



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:04 AM GMT

PDB ID : 3O06  
Title : Crystal Structure of yeast pyridoxal 5-phosphate synthase Snz1  
Authors : Teng, Y.B.; Zhang, X.; Zhou, C.Z.; Hu, H.X.  
Deposited on : 2010-07-19  
Resolution : 2.35 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  
<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

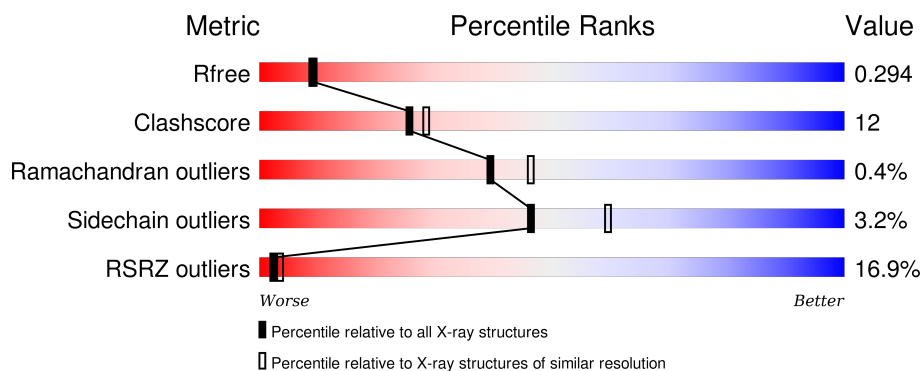
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	291	<div> <div>9%</div> <div>71%</div> <div>16%</div> <div>•</div> <div>11%</div> </div>
1	B	291	<div> <div>9%</div> <div>75%</div> <div>11%</div> <div>••</div> <div>11%</div> </div>
1	C	291	<div> <div>28%</div> <div>72%</div> <div>15%</div> <div>•</div> <div>11%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5875 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 Pyridoxine biosynthesis protein SNZ1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1933	1214	331	373	15			
1	B	258	Total	C	N	O	S	0	0	0
			1933	1214	331	373	15			
1	C	258	Total	C	N	O	S	0	0	0
			1933	1214	331	373	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	EXPRESSION TAG	UNP Q03148
A	8	HIS	-	EXPRESSION TAG	UNP Q03148
A	9	HIS	-	EXPRESSION TAG	UNP Q03148
A	10	HIS	-	EXPRESSION TAG	UNP Q03148
A	11	HIS	-	EXPRESSION TAG	UNP Q03148
A	12	HIS	-	EXPRESSION TAG	UNP Q03148
A	13	HIS	-	EXPRESSION TAG	UNP Q03148
A	14	GLY	-	EXPRESSION TAG	UNP Q03148
B	7	MET	-	EXPRESSION TAG	UNP Q03148
B	8	HIS	-	EXPRESSION TAG	UNP Q03148
B	9	HIS	-	EXPRESSION TAG	UNP Q03148
B	10	HIS	-	EXPRESSION TAG	UNP Q03148
B	11	HIS	-	EXPRESSION TAG	UNP Q03148
B	12	HIS	-	EXPRESSION TAG	UNP Q03148
B	13	HIS	-	EXPRESSION TAG	UNP Q03148
B	14	GLY	-	EXPRESSION TAG	UNP Q03148
C	7	MET	-	EXPRESSION TAG	UNP Q03148
C	8	HIS	-	EXPRESSION TAG	UNP Q03148
C	9	HIS	-	EXPRESSION TAG	UNP Q03148
C	10	HIS	-	EXPRESSION TAG	UNP Q03148
C	11	HIS	-	EXPRESSION TAG	UNP Q03148
C	12	HIS	-	EXPRESSION TAG	UNP Q03148
C	13	HIS	-	EXPRESSION TAG	UNP Q03148

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Chain	Residue	Modelled	Actual	Comment	Reference
C	14	GLY	-	EXPRESSION TAG	UNP Q03148

