



Full wwPDB X-ray Structure Validation Report

Apr 10, 2014 – 02:22 PM EDT

PDB ID : 4BHD
Title : Methanococcus jannaschii serine hydroxymethyl-transferase,apo form
Authors : Saccoccia, F.; Angelucci, F.; Ilari, A.
Deposited on : 2013-04-02
Resolution : 2.83 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

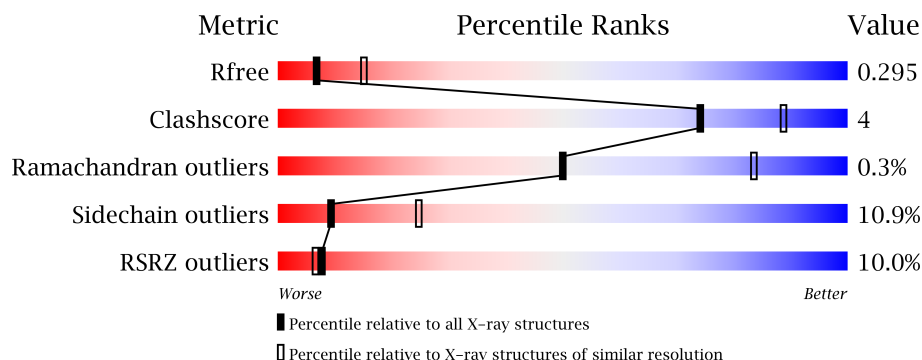
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : **FAILED**
Xtriage (Phenix) : dev-1439
EDS : stable22978
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22978

1 Overall quality at a glance

The reported resolution of this entry is 2.83 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}	66092	2270 (2.88-2.80)
Clashscore	79885	2848 (2.88-2.80)
Ramachandran outliers	78287	2786 (2.88-2.80)
Sidechain outliers	78261	2789 (2.88-2.80)
RSRZ outliers	66119	2274 (2.88-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	428	
1	B	428	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6412 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

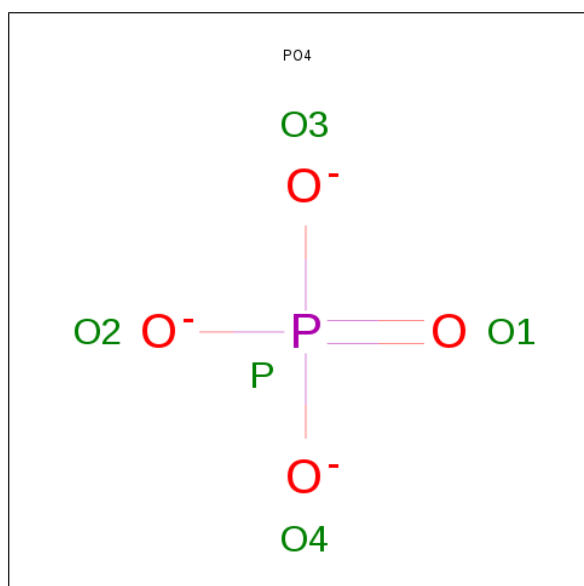
- Molecule 1 is a protein called SERINE HYDROXYMETHYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	S	0	0	0
			3269	2085	546	622	16			
1	B	395	Total	C	N	O	S	0	0	0
			3122	1991	516	598	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	EXPRESSION TAG	UNP Q58992
B	2	MET	-	EXPRESSION TAG	UNP Q58992

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

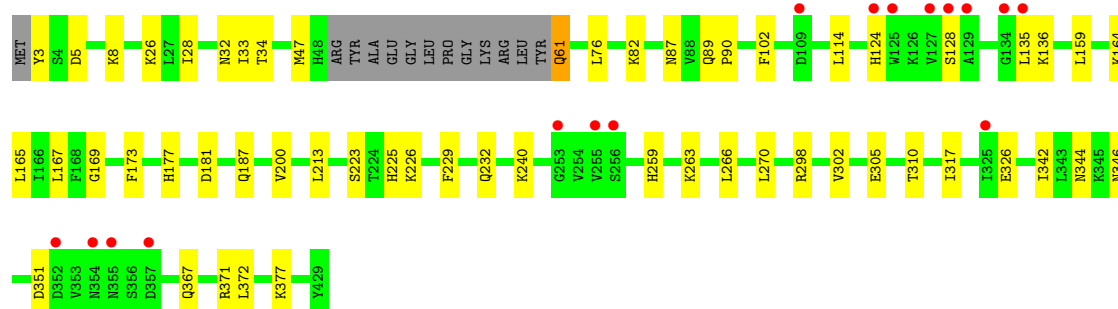
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	13	Total 13	O 13	0	0
3	B	3	Total 3	O 3	0	0

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 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 ($RSRZ > 2$). 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.

