



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 01:09 pm BST

PDB ID : 6NRP  
Title : Putative short-chain dehydrogenase/reductase (SDR) from *Acinetobacter baumannii*  
Authors : Cross, E.M.; Smith, K.M.; Shaw, K.I.; Aragao, D.; Forwood, J.K.  
Deposited on : 2019-01-23  
Resolution : 1.90 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	:	2.11
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

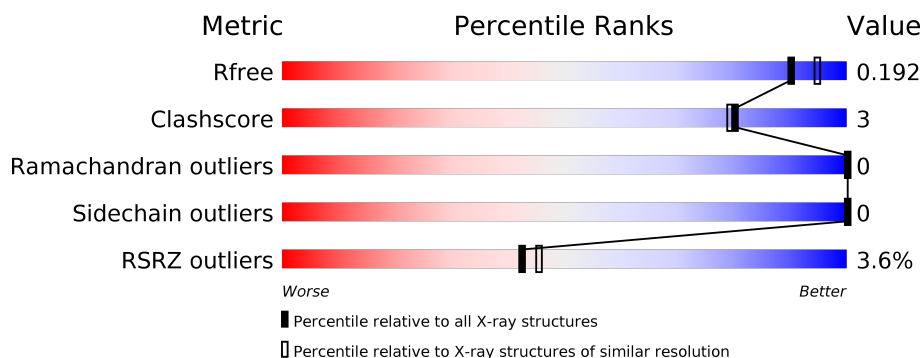
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	263	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>8%</div> <div>9%</div> </div> </div>
1	B	263	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>5%</div> <div>10%</div> </div> </div>
1	C	263	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>6%</div> <div>12%</div> </div> </div>
1	D	263	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>6%</div> <div>12%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7616 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 3-oxoacyl-ACP reductase FabG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1824	1144	324	347	9			
1	B	238	Total	C	N	O	S	0	0	0
			1808	1135	322	341	10			
1	C	231	Total	C	N	O	S	0	0	0
			1751	1100	314	329	8			
1	D	231	Total	C	N	O	S	0	0	0
			1749	1099	312	329	9			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP A0A1K1L6W4
A	-20	HIS	-	expression tag	UNP A0A1K1L6W4
A	-19	HIS	-	expression tag	UNP A0A1K1L6W4
A	-18	HIS	-	expression tag	UNP A0A1K1L6W4
A	-17	HIS	-	expression tag	UNP A0A1K1L6W4
A	-16	HIS	-	expression tag	UNP A0A1K1L6W4
A	-15	HIS	-	expression tag	UNP A0A1K1L6W4
A	-14	SER	-	expression tag	UNP A0A1K1L6W4
A	-13	SER	-	expression tag	UNP A0A1K1L6W4
A	-12	GLY	-	expression tag	UNP A0A1K1L6W4
A	-11	VAL	-	expression tag	UNP A0A1K1L6W4
A	-10	ASP	-	expression tag	UNP A0A1K1L6W4
A	-9	LEU	-	expression tag	UNP A0A1K1L6W4
A	-8	GLY	-	expression tag	UNP A0A1K1L6W4
A	-7	THR	-	expression tag	UNP A0A1K1L6W4
A	-6	GLU	-	expression tag	UNP A0A1K1L6W4
A	-5	ASN	-	expression tag	UNP A0A1K1L6W4
A	-4	LEU	-	expression tag	UNP A0A1K1L6W4
A	-3	TYR	-	expression tag	UNP A0A1K1L6W4
A	-2	PHE	-	expression tag	UNP A0A1K1L6W4
A	-1	GLN	-	expression tag	UNP A0A1K1L6W4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP A0A1K1L6W4
B	-21	MET	-	initiating methionine	UNP A0A1K1L6W4
B	-20	HIS	-	expression tag	UNP A0A1K1L6W4
B	-19	HIS	-	expression tag	UNP A0A1K1L6W4
B	-18	HIS	-	expression tag	UNP A0A1K1L6W4
B	-17	HIS	-	expression tag	UNP A0A1K1L6W4
B	-16	HIS	-	expression tag	UNP A0A1K1L6W4
B	-15	HIS	-	expression tag	UNP A0A1K1L6W4
