



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:39 pm GMT

PDB ID : 4WL2  
Title : Structure of penicillin V acylase from *Pectobacterium atrosepticum*  
Authors : Ramasamy, S.; Avinash, V.S.; Pundle, A.V.; Suresh, C.G.  
Deposited on : 2014-10-06  
Resolution : 2.50 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 : trunk28620  
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) : trunk28620

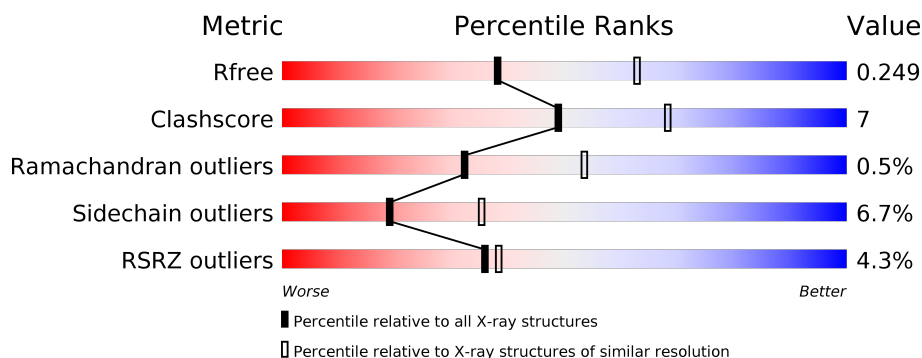
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	355	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>...</div> </div> </div>
1	B	355	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>5%</div> <div>...</div> </div> </div>
1	C	355	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>...</div> </div> </div>
1	D	355	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>...</div> </div> </div>
1	E	355	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>...</div> </div> </div>
1	F	355	<div> <div>6%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>...</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	355	<div><div></div><div>3%</div><div>85%</div><div>9%</div><div>• •</div></div>
1	H	355	<div><div></div><div>9%</div><div>82%</div><div>12%</div><div>• • •</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21734 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 exported choloylglycine hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2711	1730	462	513	6			
1	B	347	Total	C	N	O	S	0	0	0
			2711	1730	462	513	6			
1	C	347	Total	C	N	O	S	0	0	0
			2711	1730	462	513	6			
1	D	347	Total	C	N	O	S	0	0	0
			2711	1730	462	513	6			
1	E	347	Total	C	N	O	S	0	0	0
			2711	1730	462	513	6			
1	F	347	Total	C	N	O	S	0	0	0
			2711	1730	462	513	6			
1	G	347	Total	C	N	O	S	0	0	0
			2711	1730	462	513	6			
1	H	347	Total	C	N	O	S	0	0	0
			2711	1730	462	513	6			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	348	LEU	-	expression tag	UNP Q6D291
A	349	GLU	-	expression tag	UNP Q6D291
A	350	HIS	-	expression tag	UNP Q6D291
A	351	HIS	-	expression tag	UNP Q6D291
A	352	HIS	-	expression tag	UNP Q6D291
A	353	HIS	-	expression tag	UNP Q6D291
A	354	HIS	-	expression tag	UNP Q6D291
A	355	HIS	-	expression tag	UNP Q6D291
B	348	LEU	-	expression tag	UNP Q6D291
B	349	GLU	-	expression tag	UNP Q6D291
B	350	HIS	-	expression tag	UNP Q6D291
B	351	HIS	-	expression tag	UNP Q6D291
B	352	HIS	-	expression tag	UNP Q6D291

