



# Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

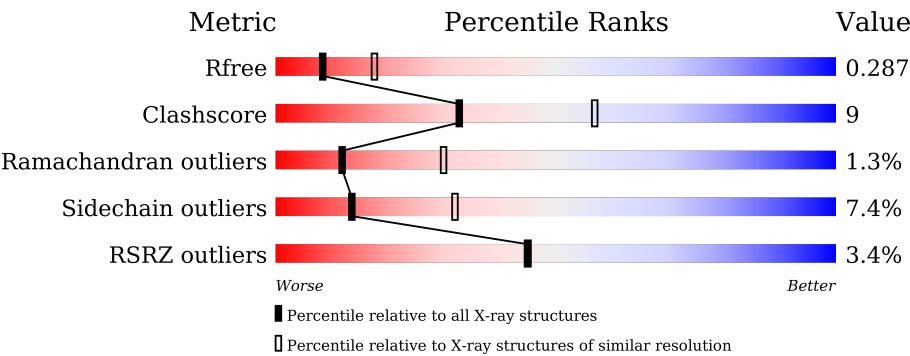
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.22
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

# 1 Overall quality at a glance i

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

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

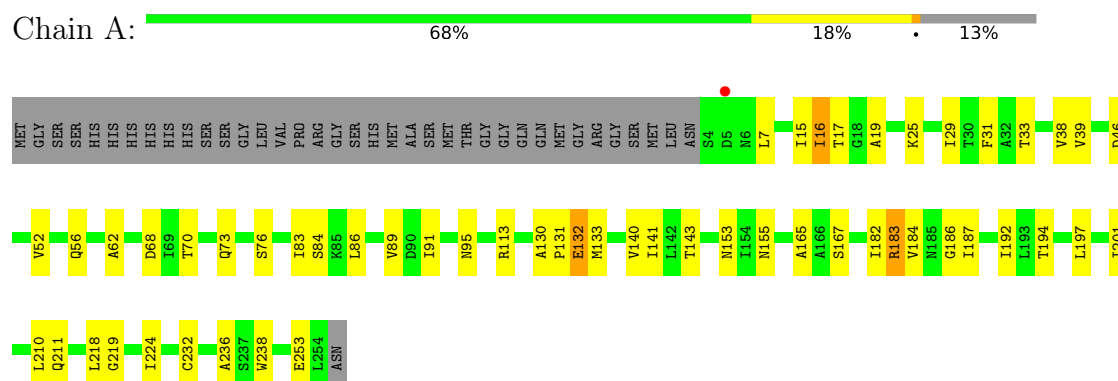
- Molecule 2 is water.

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

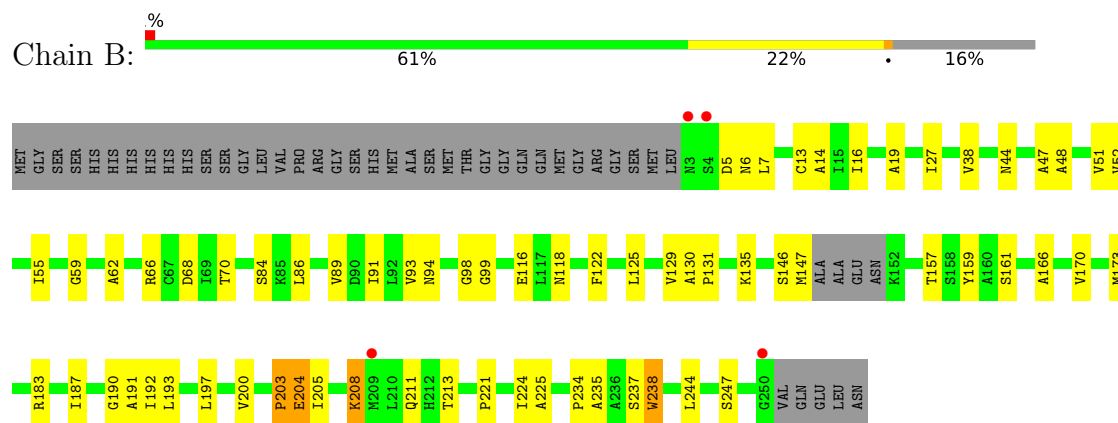
### 3 Residue-property plots

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.

