



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:35 AM UTC

PDB ID : 7ENY / pdb_00007eny
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 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

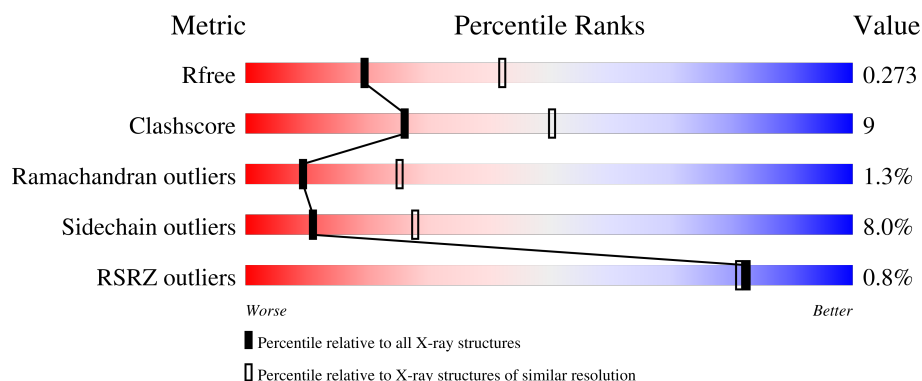
1 Overall quality at a glance

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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	% 66% 19% • 13%
1	B	289	60% 22% • 16%
1	C	289	% 65% 14% • 17%
1	D	289	63% 24% • 13%
1	E	289	% 70% 16% • 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	289	% 63%15%19%
1	G	289	% 57%22%17%
1	H	289	% 65%19%13%

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

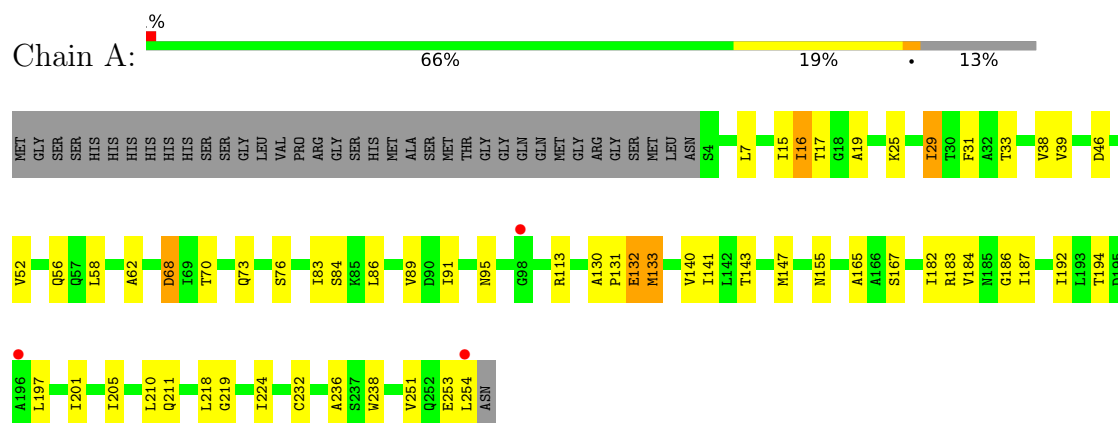
- Molecule 2 is water.

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

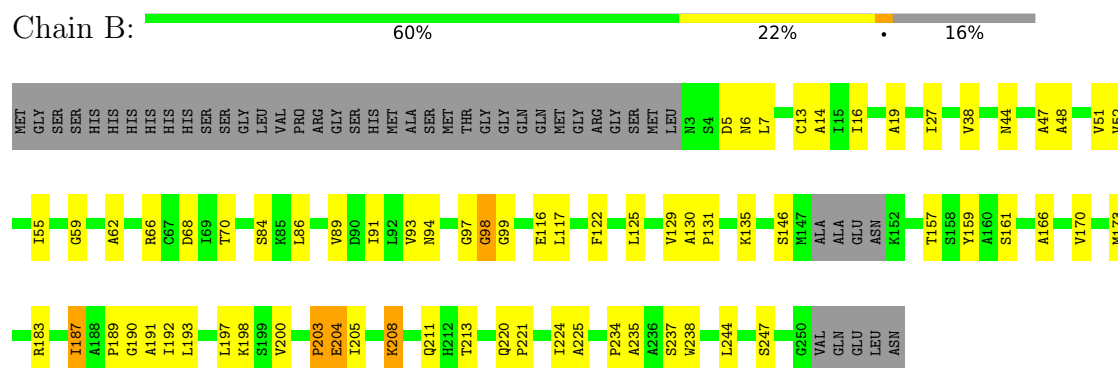
3 Residue-property plots

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.

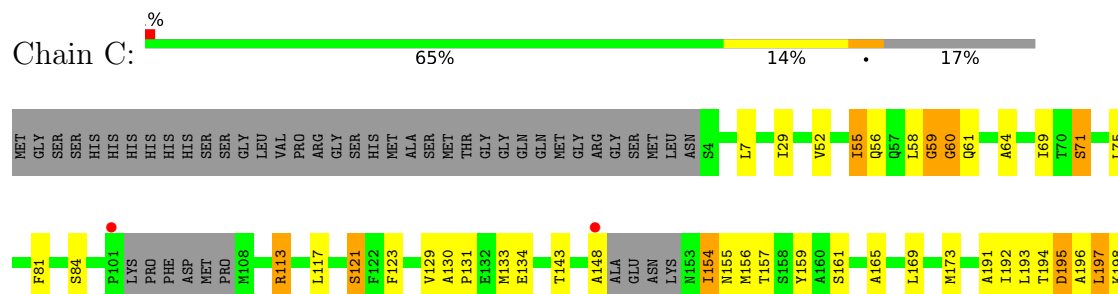
• Molecule 1: 7alpha-hydroxysteroid dehydrogenase



