



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:51 PM GMT

PDB ID : 1VH1
Title : Crystal structure of CMP-KDO synthetase
Authors : Structural GenomiX
Deposited on : 2003-12-01
Resolution : 2.60 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
<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

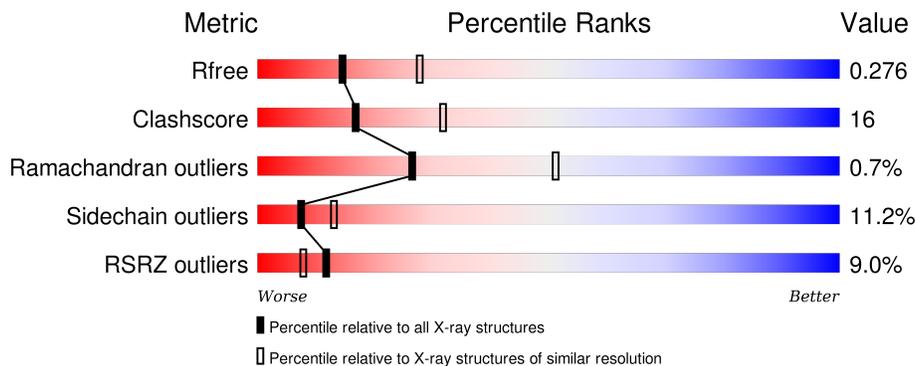
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	256	8% (Poor fit) 64% (0 outliers), 24% (1 outlier), 5% (2 outliers), 7% (3+ outliers) 64% (0 outliers), 27% (1 outlier), 8% (2 outliers), 13% (3+ outliers)
1	B	256	11% (Poor fit) 51% (0 outliers), 27% (1 outlier), 8% (2 outliers), 13% (3+ outliers) 64% (0 outliers), 22% (1 outlier), 5% (2 outliers), 9% (3+ outliers)
1	C	256	6% (Poor fit) 60% (0 outliers), 29% (1 outlier), 5% (2 outliers), 6% (3+ outliers)

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 7321 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 3-deoxy-manno-octulosonate cytidyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	239	Total 1826	C 1157	N 324	O 337	S 2	Se 6	0	0	0
1	B	224	Total 1729	C 1096	N 310	O 315	S 2	Se 6	0	0	0
1	C	233	Total 1782	C 1133	N 313	O 328	S 2	Se 6	0	0	0
1	D	241	Total 1828	C 1161	N 321	O 338	S 2	Se 6	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	cloning artifact	UNP P04951
A	29	MSE	MET	modified residue	UNP P04951
A	67	MSE	MET	modified residue	UNP P04951
A	103	MSE	MET	modified residue	UNP P04951
A	123	MSE	MET	modified residue	UNP P04951
A	208	MSE	MET	modified residue	UNP P04951
A	247	MSE	MET	modified residue	UNP P04951
A	249	GLY	-	cloning artifact	UNP P04951
A	250	SER	-	cloning artifact	UNP P04951
A	251	HIS	-	cloning artifact	UNP P04951
A	252	HIS	-	cloning artifact	UNP P04951
A	253	HIS	-	cloning artifact	UNP P04951
A	254	HIS	-	cloning artifact	UNP P04951
A	255	HIS	-	cloning artifact	UNP P04951
A	256	HIS	-	cloning artifact	UNP P04951
B	1	MSE	-	cloning artifact	UNP P04951
B	29	MSE	MET	modified residue	UNP P04951
B	67	MSE	MET	modified residue	UNP P04951
B	103	MSE	MET	modified residue	UNP P04951
B	123	MSE	MET	modified residue	UNP P04951
B	208	MSE	MET	modified residue	UNP P04951

