



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2021 – 10:16 AM JST

PDB ID : 7BTM  
Title : SDR protein/resistance protein NapW  
Authors : Wen, W.H.; Tang, G.L.  
Deposited on : 2020-04-02  
Resolution : 2.08 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	:	2.23.2
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)	:	2.23.2

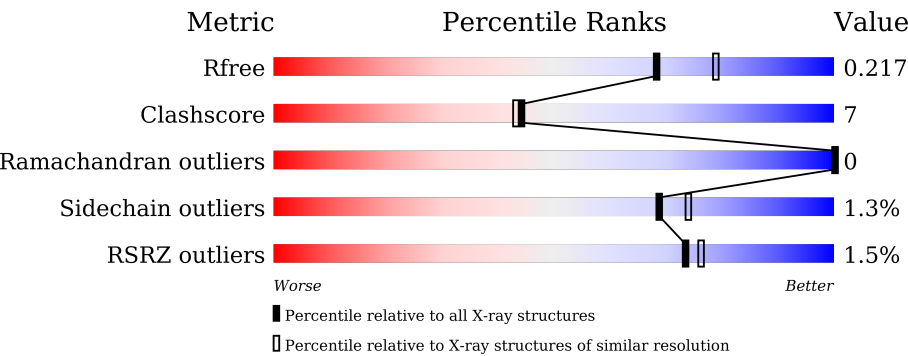
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.08 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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	331	<div><div>2%</div><div></div><div>74%</div><div>12%</div><div>14%</div></div>
1	B	331	<div><div>%</div><div></div><div>76%</div><div>9%</div><div>15%</div></div>
1	C	331	<div><div>%</div><div></div><div>80%</div><div>6%</div><div>14%</div></div>
1	D	331	<div><div>2%</div><div></div><div>76%</div><div>12%</div><div>13%</div></div>
1	E	331	<div><div>2%</div><div></div><div>76%</div><div>12%</div><div>12%</div></div>
1	F	331	<div><div>2%</div><div></div><div>79%</div><div>8%</div><div>13%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	331	<div><div>%</div><div><div></div><div>77%</div><div>11%</div><div>12%</div></div></div>
1	H	331	<div><div></div><div><div>76%</div><div>11%</div><div>12%</div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18962 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 Short chain dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2160	1347	384	421	8			
1	B	282	Total	C	N	O	S	0	0	0
			2145	1339	382	416	8			
1	C	286	Total	C	N	O	S	0	0	0
			2178	1361	387	422	8			
1	D	289	Total	C	N	O	S	0	0	0
			2207	1380	390	429	8			
1	E	292	Total	C	N	O	S	0	0	0
			2239	1402	396	433	8			
1	F	289	Total	C	N	O	S	0	0	0
			2208	1382	389	429	8			
1	G	290	Total	C	N	O	S	0	0	0
			2220	1390	391	431	8			
1	H	291	Total	C	N	O	S	0	0	0
			2226	1395	392	431	8			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP S4TKM8
A	-18	GLY	-	expression tag	UNP S4TKM8
A	-17	SER	-	expression tag	UNP S4TKM8
A	-16	SER	-	expression tag	UNP S4TKM8
A	-15	HIS	-	expression tag	UNP S4TKM8
A	-14	HIS	-	expression tag	UNP S4TKM8
A	-13	HIS	-	expression tag	UNP S4TKM8
A	-12	HIS	-	expression tag	UNP S4TKM8
A	-11	HIS	-	expression tag	UNP S4TKM8
A	-10	HIS	-	expression tag	UNP S4TKM8
A	-9	SER	-	expression tag	UNP S4TKM8
A	-8	SER	-	expression tag	UNP S4TKM8
A	-7	GLY	-	expression tag	UNP S4TKM8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP S4TKM8
A	-5	VAL	-	expression tag	UNP S4TKM8
A	-4	PRO	-	expression tag	UNP S4TKM8
A	-3	ARG	-	expression tag	UNP S4TKM8
A	-2	GLY	-	expression tag	UNP S4TKM8
A	-1	SER	-	expression tag	UNP S4TKM8
A	0	HIS	-	expression tag	UNP S4TKM8
B	-19	MET	-	expression tag	UNP S4TKM8
B	-18	GLY	-	expression tag	UNP S4TKM8
B	-17	SER	-	expression tag	UNP S4TKM8
B	-16	SER	-	expression tag	UNP S4TKM8
B	-15	HIS	-	expression tag	UNP S4TKM8
B	-14	HIS	-	expression tag	UNP S4TKM8
B	-13	HIS	-	expression tag	UNP S4TKM8
B	-12	HIS	-	expression tag	UNP S4TKM8
B	-11	HIS	-	expression tag	UNP S4TKM8
B	-10	HIS	-	expression tag	UNP S4TKM8
B	-9	SER	-	expression tag	UNP S4TKM8
B	-8	SER	-	expression tag	UNP S4TKM8
B	-7	GLY	-	expression tag	UNP S4TKM8
B	-6	LEU	-	expression tag	UNP S4TKM8
B	-5	VAL	-	expression tag	UNP S4TKM8
B	-4	PRO	-	expression tag	UNP S4TKM8
B	-3	ARG	-	expression tag	UNP S4TKM8
B	-2	GLY	-	expression tag	UNP S4TKM8
B	-1	SER	-	expression tag	UNP S4TKM8
B	0	HIS	-	expression tag	UNP S4TKM8
C	-19	MET	-	expression tag	UNP S4TKM8
C	-18	GLY	-	expression tag	UNP S4TKM8
C	-17	SER	-	expression tag	UNP S4TKM8
C	-16	SER	-	expression tag	UNP S4TKM8
C	-15	HIS	-	expression tag	UNP S4TKM8
C	-14	HIS	-	expression tag	UNP S4TKM8
C	-13	HIS	-	expression tag	UNP S4TKM8
C	-12	HIS	-	expression tag	UNP S4TKM8
C	-11	HIS	-	expression tag	UNP S4TKM8
C	-10	HIS	-	expression tag	UNP S4TKM8
C	-9	SER	-	expression tag	UNP S4TKM8
C	-8	SER	-	expression tag	UNP S4TKM8
C	-7	GLY	-	expression tag	UNP S4TKM8
C	-6	LEU	-	expression tag	UNP S4TKM8
C	-5	VAL	-	expression tag	UNP S4TKM8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP S4TKM8
C	-3	ARG	-	expression tag	UNP S4TKM8
C	-2	GLY	-	expression tag	UNP S4TKM8
C	-1	SER	-	expression tag	UNP S4TKM8
C	0	HIS	-	expression tag	UNP S4TKM8
D	-19	MET	-	expression tag	UNP S4TKM8
D	-18	GLY	-	expression tag	UNP S4TKM8
D	-17	SER	-	expression tag	UNP S4TKM8
D	-16	SER	-	expression tag	UNP S4TKM8
D	-15	HIS	-	expression tag	UNP S4TKM8
D	-14	HIS	-	expression tag	UNP S4TKM8
D	-13	HIS	-	expression tag	UNP S4TKM8
D	-12	HIS	-	expression tag	UNP S4TKM8
D	-11	HIS	-	expression tag	UNP S4TKM8
D	-10	HIS	-	expression tag	UNP S4TKM8
D	-9	SER	-	expression tag	UNP S4TKM8
D	-8	SER	-	expression tag	UNP S4TKM8
D	-7	GLY	-	expression tag	UNP S4TKM8
D	-6	LEU	-	expression tag	UNP S4TKM8
D	-5	VAL	-	expression tag	UNP S4TKM8
D	-4	PRO	-	expression tag	UNP S4TKM8
D	-3	ARG	-	expression tag	UNP S4TKM8
D	-2	GLY	-	expression tag	UNP S4TKM8
D	-1	SER	-	expression tag	UNP S4TKM8
D	0	HIS	-	expression tag	UNP S4TKM8
E	-19	MET	-	expression tag	UNP S4TKM8
E	-18	GLY	-	expression tag	UNP S4TKM8
E	-17	SER	-	expression tag	UNP S4TKM8
E	-16	SER	-	expression tag	UNP S4TKM8
E	-15	HIS	-	expression tag	UNP S4TKM8
E	-14	HIS	-	expression tag	UNP S4TKM8
E	-13	HIS	-	expression tag	UNP S4TKM8
E	-12	HIS	-	expression tag	UNP S4TKM8
E	-11	HIS	-	expression tag	UNP S4TKM8
E	-10	HIS	-	expression tag	UNP S4TKM8
E	-9	SER	-	expression tag	UNP S4TKM8
E	-8	SER	-	expression tag	UNP S4TKM8
E	-7	GLY	-	expression tag	UNP S4TKM8
E	-6	LEU	-	expression tag	UNP S4TKM8
E	-5	VAL	-	expression tag	UNP S4TKM8
E	-4	PRO	-	expression tag	UNP S4TKM8
E	-3	ARG	-	expression tag	UNP S4TKM8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP S4TKM8
E	-1	SER	-	expression tag	UNP S4TKM8
E	0	HIS	-	expression tag	UNP S4TKM8
F	-19	MET	-	expression tag	UNP S4TKM8
F	-18	GLY	-	expression tag	UNP S4TKM8
F	-17	SER	-	expression tag	UNP S4TKM8
F	-16	SER	-	expression tag	UNP S4TKM8
F	-15	HIS	-	expression tag	UNP S4TKM8
F	-14	HIS	-	expression tag	UNP S4TKM8
F	-13	HIS	-	expression tag	UNP S4TKM8
F	-12	HIS	-	expression tag	UNP S4TKM8
F	-11	HIS	-	expression tag	UNP S4TKM8
F	-10	HIS	-	expression tag	UNP S4TKM8
F	-9	SER	-	expression tag	UNP S4TKM8
F	-8	SER	-	expression tag	UNP S4TKM8
F	-7	GLY	-	expression tag	UNP S4TKM8
F	-6	LEU	-	expression tag	UNP S4TKM8
F	-5	VAL	-	expression tag	UNP S4TKM8
F	-4	PRO	-	expression tag	UNP S4TKM8
F	-3	ARG	-	expression tag	UNP S4TKM8
F	-2	GLY	-	expression tag	UNP S4TKM8
F	-1	SER	-	expression tag	UNP S4TKM8
F	0	HIS	-	expression tag	UNP S4TKM8
G	-19	MET	-	expression tag	UNP S4TKM8
G	-18	GLY	-	expression tag	UNP S4TKM8
G	-17	SER	-	expression tag	UNP S4TKM8
G	-16	SER	-	expression tag	UNP S4TKM8
G	-15	HIS	-	expression tag	UNP S4TKM8
G	-14	HIS	-	expression tag	UNP S4TKM8
G	-13	HIS	-	expression tag	UNP S4TKM8
G	-12	HIS	-	expression tag	UNP S4TKM8
G	-11	HIS	-	expression tag	UNP S4TKM8
G	-10	HIS	-	expression tag	UNP S4TKM8
G	-9	SER	-	expression tag	UNP S4TKM8
G	-8	SER	-	expression tag	UNP S4TKM8
G	-7	GLY	-	expression tag	UNP S4TKM8
G	-6	LEU	-	expression tag	UNP S4TKM8
G	-5	VAL	-	expression tag	UNP S4TKM8
G	-4	PRO	-	expression tag	UNP S4TKM8
G	-3	ARG	-	expression tag	UNP S4TKM8
G	-2	GLY	-	expression tag	UNP S4TKM8
G	-1	SER	-	expression tag	UNP S4TKM8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP S4TKM8
H	-19	MET	-	expression tag	UNP S4TKM8
H	-18	GLY	-	expression tag	UNP S4TKM8
H	-17	SER	-	expression tag	UNP S4TKM8
H	-16	SER	-	expression tag	UNP S4TKM8
H	-15	HIS	-	expression tag	UNP S4TKM8
H	-14	HIS	-	expression tag	UNP S4TKM8
H	-13	HIS	-	expression tag	UNP S4TKM8
H	-12	HIS	-	expression tag	UNP S4TKM8
H	-11	HIS	-	expression tag	UNP S4TKM8
H	-10	HIS	-	expression tag	UNP S4TKM8
H	-9	SER	-	expression tag	UNP S4TKM8
H	-8	SER	-	expression tag	UNP S4TKM8
H	-7	GLY	-	expression tag	UNP S4TKM8
H	-6	LEU	-	expression tag	UNP S4TKM8
H	-5	VAL	-	expression tag	UNP S4TKM8
H	-4	PRO	-	expression tag	UNP S4TKM8
H	-3	ARG	-	expression tag	UNP S4TKM8
H	-2	GLY	-	expression tag	UNP S4TKM8
H	-1	SER	-	expression tag	UNP S4TKM8
H	0	HIS	-	expression tag	UNP S4TKM8

- Molecule 2 is water.

