



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2017 – 09:14 PM EST

PDB ID : 4TO2  
Title : Structure basis of cellular dNTP regulation, SAMHD1-dGTP-dGTP-dGTP/  
dTTP complex  
Authors : Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.  
Deposited on : unknown  
Resolution : 2.27 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

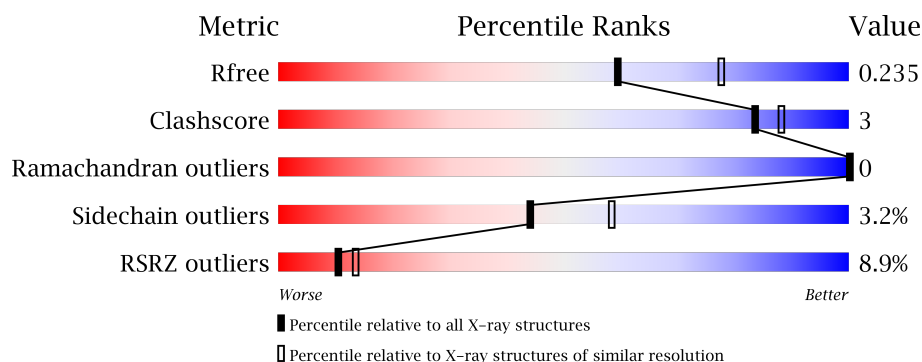
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.27 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))
$R_{free}$	100719	5609 (2.30-2.26)
Clashscore	112137	6364 (2.30-2.26)
Ramachandran outliers	110173	6281 (2.30-2.26)
Sidechain outliers	110143	6281 (2.30-2.26)
RSRZ outliers	101464	5639 (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. 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	514	<div> <div>10%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>6%</div> </div> </div>
1	B	514	<div> <div>9%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>6%</div> </div> </div>
1	C	514	<div> <div>10%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>6%</div> </div> </div>
1	D	514	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>6%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16367 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.

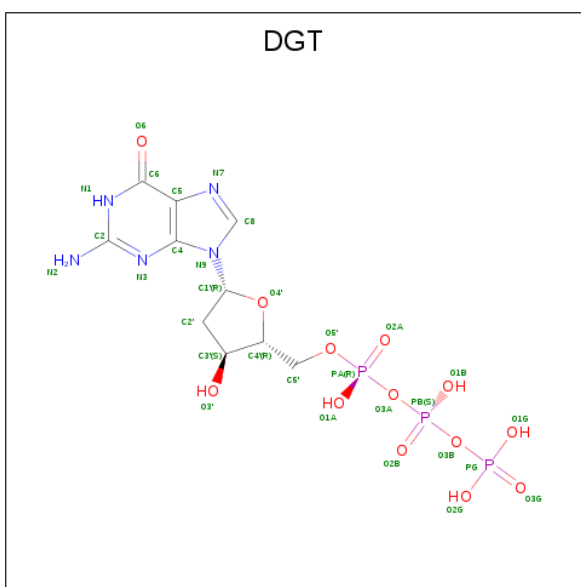
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

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<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
2	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	D	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	D	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	D	1	Total 31	C 10	N 5	O 13	P 3	0	0

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

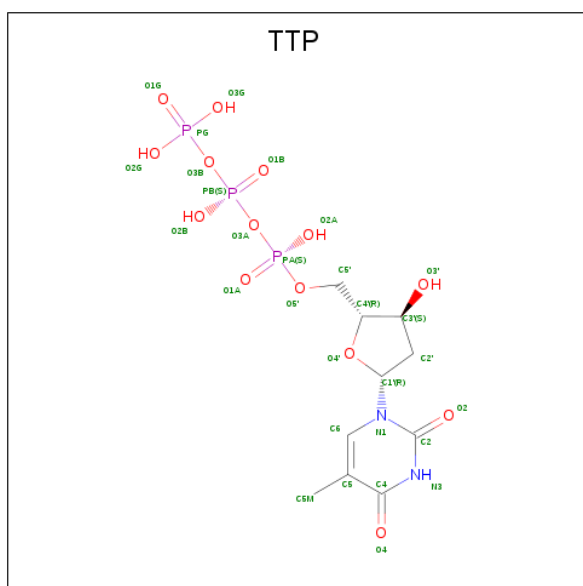
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0

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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		