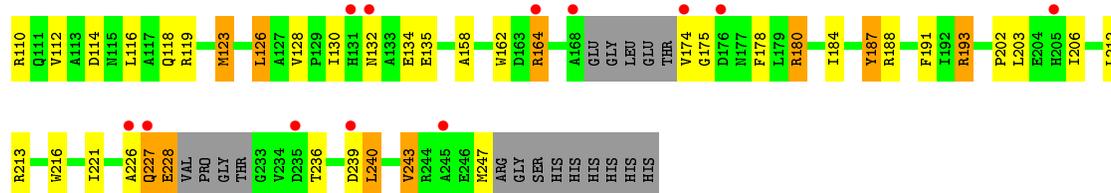
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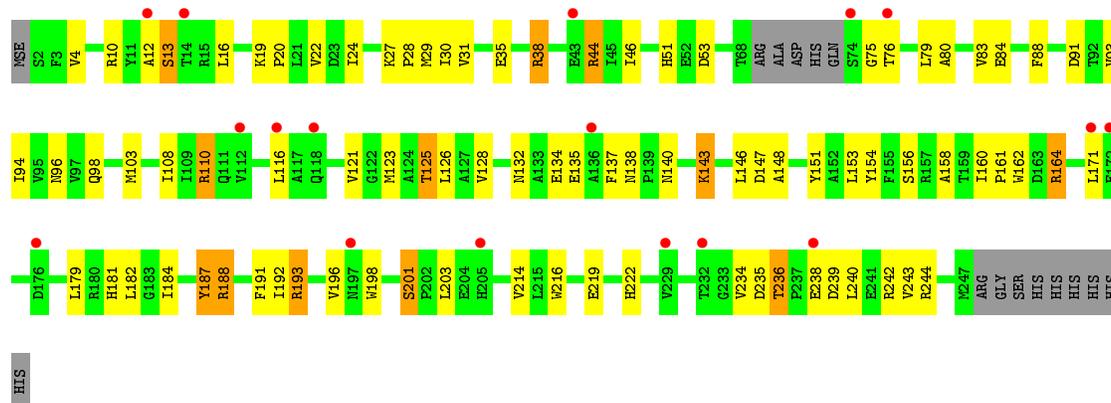
Chain	Residue	Modelled	Actual	Comment	Reference
B	247	MSE	MET	modified residue	UNP P04951
B	249	GLY	-	cloning artifact	UNP P04951
B	250	SER	-	cloning artifact	UNP P04951
B	251	HIS	-	cloning artifact	UNP P04951
B	252	HIS	-	cloning artifact	UNP P04951
B	253	HIS	-	cloning artifact	UNP P04951
B	254	HIS	-	cloning artifact	UNP P04951
B	255	HIS	-	cloning artifact	UNP P04951
B	256	HIS	-	cloning artifact	UNP P04951
C	1	MSE	-	cloning artifact	UNP P04951
C	29	MSE	MET	modified residue	UNP P04951
C	67	MSE	MET	modified residue	UNP P04951
C	103	MSE	MET	modified residue	UNP P04951
C	123	MSE	MET	modified residue	UNP P04951
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C	252	HIS	-	cloning artifact	UNP P04951
C	253	HIS	-	cloning artifact	UNP P04951
C	254	HIS	-	cloning artifact	UNP P04951
C	255	HIS	-	cloning artifact	UNP P04951
C	256	HIS	-	cloning artifact	UNP P04951
D	1	MSE	-	cloning artifact	UNP P04951
D	29	MSE	MET	modified residue	UNP P04951
D	67	MSE	MET	modified residue	UNP P04951
D	103	MSE	MET	modified residue	UNP P04951
D	123	MSE	MET	modified residue	UNP P04951
D	208	MSE	MET	modified residue	UNP P04951
D	247	MSE	MET	modified residue	UNP P04951
D	249	GLY	-	cloning artifact	UNP P04951
D	250	SER	-	cloning artifact	UNP P04951
D	251	HIS	-	cloning artifact	UNP P04951
D	252	HIS	-	cloning artifact	UNP P04951
D	253	HIS	-	cloning artifact	UNP P04951
D	254	HIS	-	cloning artifact	UNP P04951
D	255	HIS	-	cloning artifact	UNP P04951
D	256	HIS	-	cloning artifact	UNP P04951

