



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 5, 2021 – 06:24 PM JST

PDB ID : 7ENY
Title : Crystal structure of hydroxysteroid dehydrogenase from Escherichia coli
Authors : Kim, K.-H.; Lee, C.W.; Pardhe, D.P.; Hwang, J.; Do, H.; Lee, Y.M.; Lee, J.H.; Oh, T.-J.
Deposited on : 2021-04-21
Resolution : 2.70 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.22
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.22

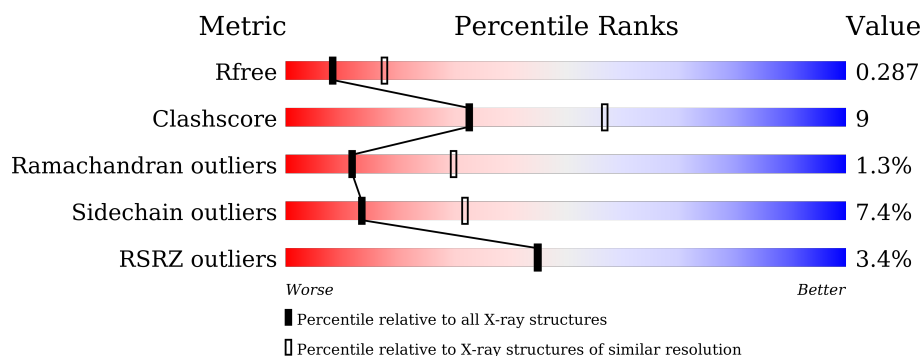
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 $\leq 5\%$. 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	289	<div> <div>68%</div> <div>18%</div> <div>•</div> <div>13%</div> </div>
1	B	289	<div> <div>%</div> <div>61%</div> <div>22%</div> <div>•</div> <div>16%</div> </div>
1	C	289	<div> <div>3%</div> <div>65%</div> <div>14%</div> <div>•</div> <div>17%</div> </div>
1	D	289	<div> <div>4%</div> <div>64%</div> <div>23%</div> <div>13%</div> </div>
1	E	289	<div> <div>%</div> <div>72%</div> <div>15%</div> <div>•</div> <div>13%</div> </div>
1	F	289	<div> <div>3%</div> <div>63%</div> <div>16%</div> <div>•</div> <div>19%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	289	<div><div></div><div>3%</div><div>58%</div><div>22%</div><div>•</div><div>17%</div></div>
1	H	289	<div><div></div><div>6%</div><div>67%</div><div>19%</div><div>•</div><div>13%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14545 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.

- Molecule 1 is a protein called 7alpha-hydroxysteroid dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			1840	1152	320	357	11			
1	B	244	Total	C	N	O	S	0	0	0
			1788	1120	312	345	11			
1	C	239	Total	C	N	O	S	0	2	0
			1759	1099	310	340	10			
1	D	252	Total	C	N	O	S	0	0	0
			1848	1156	322	359	11			
1	E	251	Total	C	N	O	S	0	0	0
			1840	1152	320	357	11			
1	F	235	Total	C	N	O	S	0	0	0
			1708	1070	297	331	10			
1	G	240	Total	C	N	O	S	0	0	0
			1767	1109	307	340	11			
1	H	252	Total	C	N	O	S	0	0	0
			1848	1156	322	359	11			

