



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 10:52 PM GMT

PDB ID : 3TB9  
Title : Structure of Yeast Ribonucleotide Reductase 1 Q288A with AMPPNP and CDP  
Authors : Ahmad, M.F.; Kaushal, P.S.; Wan, Q.; Wijeratna, S.R.; Huang, M.; Dealwis, C.D.  
Deposited on : 2011-08-05  
Resolution : 2.53 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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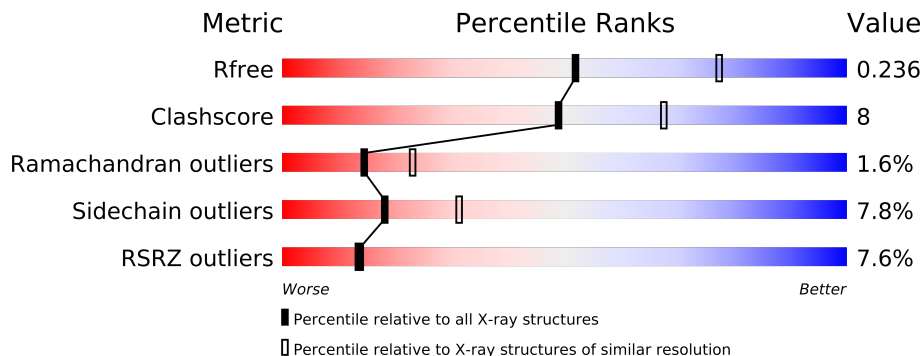
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.53 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))
$R_{free}$	66092	3240 (2.54-2.50)
Clashscore	79885	4080 (2.54-2.50)
Ramachandran outliers	78287	3990 (2.54-2.50)
Sidechain outliers	78261	3992 (2.54-2.50)
RSRZ outliers	66119	3241 (2.54-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	888	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	MG	A	891	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 5278 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

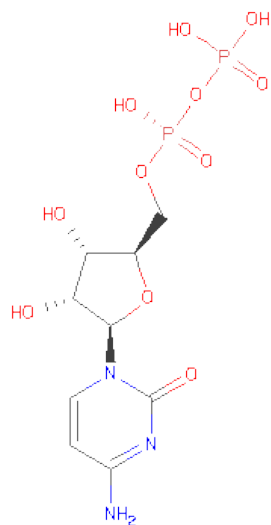
- Molecule 1 is a protein called Ribonucleoside-diphosphatereductase large chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	643	5107	3253	864	959	31	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	288	ALA	GLN	ENGINEERED MUTATION	UNP P21524

- Molecule 2 is CYTIDINE-5'-DIPHOSPHATE (three-letter code: CDP) (formula:  $C_9H_{15}N_3O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	25	9	3	11	2	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONICACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	114	Total	O	0	0
			114	114		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.89Å 116.96Å 64.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.48 – 2.53 43.27 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.48-2.53) 99.9 (43.27-2.53)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.54 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.199 , 0.237 0.199 , 0.236	Depositor DCC
$R_{free}$ test set	2793 reflections (11.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.3	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 29.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 27860 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5278	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDP, MG, ANP

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	0.60	0/5223	0.70	1/7075 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	220	LEU	CA-CB-CG	5.21	127.28	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5107	0	5013	78	0
2	A	25	0	12	1	0
3	A	31	0	13	0	0
4	A	1	0	0	0	0
5	A	114	0	0	1	0
All	All	5278	0	5038	78	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 8.

