



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:33 PM GMT

PDB ID : 4TO5  
Title : Structure basis of cellular dNTP regulation, SAMHD1-GTP-dTTP-dCTP complex  
Authors : Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.  
Deposited on : 2014-06-05  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

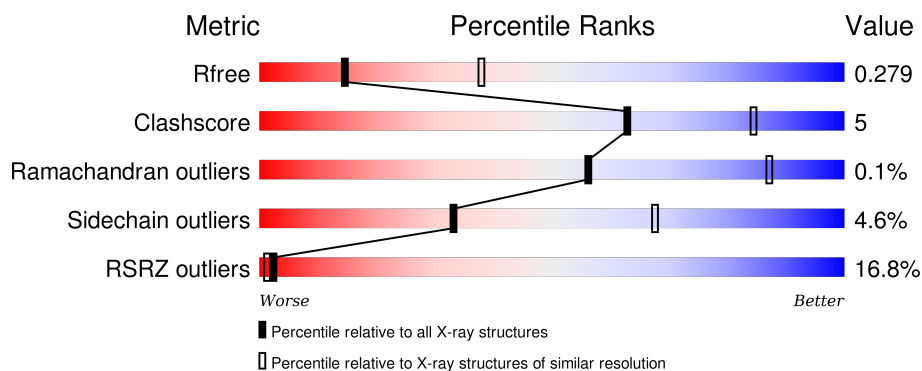
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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>17%</div> <div> <div>81%</div> <div>10%</div> <div>•</div> <div>7%</div> </div> </div>
1	B	514	<div> <div>19%</div> <div> <div>81%</div> <div>11%</div> <div>•</div> <div>7%</div> </div> </div>
1	C	514	<div> <div>11%</div> <div> <div>81%</div> <div>12%</div> <div>•</div> <div>7%</div> </div> </div>
1	D	514	<div> <div>16%</div> <div> <div>83%</div> <div>9%</div> <div>•</div> <div>7%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16073 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.

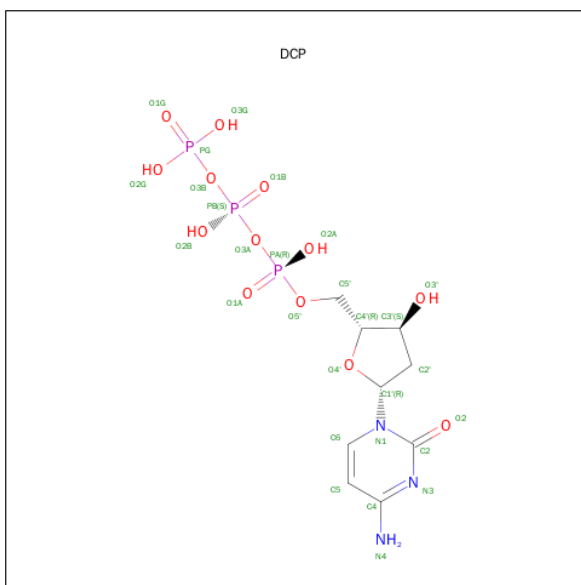
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	1	0
			3932	2517	684	711	20			
1	C	479	Total	C	N	O	S	0	1	0
			3922	2511	684	706	21			
1	D	480	Total	C	N	O	S	0	2	0
			3933	2518	684	710	21			
1	B	480	Total	C	N	O	S	0	0	0
			3922	2512	683	707	20			

There are 8 discrepancies between the modelled and reference sequences:

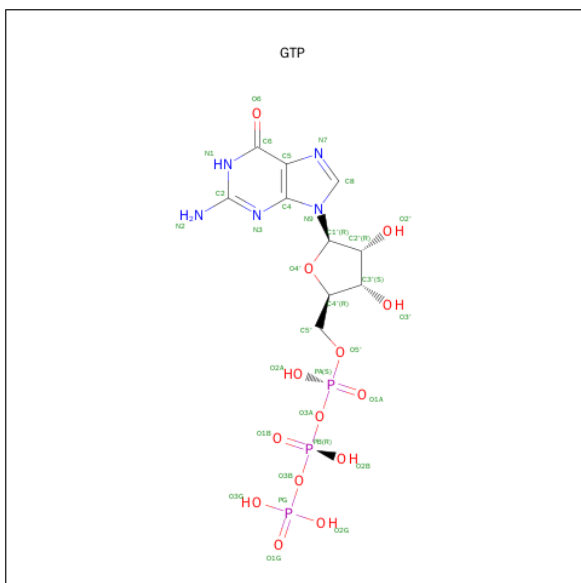
Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
D	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
D	207	ASN	ASP	engineered mutation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

- Molecule 2 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>3</sub>O<sub>13</sub>P<sub>3</sub>).



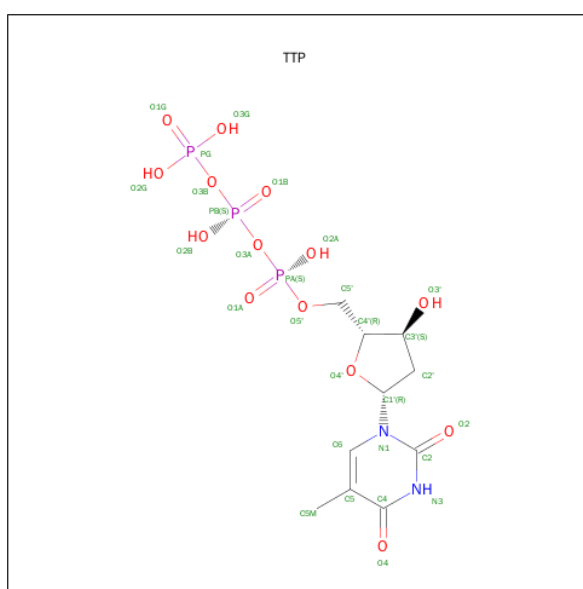
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 28	C 9	N 3	O 13	P 3	0	0
2	C	1	Total 28	C 9	N 3	O 13	P 3	0	0
2	D	1	Total 28	C 9	N 3	O 13	P 3	0	0
2	B	1	Total 28	C 9	N 3	O 13	P 3	0	0

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	5	14	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	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
4	C	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
4	D	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
4	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		