There are 280 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	initiating methionine	UNP P0AET8
A	-32	GLY	-	expression tag	UNP P0AET8
A	-31	SER	-	expression tag	UNP P0AET8
A	-30	SER	-	expression tag	UNP P0AET8
A	-29	HIS	-	expression tag	UNP P0AET8
A	-28	HIS	-	expression tag	UNP P0AET8
A	-27	HIS	-	expression tag	UNP P0AET8
A	-26	HIS	-	expression tag	UNP P0AET8
A	-25	HIS	-	expression tag	UNP P0AET8
A	-24	HIS	-	expression tag	UNP P0AET8
A	-23	SER	-	expression tag	UNP P0AET8
A	-22	SER	-	expression tag	UNP P0AET8
A	-21	GLY	-	expression tag	UNP P0AET8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	LEU	-	expression tag	UNP P0AET8
A	-19	VAL	-	expression tag	UNP P0AET8
A	-18	PRO	-	expression tag	UNP P0AET8
A	-17	ARG	-	expression tag	UNP P0AET8
A	-16	GLY	-	expression tag	UNP P0AET8
A	-15	SER	-	expression tag	UNP P0AET8
A	-14	HIS	-	expression tag	UNP P0AET8
A	-13	MET	-	expression tag	UNP P0AET8
A	-12	ALA	-	expression tag	UNP P0AET8
A	-11	SER	-	expression tag	UNP P0AET8
A	-10	MET	-	expression tag	UNP P0AET8
A	-9	THR	-	expression tag	UNP P0AET8
A	-8	GLY	-	expression tag	UNP P0AET8
A	-7	GLY	-	expression tag	UNP P0AET8
A	-6	GLN	-	expression tag	UNP P0AET8
A	-5	GLN	-	expression tag	UNP P0AET8
A	-4	MET	-	expression tag	UNP P0AET8
A	-3	GLY	-	expression tag	UNP P0AET8
A	-2	ARG	-	expression tag	UNP P0AET8
A	-1	GLY	-	expression tag	UNP P0AET8
A	0	SER	-	expression tag	UNP P0AET8
A	2	LEU	PHE	engineered mutation	UNP P0AET8
B	-33	MET	-	initiating methionine	UNP P0AET8
B	-32	GLY	-	expression tag	UNP P0AET8
B	-31	SER	-	expression tag	UNP P0AET8
B	-30	SER	-	expression tag	UNP P0AET8
B	-29	HIS	-	expression tag	UNP P0AET8
B	-28	HIS	-	expression tag	UNP P0AET8
B	-27	HIS	-	expression tag	UNP P0AET8
B	-26	HIS	-	expression tag	UNP P0AET8
B	-25	HIS	-	expression tag	UNP P0AET8
B	-24	HIS	-	expression tag	UNP P0AET8
B	-23	SER	-	expression tag	UNP P0AET8
B	-22	SER	-	expression tag	UNP P0AET8
B	-21	GLY	-	expression tag	UNP P0AET8
B	-20	LEU	-	expression tag	UNP P0AET8
B	-19	VAL	-	expression tag	UNP P0AET8
B	-18	PRO	-	expression tag	UNP P0AET8
B	-17	ARG	-	expression tag	UNP P0AET8
B	-16	GLY	-	expression tag	UNP P0AET8
B	-15	SER	-	expression tag	UNP P0AET8
B	-14	HIS	-	expression tag	UNP P0AET8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	MET	-	expression tag	UNP P0AET8
B	-12	ALA	-	expression tag	UNP P0AET8
B	-11	SER	-	expression tag	UNP P0AET8
B	-10	MET	-	expression tag	UNP P0AET8
B	-9	THR	-	expression tag	UNP P0AET8
B	-8	GLY	-	expression tag	UNP P0AET8
B	-7	GLY	-	expression tag	UNP P0AET8
B	-6	GLN	-	expression tag	UNP P0AET8
B	-5	GLN	-	expression tag	UNP P0AET8
B	-4	MET	-	expression tag	UNP P0AET8
B	-3	GLY	-	expression tag	UNP P0AET8
B	-2	ARG	-	expression tag	UNP P0AET8
B	-1	GLY	-	expression tag	UNP P0AET8
B	0	SER	-	expression tag	UNP P0AET8
B	2	LEU	PHE	engineered mutation	UNP P0AET8
C	-33	MET	-	initiating methionine	UNP P0AET8
C	-32	GLY	-	expression tag	UNP P0AET8
C	-31	SER	-	expression tag	UNP P0AET8
C	-30	SER	-	expression tag	UNP P0AET8
C	-29	HIS	-	expression tag	UNP P0AET8
C	-28	HIS	-	expression tag	UNP P0AET8
C	-27	HIS	-	expression tag	UNP P0AET8
C	-26	HIS	-	expression tag	UNP P0AET8
C	-25	HIS	-	expression tag	UNP P0AET8
C	-24	HIS	-	expression tag	UNP P0AET8
C	-23	SER	-	expression tag	UNP P0AET8
C	-22	SER	-	expression tag	UNP P0AET8
C	-21	GLY	-	expression tag	UNP P0AET8
C	-20	LEU	-	expression tag	UNP P0AET8
C	-19	VAL	-	expression tag	UNP P0AET8
C	-18	PRO	-	expression tag	UNP P0AET8
C	-17	ARG	-	expression tag	UNP P0AET8
C	-16	GLY	-	expression tag	UNP P0AET8
C	-15	SER	-	expression tag	UNP P0AET8
C	-14	HIS	-	expression tag	UNP P0AET8
C	-13	MET	-	expression tag	UNP P0AET8
C	-12	ALA	-	expression tag	UNP P0AET8
C	-11	SER	-	expression tag	UNP P0AET8