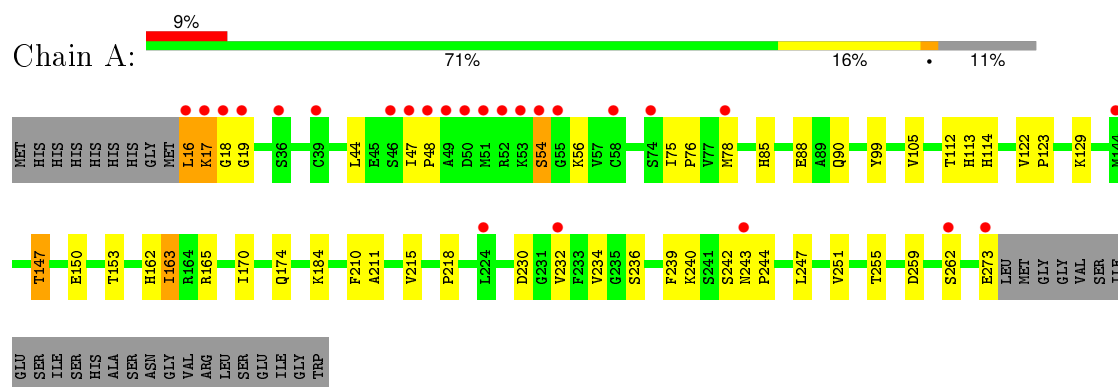
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	29	Total	O	0	0
			29	29		
2	B	20	Total	O	0	0
			20	20		
2	C	27	Total	O	0	0
			27	27		

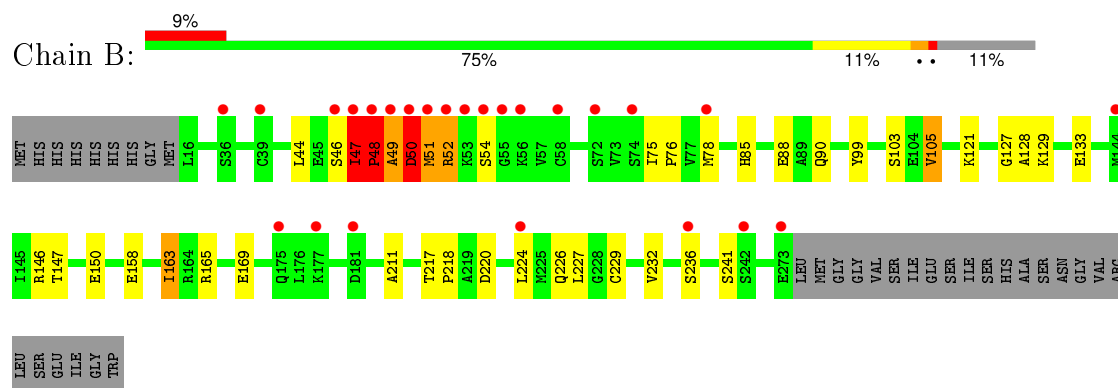
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

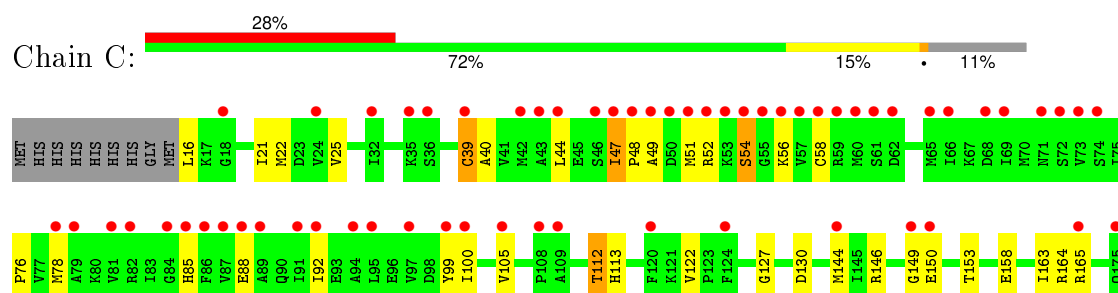
#### • Molecule 1: Pyridoxine biosynthesis protein SNZ1



