



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 01:59 PM UTC

PDB ID : 3DDM / pdb\_00003ddm  
Title : CRYSTAL STRUCTURE OF MANDELATE RACEMASE/MUCONATE  
LACTONIZING ENZYME FROM *Bordetella bronchiseptica* RB50  
Authors : Fedorov, A.A.; Fedorov, E.V.; Toro, R.; Gerlt, J.A.; Burley, S.K.; Almo, S.C.;  
New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2008-06-05  
Resolution : 2.60 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

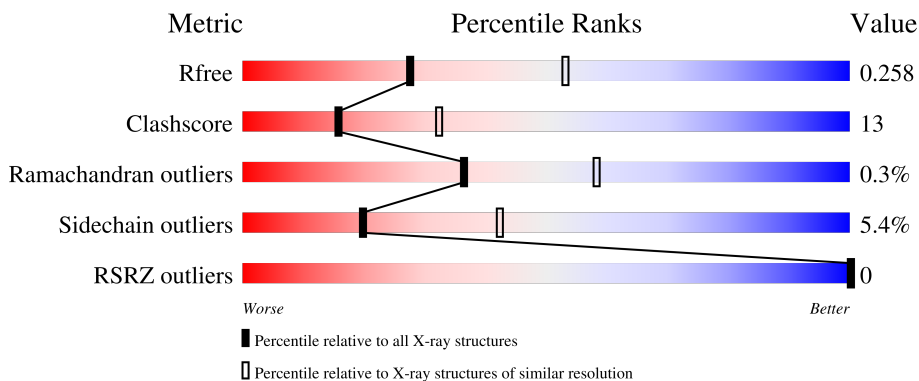
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 of 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	392	
1	B	392	
1	C	392	
1	D	392	

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 10762 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 mandelate racemase/muconate lactonizing enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	363	2672	1687	494	481	10	0	0	0
1	B	363	2672	1687	494	481	10	0	0	0
1	C	363	2672	1687	494	481	10	0	0	0
1	D	363	2672	1687	494	481	10	0	0	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q7WJN4
A	2	SER	-	expression tag	UNP Q7WJN4
A	3	LEU	-	expression tag	UNP Q7WJN4
A	336	GLY	GLU	engineered mutation	UNP Q7WJN4
A	374	LEU	-	expression tag	UNP Q7WJN4
A	375	ALA	-	expression tag	UNP Q7WJN4
A	376	ALA	-	expression tag	UNP Q7WJN4
A	377	LEU	-	expression tag	UNP Q7WJN4
A	378	ARG	-	expression tag	UNP Q7WJN4
A	379	ALA	-	expression tag	UNP Q7WJN4
A	380	ALA	-	expression tag	UNP Q7WJN4
A	381	CYS	-	expression tag	UNP Q7WJN4
A	382	ALA	-	expression tag	UNP Q7WJN4
A	383	ALA	-	expression tag	UNP Q7WJN4
A	384	ARG	-	expression tag	UNP Q7WJN4
A	385	GLU	-	expression tag	UNP Q7WJN4
A	386	GLY	-	expression tag	UNP Q7WJN4
A	387	HIS	-	expression tag	UNP Q7WJN4
A	388	HIS	-	expression tag	UNP Q7WJN4
A	389	HIS	-	expression tag	UNP Q7WJN4
A	390	HIS	-	expression tag	UNP Q7WJN4