C	-10	MET	-	expression tag	UNP P0AET8
C	-9	THR	-	expression tag	UNP P0AET8
C	-8	GLY	-	expression tag	UNP P0AET8
C	-7	GLY	-	expression tag	UNP P0AET8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	GLN	-	expression tag	UNP P0AET8
C	-5	GLN	-	expression tag	UNP P0AET8
C	-4	MET	-	expression tag	UNP P0AET8
C	-3	GLY	-	expression tag	UNP P0AET8
C	-2	ARG	-	expression tag	UNP P0AET8
C	-1	GLY	-	expression tag	UNP P0AET8
C	0	SER	-	expression tag	UNP P0AET8
C	2	LEU	PHE	engineered mutation	UNP P0AET8
D	-33	MET	-	initiating methionine	UNP P0AET8
D	-32	GLY	-	expression tag	UNP P0AET8
D	-31	SER	-	expression tag	UNP P0AET8
D	-30	SER	-	expression tag	UNP P0AET8
D	-29	HIS	-	expression tag	UNP P0AET8
D	-28	HIS	-	expression tag	UNP P0AET8
D	-27	HIS	-	expression tag	UNP P0AET8
D	-26	HIS	-	expression tag	UNP P0AET8
D	-25	HIS	-	expression tag	UNP P0AET8
D	-24	HIS	-	expression tag	UNP P0AET8
D	-23	SER	-	expression tag	UNP P0AET8
D	-22	SER	-	expression tag	UNP P0AET8
D	-21	GLY	-	expression tag	UNP P0AET8
D	-20	LEU	-	expression tag	UNP P0AET8
D	-19	VAL	-	expression tag	UNP P0AET8
D	-18	PRO	-	expression tag	UNP P0AET8
D	-17	ARG	-	expression tag	UNP P0AET8
D	-16	GLY	-	expression tag	UNP P0AET8
D	-15	SER	-	expression tag	UNP P0AET8
D	-14	HIS	-	expression tag	UNP P0AET8
D	-13	MET	-	expression tag	UNP P0AET8
D	-12	ALA	-	expression tag	UNP P0AET8
D	-11	SER	-	expression tag	UNP P0AET8
D	-10	MET	-	expression tag	UNP P0AET8
D	-9	THR	-	expression tag	UNP P0AET8
D	-8	GLY	-	expression tag	UNP P0AET8
D	-7	GLY	-	expression tag	UNP P0AET8
D	-6	GLN	-	expression tag	UNP P0AET8
D	-5	GLN	-	expression tag	UNP P0AET8
D	-4	MET	-	expression tag	UNP P0AET8
D	-3	GLY	-	expression tag	UNP P0AET8
D	-2	ARG	-	expression tag	UNP P0AET8
D	-1	GLY	-	expression tag	UNP P0AET8
D	0	SER	-	expression tag	UNP P0AET8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2	LEU	PHE	engineered mutation	UNP P0AET8
E	-33	MET	-	initiating methionine	UNP P0AET8
E	-32	GLY	-	expression tag	UNP P0AET8
E	-31	SER	-	expression tag	UNP P0AET8
E	-30	SER	-	expression tag	UNP P0AET8
E	-29	HIS	-	expression tag	UNP P0AET8
E	-28	HIS	-	expression tag	UNP P0AET8
E	-27	HIS	-	expression tag	UNP P0AET8
E	-26	HIS	-	expression tag	UNP P0AET8
E	-25	HIS	-	expression tag	UNP P0AET8
E	-24	HIS	-	expression tag	UNP P0AET8
E	-23	SER	-	expression tag	UNP P0AET8
E	-22	SER	-	expression tag	UNP P0AET8
E	-21	GLY	-	expression tag	UNP P0AET8
E	-20	LEU	-	expression tag	UNP P0AET8
E	-19	VAL	-	expression tag	UNP P0AET8
E	-18	PRO	-	expression tag	UNP P0AET8
E	-17	ARG	-	expression tag	UNP P0AET8
E	-16	GLY	-	expression tag	UNP P0AET8
E	-15	SER	-	expression tag	UNP P0AET8
E	-14	HIS	-	expression tag	UNP P0AET8
E	-13	MET	-	expression tag	UNP P0AET8
E	-12	ALA	-	expression tag	UNP P0AET8
E	-11	SER	-	expression tag	UNP P0AET8
E	-10	MET	-	expression tag	UNP P0AET8
E	-9	THR	-	expression tag	UNP P0AET8
E	-8	GLY	-	expression tag	UNP P0AET8
E	-7	GLY	-	expression tag	UNP P0AET8
E	-6	GLN	-	expression tag	UNP P0AET8
E	-5	GLN	-	expression tag	UNP P0AET8
E	-4	MET	-	expression tag	UNP P0AET8
E	-3	GLY	-	expression tag	UNP P0AET8
E	-2	ARG	-	expression tag	UNP P0AET8
E	-1	GLY	-	expression tag	UNP P0AET8
E	0	SER	-	expression tag	UNP P0AET8
E	2	LEU	PHE	engineered mutation	UNP P0AET8
F	-33	MET	-	initiating methionine	UNP P0AET8
F	-32	GLY	-	expression tag	UNP P0AET8
F	-31	SER	-	expression tag	UNP P0AET8
F	-30	SER	-	expression tag	UNP P0AET8
F	-29	HIS	-	expression tag	UNP P0AET8
F	-28	HIS	-	expression tag	UNP P0AET8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-27	HIS	-	expression tag	UNP P0AET8
F	-26	HIS	-	expression tag	UNP P0AET8
F	-25	HIS	-	expression tag	UNP P0AET8
F	-24	HIS	-	expression tag	UNP P0AET8
F	-23	SER	-	expression tag	UNP P0AET8
