



# Full wwPDB X-ray Structure Validation Report

Oct 22, 2014 – 06:11 AM EDT

PDB ID : 4TO2  
Title : Structure basis of cellular dNTP regulation, SAMHD1-dGTP-dGTP-dGTP/  
dTTPcomplex  
Authors : Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.  
Deposited on : 2014-06-05  
Resolution : 2.27 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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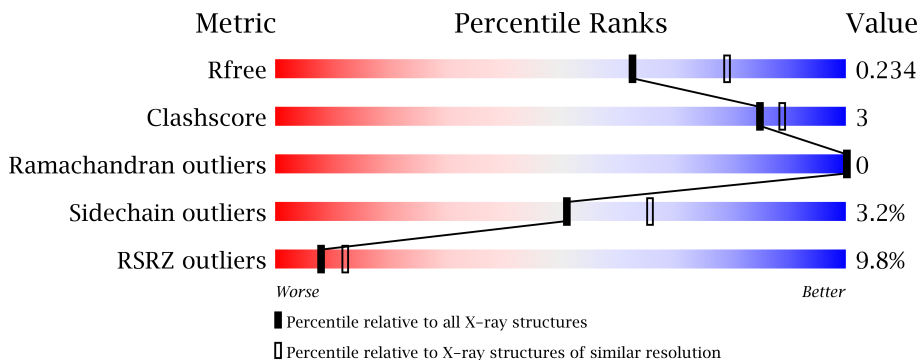
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable24103  
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) : stable24103

# 1 Overall quality at a glance

The reported resolution of this entry is 2.27 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	3861 (2.30-2.26)
Clashscore	79885	4801 (2.30-2.26)
Ramachandran outliers	78287	4729 (2.30-2.26)
Sidechain outliers	78261	4728 (2.30-2.26)
RSRZ outliers	66119	3864 (2.30-2.26)

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	514	
1	B	514	
1	C	514	
1	D	514	

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	C	705	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16367 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 Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	1	0
			3939	2520	686	712	21			
1	B	481	Total	C	N	O	S	0	1	0
			3939	2520	686	712	21			
1	C	481	Total	C	N	O	S	0	1	0
			3939	2520	686	712	21			
1	D	481	Total	C	N	O	S	0	1	0
			3939	2520	686	712	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
B	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
D	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
D	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3

- Molecule 2 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



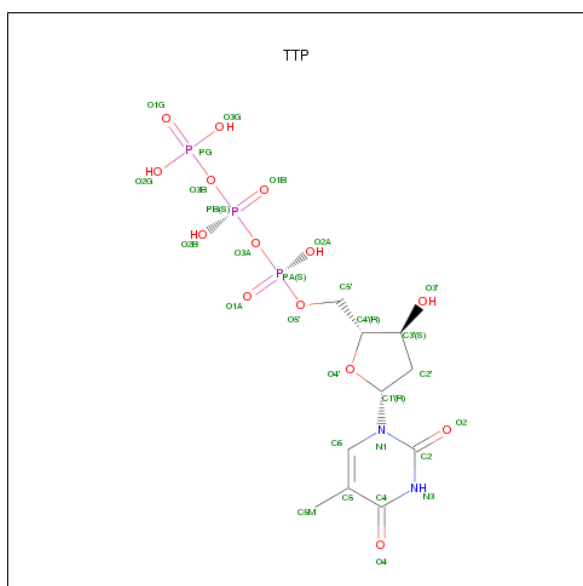
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula:  $C_{10}H_{17}N_2O_{14}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 5 is water.

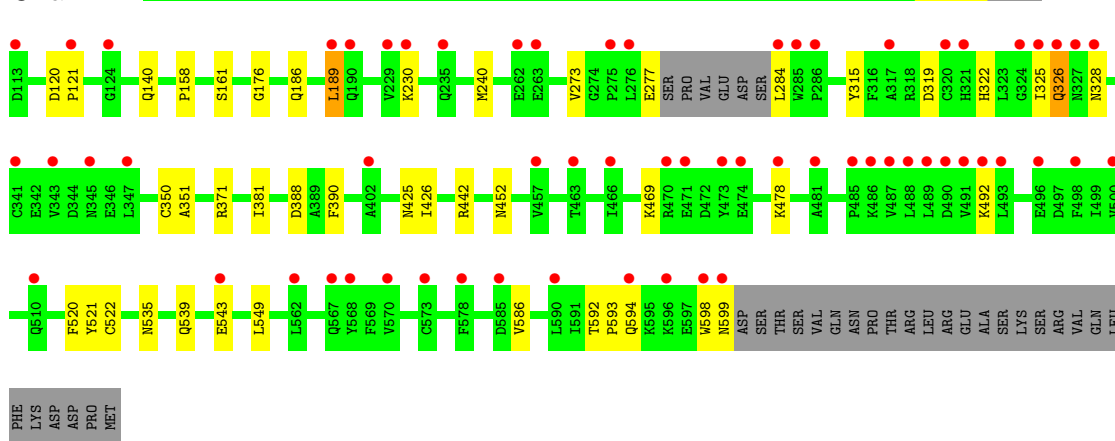
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	52	Total	O	0	0
			52	52		
5	B	56	Total	O	0	0
			56	56		
5	C	40	Total	O	0	0
			40	40		
5	D	85	Total	O	0	0
			85	85		