All (78) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:447:SER:HB3	1:A:606:MET:CE	1.87	1.05
1:A:447:SER:HB3	1:A:606:MET:HE1	1.50	0.92
1:A:620:CYS:O	1:A:620:CYS:SG	2.33	0.85
1:A:608:THR:HG22	1:A:612:SER:HB3	1.65	0.78
1:A:447:SER:HB3	1:A:606:MET:HE3	1.67	0.77
1:A:417:LYS:HE3	1:A:574:MET:HE1	1.69	0.74
1:A:417:LYS:HE3	1:A:574:MET:CE	2.21	0.70
1:A:608:THR:CG2	1:A:612:SER:HB3	2.24	0.67
1:A:486:ASP:OD2	1:A:503:ARG:NH2	2.29	0.65
1:A:413:LYS:NZ	1:A:735:GLY:O	2.31	0.64
1:A:447:SER:CB	1:A:606:MET:HE1	2.25	0.64
1:A:538:THR:HB	1:A:583:TRP:NE1	2.13	0.64
1:A:745:THR:O	1:A:746:GLN:HB2	1.97	0.64
1:A:482:ASN:HD21	1:A:503:ARG:HH11	1.47	0.62
1:A:534:GLN:O	1:A:538:THR:HG23	2.00	0.61
1:A:620:CYS:O	1:A:622:GLU:N	2.34	0.61
1:A:486:ASP:CG	1:A:503:ARG:HH22	2.03	0.61
1:A:457:SER:O	1:A:458:GLU:HB2	2.00	0.61
1:A:618:ASN:O	1:A:619:GLU:CB	2.46	0.61
1:A:482:ASN:HD22	1:A:599:ASN:HD21	1.48	0.61
1:A:482:ASN:ND2	1:A:503:ARG:HH11	1.99	0.60
1:A:608:THR:O	1:A:608:THR:HG22	2.02	0.59
1:A:126:GLU:OE1	1:A:181:ARG:NH1	2.34	0.59
1:A:482:ASN:ND2	1:A:503:ARG:NH1	2.51	0.58
1:A:560:PHE:CZ	1:A:596:GLY:HA2	2.38	0.58
1:A:297:PHE:HB2	1:A:328:LEU:HD22	1.85	0.58
1:A:520:ARG:HH22	1:A:648:ASP:CG	2.07	0.58
1:A:618:ASN:O	1:A:619:GLU:HB2	2.04	0.57
1:A:168:GLN:NE2	1:A:190:TYR:OH	2.34	0.57
1:A:619:GLU:O	1:A:620:CYS:HB3	2.03	0.56
1:A:506:ALA:HB1	1:A:604:ALA:HB3	1.87	0.55
1:A:214:GLN:HE22	1:A:216:SER:HB2	1.71	0.55
1:A:428:CYS:SG	2:A:889:CDP:H3'	2.48	0.53
1:A:512:LEU:HD12	1:A:621:PHE:HA	1.89	0.53
1:A:168:GLN:HE22	1:A:194:SER:HB2	1.73	0.53
1:A:393:LEU:HD22	1:A:724:LEU:HD13	1.91	0.53
1:A:618:ASN:O	1:A:619:GLU:CD	2.48	0.51
1:A:286:VAL:HG13	1:A:286:VAL:O	2.10	0.51
1:A:724:LEU:HD21	1:A:740:MET:HE1	1.93	0.51