F	-22	SER	-	expression tag	UNP P0AET8
F	-21	GLY	-	expression tag	UNP P0AET8
F	-20	LEU	-	expression tag	UNP P0AET8
F	-19	VAL	-	expression tag	UNP P0AET8
F	-18	PRO	-	expression tag	UNP P0AET8
F	-17	ARG	-	expression tag	UNP P0AET8
F	-16	GLY	-	expression tag	UNP P0AET8
F	-15	SER	-	expression tag	UNP P0AET8
F	-14	HIS	-	expression tag	UNP P0AET8
F	-13	MET	-	expression tag	UNP P0AET8
F	-12	ALA	-	expression tag	UNP P0AET8
F	-11	SER	-	expression tag	UNP P0AET8
F	-10	MET	-	expression tag	UNP P0AET8
F	-9	THR	-	expression tag	UNP P0AET8
F	-8	GLY	-	expression tag	UNP P0AET8
F	-7	GLY	-	expression tag	UNP P0AET8
F	-6	GLN	-	expression tag	UNP P0AET8
F	-5	GLN	-	expression tag	UNP P0AET8
F	-4	MET	-	expression tag	UNP P0AET8
F	-3	GLY	-	expression tag	UNP P0AET8
F	-2	ARG	-	expression tag	UNP P0AET8
F	-1	GLY	-	expression tag	UNP P0AET8
F	0	SER	-	expression tag	UNP P0AET8
F	2	LEU	PHE	engineered mutation	UNP P0AET8
G	-33	MET	-	initiating methionine	UNP P0AET8
G	-32	GLY	-	expression tag	UNP P0AET8
G	-31	SER	-	expression tag	UNP P0AET8
G	-30	SER	-	expression tag	UNP P0AET8
G	-29	HIS	-	expression tag	UNP P0AET8
G	-28	HIS	-	expression tag	UNP P0AET8
G	-27	HIS	-	expression tag	UNP P0AET8
G	-26	HIS	-	expression tag	UNP P0AET8
G	-25	HIS	-	expression tag	UNP P0AET8
G	-24	HIS	-	expression tag	UNP P0AET8
G	-23	SER	-	expression tag	UNP P0AET8
G	-22	SER	-	expression tag	UNP P0AET8
G	-21	GLY	-	expression tag	UNP P0AET8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-20	LEU	-	expression tag	UNP P0AET8
G	-19	VAL	-	expression tag	UNP P0AET8
G	-18	PRO	-	expression tag	UNP P0AET8
G	-17	ARG	-	expression tag	UNP P0AET8
G	-16	GLY	-	expression tag	UNP P0AET8
G	-15	SER	-	expression tag	UNP P0AET8
G	-14	HIS	-	expression tag	UNP P0AET8
G	-13	MET	-	expression tag	UNP P0AET8
G	-12	ALA	-	expression tag	UNP P0AET8
G	-11	SER	-	expression tag	UNP P0AET8
G	-10	MET	-	expression tag	UNP P0AET8
G	-9	THR	-	expression tag	UNP P0AET8
G	-8	GLY	-	expression tag	UNP P0AET8
G	-7	GLY	-	expression tag	UNP P0AET8
G	-6	GLN	-	expression tag	UNP P0AET8
G	-5	GLN	-	expression tag	UNP P0AET8
G	-4	MET	-	expression tag	UNP P0AET8
G	-3	GLY	-	expression tag	UNP P0AET8
G	-2	ARG	-	expression tag	UNP P0AET8
G	-1	GLY	-	expression tag	UNP P0AET8
G	0	SER	-	expression tag	UNP P0AET8
G	2	LEU	PHE	engineered mutation	UNP P0AET8
H	-33	MET	-	initiating methionine	UNP P0AET8
H	-32	GLY	-	expression tag	UNP P0AET8
H	-31	SER	-	expression tag	UNP P0AET8
H	-30	SER	-	expression tag	UNP P0AET8
H	-29	HIS	-	expression tag	UNP P0AET8
H	-28	HIS	-	expression tag	UNP P0AET8
H	-27	HIS	-	expression tag	UNP P0AET8
H	-26	HIS	-	expression tag	UNP P0AET8
H	-25	HIS	-	expression tag	UNP P0AET8
H	-24	HIS	-	expression tag	UNP P0AET8
H	-23	SER	-	expression tag	UNP P0AET8
H	-22	SER	-	expression tag	UNP P0AET8
H	-21	GLY	-	expression tag	UNP P0AET8
H	-20	LEU	-	expression tag	UNP P0AET8
H	-19	VAL	-	expression tag	UNP P0AET8
H	-18	PRO	-	expression tag	UNP P0AET8
H	-17	ARG	-	expression tag	UNP P0AET8
H	-16	GLY	-	expression tag	UNP P0AET8
H	-15	SER	-	expression tag	UNP P0AET8
H	-14	HIS	-	expression tag	UNP P0AET8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-13	MET	-	expression tag	UNP P0AET8
H	-12	ALA	-	expression tag	UNP P0AET8
H	-11	SER	-	expression tag	UNP P0AET8
H	-10	MET	-	expression tag	UNP P0AET8
H	-9	THR	-	expression tag	UNP P0AET8
H	-8	GLY	-	expression tag	UNP P0AET8
H	-7	GLY	-	expression tag	UNP P0AET8
H	-6	GLN	-	expression tag	UNP P0AET8
H	-5	GLN	-	expression tag	UNP P0AET8
H	-4	MET	-	expression tag	UNP P0AET8
H	-3	GLY	-	expression tag	UNP P0AET8
H	-2	ARG	-	expression tag	UNP P0AET8
H	-1	GLY	-	expression tag	UNP P0AET8
H	0	SER	-	expression tag	UNP P0AET8
H	2	LEU	PHE	engineered mutation	UNP P0AET8