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.31Å 110.38Å 156.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	110.38 – 2.35 47.14 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.5 (110.38-2.35) 99.6 (47.14-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.22 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.204 , 0.251 0.267 , 0.294	Depositor DCC
$R_{free}$ test set	2172 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.8	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 43299 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	5875	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 4.48% 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	1.05	0/1958	0.88	2/2640 (0.1%)
1	B	0.97	0/1958	0.86	3/2640 (0.1%)
1	C	1.02	3/1958 (0.2%)	0.85	0/2640
All	All	1.01	3/5874 (0.1%)	0.87	5/7920 (0.1%)

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	B	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	39	CYS	CB-SG	5.27	1.91	1.82
1	C	253	GLU	CB-CG	5.21	1.62	1.52
1	C	58	CYS	CB-SG	5.17	1.91	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	ILE	C-N-CD	-6.30	106.73	120.60
1	A	147	THR	CB-CA-C	5.82	127.30	111.60
1	A	163	ILE	CG1-CB-CG2	-5.70	98.86	111.40
1	B	163	ILE	CG1-CB-CG2	-5.44	99.43	111.40
1	B	48	PRO	C-N-CA	5.19	134.67	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	47	ILE	Mainchain,Peptide

## 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	1933	0	1989	48	0
1	B	1933	0	1989	52	0
1	C	1933	0	1989	50	0
2	A	29	0	0	1	0
2	B	20	0	0	0	0
2	C	27	0	0	0	0
All	All	5875	0	5967	147	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.