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	391	HIS	-	expression tag	UNP Q7WJN4
A	392	HIS	-	expression tag	UNP Q7WJN4
B	1	MET	-	expression tag	UNP Q7WJN4
B	2	SER	-	expression tag	UNP Q7WJN4
B	3	LEU	-	expression tag	UNP Q7WJN4
B	336	GLY	GLU	engineered mutation	UNP Q7WJN4
B	374	LEU	-	expression tag	UNP Q7WJN4
B	375	ALA	-	expression tag	UNP Q7WJN4
B	376	ALA	-	expression tag	UNP Q7WJN4
B	377	LEU	-	expression tag	UNP Q7WJN4
B	378	ARG	-	expression tag	UNP Q7WJN4
B	379	ALA	-	expression tag	UNP Q7WJN4
B	380	ALA	-	expression tag	UNP Q7WJN4
B	381	CYS	-	expression tag	UNP Q7WJN4
B	382	ALA	-	expression tag	UNP Q7WJN4
B	383	ALA	-	expression tag	UNP Q7WJN4
B	384	ARG	-	expression tag	UNP Q7WJN4
B	385	GLU	-	expression tag	UNP Q7WJN4
B	386	GLY	-	expression tag	UNP Q7WJN4
B	387	HIS	-	expression tag	UNP Q7WJN4
B	388	HIS	-	expression tag	UNP Q7WJN4
B	389	HIS	-	expression tag	UNP Q7WJN4
B	390	HIS	-	expression tag	UNP Q7WJN4
B	391	HIS	-	expression tag	UNP Q7WJN4
B	392	HIS	-	expression tag	UNP Q7WJN4
C	1	MET	-	expression tag	UNP Q7WJN4
C	2	SER	-	expression tag	UNP Q7WJN4
C	3	LEU	-	expression tag	UNP Q7WJN4
C	336	GLY	GLU	engineered mutation	UNP Q7WJN4
C	374	LEU	-	expression tag	UNP Q7WJN4
C	375	ALA	-	expression tag	UNP Q7WJN4
C	376	ALA	-	expression tag	UNP Q7WJN4
C	377	LEU	-	expression tag	UNP Q7WJN4
C	378	ARG	-	expression tag	UNP Q7WJN4
C	379	ALA	-	expression tag	UNP Q7WJN4
C	380	ALA	-	expression tag	UNP Q7WJN4
C	381	CYS	-	expression tag	UNP Q7WJN4
C	382	ALA	-	expression tag	UNP Q7WJN4
C	383	ALA	-	expression tag	UNP Q7WJN4
C	384	ARG	-	expression tag	UNP Q7WJN4
C	385	GLU	-	expression tag	UNP Q7WJN4
C	386	GLY	-	expression tag	UNP Q7WJN4

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	387	HIS	-	expression tag	UNP Q7WJN4
C	388	HIS	-	expression tag	UNP Q7WJN4
C	389	HIS	-	expression tag	UNP Q7WJN4
C	390	HIS	-	expression tag	UNP Q7WJN4
C	391	HIS	-	expression tag	UNP Q7WJN4
C	392	HIS	-	expression tag	UNP Q7WJN4
D	1	MET	-	expression tag	UNP Q7WJN4
D	2	SER	-	expression tag	UNP Q7WJN4
D	3	LEU	-	expression tag	UNP Q7WJN4
D	336	GLY	GLU	engineered mutation	UNP Q7WJN4
D	374	LEU	-	expression tag	UNP Q7WJN4
D	375	ALA	-	expression tag	UNP Q7WJN4
D	376	ALA	-	expression tag	UNP Q7WJN4
D	377	LEU	-	expression tag	UNP Q7WJN4
D	378	ARG	-	expression tag	UNP Q7WJN4
D	379	ALA	-	expression tag	UNP Q7WJN4
D	380	ALA	-	expression tag	UNP Q7WJN4
D	381	CYS	-	expression tag	UNP Q7WJN4
D	382	ALA	-	expression tag	UNP Q7WJN4
D	383	ALA	-	expression tag	UNP Q7WJN4
D	384	ARG	-	expression tag	UNP Q7WJN4
D	385	GLU	-	expression tag	UNP Q7WJN4
D	386	GLY	-	expression tag	UNP Q7WJN4
D	387	HIS	-	expression tag	UNP Q7WJN4
D	388	HIS	-	expression tag	UNP Q7WJN4
D	389	HIS	-	expression tag	UNP Q7WJN4
D	390	HIS	-	expression tag	UNP Q7WJN4
D	391	HIS	-	expression tag	UNP Q7WJN4
D	392	HIS	-	expression tag	UNP Q7WJN4

- Molecule 2 is water.

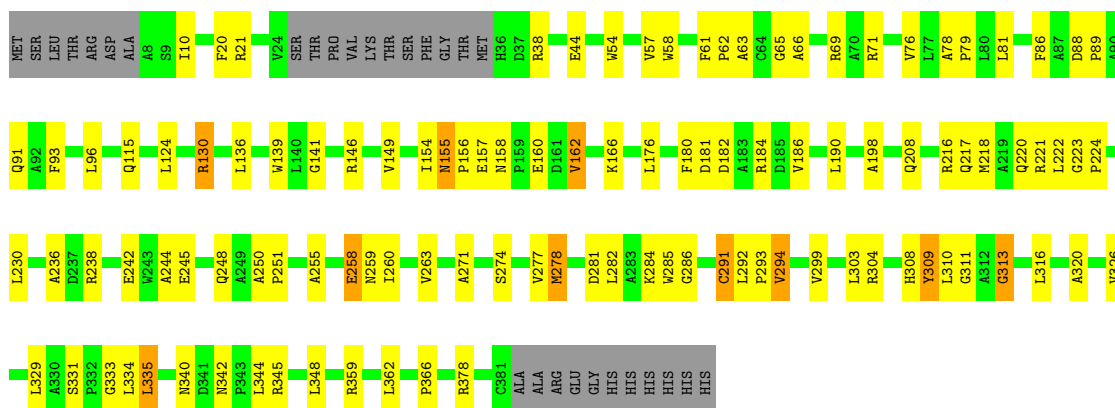
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	20	Total O 20 20	0	0
2	B	23	Total O 23 23	0	0
2	C	18	Total O 18 18	0	0
2	D	13	Total O 13 13	0	0