### 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.

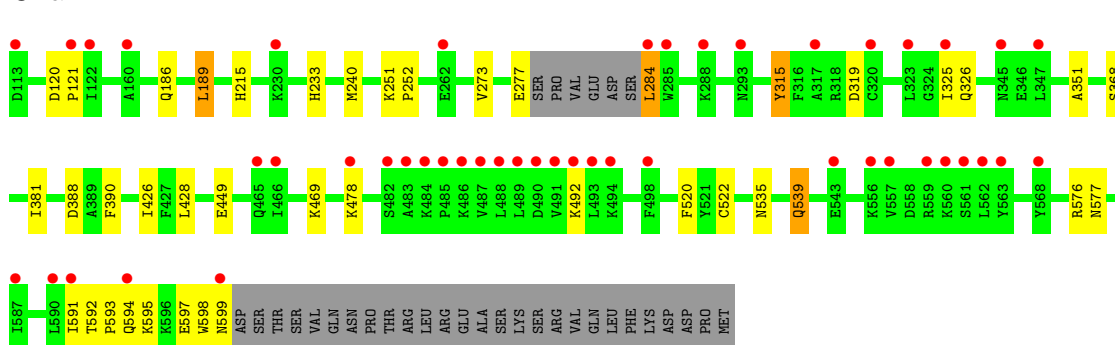
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain A:



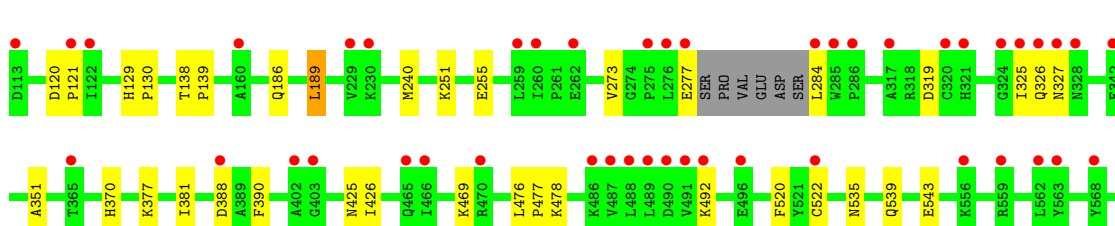
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

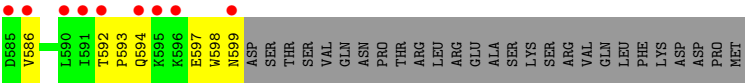
Chain B:



- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

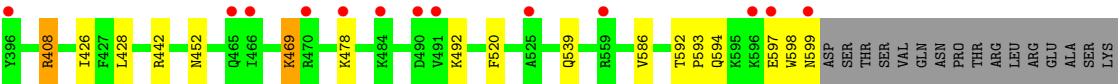
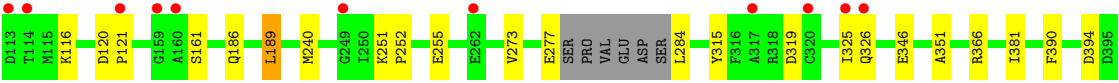
Chain C:





● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.31Å 145.80Å 98.26Å 90.00° 114.22° 90.00°	Depositor
Resolution (Å)	50.00 – 2.27 49.54 – 2.27	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-2.27) 98.3 (49.54-2.27)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.206 , 0.234 0.209 , 0.234	Depositor DCC
$R_{free}$ test set	4941 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.9	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.1	EDS
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 99163 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16367	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: MG, TTP, 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	0.69	1/4031 (0.0%)	0.74	4/5441 (0.1%)
1	B	0.75	2/4031 (0.0%)	0.74	0/5441
1	C	0.68	0/4031	0.73	2/5441 (0.0%)
1	D	0.81	2/4031 (0.0%)	0.76	2/5441 (0.0%)
All	All	0.74	5/16124 (0.0%)	0.74	8/21764 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	368	SER	CB-OG	-5.99	1.34	1.42
1	A	161	SER	CB-OG	5.21	1.49	1.42
1	D	319	ASP	CB-CG	5.20	1.62	1.51
1	B	319	ASP	CB-CG	5.10	1.62	1.51
1	D	161	SER	CB-OG	5.10	1.48	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	388	ASP	CB-CG-OD1	6.73	124.36	118.30
1	A	388	ASP	CB-CG-OD1	6.38	124.05	118.30
1	D	366	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	230	LYS	CD-CE-NZ	5.63	124.65	111.70
1	C	319	ASP	CB-CG-OD1	5.37	123.13	118.30
1	D	442	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	442	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	A	319	ASP	CB-CG-OD1	5.09	122.88	118.30

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	3939	0	3925	31	0
1	B	3939	0	3925	23	0
1	C	3939	0	3925	22	0
1	D	3939	0	3925	18	0
2	A	93	0	36	2	0
2	B	93	0	36	2	0
2	C	62	0	24	0	0
2	D	93	0	36	2	0
3	A	3	0	0	1	0
3	B	1	0	0	0	0
3	C	3	0	0	0	0
3	D	1	0	0	0	0
4	C	29	0	13	2	0
5	A	52	0	0	10	0
5	B	56	0	0	3	0
5	C	40	0	0	5	0
5	D	85	0	0	2	0
All	All	16367	0	15845	90	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 3.

