WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 28, 2014 – 10:52 PM GMT

PDB ID : 3TBA
Title : Structure of Yeast Ribonucleotide Reductase 1 Q288A with dGTP and ADP
Authors : Ahmad, M.F.; Kaushal, P.S.; Wan, Q.; Wijeratna, S.R.; Huang, M.; Dealwis, C
Deposited on : 2011-08-05
Resolution : 2.80 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 (i)

The reported resolution of this entry is 2.80 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	Percentile Ranks	Value
Rfree		0.260
Clashscore		9
Ramachandran outliers		1.5%
Sidechain outliers		11.2%
RSRZ outliers		5.0%

Worse   Better

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
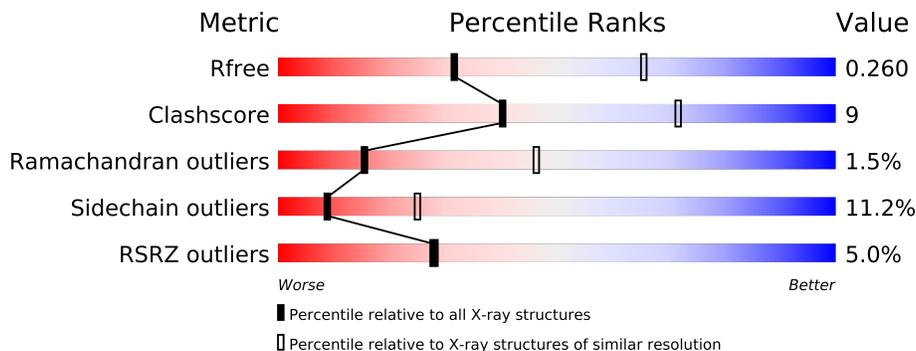
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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
2	MG	A	889	-	X

WORLDWIDE wwPDB PROTEIN DATA BANK

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5354 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	660	5234	3331	889	983	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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0

- Molecule 3 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).
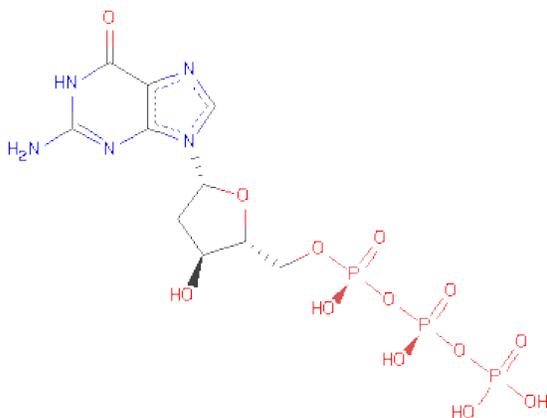
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
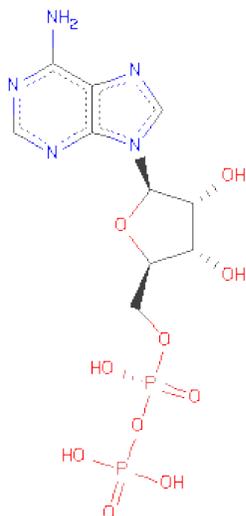
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	61	Total	O	0	0
			61	61		

