



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:32 PM GMT

PDB ID : 4TO1
Title : Structure basis of cellular dNTP regulation, SAMHD1-GTP-dATP/dCTP-dCTP complex
Authors : Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.
Deposited on : 2014-06-05
Resolution : 2.55 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

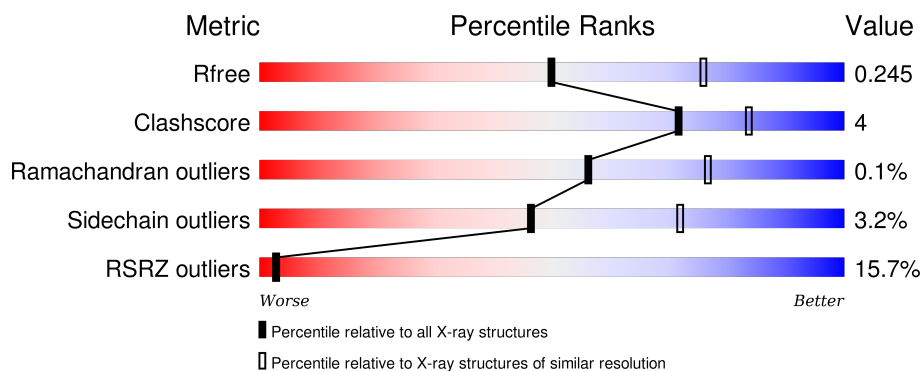
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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. 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>15%</div> <div>84%</div> <div>9%</div> <div>7%</div> </div>
1	B	514	<div> <div>23%</div> <div>86%</div> <div>7%</div> <div>7%</div> </div>
1	C	514	<div> <div>6%</div> <div>84%</div> <div>9%</div> <div>6%</div> </div>
1	D	514	<div> <div>15%</div> <div>83%</div> <div>11%</div> <div>6%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16149 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.

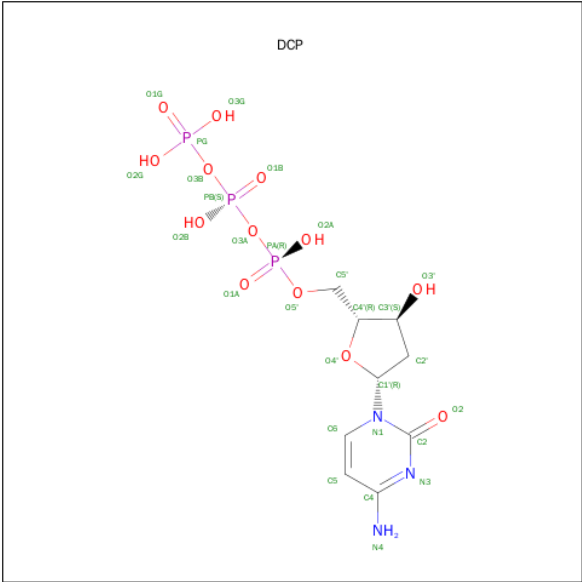
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	1	0
			3922	2511	684	706	21			
1	B	480	Total	C	N	O	S	0	0	0
			3924	2512	684	708	20			
1	C	481	Total	C	N	O	S	0	2	0
			3944	2522	687	715	20			
1	D	484	Total	C	N	O	S	0	1	0
			3961	2535	689	716	21			

There are 8 discrepancies between the modelled and reference sequences:

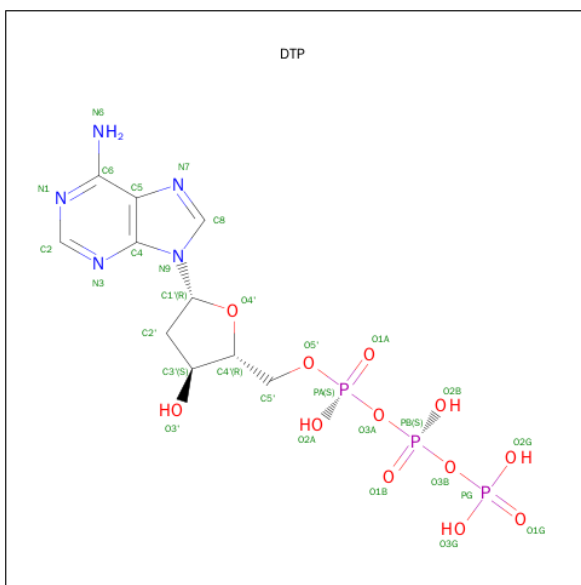
Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
B	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation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

- Molecule 2 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: $C_9H_{16}N_3O_{13}P_3$).



