



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:20 PM GMT

PDB ID : 4C5U  
Title : Structural Investigations into the Stereochemistry and Activity of a Phenylalanine-2,3-Aminomutase from *Taxus chinensis*  
Authors : Wybenga, G.G.; Szymanski, W.; Wu, B.; Feringa, B.L.; Janssen, D.B.; Dijkstra, B.W.  
Deposited on : 2013-09-16  
Resolution : 2.19 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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

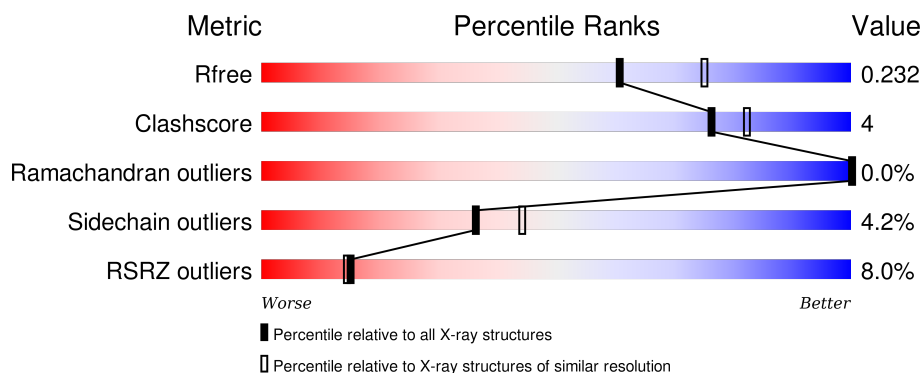
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	707	<div> <div>7%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>9%</div> </div> </div>
1	B	707	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>9%</div> <div>10%</div> </div> </div>
1	C	707	<div> <div>8%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>10%</div> </div> </div>
1	D	707	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>11%</div> <div>10%</div> </div> </div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 19779 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 PHENYLALANINE AMMONIA-LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	641	Total	C	N	O	S	0	0	0
			4962	3147	855	937	23			
1	B	636	Total	C	N	O	S	0	0	0
			4922	3120	847	932	23			
1	C	639	Total	C	N	O	S	0	0	0
			4941	3133	853	932	23			
1	D	636	Total	C	N	O	S	0	0	0
			4917	3121	848	925	23			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q68G84
A	-18	GLY	-	EXPRESSION TAG	UNP Q68G84
A	-17	SER	-	EXPRESSION TAG	UNP Q68G84
A	-16	SER	-	EXPRESSION TAG	UNP Q68G84
A	-15	HIS	-	EXPRESSION TAG	UNP Q68G84
A	-14	HIS	-	EXPRESSION TAG	UNP Q68G84
A	-13	HIS	-	EXPRESSION TAG	UNP Q68G84
A	-12	HIS	-	EXPRESSION TAG	UNP Q68G84
A	-11	HIS	-	EXPRESSION TAG	UNP Q68G84
A	-10	HIS	-	EXPRESSION TAG	UNP Q68G84
A	-9	SER	-	EXPRESSION TAG	UNP Q68G84
A	-8	SER	-	EXPRESSION TAG	UNP Q68G84
A	-7	GLY	-	EXPRESSION TAG	UNP Q68G84
A	-6	LEU	-	EXPRESSION TAG	UNP Q68G84
A	-5	VAL	-	EXPRESSION TAG	UNP Q68G84
A	-4	PRO	-	EXPRESSION TAG	UNP Q68G84
A	-3	ARG	-	EXPRESSION TAG	UNP Q68G84
A	-2	GLY	-	EXPRESSION TAG	UNP Q68G84
A	-1	SER	-	EXPRESSION TAG	UNP Q68G84
A	0	HIS	-	EXPRESSION TAG	UNP Q68G84
A	322	ALA	TYR	ENGINEERED MUTATION	UNP Q68G84

