



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 09:08 pm BST

PDB ID : 6RG0  
Title : Structure of pdxj  
Authors : Rohweder, B.; Rajendran, C.; Sterner, R.  
Deposited on : 2019-04-16  
Resolution : 3.07 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.

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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

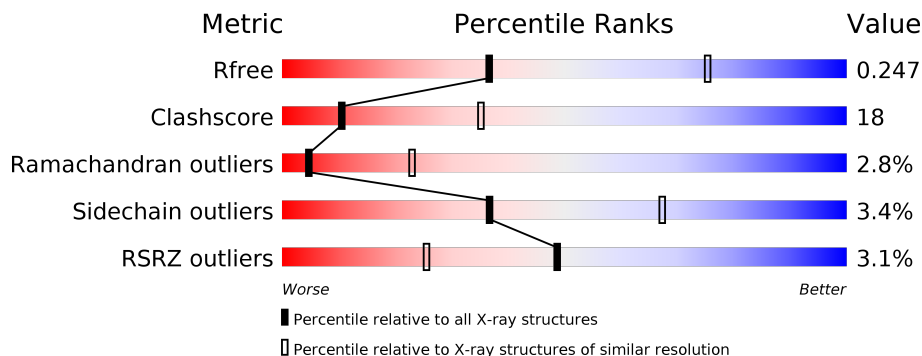
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.07 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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	268	<p>0% 64% 25% 10%</p>
1	B	268	<p>2% 57% 30% 10%</p>
1	C	268	<p>0% 65% 24% 10%</p>
1	D	268	<p>7% 52% 25% 18%</p>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6975 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 5'-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	242	1814	1129	334	340	11	0	0	0
1	B	242	1812	1128	331	342	11	0	0	0
1	C	242	1789	1115	328	335	11	0	0	0
1	D	220	1560	980	274	295	11	0	0	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P0A794
A	2	HIS	-	expression tag	UNP P0A794
A	3	HIS	-	expression tag	UNP P0A794
A	4	HIS	-	expression tag	UNP P0A794
A	5	HIS	-	expression tag	UNP P0A794
A	6	HIS	-	expression tag	UNP P0A794
A	7	HIS	-	expression tag	UNP P0A794
A	8	THR	-	expression tag	UNP P0A794
A	9	ASP	-	expression tag	UNP P0A794
A	10	PRO	-	expression tag	UNP P0A794
A	11	ALA	-	expression tag	UNP P0A794
A	12	LEU	-	expression tag	UNP P0A794
A	13	ARG	-	expression tag	UNP P0A794
A	14	ALA	-	expression tag	UNP P0A794
A	159	LYS	GLU	conflict	UNP P0A794
A	211	ARG	HIS	conflict	UNP P0A794
A	237	LEU	MET	conflict	UNP P0A794
A	242	VAL	ASP	conflict	UNP P0A794
A	257	GLY	-	expression tag	UNP P0A794
A	258	LEU	-	expression tag	UNP P0A794
A	259	GLU	-	expression tag	UNP P0A794

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Chain	Residue	Modelled	Actual	Comment	Reference
A	260	PRO	-	expression tag	UNP P0A794
A	261	LEU	-	expression tag	UNP P0A794
A	262	ARG	-	expression tag	UNP P0A794
A	263	VAL	-	expression tag	UNP P0A794
A	264	VAL	-	expression tag	UNP P0A794
A	265	SER	-	expression tag	UNP P0A794
A	266	LEU	-	expression tag	UNP P0A794
A	267	ILE	-	expression tag	UNP P0A794
A	268	SER	-	expression tag	UNP P0A794
B	1	MET	-	initiating methionine	UNP P0A794
B	2	HIS	-	expression tag	UNP P0A794
B	3	HIS	-	expression tag	UNP P0A794
B	4	HIS	-	expression tag	UNP P0A794
B	5	HIS	-	expression tag	UNP P0A794
B	6	HIS	-	expression tag	UNP P0A794
B	7	HIS	-	expression tag	UNP P0A794
B	8	THR	-	expression tag	UNP P0A794
B	9	ASP	-	expression tag	UNP P0A794
B	10	PRO	-	expression tag	UNP P0A794
B	11	ALA	-	expression tag	UNP P0A794
B	12	LEU	-	expression tag	UNP P0A794
B	13	ARG	-	expression tag	UNP P0A794
B	14	ALA	-	expression tag	UNP P0A794
B	159	LYS	GLU	conflict	UNP P0A794
B	211	ARG	HIS	conflict	UNP P0A794
B	237	LEU	MET	conflict	UNP P0A794
B	242	VAL	ASP	conflict	UNP P0A794
B	257	GLY	-	expression tag	UNP P0A794
B	258	LEU	-	expression tag	UNP P0A794
B	259	GLU	-	expression tag	UNP P0A794
B	260	PRO	-	expression tag	UNP P0A794
B	261	LEU	-	expression tag	UNP P0A794
B	262	ARG	-	expression tag	UNP P0A794
B	263	VAL	-	expression tag	UNP P0A794
B	264	VAL	-	expression tag	UNP P0A794
B	265	SER	-	expression tag	UNP P0A794
B	266	LEU	-	expression tag	UNP P0A794
B	267	ILE	-	expression tag	UNP P0A794
B	268	SER	-	expression tag	UNP P0A794
C	1	MET	-	initiating methionine	UNP P0A794
C	2	HIS	-	expression tag	UNP P0A794
C	3	HIS	-	expression tag	UNP P0A794