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

- Molecule 3 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃).

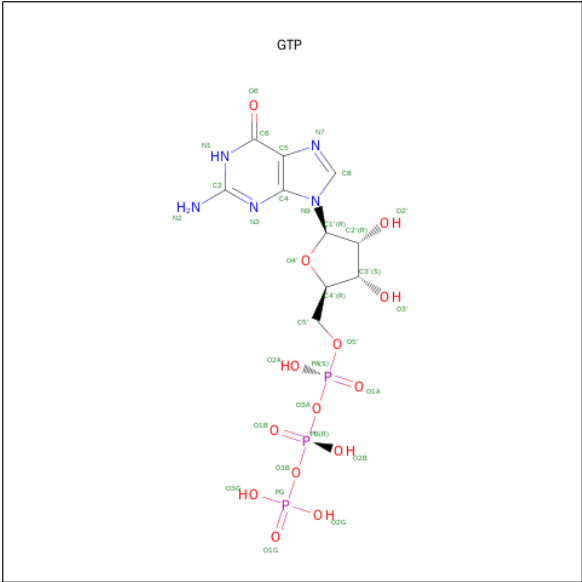


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 30	C 10	N 5	O 12	P 3	0	0
3	B	1	Total 30	C 10	N 5	O 12	P 3	0	0

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

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

- Molecule 5 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
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

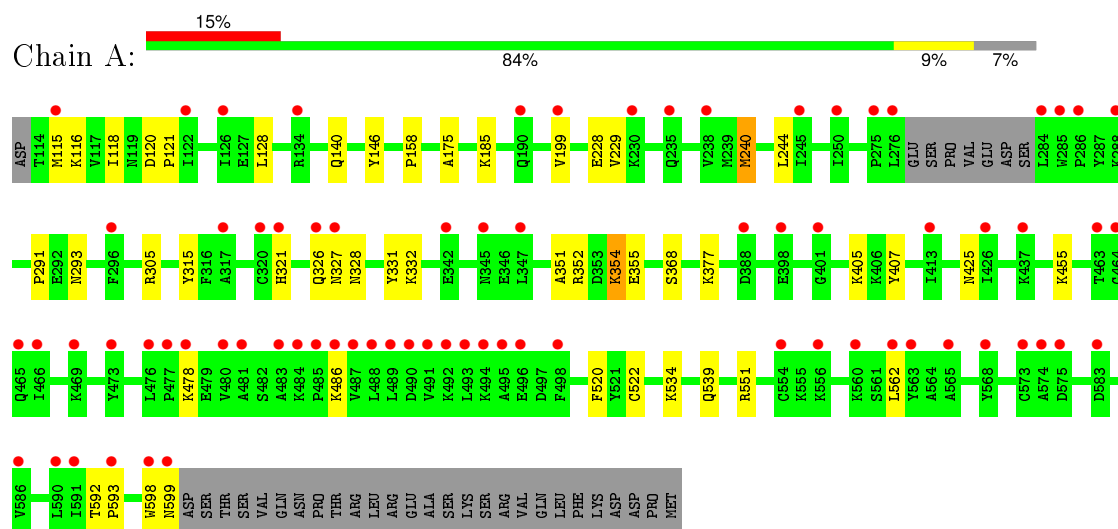
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total	O	0	0
			7	7		
6	B	6	Total	O	0	0
			6	6		
6	C	22	Total	O	0	0
			22	22		
6	D	3	Total	O	0	0
			3	3		

