



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2017 – 11:23 PM EDT

PDB ID : 2ONN  
Title : Arg475Gln Mutant of Human Mitochondrial Aldehyde Dehydrogenase, Apo form  
Authors : Larson, H.N.; Hurley, T.D.  
Deposited on : unknown  
Resolution : 2.75 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

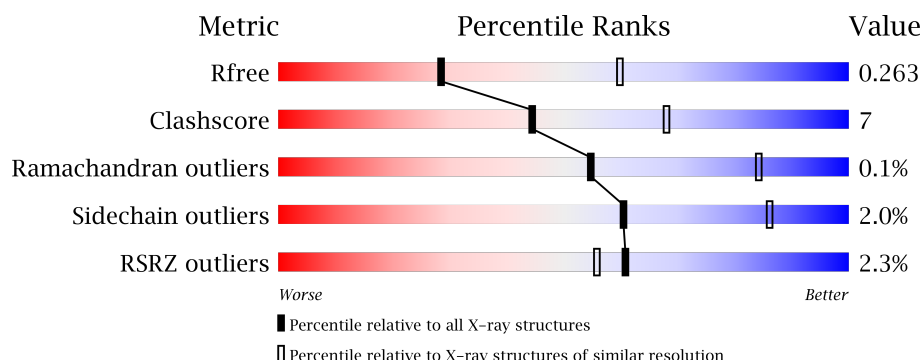
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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))
$R_{free}$	100719	3666 (2.80-2.72)
Clashscore	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)
RSRZ outliers	101464	3697 (2.80-2.72)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	500	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>18%</div> <div>..</div> </div> </div>
1	B	500	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>18%</div> <div>.</div> </div> </div>
1	C	500	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>..</div> </div> </div>
1	D	500	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>..</div> </div> </div>
1	E	500	<div> <div></div> <div> <div></div> <div>83%</div> <div>15%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	500	<div><div></div><div>84%</div><div>14%</div><div>..</div></div>
1	G	500	<div><div>%</div><div></div><div>83%</div><div>15%</div><div>..</div></div>
1	H	500	<div><div>6%</div><div></div><div>83%</div><div>15%</div><div>..</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 31105 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	B	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	C	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	D	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	E	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	F	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	G	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	H	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	475	GLN	ARG	ENGINEERED	UNP P05091
B	475	GLN	ARG	ENGINEERED	UNP P05091
C	475	GLN	ARG	ENGINEERED	UNP P05091
D	475	GLN	ARG	ENGINEERED	UNP P05091
E	475	GLN	ARG	ENGINEERED	UNP P05091
F	475	GLN	ARG	ENGINEERED	UNP P05091
G	475	GLN	ARG	ENGINEERED	UNP P05091
H	475	GLN	ARG	ENGINEERED	UNP P05091

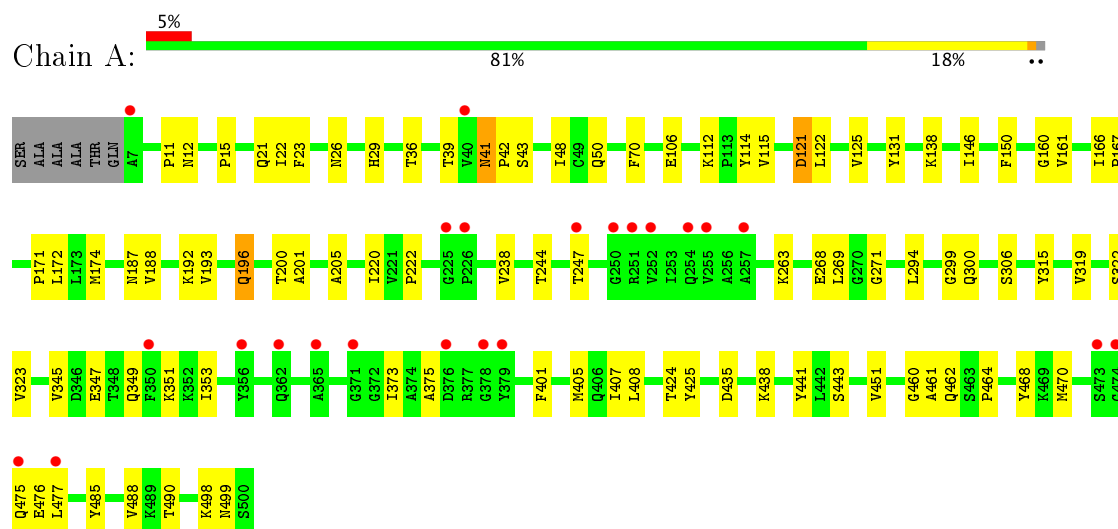
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	73	Total 73	O 73	0	0
2	B	89	Total 89	O 89	0	0
2	C	104	Total 104	O 104	0	0
2	D	82	Total 82	O 82	0	0
2	E	93	Total 93	O 93	0	0
2	F	110	Total 110	O 110	0	0
2	G	101	Total 101	O 101	0	0
2	H	85	Total 85	O 85	0	0