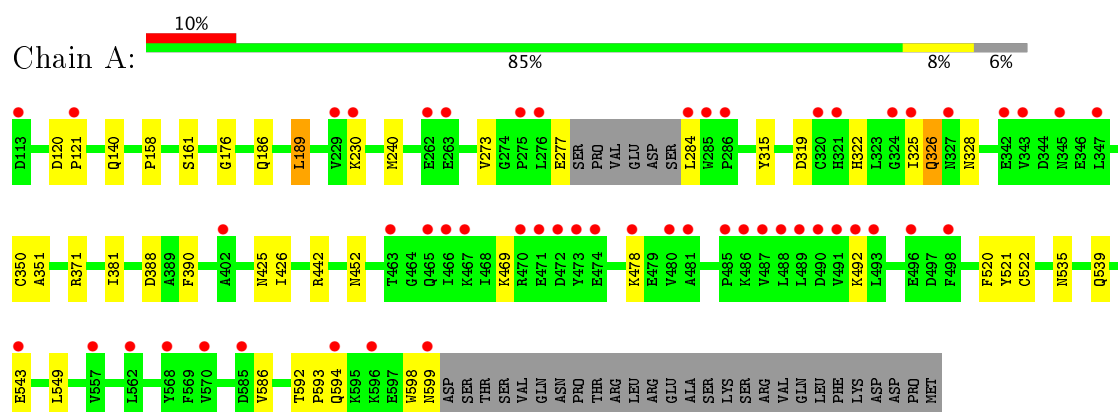
- Molecule 5 is water.

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		

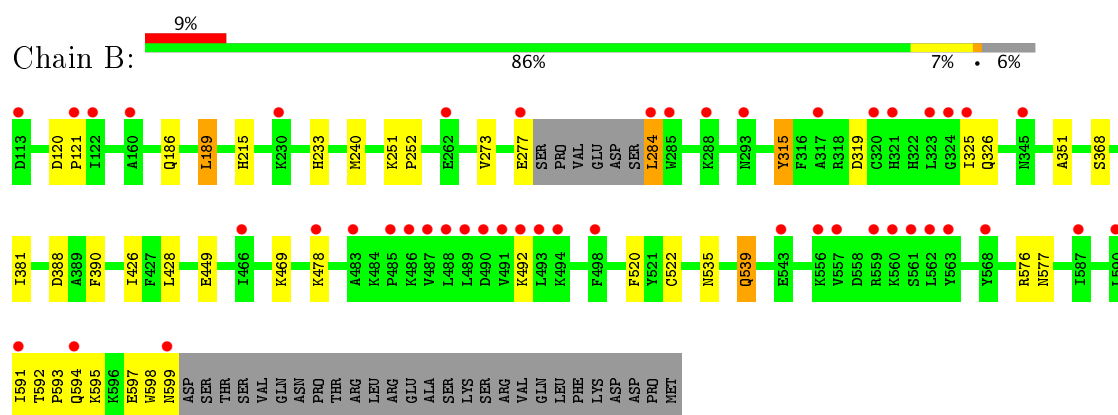
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

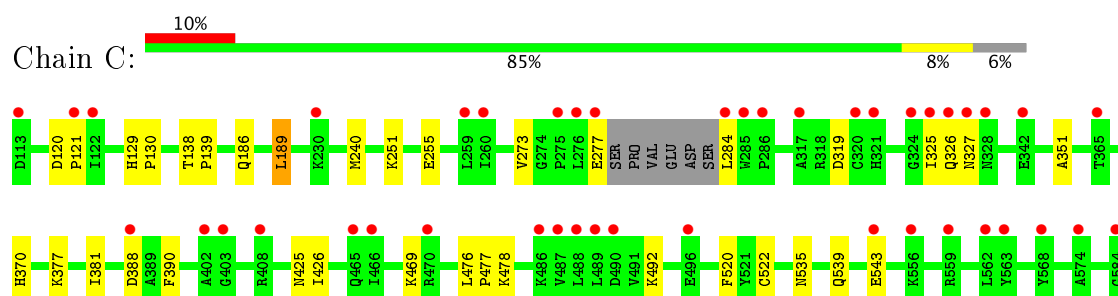
#### • Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