• Molecule 1: 7alpha-hydroxysteroid dehydrogenase



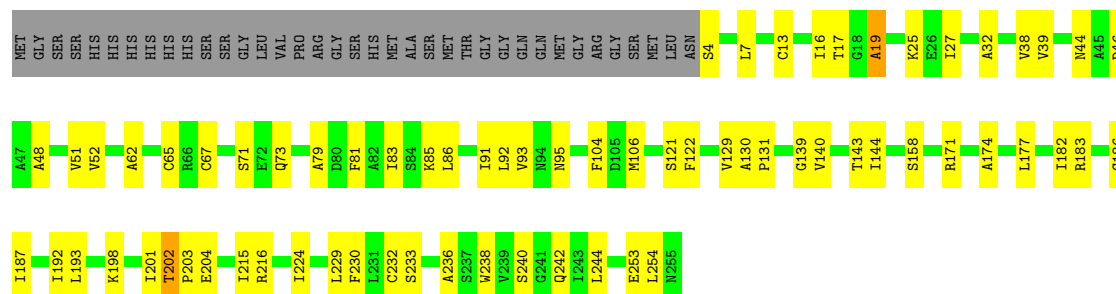
• Molecule 1: 7alpha-hydroxysteroid dehydrogenase





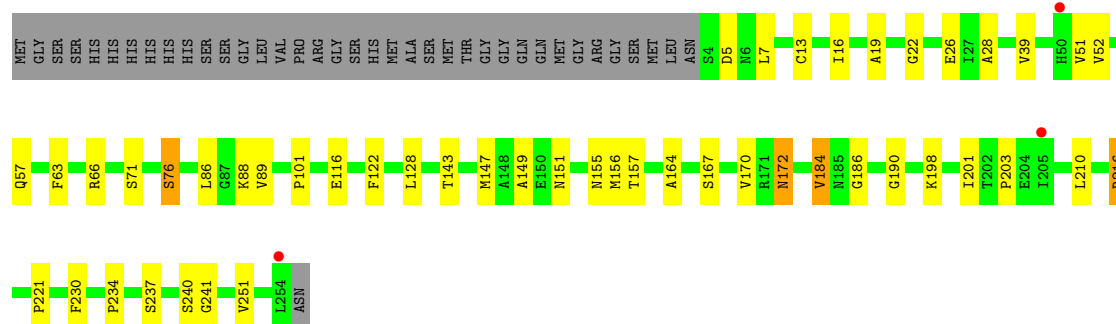
• Molecule 1: 7alpha-hydroxysteroid dehydrogenase

Chain D: 63% 24% 13%



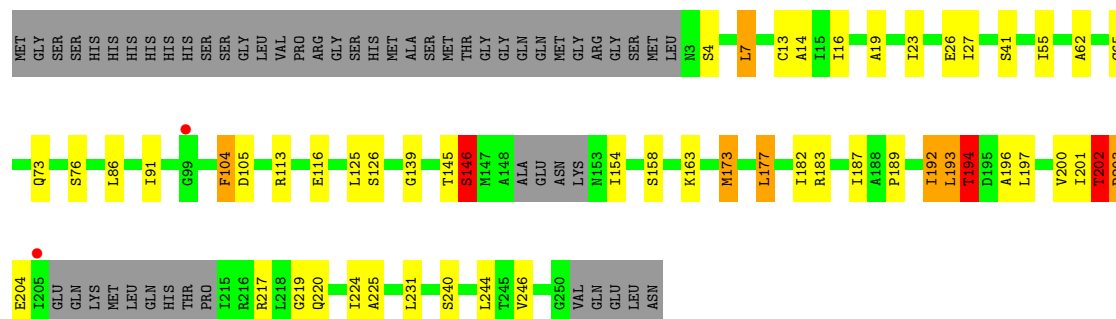
• Molecule 1: 7alpha-hydroxysteroid dehydrogenase

