



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:46 PM GMT

PDB ID : 1H6J
Title : The three-dimensional structure of capsule-specific CMP:2-keto-3-deoxy-mannono-octonic acid synthetase from Escherichia coli
Authors : Jelakovic, S.; Jann, K.; Schulz, G.E.
Deposited on : 2001-06-17
Resolution : 2.32 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

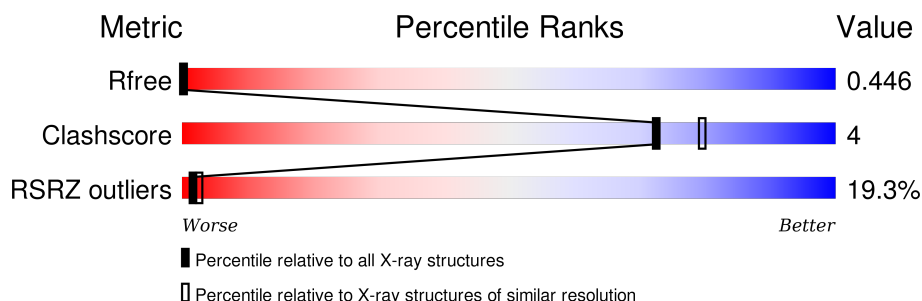
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

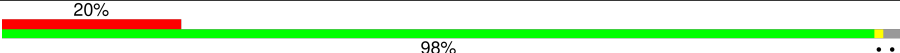
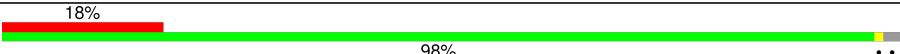
The reported resolution of this entry is 2.32 Å.

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	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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	245	
1	B	245	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 482 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.

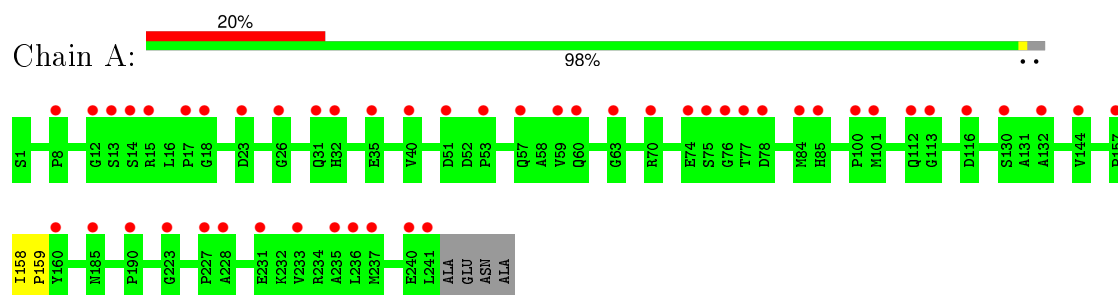
- Molecule 1 is a protein called 3-DEOXY-MANNO-OCTULOSONATE CYTIDYLYL-TRANSFERASE.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	241	Total 241	C 241	0	0	241
1	B	241	Total 241	C 241	0	0	241

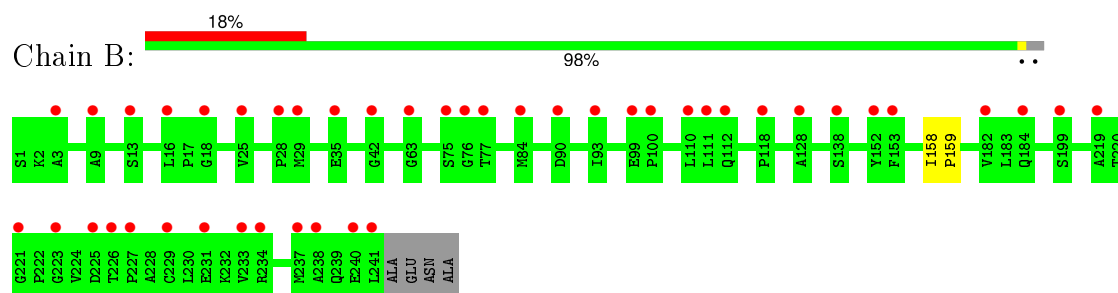
3 Residue-property plots

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: 3-DEOXY-MANNO-OCTULOSONATE CYTIDYLYLTRANSFERASE



- Molecule 1: 3-DEOXY-MANNO-OCTULOSONATE CYTIDYLYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.09 Å 133.46 Å 48.33 Å 90.00° 102.51° 90.00°	Depositor
Resolution (Å)	10.00 – 2.32 24.60 – 2.32	Depositor EDS
% Data completeness (in resolution range)	90.0 (10.00-2.32) 86.7 (24.60-2.32)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.33 Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.225 , 0.266 0.427 , 0.446	Depositor DCC
R_{free} test set	1091 reflections (5.14%)	DCC
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.71 , 461.0	EDS
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 21232 reflections	Xtriage
F_o, F_c correlation	0.49	EDS
Total number of atoms	482	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% 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](#)