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Chain	Residue	Modelled	Actual	Comment	Reference
B	353	HIS	-	expression tag	UNP Q6D291
B	354	HIS	-	expression tag	UNP Q6D291
B	355	HIS	-	expression tag	UNP Q6D291
C	348	LEU	-	expression tag	UNP Q6D291
C	349	GLU	-	expression tag	UNP Q6D291
C	350	HIS	-	expression tag	UNP Q6D291
C	351	HIS	-	expression tag	UNP Q6D291
C	352	HIS	-	expression tag	UNP Q6D291
C	353	HIS	-	expression tag	UNP Q6D291
C	354	HIS	-	expression tag	UNP Q6D291
C	355	HIS	-	expression tag	UNP Q6D291
D	348	LEU	-	expression tag	UNP Q6D291
D	349	GLU	-	expression tag	UNP Q6D291
D	350	HIS	-	expression tag	UNP Q6D291
D	351	HIS	-	expression tag	UNP Q6D291
D	352	HIS	-	expression tag	UNP Q6D291
D	353	HIS	-	expression tag	UNP Q6D291
D	354	HIS	-	expression tag	UNP Q6D291
D	355	HIS	-	expression tag	UNP Q6D291
E	348	LEU	-	expression tag	UNP Q6D291
E	349	GLU	-	expression tag	UNP Q6D291
E	350	HIS	-	expression tag	UNP Q6D291
E	351	HIS	-	expression tag	UNP Q6D291
E	352	HIS	-	expression tag	UNP Q6D291
E	353	HIS	-	expression tag	UNP Q6D291
E	354	HIS	-	expression tag	UNP Q6D291
E	355	HIS	-	expression tag	UNP Q6D291
F	348	LEU	-	expression tag	UNP Q6D291
F	349	GLU	-	expression tag	UNP Q6D291
F	350	HIS	-	expression tag	UNP Q6D291
F	351	HIS	-	expression tag	UNP Q6D291
F	352	HIS	-	expression tag	UNP Q6D291
F	353	HIS	-	expression tag	UNP Q6D291
F	354	HIS	-	expression tag	UNP Q6D291
F	355	HIS	-	expression tag	UNP Q6D291
G	348	LEU	-	expression tag	UNP Q6D291
G	349	GLU	-	expression tag	UNP Q6D291
G	350	HIS	-	expression tag	UNP Q6D291
G	351	HIS	-	expression tag	UNP Q6D291
G	352	HIS	-	expression tag	UNP Q6D291
G	353	HIS	-	expression tag	UNP Q6D291
G	354	HIS	-	expression tag	UNP Q6D291

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Chain	Residue	Modelled	Actual	Comment	Reference
G	355	HIS	-	expression tag	UNP Q6D291
H	348	LEU	-	expression tag	UNP Q6D291
H	349	GLU	-	expression tag	UNP Q6D291
H	350	HIS	-	expression tag	UNP Q6D291
H	351	HIS	-	expression tag	UNP Q6D291
H	352	HIS	-	expression tag	UNP Q6D291
H	353	HIS	-	expression tag	UNP Q6D291
H	354	HIS	-	expression tag	UNP Q6D291
H	355	HIS	-	expression tag	UNP Q6D291

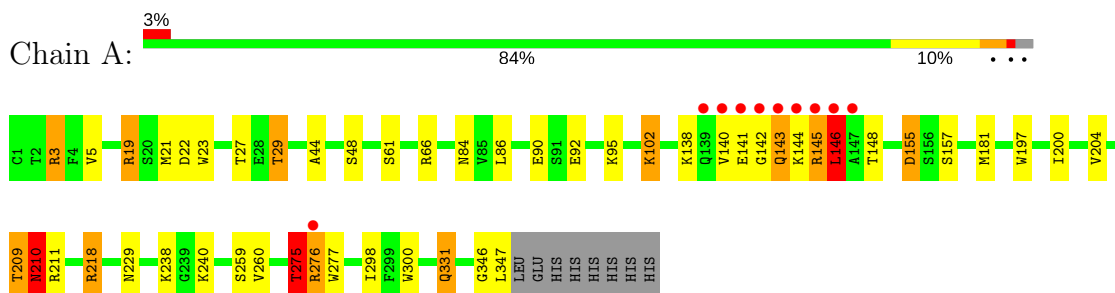
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	11	Total O 11 11	0	0
2	B	3	Total O 3 3	0	0
2	C	5	Total O 5 5	0	0
2	D	7	Total O 7 7	0	0
2	E	5	Total O 5 5	0	0
2	F	2	Total O 2 2	0	0
2	G	9	Total O 9 9	0	0
2	H	4	Total O 4 4	0	0

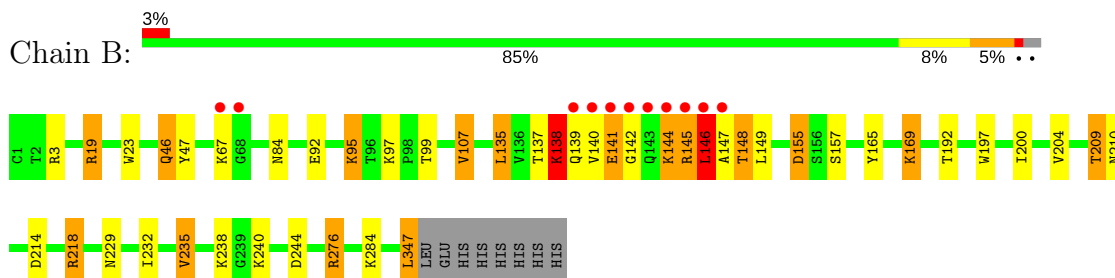
### 3 Residue-property plots

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.

