WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 21, 2023 – 04:56 AM 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)

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

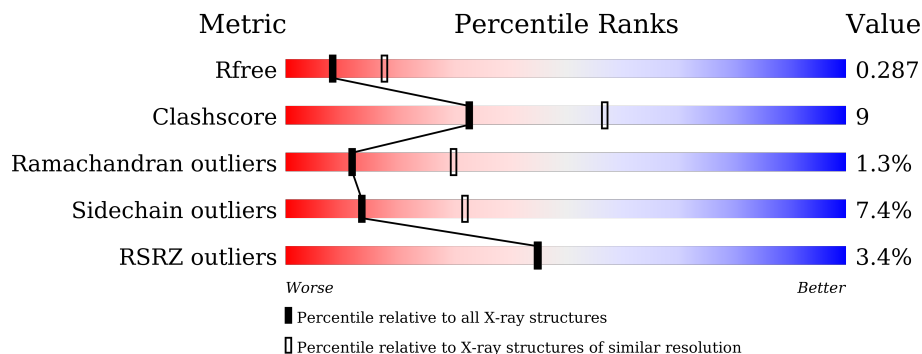|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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.
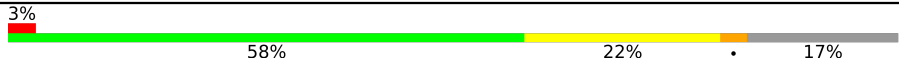
Metric	Percentile Ranks	Value
Rfree		0.287
Clashscore		9
Ramachandran outliers		1.3%
Sidechain outliers		7.4%
RSRZ outliers		3.4%

Worse | | Better

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

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 <=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	68% · · · 18% · 13%
1	B	289	% 61% · 22% · 16%
1	C	289	3% 65% · 14% · 17%
1	D	289	4% 64% · 23% · 13%
1	E	289	% 72% · 15% · 13%
1	F	289	3% 63% · 16% · 19%

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Mol	Chain	Length	Quality of chain
1	G	289	3% 58% 22% · 17%
1	H	289	6% 67% 19% · 13%

2   Entry composition (i)

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 34	O 34	0	0
2	B	17	Total 17	O 17	0	0
2	C	11	Total 11	O 11	0	0
2	D	13	Total 13	O 13	0	0
2	E	21	Total 21	O 21	0	0
2	F	20	Total 20	O 20	0	0
2	G	20	Total 20	O 20	0	0
2	H	11	Total 11	O 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.
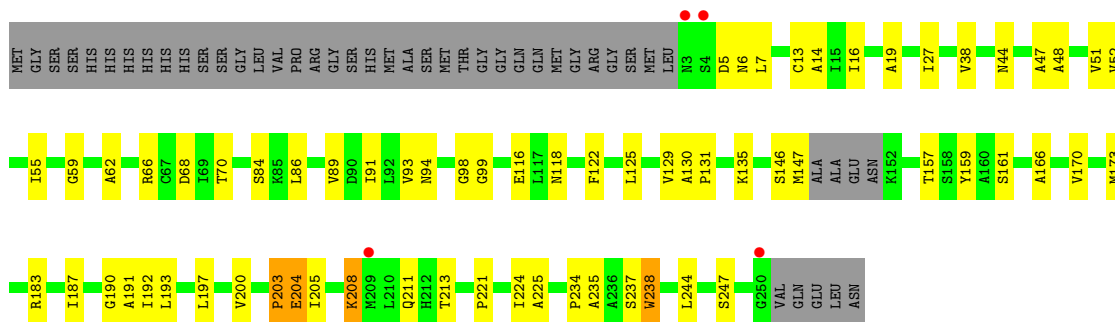
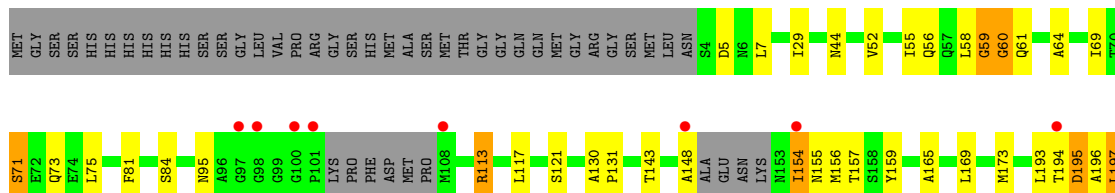• Molecule 1: 7alpha-hydroxysteroid dehydrogenase

