



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:48 AM GMT

PDB ID : 3G17  
Title : Structure of putative 2-dehydropantoate 2-reductase from staphylococcus aureus  
Authors : Ramagopal, U.A.; Toro, R.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2009-01-29  
Resolution : 2.30 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

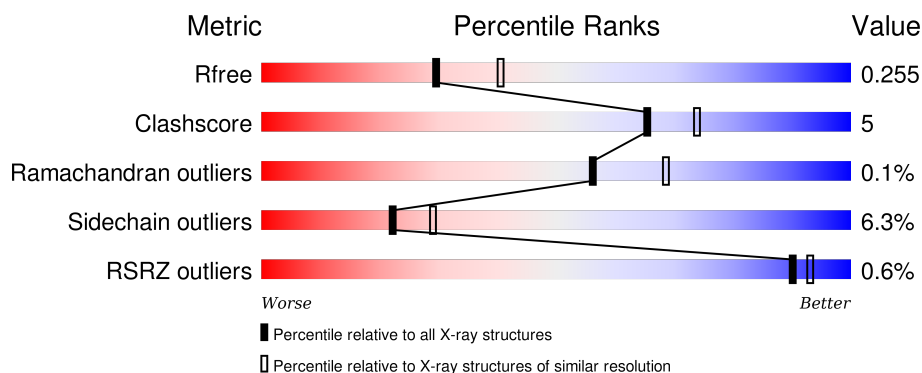
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	294	<div> <div></div> <div>85%10% ..</div> </div>
1	B	294	<div> <div></div> <div>83%13% ..</div> </div>
1	C	294	<div> <div></div> <div>80%15% ..</div> </div>
1	D	294	<div> <div></div> <div>82%14% ..</div> </div>
1	E	294	<div> <div></div> <div>86%11% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	294	
1	G	294	
1	H	294	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18687 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 Similar to 2-dehydropantoate 2-reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2268	1449	389	423	7			
1	B	286	Total	C	N	O	S	0	0	0
			2278	1453	390	428	7			
1	C	285	Total	C	N	O	S	0	1	0
			2273	1452	388	426	7			
1	D	287	Total	C	N	O	S	0	0	0
			2291	1460	395	429	7			
1	E	288	Total	C	N	O	S	0	1	0
			2303	1467	399	430	7			
1	F	282	Total	C	N	O	S	0	0	0
			2245	1430	390	418	7			
1	G	290	Total	C	N	O	S	0	0	0
			2318	1477	403	431	7			
1	H	290	Total	C	N	O	S	0	0	0
			2315	1476	402	430	7			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q99R37
A	2	SER	-	expression tag	UNP Q99R37
A	287	GLU	-	expression tag	UNP Q99R37
A	288	GLY	-	expression tag	UNP Q99R37
A	289	HIS	-	expression tag	UNP Q99R37
A	290	HIS	-	expression tag	UNP Q99R37
A	291	HIS	-	expression tag	UNP Q99R37
A	292	HIS	-	expression tag	UNP Q99R37
A	293	HIS	-	expression tag	UNP Q99R37
A	294	HIS	-	expression tag	UNP Q99R37
B	1	MET	-	expression tag	UNP Q99R37
B	2	SER	-	expression tag	UNP Q99R37
B	287	GLU	-	expression tag	UNP Q99R37

