



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 10:49 am BST

PDB ID : 3V8B  
Title : Crystal Structure of a 3-ketoacyl-ACP reductase from *Sinorhizobium meliloti* 1021  
Authors : Kumaran, D.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; Lafleur, J.; Seidel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRG)  
Deposited on : 2011-12-22  
Resolution : 2.70 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

<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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

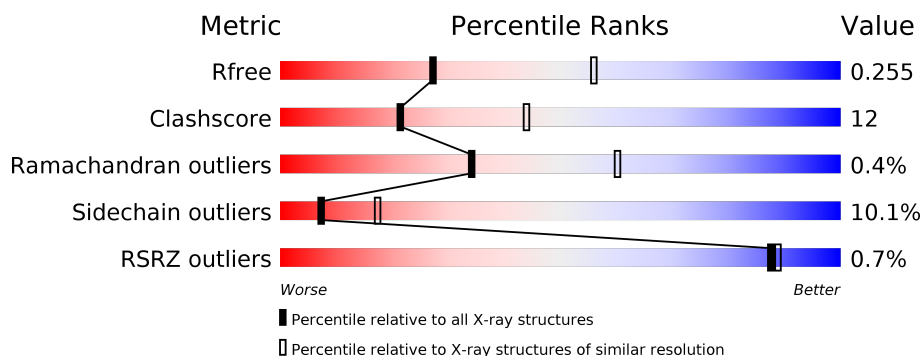
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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 on 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	283	<div> <div>65%</div> <div>23%</div> <div>•</div> <div>9%</div> </div>
1	B	283	<div> <div>68%</div> <div>18%</div> <div>5%</div> <div>9%</div> </div>
1	C	283	<div> <div>67%</div> <div>19%</div> <div>•</div> <div>10%</div> </div>
1	D	283	<div> <div>2%</div> <div>62%</div> <div>24%</div> <div>•</div> <div>10%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7663 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 Putative dehydrogenase, possibly 3-oxoacyl-[acyl-carrier protein] reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	Se	0	0	0
			1908	1198	342	366	1	1			
1	B	257	Total	C	N	O	S	Se	0	0	0
			1908	1198	342	366	1	1			
1	C	255	Total	C	N	O	S	Se	0	0	0
			1895	1190	340	363	1	1			
1	D	256	Total	C	N	O	S	Se	0	0	0
			1901	1193	341	365	1	1			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MSE	-	EXPRESSION TAG	UNP Q92U42
A	-21	HIS	-	EXPRESSION TAG	UNP Q92U42
A	-20	HIS	-	EXPRESSION TAG	UNP Q92U42
A	-19	HIS	-	EXPRESSION TAG	UNP Q92U42
A	-18	HIS	-	EXPRESSION TAG	UNP Q92U42
A	-17	HIS	-	EXPRESSION TAG	UNP Q92U42
A	-16	HIS	-	EXPRESSION TAG	UNP Q92U42
A	-15	SER	-	EXPRESSION TAG	UNP Q92U42
A	-14	SER	-	EXPRESSION TAG	UNP Q92U42
A	-13	GLY	-	EXPRESSION TAG	UNP Q92U42
A	-12	VAL	-	EXPRESSION TAG	UNP Q92U42
A	-11	ASP	-	EXPRESSION TAG	UNP Q92U42
A	-10	LEU	-	EXPRESSION TAG	UNP Q92U42
A	-9	GLY	-	EXPRESSION TAG	UNP Q92U42
A	-8	THR	-	EXPRESSION TAG	UNP Q92U42
A	-7	GLU	-	EXPRESSION TAG	UNP Q92U42
A	-6	ASN	-	EXPRESSION TAG	UNP Q92U42
A	-5	LEU	-	EXPRESSION TAG	UNP Q92U42
A	-4	TYR	-	EXPRESSION TAG	UNP Q92U42
A	-3	PHE	-	EXPRESSION TAG	UNP Q92U42