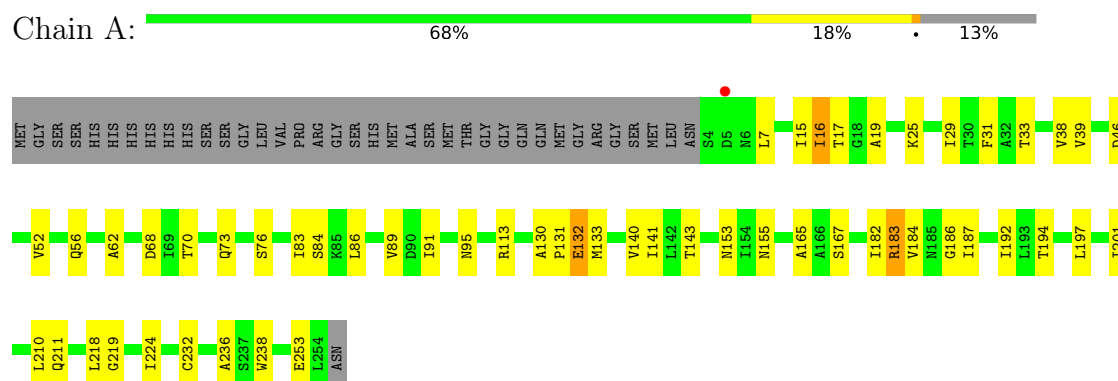
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	34	Total O 34 34	0	0
2	B	17	Total O 17 17	0	0
2	C	11	Total O 11 11	0	0
2	D	13	Total O 13 13	0	0
2	E	21	Total O 21 21	0	0
2	F	20	Total O 20 20	0	0
2	G	20	Total O 20 20	0	0
2	H	11	Total O 11 11	0	0