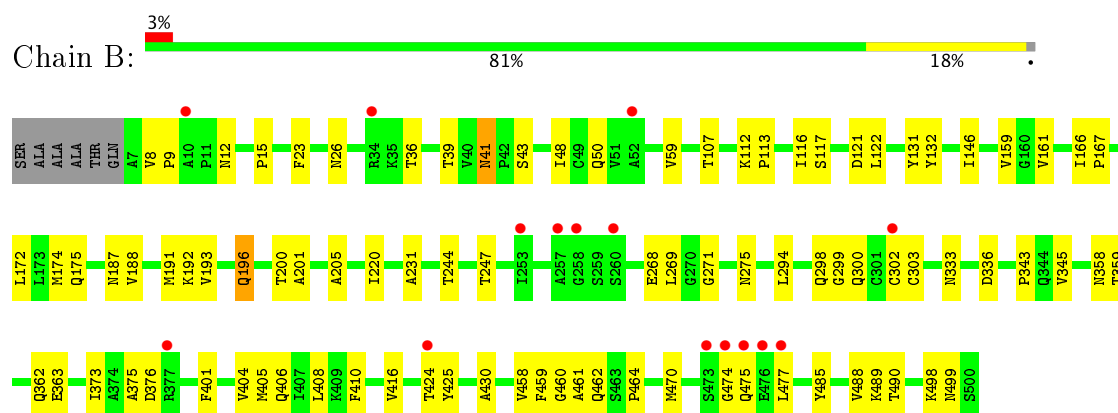
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

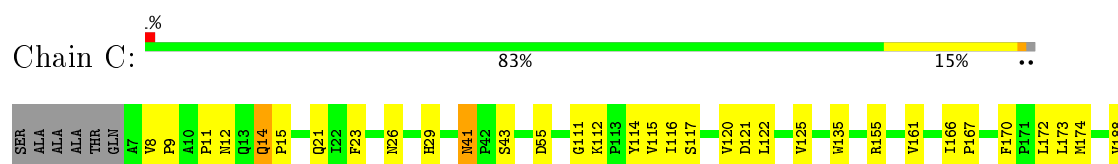
- Molecule 1: Aldehyde dehydrogenase

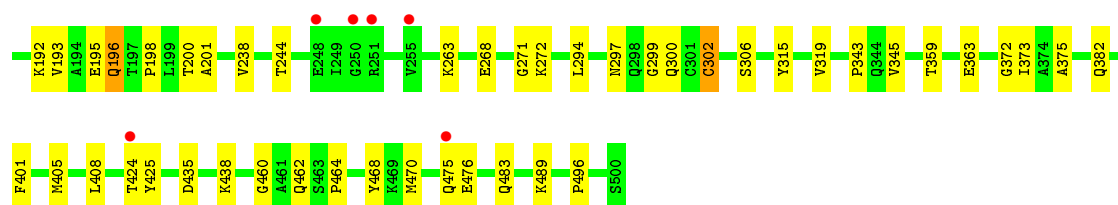


- Molecule 1: Aldehyde dehydrogenase

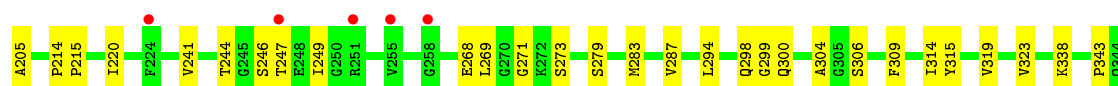
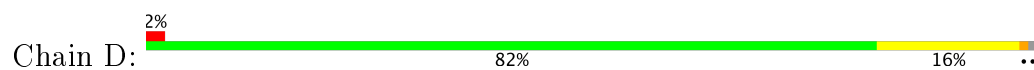


- Molecule 1: Aldehyde dehydrogenase

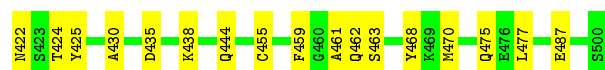
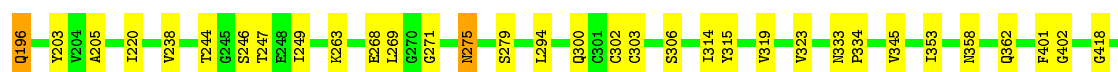
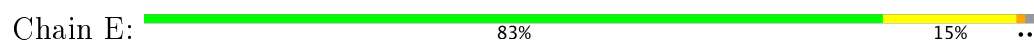




