



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:54 PM GMT

PDB ID : 3S87  
Title : Structure of Yeast Ribonucleotide Reductase 1 with dGTP and ADP  
Authors : Ahmad, M.F.; Kaushal, P.S.; Wan, Q.; Wijeratna, S.R.; Huang, M.; Dealwis, C.D.  
Deposited on : 2011-05-27  
Resolution : 2.25 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

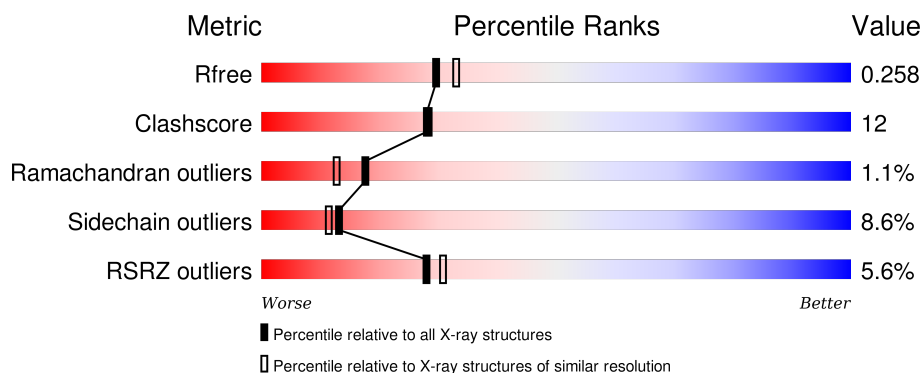
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5544 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.

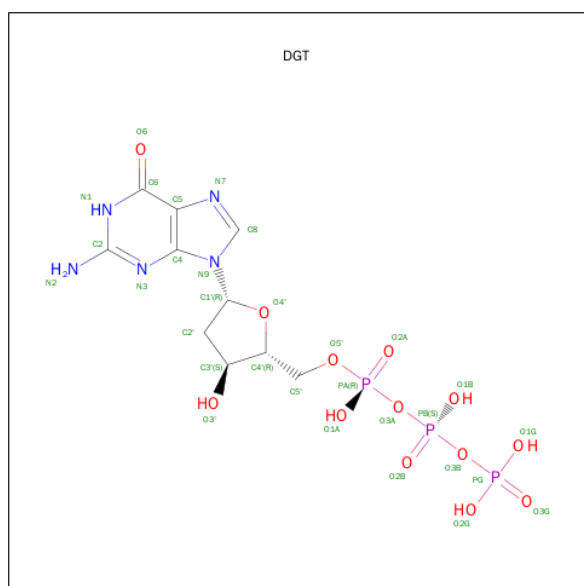
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase large chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	664	Total	C	N	O	S	0	0	0
			5283	3362	897	993	31			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

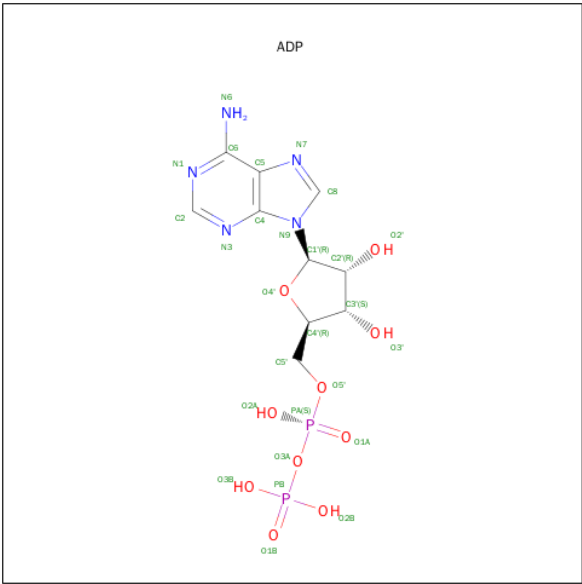
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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		

