



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 10, 2014 – 04:42 PM EDT

PDB ID : 4N8H  
Title : E61V mutant, RipA structure  
Authors : Torres, R.; Goulding, C.W.  
Deposited on : 2013-10-17  
Resolution : 2.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

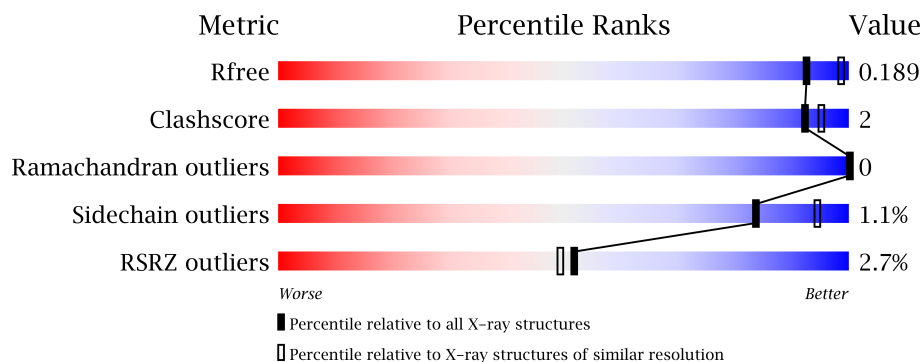
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable22978  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22978

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 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))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	476	
1	B	476	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13860 atoms, of which 6744 are hydrogens and 0 are deuterium.

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 4-hydroxybutyrate coenzyme A transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	440	Total	C	H	N	O	S	0	0	0
			6766	2134	3368	610	637	17			
1	B	440	Total	C	H	N	O	S	0	0	0
			6774	2134	3376	610	637	17			

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	INITIATING METHIONINE	UNP Q9ZC36
A	-34	GLY	-	EXPRESSION TAG	UNP Q9ZC36
A	-33	SER	-	EXPRESSION TAG	UNP Q9ZC36
A	-32	SER	-	EXPRESSION TAG	UNP Q9ZC36
A	-31	HIS	-	EXPRESSION TAG	UNP Q9ZC36
A	-30	HIS	-	EXPRESSION TAG	UNP Q9ZC36
A	-29	HIS	-	EXPRESSION TAG	UNP Q9ZC36
A	-28	HIS	-	EXPRESSION TAG	UNP Q9ZC36
A	-27	HIS	-	EXPRESSION TAG	UNP Q9ZC36
A	-26	HIS	-	EXPRESSION TAG	UNP Q9ZC36
A	-25	SER	-	EXPRESSION TAG	UNP Q9ZC36
A	-24	SER	-	EXPRESSION TAG	UNP Q9ZC36
A	-23	GLY	-	EXPRESSION TAG	UNP Q9ZC36
A	-22	LEU	-	EXPRESSION TAG	UNP Q9ZC36
A	-21	VAL	-	EXPRESSION TAG	UNP Q9ZC36
A	-20	PRO	-	EXPRESSION TAG	UNP Q9ZC36
A	-19	ARG	-	EXPRESSION TAG	UNP Q9ZC36
A	-18	GLY	-	EXPRESSION TAG	UNP Q9ZC36
A	-17	SER	-	EXPRESSION TAG	UNP Q9ZC36
A	-16	HIS	-	EXPRESSION TAG	UNP Q9ZC36
A	-15	MET	-	EXPRESSION TAG	UNP Q9ZC36
A	-14	ALA	-	EXPRESSION TAG	UNP Q9ZC36
A	-13	SER	-	EXPRESSION TAG	UNP Q9ZC36
A	-12	MET	-	EXPRESSION TAG	UNP Q9ZC36
A	-11	THR	-	EXPRESSION TAG	UNP Q9ZC36