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Chain	Residue	Modelled	Actual	Comment	Reference
B	288	GLY	-	expression tag	UNP Q99R37
B	289	HIS	-	expression tag	UNP Q99R37
B	290	HIS	-	expression tag	UNP Q99R37
B	291	HIS	-	expression tag	UNP Q99R37
B	292	HIS	-	expression tag	UNP Q99R37
B	293	HIS	-	expression tag	UNP Q99R37
B	294	HIS	-	expression tag	UNP Q99R37
C	1	MET	-	expression tag	UNP Q99R37
C	2	SER	-	expression tag	UNP Q99R37
C	287	GLU	-	expression tag	UNP Q99R37
C	288	GLY	-	expression tag	UNP Q99R37
C	289	HIS	-	expression tag	UNP Q99R37
C	290	HIS	-	expression tag	UNP Q99R37
C	291	HIS	-	expression tag	UNP Q99R37
C	292	HIS	-	expression tag	UNP Q99R37
C	293	HIS	-	expression tag	UNP Q99R37
C	294	HIS	-	expression tag	UNP Q99R37
D	1	MET	-	expression tag	UNP Q99R37
D	2	SER	-	expression tag	UNP Q99R37
D	287	GLU	-	expression tag	UNP Q99R37
D	288	GLY	-	expression tag	UNP Q99R37
D	289	HIS	-	expression tag	UNP Q99R37
D	290	HIS	-	expression tag	UNP Q99R37
D	291	HIS	-	expression tag	UNP Q99R37
D	292	HIS	-	expression tag	UNP Q99R37
D	293	HIS	-	expression tag	UNP Q99R37
D	294	HIS	-	expression tag	UNP Q99R37
E	1	MET	-	expression tag	UNP Q99R37
E	2	SER	-	expression tag	UNP Q99R37
E	287	GLU	-	expression tag	UNP Q99R37
E	288	GLY	-	expression tag	UNP Q99R37
E	289	HIS	-	expression tag	UNP Q99R37
E	290	HIS	-	expression tag	UNP Q99R37
E	291	HIS	-	expression tag	UNP Q99R37
E	292	HIS	-	expression tag	UNP Q99R37
E	293	HIS	-	expression tag	UNP Q99R37
E	294	HIS	-	expression tag	UNP Q99R37
F	1	MET	-	expression tag	UNP Q99R37
F	2	SER	-	expression tag	UNP Q99R37
F	287	GLU	-	expression tag	UNP Q99R37
F	288	GLY	-	expression tag	UNP Q99R37
F	289	HIS	-	expression tag	UNP Q99R37

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Chain	Residue	Modelled	Actual	Comment	Reference
F	290	HIS	-	expression tag	UNP Q99R37
F	291	HIS	-	expression tag	UNP Q99R37
F	292	HIS	-	expression tag	UNP Q99R37
F	293	HIS	-	expression tag	UNP Q99R37
F	294	HIS	-	expression tag	UNP Q99R37
G	1	MET	-	expression tag	UNP Q99R37
G	2	SER	-	expression tag	UNP Q99R37
G	287	GLU	-	expression tag	UNP Q99R37
G	288	GLY	-	expression tag	UNP Q99R37
G	289	HIS	-	expression tag	UNP Q99R37
G	290	HIS	-	expression tag	UNP Q99R37
G	291	HIS	-	expression tag	UNP Q99R37
G	292	HIS	-	expression tag	UNP Q99R37
G	293	HIS	-	expression tag	UNP Q99R37
G	294	HIS	-	expression tag	UNP Q99R37
H	1	MET	-	expression tag	UNP Q99R37
H	2	SER	-	expression tag	UNP Q99R37
H	287	GLU	-	expression tag	UNP Q99R37
H	288	GLY	-	expression tag	UNP Q99R37
H	289	HIS	-	expression tag	UNP Q99R37
H	290	HIS	-	expression tag	UNP Q99R37
H	291	HIS	-	expression tag	UNP Q99R37
H	292	HIS	-	expression tag	UNP Q99R37
H	293	HIS	-	expression tag	UNP Q99R37
H	294	HIS	-	expression tag	UNP Q99R37

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	74	Total O 74 74	0	0
2	B	60	Total O 60 60	0	0
2	C	51	Total O 51 51	0	0
2	D	38	Total O 38 38	0	0
2	E	31	Total O 31 31	0	0
2	F	29	Total O 29 29	0	0
2	G	60	Total O 60 60	0	0

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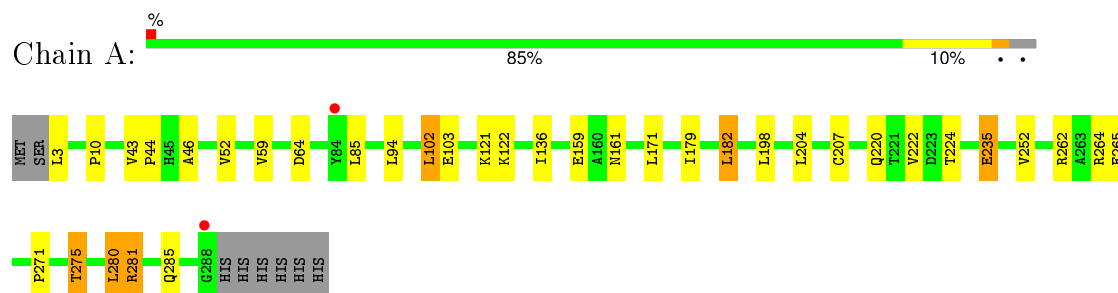
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	53	Total	O	0	0
			53	53		