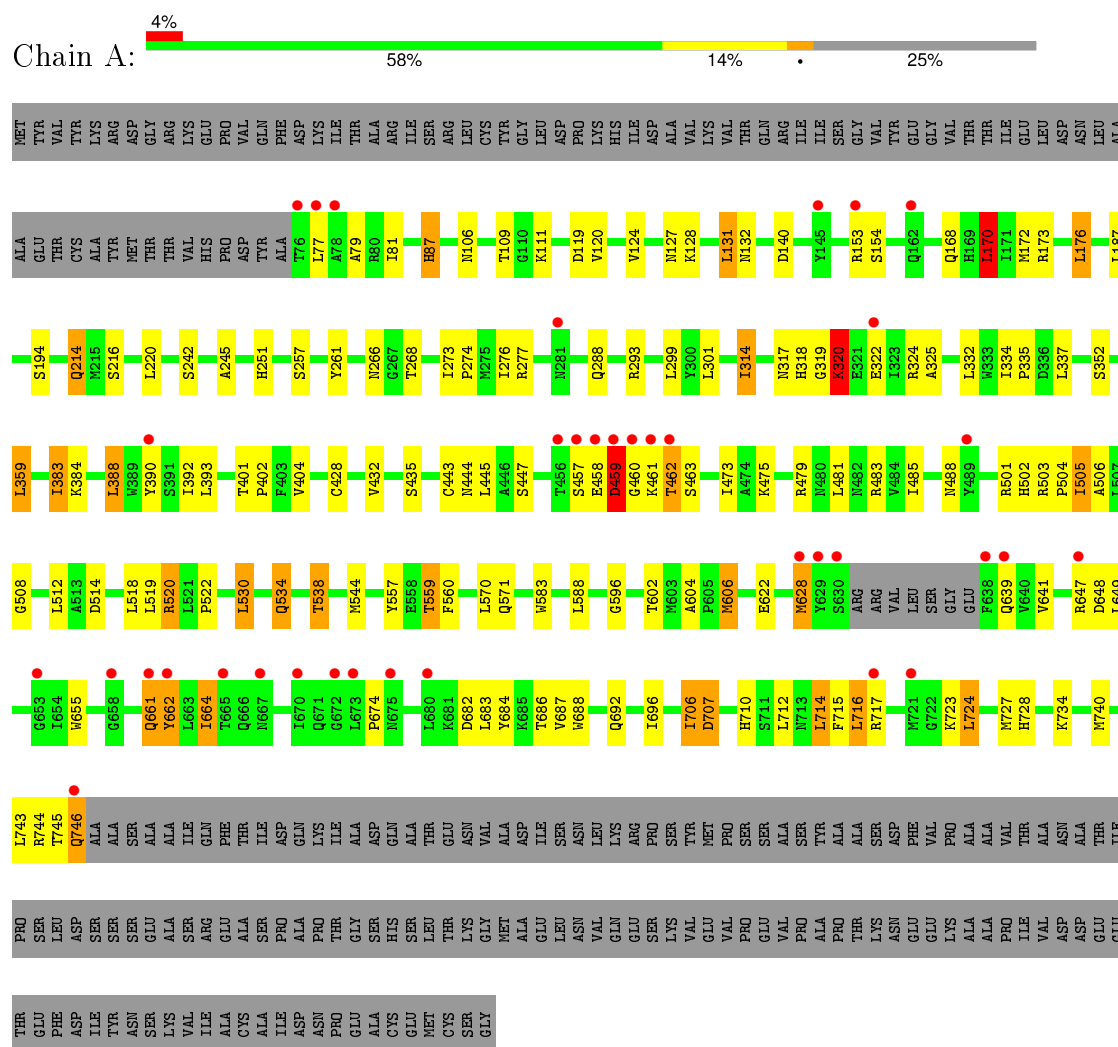
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	202	Total	O	0	0
			202	202		

### 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-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, $\alpha$ , $\beta$ , $\gamma$	107.62Å 117.19Å 65.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25 19.53 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.25) 99.7 (19.53-2.25)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.54 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.204 , 0.261 0.208 , 0.258	Depositor DCC
$R_{free}$ test set	4022 reflections (11.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.5	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 35.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 39922 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5544	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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

