



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:01 AM GMT

PDB ID : 3S8C
Title : Structure of Yeast Ribonucleotide Reductase 1 R293A with AMPPNP and CDP
Authors : Ahmad, M.F.; Kaushal, P.S.; Wan, Q.; Wijeratna, S.R.; Huang, M.; Dealwis, C.D.
Deposited on : 2011-05-27
Resolution : 2.77 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

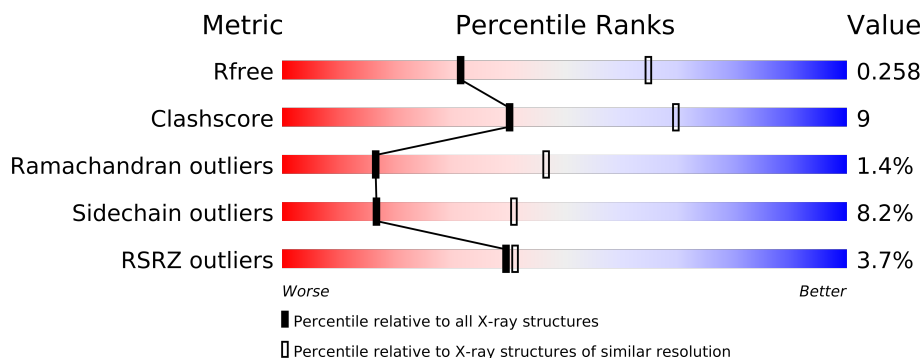
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.77 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	2193 (2.80-2.76)
Clashscore	79885	2751 (2.80-2.76)
Ramachandran outliers	78287	2699 (2.80-2.76)
Sidechain outliers	78261	2701 (2.80-2.76)
RSRZ outliers	66119	2196 (2.80-2.76)

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 ≥ 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
3	MG	A	890	-	X

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 5346 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.

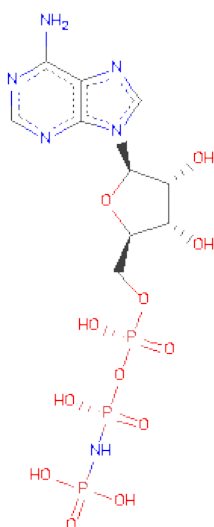
- Molecule 1 is a protein called Ribonucleoside-diphosphatereductase large chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	666	5254	3338	893	992	31	22	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	293	ALA	ARG	ENGINEERED MUTATION	UNP P21524

- Molecule 2 is PHOSPHOAMINOPHOSPHONICACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

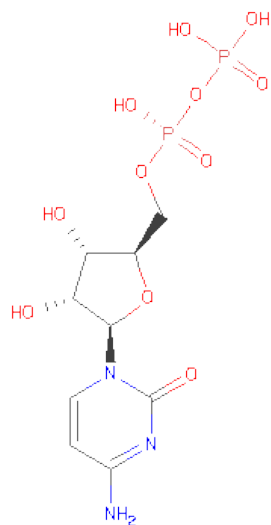


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	10	6	12	3	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is CYTIDINE-5'-DIPHOSPHATE (three-letter code: CDP) (formula: $C_9H_{15}N_3O_{11}P_2$).



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

- Molecule 5 is water.

