



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 1, 2016 – 03:32 PM EDT

PDB ID : 5ICS
Title : Crystal structure of 17beta-hydroxysteroid dehydrogenase type 14 apoenzyme.
Authors : Bertoletti, N.; Marchais-Oberwinkler, S.; Heine, A.; Klebe, G.
Deposited on : 2016-02-23
Resolution : 1.52 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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
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) : rb-20027939

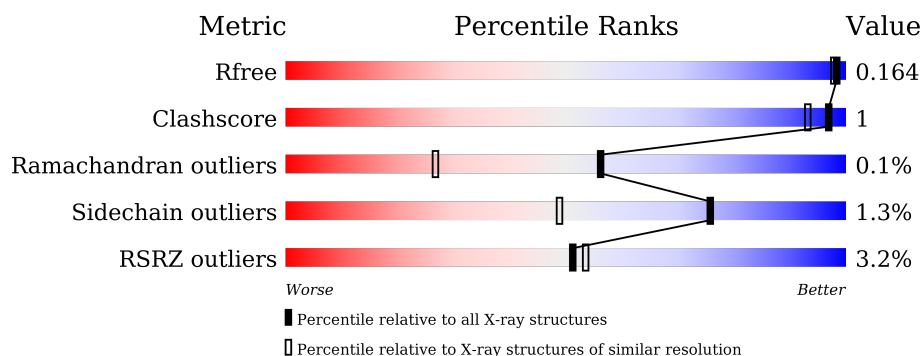
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.52 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	2658 (1.54-1.50)
Clashscore	102246	2887 (1.54-1.50)
Ramachandran outliers	100387	2818 (1.54-1.50)
Sidechain outliers	100360	2816 (1.54-1.50)
RSRZ outliers	91569	2660 (1.54-1.50)

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	274	<div> <div>2%</div> <div>91% 5%</div> </div>
1	C	274	<div> <div>5%</div> <div>91% 5%</div> </div>
1	D	274	<div> <div>5%</div> <div>89% 5% 6%</div> </div>
1	F	274	<div> <div>%</div> <div>92% 6%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15949 atoms, of which 7594 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 17-beta-hydroxysteroid dehydrogenase 14.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	259	Total	C	H	N	O	S	0	11	0
			3901	1222	1953	344	373	9			
1	C	259	Total	C	H	N	O	S	0	5	0
			3760	1193	1874	325	358	10			
1	D	258	Total	C	H	N	O	S	0	6	0
			3761	1190	1873	328	360	10			
1	F	257	Total	C	H	N	O	S	0	6	0
			3790	1196	1894	329	362	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9BPX1
A	0	HIS	-	expression tag	UNP Q9BPX1
A	205	SER	THR	conflict	UNP Q9BPX1
A	271	GLY	-	expression tag	UNP Q9BPX1
A	272	SER	-	expression tag	UNP Q9BPX1
C	-1	GLY	-	expression tag	UNP Q9BPX1
C	0	HIS	-	expression tag	UNP Q9BPX1
C	205	SER	THR	conflict	UNP Q9BPX1
C	271	GLY	-	expression tag	UNP Q9BPX1
C	272	SER	-	expression tag	UNP Q9BPX1
D	-1	GLY	-	expression tag	UNP Q9BPX1
D	0	HIS	-	expression tag	UNP Q9BPX1
D	205	SER	THR	conflict	UNP Q9BPX1
D	271	GLY	-	expression tag	UNP Q9BPX1
D	272	SER	-	expression tag	UNP Q9BPX1
F	-1	GLY	-	expression tag	UNP Q9BPX1
F	0	HIS	-	expression tag	UNP Q9BPX1
F	205	SER	THR	conflict	UNP Q9BPX1
F	271	GLY	-	expression tag	UNP Q9BPX1
F	272	SER	-	expression tag	UNP Q9BPX1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	217	Total 217	O 217	0	0
2	C	178	Total 178	O 178	0	0
2	D	152	Total 153	O 153	0	1
2	F	188	Total 189	O 189	0	1

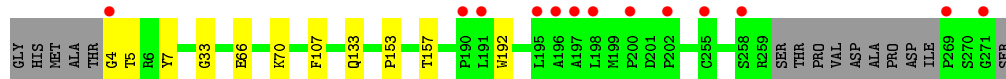
3 Residue-property plots [i](#)

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.

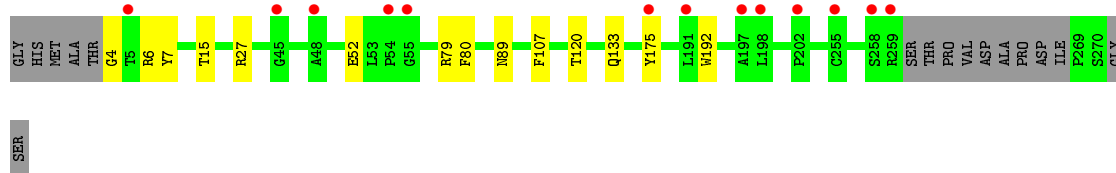
- Molecule 1: 17-beta-hydroxysteroid dehydrogenase 14



