W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2014 – 06:48 AM EDT

PDB ID	:	4TNX
Title	:	Structure basis of cellular dNTP regulation, SAMHD1-GTP-dGTP complex
Authors	:	Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.
Deposited on	:	2014-06-05
Resolution	:	2.31 Å(reported)

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 2.31 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	Percentile Ranks	Value
Rfree		0.223
Clashscore		5
Ramachandran outliers		0.1%
Sidechain outliers		2.6%
RSRZ outliers		5.6%

Worse _____ *Better*

▌Percentile relative to all X–ray structures

▯Percentile relative to X–ray structures of similar resolution
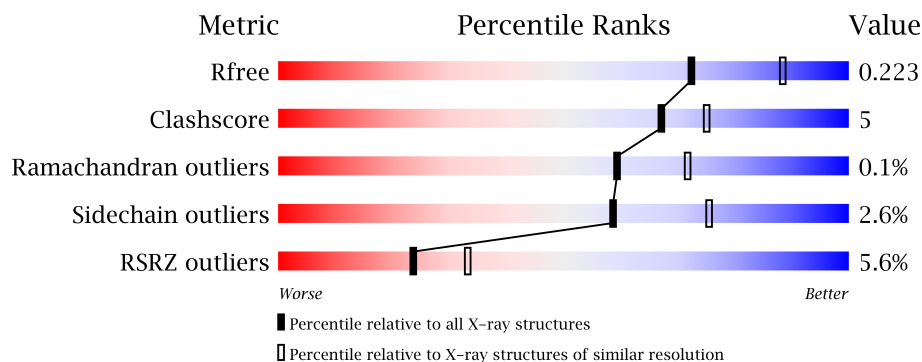
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	3293 (2.34-2.30)
Clashscore	79885	4097 (2.34-2.30)
Ramachandran outliers	78287	4055 (2.34-2.30)
Sidechain outliers	78261	4054 (2.34-2.30)
RSRZ outliers	66119	3294 (2.34-2.30)

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 >=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
5	3PO	A	705	-	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 16322 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	3	0
			3956	2529	689	717	21			
1	B	479	Total	C	N	O	S	0	3	0
			3940	2521	686	712	21			
1	C	481	Total	C	N	O	S	0	2	0
			3947	2524	688	714	21			
1	D	483	Total	C	N	O	S	0	2	0
			3961	2531	690	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
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: $C_{10}H_{16}N_5O_{13}P_3$).

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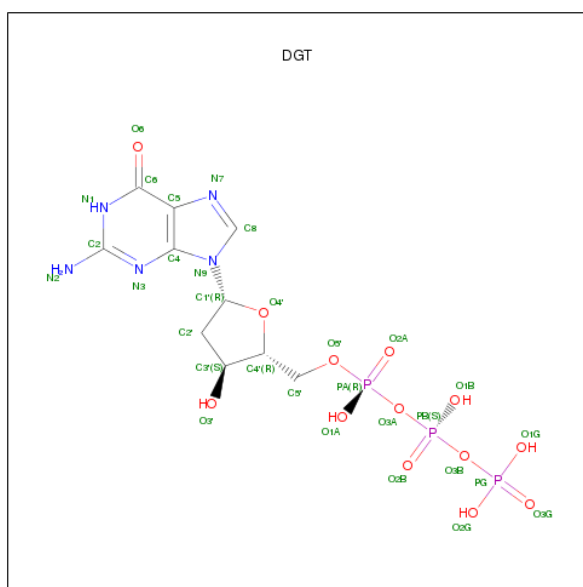
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

GTP
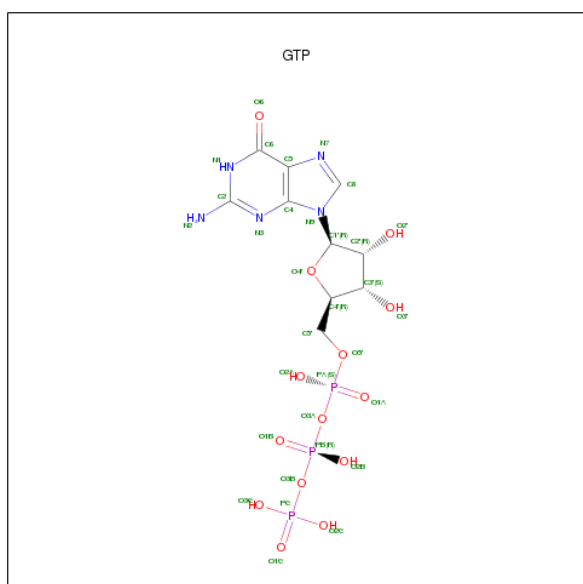
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 32	C 10	N 5	O 14	P 3	0	0
3	A	1	Total 32	C 10	N 5	O 14	P 3	0	0
3	B	1	Total 32	C 10	N 5	O 14	P 3	0	0
3	C	1	Total 32	C 10	N 5	O 14	P 3	0	0