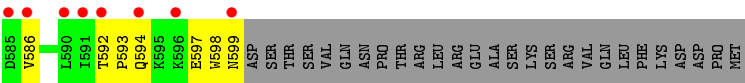


#### • Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

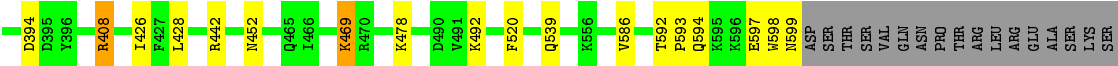
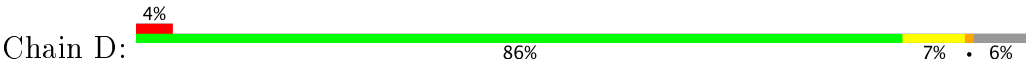


#### • Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



## 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 0.208 , 0.235	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 , 52.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	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.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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 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	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

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 3.

All (90) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:THR:C	5:C:829:HOH:O	2.52	0.46
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%)	46	61
1	B	428/459 (93%)	414 (97%)	14 (3%)	43	57
1	C	428/459 (93%)	415 (97%)	13 (3%)	46	61
1	D	428/459 (93%)	414 (97%)	14 (3%)	43	57
All	All	1712/1836 (93%)	1658 (97%)	54 (3%)	44	58

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

Mol	Chain	Res	Type
1	A	189	LEU
1	A	273	VAL

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Mol	Chain	Res	Type
1	A	277	GLU
1	A	284	LEU
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

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Mol	Chain	Res	Type
1	D	284	LEU
1	D	325	ILE
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 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 ⓘ

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	26,33,33	1.23	2 (7%)	28,52,52	1.99	7 (25%)
2	DGT	A	703	3	26,33,33	1.13	1 (3%)	28,52,52	1.62	7 (25%)
2	DGT	A	704	3	26,33,33	1.36	5 (19%)	28,52,52	2.51	9 (32%)
2	DGT	B	701	3	26,33,33	1.49	6 (23%)	28,52,52	1.72	5 (17%)
2	DGT	B	703	3	26,33,33	1.29	2 (7%)	28,52,52	2.05	8 (28%)
2	DGT	B	704	3	26,33,33	1.33	4 (15%)	28,52,52	2.35	9 (32%)
2	DGT	C	701	3	26,33,33	1.35	3 (11%)	28,52,52	1.97	7 (25%)
4	TTP	C	704	3	22,30,30	1.03	1 (4%)	25,47,47	2.13	6 (24%)
2	DGT	C	706	3	26,33,33	1.21	2 (7%)	28,52,52	2.14	9 (32%)
2	DGT	D	701	3	26,33,33	1.28	4 (15%)	28,52,52	1.77	8 (28%)
2	DGT	D	702	3	26,33,33	1.50	4 (15%)	28,52,52	1.57	4 (14%)
2	DGT	D	704	3	26,33,33	1.32	5 (19%)	28,52,52	2.07	9 (32%)