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

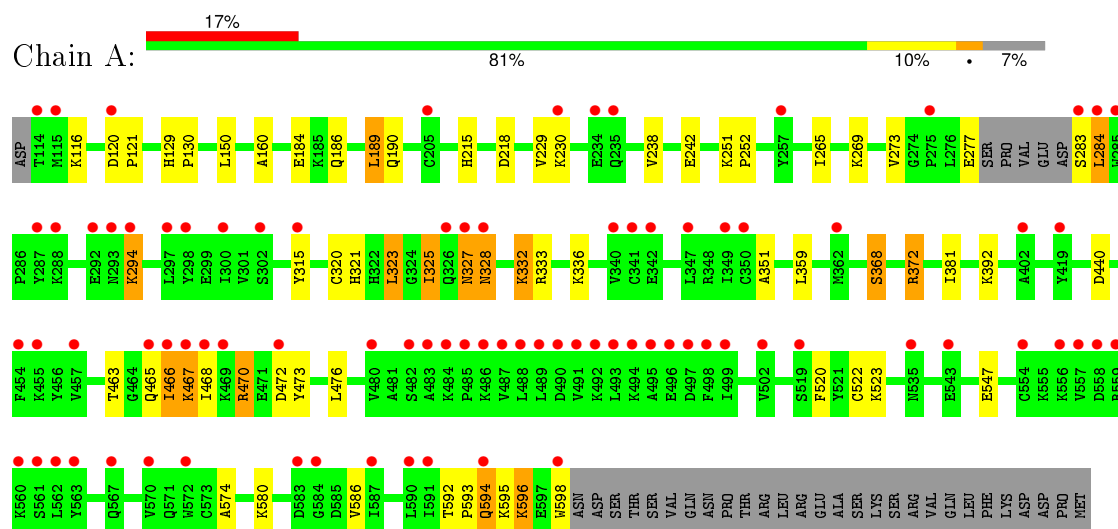
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	O 1	0	0
6	C	1	Total 1	O 1	0	0
6	D	1	Total 1	O 1	0	0
6	B	1	Total 1	O 1	0	0

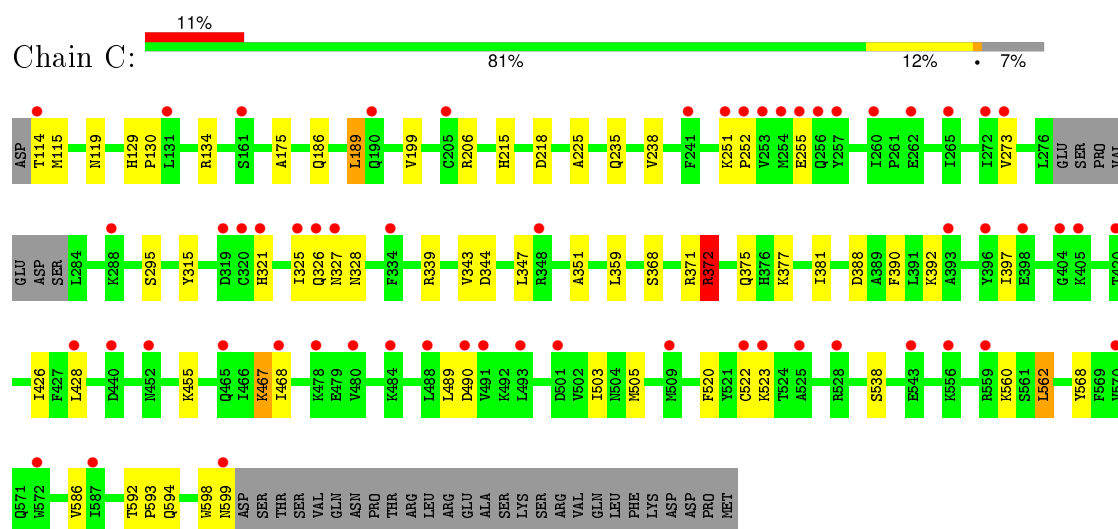
### 3 Residue-property plots

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.

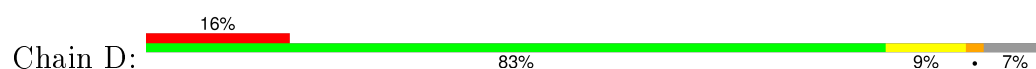
#### • Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.46Å 145.12Å 98.23Å 90.00° 114.13° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 48.39 – 2.73	Depositor EDS
% Data completeness (in resolution range)	96.6 (50.00-2.80) 96.6 (48.39-2.73)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, $R_{free}$	0.271 , 0.285 0.266 , 0.279	Depositor DCC
$R_{free}$ test set	2761 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.2	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 75.0	EDS
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 56472 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	16073	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, TTP, DCP

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	0.56	0/4024	0.70	2/5431 (0.0%)
1	B	0.60	0/4014	0.75	7/5418 (0.1%)
1	C	0.56	0/4014	0.71	3/5418 (0.1%)
1	D	0.58	0/4025	0.72	3/5433 (0.1%)
All	All	0.57	0/16077	0.72	15/21700 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	LYS	CD-CE-NZ	7.83	129.70	111.70
1	B	371	ARG	NE-CZ-NH2	7.31	123.95	120.30
1	B	352	ARG	CG-CD-NE	-7.02	97.05	111.80
1	D	352	ARG	CG-CD-NE	-6.81	97.51	111.80
1	D	470	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	C	115	MET	CG-SD-CE	6.46	110.53	100.20
1	A	372	ARG	NE-CZ-NH1	-6.19	117.21	120.30
1	B	226	ARG	CG-CD-NE	6.12	124.66	111.80
1	B	483	ALA	N-CA-C	5.70	126.38	111.00
1	B	226	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	D	470	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	C	372	ARG	CG-CD-NE	5.32	122.97	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	371	ARG	NE-CZ-NH2	5.06	122.83	120.30
1	B	371	ARG	NE-CZ-NH1	-5.01	117.80	120.30
1	B	405	LYS	N-CA-CB	-5.01	101.59	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	404	GLY	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3932	0	3920	63	0
1	B	3922	0	3913	46	0
1	C	3922	0	3915	38	1
1	D	3933	0	3916	30	1
2	A	28	0	12	7	0
2	B	28	0	12	5	0
2	C	28	0	12	0	0
2	D	28	0	12	1	0
3	A	32	0	12	1	0
3	B	64	0	24	0	0
3	D	32	0	12	2	0
4	A	29	0	13	2	0
4	B	29	0	13	2	0
4	C	29	0	13	1	0
4	D	29	0	13	1	0
5	A	2	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	1	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
All	All	16073	0	15812	169	1

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 5.