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

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

- Molecule 5 is TRIPHOSPHATE (three-letter code: 3PO) (formula: $H_5O_{10}P_3$).
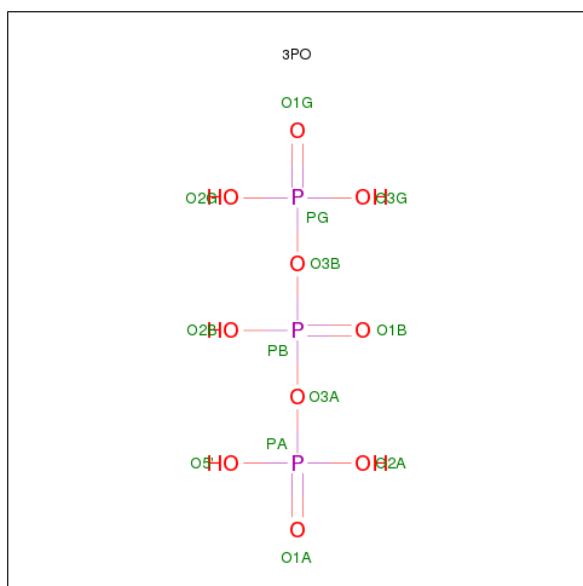
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 13	O 10	P 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	80	Total 80	O 80	0	0
6	B	49	Total 49	O 49	0	0
6	C	47	Total 47	O 47	0	0
6	D	73	Total 73	O 73	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:
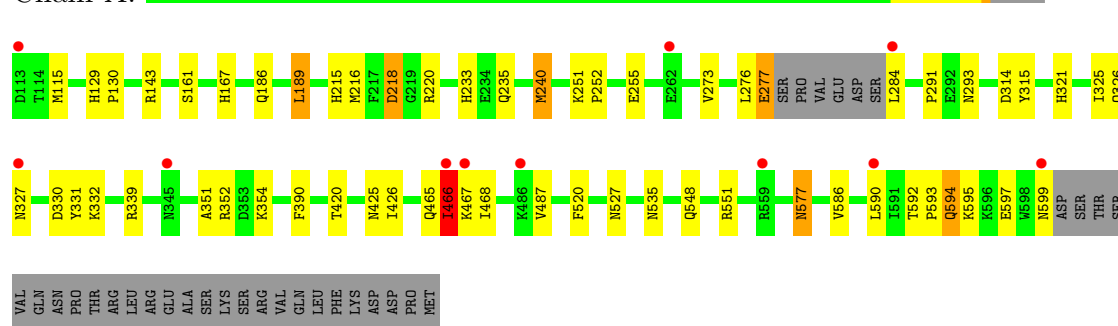
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain B:
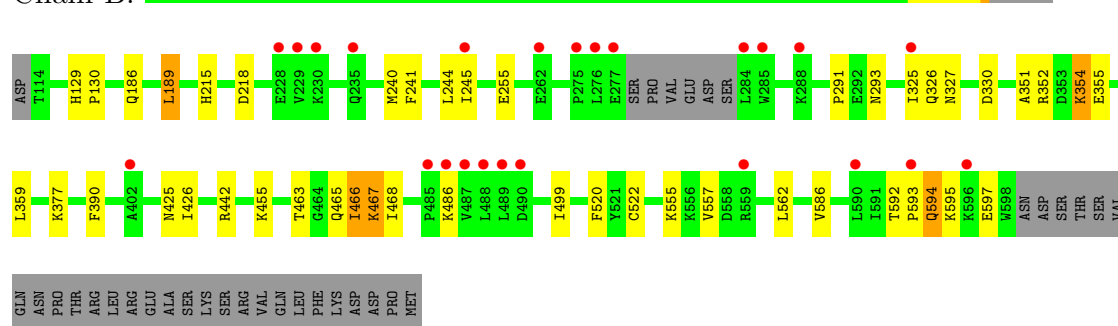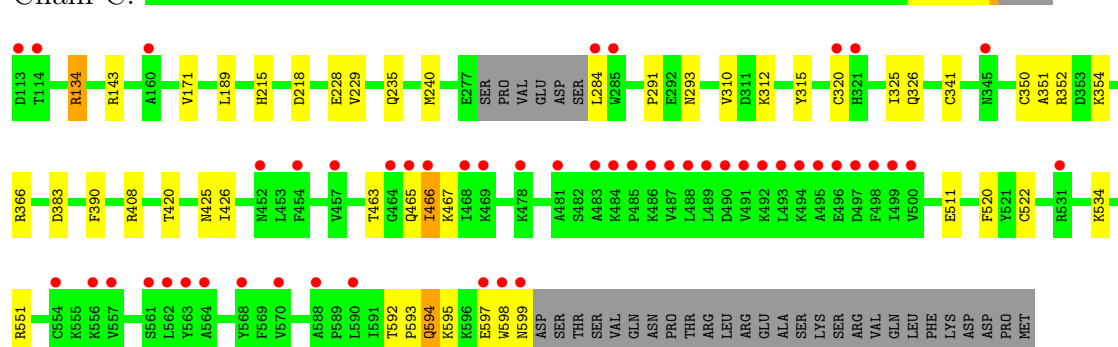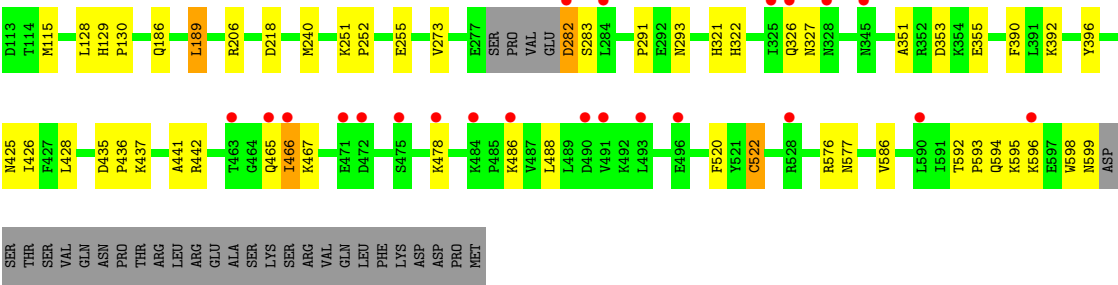

- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

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, α, β, γ	80.89Å 140.73Å 97.60Å 90.00° 114.71° 90.00°	Depositor
Resolution (Å)	50.00 – 2.31 47.82 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.31) 99.2 (47.82-2.31)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.188 , 0.226 0.192 , 0.223	Depositor DCC
R_{free} test set	4335 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	40.8	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.4	EDS
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
L-test for twinning	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Outliers	1 of 86352 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16322	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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: GTP, MG, DGT, 3PO

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	0.76	1/4048 (0.0%)	0.81	5/5464 (0.1%)
1	B	0.69	1/4032 (0.0%)	0.77	4/5442 (0.1%)
1	C	0.65	0/4039	0.76	5/5452 (0.1%)
1	D	0.76	1/4053 (0.0%)	0.82	7/5471 (0.1%)
All	All	0.72	3/16172 (0.0%)	0.79	21/21829 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	355	GLU	CD-OE2	6.14	1.32	1.25
1	A	161	SER	CB-OG	5.90	1.50	1.42
1	D	355	GLU	CD-OE1	5.41	1.31	1.25