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	45	Total 45	O 45	0	0
2	B	34	Total 34	O 34	0	0
2	C	42	Total 42	O 42	0	0
2	D	35	Total 35	O 35	0	0



• Molecule 1: 3-deoxy-manno-octulosonate cytidyltransferase



HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.59Å 130.81Å 159.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.60 19.92 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.92-2.60) 100.0 (19.92-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.88 (at 2.59Å)	Xtriage
Refinement program	REFMAC 4	Depositor
R, R_{free}	0.240 , 0.302 0.220 , 0.276	Depositor DCC
R_{free} test set	1718 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 33904 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7321	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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](#)

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	0.61	0/1856	1.11	13/2517 (0.5%)
1	B	0.60	0/1755	1.15	14/2374 (0.6%)
1	C	0.62	0/1810	1.12	9/2453 (0.4%)
1	D	0.61	0/1859	1.15	12/2525 (0.5%)
All	All	0.61	0/7280	1.13	48/9869 (0.5%)

There are no bond length outliers.

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	38	ARG	CD-NE-CZ	12.28	140.79	123.60
1	C	193	ARG	CD-NE-CZ	10.70	138.58	123.60
1	D	38	ARG	NE-CZ-NH1	10.33	125.46	120.30
1	A	78	ARG	CD-NE-CZ	10.05	137.67	123.60
1	D	188	ARG	NE-CZ-NH1	-9.77	115.42	120.30

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	1826	0	1785	45	0
1	B	1729	0	1693	80	0
1	C	1782	0	1741	54	0
1	D	1828	0	1786	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	45	0	0	2	0
2	B	34	0	0	4	0
2	C	42	0	0	3	0
2	D	35	0	0	5	0
All	All	7321	0	7005	232	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 16.

The worst 5 of 232 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:C:103:MSE:HG3	1:C:247:MSE:HE2	1.46	0.97
1:B:49:THR:HG21	1:B:54:VAL:HB	1.54	0.89
1:D:236:THR:HG22	1:D:239:ASP:H	1.37	0.88
1:B:125:THR:HG21	1:B:181:HIS:HE1	1.40	0.87
1:A:29:MSE:HG3	1:A:102:PRO:HG3	1.57	0.86

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	233/256 (91%)	225 (97%)	8 (3%)	0	100	100
1	B	216/256 (84%)	202 (94%)	11 (5%)	3 (1%)	14	28
1	C	225/256 (88%)	215 (96%)	9 (4%)	1 (0%)	39	65
1	D	237/256 (93%)	230 (97%)	5 (2%)	2 (1%)	24	46
All	All	911/1024 (89%)	872 (96%)	33 (4%)	6 (1%)	26	51

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	227	GLN
1	D	13	SER
1	B	96	ASN
1	B	97	VAL
1	D	75	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	185/203 (91%)	166 (90%)	19 (10%)	9 16
1	B	174/203 (86%)	143 (82%)	31 (18%)	2 3
1	C	180/203 (89%)	165 (92%)	15 (8%)	14 27
1	D	185/203 (91%)	169 (91%)	16 (9%)	13 25
All	All	724/812 (89%)	643 (89%)	81 (11%)	7 13

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	143	LYS
1	B	203	LEU
1	D	146	LEU
1	B	146	LEU
1	B	166	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	120	GLN
1	B	181	HIS
1	C	98	GLN
1	B	115	ASN
1	C	120	GLN

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	233/256 (91%)	0.51	21 (9%) 12 8	51, 64, 94, 120	0
1	B	218/256 (85%)	0.70	29 (13%) 4 3	49, 68, 101, 124	0
1	C	227/256 (88%)	0.42	15 (6%) 22 16	49, 63, 95, 104	0
1	D	235/256 (91%)	0.55	17 (7%) 18 13	51, 68, 99, 111	0
All	All	913/1024 (89%)	0.54	82 (8%) 12 8	49, 66, 98, 124	0

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	74	SER	6.0
1	B	24	ILE	5.4
1	D	14	THR	5.1
1	C	73	GLN	5.1
1	D	176	ASP	4.6

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

There are no such residues in this entry.