



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2024 – 09:05 PM EDT

PDB ID : 1YDN
Title : Crystal Structure of the HMG-CoA Lyase from Brucella melitensis, Northeast Structural Genomics Target LR35.
Authors : Forouhar, F.; Abashidze, M.; Hussain, M.; Vorobiev, S.M.; Xiao, R.; Ciano, M.; Acton, T.B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2004-12-24
Resolution : 2.30 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

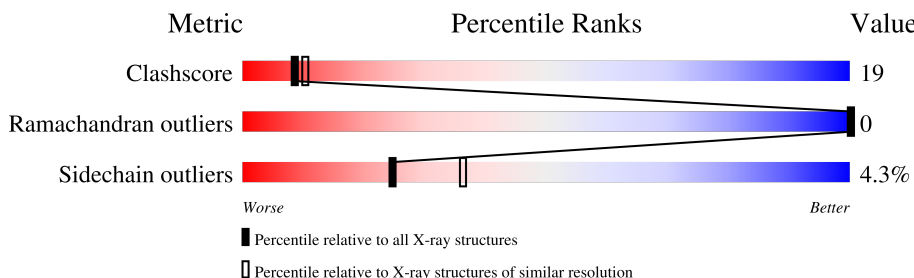
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	295	 62% 32% . .
1	B	295	 65% 30% . .
1	C	295	 66% 27% . .
1	D	295	 62% 32% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8972 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 HYDROXYMETHYLGLUTARYL-COA LYASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	Se	0	0	0
			2093	1306	370	405	6	6			
1	B	283	Total	C	N	O	S	Se	0	0	0
			2093	1306	370	405	6	6			
1	C	283	Total	C	N	O	S	Se	0	0	0
			2093	1306	370	405	6	6			
1	D	283	Total	C	N	O	S	Se	0	0	0
			2093	1306	370	405	6	6			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	MSE	MET	modified residue	UNP Q8YEF2
A	64	MSE	MET	modified residue	UNP Q8YEF2
A	82	MSE	MET	modified residue	UNP Q8YEF2
A	189	MSE	MET	modified residue	UNP Q8YEF2
A	256	MSE	MET	modified residue	UNP Q8YEF2
A	260	MSE	MET	modified residue	UNP Q8YEF2
A	288	LEU	-	cloning artifact	UNP Q8YEF2
A	289	GLU	-	cloning artifact	UNP Q8YEF2
A	290	HIS	-	expression tag	UNP Q8YEF2
A	291	HIS	-	expression tag	UNP Q8YEF2
A	292	HIS	-	expression tag	UNP Q8YEF2
A	293	HIS	-	expression tag	UNP Q8YEF2
A	294	HIS	-	expression tag	UNP Q8YEF2
A	295	HIS	-	expression tag	UNP Q8YEF2
B	10	MSE	MET	modified residue	UNP Q8YEF2
B	64	MSE	MET	modified residue	UNP Q8YEF2
B	82	MSE	MET	modified residue	UNP Q8YEF2
B	189	MSE	MET	modified residue	UNP Q8YEF2
B	256	MSE	MET	modified residue	UNP Q8YEF2
B	260	MSE	MET	modified residue	UNP Q8YEF2
B	288	LEU	-	cloning artifact	UNP Q8YEF2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	289	GLU	-	cloning artifact	UNP Q8YEF2
B	290	HIS	-	expression tag	UNP Q8YEF2
B	291	HIS	-	expression tag	UNP Q8YEF2
B	292	HIS	-	expression tag	UNP Q8YEF2
B	293	HIS	-	expression tag	UNP Q8YEF2
B	294	HIS	-	expression tag	UNP Q8YEF2
B	295	HIS	-	expression tag	UNP Q8YEF2
C	10	MSE	MET	modified residue	UNP Q8YEF2
C	64	MSE	MET	modified residue	UNP Q8YEF2
C	82	MSE	MET	modified residue	UNP Q8YEF2
C	189	MSE	MET	modified residue	UNP Q8YEF2
C	256	MSE	MET	modified residue	UNP Q8YEF2
C	260	MSE	MET	modified residue	UNP Q8YEF2
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C	291	HIS	-	expression tag	UNP Q8YEF2
C	292	HIS	-	expression tag	UNP Q8YEF2
C	293	HIS	-	expression tag	UNP Q8YEF2
C	294	HIS	-	expression tag	UNP Q8YEF2
C	295	HIS	-	expression tag	UNP Q8YEF2
D	10	MSE	MET	modified residue	UNP Q8YEF2
D	64	MSE	MET	modified residue	UNP Q8YEF2
D	82	MSE	MET	modified residue	UNP Q8YEF2
D	189	MSE	MET	modified residue	UNP Q8YEF2
D	256	MSE	MET	modified residue	UNP Q8YEF2
D	260	MSE	MET	modified residue	UNP Q8YEF2
D	288	LEU	-	cloning artifact	UNP Q8YEF2
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D	290	HIS	-	expression tag	UNP Q8YEF2
D	291	HIS	-	expression tag	UNP Q8YEF2
D	292	HIS	-	expression tag	UNP Q8YEF2
D	293	HIS	-	expression tag	UNP Q8YEF2
D	294	HIS	-	expression tag	UNP Q8YEF2
D	295	HIS	-	expression tag	UNP Q8YEF2