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	240	MET	CG-SD-CE	-8.38	86.80	100.20
1	A	551	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	D	218	ASP	CB-CG-OD2	6.76	124.39	118.30
1	A	218	ASP	CB-CG-OD2	6.55	124.19	118.30
1	B	330	ASP	CB-CG-OD2	-6.45	112.49	118.30
1	B	330	ASP	CB-CG-OD1	6.33	124.00	118.30
1	D	442	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	442	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	C	551	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	A	218	ASP	CB-CG-OD1	-5.93	112.96	118.30
1	D	353	ASP	CB-CG-OD1	5.68	123.42	118.30
1	D	442	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	354	LYS	CD-CE-NZ	-5.46	99.14	111.70
1	C	383	ASP	CB-CG-OD1	5.35	123.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	206	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	C	383	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	D	218	ASP	CB-CG-OD1	-5.25	113.57	118.30
1	C	366	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	D	576	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	A	330	ASP	CB-CG-OD1	5.05	122.85	118.30
1	C	551	ARG	NE-CZ-NH1	-5.00	117.80	120.30

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	3956	0	3935	56	0
1	B	3940	0	3925	35	0
1	C	3947	0	3930	34	0
1	D	3961	0	3939	47	0
2	A	31	0	12	4	0
2	B	31	0	12	1	0
2	C	31	0	12	1	0
2	D	31	0	12	2	0
3	A	64	0	24	0	0
3	B	32	0	12	0	0
3	C	32	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
5	A	13	0	0	1	0
6	A	80	0	0	4	0
6	B	49	0	0	0	0
6	C	47	0	0	2	0
6	D	73	0	0	6	0
All	All	16322	0	15825	158	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 5.