All (90) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:350:CYS:HB3	5:A:850:HOH:O	1.49	1.09
1:B:449:GLU:HB3	5:C:829:HOH:O	1.53	1.08
1:A:140:GLN:HB3	1:A:240:MET:HE1	1.50	0.93
1:D:346:GLU:HA	5:D:860:HOH:O	1.68	0.92
1:A:140:GLN:CB	1:A:240:MET:HE1	2.12	0.78
1:B:577:ASN:OD1	1:B:595:LYS:NZ	2.17	0.77
1:A:158:PRO:HG2	5:A:843:HOH:O	1.85	0.77
1:A:140:GLN:HB3	1:A:240:MET:CE	2.19	0.72
1:C:139:PRO:N	5:C:829:HOH:O	2.31	0.64
2:A:704:DGT:O1G	3:A:705:MG:MG	1.41	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:284:LEU:N	1:B:284:LEU:CD1	2.61	0.63
1:A:176:GLY:HA3	5:A:844:HOH:O	1.99	0.61
1:A:535:ASN:N	1:A:535:ASN:OD1	2.34	0.60
1:A:520:PHE:C	5:A:850:HOH:O	2.40	0.60
1:B:522[A]:CYS:SG	1:D:586:VAL:HG11	2.42	0.59
1:D:469:LYS:HE2	5:D:881:HOH:O	2.02	0.59
1:B:535:ASN:OD1	1:B:535:ASN:N	2.32	0.58
1:A:350:CYS:CB	5:A:850:HOH:O	2.28	0.55
2:D:702:DGT:O3G	2:D:702:DGT:O1B	2.23	0.55
1:A:543:GLU:HG3	1:C:543:GLU:HG3	1.89	0.55
1:A:120:ASP:OD1	1:A:121:PRO:HD2	2.06	0.55
1:A:140:GLN:CG	1:A:240:MET:HE1	2.38	0.54
1:B:120:ASP:OD1	1:B:121:PRO:HD2	2.08	0.54
1:A:322:HIS:NE2	5:A:834:HOH:O	2.33	0.53
1:C:535:ASN:N	1:C:535:ASN:OD1	2.34	0.53
1:B:390:PHE:CE2	1:B:426:ILE:HD11	2.43	0.53
1:B:539:GLN:HG3	5:B:843:HOH:O	2.07	0.53
1:A:158:PRO:HB3	5:A:849:HOH:O	2.09	0.53
1:B:315:TYR:CE2	2:B:701:DGT:H5'	2.43	0.53
1:C:186:GLN:HB2	1:C:189:LEU:HD22	1.91	0.52
1:A:390:PHE:CE2	1:A:426:ILE:HD11	2.46	0.51
1:C:370:HIS:HE1	4:C:704:TTP:HM53	1.76	0.51
4:C:704:TTP:O2B	4:C:704:TTP:O1G	2.28	0.51
1:C:120:ASP:OD1	1:C:121:PRO:HD2	2.11	0.50
1:D:390:PHE:CE2	1:D:426:ILE:HD11	2.46	0.50
1:A:186:GLN:HB2	1:A:189:LEU:HD22	1.94	0.50
1:A:371:ARG:NH1	1:A:549:LEU:HD21	2.27	0.49
1:B:233:HIS:HB2	5:B:849:HOH:O	2.11	0.49
1:A:140:GLN:CG	1:A:240:MET:CE	2.91	0.49
1:B:186:GLN:HB2	1:B:189:LEU:HD22	1.95	0.49
1:D:394:ASP:O	1:D:408:ARG:HD3	2.12	0.49
1:D:120:ASP:OD1	1:D:121:PRO:HD2	2.12	0.49
1:D:186:GLN:HB2	1:D:189:LEU:HD22	1.94	0.49
1:C:390:PHE:CE2	1:C:426:ILE:HD11	2.49	0.48
1:A:240:MET:HB3	1:A:240:MET:HE2	1.66	0.48
1:A:522[A]:CYS:SG	1:C:586:VAL:HG11	2.54	0.48
1:B:284:LEU:N	1:B:284:LEU:HD12	2.29	0.48
1:A:322:HIS:CE1	5:A:834:HOH:O	2.66	0.47
1:D:597:GLU:OE1	1:D:597:GLU:N	2.33	0.47
1:A:521:TYR:HB3	5:A:850:HOH:O	2.14	0.47
1:B:351:ALA:O	1:B:520:PHE:HA	2.14	0.47
1:C:138:THR:C	5:C:829:HOH:O	2.52	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:425:ASN:HB2	1:D:428:LEU:HD13	1.97	0.46
1:C:139:PRO:CA	5:C:829:HOH:O	2.64	0.46
1:C:351:ALA:O	1:C:520:PHE:HA	2.16	0.45
1:A:351:ALA:O	1:A:520:PHE:HA	2.16	0.45
2:A:703:DGT:O3G	1:D:116:LYS:NZ	2.41	0.45
1:D:351:ALA:O	1:D:520:PHE:HA	2.17	0.44
1:C:598:TRP:O	1:C:599:ASN:HB2	2.18	0.44
1:A:140:GLN:HG2	1:A:240:MET:HE3	2.00	0.44
1:D:315:TYR:CE2	2:D:702:DGT:H5'	2.52	0.44
1:B:215:HIS:CE1	2:B:701:DGT:O2A	2.70	0.44
1:C:381:ILE:HD12	1:C:381:ILE:HA	1.91	0.44
1:C:592:THR:N	1:C:593:PRO:CD	2.81	0.43
1:D:381:ILE:HA	1:D:381:ILE:HD12	1.90	0.43
1:B:390:PHE:CE2	1:B:426:ILE:CD1	3.01	0.43
1:B:597:GLU:OE1	1:B:597:GLU:N	2.35	0.43
1:B:598:TRP:O	1:B:599:ASN:HB2	2.18	0.43
1:A:586:VAL:HG11	1:C:522[A]:CYS:SG	2.59	0.43
1:A:592:THR:N	1:A:593:PRO:CD	2.82	0.43
1:B:591:ILE:HG12	5:B:847:HOH:O	2.18	0.42
1:B:592:THR:N	1:B:593:PRO:CD	2.82	0.42
1:D:592:THR:N	1:D:593:PRO:CD	2.82	0.42
1:C:139:PRO:HA	5:C:829:HOH:O	2.20	0.42
1:B:576:ARG:O	1:B:577:ASN:HB2	2.20	0.42
1:A:598:TRP:O	1:A:599:ASN:HB2	2.19	0.42
1:D:598:TRP:O	1:D:599:ASN:HB2	2.19	0.42
1:D:251:LYS:HB2	1:D:252:PRO:HD3	2.02	0.42
1:B:251:LYS:HB2	1:B:252:PRO:HD3	2.01	0.41
1:A:326:GLN:HG2	1:C:327:ASN:O	2.21	0.41
1:A:381:ILE:HA	1:A:381:ILE:HD12	1.87	0.41
1:C:476:LEU:N	1:C:477:PRO:CD	2.83	0.41
1:C:597:GLU:OE1	1:C:597:GLU:N	2.36	0.41
1:B:381:ILE:HD12	1:B:381:ILE:HA	1.92	0.41
1:B:428:LEU:HD13	1:C:425:ASN:HB2	2.02	0.41
1:C:251:LYS:O	1:C:255:GLU:HG2	2.22	0.40
1:D:390:PHE:CE2	1:D:426:ILE:CD1	3.04	0.40
1:A:328:ASN:HB3	5:A:830:HOH:O	2.21	0.40
1:C:129:HIS:CG	1:C:130:PRO:HD2	2.57	0.40
1:D:251:LYS:O	1:D:255:GLU:HG2	2.21	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	478/514 (93%)	472 (99%)	6 (1%)	0	100	100
1	B	478/514 (93%)	471 (98%)	7 (2%)	0	100	100
1	C	478/514 (93%)	471 (98%)	7 (2%)	0	100	100
1	D	478/514 (93%)	471 (98%)	7 (2%)	0	100	100
All	All	1912/2056 (93%)	1885 (99%)	27 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	428/459 (93%)	415 (97%)	13 (3%)	53	68
1	B	428/459 (93%)	414 (97%)	14 (3%)	50	64
1	C	428/459 (93%)	415 (97%)	13 (3%)	53	68
1	D	428/459 (93%)	414 (97%)	14 (3%)	50	64
All	All	1712/1836 (93%)	1658 (97%)	54 (3%)	51	66

