



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:57 PM GMT

PDB ID : 3DHE
Title : ESTROGENIC 17-BETA HYDROXYSTEROID DEHYDROGENASE COM-
PLEXED DEHYDROEPIANDROSTERONE
Authors : Han, Q.; Campbell, R.L.; Gangloff, A.; Lin, S.X.
Deposited on : 1998-03-25
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

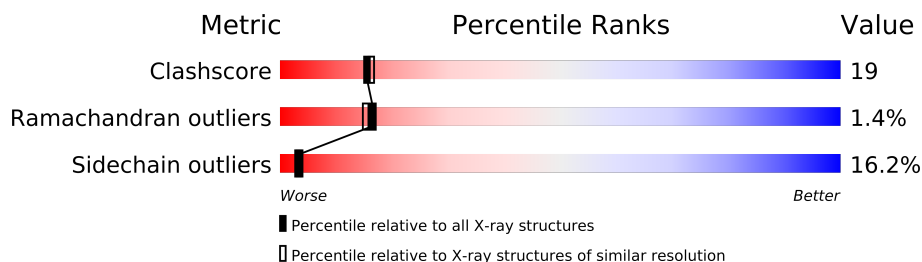
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	327	

2 Entry composition i

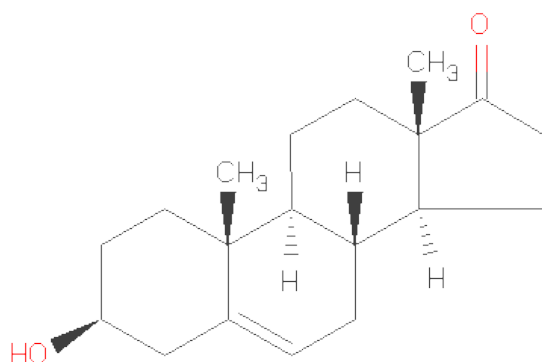
There are 3 unique types of molecules in this entry. The entry contains 2236 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ESTROGENIC 17-BETA HYDROXYSTEROID DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	284	2177	1382	385	398	12	0	0	0

- Molecule 2 is 3-BETA-HYDROXY-5-ANDROSTEN-17-ONE (three-letter code: AND) (formula: C₁₉H₂₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	21	19	2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total	O	0	0
			38	38		

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.66Å 45.19Å 61.30Å 90.00° 99.10° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	95.0 (8.00-2.30)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.184 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2236	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
AND

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	0.46	1/2218 (0.0%)	0.67	4/3009 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	ASP	CG-OD2	5.12	1.37	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	ARG	NE-CZ-NH2	7.14	123.87	120.30
1	A	206	ARG	NE-CZ-NH2	6.86	123.73	120.30
1	A	112	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	A	112	ASP	CB-CG-OD1	5.22	123.00	118.30

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	2177	0	2218	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	21	0	27	15	0
3	A	38	0	0	7	0
All	All	2236	0	2245	82	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 19.