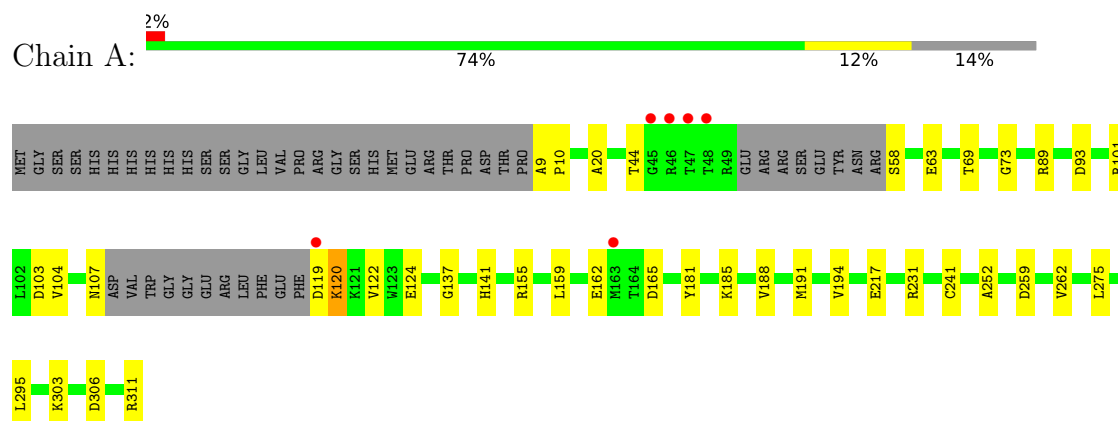
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	181	Total	O	0	0
			181	181		
2	B	201	Total	O	0	0
			201	201		
2	C	158	Total	O	0	0
			158	158		
2	D	143	Total	O	0	0
			143	143		
2	E	187	Total	O	0	0
			187	187		
2	F	153	Total	O	0	0
			153	153		
2	G	184	Total	O	0	0
			184	184		
2	H	172	Total	O	0	0
			172	172		



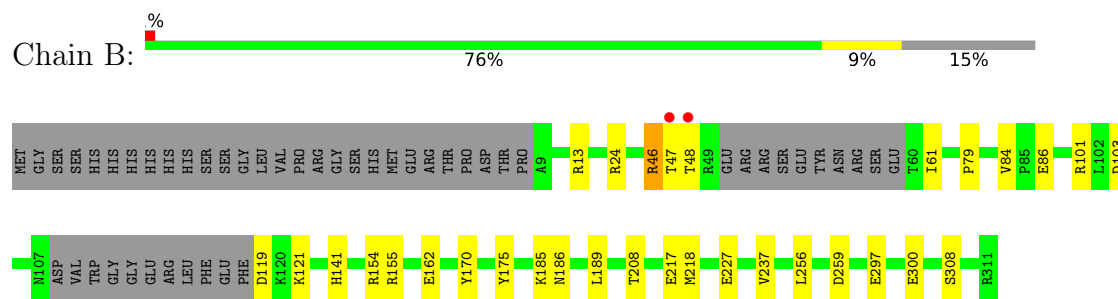
### 3 Residue-property plots [i](#)

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.