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	LEU
1	A	273	VAL
1	A	277	GLU
1	A	284	LEU

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Mol	Chain	Res	Type
1	A	315	TYR
1	A	325	ILE
1	A	326	GLN
1	A	452	ASN
1	A	469	LYS
1	A	478	LYS
1	A	492	LYS
1	A	539	GLN
1	A	594	GLN
1	B	189	LEU
1	B	240	MET
1	B	273	VAL
1	B	277	GLU
1	B	284	LEU
1	B	315	TYR
1	B	325	ILE
1	B	326	GLN
1	B	388	ASP
1	B	469	LYS
1	B	478	LYS
1	B	492	LYS
1	B	539	GLN
1	B	594	GLN
1	C	189	LEU
1	C	240	MET
1	C	273	VAL
1	C	277	GLU
1	C	284	LEU
1	C	325	ILE
1	C	326	GLN
1	C	377	LYS
1	C	469	LYS
1	C	478	LYS
1	C	492	LYS
1	C	539	GLN
1	C	594	GLN
1	D	189	LEU
1	D	240	MET
1	D	273	VAL
1	D	277	GLU
1	D	284	LEU
1	D	325	ILE

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Mol	Chain	Res	Type
1	D	326	GLN
1	D	408	ARG
1	D	452	ASN
1	D	469	LYS
1	D	478	LYS
1	D	492	LYS
1	D	539	GLN
1	D	594	GLN

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	235	GLN
1	A	425	ASN
1	B	215	HIS
1	B	326	GLN
1	B	425	ASN
1	C	215	HIS
1	C	235	GLN
1	C	326	GLN
1	C	425	ASN
1	D	235	GLN
1	D	425	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 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	DGT	A	701	3	33,33,33	1.46	5 (15%)	50,52,52	2.75	9 (18%)
2	DGT	A	703	3	33,33,33	1.82	5 (15%)	50,52,52	1.57	9 (18%)
2	DGT	A	704	3	33,33,33	2.08	8 (24%)	50,52,52	2.46	12 (24%)
2	DGT	B	701	3	33,33,33	1.74	8 (24%)	50,52,52	2.16	8 (16%)
2	DGT	B	703	3	33,33,33	1.54	6 (18%)	50,52,52	2.99	13 (26%)
2	DGT	B	704	3	33,33,33	1.94	8 (24%)	50,52,52	2.12	12 (24%)
2	DGT	C	701	3	33,33,33	1.41	6 (18%)	50,52,52	3.22	14 (28%)
4	TTP	C	704	3	30,30,30	1.40	5 (16%)	42,47,47	1.98	9 (21%)
2	DGT	C	706	3	33,33,33	1.82	8 (24%)	50,52,52	2.10	11 (22%)
2	DGT	D	701	3	33,33,33	1.48	4 (12%)	50,52,52	1.70	15 (30%)
2	DGT	D	702	3	33,33,33	1.98	7 (21%)	50,52,52	2.22	8 (16%)
2	DGT	D	704	3	33,33,33	1.71	7 (21%)	50,52,52	2.08	12 (24%)

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	DGT	A	701	3	-	0/20/34/34	0/3/3/3
2	DGT	A	703	3	-	0/20/34/34	0/3/3/3
2	DGT	A	704	3	-	0/20/34/34	0/3/3/3
2	DGT	B	701	3	-	0/20/34/34	0/3/3/3
2	DGT	B	703	3	-	0/20/34/34	0/3/3/3
2	DGT	B	704	3	-	0/20/34/34	0/3/3/3
2	DGT	C	701	3	-	0/20/34/34	0/3/3/3
4	TTP	C	704	3	-	0/19/34/34	0/2/2/2
2	DGT	C	706	3	-	0/20/34/34	0/3/3/3
2	DGT	D	701	3	-	0/20/34/34	0/3/3/3
2	DGT	D	702	3	-	0/20/34/34	0/3/3/3
2	DGT	D	704	3	-	0/20/34/34	0/3/3/3