### 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	0.68	0/5404	0.75	4/7320 (0.1%)

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	5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	359	LEU	CA-CB-CG	5.55	128.06	115.30
1	A	359	LEU	CB-CG-CD1	5.26	119.94	111.00
1	A	707	ASP	CB-CG-OD1	-5.25	113.58	118.30
1	A	170	LEU	CA-CB-CG	5.16	127.17	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	318	HIS	Peptide
1	A	459	ASP	Peptide
1	A	460	GLY	Peptide
1	A	461	LYS	Peptide
1	A	706	ILE	Peptide

## 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	5283	0	5194	124	0
2	A	1	0	0	0	0
3	A	31	0	12	0	0
4	A	27	0	12	1	0
5	A	202	0	0	15	0
All	All	5544	0	5218	124	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 12.

All (124) 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:106:ASN:OD1	1:A:109:THR:HG22	1.54	1.08
1:A:706:ILE:HG13	5:A:965:HOH:O	1.59	1.01
1:A:508:GLY:HA3	1:A:606:MET:HE1	1.49	0.92
1:A:445:LEU:HD22	1:A:506:ALA:HB3	1.54	0.90
1:A:393:LEU:HD22	1:A:724:LEU:HD13	1.55	0.87
1:A:686:THR:HG22	1:A:688:TRP:H	1.41	0.83
1:A:710:HIS:HD2	5:A:1092:HOH:O	1.63	0.81
1:A:706:ILE:CD1	5:A:965:HOH:O	2.28	0.79
1:A:706:ILE:CG1	5:A:965:HOH:O	2.23	0.78
1:A:534:GLN:O	1:A:538:THR:HG22	1.84	0.78
1:A:457:SER:HB3	1:A:462:THR:HG22	1.64	0.78
1:A:723:LYS:HG3	5:A:929:HOH:O	1.84	0.76
1:A:314:ILE:HG12	1:A:325:ALA:HB3	1.66	0.76
1:A:538:THR:HB	1:A:583:TRP:HE1	1.53	0.73
1:A:106:ASN:OD1	1:A:109:THR:CG2	2.35	0.73
1:A:724:LEU:HA	1:A:727:MET:HE3	1.71	0.73
1:A:662:TYR:CD1	1:A:662:TYR:O	2.43	0.71
1:A:538:THR:HB	1:A:583:TRP:NE1	2.06	0.70
1:A:109:THR:HG23	1:A:111:LYS:H	1.56	0.70
1:A:485:ILE:HD11	1:A:505:ILE:CD1	2.22	0.69
1:A:459:ASP:C	1:A:459:ASP:OD2	2.30	0.69
1:A:501:ARG:HG2	1:A:501:ARG:HH11	1.58	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:MET:SD	1:A:743:LEU:HB2	2.33	0.67
1:A:485:ILE:HD11	1:A:505:ILE:HD12	1.77	0.67
1:A:319:GLY:O	1:A:320:LYS:HB2	1.94	0.66
1:A:706:ILE:HD11	5:A:965:HOH:O	1.93	0.65
1:A:557:TYR:CD1	1:A:559:THR:HG22	2.32	0.65
1:A:505:ILE:HG22	1:A:602:THR:HA	1.78	0.64
1:A:502:HIS:ND1	1:A:559:THR:HG21	2.12	0.64