All (169) 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:D:390:PHE:CZ	1:D:426:ILE:HD11	1.78	1.18
1:A:283:SER:HB2	1:A:284:LEU:CA	1.84	1.07
1:A:283:SER:CB	1:A:284:LEU:HA	1.89	1.03
1:A:466:ILE:H	1:A:466:ILE:HD12	0.90	1.03
1:D:390:PHE:CE2	1:D:426:ILE:HD11	1.94	1.02
1:A:466:ILE:H	1:A:466:ILE:CD1	1.70	1.02
1:A:283:SER:HB2	1:A:284:LEU:HA	1.04	1.00
1:A:466:ILE:N	1:A:466:ILE:HD12	1.74	1.00
1:A:463:THR:O	1:A:466:ILE:HD13	1.63	0.98
1:A:470:ARG:NH1	1:A:470:ARG:HB2	1.87	0.90
1:D:390:PHE:CZ	1:D:426:ILE:CD1	2.55	0.89
1:A:328:ASN:HD21	1:C:326:GLN:HE21	1.20	0.89
1:A:215:HIS:HE1	2:A:701:DCP:O4'	1.56	0.88
1:C:490:ASP:OD2	1:C:560:LYS:HE2	1.74	0.86
1:A:473:TYR:HA	1:A:476:LEU:CD1	2.06	0.85
1:B:463:THR:O	1:B:466:ILE:HG12	1.76	0.84
1:A:463:THR:O	1:A:466:ILE:CD1	2.26	0.84
1:A:215:HIS:CE1	2:A:701:DCP:O4'	2.33	0.81
1:B:466:ILE:HD13	1:B:466:ILE:N	1.95	0.81
1:D:115:MET:SD	1:D:115:MET:C	2.59	0.80
1:A:473:TYR:HA	1:A:476:LEU:HD13	1.64	0.80
1:D:377:LYS:NZ	4:B:702:TTP:O2B	2.16	0.78
1:B:215:HIS:CD2	2:B:703:DCP:C6	2.67	0.77
1:A:470:ARG:CZ	1:A:470:ARG:HB2	2.14	0.76
1:A:522:CYS:SG	1:C:586:VAL:HG11	2.28	0.73
1:D:466:ILE:N	1:D:466:ILE:HD13	2.05	0.72
1:A:470:ARG:HA	1:A:473:TYR:CE2	2.24	0.72
1:A:328:ASN:C	1:A:328:ASN:HD22	1.94	0.71
1:C:327:ASN:O	1:C:328:ASN:HB2	1.92	0.70
1:B:390:PHE:CE2	1:B:426:ILE:HD11	2.26	0.70
1:A:472:ASP:O	1:A:476:LEU:HD12	1.92	0.69
1:A:215:HIS:CE1	2:A:701:DCP:C6	2.76	0.69
4:A:703:TTP:O4	1:C:372:ARG:HG2	1.94	0.67
1:B:326:GLN:HG3	1:B:326:GLN:O	1.94	0.67
1:A:470:ARG:CZ	1:A:470:ARG:CB	2.73	0.66
1:A:320:CYS:SG	1:A:327:ASN:O	2.53	0.65
1:A:190:GLN:O	1:A:294:LYS:NZ	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:GLU:OE2	1:D:406:LYS:HD3	1.98	0.64
1:D:326:GLN:O	1:D:327:ASN:CB	2.47	0.63
1:A:265:ILE:O	1:A:269:LYS:HG3	1.98	0.63
1:D:490:ASP:OD2	1:D:560:LYS:HD3	2.00	0.62
1:A:238:VAL:O	1:A:242:GLU:HG3	2.00	0.62
1:A:328:ASN:ND2	1:A:328:ASN:C	2.52	0.62
1:B:466:ILE:HD13	1:B:466:ILE:H	1.65	0.61
1:B:215:HIS:CE1	2:B:703:DCP:O2A	2.52	0.61
1:B:466:ILE:CD1	1:B:466:ILE:N	2.62	0.61
1:A:586:VAL:HG11	1:C:522[A]:CYS:SG	2.40	0.60
1:D:535:ASN:OD1	1:D:535:ASN:N	2.31	0.60
1:A:596:LYS:N	1:A:596:LYS:CD	2.63	0.60
1:C:235:GLN:O	1:C:238:VAL:HG22	2.01	0.60
1:A:215:HIS:ND1	2:A:701:DCP:C6	2.65	0.59
1:B:327:ASN:HD22	1:B:328:ASN:N	1.99	0.59
1:A:392:LYS:NZ	1:A:440:ASP:OD1	2.35	0.59
1:C:321:HIS:CE1	1:B:321:HIS:CE1	2.91	0.59
4:A:703:TTP:O1B	1:C:377:LYS:NZ	2.34	0.58
1:A:472:ASP:O	1:A:476:LEU:CD1	2.51	0.57
1:C:372:ARG:HH21	1:C:372:ARG:HG2	1.68	0.57
1:A:473:TYR:CA	1:A:476:LEU:CD1	2.81	0.57
1:B:413:ILE:CD1	1:B:419:TYR:CE1	2.88	0.56
1:D:215:HIS:CD2	2:D:702:DCP:C6	2.89	0.56
1:C:375:GLN:HG3	1:C:505:MET:CE	2.36	0.55
1:A:470:ARG:HA	1:A:473:TYR:CD2	2.42	0.55
1:D:390:PHE:CE1	1:D:426:ILE:CD1	2.89	0.55
1:A:116:LYS:NZ	3:D:703:GTP:O2A	2.39	0.55
1:C:388:ASP:OD2	1:C:392:LYS:HE3	2.06	0.55
1:C:455:LYS:HG3	1:C:562:LEU:HD11	1.89	0.55
1:D:465:GLN:OE1	1:D:465:GLN:HA	2.07	0.55
1:C:119:ASN:ND2	1:B:323:LEU:O	2.40	0.55
1:D:522[A]:CYS:SG	1:B:586:VAL:HG11	2.47	0.54
1:A:596:LYS:HD3	1:A:596:LYS:N	2.22	0.54
1:C:467:LYS:HG3	1:C:468:ILE:N	2.24	0.53
6:A:801:HOH:O	1:B:116:LYS:HE2	2.08	0.53
1:A:547:GLU:OE1	1:C:538:SER:OG	2.24	0.52
1:B:467:LYS:HG3	1:B:468:ILE:N	2.24	0.52
4:D:704:TTP:O1B	1:B:377:LYS:NZ	2.42	0.51
1:B:327:ASN:HD22	1:B:328:ASN:H	1.58	0.51
1:C:428:LEU:HD13	1:B:425:ASN:HB2	1.93	0.51
1:A:238:VAL:HG13	1:A:269:LYS:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:GLN:CG	1:B:326:GLN:O	2.59	0.50
1:A:592:THR:OG1	1:A:593:PRO:HD3	2.12	0.50
1:A:467:LYS:HG3	1:A:468:ILE:N	2.27	0.50
1:D:467:LYS:HG3	1:D:468:ILE:N	2.26	0.49
1:A:476:LEU:HD12	1:A:476:LEU:H	1.76	0.49
1:D:390:PHE:CE1	1:D:426:ILE:HD12	2.47	0.49
1:A:129:HIS:CG	1:A:130:PRO:HD2	2.47	0.49
