



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:30 PM GMT

PDB ID : 1XJJ  
Title : Structural mechanism of allosteric substrate specificity in a ribonucleotide reductase: dGTP complex  
Authors : Larsson, K.-M.; Jordan, A.; Eliasson, R.; Reichard, P.; Logan, D.T.; Nordlund, P.  
Deposited on : 2004-09-23  
Resolution : 1.86 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.

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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 : 1.7 (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

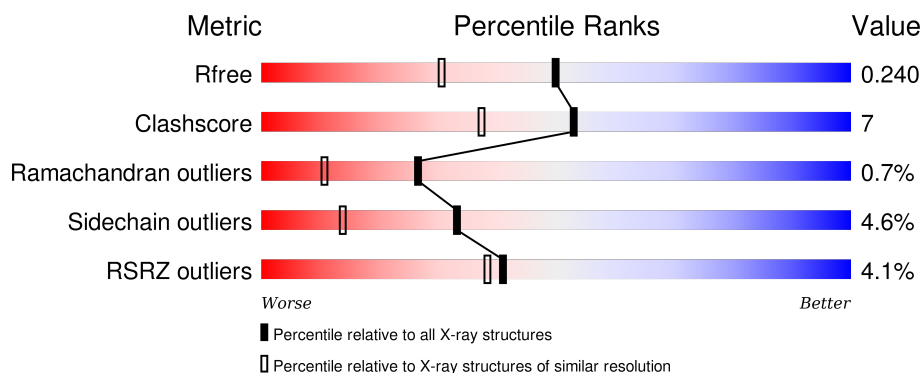
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.86 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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	644	<div> <div>3%</div> <div>81%</div> <div>14%</div> <div>• •</div> </div>
1	B	644	<div> <div>4%</div> <div>78%</div> <div>14%</div> <div>• 5%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10591 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 ribonucleotide reductase, B12-dependent.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	623	Total	C	N	O	S	0	0	0
			5005	3208	848	929	20			
1	B	611	Total	C	N	O	S	0	0	0
			4910	3149	833	908	20			

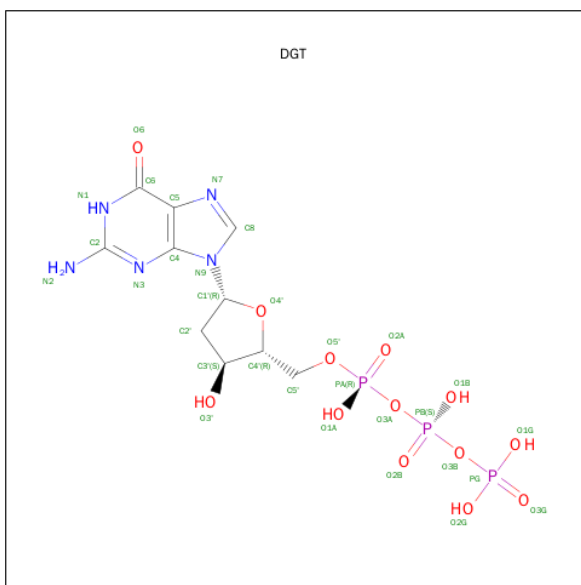
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	SER	TYR	SEE REMARK 999	UNP O33839
B	205	SER	TYR	SEE REMARK 999	UNP O33839

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
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 31	C 10	N 5	O 13	P 3	0	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

