

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	8QPM
Title	:	Structure of methylene-tetrahydromethanopterin reductase from Methanocal-
		dococcus jannaschii
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Deposited on	:	2023-10-02
Resolution	:	1.80 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 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	:	2.36.2
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)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.80 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.



Matria	Whole archive	Similar resolution			
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$			
R_{free}	130704	5950(1.80-1.80)			
Clashscore	141614	6793 (1.80-1.80)			
Ramachandran outliers	138981	6697 (1.80-1.80)			
Sidechain outliers	138945	6696 (1.80-1.80)			
RSRZ outliers	127900	5850 (1.80-1.80)			

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 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	А	335	93%	5% ••				
1	В	335	93%	6% ·				
1	С	335	86%	12% •				
1	D	335	87%	11% ••				



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2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 20639 atoms, of which 10151 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.

Mol	Chain	Residues			Atom	s			ZeroOcc	AltConf	Trace
1	Δ	320	Total	С	Η	Ν	0	\mathbf{S}	0	0	0
1	Π	525	5006	1576	2545	409	461	15	0	0	0
1	В	320	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
1		529	5006	1576	2545	409	461	15	0	0	0
1	С	397	Total	С	Η	Ν	0	S	0	0	0
	321	4977	1567	2529	407	459	15	0	0		
1	Л	320	Total	С	Н	Ν	0	S	0	0	0
	D	529	4993	1576	2532	409	461	51 15	0	0	U

• Molecule 1 is a protein called 5,10-methylenetetrahydromethanopterin reductase.

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	332	ALA	-	expression tag	UNP A0A832SYB5
А	333	LEU	-	expression tag	UNP A0A832SYB5
А	334	LYS	-	expression tag	UNP A0A832SYB5
А	335	GLU	-	expression tag	UNP A0A832SYB5
В	332	ALA	-	expression tag	UNP A0A832SYB5
В	333	LEU	-	expression tag	UNP A0A832SYB5
В	334	LYS	-	expression tag	UNP A0A832SYB5
В	335	GLU	-	expression tag	UNP A0A832SYB5
С	332	ALA	-	expression tag	UNP A0A832SYB5
С	333	LEU	-	expression tag	UNP A0A832SYB5
С	334	LYS	-	expression tag	UNP A0A832SYB5
С	335	GLU	-	expression tag	UNP A0A832SYB5
D	332	ALA	-	expression tag	UNP A0A832SYB5
D	333	LEU	-	expression tag	UNP A0A832SYB5
D	334	LYS	-	expression tag	UNP A0A832SYB5
D	335	GLU	-	expression tag	UNP A0A832SYB5

• Molecule 2 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	213	Total O 213 213	0	0
2	В	210	Total O 210 210	0	0
2	С	126	Total O 126 126	0	0
2	D	108	Total O 108 108	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: 5,10-methylenetetrahydromethanopterin reductase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	96.66Å 96.28Å 166.78Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	48.33 - 1.80	Depositor
Resolution (A)	48.33 - 1.80	EDS
% Data completeness	99.8 (48.33-1.80)	Depositor
(in resolution range)	98.8(48.33-1.80)	EDS
R_{merge}	0.11	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.75 (at 1.79 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
D D.	0.180 , 0.202	Depositor
Π, Π_{free}	0.180 , 0.203	DCC
R_{free} test set	2003 reflections $(1.39%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	33.7	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.40 , 52.5	EDS
L-test for $twinning^2$	$< L >=0.49, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.407 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20639	wwPDB-VP
Average B, all atoms $(Å^2)$	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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	Bond	lengths	Bond angles		
10101	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.45	0/2505	0.63	0/3394	
1	В	0.44	0/2505	0.64	1/3394~(0.0%)	
1	С	0.40	0/2492	0.59	0/3376	
1	D	0.46	0/2505	0.65	0/3394	
All	All	0.44	0/10007	0.63	1/13558~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	251	GLU	CA-CB-CG	-6.07	100.05	113.40

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	А	2461	2545	2545	18	0
1	В	2461	2545	2545	9	0
1	С	2448	2529	2529	29	0
1	D	2461	2532	2545	23	0
2	А	213	0	0	1	0
2	В	210	0	0	0	0
2	С	126	0	0	0	0
2	D	108	0	0	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10488	10151	10164	78	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.

