



# Full wwPDB X-ray Structure Validation Report

Oct 22, 2014 – 06:49 AM EDT

PDB ID : 4TNY  
Title : Structural basis of cellular dNTP regulation, SAMHD1-dGTP-dATP-dGT  
Pcomplex  
Authors : Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.  
Deposited on : 2014-06-05  
Resolution : 2.60 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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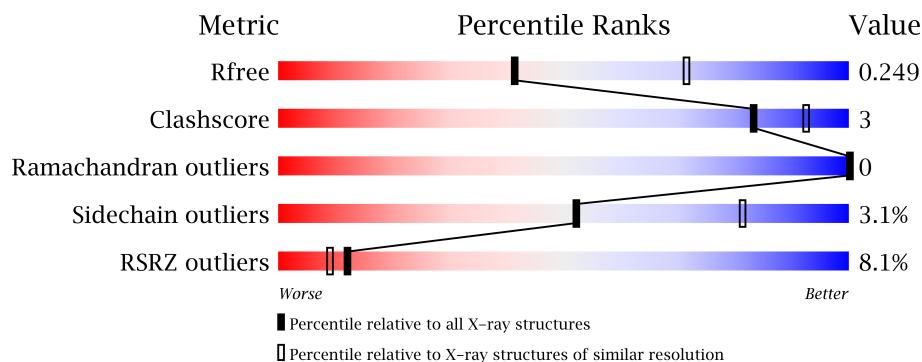
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.60 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	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16275 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.

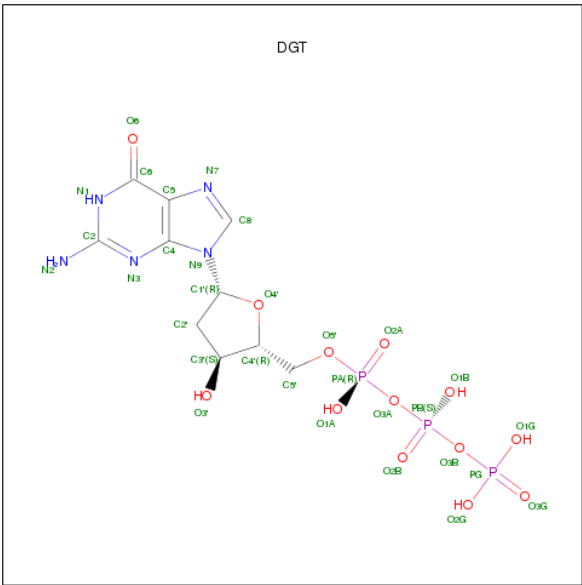
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	5	0
			3974	2539	693	721	21			
1	C	481	Total	C	N	O	S	0	5	0
			3974	2539	693	721	21			
1	B	481	Total	C	N	O	S	0	5	0
			3974	2539	693	721	21			
1	D	481	Total	C	N	O	S	0	4	0
			3966	2535	691	719	21			

There are 8 discrepancies between the modelled and reference sequences:

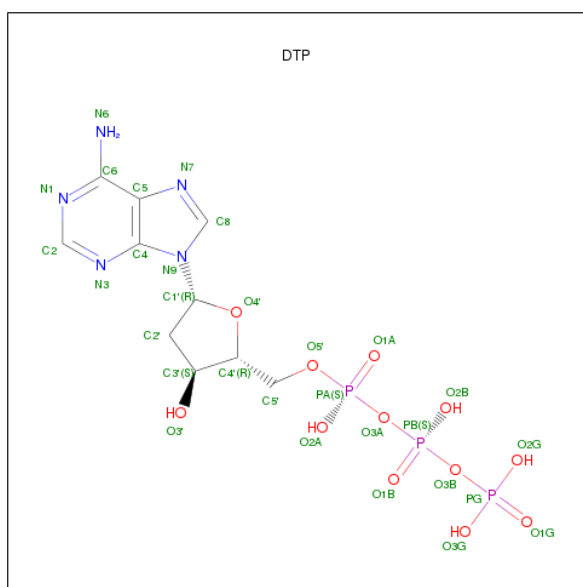
Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
B	207	ASN	ASP	engineered mutation	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:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

- Molecule 3 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	O	0	0
			7	7		

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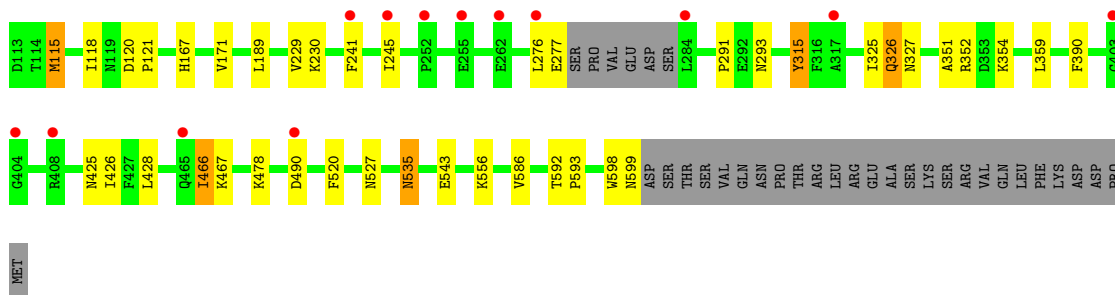
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	3	Total 3	O 3	0	0
5	B	1	Total 1	O 1	0	0
5	D	4	Total 4	O 4	0	0