All (158) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:577:ASN:ND2	1:D:595:LYS:HZ1	1.60	1.00
1:D:596:LYS:HB3	6:D:907:HOH:O	1.63	0.98
1:A:597:GLU:OE1	1:A:597:GLU:N	1.97	0.96
1:A:216:MET:HA	6:A:869:HOH:O	1.67	0.94
1:D:577:ASN:ND2	1:D:595:LYS:NZ	2.19	0.89
1:C:465:GLN:HG2	1:C:466:ILE:HD13	1.56	0.87
1:C:390:PHE:CE2	1:C:426:ILE:HD11	2.10	0.87
1:A:327:ASN:O	1:C:326:GLN:HG2	1.75	0.86
1:D:577:ASN:HD22	1:D:595:LYS:NZ	1.75	0.85
1:C:465:GLN:CG	1:C:466:ILE:HD13	2.08	0.84
1:D:390:PHE:CE2	1:D:426:ILE:HD11	2.11	0.84
1:A:390:PHE:CE2	1:A:426:ILE:HD11	2.17	0.80
2:A:701:DGT:H5'A	6:D:971:HOH:O	1.81	0.80
1:A:467:LYS:HB2	1:A:548:GLN:CD	2.04	0.78
2:A:701:DGT:C5'	6:D:971:HOH:O	2.31	0.77
1:D:466:ILE:HD13	1:D:466:ILE:N	2.01	0.76
1:C:466:ILE:N	1:C:466:ILE:HD13	2.01	0.74
1:A:467:LYS:HG3	1:A:468:ILE:N	2.00	0.74
1:B:466:ILE:HD13	1:B:466:ILE:N	2.00	0.74
1:A:467:LYS:HG3	1:A:468:ILE:H	1.53	0.71
1:A:593:PRO:HA	1:A:599:ASN:HD21	1.52	0.71
1:A:467:LYS:HB2	1:A:548:GLN:OE1	1.91	0.71
1:B:325:ILE:HG22	2:D:800:DGT:N2	2.06	0.71
1:B:377:LYS:NZ	2:D:800:DGT:O2G	2.24	0.70
1:A:277:GLU:O	1:A:277:GLU:CG	2.39	0.70
1:B:390:PHE:CE2	1:B:426:ILE:HD11	2.26	0.69
1:C:465:GLN:CG	1:C:466:ILE:CD1	2.70	0.69
1:C:408:ARG:NH2	6:C:801:HOH:O	2.25	0.69
1:D:577:ASN:HD22	1:D:595:LYS:HZ1	1.33	0.69
1:D:465:GLN:HG3	1:D:466:ILE:CD1	2.26	0.66
1:C:465:GLN:HG2	1:C:466:ILE:CD1	2.26	0.66
1:A:425:ASN:ND2	1:D:425:ASN:HD22	1.94	0.65
1:A:167:HIS:HD2	1:A:314:ASP:OD2	1.79	0.65
1:C:390:PHE:CE2	1:C:426:ILE:CD1	2.80	0.65
1:A:390:PHE:CE2	1:A:426:ILE:CD1	2.80	0.64
1:D:390:PHE:CE2	1:D:426:ILE:CD1	2.80	0.64
1:A:425:ASN:HD21	1:D:425:ASN:ND2	1.94	0.64
1:C:465:GLN:HG3	1:C:466:ILE:CD1	2.28	0.64
1:A:592:THR:OG1	1:A:593:PRO:HD3	1.98	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:425:ASN:HD21	1:D:425:ASN:HD22	1.48	0.60
1:B:597:GLU:OE1	1:B:597:GLU:N	2.27	0.60
1:D:465:GLN:HG3	1:D:466:ILE:HD13	1.84	0.59
2:A:701:DGT:H5'	6:D:971:HOH:O	2.00	0.59
1:A:586:VAL:HG11	1:C:522[A]:CYS:SG	2.41	0.59
1:B:390:PHE:CE2	1:B:426:ILE:CD1	2.85	0.59
1:A:465:GLN:C	1:A:466:ILE:HG23	2.23	0.59
1:B:522[A]:CYS:SG	1:D:586:VAL:HG11	2.43	0.59
1:A:466:ILE:O	1:A:467:LYS:HG2	2.03	0.58
1:D:115:MET:HG3	1:D:128:LEU:O	2.04	0.58
1:B:592:THR:OG1	1:B:593:PRO:HD3	2.04	0.58
1:A:339:ARG:NH1	1:A:527:ASN:OD1	2.24	0.58
1:A:597:GLU:CD	1:A:597:GLU:H	2.02	0.58
1:B:465:GLN:CG	1:B:466:ILE:HD13	2.34	0.58
1:C:325:ILE:HG22	2:C:703:DGT:N2	2.19	0.57
1:C:592:THR:OG1	1:C:593:PRO:HD3	2.05	0.57
1:A:321:HIS:CE1	1:D:321:HIS:CE1	2.93	0.56
1:A:465:GLN:O	1:A:466:ILE:HG23	2.05	0.56
1:C:465:GLN:HG3	1:C:466:ILE:HD13	1.82	0.56
1:D:466:ILE:N	1:D:466:ILE:CD1	2.69	0.56
1:A:277:GLU:O	1:A:277:GLU:HG3	2.05	0.56
1:A:535:ASN:N	1:A:535:ASN:OD1	2.35	0.55
1:D:465:GLN:CG	1:D:466:ILE:HD13	2.35	0.55
1:B:425:ASN:ND2	1:C:425:ASN:ND2	2.54	0.55
1:A:390:PHE:CZ	1:A:426:ILE:CD1	2.91	0.54
1:D:592:THR:OG1	1:D:593:PRO:HD3	2.07	0.54
1:D:291:PRO:HG2	1:D:293:ASN:OD1	2.07	0.54
1:B:291:PRO:HG2	1:B:293:ASN:OD1	2.07	0.54
1:B:465:GLN:HG2	1:B:466:ILE:HD13	1.88	0.53
1:A:143:ARG:HD3	6:A:819:HOH:O	2.08	0.53
1:D:465:GLN:CG	1:D:466:ILE:CD1	2.87	0.53
1:C:594:GLN:HG2	1:C:595:LYS:N	2.23	0.52
1:D:322:HIS:HE1	6:D:944:HOH:O	1.92	0.52
1:D:186:GLN:HB2	1:D:189:LEU:HD22	1.91	0.52
1:B:327:ASN:O	1:D:326:GLN:HG2	2.10	0.52
1:C:291:PRO:HG2	1:C:293:ASN:OD1	2.10	0.52
1:A:467:LYS:CG	1:A:468:ILE:H	2.21	0.51
1:A:594:GLN:HG2	1:A:595:LYS:N	2.25	0.51
1:D:322:HIS:CE1	6:D:944:HOH:O	2.63	0.50
1:C:592:THR:N	1:C:593:PRO:CD	2.75	0.50
1:C:134:ARG:HA	1:C:134:ARG:NE	2.27	0.49
1:A:186:GLN:HB2	1:A:189:LEU:HD22	1.93	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:351:ALA:O	1:A:520:PHE:HA	2.13	0.49
1:B:465:GLN:HG2	1:B:466:ILE:CD1	2.43	0.49
1:A:327:ASN:O	1:C:326:GLN:CG	2.54	0.49
1:D:577:ASN:ND2	1:D:595:LYS:HZ3	2.07	0.49
1:A:325:ILE:HG22	2:A:701:DGT:N2	2.28	0.49
1:B:592:THR:N	1:B:593:PRO:CD	2.76	0.48
1:A:220:ARG:HG3	6:A:869:HOH:O	2.14	0.48
1:D:577:ASN:HD21	1:D:595:LYS:HZ1	1.55	0.48
1:B:465:GLN:CG	1:B:466:ILE:CD1	2.91	0.48
1:B:326:GLN:HG3	1:D:326:GLN:CG	2.44	0.48
1:B:351:ALA:O	1:B:520:PHE:HA	2.13	0.48
1:C:598:TRP:O	1:C:599:ASN:CB	2.62	0.47
1:A:216:MET:CA	6:A:869:HOH:O	2.43	0.47
1:D:351:ALA:O	1:D:520:PHE:HA	2.14	0.47
1:A:487:VAL:HG13	1:A:590:LEU:HD12	1.95	0.47
1:D:598:TRP:O	1:D:599:ASN:CB	2.62	0.47
1:B:352:ARG:HG3	1:B:354:LYS:HG2	1.97	0.46
1:C:351:ALA:O	1:C:520:PHE:HA	2.15	0.46
1:D:282:ASP:N	1:D:282:ASP:OD2	2.48	0.46
1:A:466:ILE:O	1:A:466:ILE:HD12	2.14	0.46
1:A:425:ASN:HB2	1:D:428:LEU:HD13	1.97	0.46
1:C:228:GLU:OE2	1:C:229:VAL:HG23	2.15	0.46
1:D:592:THR:N	1:D:593:PRO:CD	2.78	0.46
1:B:186:GLN:HB2	1:B:189:LEU:HD22	1.97	0.46
1:A:215:HIS:HA	1:A:218:ASP:OD2	2.15	0.46
1:A:390:PHE:CZ	1:A:426:ILE:HD11	2.51	0.45
1:B:390:PHE:CZ	1:B:426:ILE:CD1	3.00	0.45
1:C:352:ARG:HG3	1:C:354:LYS:HG2	1.97	0.45
1:A:115:MET:C	1:A:115:MET:SD	2.94	0.45
1:B:326:GLN:HG3	1:D:326:GLN:HG2	1.97	0.45
1:A:331:TYR:CE1	1:A:332:LYS:HG3	2.52	0.45
1:A:277:GLU:O	1:A:277:GLU:HG2	2.15	0.45
1:C:215:HIS:HA	1:C:218:ASP:OD2	2.17	0.45
1:A:291:PRO:HG2	1:A:293:ASN:OD1	2.17	0.44
1:B:594:GLN:HG2	1:B:595:LYS:N	2.33	0.44
1:D:392:LYS:HB3	1:D:441:ALA:HB2	2.00	0.44
1:D:396:TYR:CD1	1:D:437:LYS:HD2	2.52	0.44
1:A:143:ARG:HD2	1:A:420:THR:HA	2.00	0.44
1:A:251:LYS:HB2	1:A:252:PRO:HD3	2.00	0.44
1:A:577:ASN:ND2	1:A:595:LYS:NZ	2.66	0.44
1:B:467:LYS:HG3	1:B:468:ILE:N	2.32	0.43
1:B:499:ILE:HD11	1:B:555:LYS:HE2	1.99	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:129:HIS:CG	1:A:130:PRO:HD2	2.53	0.43
1:A:352:ARG:HG3	1:A:354:LYS:HG2	2.00	0.43
1:C:390:PHE:CZ	1:C:426:ILE:CD1	3.01	0.43
1:D:390:PHE:CZ	1:D:426:ILE:CD1	3.01	0.43
1:B:129:HIS:CG	1:B:130:PRO:HD2	2.53	0.43
1:B:465:GLN:HG3	1:B:466:ILE:CD1	2.48	0.43
1:D:251:LYS:HB2	1:D:252:PRO:HD3	1.99	0.43
1:C:320:CYS:HB3	1:C:325:ILE:O	2.19	0.43
1:D:115:MET:CE	1:D:129:HIS:HA	2.48	0.43
1:B:326:GLN:HB3	1:D:327:ASN:O	2.19	0.43
1:B:562:LEU:HA	1:B:562:LEU:HD12	1.87	0.42
1:C:171:VAL:HG13	1:C:310:VAL:HG23	2.01	0.42
1:D:129:HIS:CG	1:D:130:PRO:HD2	2.53	0.42
1:D:488:LEU:HA	1:D:488:LEU:HD13	1.78	0.42
1:D:390:PHE:CZ	1:D:426:ILE:HG13	2.54	0.42
1:A:592:THR:N	1:A:593:PRO:CD	2.83	0.42
1:B:241:PHE:O	1:B:245:ILE:HG12	2.20	0.42
1:D:577:ASN:HD21	1:D:595:LYS:NZ	2.09	0.42
1:C:341:CYS:HB2	1:C:350:CYS:SG	2.59	0.42
1:D:435:ASP:HA	1:D:436:PRO:HD3	1.90	0.42
1:C:597:GLU:OE1	1:C:597:GLU:N	2.37	0.42
1:C:598:TRP:O	1:C:599:ASN:HB2	2.20	0.41
1:B:215:HIS:HA	1:B:218:ASP:OD2	2.20	0.41
1:C:143:ARG:HD2	1:C:420:THR:HA	2.02	0.41
1:A:326:GLN:HG3	1:C:326:GLN:CG	2.51	0.41
1:A:425:ASN:ND2	1:D:425:ASN:ND2	2.59	0.41
1:A:167:HIS:CD2	1:A:314:ASP:OD2	2.67	0.41
1:B:455:LYS:HG2	1:B:557:VAL:HG12	2.02	0.41
1:B:244:LEU:HD23	1:B:244:LEU:C	2.42	0.41
1:A:233:HIS:NE2	5:A:705:3PO:O2G	2.54	0.40
1:C:312:LYS:HG3	6:C:836:HOH:O	2.20	0.40
1:B:586:VAL:HG11	1:D:522[A]:CYS:SG	2.61	0.40
1:A:276:LEU:O	1:A:277:GLU:C	2.59	0.40
1:B:354:LYS:HZ1	2:B:703:DGT:PA	2.41	0.40
1:A:390:PHE:CZ	1:A:426:ILE:HG13	2.57	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	480/514 (93%)	474 (99%)	5 (1%)	1 (0%)	56	67
1	B	478/514 (93%)	470 (98%)	8 (2%)	0	100	100
1	C	479/514 (93%)	474 (99%)	5 (1%)	0	100	100
1	D	481/514 (94%)	474 (98%)	7 (2%)	0	100	100
All	All	1918/2056 (93%)	1892 (99%)	25 (1%)	1 (0%)	59	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	466	ILE

