



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 10:31 PM GMT

PDB ID : 5DH1  
Title : Structure of the siderophore periplasmic binding protein from the fuscachelin gene cluster of *Thermobifida fusca* in P21  
Authors : Li, K.; Bruner, S.D.  
Deposited on : 2015-08-29  
Resolution : 2.84 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 : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

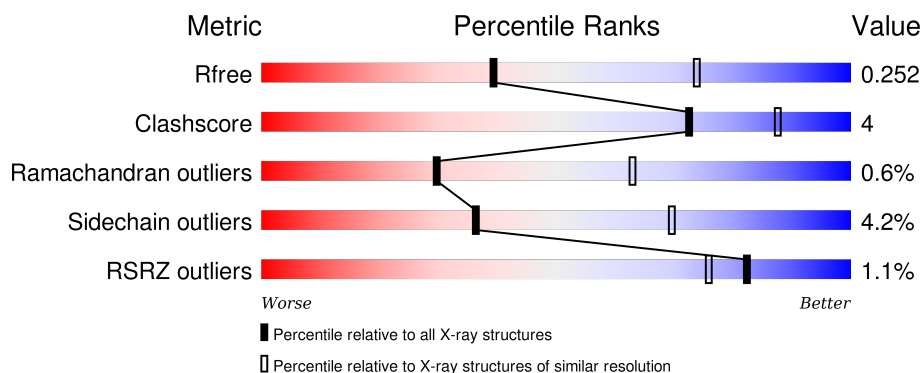
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.84 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	3170 (2.88-2.80)
Clashscore	102246	3658 (2.88-2.80)
Ramachandran outliers	100387	3591 (2.88-2.80)
Sidechain outliers	100360	3594 (2.88-2.80)
RSRZ outliers	91569	3184 (2.88-2.80)