### 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.

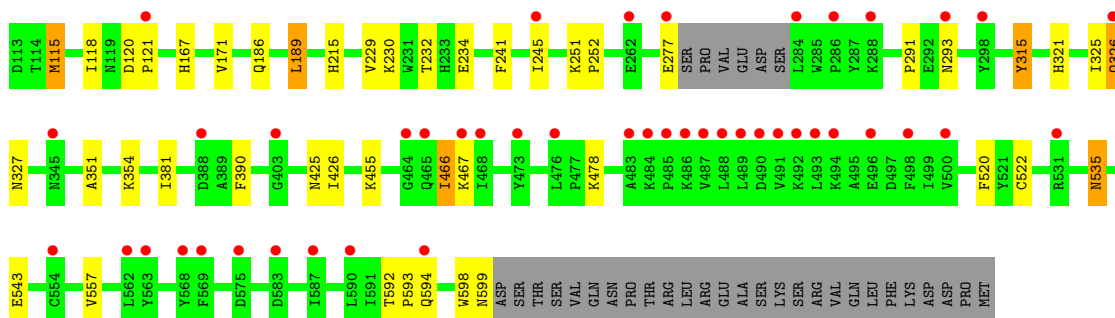
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain A: 



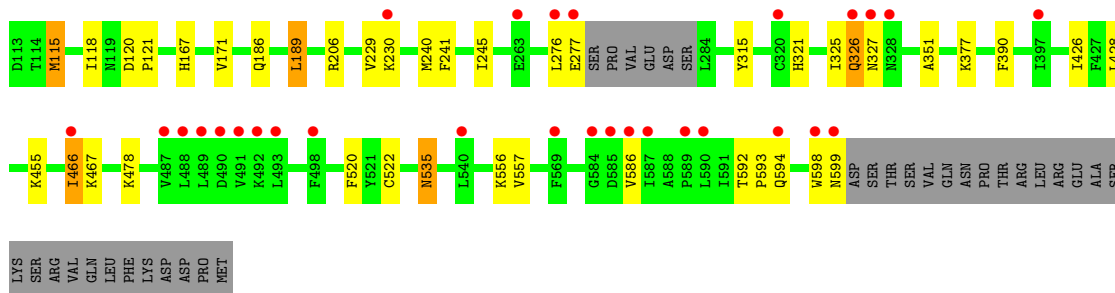
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain C: 



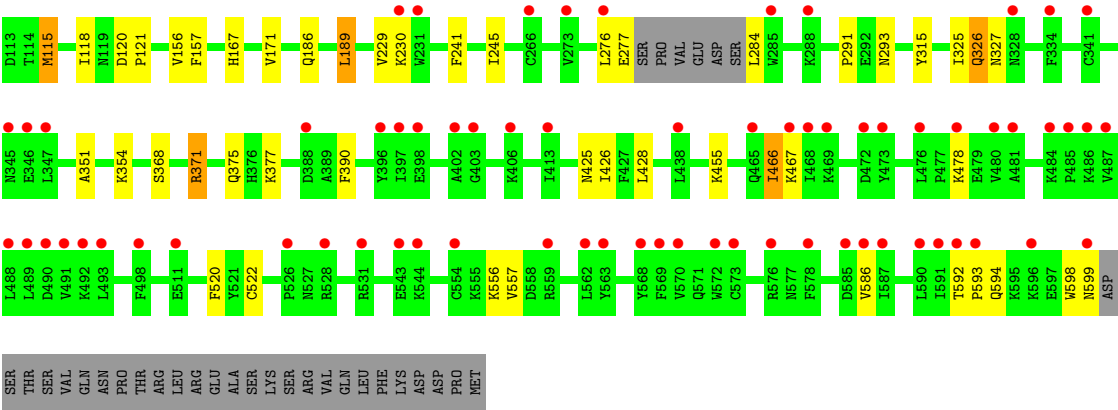
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain B: 



● 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, $\alpha$ , $\beta$ , $\gamma$	86.25Å 141.87Å 98.33Å 90.00° 116.38° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 48.69 – 2.58	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-2.60) 98.8 (48.69-2.58)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.214 , 0.244 0.222 , 0.249	Depositor DCC
$R_{free}$ test set	3322 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.1	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.6	EDS
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 65672 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16275	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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, DTP, 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	0.63	0/4067	0.71	0/5490
1	B	0.61	0/4067	0.70	0/5490
1	C	0.60	0/4067	0.71	0/5490
1	D	0.58	0/4059	0.70	0/5479
All	All	0.61	0/16260	0.71	0/21949

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	1
1	B	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	276	LEU	Peptide
1	B	276	LEU	Peptide
1	D	276	LEU	Peptide

## 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	3974	0	3944	24	1
1	B	3974	0	3944	23	0
1	C	3974	0	3944	30	0
1	D	3966	0	3939	26	0
2	A	31	0	12	2	0
2	B	62	0	24	1	0
2	C	62	0	24	4	0
2	D	93	0	36	8	0
3	A	30	0	12	2	0
3	B	30	0	12	2	0
3	C	30	0	12	2	0
3	D	30	0	12	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	7	0	0	0	0
5	B	1	0	0	0	0
5	C	3	0	0	0	0
5	D	4	0	0	0	0
All	All	16275	0	15915	98	1

