



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:34 AM GMT

PDB ID : 3PAW  
Title : Low resolution X-ray crystal structure of Yeast Rnr1p with dATP bound in the A-site  
Authors : Fairman, J.W.; Wijerathna, S.R.; Dealwis, C.G.  
Deposited on : 2010-10-19  
Resolution : 6.61 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

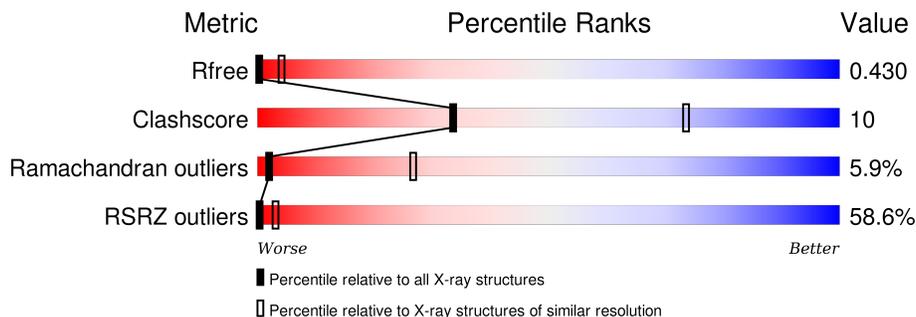
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 6.61 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	1014 (9.50-3.66)
Clashscore	102246	1062 (9.50-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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	888	
1	B	888	
1	C	888	
1	D	888	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14596 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.

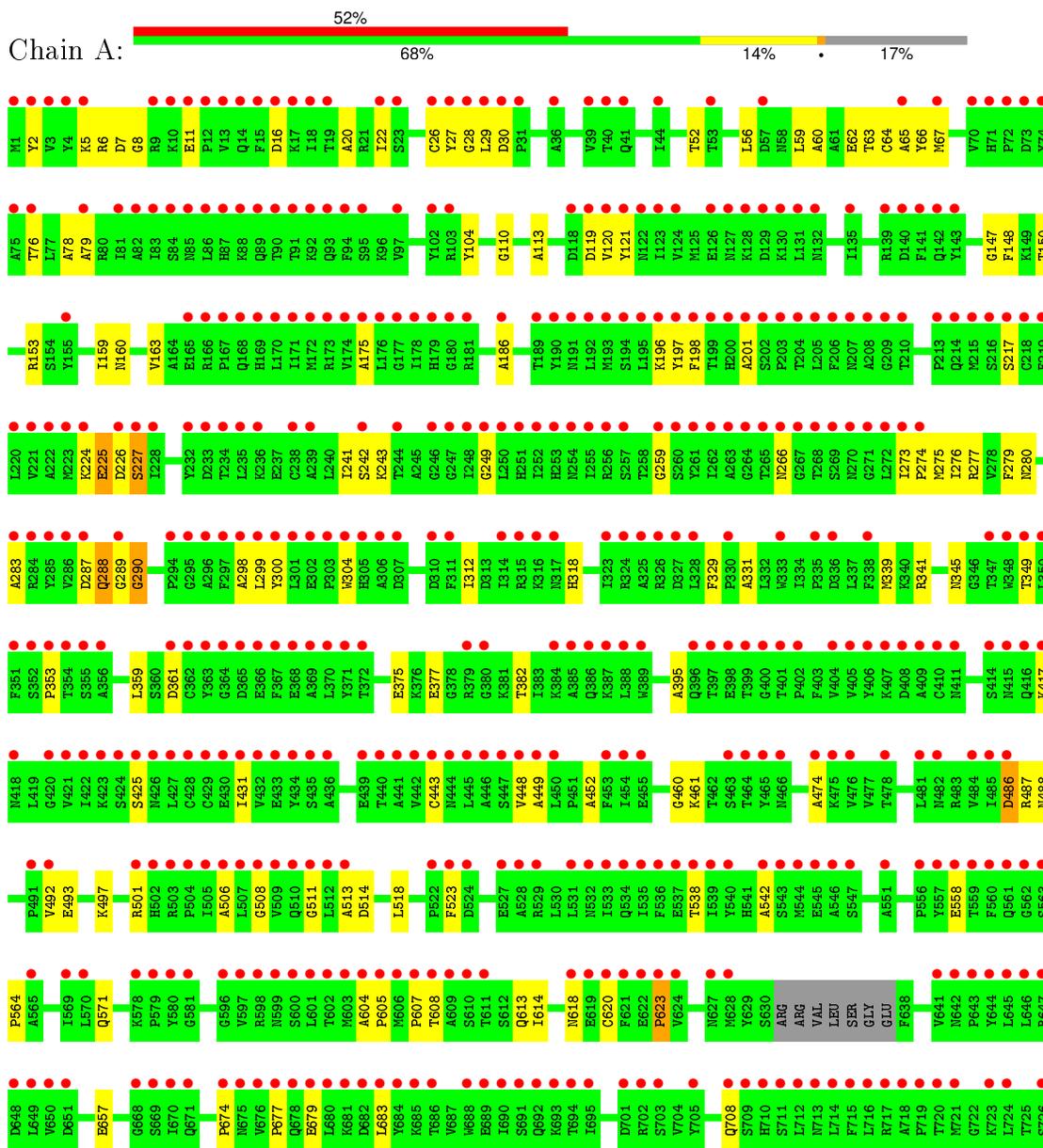
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase large chain 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	739	3649	2171	739	739	0	0	0
1	B	739	3649	2171	739	739	0	0	0
1	C	739	3649	2171	739	739	0	0	0
1	D	739	3649	2171	739	739	0	0	0