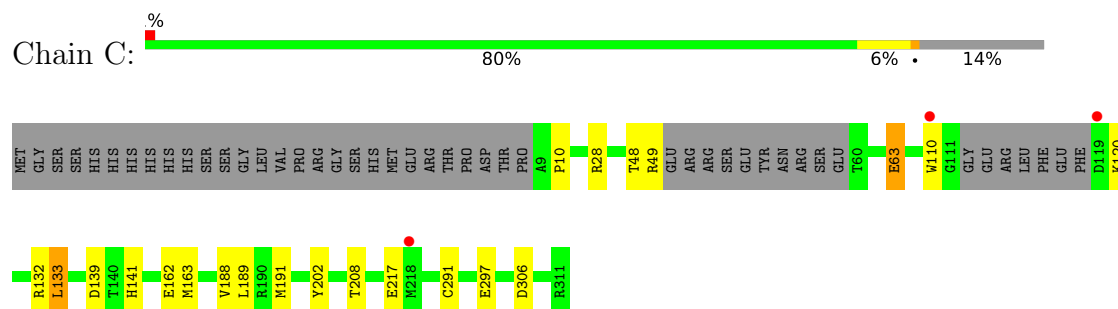
- Molecule 1: Short chain dehydrogenase



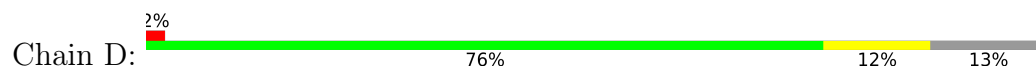
- Molecule 1: Short chain dehydrogenase

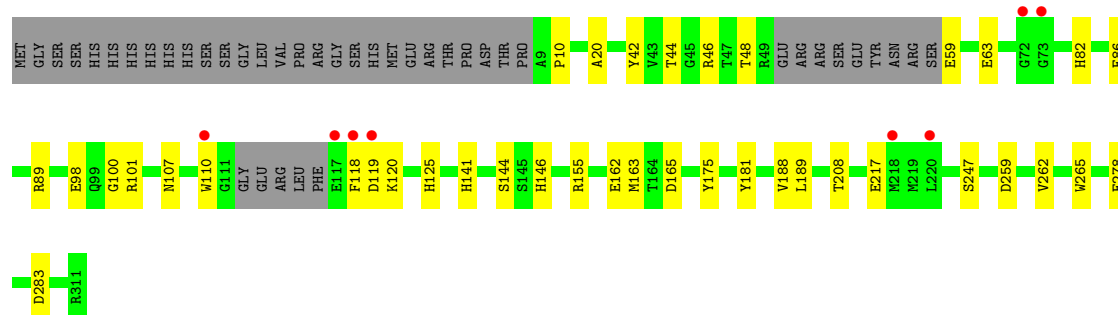


- Molecule 1: Short chain dehydrogenase

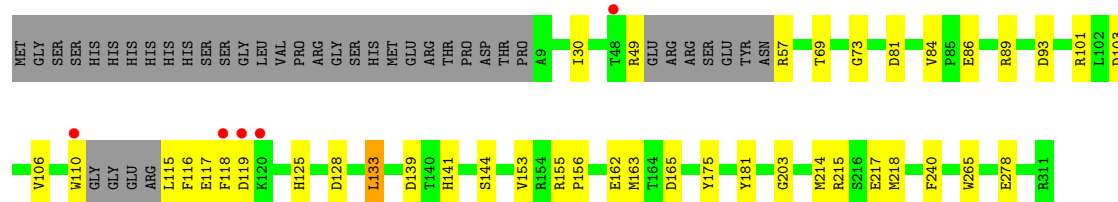
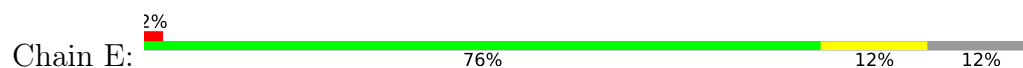


- Molecule 1: Short chain dehydrogenase

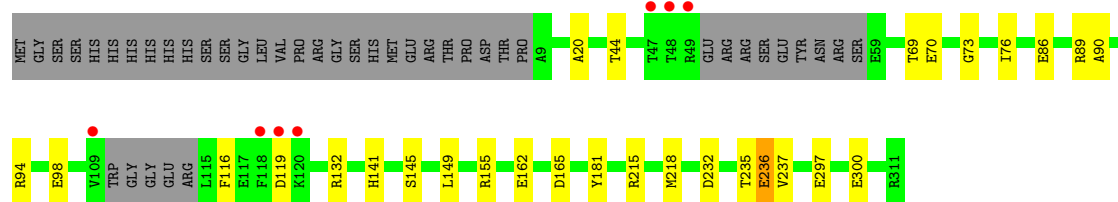
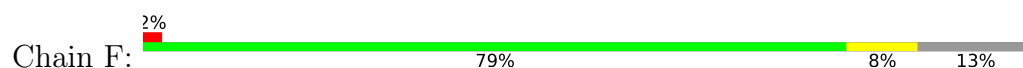




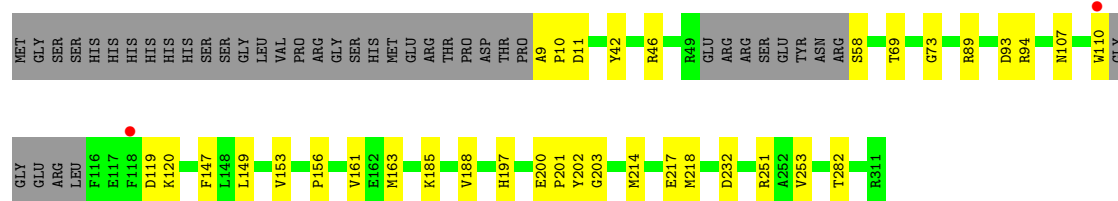
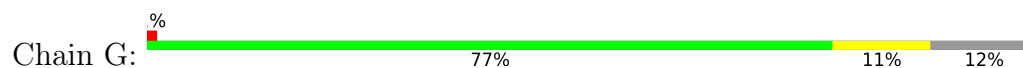
- Molecule 1: Short chain dehydrogenase



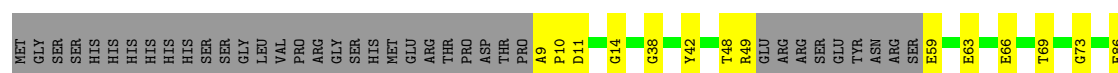
- Molecule 1: Short chain dehydrogenase

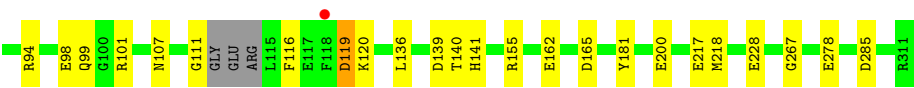


- Molecule 1: Short chain dehydrogenase



- Molecule 1: Short chain dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.15Å 134.44Å 117.22Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	41.33 – 2.08 48.85 – 2.08	Depositor EDS
% Data completeness (in resolution range)	98.5 (41.33-2.08) 98.4 (48.85-2.08)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.210 , 0.249 0.184 , 0.217	Depositor DCC
$R_{free}$ test set	10999 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.2	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 36.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.450 for l,k,-h 0.460 for h,-k,-l 0.457 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18962	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	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 63.79 % 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 9.1646e-06. 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	0.49	0/2201	0.60	0/2992
1	B	0.48	0/2186	0.62	0/2972
1	C	0.46	0/2221	0.60	0/3021
1	D	0.48	0/2251	0.60	0/3061
1	E	0.49	0/2284	0.60	0/3105
1	F	0.47	0/2251	0.62	1/3060 (0.0%)
1	G	0.48	0/2265	0.59	0/3080
1	H	0.48	0/2271	0.58	0/3088
All	All	0.48	0/17930	0.60	1/24379 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	155	ARG	NE-CZ-NH2	-5.66	117.47	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2160	0	2105	36	0
1	B	2145	0	2094	31	0
1	C	2178	0	2120	18	0
1	D	2207	0	2141	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2239	0	2176	34	0
1	F	2208	0	2148	23	0
1	G	2220	0	2152	31	0
1	H	2226	0	2161	33	0
2	A	181	0	0	12	0
2	B	201	0	0	10	0
2	C	158	0	0	9	0
2	D	143	0	0	6	0
2	E	187	0	0	16	4
2	F	153	0	0	15	3
2	G	184	0	0	16	3
2	H	172	0	0	20	4
All	All	18962	0	17097	228	7

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 7.