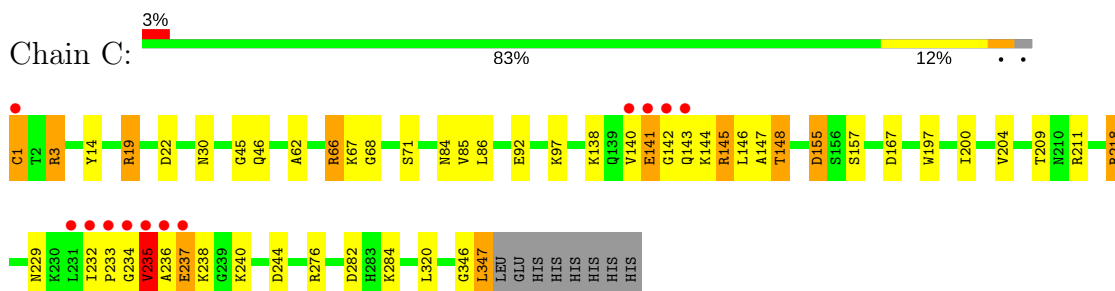
#### • Molecule 1: Putative exported choloylglycine hydrolase



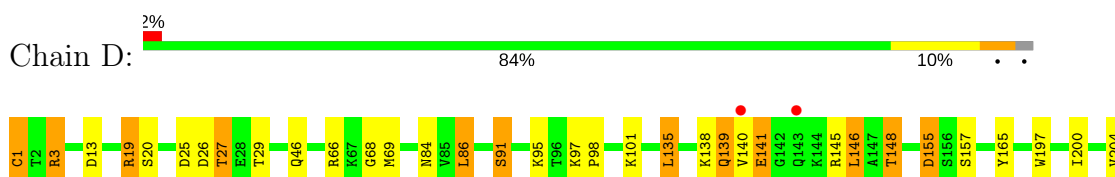
#### • Molecule 1: Putative exported choloylglycine hydrolase

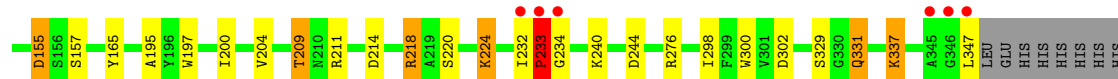


#### • Molecule 1: Putative exported choloylglycine hydrolase



#### • Molecule 1: Putative exported choloylglycine hydrolase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.45Å 150.21Å 185.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.43 – 2.50 63.43 – 2.50	Depositor EDS
% Data completeness (in resolution range)	88.0 (63.43-2.50) 88.0 (63.43-2.50)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.218 , 0.248 0.221 , 0.249	Depositor DCC
$R_{free}$ test set	5077 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.2	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 33.7	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	21734	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% 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

### 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	0.68	0/2781	0.92	17/3779 (0.4%)
1	B	0.66	0/2781	0.83	7/3779 (0.2%)
1	C	0.73	2/2781 (0.1%)	0.86	10/3779 (0.3%)
1	D	0.67	1/2781 (0.0%)	0.86	10/3779 (0.3%)
1	E	0.70	2/2781 (0.1%)	0.89	10/3779 (0.3%)
1	F	0.65	1/2781 (0.0%)	0.84	9/3779 (0.2%)
1	G	0.62	0/2781	0.82	4/3779 (0.1%)
1	H	0.74	3/2781 (0.1%)	0.90	12/3779 (0.3%)
All	All	0.68	9/22248 (0.0%)	0.87	79/30232 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	1
1	F	0	2
1	H	0	2
All	All	0	10

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	233	PRO	CA-C	10.92	1.74	1.52
1	C	235	VAL	N-CA	10.70	1.67	1.46
1	H	233	PRO	N-CA	8.77	1.62	1.47
1	E	234	GLY	N-CA	6.78	1.56	1.46
1	E	184	SER	CA-CB	-6.53	1.43	1.52

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	ARG	NE-CZ-NH2	17.32	128.96	120.30
1	E	184	SER	C-N-CD	11.51	152.56	128.40
1	G	150	HIS	CB-CA-C	-11.24	87.91	110.40
1	F	184	SER	C-N-CD	10.76	150.99	128.40
1	D	276	ARG	NE-CZ-NH1	8.69	124.64	120.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	346	GLY	Peptide
1	B	137	THR	Peptide
1	C	346	GLY	Peptide
1	D	1	CYS	Peptide
1	D	139	GLN	Peptide