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	704	DGT	C4-N9	-6.52	1.28	1.37
2	A	704	DGT	C4-N9	-5.82	1.29	1.37
2	D	704	DGT	C4-N9	-5.43	1.29	1.37
2	D	702	DGT	C2-N2	5.34	1.40	1.32
2	A	704	DGT	C5-N7	-5.28	1.31	1.38
2	A	703	DGT	C5-N7	-5.17	1.32	1.38
2	B	704	DGT	C5-N7	-5.06	1.32	1.38
2	C	706	DGT	C5-N7	-5.01	1.32	1.38
2	D	702	DGT	C4-N9	-4.76	1.30	1.37
2	A	703	DGT	C4-N9	-4.52	1.31	1.37
2	D	704	DGT	C5-N7	-4.41	1.32	1.38
2	A	704	DGT	C6-N1	-4.16	1.30	1.36
2	A	703	DGT	C6-N1	-4.14	1.30	1.36
2	B	701	DGT	C2-N2	4.13	1.38	1.32
4	C	704	TTP	C4-C5	4.13	1.50	1.40
2	A	703	DGT	C2-N3	4.04	1.38	1.33
2	C	706	DGT	C4-N9	-4.03	1.31	1.37
2	B	701	DGT	C2-N3	3.98	1.38	1.33
2	A	704	DGT	C2-N2	3.92	1.38	1.32
2	D	701	DGT	C4-N9	-3.91	1.32	1.37
2	A	701	DGT	C4-N9	-3.88	1.32	1.37
2	D	701	DGT	C2-N2	3.87	1.38	1.32
2	C	706	DGT	C2-N2	3.80	1.38	1.32
2	D	702	DGT	C5-C4	3.75	1.49	1.40
2	B	701	DGT	C5-C4	3.72	1.48	1.40
2	B	701	DGT	C4-N9	-3.70	1.32	1.37
2	D	702	DGT	C2-N3	3.54	1.37	1.33
2	B	703	DGT	C5-C4	3.48	1.48	1.40
2	A	701	DGT	C2-N3	3.47	1.37	1.33
2	B	703	DGT	C5-N7	-3.44	1.34	1.38
2	B	704	DGT	C4-N3	-3.43	1.30	1.35
2	A	701	DGT	C2-N2	3.36	1.37	1.32
2	C	706	DGT	C5-C4	3.26	1.47	1.40
2	D	702	DGT	PB-O3B	3.25	1.65	1.59
2	C	701	DGT	C6-N1	-3.19	1.32	1.36
4	C	704	TTP	C2-N1	3.17	1.41	1.38
2	D	702	DGT	PA-O3A	3.11	1.65	1.59
2	B	703	DGT	C4-N9	-3.07	1.33	1.37
2	A	701	DGT	C5-C4	3.05	1.47	1.40
2	C	701	DGT	C2-N2	3.05	1.36	1.32
2	A	704	DGT	PG-O3B	3.04	1.65	1.60
2	B	703	DGT	C2-N2	3.02	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	DGT	PA-O3A	2.86	1.65	1.59
2	C	706	DGT	C6-N1	-2.84	1.32	1.36
2	D	704	DGT	C5-C4	2.77	1.46	1.40
2	C	706	DGT	PB-O3B	2.76	1.64	1.59
2	A	704	DGT	C5-C4	2.73	1.46	1.40
2	C	706	DGT	PA-O3A	-2.69	1.55	1.59
2	C	701	DGT	C4-N9	-2.68	1.33	1.37
2	B	703	DGT	PA-O3A	-2.67	1.55	1.59
2	B	703	DGT	C6-N1	-2.65	1.33	1.36
2	A	703	DGT	C2-N2	2.60	1.36	1.32
2	D	704	DGT	C6-N1	-2.57	1.33	1.36
2	D	701	DGT	C4-N3	-2.54	1.31	1.35
2	B	704	DGT	C2-N2	2.50	1.36	1.32
2	D	702	DGT	C2-N1	2.47	1.40	1.36
2	C	701	DGT	C5-C4	2.45	1.46	1.40
2	A	704	DGT	C4-N3	-2.42	1.31	1.35
2	B	701	DGT	PB-O3B	2.39	1.64	1.59
2	C	701	DGT	PB-O3A	2.25	1.63	1.59
2	B	704	DGT	C8-N9	-2.25	1.33	1.36
2	D	704	DGT	C4-N3	-2.25	1.32	1.35
2	C	701	DGT	C4-N3	-2.21	1.32	1.35
4	C	704	TTP	O4'-C4'	-2.21	1.39	1.45
2	A	704	DGT	C2-N3	-2.20	1.30	1.33
2	D	701	DGT	PB-O3A	2.20	1.63	1.59
2	B	704	DGT	O4'-C4'	-2.17	1.40	1.45
4	C	704	TTP	O2-C2	2.16	1.24	1.21
2	B	704	DGT	PA-O1A	-2.12	1.45	1.55
2	C	706	DGT	PG-O1G	-2.11	1.47	1.54
2	B	704	DGT	PG-O3B	2.09	1.63	1.60
2	B	701	DGT	C8-N7	2.07	1.38	1.34
2	D	704	DGT	C8-N7	2.06	1.38	1.34
2	B	701	DGT	C5-N7	-2.05	1.35	1.38
2	D	704	DGT	PG-O3B	2.03	1.63	1.60
2	A	701	DGT	PA-O3A	2.03	1.63	1.59
4	C	704	TTP	PA-O3A	2.02	1.63	1.59