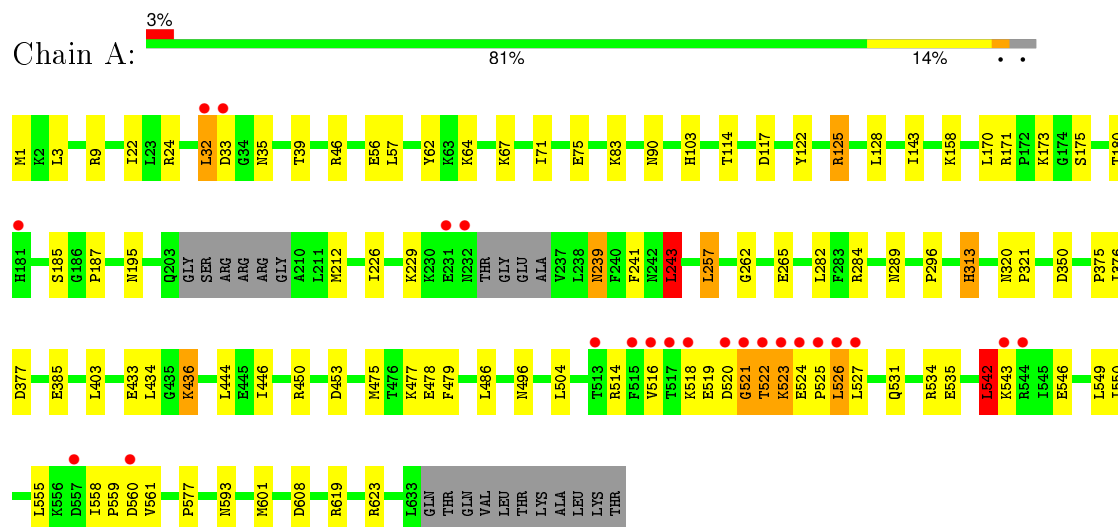
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	292	Total O 292 292	0	0
4	B	258	Total O 258 258	0	0

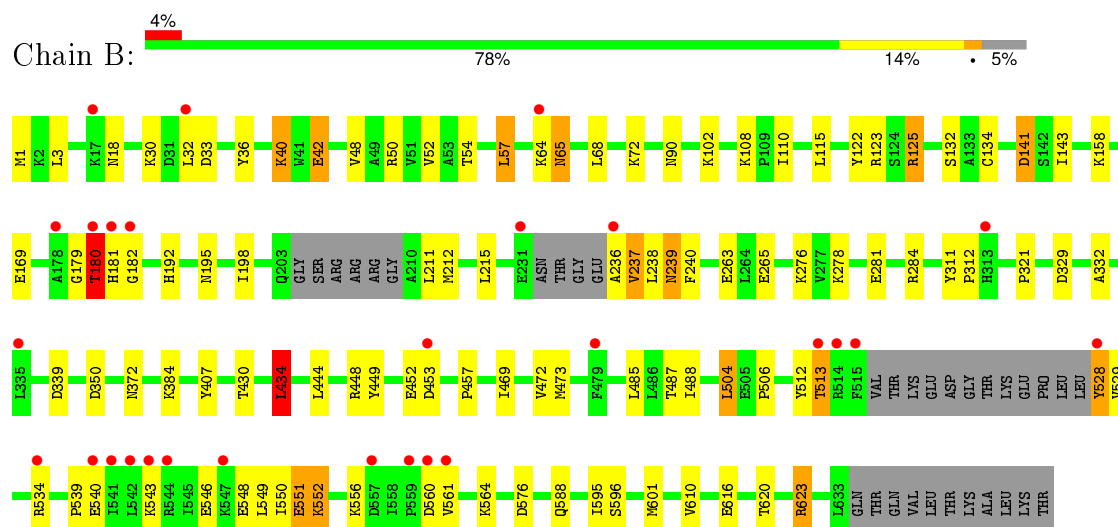
### 3 Residue-property plots [i](#)

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: ribonucleotide reductase, B12-dependent



- Molecule 1: ribonucleotide reductase, B12-dependent



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.07Å 123.88Å 106.30Å 90.00° 103.70° 90.00°	Depositor
Resolution (Å)	42.26 – 1.86 42.08 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.26-1.86) 99.9 (42.08-1.86)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.196 , 0.241 0.195 , 0.240	Depositor DCC
$R_{free}$ test set	6217 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 124129 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10591	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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, 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	0.87	0/5104	0.87	7/6891 (0.1%)
1	B	0.83	0/5007	0.89	7/6758 (0.1%)
All	All	0.85	0/10111	0.88	14/13649 (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	B	0	2

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	623	ARG	NE-CZ-NH1	14.35	127.48	120.30
1	B	623	ARG	NE-CZ-NH2	-12.18	114.21	120.30
1	A	623	ARG	NE-CZ-NH1	-7.38	116.61	120.30
1	A	377	ASP	CB-CG-OD1	6.68	124.31	118.30
1	B	125	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	243	LEU	CB-CG-CD1	5.46	120.27	111.00
1	A	125	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	B	576	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	329	ASP	CB-CG-OD1	-5.25	113.57	118.30
1	B	141	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	125	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	403	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	B	434	LEU	CB-CG-CD1	5.07	119.61	111.00
1	A	542	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	237	VAL	Peptide
1	B	560	ASP	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	5005	0	5057	64	0
1	B	4910	0	4958	75	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	62	0	24	0	0
3	B	62	0	24	0	0
4	A	292	0	0	6	0
4	B	258	0	0	3	0
All	All	10591	0	10063	133	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 7.