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	EXPRESSION TAG	UNP Q68G84
B	-18	GLY	-	EXPRESSION TAG	UNP Q68G84
B	-17	SER	-	EXPRESSION TAG	UNP Q68G84
B	-16	SER	-	EXPRESSION TAG	UNP Q68G84
B	-15	HIS	-	EXPRESSION TAG	UNP Q68G84
B	-14	HIS	-	EXPRESSION TAG	UNP Q68G84
B	-13	HIS	-	EXPRESSION TAG	UNP Q68G84
B	-12	HIS	-	EXPRESSION TAG	UNP Q68G84
B	-11	HIS	-	EXPRESSION TAG	UNP Q68G84
B	-10	HIS	-	EXPRESSION TAG	UNP Q68G84
B	-9	SER	-	EXPRESSION TAG	UNP Q68G84
B	-8	SER	-	EXPRESSION TAG	UNP Q68G84
B	-7	GLY	-	EXPRESSION TAG	UNP Q68G84
B	-6	LEU	-	EXPRESSION TAG	UNP Q68G84
B	-5	VAL	-	EXPRESSION TAG	UNP Q68G84
B	-4	PRO	-	EXPRESSION TAG	UNP Q68G84
B	-3	ARG	-	EXPRESSION TAG	UNP Q68G84
B	-2	GLY	-	EXPRESSION TAG	UNP Q68G84
B	-1	SER	-	EXPRESSION TAG	UNP Q68G84
B	0	HIS	-	EXPRESSION TAG	UNP Q68G84
B	322	ALA	TYR	ENGINEERED MUTATION	UNP Q68G84
C	-19	MET	-	EXPRESSION TAG	UNP Q68G84
C	-18	GLY	-	EXPRESSION TAG	UNP Q68G84
C	-17	SER	-	EXPRESSION TAG	UNP Q68G84
C	-16	SER	-	EXPRESSION TAG	UNP Q68G84
C	-15	HIS	-	EXPRESSION TAG	UNP Q68G84
C	-14	HIS	-	EXPRESSION TAG	UNP Q68G84
C	-13	HIS	-	EXPRESSION TAG	UNP Q68G84
C	-12	HIS	-	EXPRESSION TAG	UNP Q68G84
C	-11	HIS	-	EXPRESSION TAG	UNP Q68G84
C	-10	HIS	-	EXPRESSION TAG	UNP Q68G84
C	-9	SER	-	EXPRESSION TAG	UNP Q68G84
C	-8	SER	-	EXPRESSION TAG	UNP Q68G84
C	-7	GLY	-	EXPRESSION TAG	UNP Q68G84
C	-6	LEU	-	EXPRESSION TAG	UNP Q68G84
C	-5	VAL	-	EXPRESSION TAG	UNP Q68G84
C	-4	PRO	-	EXPRESSION TAG	UNP Q68G84
C	-3	ARG	-	EXPRESSION TAG	UNP Q68G84
C	-2	GLY	-	EXPRESSION TAG	UNP Q68G84
C	-1	SER	-	EXPRESSION TAG	UNP Q68G84
C	0	HIS	-	EXPRESSION TAG	UNP Q68G84
C	322	ALA	TYR	ENGINEERED MUTATION	UNP Q68G84

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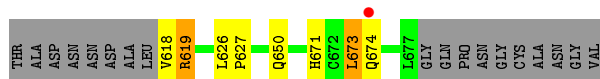
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	EXPRESSION TAG	UNP Q68G84
D	-18	GLY	-	EXPRESSION TAG	UNP Q68G84
D	-17	SER	-	EXPRESSION TAG	UNP Q68G84
D	-16	SER	-	EXPRESSION TAG	UNP Q68G84
D	-15	HIS	-	EXPRESSION TAG	UNP Q68G84
D	-14	HIS	-	EXPRESSION TAG	UNP Q68G84
D	-13	HIS	-	EXPRESSION TAG	UNP Q68G84
D	-12	HIS	-	EXPRESSION TAG	UNP Q68G84
D	-11	HIS	-	EXPRESSION TAG	UNP Q68G84
D	-10	HIS	-	EXPRESSION TAG	UNP Q68G84
D	-9	SER	-	EXPRESSION TAG	UNP Q68G84
D	-8	SER	-	EXPRESSION TAG	UNP Q68G84
D	-7	GLY	-	EXPRESSION TAG	UNP Q68G84
D	-6	LEU	-	EXPRESSION TAG	UNP Q68G84
D	-5	VAL	-	EXPRESSION TAG	UNP Q68G84
D	-4	PRO	-	EXPRESSION TAG	UNP Q68G84
D	-3	ARG	-	EXPRESSION TAG	UNP Q68G84
D	-2	GLY	-	EXPRESSION TAG	UNP Q68G84
D	-1	SER	-	EXPRESSION TAG	UNP Q68G84
D	0	HIS	-	EXPRESSION TAG	UNP Q68G84
D	322	ALA	TYR	ENGINEERED MUTATION	UNP Q68G84