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	DGT	C6-C5-N7	19.15	136.72	134.14
2	B	703	DGT	C6-C5-N7	15.66	136.25	134.14
2	A	701	DGT	C6-C5-N7	14.48	136.09	134.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	704	DGT	C6-N1-C2	11.48	126.69	120.20
2	D	702	DGT	C6-C5-N7	-11.42	132.60	134.14
2	B	701	DGT	C6-C5-N7	9.32	135.40	134.14
2	A	704	DGT	C6-C5-N7	8.19	135.24	134.14
2	C	706	DGT	C6-N1-C2	7.91	124.67	120.20
4	C	704	TTP	N3-C2-N1	6.26	121.19	115.97
2	B	704	DGT	N2-C2-N3	-6.23	112.18	120.28
2	B	704	DGT	N2-C2-N1	6.16	124.42	117.82
2	B	703	DGT	C5-C4-N3	-6.06	119.09	126.07
2	D	704	DGT	C5-C4-N3	-6.05	119.10	126.07
2	D	704	DGT	C6-C5-N7	6.02	134.95	134.14
2	B	703	DGT	C6-N1-C2	5.82	123.48	120.20
2	B	701	DGT	PB-O3B-PG	-5.68	116.21	131.93
2	A	703	DGT	C5-C4-N3	-5.26	120.02	126.07
2	C	706	DGT	PA-O3A-PB	-5.21	117.51	131.93
2	A	701	DGT	PB-O3B-PG	-5.17	117.61	131.93
2	D	702	DGT	PB-O3B-PG	-5.16	117.64	131.93
4	C	704	TTP	PB-O3B-PG	-5.10	117.80	131.93
2	B	704	DGT	C5-C4-N3	-5.07	120.23	126.07
2	A	703	DGT	N3-C4-N9	4.87	134.06	126.91
2	C	706	DGT	PB-O3B-PG	-4.79	118.66	131.93
2	B	703	DGT	PA-O3A-PB	-4.79	118.68	131.93
4	C	704	TTP	C6-N1-C2	-4.78	121.05	122.41
2	C	701	DGT	O3A-PB-O3B	-4.68	92.15	101.66
2	C	701	DGT	N2-C2-N3	-4.65	114.24	120.28
2	B	701	DGT	PA-O3A-PB	-4.59	119.22	131.93
2	C	706	DGT	C5-C4-N3	-4.52	120.87	126.07
2	A	701	DGT	C5-C4-N3	-4.49	120.90	126.07
2	D	704	DGT	C2-N3-C4	4.45	120.64	115.30
2	D	704	DGT	C6-N1-C2	4.41	122.69	120.20
2	A	701	DGT	N3-C4-N9	4.41	133.38	126.91
2	C	706	DGT	N3-C4-N9	4.34	133.27	126.91
2	B	703	DGT	N3-C4-N9	4.21	133.09	126.91
2	A	701	DGT	C2-N3-C4	4.21	120.35	115.30
2	B	701	DGT	C5-C4-N3	-4.14	121.30	126.07
2	D	702	DGT	N3-C4-N9	4.11	132.94	126.91
2	B	703	DGT	C2-N3-C4	4.11	120.22	115.30
2	A	701	DGT	O2G-PG-O1G	4.01	122.42	107.38
2	D	704	DGT	PB-O3B-PG	-3.99	120.88	131.93
2	D	702	DGT	PA-O3A-PB	-3.80	121.41	131.93
2	D	701	DGT	N2-C2-N3	-3.80	115.35	120.28
4	C	704	TTP	C5M-C5-C4	3.79	125.10	121.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	DGT	PA-O3A-PB	-3.78	121.46	131.93
4	C	704	TTP	PB-O3A-PA	-3.75	121.54	131.93
2	B	704	DGT	C6-C5-N7	3.71	134.64	134.14
2	B	701	DGT	N3-C4-N9	3.71	132.35	126.91
2	B	704	DGT	C4-C5-N7	-3.69	105.84	109.41
2	D	701	DGT	O1G-PG-O3G	3.69	122.42	110.36
2	B	704	DGT	C2-N3-C4	3.68	119.71	115.30
2	D	704	DGT	PA-O3A-PB	-3.62	121.90	131.93
2	D	704	DGT	N3-C4-N9	3.60	132.18	126.91
2	A	701	DGT	C8-N9-C4	3.50	109.80	106.96
2	B	704	DGT	C6-N1-C2	3.47	122.16	120.20
2	A	704	DGT	O2G-PG-O1G	3.36	120.00	107.38
2	B	701	DGT	C2-N3-C4	3.35	119.31	115.30
2	A	704	DGT	C8-N9-C1'	3.23	132.24	126.15
2	C	701	DGT	C5-C4-N3	-3.22	122.36	126.07
2	B	703	DGT	N2-C2-N3	-3.14	116.20	120.28
2	D	701	DGT	C6-C5-N7	-3.13	133.72	134.14
2	D	701	DGT	N3-C4-N9	3.07	131.41	126.91
2	C	701	DGT	C8-N9-C1'	3.06	131.92	126.15
2	C	701	DGT	C4-C5-N7	-3.04	106.47	109.41
2	A	703	DGT	O2G-PG-O3G	3.01	120.19	110.36