1:C:592:THR:OG1	1:C:593:PRO:HD3	2.12	0.49
1:D:592:THR:OG1	1:D:593:PRO:HD3	2.13	0.49
1:B:351:ALA:O	1:B:520:PHE:HA	2.13	0.49
1:A:368:SER:O	1:A:372:ARG:HG3	2.12	0.48
1:B:592:THR:OG1	1:B:593:PRO:HD3	2.13	0.48
3:A:702:GTP:O2A	1:D:116:LYS:HE3	2.13	0.48
1:C:489:LEU:CD1	1:C:568:TYR:HE2	2.27	0.48
1:A:215:HIS:NE2	2:A:701:DCP:O1A	2.46	0.48
1:C:129:HIS:CG	1:C:130:PRO:HD2	2.49	0.47
1:D:351:ALA:O	1:D:520:PHE:HA	2.15	0.47
1:D:115:MET:SD	1:D:115:MET:O	2.72	0.47
1:B:463:THR:O	1:B:466:ILE:CG1	2.54	0.47
1:B:129:HIS:CG	1:B:130:PRO:HD2	2.50	0.47
1:D:186:GLN:HB2	1:D:189:LEU:HD22	1.97	0.47
1:D:129:HIS:CG	1:D:130:PRO:HD2	2.50	0.47
2:A:701:DCP:O2G	2:A:701:DCP:O2B	2.32	0.46
1:B:226:ARG:NH2	1:B:229:VAL:HG21	2.30	0.46
1:D:466:ILE:N	1:D:466:ILE:CD1	2.74	0.46
1:A:320:CYS:HB3	1:A:325:ILE:O	2.16	0.46
1:B:390:PHE:CE2	1:B:426:ILE:CD1	2.98	0.46
1:A:215:HIS:ND1	2:A:701:DCP:N1	2.64	0.46
1:B:390:PHE:CZ	1:B:426:ILE:CD1	2.99	0.46
1:B:390:PHE:CZ	1:B:426:ILE:HD11	2.51	0.46
1:C:397:ILE:HG21	1:C:426:ILE:HD11	1.96	0.45
1:A:351:ALA:O	1:A:520:PHE:HA	2.16	0.45
1:C:598:TRP:O	1:C:599:ASN:CB	2.64	0.45
1:A:277:GLU:O	1:A:277:GLU:HG3	2.16	0.45
1:A:150:LEU:CD1	1:A:323:LEU:HD21	2.47	0.45
1:C:351:ALA:O	1:C:520:PHE:HA	2.16	0.45
1:A:574:ALA:HB1	1:A:595:LYS:HD2	1.99	0.45
1:B:186:GLN:HB2	1:B:189:LEU:HD22	1.98	0.45
1:B:320:CYS:SG	1:B:327:ASN:O	2.72	0.45
1:A:251:LYS:HB2	1:A:252:PRO:HD3	1.99	0.45
1:D:592:THR:N	1:D:593:PRO:CD	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ALA:HB2	1:A:323:LEU:HD22	1.99	0.45
1:A:592:THR:N	1:A:593:PRO:CD	2.80	0.44
1:B:592:THR:N	1:B:593:PRO:CD	2.81	0.44
1:A:215:HIS:HA	1:A:218:ASP:OD2	2.17	0.44
1:C:598:TRP:O	1:C:599:ASN:HB2	2.17	0.44
1:B:120:ASP:OD2	1:B:121:PRO:HD2	2.17	0.44
1:C:186:GLN:HB2	1:C:189:LEU:HD22	1.98	0.44
1:D:320:CYS:HB3	1:D:325:ILE:O	2.18	0.44
1:D:251:LYS:HB2	1:D:252:PRO:HD3	2.00	0.44
1:B:320:CYS:HB3	1:B:325:ILE:O	2.18	0.44
1:C:592:THR:N	1:C:593:PRO:CD	2.81	0.44
1:C:390:PHE:CZ	1:C:426:ILE:CG2	3.01	0.44
1:B:251:LYS:HB2	1:B:252:PRO:HD3	2.00	0.44
1:D:352:ARG:HG3	1:D:354:LYS:HG2	2.00	0.44
1:C:372:ARG:HH21	1:C:372:ARG:CG	2.31	0.43
1:C:215:HIS:HA	1:C:218:ASP:OD2	2.18	0.43
1:C:327:ASN:O	1:C:328:ASN:CB	2.59	0.43
1:B:215:HIS:CD2	2:B:703:DCP:N1	2.86	0.43
1:A:186:GLN:HB2	1:A:189:LEU:HD22	1.99	0.43
1:A:332:LYS:NZ	1:A:336:LYS:HE2	2.34	0.43
1:B:352:ARG:HG3	1:B:354:LYS:HG2	2.00	0.43
1:C:343:VAL:O	1:C:344:ASP:HB2	2.18	0.43
1:C:375:GLN:HG3	1:C:505:MET:HE2	1.99	0.43
1:A:120:ASP:OD2	1:A:121:PRO:HD2	2.19	0.43
1:B:215:HIS:HE2	2:B:703:DCP:PA	2.41	0.43
1:A:372:ARG:HD2	4:C:701:TTP:O4	2.18	0.43
1:B:175:ALA:HB1	1:B:199:VAL:HG12	2.01	0.43
1:B:215:HIS:HA	1:B:218:ASP:OD2	2.19	0.42
1:C:295:SER:OG	1:C:347:LEU:O	2.37	0.42
1:B:598:TRP:O	1:B:599:ASN:CB	2.67	0.42
1:B:215:HIS:NE2	2:B:703:DCP:O2A	2.52	0.42
1:B:480:VAL:HG22	1:B:572:TRP:CD2	2.55	0.42
1:B:479:GLU:HB3	1:B:572:TRP:HE1	1.85	0.42
1:C:375:GLN:HG3	1:C:505:MET:HE1	2.02	0.42
1:B:598:TRP:O	1:B:599:ASN:HB2	2.20	0.41
1:A:381:ILE:HD12	1:A:381:ILE:HA	1.93	0.41
1:A:283:SER:HB2	1:A:284:LEU:C	2.35	0.41
1:D:175:ALA:HB1	1:D:199:VAL:HG12	2.03	0.41
1:A:333:ARG:HB2	1:B:125:HIS:CE1	2.56	0.41
1:A:321:HIS:CE1	1:D:321:HIS:NE2	2.89	0.41
1:C:251:LYS:HB2	1:C:252:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:ALA:HB1	1:C:199:VAL:HG12	2.02	0.41
3:D:703:GTP:H5''	4:B:702:TTP:O1B	2.20	0.41
1:D:327:ASN:O	1:D:365:THR:HG21	2.21	0.41
1:A:580:LYS:HD2	1:A:598:TRP:HB3	2.03	0.41
1:A:594:GLN:O	1:A:596:LYS:HE2	2.21	0.41
1:C:503:ILE:HG21	1:C:505:MET:HE2	2.02	0.41
1:C:381:ILE:HA	1:C:381:ILE:HD12	1.94	0.41
1:B:597:GLU:OE1	1:B:597:GLU:N	2.37	0.40
1:B:580:LYS:HD2	1:B:598:TRP:HB3	2.04	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	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:ALA:O	1:D:494:LYS:NZ[1_656]	1.87	0.33