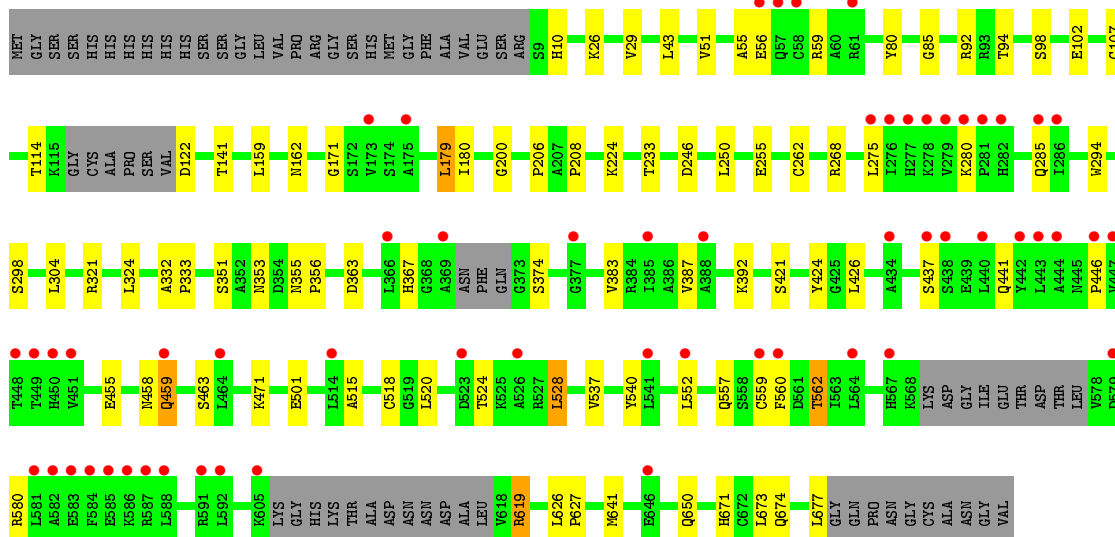
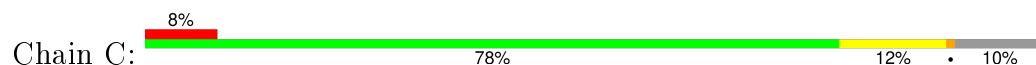
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	15	Total O 15 15	0	0
2	B	6	Total O 6 6	0	0
2	C	10	Total O 10 10	0	0
2	D	6	Total O 6 6	0	0

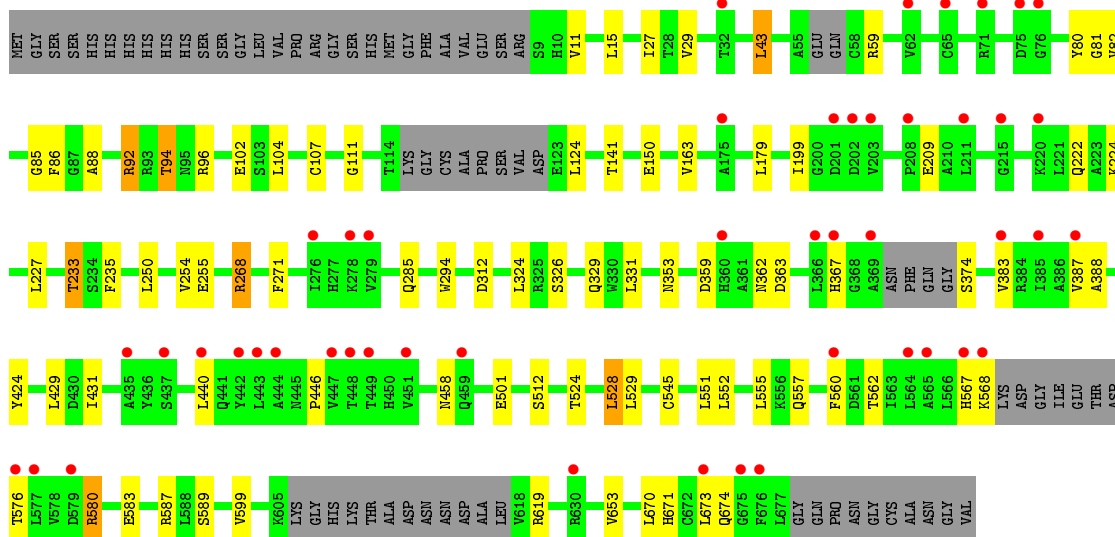
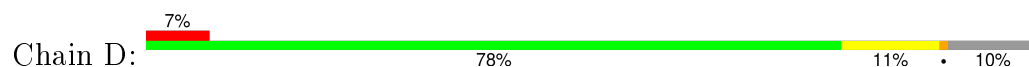