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total 1	Ca 1	0	0
2	D	1	Total 1	Ca 1	0	0

- Molecule 3 is water.

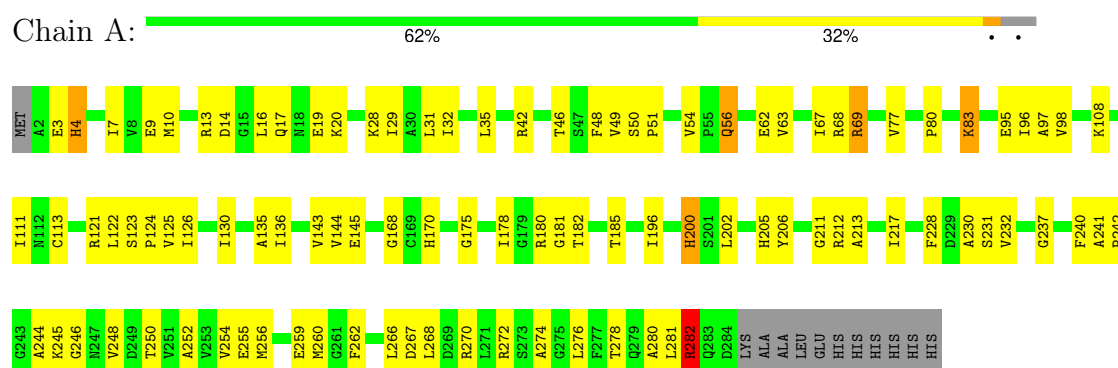
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	197	Total 197	O 197	0	0
3	B	131	Total 131	O 131	0	0
3	C	143	Total 143	O 143	0	0
3	D	125	Total 125	O 125	0	0

3 Residue-property plots

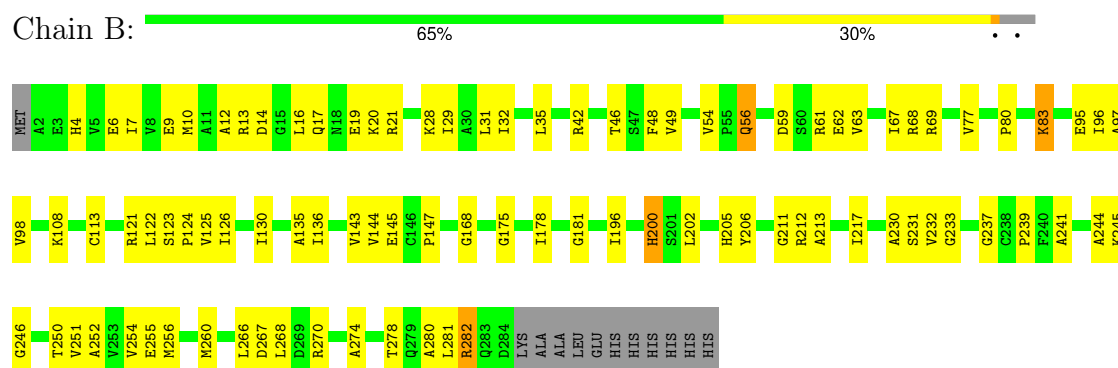
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

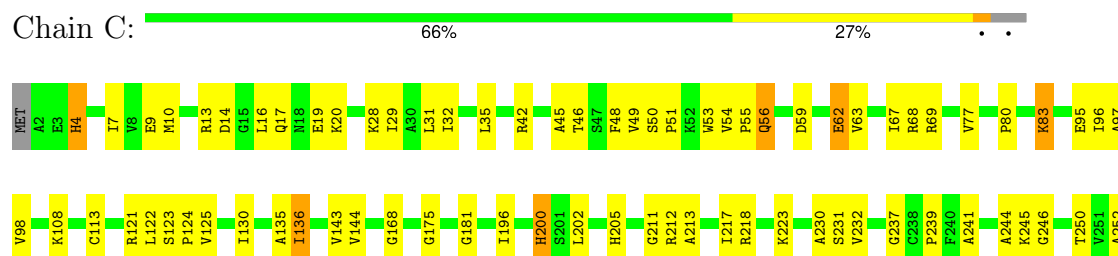
• Molecule 1: HYDROXYMETHYLGLUTARYL-COA LYASE