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

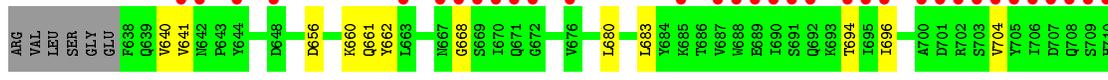
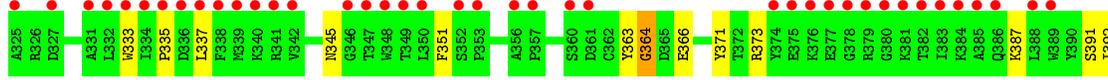
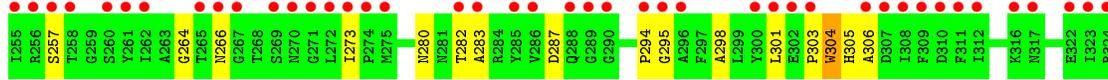
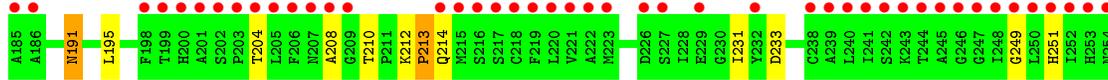
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Ribonucleoside-diphosphate reductase large chain 1