1:A:501:ARG:HG2	1:A:501:ARG:NH1	2.12	0.64
1:A:273:ILE:HB	1:A:274:PRO:HD3	1.80	0.64
1:A:214:GLN:HE22	1:A:216:SER:HB2	1.63	0.63
1:A:745:THR:O	1:A:746:GLN:HB2	1.98	0.63
1:A:520:ARG:HH22	1:A:648:ASP:CG	2.02	0.63
1:A:168:GLN:HE22	1:A:194:SER:HB2	1.65	0.62
1:A:522:PRO:HB3	1:A:682:ASP:O	2.00	0.62
1:A:716:LEU:HG	1:A:727:MET:HE1	1.80	0.61
1:A:534:GLN:O	1:A:538:THR:CG2	2.48	0.61
1:A:746:GLN:HA	5:A:926:HOH:O	2.00	0.61
1:A:710:HIS:CD2	5:A:1092:HOH:O	2.46	0.61
1:A:332:LEU:HD11	1:A:392:ILE:HD12	1.82	0.60
1:A:557:TYR:CE1	1:A:559:THR:HG22	2.36	0.60
1:A:447:SER:HB3	1:A:606:MET:HE3	1.85	0.59
1:A:485:ILE:CD1	1:A:505:ILE:CD1	2.81	0.59
1:A:170:LEU:HD22	1:A:173:ARG:NH2	2.19	0.58
1:A:314:ILE:CG1	1:A:325:ALA:HB3	2.33	0.57
1:A:140:ASP:OD2	1:A:168:GLN:HG2	2.05	0.57
1:A:475:LYS:O	1:A:479:ARG:HG3	2.05	0.56
1:A:724:LEU:HA	1:A:727:MET:CE	2.34	0.56
1:A:622:GLU:HG3	5:A:932:HOH:O	2.05	0.56
1:A:483:ARG:HD3	5:A:949:HOH:O	2.06	0.55
1:A:686:THR:HG22	1:A:687:VAL:N	2.22	0.55
1:A:277:ARG:HD2	1:A:322:GLU:O	2.06	0.55
1:A:242:SER:O	1:A:288:GLN:HA	2.07	0.55
1:A:251:HIS:HD2	5:A:1080:HOH:O	1.88	0.54
1:A:444:ASN:C	1:A:445:LEU:HD23	2.28	0.54
1:A:457:SER:CB	1:A:462:THR:HG22	2.37	0.54
1:A:458:GLU:O	1:A:459:ASP:HB3	2.08	0.54
1:A:692:GLN:O	1:A:696:ILE:HG12	2.08	0.54
1:A:383:ILE:CG1	1:A:384:LYS:H	2.22	0.53
1:A:428:CYS:SG	4:A:1002:ADP:H3'	2.49	0.53
1:A:683:LEU:HD23	1:A:684:TYR:CZ	2.45	0.52
1:A:686:THR:CG2	1:A:687:VAL:N	2.73	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:THR:HB	1:A:402:PRO:HA	1.92	0.51
1:A:662:TYR:O	1:A:662:TYR:HD1	1.94	0.51
1:A:481:LEU:HB3	1:A:505:ILE:CG1	2.40	0.51
1:A:686:THR:HG22	1:A:688:TRP:N	2.20	0.51
1:A:459:ASP:O	1:A:459:ASP:OD2	2.30	0.49
1:A:692:GLN:NE2	1:A:715:PHE:H	2.10	0.48
1:A:530:LEU:O	1:A:534:GLN:HG2	2.13	0.48
1:A:504:PRO:O	1:A:505:ILE:HD12	2.13	0.48
1:A:481:LEU:HB3	1:A:505:ILE:HG13	1.95	0.48
1:A:170:LEU:C	1:A:170:LEU:CD1	2.82	0.48
1:A:127:ASN:HB2	1:A:131:LEU:HD22	1.96	0.47
1:A:724:LEU:HD21	1:A:740:MET:HE1	1.96	0.47
1:A:257:SER:OG	1:A:352:SER:HB2	2.15	0.47
1:A:560:PHE:CZ	1:A:596:GLY:HA2	2.50	0.47
1:A:170:LEU:C	1:A:170:LEU:HD13	2.35	0.47