1:A:549:GLU:O	1:A:553:LYS:HG3	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:530:LEU:O	1:A:534:GLN:HG3	2.11	0.50
1:A:692:GLN:NE2	1:A:715:PHE:H	2.09	0.50
1:A:510:GLN:HB3	1:A:608:THR:HG21	1.94	0.49
1:A:251:HIS:HE1	1:A:435:SER:OG	1.96	0.49
1:A:608:THR:HB	1:A:619:GLU:O	2.13	0.49
1:A:334:ILE:HD12	1:A:404:VAL:HG13	1.94	0.48
1:A:713:ASN:ND2	1:A:742:TYR:HB2	2.29	0.48
1:A:178:ILE:O	1:A:487:ARG:HD3	2.14	0.48
1:A:482:ASN:HD21	1:A:503:ARG:NH1	2.08	0.47
1:A:702:ARG:HH11	1:A:710:HIS:HE1	1.62	0.47
1:A:142:GLN:HE22	1:A:195:LEU:HD12	1.79	0.46
1:A:656:ASP:H	1:A:659:MET:HB2	1.80	0.46
1:A:608:THR:HG22	1:A:612:SER:CB	2.41	0.46
1:A:538:THR:HB	1:A:583:TRP:HE1	1.78	0.46
1:A:534:GLN:O	1:A:538:THR:CG2	2.63	0.45
1:A:510:GLN:OE1	1:A:612:SER:HA	2.16	0.45
1:A:457:SER:O	1:A:458:GLU:CB	2.65	0.45
1:A:338:PHE:O	1:A:342:VAL:HG23	2.16	0.45
1:A:460:GLY:O	1:A:462:THR:N	2.48	0.44
1:A:146:PHE:HE1	1:A:613:GLN:HE21	1.65	0.44
1:A:620:CYS:O	1:A:621:PHE:CG	2.71	0.44
1:A:683:LEU:HD23	1:A:684:TYR:CZ	2.51	0.44
1:A:273:ILE:HD12	1:A:314:ILE:HD11	2.00	0.44
1:A:519:LEU:O	1:A:520:ARG:HB2	2.18	0.43
1:A:172:MET:O	1:A:176:LEU:HD22	2.18	0.43
1:A:618:ASN:O	1:A:619:GLU:OE2	2.37	0.43
1:A:135:ILE:HG23	1:A:168:GLN:HB3	2.01	0.43
1:A:273:ILE:HB	1:A:274:PRO:HD3	2.01	0.43
1:A:146:PHE:CE1	1:A:613:GLN:NE2	2.86	0.43
1:A:337:LEU:HG	1:A:368:GLU:HG2	2.00	0.43
1:A:273:ILE:HG21	1:A:323:ILE:HA	2.01	0.42
1:A:505:ILE:HG13	1:A:602:THR:HA	2.01	0.41
1:A:686:THR:HB	1:A:689:GLU:OE1	2.20	0.41
1:A:487:ARG:HD2	5:A:997:HOH:O	2.20	0.41
1:A:717:ARG:O	1:A:719:PRO:HD3	2.20	0.41
1:A:356:ALA:HB1	1:A:374:TYR:CD1	2.55	0.41
1:A:146:PHE:CZ	1:A:613:GLN:NE2	2.89	0.41
1:A:223:MET:HG2	1:A:255:ILE:HD11	2.01	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	637/888 (72%)	613 (96%)	14 (2%)	10 (2%)	14 23