All (147) 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:47:ILE:CD1	1:C:236:SER:HB2	1.60	1.28
1:B:48:PRO:HG2	1:B:105:VAL:CG1	1.71	1.21
1:C:47:ILE:HD12	1:C:236:SER:CB	1.72	1.17
1:B:48:PRO:CG	1:B:105:VAL:HG12	1.74	1.16
1:B:211:ALA:HB3	1:B:232:VAL:HG22	1.22	1.09
1:C:47:ILE:HD12	1:C:236:SER:HB2	1.21	1.08
1:C:47:ILE:CD1	1:C:236:SER:CB	2.30	1.04
1:C:48:PRO:HG2	1:C:105:VAL:HG12	1.38	1.01
1:B:48:PRO:HG2	1:B:105:VAL:HG12	1.32	1.01
1:B:48:PRO:CG	1:B:105:VAL:CG1	2.38	0.99
1:B:47:ILE:HG21	1:B:236:SER:OG	1.64	0.97
1:C:48:PRO:HG2	1:C:105:VAL:CG1	1.96	0.94
1:A:17:LYS:H	1:A:17:LYS:HE3	1.32	0.91
1:A:16:LEU:HB3	1:A:99:TYR:OH	1.72	0.90
1:C:149:GLY:HA2	1:C:158:GLU:HB3	1.53	0.90
1:B:211:ALA:HB3	1:B:232:VAL:CG2	2.03	0.89
1:A:147:THR:HG23	1:A:162:HIS:HB2	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:PRO:HG3	1:B:105:VAL:HG12	1.56	0.86
1:A:16:LEU:N	1:A:16:LEU:HD23	1.91	0.86
1:B:48:PRO:HG2	1:B:105:VAL:HG11	1.59	0.83
1:A:242:SER:OG	1:A:273:GLU:HB3	1.78	0.82
1:B:47:ILE:CG2	1:B:236:SER:OG	2.26	0.82
1:A:19:GLY:O	1:A:255:THR:HG21	1.81	0.81
1:C:47:ILE:HD12	1:C:236:SER:OG	1.80	0.81
1:A:54:SER:HB2	1:A:56:LYS:HG2	1.64	0.80
1:B:103:SER:OG	1:B:105:VAL:HG23	1.83	0.78
1:A:211:ALA:HB3	1:A:232:VAL:HG22	1.69	0.73
1:C:47:ILE:HD11	1:C:236:SER:H	1.55	0.72
1:C:47:ILE:HD11	1:C:236:SER:CB	2.20	0.71
1:B:163:ILE:CD1	1:B:227:LEU:HB3	2.21	0.70
1:C:78:MET:HG2	1:C:99:TYR:HB2	1.72	0.69
1:B:47:ILE:O	1:B:48:PRO:C	2.30	0.68
1:A:147:THR:CG2	1:A:162:HIS:HB2	2.22	0.68
1:B:47:ILE:O	1:B:49:ALA:N	2.26	0.68
1:A:47:ILE:HD13	1:A:240:LYS:NZ	2.08	0.68
1:A:90:GLN:HE22	1:B:226:GLN:HE22	1.40	0.67
1:B:47:ILE:HG21	1:B:236:SER:CB	2.25	0.67
1:B:90:GLN:HE22	1:C:226:GLN:HE22	1.42	0.67
1:B:49:ALA:O	1:B:52:ARG:N	2.28	0.66
1:C:211:ALA:CB	1:C:224:LEU:HD13	2.26	0.65
1:C:215:VAL:HG11	1:C:232:VAL:HG11	1.79	0.65
1:A:147:THR:HG23	1:A:162:HIS:CB	2.26	0.65
1:B:163:ILE:HD11	1:B:227:LEU:HB3	1.79	0.64
1:B:49:ALA:O	1:B:51:MET:N	2.30	0.64
1:A:17:LYS:O	1:A:210:PHE:CZ	2.51	0.64
1:B:165:ARG:NE	1:B:169:GLU:OE2	2.30	0.64
1:A:47:ILE:HD13	1:A:240:LYS:HZ1	1.61	0.64
1:C:47:ILE:HD11	1:C:236:SER:HB2	1.73	0.64
1:A:17:LYS:HE3	1:A:17:LYS:N	2.10	0.64
1:C:47:ILE:CD1	1:C:236:SER:OG	2.41	0.63
1:C:150:GLU:OE2	1:C:153:THR:HG21	1.97	0.63