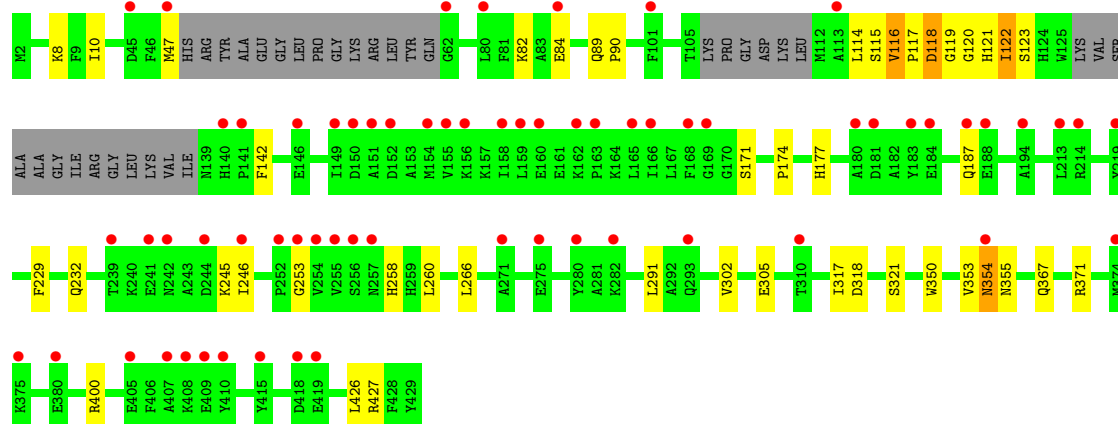
• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

Chain A: 



• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.59Å 110.16Å 110.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.83 49.45 – 2.82	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-2.83) 97.9 (49.45-2.82)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.242 , 0.298 0.243 , 0.295	Depositor DCC
R_{free} test set	1293 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	70.5	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.3	EDS
Estimated twinning fraction	0.026 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 25490 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6412	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.35	0/3341	0.56	3/4505 (0.1%)
1	B	0.36	0/3190	0.55	3/4300 (0.1%)
All	All	0.36	0/6531	0.56	6/8805 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	SER	N-CA-C	10.54	139.45	111.00
1	B	121	HIS	N-CA-C	8.01	132.62	111.00
1	B	121	HIS	CB-CA-C	-6.17	98.06	110.40
1	B	253	GLY	N-CA-C	-5.53	99.27	113.10
1	A	226	LYS	N-CA-C	5.41	125.59	111.00
1	A	128	SER	CB-CA-C	-5.23	100.16	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3269	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3122	0	0	17	0
2	B	5	0	0	0	0
3	A	13	0	0	0	0
3	B	3	0	0	0	0
All	All	6412	0	0	26	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (26) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:118:ASP:OD2	1:B:142:PHE:CD2	2.19	0.95
1:B:116:VAL:CG1	1:B:117:PRO:N	2.30	0.94
1:B:116:VAL:N	1:B:117:PRO:CD	2.30	0.94
1:B:118:ASP:OD2	1:B:142:PHE:CG	2.28	0.86
1:A:61:GLN:C	1:A:61:GLN:NE2	2.30	0.86
1:A:223:SER:OG	1:A:225:HIS:CD2	2.35	0.80
1:B:115:SER:OG	1:B:117:PRO:CD	2.30	0.79
1:B:115:SER:C	1:B:117:PRO:CD	2.63	0.66
1:B:122:ILE:O	1:B:122:ILE:CG1	2.44	0.65
1:B:116:VAL:O	1:B:120:GLY:N	2.30	0.65
1:A:61:GLN:O	1:A:61:GLN:NE2	2.30	0.65
1:A:223:SER:OG	1:A:225:HIS:NE2	2.31	0.63
1:B:353:VAL:O	1:B:355:ASN:N	2.31	0.63
1:B:115:SER:CB	1:B:117:PRO:CD	2.76	0.63
1:B:115:SER:OG	1:B:118:ASP:N	2.36	0.59
1:B:118:ASP:OD2	1:B:142:PHE:CB	2.50	0.59
1:B:115:SER:OG	1:B:117:PRO:CG	2.51	0.58
1:A:200:VAL:CG1	1:A:200:VAL:O	2.56	0.53
1:A:169:GLY:N	1:A:177:HIS:CD2	2.81	0.49
1:A:89:GLN:N	1:A:90:PRO:CD	2.77	0.48
1:A:47:MET:SD	1:A:47:MET:N	2.89	0.46
1:B:119:GLY:O	1:B:171:SER:N	2.50	0.45
1:B:89:GLN:N	1:B:90:PRO:CD	2.81	0.44
1:B:318:ASP:OD2	1:B:321:SER:OG	2.37	0.43
1:B:115:SER:OG	1:B:118:ASP:CB	2.68	0.41
1:A:32:ASN:OD1	1:A:33:ILE:N	2.54	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	411/428 (96%)	384 (93%)	27 (7%)	0	100	100
1	B	387/428 (90%)	347 (90%)	38 (10%)	2 (0%)	38	75
All	All	798/856 (93%)	731 (92%)	65 (8%)	2 (0%)	50	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	354	ASN
1	B	174	PRO

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	348/358 (97%)	304 (87%)	44 (13%)	7	18
1	B	333/358 (93%)	303 (91%)	30 (9%)	14	36
All	All	681/716 (95%)	607 (89%)	74 (11%)	9	25