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	430/459 (94%)	419 (97%)	11 (3%)	59	75
1	B	428/459 (93%)	419 (98%)	9 (2%)	66	82
1	C	429/459 (94%)	417 (97%)	12 (3%)	56	72
1	D	431/459 (94%)	418 (97%)	13 (3%)	53	70
All	All	1718/1836 (94%)	1673 (97%)	45 (3%)	59	75

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	LEU

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Mol	Chain	Res	Type
1	A	235	GLN
1	A	240	MET
1	A	255	GLU
1	A	273	VAL
1	A	277	GLU
1	A	284	LEU
1	A	315	TYR
1	A	466	ILE
1	A	577	ASN
1	A	594	GLN
1	B	189	LEU
1	B	240	MET
1	B	255	GLU
1	B	359	LEU
1	B	463	THR
1	B	466	ILE
1	B	467	LYS
1	B	486	LYS
1	B	594	GLN
1	C	134	ARG
1	C	189	LEU
1	C	235	GLN
1	C	240	MET
1	C	284	LEU
1	C	315	TYR
1	C	463	THR
1	C	466	ILE
1	C	467	LYS
1	C	511	GLU
1	C	534	LYS
1	C	594	GLN
1	D	189	LEU
1	D	240	MET
1	D	255	GLU
1	D	273	VAL
1	D	282	ASP
1	D	283	SER
1	D	466	ILE
1	D	467	LYS
1	D	478	LYS
1	D	486	LYS
1	D	522[A]	CYS