• Molecule 1: PHENYLALANINE AMMONIA-LYASE



• Molecule 1: PHENYLALANINE AMMONIA-LYASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.48Å 147.27Å 99.77Å 90.00° 99.80° 90.00°	Depositor
Resolution (Å)	48.38 – 2.19 48.38 – 2.19	Depositor EDS
% Data completeness (in resolution range)	94.3 (48.38-2.19) 98.1 (48.38-2.19)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.83 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.189 , 0.224 0.194 , 0.232	Depositor DCC
$R_{free}$ test set	7176 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.4	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 34.3	EDS
Estimated twinning fraction	0.865 for H, K, L 0.135 for L, -K, H 0.000 for l,-k,h	Xtriage
Reported twinning fraction	0.865 for H, K, L 0.135 for L, -K, H	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	1 of 141777 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19779	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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 ⓘ

### 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	0.57	1/5045 (0.0%)	0.69	1/6843 (0.0%)
1	B	0.54	2/5002 (0.0%)	0.65	1/6782 (0.0%)
1	C	0.55	1/5024 (0.0%)	0.67	1/6813 (0.0%)
1	D	0.55	1/4999 (0.0%)	0.68	0/6780
All	All	0.56	5/20070 (0.0%)	0.67	3/27218 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	294	TRP	CD2-CE2	5.71	1.48	1.41
1	B	68	TRP	CD2-CE2	5.47	1.48	1.41
1	B	294	TRP	CD2-CE2	5.26	1.47	1.41
1	A	68	TRP	CD2-CE2	5.07	1.47	1.41
1	D	294	TRP	CD2-CE2	5.06	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	619	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	619	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	C	321	ARG	NE-CZ-NH2	-5.37	117.62	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts ⓘ

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	4962	0	5044	50	0
1	B	4922	0	4993	40	0
1	C	4941	0	5021	45	0
1	D	4917	0	5004	40	0
2	A	15	0	0	0	0
2	B	6	0	0	0	0
2	C	10	0	0	0	0
2	D	6	0	0	0	0
All	All	19779	0	20062	151	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 151 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:29:VAL:HG12	1:A:141:THR:HG21	1.58	0.85
1:D:580:ARG:HH11	1:D:580:ARG:CG	2.01	0.74
1:A:80:TYR:HB3	1:A:367:HIS:HD2	1.52	0.73
1:B:671:HIS:O	1:B:674:GLN:HG2	1.89	0.72
1:D:29:VAL:HG12	1:D:141:THR:HG21	1.71	0.71

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	631/707 (89%)	616 (98%)	14 (2%)	1 (0%)	52	59
1	B	622/707 (88%)	603 (97%)	19 (3%)	0	100	100
1	C	629/707 (89%)	609 (97%)	20 (3%)	0	100	100
1	D	624/707 (88%)	610 (98%)	14 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2506/2828 (89%)	2438 (97%)	67 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	ALA

### 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	543/592 (92%)	516 (95%)	27 (5%)	30	35
1	B	538/592 (91%)	522 (97%)	16 (3%)	48	60
1	C	539/592 (91%)	516 (96%)	23 (4%)	35	43
1	D	537/592 (91%)	512 (95%)	25 (5%)	32	39
All	All	2157/2368 (91%)	2066 (96%)	91 (4%)	36	44

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	618	VAL
1	C	107	CYS
1	D	562	THR
1	B	673	LEU
1	C	92	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	336	GLN
1	D	674	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	641/707 (90%)	0.54	53 (8%) 14 13	20, 37, 61, 92	0
1	B	636/707 (89%)	0.51	45 (7%) 19 18	20, 40, 66, 81	0
1	C	639/707 (90%)	0.55	58 (9%) 11 11	19, 39, 72, 93	0
1	D	636/707 (89%)	0.56	47 (7%) 17 17	20, 39, 64, 85	0
All	All	2552/2828 (90%)	0.54	203 (7%) 15 14	19, 39, 66, 93	0

The worst 5 of 203 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	276	ILE	7.3
1	C	279	VAL	7.3
1	C	275	LEU	6.6
1	B	276	ILE	5.5
1	C	369	ALA	5.5

### 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.