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

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	241	0	0	1	0
1	B	241	0	0	1	0
All	All	482	0	0	2	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 (2) 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:158:ILE:CA	1:B:159:PRO:CA	2.91	0.48
1:A:158:ILE:CA	1:A:159:PRO:CA	2.91	0.48

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 ⓘ

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	241/245 (98%)	1.26	49 (20%) 1 2	2, 11, 40, 49	0
1	B	241/245 (98%)	1.06	44 (18%) 2 3	2, 10, 37, 47	0
All	All	482/490 (98%)	1.16	93 (19%) 2 2	2, 11, 39, 49	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	77	THR	26.6
1	A	231	GLU	20.6
1	A	240	GLU	19.3
1	A	17	PRO	17.9
1	A	237	MET	10.3
1	A	228	ALA	10.0
1	A	236	LEU	9.6
1	B	42	GLY	8.2
1	A	26	GLY	8.2
1	B	231	GLU	7.8
1	B	241	LEU	7.5
1	A	235	ALA	7.1
1	A	18	GLY	7.1
1	B	234	ARG	6.8
1	B	237	MET	6.5
1	A	223	GLY	6.1
1	B	99	GLU	5.8
1	A	60	GLN	5.4
1	A	32	HIS	5.4
1	B	112	GLN	5.3
1	B	238	ALA	5.2
1	B	13	SER	5.1
1	A	116	ASP	4.9
1	A	63	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	227	PRO	4.7
1	A	130	SER	4.7
1	A	53	PRO	4.6
1	B	28	PRO	4.5
1	A	77	THR	4.5
1	B	63	GLY	4.1
1	A	59	VAL	4.1
1	A	15	ARG	4.0
1	A	233	VAL	4.0
1	A	227	PRO	4.0
1	B	75	SER	3.9
1	A	190	PRO	3.8
1	A	14	SER	3.7
1	A	74	GLU	3.7
1	A	70	ARG	3.7
1	B	118	PRO	3.6
1	A	57	GLN	3.6
1	A	84	MET	3.5
1	B	229	CYS	3.4
1	B	223	GLY	3.4
1	B	93	ILE	3.3
1	A	13	SER	3.3
1	B	84	MET	3.3
1	A	75	SER	3.2
1	A	12	GLY	3.2
1	A	160	TYR	3.2
1	A	100	PRO	3.1
1	A	101	MET	3.1
1	B	35	GLU	2.9
1	B	152	TYR	2.9
1	A	241	LEU	2.9
1	A	23	ASP	2.9
1	A	40	VAL	2.9
1	B	90	ASP	2.9
1	A	35	GLU	2.8
1	A	113	GLY	2.8
1	B	240	GLU	2.8
1	A	78	ASP	2.8
1	B	226	THR	2.8
1	A	132	ALA	2.7
1	B	111	LEU	2.7
1	B	184	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	144	VAL	2.6
1	B	199	SER	2.5
1	B	18	GLY	2.5
1	A	31	GLN	2.5
1	B	100	PRO	2.5
1	B	182	VAL	2.4
1	B	153	PHE	2.4
1	A	157	PRO	2.4
1	B	25	VAL	2.4
1	B	233	VAL	2.4
1	B	76	GLY	2.4
1	A	51	ASP	2.4
1	B	219	ALA	2.4
1	B	225	ASP	2.3
1	B	221	GLY	2.2
1	B	3	ALA	2.2
1	B	138	SER	2.2
1	A	112	GLN	2.2
1	B	110	LEU	2.2
1	B	128	ALA	2.2
1	B	29	MET	2.2
1	A	76	GLY	2.1
1	B	16	LEU	2.1
1	A	185	ASN	2.1
1	A	8	PRO	2.1
1	B	9	ALA	2.1
1	A	85	HIS	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](#)

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.