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	EXPRESSION TAG	UNP Q9ZC36
A	-9	GLY	-	EXPRESSION TAG	UNP Q9ZC36
A	-8	GLN	-	EXPRESSION TAG	UNP Q9ZC36
A	-7	GLN	-	EXPRESSION TAG	UNP Q9ZC36
A	-6	MET	-	EXPRESSION TAG	UNP Q9ZC36
A	-5	GLY	-	EXPRESSION TAG	UNP Q9ZC36
A	-4	ARG	-	EXPRESSION TAG	UNP Q9ZC36
A	-3	GLY	-	EXPRESSION TAG	UNP Q9ZC36
A	-2	SER	-	EXPRESSION TAG	UNP Q9ZC36
A	-1	GLU	-	EXPRESSION TAG	UNP Q9ZC36
A	0	PHE	-	EXPRESSION TAG	UNP Q9ZC36
A	61	VAL	GLU	ENGINEERED MUTATION	UNP Q9ZC36
B	-35	MET	-	INITIATING METHIONINE	UNP Q9ZC36
B	-34	GLY	-	EXPRESSION TAG	UNP Q9ZC36
B	-33	SER	-	EXPRESSION TAG	UNP Q9ZC36
B	-32	SER	-	EXPRESSION TAG	UNP Q9ZC36
B	-31	HIS	-	EXPRESSION TAG	UNP Q9ZC36
B	-30	HIS	-	EXPRESSION TAG	UNP Q9ZC36
B	-29	HIS	-	EXPRESSION TAG	UNP Q9ZC36
B	-28	HIS	-	EXPRESSION TAG	UNP Q9ZC36
B	-27	HIS	-	EXPRESSION TAG	UNP Q9ZC36
B	-26	HIS	-	EXPRESSION TAG	UNP Q9ZC36
B	-25	SER	-	EXPRESSION TAG	UNP Q9ZC36
B	-24	SER	-	EXPRESSION TAG	UNP Q9ZC36
B	-23	GLY	-	EXPRESSION TAG	UNP Q9ZC36
B	-22	LEU	-	EXPRESSION TAG	UNP Q9ZC36
B	-21	VAL	-	EXPRESSION TAG	UNP Q9ZC36
B	-20	PRO	-	EXPRESSION TAG	UNP Q9ZC36
B	-19	ARG	-	EXPRESSION TAG	UNP Q9ZC36
B	-18	GLY	-	EXPRESSION TAG	UNP Q9ZC36
B	-17	SER	-	EXPRESSION TAG	UNP Q9ZC36
B	-16	HIS	-	EXPRESSION TAG	UNP Q9ZC36
B	-15	MET	-	EXPRESSION TAG	UNP Q9ZC36
B	-14	ALA	-	EXPRESSION TAG	UNP Q9ZC36
B	-13	SER	-	EXPRESSION TAG	UNP Q9ZC36
B	-12	MET	-	EXPRESSION TAG	UNP Q9ZC36
B	-11	THR	-	EXPRESSION TAG	UNP Q9ZC36
B	-10	GLY	-	EXPRESSION TAG	UNP Q9ZC36
B	-9	GLY	-	EXPRESSION TAG	UNP Q9ZC36
B	-8	GLN	-	EXPRESSION TAG	UNP Q9ZC36
B	-7	GLN	-	EXPRESSION TAG	UNP Q9ZC36
B	-6	MET	-	EXPRESSION TAG	UNP Q9ZC36

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLY	-	EXPRESSION TAG	UNP Q9ZC36
B	-4	ARG	-	EXPRESSION TAG	UNP Q9ZC36
B	-3	GLY	-	EXPRESSION TAG	UNP Q9ZC36
B	-2	SER	-	EXPRESSION TAG	UNP Q9ZC36
B	-1	GLU	-	EXPRESSION TAG	UNP Q9ZC36
B	0	PHE	-	EXPRESSION TAG	UNP Q9ZC36
B	61	VAL	GLU	ENGINEERED MUTATION	UNP Q9ZC36

- Molecule 2 is water.

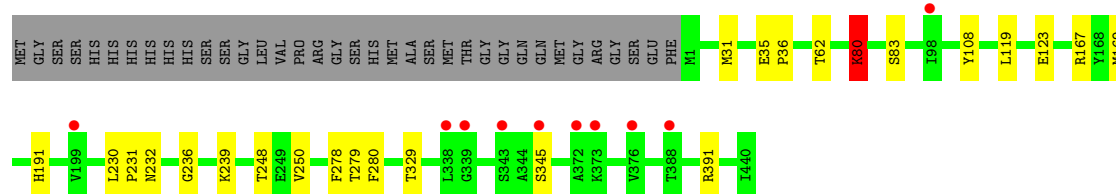
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	177	Total 177	O 177	0	0
2	B	143	Total 143	O 143	0	0

### 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.

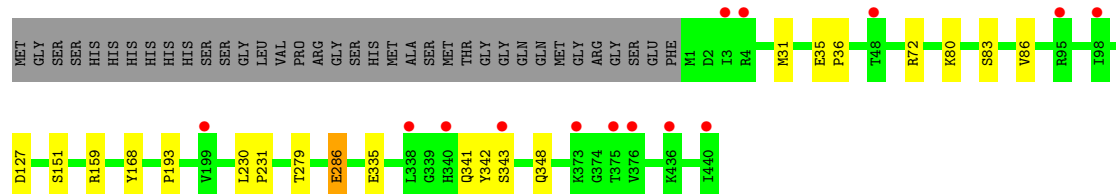
- Molecule 1: 4-hydroxybutyrate coenzyme A transferase

Chain A: 