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	TYR
1	A	5	ASP
1	A	8	LYS
1	A	26	LYS
1	A	28	ILE
1	A	34	THR
1	A	61	GLN

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Mol	Chain	Res	Type
1	A	76	LEU
1	A	82	LYS
1	A	87	ASN
1	A	102	PHE
1	A	114	LEU
1	A	124	HIS
1	A	135	LEU
1	A	136	LYS
1	A	159	LEU
1	A	164	LYS
1	A	165	LEU
1	A	167	LEU
1	A	173	PHE
1	A	181	ASP
1	A	187	GLN
1	A	213	LEU
1	A	229	PHE
1	A	232	GLN
1	A	240	LYS
1	A	259	HIS
1	A	263	LYS
1	A	266	LEU
1	A	270	LEU
1	A	298	ARG
1	A	302	VAL
1	A	305	GLU
1	A	310	THR
1	A	317	ILE
1	A	326	GLU
1	A	342	ILE
1	A	344	ASN
1	A	346	ASN
1	A	351	ASP
1	A	367	GLN
1	A	371	ARG
1	A	372	LEU
1	A	377	LYS
1	B	8	LYS
1	B	10	ILE
1	B	47	MET
1	B	82	LYS
1	B	84	GLU

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Mol	Chain	Res	Type
1	B	114	LEU
1	B	116	VAL
1	B	118	ASP
1	B	122	ILE
1	B	123	SER
1	B	177	HIS
1	B	187	GLN
1	B	229	PHE
1	B	232	GLN
1	B	245	LYS
1	B	246	ILE
1	B	258	HIS
1	B	260	LEU
1	B	266	LEU
1	B	291	LEU
1	B	302	VAL
1	B	305	GLU
1	B	317	ILE
1	B	350	TRP
1	B	354	ASN
1	B	367	GLN
1	B	371	ARG
1	B	400	ARG
1	B	426	LEU
1	B	427	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

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, 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	415/428 (96%)	0.34	16 (3%) 37 39	44, 66, 104, 130	0
1	B	395/428 (92%)	0.96	65 (16%) 2 2	56, 94, 166, 204	0
All	All	810/856 (94%)	0.64	81 (10%) 8 6	44, 79, 147, 204	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	352	ASP	7.7
1	B	241	GLU	7.4
1	B	183	TYR	7.3
1	B	155	VAL	6.7
1	B	244	ASP	6.1
1	B	159	LEU	6.0
1	B	149	ILE	6.0
1	B	180	ALA	5.6
1	B	156	LYS	5.6
1	B	194	ALA	5.5
1	B	151	ALA	5.4
1	B	113	ALA	5.3
1	B	162	LYS	5.3
1	B	163	PRO	5.1
1	A	255	VAL	4.7
1	A	355	ASN	4.5
1	B	146	GLU	4.4
1	B	165	LEU	4.4
1	B	257	ASN	4.4
1	B	181	ASP	4.2
1	B	252	PRO	4.1
1	B	158	ILE	4.0
1	B	184	GLU	4.0
1	B	419	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	124	HIS	3.9
1	B	242	ASN	3.9
1	A	134	GLY	3.8
1	B	219	TYR	3.8
1	A	325	ILE	3.8
1	B	256	SER	3.7
1	B	415	TYR	3.7
1	B	166	ILE	3.7
1	A	253	GLY	3.7
1	B	152	ASP	3.6
1	B	80	LEU	3.5
1	B	354	ASN	3.5
1	A	354	ASN	3.4
1	A	357	ASP	3.4
1	B	418	ASP	3.4
1	B	187	GLN	3.4
1	B	101	PHE	3.3
1	B	154	MET	3.2
1	B	374	MET	3.2
1	A	125	TRP	3.1
1	B	141	PRO	3.1
1	A	128	SER	3.0
1	A	135	LEU	3.0
1	B	408	LYS	2.9
1	B	62	GLY	2.9
1	B	84	GLU	2.9
1	B	168	PHE	2.8
1	B	280	TYR	2.7
1	A	256	SER	2.7
1	B	254	VAL	2.7
1	B	160	GLU	2.6
1	A	109	ASP	2.6
1	B	47	MET	2.6
1	B	375	LYS	2.6
1	B	310	THR	2.5
1	B	150	ASP	2.5
1	B	407	ALA	2.5
1	B	282	LYS	2.5
1	A	129	ALA	2.4
1	B	405	GLU	2.4
1	B	410	TYR	2.4
1	B	45	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	213	LEU	2.4
1	B	293	GLN	2.4
1	B	255	VAL	2.2
1	B	140	HIS	2.2
1	B	271	ALA	2.2
1	B	380	GLU	2.2
1	B	409	GLU	2.2
1	B	239	THR	2.2
1	B	214	ARG	2.2
1	B	246	ILE	2.1
1	B	188	GLU	2.1
1	B	275	GLU	2.0
1	A	127	VAL	2.0
1	B	169	GLY	2.0
1	B	253	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	PO4	B	1430	5/5	0.26	-0.11	54,54,55,55	5

6.5 Other polymers ⓘ

There are no such residues in this entry.