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	HIS	-	expression tag	UNP P0A794
C	5	HIS	-	expression tag	UNP P0A794
C	6	HIS	-	expression tag	UNP P0A794
C	7	HIS	-	expression tag	UNP P0A794
C	8	THR	-	expression tag	UNP P0A794
C	9	ASP	-	expression tag	UNP P0A794
C	10	PRO	-	expression tag	UNP P0A794
C	11	ALA	-	expression tag	UNP P0A794
C	12	LEU	-	expression tag	UNP P0A794
C	13	ARG	-	expression tag	UNP P0A794
C	14	ALA	-	expression tag	UNP P0A794
C	159	LYS	GLU	conflict	UNP P0A794
C	211	ARG	HIS	conflict	UNP P0A794
C	237	LEU	MET	conflict	UNP P0A794
C	242	VAL	ASP	conflict	UNP P0A794
C	257	GLY	-	expression tag	UNP P0A794
C	258	LEU	-	expression tag	UNP P0A794
C	259	GLU	-	expression tag	UNP P0A794
C	260	PRO	-	expression tag	UNP P0A794
C	261	LEU	-	expression tag	UNP P0A794
C	262	ARG	-	expression tag	UNP P0A794
C	263	VAL	-	expression tag	UNP P0A794
C	264	VAL	-	expression tag	UNP P0A794
C	265	SER	-	expression tag	UNP P0A794
C	266	LEU	-	expression tag	UNP P0A794
C	267	ILE	-	expression tag	UNP P0A794
C	268	SER	-	expression tag	UNP P0A794
D	1	MET	-	initiating methionine	UNP P0A794
D	2	HIS	-	expression tag	UNP P0A794
D	3	HIS	-	expression tag	UNP P0A794
D	4	HIS	-	expression tag	UNP P0A794
D	5	HIS	-	expression tag	UNP P0A794
D	6	HIS	-	expression tag	UNP P0A794
D	7	HIS	-	expression tag	UNP P0A794
D	8	THR	-	expression tag	UNP P0A794
D	9	ASP	-	expression tag	UNP P0A794
D	10	PRO	-	expression tag	UNP P0A794
D	11	ALA	-	expression tag	UNP P0A794
D	12	LEU	-	expression tag	UNP P0A794
D	13	ARG	-	expression tag	UNP P0A794
D	14	ALA	-	expression tag	UNP P0A794
D	159	LYS	GLU	conflict	UNP P0A794