All (133) 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:522:THR:HB	1:A:523:LYS:HA	1.41	1.02
1:A:128:LEU:HD13	1:B:179:GLY:HA2	1.47	0.95
1:B:180:THR:HG22	1:B:181:HIS:H	1.30	0.94
1:B:487:THR:O	1:B:488:ILE:HD13	1.64	0.94
1:A:128:LEU:CD1	1:B:179:GLY:HA2	2.00	0.92
1:B:449:TYR:HE1	1:B:473:MET:CE	1.83	0.91
1:B:195:ASN:HD21	1:B:240:PHE:H	1.14	0.87
1:B:449:TYR:HE1	1:B:473:MET:HE1	1.40	0.85
1:B:551:GLU:O	1:B:552:LYS:HB2	1.78	0.81
1:B:512:TYR:O	1:B:513:THR:HG23	1.81	0.80
1:A:542:LEU:O	1:A:546:GLU:HG3	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:GLU:OE1	4:A:1262:HOH:O	2.05	0.75
1:B:64:LYS:O	1:B:65:ASN:HB2	1.88	0.72
1:A:522:THR:CB	1:A:523:LYS:HA	2.18	0.72
1:B:1:MET:HB3	1:B:350:ASP:OD2	1.89	0.72
1:B:239:ASN:H	1:B:239:ASN:HD22	1.37	0.71
1:B:180:THR:HG22	1:B:181:HIS:N	2.04	0.70
1:A:524:GLU:HG2	1:A:525:PRO:HD2	1.74	0.70
1:A:619:ARG:NH1	4:A:1204:HOH:O	2.26	0.69
1:A:241:PHE:HB3	1:A:243:LEU:HD13	1.75	0.69
1:B:457:PRO:HD3	1:B:473:MET:CE	2.24	0.68
1:A:1:MET:HB3	1:A:350:ASP:OD2	1.96	0.66
1:B:180:THR:CG2	1:B:181:HIS:H	2.09	0.65
1:B:623:ARG:HD2	4:B:1017:HOH:O	1.97	0.64
1:B:263:GLU:HG2	1:B:278:LYS:HD3	1.80	0.64
1:A:475:MET:O	1:A:478:GLU:HG2	1.98	0.64
1:B:449:TYR:CE1	1:B:473:MET:CE	2.74	0.63
1:B:122:TYR:O	1:B:125:ARG:HD3	1.99	0.63
1:B:212:MET:HB2	1:B:321:PRO:HA	1.81	0.62
1:B:449:TYR:CE1	1:B:473:MET:HE1	2.30	0.62
1:B:192:HIS:HE1	1:B:236:ALA:O	1.82	0.62
1:A:24:ARG:HH22	1:A:39:THR:HB	1.64	0.62
1:B:449:TYR:HE1	1:B:473:MET:HE3	1.65	0.60
1:A:284:ARG:NH2	1:A:608:ASP:OD1	2.27	0.59
1:B:18:ASN:ND2	1:B:528:TYR:OH	2.35	0.59
1:B:457:PRO:HD3	1:B:473:MET:HE1	1.83	0.59
1:A:549:LEU:HD13	1:A:555:LEU:HD23	1.84	0.59
1:A:226:ILE:HG22	1:A:289:ASN:HD22	1.67	0.58
1:B:539:PRO:O	1:B:540:GLU:HB2	2.03	0.58
1:A:257:LEU:HD22	1:A:262:GLY:HA3	1.85	0.58
1:B:601:MET:HE1	1:B:610:VAL:HG22	1.85	0.58
1:B:64:LYS:HE3	1:B:115:LEU:HD21	1.86	0.58
1:B:449:TYR:CE1	1:B:473:MET:HE3	2.39	0.57
1:A:577:PRO:HG3	1:A:601:MET:HG2	1.86	0.57
1:A:128:LEU:HD11	1:B:179:GLY:HA2	1.84	0.57
1:A:518:LYS:H	1:A:522:THR:CG2	2.18	0.57
1:B:40:LYS:HB3	1:B:40:LYS:NZ	2.20	0.57
1:B:265:GLU:OE1	1:B:276:LYS:HG2	2.05	0.56
1:A:195:ASN:HD21	1:A:239:ASN:ND2	2.04	0.55
1:B:180:THR:CG2	1:B:181:HIS:N	2.67	0.55
1:B:548:GLU:O	1:B:551:GLU:O	2.23	0.55
1:B:40:LYS:CB	1:B:40:LYS:NZ	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:GLY:HA3	1:A:522:THR:O	2.06	0.54
1:A:212:MET:HB2	1:A:321:PRO:HA	1.89	0.54
1:B:50:ARG:NH1	1:B:108:LYS:O	2.37	0.54
1:A:229:LYS:HG3	1:A:243:LEU:HD22	1.90	0.54
1:A:313:HIS:HD2	1:A:446:ILE:HD12	1.73	0.53
1:B:64:LYS:O	1:B:65:ASN:CB	2.57	0.53
1:B:601:MET:CE	1:B:610:VAL:HG22	2.39	0.52
1:A:523:LYS:HB3	1:A:524:GLU:HA	1.90	0.52
1:B:195:ASN:ND2	1:B:240:PHE:H	1.96	0.52
1:A:239:ASN:HD22	1:A:239:ASN:H	1.57	0.52
1:B:457:PRO:HD3	1:B:473:MET:HE2	1.93	0.51
1:A:516:VAL:HG23	1:A:526:LEU:HD22	1.94	0.50
1:A:103:HIS:HE1	4:A:1191:HOH:O	1.94	0.50
1:B:134:CYS:O	1:B:332:ALA:HA	2.12	0.50
1:B:488:ILE:HG21	1:B:504:LEU:HG	1.93	0.50
1:A:453:ASP:HA	4:A:1233:HOH:O	2.13	0.49