Chain A:
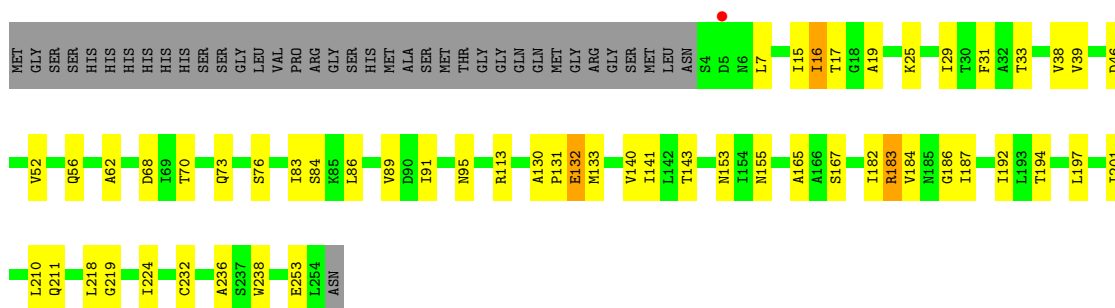
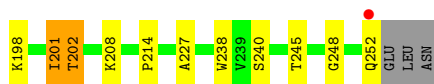
• Molecule 1: 7alpha-hydroxysteroid dehydrogenase

Chain B:

• Molecule 1: 7alpha-hydroxysteroid dehydrogenase

Chain C:
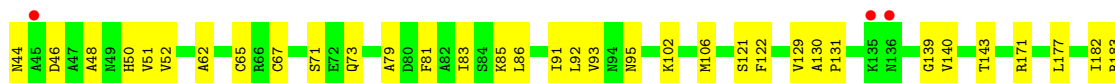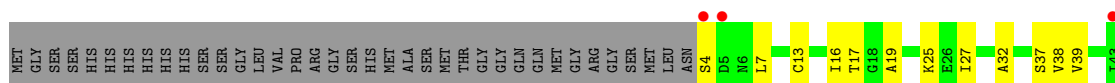
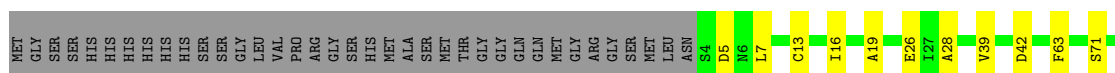K198 I201 T202 K208 P214 A227 W238 V239 S240 T245 G248 Q252 GLU LEU ASN

● Molecule 1: 7alpha-hydroxysteroid dehydrogenase

Chain D:

4%

64% 23% 13%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA SER MET THR GLY GLY GLN MET GLY ARG GLY SER MET LEU ASN S4 D5 N6 L7 C13 I16 T17 G18 A19 K25 E26 I27 A32 S37 V38 V39 I43

N44 A45 D46 A47 A48 N49 H50 V51 V52 A62 C65 R66 C67 S71 E72 Q73 A79 D80 F81 A82 I83 S84 K85 L86 I91 L92 V93 N94 N95 K102 M106 S121 F122 V129 A130 P131 K135 N136 G139 V140 T143 R171 L177 I182 R183

G186 I187 I192 L193 T194 D195 K198 S199 V200 I201 T202 P203 H212 R216 I224 L229 F230 L231 C232 S233 A236 S237 W238 V239 S240 Q242 I243 L244 E253 L254 N255
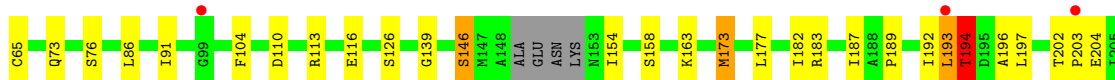
● Molecule 1: 7alpha-hydroxysteroid dehydrogenase

Chain E:

%

72% 15% • 13%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA SER MET THR GLY GLY GLN MET GLY ARG GLY SER MET LEU ASN S4 D5 N6 L7 C13 I16 A19 E26 I27 A28 V39 D42 F63 S71

S76 L86 G87 K88 P101 E116 F122 S126 Q127 L128 T143 M147 A148 A149 E150 N151 N155 A164 S167 V170 R171 N172 F175 D176 V184 M185 G186 G190 K198 I201 T202 P203 E204 I205 K208 M209 L210 R216 P221 P234