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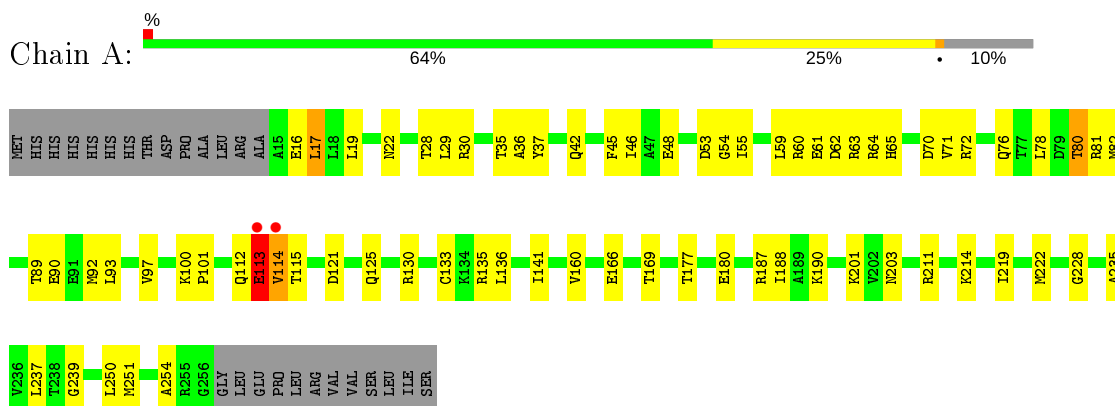
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Chain	Residue	Modelled	Actual	Comment	Reference
D	211	ARG	HIS	conflict	UNP P0A794
D	237	LEU	MET	conflict	UNP P0A794
D	242	VAL	ASP	conflict	UNP P0A794
D	257	GLY	-	expression tag	UNP P0A794
D	258	LEU	-	expression tag	UNP P0A794
D	259	GLU	-	expression tag	UNP P0A794
D	260	PRO	-	expression tag	UNP P0A794
D	261	LEU	-	expression tag	UNP P0A794
D	262	ARG	-	expression tag	UNP P0A794
D	263	VAL	-	expression tag	UNP P0A794
D	264	VAL	-	expression tag	UNP P0A794
D	265	SER	-	expression tag	UNP P0A794
D	266	LEU	-	expression tag	UNP P0A794
D	267	ILE	-	expression tag	UNP P0A794
D	268	SER	-	expression tag	UNP P0A794

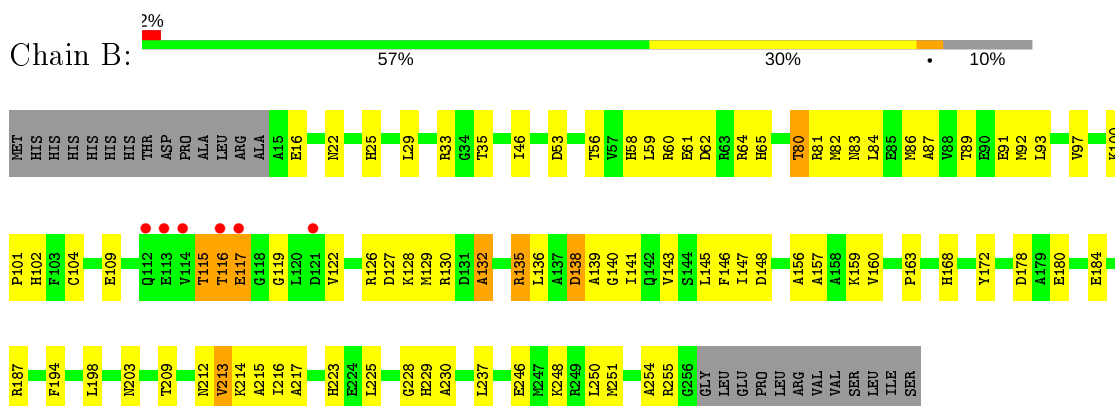
### 3 Residue-property plots [i](#)

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.

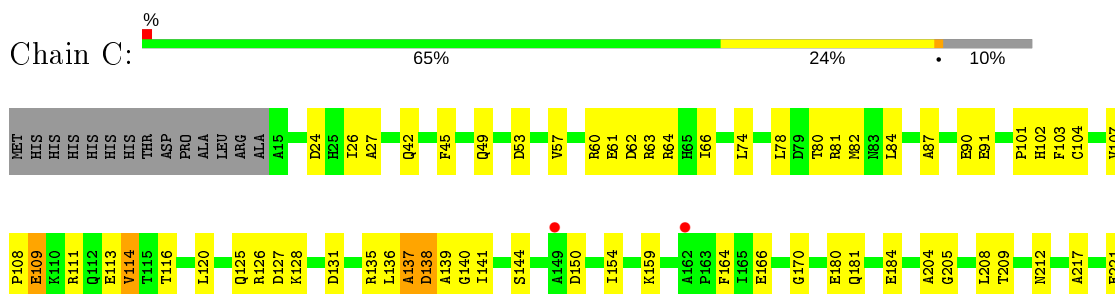
- Molecule 1: Pyridoxine 5'-phosphate synthase