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	-	0/18/34/34	0/3/3/3
2	DGT	A	703	3	-	0/18/34/34	0/3/3/3
2	DGT	A	704	3	-	0/18/34/34	0/3/3/3
2	DGT	B	701	3	-	0/18/34/34	0/3/3/3
2	DGT	B	703	3	-	0/18/34/34	0/3/3/3
2	DGT	B	704	3	-	0/18/34/34	0/3/3/3
2	DGT	C	701	3	-	0/18/34/34	0/3/3/3
4	TTP	C	704	3	-	0/18/34/34	0/2/2/2
2	DGT	C	706	3	-	0/18/34/34	0/3/3/3
2	DGT	D	701	3	-	0/18/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DGT	D	702	3	-	0/18/34/34	0/3/3/3
2	DGT	D	704	3	-	0/18/34/34	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	704	DGT	C4-N3	-3.45	1.30	1.35
2	D	701	DGT	C4-N3	-2.55	1.31	1.35
2	A	704	DGT	C4-N3	-2.43	1.31	1.35
4	C	704	TTP	O4'-C4'	-2.26	1.39	1.45
2	D	704	DGT	C4-N3	-2.25	1.32	1.35
2	B	704	DGT	O4'-C4'	-2.22	1.40	1.45
2	C	701	DGT	C4-N3	-2.22	1.32	1.35
2	D	701	DGT	C2-N2	2.02	1.38	1.34
2	A	704	DGT	C2-N2	2.05	1.38	1.34
2	D	704	DGT	C8-N7	2.07	1.38	1.34
2	B	701	DGT	C8-N7	2.08	1.38	1.34
2	D	701	DGT	C2-N1	2.10	1.39	1.35
2	D	704	DGT	PG-O3B	2.21	1.63	1.60
2	B	701	DGT	C2-N2	2.21	1.38	1.34
2	B	704	DGT	PG-O3B	2.27	1.63	1.60
2	B	704	DGT	C6-C5	2.29	1.45	1.41
2	D	702	DGT	C6-C5	2.30	1.45	1.41
2	B	701	DGT	C6-N1	2.31	1.37	1.33
2	A	704	DGT	C6-C5	2.32	1.45	1.41
2	B	701	DGT	C2-N1	2.42	1.39	1.35
2	C	701	DGT	C5-C4	2.45	1.46	1.40
2	A	704	DGT	C5-C4	2.73	1.46	1.40
2	D	704	DGT	C5-C4	2.77	1.46	1.40
2	D	702	DGT	C2-N1	2.83	1.40	1.35
2	D	701	DGT	C6-C5	2.88	1.46	1.41
2	C	706	DGT	C6-C5	3.01	1.47	1.41
2	A	701	DGT	C5-C4	3.05	1.47	1.40
2	D	702	DGT	C2-N2	3.07	1.40	1.34
2	A	704	DGT	PG-O3B	3.26	1.65	1.60
2	C	706	DGT	C5-C4	3.26	1.47	1.40
2	A	701	DGT	C6-C5	3.38	1.47	1.41
2	B	703	DGT	C5-C4	3.48	1.48	1.40
2	D	704	DGT	C6-C5	3.55	1.48	1.41
2	B	701	DGT	C6-C5	3.72	1.48	1.41
2	B	701	DGT	C5-C4	3.72	1.48	1.40
2	D	702	DGT	C5-C4	3.75	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	703	DGT	C6-C5	3.79	1.48	1.41
2	C	701	DGT	C6-C5	4.09	1.49	1.41
2	B	703	DGT	C6-C5	4.18	1.49	1.41