Chain E: 70% 16% 13%



• Molecule 1: 7alpha-hydroxysteroid dehydrogenase

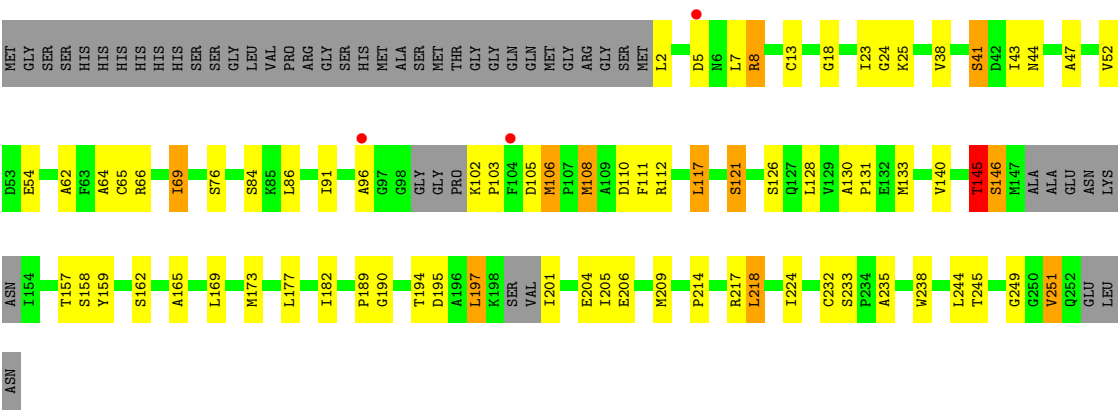
Chain F: 63% 15% 19%



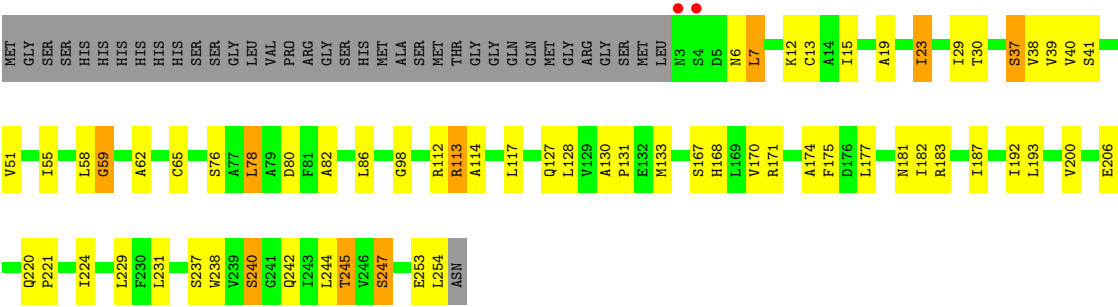
• Molecule 1: 7alpha-hydroxysteroid dehydrogenase

Chain G: 57% 22% 17%





• 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 38.09 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (38.09-2.70) 98.3 (38.09-2.70)	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 (Not available) , 0.273	Depositor DCC
R_{free} test set	2490 reflections (4.90%)	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 , 25.6	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	0.95	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

5.1 Standard geometry

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	1.13	0/1866	1.53	1/2526 (0.0%)
1	B	1.12	0/1813	1.52	1/2452 (0.0%)
1	C	1.12	0/1783	1.56	6/2410 (0.2%)
1	D	1.10	0/1874	1.56	5/2537 (0.2%)
1	E	1.11	0/1866	1.49	3/2526 (0.1%)
1	F	1.15	0/1730	1.57	10/2340 (0.4%)
1	G	1.10	0/1789	1.57	1/2417 (0.0%)
1	H	1.11	0/1874	1.50	1/2537 (0.0%)
All	All	1.12	0/14595	1.54	28/19745 (0.1%)

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

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	202	THR	CB-CA-C	6.32	118.36	108.88
1	D	215	ILE	CA-C-O	-6.09	117.33	122.63
1	F	177	LEU	CA-C-N	5.91	126.54	119.98
1	F	177	LEU	C-N-CA	5.91	126.54	119.98
1	C	134	GLU	CA-C-N	5.81	128.34	120.38
1	C	134	GLU	C-N-CA	5.81	128.34	120.38
1	D	174	ALA	CA-C-N	5.49	127.90	120.44
1	D	174	ALA	C-N-CA	5.49	127.90	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	121	SER	CA-C-N	5.44	127.57	120.28
1	C	121	SER	C-N-CA	5.44	127.57	120.28
1	A	68	ASP	CA-CB-CG	5.41	118.01	112.60
1	D	19	ALA	CA-C-N	5.38	125.96	119.98
1	D	19	ALA	C-N-CA	5.38	125.96	119.98
1	F	192	ILE	CA-C-N	5.36	129.17	120.60
1	F	192	ILE	C-N-CA	5.36	129.17	120.60
1	B	189	PRO	CA-C-O	-5.32	115.52	122.12
1	H	245	THR	CB-CA-C	5.31	119.09	110.22
1	F	104	PHE	CA-C-N	5.20	131.48	121.54
1	F	104	PHE	C-N-CA	5.20	131.48	121.54
1	E	22	GLY	CA-C-N	5.13	127.22	120.60
1	E	22	GLY	C-N-CA	5.13	127.22	120.60
1	C	161	SER	CA-C-N	5.11	127.13	120.28
1	C	161	SER	C-N-CA	5.11	127.13	120.28
1	E	230	PHE	CA-CB-CG	-5.11	108.69	113.80
1	F	225	ALA	CA-C-N	5.10	127.42	120.54
1	F	225	ALA	C-N-CA	5.10	127.42	120.54
1	F	105	ASP	CA-CB-CG	5.08	117.68	112.60
1	G	145	THR	CB-CA-C	5.02	118.73	110.95

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	34	0
1	B	1788	0	1798	37	0
1	C	1759	0	1771	29	0
1	D	1848	0	1855	38	0
1	E	1840	0	1849	21	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1708	0	1713	26	0
1	G	1767	0	1778	57	0
1	H	1848	0	1855	49	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	270	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.