All (228) 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:191:MET:SD	2:C:421:HOH:O	2.12	1.05
1:H:99:GLN:O	1:H:101:ARG:NH1	2.02	0.92
1:A:101:ARG:NH2	2:A:402:HOH:O	2.03	0.90
1:G:107:ASN:O	2:G:401:HOH:O	1.90	0.89
1:D:283:ASP:OD2	2:D:401:HOH:O	1.93	0.86
1:F:98:GLU:OE1	2:F:401:HOH:O	1.93	0.85
1:H:98:GLU:OE2	2:H:401:HOH:O	1.97	0.82
1:G:214:MET:SD	2:G:561:HOH:O	2.37	0.82
1:C:110:TRP:HH2	1:C:188:VAL:HG21	1.45	0.82
1:A:103:ASP:O	2:A:401:HOH:O	1.99	0.81
1:B:119:ASP:OD2	2:B:401:HOH:O	1.98	0.81
1:H:42:TYR:OH	1:H:98:GLU:OE1	1.97	0.80
1:G:197:HIS:O	2:G:402:HOH:O	1.99	0.80
1:F:86:GLU:O	2:F:402:HOH:O	2.00	0.80
1:D:59:GLU:N	1:D:63:GLU:OE2	2.14	0.80
1:B:46:ARG:HD3	1:B:46:ARG:H	1.45	0.80
1:C:10:PRO:O	2:C:401:HOH:O	1.99	0.79
1:E:101:ARG:HB2	1:E:155:ARG:HH22	1.46	0.79
1:B:256:LEU:O	2:B:402:HOH:O	2.03	0.75
1:H:120:LYS:NZ	2:H:409:HOH:O	2.19	0.75
1:F:300:GLU:OE1	2:F:404:HOH:O	2.04	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:ARG:O	2:E:401:HOH:O	2.04	0.74
1:G:46:ARG:NH2	2:G:409:HOH:O	2.22	0.73
1:F:215:ARG:NH2	2:F:407:HOH:O	2.21	0.72
1:G:94:ARG:NE	2:G:407:HOH:O	2.22	0.72
1:B:13:ARG:NH1	2:B:409:HOH:O	2.21	0.72
1:H:107:ASN:ND2	2:H:404:HOH:O	2.09	0.72
1:G:200:GLU:OE1	2:G:403:HOH:O	2.06	0.71
1:H:69:THR:O	2:H:403:HOH:O	2.08	0.71
1:E:139:ASP:OD2	2:E:402:HOH:O	2.09	0.71
1:A:103:ASP:OD1	2:A:403:HOH:O	2.07	0.70
1:C:139:ASP:OD2	2:C:402:HOH:O	2.08	0.70
1:D:82:HIS:ND1	2:D:402:HOH:O	2.02	0.70
1:H:155:ARG:NH2	2:H:415:HOH:O	2.24	0.70
1:F:141:HIS:ND1	1:F:162:GLU:OE1	2.23	0.70
1:D:141:HIS:ND1	1:D:162:GLU:OE1	2.24	0.70
1:F:94:ARG:NE	2:F:401:HOH:O	2.22	0.69
1:G:11:ASP:O	2:G:404:HOH:O	2.11	0.69
1:F:145:SER:OG	2:F:405:HOH:O	2.11	0.69
1:B:297:GLU:OE2	2:B:404:HOH:O	2.10	0.68
1:E:101:ARG:HB3	1:E:155:ARG:HH12	1.58	0.68
1:E:214:MET:SD	2:E:561:HOH:O	2.51	0.68
1:E:86:GLU:OE2	2:E:404:HOH:O	2.11	0.67
1:E:93:ASP:OD2	2:E:403:HOH:O	2.11	0.67
1:H:119:ASP:OD2	1:H:119:ASP:N	2.27	0.67
1:B:259:ASP:O	2:B:402:HOH:O	2.12	0.67
1:G:200:GLU:N	2:G:402:HOH:O	2.22	0.67
1:E:153:VAL:O	2:E:405:HOH:O	2.13	0.67
1:C:306:ASP:OD2	2:C:403:HOH:O	2.14	0.66
1:C:297:GLU:O	2:C:404:HOH:O	2.14	0.66
1:A:101:ARG:HD2	1:A:155:ARG:HH22	1.60	0.66
1:H:139:ASP:OD2	2:H:405:HOH:O	2.13	0.66
1:A:303:LYS:O	2:A:404:HOH:O	2.14	0.66
1:C:110:TRP:CH2	1:C:188:VAL:HG21	2.31	0.65
1:A:155:ARG:NH2	2:A:421:HOH:O	2.30	0.65
1:F:90:ALA:N	2:F:402:HOH:O	2.28	0.65
1:E:103:ASP:OD1	2:E:406:HOH:O	2.15	0.64
1:D:247:SER:OG	2:D:404:HOH:O	2.15	0.64
1:G:93:ASP:OD2	2:G:405:HOH:O	2.15	0.64
1:F:297:GLU:OE2	2:F:406:HOH:O	2.14	0.63
1:D:110:TRP:HH2	1:D:188:VAL:HG21	1.64	0.63
1:A:137:GLY:O	2:A:405:HOH:O	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:GLU:OE1	2:B:405:HOH:O	2.16	0.62
1:H:49:ARG:NH1	2:H:416:HOH:O	2.24	0.62
1:B:48:THR:HG22	1:B:61:ILE:HG22	1.82	0.62
1:D:119:ASP:OD1	1:D:119:ASP:N	2.31	0.62
1:A:89:ARG:NH1	1:A:93:ASP:OD2	2.33	0.61
1:H:11:ASP:HA	2:H:417:HOH:O	1.99	0.61
1:A:93:ASP:OD2	2:A:407:HOH:O	2.16	0.61
1:D:10:PRO:O	2:D:405:HOH:O	2.16	0.61
1:D:144:SER:HB2	2:D:402:HOH:O	2.01	0.61
1:A:306:ASP:OD2	2:A:406:HOH:O	2.16	0.60
1:G:201:PRO:HD3	2:G:402:HOH:O	2.00	0.60
1:A:107:ASN:ND2	1:A:162:GLU:OE2	2.33	0.60
1:E:49:ARG:O	2:E:408:HOH:O	2.16	0.60
1:H:141:HIS:ND1	1:H:162:GLU:OE1	2.27	0.60
1:H:278:GLU:OE1	2:H:406:HOH:O	2.16	0.59
1:A:165:ASP:OD2	1:A:181:TYR:OH	2.16	0.59
1:H:94:ARG:NE	2:H:401:HOH:O	2.36	0.58