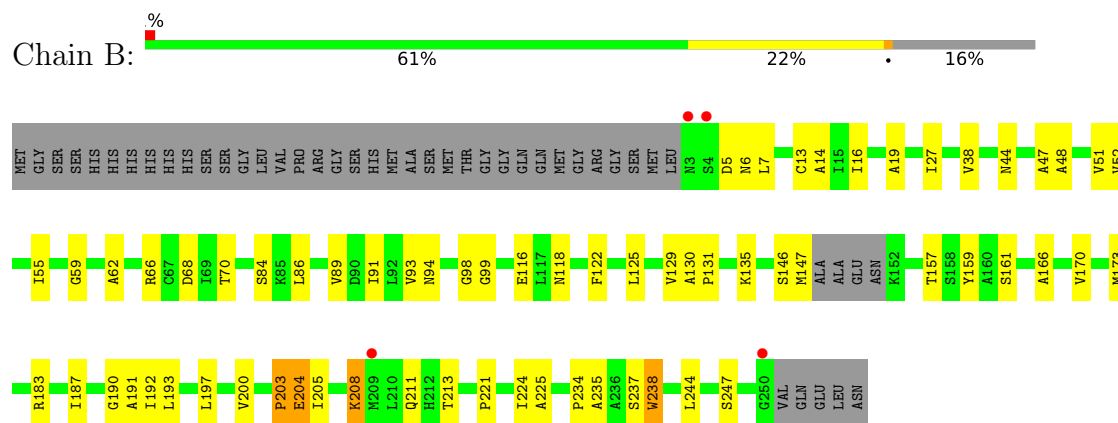
3 Residue-property plots

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.

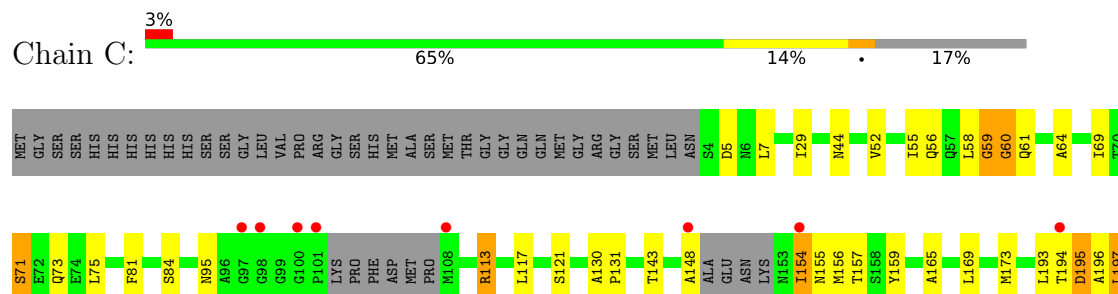
• Molecule 1: 7alpha-hydroxysteroid dehydrogenase