All (270) 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
1:B:55:ILE:HG21	1:B:62:ALA:HB2	1.73	0.70
1:C:69:ILE:O	1:C:75:LEU:HD11	1.91	0.70
1:A:39:VAL:HG23	1:A:86:LEU:HD11	1.74	0.70
1:D:44:ASN:OD1	1:D:46:ASP:HB2	1.93	0.69
1:A:17:THR:O	1:A:95:ASN:HB3	1.92	0.69
1:F:220:GLN:N	1:F:220:GLN:OE1	2.26	0.69
1:G:217:ARG:O	1:G:218:LEU:HB2	1.93	0.69
1:C:59:GLY:O	1:C:60:GLY:O	2.12	0.67
1:G:214:PRO:HB3	1:H:174:ALA:O	1.95	0.67
1:C:154:ILE:O	1:C:156:MET:N	2.28	0.67
1:H:6:ASN:HB2	2:H:310:HOH:O	1.96	0.66
1:A:143:THR:O	1:A:186:GLY:HA2	1.95	0.66
1:B:70:THR:HG22	1:B:116:GLU:HB3	1.78	0.65
1:F:193:LEU:O	1:F:194:THR:O	2.15	0.65
1:F:194:THR:HG22	1:F:197:LEU:HB2	1.80	0.64
1:B:27:ILE:CD1	1:B:225:ALA:HA	2.28	0.63
1:G:8:ARG:HH11	1:G:8:ARG:HG2	1.62	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:183:ARG:NH2	1:F:231:LEU:O	2.31	0.63
1:A:16:ILE:HG22	1:A:19:ALA:HB2	1.80	0.63
1:B:6:ASN:HB3	1:B:235:ALA:HB2	1.80	0.63
1:C:61[A]:GLN:OE1	1:C:61[A]:GLN:HA	1.97	0.62
1:E:7:LEU:HG	1:F:7:LEU:HG	1.80	0.62
1:E:116:GLU:OE2	1:G:112:ARG:NH1	2.33	0.62
1:C:71:SER:O	1:C:75:LEU:HD12	1.98	0.62
1:E:39:VAL:HG23	1:E:86:LEU:HD11	1.82	0.62
1:D:106:MET:HE1	1:D:158:SER:OG	2.01	0.61
1:G:91:ILE:HG12	1:G:140:VAL:HG12	1.83	0.60
1:H:23:ILE:HD11	1:H:192:ILE:HG13	1.82	0.60
1:H:55:ILE:HG21	1:H:62:ALA:HB2	1.82	0.60
1:E:26:GLU:HG2	1:E:221:PRO:HB2	1.84	0.59
1:B:27:ILE:HG21	1:B:93:VAL:HG11	1.84	0.59
1:G:23:ILE:HG21	1:G:224:ILE:HG21	1.84	0.59
1:G:5:ASP:HA	1:G:8:ARG:HB2	1.85	0.58
1:G:108:MET:HE2	1:G:108:MET:HA	1.85	0.58
1:A:68:ASP:OD1	1:A:70:THR:OG1	2.14	0.58
1:D:130:ALA:HB3	1:D:131:PRO:HD3	1.86	0.58
1:D:79:ALA:O	1:D:83:ILE:HG12	2.02	0.58
1:F:14:ALA:HA	1:F:91:ILE:O	2.03	0.58
1:C:81:PHE:O	1:C:84:SER:OG	2.19	0.57
1:E:16:ILE:HG22	1:E:19:ALA:HB2	1.86	0.57
1:H:177:LEU:HB3	1:H:182:ILE:HB	1.86	0.57
1:B:125:LEU:O	1:B:129:VAL:HG23	2.05	0.57
1:B:89:VAL:HG11	1:B:129:VAL:CG1	2.35	0.57
1:D:39:VAL:HG23	1:D:86:LEU:HD11	1.87	0.57
1:F:194:THR:HG22	1:F:197:LEU:CB	2.35	0.56
1:A:38:VAL:O	1:A:62:ALA:HA	2.05	0.56
1:G:133:MET:HB2	1:G:182:ILE:HD11	1.88	0.56
1:G:106:MET:HE2	1:G:111:PHE:HB2	1.88	0.56
1:B:204:GLU:OE1	1:B:204:GLU:O	2.24	0.55
1:G:23:ILE:CG2	1:G:224:ILE:HG21	2.36	0.55
1:G:106:MET:HE1	1:G:158:SER:HB2	1.88	0.55
1:G:233:SER:OG	1:G:235:ALA:HB3	2.07	0.55
1:A:29:ILE:O	1:A:33:THR:HG23	2.07	0.55
1:G:169:LEU:O	1:G:173:MET:HB2	2.06	0.55
1:G:18:GLY:O	1:G:24:GLY:HA3	2.07	0.55
1:G:111:PHE:HA	1:G:158:SER:OG	2.07	0.55
1:H:183:ARG:NH2	1:H:231:LEU:O	2.40	0.55
1:A:133:MET:CE	1:A:182:ILE:HD13	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:VAL:HG11	1:B:129:VAL:HG13	1.89	0.54
1:H:245:THR:HG22	1:H:247:SER:HB2	1.89	0.54
1:B:204:GLU:O	1:B:204:GLU:CD	2.51	0.54
1:B:13:CYS:HB3	1:B:86:LEU:HD13	1.91	0.53
1:C:193:LEU:O	1:C:195:ASP:N	2.41	0.53
1:A:52:VAL:O	1:A:56:GLN:HG3	2.08	0.53
1:H:19:ALA:O	1:H:51:VAL:HG21	2.08	0.53
1:G:43:ILE:N	1:G:43:ILE:HD12	2.24	0.53
1:H:80:ASP:C	1:H:82:ALA:H	2.16	0.53
1:A:140:VAL:HG21	1:A:232:CYS:HA	1.91	0.53
1:E:16:ILE:HD12	1:E:28:ALA:HA	1.90	0.52
1:F:13:CYS:HB3	1:F:86:LEU:HD13	1.91	0.52
1:F:73:GLN:NE2	2:F:301:HOH:O	2.42	0.52
1:H:19:ALA:HB3	1:H:40:VAL:HG13	1.92	0.52
1:D:25:LYS:HD2	1:D:51:VAL:HG22	1.91	0.52
1:F:192:ILE:HG22	1:F:194:THR:H	1.74	0.52
1:D:38:VAL:O	1:D:62:ALA:HA	2.09	0.52
1:G:249:GLY:CA	1:H:240:SER:HB3	2.40	0.52
1:H:38:VAL:HG23	1:H:38:VAL:O	2.10	0.52
1:H:65:CYS:SG	1:H:78:LEU:HD12	2.50	0.52
1:G:103:PRO:O	1:G:106:MET:SD	2.68	0.52
1:D:140:VAL:HG21	1:D:232:CYS:HA	1.90	0.52
1:E:147:MET:HE1	1:E:251:VAL:HA	1.91	0.52
1:C:113[A]:ARG:NH2	1:C:159:TYR:OH	2.42	0.52
1:D:16:ILE:HD13	1:D:27:ILE:HG22	1.91	0.51
1:F:55:ILE:HG21	1:F:62:ALA:HB2	1.93	0.51
1:H:41:SER:HA	1:H:65:CYS:O	2.10	0.51
1:A:192:ILE:HG22	1:A:194:THR:HG23	1.92	0.51
1:D:86:LEU:HA	2:D:302:HOH:O	2.10	0.51
1:E:13:CYS:SG	1:E:86:LEU:HB3	2.50	0.51
1:B:192:ILE:HD11	1:B:224:ILE:HD11	1.93	0.51
1:D:81:PHE:CZ	1:D:85:LYS:HE3	2.46	0.51
1:H:38:VAL:O	1:H:62:ALA:HA	2.10	0.51
