



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 03:01 am GMT

PDB ID : 2CVS  
Title : Structures of Yeast Ribonucleotide Reductase I  
Authors : Xu, H.; Faber, C.; Uchiki, T.; Fairman, J.W.; Racca, J.; Dealwis, C.  
Deposited on : 2005-06-14  
Resolution : 2.60 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

<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 : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

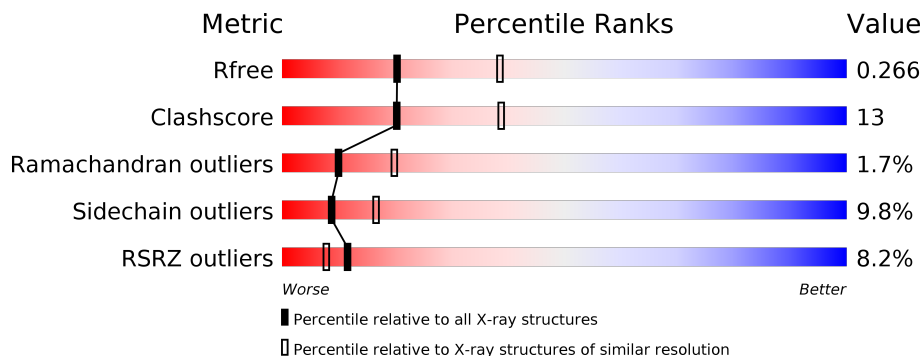
# 1 Overall quality at a glance

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))
$R_{free}$	111664	2767 (2.60-2.60)
Clashscore	122126	3110 (2.60-2.60)
Ramachandran outliers	120053	3062 (2.60-2.60)
Sidechain outliers	120020	3062 (2.60-2.60)
RSRZ outliers	108989	2706 (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 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	<div> <div>6%</div> <div>50%</div> <div>20%</div> <div>•</div> <div>26%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5435 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
1	A	657	Total	C	N	O	S	0	0	0
			5254	3349	890	984	31			