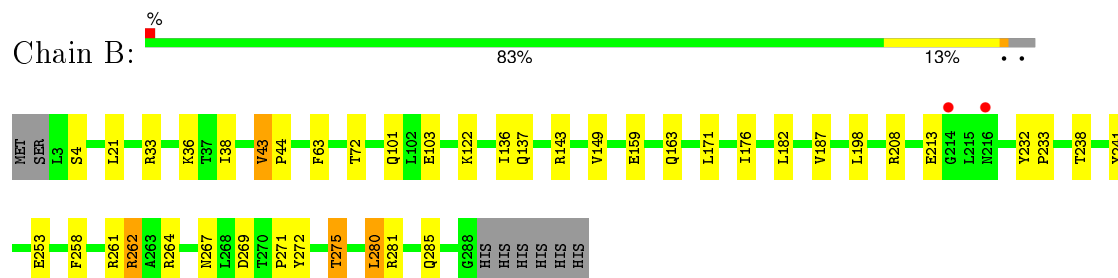
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

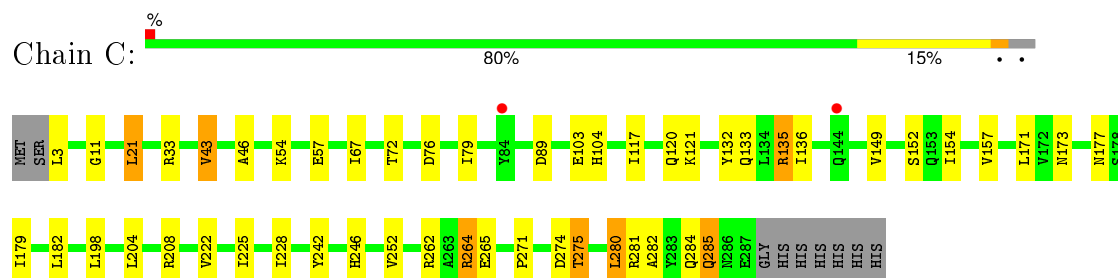
- Molecule 1: Similar to 2-dehydropantoate 2-reductase



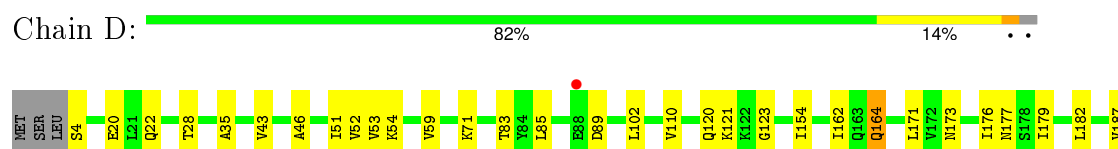
- Molecule 1: Similar to 2-dehydropantoate 2-reductase



- Molecule 1: Similar to 2-dehydropantoate 2-reductase



- Molecule 1: Similar to 2-dehydropantoate 2-reductase







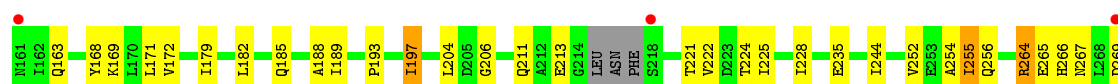
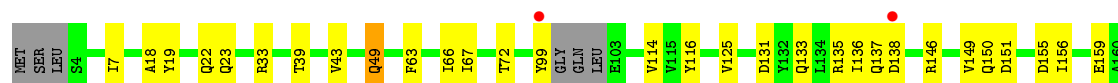
- Molecule 1: Similar to 2-dehydropantoate 2-reductase

Chain E: 86% 11% ..



- Molecule 1: Similar to 2-dehydropantoate 2-reductase

Chain F: 2% 73% 21% ..



- Molecule 1: Similar to 2-dehydropantoate 2-reductase

Chain G: 89% 9% ..



- Molecule 1: Similar to 2-dehydropantoate 2-reductase

Chain H: 86% 11% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.24Å 99.64Å 100.26Å 103.66° 105.23° 102.26°	Depositor
Resolution (Å)	50.00 – 2.30 37.55 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.30) 87.9 (37.55-2.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, $R_{free}$	0.200 , 0.260 0.198 , 0.255	Depositor DCC
$R_{free}$ test set	5744 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.0	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.6	EDS
Estimated twinning fraction	0.007 for -h,-l,-k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 113882 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18687	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.61	0/2314	0.68	0/3155
1	B	0.63	0/2324	0.67	0/3168
1	C	0.56	0/2322	0.65	0/3166
1	D	0.63	0/2339	0.69	0/3188
1	E	0.62	0/2355	0.66	0/3210
1	F	0.54	0/2291	0.65	0/3121
1	G	0.63	1/2368 (0.0%)	0.70	1/3228 (0.0%)
1	H	0.58	0/2365	0.66	0/3224
All	All	0.60	1/18678 (0.0%)	0.67	1/25460 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	111	CYS	CB-SG	-5.72	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	226	MET	CA-CB-CG	-5.34	104.22	113.30