1:A:508:GLY:HA3	1:A:606:MET:CE	2.34	0.47
1:A:501:ARG:CG	1:A:501:ARG:HH11	2.27	0.46
1:A:557:TYR:HD1	1:A:559:THR:HG22	1.79	0.46
1:A:393:LEU:CD2	1:A:724:LEU:HD13	2.38	0.46
1:A:388:LEU:O	1:A:392:ILE:HG12	2.15	0.46
1:A:214:GLN:HE21	1:A:488:ASN:HD21	1.63	0.46
1:A:79:ALA:C	1:A:81:ILE:H	2.19	0.46
1:A:288:GLN:HG3	1:A:293:ARG:O	2.16	0.45
1:A:570:LEU:O	1:A:571:GLN:C	2.55	0.45
1:A:649:LEU:HB3	1:A:655:TRP:HB2	1.98	0.45
1:A:744:ARG:NH1	5:A:977:HOH:O	2.50	0.45
1:A:503:ARG:N	1:A:504:PRO:CD	2.79	0.45
1:A:322:GLU:HG2	5:A:935:HOH:O	2.16	0.45
1:A:544:MET:HB2	1:A:588:LEU:HD21	1.98	0.45
1:A:734:LYS:HA	1:A:734:LYS:HD2	1.82	0.45
1:A:686:THR:HG21	1:A:688:TRP:HD1	1.82	0.45
1:A:519:LEU:O	1:A:520:ARG:HB2	2.17	0.45
1:A:332:LEU:CD1	1:A:392:ILE:HD12	2.46	0.45
1:A:383:ILE:HD12	1:A:384:LYS:H	1.80	0.45
1:A:276:ILE:HD12	1:A:299:LEU:HD13	1.99	0.44
1:A:383:ILE:CG1	1:A:384:LYS:N	2.80	0.44
1:A:664:ILE:HG13	5:A:1044:HOH:O	2.17	0.44
1:A:383:ILE:CD1	1:A:384:LYS:H	2.30	0.44
1:A:661:GLN:HG2	5:A:1044:HOH:O	2.17	0.43
1:A:696:ILE:HD11	1:A:714:LEU:HD11	1.99	0.43
1:A:485:ILE:CD1	1:A:505:ILE:HD11	2.49	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LYS:O	1:A:132:ASN:HB2	2.19	0.43
1:A:683:LEU:HD23	1:A:684:TYR:CE1	2.54	0.43
1:A:724:LEU:HD22	1:A:728:HIS:NE2	2.34	0.42
1:A:251:HIS:HE1	1:A:435:SER:OG	2.03	0.42
1:A:508:GLY:CA	1:A:606:MET:HE1	2.33	0.42
1:A:334:ILE:HD12	1:A:404:VAL:HG13	2.02	0.42
1:A:481:LEU:CB	1:A:505:ILE:HG12	2.50	0.41
1:A:334:ILE:HG22	1:A:335:PRO:O	2.20	0.41
1:A:481:LEU:HB3	1:A:505:ILE:HG12	2.02	0.41
1:A:383:ILE:HG13	1:A:384:LYS:H	1.85	0.41
1:A:120:VAL:O	1:A:124:VAL:HG23	2.20	0.41
1:A:686:THR:HG21	1:A:688:TRP:CD1	2.56	0.41
1:A:716:LEU:HG	1:A:727:MET:CE	2.49	0.41
1:A:131:LEU:HD12	1:A:131:LEU:HA	1.94	0.41
1:A:261:TYR:HE2	1:A:266:ASN:HD22	1.67	0.41
1:A:87:HIS:HE1	1:A:140:ASP:OD1	2.05	0.41
1:A:557:TYR:HE1	1:A:559:THR:CG2	2.34	0.40
1:A:628:MET:SD	1:A:664:ILE:HG23	2.62	0.40
1:A:172:MET:HG3	1:A:176:LEU:HD22	2.04	0.40
1:A:506:ALA:HB1	1:A:604:ALA:HB3	2.03	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	660/888 (74%)	620 (94%)	33 (5%)	7 (1%)	17 13