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:377:LYS:NZ	3:D:703:DTP:O2B	2.09	0.85
1:A:535:ASN:N	1:A:535:ASN:OD1	2.21	0.71
1:A:586:VAL:HG11	1:C:522[A]:CYS:SG	2.32	0.68
1:B:535:ASN:OD1	1:B:535:ASN:N	2.22	0.66
1:C:535:ASN:N	1:C:535:ASN:OD1	2.21	0.66
2:D:704:DGT:O3G	2:D:704:DGT:PA	2.54	0.66
1:C:390:PHE:CE2	1:C:426:ILE:HD11	2.36	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:354:LYS:NZ	3:C:701:DTP:O1A	2.32	0.60
1:D:390:PHE:CE2	1:D:426:ILE:HD11	2.37	0.60
1:A:120:ASP:OD1	1:A:121:PRO:HD2	2.00	0.60
1:A:390:PHE:CE2	1:A:426:ILE:HD11	2.37	0.59
1:B:120:ASP:OD1	1:B:121:PRO:HD2	2.03	0.57
1:B:390:PHE:CE2	1:B:426:ILE:HD11	2.39	0.57
1:B:206:ARG:NH2	2:B:702:DGT:O2B	2.34	0.57
1:D:466:ILE:HD13	1:D:466:ILE:N	2.21	0.56
1:A:327:ASN:O	1:C:326:GLN:HG2	2.06	0.56
1:B:598:TRP:O	1:B:599:ASN:HB2	2.07	0.55
1:C:598:TRP:O	1:C:599:ASN:HB2	2.06	0.55
1:B:326:GLN:HG2	1:D:327:ASN:O	2.07	0.54
1:A:326:GLN:HG2	1:C:327:ASN:O	2.07	0.54
1:B:466:ILE:N	1:B:466:ILE:HD13	2.23	0.54
1:A:598:TRP:O	1:A:599:ASN:HB2	2.07	0.54
1:C:215:HIS:NE2	2:C:702:DGT:O2A	2.40	0.54
1:D:598:TRP:O	1:D:599:ASN:HB2	2.08	0.54
1:C:466:ILE:HD13	1:C:466:ILE:N	2.22	0.53
3:B:704:DTP:O2B	1:D:377:LYS:NZ	2.32	0.53
2:C:702:DGT:H4'	2:C:702:DGT:O1A	2.09	0.53
1:A:466:ILE:N	1:A:466:ILE:HD13	2.24	0.52
1:C:120:ASP:OD1	1:C:121:PRO:HD2	2.12	0.50
1:A:428:LEU:HD13	1:D:425:ASN:HB2	1.93	0.49
1:B:586:VAL:HG11	1:D:522[A]:CYS:SG	2.53	0.49
1:A:315:TYR:CD1	2:A:701:DGT:H3'	2.47	0.48
1:A:425:ASN:HB2	1:D:428:LEU:HD13	1.95	0.48
1:D:351:ALA:O	1:D:520:PHE:HA	2.13	0.48
1:D:598:TRP:O	1:D:599:ASN:CB	2.62	0.48
1:B:351:ALA:O	1:B:520:PHE:HA	2.14	0.48
1:B:327:ASN:O	1:D:326:GLN:HG2	2.13	0.48
1:C:351:ALA:O	1:C:520:PHE:HA	2.14	0.48
1:A:598:TRP:O	1:A:599:ASN:CB	2.61	0.48
1:D:241:PHE:O	1:D:245:ILE:HG12	2.14	0.48
2:D:704:DGT:O1A	2:D:704:DGT:PG	2.72	0.47
1:B:241:PHE:O	1:B:245:ILE:HG12	2.14	0.47
1:B:598:TRP:O	1:B:599:ASN:CB	2.61	0.47
1:C:241:PHE:O	1:C:245:ILE:HG12	2.14	0.47
1:C:598:TRP:O	1:C:599:ASN:CB	2.61	0.47
1:A:354:LYS:NZ	3:A:702:DTP:O1A	2.42	0.47
1:A:315:TYR:CE2	2:A:701:DGT:H5'	2.48	0.47
1:A:241:PHE:O	1:A:245:ILE:HG12	2.14	0.47
1:D:167:HIS:O	1:D:171:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:120:ASP:OD1	1:D:121:PRO:HD2	2.14	0.47
1:A:167:HIS:O	1:A:171:VAL:HG23	2.16	0.46
1:A:592:THR:N	1:A:593:PRO:CD	2.78	0.46
1:C:167:HIS:O	1:C:171:VAL:HG23	2.16	0.46
1:A:351:ALA:O	1:A:520:PHE:HA	2.16	0.46
1:B:167:HIS:O	1:B:171:VAL:HG23	2.15	0.46
1:D:156:VAL:O	2:D:705:DGT:H8	2.16	0.46
1:A:543:GLU:HG2	1:C:543:GLU:HG2	1.98	0.45
1:B:592:THR:N	1:B:593:PRO:CD	2.80	0.45
1:B:229:VAL:HG12	1:B:230:LYS:N	2.32	0.45
1:C:229:VAL:HG12	1:C:230:LYS:N	2.32	0.45
1:C:592:THR:N	1:C:593:PRO:CD	2.80	0.45
1:C:115:MET:SD	1:C:115:MET:C	2.96	0.45
1:B:115:MET:C	1:B:115:MET:SD	2.94	0.45
1:D:592:THR:N	1:D:593:PRO:CD	2.80	0.44
2:D:705:DGT:H3'	2:D:705:DGT:PA	2.57	0.44
1:D:115:MET:SD	1:D:115:MET:C	2.96	0.44
1:A:115:MET:C	1:A:115:MET:SD	2.95	0.44
1:C:381:ILE:HD12	1:C:381:ILE:HA	1.89	0.44
1:A:229:VAL:HG12	1:A:230:LYS:N	2.33	0.44
1:D:229:VAL:HG12	1:D:230:LYS:N	2.32	0.44
3:C:701:DTP:O1B	2:D:702:DGT:H5'A	2.18	0.44
1:D:186:GLN:HB2	1:D:189:LEU:HD22	2.00	0.43
1:D:455:LYS:HG2	1:D:557:VAL:HG12	2.00	0.43
1:D:368:SER:HA	1:D:371:ARG:HD2	1.99	0.43
1:C:455:LYS:HG2	1:C:557:VAL:HG12	2.00	0.43
2:D:704:DGT:O1A	2:D:704:DGT:O1G	2.36	0.43
1:B:455:LYS:HG2	1:B:557:VAL:HG12	2.01	0.43
1:B:230:LYS:HA	1:B:230:LYS:HD2	1.88	0.43
1:C:230:LYS:HA	1:C:230:LYS:HD2	1.85	0.43
1:B:186:GLN:HB2	1:B:189:LEU:HD22	2.00	0.42
1:B:522[A]:CYS:SG	1:D:586:VAL:HG11	2.59	0.42
1:D:291:PRO:HG2	1:D:293:ASN:OD1	2.19	0.42
1:C:186:GLN:HB2	1:C:189:LEU:HD22	2.01	0.42
2:D:705:DGT:H2'A	2:D:705:DGT:N3	2.34	0.42
1:C:251:LYS:HB2	1:C:252:PRO:HD3	2.00	0.42
1:C:291:PRO:HG2	1:C:293:ASN:OD1	2.20	0.42
1:C:425:ASN:HB2	1:B:428:LEU:HD13	2.01	0.42
1:C:390:PHE:CE2	1:C:426:ILE:CD1	3.03	0.41
2:C:702:DGT:O1B	2:C:702:DGT:O3G	2.36	0.41
1:A:352:ARG:HH22	3:A:702:DTP:PG	2.44	0.41
3:B:704:DTP:H2'1	1:D:157:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:315:TYR:CE2	2:C:702:DGT:H5'	2.56	0.41
1:A:291:PRO:HG2	1:A:293:ASN:OD1	2.21	0.41
1:D:375:GLN:NE2	2:D:704:DGT:O6	2.45	0.41
1:C:321:HIS:CE1	1:B:321:HIS:CE1	3.09	0.40
1:D:354:LYS:NZ	3:D:703:DTP:O1A	2.53	0.40
1:A:543:GLU:HG3	1:C:543:GLU:HG3	2.03	0.40
1:C:232:THR:HB	1:C:234:GLU:OE1	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:490:ASP:OD1	1:A:527:ASN:O[2.545]	2.17	0.03