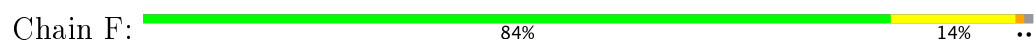
• Molecule 1: Aldehyde dehydrogenase



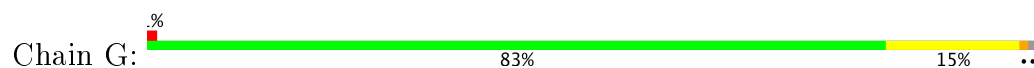
• Molecule 1: Aldehyde dehydrogenase

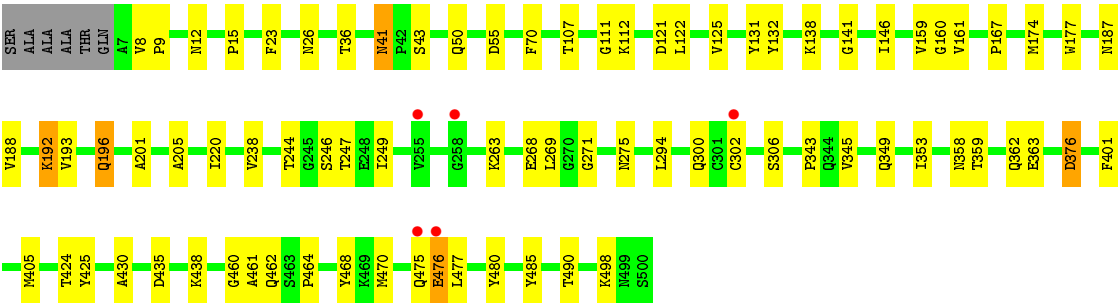


• Molecule 1: Aldehyde dehydrogenase

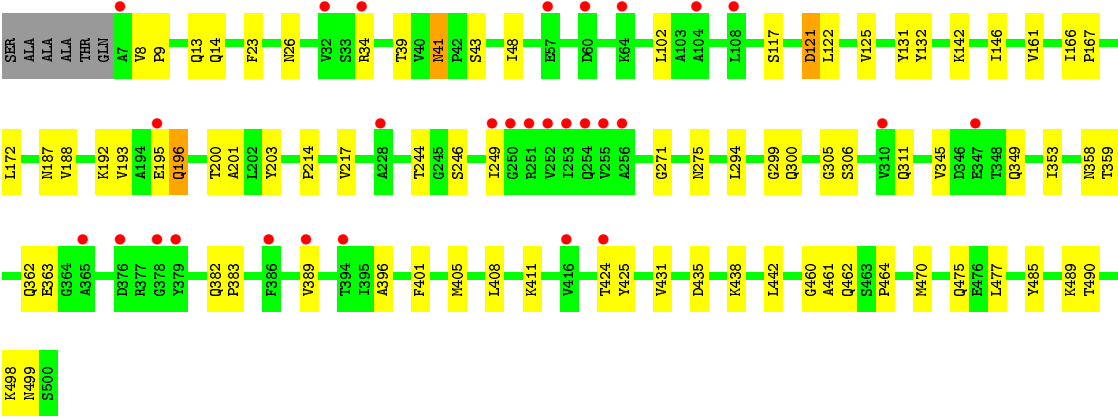
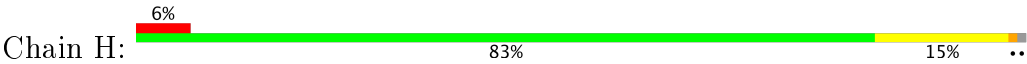


• Molecule 1: Aldehyde dehydrogenase





● Molecule 1: Aldehyde dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.78Å 150.86Å 177.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.50 – 2.75 38.29 – 2.75	Depositor EDS
% Data completeness (in resolution range)	96.6 (37.50-2.75) 96.3 (38.29-2.75)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.226 , 0.268 0.223 , 0.263	Depositor DCC
$R_{free}$ test set	4795 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.9	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 34.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	31105	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	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 76.16 % 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 1.0993e-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 ⓘ