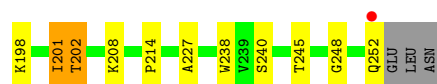


• Molecule 1: 7alpha-hydroxysteroid dehydrogenase

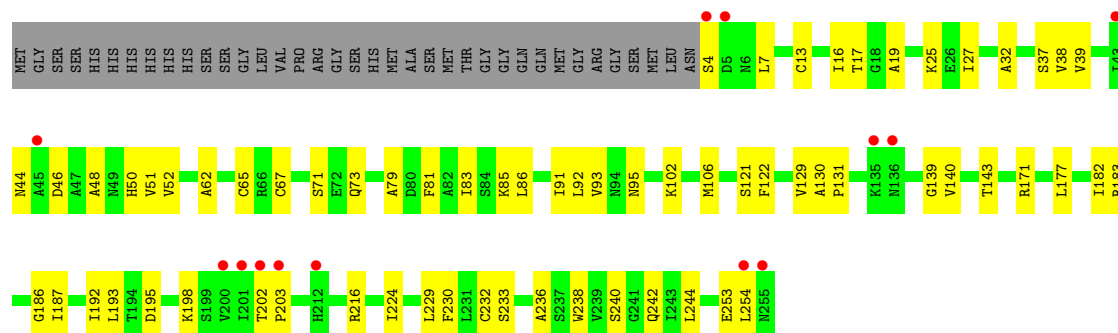


• Molecule 1: 7alpha-hydroxysteroid dehydrogenase

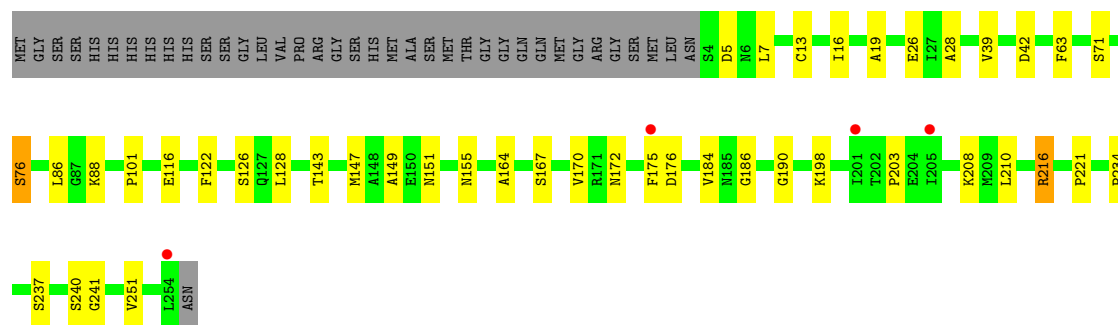




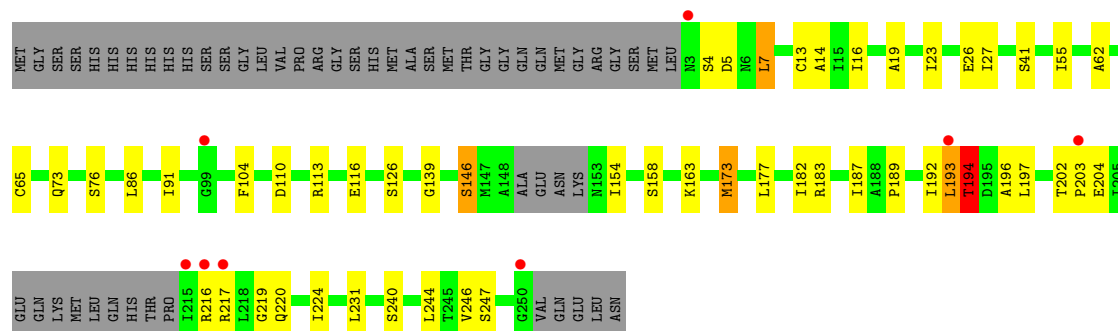
- Molecule 1: 7alpha-hydroxysteroid dehydrogenase



- Molecule 1: 7alpha-hydroxysteroid dehydrogenase

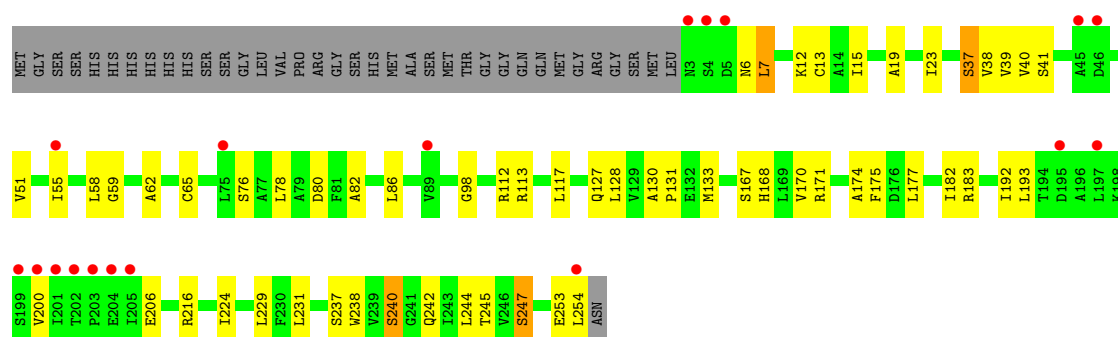


- Molecule 1: 7alpha-hydroxysteroid dehydrogenase



- Molecule 1: 7alpha-hydroxysteroid dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.83Å 100.19Å 160.22Å 90.00° 95.57° 90.00°	Depositor
Resolution (Å)	38.09 – 2.70 38.06 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (38.09-2.70) 98.4 (38.06-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.69 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.198 , 0.293 0.199 , 0.287	Depositor DCC
R_{free} test set	2490 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14545	wwPDB-VP
Average B, all atoms (Å ²)	63.0	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 38.75 % 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 3.5155e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.74	0/1866	0.88	1/2526 (0.0%)
1	B	0.75	0/1813	0.85	0/2452
1	C	0.75	0/1783	0.87	0/2410
1	D	0.73	0/1874	0.86	0/2537
1	E	0.73	0/1866	0.84	0/2526
1	F	0.77	1/1730 (0.1%)	0.88	0/2340
1	G	0.73	0/1789	0.90	0/2417
1	H	0.72	0/1874	0.84	0/2537
All	All	0.74	1/14595 (0.0%)	0.87	1/19745 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
1	H	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	247	SER	CA-CB	-5.24	1.45	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	ARG	NE-CZ-NH1	-5.44	117.58	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	202	THR	Peptide
1	H	253	GLU	Peptide