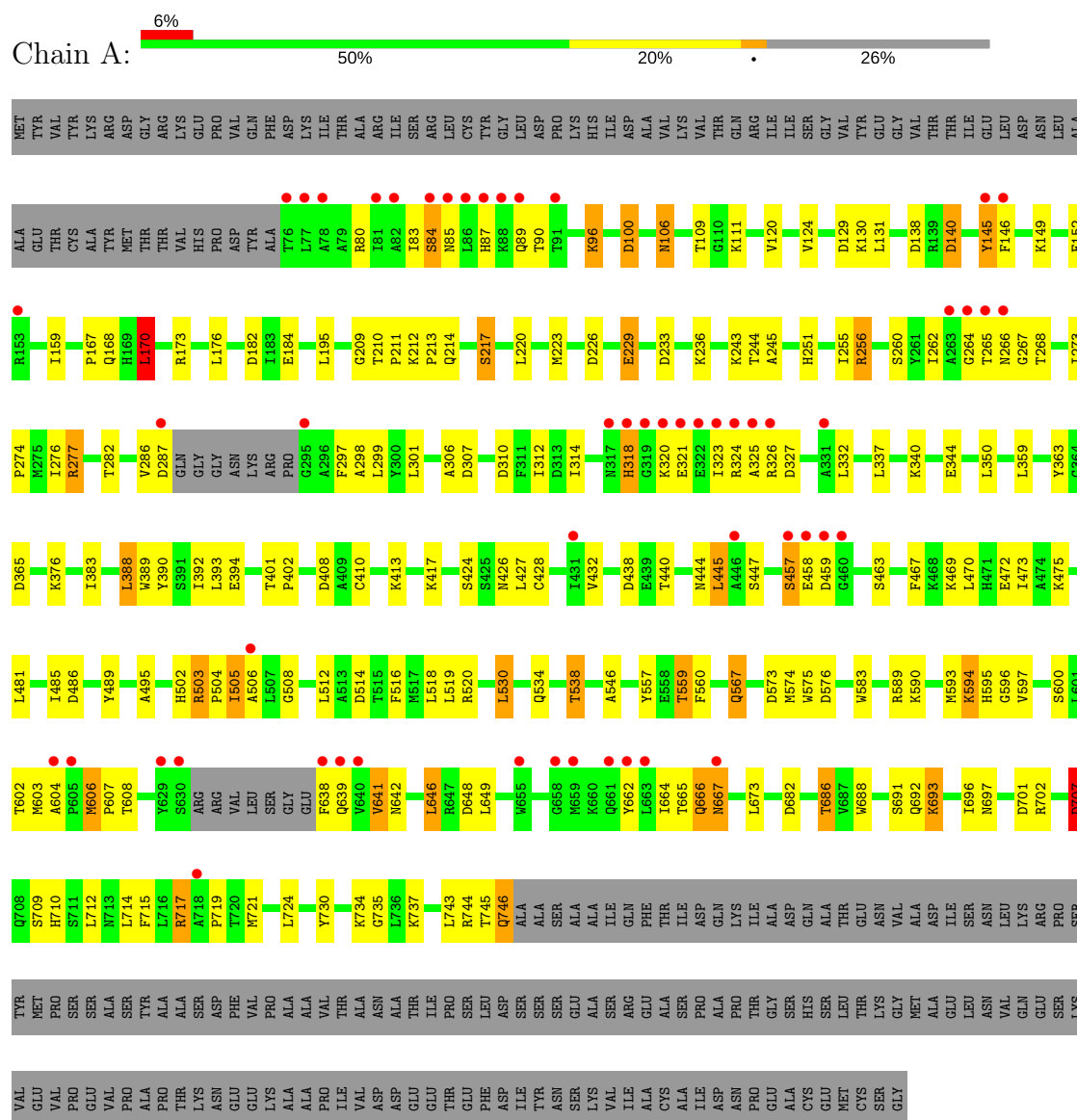
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	181	Total	O	0	0
			181	181		

### 3 Residue-property plots

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: Ribonucleoside-diphosphate reductase large chain 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.51Å 117.17Å 63.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 40.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-2.60) 97.4 (40.00-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0007	Depositor
R, $R_{free}$	0.204 , 0.267 0.203 , 0.266	Depositor DCC
$R_{free}$ test set	3208 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.1	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 48.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5435	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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	0.62	0/5374	0.85	21/7275 (0.3%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	ASP	CB-CG-OD2	8.45	125.91	118.30
1	A	226	ASP	CB-CG-OD2	8.06	125.56	118.30
1	A	707	ASP	CB-CG-OD2	7.37	124.94	118.30
1	A	100	ASP	CB-CG-OD2	6.92	124.53	118.30
1	A	182	ASP	CB-CG-OD2	6.39	124.06	118.30
1	A	459	ASP	CB-CG-OD2	6.35	124.02	118.30
1	A	129	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	307	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	287	ASP	CB-CG-OD2	6.07	123.76	118.30
1	A	233	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	140	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	573	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	682	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	576	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	438	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	514	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	701	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	445	LEU	CA-CB-CG	5.10	127.04	115.30
1	A	648	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	503	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	A	170	LEU	CA-CB-CG	5.00	126.81	115.30

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	5254	0	5189	140	0
2	A	181	0	0	13	0
All	All	5435	0	5189	140	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.