- Molecule 1: 4-hydroxybutyrate coenzyme A transferase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.91Å 109.00Å 85.01Å 90.00° 120.07° 90.00°	Depositor
Resolution (Å)	39.70 – 2.40 39.70 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (39.70-2.40) 98.5 (39.70-2.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	10.50 (at 2.39Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.3_1479)	Depositor
R, $R_{free}$	0.151 , 0.192 0.153 , 0.189	Depositor DCC
$R_{free}$ test set	1986 reflections (5.48%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.2	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 27.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 36693 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13860	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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	0.59	0/3463	0.53	2/4699 (0.0%)
1	B	0.59	1/3463 (0.0%)	0.53	1/4699 (0.0%)
All	All	0.59	1/6926 (0.0%)	0.53	3/9398 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	151	SER	CB-OG	-5.51	1.35	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	LYS	C-N-CD	5.92	140.83	128.40
1	B	80	LYS	C-N-CD	5.67	140.31	128.40
1	A	169	MET	C-N-CD	5.20	139.32	128.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3398	3368	18	12	0
1	B	3398	3376	9	12	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	177	0	0	0	0
2	B	143	0	0	2	0
All	All	7116	6744	27	24	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (24) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:335:GLU:HB2	1:B:343:SER:HG	1.41	0.86
1:A:108:TYR:OH	1:A:345:SER:OG	2.16	0.64
1:B:341:GLN:OE1	1:B:343:SER:HB2	2.04	0.58
1:B:86:VAL:HG21	1:B:342:TYR:CD1	2.42	0.55
1:B:335:GLU:CB	1:B:343:SER:HG	2.18	0.53
1:A:236:GLY:O	1:A:239:LYS:NZ	2.40	0.53
1:A:230:LEU:HB3	1:A:231:PRO:HD3	1.91	0.53
1:B:335:GLU:HB2	1:B:343:SER:OG	2.07	0.51
1:B:127:ASP:OD1	1:B:159:ARG:NH2	2.46	0.49
1:B:230:LEU:HB3	1:B:231:PRO:HD3	1.96	0.46
1:B:168:TYR:CD2	1:B:193:PRO:HA	2.50	0.45
1:A:167:ARG:HG2	1:A:191:HIS:ND1	2.32	0.45
1:A:35:GLU:HA	1:A:36:PRO:HD3	1.85	0.43
1:B:286:GLU:HG2	2:B:621:HOH:O	2.17	0.43
1:B:31:MET:HE2	1:B:31:MET:HB3	1.85	0.43
1:A:250:VAL:HG22	1:A:280:PHE:CE1	2.54	0.42
1:A:80:LYS:HG3	1:A:80:LYS:HZ2	1.69	0.42
1:B:348:GLN:NE2	2:B:534:HOH:O	2.47	0.42
1:A:31:MET:HB3	1:A:31:MET:HE2	1.84	0.42
1:A:329:THR:HB	1:A:391:ARG:HD3	2.03	0.41
1:A:35:GLU:OE2	1:A:62:THR:HA	2.22	0.40
1:B:35:GLU:HA	1:B:36:PRO:HD3	1.95	0.40
1:A:119:LEU:HD12	1:A:123:GLU:HG3	2.02	0.40
1:A:248:THR:O	1:A:278:PHE:HA	2.21	0.40

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 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	438/476 (92%)	427 (98%)	11 (2%)	0	100	100
1	B	438/476 (92%)	426 (97%)	12 (3%)	0	100	100
All	All	876/952 (92%)	853 (97%)	23 (3%)	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	366/394 (93%)	362 (99%)	4 (1%)	84	94
1	B	366/394 (93%)	362 (99%)	4 (1%)	84	94
All	All	732/788 (93%)	724 (99%)	8 (1%)	84	94

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LYS
1	A	83	SER
1	A	232	ASN
1	A	279	THR
1	B	72	ARG
1	B	83	SER
1	B	279	THR
1	B	286	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	ASN
1	A	224	GLN
1	A	306	ASN
1	A	316	ASN
1	A	333	ASN
1	A	341	GLN
1	A	348	GLN
1	B	76	ASN
1	B	190	ASN
1	B	306	ASN
1	B	316	ASN
1	B	333	ASN
1	B	341	GLN
1	B	348	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	440/476 (92%)	-0.19	10 (2%) 57 55	15, 27, 59, 106	0
1	B	440/476 (92%)	-0.11	14 (3%) 45 43	16, 31, 66, 99	0
All	All	880/952 (92%)	-0.15	24 (2%) 52 49	15, 29, 61, 106	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	338	LEU	5.8
1	B	343	SER	4.2
1	A	338	LEU	4.1
1	B	376	VAL	4.0
1	A	339	GLY	3.6
1	A	345	SER	3.5
1	A	98	ILE	3.5
1	B	440	ILE	3.3
1	B	375	THR	3.0
1	B	373	LYS	2.9
1	B	98	ILE	2.8
1	B	340	HIS	2.8
1	A	343	SER	2.7
1	A	199	VAL	2.6
1	A	376	VAL	2.5
1	B	199	VAL	2.4
1	B	95	ARG	2.3
1	A	373	LYS	2.2
1	B	436	LYS	2.2
1	A	372	ALA	2.2
1	B	48	THR	2.2
1	A	388	THR	2.1
1	B	4	ARG	2.1
1	B	3	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.