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	320	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	459	ASP
1	A	662	TYR
1	A	674	PRO
1	A	707	ASP
1	A	245	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	569/761 (75%)	520 (91%)	49 (9%)	13	11

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LEU
1	A	87	HIS
1	A	119	ASP
1	A	131	LEU
1	A	153	ARG
1	A	154	SER
1	A	170	LEU
1	A	176	LEU
1	A	187	LEU
1	A	214	GLN
1	A	220	LEU
1	A	268	THR
1	A	301	LEU
1	A	314	ILE
1	A	317	ASN
1	A	320	LYS
1	A	324	ARG
1	A	337	LEU
1	A	359	LEU
1	A	383	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	388	LEU
1	A	390	TYR
1	A	432	VAL
1	A	443	CYS
1	A	459	ASP
1	A	462	THR
1	A	463	SER
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	534	GLN
1	A	538	THR
1	A	559	THR
1	A	606	MET
1	A	628	MET
1	A	639	GLN
1	A	641	VAL
1	A	647	ARG
1	A	661	GLN
1	A	664	ILE
1	A	712	LEU
1	A	714	LEU
1	A	716	LEU
1	A	724	LEU
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	87	HIS
1	A	168	GLN
1	A	214	GLN
1	A	251	HIS
1	A	266	ASN
1	A	270	ASN
1	A	317	ASN
1	A	534	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	561	GLN
1	A	613	GLN
1	A	692	GLN
1	A	710	HIS
1	A	713	ASN

### 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](#)

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	1001	2	25,33,33	1.11	2 (8%)	35,52,52	1.52	6 (17%)
4	ADP	A	1002	-	22,29,29	1.01	1 (4%)	27,45,45	2.42	6 (22%)

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	1001	2	-	0/18/34/34	0/3/3/3
4	ADP	A	1002	-	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	DGT	C6-C5	2.97	1.47	1.41
3	A	1001	DGT	C5-C4	2.99	1.47	1.40
4	A	1002	ADP	C5-C4	3.22	1.47	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	ADP	N3-C2-N1	-8.48	122.40	128.89
4	A	1002	ADP	C2'-C1'-N9	-6.13	104.92	114.29
3	A	1001	DGT	C6-C5-C4	-3.11	117.19	120.90
3	A	1001	DGT	C5-C6-N1	-3.10	119.35	123.59
4	A	1002	ADP	O3A-PA-O5'	-3.04	94.88	102.94
3	A	1001	DGT	PA-O3A-PB	-2.92	124.52	132.73
3	A	1001	DGT	N3-C2-N1	-2.84	123.12	127.44
4	A	1002	ADP	C1'-N9-C4	-2.84	122.66	126.94
3	A	1001	DGT	PB-O3B-PG	-2.25	125.12	132.67
4	A	1002	ADP	O3B-PB-O1B	2.06	117.20	110.58
4	A	1002	ADP	C2-N1-C6	2.47	123.19	118.77
3	A	1001	DGT	C6-N1-C2	4.21	121.78	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	ADP	1	0

## 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	664/888 (74%)	0.10	37 (5%)	28 31	27, 41, 79, 96	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	638	PHE	7.0
1	A	630	SER	5.9
1	A	458	GLU	4.8
1	A	459	ASP	4.8
1	A	77	LEU	4.8
1	A	629	TYR	4.3
1	A	672	GLY	4.3
1	A	457	SER	4.2
1	A	717	ARG	4.2
1	A	76	THR	4.1
1	A	390	TYR	4.1
1	A	746	GLN	4.0
1	A	661	GLN	3.5
1	A	462	THR	3.5
1	A	460	GLY	3.4
1	A	489	TYR	3.4
1	A	639	GLN	3.3
1	A	665	THR	3.1
1	A	145	TYR	3.0
1	A	673	LEU	2.9
1	A	653	GLY	2.9
1	A	153	ARG	2.8
1	A	628	MET	2.7
1	A	78	ALA	2.6
1	A	667	ASN	2.6
1	A	162	GLN	2.5
1	A	322	GLU	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	658	GLY	2.3
1	A	647	ARG	2.3
1	A	721	MET	2.3
1	A	281	ASN	2.3
1	A	461	LYS	2.2
1	A	675	ASN	2.1
1	A	456	THR	2.1
1	A	670	ILE	2.1
1	A	680	LEU	2.1
1	A	662	TYR	2.1

## 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](#)

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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ADP	A	1002	27/27	0.97	0.09	-0.72	35,39,41,43	0
3	DGT	A	1001	31/31	0.96	0.09	-0.80	29,32,37,39	0
2	MG	A	2001	1/1	0.98	0.03	-	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.