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:
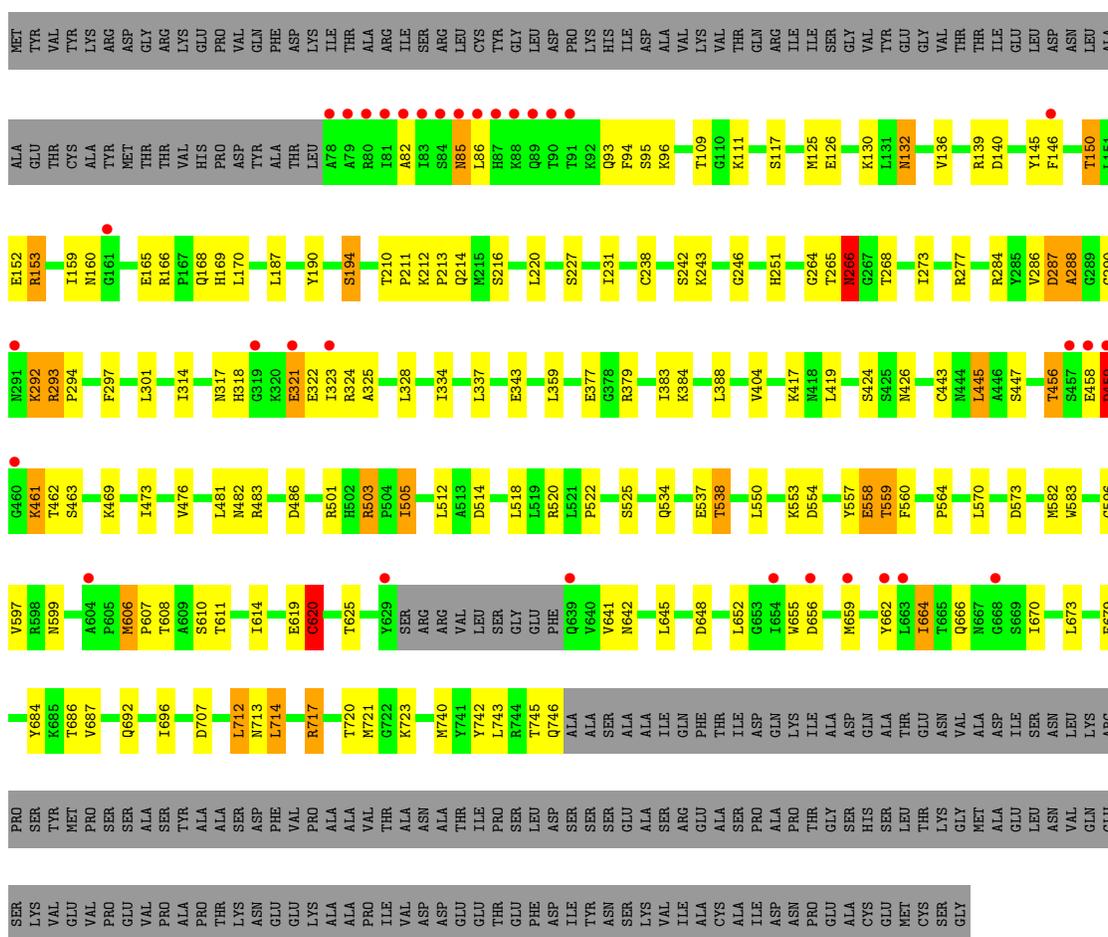
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	107.77Å 118.09Å 67.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.13 – 2.80 41.13 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.1 (41.13-2.80) 96.1 (41.13-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	6.49 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.264 0.195 , 0.260	Depositor DCC
R_{free} test set	2122 reflections (11.20%)	DCC
Wilson B-factor (Å^2)	56.9	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 31.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 21065 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5354	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.37% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]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: MG, ADP, DGT