All (82) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:193:MET:CE	2:A:400:AND:H151	1.43	1.47
1:A:189:HIS:CE1	3:A:1081:HOH:O	1.90	1.24
1:A:189:HIS:NE2	3:A:1081:HOH:O	1.73	1.20
1:A:193:MET:HE3	2:A:400:AND:C15	1.69	1.17
1:A:193:MET:HE1	2:A:400:AND:C15	1.77	1.07
1:A:193:MET:HE3	2:A:400:AND:H152	1.38	1.05
1:A:197:LEU:HB2	1:A:219:LEU:HD22	1.41	1.02
1:A:35:THR:HG22	3:A:1088:HOH:O	1.58	1.01
1:A:60:GLU:HG3	3:A:1093:HOH:O	1.68	0.93
1:A:122:LEU:O	1:A:126:LEU:HB2	1.75	0.86
1:A:149:LEU:HD22	2:A:400:AND:H193	1.58	0.84
1:A:193:MET:HE1	2:A:400:AND:H151	0.85	0.84
1:A:197:LEU:O	1:A:197:LEU:HD12	1.79	0.83
1:A:67:ARG:HG2	1:A:112:ASP:OD2	1.81	0.80
1:A:149:LEU:HD22	2:A:400:AND:C19	2.12	0.79
1:A:282:GLU:HG2	1:A:282:GLU:O	1.84	0.77
1:A:35:THR:CG2	3:A:1088:HOH:O	2.22	0.76
1:A:222:SER:HB2	2:A:400:AND:H6	1.68	0.76
1:A:44:ARG:HD3	3:A:1097:HOH:O	1.87	0.75
1:A:197:LEU:HB2	1:A:219:LEU:CD2	2.18	0.73
1:A:35:THR:HG23	1:A:64:LEU:HB3	1.70	0.73
1:A:281:ARG:NE	1:A:281:ARG:HA	2.04	0.72
1:A:149:LEU:HD13	2:A:400:AND:C19	2.23	0.68
1:A:149:LEU:HD13	2:A:400:AND:H193	1.76	0.67
1:A:282:GLU:O	1:A:282:GLU:CG	2.41	0.67
1:A:149:LEU:CD2	2:A:400:AND:H193	2.26	0.66
1:A:44:ARG:CD	3:A:1097:HOH:O	2.40	0.65
1:A:260:LEU:N	1:A:261:PRO:HD2	2.13	0.64
1:A:136:ARG:NH2	1:A:246:ALA:O	2.31	0.64
1:A:90:ASN:HA	1:A:140:THR:HG23	1.80	0.63
1:A:214:ARG:HD3	1:A:284:PHE:CE1	2.34	0.62
1:A:67:ARG:CG	1:A:112:ASP:OD2	2.50	0.58
1:A:192:PHE:O	1:A:196:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:201:GLU:HG2	1:A:202:GLU:N	2.18	0.58
1:A:67:ARG:HD2	1:A:112:ASP:OD2	2.05	0.57
1:A:257:GLU:H	1:A:257:GLU:CD	2.09	0.56
1:A:67:ARG:CD	1:A:112:ASP:OD2	2.53	0.56
1:A:209:ILE:O	1:A:209:ILE:HG13	2.06	0.55
1:A:146:LEU:HB3	1:A:263:LEU:HD11	1.90	0.53
1:A:149:LEU:CD1	2:A:400:AND:H193	2.39	0.52
1:A:224:GLN:HE22	1:A:227:ARG:NH1	2.07	0.52
1:A:200:PRO:O	1:A:212:PHE:CE1	2.63	0.52
1:A:193:MET:CE	2:A:400:AND:C16	2.86	0.52
1:A:22:LEU:CD1	1:A:241:LEU:HD21	2.40	0.51
1:A:7:ILE:HD13	1:A:18:LEU:HD12	1.92	0.51
1:A:229:ALA:HB2	1:A:258:ARG:CZ	2.40	0.51
1:A:258:ARG:O	1:A:261:PRO:HD2	2.12	0.50
1:A:221:HIS:CE1	1:A:282:GLU:O	2.65	0.50
1:A:37:ARG:NH2	1:A:67:ARG:HH22	2.10	0.49
1:A:149:LEU:HD13	2:A:400:AND:H191	1.94	0.49
1:A:118:THR:HG21	1:A:162:LEU:HD21	1.93	0.49
1:A:22:LEU:HD13	1:A:241:LEU:HD21	1.95	0.48
1:A:188:VAL:O	1:A:190:THR:N	2.46	0.48
1:A:83:ARG:HG2	1:A:84:VAL:N	2.29	0.47
1:A:83:ARG:HE	1:A:83:ARG:HB3	1.46	0.47
1:A:5:VAL:HG22	1:A:86:VAL:HB	1.97	0.47
1:A:35:THR:CG2	1:A:64:LEU:HB3	2.43	0.46
1:A:7:ILE:O	1:A:35:THR:HB	2.16	0.46
1:A:189:HIS:CE1	1:A:230:ALA:HB3	2.50	0.46
1:A:200:PRO:O	1:A:212:PHE:HE1	1.98	0.46
1:A:201:GLU:HG2	1:A:202:GLU:H	1.80	0.46
1:A:125:PHE:O	1:A:129:MET:HG3	2.15	0.46
1:A:205:ASP:OD1	1:A:205:ASP:O	2.34	0.46
1:A:18:LEU:HD13	1:A:22:LEU:HD22	1.98	0.45
1:A:260:LEU:N	1:A:261:PRO:CD	2.79	0.45
1:A:273:SER:O	1:A:277:THR:HG23	2.17	0.45
1:A:204:LEU:O	1:A:204:LEU:HG	2.16	0.44
1:A:39:LEU:O	1:A:42:GLN:HG2	2.18	0.44
1:A:37:ARG:HG2	1:A:37:ARG:HH11	1.82	0.44
1:A:37:ARG:NH2	1:A:67:ARG:NH2	2.66	0.44
1:A:83:ARG:HD2	1:A:85:ASP:OD1	2.18	0.43
1:A:224:GLN:NE2	1:A:227:ARG:NH1	2.67	0.43
1:A:188:VAL:HG22	1:A:236:VAL:HG21	1.99	0.43
1:A:31:LYS:NZ	1:A:60:GLU:HG2	2.34	0.42
1:A:39:LEU:C	1:A:41:THR:H	2.21	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:149:LEU:HD22	2:A:400:AND:H192	1.94	0.41
1:A:234:GLU:HG2	1:A:234:GLU:H	1.65	0.41
1:A:110:VAL:O	1:A:114:ASN:HB2	2.21	0.41
1:A:283:VAL:O	1:A:283:VAL:HG12	2.21	0.41
1:A:11:SER:O	1:A:12:SER:HB3	2.21	0.41
1:A:174:LEU:HB3	1:A:175:PRO:HD3	2.03	0.41
1:A:119:VAL:O	1:A:123:GLN:HG3	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	282/327 (86%)	269 (95%)	9 (3%)	4 (1%)	16 15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	HIS
1	A	198	GLY
1	A	200	PRO
1	A	3	THR