1:D:92:LEU:HD22	1:D:129:VAL:HG21	1.93	0.51
1:D:193:LEU:HG	1:D:198:LYS:HG3	1.93	0.51
1:F:187:ILE:HG23	1:F:246:VAL:HG23	1.92	0.51
1:G:8:ARG:HH11	1:G:8:ARG:CG	2.23	0.51
1:F:139:GLY:O	1:F:182:ILE:HA	2.11	0.50
1:D:143:THR:O	1:D:186:GLY:HA2	2.11	0.50
1:G:41:SER:HA	1:G:65:CYS:O	2.10	0.50
1:G:214:PRO:HG3	1:H:175:PHE:HA	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ILE:HD11	1:A:132:GLU:HG2	1.92	0.50
1:C:169:LEU:O	1:C:173:MET:HB2	2.12	0.50
1:F:126:SER:OG	1:F:173:MET:HE1	2.11	0.50
1:D:13:CYS:HB3	1:D:86:LEU:HD13	1.94	0.50
1:B:187:ILE:HA	1:B:244:LEU:O	2.10	0.50
1:G:245:THR:HB	1:H:242:GLN:OE1	2.12	0.50
1:G:2:LEU:HD23	1:H:229:LEU:HD21	1.94	0.49
1:E:76:SER:HA	1:E:128:LEU:HD13	1.94	0.49
1:D:183:ARG:CZ	1:D:236:ALA:O	2.59	0.49
1:A:15:ILE:C	1:A:16:ILE:HD12	2.38	0.49
1:B:48:ALA:O	1:B:52:VAL:HG23	2.13	0.49
1:B:221:PRO:HG2	2:B:317:HOH:O	2.13	0.49
1:D:17:THR:O	1:D:95:ASN:HB3	2.12	0.49
1:A:31:PHE:HE2	1:A:91:ILE:HG21	1.77	0.49
1:G:189:PRO:HB3	1:G:224:ILE:HD11	1.94	0.49
1:B:166:ALA:O	1:B:170:VAL:HG23	2.13	0.48
1:G:25:LYS:NZ	1:G:54:GLU:OE2	2.46	0.48
1:G:177:LEU:HB3	1:G:182:ILE:HB	1.95	0.48
1:F:177:LEU:HB3	1:F:182:ILE:HB	1.95	0.48
1:D:177:LEU:HB3	1:D:182:ILE:HB	1.96	0.48
1:A:155:ASN:HA	2:A:305:HOH:O	2.13	0.48
1:B:200:VAL:HG12	1:B:200:VAL:O	2.12	0.48
1:G:205:ILE:O	1:G:205:ILE:HD12	2.14	0.48
1:D:27:ILE:HG21	1:D:93:VAL:HG11	1.96	0.48
1:B:68:ASP:OD2	1:B:70:THR:OG1	2.25	0.48
1:B:187:ILE:HG21	1:B:224:ILE:HG23	1.95	0.48
1:E:143:THR:O	1:E:186:GLY:HA2	2.14	0.48
1:F:192:ILE:HA	1:F:219:GLY:O	2.14	0.48
1:H:37:SER:HB2	1:H:86:LEU:HD22	1.96	0.48
1:H:78:LEU:C	1:H:80:ASP:H	2.20	0.48
1:F:189:PRO:HB3	1:F:224:ILE:HD12	1.96	0.47
1:D:32:ALA:HB2	1:D:38:VAL:HG21	1.96	0.47
1:G:52:VAL:HG21	1:G:64:ALA:HB2	1.94	0.47
1:A:210:LEU:HD21	1:A:218:LEU:HD23	1.96	0.47
1:E:101:PRO:HA	1:E:155:ASN:O	2.14	0.47
1:A:16:ILE:HD12	1:A:16:ILE:N	2.30	0.47
1:C:129:VAL:CG1	1:C:133:MET:HE3	2.44	0.47
1:G:244:LEU:HD13	1:H:244:LEU:HD13	1.95	0.47
1:C:245:THR:HB	1:D:242:GLN:OE1	2.14	0.47
1:G:249:GLY:HA3	1:H:240:SER:HB3	1.97	0.47
1:E:210:LEU:HB3	1:E:216:ARG:HG3	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:VAL:O	1:B:200:VAL:CG1	2.63	0.47
1:E:149:ALA:HB1	1:E:164:ALA:HA	1.97	0.47
1:H:76:SER:HA	1:H:128:LEU:HD13	1.97	0.47
1:C:143:THR:HG21	2:C:301:HOH:O	2.15	0.47
1:C:56:GLN:HA	1:C:60:GLY:HA2	1.96	0.46
1:C:148:ALA:CB	1:C:159:TYR:HB3	2.46	0.46
1:D:16:ILE:HG22	1:D:19:ALA:HB2	1.97	0.46
1:H:192:ILE:HD11	1:H:224:ILE:HD11	1.96	0.46
1:A:39:VAL:HG23	1:A:86:LEU:CD1	2.43	0.46
1:F:16:ILE:HG22	1:F:19:ALA:HB2	1.96	0.46
1:G:189:PRO:HB3	1:G:224:ILE:CD1	2.45	0.46
1:B:183:ARG:HD3	1:B:237:SER:O	2.16	0.46
1:A:238:TRP:HZ2	1:B:191:ALA:HB3	1.81	0.45
1:B:55:ILE:O	1:B:59:GLY:O	2.34	0.45
1:C:123:PHE:HD1	1:C:173:MET:HE2	1.81	0.45
1:F:116:GLU:OE1	1:H:112:ARG:NH1	2.49	0.45
1:H:130:ALA:HB3	1:H:131:PRO:HD3	1.98	0.45
1:A:197:LEU:HG	1:A:201:ILE:HG13	1.99	0.45
1:H:133:MET:HE3	1:H:182:ILE:HD13	1.98	0.45
1:C:130:ALA:N	1:C:131:PRO:CD	2.80	0.45
1:H:168:HIS:HA	1:H:171:ARG:HD3	1.98	0.45
1:B:16:ILE:HD13	1:B:38:VAL:HG13	1.98	0.45
1:D:91:ILE:HA	1:D:140:VAL:O	2.16	0.45
1:H:80:ASP:C	1:H:82:ALA:N	2.74	0.45
1:H:38:VAL:O	1:H:38:VAL:CG2	2.65	0.45
1:C:29:ILE:HA	1:C:55:ILE:HD13	1.99	0.44
1:G:249:GLY:HA2	1:H:240:SER:C	2.42	0.44
1:B:94:ASN:ND2	1:B:122:PHE:HB2	2.33	0.44
1:G:106:MET:HE2	1:G:111:PHE:CB	2.47	0.44
1:C:227:ALA:HA	1:D:230:PHE:CZ	2.51	0.44
1:E:234:PRO:O	1:E:237:SER:HB3	2.17	0.44
1:G:13:CYS:HB3	1:G:86:LEU:HD22	1.97	0.44
1:H:19:ALA:CB	1:H:40:VAL:HG13	2.46	0.44
1:C:197:LEU:HD22	1:C:201:ILE:HG12	1.99	0.44
1:B:208:LYS:HA	1:B:211:GLN:NE2	2.32	0.44
1:G:96:ALA:HB1	1:G:117:LEU:HD12	1.99	0.44
1:B:27:ILE:HD12	1:B:225:ALA:HA	1.97	0.44
1:G:206:GLU:O	1:G:209:MET:N	2.50	0.44
1:C:191:ALA:HB1	1:C:209:MET:HE3	1.99	0.44
1:A:165:ALA:HB2	1:C:165:ALA:HB2	2.00	0.44
1:D:104:PHE:CD1	1:D:104:PHE:C	2.95	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:ILE:HD13	1:F:27:ILE:HG22	2.00	0.44
1:A:219:GLY:HA3	1:B:238:TRP:CZ3	2.53	0.44