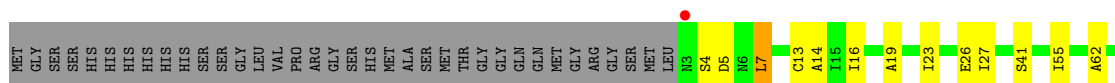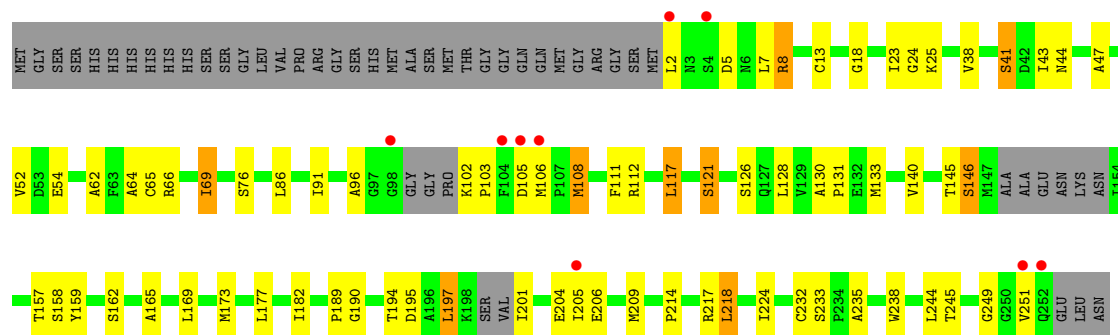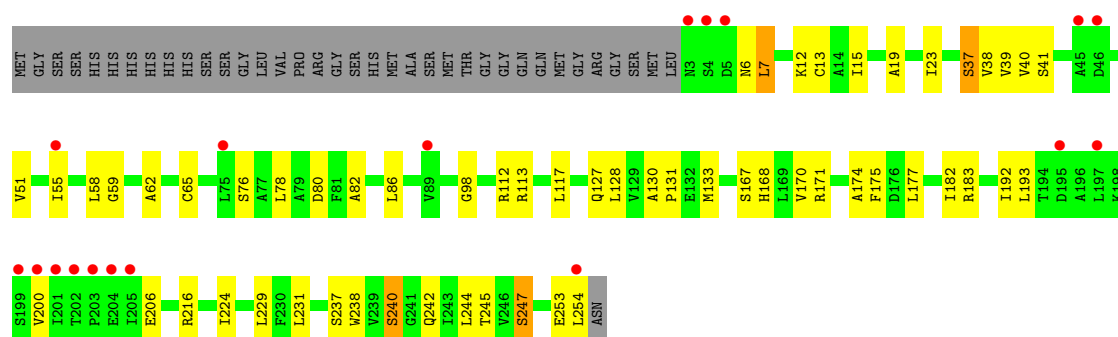S237 S240 G241 V251 L254 ASN

● Molecule 1: 7alpha-hydroxysteroid dehydrogenase

Chain F:

3%

63% 16% • 19%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA SER MET THR GLY GLY GLN MET ARG GLY SER MET LEU N3 S4 D5 N6 L7 C13 A14 I15 I16 A19 I23 E26 I27 S41 I55 A62

C65 Q73 S76 L86 I91 G99 F104 D110 R113 E116 S126 G139 S146 M147 A148 ALA GLU ASN LYS N153 I154 S158 K163 M173 L177 I182 R183 I187 A188 P189 I192 L193 T194 D195 A196 L197 T202 P203 E204 I205

GLU GLN LYS MET LEU GLN HIS THR PRO I215 R216 R217 L218 G219 Q220 I224 L231 S240 L244 T245 V246 S247 G250 VAL GLN GLU LEU ASN

● Molecule 1: 7alpha-hydroxysteroid dehydrogenase

Chain G:

3%

58% 22% • 17%

• Molecule 1: 7alpha-hydroxysteroid dehydrogenase

Chain H:

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
$< I/\sigma(I) >$ [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]	$< |L| > = 0.51$, $< L^2 > = 0.34$	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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(^{o})	Ideal(^{o})
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 (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	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 ⓘ

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	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 ⓘ

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 ⓘ

There are no monosaccharides 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(Å²)	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 ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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.