## 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	477/514 (93%)	469 (98%)	8 (2%)	0	100	100
1	B	476/514 (93%)	468 (98%)	8 (2%)	0	100	100
1	C	476/514 (93%)	468 (98%)	8 (2%)	0	100	100
1	D	478/514 (93%)	470 (98%)	7 (2%)	1 (0%)	52	84
All	All	1907/2056 (93%)	1875 (98%)	31 (2%)	1 (0%)	56	87

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	327	ASN



### 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	427/459 (93%)	406 (95%)	21 (5%)	31	65
1	B	425/459 (93%)	406 (96%)	19 (4%)	34	68
1	C	426/459 (93%)	410 (96%)	16 (4%)	40	74
1	D	426/459 (93%)	404 (95%)	22 (5%)	29	62
All	All	1704/1836 (93%)	1626 (95%)	78 (5%)	33	67

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	GLU
1	A	189	LEU
1	A	229	VAL
1	A	230	LYS
1	A	273	VAL
1	A	284	LEU
1	A	315	TYR
1	A	323	LEU
1	A	325	ILE
1	A	327	ASN
1	A	328	ASN
1	A	332	LYS
1	A	359	LEU
1	A	368	SER
1	A	465	GLN
1	A	466	ILE
1	A	467	LYS
1	A	470	ARG
1	A	523	LYS
1	A	594	GLN
1	A	596	LYS
1	C	114	THR
1	C	134	ARG
1	C	189	LEU

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Mol	Chain	Res	Type
1	C	206	ARG
1	C	255	GLU
1	C	273	VAL
1	C	315	TYR
1	C	325	ILE
1	C	339	ARG
1	C	359	LEU
1	C	368	SER
1	C	372	ARG
1	C	467	LYS
1	C	523	LYS
1	C	562	LEU
1	C	594	GLN
1	D	114	THR
1	D	115	MET
1	D	185	LYS
1	D	189	LEU
1	D	190	GLN
1	D	206	ARG
1	D	228	GLU
1	D	229	VAL
1	D	240	MET
1	D	255	GLU
1	D	315	TYR
1	D	325	ILE
1	D	359	LEU
1	D	368	SER
1	D	408	ARG
1	D	465	GLN
1	D	466	ILE
1	D	467	LYS
1	D	478	LYS
1	D	509	MET
1	D	535	ASN
1	D	594	GLN
1	B	115	MET
1	B	116	LYS
1	B	189	LEU
1	B	206	ARG
1	B	240	MET
1	B	277	GLU
1	B	284	LEU

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Mol	Chain	Res	Type
1	B	315	TYR
1	B	326	GLN
1	B	327	ASN
1	B	332	LYS
1	B	345	ASN
1	B	359	LEU
1	B	368	SER
1	B	413	ILE
1	B	466	ILE
1	B	467	LYS
1	B	540	LEU
1	B	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	215	HIS
1	A	327	ASN
1	A	328	ASN
1	A	425	ASN
1	C	425	ASN
1	D	190	GLN
1	D	322	HIS
1	D	425	ASN
1	B	233	HIS
1	B	327	ASN
1	B	425	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	DCP	A	701	-	21,29,29	0.63	0	33,45,45	1.47	3 (9%)
3	GTP	A	702	5	25,34,34	1.24	3 (12%)	34,54,54	1.91	9 (26%)
4	TTP	A	703	5	21,30,30	0.77	0	31,47,47	2.44	6 (19%)
3	GTP	B	701	5	25,34,34	1.36	3 (12%)	34,54,54	1.63	7 (20%)
4	TTP	B	702	5	21,30,30	0.71	0	31,47,47	2.31	5 (16%)
2	DCP	B	703	-	21,29,29	0.56	0	33,45,45	1.32	5 (15%)
3	GTP	B	704	5	25,34,34	1.16	2 (8%)	34,54,54	1.86	8 (23%)
4	TTP	C	701	5	21,30,30	0.62	0	31,47,47	2.47	7 (22%)
2	DCP	C	702	-	21,29,29	0.57	0	33,45,45	1.33	3 (9%)
2	DCP	D	702	-	21,29,29	0.57	0	33,45,45	1.36	4 (12%)
3	GTP	D	703	5	25,34,34	1.15	2 (8%)	34,54,54	1.87	10 (29%)
4	TTP	D	704	5	21,30,30	0.68	0	31,47,47	2.38	7 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DCP	A	701	-	-	0/18/34/34	0/2/2/2
3	GTP	A	702	5	-	0/18/38/38	0/3/3/3
4	TTP	A	703	5	-	0/18/34/34	0/2/2/2
3	GTP	B	701	5	-	0/18/38/38	0/3/3/3
4	TTP	B	702	5	-	0/18/34/34	0/2/2/2
2	DCP	B	703	-	-	0/18/34/34	0/2/2/2
3	GTP	B	704	5	-	0/18/38/38	0/3/3/3
4	TTP	C	701	5	-	0/18/34/34	0/2/2/2
2	DCP	C	702	-	-	0/18/34/34	0/2/2/2
2	DCP	D	702	-	-	0/18/34/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	D	703	5	-	0/18/38/38	0/3/3/3
4	TTP	D	704	5	-	0/18/34/34	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	703	GTP	O4'-C1'	2.08	1.43	1.41
3	A	702	GTP	O4'-C1'	2.16	1.43	1.41
3	B	701	GTP	C8-N7	2.32	1.39	1.34
3	B	701	GTP	C5-C4	2.53	1.46	1.40
3	D	703	GTP	C5-C4	2.81	1.46	1.40
3	A	702	GTP	C5-C4	2.94	1.47	1.40
3	B	704	GTP	C5-C4	3.01	1.47	1.40
3	A	702	GTP	C6-C5	3.57	1.48	1.41
3	B	704	GTP	C6-C5	3.62	1.48	1.41
3	B	701	GTP	O4'-C1'	4.06	1.46	1.41