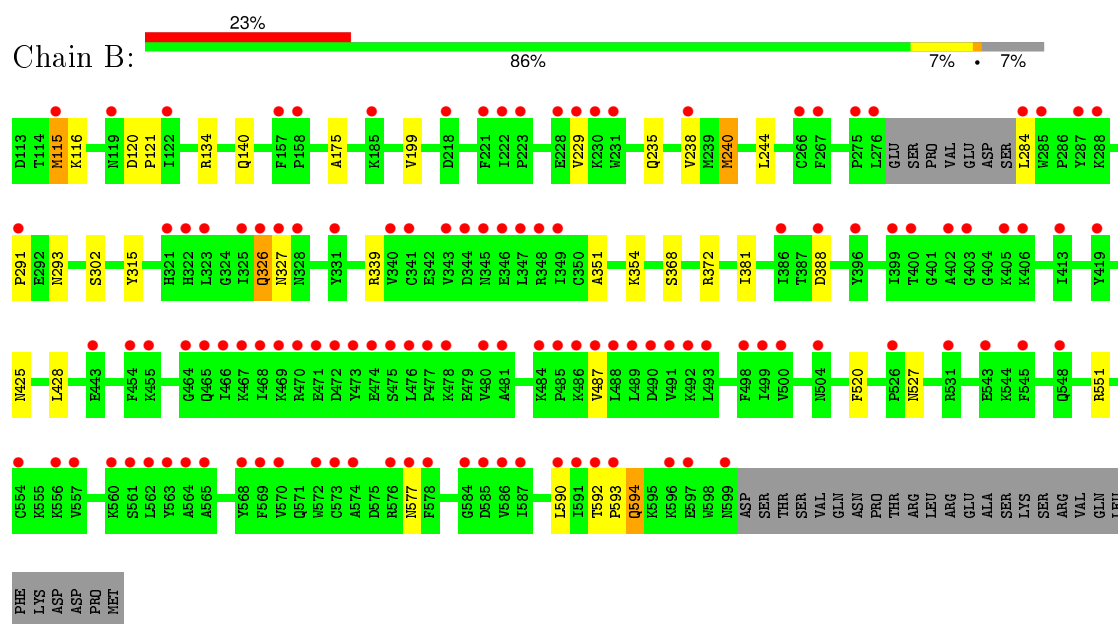
3 Residue-property plots

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.

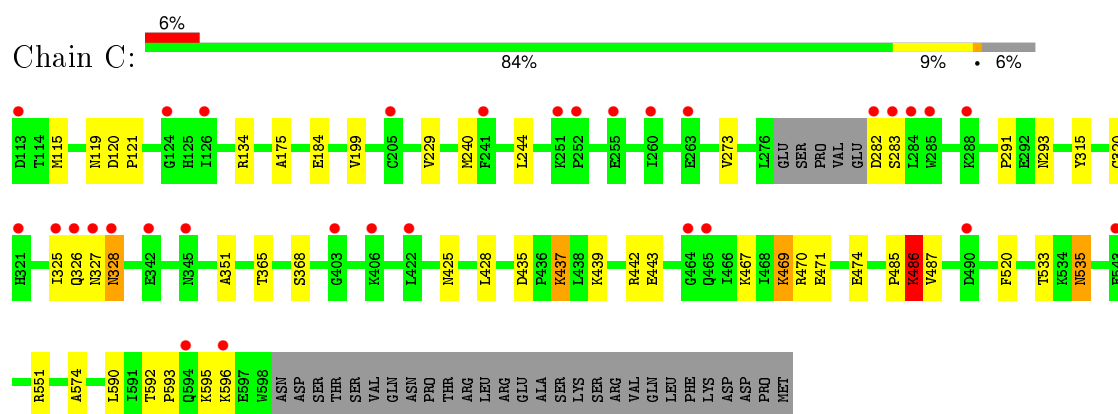
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