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	0.61	1/5354 (0.0%)	0.74	5/7255 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	620	CYS	CB-SG	-5.44	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	170	LEU	CA-CB-CG	6.79	130.92	115.30
1	A	620	CYS	CB-CA-C	-5.80	98.81	110.40
1	A	445	LEU	CA-CB-CG	5.68	128.37	115.30
1	A	503	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	712	LEU	CA-CB-CG	5.15	127.15	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	5234	0	5138	96	0
2	A	1	0	0	0	0
3	A	31	0	12	1	0
4	A	27	0	12	4	0
5	A	61	0	0	2	0
All	All	5354	0	5162	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:109:THR:CG2	1:A:111:LYS:HG2	1.99	0.93
1:A:557:TYR:HE1	1:A:559:THR:HG22	1.34	0.93
1:A:109:THR:HG22	1:A:111:LYS:HG2	1.55	0.88
1:A:717:ARG:HB2	5:A:934:HOH:O	1.73	0.87
1:A:557:TYR:CE1	1:A:559:THR:HG22	2.09	0.85
1:A:482:ASN:HD22	1:A:599:ASN:HD21	1.26	0.81
1:A:458:GLU:O	1:A:459:ASP:HB3	1.82	0.78
1:A:619:GLU:O	1:A:620:CYS:CB	2.33	0.77
1:A:481:LEU:HB3	1:A:505:ILE:HD12	1.66	0.77
1:A:153:ARG:HH11	1:A:153:ARG:HB2	1.50	0.76
1:A:619:GLU:O	1:A:620:CYS:HB2	1.83	0.76
1:A:109:THR:HG21	1:A:111:LYS:HG2	1.73	0.70
1:A:140:ASP:OD2	1:A:168:GLN:HG2	1.94	0.67
1:A:538:THR:HB	1:A:583:TRP:HE1	1.59	0.67
1:A:461:LYS:N	1:A:461:LYS:HE3	2.09	0.67
1:A:692:GLN:O	1:A:696:ILE:HD13	1.96	0.66
1:A:447:SER:HB3	1:A:606:MET:CE	2.26	0.66
4:A:891:ADP:H5'2	4:A:891:ADP:H8	1.61	0.65
1:A:287:ASP:HA	1:A:294:PRO:HA	1.80	0.62
1:A:538:THR:HB	1:A:583:TRP:NE1	2.15	0.62
1:A:159:ILE:HG23	1:A:160:ASN:H	1.65	0.62
1:A:159:ILE:HG23	1:A:160:ASN:N	2.14	0.62
1:A:534:GLN:O	1:A:538:THR:HG22	2.01	0.60
1:A:251:HIS:HB3	1:A:424:SER:HB3	1.84	0.59
1:A:288:ALA:O	1:A:292:LYS:HB2	2.02	0.59
1:A:277:ARG:NH2	1:A:322:GLU:HA	2.18	0.58
1:A:238:CYS:O	1:A:242:SER:HB2	2.03	0.57
1:A:745:THR:HG23	1:A:746:GLN:HG3	1.85	0.56
1:A:447:SER:HB3	1:A:606:MET:HE3	1.86	0.56
1:A:486:ASP:CG	1:A:503:ARG:HH22	2.10	0.55
1:A:166:ARG:HB2	1:A:169:HIS:ND1	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:447:SER:HB3	1:A:606:MET:HE1	1.89	0.54
1:A:655:TRP:HA	1:A:659:MET:HG3	1.89	0.54
1:A:277:ARG:NH2	1:A:321:GLU:O	2.41	0.53
1:A:456:THR:HA	1:A:463:SER:HA	1.90	0.52
1:A:220:LEU:HD21	1:A:426:ASN:HB3	1.91	0.52
1:A:286:VAL:O	1:A:286:VAL:HG12	2.08	0.52
1:A:220:LEU:CD2	1:A:426:ASN:HB3	2.40	0.52
1:A:662:TYR:CD1	1:A:673:LEU:HG	2.44	0.52
1:A:377:GLU:OE1	1:A:379:ARG:NH1	2.35	0.52
1:A:550:LEU:HD23	1:A:553:LYS:NZ	2.25	0.51
1:A:85:ASN:C	1:A:85:ASN:HD22	2.14	0.51
1:A:334:ILE:HD12	1:A:404:VAL:HG13	1.91	0.51
1:A:714:LEU:HD22	1:A:740:MET:HG3	1.93	0.51
1:A:251:HIS:HD2	5:A:894:HOH:O	1.93	0.50
1:A:95:SER:H	1:A:132:ASN:HD21	1.60	0.49
1:A:159:ILE:CG2	1:A:160:ASN:H	2.24	0.49
1:A:168:GLN:NE2	1:A:190:TYR:OH	2.43	0.49
1:A:560:PHE:CZ	1:A:596:GLY:HA2	2.48	0.48
1:A:461:LYS:HE3	1:A:461:LYS:H	1.78	0.48
1:A:277:ARG:HH21	1:A:322:GLU:HA	1.79	0.48
1:A:642:ASN:HB3	1:A:645:LEU:HB3	1.95	0.48
1:A:159:ILE:CG2	1:A:160:ASN:N	2.77	0.48
1:A:625:THR:HA	1:A:687:VAL:HG12	1.96	0.48
1:A:94:PHE:HD1	1:A:169:HIS:HD2	1.60	0.47
1:A:606:MET:HB2	1:A:607:PRO:CD	2.45	0.47
1:A:656:ASP:H	1:A:659:MET:HB2	1.79	0.47
1:A:662:TYR:CZ	1:A:666:GLN:HG3	2.50	0.47
1:A:570:LEU:O	1:A:573:ASP:HB2	2.14	0.47
1:A:292:LYS:C	1:A:293:ARG:HG3	2.35	0.47
1:A:662:TYR:CZ	1:A:666:GLN:CG	2.98	0.47
1:A:93:GLN:HG3	1:A:132:ASN:OD1	2.14	0.47
1:A:648:ASP:O	1:A:652:LEU:HD23	2.14	0.47
1:A:662:TYR:CD1	1:A:662:TYR:O	2.68	0.47
1:A:264:GLY:HA3	3:A:890:DGT:O2B	2.15	0.47
1:A:117:SER:HB3	1:A:211:PRO:HA	1.97	0.46
1:A:537:GLU:OE1	1:A:582:MET:HB2	2.16	0.46
1:A:419:LEU:HD21	1:A:559:THR:HG21	1.98	0.46
4:A:891:ADP:C8	4:A:891:ADP:H5'2	2.47	0.46
1:A:227:SER:O	1:A:231:ILE:HG13	2.16	0.45
1:A:608:THR:N	4:A:891:ADP:O2A	2.51	0.44
1:A:611:THR:HA	1:A:614:ILE:HD12	2.00	0.44
1:A:740:MET:HE1	1:A:743:LEU:HD23	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:417:LYS:HD2	1:A:564:PRO:HG3	1.98	0.44
1:A:501:ARG:HA	1:A:558:GLU:OE1	2.17	0.43
1:A:165:GLU:HG2	1:A:169:HIS:HB2	2.00	0.43
1:A:383:ILE:HA	1:A:383:ILE:HD12	1.86	0.43
1:A:212:LYS:HA	1:A:213:PRO:HD3	1.62	0.43
1:A:82:ALA:HA	1:A:85:ASN:OD1	2.19	0.42
1:A:550:LEU:HD23	1:A:553:LYS:HZ1	1.85	0.42
1:A:740:MET:CE	1:A:743:LEU:HD23	2.49	0.42
1:A:210:THR:HB	1:A:211:PRO:CD	2.50	0.42
1:A:318:HIS:O	1:A:324:ARG:NH1	2.53	0.42
1:A:210:THR:HB	1:A:211:PRO:HD2	2.02	0.41
1:A:713:ASN:HD22	1:A:742:TYR:H	1.68	0.41
1:A:146:PHE:O	1:A:150:THR:OG1	2.38	0.41
1:A:419:LEU:HD21	1:A:559:THR:CG2	2.50	0.41
1:A:265:THR:O	1:A:266:ASN:C	2.59	0.41
1:A:664:ILE:HG13	1:A:664:ILE:H	1.72	0.41
1:A:190:TYR:O	1:A:194:SER:OG	2.39	0.41
1:A:608:THR:HA	4:A:891:ADP:O2A	2.21	0.41
1:A:522:PRO:HG2	1:A:525:SER:HB3	2.02	0.41
1:A:670:ILE:HD11	1:A:684:TYR:HB2	2.02	0.41
1:A:136:VAL:HB	1:A:139:ARG:HD2	2.03	0.40
1:A:297:PHE:HB2	1:A:328:LEU:HD22	2.01	0.40
1:A:266:ASN:HA	1:A:266:ASN:HD22	1.73	0.40
1:A:287:ASP:O	1:A:288:ALA:C	2.60	0.40
1:A:85:ASN:ND2	1:A:86:LEU:N	2.70	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	656/888 (74%)	602 (92%)	44 (7%)	10 (2%)	15	46