1:B:24:ARG:HH22	1:B:46:ARG:NH2	2.02	0.58
1:H:165:ASP:OD2	1:H:181:TYR:OH	2.21	0.58
1:E:110:TRP:HZ2	1:E:163:MET:O	1.87	0.57
1:F:236:GLU:HG3	1:F:237:VAL:HG23	1.86	0.57
1:E:117:GLU:HB2	1:E:125:HIS:CD2	2.40	0.57
1:H:200:GLU:O	2:H:407:HOH:O	2.18	0.56
1:E:155:ARG:NH1	2:E:425:HOH:O	2.38	0.56
1:F:165:ASP:OD2	1:F:181:TYR:OH	2.15	0.56
1:C:110:TRP:HZ2	1:C:163:MET:O	1.89	0.56
1:C:188:VAL:HG22	2:C:421:HOH:O	2.04	0.56
1:G:232:ASP:OD2	2:G:406:HOH:O	2.18	0.56
1:G:251:ARG:NH1	1:G:282:THR:O	2.39	0.55
1:H:285:ASP:OD2	2:H:408:HOH:O	2.18	0.55
1:A:89:ARG:NH1	2:A:407:HOH:O	2.33	0.55
1:B:48:THR:HG21	1:B:79:PRO:HG3	1.88	0.55
1:A:58:SER:HB3	1:A:63:GLU:HB2	1.88	0.55
1:A:188:VAL:HA	1:A:191:MET:HE2	1.88	0.55
1:D:189:LEU:HA	1:D:208:THR:HG21	1.89	0.55
1:E:128:ASP:OD1	2:E:409:HOH:O	2.18	0.55
1:D:110:TRP:CH2	1:D:188:VAL:HG21	2.41	0.54
1:B:217:GLU:H	1:B:217:GLU:CD	2.10	0.54
1:G:163:MET:N	2:G:401:HOH:O	2.13	0.54
1:G:119:ASP:OD1	1:G:119:ASP:N	2.32	0.54
1:C:141:HIS:ND1	1:C:162:GLU:OE1	2.30	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:SER:O	2:B:407:HOH:O	2.19	0.53
1:A:231:ARG:HD2	2:A:426:HOH:O	2.08	0.53
1:A:217:GLU:H	1:A:217:GLU:CD	2.13	0.52
1:E:101:ARG:CB	1:E:155:ARG:HH22	2.21	0.52
1:E:144:SER:OG	2:E:410:HOH:O	2.18	0.52
1:E:217:GLU:HG2	1:E:218:MET:N	2.26	0.51
1:G:89:ARG:NH1	2:G:425:HOH:O	2.39	0.51
1:D:265:TRP:HZ2	1:D:278:GLU:HG2	1.75	0.51
1:D:165:ASP:OD2	1:D:181:TYR:OH	2.23	0.51
1:E:155:ARG:NH2	2:E:428:HOH:O	2.43	0.51
1:G:110:TRP:HH2	1:G:188:VAL:HG21	1.76	0.51
1:E:81:ASP:OD1	2:E:411:HOH:O	2.19	0.50
1:B:24:ARG:HH22	1:B:46:ARG:HH22	1.59	0.50
1:D:100:GLY:O	1:D:155:ARG:NH1	2.44	0.50
1:G:217:GLU:CD	1:G:217:GLU:H	2.14	0.50
1:H:217:GLU:H	1:H:217:GLU:CD	2.13	0.50
1:B:300:GLU:OE1	2:B:408:HOH:O	2.20	0.50
1:G:69:THR:HA	1:G:73:GLY:O	2.11	0.50
1:H:38:GLY:O	2:H:410:HOH:O	2.19	0.50
1:E:103:ASP:O	2:E:412:HOH:O	2.20	0.49
1:A:120:LYS:HG3	1:A:124:GLU:HB2	1.95	0.49
1:E:116:PHE:HD1	1:E:133:LEU:HD11	1.77	0.49
1:F:76:ILE:HG21	2:F:401:HOH:O	2.11	0.49
1:B:154:ARG:HD2	1:B:155:ARG:HH22	1.78	0.49
1:D:86:GLU:OE2	1:D:89:ARG:NH2	2.28	0.49
1:B:189:LEU:HA	1:B:208:THR:HG21	1.93	0.49
1:G:156:PRO:HB3	1:G:203:GLY:HA3	1.93	0.49
1:H:49:ARG:HH22	1:H:66:GLU:CD	2.16	0.49
1:B:121:LYS:HE3	1:C:202:TYR:HE2	1.77	0.49
1:E:116:PHE:HE1	1:E:133:LEU:HD21	1.78	0.49
1:F:232:ASP:O	2:F:403:HOH:O	2.20	0.48
1:B:48:THR:HG21	1:B:79:PRO:CG	2.42	0.48
1:E:119:ASP:OD2	1:E:119:ASP:N	2.46	0.48
1:H:59:GLU:N	1:H:63:GLU:OE1	2.46	0.48
1:H:140:THR:O	2:H:411:HOH:O	2.20	0.48
1:A:101:ARG:HB3	1:A:155:ARG:HH12	1.78	0.48
1:B:24:ARG:HH12	1:B:46:ARG:NH2	2.12	0.48
1:C:132:ARG:NH2	2:C:405:HOH:O	2.30	0.48
1:B:46:ARG:H	1:B:46:ARG:HH11	1.61	0.48
1:B:84:VAL:HG12	1:B:86:GLU:HG2	1.95	0.48
1:D:46:ARG:NH1	2:D:419:HOH:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:TYR:OH	1:B:300:GLU:OE2	2.24	0.47
1:B:185:LYS:HA	1:B:185:LYS:HD3	1.68	0.47
1:A:69:THR:HA	1:A:73:GLY:O	2.14	0.47
1:A:194:VAL:HG13	1:D:175:TYR:HE2	1.80	0.47
1:E:141:HIS:ND1	1:E:162:GLU:OE1	2.37	0.47
1:B:141:HIS:ND1	1:B:162:GLU:OE1	2.32	0.47
1:E:265:TRP:HZ2	1:E:278:GLU:HG2	1.79	0.47
1:A:259:ASP:HB3	1:A:262:VAL:HB	1.96	0.46
1:F:89:ARG:HB3	2:F:402:HOH:O	2.13	0.46
1:G:42:TYR:HE2	2:G:407:HOH:O	1.96	0.46
1:B:186:ASN:HB3	2:B:557:HOH:O	2.15	0.46
1:D:217:GLU:H	1:D:217:GLU:CD	2.18	0.46
1:G:110:TRP:CH2	1:G:188:VAL:HG21	2.50	0.46