1:A:16:LEU:N	1:A:17:LYS:HE3	2.13	0.62
1:A:112:THR:HB	1:A:113:HIS:HD2	1.63	0.62
1:A:85:HIS:CD2	1:A:88:GLU:H	2.18	0.62
1:B:165:ARG:NH2	1:B:169:GLU:OE2	2.33	0.62
1:B:211:ALA:HB1	1:B:224:LEU:HD13	1.82	0.61
1:A:16:LEU:N	1:A:16:LEU:CD2	2.63	0.61
1:A:112:THR:HB	1:A:113:HIS:CD2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ILE:HD11	1:B:227:LEU:CB	2.31	0.60
1:A:54:SER:HB2	1:A:56:LYS:CG	2.33	0.58
1:B:44:LEU:N	1:B:44:LEU:HD23	2.19	0.58
1:C:44:LEU:HD12	1:C:44:LEU:O	2.05	0.57
1:C:48:PRO:CG	1:C:105:VAL:HG12	2.25	0.57
1:C:48:PRO:CG	1:C:105:VAL:CG1	2.78	0.57
1:C:47:ILE:HG22	1:C:49:ALA:H	1.69	0.57
1:C:211:ALA:HB1	1:C:224:LEU:HD13	1.86	0.57
1:B:163:ILE:HD11	1:B:227:LEU:HD13	1.85	0.56
1:A:170:ILE:O	1:A:174:GLN:HG3	2.06	0.56
1:B:48:PRO:CG	1:B:105:VAL:HG11	2.25	0.56
1:C:100:ILE:HD12	1:C:122:VAL:HG11	1.85	0.56
1:C:130:ASP:HB3	1:C:165:ARG:HD3	1.87	0.56
1:B:47:ILE:HG12	1:B:47:ILE:O	2.07	0.55
1:C:85:HIS:CD2	1:C:88:GLU:H	2.23	0.55
1:A:17:LYS:O	1:A:210:PHE:CE2	2.60	0.55
1:C:112:THR:HB	1:C:113:HIS:CD2	2.42	0.55
1:A:112:THR:HG22	1:A:112:THR:O	2.08	0.54
1:C:92:ILE:HG21	1:C:100:ILE:HG12	1.88	0.54
1:C:47:ILE:HD13	1:C:236:SER:HB2	1.78	0.54
1:B:165:ARG:CZ	1:B:169:GLU:OE2	2.57	0.53
1:C:48:PRO:HB2	1:C:105:VAL:HG13	1.90	0.53
1:A:85:HIS:CD2	1:A:88:GLU:HG3	2.43	0.53
1:A:48:PRO:HG2	1:A:105:VAL:HG11	1.91	0.53
1:C:51:MET:O	1:C:54:SER:N	2.42	0.53
1:A:150:GLU:OE2	1:A:153:THR:HG21	2.10	0.52
1:A:17:LYS:CE	1:A:17:LYS:H	2.13	0.52
1:B:85:HIS:CD2	1:B:88:GLU:H	2.27	0.52
1:C:21:ILE:HG12	1:C:40:ALA:HB3	1.93	0.51
1:B:78:MET:HG2	1:B:99:TYR:HB2	1.92	0.50
1:B:49:ALA:C	1:B:51:MET:N	2.64	0.50
1:A:247:LEU:O	1:A:251:VAL:HG23	2.11	0.50
1:A:17:LYS:O	1:A:210:PHE:HZ	1.94	0.50
1:C:215:VAL:HG21	1:C:232:VAL:CG1	2.42	0.50
1:A:242:SER:HG	1:A:273:GLU:HB3	1.75	0.49
1:A:16:LEU:HB3	1:A:99:TYR:HH	1.73	0.49
1:C:47:ILE:CG2	1:C:49:ALA:HB3	2.41	0.49
1:C:149:GLY:HA2	1:C:158:GLU:CB	2.33	0.49
1:C:149:GLY:CA	1:C:158:GLU:HB3	2.35	0.49
1:A:85:HIS:HD2	1:A:88:GLU:H	1.57	0.49
1:B:50:ASP:O	1:B:54:SER:OG	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:HIS:HE1	2:A:317:HOH:O	1.96	0.48
1:A:122:VAL:HG23	1:A:123:PRO:HD2	1.95	0.48
1:B:163:ILE:CD1	1:B:227:LEU:CB	2.91	0.48
1:A:215:VAL:HG11	1:A:232:VAL:HG11	1.96	0.47