All (140) 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:691:SER:OG	1:A:693:LYS:HD3	1.53	1.08
1:A:327:ASP:HA	2:A:941:HOH:O	1.70	0.92
1:A:662:TYR:CD1	1:A:673:LEU:HD21	2.14	0.83
1:A:276:ILE:HD12	1:A:299:LEU:HD13	1.62	0.82
1:A:390:TYR:O	1:A:394:GLU:HG3	1.83	0.78
1:A:262:ILE:H	1:A:267:GLY:HA2	1.49	0.77
1:A:693:LYS:H	1:A:693:LYS:HD2	1.47	0.77
1:A:557:TYR:CE1	1:A:559:THR:HG22	2.20	0.77
1:A:214:GLN:HG3	2:A:891:HOH:O	1.86	0.75
1:A:120:VAL:O	1:A:124:VAL:HG23	1.87	0.75
1:A:691:SER:HG	1:A:693:LYS:HD3	1.53	0.74
1:A:445:LEU:HD13	1:A:506:ALA:HB3	1.71	0.71
1:A:589:ARG:O	1:A:593:MET:HG3	1.89	0.71
1:A:595:HIS:HD2	2:A:1064:HOH:O	1.72	0.69
1:A:417:LYS:HE3	1:A:574:MET:HE1	1.73	0.69
1:A:256:ARG:HG2	1:A:260:SER:HB2	1.73	0.69
1:A:212:LYS:HD2	1:A:489:TYR:CZ	2.29	0.67
1:A:277:ARG:HH11	1:A:277:ARG:HG2	1.60	0.66
1:A:691:SER:OG	1:A:693:LYS:CD	2.39	0.66
1:A:320:LYS:HG2	1:A:321:GLU:H	1.61	0.65
1:A:170:LEU:HD22	1:A:173:ARG:NH2	2.11	0.65
1:A:692:GLN:O	1:A:696:ILE:HG12	1.97	0.65
1:A:376:LYS:HD3	2:A:980:HOH:O	1.97	0.65
1:A:557:TYR:HE1	1:A:559:THR:HG22	1.61	0.64
1:A:80:ARG:O	1:A:84:SER:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:THR:HB	1:A:402:PRO:HA	1.80	0.64
1:A:427:LEU:HB3	2:A:1012:HOH:O	1.98	0.63
1:A:730:TYR:O	1:A:734:LYS:HG2	2.00	0.61
1:A:276:ILE:HD12	1:A:299:LEU:CD1	2.30	0.61
1:A:693:LYS:H	1:A:693:LYS:CD	2.09	0.61
1:A:717:ARG:O	1:A:719:PRO:HD3	2.01	0.60
1:A:332:LEU:HD11	1:A:392:ILE:HD12	1.84	0.60
1:A:557:TYR:CD1	1:A:559:THR:HG22	2.38	0.59
1:A:220:LEU:HD21	1:A:426:ASN:HB3	1.85	0.58
1:A:306:ALA:HA	1:A:350:LEU:HB3	1.84	0.58
1:A:467:PHE:HD2	1:A:538:THR:HG21	1.69	0.58
1:A:140:ASP:OD2	1:A:167:PRO:HB2	2.04	0.57
1:A:277:ARG:NH1	1:A:277:ARG:HG2	2.18	0.57
1:A:390:TYR:CD2	1:A:394:GLU:OE1	2.58	0.57
1:A:595:HIS:CD2	2:A:1064:HOH:O	2.52	0.56
1:A:665:THR:HG22	1:A:666:GLN:NE2	2.21	0.56
1:A:273:ILE:HD11	1:A:310:ASP:HB3	1.86	0.55
1:A:223:MET:HG2	1:A:255:ILE:HD11	1.88	0.55
1:A:534:GLN:O	1:A:538:THR:CG2	2.54	0.55
1:A:534:GLN:O	1:A:538:THR:HG23	2.06	0.55
1:A:606:MET:HB2	1:A:607:PRO:HD2	1.88	0.55