1:A:433:GLU:CA	1:A:436:LYS:HE3	2.43	0.49
1:B:453:ASP:HA	4:B:1211:HOH:O	2.12	0.49
1:A:128:LEU:HD13	1:B:179:GLY:CA	2.32	0.49
1:B:469:ILE:O	1:B:473:MET:HG2	2.14	0.48
1:B:239:ASN:N	1:B:239:ASN:HD22	2.09	0.48
1:B:430:THR:HG22	1:B:434:LEU:HD22	1.95	0.48
1:A:143:ILE:HG13	1:B:158:LYS:HD2	1.95	0.48
1:B:50:ARG:NH2	1:B:108:LYS:O	2.46	0.48
1:A:433:GLU:HA	1:A:436:LYS:HE3	1.95	0.47
1:A:46:ARG:HH21	1:A:75:GLU:HG2	1.78	0.47
1:B:30:LYS:HE2	1:B:36:TYR:CE1	2.49	0.47
1:A:56:GLU:HB2	1:A:71:ILE:HG12	1.95	0.47
1:B:529:VAL:HB	1:B:534:ARG:NH2	2.30	0.47
1:B:448:ARG:O	1:B:452:GLU:HB2	2.15	0.46
1:A:313:HIS:CD2	1:A:446:ILE:HD12	2.51	0.46
1:A:122:TYR:O	1:A:125:ARG:HD3	2.15	0.46
1:B:311:TYR:CD1	1:B:312:PRO:HA	2.51	0.46
1:A:531:GLN:HE21	1:A:534:ARG:HH21	1.62	0.46
1:A:62:TYR:HB2	1:A:67:LYS:HE3	1.97	0.46
1:B:54:THR:O	1:B:57:LEU:HB2	2.15	0.45
1:A:22:ILE:CD1	1:A:496:ASN:HB3	2.47	0.45
1:B:68:LEU:O	1:B:72:LYS:HG3	2.17	0.45
1:A:320:ASN:HB2	1:A:321:PRO:HD2	1.99	0.44
1:A:375:PRO:C	1:A:376:ILE:HG13	2.38	0.44
1:B:265:GLU:OE2	1:B:276:LYS:HE3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:HD12	1:A:187:PRO:HA	1.99	0.44
1:B:588:GLN:HB2	1:B:595:ILE:HD12	1.99	0.44
1:A:450:ARG:HA	1:A:477:LYS:HG3	1.99	0.44
1:A:33:ASP:HB2	1:A:35:ASN:HD22	1.83	0.43
1:B:72:LYS:O	1:B:110:ILE:HD11	2.18	0.43
1:B:237:VAL:HA	1:B:238:LEU:HB2	1.99	0.43
1:A:478:GLU:HG3	1:A:479:PHE:CD2	2.54	0.43
1:A:527:LEU:CD1	1:A:550:ILE:HD11	2.47	0.43
1:A:527:LEU:HD12	1:A:550:ILE:HD11	1.99	0.43
1:A:114:THR:O	1:A:117:ASP:HB2	2.18	0.43
1:B:616:GLU:O	1:B:620:THR:HG23	2.19	0.43
1:A:226:ILE:HG22	1:A:289:ASN:ND2	2.32	0.43
1:B:181:HIS:HB3	1:B:182:GLY:HA2	2.00	0.42
1:A:9:ARG:NH2	4:A:1095:HOH:O	2.52	0.42
1:A:83:LYS:NZ	4:A:1202:HOH:O	2.53	0.42
1:B:384:LYS:HG3	4:B:1123:HOH:O	2.19	0.42
1:A:523:LYS:H	1:A:524:GLU:CB	2.32	0.42
1:A:486:LEU:O	1:A:593:ASN:HB2	2.20	0.42
1:A:313:HIS:N	1:A:313:HIS:ND1	2.68	0.41
1:B:546:GLU:O	1:B:550:ILE:HG13	2.19	0.41
1:B:215:LEU:HA	1:B:215:LEU:HD12	1.90	0.41
1:B:469:ILE:O	1:B:472:VAL:HG12	2.20	0.41
1:A:32:LEU:H	1:A:32:LEU:HG	1.69	0.41
1:B:239:ASN:ND2	1:B:239:ASN:H	2.09	0.41
1:A:173:LYS:HG3	1:A:185:SER:O	2.20	0.41
1:B:339:ASP:C	1:B:339:ASP:OD1	2.59	0.41
1:A:518:LYS:H	1:A:522:THR:HG22	1.85	0.41
1:B:40:LYS:HG3	1:B:42:GLU:HG2	2.02	0.41
1:B:198:ILE:HG13	1:B:211:LEU:HD11	2.03	0.41
1:A:518:LYS:O	1:A:522:THR:HG23	2.21	0.41
1:A:158:LYS:HD2	1:B:143:ILE:HG13	2.03	0.41
1:A:171:ARG:HG3	1:A:175:SER:HB2	2.02	0.41
1:A:22:ILE:HD13	1:A:496:ASN:HB3	2.03	0.41
1:B:588:GLN:CD	1:B:623:ARG:HD3	2.41	0.41
1:B:141:ASP:HB2	1:B:169:GLU:O	2.20	0.40
1:A:558:ILE:HA	1:A:559:PRO:HD2	1.96	0.40
1:B:48:VAL:O	1:B:52:VAL:HG23	2.21	0.40
1:B:132:SER:OG	1:B:372:ASN:ND2	2.53	0.40
1:B:407:TYR:CZ	1:B:506:PRO:HD3	2.56	0.40
1:A:433:GLU:O	1:A:436:LYS:HE3	2.22	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	617/644 (96%)	595 (96%)	20 (3%)	2 (0%)	46	29
1	B	603/644 (94%)	574 (95%)	23 (4%)	6 (1%)	19	6
All	All	1220/1288 (95%)	1169 (96%)	43 (4%)	8 (1%)	26	11