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	704	DGT	C5-C6-N1	-6.85	113.73	123.48
2	B	704	DGT	C5-C6-N1	-6.08	114.83	123.48
2	C	706	DGT	C5-C6-N1	-5.82	115.19	123.48
4	C	704	TTP	C5-C4-N3	-5.49	119.19	125.24
2	A	701	DGT	C6-C5-C4	-5.46	115.42	120.84
2	D	704	DGT	C5-C6-N1	-4.95	116.43	123.48
2	C	701	DGT	C5-C6-N1	-4.75	116.72	123.48
2	A	704	DGT	C6-C5-C4	-4.49	116.38	120.84
2	B	703	DGT	C5-C6-N1	-4.47	117.11	123.48
2	D	702	DGT	C6-C5-C4	-4.20	116.66	120.84
2	C	701	DGT	C6-C5-C4	-4.12	116.75	120.84
2	B	701	DGT	C6-C5-C4	-3.97	116.89	120.84
2	D	701	DGT	C6-C5-C4	-3.84	117.02	120.84
2	D	701	DGT	C5-C6-N1	-3.83	118.03	123.48
2	B	701	DGT	C5-C6-N1	-3.78	118.09	123.48
2	B	703	DGT	C6-C5-C4	-3.75	117.12	120.84
2	D	702	DGT	C5-C6-N1	-3.71	118.20	123.48
2	B	704	DGT	C4-C5-N7	-3.69	105.84	109.41
2	A	703	DGT	C5-C6-N1	-3.66	118.27	123.48
2	D	704	DGT	C6-C5-C4	-3.44	117.42	120.84
2	A	701	DGT	N3-C2-N1	-3.40	122.49	127.46
2	C	706	DGT	C6-C5-C4	-3.34	117.53	120.84
2	D	701	DGT	O3B-PG-O3G	-3.33	90.95	111.44
2	A	704	DGT	N3-C2-N1	-3.29	122.66	127.46
2	A	703	DGT	C6-C5-C4	-3.17	117.69	120.84
2	B	703	DGT	N3-C2-N1	-3.11	122.91	127.46
2	C	701	DGT	C4-C5-N7	-3.04	106.47	109.41
2	B	704	DGT	N2-C2-N3	-3.02	112.18	117.75
2	B	701	DGT	N3-C2-N1	-2.98	123.10	127.46
2	B	704	DGT	O4'-C1'-N9	-2.97	102.78	107.78
2	B	703	DGT	C4-C5-N7	-2.88	106.63	109.41
2	B	704	DGT	N3-C2-N1	-2.78	123.40	127.46
2	D	704	DGT	N3-C2-N1	-2.66	123.57	127.46
2	C	706	DGT	N3-C2-N1	-2.60	123.67	127.46
2	D	701	DGT	O5'-PA-O2A	-2.59	98.79	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	702	DGT	N3-C2-N1	-2.58	123.69	127.46
2	A	703	DGT	O5'-PA-O2A	-2.52	99.07	109.25
2	A	701	DGT	C5-C6-N1	-2.50	119.93	123.48
2	A	704	DGT	O4'-C1'-N9	-2.50	103.57	107.78
2	C	706	DGT	O3B-PG-O3G	-2.46	96.31	111.44
2	C	701	DGT	O4'-C1'-N9	-2.33	103.86	107.78
2	C	701	DGT	O3B-PG-O3G	-2.13	98.32	111.44
2	D	704	DGT	O5'-PA-O2A	-2.06	100.93	109.25
2	D	701	DGT	C2-N3-C4	2.02	117.52	115.16
2	D	704	DGT	O1G-PG-O3G	2.03	118.43	110.50
2	D	704	DGT	O2G-PG-O1G	2.04	115.83	107.61
2	B	703	DGT	O2G-PG-O1G	2.08	115.99	107.61
2	D	704	DGT	O1A-PA-O5'	2.11	118.08	108.14
2	A	704	DGT	N2-C2-N1	2.17	120.71	117.24
2	D	701	DGT	O1B-PB-O2B	2.19	123.63	112.28
2	A	704	DGT	O1B-PB-O2B	2.22	123.79	112.28
2	D	701	DGT	C6-N1-C2	2.23	119.27	116.06
2	C	701	DGT	O1A-PA-O2A	2.24	123.89	112.28
2	C	706	DGT	O1B-PB-O2B	2.25	123.92	112.28
2	B	703	DGT	N2-C2-N1	2.25	120.84	117.24
2	C	706	DGT	O1G-PG-O3G	2.30	119.52	110.50
2	A	704	DGT	O2G-PG-O3G	2.31	119.55	110.50
2	B	704	DGT	O2G-PG-O1G	2.32	116.96	107.61
2	A	701	DGT	O1A-PA-O2A	2.33	124.31	112.28
2	C	706	DGT	O2G-PG-O3G	2.33	119.61	110.50
4	C	704	TTP	O2B-PB-O1B	2.36	124.49	112.28
4	C	704	TTP	O2G-PG-O1G	2.41	119.95	110.50
2	C	706	DGT	C2-N3-C4	2.47	118.04	115.16
4	C	704	TTP	O4'-C1'-N1	2.47	111.95	107.78
2	A	703	DGT	O2G-PG-O3G	2.48	120.19	110.50
2	A	703	DGT	C2-N3-C4	2.50	118.08	115.16
2	A	703	DGT	O1A-PA-O5'	2.51	119.98	108.14
2	D	701	DGT	O1G-PG-O3G	3.05	122.42	110.50
2	A	704	DGT	O2G-PG-O1G	3.07	120.00	107.61
2	A	701	DGT	C6-N1-C2	3.31	120.82	116.06
2	A	703	DGT	C6-N1-C2	3.42	120.98	116.06
2	D	702	DGT	C6-N1-C2	3.43	120.99	116.06
2	B	701	DGT	C2-N3-C4	3.56	119.31	115.16
2	B	701	DGT	C6-N1-C2	3.61	121.25	116.06
2	C	701	DGT	C6-N1-C2	3.63	121.28	116.06
2	A	701	DGT	O2G-PG-O1G	3.67	122.42	107.61
2	B	704	DGT	C2-N3-C4	3.90	119.71	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	704	DGT	C6-N1-C2	4.24	122.16	116.06
4	C	704	TTP	C5M-C5-C4	4.27	125.10	120.17
2	B	703	DGT	C2-N3-C4	4.34	120.22	115.16
2	A	701	DGT	C2-N3-C4	4.44	120.35	115.16
2	B	704	DGT	N2-C2-N1	4.49	124.42	117.24
2	D	704	DGT	C6-N1-C2	4.61	122.69	116.06
2	D	704	DGT	C2-N3-C4	4.69	120.64	115.16
2	B	703	DGT	C6-N1-C2	5.16	123.48	116.06
4	C	704	TTP	C4-N3-C2	5.41	119.89	115.16
2	C	706	DGT	C6-N1-C2	5.98	124.67	116.06
2	A	704	DGT	C6-N1-C2	7.39	126.69	116.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	703	DGT	1	0
2	A	704	DGT	1	0
2	B	701	DGT	2	0
4	C	704	TTP	2	0
2	D	702	DGT	2	0