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLN	-	EXPRESSION TAG	UNP Q92U42
A	-1	SER	-	EXPRESSION TAG	UNP Q92U42
A	0	MSE	-	EXPRESSION TAG	UNP Q92U42
B	-22	MSE	-	EXPRESSION TAG	UNP Q92U42
B	-21	HIS	-	EXPRESSION TAG	UNP Q92U42
B	-20	HIS	-	EXPRESSION TAG	UNP Q92U42
B	-19	HIS	-	EXPRESSION TAG	UNP Q92U42
B	-18	HIS	-	EXPRESSION TAG	UNP Q92U42
B	-17	HIS	-	EXPRESSION TAG	UNP Q92U42
B	-16	HIS	-	EXPRESSION TAG	UNP Q92U42
B	-15	SER	-	EXPRESSION TAG	UNP Q92U42
B	-14	SER	-	EXPRESSION TAG	UNP Q92U42
B	-13	GLY	-	EXPRESSION TAG	UNP Q92U42
B	-12	VAL	-	EXPRESSION TAG	UNP Q92U42
B	-11	ASP	-	EXPRESSION TAG	UNP Q92U42
B	-10	LEU	-	EXPRESSION TAG	UNP Q92U42
B	-9	GLY	-	EXPRESSION TAG	UNP Q92U42
B	-8	THR	-	EXPRESSION TAG	UNP Q92U42
B	-7	GLU	-	EXPRESSION TAG	UNP Q92U42
B	-6	ASN	-	EXPRESSION TAG	UNP Q92U42
B	-5	LEU	-	EXPRESSION TAG	UNP Q92U42
B	-4	TYR	-	EXPRESSION TAG	UNP Q92U42
B	-3	PHE	-	EXPRESSION TAG	UNP Q92U42
B	-2	GLN	-	EXPRESSION TAG	UNP Q92U42
B	-1	SER	-	EXPRESSION TAG	UNP Q92U42
B	0	MSE	-	EXPRESSION TAG	UNP Q92U42
C	-22	MSE	-	EXPRESSION TAG	UNP Q92U42
C	-21	HIS	-	EXPRESSION TAG	UNP Q92U42
C	-20	HIS	-	EXPRESSION TAG	UNP Q92U42
C	-19	HIS	-	EXPRESSION TAG	UNP Q92U42
C	-18	HIS	-	EXPRESSION TAG	UNP Q92U42
C	-17	HIS	-	EXPRESSION TAG	UNP Q92U42
C	-16	HIS	-	EXPRESSION TAG	UNP Q92U42
C	-15	SER	-	EXPRESSION TAG	UNP Q92U42
C	-14	SER	-	EXPRESSION TAG	UNP Q92U42
C	-13	GLY	-	EXPRESSION TAG	UNP Q92U42
C	-12	VAL	-	EXPRESSION TAG	UNP Q92U42
C	-11	ASP	-	EXPRESSION TAG	UNP Q92U42
C	-10	LEU	-	EXPRESSION TAG	UNP Q92U42
C	-9	GLY	-	EXPRESSION TAG	UNP Q92U42
C	-8	THR	-	EXPRESSION TAG	UNP Q92U42
C	-7	GLU	-	EXPRESSION TAG	UNP Q92U42

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	ASN	-	EXPRESSION TAG	UNP Q92U42
C	-5	LEU	-	EXPRESSION TAG	UNP Q92U42
C	-4	TYR	-	EXPRESSION TAG	UNP Q92U42
C	-3	PHE	-	EXPRESSION TAG	UNP Q92U42
C	-2	GLN	-	EXPRESSION TAG	UNP Q92U42
C	-1	SER	-	EXPRESSION TAG	UNP Q92U42
C	0	MSE	-	EXPRESSION TAG	UNP Q92U42
D	-22	MSE	-	EXPRESSION TAG	UNP Q92U42
D	-21	HIS	-	EXPRESSION TAG	UNP Q92U42
D	-20	HIS	-	EXPRESSION TAG	UNP Q92U42
D	-19	HIS	-	EXPRESSION TAG	UNP Q92U42
D	-18	HIS	-	EXPRESSION TAG	UNP Q92U42
D	-17	HIS	-	EXPRESSION TAG	UNP Q92U42
D	-16	HIS	-	EXPRESSION TAG	UNP Q92U42
D	-15	SER	-	EXPRESSION TAG	UNP Q92U42
D	-14	SER	-	EXPRESSION TAG	UNP Q92U42
D	-13	GLY	-	EXPRESSION TAG	UNP Q92U42
D	-12	VAL	-	EXPRESSION TAG	UNP Q92U42
D	-11	ASP	-	EXPRESSION TAG	UNP Q92U42
D	-10	LEU	-	EXPRESSION TAG	UNP Q92U42
D	-9	GLY	-	EXPRESSION TAG	UNP Q92U42
D	-8	THR	-	EXPRESSION TAG	UNP Q92U42
D	-7	GLU	-	EXPRESSION TAG	UNP Q92U42
D	-6	ASN	-	EXPRESSION TAG	UNP Q92U42
D	-5	LEU	-	EXPRESSION TAG	UNP Q92U42
D	-4	TYR	-	EXPRESSION TAG	UNP Q92U42
D	-3	PHE	-	EXPRESSION TAG	UNP Q92U42
D	-2	GLN	-	EXPRESSION TAG	UNP Q92U42
D	-1	SER	-	EXPRESSION TAG	UNP Q92U42
D	0	MSE	-	EXPRESSION TAG	UNP Q92U42