B	-14	SER	-	expression tag	UNP A0A1K1L6W4
B	-13	SER	-	expression tag	UNP A0A1K1L6W4
B	-12	GLY	-	expression tag	UNP A0A1K1L6W4
B	-11	VAL	-	expression tag	UNP A0A1K1L6W4
B	-10	ASP	-	expression tag	UNP A0A1K1L6W4
B	-9	LEU	-	expression tag	UNP A0A1K1L6W4
B	-8	GLY	-	expression tag	UNP A0A1K1L6W4
B	-7	THR	-	expression tag	UNP A0A1K1L6W4
B	-6	GLU	-	expression tag	UNP A0A1K1L6W4
B	-5	ASN	-	expression tag	UNP A0A1K1L6W4
B	-4	LEU	-	expression tag	UNP A0A1K1L6W4
B	-3	TYR	-	expression tag	UNP A0A1K1L6W4
B	-2	PHE	-	expression tag	UNP A0A1K1L6W4
B	-1	GLN	-	expression tag	UNP A0A1K1L6W4
B	0	SER	-	expression tag	UNP A0A1K1L6W4
C	-21	MET	-	initiating methionine	UNP A0A1K1L6W4
C	-20	HIS	-	expression tag	UNP A0A1K1L6W4
C	-19	HIS	-	expression tag	UNP A0A1K1L6W4
C	-18	HIS	-	expression tag	UNP A0A1K1L6W4
C	-17	HIS	-	expression tag	UNP A0A1K1L6W4
C	-16	HIS	-	expression tag	UNP A0A1K1L6W4
C	-15	HIS	-	expression tag	UNP A0A1K1L6W4
C	-14	SER	-	expression tag	UNP A0A1K1L6W4
C	-13	SER	-	expression tag	UNP A0A1K1L6W4
C	-12	GLY	-	expression tag	UNP A0A1K1L6W4
C	-11	VAL	-	expression tag	UNP A0A1K1L6W4
C	-10	ASP	-	expression tag	UNP A0A1K1L6W4
C	-9	LEU	-	expression tag	UNP A0A1K1L6W4
C	-8	GLY	-	expression tag	UNP A0A1K1L6W4
C	-7	THR	-	expression tag	UNP A0A1K1L6W4
C	-6	GLU	-	expression tag	UNP A0A1K1L6W4
C	-5	ASN	-	expression tag	UNP A0A1K1L6W4
C	-4	LEU	-	expression tag	UNP A0A1K1L6W4
C	-3	TYR	-	expression tag	UNP A0A1K1L6W4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	PHE	-	expression tag	UNP A0A1K1L6W4
C	-1	GLN	-	expression tag	UNP A0A1K1L6W4
C	0	SER	-	expression tag	UNP A0A1K1L6W4
D	-21	MET	-	initiating methionine	UNP A0A1K1L6W4
D	-20	HIS	-	expression tag	UNP A0A1K1L6W4
D	-19	HIS	-	expression tag	UNP A0A1K1L6W4
D	-18	HIS	-	expression tag	UNP A0A1K1L6W4
D	-17	HIS	-	expression tag	UNP A0A1K1L6W4
D	-16	HIS	-	expression tag	UNP A0A1K1L6W4
D	-15	HIS	-	expression tag	UNP A0A1K1L6W4
D	-14	SER	-	expression tag	UNP A0A1K1L6W4
D	-13	SER	-	expression tag	UNP A0A1K1L6W4
D	-12	GLY	-	expression tag	UNP A0A1K1L6W4
D	-11	VAL	-	expression tag	UNP A0A1K1L6W4
D	-10	ASP	-	expression tag	UNP A0A1K1L6W4
D	-9	LEU	-	expression tag	UNP A0A1K1L6W4
D	-8	GLY	-	expression tag	UNP A0A1K1L6W4
D	-7	THR	-	expression tag	UNP A0A1K1L6W4
D	-6	GLU	-	expression tag	UNP A0A1K1L6W4
D	-5	ASN	-	expression tag	UNP A0A1K1L6W4
D	-4	LEU	-	expression tag	UNP A0A1K1L6W4
D	-3	TYR	-	expression tag	UNP A0A1K1L6W4
D	-2	PHE	-	expression tag	UNP A0A1K1L6W4
D	-1	GLN	-	expression tag	UNP A0A1K1L6W4
D	0	SER	-	expression tag	UNP A0A1K1L6W4

