

wwPDB X-ray Structure Validation Summary Report (i)

Feb 15, 2024 – 03:32 AM EST

PDB ID : 3O3M

Title : (R)-2-Hydroxyisocaproyl-CoA Dehydratase Authors : Knauer, S.H.; Buckel, W.; Dobbek, H.

Deposited on : 2010-07-25

Resolution : 1.82 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 (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

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

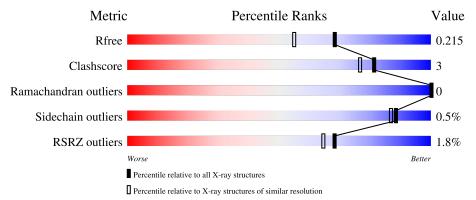
Validation Pipeline (wwPDB-VP) : 2.36

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 1.82 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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	A	408	91%	7% •
1	С	408	90%	8% •
2	В	385	92%	5% •
2	D	385	92%	5% •



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 26633 atoms, of which 12460 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 alpha subunit 2-hydroxyisocaproyl-CoA dehydratase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
1	A	399	Total 6410	C 2050	H 3188	N 526	O 616	S 30	0	11	0
1	С	401	Total 6448	C 2060	H 3209	N 529	O 619	S 31	0	11	0

• Molecule 2 is a protein called beta subunit 2-hydroxyacyl-CoA dehydratase.

Mol	Chain	Residues	\mathbf{Atoms}			ZeroOcc	AltConf	Trace			
2	В	373	Total 5975	C 1886	H 3004	N 492	O 570	S 23	0	4	0
2	D	375	Total 6063	C 1910	H 3059	N 496	O 575	S 23	11	8	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	376	SER	-	expression tag	UNP Q5U923
В	377	ALA	-	expression tag	UNP Q5U923
В	378	TRP	-	expression tag	UNP Q5U923
В	379	SER	-	expression tag	UNP Q5U923
В	380	HIS	-	expression tag	UNP Q5U923
В	381	PRO	-	expression tag	UNP Q5U923
В	382	GLN	-	expression tag	UNP Q5U923
В	383	PHE	-	expression tag	UNP Q5U923
В	384	GLU	-	expression tag	UNP Q5U923
В	385	LYS	-	expression tag	UNP Q5U923
D	376	SER	-	expression tag	UNP Q5U923
D	377	ALA	-	expression tag	UNP Q5U923
D	378	TRP	-	expression tag	UNP Q5U923
D	379	SER	-	expression tag	UNP Q5U923
D	380	HIS	-	expression tag	UNP Q5U923
D	381	PRO	-	expression tag	UNP Q5U923

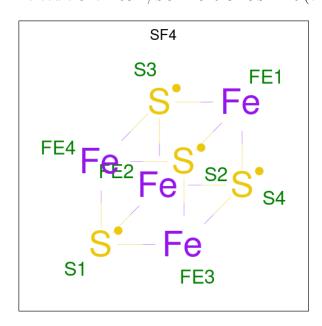
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Chain	Residue	Modelled	Actual	Comment	Reference
D	382	GLN	-	expression tag	UNP Q5U923
D	383	PHE	-	expression tag	UNP Q5U923
D	384	GLU	-	expression tag	UNP Q5U923
D	385	LYS	-	expression tag	UNP Q5U923

 \bullet Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
3	Λ	1	Total Fe S	0	0	
3	Λ	1	8 4 4		0	
3	В	1	Total Fe S	0	0	
3	Ъ	1	8 4 4			
2	С	1	Total Fe S	0	0	
3		1	8 4 4	0	U	
3	D	1	Total Fe S	0	0	
3	3 D	1	8 4 4		U	

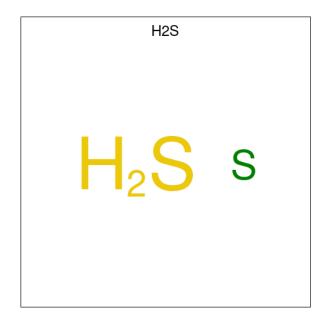
 \bullet Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: $\mathrm{O_4S}).$





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	С	1	Total O S 5 4 1	0	0

 \bullet Molecule 5 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: $\rm H_2S).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total S 1 1	0	0
5	D	1	Total S 1 1	0	0



• Molecule 6 is water.

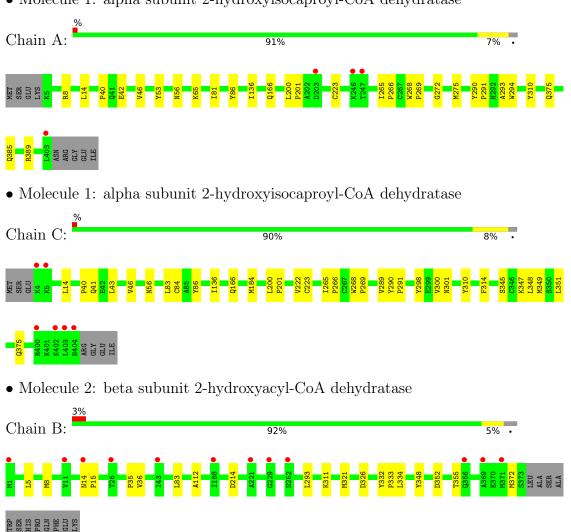
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	436	Total O 442 442	0	6
6	В	349	Total O 349 349	0	0
6	С	482	Total O 484 484	0	2
6	D	416	Total O 418 418	1	2



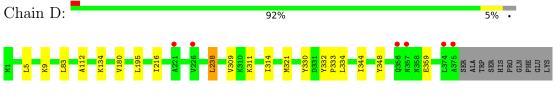
3 Residue-property plots (i)