All (78) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:282:ILE:HG22	1:D:289:VAL:HG13	1.65	0.79
1:A:151:LYS:H	1:A:151:LYS:HE2	1.51	0.76
1:A:240:PRO:O	1:A:244:GLU:HG3	1.93	0.68
1:D:285:THR:O	1:D:289:VAL:HG23	1.95	0.67
1:A:151:LYS:H	1:A:151:LYS:CE	2.09	0.65
1:C:259:ALA:HB3	1:C:268:ALA:HB2	1.79	0.65
1:C:231:VAL:HG21	1:C:277:LEU:HD23	1.81	0.63
1:A:151:LYS:H	1:A:151:LYS:CD	2.13	0.62
1:C:151:LYS:HD2	1:C:152:ALA:H	1.64	0.62
1:D:231:VAL:HG21	1:D:277:LEU:HD23	1.82	0.61
1:D:181:ASN:ND2	1:D:279:ALA:HB1	2.15	0.61
1:C:161:GLY:O	1:C:165:LEU:HD12	2.01	0.61
1:D:256:ILE:HG23	1:D:268:ALA:HB1	1.81	0.60
1:D:181:ASN:HD22	1:D:246:HIS:CE1	2.19	0.60
1:C:162:PRO:HA	1:C:165:LEU:HD13	1.86	0.58
1:D:162:PRO:HA	1:D:191:LEU:HD22	1.85	0.57
1:C:216:VAL:HG22	1:C:289:VAL:HG21	1.87	0.57
1:A:163:LYS:H	1:A:163:LYS:CD	2.19	0.56
1:C:287:GLU:OE1	1:C:287:GLU:N	2.26	0.55
1:A:163:LYS:H	1:A:163:LYS:HE2	1.72	0.53
1:A:219:ASN:HB3	1:A:222:LYS:HG3	1.91	0.53
1:C:133:GLU:OE1	1:C:138:LYS:HE3	2.09	0.53
1:D:266:PRO:O	1:D:270:LYS:HG3	2.08	0.52
1:D:222:LYS:HE2	1:D:312:PRO:HB3	1.92	0.51
1:D:181:ASN:HD21	1:D:280:PHE:H	1.57	0.51
1:C:326:ILE:N	1:C:327:PRO:HD2	2.26	0.51
1:C:166:GLU:OE2	1:C:191:LEU:HD23	2.12	0.50
1:D:273:ASP:OD1	1:D:276:MET:HG3	2.12	0.50
1:D:288:ASP:O	1:D:292:LYS:HG3	2.12	0.49
1:A:163:LYS:H	1:A:163:LYS:HD3	1.76	0.49
1:A:163:LYS:H	1:A:163:LYS:CE	2.25	0.49
1:C:165:LEU:HD12	1:C:165:LEU:H	1.77	0.49
1:A:202:SER:O	1:A:205:GLU:HG2	2.13	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:235:ALA:HA	1:C:280:PHE:HE2	1.78	0.49
1:D:282:ILE:CG2	1:D:289:VAL:HG13	2.39	0.48
1:D:276:MET:O	1:D:279:ALA:O	2.32	0.48
1:C:242:VAL:HG22	1:C:245:ARG:HH21	1.79	0.47
1:C:165:LEU:CD2	1:C:188:ALA:HB1	2.45	0.46