1:A:104:VAL:HG22	2:A:401:HOH:O	2.15	0.46
1:F:119:ASP:OD2	1:F:119:ASP:N	2.49	0.46
1:A:58:SER:O	1:A:63:GLU:HG2	2.15	0.46
1:A:159:LEU:HB3	2:A:401:HOH:O	2.15	0.46
1:C:28:ARG:NH2	1:C:63:GLU:HG2	2.31	0.46
1:A:191:MET:HE2	1:A:191:MET:HB2	1.66	0.46
1:E:69:THR:HA	1:E:73:GLY:O	2.16	0.45
1:E:84:VAL:HG12	1:E:86:GLU:HG2	1.98	0.45
1:B:297:GLU:O	2:B:410:HOH:O	2.21	0.45
1:H:101:ARG:HD2	2:H:415:HOH:O	2.16	0.45
1:E:115:LEU:HB2	1:E:133:LEU:HG	1.98	0.45
1:E:156:PRO:HB3	1:E:203:GLY:HA3	1.99	0.45
1:H:94:ARG:CZ	2:H:401:HOH:O	2.64	0.45
1:H:200:GLU:OE2	2:H:413:HOH:O	2.21	0.45
1:D:110:TRP:HZ2	1:D:163:MET:O	1.99	0.45
1:D:42:TYR:OH	1:D:98:GLU:OE1	2.24	0.44
1:F:149:LEU:HD23	1:F:149:LEU:HA	1.84	0.44
1:F:236:GLU:CG	1:F:237:VAL:HG23	2.47	0.44
1:C:217:GLU:CD	1:C:217:GLU:H	2.21	0.44
1:A:107:ASN:HD22	1:A:162:GLU:CD	2.21	0.44
1:B:46:ARG:HD3	1:B:46:ARG:N	2.22	0.44
1:H:14:GLY:O	2:H:412:HOH:O	2.20	0.43
1:C:133:LEU:HD12	2:C:489:HOH:O	2.17	0.43
1:F:235:THR:HA	2:F:456:HOH:O	2.17	0.43
1:B:119:ASP:OD2	1:B:119:ASP:N	2.51	0.43
1:A:252:ALA:HB1	1:A:275:LEU:HD12	2.01	0.43
1:A:119:ASP:N	1:A:119:ASP:OD1	2.52	0.43
1:C:291:CYS:HB2	2:C:423:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:ARG:O	2:E:413:HOH:O	2.21	0.43
1:G:161:VAL:HG21	1:G:253:VAL:HG13	2.00	0.43
1:G:185:LYS:HA	1:G:185:LYS:HD3	1.87	0.42
1:H:86:GLU:H	1:H:86:GLU:CD	2.22	0.42
1:A:9:ALA:HA	1:A:10:PRO:HD3	1.94	0.42
1:G:58:SER:N	2:G:435:HOH:O	2.52	0.42
1:A:295:LEU:HD23	1:A:295:LEU:HA	1.75	0.42
1:G:120:LYS:HA	1:G:120:LYS:HD2	1.64	0.42
1:H:228:GLU:OE1	1:H:228:GLU:N	2.47	0.42
1:A:122:VAL:O	1:D:146:HIS:HD2	2.01	0.42
1:B:46:ARG:CZ	1:B:47:THR:HG23	2.50	0.42
1:E:30:ILE:HG21	1:E:106:VAL:HG11	2.01	0.42
1:F:235:THR:HG23	2:F:472:HOH:O	2.19	0.42
1:H:267:GLY:O	2:H:414:HOH:O	2.21	0.42
1:E:215:ARG:HG2	1:E:240:PHE:CZ	2.54	0.42
1:H:111:GLY:HA3	1:H:136:LEU:HD13	2.02	0.42
1:A:20:ALA:HA	1:A:44:THR:OG1	2.20	0.42
1:B:101:ARG:HA	1:B:155:ARG:NH1	2.35	0.42
1:D:101:ARG:HA	1:D:155:ARG:HH11	1.84	0.42
1:A:185:LYS:HA	1:A:185:LYS:HD3	1.77	0.41
1:D:20:ALA:HA	1:D:44:THR:OG1	2.20	0.41
1:F:70:GLU:HG3	2:F:481:HOH:O	2.20	0.41
1:E:165:ASP:OD2	1:E:181:TYR:OH	2.20	0.41
1:C:189:LEU:HA	1:C:208:THR:HG21	2.03	0.41
1:H:9:ALA:HA	1:H:10:PRO:HD3	1.90	0.41
1:A:241:CYS:O	1:A:311:ARG:NH2	2.51	0.41
1:G:9:ALA:HA	1:G:10:PRO:HD3	1.92	0.41
1:C:48:THR:OG1	1:C:49:ARG:N	2.54	0.41
1:D:120:LYS:HE3	1:D:125:HIS:HA	2.03	0.41
1:F:20:ALA:HA	1:F:44:THR:OG1	2.21	0.41
1:G:89:ARG:HB2	1:G:147:PHE:CE1	2.55	0.41
1:G:93:ASP:OD2	2:G:408:HOH:O	2.22	0.41
1:G:153:VAL:HB	1:G:202:TYR:CG	2.56	0.41
1:F:94:ARG:NH2	2:F:401:HOH:O	2.54	0.41
1:G:149:LEU:HD23	1:G:149:LEU:HA	1.89	0.41
1:E:89:ARG:NH1	2:E:418:HOH:O	2.32	0.40
1:B:101:ARG:NH1	1:B:103:ASP:OD2	2.54	0.40
1:F:69:THR:HA	1:F:73:GLY:O	2.21	0.40
1:H:267:GLY:C	2:H:414:HOH:O	2.59	0.40
1:D:259:ASP:HB3	1:D:262:VAL:HB	2.03	0.40
1:G:110:TRP:HZ2	1:G:163:MET:O	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:HIS:ND1	1:A:162:GLU:OE1	2.29	0.40
1:H:69:THR:HA	1:H:73:GLY:O	2.21	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:503:HOH:O	2:G:544:HOH:O[2_855]	1.96	0.24
2:E:555:HOH:O	2:H:556:HOH:O[2_855]	1.98	0.22
2:E:563:HOH:O	2:H:554:HOH:O[2_855]	2.01	0.19
2:F:507:HOH:O	2:G:535:HOH:O[2_855]	2.04	0.16
2:E:521:HOH:O	2:H:502:HOH:O[2_855]	2.08	0.12
2:E:445:HOH:O	2:H:537:HOH:O[2_855]	2.15	0.05
2:F:547:HOH:O	2:G:569:HOH:O[2_855]	2.16	0.04