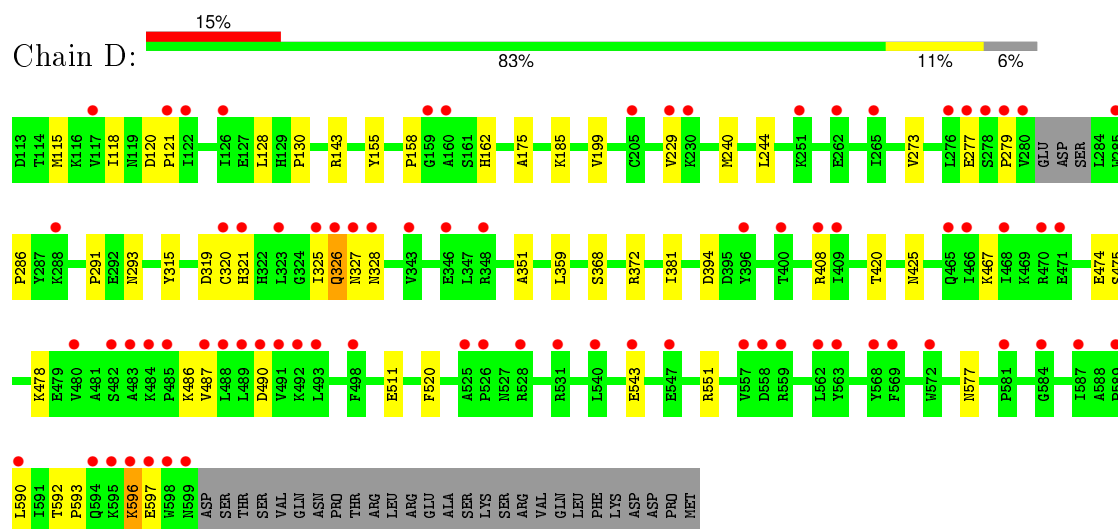
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



- 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, α , β , γ	86.20Å 141.59Å 98.19Å 90.00° 115.79° 90.00°	Depositor
Resolution (Å)	50.00 – 2.55 48.75 – 2.54	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-2.55) 95.1 (48.75-2.54)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.221 , 0.235 0.233 , 0.245	Depositor DCC
R_{free} test set	3199 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.877	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.9	EDS
Estimated twinning fraction	0.038 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	14 of 66501 reflections (0.021%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16149	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, DTP, 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	0.54	0/4014	0.72	3/5418 (0.1%)
1	B	0.52	0/4016	0.70	2/5421 (0.0%)
1	C	0.63	0/4036	0.74	2/5448 (0.0%)
1	D	0.55	0/4054	0.71	3/5473 (0.1%)
All	All	0.56	0/16120	0.72	10/21760 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	551	ARG	NE-CZ-NH2	5.79	123.20	120.30
1	B	134	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	A	551	ARG	NE-CZ-NH2	5.65	123.13	120.30
1	C	551	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	A	305	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	B	551	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	A	305	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	C	442	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	D	115[A]	MET	CG-SD-CE	5.01	108.22	100.20
1	D	115[B]	MET	CG-SD-CE	5.01	108.22	100.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3922	0	3915	39	0
1	B	3924	0	3915	37	0
1	C	3944	0	3927	47	0
1	D	3961	0	3950	31	0
2	A	28	0	12	1	0
2	B	28	0	12	1	0
2	C	56	0	24	1	0
2	D	56	0	24	1	0
3	A	30	0	12	0	0
3	B	30	0	12	1	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
5	C	64	0	24	0	0
5	D	64	0	24	0	0
6	A	7	0	0	4	0
6	B	6	0	0	1	0
6	C	22	0	0	1	0
6	D	3	0	0	1	0
All	All	16149	0	15851	137	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 4.