• Molecule 1: HYDROXYMETHYLGLUTARYL-COA LYASE

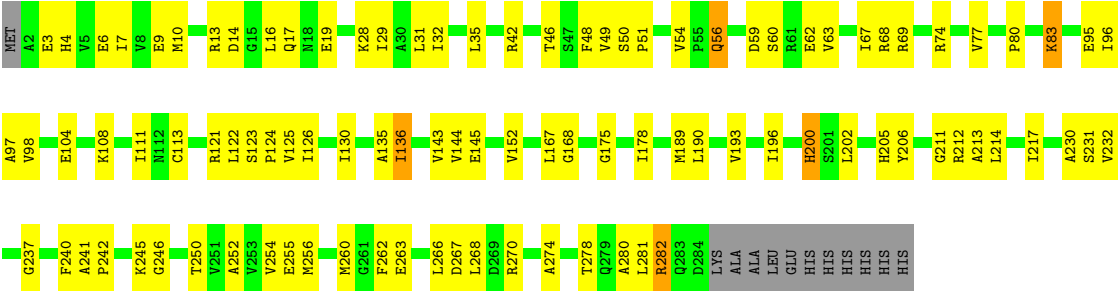


• Molecule 1: HYDROXYMETHYLGLUTARYL-COA LYASE





● Molecule 1: HYDROXYMETHYLGLUTARYL-COA LYASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.27Å 86.40Å 87.68Å 90.00° 118.70° 90.00°	Depositor
Resolution (Å)	28.94 – 2.30	Depositor
% Data completeness (in resolution range)	94.5 (28.94-2.30)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.271 , 0.304	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8972	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

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:
CA

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	0.40	0/2122	1.00	6/2871 (0.2%)
1	B	0.38	0/2122	0.61	4/2871 (0.1%)
1	C	0.37	0/2122	0.62	4/2871 (0.1%)
1	D	0.37	0/2122	0.62	3/2871 (0.1%)
All	All	0.38	0/8488	0.73	17/11484 (0.1%)

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ARG	NE-CZ-NH1	-23.89	108.36	120.30
1	A	69	ARG	NE-CZ-NH2	21.20	130.90	120.30
1	A	282	ARG	NE-CZ-NH2	-19.27	110.66	120.30
1	A	282	ARG	NE-CZ-NH1	19.09	129.84	120.30
1	A	69	ARG	CD-NE-CZ	9.99	137.59	123.60

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	2093	0	2071	81	0
1	B	2093	0	2071	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2093	0	2071	78	0
1	D	2093	0	2071	84	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	197	0	0	12	0
3	B	131	0	0	10	0
3	C	143	0	0	10	0
3	D	125	0	0	15	0
All	All	8972	0	8284	309	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 19.

The worst 5 of 309 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:A:7:ILE:HD11	1:A:230:ALA:HB3	1.59	0.85
1:B:7:ILE:HD11	1:B:230:ALA:HB3	1.59	0.85
1:C:7:ILE:HD11	1:C:230:ALA:HB3	1.60	0.84
1:A:259:GLU:HA	3:A:674:HOH:O	1.78	0.82
1:D:7:ILE:HD11	1:D:230:ALA:HB3	1.60	0.81

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	281/295 (95%)	264 (94%)	17 (6%)	0	100	100
1	B	281/295 (95%)	265 (94%)	16 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	281/295 (95%)	264 (94%)	17 (6%)	0	100	100
1	D	281/295 (95%)	264 (94%)	17 (6%)	0	100	100
All	All	1124/1180 (95%)	1057 (94%)	67 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	217/221 (98%)	206 (95%)	11 (5%)	20	29
1	B	217/221 (98%)	209 (96%)	8 (4%)	29	43
1	C	217/221 (98%)	208 (96%)	9 (4%)	26	39
1	D	217/221 (98%)	208 (96%)	9 (4%)	26	39
All	All	868/884 (98%)	831 (96%)	37 (4%)	25	36

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	4	HIS
1	D	202	LEU
1	D	56	GLN
1	D	83	LYS
1	B	56	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	56	GLN
1	D	163	GLN
1	D	200	HIS
1	D	112	ASN
1	B	283	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.