## 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	278/331 (84%)	273 (98%)	5 (2%)	0	100	100
1	B	276/331 (83%)	272 (99%)	4 (1%)	0	100	100
1	C	280/331 (85%)	275 (98%)	5 (2%)	0	100	100
1	D	283/331 (86%)	279 (99%)	4 (1%)	0	100	100
1	E	286/331 (86%)	281 (98%)	5 (2%)	0	100	100
1	F	283/331 (86%)	278 (98%)	5 (2%)	0	100	100
1	G	284/331 (86%)	279 (98%)	5 (2%)	0	100	100
1	H	285/331 (86%)	279 (98%)	6 (2%)	0	100	100
All	All	2255/2648 (85%)	2216 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	223/265 (84%)	222 (100%)	1 (0%)	91	93
1	B	221/265 (83%)	217 (98%)	4 (2%)	59	63
1	C	224/265 (84%)	221 (99%)	3 (1%)	69	74
1	D	227/265 (86%)	224 (99%)	3 (1%)	69	74
1	E	231/265 (87%)	227 (98%)	4 (2%)	60	65
1	F	228/265 (86%)	224 (98%)	4 (2%)	59	63
1	G	229/265 (86%)	228 (100%)	1 (0%)	91	93
1	H	229/265 (86%)	225 (98%)	4 (2%)	60	65
All	All	1812/2120 (86%)	1788 (99%)	24 (1%)	69	74