1:A:273:ILE:HG21	1:A:323:ILE:HA	1.89	0.54
1:A:389:TRP:HE1	1:A:393:LEU:HD11	1.73	0.53
1:A:184:GLU:OE2	1:A:184:GLU:HA	2.09	0.53
1:A:413:LYS:NZ	1:A:735:GLY:O	2.43	0.52
1:A:481:LEU:HB3	1:A:505:ILE:HD12	1.92	0.52
1:A:106:ASN:HB3	1:A:109:THR:HG22	1.91	0.52
1:A:426:ASN:ND2	1:A:428:CYS:H	2.08	0.52
1:A:109:THR:HG23	1:A:111:LYS:H	1.75	0.51
1:A:96:LYS:HD2	2:A:1024:HOH:O	2.09	0.51
1:A:702:ARG:HH11	1:A:710:HIS:HE1	1.58	0.51
1:A:646:LEU:HA	1:A:649:LEU:HD12	1.93	0.50
1:A:662:TYR:CG	1:A:673:LEU:HD21	2.47	0.50
1:A:594:LYS:HE3	1:A:594:LYS:HA	1.93	0.50
1:A:686:THR:CG2	1:A:688:TRP:HD1	2.25	0.50
1:A:538:THR:HB	1:A:583:TRP:NE1	2.26	0.49
1:A:447:SER:HB3	1:A:606:MET:CE	2.42	0.49
1:A:662:TYR:HA	1:A:665:THR:HB	1.95	0.49
1:A:109:THR:HG23	1:A:111:LYS:HG3	1.95	0.49
1:A:262:ILE:HB	1:A:266:ASN:O	2.13	0.49
1:A:692:GLN:NE2	1:A:715:PHE:H	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:MET:H	1:A:707:ASP:HB2	1.76	0.49
1:A:516:PHE:HB2	2:A:956:HOH:O	2.13	0.49
1:A:475:LYS:HD2	1:A:546:ALA:HB2	1.95	0.48
1:A:469:LYS:O	1:A:473:ILE:HG12	2.11	0.48
1:A:298:ALA:HB2	1:A:427:LEU:HA	1.95	0.48
1:A:444:ASN:ND2	1:A:504:PRO:O	2.45	0.48
1:A:83:ILE:O	1:A:87:HIS:N	2.46	0.48
1:A:332:LEU:CD1	1:A:392:ILE:HD12	2.43	0.48
1:A:390:TYR:HD2	1:A:394:GLU:OE1	1.95	0.47
1:A:557:TYR:CZ	1:A:600:SER:HA	2.49	0.47
1:A:312:ILE:HG22	1:A:402:PRO:HG3	1.96	0.47
1:A:606:MET:HG2	1:A:608:THR:CG2	2.45	0.47
1:A:83:ILE:O	1:A:87:HIS:HB2	2.14	0.47
1:A:140:ASP:OD2	1:A:168:GLN:HG2	2.14	0.47
1:A:502:HIS:ND1	1:A:559:THR:HG21	2.29	0.47
1:A:320:LYS:HB3	1:A:323:ILE:CG2	2.45	0.47
1:A:506:ALA:HB1	1:A:604:ALA:HB3	1.95	0.47
1:A:326:ARG:HG2	1:A:326:ARG:O	2.16	0.46
1:A:686:THR:CG2	1:A:688:TRP:H	2.28	0.46
1:A:229:GLU:HB2	2:A:1058:HOH:O	2.15	0.46
1:A:702:ARG:HH11	1:A:710:HIS:CE1	2.34	0.46
1:A:641:VAL:HG13	1:A:646:LEU:HD22	1.99	0.45
1:A:673:LEU:HA	1:A:673:LEU:HD23	1.63	0.45
1:A:447:SER:HB3	1:A:606:MET:HE3	1.98	0.45
1:A:686:THR:HG23	1:A:688:TRP:H	1.82	0.45
1:A:481:LEU:O	1:A:485:ILE:HG13	2.17	0.45
1:A:745:THR:O	1:A:746:GLN:CB	2.64	0.45
1:A:85:ASN:O	1:A:89:GLN:HG2	2.17	0.45
1:A:745:THR:O	1:A:746:GLN:HB2	2.18	0.44