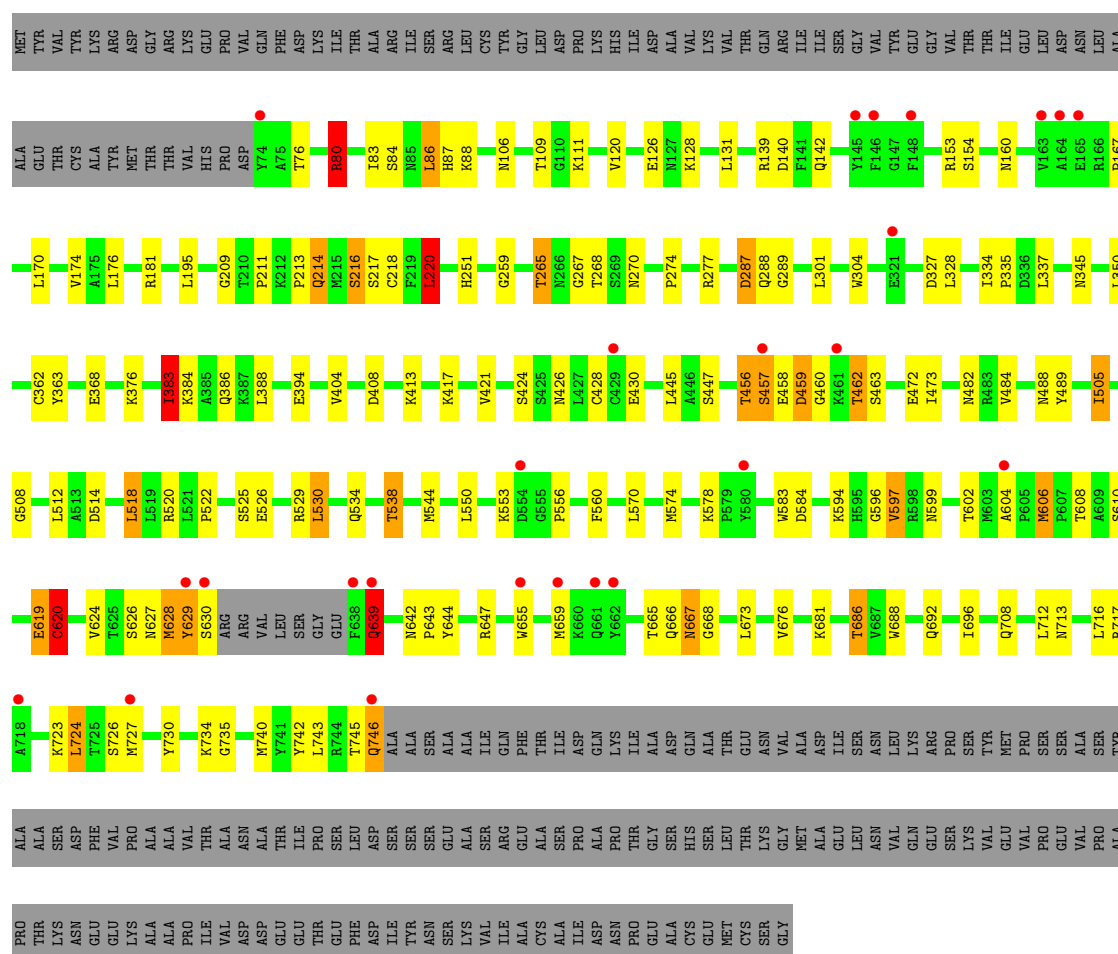
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	35	Total	O	0	0
			35	35		

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 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-diphosphatereductase large chain 1

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.78Å 116.81Å 64.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.29 – 2.77 40.08 – 2.77	Depositor EDS
% Data completeness (in resolution range)	98.3 (40.29-2.77) 98.3 (40.08-2.77)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.256 0.202 , 0.258	Depositor DCC
R_{free} test set	2086 reflections (11.15%)	DCC
Wilson B-factor (Å ²)	52.1	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 22.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 20790 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5346	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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	0.90	6/5373 (0.1%)	0.88	11/7284 (0.2%)