## 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	482/514 (94%)	476 (99%)	6 (1%)	0	100	100
1	B	482/514 (94%)	477 (99%)	5 (1%)	0	100	100
1	C	482/514 (94%)	475 (98%)	7 (2%)	0	100	100
1	D	481/514 (94%)	476 (99%)	5 (1%)	0	100	100
All	All	1927/2056 (94%)	1904 (99%)	23 (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	432/459 (94%)	419 (97%)	13 (3%)	53	82
1	B	432/459 (94%)	418 (97%)	14 (3%)	51	80
1	C	432/459 (94%)	420 (97%)	12 (3%)	56	84
1	D	431/459 (94%)	417 (97%)	14 (3%)	51	80
All	All	1727/1836 (94%)	1674 (97%)	53 (3%)	52	81

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	MET
1	A	118	ILE
1	A	189	LEU
1	A	277	GLU
1	A	315	TYR
1	A	325	ILE
1	A	326	GLN
1	A	359	LEU
1	A	466	ILE
1	A	467	LYS
1	A	478	LYS
1	A	535	ASN
1	A	556	LYS
1	C	115	MET
1	C	118	ILE
1	C	189	LEU
1	C	277	GLU
1	C	315	TYR
1	C	325	ILE
1	C	326	GLN
1	C	466	ILE
1	C	467	LYS
1	C	478	LYS
1	C	535	ASN
1	C	594	GLN
1	B	115	MET
1	B	118	ILE
1	B	189	LEU
1	B	240	MET
1	B	277	GLU
1	B	315	TYR
1	B	325	ILE
1	B	326	GLN