1:A:47:ILE:HG12	1:A:236:SER:CB	2.45	0.47
1:B:147:THR:HG21	1:B:163:ILE:HG23	1.96	0.46
1:C:100:ILE:CD1	1:C:122:VAL:HG11	2.45	0.46
1:C:163:ILE:HG23	1:C:164:ARG:N	2.31	0.46
1:A:129:LYS:HB2	1:A:162:HIS:CD2	2.51	0.46
1:C:146:ARG:HA	1:C:210:PHE:O	2.15	0.46
1:C:238:ILE:HG21	1:C:248:ALA:HB2	1.97	0.46
1:A:85:HIS:HE1	1:B:220:ASP:OD1	1.98	0.46
1:B:44:LEU:HG	1:B:46:SER:O	2.16	0.46
1:A:150:GLU:CD	1:A:153:THR:HG21	2.35	0.46
1:A:78:MET:HG2	1:A:99:TYR:HB2	1.99	0.45
1:C:100:ILE:HD12	1:C:122:VAL:CG1	2.45	0.45
1:B:129:LYS:N	1:B:133:GLU:OE1	2.47	0.45
1:B:44:LEU:N	1:B:44:LEU:CD2	2.80	0.44
1:A:17:LYS:HB2	1:A:18:GLY:H	1.50	0.44
1:B:150:GLU:HB2	1:B:158:GLU:HG3	1.99	0.44
1:B:48:PRO:HG3	1:B:105:VAL:CG1	2.24	0.43
1:C:211:ALA:HB3	1:C:232:VAL:HG22	2.01	0.43
1:A:234:VAL:HG11	1:A:251:VAL:HG11	1.99	0.43
1:B:163:ILE:HG21	1:B:229:CYS:SG	2.58	0.43
1:A:243:ASN:HA	1:A:244:PRO:HD3	1.76	0.43
1:B:163:ILE:HD11	1:B:227:LEU:CD1	2.48	0.43
1:C:25:VAL:HG12	1:C:44:LEU:HD12	2.00	0.43
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.68	0.43
1:B:49:ALA:O	1:B:50:ASP:C	2.56	0.43
1:B:128:ALA:HA	1:B:133:GLU:OE1	2.19	0.43
1:C:22:MET:HG2	1:C:234:VAL:CG2	2.49	0.43
1:A:75:ILE:HB	1:A:76:PRO:CD	2.49	0.42
1:C:215:VAL:HG21	1:C:232:VAL:HG13	2.01	0.42
1:C:16:LEU:HD12	1:C:144:MET:HE1	2.00	0.42
1:C:39:CYS:O	1:C:76:PRO:HD2	2.20	0.42
1:B:103:SER:HG	1:B:105:VAL:HG23	1.83	0.42
1:B:75:ILE:HB	1:B:76:PRO:HD2	2.00	0.42
1:B:127:GLY:HA2	1:B:146:ARG:O	2.20	0.42
1:C:92:ILE:CG2	1:C:100:ILE:HG12	2.49	0.42
1:B:49:ALA:C	1:B:51:MET:H	2.23	0.41
1:C:92:ILE:HA	1:C:92:ILE:HD13	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:PRO:HB2	1:B:49:ALA:H	1.61	0.41
1:A:236:SER:O	1:A:239:PHE:N	2.51	0.41
1:B:217:THR:HB	1:B:218:PRO:HD2	2.02	0.41
1:C:127:GLY:HA2	1:C:146:ARG:O	2.20	0.41
1:C:47:ILE:HD11	1:C:236:SER:N	2.30	0.40
1:A:18:GLY:CA	1:A:230:ASP:O	2.70	0.40
1:B:121:LYS:HD2	1:B:121:LYS:HA	1.90	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	256/291 (88%)	243 (95%)	13 (5%)	0	100	100
1	B	256/291 (88%)	245 (96%)	8 (3%)	3 (1%)	16	15
1	C	256/291 (88%)	249 (97%)	7 (3%)	0	100	100
All	All	768/873 (88%)	737 (96%)	28 (4%)	3 (0%)	39	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	48	PRO
1	B	49	ALA
1	B	50	ASP