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	TTP	C5-C4-N3	-7.56	116.72	125.14
4	C	701	TTP	C5-C4-N3	-7.40	116.90	125.14
4	B	702	TTP	C5-C4-N3	-6.95	117.39	125.14
4	D	704	TTP	C5-C4-N3	-6.93	117.42	125.14
3	B	704	GTP	PA-O3A-PB	-5.89	116.18	132.73
3	D	703	GTP	PA-O3A-PB	-4.81	119.23	132.73
4	A	703	TTP	PB-O3A-PA	-4.28	120.70	132.73
4	B	702	TTP	PB-O3A-PA	-4.22	120.89	132.73
3	A	702	GTP	PA-O3A-PB	-4.15	121.06	132.73
3	D	703	GTP	C5-C6-N1	-4.12	117.95	123.59
3	A	702	GTP	C5-C6-N1	-3.95	118.19	123.59
2	A	701	DCP	PB-O3B-PG	-3.93	119.47	132.67
2	A	701	DCP	PB-O3A-PA	-3.92	121.72	132.73
3	B	704	GTP	C5-C6-N1	-3.88	118.29	123.59
3	B	701	GTP	PA-O3A-PB	-3.86	121.89	132.73
2	D	702	DCP	PB-O3A-PA	-3.74	122.22	132.73
2	C	702	DCP	PB-O3A-PA	-3.74	122.23	132.73
4	C	701	TTP	PB-O3A-PA	-3.74	122.24	132.73
4	A	703	TTP	PB-O3B-PG	-3.71	120.21	132.67
3	D	703	GTP	PB-O3B-PG	-3.66	120.39	132.67
2	D	702	DCP	PB-O3B-PG	-3.57	120.71	132.67
3	B	701	GTP	C5-C6-N1	-3.47	118.85	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	702	DCP	PB-O3B-PG	-3.45	121.11	132.67
2	B	703	DCP	PB-O3B-PG	-3.40	121.26	132.67
4	D	704	TTP	PB-O3A-PA	-3.35	123.32	132.73
4	C	701	TTP	PB-O3B-PG	-3.34	121.45	132.67
3	B	701	GTP	C6-C5-C4	-3.31	116.94	120.90
3	A	702	GTP	C6-C5-C4	-3.26	117.00	120.90
4	D	704	TTP	PB-O3B-PG	-3.25	121.76	132.67
2	B	703	DCP	PB-O3A-PA	-3.25	123.60	132.73
3	A	702	GTP	N3-C2-N1	-3.20	122.58	127.44
3	B	704	GTP	C6-C5-C4	-3.01	117.30	120.90
3	A	702	GTP	PB-O3B-PG	-2.98	122.67	132.67
4	B	702	TTP	PB-O3B-PG	-2.93	122.83	132.67
3	B	704	GTP	N3-C2-N1	-2.89	123.05	127.44
3	B	701	GTP	PB-O3B-PG	-2.88	123.01	132.67
3	D	703	GTP	N3-C2-N1	-2.75	123.26	127.44
3	B	704	GTP	C4-C5-N7	-2.71	106.99	109.48
3	A	702	GTP	C4-C5-N7	-2.64	107.05	109.48
3	D	703	GTP	O3A-PA-O5'	-2.63	95.96	102.94
3	B	701	GTP	N3-C2-N1	-2.62	123.45	127.44
3	D	703	GTP	C6-C5-C4	-2.51	117.89	120.90
3	B	704	GTP	PB-O3B-PG	-2.37	124.72	132.67
3	A	702	GTP	O3A-PA-O5'	-2.37	96.65	102.94
4	D	704	TTP	O4'-C1'-N1	-2.35	103.65	107.72
3	D	703	GTP	C2'-C1'-N9	-2.31	110.76	114.29
2	D	702	DCP	C2'-C1'-N1	-2.11	109.02	114.16
3	B	701	GTP	O4'-C4'-C3'	-2.03	101.06	105.15
4	C	701	TTP	O3A-PA-O5'	-2.00	97.63	102.94
4	A	703	TTP	O3G-PG-O2G	2.01	115.03	107.38
3	D	703	GTP	O4'-C1'-N9	2.06	112.41	108.10
2	B	703	DCP	O3G-PG-O1G	2.09	117.31	110.58
4	D	704	TTP	O2A-PA-O1A	2.12	124.01	112.53
4	A	703	TTP	C2'-C3'-C4'	2.17	107.28	102.77
2	B	703	DCP	O4'-C1'-N1	2.19	111.51	107.72
4	C	701	TTP	O2A-PA-O1A	2.23	124.62	112.53
3	D	703	GTP	O3G-PG-O2G	2.27	116.03	107.38
3	B	704	GTP	N2-C2-N1	2.30	121.01	117.20
3	A	702	GTP	O3G-PG-O2G	2.50	116.91	107.38
4	D	704	TTP	O2G-PG-O1G	2.63	119.03	110.58
2	D	702	DCP	C2-N3-C4	2.98	119.81	115.61
2	C	702	DCP	C2-N3-C4	3.08	119.95	115.61
4	B	702	TTP	O3G-PG-O2G	3.16	119.41	107.38
2	B	703	DCP	C2-N3-C4	3.17	120.08	115.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	GTP	C6-N1-C2	3.71	121.08	115.94
2	A	701	DCP	C2-N3-C4	3.75	120.90	115.61
3	D	703	GTP	C6-N1-C2	3.93	121.39	115.94
3	B	704	GTP	C6-N1-C2	4.02	121.51	115.94
3	A	702	GTP	C6-N1-C2	4.33	121.95	115.94
4	C	701	TTP	O2G-PG-O1G	5.06	126.87	110.58
4	C	701	TTP	C4-N3-C2	7.55	121.77	115.25
4	B	702	TTP	C4-N3-C2	7.82	122.01	115.25
4	A	703	TTP	C4-N3-C2	8.51	122.61	115.25
4	D	704	TTP	C4-N3-C2	8.75	122.81	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	DCP	7	0
3	A	702	GTP	1	0
4	A	703	TTP	2	0
4	B	702	TTP	2	0
2	B	703	DCP	5	0
4	C	701	TTP	1	0
2	D	702	DCP	1	0
3	D	703	GTP	2	0
4	D	704	TTP	1	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	480/514 (93%)	1.15	85 (17%) <b>2</b> <b>1</b>	74, 96, 122, 142	0
1	B	480/514 (93%)	1.23	96 (20%) <b>1</b> <b>1</b>	74, 96, 126, 152	0
1	C	479/514 (93%)	0.99	58 (12%) <b>6</b> <b>3</b>	68, 92, 110, 121	0
1	D	480/514 (93%)	1.11	83 (17%) <b>2</b> <b>1</b>	86, 108, 134, 148	0
All	All	1919/2056 (93%)	1.12	322 (16%) <b>2</b> <b>1</b>	68, 98, 127, 152	0