1:A:170:LEU:HD22	1:A:173:ARG:HH21	1.80	0.44
1:A:120:VAL:HG21	1:A:209:GLY:HA2	1.98	0.44
1:A:567:GLN:HA	1:A:567:GLN:HE21	1.83	0.44
1:A:213:PRO:HD2	1:A:489:TYR:HB2	2.00	0.44
1:A:472:GLU:HG2	2:A:1051:HOH:O	2.18	0.44
1:A:467:PHE:CD2	1:A:538:THR:HG21	2.52	0.44
1:A:662:TYR:CD1	1:A:662:TYR:O	2.71	0.44
1:A:251:HIS:HD2	2:A:902:HOH:O	2.01	0.44
1:A:273:ILE:HD11	1:A:310:ASP:CB	2.48	0.44
1:A:457:SER:O	1:A:458:GLU:HB2	2.18	0.44
1:A:606:MET:HG2	1:A:608:THR:HG23	1.98	0.44
1:A:276:ILE:CD1	1:A:299:LEU:HD13	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:ASP:CG	1:A:503:ARG:HH22	2.22	0.43
1:A:363:TYR:HB2	1:A:408:ASP:OD1	2.18	0.43
1:A:388:LEU:O	1:A:392:ILE:HG12	2.18	0.43
1:A:560:PHE:CZ	1:A:596:GLY:HA2	2.53	0.43
1:A:210:THR:HB	1:A:211:PRO:HD2	2.01	0.43
1:A:212:LYS:HD2	1:A:489:TYR:CE2	2.54	0.43
1:A:697:ASN:OD1	1:A:734:LYS:HE2	2.19	0.43
1:A:314:ILE:HD12	1:A:314:ILE:HA	1.84	0.43
1:A:530:LEU:O	1:A:534:GLN:HG3	2.19	0.43
1:A:519:LEU:O	1:A:520:ARG:HB2	2.18	0.42
1:A:428:CYS:SG	1:A:607:PRO:HG2	2.59	0.42
1:A:389:TRP:NE1	1:A:393:LEU:HD11	2.34	0.42
1:A:413:LYS:HE2	1:A:575:TRP:CE2	2.54	0.42
1:A:282:THR:O	1:A:286:VAL:HG23	2.20	0.42
1:A:410:CYS:SG	1:A:737:LYS:HB3	2.60	0.42
1:A:709:SER:OG	1:A:710:HIS:N	2.53	0.42
1:A:602:THR:N	1:A:707:ASP:OD2	2.53	0.41
1:A:508:GLY:HA3	1:A:606:MET:HE1	2.02	0.41
1:A:100:ASP:HB3	1:A:159:ILE:HD11	2.01	0.41
1:A:320:LYS:HB3	1:A:323:ILE:HG22	2.02	0.41
1:A:273:ILE:HB	1:A:274:PRO:HD3	2.03	0.41
1:A:642:ASN:O	1:A:646:LEU:HD23	2.21	0.41
1:A:130:LYS:HB2	2:A:933:HOH:O	2.21	0.41
1:A:251:HIS:HB3	1:A:424:SER:HB3	2.03	0.41
1:A:389:TRP:CZ2	1:A:393:LEU:HD21	2.55	0.41
1:A:440:THR:O	1:A:495:ALA:HA	2.21	0.40
1:A:470:LEU:HD23	1:A:538:THR:OG1	2.21	0.40
1:A:606:MET:HE3	1:A:608:THR:CG2	2.52	0.40
1:A:243:LYS:C	1:A:245:ALA:H	2.24	0.40
1:A:417:LYS:HE2	1:A:417:LYS:HB3	1.88	0.40
1:A:340:LYS:O	1:A:344:GLU:HG3	2.22	0.40
1:A:427:LEU:CB	2:A:1012:HOH:O	2.63	0.40
1:A:298:ALA:CB	1:A:427:LEU:HA	2.51	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	651/888 (73%)	598 (92%)	42 (6%)	11 (2%)	10	20