### 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	211/238 (89%)	202 (96%)	9 (4%)	35	45
1	B	211/238 (89%)	205 (97%)	6 (3%)	51	65
1	C	211/238 (89%)	206 (98%)	5 (2%)	57	71
All	All	633/714 (89%)	613 (97%)	20 (3%)	46	59

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	17	LYS
1	A	54	SER
1	A	163	ILE
1	A	165	ARG
1	A	184	LYS
1	A	218	PRO
1	A	259	ASP
1	A	262	SER
1	B	47	ILE
1	B	50	ASP
1	B	51	MET
1	B	52	ARG
1	B	105	VAL
1	B	241	SER
1	C	47	ILE
1	C	52	ARG
1	C	54	SER
1	C	56	LYS
1	C	112	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	113	HIS
1	A	114	HIS
1	A	226	GLN
1	B	85	HIS
1	B	113	HIS

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Mol	Chain	Res	Type
1	B	226	GLN
1	C	85	HIS
1	C	113	HIS
1	C	226	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	258/291 (88%)	0.33	25 (9%) 10 16	10, 25, 57, 99	15 (5%)
1	B	258/291 (88%)	0.49	25 (9%) 10 16	9, 27, 60, 99	15 (5%)
1	C	258/291 (88%)	1.89	81 (31%) 1 0	31, 60, 96, 123	15 (5%)
All	All	774/873 (88%)	0.90	131 (16%) 2 3	9, 35, 87, 123	45 (5%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	51	MET	16.7
1	A	51	MET	15.2
1	C	47	ILE	13.7
1	B	48	PRO	13.5
1	B	47	ILE	12.4
1	C	49	ALA	11.6
1	C	48	PRO	10.9
1	B	49	ALA	9.8
1	C	58	CYS	9.4
1	A	48	PRO	9.3
1	B	51	MET	9.2
1	C	52	ARG	8.9
1	A	47	ILE	8.4
1	C	50	ASP	8.1
1	B	54	SER	7.9
1	B	46	SER	7.7
1	C	46	SER	7.6
1	A	49	ALA	7.6
1	B	50	ASP	7.5
1	A	52	ARG	6.8
1	B	52	ARG	6.2
1	A	50	ASP	5.9
1	C	262	SER	5.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	39	CYS	5.7
1	C	55	GLY	5.6
1	C	224	LEU	5.6
1	B	39	CYS	5.5
1	C	53	LYS	5.5
1	C	78	MET	5.4
1	A	54	SER	5.3
1	A	224	LEU	5.3
1	C	36	SER	5.1
1	A	53	LYS	5.0
1	B	53	LYS	5.0
1	C	72	SER	4.9
1	A	262	SER	4.9
1	A	39	CYS	4.7
1	B	58	CYS	4.4
1	C	54	SER	4.4
1	B	78	MET	4.3
1	C	144	MET	4.3
1	B	273	GLU	4.2
1	C	87	VAL	3.8
1	C	74	SER	3.6
1	B	144	MET	3.6
1	C	18	GLY	3.6
1	C	150	GLU	3.6
1	C	240	LYS	3.6
1	A	58	CYS	3.5
1	B	242	SER	3.5
1	A	36	SER	3.5
1	C	89	ALA	3.4
1	B	72	SER	3.4
1	C	176	LEU	3.4
1	B	175	GLN	3.4
1	C	43	ALA	3.4
1	C	232	VAL	3.4
1	B	177	LYS	3.3
1	B	36	SER	3.3
1	C	109	ALA	3.3
1	B	224	LEU	3.3
1	C	193	VAL	3.3
1	A	243	ASN	3.3
1	C	57	VAL	3.3
1	C	56	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	19	GLY	3.2
1	B	55	GLY	3.2
1	A	144	MET	3.2
1	C	177	LYS	3.2
1	C	44	LEU	3.0
1	C	60	MET	3.0
1	C	85	HIS	3.0
1	A	78	MET	3.0
1	C	65	MET	3.0
1	C	97	VAL	3.0
1	C	185	VAL	3.0
1	A	46	SER	2.9
1	C	238	ILE	2.9
1	A	17	LYS	2.8
1	C	59	ARG	2.8
1	C	91	ILE	2.8
1	A	74	SER	2.8
1	C	105	VAL	2.7
1	C	92	ILE	2.7
1	B	74	SER	2.7
1	C	61	SER	2.7
1	C	94	ALA	2.7
1	A	55	GLY	2.6
1	C	62	ASP	2.6
1	C	86	PHE	2.6
1	C	79	ALA	2.5
1	C	265	LEU	2.5
1	A	273	GLU	2.5
1	A	16	LEU	2.5
1	C	217	THR	2.5
1	C	84	GLY	2.5
1	C	32	ILE	2.5
1	C	100	ILE	2.4
1	C	73	VAL	2.4
1	C	35	LYS	2.4
1	C	24	VAL	2.3
1	C	81	VAL	2.3
1	C	245	VAL	2.3
1	B	236	SER	2.3
1	C	269	SER	2.3
1	C	68	ASP	2.3
1	C	71	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	219	ALA	2.3
1	C	165	ARG	2.2
1	C	184	LYS	2.2
1	B	181	ASP	2.2
1	C	181	ASP	2.2
1	C	182	ILE	2.2
1	C	270	ASP	2.2
1	C	124	PHE	2.2
1	A	18	GLY	2.2
1	C	149	GLY	2.2
1	C	82	ARG	2.2
1	C	120	PHE	2.2
1	C	42	MET	2.2
1	C	99	TYR	2.1
1	C	108	PRO	2.1
1	C	88	GLU	2.1
1	C	189	MET	2.1
1	A	232	VAL	2.1
1	C	95	LEU	2.1
1	C	66	ILE	2.1
1	B	56	LYS	2.1
1	C	69	ILE	2.1
1	C	187	GLU	2.1
1	C	175	GLN	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.