1:D:272:VAL:HA	1:D:276:MET:SD	2.55	0.46
1:D:326:ILE:N	1:D:327:PRO:CD	2.79	0.46
1:A:230:VAL:HG23	2:A:423:HOH:O	2.16	0.45
1:A:293:CYS:SG	1:A:304:ILE:HD13	2.56	0.45
1:B:216:VAL:HG22	1:B:289:VAL:HG21	1.97	0.45
1:A:151:LYS:CD	1:A:151:LYS:N	2.79	0.45
1:C:151:LYS:HD2	1:C:152:ALA:N	2.30	0.45
1:C:295:LYS:N	1:C:295:LYS:HD3	2.32	0.45
1:A:115:LYS:NZ	1:A:119:GLU:OE1	2.50	0.45
1:B:22:LEU:HD11	1:B:319:LYS:HE3	1.99	0.44
1:A:220:ALA:HB2	1:A:285:THR:HG23	1.99	0.44
1:C:111:VAL:HG22	1:C:164:MET:CE	2.46	0.44
1:C:55:LYS:HE2	1:C:55:LYS:HB2	1.81	0.44
1:D:135:LYS:HB3	1:D:135:LYS:HE3	1.79	0.44
1:C:235:ALA:CB	1:C:276:MET:CE	2.96	0.43
1:D:6:GLU:HG3	1:D:211:TYR:OH	2.19	0.43
1:B:326:ILE:N	1:B:327:PRO:CD	2.81	0.43
1:C:278:GLU:O	1:C:278:GLU:HG3	2.18	0.43
1:C:256:ILE:HG23	1:C:268:ALA:HB1	2.00	0.43
1:C:51:MET:CE	1:D:51:MET:CE	2.96	0.43
1:C:258:ASN:HA	1:C:261:LYS:CD	2.50	0.42
1:D:108:VAL:O	1:D:109:LYS:C	2.58	0.42
1:B:294:LYS:O	1:B:298:GLU:HG3	2.20	0.42
1:C:280:PHE:CD1	1:C:280:PHE:N	2.88	0.42
1:D:286:PRO:O	1:D:290:VAL:HG23	2.20	0.42
1:A:217:ASP:O	1:A:285:THR:HA	2.19	0.42
1:B:166:GLU:O	1:B:170:MET:HG3	2.20	0.42
1:C:258:ASN:HA	1:C:261:LYS:HD2	2.02	0.41
1:A:202:SER:O	1:A:205:GLU:CG	2.69	0.41
1:B:202:SER:O	1:B:205:GLU:HG2	2.20	0.41
1:C:222:LYS:HE2	1:C:312:PRO:HB3	2.02	0.41
1:B:193:LYS:HD2	1:B:197:GLU:HG2	2.03	0.41
1:D:292:LYS:O	1:D:296:LEU:CD1	2.68	0.41
1:B:189:ILE:HD12	1:B:299:MET:O	2.21	0.40
1:B:265:PHE:N	1:B:266:PRO:CD	2.83	0.40
1:C:111:VAL:HG22	1:C:164:MET:HE2	2.02	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LYS:HD3	1:A:163:LYS:N	2.36	0.40
1:C:280:PHE:N	1:C:280:PHE:HD1	2.19	0.40
1:C:285:THR:HB	1:C:286:PRO:HD2	2.03	0.40
1:D:193:LYS:HD2	1:D:197:GLU:HG2	2.03	0.40