- Molecule 1: 17-beta-hydroxysteroid dehydrogenase 14



- Molecule 1: 17-beta-hydroxysteroid dehydrogenase 14



SER

- Molecule 1: 17-beta-hydroxysteroid dehydrogenase 14



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.04Å 92.19Å 87.28Å 90.00° 114.98° 90.00°	Depositor
Resolution (Å)	43.95 – 1.52 43.95 – 1.52	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.95-1.52) 99.7 (43.95-1.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 1.52Å)	Xtriage
Refinement program	PHENIX (1.10.1-2155_1492: ???)	Depositor
R, R_{free}	0.129 , 0.164 0.128 , 0.164	Depositor DCC
R_{free} test set	8465 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	13.7	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15949	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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, 0.333 respectively for untwinned datasets, and 0.375, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.45	0/2011	0.63	1/2732 (0.0%)
1	C	0.41	0/1942	0.62	0/2639
1	D	0.41	0/1935	0.62	0/2633
1	F	0.45	0/1952	0.64	1/2654 (0.0%)
All	All	0.43	0/7840	0.63	2/10658 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	F	217	ARG	NE-CZ-NH2	-5.32	117.64	120.30

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	1948	1953	1923	5	0
1	C	1886	1874	1865	6	0
1	D	1888	1873	1850	7	0
1	F	1896	1894	1881	2	0
2	A	217	0	0	1	0
2	C	178	0	0	1	0
2	D	153	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	189	0	0	0	0
All	All	8355	7594	7519	19	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 1.

All (19) 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:D:6:ARG:NH1	1:F:234:GLU:OE2	2.28	0.67
1:C:4:GLY:N	1:C:5:THR:HA	2.18	0.57
1:A:41:LYS:NZ	2:A:301:HOH:O	2.17	0.57
1:D:4:GLY:N	2:D:304:HOH:O	2.43	0.51
1:C:133:GLN:OE1	2:C:301:HOH:O	2.19	0.50
1:A:41:LYS:CE	1:A:62:ASP:CG	2.82	0.48
1:A:41:LYS:HE2	1:A:62:ASP:CG	2.33	0.48
1:D:27:ARG:HH12	1:D:52:GLU:CD	2.17	0.47
1:D:133:GLN:NE2	1:D:175:TYR:O	2.42	0.46
1:C:66:GLU:HG2	1:C:70:LYS:HE3	1.99	0.45
1:C:153:PRO:O	1:C:157:THR:HG23	2.18	0.44
1:C:4:GLY:HA3	1:C:33:GLY:HA3	2.00	0.43
1:D:15:THR:O	1:D:89:ASN:HB3	2.19	0.43
1:C:4:GLY:HA3	1:C:33:GLY:CA	2.49	0.43
1:F:27:ARG:HH12	1:F:52:GLU:CD	2.22	0.42
1:A:15:THR:O	1:A:89:ASN:HB3	2.20	0.41
1:D:79:ARG:HD2	1:D:80:PHE:CE2	2.55	0.41
1:D:120[A]:THR:HG22	2:D:420:HOH:O	2.20	0.41
1:A:153:PRO:O	1:A:157:THR:HG23	2.21	0.40

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	267/274 (97%)	262 (98%)	4 (2%)	1 (0%)	39	14
1	C	262/274 (96%)	258 (98%)	4 (2%)	0	100	100
1	D	260/274 (95%)	256 (98%)	4 (2%)	0	100	100
1	F	259/274 (94%)	254 (98%)	5 (2%)	0	100	100
All	All	1048/1096 (96%)	1030 (98%)	17 (2%)	1 (0%)	56	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	GLY

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	203/210 (97%)	201 (99%)	2 (1%)	82	61
1	C	193/210 (92%)	190 (98%)	3 (2%)	70	40
1	D	191/210 (91%)	188 (98%)	3 (2%)	70	40
1	F	196/210 (93%)	194 (99%)	2 (1%)	82	61
All	All	783/840 (93%)	773 (99%)	10 (1%)	76	49

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	TYR
1	A	107	PHE
1	C	7	TYR
1	C	107	PHE
1	C	192	TRP
1	D	7	TYR
1	D	107	PHE
1	D	192	TRP
1	F	7	TYR
1	F	107	PHE

Some 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 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, 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	259/274 (94%)	-0.22	5 (1%) 70 73	9, 15, 30, 45	0
1	C	259/274 (94%)	-0.20	13 (5%) 32 33	9, 16, 36, 49	0
1	D	258/274 (94%)	-0.03	13 (5%) 32 33	9, 18, 40, 54	0
1	F	257/274 (93%)	-0.26	2 (0%) 87 89	9, 16, 28, 43	0
All	All	1033/1096 (94%)	-0.18	33 (3%) 51 53	9, 16, 35, 54	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	54	PRO	4.8
1	A	2	ALA	4.3
1	C	191	LEU	4.1
1	D	259	ARG	3.8
1	D	55	GLY	3.3
1	A	261	THR	3.3
1	F	261	THR	3.1
1	C	200	PRO	3.1
1	C	197	ALA	3.1
1	D	175	TYR	3.1
1	D	191	LEU	3.0
1	C	198	LEU	2.9
1	F	257	ALA	2.8
1	C	271	GLY	2.8
1	D	45	GLY	2.8
1	C	195	LEU	2.7
1	D	197	ALA	2.7
1	C	190	PRO	2.6
1	C	4	GLY	2.6
1	C	196	ALA	2.6
1	C	258	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	5	THR	2.5
1	A	259	ARG	2.5
1	D	48	ALA	2.4
1	D	258	SER	2.4
1	A	262	PRO	2.4
1	C	255	CYS	2.4
1	D	202	PRO	2.2
1	C	269	PRO	2.2
1	D	255	CYS	2.1
1	C	202	PRO	2.1
1	D	198	LEU	2.1
1	A	105	GLN	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 [i](#)

There are no such residues in this entry.