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Mol	Chain	Res	Type
1	B	466	ILE
1	B	467	LYS
1	B	478	LYS
1	B	535	ASN
1	B	556	LYS
1	B	594	GLN
1	D	115	MET
1	D	118	ILE
1	D	189	LEU
1	D	277	GLU
1	D	284	LEU
1	D	315	TYR
1	D	325	ILE
1	D	326	GLN
1	D	371	ARG
1	D	466	ILE
1	D	467	LYS
1	D	478	LYS
1	D	556	LYS
1	D	594	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	364	HIS
1	A	425	ASN
1	C	364	HIS
1	C	425	ASN
1	B	364	HIS
1	B	425	ASN
1	D	364	HIS
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 16 ligands modelled in this entry, 4 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	-	33,33,33	1.43	5 (15%)	50,52,52	2.98	12 (24%)
3	DTP	A	702	4	32,32,32	1.06	3 (9%)	50,50,50	2.52	16 (32%)
2	DGT	B	702	-	33,33,33	1.36	6 (18%)	50,52,52	4.14	13 (26%)
2	DGT	B	703	4	33,33,33	1.68	6 (18%)	50,52,52	2.50	11 (22%)
3	DTP	B	704	4	32,32,32	1.06	2 (6%)	50,50,50	2.39	14 (28%)
3	DTP	C	701	4	32,32,32	1.18	4 (12%)	50,50,50	2.36	12 (24%)
2	DGT	C	702	-	33,33,33	1.30	5 (15%)	50,52,52	3.37	10 (20%)
2	DGT	C	703	4	33,33,33	1.68	5 (15%)	50,52,52	1.67	6 (12%)
2	DGT	D	702	4	33,33,33	1.51	5 (15%)	50,52,52	2.20	9 (18%)
3	DTP	D	703	4	32,32,32	1.19	6 (18%)	50,50,50	2.23	12 (24%)
2	DGT	D	704	-	33,33,33	1.24	4 (12%)	50,52,52	4.54	12 (24%)
2	DGT	D	705	4	33,33,33	1.58	5 (15%)	50,52,52	2.77	8 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DGT	A	701	-	-	0/20/34/34	0/3/3/3
3	DTP	A	702	4	-	0/20/34/34	0/3/3/3
2	DGT	B	702	-	-	0/20/34/34	0/3/3/3
2	DGT	B	703	4	-	0/20/34/34	0/3/3/3
3	DTP	B	704	4	-	0/20/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DTP	C	701	4	-	0/20/34/34	0/3/3/3
2	DGT	C	702	-	-	0/20/34/34	0/3/3/3
2	DGT	C	703	4	-	0/20/34/34	0/3/3/3
2	DGT	D	702	4	-	0/20/34/34	0/3/3/3
3	DTP	D	703	4	-	0/20/34/34	0/3/3/3
2	DGT	D	704	-	-	0/20/34/34	0/3/3/3
2	DGT	D	705	4	-	0/20/34/34	0/3/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	703	DGT	C5-N7	-5.60	1.31	1.38
2	C	703	DGT	C4-N9	-4.65	1.31	1.37
2	D	705	DGT	C4-N9	-4.48	1.31	1.37
2	D	705	DGT	C5-N7	-4.28	1.33	1.38
2	D	702	DGT	C6-N1	-4.08	1.31	1.36
2	A	701	DGT	C5-C4	3.91	1.49	1.40
2	B	703	DGT	C6-N1	-3.89	1.31	1.36
2	D	702	DGT	C5-N7	-3.85	1.33	1.38
2	B	703	DGT	C5-N7	-3.83	1.33	1.38
2	B	702	DGT	C5-C4	3.75	1.49	1.40
2	A	701	DGT	C4-N9	-3.68	1.32	1.37
2	B	703	DGT	C2-N2	3.53	1.37	1.32
2	D	702	DGT	C4-N9	-3.53	1.32	1.37
2	D	705	DGT	C5-C4	3.52	1.48	1.40
2	B	703	DGT	C5-C4	3.44	1.48	1.40
2	B	703	DGT	C4-N9	-3.40	1.32	1.37
2	C	702	DGT	C5-C4	3.38	1.48	1.40
2	D	704	DGT	C5-C4	3.37	1.48	1.40
2	B	703	DGT	C2-N3	3.31	1.37	1.33
2	C	703	DGT	C2-N3	3.25	1.37	1.33
3	C	701	DTP	C8-N9	-3.00	1.32	1.36
2	C	703	DGT	C5-C4	2.91	1.47	1.40
3	B	704	DTP	C4-N9	-2.90	1.33	1.37
3	A	702	DTP	C4-N9	-2.83	1.33	1.37
2	A	701	DGT	O4'-C4'	-2.62	1.38	1.45
3	B	704	DTP	C5-C4	2.59	1.46	1.40
2	B	702	DGT	C4-N9	-2.57	1.34	1.37
2	A	701	DGT	C5-N7	-2.55	1.35	1.38
2	B	702	DGT	C5-N7	-2.55	1.35	1.38
2	C	702	DGT	C5-N7	-2.51	1.35	1.38
2	C	703	DGT	C2-N2	2.51	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	702	DGT	C4-N9	-2.46	1.34	1.37
3	C	701	DTP	C4-N9	-2.44	1.34	1.37
3	D	703	DTP	C4-N9	-2.41	1.34	1.37
3	A	702	DTP	C5-C4	2.40	1.45	1.40
2	A	701	DGT	C2-N2	2.40	1.36	1.32
2	D	704	DGT	C4-N9	-2.39	1.34	1.37
3	D	703	DTP	O4'-C4'	-2.36	1.39	1.45
3	D	703	DTP	C8-N9	-2.34	1.33	1.36
2	D	704	DGT	C2-N3	2.26	1.36	1.33
2	D	705	DGT	C2-N3	2.26	1.36	1.33
2	D	705	DGT	C2-N2	2.25	1.35	1.32
2	C	702	DGT	C2-N3	2.24	1.36	1.33
2	C	702	DGT	C2-N2	2.23	1.35	1.32
2	D	704	DGT	C2-N2	2.23	1.35	1.32
2	D	702	DGT	C2-N2	2.23	1.35	1.32
3	D	703	DTP	PA-O3A	2.21	1.63	1.59
3	D	703	DTP	C5-C4	2.19	1.45	1.40
3	C	701	DTP	C2-N3	2.19	1.35	1.32
2	D	702	DGT	C2-N1	-2.11	1.33	1.36
3	C	701	DTP	C5-C4	2.05	1.45	1.40
2	B	702	DGT	C8-N7	2.05	1.38	1.34
3	A	702	DTP	C8-N9	-2.02	1.33	1.36
2	B	702	DGT	C2-N2	2.02	1.35	1.32
2	B	702	DGT	PB-O3B	2.01	1.63	1.59
3	D	703	DTP	C2-N3	2.00	1.35	1.32