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Mol	Chain	Res	Type
1	D	522[B]	CYS
1	D	594	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	HIS
1	A	364	HIS
1	A	425	ASN
1	A	577	ASN
1	B	425	ASN
1	C	322	HIS
1	C	425	ASN
1	D	322	HIS
1	D	577	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 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	4	33,33,33	1.47	6 (18%)	50,52,52	4.44	9 (18%)
3	GTP	A	702	4	34,34,34	1.40	5 (14%)	52,54,54	2.61	11 (21%)
3	GTP	A	704	4	34,34,34	1.55	6 (17%)	52,54,54	2.30	12 (23%)
5	3PO	A	705	-	12,12,12	1.27	2 (16%)	20,20,20	1.50	5 (25%)
3	GTP	B	701	4	34,34,34	1.57	6 (17%)	52,54,54	3.24	12 (23%)
2	DGT	B	703	4	33,33,33	1.88	8 (24%)	50,52,52	4.00	11 (22%)
2	DGT	C	703	4	33,33,33	1.47	5 (15%)	50,52,52	3.98	11 (22%)
3	GTP	C	704	4	34,34,34	1.25	4 (11%)	52,54,54	2.70	14 (26%)
2	DGT	D	800	4	33,33,33	1.49	5 (15%)	50,52,52	3.31	13 (26%)

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	4	-	0/20/34/34	0/3/3/3
3	GTP	A	702	4	-	0/22/38/38	0/3/3/3
3	GTP	A	704	4	-	0/22/38/38	0/3/3/3
5	3PO	A	705	-	-	0/12/12/12	0/0/0/0
3	GTP	B	701	4	-	0/22/38/38	0/3/3/3
2	DGT	B	703	4	-	0/20/34/34	0/3/3/3
2	DGT	C	703	4	-	0/20/34/34	0/3/3/3
3	GTP	C	704	4	-	0/22/38/38	0/3/3/3
2	DGT	D	800	4	-	0/20/34/34	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	703	DGT	C4-N9	-4.99	1.30	1.37
2	B	703	DGT	C5-N7	-4.94	1.32	1.38
3	A	704	GTP	C5-N7	-4.59	1.32	1.38
2	A	701	DGT	C4-N9	-4.12	1.31	1.37
3	B	701	GTP	C5-N7	-4.11	1.33	1.38
3	A	702	GTP	C5-C4	3.99	1.49	1.40
2	C	703	DGT	C4-N9	-3.95	1.32	1.37
2	D	800	DGT	C4-N9	-3.86	1.32	1.37
2	C	703	DGT	PG-O3B	3.85	1.66	1.60
3	B	701	GTP	C4-N9	-3.67	1.32	1.37
3	A	704	GTP	C5-C4	3.55	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	DGT	C5-C4	3.53	1.48	1.40
3	B	701	GTP	C5-C4	3.47	1.48	1.40
2	B	703	DGT	C2-N1	-3.38	1.31	1.36
3	A	702	GTP	C4-N9	-3.37	1.32	1.37
3	C	704	GTP	C5-N7	-3.27	1.34	1.38
2	B	703	DGT	PG-O3B	3.22	1.65	1.60
2	D	800	DGT	C5-N7	-3.13	1.34	1.38
2	D	800	DGT	C6-N1	-3.06	1.32	1.36
3	C	704	GTP	C2-N2	2.98	1.36	1.32
3	A	702	GTP	PB-O3B	2.97	1.65	1.59
2	C	703	DGT	C5-N7	-2.96	1.34	1.38
3	C	704	GTP	C5-C4	2.96	1.47	1.40
3	B	701	GTP	PB-O3A	2.95	1.65	1.59
2	C	703	DGT	C5-C4	2.90	1.47	1.40
2	D	800	DGT	C5-C4	2.86	1.47	1.40
3	B	701	GTP	O4'-C1'	2.84	1.44	1.41
2	A	701	DGT	C2-N2	2.73	1.36	1.32
2	A	701	DGT	PG-O3B	2.67	1.64	1.60
2	B	703	DGT	C5-C4	2.63	1.46	1.40
2	B	703	DGT	C6-N1	-2.63	1.33	1.36
3	A	702	GTP	C5-N7	-2.56	1.35	1.38
2	C	703	DGT	PB-O3B	2.56	1.64	1.59
2	A	701	DGT	C5-N7	-2.49	1.35	1.38
5	A	705	3PO	PB-O3B	2.47	1.64	1.59
2	D	800	DGT	C2-N2	2.46	1.36	1.32
3	A	704	GTP	C2-N2	2.39	1.35	1.32
3	A	704	GTP	O4'-C1'	2.33	1.44	1.41
2	A	701	DGT	O4'-C4'	-2.31	1.39	1.45
5	A	705	3PO	PB-O3A	2.30	1.64	1.59
3	C	704	GTP	C4-N9	-2.27	1.34	1.37
3	B	701	GTP	PA-O3A	2.19	1.63	1.59
2	B	703	DGT	PA-O3A	2.19	1.63	1.59
3	A	702	GTP	PG-O2G	-2.13	1.47	1.54
2	B	703	DGT	PB-O3A	2.11	1.63	1.59
3	A	704	GTP	PB-O3B	-2.08	1.56	1.59
3	A	704	GTP	C2'-C1'	-2.03	1.50	1.53