### 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	0.42	0/3880	0.60	0/5265
1	B	0.43	0/3880	0.62	0/5265
1	C	0.52	2/3880 (0.1%)	0.66	2/5265 (0.0%)
1	D	0.40	0/3880	0.60	0/5265
1	E	0.39	0/3880	0.59	0/5265
1	F	0.43	0/3880	0.61	0/5265
1	G	0.43	0/3880	0.61	1/5265 (0.0%)
1	H	0.41	0/3880	0.60	2/5265 (0.0%)
All	All	0.43	2/31040 (0.0%)	0.61	5/42120 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	476	GLU	CD-OE1	-17.19	1.06	1.25
1	C	302	CYS	CB-SG	5.09	1.91	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	476	GLU	OE1-CD-OE2	-15.63	104.54	123.30
1	C	476	GLU	CG-CD-OE1	9.45	137.20	118.30
1	H	34	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	G	476	GLU	OE1-CD-OE2	5.21	129.55	123.30
1	H	34	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3796	0	3740	67	0
1	B	3796	0	3740	67	0
1	C	3796	0	3740	61	0
1	D	3796	0	3740	61	0
1	E	3796	0	3740	55	0
1	F	3796	0	3740	57	0
1	G	3796	0	3740	56	0
1	H	3796	0	3740	56	0
2	A	73	0	0	2	0
2	B	89	0	0	0	0
2	C	104	0	0	2	0
2	D	82	0	0	0	0
2	E	93	0	0	1	0
2	F	110	0	0	0	0
2	G	101	0	0	1	0
2	H	85	0	0	0	0
All	All	31105	0	29920	451	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 7.

The worst 5 of 451 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:H:196:GLN:HE21	1:H:196:GLN:H	1.05	0.97
1:F:196:GLN:H	1:F:196:GLN:HE21	1.11	0.96
1:C:196:GLN:H	1:C:196:GLN:HE21	1.06	0.93
1:E:196:GLN:H	1:E:196:GLN:HE21	1.16	0.89
1:A:196:GLN:H	1:A:196:GLN:HE21	1.18	0.87

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	492/500 (98%)	470 (96%)	22 (4%)	0	100	100
1	B	492/500 (98%)	468 (95%)	24 (5%)	0	100	100
1	C	492/500 (98%)	469 (95%)	22 (4%)	1 (0%)	51	81
1	D	492/500 (98%)	472 (96%)	20 (4%)	0	100	100
1	E	492/500 (98%)	472 (96%)	20 (4%)	0	100	100
1	F	492/500 (98%)	474 (96%)	17 (4%)	1 (0%)	51	81
1	G	492/500 (98%)	469 (95%)	23 (5%)	0	100	100
1	H	492/500 (98%)	469 (95%)	23 (5%)	0	100	100
All	All	3936/4000 (98%)	3763 (96%)	171 (4%)	2 (0%)	55	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	198	PRO
1	F	198	PRO

### 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	399/402 (99%)	393 (98%)	6 (2%)	70	90
1	B	399/402 (99%)	392 (98%)	7 (2%)	64	87
1	C	399/402 (99%)	390 (98%)	9 (2%)	56	84
1	D	399/402 (99%)	389 (98%)	10 (2%)	53	82
1	E	399/402 (99%)	390 (98%)	9 (2%)	56	84
1	F	399/402 (99%)	393 (98%)	6 (2%)	70	90
1	G	399/402 (99%)	390 (98%)	9 (2%)	56	84
1	H	399/402 (99%)	391 (98%)	8 (2%)	60	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3192/3216 (99%)	3128 (98%)	64 (2%)	60 86

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	338	LYS
1	E	196	GLN
1	H	192	LYS
1	D	401	PHE
1	E	41	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	196	GLN
1	E	41	ASN
1	H	26	ASN
1	D	275	ASN
1	E	13	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	494/500 (98%)	0.24	23 (4%) 32 26	5, 38, 68, 83	0
1	B	494/500 (98%)	-0.07	15 (3%) 51 45	7, 27, 64, 76	0
1	C	494/500 (98%)	-0.40	6 (1%) 79 76	5, 20, 50, 71	0
1	D	494/500 (98%)	0.03	11 (2%) 62 57	6, 35, 62, 76	0
1	E	494/500 (98%)	-0.20	0 100 100	6, 29, 55, 69	0
1	F	494/500 (98%)	-0.45	1 (0%) 94 95	6, 20, 45, 67	0
1	G	494/500 (98%)	-0.24	5 (1%) 82 80	5, 25, 56, 71	0
1	H	494/500 (98%)	0.30	29 (5%) 23 18	6, 40, 67, 79	0
All	All	3952/4000 (98%)	-0.10	90 (2%) 61 56	5, 28, 62, 83	0

The worst 5 of 90 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	VAL	11.2
1	A	247	THR	7.1
1	B	253	ILE	5.4
1	A	251	ARG	5.3
1	H	249	ILE	5.1

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates 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.