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	A	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	80	ARG	CD-NE	-12.15	1.25	1.46
1	A	620	CYS	CB-SG	-10.46	1.64	1.82
1	A	553	LYS	CB-CG	-9.83	1.26	1.52
1	A	376	LYS	CG-CD	7.94	1.79	1.52
1	A	578	LYS	CG-CD	-6.71	1.29	1.52
1	A	472	GLU	CG-CD	5.68	1.60	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	553	LYS	CA-CB-CG	8.41	131.91	113.40
1	A	584	ASP	CB-CG-OD1	7.17	124.76	118.30
1	A	578	LYS	CB-CG-CD	6.75	129.14	111.60
1	A	594	LYS	CG-CD-CE	-6.46	92.52	111.90
1	A	620	CYS	N-CA-CB	-6.36	99.15	110.60
1	A	594	LYS	CD-CE-NZ	-6.30	97.21	111.70
1	A	220	LEU	CA-CB-CG	6.23	129.63	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	ARG	CD-NE-CZ	-6.15	114.99	123.60
1	A	80	ARG	CG-CD-NE	6.15	124.71	111.80
1	A	383	ILE	CG1-CB-CG2	5.21	122.86	111.40
1	A	376	LYS	CB-CG-CD	-5.12	98.29	111.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	619	GLU	Peptide
1	A	80	ARG	Sidechain

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	5254	0	5133	96	0
2	A	31	0	13	1	0
3	A	1	0	0	0	0
4	A	25	0	12	1	0
5	A	35	0	0	2	0
All	All	5346	0	5158	98	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 9.