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	65	ASN
1	B	180	THR
1	B	32	LEU
1	B	513	THR
1	B	552	LYS
1	A	522	THR
1	B	556	LYS
1	A	521	GLY

### 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	550/566 (97%)	523 (95%)	27 (5%)	31	12
1	B	538/566 (95%)	515 (96%)	23 (4%)	35	16
All	All	1088/1132 (96%)	1038 (95%)	50 (5%)	33	14

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	32	LEU
1	A	57	LEU
1	A	64	LYS
1	A	90	ASN
1	A	180	THR
1	A	239	ASN
1	A	243	LEU
1	A	257	LEU
1	A	265	GLU
1	A	282	LEU
1	A	296	PRO
1	A	313	HIS
1	A	434	LEU
1	A	436	LYS
1	A	444	LEU
1	A	504	LEU
1	A	514	ARG
1	A	519	GLU
1	A	520	ASP
1	A	523	LYS
1	A	526	LEU
1	A	535	GLU
1	A	542	LEU
1	A	543	LYS
1	A	560	ASP
1	A	561	VAL
1	B	3	LEU
1	B	33	ASP
1	B	40	LYS
1	B	42	GLU
1	B	57	LEU
1	B	90	ASN
1	B	102	LYS
1	B	123	ARG
1	B	180	THR
1	B	239	ASN
1	B	281	GLU
1	B	284	ARG
1	B	434	LEU
1	B	444	LEU
1	B	485	LEU
1	B	504	LEU