## 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	481/514 (93%)	0.65	53 (11%) 6 8	41, 72, 118, 145	0
1	B	481/514 (93%)	0.51	46 (9%) 9 11	41, 61, 100, 130	0
1	C	481/514 (93%)	0.66	51 (10%) 7 9	45, 75, 112, 148	0
1	D	481/514 (93%)	0.33	22 (4%) 33 39	42, 54, 81, 108	0
All	All	1924/2056 (93%)	0.54	172 (8%) 10 13	41, 64, 109, 148	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	488	LEU	7.8
1	A	488	LEU	6.8
1	B	489	LEU	6.7
1	B	490	ASP	6.3
1	C	488	LEU	6.3
1	A	487	VAL	5.7
1	B	486	LYS	5.4
1	C	590	LEU	5.4
1	C	490	ASP	5.1
1	B	599	ASN	5.1
1	C	487	VAL	4.7
1	C	465	GLN	4.6
1	A	471	GLU	4.5
1	A	466	ILE	4.5
1	A	486	LYS	4.5
1	B	591	ILE	4.5
1	D	491	VAL	4.4
1	C	276	LEU	4.3
1	A	345	ASN	4.3
1	C	599	ASN	4.3
1	C	594	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	491	VAL	4.1
1	A	230	LYS	4.1
1	A	489	LEU	4.0
1	C	596	LYS	4.0
1	A	562	LEU	4.0
1	C	326	GLN	3.9
1	B	561	SER	3.9
1	A	490	ASP	3.9
1	B	557	VAL	3.9
1	A	568	TYR	3.8
1	B	492	LYS	3.8
1	C	470	ARG	3.8
1	D	490	ASP	3.8
1	A	285	TRP	3.7
1	D	465	GLN	3.7
1	B	560	LYS	3.7
1	B	562	LEU	3.7
1	A	473	TYR	3.7
1	B	325	ILE	3.7
1	A	276	LEU	3.6
1	A	481	ALA	3.5
1	B	590	LEU	3.5
1	C	562	LEU	3.5
1	B	285	TRP	3.5
1	B	487	VAL	3.4
1	C	489	LEU	3.4
1	B	284	LEU	3.4
1	C	325	ILE	3.4
1	B	262	GLU	3.3
1	D	262	GLU	3.3
1	C	122	ILE	3.3
1	B	559	ARG	3.3
1	C	592	THR	3.2
1	A	585	ASP	3.2
1	A	286	PRO	3.2
1	B	587	ILE	3.2
1	B	478	LYS	3.2
1	B	483	ALA	3.1
1	A	599	ASN	3.1
1	B	594	GLN	3.1
1	C	277	GLU	3.1
1	A	343	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	563	TYR	3.0
1	C	113	ASP	3.0
1	A	275	PRO	3.0
1	B	543	GLU	3.0
1	B	498	PHE	3.0
1	A	113	ASP	3.0
1	D	249	GLY	2.9
1	C	466	ILE	2.9
1	B	485	PRO	2.9
1	B	556	LYS	2.8
1	A	263	GLU	2.8
1	C	317	ALA	2.8
1	A	284	LEU	2.7
1	C	403	GLY	2.7
1	A	491	VAL	2.7
1	C	556	LYS	2.7
1	B	121	PRO	2.7
1	A	570	VAL	2.7
1	B	493	LEU	2.7
1	C	563	TYR	2.7
1	B	230	LYS	2.7
1	C	121	PRO	2.6
1	C	275	PRO	2.6
1	A	596	LYS	2.6
1	C	327	ASN	2.6
1	D	317	ALA	2.6
1	D	466	ILE	2.6
1	C	559	ARG	2.6
1	D	478	LYS	2.6
1	C	591	ILE	2.6
1	C	496	GLU	2.6
1	A	463	THR	2.6
1	A	478	LYS	2.6
1	A	402	ALA	2.5
1	B	345	ASN	2.5
1	B	323	LEU	2.5
1	B	293	ASN	2.5
1	C	320	CYS	2.5
1	C	568	TYR	2.5
1	B	288	LYS	2.4
1	B	317	ALA	2.4
1	D	121	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	321	HIS	2.4