All (137) 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:C:574:ALA:O	1:C:595:LYS:NZ	1.67	1.26
2:B:701:DCP:N3	6:B:801:HOH:O	1.91	1.01
1:B:115:MET:HE2	1:B:116:LYS:N	1.75	1.00
1:C:328:ASN:ND2	1:C:365:THR:OG1	1.96	0.99
1:B:115:MET:HE2	1:B:116:LYS:CA	1.94	0.96
1:C:439:LYS:O	1:C:443:GLU:HG3	1.63	0.96
1:C:435:ASP:OD1	1:C:437:LYS:HG2	1.69	0.93
1:B:115:MET:C	1:B:115:MET:HE2	1.90	0.92
1:C:533:THR:OG1	1:C:535[A]:ASN:ND2	2.03	0.92
1:B:115:MET:HE1	1:B:116:LYS:O	1.70	0.90
1:B:115:MET:CE	1:B:116:LYS:N	2.35	0.88
1:B:115:MET:CE	1:B:116:LYS:C	2.41	0.88
1:C:535[A]:ASN:HD22	1:C:535[A]:ASN:H	1.23	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:MET:CE	1:B:115:MET:C	2.44	0.85
1:C:435:ASP:CG	1:C:437:LYS:HG3	1.98	0.83
1:B:115:MET:CE	1:B:116:LYS:O	2.28	0.82
1:C:467:LYS:CE	1:C:469:LYS:HE3	2.12	0.80
1:B:115:MET:HE2	1:B:116:LYS:C	1.99	0.79
1:C:485:PRO:O	1:C:486:LYS:HB2	1.81	0.79
1:C:435:ASP:CG	1:C:437:LYS:CG	2.52	0.78
1:A:326:GLN:NE2	1:C:326:GLN:HE21	1.81	0.77
1:C:435:ASP:OD2	1:C:437:LYS:HD2	1.85	0.76
1:A:326:GLN:NE2	1:C:326:GLN:NE2	2.33	0.75
1:C:435:ASP:OD1	1:C:437:LYS:CG	2.33	0.75
1:C:535[A]:ASN:HD22	1:C:535[A]:ASN:N	1.86	0.73
1:A:326:GLN:HE22	1:C:326:GLN:NE2	1.86	0.72
1:C:467:LYS:HE2	1:C:469:LYS:HE3	1.70	0.72
1:A:326:GLN:HE22	1:C:326:GLN:HE21	1.37	0.72
1:A:327:ASN:O	1:C:326:GLN:HB2	1.92	0.70
1:A:140:GLN:HG3	1:A:240:MET:CE	2.21	0.70
1:B:594:GLN:OE1	1:B:594:GLN:N	2.25	0.70
1:B:372:ARG:HH22	1:D:328:ASN:HD21	1.39	0.69
1:B:115:MET:HE1	1:B:116:LYS:C	2.09	0.68
1:D:596:LYS:HE2	1:D:597:GLU:OE1	1.93	0.68
1:B:140:GLN:HG3	1:B:240:MET:CE	2.25	0.67
1:B:425:ASN:ND2	1:C:425:ASN:OD1	2.30	0.64
1:C:470:ARG:HB2	1:C:470:ARG:CZ	2.27	0.64
1:B:327:ASN:O	1:D:326:GLN:HB2	1.96	0.64
1:B:326:GLN:HB2	1:D:327:ASN:O	2.01	0.61
1:A:331:TYR:OH	6:A:801:HOH:O	2.13	0.60
1:B:339:ARG:HH11	1:B:527:ASN:HD21	1.47	0.60
1:A:425:ASN:OD1	1:D:425:ASN:ND2	2.34	0.60
1:C:435:ASP:OD2	1:C:437:LYS:CD	2.49	0.59
1:C:435:ASP:OD2	1:C:437:LYS:CG	2.51	0.58
1:A:405:LYS:HD3	1:A:407:TYR:OH	2.04	0.58
1:A:146:TYR:HH	1:D:155:TYR:HH	1.53	0.56
1:B:115:MET:HE3	1:B:116:LYS:N	2.19	0.56
1:A:140:GLN:CG	1:A:240:MET:CE	2.84	0.56