1:F:202:THR:O	1:F:203:PRO:C	2.60	0.44
1:H:13:CYS:HA	1:H:37:SER:O	2.18	0.44
1:G:197:LEU:HD13	1:G:197:LEU:HA	1.82	0.43
1:F:145:THR:O	1:F:146:SER:C	2.61	0.43
1:G:197:LEU:HB3	1:G:201:ILE:HA	2.00	0.43
1:A:253:GLU:N	1:A:253:GLU:OE1	2.51	0.43
1:E:172:ASN:HB3	1:G:157:THR:HG22	2.01	0.43
1:G:69:ILE:HD13	1:G:69:ILE:HA	1.85	0.43
1:B:130:ALA:HB3	1:B:131:PRO:HD3	2.01	0.43
1:D:19:ALA:O	1:D:25:LYS:HA	2.18	0.43
1:D:81:PHE:CE1	1:D:85:LYS:HG3	2.53	0.43
1:D:183:ARG:NH1	1:D:236:ALA:O	2.51	0.43
1:E:151:ASN:ND2	2:E:304:HOH:O	2.46	0.43
1:E:167:SER:O	1:E:170:VAL:HB	2.18	0.43
1:F:41:SER:HA	1:F:65:CYS:O	2.19	0.43
1:B:19:ALA:O	1:B:51:VAL:HG21	2.18	0.43
1:C:214:PRO:HD2	1:C:248:GLY:O	2.19	0.43
1:G:102:LYS:N	1:G:103:PRO:CD	2.82	0.43
1:A:141:ILE:O	1:A:184:VAL:HA	2.19	0.42
1:B:97:GLY:O	1:B:98:GLY:C	2.61	0.42
1:D:139:GLY:O	1:D:182:ILE:HA	2.18	0.42
1:G:106:MET:HE3	1:G:110:ASP:HB3	2.01	0.42
1:H:167:SER:O	1:H:170:VAL:HB	2.18	0.42
1:E:156:MET:O	1:E:157:THR:C	2.62	0.42
1:G:106:MET:HE2	1:G:111:PHE:CA	2.49	0.42
1:A:16:ILE:N	1:A:16:ILE:CD1	2.82	0.42
1:A:147:MET:HE2	1:A:147:MET:HB3	1.85	0.42
1:B:14:ALA:HA	1:B:91:ILE:O	2.19	0.42
1:B:44:ASN:HD22	1:B:47:ALA:H	1.67	0.42
1:D:73:GLN:OE1	1:D:73:GLN:N	2.52	0.42
1:E:184:VAL:O	1:E:241:GLY:N	2.47	0.42
1:G:2:LEU:CD2	1:H:7:LEU:HD23	2.50	0.42
1:H:127:GLN:O	1:H:131:PRO:HD3	2.19	0.42
1:G:197:LEU:CD1	2:G:315:HOH:O	2.67	0.42
1:H:15:ILE:HA	1:H:39:VAL:CG1	2.50	0.42
1:B:198:LYS:C	1:B:200:VAL:H	2.28	0.42
1:H:220:GLN:O	1:H:221:PRO:C	2.61	0.42
1:D:192:ILE:HD11	1:D:224:ILE:HD11	2.01	0.42
1:D:65:CYS:HB2	1:D:81:PHE:CD1	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:69:ILE:HG23	1:G:121:SER:CB	2.50	0.42
1:A:210:LEU:HD21	1:A:218:LEU:CD2	2.50	0.41
1:G:44:ASN:OD1	1:G:47:ALA:N	2.44	0.41
1:C:52:VAL:HG21	1:C:64:ALA:HB2	2.02	0.41
1:E:51:VAL:O	1:E:52:VAL:C	2.61	0.41
1:F:104:PHE:CE2	1:H:127:GLN:HA	2.55	0.41
1:G:197:LEU:HD13	2:G:315:HOH:O	2.21	0.41
1:H:58:LEU:O	1:H:59:GLY:C	2.63	0.41
1:G:130:ALA:N	1:G:131:PRO:HD2	2.34	0.41
1:H:41:SER:HB2	1:H:78:LEU:HD11	2.02	0.41
1:A:133:MET:HE3	1:A:182:ILE:HG12	2.02	0.41
1:C:7:LEU:HD22	1:D:7:LEU:HD22	2.03	0.41
1:C:29:ILE:HA	1:C:55:ILE:CD1	2.51	0.41
1:A:130:ALA:N	1:A:131:PRO:HD2	2.36	0.41
1:B:99:GLY:HA2	1:B:159:TYR:CZ	2.56	0.41
1:D:48:ALA:O	1:D:52:VAL:HG23	2.20	0.41
1:A:183:ARG:NH2	1:A:236:ALA:O	2.54	0.41
1:D:121:SER:OG	1:D:122:PHE:N	2.54	0.41
1:G:38:VAL:O	1:G:62:ALA:HA	2.20	0.41
1:H:29:ILE:O	1:H:30:THR:C	2.63	0.41
1:H:183:ARG:HD2	1:H:237:SER:O	2.21	0.41
1:A:25:LYS:NZ	2:A:307:HOH:O	2.54	0.41
1:A:187:ILE:HG21	1:A:224:ILE:HG23	2.03	0.41
1:B:157:THR:O	1:B:161:SER:HB2	2.21	0.41
1:B:190:GLY:HA3	1:B:247:SER:CB	2.51	0.41
1:G:162:SER:O	1:G:165:ALA:HB3	2.19	0.41
1:D:229:LEU:O	1:D:233:SER:HB3	2.21	0.41
1:G:140:VAL:HG21	1:G:232:CYS:HA	2.03	0.41
1:H:23:ILE:CD1	1:H:192:ILE:HG13	2.49	0.40
1:A:83:ILE:CD1	1:A:89:VAL:HG23	2.51	0.40
1:A:238:TRP:HA	1:A:238:TRP:CE3	2.56	0.40
1:D:187:ILE:HA	1:D:244:LEU:O	2.21	0.40
1:D:202:THR:C	1:D:204:GLU:H	2.30	0.40
1:E:122:PHE:CE1	1:E:143:THR:HB	2.56	0.40
1:G:126:SER:O	1:G:130:ALA:HB2	2.22	0.40
1:G:145:THR:O	1:G:146:SER:CB	2.69	0.40
1:H:98:GLY:H	1:H:117:LEU:HB3	1.86	0.40
1:F:23:ILE:HD12	1:F:224:ILE:HG13	2.03	0.40
1:F:187:ILE:HA	1:F:244:LEU:O	2.21	0.40
1:G:76:SER:HA	1:G:128:LEU:HD13	2.04	0.40
1:H:15:ILE:HA	1:H:39:VAL:HG13	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:LEU:O	1:C:121:SER:OG	2.40	0.40
1:H:113:ARG:O	1:H:114:ALA:C	2.65	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	249/289 (86%)	230 (92%)	19 (8%)	0	100	100
1	B	240/289 (83%)	219 (91%)	17 (7%)	4 (2%)	7	19
1	C	235/289 (81%)	209 (89%)	18 (8%)	8 (3%)	3	7
1	D	250/289 (86%)	233 (93%)	15 (6%)	2 (1%)	16	37
1	E	249/289 (86%)	233 (94%)	14 (6%)	2 (1%)	16	37
1	F	229/289 (79%)	214 (93%)	11 (5%)	4 (2%)	7	19
1	G	232/289 (80%)	210 (90%)	17 (7%)	5 (2%)	5	14
1	H	250/289 (86%)	218 (87%)	31 (12%)	1 (0%)	30	54
All	All	1934/2312 (84%)	1766 (91%)	142 (7%)	26 (1%)	9	25