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

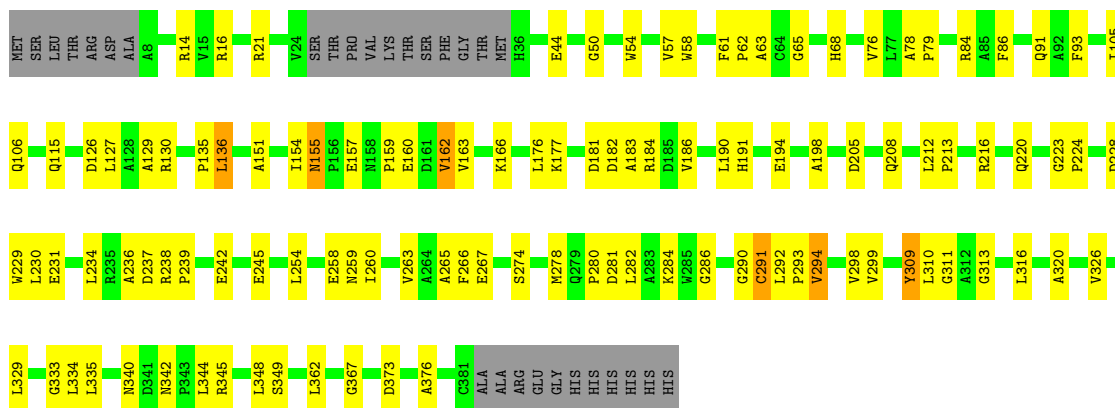
- Molecule 1: Putative mandelate racemase/muconate lactonizing enzyme

Chain A: 



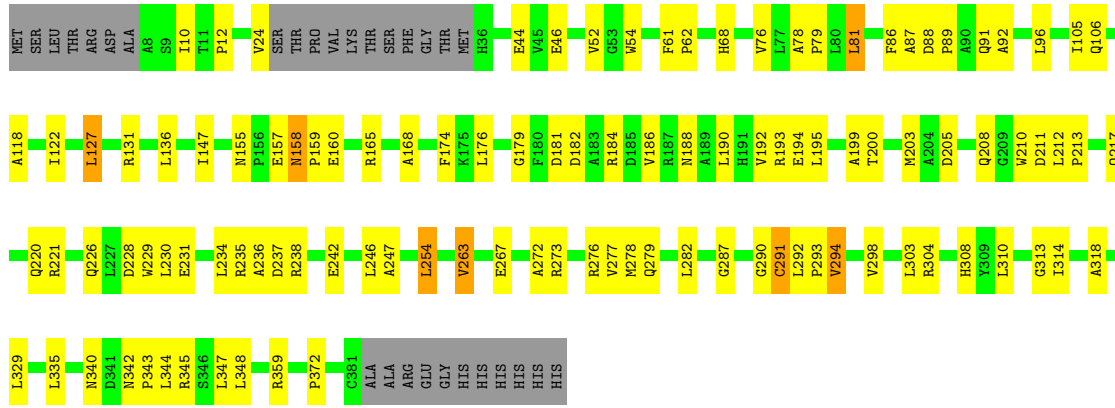
- Molecule 1: Putative mandelate racemase/muconate lactonizing enzyme

Chain B: 

