



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:07 PM GMT

PDB ID : 4HAC
Title : Crystal Structure of the Mevalonate Kinase from an Archaeon Methanosarcina mazei
Authors : Zhuang, N.; Lee, K.H.
Deposited on : 2012-09-26
Resolution : 1.92 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

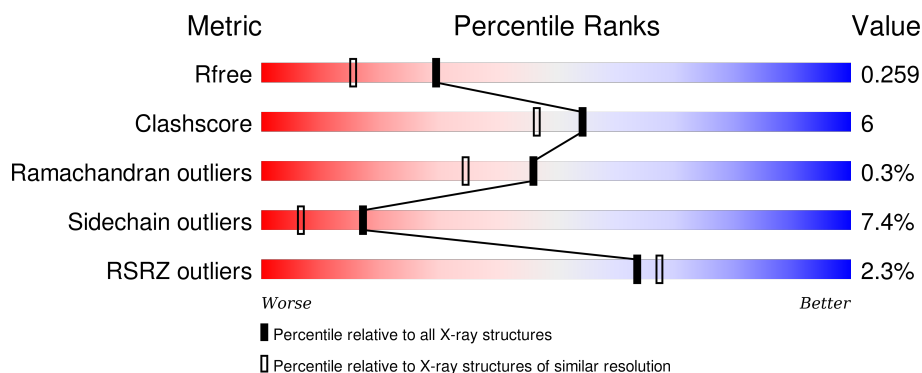
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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}	91344	5832 (1.94-1.90)
Clashscore	102246	6540 (1.94-1.90)
Ramachandran outliers	100387	6464 (1.94-1.90)
Sidechain outliers	100360	6465 (1.94-1.90)
RSRZ outliers	91569	5846 (1.94-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	321	
2	B	321	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4710 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 Mevalonate kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	312	2281	1435	394	442	6	4	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q8PW39
A	-18	GLY	-	EXPRESSION TAG	UNP Q8PW39
A	-17	SER	-	EXPRESSION TAG	UNP Q8PW39
A	-16	SER	-	EXPRESSION TAG	UNP Q8PW39
A	-15	HIS	-	EXPRESSION TAG	UNP Q8PW39
A	-14	HIS	-	EXPRESSION TAG	UNP Q8PW39
A	-13	HIS	-	EXPRESSION TAG	UNP Q8PW39
A	-12	HIS	-	EXPRESSION TAG	UNP Q8PW39
A	-11	HIS	-	EXPRESSION TAG	UNP Q8PW39
A	-10	HIS	-	EXPRESSION TAG	UNP Q8PW39
A	-9	SER	-	EXPRESSION TAG	UNP Q8PW39
A	-8	SER	-	EXPRESSION TAG	UNP Q8PW39
A	-7	GLY	-	EXPRESSION TAG	UNP Q8PW39
A	-6	LEU	-	EXPRESSION TAG	UNP Q8PW39
A	-5	VAL	-	EXPRESSION TAG	UNP Q8PW39
A	-4	PRO	-	EXPRESSION TAG	UNP Q8PW39
A	-3	ARG	-	EXPRESSION TAG	UNP Q8PW39
A	-2	GLY	-	EXPRESSION TAG	UNP Q8PW39
A	-1	SER	-	EXPRESSION TAG	UNP Q8PW39
A	0	HIS	-	EXPRESSION TAG	UNP Q8PW39

- Molecule 2 is a protein called Mevalonate kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	308	2261	1424	389	438	5	5	0	1	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	EXPRESSION TAG	UNP Q8PW39
B	-18	GLY	-	EXPRESSION TAG	UNP Q8PW39
B	-17	SER	-	EXPRESSION TAG	UNP Q8PW39
B	-16	SER	-	EXPRESSION TAG	UNP Q8PW39
B	-15	HIS	-	EXPRESSION TAG	UNP Q8PW39
B	-14	HIS	-	EXPRESSION TAG	UNP Q8PW39
B	-13	HIS	-	EXPRESSION TAG	UNP Q8PW39
B	-12	HIS	-	EXPRESSION TAG	UNP Q8PW39
B	-11	HIS	-	EXPRESSION TAG	UNP Q8PW39
B	-10	HIS	-	EXPRESSION TAG	UNP Q8PW39
B	-9	SER	-	EXPRESSION TAG	UNP Q8PW39
B	-8	SER	-	EXPRESSION TAG	UNP Q8PW39
B	-7	GLY	-	EXPRESSION TAG	UNP Q8PW39
B	-6	LEU	-	EXPRESSION TAG	UNP Q8PW39
B	-5	VAL	-	EXPRESSION TAG	UNP Q8PW39
B	-4	PRO	-	EXPRESSION TAG	UNP Q8PW39
B	-3	ARG	-	EXPRESSION TAG	UNP Q8PW39
B	-2	GLY	-	EXPRESSION TAG	UNP Q8PW39
B	-1	SER	-	EXPRESSION TAG	UNP Q8PW39
B	0	HIS	-	EXPRESSION TAG	UNP Q8PW39