All (98) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:724:LEU:HA	1:A:727:MET:HE3	1.43	0.98
1:A:619:GLU:O	1:A:620:CYS:HB3	1.71	0.89
1:A:665:THR:HG23	1:A:666:GLN:HE21	1.43	0.84
1:A:270:ASN:HB3	1:A:274:PRO:HG2	1.62	0.80
1:A:459:ASP:OD1	1:A:460:GLY:N	2.19	0.76
1:A:530:LEU:O	1:A:534:GLN:HG3	1.88	0.74
1:A:417:LYS:HE3	1:A:574:MET:HE1	1.69	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:716:LEU:HD11	1:A:727:MET:HE2	1.72	0.72
1:A:724:LEU:HA	1:A:727:MET:CE	2.22	0.69
1:A:505:ILE:HG22	1:A:602:THR:HA	1.75	0.68
1:A:716:LEU:HD11	1:A:727:MET:CE	2.24	0.68
1:A:345:ASN:HD22	1:A:386:GLN:CD	1.98	0.66
1:A:619:GLU:O	1:A:620:CYS:CB	2.36	0.66
1:A:214:GLN:NE2	1:A:216:SER:H	1.94	0.66
1:A:560:PHE:CZ	1:A:596:GLY:HA2	2.30	0.64
1:A:106:ASN:HB3	1:A:109:THR:HG22	1.80	0.63
1:A:265:THR:HB	1:A:267:GLY:H	1.63	0.63
1:A:214:GLN:HE22	1:A:216:SER:H	1.48	0.62
1:A:109:THR:HG23	1:A:111:LYS:H	1.65	0.62
1:A:251:HIS:HB3	1:A:424:SER:HB3	1.82	0.61
1:A:139:ARG:O	1:A:142:GLN:HG2	2.01	0.60
1:A:383:ILE:HG22	5:A:913:HOH:O	2.01	0.60
1:A:522:PRO:HG2	1:A:525:SER:HB3	1.84	0.59
1:A:686:THR:HG23	1:A:688:TRP:HD1	1.68	0.59
1:A:508:GLY:HA3	1:A:606:MET:HE1	1.87	0.57
1:A:126:GLU:OE1	1:A:181:ARG:NH1	2.33	0.57
1:A:120:VAL:HG21	1:A:209:GLY:HA2	1.85	0.57
1:A:428:CYS:HB2	1:A:430:GLU:OE2	2.05	0.56
1:A:655:TRP:HA	1:A:659:MET:HG3	1.87	0.56
1:A:170:LEU:O	1:A:174:VAL:HG23	2.05	0.56
1:A:534:GLN:O	1:A:538:THR:HG23	2.07	0.55
1:A:447:SER:HB3	1:A:606:MET:CE	2.37	0.55
1:A:619:GLU:HB3	1:A:620:CYS:HB2	1.89	0.54
1:A:220:LEU:HD21	1:A:426:ASN:HB3	1.89	0.54
1:A:334:ILE:HD12	1:A:404:VAL:HG13	1.90	0.53
1:A:482:ASN:HD22	1:A:599:ASN:HD21	1.55	0.53
2:A:889:ANP:H8	2:A:889:ANP:O5'	2.09	0.53
1:A:106:ASN:OD1	1:A:109:THR:HG22	2.09	0.53
1:A:518:LEU:HD13	1:A:644:TYR:CE2	2.44	0.52
1:A:627:ASN:ND2	1:A:668:GLY:O	2.43	0.51
1:A:345:ASN:HD22	1:A:386:GLN:NE2	2.07	0.51
1:A:383:ILE:CG2	5:A:913:HOH:O	2.58	0.51
1:A:383:ILE:CD1	1:A:384:LYS:H	2.23	0.51
1:A:482:ASN:ND2	1:A:599:ASN:HD21	2.09	0.51
1:A:213:PRO:HD2	1:A:489:TYR:HB2	1.93	0.51
1:A:84:SER:O	1:A:88:LYS:HG3	2.10	0.51
1:A:604:ALA:HB2	1:A:708:GLN:HB2	1.92	0.50
1:A:456:THR:O	1:A:458:GLU:HG3	2.11	0.50
1:A:713:ASN:ND2	1:A:742:TYR:HB2	2.27	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:560:PHE:CE2	1:A:596:GLY:HA2	2.47	0.50
1:A:84:SER:HA	1:A:87:HIS:HD2	1.77	0.50
1:A:740:MET:SD	1:A:743:LEU:HB2	2.52	0.49
1:A:692:GLN:O	1:A:696:ILE:HG12	2.13	0.49
1:A:265:THR:HB	1:A:267:GLY:N	2.26	0.49
1:A:106:ASN:HB3	1:A:109:THR:CG2	2.43	0.49
1:A:686:THR:HG23	1:A:688:TRP:CD1	2.47	0.48
1:A:447:SER:HB3	1:A:606:MET:HE3	1.95	0.48
1:A:676:VAL:HB	1:A:681:LYS:HE3	1.96	0.48
1:A:627:ASN:H	1:A:668:GLY:HA3	1.77	0.48
1:A:686:THR:CG2	1:A:688:TRP:HD1	2.25	0.48
1:A:327:ASP:O	1:A:328:LEU:HD23	2.14	0.47
1:A:723:LYS:O	1:A:727:MET:HG3	2.14	0.47
1:A:83:ILE:O	1:A:86:LEU:HB3	2.15	0.47
1:A:217:SER:HB2	1:A:445:LEU:HD13	1.96	0.47
1:A:606:MET:HE3	1:A:608:THR:CG2	2.44	0.47
1:A:526:GLU:OE2	1:A:529:ARG:NH1	2.46	0.46
1:A:544:MET:CE	1:A:570:LEU:HD22	2.45	0.46
1:A:140:ASP:OD2	1:A:167:PRO:HB2	2.14	0.46
1:A:84:SER:HA	1:A:87:HIS:CD2	2.51	0.46
1:A:538:THR:HB	1:A:583:TRP:NE1	2.32	0.45
1:A:334:ILE:HA	1:A:335:PRO:HD2	1.85	0.45
1:A:456:THR:HA	1:A:463:SER:HA	1.99	0.45
1:A:534:GLN:O	1:A:538:THR:CG2	2.65	0.44
1:A:458:GLU:OE1	1:A:462:THR:HB	2.17	0.44
1:A:630:SER:HB2	1:A:639:GLN:NE2	2.32	0.44
1:A:362:CYS:HA	1:A:421:VAL:HG21	1.99	0.43
4:A:891:CDP:H6	4:A:891:CDP:H5'2	1.83	0.43
1:A:550:LEU:HA	1:A:550:LEU:HD23	1.89	0.43
1:A:556:PRO:HA	1:A:597:VAL:O	2.17	0.43
1:A:287:ASP:O	1:A:289:GLY:N	2.51	0.43
1:A:214:GLN:HE21	1:A:488:ASN:HD21	1.67	0.43
1:A:417:LYS:HE3	1:A:574:MET:CE	2.43	0.43
1:A:363:TYR:HB2	1:A:408:ASP:OD1	2.19	0.43
1:A:726:SER:O	1:A:730:TYR:HB2	2.19	0.42
1:A:128:LYS:HB3	1:A:128:LYS:HE2	1.81	0.42
1:A:447:SER:HB3	1:A:606:MET:HE1	2.01	0.42
1:A:716:LEU:HD11	1:A:727:MET:HE1	2.01	0.42
1:A:484:VAL:O	1:A:488:ASN:HB2	2.20	0.41
1:A:211:PRO:O	1:A:213:PRO:HD3	2.21	0.41
1:A:745:THR:HG23	1:A:746:GLN:H	1.85	0.41
1:A:259:GLY:HA2	1:A:268:THR:OG1	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:413:LYS:NZ	1:A:735:GLY:O	2.47	0.41
1:A:538:THR:HB	1:A:583:TRP:HE1	1.85	0.41
1:A:730:TYR:O	1:A:734:LYS:HG2	2.21	0.41
1:A:304:TRP:O	1:A:350:LEU:HA	2.21	0.40
1:A:628:MET:O	1:A:629:TYR:C	2.60	0.40
1:A:642:ASN:HA	1:A:643:PRO:HD3	1.96	0.40
1:A:606:MET:CE	1:A:608:THR:HG23	2.51	0.40