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	Perce	entiles
1	А	327/335~(98%)	321 (98%)	6 (2%)	0	100	100
1	В	327/335~(98%)	320 (98%)	7 (2%)	0	100	100
1	С	325/335~(97%)	315~(97%)	10 (3%)	0	100	100
1	D	327/335~(98%)	317 (97%)	10 (3%)	0	100	100
All	All	1306/1340~(98%)	1273 (98%)	33 (2%)	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	Outliers	Percentiles
1	А	258/263~(98%)	254 (98%)	4 (2%)	62 54
1	В	258/263~(98%)	258 (100%)	0	100 100



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	С	257/263~(98%)	253~(98%)	4 (2%)	62	54
1	D	258/263~(98%)	253~(98%)	5 (2%)	57	46
All	All	1031/1052~(98%)	1018 (99%)	13 (1%)	69	62

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	147	LYS
1	А	151	LYS
1	А	163	LYS
1	А	261	LYS
1	С	151	LYS
1	С	211	TYR
1	С	274	ASP
1	С	281	SER
1	D	151	LYS
1	D	180	SER
1	D	191	LEU
1	D	211	TYR
1	D	221	ASP

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such side chains are listed below:

Mol	Chain	Res	Type
1	С	181	ASN
1	D	181	ASN
1	D	246	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)

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, 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>2	$OWAB(Å^2)$	Q<0.9
1	А	329/335~(98%)	-0.18	1 (0%) 94 92	24, 37, 57, 75	0
1	В	329/335~(98%)	-0.24	1 (0%) 94 92	25, 38, 59, 82	0
1	С	327/335~(97%)	0.46	35 (10%) 6 4	28, 57, 122, 154	0
1	D	329/335~(98%)	0.74	53 (16%) 1 1	30, 56, 148, 174	0
All	All	1314/1340~(98%)	0.19	90 (6%) 17 13	24, 45, 117, 174	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	248	ILE	10.3
1	D	260	LEU	9.3
1	D	257	ARG	9.2
1	D	242	VAL	7.8
1	D	271	ASN	7.6
1	D	234	ILE	7.3
1	С	248	ILE	7.0
1	D	277	LEU	6.4
1	D	275	THR	6.0
1	D	230	VAL	5.8
1	D	183	LYS	5.8
1	D	262	SER	5.6
1	D	268	ALA	5.6
1	D	280	PHE	5.5
1	D	181	ASN	5.5
1	D	233	PHE	5.3
1	С	256	ILE	5.2
1	С	260	LEU	5.2
1	С	277	LEU	5.1
1	D	272	VAL	5.1
1	D	239	PRO	4.8



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Mol	Chain	Res	Type	RSRZ
1	D	236	ALA	4.7
1	С	230	VAL	4.6
1	D	254	GLU	4.6
1	С	261	LYS	4.6
1	D	246	HIS	4.4
1	D	283	TYR	4.3
1	D	178	ASN	4.2
1	С	268	ALA	4.2
1	С	280	PHE	4.2
1	С	160	GLN	4.2
1	D	276	MET	4.1
1	С	283	TYR	4.1
1	D	261	LYS	3.9
1	D	185	PHE	3.9
1	С	233	PHE	3.8
1	D	258	ASN	3.8
1	С	250	MET	3.7
1	D	269	PHE	3.7
1	D	243	LEU	3.7
1	D	253	VAL	3.6
1	D	329	LEU	3.5
1	С	234	ILE	3.5
1	D	282	ILE	3.3
1	D	279	ALA	3.3
1	D	256	ILE	3.3
1	D	255	ALA	3.3
1	С	276	MET	3.3
1	С	183	LYS	3.2
1	D	265	PHE	3.1
1	С	236	ALA	3.1
1	С	251	GLU	3.0
1	C	185	PHE	3.0
1	C	239	PRO	3.0
1	C	246	HIS	3.0
1	D	300	GLY	2.9
1	D	278	GLU	2.9
1	D	237	GLY	2.9
1	С	242	VAL	2.8
1	D	199	ALA	2.7
1	С	161	GLY	2.7
1	D	232	ALA	2.7
1	С	271	ASN	2.7



Mol	Chain	Res	Type	RSRZ
1	D	211	TYR	2.7
1	С	259	ALA	2.6
1	С	257	ARG	2.6
1	D	297	ALA	2.6
1	D	247	GLY	2.5
1	С	244	GLU	2.5
1	С	241	VAL	2.5
1	D	264	ASN	2.5
1	А	31	CYS	2.4
1	С	272	VAL	2.4
1	D	301	VAL	2.4
1	D	184	ASP	2.4
1	D	244	GLU	2.3
1	С	273	ASP	2.3
1	С	253	VAL	2.3
1	D	229	PRO	2.2
1	D	192	ILE	2.2
1	D	250	MET	2.2
1	В	329	LEU	2.2
1	С	258	ASN	2.2
1	D	290	VAL	2.2
1	С	232	ALA	2.2
1	С	262	SER	2.1
1	С	192	ILE	2.1
1	D	267	GLU	2.1
1	D	108	VAL	2.1
1	С	238	SER	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)

There are no ligands in this entry.



6.5 Other polymers (i)

There are no such residues in this entry.