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	55	Total O 55 55	0	0
4	B	111	Total O 111 111	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	97.30 Å 135.36 Å 45.87 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.93 – 1.92 40.93 – 1.92	Depositor EDS
% Data completeness (in resolution range)	98.9 (40.93-1.92) 98.9 (40.93-1.92)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 1.91 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.211 , 0.263 0.209 , 0.259	Depositor DCC
R_{free} test set	2382 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 47017 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4710	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.26% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG

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	0.97	1/2308 (0.0%)	0.97	5/3116 (0.2%)
2	B	1.11	1/2289 (0.0%)	0.99	5/3089 (0.2%)
All	All	1.04	2/4597 (0.0%)	0.98	10/6205 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6	ALA	CA-CB	6.18	1.65	1.52
1	A	234	VAL	CB-CG2	5.04	1.63	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	ARG	NE-CZ-NH2	-14.96	112.82	120.30
1	A	32	ARG	NE-CZ-NH1	11.74	126.17	120.30
2	B	32	ARG	NE-CZ-NH2	-8.67	115.96	120.30
2	B	106	LEU	CB-CG-CD1	6.42	121.92	111.00
1	A	32	ARG	CG-CD-NE	-5.97	99.26	111.80
2	B	218	ILE	CG1-CB-CG2	-5.69	98.88	111.40
2	B	54	LEU	CB-CG-CD2	5.42	120.22	111.00
1	A	184	LEU	CA-CB-CG	5.19	127.23	115.30
2	B	230	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	32	ARG	CD-NE-CZ	5.07	130.70	123.60

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	2281	0	2341	21	0
2	B	2261	0	2330	39	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	55	0	0	2	0
4	B	111	0	0	7	0
All	All	4710	0	4671	59	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 6.

All (59) 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)
2:B:185:ARG:HH11	2:B:185:ARG:HG2	1.03	1.20
2:B:90:SER:HB2	4:B:752:HOH:O	1.50	1.11
2:B:90:SER:O	2:B:92:LEU:N	1.95	0.98
2:B:185:ARG:NH1	2:B:185:ARG:HG2	1.83	0.90
2:B:107:ASN:HD21	2:B:114:LEU:H	1.19	0.85
2:B:107:ASN:HD22	2:B:112:PHE:HB2	1.41	0.84
1:A:22:GLU:HG3	1:A:200:GLY:HA3	1.59	0.82
1:A:107:ASN:HD21	1:A:114:LEU:H	1.30	0.78
1:A:48:GLN:HG2	4:A:714:HOH:O	1.85	0.76
2:B:201:LYS:HD2	2:B:204:ARG:HH12	1.50	0.75
1:A:107:ASN:HD22	1:A:112:PHE:HB2	1.52	0.74
1:A:30:GLU:OE2	1:A:32:ARG:HD2	1.88	0.73
2:B:207:GLU:O	2:B:211:LEU:HD22	1.87	0.73
2:B:91:GLY:CA	4:B:769:HOH:O	2.40	0.70
2:B:185:ARG:CG	2:B:185:ARG:HH11	1.94	0.69
2:B:39:LEU:HD22	2:B:109:LEU:HD11	1.75	0.68
2:B:15:GLU:O	4:B:701:HOH:O	2.13	0.67
1:A:22:GLU:HG3	1:A:200:GLY:CA	2.24	0.67
2:B:16:HIS:HE1	2:B:259:ALA:O	1.79	0.65
1:A:40:ASN:HD22	1:A:42:SER:H	1.46	0.61
2:B:39:LEU:CD2	2:B:109:LEU:HD11	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:TYR:CE2	2:B:221:LEU:HD11	2.37	0.59
2:B:239:LEU:HD13	2:B:256:ILE:HG12	1.83	0.59
2:B:91:GLY:N	4:B:769:HOH:O	2.36	0.58
2:B:275[B]:ASN:ND2	2:B:279:GLU:OE2	2.37	0.58
2:B:204:ARG:NH2	4:B:744:HOH:O	2.37	0.57
2:B:89:GLY:O	2:B:90:SER:CB	2.54	0.56
2:B:107:ASN:ND2	2:B:112:PHE:HB2	2.17	0.55
1:A:182:ARG:NH2	1:A:186:GLU:OE2	2.39	0.55
2:B:-6:LEU:HD23	2:B:-5:VAL:H	1.72	0.55
1:A:189:PRO:O	1:A:193:GLU:HG3	2.06	0.55
2:B:14:GLY:H	2:B:225:ASN:HD21	1.55	0.54
2:B:23:THR:HG21	2:B:204:ARG:HG3	1.88	0.54
1:A:172:SER:HB3	1:A:261:GLY:O	2.08	0.53
1:A:23:THR:HG23	1:A:150:ILE:O	2.07	0.53
1:A:204:ARG:HH11	1:A:204:ARG:HG3	1.74	0.51
2:B:-1:SER:HA	2:B:39:LEU:HD23	1.92	0.51
2:B:201:LYS:HD2	2:B:204:ARG:NH1	2.24	0.50
2:B:12:LEU:O	2:B:255:LYS:HE2	2.12	0.49
1:A:141:VAL:HG22	1:A:148:VAL:HG11	1.94	0.49
2:B:174:THR:O	2:B:178:VAL:HG23	2.12	0.49
2:B:12:LEU:O	2:B:255:LYS:CE	2.62	0.48
1:A:155:LYS:HG3	4:A:754:HOH:O	2.14	0.47
2:B:89:GLY:O	2:B:90:SER:HB3	2.15	0.47
2:B:61:TYR:CZ	2:B:95:SER:HB2	2.50	0.46
2:B:91:GLY:HA3	4:B:769:HOH:O	2.07	0.46
2:B:188:TYR:N	2:B:189:PRO:HD3	2.31	0.46
2:B:207:GLU:O	2:B:211:LEU:CD2	2.63	0.45
1:A:204:ARG:HG3	1:A:204:ARG:NH1	2.32	0.45
2:B:16:HIS:HD2	4:B:760:HOH:O	2.00	0.44
2:B:154:ARG:NH2	2:B:207:GLU:OE2	2.52	0.43
1:A:14:GLY:H	1:A:225:ASN:HD21	1.66	0.43
1:A:236:ILE:HD11	1:A:262:GLY:HA2	2.01	0.42
2:B:-2:GLY:O	2:B:39:LEU:HD21	2.19	0.42
2:B:154:ARG:CZ	2:B:154:ARG:CB	2.98	0.41
2:B:152:GLU:H	2:B:152:GLU:CD	2.22	0.41
1:A:217:SER:OG	1:A:220:ARG:NH2	2.54	0.41
1:A:73:ILE:HB	1:A:112:PHE:CZ	2.56	0.41
1:A:193:GLU:HB2	1:A:194:PRO:HD3	2.03	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	310/321 (97%)	303 (98%)	7 (2%)	0	100	100
2	B	307/321 (96%)	295 (96%)	10 (3%)	2 (1%)	26	13
All	All	617/642 (96%)	598 (97%)	17 (3%)	2 (0%)	46	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	90	SER
2	B	91	GLY