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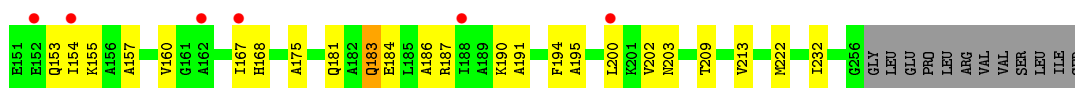
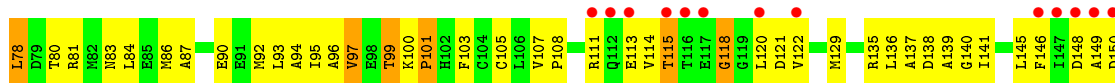
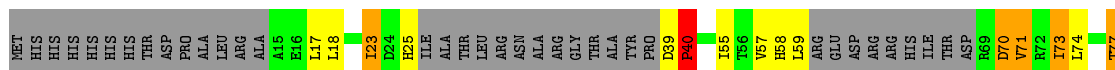


- Molecule 1: Pyridoxine 5'-phosphate synthase





- Molecule 1: Pyridoxine 5'-phosphate synthase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.05Å 188.12Å 192.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.44 – 3.07 48.44 – 3.07	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.44-3.07) 99.1 (48.44-3.07)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 3.07Å)	Xtrriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, $R_{free}$	0.182 , 0.248 0.185 , 0.247	Depositor DCC
$R_{free}$ test set	1367 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	85.5	Xtrriage
Anisotropy	0.258	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 63.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6975	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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	0.65	1/1835 (0.1%)	0.78	1/2481 (0.0%)
1	B	0.56	0/1833	0.73	1/2479 (0.0%)
1	C	0.52	0/1810	0.69	0/2452
1	D	0.55	0/1575	0.74	0/2138
All	All	0.57	1/7053 (0.0%)	0.73	2/9550 (0.0%)

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	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	CYS	CB-SG	-5.47	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	VAL	N-CA-C	5.30	125.30	111.00
1	A	17	LEU	CB-CG-CD2	-5.00	102.49	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	127	ASP	Peptide
1	B	135	ARG	Peptide
1	B	61	GLU	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	1814	0	1838	63	0
1	B	1812	0	1831	67	0
1	C	1789	0	1793	50	0
1	D	1560	0	1534	90	0
All	All	6975	0	6996	258	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 18.

The worst 5 of 258 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:D:108:PRO:HB3	1:D:113:GLU:CB	1.42	1.45
1:D:93:LEU:O	1:D:97:VAL:CG2	1.73	1.37
1:D:94:ALA:C	1:D:97:VAL:HG23	1.51	1.30
1:D:94:ALA:O	1:D:97:VAL:HG23	1.16	1.27
1:D:114:VAL:O	1:D:115:THR:OG1	1.55	1.22

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	240/268 (90%)	224 (93%)	13 (5%)	3 (1%)	12 40
1	B	240/268 (90%)	206 (86%)	26 (11%)	8 (3%)	4 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	240/268 (90%)	212 (88%)	24 (10%)	4 (2%)	9 34
1	D	214/268 (80%)	174 (81%)	29 (14%)	11 (5%)	2 11
All	All	934/1072 (87%)	816 (87%)	92 (10%)	26 (3%)	5 23

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	B	140	GLY
1	B	213	VAL
1	D	40	PRO
1	B	138	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	180/208 (86%)	175 (97%)	5 (3%)	43 71
1	B	180/208 (86%)	178 (99%)	2 (1%)	73 88
1	C	174/208 (84%)	168 (97%)	6 (3%)	37 67
1	D	146/208 (70%)	136 (93%)	10 (7%)	16 44
All	All	680/832 (82%)	657 (97%)	23 (3%)	37 67

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	138	ASP
1	C	234	ARG
1	D	99	THR
1	C	181	GLN
1	D	23	ILE

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

Mol	Chain	Res	Type
1	B	102	HIS
1	C	125	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	242/268 (90%)	-0.36	2 (0%) 86 71	40, 64, 118, 196	0
1	B	242/268 (90%)	-0.08	6 (2%) 57 33	42, 86, 152, 213	0
1	C	242/268 (90%)	-0.15	2 (0%) 86 71	55, 91, 157, 196	0
1	D	220/268 (82%)	0.27	19 (8%) 10 4	60, 130, 192, 225	0
All	All	946/1072 (88%)	-0.09	29 (3%) 49 25	40, 89, 171, 225	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	116	THR	7.4
1	D	115	THR	7.0
1	D	120	LEU	4.4
1	D	152	GLU	4.0
1	D	113	GLU	3.6

### 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

There are no such residues in this entry.