All (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
1	F	194	THR
1	F	203	PRO
1	G	146	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	194	THR
1	B	98	GLY
1	C	196	ALA
1	G	190	GLY
1	C	202	THR
1	F	196	ALA
1	H	59	GLY
1	B	146	SER
1	C	198	LYS
1	C	195	ASP
1	E	203	PRO
1	B	193	LEU
1	D	203	PRO
1	G	218	LEU
1	C	59	GLY
1	B	203	PRO
1	E	190	GLY
1	G	251	VAL

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%)	177 (92%)	16 (8%)	10	26
1	B	188/223 (84%)	172 (92%)	16 (8%)	10	25
1	C	184/223 (82%)	171 (93%)	13 (7%)	13	33
1	D	194/223 (87%)	183 (94%)	11 (6%)	18	43
1	E	193/223 (86%)	179 (93%)	14 (7%)	13	32
1	F	178/223 (80%)	160 (90%)	18 (10%)	7	18
1	G	186/223 (83%)	168 (90%)	18 (10%)	8	20
1	H	194/223 (87%)	179 (92%)	15 (8%)	12	30
All	All	1510/1784 (85%)	1389 (92%)	121 (8%)	11	28

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	16	ILE
1	A	29	ILE
1	A	46	ASP
1	A	58	LEU
1	A	73	GLN
1	A	76	SER
1	A	84	SER
1	A	113	ARG
1	A	132	GLU
1	A	133	MET
1	A	167	SER
1	A	205	ILE
1	A	211	GLN
1	A	251	VAL
1	A	254	LEU
1	B	5	ASP
1	B	7	LEU
1	B	66	ARG
1	B	84	SER
1	B	117	LEU
1	B	135	LYS
1	B	173	MET
1	B	187	ILE
1	B	197	LEU
1	B	203	PRO
1	B	204	GLU
1	B	205	ILE
1	B	208	LYS
1	B	213	THR
1	B	220	GLN
1	B	234	PRO
1	C	55	ILE
1	C	58	LEU
1	C	71	SER
1	C	113[A]	ARG
1	C	113[B]	ARG
1	C	154	ILE
1	C	157	THR
1	C	192	ILE
1	C	197	LEU
1	C	201	ILE
1	C	202	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	240	SER
1	C	252	GLN
1	D	4	SER
1	D	67	CYS
1	D	71	SER
1	D	144	ILE
1	D	171	ARG
1	D	201	ILE
1	D	202	THR
1	D	238	TRP
1	D	240	SER
1	D	253	GLU
1	D	254	LEU
1	E	5	ASP
1	E	57	GLN
1	E	63	PHE
1	E	66	ARG
1	E	71	SER
1	E	76	SER
1	E	88	LYS
1	E	89	VAL
1	E	172	ASN
1	E	184	VAL
1	E	198	LYS
1	E	201	ILE
1	E	216	ARG
1	E	240	SER
1	F	4	SER
1	F	7	LEU
1	F	26	GLU
1	F	76	SER
1	F	113	ARG
1	F	125	LEU
1	F	146	SER
1	F	154	ILE
1	F	158	SER
1	F	163	LYS
1	F	173	MET
1	F	193	LEU
1	F	194	THR
1	F	200	VAL
1	F	201	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	204	GLU
1	F	217	ARG
1	F	240	SER
1	G	7	LEU
1	G	8	ARG
1	G	41	SER
1	G	66	ARG
1	G	69	ILE
1	G	84	SER
1	G	105	ASP
1	G	106	MET
1	G	108	MET
1	G	117	LEU
1	G	121	SER
1	G	145	THR
1	G	159	TYR
1	G	195	ASP
1	G	197	LEU
1	G	204	GLU
1	G	238	TRP
1	G	251	VAL
1	H	7	LEU
1	H	12	LYS
1	H	23	ILE
1	H	37	SER
1	H	78	LEU
1	H	113	ARG
1	H	181	ASN
1	H	187	ILE
1	H	193	LEU
1	H	200	VAL
1	H	206	GLU
1	H	238	TRP
1	H	240	SER
1	H	247	SER
1	H	254	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	136	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	168	HIS
1	A	211	GLN
1	A	220	GLN
1	B	44	ASN
1	B	172	ASN
1	B	211	GLN
1	B	212	HIS
1	C	153	ASN
1	C	220	GLN
1	D	127	GLN
1	D	168	HIS
1	D	185	ASN
1	D	220	GLN
1	E	95	ASN
1	E	127	GLN
1	F	3	ASN
1	F	136	ASN
1	F	155	ASN
1	F	222	GLN
1	F	226	ASN
1	G	57	GLN
1	G	118	ASN
1	G	124	HIS
1	G	211	GLN
1	G	212	HIS
1	H	127	GLN