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	DGT	C6-C5-N7	28.09	137.92	134.14
2	B	703	DGT	C6-C5-N7	24.74	137.47	134.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	703	DGT	C6-C5-N7	24.40	137.43	134.14
2	D	800	DGT	C6-C5-N7	19.81	136.81	134.14
3	B	701	GTP	C6-C5-N7	17.85	136.54	134.14
3	A	702	GTP	C6-C5-N7	13.58	135.97	134.14
3	C	704	GTP	C6-C5-N7	12.54	135.83	134.14
2	B	703	DGT	C6-N1-C2	8.70	125.11	120.20
3	A	704	GTP	C6-C5-N7	7.17	135.11	134.14
3	A	704	GTP	C6-N1-C2	7.04	124.17	120.20
3	B	701	GTP	C5-C4-N3	-6.54	118.54	126.07
2	C	703	DGT	N2-C2-N1	6.02	124.28	117.82
2	A	701	DGT	N2-C2-N3	-5.87	112.65	120.28
3	C	704	GTP	C5-C4-N3	-5.81	119.37	126.07
3	A	702	GTP	C6-N1-C2	5.74	123.44	120.20
2	A	701	DGT	N2-C2-N1	5.72	123.95	117.82
2	C	703	DGT	C2-N3-C4	5.59	122.00	115.30
2	D	800	DGT	C6-N1-C2	5.46	123.28	120.20
3	A	704	GTP	C5-C4-N3	-5.39	119.86	126.07
3	A	702	GTP	N3-C4-N9	5.34	134.74	126.91
2	C	703	DGT	N2-C2-N3	-5.17	113.56	120.28
3	B	701	GTP	N2-C2-N3	-4.98	113.81	120.28
3	A	704	GTP	N3-C4-N9	4.95	134.16	126.91
3	C	704	GTP	N3-C4-N9	4.90	134.09	126.91
3	C	704	GTP	C2-N3-C4	4.88	121.16	115.30
3	B	701	GTP	C2-N3-C4	4.73	120.97	115.30
2	A	701	DGT	C5-C4-N3	-4.73	120.63	126.07
3	A	702	GTP	C5-C4-N3	-4.71	120.65	126.07
2	C	703	DGT	C5-C4-N3	-4.63	120.74	126.07
3	B	701	GTP	N3-C4-N9	4.58	133.62	126.91
2	A	701	DGT	C6-N1-C2	4.51	122.75	120.20
2	A	701	DGT	C2-N3-C4	4.51	120.70	115.30
3	B	701	GTP	PA-O3A-PB	-4.41	119.71	131.93
3	C	704	GTP	C3'-C2'-C1'	4.28	107.63	100.92
3	B	701	GTP	N2-C2-N1	4.20	122.33	117.82
2	D	800	DGT	C5-C4-N3	-4.15	121.29	126.07
2	D	800	DGT	N3-C4-N9	4.14	132.97	126.91
3	A	704	GTP	C2-N3-C4	4.13	120.26	115.30
3	C	704	GTP	C6-N1-C2	4.09	122.51	120.20
2	C	703	DGT	N3-C4-N9	4.08	132.90	126.91
3	C	704	GTP	PA-O3A-PB	-4.02	120.79	131.93
2	A	701	DGT	N3-C4-N9	3.86	132.56	126.91
3	A	702	GTP	C2-N3-C4	3.76	119.81	115.30
2	B	703	DGT	C5-C4-N3	-3.70	121.81	126.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	704	GTP	N2-C2-N1	3.67	121.76	117.82
3	A	704	GTP	N2-C2-N3	-3.67	115.52	120.28
3	B	701	GTP	C3'-C2'-C1'	3.61	106.58	100.92
3	C	704	GTP	PB-O3B-PG	-3.54	122.12	131.93
3	B	701	GTP	C6-N1-C2	3.52	122.19	120.20
3	A	704	GTP	C3'-C2'-C1'	3.52	106.44	100.92
3	A	704	GTP	PA-O3A-PB	-3.45	122.37	131.93
3	A	702	GTP	PA-O3A-PB	-3.43	122.42	131.93
2	D	800	DGT	C2-N3-C4	3.27	119.23	115.30
2	B	703	DGT	N3-C4-N9	3.26	131.69	126.91
3	A	702	GTP	O2G-PG-O1G	3.23	120.92	110.36
3	C	704	GTP	N2-C2-N1	3.16	121.21	117.82
5	A	705	3PO	PB-O3B-PG	-3.09	123.38	131.93
2	B	703	DGT	O1B-PB-O2B	3.08	129.17	112.14
3	C	704	GTP	N2-C2-N3	-3.08	116.28	120.28
3	B	701	GTP	C4-C5-N7	-3.07	106.44	109.41
2	D	800	DGT	O2G-PG-O1G	2.97	118.53	107.38
2	B	703	DGT	O1G-PG-O3G	2.93	119.95	110.36
2	A	701	DGT	C4-C5-N7	-2.91	106.59	109.41
3	A	702	GTP	PB-O3B-PG	-2.89	123.94	131.93
3	C	704	GTP	O3A-PA-O5'	-2.86	95.33	102.91
3	A	702	GTP	C3'-C2'-C1'	2.80	105.31	100.92
2	C	703	DGT	C6-N1-C2	2.77	121.76	120.20
3	A	704	GTP	O2'-C2'-C1'	-2.73	102.84	111.49
3	C	704	GTP	C4-C5-N7	-2.70	106.80	109.41
5	A	705	3PO	PB-O3A-PA	-2.63	124.65	131.93
3	C	704	GTP	O2G-PG-O1G	2.62	118.92	110.36
2	B	703	DGT	C2-N3-C4	2.60	118.42	115.30
3	A	704	GTP	O3G-PG-O2G	2.57	117.04	107.38
2	A	701	DGT	O2G-PG-O1G	2.51	116.80	107.38
3	B	701	GTP	PB-O3B-PG	-2.50	125.00	131.93
3	A	702	GTP	C8-N9-C4	2.49	108.98	106.96
2	D	800	DGT	C2'-C3'-C4'	2.48	108.25	102.73
2	D	800	DGT	O1G-PG-O3G	2.48	118.47	110.36
5	A	705	3PO	O3G-PG-O2G	2.40	116.38	107.38
2	B	703	DGT	C8-N9-C4	2.40	108.91	106.96
3	A	702	GTP	O2A-PA-O3A	2.38	116.44	105.14
2	D	800	DGT	N2-C2-N3	-2.36	117.22	120.28
3	A	704	GTP	O3A-PA-O5'	-2.34	96.71	102.91
2	B	703	DGT	C1'-N9-C4	-2.30	121.25	126.84
2	D	800	DGT	N2-C2-N1	2.29	120.28	117.82
2	B	703	DGT	C2'-C3'-C4'	2.29	107.81	102.73