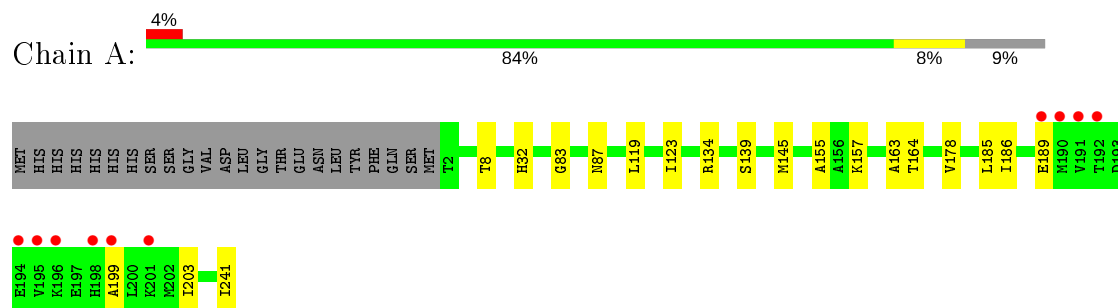
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	131	Total O 131 131	0	0
2	B	124	Total O 124 124	0	0
2	C	117	Total O 117 117	0	0
2	D	112	Total O 112 112	0	0

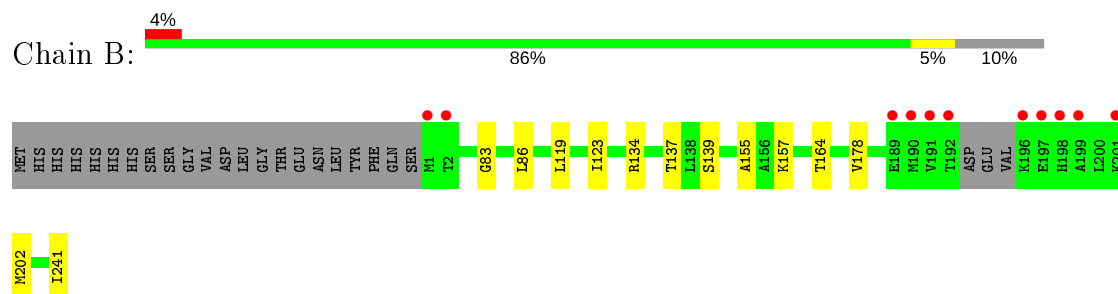
### 3 Residue-property plots [i](#)

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.

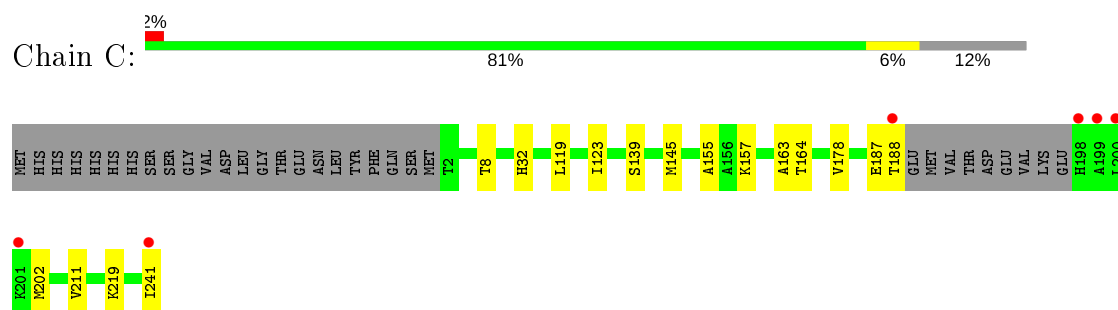
#### • Molecule 1: 3-oxoacyl-ACP reductase FabG