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Mol	Chain	Res	Type
1	B	528	TYR
1	B	543	LYS
1	B	549	LEU
1	B	551	GLU
1	B	561	VAL
1	B	564	LYS
1	B	596	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	127	HIS
1	A	181	HIS
1	A	239	ASN
1	A	345	ASN
1	A	355	GLN
1	A	359	GLN
1	A	531	GLN
1	A	584	GLN
1	A	603	GLN
1	B	18	ASN
1	B	127	HIS
1	B	192	HIS
1	B	195	ASN
1	B	239	ASN
1	B	345	ASN
1	B	346	ASN
1	B	359	GLN
1	B	464	ASN
1	B	584	GLN
1	B	603	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](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	1.72	5 (20%)	35,52,52	1.78	8 (22%)
3	DGT	A	1003	-	25,33,33	1.53	3 (12%)	35,52,52	2.02	14 (40%)
3	DGT	B	1002	2	25,33,33	1.50	3 (12%)	35,52,52	2.18	9 (25%)
3	DGT	B	1004	-	25,33,33	1.55	3 (12%)	35,52,52	1.77	8 (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
3	DGT	A	1003	-	-	0/18/34/34	0/3/3/3
3	DGT	B	1002	2	-	0/18/34/34	0/3/3/3
3	DGT	B	1004	-	-	0/18/34/34	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	DGT	PG-O1G	-2.59	1.45	1.54
3	A	1001	DGT	C6-C5	-2.01	1.37	1.41
3	A	1003	DGT	PG-O3G	2.06	1.57	1.51
3	B	1002	DGT	C2-N1	2.10	1.39	1.35
3	A	1001	DGT	PG-O3G	2.55	1.59	1.51
3	B	1002	DGT	C6-N1	2.71	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1004	DGT	PG-O3G	3.16	1.61	1.51
3	A	1001	DGT	C6-N1	3.23	1.39	1.33
3	B	1004	DGT	C2-N1	3.57	1.41	1.35
3	B	1002	DGT	PG-O3G	3.72	1.63	1.51
3	A	1003	DGT	C2-N1	3.78	1.42	1.35
3	A	1001	DGT	C2-N1	4.39	1.43	1.35
3	B	1004	DGT	C6-N1	4.89	1.42	1.33
3	A	1003	DGT	C6-N1	5.03	1.42	1.33