1	C	342	GLU	2.4
1	D	396	TYR	2.4
1	A	325	ILE	2.4
1	A	493	LEU	2.4
1	C	328	ASN	2.4
1	D	326	GLN	2.4
1	A	498	PHE	2.4
1	D	320	CYS	2.4
1	C	486	LYS	2.4
1	D	470	ARG	2.4
1	A	594	GLN	2.3
1	A	324	GLY	2.3
1	C	284	LEU	2.3
1	D	325	ILE	2.3
1	B	494	LYS	2.3
1	B	324	GLY	2.3
1	C	584	GLY	2.3
1	C	230	LYS	2.3
1	A	465	GLN	2.3
1	B	320	CYS	2.2
1	C	585	ASP	2.2
1	A	480	VAL	2.2
1	A	543	GLU	2.2
1	A	474	GLU	2.2
1	A	467	LYS	2.2
1	C	365	THR	2.2
1	C	574	ALA	2.2
1	D	160	ALA	2.2
1	A	347	LEU	2.2
1	C	388	ASP	2.2
1	B	122	ILE	2.2
1	B	568	TYR	2.2
1	A	321	HIS	2.2
1	C	260	ILE	2.2
1	D	596	LYS	2.2
1	A	262	GLU	2.2
1	B	466	ILE	2.2
1	C	259	LEU	2.2
1	D	159	GLY	2.2
1	B	321	HIS	2.1
1	C	408	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	342	GLU	2.1
1	C	586	VAL	2.1
1	C	324	GLY	2.1
1	A	492	LYS	2.1
1	D	162	HIS	2.1
1	A	472	ASP	2.1
1	A	470	ARG	2.1
1	A	327	ASN	2.1
1	A	496	GLU	2.1
1	C	286	PRO	2.1
1	B	113	ASP	2.1
1	C	543	GLU	2.1
1	A	229	VAL	2.1
1	C	285	TRP	2.1
1	A	121	PRO	2.1
1	B	277	GLU	2.0
1	D	556	LYS	2.0
1	B	160	ALA	2.0
1	C	402	ALA	2.0
1	A	320	CYS	2.0
1	D	599	ASN	2.0
1	A	485	PRO	2.0
1	A	557	VAL	2.0
1	D	323	LEU	2.0
1	D	114	THR	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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	DGT	D	702	31/31	0.87	0.15	-0.37	49,59,84,86	0
2	DGT	D	704	31/31	0.98	0.14	-0.44	44,45,47,47	0
2	DGT	B	704	31/31	0.98	0.16	-0.44	42,43,45,45	0
4	TTP	C	704	29/29	0.88	0.16	-0.53	59,72,97,101	0
2	DGT	A	701	31/31	0.89	0.13	-0.61	58,75,92,93	0
2	DGT	D	701	31/31	0.98	0.15	-0.85	41,42,45,46	0
2	DGT	A	704	31/31	0.97	0.14	-0.90	47,49,54,55	0
2	DGT	B	701	31/31	0.93	0.12	-0.97	53,57,77,81	0
2	DGT	C	706	31/31	0.98	0.12	-0.99	49,50,58,60	0
2	DGT	C	701	31/31	0.97	0.15	-1.17	44,46,53,53	0
2	DGT	A	703	31/31	0.97	0.11	-1.71	45,47,56,59	0
2	DGT	B	703	31/31	0.97	0.11	-1.81	46,47,55,55	0
3	MG	C	705	1/1	0.80	0.31	-	92,92,92,92	0
3	MG	A	702	1/1	0.95	0.07	-	81,81,81,81	0
3	MG	C	702	1/1	0.95	0.05	-	50,50,50,50	0
3	MG	B	702	1/1	0.97	0.07	-	74,74,74,74	0
3	MG	A	706	1/1	0.98	0.04	-	45,45,45,45	0
3	MG	A	705	1/1	0.98	0.06	-	58,58,58,58	0
3	MG	C	703	1/1	0.86	0.05	-	48,48,48,48	0
3	MG	D	703	1/1	0.99	0.03	-	65,65,65,65	0

## 6.5 Other polymers

There are no such residues in this entry.