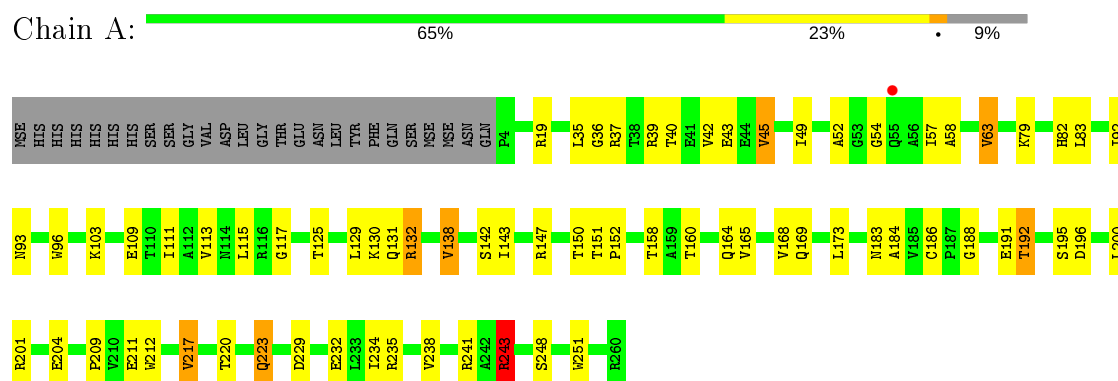
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	11	Total O 11 11	0	0
2	B	16	Total O 16 16	0	0
2	C	9	Total O 9 9	0	0
2	D	15	Total O 15 15	0	0

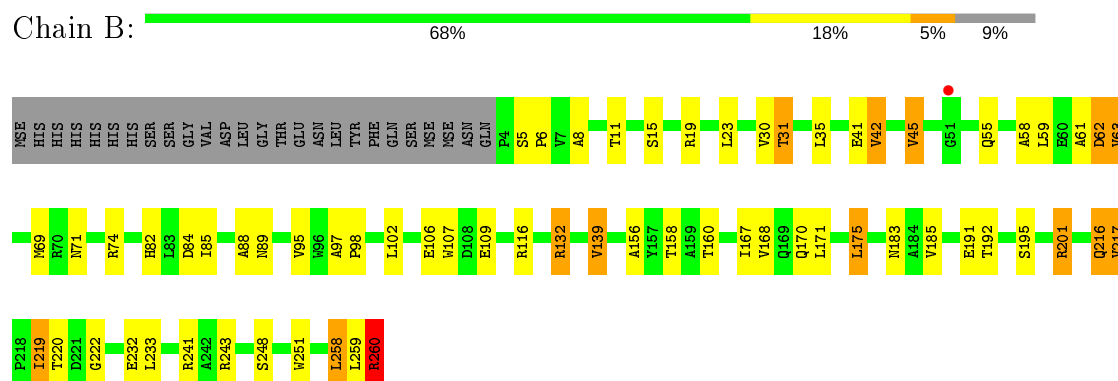
### 3 Residue-property plots

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.

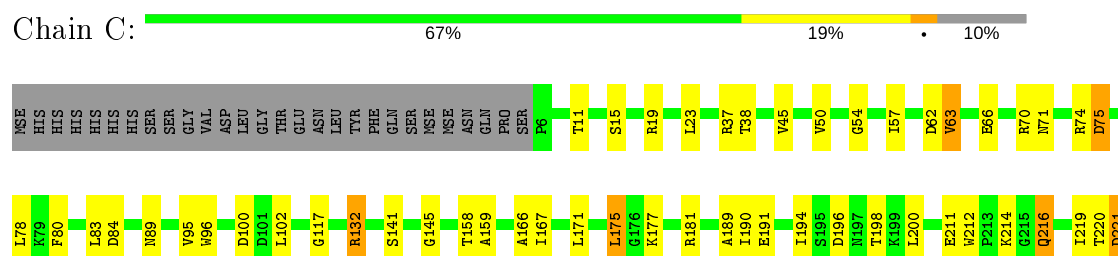
- Molecule 1: Putative dehydrogenase, possibly 3-oxoacyl-[acyl-carrier protein] reductase

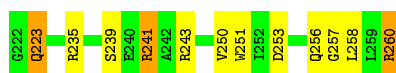


- Molecule 1: Putative dehydrogenase, possibly 3-oxoacyl-[acyl-carrier protein] reductase