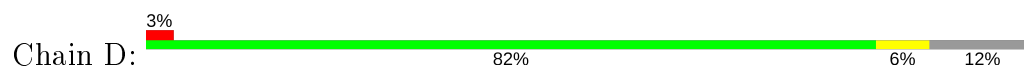
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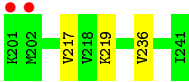
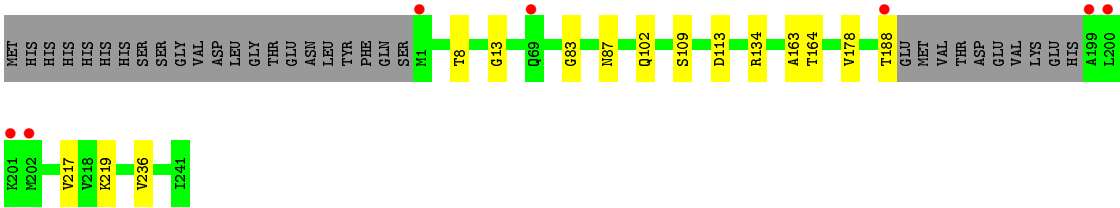


#### • Molecule 1: 3-oxoacyl-ACP reductase FabG



#### • Molecule 1: 3-oxoacyl-ACP reductase FabG





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.48 Å 89.48 Å 239.47 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.99 – 1.90 24.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.99-1.90) 99.9 (24.99-1.90)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 1.90 Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.170 , 0.192 0.170 , 0.192	Depositor DCC
$R_{free}$ test set	4504 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.9	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 45.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7616	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.41% 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	0.41	0/1847	0.57	0/2495
1	B	0.38	0/1830	0.53	0/2469
1	C	0.37	0/1773	0.54	0/2394
1	D	0.38	0/1770	0.53	0/2389
All	All	0.38	0/7220	0.55	0/9747

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	1824	0	1861	12	0
1	B	1808	0	1853	8	0
1	C	1751	0	1791	12	0
1	D	1749	0	1796	10	0
2	A	131	0	0	0	0
2	B	124	0	0	0	0
2	C	117	0	0	0	0
2	D	112	0	0	1	0
All	All	7616	0	7301	39	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 3.