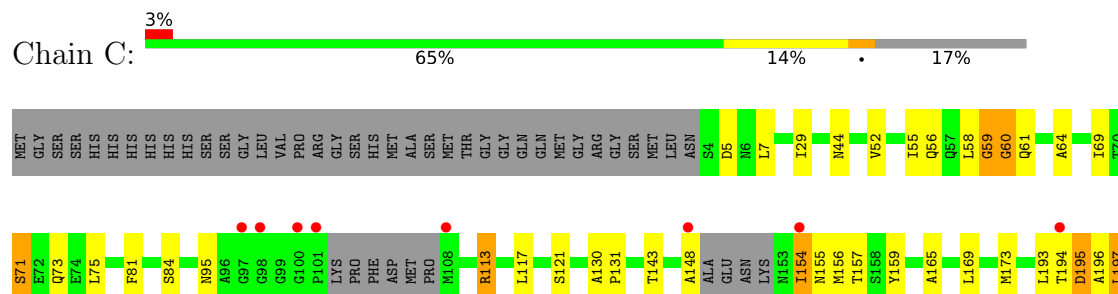
#### • Molecule 1: 7alpha-hydroxysteroid dehydrogenase

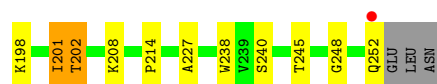


#### • Molecule 1: 7alpha-hydroxysteroid dehydrogenase

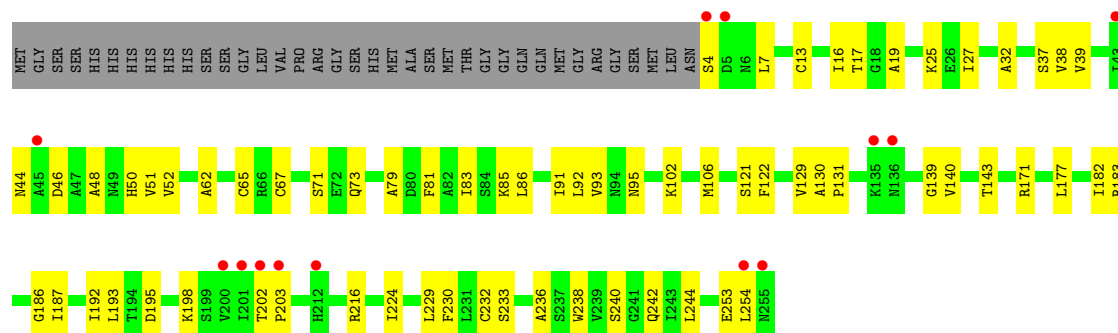


#### • Molecule 1: 7alpha-hydroxysteroid dehydrogenase

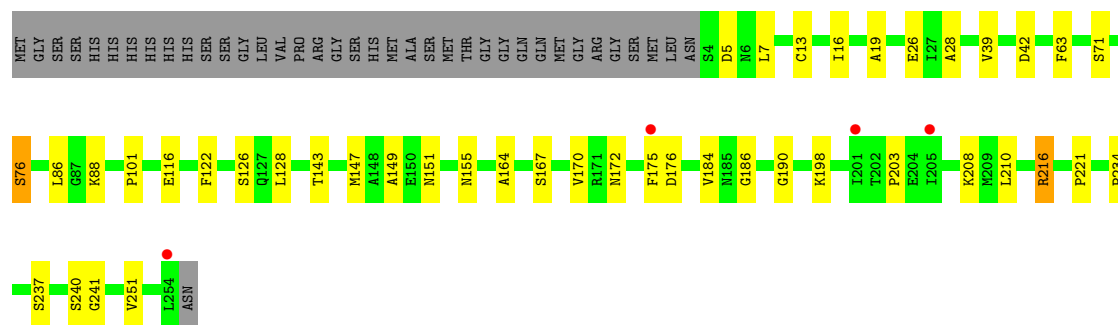




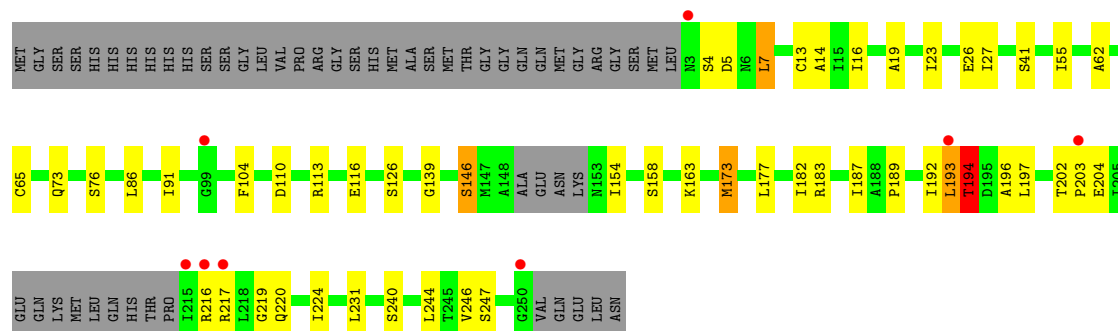
• Molecule 1: 7alpha-hydroxysteroid dehydrogenase