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	459	ASP
1	A	287	ASP
1	A	288	ALA
1	A	290	GLY
1	A	145	TYR
1	A	246	GLY
1	A	266	ASN
1	A	620	CYS
1	A	325	ALA
1	A	717	ARG

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%)	499 (89%)	63 (11%)	9	25

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	96	LYS
1	A	125	MET
1	A	126	GLU
1	A	130	LYS
1	A	132	ASN
1	A	150	THR
1	A	152	GLU
1	A	153	ARG
1	A	187	LEU
1	A	194	SER
1	A	214	GLN
1	A	216	SER
1	A	243	LYS
1	A	266	ASN
1	A	268	THR
1	A	273	ILE
1	A	284	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	292	LYS
1	A	293	ARG
1	A	301	LEU
1	A	314	ILE
1	A	317	ASN
1	A	321	GLU
1	A	323	ILE
1	A	337	LEU
1	A	343	GLU
1	A	359	LEU
1	A	384	LYS
1	A	388	LEU
1	A	443	CYS
1	A	445	LEU
1	A	456	THR
1	A	459	ASP
1	A	461	LYS
1	A	462	THR
1	A	469	LYS
1	A	473	ILE
1	A	476	VAL
1	A	483	ARG
1	A	505	ILE
1	A	512	LEU
1	A	514	ASP
1	A	518	LEU
1	A	520	ARG
1	A	538	THR
1	A	554	ASP
1	A	558	GLU
1	A	559	THR
1	A	597	VAL
1	A	606	MET
1	A	610	SER
1	A	620	CYS
1	A	641	VAL
1	A	664	ILE
1	A	679	GLU
1	A	686	THR
1	A	707	ASP
1	A	712	LEU
1	A	714	LEU

Continued from previous page...