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	LYS
1	B	46	ARG
1	B	175	TYR
1	B	218	MET
1	B	237	VAL
1	C	63	GLU
1	C	120	LYS
1	C	133	LEU
1	D	48	THR
1	D	107	ASN
1	D	118	PHE
1	E	57	ARG
1	E	118	PHE
1	E	133	LEU
1	E	175	TYR
1	F	116	PHE

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Mol	Chain	Res	Type
1	F	132	ARG
1	F	218	MET
1	F	236	GLU
1	G	218	MET
1	H	48	THR
1	H	116	PHE
1	H	119	ASP
1	H	218	MET

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

Mol	Chain	Res	Type
1	D	146	HIS

### 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	284/331 (85%)	-0.14	6 (2%) 63 67	11, 18, 37, 391	0
1	B	282/331 (85%)	-0.26	2 (0%) 87 89	9, 17, 32, 68	0
1	C	286/331 (86%)	-0.20	3 (1%) 82 84	9, 17, 30, 217	0
1	D	289/331 (87%)	-0.05	8 (2%) 53 58	10, 17, 47, 407	0
1	E	292/331 (88%)	-0.16	5 (1%) 70 73	9, 17, 32, 387	0
1	F	289/331 (87%)	-0.09	7 (2%) 59 63	10, 18, 37, 387	0
1	G	290/331 (87%)	-0.24	2 (0%) 87 89	10, 17, 31, 64	0
1	H	291/331 (87%)	-0.25	1 (0%) 94 94	10, 17, 30, 39	0
All	All	2303/2648 (86%)	-0.17	34 (1%) 73 76	9, 17, 33, 407	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	118	PHE	16.1
1	E	118	PHE	12.0
1	F	118	PHE	11.0
1	F	119	ASP	10.0
1	F	48	THR	8.5
1	E	119	ASP	8.4
1	D	73	GLY	8.3
1	D	117	GLU	7.8
1	F	109	VAL	7.7
1	E	110	TRP	7.5
1	A	47	THR	7.4
1	F	49	ARG	6.9
1	E	120	LYS	6.2
1	A	119	ASP	6.0
1	D	220	LEU	6.0
1	F	47	THR	5.9

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Mol	Chain	Res	Type	RSRZ
1	D	72	GLY	5.6
1	A	46	ARG	5.5
1	C	110	TRP	5.3
1	A	48	THR	4.8
1	C	119	ASP	4.7
1	D	119	ASP	4.1
1	F	120	LYS	4.0
1	E	48	THR	3.1
1	B	48	THR	3.0
1	D	218	MET	3.0
1	G	118	PHE	2.9
1	H	118	PHE	2.8
1	A	45	GLY	2.7
1	B	47	THR	2.7
1	D	110	TRP	2.5
1	A	163	MET	2.5
1	G	110	TRP	2.3
1	C	218	MET	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.