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	458	GLU
1	A	461	LYS
1	A	620	CYS
1	A	619	GLU
1	A	621	PHE
1	A	717	ARG
1	A	296	ALA
1	A	457	SER
1	A	639	GLN
1	A	667	ASN

### 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	550/760 (72%)	507 (92%)	43 (8%)	18 31

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	LYS
1	A	131	LEU
1	A	149	LYS
1	A	153	ARG

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Mol	Chain	Res	Type
1	A	176	LEU
1	A	195	LEU
1	A	214	GLN
1	A	220	LEU
1	A	242	SER
1	A	265	THR
1	A	301	LEU
1	A	314	ILE
1	A	324	ARG
1	A	326	ARG
1	A	337	LEU
1	A	359	LEU
1	A	388	LEU
1	A	423	LYS
1	A	443	CYS
1	A	458	GLU
1	A	459	ASP
1	A	462	THR
1	A	472	GLU
1	A	512	LEU
1	A	518	LEU
1	A	530	LEU
1	A	538	THR
1	A	606	MET
1	A	619	GLU
1	A	626	SER
1	A	647	ARG
1	A	656	ASP
1	A	665	THR
1	A	667	ASN
1	A	673	LEU
1	A	686	THR
1	A	712	LEU
1	A	714	LEU
1	A	716	LEU
1	A	721	MET
1	A	724	LEU
1	A	743	LEU
1	A	746	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	142	GLN
1	A	168	GLN
1	A	214	GLN
1	A	251	HIS
1	A	444	ASN
1	A	482	ASN
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 chains 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	CDP	A	889	-	26,26,26	1.14	2 (7%)	37,40,40	1.20	3 (8%)
3	ANP	A	890	4	33,33,33	3.66	7 (21%)	51,52,52	2.13	14 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CDP	A	889	-	-	0/14/32/32	0/2/2/2
3	ANP	A	890	4	-	0/18/38/38	0/1/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	890	ANP	PB-N3B	13.70	1.76	1.64
3	A	890	ANP	PG-N3B	12.82	1.75	1.64
3	A	890	ANP	PB-O1B	5.43	1.52	1.46
3	A	890	ANP	PG-O1G	4.37	1.51	1.46
2	A	889	CDP	C2-N1	4.11	1.42	1.38
3	A	890	ANP	C5-C4	3.34	1.48	1.40
3	A	890	ANP	C4-N9	-2.86	1.33	1.37
3	A	890	ANP	PB-O3A	2.50	1.62	1.59
2	A	889	CDP	O4'-C1'	2.12	1.44	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	890	ANP	N3-C2-N1	-7.82	122.17	128.71
3	A	890	ANP	N3-C4-N9	5.04	134.53	125.43
3	A	890	ANP	PB-N3B-PG	-4.53	122.46	130.07
3	A	890	ANP	O1G-PG-N3B	-4.22	105.45	111.83
3	A	890	ANP	O2B-PB-O1B	4.17	119.52	109.89
2	A	889	CDP	C2-N3-C4	4.04	121.42	115.57
3	A	890	ANP	O3G-PG-O2G	3.33	117.21	107.66
3	A	890	ANP	C8-N9-C4	3.32	109.43	106.90
2	A	889	CDP	C6-C5-C4	3.25	118.82	117.47
3	A	890	ANP	O1B-PB-N3B	-2.77	107.64	111.83
3	A	890	ANP	C2-N1-C6	2.53	123.34	118.77
3	A	890	ANP	C5-C4-N3	-2.46	120.35	125.70
3	A	890	ANP	C2-N3-C4	2.34	120.66	114.01
3	A	890	ANP	C3'-C2'-C1'	2.17	104.31	100.91
3	A	890	ANP	C4-C5-N7	-2.13	107.70	109.52
2	A	889	CDP	N4-C4-N3	2.09	120.61	116.59
3	A	890	ANP	C2'-C1'-N9	-2.03	108.06	113.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	643/888 (72%)	0.45	49 (7%) 14 13	22, 37, 64, 78	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	638	PHE	8.9
1	A	639	GLN	5.4
1	A	318	HIS	4.9
1	A	145	TYR	4.6
1	A	323	ILE	4.6
1	A	91	THR	4.2
1	A	321	GLU	4.2
1	A	457	SER	4.0
1	A	163	VAL	4.0
1	A	319	GLY	4.0
1	A	654	ILE	3.9
1	A	746	GLN	3.9
1	A	652	LEU	3.6
1	A	317	ASN	3.5
1	A	620	CYS	3.5
1	A	390	TYR	3.4
1	A	322	GLU	3.4
1	A	460	GLY	3.4
1	A	146	PHE	3.3
1	A	663	LEU	3.3
1	A	640	VAL	3.2
1	A	428	CYS	3.2
1	A	462	THR	3.1
1	A	461	LYS	3.1
1	A	459	ASP	3.0
1	A	320	LYS	2.9
1	A	326	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	655	TRP	2.8
1	A	148	PHE	2.7
1	A	89	GLN	2.7
1	A	605	PRO	2.6
1	A	651	ASP	2.5
1	A	456	THR	2.5
1	A	604	ALA	2.5
1	A	119	ASP	2.4
1	A	164	ALA	2.3
1	A	429	CYS	2.3
1	A	162	GLN	2.3
1	A	159	ILE	2.3
1	A	152	GLU	2.3
1	A	268	THR	2.2
1	A	160	ASN	2.2
1	A	444	ASN	2.2
1	A	628	MET	2.2
1	A	426	ASN	2.2
1	A	659	MET	2.2
1	A	649	LEU	2.1
1	A	161	GLY	2.1
1	A	711	SER	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.



Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	A	891	1/1	0.20	8.16	57,57,57,57	0
3	ANP	A	890	31/31	0.16	-0.04	43,45,50,51	0
2	CDP	A	889	25/25	0.14	-1.47	42,47,55,56	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.