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	309	<div> <div>80%</div> <div>9%</div> <div>10%</div> </div>
1	B	309	<div> <div>2%</div> <div>76%</div> <div>13%</div> <div>11%</div> </div>
1	C	309	<div> <div>%</div> <div>76%</div> <div>11%</div> <div>11%</div> </div>
1	D	309	<div> <div>%</div> <div>76%</div> <div>13%</div> <div>11%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8547 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 siderophore periplasmic binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2141	1353	350	436	2			
1	B	276	Total	C	N	O	S	0	0	0
			2134	1349	350	433	2			
1	C	274	Total	C	N	O	S	0	0	0
			2121	1340	344	435	2			
1	D	276	Total	C	N	O	S	0	0	0
			2128	1347	347	432	2			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	MET	-	initiating methionine	UNP Q47NS2
A	54	GLY	-	expression tag	UNP Q47NS2
A	55	SER	-	expression tag	UNP Q47NS2
A	56	SER	-	expression tag	UNP Q47NS2
A	57	HIS	-	expression tag	UNP Q47NS2
A	58	HIS	-	expression tag	UNP Q47NS2
A	59	HIS	-	expression tag	UNP Q47NS2
A	60	HIS	-	expression tag	UNP Q47NS2
A	61	HIS	-	expression tag	UNP Q47NS2
A	62	HIS	-	expression tag	UNP Q47NS2
A	63	SER	-	expression tag	UNP Q47NS2
A	64	SER	-	expression tag	UNP Q47NS2
A	65	GLY	-	expression tag	UNP Q47NS2
A	66	LEU	-	expression tag	UNP Q47NS2
A	67	VAL	-	expression tag	UNP Q47NS2
A	68	PRO	-	expression tag	UNP Q47NS2
A	69	ARG	-	expression tag	UNP Q47NS2
A	70	GLY	-	expression tag	UNP Q47NS2
A	71	SER	-	expression tag	UNP Q47NS2
A	72	HIS	-	expression tag	UNP Q47NS2
A	73	MET	-	expression tag	UNP Q47NS2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ALA	-	expression tag	UNP Q47NS2
A	75	SER	-	expression tag	UNP Q47NS2
A	76	MET	-	expression tag	UNP Q47NS2
A	77	THR	-	expression tag	UNP Q47NS2
A	78	GLY	-	expression tag	UNP Q47NS2
A	79	GLY	-	expression tag	UNP Q47NS2
A	80	GLN	-	expression tag	UNP Q47NS2
A	81	GLN	-	expression tag	UNP Q47NS2
A	82	MET	-	expression tag	UNP Q47NS2
A	83	GLY	-	expression tag	UNP Q47NS2
A	84	ARG	-	expression tag	UNP Q47NS2
A	85	GLY	-	expression tag	UNP Q47NS2
A	86	SER	-	expression tag	UNP Q47NS2
B	53	MET	-	initiating methionine	UNP Q47NS2
B	54	GLY	-	expression tag	UNP Q47NS2
B	55	SER	-	expression tag	UNP Q47NS2
B	56	SER	-	expression tag	UNP Q47NS2
B	57	HIS	-	expression tag	UNP Q47NS2
B	58	HIS	-	expression tag	UNP Q47NS2
B	59	HIS	-	expression tag	UNP Q47NS2
B	60	HIS	-	expression tag	UNP Q47NS2
B	61	HIS	-	expression tag	UNP Q47NS2
B	62	HIS	-	expression tag	UNP Q47NS2
B	63	SER	-	expression tag	UNP Q47NS2
B	64	SER	-	expression tag	UNP Q47NS2
B	65	GLY	-	expression tag	UNP Q47NS2
B	66	LEU	-	expression tag	UNP Q47NS2
B	67	VAL	-	expression tag	UNP Q47NS2
B	68	PRO	-	expression tag	UNP Q47NS2
B	69	ARG	-	expression tag	UNP Q47NS2
B	70	GLY	-	expression tag	UNP Q47NS2
B	71	SER	-	expression tag	UNP Q47NS2
B	72	HIS	-	expression tag	UNP Q47NS2
B	73	MET	-	expression tag	UNP Q47NS2
B	74	ALA	-	expression tag	UNP Q47NS2
B	75	SER	-	expression tag	UNP Q47NS2
B	76	MET	-	expression tag	UNP Q47NS2
B	77	THR	-	expression tag	UNP Q47NS2
B	78	GLY	-	expression tag	UNP Q47NS2
B	79	GLY	-	expression tag	UNP Q47NS2
B	80	GLN	-	expression tag	UNP Q47NS2
B	81	GLN	-	expression tag	UNP Q47NS2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	82	MET	-	expression tag	UNP Q47NS2
B	83	GLY	-	expression tag	UNP Q47NS2
B	84	ARG	-	expression tag	UNP Q47NS2
B	85	GLY	-	expression tag	UNP Q47NS2
B	86	SER	-	expression tag	UNP Q47NS2
C	53	MET	-	initiating methionine	UNP Q47NS2
C	54	GLY	-	expression tag	UNP Q47NS2
C	55	SER	-	expression tag	UNP Q47NS2
C	56	SER	-	expression tag	UNP Q47NS2
C	57	HIS	-	expression tag	UNP Q47NS2
C	58	HIS	-	expression tag	UNP Q47NS2
C	59	HIS	-	expression tag	UNP Q47NS2
C	60	HIS	-	expression tag	UNP Q47NS2
C	61	HIS	-	expression tag	UNP Q47NS2
C	62	HIS	-	expression tag	UNP Q47NS2
C	63	SER	-	expression tag	UNP Q47NS2
C	64	SER	-	expression tag	UNP Q47NS2
C	65	GLY	-	expression tag	UNP Q47NS2
C	66	LEU	-	expression tag	UNP Q47NS2
C	67	VAL	-	expression tag	UNP Q47NS2
C	68	PRO	-	expression tag	UNP Q47NS2
C	69	ARG	-	expression tag	UNP Q47NS2
C	70	GLY	-	expression tag	UNP Q47NS2
C	71	SER	-	expression tag	UNP Q47NS2
C	72	HIS	-	expression tag	UNP Q47NS2
C	73	MET	-	expression tag	UNP Q47NS2
C	74	ALA	-	expression tag	UNP Q47NS2
C	75	SER	-	expression tag	UNP Q47NS2
C	76	MET	-	expression tag	UNP Q47NS2
C	77	THR	-	expression tag	UNP Q47NS2
C	78	GLY	-	expression tag	UNP Q47NS2
C	79	GLY	-	expression tag	UNP Q47NS2
C	80	GLN	-	expression tag	UNP Q47NS2
C	81	GLN	-	expression tag	UNP Q47NS2
C	82	MET	-	expression tag	UNP Q47NS2
C	83	GLY	-	expression tag	UNP Q47NS2
C	84	ARG	-	expression tag	UNP Q47NS2
C	85	GLY	-	expression tag	UNP Q47NS2
C	86	SER	-	expression tag	UNP Q47NS2
D	53	MET	-	initiating methionine	UNP Q47NS2
D	54	GLY	-	expression tag	UNP Q47NS2
D	55	SER	-	expression tag	UNP Q47NS2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	56	SER	-	expression tag	UNP Q47NS2
D	57	HIS	-	expression tag	UNP Q47NS2
D	58	HIS	-	expression tag	UNP Q47NS2
D	59	HIS	-	expression tag	UNP Q47NS2
D	60	HIS	-	expression tag	UNP Q47NS2
D	61	HIS	-	expression tag	UNP Q47NS2
D	62	HIS	-	expression tag	UNP Q47NS2
D	63	SER	-	expression tag	UNP Q47NS2
D	64	SER	-	expression tag	UNP Q47NS2
D	65	GLY	-	expression tag	UNP Q47NS2
D	66	LEU	-	expression tag	UNP Q47NS2
D	67	VAL	-	expression tag	UNP Q47NS2
D	68	PRO	-	expression tag	UNP Q47NS2
D	69	ARG	-	expression tag	UNP Q47NS2
D	70	GLY	-	expression tag	UNP Q47NS2
D	71	SER	-	expression tag	UNP Q47NS2
D	72	HIS	-	expression tag	UNP Q47NS2
D	73	MET	-	expression tag	UNP Q47NS2
D	74	ALA	-	expression tag	UNP Q47NS2
D	75	SER	-	expression tag	UNP Q47NS2
D	76	MET	-	expression tag	UNP Q47NS2
D	77	THR	-	expression tag	UNP Q47NS2
D	78	GLY	-	expression tag	UNP Q47NS2
D	79	GLY	-	expression tag	UNP Q47NS2
D	80	GLN	-	expression tag	UNP Q47NS2
D	81	GLN	-	expression tag	UNP Q47NS2
D	82	MET	-	expression tag	UNP Q47NS2
D	83	GLY	-	expression tag	UNP Q47NS2
D	84	ARG	-	expression tag	UNP Q47NS2
D	85	GLY	-	expression tag	UNP Q47NS2
D	86	SER	-	expression tag	UNP Q47NS2