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	235/257 (91%)	197 (84%)	38 (16%)	3 3

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	18	LEU
1	A	22	LEU
1	A	36	LEU
1	A	37	ARG
1	A	40	LYS
1	A	44	ARG
1	A	47	GLU
1	A	50	ARG
1	A	64	LEU
1	A	78	ARG
1	A	83	ARG
1	A	93	LEU
1	A	99	LEU
1	A	102	LEU
1	A	112	ASP
1	A	118	THR
1	A	126	LEU
1	A	131	ARG
1	A	136	ARG
1	A	138	LEU
1	A	140	THR
1	A	178	VAL
1	A	202	GLU
1	A	205	ASP
1	A	209	ILE
1	A	214	ARG
1	A	226	PHE
1	A	227	ARG
1	A	228	GLU
1	A	231	GLN
1	A	234	GLU
1	A	235	GLU
1	A	241	LEU
1	A	257	GLU
1	A	260	LEU
1	A	264	ARG
1	A	273	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	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 ⓘ

1 ligand is modelled in this entry.

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	AND	A	400	1	24,24,24	3.56	12 (50%)	39,39,39	5.17	11 (28%)

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
2	AND	A	400	1	-	0/0/58/58	0/0/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	AND	O17-C17	13.27	1.45	1.21
2	A	400	AND	C1-C10	3.78	1.61	1.54
2	A	400	AND	C13-C17	3.63	1.57	1.52
2	A	400	AND	C16-C17	3.60	1.57	1.51
2	A	400	AND	C10-C9	3.49	1.62	1.56
2	A	400	AND	C10-C5	2.94	1.59	1.52
2	A	400	AND	C8-C9	2.89	1.59	1.53
2	A	400	AND	C8-C14	2.89	1.59	1.53
2	A	400	AND	C12-C13	2.85	1.59	1.54
2	A	400	AND	C7-C6	2.25	1.55	1.50
2	A	400	AND	C7-C8	2.24	1.57	1.53
2	A	400	AND	C11-C9	2.17	1.57	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	AND	O17-C17-C16	18.67	149.85	125.72
2	A	400	AND	O17-C17-C13	-17.57	100.35	125.99
2	A	400	AND	C15-C14-C13	14.42	116.55	104.06
2	A	400	AND	C15-C16-C17	6.33	112.23	105.67
2	A	400	AND	C12-C13-C17	5.54	125.73	116.62
2	A	400	AND	C18-C13-C17	-5.39	94.35	105.21
2	A	400	AND	C15-C14-C8	4.51	126.20	119.03
2	A	400	AND	C18-C13-C14	3.27	118.19	112.94
2	A	400	AND	C11-C9-C8	2.73	115.67	111.73
2	A	400	AND	C11-C9-C10	2.66	116.76	113.08
2	A	400	AND	C19-C10-C5	-2.32	104.66	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.