● Molecule 1: Ribonucleoside-diphosphate reductase large chain 1





VAL	GLU	TTR	HT10	R647	M800	C429	B361	L298	E237	H169	D73	M1
GLU	VAL	MET	S711	D648	R501	E430	C362	L299	C238	L170	T74	I2
VAL	VAL	PRO	L712	L649	H502	I431	Y363	Y300	A239	V174	A75	V3
PRO	PRO	SER	N713	M650	R503	V432	G364	L301	L240	L176	T76	Y4
GLU	VAL	SER	N714	D651	G581	E433	D365	D302	I241	L175	L77	K5
VAL	ALA	ALA	L715	M652	P504	D851	D366	P303	S242	L176	A78	R6
PRO	SER	SER	L716	G653	I505	M583	F367	R304	K243	L177	A79	D7
ALA	ALA	TTR	P719	I654	L506	S435	E368	H305	T244	I178	A82	G8
PRO	ALA	ALA	D586	M585	L507	A436	E369	R306	G245	G180		R9
ALA	ALA	ALA	D586	M586	G508	P437	L370	D307	G246	G181		R10
THR	THR	SER	I592	M659	V509	D438	Y371	I308	G247	R181		E11
LYS	LYS	ASP	L511	G511	Q510	T440	T372	F309	I248	D182		E12
ASN	ASN	ASP	L512	H595	G511	A441	R373	H310	G249	T90		P13
GLU	GLU	PHE	A513	G596	D514	V442	Y374	F311	L250	T91		P14
GLU	VAL	VAL	T515	M597	T515	C443	E375	I312	H251	T91		Q14
ALA	ALA	ALA	L518	M599	L518	M444		D313	R252	T91		F15
ALA	ALA	ALA	L518	M599	L518	M444		D314	R253	T91		D16
PRO	PRO	VAL	L518	M599	L518	M444		D315	R254	G249		H16
ILE	ILE	THR	L518	M599	L518	M444		D316	R255	G249		F16
THR	THR	THR	L518	M599	L518	M444		D317	R256	G249		D17
ALA	ALA	ALA	L518	M599	L518	M444		D318	R257	G249		H17
VAL	VAL	ALA	L518	M599	L518	M444		D319	R258	G249		F17
ASP	ASP	ASN	L518	M599	L518	M444		D320	R259	G249		R18
ASP	ASP	ALA	L518	M599	L518	M444		D321	R260	G249		E13
ALA	ALA	ALA	L518	M599	L518	M444		D322	R261	G249		D18
THR	THR	THR	L518	M599	L518	M444		D323	R262	G249		D19
ILE	ILE	ILE	L518	M599	L518	M444		D324	R263	G249		D20
VAL	VAL	VAL	L518	M599	L518	M444		D325	R264	G249		A36
VAL	VAL	VAL	L518	M599	L518	M444		D326	R265	G249		V37
ASP	ASP	ASP	L518	M599	L518	M444		D327	R266	G249		V38
LYS	LYS	LYS	L518	M599	L518	M444		D328	R267	G249		V39
ASN	ASN	ASN	L518	M599	L518	M444		D329	R268	G249		T40
SER	SER	SER	L518	M599	L518	M444		D330	R269	G249		Q41
SER	SER	SER	L518	M599	L518	M444		D331	R270	G249		R42
GLU	GLU	GLU	L518	M599	L518	M444		D332	R271	G249		I43
LYS	LYS	LYS	L518	M599	L518	M444		D333	R272	G249		I44
VAL	VAL	VAL	L518	M599	L518	M444		D334	R273	G249		I45
ILE	ILE	ILE	L518	M599	L518	M444		D335	R274	G249		G46
ILE	ILE	ILE	L518	M599	L518	M444		D336	R275	G249		V47
CYS	CYS	CYS	L518	M599	L518	M444		D337	R276	G249		Y48
ALA	ALA	ALA	L518	M599	L518	M444		D338	R277	G249		E49
ILE	ILE	ILE	L518	M599	L518	M444		D339	R278	G249		G50
ASP	ASP	ASP	L518	M599	L518	M444		D340	R279	G249		V51
ASN	ASN	ASN	L518	M599	L518	M444		D341	R280	G249		T52
PRO	PRO	PRO	L518	M599	L518	M444		D342	R281	G249		T53
GLY	GLY	GLY	L518	M599	L518	M444		D343	R282	G249		L56
ALA	ALA	ALA	L518	M599	L518	M444		D344	R283	G249		A60
CYS	CYS	CYS	L518	M599	L518	M444		D345	R284	G249		E62
GLU	GLU	GLU	L518	M599	L518	M444		D346	R285	G249		T63
GLU	GLU	GLU	L518	M599	L518	M444		D347	R286	G249		A65
CYS	CYS	CYS	L518	M599	L518	M444		D348	R287	G249		Y66
MET	MET	MET	L518	M599	L518	M444		D349	R288	G249		M67
SER	SER	SER	L518	M599	L518	M444		D350	R289	G249		T68
GLY	GLY	GLY	L518	M599	L518	M444		D351	R290	G249		T69
ALA	ALA	ALA	L518	M599	L518	M444		D352	R291	G249		V70
ASP	ASP	ASP	L518	M599	L518	M444		D353	R292	G249		H71
ALA	ALA	ALA	L518	M599	L518	M444		D354	R293	G249		P72
ILE	ILE	ILE	L518	M599	L518	M444		D355	R294	G249		
ILE	ILE	ILE	L518	M599	L518	M444		D356	R295	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D357	R296	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D358	R297	G249		
CYS	CYS	CYS	L518	M599	L518	M444		D359	R298	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D360	R299	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D361	R300	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D362	R301	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D363	R302	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D364	R303	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D365	R304	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D366	R305	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D367	R306	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D368	R307	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D369	R308	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D370	R309	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D371	R310	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D372	R311	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D373	R312	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D374	R313	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D375	R314	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D376	R315	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D377	R316	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D378	R317	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D379	R318	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D380	R319	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D381	R320	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D382	R321	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D383	R322	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D384	R323	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D385	R324	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D386	R325	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D387	R326	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D388	R327	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D389	R328	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D390	R329	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D391	R330	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D392	R331	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D393	R332	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D394	R333	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D395	R334	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D396	R335	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D397	R336	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D398	R337	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D399	R338	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D400	R339	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D401	R340	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D402	R341	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D403	R342	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D404	R343	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D405	R344	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D406	R345	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D407	R346	G249		
GLU	GLU	GLU	L518	M599	L518	M444		D408	R347	G249		
GLU	GLU	GLU	L518									