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	704	DGT	C6-C5-N7	28.70	138.00	134.14
2	B	702	DGT	C6-C5-N7	25.70	137.60	134.14
2	C	702	DGT	C6-C5-N7	19.49	136.76	134.14
2	A	701	DGT	C6-C5-N7	16.74	136.39	134.14
2	D	705	DGT	C6-C5-N7	15.19	136.19	134.14
2	B	703	DGT	C6-C5-N7	10.16	135.51	134.14
3	A	702	DTP	N3-C2-N1	-10.13	119.97	128.89
3	B	704	DTP	N3-C2-N1	-8.99	120.98	128.89
2	D	702	DGT	C6-C5-N7	8.85	135.33	134.14
3	C	701	DTP	C5-C4-N3	-8.45	117.74	125.98
3	D	703	DTP	C5-C4-N3	-8.18	118.01	125.98
2	B	703	DGT	C5-C4-N3	-7.37	117.59	126.07
3	D	703	DTP	N3-C2-N1	-6.78	122.93	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	701	DTP	N3-C4-N9	6.58	136.67	125.39
3	D	703	DTP	N3-C4-N9	6.22	136.06	125.39
2	C	702	DGT	C5-C4-N3	-6.10	119.05	126.07
2	D	702	DGT	C5-C4-N3	-6.08	119.07	126.07
2	D	704	DGT	C5-C4-N3	-6.01	119.15	126.07
3	C	701	DTP	N3-C2-N1	-5.65	123.92	128.89
3	A	702	DTP	C8-N9-C4	5.53	111.45	106.96
3	B	704	DTP	PB-O3B-PG	-5.44	116.86	131.93
2	D	705	DGT	C5-C4-N3	-5.40	119.85	126.07
2	B	703	DGT	N3-C4-N9	5.39	134.82	126.91
2	C	702	DGT	PB-O3B-PG	-5.28	117.31	131.93
3	B	704	DTP	C5-C4-N3	-5.28	120.83	125.98
2	C	703	DGT	C5-C4-N3	-5.20	120.08	126.07
2	C	702	DGT	N3-C4-N9	5.03	134.29	126.91
2	D	704	DGT	PB-O3B-PG	-5.02	118.02	131.93
2	B	702	DGT	C5-C4-N3	-5.00	120.31	126.07
2	D	702	DGT	N3-C4-N9	5.00	134.24	126.91
2	B	702	DGT	C6-N1-C2	4.97	123.01	120.20
2	B	702	DGT	PA-O3A-PB	-4.94	118.24	131.93
2	C	703	DGT	N3-C4-N9	4.92	134.13	126.91
3	A	702	DTP	N3-C4-N9	4.87	133.74	125.39
2	A	701	DGT	PA-O3A-PB	-4.81	118.60	131.93
2	C	703	DGT	PA-O3A-PB	-4.77	118.73	131.93
2	D	704	DGT	PA-O3A-PB	-4.73	118.84	131.93
2	D	704	DGT	C2-N3-C4	4.71	120.95	115.30
2	D	704	DGT	N3-C4-N9	4.61	133.67	126.91
2	D	705	DGT	C2-N3-C4	4.50	120.69	115.30
3	A	702	DTP	C5-C4-N3	-4.48	121.61	125.98
2	D	705	DGT	N3-C4-N9	4.47	133.47	126.91
2	D	705	DGT	PA-O3A-PB	-4.45	119.61	131.93
2	C	702	DGT	PA-O3A-PB	-4.42	119.70	131.93
2	B	703	DGT	PA-O3A-PB	-4.39	119.78	131.93
2	A	701	DGT	PB-O3B-PG	-4.36	119.87	131.93
2	B	703	DGT	C2-N3-C4	4.33	120.49	115.30
3	B	704	DTP	N3-C4-N9	4.31	132.78	125.39
3	B	704	DTP	C4-C5-N7	-4.30	105.25	109.41
2	B	702	DGT	C2-N3-C4	4.28	120.44	115.30
3	C	701	DTP	C8-N9-C4	4.24	110.40	106.96
3	C	701	DTP	C4-C5-N7	-4.20	105.35	109.41
2	A	701	DGT	C5-C4-N3	-4.12	121.32	126.07
2	C	702	DGT	C2-N3-C4	4.11	120.22	115.30
3	A	702	DTP	C2-N1-C6	4.05	125.97	118.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	702	DGT	PA-O3A-PB	-3.98	120.91	131.93
2	D	702	DGT	C2-N3-C4	3.89	119.96	115.30
2	D	705	DGT	PB-O3B-PG	-3.87	121.21	131.93
3	C	701	DTP	O5'-PA-O1A	-3.81	94.45	109.37
2	A	701	DGT	N2-C2-N3	-3.79	115.36	120.28
2	D	705	DGT	C6-N1-C2	3.72	122.30	120.20
3	B	704	DTP	C2-N1-C6	3.72	125.38	118.76
2	A	701	DGT	N3-C4-N9	3.65	132.26	126.91
2	B	703	DGT	C6-N1-C2	3.64	122.26	120.20
2	D	704	DGT	C4-C5-N7	-3.63	105.90	109.41
2	B	702	DGT	N2-C2-N1	3.57	121.65	117.82
2	A	701	DGT	C6-N1-C2	3.54	122.20	120.20