All (322) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	489	LEU	8.2
1	D	522[A]	CYS	7.5
1	A	490	ASP	6.7
1	A	488	LEU	6.3
1	B	486	LYS	6.3
1	B	286	PRO	6.2
1	A	288	LYS	6.2
1	D	590	LEU	6.0
1	B	404	GLY	5.9
1	A	487	VAL	5.8
1	A	563	TYR	5.7
1	C	251	LYS	5.7
1	A	491	VAL	5.4
1	B	570	VAL	5.4
1	B	465	GLN	5.1
1	D	276	LEU	5.1
1	A	115	MET	5.0
1	D	490	ASP	5.0
1	A	486	LYS	4.9
1	D	326	GLN	4.9
1	C	490	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	498	PHE	4.7
1	A	347	LEU	4.6
1	B	488	LEU	4.4
1	B	487	VAL	4.4
1	C	522[A]	CYS	4.4
1	A	205	CYS	4.4
1	B	500	VAL	4.3
1	A	554	CYS	4.3
1	A	557	VAL	4.2
1	D	269	LYS	4.2
1	D	230	LYS	4.2
1	C	257	TYR	4.2
1	B	360	TYR	4.1
1	A	327	ASN	4.1
1	B	586	VAL	4.0
1	B	313	TRP	4.0
1	B	272	ILE	4.0
1	C	543	GLU	4.0
1	B	499	ILE	4.0
1	B	598	TRP	3.9
1	D	543	GLU	3.9
1	C	131	LEU	3.9
1	B	583	ASP	3.9
1	A	284	LEU	3.8
1	D	113	ASP	3.8
1	B	406	LYS	3.8
1	D	491	VAL	3.8
1	A	485	PRO	3.8
1	A	350	CYS	3.8
1	B	285	TRP	3.7
1	D	341	CYS	3.7
1	B	483	ALA	3.7
1	D	241	PHE	3.7
1	C	523	LYS	3.7
1	B	276	LEU	3.7
1	A	467	LYS	3.7
1	B	328	ASN	3.6
1	A	492	LYS	3.6
1	B	213	PHE	3.6
1	B	493	LEU	3.6
1	B	472	ASP	3.6
1	A	591	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	585	ASP	3.6
1	C	468	ILE	3.6
1	A	465	GLN	3.6
1	B	471	GLU	3.5
1	D	562	LEU	3.5
1	B	563	TYR	3.5
1	D	405	LYS	3.5
1	B	480	VAL	3.5
1	D	272	ILE	3.5
1	D	268	ILE	3.5
1	B	568	TYR	3.5
1	A	493	LEU	3.5
1	C	493	LEU	3.5
1	D	568	TYR	3.4
1	D	498	PHE	3.4
1	B	468	ILE	3.4
1	A	419	TYR	3.4
1	B	484	LYS	3.4
1	A	326	GLN	3.4
1	B	476	LEU	3.4
1	A	285	TRP	3.4
1	D	587	ILE	3.4
1	B	485	PRO	3.4
1	C	398	GLU	3.3
1	B	562	LEU	3.3
1	A	495	ALA	3.3
1	C	326	GLN	3.3
1	A	584	GLY	3.3
1	D	327	ASN	3.3
1	D	390	PHE	3.3
1	B	592	THR	3.3
1	D	488	LEU	3.3
1	A	230	LYS	3.2
1	D	321	HIS	3.2
1	D	465	GLN	3.2
1	A	468	ILE	3.2
1	D	592	THR	3.2
1	D	496	GLU	3.1
1	D	489	LEU	3.1
1	B	241	PHE	3.1
1	B	114	THR	3.1
1	C	241	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	262	GLU	3.1
1	D	581	PRO	3.0
1	B	287	TYR	3.0
1	D	328	ASN	3.0
1	B	459	GLU	3.0
1	D	556	LYS	3.0
1	B	250	ILE	3.0
1	D	572	TRP	3.0
1	D	313	TRP	2.9
1	B	489	LEU	2.9
1	D	297	LEU	2.9
1	A	567	GLN	2.9
1	B	573	CYS	2.9
1	A	498	PHE	2.9
1	C	327	ASN	2.9
1	B	304	LYS	2.9
1	B	231	TRP	2.9
1	B	569	PHE	2.9
1	C	393	ALA	2.9
1	B	238	VAL	2.9
1	B	474	GLU	2.9
1	D	557	VAL	2.8
1	B	275	PRO	2.8
1	A	483	ALA	2.8
1	A	535	ASN	2.8
1	A	257	TYR	2.8
1	A	556	LYS	2.8
1	B	347	LEU	2.8
1	D	204	LEU	2.8
1	C	572	TRP	2.8
1	A	562	LEU	2.8
1	C	253	VAL	2.8
1	C	484	LYS	2.8
1	B	235	GLN	2.8
1	D	444	ILE	2.7
1	D	154	TYR	2.7
1	B	594	GLN	2.7
1	B	501	ASP	2.7
1	B	320	CYS	2.7
1	D	383	ASP	2.7
1	A	543	GLU	2.7
1	A	454	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	589	PRO	2.7
1	B	388	ASP	2.7
1	A	587	ILE	2.7
1	D	386	ILE	2.7
1	B	349	ILE	2.7
1	A	292	GLU	2.7
1	B	457	VAL	2.7
1	A	297	LEU	2.7
1	D	569	PHE	2.7
1	C	570	VAL	2.7
1	D	317	ALA	2.7
1	B	567	GLN	2.7
1	D	554	CYS	2.6
1	D	134	ARG	2.6
1	D	471	GLU	2.6
1	A	482	SER	2.6
1	B	301	VAL	2.6
1	C	273	VAL	2.6
1	A	287	TYR	2.6
1	C	465	GLN	2.6
1	C	420	THR	2.6
1	D	364	HIS	2.6
1	C	256	GLN	2.6
1	D	584	GLY	2.6
1	A	469	LYS	2.6
1	C	265	ILE	2.6
1	C	525	ALA	2.6
1	B	566	ARG	2.5
1	A	519	SER	2.5
1	B	466	ILE	2.5
1	A	457	VAL	2.5
1	B	491	VAL	2.5
1	B	552	VAL	2.5
1	B	576	ARG	2.5
1	D	288	LYS	2.5
1	B	467	LYS	2.5
1	A	583	ASP	2.5
1	D	222	ILE	2.5
1	B	409	ILE	2.5
1	C	528	ARG	2.5
