

wwPDB X-ray Structure Validation Summary Report (i)

Aug 3, 2023 – 02:13 AM EDT

PDB ID	:	1HXH
Title	:	COMAMONAS TESTOSTERONI 3BETA/17BETA HYDROXYSTEROID
		DEHYDROGENASE
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Deposited on		
Resolution	:	1.22 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:

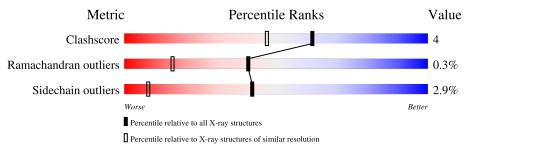
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.22 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
Clashscore	141614	1294 (1.24-1.20)		
Ramachandran outliers	138981	1251 (1.24-1.20)		
Sidechain outliers	138945	1250 (1.24-1.20)		

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	А	253	85%	13% •	•
1	В	253	87%	10% •	•
1	С	253	90%	9%	•
1	D	253	88%	10% •	•



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9110 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.

 \bullet Molecule 1 is a protein called 3BETA/17BETA-HYDROXYSTEROID DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	۸	253	Total	С	Ν	0	S	0	17	0
	А	200	1959	1220	350	375	14	0		
1	P	253	Total	С	Ν	0	S	0	18	0
	D	200	1971	1229	355	372	15	0	10	0
1	С	252	Total	С	Ν	0	S	0	17	0
	U	253	1961	1221	347	378	15	0	17	0
1	Л	952	Total	С	Ν	0	S	0	17	0
	I D	253	1963	1225	346	378	14	U	17	0

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	284	Total O 284 284	0	0
2	В	323	Total O 323 323	0	0
2	С	350	Total O 350 350	0	0
2	D	299	Total O 299 299	0	0



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. 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: 3BETA/17BETA-HYDROXYSTEROID DEHYDROGENASE



4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	80.02Å 110.59Å 115.14Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	20.00 - 1.22	Depositor	
% Data completeness	96.6 (20.00-1.22)	Depositor	
(in resolution range)	50.0 (20.00-1.22)		
R_{merge}	0.07	Depositor	
R _{sym}	(Not available)	Depositor	
Refinement program	REFMAC, CNS, SHELXL-97	Depositor	
R, R_{free}	0.146 , 0.180	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	9110	wwPDB-VP	
Average B, all atoms $(Å^2)$	19.0	wwPDB-VP	



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	Bo	nd lengths	Bond angles		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.70	1/2034~(0.0%)	1.35	22/2741~(0.8%)	
1	В	0.68	1/2055~(0.0%)	1.28	18/2765~(0.7%)	
1	С	0.69	0/2035	1.16	9/2742~(0.3%)	
1	D	0.72	2/2032~(0.1%)	1.32	16/2739~(0.6%)	
All	All	0.70	4/8156~(0.0%)	1.28	65/10987~(0.6%)	

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
1	D	253	LEU	C-O	9.82	1.42	1.23
1	А	253	LEU	C-OXT	5.66	1.34	1.23
1	В	253	LEU	C-OXT	5.42	1.33	1.23
1	D	253	LEU	C-OXT	-5.23	1.13	1.23

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	76	ARG	CD-NE-CZ	16.25	146.36	123.60
1	А	76	ARG	NE-CZ-NH2	-12.40	114.10	120.30
1	А	3	ARG	NE-CZ-NH2	-10.98	114.81	120.30
1	А	106[A]	ARG	NE-CZ-NH1	10.91	125.76	120.30
1	А	106[B]	ARG	NE-CZ-NH1	10.91	125.76	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	А	1959	0	2006	25	0
1	В	1971	0	2038	17	0
1	С	1961	0	2005	15	0
1	D	1963	0	2013	18	0
2	А	284	0	0	10	0
2	В	323	0	0	6	0
2	С	350	0	0	13	0
2	D	299	0	0	12	0
All	All	9110	0	8062	71	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.

The worst 5 of 71 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:192:GLN:HG3	2:C:599:HOH:O	1.84	0.78
1:B:76:ARG:HG3	2:B:550:HOH:O	1.86	0.75
1:B:96:MET:O	1:D:120[B]:GLN:HG2	1.88	0.73
1:A:76:ARG:HG3	2:A:495:HOH:O	1.92	0.67
1:B:40:GLU:OE2	1:B:58:ARG:HG3	1.97	0.65

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	Perce	ntiles
1	А	268/253~(106%)	263~(98%)	4 (2%)	1 (0%)	34	11
1	В	269/253~(106%)	263~(98%)	6 (2%)	0	100	100
1	С	268/253~(106%)	262~(98%)	5 (2%)	1 (0%)	34	11
1	D	268/253~(106%)	263~(98%)	4 (2%)	1 (0%)	34	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percen	tiles
All	All	1073/1012~(106%)	1051 (98%)	19 (2%)	3~(0%)	41	16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	184	ASP
1	А	184	ASP
1	С	184	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentil	es
1	А	214/198~(108%)	211~(99%)	3 (1%)	67 32	
1	В	216/198~(109%)	202 (94%)	14 (6%)	17 1	
1	С	215/198~(109%)	208~(97%)	7(3%)	38 6	
1	D	215/198~(109%)	212~(99%)	3 (1%)	67 32	
All	All	860/792~(109%)	833~(97%)	27 (3%)	42 7	

5 of 27 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	В	190	MET
1	С	1	THR
1	D	44	GLN
1	В	211	ASN
1	С	3	ARG

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such side chains are listed below:

Mol	Chain	Res	Type
1	С	192	GLN
1	D	211	ASN

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Mol	Chain	Res	Type
1	С	211	ASN
1	D	224	GLN
1	D	45	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)

There are no ligands in this entry.

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