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	TYR
1	A	318	HIS
1	A	457	SER
1	A	667	ASN
1	A	217	SER
1	A	264	GLY
1	A	268	THR
1	A	639	GLN
1	A	325	ALA
1	A	717	ARG
1	A	256	ARG

### 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	570/761 (75%)	514 (90%)	56 (10%)	9	16

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	SER
1	A	90	THR
1	A	96	LYS
1	A	106	ASN
1	A	131	LEU
1	A	138	ASP
1	A	145	TYR
1	A	146	PHE
1	A	149	LYS
1	A	152	GLU
1	A	170	LEU
1	A	176	LEU
1	A	195	LEU
1	A	217	SER
1	A	229	GLU
1	A	236	LYS
1	A	244	THR
1	A	265	THR
1	A	277	ARG
1	A	297	PHE
1	A	301	LEU
1	A	318	HIS
1	A	324	ARG
1	A	337	LEU
1	A	359	LEU
1	A	383	ILE
1	A	388	LEU
1	A	432	VAL
1	A	463	SER
1	A	505	ILE
1	A	512	LEU
1	A	518	LEU
1	A	530	LEU
1	A	538	THR
1	A	559	THR
1	A	567	GLN
1	A	590	LYS
1	A	594	LYS
1	A	597	VAL
1	A	606	MET
1	A	638	PHE
1	A	641	VAL
1	A	646	LEU

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Mol	Chain	Res	Type
1	A	664	ILE
1	A	666	GLN
1	A	667	ASN
1	A	686	THR
1	A	693	LYS
1	A	707	ASP
1	A	712	LEU
1	A	714	LEU
1	A	721	MET
1	A	724	LEU
1	A	743	LEU
1	A	744	ARG
1	A	746	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	127	ASN
1	A	160	ASN
1	A	251	HIS
1	A	567	GLN
1	A	613	GLN
1	A	618	ASN
1	A	639	GLN
1	A	661	GLN
1	A	666	GLN
1	A	692	GLN
1	A	710	HIS
1	A	713	ASN
1	A	746	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	657/888 (73%)	0.19	54 (8%) 11 8	29, 47, 87, 112	1 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	GLY	5.9
1	A	321	GLU	5.7
1	A	325	ALA	5.7
1	A	318	HIS	5.6
1	A	457	SER	5.4
1	A	662	TYR	4.9
1	A	629	TYR	4.8
1	A	638	PHE	4.7
1	A	459	ASP	4.6
1	A	630	SER	4.3
1	A	323	ILE	4.2
1	A	264	GLY	4.1
1	A	146	PHE	3.9
1	A	640	VAL	3.9
1	A	82	ALA	3.8
1	A	458	GLU	3.8
1	A	295	GLY	3.8
1	A	663	LEU	3.8
1	A	88	LYS	3.8
1	A	85	ASN	3.7
1	A	77	LEU	3.6
1	A	81	ILE	3.6
1	A	78	ALA	3.6
1	A	667	ASN	3.5
1	A	86	LEU	3.3
1	A	326	ARG	3.2
1	A	287	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	84	SER	3.2
1	A	320	LYS	3.1
1	A	639	GLN	3.1
1	A	659	MET	3.0
1	A	265	THR	2.9
1	A	145	TYR	2.9
1	A	658	GLY	2.9
1	A	87	HIS	2.8
1	A	324	ARG	2.6
1	A	604	ALA	2.6
1	A	317	ASN	2.6
1	A	76	THR	2.4
1	A	506	ALA	2.4
1	A	431	ILE	2.4
1	A	266	ASN	2.4
1	A	460	GLY	2.4
1	A	446	ALA	2.3
1	A	153	ARG	2.3
1	A	322	GLU	2.3
1	A	91	THR	2.3
1	A	331	ALA	2.2
1	A	655	TRP	2.2
1	A	661	GLN	2.2
1	A	89	GLN	2.1
1	A	263	ALA	2.1
1	A	605	PRO	2.0
1	A	718	ALA	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.