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 oligosaccharides 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	251/289 (86%)	-0.38	3 (1%) 76 75	34, 49, 85, 111	0
1	B	244/289 (84%)	-0.29	0 100 100	31, 53, 99, 122	0
1	C	239/289 (82%)	-0.25	2 (0%) 82 81	25, 57, 118, 171	2 (0%)
1	D	252/289 (87%)	-0.32	0 100 100	38, 60, 93, 140	0
1	E	251/289 (86%)	-0.33	3 (1%) 76 75	35, 53, 93, 126	0
1	F	235/289 (81%)	-0.28	2 (0%) 81 80	36, 53, 94, 143	0
1	G	240/289 (83%)	-0.05	3 (1%) 75 73	35, 62, 125, 164	0
1	H	252/289 (87%)	-0.08	2 (0%) 82 81	43, 69, 115, 152	0
All	All	1964/2312 (84%)	-0.25	15 (0%) 82 81	25, 57, 107, 171	2 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	205	ILE	3.3
1	C	101	PRO	3.3
1	E	50	HIS	3.0
1	E	254	LEU	2.9
1	H	4	SER	2.8
1	G	5	ASP	2.7
1	G	96	ALA	2.5
1	F	99	GLY	2.4
1	C	148	ALA	2.4
1	G	104	PHE	2.4
1	A	196	ALA	2.2
1	E	205	ILE	2.2
1	A	254	LEU	2.1
1	A	98	GLY	2.1
1	H	3	ASN	2.1

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 oligosaccharides 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.