2	D	702	DGT	C8-N9-C4	2.94	109.35	106.96
4	C	704	TTP	O2G-PG-O1G	2.93	119.95	110.36
2	B	703	DGT	PB-O3B-PG	-2.88	123.95	131.93
2	B	703	DGT	C4-C5-N7	-2.88	106.63	109.41
2	D	701	DGT	O3B-PG-O3G	-2.84	90.95	110.43
2	C	706	DGT	O2G-PG-O3G	2.83	119.61	110.36
2	C	701	DGT	C1'-N9-C4	-2.83	119.97	126.84
2	B	703	DGT	N2-C2-N1	2.82	120.84	117.82
2	D	704	DGT	N2-C2-N3	-2.82	116.62	120.28
2	A	704	DGT	O2G-PG-O3G	2.81	119.55	110.36
2	A	704	DGT	N2-C2-N3	-2.80	116.64	120.28
2	C	706	DGT	O1G-PG-O3G	2.80	119.52	110.36
2	D	702	DGT	C5-C4-N3	-2.79	122.86	126.07
2	B	704	DGT	O1A-PA-O3A	2.73	118.08	105.14
2	D	704	DGT	O3A-PB-O3B	-2.72	96.14	101.66
2	B	704	DGT	O4'-C1'-N9	-2.71	102.78	107.66
2	D	701	DGT	O5'-PA-O2A	-2.70	98.79	109.37
2	C	701	DGT	N1-C2-N3	2.69	125.42	121.78
2	A	704	DGT	PB-O3B-PG	-2.69	124.47	131.93
2	A	704	DGT	N2-C2-N1	2.69	120.71	117.82
4	C	704	TTP	C4-N3-C2	-2.68	119.89	125.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	703	DGT	O5'-PA-O2A	-2.63	99.07	109.37
2	D	701	DGT	C1'-N9-C4	-2.58	120.56	126.84
2	A	703	DGT	PB-O3B-PG	-2.56	124.85	131.93
2	B	701	DGT	O3A-PB-O3B	-2.55	96.47	101.66
2	B	704	DGT	O2G-PG-O1G	2.55	116.96	107.38
2	D	701	DGT	O1A-PA-O3A	2.55	117.24	105.14
2	D	701	DGT	C5-C4-N3	-2.55	123.14	126.07
2	A	704	DGT	PA-O3A-PB	-2.53	124.93	131.93
2	B	703	DGT	O1A-PA-O3A	2.48	116.91	105.14
2	D	704	DGT	O1G-PG-O3G	2.47	118.43	110.36
2	A	703	DGT	PA-O3A-PB	-2.46	125.13	131.93
2	C	706	DGT	O3A-PB-O2B	-2.45	93.68	110.43
2	B	701	DGT	C8-N9-C4	2.42	108.93	106.96
2	C	701	DGT	O1G-PG-O3G	2.41	118.23	110.36
2	B	703	DGT	O3A-PA-O5'	-2.40	96.54	102.91
4	C	704	TTP	O4'-C1'-N1	2.38	111.95	107.66
2	D	701	DGT	N1-C2-N3	2.38	124.99	121.78
2	D	701	DGT	C8-N9-C1'	2.37	130.62	126.15
2	C	701	DGT	N2-C2-N1	2.35	120.34	117.82
2	A	703	DGT	N1-C2-N3	2.32	124.92	121.78
2	A	703	DGT	C2-N3-C4	2.32	118.08	115.30
2	B	703	DGT	O2G-PG-O1G	2.29	115.99	107.38
2	C	706	DGT	C2-N3-C4	2.28	118.04	115.30
2	A	703	DGT	O1A-PA-O5'	2.28	119.98	108.51
2	B	704	DGT	N3-C4-N9	2.27	130.24	126.91
2	A	704	DGT	O4'-C1'-N9	-2.27	103.57	107.66
2	D	704	DGT	O2G-PG-O1G	2.25	115.83	107.38
2	D	701	DGT	C8-N9-C4	2.25	108.78	106.96
4	C	704	TTP	O2B-PB-O1B	2.23	124.49	112.14
2	A	704	DGT	C1'-N9-C4	-2.23	121.42	126.84
2	C	701	DGT	N3-C4-N9	2.21	130.15	126.91
2	A	701	DGT	O1A-PA-O2A	2.20	124.31	112.14
2	D	702	DGT	N2-C2-N3	-2.17	117.46	120.28
2	D	704	DGT	O5'-PA-O2A	-2.16	100.93	109.37
2	D	701	DGT	PB-O3B-PG	-2.14	126.01	131.93
2	C	706	DGT	O1B-PB-O2B	2.13	123.92	112.14
2	C	701	DGT	O1A-PA-O2A	2.12	123.89	112.14
2	C	701	DGT	O4'-C1'-N9	-2.11	103.86	107.66
2	A	704	DGT	O1B-PB-O2B	2.10	123.79	112.14
2	D	702	DGT	C5-C4-N9	-2.08	104.20	107.09
2	B	704	DGT	PB-O3B-PG	-2.08	126.17	131.93
2	D	701	DGT	O1B-PB-O2B	2.08	123.63	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	706	DGT	O3B-PG-O3G	-2.06	96.31	110.43
2	C	701	DGT	O1B-PB-O3A	2.04	114.80	105.14
2	D	701	DGT	O1B-PB-O3A	2.03	114.79	105.14

