48, 78, 102, 108	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	90	ASP	3.6
1	D	290	ASP	2.7
1	B	230	THR	2.6
1	B	270	TRP	2.5
1	C	47	GLU	2.3

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.