5.2 Too-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 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	1840	0	1849	33	0
1	B	1788	0	1798	35	0
1	C	1759	0	1771	26	0
1	D	1848	0	1855	36	0
1	E	1840	0	1849	19	0
1	F	1708	0	1713	24	0
1	G	1767	0	1778	52	0
1	H	1848	0	1855	45	0
2	A	34	0	0	2	0
2	B	17	0	0	1	0
2	C	11	0	0	1	0
2	D	13	0	0	1	0
2	E	21	0	0	1	0
2	F	20	0	0	1	0
2	G	20	0	0	2	0
2	H	11	0	0	1	0
All	All	14545	0	14468	250	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 9.

The worst 5 of 250 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:113[A]:ARG:HH21	1:C:113[A]:ARG:HG2	0.94	1.09
1:C:113[A]:ARG:HG2	1:C:113[A]:ARG:NH2	1.64	1.01
1:C:113[A]:ARG:HH21	1:C:113[A]:ARG:CG	1.75	0.99
1:H:58:LEU:HD23	1:H:58:LEU:O	1.84	0.77
1:G:249:GLY:HA2	1:H:240:SER:O	1.86	0.75

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	249/289 (86%)	230 (92%)	19 (8%)	0	100	100
1	B	240/289 (83%)	219 (91%)	17 (7%)	4 (2%)	9	23
1	C	235/289 (81%)	209 (89%)	18 (8%)	8 (3%)	3	8
1	D	250/289 (86%)	233 (93%)	15 (6%)	2 (1%)	19	43
1	E	249/289 (86%)	233 (94%)	14 (6%)	2 (1%)	19	43
1	F	229/289 (79%)	214 (93%)	11 (5%)	4 (2%)	9	23
1	G	232/289 (80%)	210 (90%)	17 (7%)	5 (2%)	6	17
1	H	250/289 (86%)	218 (87%)	31 (12%)	1 (0%)	34	60
All	All	1934/2312 (84%)	1766 (91%)	142 (7%)	26 (1%)	12	30

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	60	GLY
1	C	155	ASN
1	C	194	THR
1	D	216	ARG
1	F	146	SER

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	Percentiles	
1	A	193/223 (86%)	182 (94%)	11 (6%)	20	44
1	B	188/223 (84%)	172 (92%)	16 (8%)	10	24
1	C	184/223 (82%)	167 (91%)	17 (9%)	9	21
1	D	194/223 (87%)	182 (94%)	12 (6%)	18	40
1	E	193/223 (86%)	180 (93%)	13 (7%)	16	37
1	F	178/223 (80%)	160 (90%)	18 (10%)	7	17
1	G	186/223 (83%)	172 (92%)	14 (8%)	13	31
1	H	194/223 (87%)	182 (94%)	12 (6%)	18	40
All	All	1510/1784 (85%)	1397 (92%)	113 (8%)	13	31

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	42	ASP
1	H	240	SER
1	F	7	LEU
1	H	238	TRP
1	G	204	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	220	GLN
1	D	127	GLN
1	H	151	ASN
1	E	242	GLN
1	F	3	ASN

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 [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](#)

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	251/289 (86%)	-0.39	1 (0%) 92 93	34, 49, 85, 111	0
1	B	244/289 (84%)	-0.34	4 (1%) 72 74	31, 53, 99, 122	0
1	C	239/289 (82%)	-0.17	9 (3%) 40 39	38, 57, 118, 171	0
1	D	252/289 (87%)	-0.08	13 (5%) 27 25	38, 60, 93, 140	0
1	E	251/289 (86%)	-0.23	4 (1%) 72 74	35, 53, 93, 126	0
1	F	235/289 (81%)	-0.35	8 (3%) 45 45	36, 53, 94, 143	0
1	G	240/289 (83%)	-0.05	9 (3%) 40 39	35, 62, 125, 164	0
1	H	252/289 (87%)	0.14	18 (7%) 16 14	43, 69, 115, 152	0
All	All	1964/2312 (84%)	-0.18	66 (3%) 45 45	31, 57, 107, 171	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	105	ASP	9.5
1	C	194	THR	6.3
1	G	104	PHE	5.6
1	H	254	LEU	4.7
1	B	3	ASN	4.7

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.