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	481/514 (93%)	0.78	63 (13%) 4 6	41, 72, 118, 145	0
1	B	481/514 (93%)	0.61	47 (9%) 8 12	41, 61, 100, 130	0
1	C	481/514 (93%)	0.75	54 (11%) 6 9	45, 75, 112, 148	0
1	D	481/514 (93%)	0.43	24 (4%) 28 36	42, 54, 81, 108	0
All	All	1924/2056 (93%)	0.64	188 (9%) 8 12	41, 64, 109, 148	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	488	LEU	8.9
1	B	489	LEU	8.0
1	B	490	ASP	7.4
1	A	488	LEU	6.1
1	B	591	ILE	6.0
1	C	488	LEU	5.9
1	B	486	LYS	5.8
1	B	599	ASN	5.8
1	A	466	ILE	5.6
1	C	490	ASP	5.6
1	C	487	VAL	5.4
1	C	594	GLN	5.3
1	C	276	LEU	5.2
1	A	568	TYR	5.1
1	A	487	VAL	5.1
1	B	491	VAL	5.1
1	D	491	VAL	4.9
1	C	599	ASN	4.8
1	C	590	LEU	4.8
1	A	490	ASP	4.8
1	B	562	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	486	LYS	4.7
1	B	590	LEU	4.5
1	B	559	ARG	4.5
1	C	489	LEU	4.4
1	B	560	LYS	4.4
1	B	487	VAL	4.3
1	A	471	GLU	4.3
1	A	230	LYS	4.3
1	A	489	LEU	4.2
1	C	470	ARG	4.2
1	A	345	ASN	4.2
1	C	562	LEU	4.2
1	A	491	VAL	4.1
1	A	286	PRO	4.0
1	B	557	VAL	4.0
1	A	562	LEU	3.9
1	B	483	ALA	3.9
1	C	465	GLN	3.8
1	A	276	LEU	3.8
1	C	596	LYS	3.8
1	B	561	SER	3.8
1	B	325	ILE	3.8
1	B	563	TYR	3.7
1	B	492	LYS	3.7
1	B	543	GLU	3.7
1	A	599	ASN	3.6
1	A	285	TRP	3.6
1	A	493	LEU	3.6
1	C	326	GLN	3.6
1	A	481	ALA	3.5
1	A	585	ASP	3.5
1	C	277	GLU	3.4
1	B	493	LEU	3.4
1	A	570	VAL	3.4
1	C	275	PRO	3.3
1	C	122	ILE	3.3
1	D	490	ASP	3.3
1	C	113	ASP	3.3
1	B	285	TRP	3.3
1	C	492	LYS	3.3
1	A	263	GLU	3.2
1	B	594	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	465	GLN	3.2
1	D	262	GLU	3.2
1	C	325	ILE	3.1
1	C	284	LEU	3.1
1	B	121	PRO	3.1
1	A	343	VAL	3.1
1	C	403	GLY	3.0
1	D	466	ILE	3.0
1	A	284	LEU	3.0
1	C	260	ILE	3.0
1	C	466	ILE	3.0
1	D	249	GLY	3.0
1	D	470	ARG	2.9
1	B	284	LEU	2.9
1	A	113	ASP	2.9
1	C	327	ASN	2.9
1	D	317	ALA	2.9
1	A	498	PHE	2.9
1	C	230	LYS	2.9
1	C	317	ALA	2.9
1	B	587	ILE	2.8
1	B	262	GLU	2.8
1	B	478	LYS	2.8
1	B	230	LYS	2.8
1	B	485	PRO	2.8
1	C	496	GLU	2.8
1	A	492	LYS	2.7
1	A	596	LYS	2.7
1	A	275	PRO	2.7
1	A	325	ILE	2.7
1	B	466	ILE	2.7
1	C	121	PRO	2.7
1	B	494	LYS	2.7
1	C	559	ARG	2.7
1	C	592	THR	2.7
1	A	327	ASN	2.7
1	D	478	LYS	2.7
1	A	463	THR	2.7
1	C	486	LYS	2.6
1	C	324	GLY	2.6
1	C	568	TYR	2.6
1	C	522[A]	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	473	TYR	2.6
1	A	470	ARG	2.6
1	A	262	GLU	2.6
1	A	474	GLU	2.6
1	A	324	GLY	2.6
1	C	328	ASN	2.6
1	B	568	TYR	2.5
1	A	543	GLU	2.5
1	A	320	CYS	2.5
1	C	259	LEU	2.5
1	A	402	ALA	2.5
1	D	121	PRO	2.5
1	C	286	PRO	2.5
1	C	491	VAL	2.5
1	A	478	LYS	2.5
1	A	229	VAL	2.5
1	C	388	ASP	2.5
1	C	563	TYR	2.4
1	A	500	VAL	2.4
1	C	285	TRP	2.4
1	A	573	CYS	2.4
1	C	321	HIS	2.4
1	B	345	ASN	2.4
1	B	113	ASP	2.4
1	D	325	ILE	2.4
1	A	190	GLN	2.4
1	B	556	LYS	2.4
1	D	114	THR	2.4
1	B	465	GLN	2.3
1	A	578	PHE	2.3
1	A	598	TRP	2.3
1	B	323	LEU	2.3
1	D	320	CYS	2.3
1	C	585	ASP	2.3
1	B	347	LEU	2.3
1	D	597	GLU	2.3
1	B	317	ALA	2.3
1	C	320	CYS	2.3
1	A	347	LEU	2.3
1	C	595	LYS	2.3
1	C	591	ILE	2.3
1	B	320	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	482	SER	2.3
1	A	594	GLN	2.3
1	B	288	LYS	2.2
1	B	293	ASN	2.2
1	D	599	ASN	2.2
1	A	496	GLU	2.2
1	C	229	VAL	2.2
1	D	396	TYR	2.2
1	B	122	ILE	2.2
1	B	498	PHE	2.2
1	A	121	PRO	2.2
1	D	326	GLN	2.2
1	A	328	ASN	2.2
1	A	326	GLN	2.2
1	D	559	ARG	2.2
1	C	556	LYS	2.1
1	D	596	LYS	2.1
1	D	159	GLY	2.1
1	A	189	LEU	2.1
1	A	321	HIS	2.1
1	A	317	ALA	2.1
1	A	235	GLN	2.1
1	A	341	CYS	2.1
1	C	160	ALA	2.1
1	A	590	LEU	2.1
1	A	567	GLN	2.1
1	B	160	ALA	2.1
1	A	124	GLY	2.1
1	A	510	GLN	2.1
1	C	586	VAL	2.1
1	A	457	VAL	2.0
1	B	484	LYS	2.0
1	D	113	ASP	2.0
1	C	365	THR	2.0
1	C	402	ALA	2.0
1	D	160	ALA	2.0
1	A	485	PRO	2.0
1	D	484	LYS	2.0
1	C	262	GLU	2.0
1	D	525	ALA	2.0
1	C	342	GLU	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, 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(Å <sup>2</sup> )	Q<0.9
3	MG	C	705	1/1	0.26	3.37	92,92,92,92	0
2	DGT	D	702	31/31	0.15	-0.31	49,59,84,86	0
2	DGT	B	704	31/31	0.16	-0.41	42,43,45,45	0
2	DGT	D	704	31/31	0.14	-0.57	44,45,47,47	0
4	TTP	C	704	29/29	0.15	-0.57	59,72,97,101	0
2	DGT	A	701	31/31	0.13	-0.64	58,75,92,93	0
2	DGT	D	701	31/31	0.15	-0.87	41,42,45,46	0
2	DGT	B	701	31/31	0.12	-0.88	53,57,77,81	0
2	DGT	A	704	31/31	0.14	-0.98	47,49,54,55	0
2	DGT	C	706	31/31	0.12	-1.14	49,50,58,60	0
2	DGT	C	701	31/31	0.14	-1.31	44,46,53,53	0
2	DGT	B	703	31/31	0.11	-1.67	46,47,55,55	0
2	DGT	A	703	31/31	0.11	-1.94	45,47,56,59	0
3	MG	B	702	1/1	0.06	-2.35	74,74,74,74	0
3	MG	A	702	1/1	0.07	-4.18	81,81,81,81	0
3	MG	C	702	1/1	0.04	-4.78	50,50,50,50	0
3	MG	D	703	1/1	0.03	-5.09	65,65,65,65	0
3	MG	C	703	1/1	0.05	-11.59	48,48,48,48	0
3	MG	A	706	1/1	0.06	-15.67	45,45,45,45	0
3	MG	A	705	1/1	0.08	-19.67	58,58,58,58	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.