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	662/888 (74%)	622 (94%)	31 (5%)	9 (1%)	16 47

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	457	SER
1	A	459	ASP
1	A	629	TYR
1	A	717	ARG
1	A	287	ASP
1	A	620	CYS
1	A	639	GLN
1	A	667	ASN
1	A	288	GLN

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	562/760 (74%)	516 (92%)	46 (8%)	17	41

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	THR
1	A	80	ARG
1	A	86	LEU
1	A	131	LEU
1	A	153	ARG
1	A	154	SER
1	A	160	ASN
1	A	176	LEU
1	A	195	LEU
1	A	214	GLN
1	A	216	SER
1	A	218	CYS
1	A	220	LEU
1	A	265	THR
1	A	277	ARG
1	A	301	LEU
1	A	337	LEU
1	A	368	GLU
1	A	383	ILE
1	A	388	LEU
1	A	394	GLU
1	A	456	THR
1	A	457	SER
1	A	462	THR
1	A	473	ILE
1	A	505	ILE
1	A	512	LEU
1	A	514	ASP
1	A	518	LEU
1	A	520	ARG
1	A	530	LEU
1	A	538	THR
1	A	597	VAL
1	A	606	MET
1	A	610	SER
1	A	624	VAL
1	A	626	SER
1	A	628	MET

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Mol	Chain	Res	Type
1	A	639	GLN
1	A	647	ARG
1	A	667	ASN
1	A	673	LEU
1	A	686	THR
1	A	712	LEU
1	A	724	LEU
1	A	746	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	GLN
1	A	214	GLN
1	A	251	HIS
1	A	345	ASN
1	A	482	ASN
1	A	613	GLN
1	A	666	GLN
1	A	692	GLN
1	A	713	ASN

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	ANP	A	889	3	33,33,33	3.38	7 (21%)	51,52,52	2.32	14 (27%)
4	CDP	A	891	-	26,26,26	2.07	8 (30%)	37,40,40	1.66	6 (16%)