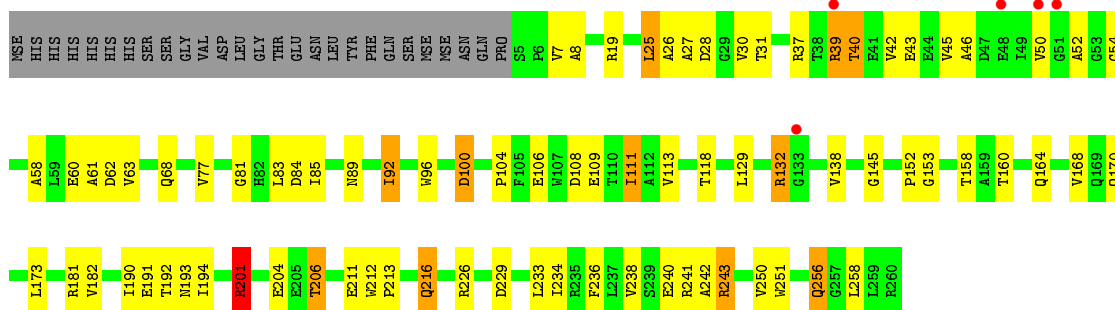


- Molecule 1: Putative dehydrogenase, possibly 3-oxoacyl-[acyl-carrier protein] reductase





- Molecule 1: Putative dehydrogenase, possibly 3-oxoacyl-[acyl-carrier protein] reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.79 Å   143.92 Å   66.71 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	48.92 – 2.70 48.92 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.92-2.70) 99.8 (48.92-2.70)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.59 (at 2.69 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.187   ,   0.255 0.188   ,   0.255	Depositor DCC
$R_{free}$ test set	1565 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.3	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 33.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7663	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% 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, 0.333 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	0.69	1/1939 (0.1%)	0.82	3/2643 (0.1%)
1	B	0.72	2/1939 (0.1%)	0.87	3/2643 (0.1%)
1	C	0.69	1/1925 (0.1%)	0.83	1/2623 (0.0%)
1	D	0.69	3/1931 (0.2%)	0.84	3/2632 (0.1%)
All	All	0.70	7/7734 (0.1%)	0.84	10/10541 (0.1%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	251	TRP	CD2-CE2	6.40	1.49	1.41
1	B	251	TRP	CD2-CE2	5.62	1.48	1.41
1	D	212	TRP	CD2-CE2	5.56	1.48	1.41
1	C	251	TRP	CD2-CE2	5.55	1.48	1.41
1	D	96	TRP	CD2-CE2	5.32	1.47	1.41

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	B	260	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	D	201	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	D	108	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	116	ARG	NE-CZ-NH1	5.49	123.04	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	1908	0	1928	45	0
1	B	1908	0	1928	52	0
1	C	1895	0	1916	37	0
1	D	1901	0	1920	64	0
2	A	11	0	0	0	0
2	B	16	0	0	0	0
2	C	9	0	0	0	0
2	D	15	0	0	0	0
All	All	7663	0	7692	183	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 12.

The worst 5 of 183 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:260:ARG:HG2	1:C:260:ARG:HH11	1.23	0.98
1:D:118:THR:HG21	1:D:164:GLN:HE21	1.26	0.97
1:B:31:THR:HB	1:B:55:GLN:HB2	1.42	0.97
1:B:260:ARG:HH11	1:B:260:ARG:HG2	1.29	0.96
1:B:35:LEU:HD21	1:B:69:MSE:HE1	1.46	0.94

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	255/283 (90%)	245 (96%)	10 (4%)	0	100	100
1	B	255/283 (90%)	240 (94%)	15 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	253/283 (89%)	237 (94%)	13 (5%)	3 (1%)	13	32
1	D	254/283 (90%)	233 (92%)	20 (8%)	1 (0%)	34	60
All	All	1017/1132 (90%)	955 (94%)	58 (6%)	4 (0%)	34	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	221	ASP
1	D	27	ALA
1	C	191	GLU
1	C	198	THR

### 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	198/218 (91%)	180 (91%)	18 (9%)	9	21
1	B	198/218 (91%)	177 (89%)	21 (11%)	6	15
1	C	196/218 (90%)	176 (90%)	20 (10%)	7	17
1	D	197/218 (90%)	176 (89%)	21 (11%)	6	15
All	All	789/872 (90%)	709 (90%)	80 (10%)	7	17

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	258	LEU
1	C	83	LEU
1	D	201	ARG
1	B	259	LEU
1	C	37	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	71	ASN
1	B	169	GLN
1	D	68	GLN
1	A	223	GLN
1	C	223	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 [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	256/283 (90%)	-0.23	1 (0%) 92 93	16, 27, 49, 78	0
1	B	256/283 (90%)	-0.31	1 (0%) 92 93	15, 26, 50, 66	0
1	C	254/283 (89%)	-0.40	0 100 100	17, 29, 53, 63	0
1	D	255/283 (90%)	-0.09	5 (1%) 65 67	17, 32, 58, 74	0
All	All	1021/1132 (90%)	-0.26	7 (0%) 87 89	15, 29, 54, 78	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	51	GLY	4.1
1	A	55	GLN	2.6
1	D	133	GLY	2.4
1	D	39	ARG	2.2
1	D	48	GLU	2.1

### 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.