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	166.51Å 166.51Å 381.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	192.45 – 6.61 36.56 – 6.61	Depositor EDS
% Data completeness (in resolution range)	87.8 (192.45-6.61) 88.3 (36.56-6.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 6.63Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.391 , 0.442 0.370 , 0.430	Depositor DCC
$R_{free}$ test set	469 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	225.0	Xtriage
Anisotropy	0.669	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 170.6	EDS
Estimated twinning fraction	0.437 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 9847 reflections	Xtriage
$F_o, F_c$ correlation	0.64	EDS
Total number of atoms	14596	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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 [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	0.52	0/3647	0.65	0/5075
1	B	0.52	0/3647	0.65	0/5075
1	C	0.53	0/3647	0.66	0/5075
1	D	0.53	0/3647	0.63	0/5075
All	All	0.52	0/14588	0.65	0/20300

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3649	0	1652	61	0
1	B	3649	0	1652	55	0
1	C	3649	0	1652	58	0
1	D	3649	0	1652	44	0
All	All	14596	0	6608	217	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 10.

The worst 5 of 217 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:147:GLY:HA3	1:A:614:ILE:HA	1.42	0.99
1:D:147:GLY:HA2	1:D:614:ILE:HA	1.48	0.95
1:C:603:MET:CB	1:C:706:ILE:HA	1.99	0.92
1:A:147:GLY:CA	1:A:614:ILE:HA	2.02	0.90
1:D:147:GLY:CA	1:D:614:ILE:HA	2.07	0.85

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	735/888 (83%)	533 (72%)	157 (21%)	45 (6%)	2	26
1	B	735/888 (83%)	518 (70%)	180 (24%)	37 (5%)	3	31
1	C	735/888 (83%)	536 (73%)	154 (21%)	45 (6%)	2	26
1	D	735/888 (83%)	542 (74%)	148 (20%)	45 (6%)	2	26
All	All	2940/3552 (83%)	2129 (72%)	639 (22%)	172 (6%)	2	27

5 of 172 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	GLU
1	A	227	SER
1	A	288	GLN
1	A	461	LYS
1	A	486	ASP

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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	739/888 (83%)	3.34	458 (61%) 0 3	39, 81, 170, 183	0
1	B	739/888 (83%)	2.85	388 (52%) 0 4	52, 74, 175, 188	0
1	C	739/888 (83%)	3.11	403 (54%) 0 3	51, 73, 173, 194	0
1	D	739/888 (83%)	3.55	483 (65%) 0 3	58, 80, 175, 186	0
All	All	2956/3552 (83%)	3.21	1732 (58%) 0 3	39, 78, 173, 194	0

The worst 5 of 1732 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	711	SER	18.8
1	C	433	GLU	18.8
1	B	415	ASN	18.6
1	B	414	SER	17.5
1	D	218	CYS	17.2

### 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.