3	A	702	DTP	O5'-PA-O1A	-3.54	95.50	109.37
3	B	704	DTP	C8-N9-C4	3.53	109.83	106.96
2	D	702	DGT	C6-N1-C2	3.53	122.19	120.20
2	B	702	DGT	N2-C2-N3	-3.52	115.70	120.28
2	B	703	DGT	C4-C5-N7	-3.46	106.06	109.41
2	B	702	DGT	O4'-C1'-N9	3.45	113.87	107.66
2	B	702	DGT	N3-C4-N9	3.41	131.90	126.91
3	B	704	DTP	PA-O3A-PB	-3.22	123.02	131.93
2	C	702	DGT	C4-C5-N7	-3.21	106.30	109.41
3	D	703	DTP	C4-C5-N7	-3.16	106.36	109.41
2	B	702	DGT	PB-O3B-PG	-3.15	123.21	131.93
3	C	701	DTP	PA-O3A-PB	-3.14	123.23	131.93
3	A	702	DTP	O2G-PG-O1G	3.10	120.49	110.36
2	C	702	DGT	C6-N1-C2	3.09	121.95	120.20
3	D	703	DTP	O3G-PG-O1G	3.09	120.47	110.36
2	C	703	DGT	PB-O3B-PG	-3.07	123.43	131.93
2	C	703	DGT	C6-N1-C2	3.07	121.93	120.20
2	B	703	DGT	PB-O3B-PG	-3.00	123.62	131.93
2	C	703	DGT	C2-N3-C4	2.96	118.85	115.30
2	A	701	DGT	C2-N3-C4	2.96	118.84	115.30
2	B	702	DGT	C4-C5-N7	-2.94	106.57	109.41
3	A	702	DTP	PB-O3B-PG	-2.92	123.83	131.93
3	D	703	DTP	C2-N3-C4	2.87	121.53	113.27
3	B	704	DTP	O5'-PA-O1A	-2.85	98.22	109.37
3	C	701	DTP	O3G-PG-O1G	2.81	119.56	110.36
3	B	704	DTP	C2-N3-C4	2.81	121.35	113.27
3	C	701	DTP	PB-O3B-PG	-2.78	124.22	131.93
3	C	701	DTP	O3A-PB-O3B	2.78	107.31	101.66
3	D	703	DTP	O3B-PG-O1G	-2.78	91.42	110.43
2	D	702	DGT	PB-O3B-PG	-2.78	124.24	131.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	704	DGT	O4'-C1'-N9	2.76	112.64	107.66
3	A	702	DTP	C4-C5-N7	-2.75	106.75	109.41
3	D	703	DTP	C8-N9-C4	2.72	109.17	106.96
2	D	704	DGT	N2-C2-N3	-2.72	116.75	120.28
2	A	701	DGT	N2-C2-N1	2.71	120.72	117.82
3	A	702	DTP	PA-O3A-PB	-2.70	124.45	131.93
3	A	702	DTP	C1'-N9-C4	-2.65	120.39	126.84
2	D	702	DGT	O1G-PG-O3G	2.63	118.98	110.36
3	C	701	DTP	C2-N3-C4	2.62	120.83	113.27
3	D	703	DTP	C2'-C3'-C4'	2.59	108.47	102.73
3	A	702	DTP	C2-N3-C4	2.57	120.68	113.27
2	B	702	DGT	O2G-PG-O3G	2.56	118.75	110.36
3	D	703	DTP	PB-O3B-PG	-2.54	124.88	131.93
2	B	703	DGT	N2-C2-N1	-2.50	115.14	117.82
3	A	702	DTP	C6-C5-C4	-2.47	114.77	117.55
3	A	702	DTP	O3A-PA-O5'	2.47	109.46	102.91
2	B	702	DGT	C8-N9-C1'	2.43	130.72	126.15
3	A	702	DTP	O4'-C1'-N9	-2.39	103.35	107.66
2	D	705	DGT	O3A-PB-O3B	2.37	106.48	101.66
2	C	702	DGT	O1G-PG-O3G	2.35	118.06	110.36
2	A	701	DGT	O2G-PG-O1G	2.32	116.07	107.38
2	A	701	DGT	O4'-C1'-N9	2.31	111.82	107.66
2	D	704	DGT	C6-N1-C2	2.30	121.50	120.20
2	A	701	DGT	C4-C5-N7	-2.28	107.21	109.41
3	B	704	DTP	C1'-N9-C4	-2.28	121.30	126.84
2	C	702	DGT	O4'-C1'-N9	2.26	111.73	107.66
2	B	703	DGT	O3A-PA-O5'	-2.25	96.95	102.91
2	B	703	DGT	O1G-PG-O3G	2.25	117.71	110.36
3	B	704	DTP	C5-C6-N6	2.23	125.76	120.72
2	D	702	DGT	C4-C5-N7	-2.12	107.36	109.41
3	D	703	DTP	O3A-PB-O3B	2.11	105.95	101.66
3	B	704	DTP	C6-C5-N7	2.09	139.34	131.34
3	D	703	DTP	O2B-PB-O1B	2.07	123.61	112.14
3	B	704	DTP	O2A-PA-O1A	2.06	123.56	112.14
2	D	704	DGT	O1G-PG-O3G	2.05	117.08	110.36
3	C	701	DTP	C8-N7-C5	2.03	109.89	103.58
3	A	702	DTP	O3B-PG-O1G	-2.01	96.64	110.43
2	D	704	DGT	O3A-PB-O3B	2.01	105.75	101.66