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1002	DGT	PA-O3A-PB	-5.61	116.98	132.73
3	A	1003	DGT	N3-C2-N1	-5.23	119.47	127.44
3	B	1002	DGT	C2'-C1'-N9	-4.99	102.02	114.16
3	B	1004	DGT	N3-C2-N1	-4.96	119.89	127.44
3	B	1002	DGT	N3-C2-N1	-4.79	120.15	127.44
3	A	1001	DGT	N3-C2-N1	-4.41	120.72	127.44
3	B	1002	DGT	C5-C6-N1	-3.81	118.38	123.59
3	A	1003	DGT	O4'-C4'-C5'	-3.60	96.43	109.32
3	A	1001	DGT	O3A-PA-O5'	-3.57	93.46	102.94
3	A	1003	DGT	C1'-N9-C4	-3.56	121.13	127.16
3	B	1004	DGT	C5-C6-N1	-3.49	118.82	123.59
3	A	1001	DGT	C5-C6-N1	-3.43	118.91	123.59
3	B	1002	DGT	C6-C5-C4	-3.08	117.22	120.90
3	A	1003	DGT	PB-O3B-PG	-2.94	122.81	132.67
3	A	1001	DGT	PA-O3A-PB	-2.94	124.47	132.73
3	A	1003	DGT	C5-C6-N1	-2.94	119.57	123.59
3	B	1004	DGT	C4'-O4'-C1'	-2.91	102.11	109.47
3	A	1003	DGT	O4'-C1'-N9	-2.79	102.88	107.72
3	B	1002	DGT	PB-O3B-PG	-2.73	123.52	132.67
3	A	1001	DGT	C2'-C1'-N9	-2.64	107.75	114.16
3	B	1002	DGT	O4'-C1'-C2'	-2.59	101.10	106.27
3	A	1003	DGT	C4-C5-N7	-2.47	107.21	109.48
3	A	1003	DGT	C6-C5-C4	-2.25	118.20	120.90
3	A	1003	DGT	O1G-PG-O3G	-2.18	103.56	110.58
3	A	1003	DGT	C4'-O4'-C1'	-2.13	104.08	109.47
3	B	1004	DGT	O4'-C1'-C2'	-2.07	102.14	106.27
3	A	1001	DGT	O2G-PG-O3G	-2.01	104.10	110.58
3	A	1003	DGT	O1A-PA-O3A	2.03	114.29	105.09
3	A	1003	DGT	O2G-PG-O3B	2.19	115.01	105.09
3	A	1001	DGT	C6-N1-C2	2.35	119.20	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	DGT	C6-N1-C2	2.39	119.26	115.94
3	B	1004	DGT	C6-N1-C2	2.48	119.38	115.94
3	B	1004	DGT	O1A-PA-O3A	2.57	116.75	105.09
3	A	1003	DGT	O2G-PG-O1G	2.74	117.80	107.38
3	B	1004	DGT	O2G-PG-O1G	2.91	118.47	107.38
3	A	1001	DGT	O2G-PG-O1G	3.29	119.90	107.38
3	B	1002	DGT	O2G-PG-O1G	3.40	120.33	107.38
3	B	1002	DGT	C6-N1-C2	3.43	120.70	115.94
3	B	1004	DGT	O4'-C1'-N9	3.59	113.94	107.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	623/644 (96%)	-0.10	22 (3%)	48 45	15, 27, 56, 88	0
1	B	611/644 (94%)	0.02	28 (4%)	36 34	17, 29, 59, 75	0
All	All	1234/1288 (95%)	-0.04	50 (4%)	41 38	15, 28, 58, 88	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	521	GLY	6.9
1	A	516	VAL	6.5
1	B	236	ALA	5.8
1	A	523	LYS	5.6
1	A	517	THR	5.3
1	A	522	THR	5.0
1	A	515	PHE	5.0
1	A	520	ASP	4.6
1	B	515	PHE	4.5
1	B	559	PRO	4.4
1	A	526	LEU	4.2
1	A	524	GLU	4.0
1	A	560	ASP	4.0
1	B	181	HIS	4.0
1	B	528	TYR	3.8
1	A	527	LEU	3.7
1	A	525	PRO	3.5
1	B	453	ASP	3.3
1	A	232	ASN	3.2
1	B	231	GLU	3.0
1	B	182	GLY	3.0
1	B	547	LYS	2.9
1	B	514	ARG	2.9
1	A	32	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	231	GLU	2.7
1	B	540	GLU	2.7
1	B	561	VAL	2.7
1	B	180	THR	2.7
1	B	557	ASP	2.6
1	B	64	LYS	2.6
1	B	544	ARG	2.6
1	A	33	ASP	2.5
1	A	518	LYS	2.5
1	B	32	LEU	2.5
1	B	560	ASP	2.5
1	A	513	THR	2.3
1	B	543	LYS	2.3
1	B	541	ILE	2.3
1	B	513	THR	2.3
1	B	542	LEU	2.2
1	A	181	HIS	2.2
1	A	557	ASP	2.2
1	B	534	ARG	2.1
1	A	543	LYS	2.1
1	B	479	PHE	2.1
1	B	178	ALA	2.1
1	B	313	HIS	2.1
1	A	544	ARG	2.1
1	B	335	LEU	2.1
1	B	17	LYS	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](#)

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
3	DGT	A	1003	31/31	0.94	0.14	0.86	26,63,75,75	0
3	DGT	B	1004	31/31	0.93	0.14	0.19	33,62,73,74	0
3	DGT	B	1002	31/31	0.96	0.08	-0.56	14,21,44,44	0
3	DGT	A	1001	31/31	0.98	0.06	-0.76	17,25,32,34	0
2	MG	A	1006	1/1	0.99	0.02	-	26,26,26,26	0
2	MG	B	1005	1/1	0.95	0.08	-	36,36,36,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.