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: alpha subunit 2-hydroxyisocaproyl-CoA dehydratase



• Molecule 2: beta subunit 2-hydroxyacyl-CoA dehydratase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	70.76Å 129.19Å 179.17Å	Donogiton
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.70 - 1.82	Depositor
Resolution (A)	19.70 - 1.82	EDS
% Data completeness	99.2 (19.70-1.82)	Depositor
(in resolution range)	99.2 (19.70-1.82)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) > 1$	2.71 (at 1.82Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
D D.	0.173 , 0.220	Depositor
R, R_{free}	0.168 , 0.215	DCC
R_{free} test set	7311 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.610	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.37, 70.3	EDS
L-test for twinning ²	$< L >=0.45, < L^2>=0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	26633	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 38.64 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5787e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical values of <|L|>, $<L^2>$ 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)

Bond lengths and bond angles in the following residue types are not validated in this section: H2S, SO4, SF4

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		
IVIOI	Moi Chain		# Z > 5	RMSZ	# Z > 5	
1	A	0.24	0/3319	0.39	0/4476	
1	С	0.25	0/3335	0.40	0/4495	
2	В	0.23	0/3038	0.39	0/4094	
2	D	0.24	0/3080	0.39	0/4149	
All	All	0.24	0/12772	0.39	0/17214	

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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	3222	3188	3176	17	0
1	С	3239	3209	3207	23	0
2	В	2971	3004	2990	13	0
2	D	3004	3059	3052	15	0
3	A	8	0	0	0	0
3	В	8	0	0	0	0
3	С	8	0	0	0	0
3	D	8	0	0	0	0
4	A	5	0	0	0	0

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Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	С	5	0	0	0	0
5	В	1	0	0	1	0
5	D	1	0	0	0	0
6	A	442	0	0	2	0
6	В	349	0	0	1	0
6	С	484	0	0	0	0
6	D	418	0	0	2	0
All	All	14173	12460	12425	65	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 3.

The worst 5 of 65 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:84:CYS:HA	1:C:345[B]:SER:HB2	1.83	0.61
2:D:83:LEU:HD21	2:D:112:ALA:HB1	1.83	0.59
2:D:134[B]:LYS:HG2	6:D:1034:HOH:O	2.02	0.59
2:D:321:MET:HG3	2:D:348:TYR:CE1	2.40	0.56
2:B:35:PRO:HB2	5:B:387:H2S:S	2.44	0.56

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	Percei	ntiles
1	A	408/408 (100%)	400 (98%)	8 (2%)	0	100	100
1	С	410/408 (100%)	401 (98%)	9 (2%)	0	100	100
2	В	375/385~(97%)	365 (97%)	10 (3%)	0	100	100
2	D	381/385 (99%)	372 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentile	\mathbf{s}
All	All	1574/1586 (99%)	1538 (98%)	36 (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	Perce	ntiles
1	A	351/348~(101%)	348 (99%)	3 (1%)	78	74
1	С	353/348~(101%)	352 (100%)	1 (0%)	92	91
2	В	330/336~(98%)	327 (99%)	3 (1%)	78	74
2	D	$335/336\ (100\%)$	334 (100%)	1 (0%)	92	91
All	All	$1369/1368\ (100\%)$	1361 (99%)	8 (1%)	88	83

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	238	LEU
1	С	41	GLN
2	В	326	ASP
2	В	214	ASP
2	В	372	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	С	41	GLN
1	С	357	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are modelled with single atom - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Trino	Chain	Dag	T inle	В	ond leng	$_{ m gths}$	В	ond ang	gles
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
3	SF4	С	409	1,6	0,12,12	-	-	-		
3	SF4	D	386	5,2	0,12,12	-	-	-		
4	SO4	A	410	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	С	410	-	4,4,4	0.15	0	6,6,6	0.05	0
3	SF4	В	386	5,2	0,12,12	-	-	-		
3	SF4	A	409	1,6	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	D	386	5,2	-	-	0/6/5/5
3	SF4	A	409	1,6	-	-	0/6/5/5
3	SF4	В	386	5,2	-	-	0/6/5/5
3	SF4	С	409	1,6	-	-	0/6/5/5

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 (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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	399/408 (97%)	-0.30	4 (1%) 82 80	14, 28, 51, 92	0
1	С	401/408 (98%)	-0.37	6 (1%) 73 70	13, 24, 42, 125	0
2	В	373/385 (96%)	-0.04	12 (3%) 47 42	15, 34, 71, 175	0
2	D	375/385 (97%)	-0.30	6 (1%) 72 68	14, 26, 52, 156	0
All	All	1548/1586 (97%)	-0.25	28 (1%) 68 64	13, 27, 58, 175	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	356	GLN	8.3
1	С	403	LEU	4.9
2	В	356	GLN	4.5
2	D	357	ASN	4.5
1	С	4	LYS	4.5

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
5	H2S	В	387	1/1	0.81	0.13	26,26,26,26	0
4	SO4	С	410	5/5	0.85	0.20	53,54,55,58	5
4	SO4	A	410	5/5	0.89	0.17	56,56,61,61	5
5	H2S	D	387	1/1	0.94	0.12	22,22,22,22	0
3	SF4	A	409	8/8	0.97	0.06	19,23,31,32	1
3	SF4	С	409	8/8	0.98	0.05	18,25,30,30	1
3	SF4	В	386	8/8	0.99	0.05	16,17,19,21	0
3	SF4	D	386	8/8	0.99	0.06	14,15,16,18	0

6.5 Other polymers (i)

There are no such residues in this entry.