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%)	0.16	13 (2%) 52 49	35, 63, 104, 133	0
1	B	481/514 (93%)	0.39	29 (6%) 21 18	37, 75, 119, 156	0
1	C	481/514 (93%)	0.49	45 (9%) 9 6	36, 74, 121, 156	0
1	D	481/514 (93%)	0.88	69 (14%) 3 2	41, 100, 169, 208	0
All	All	1924/2056 (93%)	0.48	156 (8%) 12 9	35, 76, 139, 208	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	490	ASP	6.6
1	C	489	LEU	6.6
1	D	569	PHE	6.5
1	C	488	LEU	6.4
1	D	488	LEU	6.3
1	D	554	CYS	6.2
1	D	599	ASN	6.1
1	D	562	LEU	6.0
1	D	493	LEU	5.3
1	D	480	VAL	5.3
1	C	493	LEU	5.2
1	C	490	ASP	5.2
1	B	488	LEU	5.0
1	D	489	LEU	5.0
1	D	476	LEU	5.0
1	B	540	LEU	5.0
1	D	585	ASP	5.0
1	C	491	VAL	4.9
1	D	397	ILE	4.8
1	D	487	VAL	4.8
1	D	341	CYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	276	LEU	4.4
1	D	478	LYS	4.4
1	D	572	TRP	4.4
1	D	481	ALA	4.2
1	D	345	ASN	4.2
1	D	347	LEU	4.2
1	D	472	ASP	4.1
1	D	563	TYR	4.1
1	C	492	LYS	4.0
1	D	592	THR	3.9
1	D	273	VAL	3.9
1	D	570	VAL	3.9
1	D	587	ILE	3.9
1	D	590	LEU	3.8
1	C	486	LYS	3.8
1	B	590	LEU	3.8
1	C	284	LEU	3.8
1	D	469	LYS	3.8
1	D	573	CYS	3.7
1	D	230	LYS	3.6
1	C	468	ILE	3.6
1	B	491	VAL	3.5
1	B	397	ILE	3.5
1	D	396	TYR	3.5
1	B	489	LEU	3.5
1	D	526	PRO	3.5
1	D	467	LYS	3.5
1	D	485	PRO	3.5
1	C	277	GLU	3.4
1	C	487	VAL	3.4
1	D	468	ILE	3.3
1	A	490	ASP	3.3
1	D	388[A]	ASP	3.2
1	D	402	ALA	3.2
1	A	245	ILE	3.2
1	C	484	LYS	3.2
1	D	491	VAL	3.2
1	D	473	TYR	3.2
1	D	531	ARG	3.2
1	D	586	VAL	3.2
1	B	328	ASN	3.2
1	B	492	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	262	GLU	3.0
1	C	562	LEU	3.0
1	C	568	TYR	3.0
1	B	598	TRP	2.9
1	C	473	TYR	2.9
1	C	345	ASN	2.9
1	C	594	GLN	2.9
1	D	492	LYS	2.9
1	D	511[A]	GLU	2.9
1	C	286	PRO	2.9
1	A	276	LEU	2.8
1	A	403	GLY	2.8
1	D	438	LEU	2.8
1	C	498	PHE	2.8
1	D	328	ASN	2.8
1	C	326	GLN	2.7
1	D	559	ARG	2.7
1	A	252	PRO	2.7
1	C	403	GLY	2.7
1	D	490	ASP	2.7
1	C	262	GLU	2.6
1	A	241	PHE	2.6
1	D	544	LYS	2.6
1	D	266	CYS	2.6
1	C	569	PHE	2.6
1	C	464	GLY	2.6
1	C	476	LEU	2.6
1	B	584	GLY	2.6
1	A	404	GLY	2.6
1	B	230	LYS	2.6
1	B	320	CYS	2.5
1	D	591	ILE	2.5
1	C	531	ARG	2.5
1	B	589	PRO	2.5
1	D	498	PHE	2.5
1	B	594	GLN	2.5
1	D	403	GLY	2.5
1	D	465	GLN	2.5
1	B	586	VAL	2.5
1	A	465	GLN	2.5
1	A	255	GLU	2.5
1	C	467	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	596	LYS	2.5
1	C	496	GLU	2.4
1	D	593	PRO	2.4
1	B	326	GLN	2.4
1	D	568	TYR	2.4
1	B	277	GLU	2.4
1	B	487	VAL	2.4
1	C	587	ILE	2.4
1	C	483	ALA	2.4
1	D	576	ARG	2.4
1	D	231	TRP	2.4
1	D	346	GLU	2.3
1	D	486	LYS	2.3
1	C	121	PRO	2.3
1	C	494	LYS	2.3
1	B	587	ILE	2.3
1	C	563	TYR	2.3
1	B	599	ASN	2.3
1	D	406	LYS	2.3
1	B	493	LEU	2.3
1	B	263	GLU	2.3
1	A	408	ARG	2.3
1	C	590	LEU	2.2
1	C	485	PRO	2.2
1	B	327	ASN	2.2
1	D	288	LYS	2.2
1	B	498	PHE	2.2
1	C	500	VAL	2.2
1	C	465	GLN	2.2
1	C	298	TYR	2.2
1	D	413	ILE	2.2
1	D	398	GLU	2.2
1	D	543	GLU	2.2
1	D	578	PHE	2.2
1	C	388[A]	ASP	2.2
1	C	575	ASP	2.2
1	D	285	TRP	2.1
1	C	583	ASP	2.1
1	B	569	PHE	2.1
1	C	245	ILE	2.1
1	B	466	ILE	2.1
1	C	293	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	585	ASP	2.1
1	C	288	LYS	2.1
1	B	276	LEU	2.1
1	A	284	LEU	2.1
1	D	484	LYS	2.0
1	D	334	PHE	2.0
1	C	554	CYS	2.0
1	D	528	ARG	2.0
1	A	317	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, 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
2	DGT	B	702	31/31	0.14	-0.97	41,57,111,116	0
3	DTP	C	701	30/30	0.14	-1.33	24,27,33,34	0
2	DGT	A	701	31/31	0.13	-1.51	36,58,89,98	0
2	DGT	B	703	31/31	0.11	-1.65	24,30,34,36	0
2	DGT	D	704	31/31	0.14	-1.67	47,54,88,94	0
2	DGT	C	702	31/31	0.13	-1.72	45,58,92,100	0
2	DGT	C	703	31/31	0.12	-1.73	25,27,34,34	0
3	DTP	D	703	30/30	0.12	-1.75	23,29,34,36	0
2	DGT	D	705	31/31	0.13	-1.79	25,28,30,35	0
3	DTP	A	702	30/30	0.11	-2.10	23,27,33,34	0
2	DGT	D	702	31/31	0.11	-2.35	21,27,30,35	0
3	DTP	B	704	30/30	0.11	-2.55	20,24,34,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	A	703	1/1	0.09	-5.38	28,28,28,28	0
4	MG	D	701	1/1	0.07	-6.69	30,30,30,30	0
4	MG	C	704	1/1	0.10	-14.73	45,45,45,45	0
4	MG	B	701	1/1	0.07	-58.50	32,32,32,32	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.