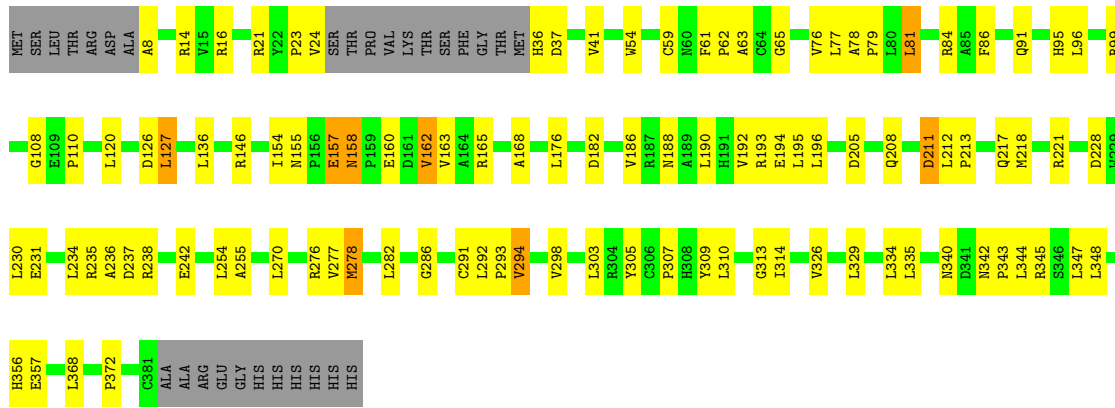


- Molecule 1: Putative mandelate racemase/muconate lactonizing enzyme

Chain C: 



● Molecule 1: Putative mandelate racemase/muconate lactonizing enzyme



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.60Å 122.64Å 164.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.58 – 2.60 24.58 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (24.58-2.60) 99.9 (24.58-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 2.39Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.224 , 0.258 0.224 , 0.258	Depositor DCC
$R_{free}$ test set	4732 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.8	Xtrriage
Anisotropy	0.210	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 24.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.480 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10762	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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	0.45	0/2734	0.99	14/3735 (0.4%)
1	B	0.46	0/2734	0.99	13/3735 (0.3%)
1	C	0.45	0/2734	0.92	6/3735 (0.2%)
1	D	0.46	0/2734	0.94	11/3735 (0.3%)
All	All	0.46	0/10936	0.96	44/14940 (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	D	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	155	ASN	CA-C-N	8.94	128.68	119.56
1	D	155	ASN	C-N-CA	8.94	128.68	119.56
1	B	326	VAL	CA-C-N	8.63	128.22	119.24
1	B	326	VAL	C-N-CA	8.63	128.22	119.24
1	A	155	ASN	CA-C-N	8.40	128.05	119.56

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	309	TYR	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	B	309	TYR	Sidechain
1	D	309	TYR	Sidechain

## 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	2672	0	2665	71	0
1	B	2672	0	2665	78	0
1	C	2672	0	2665	84	0
1	D	2672	0	2665	64	0
2	A	20	0	0	1	0
2	B	23	0	0	3	0
2	C	18	0	0	1	0
2	D	13	0	0	0	0
All	All	10762	0	10660	284	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 13.

The worst 5 of 284 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:208:GLN:HE21	1:C:236:ALA:H	1.07	0.95
1:D:208:GLN:HE21	1:D:236:ALA:H	1.13	0.95
1:B:208:GLN:HE21	1:B:236:ALA:H	1.15	0.94
1:A:208:GLN:HE21	1:A:236:ALA:H	1.11	0.94
1:B:14:ARG:HH21	1:B:16:ARG:HH11	1.23	0.84

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	359/392 (92%)	342 (95%)	16 (4%)	1 (0%)	36	58
1	B	359/392 (92%)	342 (95%)	16 (4%)	1 (0%)	36	58
1	C	359/392 (92%)	336 (94%)	22 (6%)	1 (0%)	36	58
1	D	359/392 (92%)	339 (94%)	18 (5%)	2 (1%)	21	42
All	All	1436/1568 (92%)	1359 (95%)	72 (5%)	5 (0%)	36	58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	157	GLU
1	D	157	GLU
1	A	198	ALA
1	B	198	ALA
1	D	286	GLY

### 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	254/278 (91%)	241 (95%)	13 (5%)	21	45
1	B	254/278 (91%)	243 (96%)	11 (4%)	26	51
1	C	254/278 (91%)	240 (94%)	14 (6%)	19	41
1	D	254/278 (91%)	237 (93%)	17 (7%)	15	33
All	All	1016/1112 (91%)	961 (95%)	55 (5%)	20	42

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	158	ASN
1	C	294	VAL
1	D	335	LEU
1	D	278	MET
1	C	220	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	91	GLN
1	D	208	GLN
1	D	342	ASN
1	B	191	HIS
1	B	158	ASN

### 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 oligosaccharides 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 [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	363/392 (92%)	-1.52	0 100 100	31, 46, 68, 78	0
1	B	363/392 (92%)	-1.52	0 100 100	32, 46, 68, 79	0
1	C	363/392 (92%)	-1.52	0 100 100	30, 46, 73, 84	0
1	D	363/392 (92%)	-1.51	0 100 100	29, 47, 73, 85	0
All	All	1452/1568 (92%)	-1.52	0 100 100	29, 46, 70, 85	0

There are no RSRZ outliers to report.

### 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 oligosaccharides 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.