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	ANP	A	889	3	-	0/18/38/38	0/1/3/3
4	CDP	A	891	-	-	0/14/32/32	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	889	ANP	PB-N3B	13.17	1.75	1.64
2	A	889	ANP	PG-N3B	11.29	1.74	1.64
4	A	891	CDP	C6-N1	4.55	1.43	1.35
2	A	889	ANP	PG-O1G	4.28	1.51	1.46
4	A	891	CDP	C4-N3	4.07	1.43	1.35
4	A	891	CDP	PB-O1B	3.89	1.64	1.51
2	A	889	ANP	PB-O1B	3.61	1.50	1.46
4	A	891	CDP	PA-O3A	3.60	1.66	1.59
4	A	891	CDP	C2-N1	3.58	1.42	1.38
2	A	889	ANP	PB-O3A	3.26	1.63	1.59
2	A	889	ANP	C4-N9	-3.06	1.33	1.37
2	A	889	ANP	C5-C4	2.96	1.47	1.40
4	A	891	CDP	O4'-C1'	2.87	1.45	1.41
4	A	891	CDP	C2-N3	2.53	1.42	1.35
4	A	891	CDP	PB-O3A	2.50	1.64	1.60

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	889	ANP	O1G-PG-N3B	-7.04	101.19	111.83
2	A	889	ANP	PB-N3B-PG	-5.97	120.04	130.07
2	A	889	ANP	N3-C2-N1	-5.45	124.15	128.71
2	A	889	ANP	N3-C4-N9	5.31	135.02	125.43
4	A	891	CDP	O4'-C1'-N1	4.73	118.04	108.06
2	A	889	ANP	O1B-PB-N3B	-4.37	105.22	111.83
2	A	889	ANP	C3'-C2'-C1'	4.11	107.33	100.91
4	A	891	CDP	C2-N3-C4	3.62	120.82	115.57
2	A	889	ANP	C2'-C1'-N9	-3.52	104.24	113.27
2	A	889	ANP	O2B-PB-O1B	3.50	117.96	109.89
4	A	891	CDP	PA-O3A-PB	-3.30	122.00	131.68
4	A	891	CDP	O4'-C1'-C2'	-3.08	102.05	106.77
2	A	889	ANP	PA-O3A-PB	-2.86	122.05	131.81
2	A	889	ANP	C5-C4-N3	-2.75	119.71	125.70
2	A	889	ANP	O4'-C1'-N9	-2.63	106.00	108.44
4	A	891	CDP	O3B-PB-O3A	2.26	115.84	105.14
2	A	889	ANP	C2-N3-C4	2.23	120.37	114.01
4	A	891	CDP	C4'-O4'-C1'	-2.18	107.38	109.75
2	A	889	ANP	O2B-PB-N3B	2.17	112.49	106.61
2	A	889	ANP	C4'-O4'-C1'	2.04	111.97	109.75

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, 95th 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 ²)	Q<0.9
1	A	666/888 (75%)	0.09	25 (3%)	38 40	24, 54, 85, 100	7 (1%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	659	MET	5.6
1	A	146	PHE	4.9
1	A	638	PHE	4.5
1	A	145	TYR	4.2
1	A	629	TYR	3.5
1	A	457	SER	3.5
1	A	718	ALA	3.4
1	A	165	GLU	3.2
1	A	163	VAL	3.1
1	A	164	ALA	2.9
1	A	662	TYR	2.9
1	A	321	GLU	2.6
1	A	727	MET	2.5
1	A	461	LYS	2.5
1	A	639	GLN	2.5
1	A	148	PHE	2.5
1	A	630	SER	2.4
1	A	604	ALA	2.3
1	A	429	CYS	2.2
1	A	580	TYR	2.2
1	A	554	ASP	2.1
1	A	655	TRP	2.1
1	A	661	GLN	2.1
1	A	74	TYR	2.1
1	A	746	GLN	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, 95th 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(Å ²)	Q<0.9
3	MG	A	890	1/1	0.26	101.00	67,67,67,67	0
4	CDP	A	891	25/25	0.24	0.76	64,74,77,79	0
2	ANP	A	889	31/31	0.13	-0.45	53,57,62,63	0

6.5 Other polymers ⓘ

There are no such residues in this entry.