• Molecule 1: 7alpha-hydroxysteroid dehydrogenase

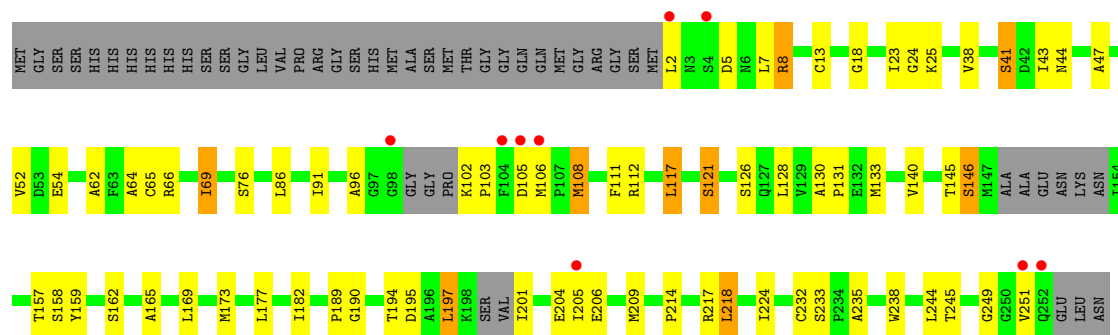


• Molecule 1: 7alpha-hydroxysteroid dehydrogenase

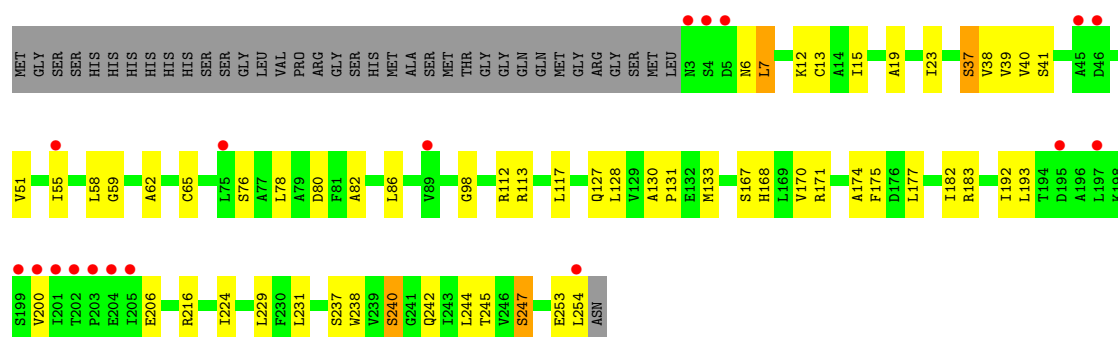


• Molecule 1: 7alpha-hydroxysteroid dehydrogenase





- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	53.1	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 33.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [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.

All (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
1:B:55:ILE:HG21	1:B:62:ALA:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:102:LYS:HB2	1:D:106:MET:HE1	1.75	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:A:68:ASP:OD1	1:A:70:THR:OG1	2.14	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:108:MET:HE2	1:G:108:MET:HA	1.86	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: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: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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:H:133:MET:HE3	1:H:182:ILE:HD13	1.94	0.49
1:B:48:ALA:O	1:B:52:VAL:HG23	2.13	0.49
1:B:204:GLU:O	1:B:204:GLU:CD	2.51	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:H:80:ASP:C	1:H:82:ALA:H	2.16	0.48
1:B:200:VAL:HG12	1:B:200:VAL:O	2.12	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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: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:B:94:ASN:ND2	1:B:122:PHE:HB2	2.33	0.44
1:A:15:ILE:C	1:A:16:ILE:HD12	2.38	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:F:126:SER:HB3	1:F:173:MET:HE3	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:165:ALA:HB2	1:C:165:ALA:HB2	2.00	0.44
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:G:106:MET:HE2	1:G:111:PHE:N	2.33	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: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:H:78:LEU:C	1:H:80:ASP:H	2.20	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:147:MET:HE3	1:E:251:VAL:HG13	2.01	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:D:139:GLY:O	1:D:182:ILE:HA	2.18	0.42
1:H:167:SER:O	1:H:170:VAL:HB	2.18	0.42
1:A:16:ILE:N	1:A:16:ILE:CD1	2.82	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: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
1:G:69:ILE:HG23	1:G:121:SER:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:133:MET:HE2	1:A:182:ILE:HD13	2.02	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: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:133:MET:HE3	1:H:182:ILE:CD1	2.50	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: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:80:ASP:C	1:H:82:ALA:N	2.74	0.40
1:H:15:ILE:HA	1:H:39:VAL:HG13	2.02	0.40
1:C:117:LEU:O	1:C:121:SER:OG	2.40	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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
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