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Mol	Chain	Res	Type	Atoms	Z	Observed($°$)	Ideal($°$)
3	B	701	GTP	O2G-PG-O1G	2.25	117.72	110.36
2	C	703	DGT	PA-O3A-PB	-2.21	125.80	131.93
2	D	800	DGT	O1B-PB-O2B	2.20	124.31	112.14
3	C	704	GTP	O2A-PA-O3A	2.19	115.51	105.14
5	A	705	3PO	O5'-PA-O2A	2.17	115.50	107.38
2	C	703	DGT	PB-O3B-PG	-2.13	126.02	131.93
2	D	800	DGT	O3A-PA-O5'	-2.10	97.36	102.91
5	A	705	3PO	O3A-PB-O3B	-2.09	97.41	101.66
2	D	800	DGT	O1A-PA-O2A	2.08	123.65	112.14
2	C	703	DGT	O2G-PG-O3B	-2.05	95.39	105.14
2	C	703	DGT	O2G-PG-O3G	2.04	117.03	110.36
2	B	703	DGT	O2G-PG-O3B	-2.03	95.50	105.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

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, 95th 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(Å²)	Q<0.9
1	A	481/514 (93%)	0.06	11 (2%)	57	68	27, 44, 71, 98	0
1	B	479/514 (93%)	0.27	24 (5%)	28	38	32, 54, 86, 113	0
1	C	481/514 (93%)	0.51	51 (10%)	7	11	32, 55, 101, 129	0
1	D	483/514 (93%)	0.14	22 (4%)	31	41	28, 45, 86, 112	0
All	All	1924/2056 (93%)	0.25	108 (5%)	24	33	27, 50, 88, 129	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	488	LEU	7.4
1	C	490	ASP	7.3
1	C	491	VAL	6.8
1	A	466	ILE	6.6
1	C	493	LEU	6.3
1	C	485	PRO	6.1
1	B	284	LEU	6.1
1	C	489	LEU	5.7
1	B	488	LEU	5.7
1	C	484	LYS	5.5
1	C	486	LYS	5.4
1	C	562	LEU	5.2
1	C	554	CYS	4.5
1	C	563	TYR	4.5
1	B	230	LYS	4.3
1	D	465	GLN	4.3
1	D	490	ASP	4.1
1	C	599	ASN	4.1
1	C	464	GLY	4.0
1	B	490	ASP	4.0
1	C	590	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	487	VAL	3.9
1	C	495	ALA	3.9
1	B	590	LEU	3.8
1	A	284	LEU	3.8
1	C	500	VAL	3.8
1	B	229	VAL	3.7
1	C	113	ASP	3.7
1	C	496	GLU	3.6
1	C	492	LYS	3.6
1	C	494	LYS	3.5
1	C	284	LEU	3.3
1	B	402	ALA	3.3
1	C	483	ALA	3.3
1	B	277	GLU	3.2
1	B	559	ARG	3.1
1	D	475	SER	3.1
1	C	452[A]	ASN	3.0
1	C	457	VAL	3.0
1	B	489	LEU	3.0
1	D	491	VAL	3.0
1	D	466	ILE	3.0
1	D	486	LYS	3.0
1	D	472	ASP	3.0
1	A	486	LYS	2.9
1	D	596	LYS	2.9
1	D	345	ASN	2.9
1	D	471	GLU	2.9
1	D	284	LEU	2.9
1	C	468	ILE	2.9
1	C	568	TYR	2.9
1	C	345	ASN	2.8
1	D	496	GLU	2.8
1	A	590	LEU	2.8
1	B	276	LEU	2.8
1	C	498	PHE	2.8
1	A	345	ASN	2.8
1	C	588	ALA	2.8
1	C	556	LYS	2.8
1	D	493	LEU	2.7
1	C	466	ILE	2.6
1	C	557	VAL	2.6
1	A	467	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	113	ASP	2.6
1	C	497	ASP	2.6
1	C	478	LYS	2.5
1	B	486	LYS	2.5
1	A	599	ASN	2.5
1	D	326	GLN	2.5
1	B	325	ILE	2.5
1	D	463	THR	2.5
1	C	561	SER	2.5
1	C	481	ALA	2.5
1	C	597	GLU	2.4
1	C	160	ALA	2.4
1	C	114	THR	2.4
1	C	465	GLN	2.4
1	C	531	ARG	2.4
1	A	327	ASN	2.4
1	C	469	LYS	2.4
1	C	320	CYS	2.3
1	B	262	GLU	2.3
1	C	570	VAL	2.3
1	A	559	ARG	2.3
1	C	598	TRP	2.3
1	C	499	ILE	2.3
1	B	288	LYS	2.3
1	D	478	LYS	2.2
1	B	596	LYS	2.2
1	C	285	TRP	2.2
1	B	228	GLU	2.2
1	B	275	PRO	2.2
1	D	484	LYS	2.2
1	A	262	GLU	2.2
1	B	593	PRO	2.2
1	D	528	ARG	2.1
1	D	325	ILE	2.1
1	C	321	HIS	2.1
1	B	285	TRP	2.1
1	B	235	GLN	2.1
1	D	282	ASP	2.1
1	D	590	LEU	2.1
1	C	487	VAL	2.1
1	B	485	PRO	2.1
1	D	328	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	245	ILE	2.0
1	C	454	PHE	2.0
1	C	564	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, 95th 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($Å^2$)	Q<0.9
5	3PO	A	705	13/13	0.21	2.26	62,89,154,155	0
4	MG	C	702	1/1	0.10	0.21	49,49,49,49	0
2	DGT	B	703	31/31	0.14	-0.08	29,30,34,36	0
2	DGT	D	800	31/31	0.14	-0.14	34,36,38,38	0
4	MG	A	703	1/1	0.12	-0.24	34,34,34,34	0
2	DGT	A	701	31/31	0.14	-0.56	31,34,38,39	0
2	DGT	C	703	31/31	0.15	-0.63	37,40,48,49	0
3	GTP	C	704	32/32	0.12	-0.84	36,43,49,50	0
4	MG	B	702	1/1	0.12	-1.00	49,49,49,49	0
3	GTP	A	702	32/32	0.10	-1.24	30,31,34,35	0
3	GTP	A	704	32/32	0.11	-1.26	29,30,32,32	0
3	GTP	B	701	32/32	0.10	-1.37	37,40,44,45	0
4	MG	C	701	1/1	0.09	-3.63	43,43,43,43	0

6.5 Other polymers ⓘ

There are no such residues in this entry.