Full wwPDB EM Validation Report ⓘ

Mar 1, 2025 – 06:04 am GMT

PDB ID	:	8S6B
EMDB ID	:	EMD-19757
Title	:	CryoEM structure of Apo form of catalytic domain of human HMG-CoA reductase
Authors	:	Manikandan, K.; Van Rooyen, J.
Deposited on	:	2024-02-27
Resolution	:	2.06 Å(reported)
Based on initial model	:	1hwk

The following versions of software and data (see references ⓘ) were used in the production of this report:

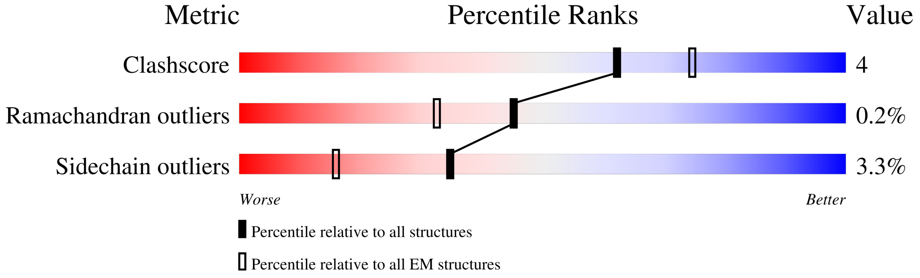
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.06 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	A	423	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3151 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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-hydroxy-3-methylglutaryl-coenzyme A reductase.

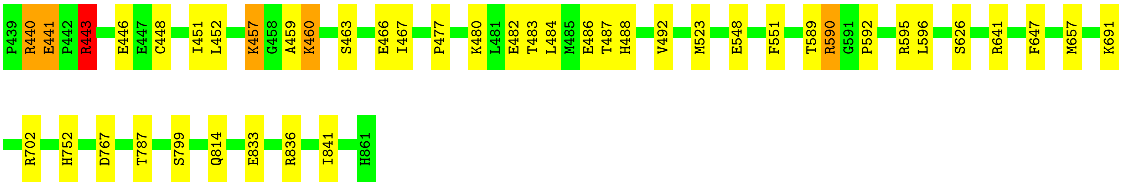
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	423	3151	1961	556	603	31	0	0

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.

- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase

Chain A:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	1066707	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\mathring{A}^2$)	54.8	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

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	0.34	0/3198	0.57	2/4322 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	443	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	A	443	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	440	ARG	Sidechain
1	A	443	ARG	Sidechain
1	A	590	ARG	Sidechain
1	A	595	ARG	Sidechain

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	3151	0	3186	26	0
All	All	3151	0	3186	26	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 (26) 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:440:ARG:HG2	1:A:441:GLU:H	1.15	1.05
1:A:440:ARG:HG2	1:A:441:GLU:N	1.92	0.83
1:A:440:ARG:CG	1:A:441:GLU:H	1.97	0.77
1:A:833:GLU:OE1	1:A:836:ARG:NH1	2.31	0.63
1:A:459:ALA:O	1:A:460:LYS:HB2	2.06	0.55
1:A:443:ARG:NH1	1:A:466:GLU:OE1	2.37	0.55
1:A:596:LEU:O	1:A:641:ARG:NH1	2.39	0.55
1:A:814:GLN:N	1:A:814:GLN:OE1	2.40	0.55
1:A:482:GLU:HB2	1:A:523:MET:SD	2.51	0.51
1:A:477:PRO:HG2	1:A:480:LYS:HB2	1.92	0.50
1:A:590:ARG:HG3	1:A:592:PRO:HD3	1.93	0.49
1:A:548:GLU:OE2	1:A:548:GLU:HA	2.16	0.46
1:A:551:PHE:CE1	1:A:841:ILE:HD11	2.51	0.45
1:A:457:LYS:HE2	1:A:457:LYS:HB3	1.57	0.45
1:A:691:LYS:CE	1:A:767:ASP:OD2	2.65	0.44
1:A:787:THR:HG22	1:A:787:THR:O	2.18	0.44
1:A:459:ALA:O	1:A:460:LYS:CB	2.65	0.44
1:A:488:HIS:CE1	1:A:523:MET:HE1	2.53	0.43
1:A:702:ARG:O	1:A:799:SER:HA	2.18	0.43
1:A:787:THR:O	1:A:787:THR:CG2	2.67	0.43
1:A:691:LYS:HE2	1:A:767:ASP:OD2	2.19	0.42
1:A:657:MET:CE	1:A:657:MET:HA	2.49	0.42
1:A:448:CYS:SG	1:A:466:GLU:OE2	2.77	0.42
1:A:463:SER:O	1:A:467:ILE:HG12	2.20	0.41
1:A:589:THR:HA	1:A:647:PHE:O	2.20	0.41
1:A:451:ILE:HG13	1:A:457:LYS:HE3	2.02	0.41

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 PDB entries followed by that with respect to all EM entries.

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	421/423 (100%)	406 (96%)	14 (3%)	1 (0%)	44 38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	460	LYS

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 PDB entries followed by that with respect to all EM entries.

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	337/337 (100%)	326 (97%)	11 (3%)	33 27

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	441	GLU
1	A	446	GLU
1	A	452	LEU
1	A	457	LYS
1	A	483	THR
1	A	484	LEU
1	A	486	GLU
1	A	487	THR
1	A	492	VAL
1	A	626	SER

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Mol	Chain	Res	Type
1	A	752	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.