All (39) 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:145:MET:SD	1:C:241:ILE:HG21	2.23	0.78
1:B:202:MET:HA	1:B:202:MET:HE3	1.86	0.57
1:B:139:SER:HA	1:B:157:LYS:HD2	1.92	0.51
1:D:164:THR:HG23	1:D:178:VAL:HG12	1.94	0.50
1:C:202:MET:HA	1:C:202:MET:HE3	1.93	0.50
1:A:145:MET:SD	1:A:241:ILE:HG21	2.52	0.50
1:C:139:SER:HA	1:C:157:LYS:HD2	1.93	0.50
1:C:164:THR:HG23	1:C:178:VAL:HG12	1.95	0.49
1:C:188:THR:CG2	1:C:211:VAL:CG1	2.91	0.49
1:B:155:ALA:HB2	1:D:163:ALA:HB2	1.95	0.48
1:A:83:GLY:HA2	1:A:134:ARG:O	2.14	0.47
1:A:164:THR:HG23	1:A:178:VAL:HG12	1.96	0.47
1:A:163:ALA:HB2	1:C:155:ALA:HB2	1.97	0.47
1:D:109:SER:O	1:D:113:ASP:HB2	2.15	0.46
1:D:13:GLY:HA2	1:D:188:THR:HG21	1.98	0.45
1:D:83:GLY:HA2	1:D:134:ARG:O	2.16	0.45
1:B:83:GLY:HA2	1:B:134:ARG:O	2.17	0.45
1:C:119:LEU:O	1:C:123:ILE:HG12	2.17	0.44
1:C:187:GLU:O	1:C:188:THR:HG23	2.17	0.44
1:A:185:LEU:HD22	1:A:199:ALA:HB3	1.99	0.44
1:B:164:THR:HG23	1:B:178:VAL:HG12	1.98	0.44
1:D:8:THR:O	1:D:87:ASN:HB3	2.18	0.44
1:C:145:MET:SD	1:C:241:ILE:CG2	3.01	0.43
1:A:199:ALA:O	1:A:203:ILE:HG13	2.18	0.43
1:A:186:ILE:HB	1:A:189:GLU:HG3	2.01	0.43
1:B:119:LEU:O	1:B:123:ILE:HG12	2.19	0.43
1:C:219:LYS:HB3	1:C:219:LYS:HE2	1.81	0.43
1:D:102:GLN:HG2	2:D:303:HOH:O	2.18	0.42
1:A:119:LEU:O	1:A:123:ILE:HG12	2.19	0.42
1:D:217:VAL:HG21	1:D:236:VAL:CG2	2.49	0.42
1:A:139:SER:HA	1:A:157:LYS:HD2	2.02	0.42
1:C:8:THR:HA	1:C:32:HIS:HB3	2.00	0.42
1:A:8:THR:O	1:A:87:ASN:HB3	2.20	0.42
1:A:8:THR:HA	1:A:32:HIS:HB3	2.02	0.41
1:D:219:LYS:HE2	1:D:219:LYS:HB3	1.94	0.41
1:B:86:LEU:HD12	1:B:137:THR:HG22	2.03	0.41
1:B:241:ILE:HA	1:B:241:ILE:HD12	1.92	0.40
1:A:155:ALA:HB2	1:C:163:ALA:HB2	2.01	0.40
1:D:217:VAL:HG21	1:D:236:VAL:HG21	2.02	0.40

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	238/263 (90%)	229 (96%)	9 (4%)	0	100	100
1	B	234/263 (89%)	226 (97%)	8 (3%)	0	100	100
1	C	227/263 (86%)	220 (97%)	7 (3%)	0	100	100
1	D	227/263 (86%)	219 (96%)	8 (4%)	0	100	100
All	All	926/1052 (88%)	894 (96%)	32 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	196/217 (90%)	196 (100%)	0	100	100
1	B	194/217 (89%)	194 (100%)	0	100	100
1	C	187/217 (86%)	187 (100%)	0	100	100
1	D	187/217 (86%)	187 (100%)	0	100	100
All	All	764/868 (88%)	764 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	D	42	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	240/263 (91%)	-0.21	10 (4%) 36 39	12, 18, 38, 57	0
1	B	238/263 (90%)	-0.14	11 (4%) 32 35	13, 19, 38, 58	0
1	C	231/263 (87%)	-0.29	6 (2%) 56 58	13, 19, 31, 64	0
1	D	231/263 (87%)	-0.21	7 (3%) 50 53	13, 20, 35, 59	0
All	All	940/1052 (89%)	-0.21	34 (3%) 42 45	12, 19, 36, 64	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	190	MET	6.2
1	B	1	MET	5.9
1	A	191	VAL	5.3
1	C	199	ALA	5.3
1	A	190	MET	5.3
1	B	198	HIS	5.3
1	B	191	VAL	5.0
1	D	1	MET	4.7
1	B	197	GLU	4.6
1	A	194	GLU	4.4
1	C	198	HIS	4.1
1	D	199	ALA	3.8
1	D	200	LEU	3.6
1	B	192	THR	3.4
1	C	201	LYS	3.4
1	C	200	LEU	3.1
1	A	198	HIS	3.1
1	A	201	LYS	3.1
1	A	196	LYS	3.0
1	D	201	LYS	3.0
1	B	199	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	192	THR	2.7
1	B	201	LYS	2.6
1	A	189	GLU	2.5
1	A	195	VAL	2.4
1	B	196	LYS	2.3
1	C	188	THR	2.3
1	D	202	MET	2.2
1	A	199	ALA	2.2
1	B	189	GLU	2.2
1	B	2	THR	2.1
1	D	188	THR	2.1
1	D	69	GLN	2.1
1	C	241	ILE	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 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.