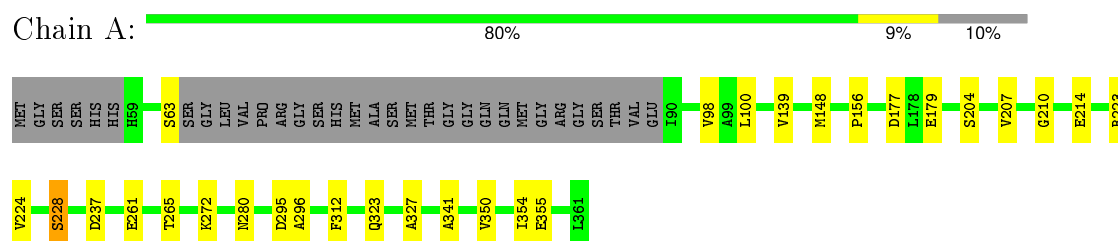
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total O 5 5	0	0
2	B	5	Total O 5 5	0	0
2	C	4	Total O 4 4	0	0
2	D	9	Total O 9 9	0	0

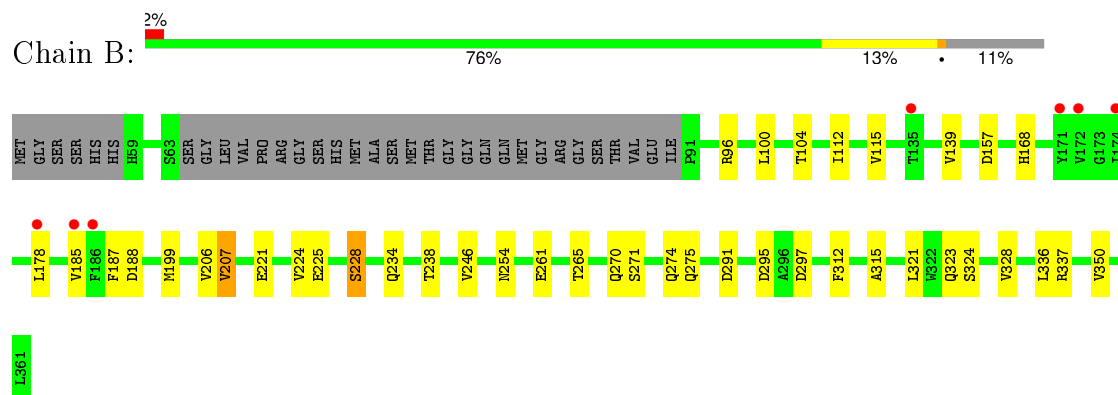
### 3 Residue-property plots [i](#)