Mol	Chain	Res	Type
1	A	720	THR
1	A	721	MET
1	A	723	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	168	GLN
1	A	214	GLN
1	A	251	HIS
1	A	266	ASN
1	A	270	ASN
1	A	482	ASN
1	A	613	GLN
1	A	675	ASN
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	#$|Z| > 2$
3	DGT	A	890	2	33,33,33	1.50	3 (9%)	49,52,52	2.57	10 (20%)
4	ADP	A	891	-	29,29,29	1.26	4 (13%)	45,45,45	1.81	6 (13%)

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
3	DGT	A	890	2	-	0/20/34/34	0/1/3/3
4	ADP	A	891	-	-	0/16/32/32	0/1/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	890	DGT	C6-C5	5.30	1.49	1.41
4	A	891	ADP	C5-C4	3.57	1.48	1.40
3	A	890	DGT	C2-N3	3.32	1.37	1.33
3	A	890	DGT	C5-C4	3.24	1.47	1.40
4	A	891	ADP	PA-O3A	2.60	1.64	1.59
4	A	891	ADP	PB-O3A	2.42	1.64	1.60
4	A	891	ADP	C4-N9	-2.07	1.34	1.37

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	890	DGT	C6-C5-N7	12.76	135.86	134.14
4	A	891	ADP	N3-C2-N1	-7.24	122.65	128.71
3	A	890	DGT	N3-C4-N9	6.41	136.31	126.91
4	A	891	ADP	N3-C4-N9	5.14	134.72	125.43
3	A	890	DGT	C5-C4-N3	-5.08	118.58	125.94
3	A	890	DGT	C2-N3-C4	3.88	120.54	115.09
3	A	890	DGT	C8-N9-C4	3.61	109.66	106.90
3	A	890	DGT	C4-C5-N7	-3.33	106.67	109.52
4	A	891	ADP	C5-C4-N3	-3.13	118.89	125.70
4	A	891	ADP	C4-C5-N7	-2.96	106.99	109.52
4	A	891	ADP	C3'-C2'-C1'	2.83	105.34	100.91
4	A	891	ADP	C2-N3-C4	2.69	121.68	114.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	890	DGT	PA-O3A-PB	-2.52	124.29	131.68
3	A	890	DGT	C2'-C1'-N9	-2.51	107.57	114.08
3	A	890	DGT	PB-O3B-PG	-2.24	125.10	131.68
3	A	890	DGT	O2G-PG-O3G	2.03	117.06	110.44

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	660/888 (74%)	-0.04	33 (5%)	28	28	35, 51, 87, 118	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	81	ILE	7.2
1	A	82	ALA	6.2
1	A	78	ALA	6.2
1	A	87	HIS	5.0
1	A	79	ALA	4.8
1	A	85	ASN	4.5
1	A	659	MET	4.2
1	A	291	ASN	4.2
1	A	662	TYR	4.1
1	A	460	GLY	4.0
1	A	86	LEU	3.8
1	A	459	ASP	3.7
1	A	89	GLN	3.6
1	A	88	LYS	3.5
1	A	323	ILE	3.4
1	A	90	THR	3.2
1	A	83	ILE	3.2
1	A	161	GLY	2.8
1	A	457	SER	2.8
1	A	84	SER	2.8
1	A	146	PHE	2.5
1	A	639	GLN	2.4
1	A	319	GLY	2.4
1	A	91	THR	2.4
1	A	663	LEU	2.4
1	A	80	ARG	2.4
1	A	321	GLU	2.3

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	654	ILE	2.2
1	A	629	TYR	2.2
1	A	458	GLU	2.1
1	A	668	GLY	2.0
1	A	656	ASP	2.0
1	A	604	ALA	2.0

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
2	MG	A	889	1/1	0.24	17.00	69,69,69,69	0
4	ADP	A	891	27/27	0.20	-0.25	78,83,84,84	0
3	DGT	A	890	31/31	0.12	-0.88	44,49,60,62	0

6.5 Other polymers ⓘ

There are no such residues in this entry.