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	2268	0	2254	23	0
1	B	2278	0	2264	20	0
1	C	2273	0	2259	33	0
1	D	2291	0	2269	22	0
1	E	2303	0	2281	20	0
1	F	2245	0	2218	40	0
1	G	2318	0	2294	14	0
1	H	2315	0	2290	25	0
2	A	74	0	0	2	0
2	B	60	0	0	0	0
2	C	51	0	0	0	0
2	D	38	0	0	0	0
2	E	31	0	0	0	0
2	F	29	0	0	1	0
2	G	60	0	0	0	0
2	H	53	0	0	0	0
All	All	18687	0	18129	182	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 5.

The worst 5 of 182 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:B:262:ARG:HH11	1:B:262:ARG:HG3	1.19	1.01
1:H:137:GLN:O	1:H:142:THR:HG21	1.68	0.91
1:F:137:GLN:HE21	1:F:138:ASP:H	1.16	0.89
1:B:262:ARG:NH1	1:B:262:ARG:HG3	1.85	0.88
1:F:171:LEU:HD11	1:F:206:GLY:HA3	1.56	0.86

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	284/294 (97%)	273 (96%)	11 (4%)	0	100	100
1	B	284/294 (97%)	269 (95%)	15 (5%)	0	100	100
1	C	284/294 (97%)	270 (95%)	14 (5%)	0	100	100
1	D	285/294 (97%)	275 (96%)	10 (4%)	0	100	100
1	E	287/294 (98%)	276 (96%)	11 (4%)	0	100	100
1	F	276/294 (94%)	255 (92%)	19 (7%)	2 (1%)	26	31
1	G	288/294 (98%)	278 (96%)	10 (4%)	0	100	100
1	H	288/294 (98%)	276 (96%)	12 (4%)	0	100	100
All	All	2276/2352 (97%)	2172 (95%)	102 (4%)	2 (0%)	56	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	188	ALA
1	F	255	ILE

### 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	244/256 (95%)	230 (94%)	14 (6%)	25	34
1	B	247/256 (96%)	227 (92%)	20 (8%)	15	18
1	C	246/256 (96%)	227 (92%)	19 (8%)	16	20
1	D	248/256 (97%)	230 (93%)	18 (7%)	17	22
1	E	250/256 (98%)	239 (96%)	11 (4%)	35	46
1	F	242/256 (94%)	220 (91%)	22 (9%)	12	13
1	G	251/256 (98%)	243 (97%)	8 (3%)	46	62
1	H	250/256 (98%)	237 (95%)	13 (5%)	29	38
All	All	1978/2048 (97%)	1853 (94%)	125 (6%)	22	29

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	71	LYS
1	D	275	THR
1	H	71	LYS
1	D	89	ASP
1	D	179	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	164	GLN
1	F	137	GLN
1	H	177	ASN
1	F	96	GLN
1	F	144	GLN

### 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 carbohydrates 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	286/294 (97%)	-0.29	2 (0%) 89 92	22, 32, 47, 53	0
1	B	286/294 (97%)	-0.14	2 (0%) 89 92	22, 36, 59, 64	0
1	C	285/294 (96%)	-0.16	2 (0%) 89 92	25, 39, 54, 61	0
1	D	287/294 (97%)	-0.24	1 (0%) 94 96	20, 33, 51, 60	0
1	E	288/294 (97%)	-0.35	0 100 100	20, 33, 48, 62	0
1	F	282/294 (95%)	0.02	5 (1%) 71 78	27, 44, 63, 66	0
1	G	290/294 (98%)	-0.32	1 (0%) 94 96	20, 31, 45, 59	0
1	H	290/294 (98%)	-0.34	1 (0%) 94 96	23, 35, 48, 57	0
All	All	2294/2352 (97%)	-0.23	14 (0%) 90 93	20, 35, 56, 66	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	288	GLY	3.1
1	F	218	SER	3.0
1	B	216	ASN	2.9
1	A	84	TYR	2.7
1	F	138	ASP	2.7

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.