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	244/249 (98%)	229 (94%)	15 (6%)	23	11
2	B	243/248 (98%)	222 (91%)	21 (9%)	13	4
All	All	487/497 (98%)	451 (93%)	36 (7%)	17	7

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	22	GLU
1	A	40	ASN
1	A	90	SER

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Mol	Chain	Res	Type
1	A	106	LEU
1	A	131	GLN
1	A	175	LYS
1	A	183	GLN
1	A	184	LEU
1	A	191	LEU
1	A	195	LEU
1	A	211	LEU
1	A	237	LEU
1	A	274	CYS
1	A	295	GLU
2	B	-6	LEU
2	B	9	LYS
2	B	15	GLU
2	B	19	VAL
2	B	39	LEU
2	B	49	ILE
2	B	54	LEU
2	B	57	GLU
2	B	106	LEU
2	B	152	GLU
2	B	172	SER
2	B	183	GLN
2	B	185	ARG
2	B	187	SER
2	B	190	ASP
2	B	191	LEU
2	B	193	GLU
2	B	201	LYS
2	B	211	LEU
2	B	232	LEU
2	B	237	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-10	HIS
1	A	0	HIS
1	A	16	HIS
1	A	40	ASN
1	A	48	GLN
1	A	107	ASN

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Mol	Chain	Res	Type
1	A	124	HIS
1	A	131	GLN
1	A	225	ASN
1	A	235	ASN
1	A	276	GLN
2	B	16	HIS
2	B	76	ASN
2	B	107	ASN
2	B	131	GLN
2	B	225	ASN
2	B	235	ASN
2	B	241	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 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	308/321 (95%)	0.13	7 (2%) 64 67	27, 42, 61, 71	0
2	B	303/321 (94%)	0.22	7 (2%) 64 67	24, 37, 55, 65	0
All	All	611/642 (95%)	0.18	14 (2%) 64 67	24, 40, 59, 71	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	88	VAL	4.9
2	B	182	ARG	4.2
2	B	-6	LEU	4.0
2	B	177	LEU	3.2
1	A	171	PHE	2.9
2	B	181	VAL	2.9
1	A	50	GLY	2.5
1	A	211	LEU	2.5
1	A	41	ASP	2.4
1	A	182	ARG	2.4
1	A	51	ARG	2.4
1	A	88	VAL	2.2
2	B	180	ASN	2.1
2	B	171	PHE	2.0

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](#)

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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	B	601	1/1	0.99	0.14	0.85	30,30,30,30	0
3	MG	A	601	1/1	0.99	0.14	0.43	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.