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Mol	Chain	Res	Type
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%)	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

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	16	ILE
1	A	46	ASP
1	A	73	GLN
1	A	76	SER
1	A	84	SER

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Mol	Chain	Res	Type
1	A	113	ARG
1	A	132	GLU
1	A	153	ASN
1	A	167	SER
1	A	211	GLN
1	B	5	ASP
1	B	7	LEU
1	B	66	ARG
1	B	84	SER
1	B	118	ASN
1	B	135	LYS
1	B	147	MET
1	B	173	MET
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	234	PRO
1	B	238	TRP
1	C	5	ASP
1	C	44	ASN
1	C	58	LEU
1	C	71	SER
1	C	73	GLN
1	C	95	ASN
1	C	113[A]	ARG
1	C	113[B]	ARG
1	C	154	ILE
1	C	157	THR
1	C	197	LEU
1	C	201	ILE
1	C	202	THR
1	C	208	LYS
1	C	238	TRP
1	C	240	SER
1	C	252	GLN
1	D	4	SER
1	D	37	SER
1	D	50	HIS
1	D	67	CYS

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Mol	Chain	Res	Type
1	D	71	SER
1	D	171	ARG
1	D	195	ASP
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	42	ASP
1	E	63	PHE
1	E	71	SER
1	E	76	SER
1	E	88	LYS
1	E	126	SER
1	E	175	PHE
1	E	176	ASP
1	E	198	LYS
1	E	208	LYS
1	E	216	ARG
1	E	240	SER
1	F	4	SER
1	F	5	ASP
1	F	7	LEU
1	F	26	GLU
1	F	76	SER
1	F	110	ASP
1	F	113	ARG
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	204	GLU
1	F	216	ARG
1	F	217	ARG
1	F	240	SER
1	G	7	LEU
1	G	8	ARG
1	G	41	SER

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Mol	Chain	Res	Type
1	G	66	ARG
1	G	69	ILE
1	G	105	ASP
1	G	108	MET
1	G	117	LEU
1	G	121	SER
1	G	159	TYR
1	G	195	ASP
1	G	197	LEU
1	G	204	GLU
1	G	238	TRP
1	H	7	LEU
1	H	12	LYS
1	H	37	SER
1	H	113	ARG
1	H	193	LEU
1	H	200	VAL
1	H	206	GLU
1	H	216	ARG
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 (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	168	HIS
1	A	222	GLN
1	B	44	ASN
1	B	211	GLN
1	B	222	GLN
1	C	153	ASN
1	C	220	GLN
1	D	127	GLN
1	D	220	GLN
1	E	127	GLN
1	E	242	GLN
1	F	3	ASN
1	H	151	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	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

All (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
1	D	5	ASP	4.6
1	H	197	LEU	4.5
1	G	98	GLY	4.4
1	E	254	LEU	4.3
1	F	216	ARG	4.3
1	C	252	GLN	3.9
1	E	205	ILE	3.7
1	H	203	PRO	3.6
1	C	148	ALA	3.5
1	D	136	ASN	3.4
1	C	101	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	4	SER	3.3
1	H	3	ASN	3.3
1	F	99	GLY	3.3
1	D	254	LEU	3.2
1	H	5	ASP	3.2
1	F	215	ILE	3.2
1	F	250	GLY	3.2
1	H	200	VAL	3.1
1	D	255	ASN	3.0
1	H	204	GLU	3.0
1	H	75	LEU	2.9
1	G	205	ILE	2.9
1	D	201	ILE	2.9
1	D	43	ILE	2.8
1	G	4	SER	2.7
1	H	4	SER	2.7
1	F	203	PRO	2.7
1	H	45	ALA	2.7
1	H	199	SER	2.7
1	E	201	ILE	2.6
1	D	200	VAL	2.6
1	H	201	ILE	2.5
1	G	2	LEU	2.5
1	B	209	MET	2.5
1	H	205	ILE	2.5
1	G	252	GLN	2.4
1	H	195	ASP	2.4
1	B	4	SER	2.4
1	D	135	LYS	2.4
1	G	251	VAL	2.4
1	A	5	ASP	2.4
1	H	202	THR	2.3
1	C	100	GLY	2.3
1	F	217	ARG	2.3
1	F	3	ASN	2.3
1	F	193	LEU	2.3
1	C	154	ILE	2.3
1	G	106	MET	2.2
1	D	203	PRO	2.2
1	D	202	THR	2.2
1	C	97	GLY	2.2
1	E	175	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	89	VAL	2.1
1	D	212	HIS	2.1
1	H	55	ILE	2.1
1	C	108	MET	2.1
1	C	98	GLY	2.1
1	D	45	ALA	2.0
1	H	46	ASP	2.0
1	B	250	GLY	2.0

## 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.