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

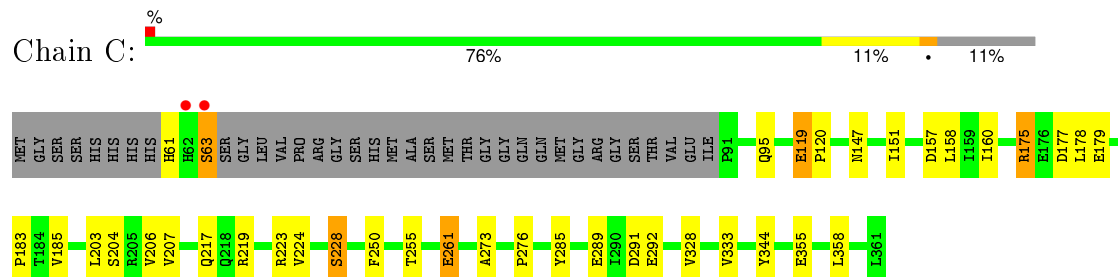
- Molecule 1: siderophore periplasmic binding protein



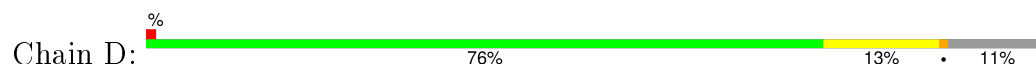
- Molecule 1: siderophore periplasmic binding protein



- Molecule 1: siderophore periplasmic binding protein



- Molecule 1: siderophore periplasmic binding protein







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.41Å 135.56Å 80.94Å 90.00° 91.98° 90.00°	Depositor
Resolution (Å)	46.53 – 2.84 47.93 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.53-2.84) 99.7 (47.93-2.84)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.183 , 0.247 0.191 , 0.252	Depositor DCC
$R_{free}$ test set	1624 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.9	Xtriage
Anisotropy	0.621	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 33.3	EDS
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 32606 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8547	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.32% 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	0.60	0/2184	0.69	0/2976
1	B	0.58	0/2177	0.66	0/2964
1	C	0.61	0/2162	0.66	0/2943
1	D	0.61	0/2170	0.70	0/2956
All	All	0.60	0/8693	0.68	0/11839

There are no bond length outliers.

There are no bond angle outliers.

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	2141	0	2023	13	0
1	B	2134	0	2022	19	0
1	C	2121	0	2014	21	0
1	D	2128	0	2019	19	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	4	0	0	0	0
2	D	9	0	0	0	0
All	All	8547	0	8078	69	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 4.

The worst 5 of 69 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:A:223:ARG:NH2	1:A:355:GLU:OE1	2.31	0.62
1:A:280:ASN:HB3	1:C:63:SER:HB3	1.83	0.61
1:B:185:VAL:HG11	1:B:206:VAL:HG21	1.83	0.61
1:B:323:GLN:HA	1:B:328:VAL:HG11	1.85	0.58
1:B:224:VAL:O	1:B:228:SER:HB3	2.04	0.58

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	273/309 (88%)	259 (95%)	12 (4%)	2 (1%)	26	59
1	B	272/309 (88%)	255 (94%)	14 (5%)	3 (1%)	17	47
1	C	270/309 (87%)	255 (94%)	15 (6%)	0	100	100
1	D	272/309 (88%)	246 (90%)	24 (9%)	2 (1%)	26	59
All	All	1087/1236 (88%)	1015 (93%)	65 (6%)	7 (1%)	30	63

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	265	THR
1	B	271	SER
1	B	295	ASP
1	D	271	SER
1	B	100	LEU

### 5.3.2 Protein sidechains [i](#)

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	222/249 (89%)	215 (97%)	7 (3%)	46	79
1	B	221/249 (89%)	213 (96%)	8 (4%)	42	75
1	C	221/249 (89%)	212 (96%)	9 (4%)	37	70
1	D	220/249 (88%)	207 (94%)	13 (6%)	24	54
All	All	884/996 (89%)	847 (96%)	37 (4%)	36	69

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	63	SER
1	C	178	LEU
1	D	291	ASP
1	C	119	GLU
1	C	175	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	277/309 (89%)	-0.20	0	100	100	21, 35, 55, 68	0
1	B	276/309 (89%)	-0.02	7 (2%)	61	50	23, 42, 69, 79	0
1	C	274/309 (88%)	-0.15	2 (0%)	89	85	20, 38, 67, 77	0
1	D	276/309 (89%)	-0.16	3 (1%)	82	76	19, 35, 67, 92	0
All	All	1103/1236 (89%)	-0.13	12 (1%)	82	76	19, 37, 66, 92	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	171	TYR	3.7
1	B	172	VAL	3.6
1	B	185	VAL	3.1
1	B	135	THR	2.9
1	D	173	GLY	2.3

### 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 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.