1	C	252	PRO	2.5
1	C	288	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	319	ASP	2.5
1	B	343	VAL	2.5
1	A	455	LYS	2.5
1	D	131	LEU	2.5
1	C	255	GLU	2.5
1	D	339	ARG	2.5
1	D	267	PHE	2.5
1	A	561	SER	2.5
1	C	452	ASN	2.4
1	D	229	VAL	2.4
1	C	405	LYS	2.4
1	D	161	SER	2.4
1	B	542	PRO	2.4
1	B	345	ASN	2.4
1	C	556	LYS	2.4
1	A	294	LYS	2.4
1	A	558	ASP	2.4
1	B	522	CYS	2.4
1	B	496	GLU	2.4
1	C	254	MET	2.4
1	C	321	HIS	2.4
1	B	262	GLU	2.4
1	B	277	GLU	2.4
1	A	275	PRO	2.4
1	D	524	THR	2.4
1	A	494	LYS	2.4
1	B	402	ALA	2.4
1	A	293	ASN	2.4
1	B	305	ARG	2.4
1	A	484	LYS	2.4
1	B	288	LYS	2.4
1	C	559	ARG	2.4
1	B	292	GLU	2.3
1	A	114	THR	2.3
1	D	125	HIS	2.3
1	B	543	GLU	2.3
1	D	381	ILE	2.3
1	A	572	TRP	2.3
1	D	200	GLN	2.3
1	B	341	CYS	2.3
1	A	300	ILE	2.3
1	A	349	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	499	ILE	2.3
1	C	587	ILE	2.3
1	B	139	PRO	2.3
1	C	440	ASP	2.3
1	B	383	ASP	2.3
1	D	367	ASN	2.3
1	B	473	TYR	2.3
1	D	160	ALA	2.3
1	A	598	TRP	2.3
1	D	334	PHE	2.3
1	D	440	ASP	2.3
1	C	334	PHE	2.3
1	C	404	GLY	2.3
1	A	234	GLU	2.3
1	A	362	MET	2.3
1	D	198	CYS	2.3
1	B	545	PHE	2.3
1	D	340	VAL	2.3
1	A	340	VAL	2.2
1	A	570	VAL	2.2
1	B	431	LEU	2.2
1	B	481	ALA	2.2
1	D	189	LEU	2.2
1	D	531	ARG	2.2
1	A	283	SER	2.2
1	D	528	ARG	2.2
1	A	472	ASP	2.2
1	D	525	ALA	2.2
1	D	119	ASN	2.2
1	C	190	GLN	2.2
1	B	264	ASP	2.2
1	C	491	VAL	2.2
1	A	341	CYS	2.2
1	B	490	ASP	2.2
1	B	263	GLU	2.2
1	B	458	GLY	2.2
1	A	590	LEU	2.2
1	C	320	CYS	2.2
1	A	466	ILE	2.2
1	D	403	GLY	2.2
1	D	594	GLN	2.2
1	B	326	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	502	VAL	2.1
1	B	269	LYS	2.1
1	C	428	LEU	2.1
1	D	404	GLY	2.1
1	A	560	LYS	2.1
1	D	393	ALA	2.1
1	A	302	SER	2.1
1	C	348	ARG	2.1
1	C	488	LEU	2.1
1	D	284	LEU	2.1
1	C	114	THR	2.1
1	A	497	ASP	2.1
1	D	330	ASP	2.1
1	C	161	SER	2.1
1	C	325	ILE	2.1
1	A	559	ARG	2.1
1	A	120	ASP	2.1
1	C	501	ASP	2.1
1	B	257	TYR	2.1
1	C	260	ILE	2.1
1	A	315	TYR	2.1
1	C	272	ILE	2.1
1	B	299	GLU	2.1
1	D	542	PRO	2.1
1	C	205	CYS	2.1
1	C	509	MET	2.1
1	B	497	ASP	2.1
1	A	235	GLN	2.1
1	A	594	GLN	2.1
1	A	480	VAL	2.1
1	A	402	ALA	2.1
1	A	342	GLU	2.0
1	C	396	TYR	2.0
1	D	504	ASN	2.0
1	D	354	LYS	2.0
1	D	114	THR	2.0
1	D	338	ALA	2.0
1	D	357	GLY	2.0
1	A	496	GLU	2.0
1	A	298	TYR	2.0
1	D	553	TYR	2.0
1	A	328	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	480	VAL	2.0
1	C	599	ASN	2.0
1	B	199	VAL	2.0
1	D	412	ALA	2.0
1	C	478	LYS	2.0
1	B	236	GLY	2.0
1	D	520	PHE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	DCP	D	702	28/28	0.75	0.30	0.84	93,106,131,133	0
2	DCP	A	701	28/28	0.71	0.27	0.18	84,95,129,131	0
2	DCP	C	702	28/28	0.76	0.27	0.16	112,120,135,137	0
2	DCP	B	703	28/28	0.71	0.25	0.03	90,106,123,126	0
4	TTP	A	703	29/29	0.92	0.25	-0.34	70,85,98,106	0
3	GTP	B	701	32/32	0.87	0.25	-0.39	48,78,103,108	0
3	GTP	D	703	32/32	0.85	0.22	-0.88	59,78,98,106	0
3	GTP	A	702	32/32	0.89	0.19	-1.03	70,84,97,103	0
4	TTP	D	704	29/29	0.91	0.20	-1.03	79,89,100,102	0
4	TTP	B	702	29/29	0.91	0.23	-1.12	56,83,101,106	0
4	TTP	C	701	29/29	0.91	0.18	-1.15	66,81,100,103	0
3	GTP	B	704	32/32	0.91	0.18	-1.36	80,87,111,114	0
5	MG	C	703	1/1	0.81	0.10	-	101,101,101,101	0
5	MG	A	704	1/1	0.56	0.10	-	148,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MG	D	701	1/1	0.77	0.16	-	85,85,85,85	0
5	MG	A	705	1/1	0.31	0.18	-	93,93,93,93	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.