## 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	2711	0	2660	72	0
1	B	2711	0	2660	43	0
1	C	2711	0	2660	30	18
1	D	2711	0	2658	44	18
1	E	2711	0	2660	27	13
1	F	2711	0	2659	22	0
1	G	2711	0	2660	27	0
1	H	2711	0	2660	39	13
2	A	11	0	0	2	0
2	B	3	0	0	0	0
2	C	5	0	0	2	0
2	D	7	0	0	4	0
2	E	5	0	0	0	0
2	F	2	0	0	0	0
2	G	9	0	0	1	0
2	H	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	21734	0	21277	291	31

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 291 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:235:VAL:N	1:C:235:VAL:CA	1.67	1.56
1:H:233:PRO:CA	1:H:233:PRO:C	1.74	1.54
1:D:68:GLY:O	1:D:138:LYS:NZ	1.57	1.34
1:A:3:ARG:NH1	1:A:181:MET:SD	2.03	1.31
1:B:209:THR:HG22	1:B:214:ASP:OD2	1.21	1.28

The worst 5 of 31 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:VAL:N	1:D:234:GLY:C[4_555]	0.89	1.31
1:C:235:VAL:N	1:D:234:GLY:CA[4_555]	1.01	1.19
1:C:234:GLY:O	1:D:234:GLY:O[4_555]	1.05	1.15
1:E:233:PRO:C	1:H:233:PRO:N[4_455]	1.06	1.14
1:E:233:PRO:O	1:H:233:PRO:N[4_455]	1.13	1.07

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	345/355 (97%)	334 (97%)	8 (2%)	3 (1%)	20	36
1	B	345/355 (97%)	336 (97%)	7 (2%)	2 (1%)	28	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	345/355 (97%)	338 (98%)	6 (2%)	1 (0%)	44	66
1	D	345/355 (97%)	338 (98%)	7 (2%)	0	100	100
1	E	345/355 (97%)	337 (98%)	6 (2%)	2 (1%)	28	48
1	F	345/355 (97%)	336 (97%)	7 (2%)	2 (1%)	28	48
1	G	345/355 (97%)	337 (98%)	7 (2%)	1 (0%)	44	66
1	H	345/355 (97%)	332 (96%)	11 (3%)	2 (1%)	28	48
All	All	2760/2840 (97%)	2688 (97%)	59 (2%)	13 (0%)	32	53

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	147	ALA
1	H	138	LYS
1	H	44	ALA
1	A	143	GLN
1	A	210	ASN

### 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	289/297 (97%)	272 (94%)	17 (6%)	23	42
1	B	289/297 (97%)	268 (93%)	21 (7%)	16	31
1	C	289/297 (97%)	272 (94%)	17 (6%)	23	42
1	D	289/297 (97%)	270 (93%)	19 (7%)	19	36
1	E	289/297 (97%)	264 (91%)	25 (9%)	12	23
1	F	289/297 (97%)	270 (93%)	19 (7%)	19	36
1	G	289/297 (97%)	271 (94%)	18 (6%)	21	39
1	H	289/297 (97%)	271 (94%)	18 (6%)	21	39
All	All	2312/2376 (97%)	2158 (93%)	154 (7%)	19	35

5 of 154 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	148	THR
1	E	135	LEU
1	H	95	LYS
1	D	276	ARG
1	E	66	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	D	139	GLN
1	E	340	GLN
1	H	36	GLN
1	C	179	GLN
1	G	36	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 ⓘ

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	347/355 (97%)	0.16	10 (2%) 52 55	19, 34, 75, 172	0
1	B	347/355 (97%)	0.21	11 (3%) 48 51	18, 36, 77, 175	0
1	C	347/355 (97%)	0.06	12 (3%) 44 47	20, 34, 73, 201	0
1	D	347/355 (97%)	0.01	6 (1%) 70 72	18, 33, 69, 128	0
1	E	347/355 (97%)	0.19	16 (4%) 33 35	18, 34, 81, 182	0
1	F	347/355 (97%)	0.31	20 (5%) 24 24	20, 39, 83, 163	0
1	G	347/355 (97%)	0.20	12 (3%) 44 47	21, 39, 75, 199	0
1	H	347/355 (97%)	0.48	33 (9%) 9 8	21, 41, 86, 149	0
All	All	2776/2840 (97%)	0.20	120 (4%) 36 38	18, 36, 80, 201	0

The worst 5 of 120 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	143	GLN	14.9
1	G	144	LYS	13.8
1	A	140	VAL	13.6
1	E	140	VAL	13.5
1	H	143	GLN	13.5

### 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.