1:B:487:VAL:HG23	1:B:590:LEU:HD12	1.89	0.55
1:D:487:VAL:HG23	1:D:590:LEU:HD12	1.89	0.54
1:A:326:GLN:HE21	1:A:327:ASN:H	1.55	0.54
1:C:487:VAL:HG23	1:C:590:LEU:HD12	1.89	0.54
1:A:326:GLN:HE21	1:A:327:ASN:N	2.05	0.53
1:B:339:ARG:HH11	1:B:527:ASN:ND2	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:535[A]:ASN:ND2	1:C:535[A]:ASN:H	2.01	0.53
1:C:485:PRO:O	1:C:486:LYS:CB	2.51	0.53
1:D:162:HIS:HE1	1:D:319:ASP:OD1	1.91	0.53
1:A:140:GLN:CG	1:A:240:MET:HE3	2.39	0.52
1:B:140:GLN:CG	1:B:240:MET:CE	2.87	0.52
1:A:331:TYR:CD1	1:A:331:TYR:C	2.83	0.52
1:C:535[A]:ASN:ND2	1:C:535[A]:ASN:N	2.56	0.52
1:A:355:GLU:OE1	6:A:806:HOH:O	2.19	0.51
1:A:228:GLU:N	1:A:228:GLU:OE1	2.41	0.51
1:C:469:LYS:HB3	1:C:471:GLU:OE1	2.11	0.51
1:C:435:ASP:OD2	1:C:437:LYS:HG3	2.10	0.51
1:A:377:LYS:HE2	6:D:801:HOH:O	2.10	0.51
1:B:235:GLN:O	1:B:238:VAL:HG22	2.11	0.50
1:A:116:LYS:NZ	6:A:805:HOH:O	2.44	0.50
1:B:140:GLN:CG	1:B:240:MET:HE3	2.42	0.49
1:C:467:LYS:HE3	1:C:469:LYS:HE3	1.93	0.49
1:A:352:ARG:CZ	1:A:354:LYS:HD3	2.43	0.49
1:C:574:ALA:C	1:C:595:LYS:NZ	2.56	0.49
1:D:394:ASP:O	1:D:408:ARG:HD2	2.14	0.48
1:C:467:LYS:CE	1:C:469:LYS:CE	2.90	0.47
1:B:120:ASP:OD1	1:B:121:PRO:HD2	2.15	0.47
1:D:474:GLU:O	1:D:478:LYS:NZ	2.37	0.47
1:D:592:THR:N	1:D:593:PRO:CD	2.78	0.47
1:C:592:THR:N	1:C:593:PRO:CD	2.78	0.47
1:D:351:ALA:O	1:D:520:PHE:HA	2.15	0.47
1:A:321:HIS:CE1	1:D:321:HIS:CE1	3.03	0.46
1:A:405:LYS:HD3	1:A:407:TYR:CZ	2.50	0.46
1:A:522:CYS:HB3	6:A:804:HOH:O	2.16	0.46
1:C:467:LYS:HE3	1:C:469:LYS:CE	2.46	0.46
1:D:475:SER:HA	1:D:478:LYS:HE2	1.98	0.45
1:B:351:ALA:O	1:B:520:PHE:HA	2.16	0.45
1:B:326:GLN:O	1:D:328:ASN:ND2	2.49	0.45
1:A:592:THR:N	1:A:593:PRO:CD	2.79	0.45
1:C:351:ALA:O	1:C:520:PHE:HA	2.16	0.45
1:D:381:ILE:HA	1:D:381:ILE:HD12	1.90	0.45
1:B:592:THR:N	1:B:593:PRO:CD	2.79	0.45
1:D:279:PRO:HG3	1:D:286:PRO:HB3	1.99	0.45
1:A:293:ASN:N	1:A:293:ASN:OD1	2.47	0.44
1:D:118:ILE:HD12	1:D:128:LEU:HD11	1.98	0.44
1:B:115:MET:HE3	1:B:115:MET:HB2	1.64	0.44
1:D:118:ILE:HD13	1:D:118:ILE:HG21	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ILE:HD12	1:A:128:LEU:HD11	2.00	0.44
1:D:511:GLU:H	1:D:511:GLU:CD	2.22	0.44
1:A:328:ASN:ND2	1:C:326:GLN:O	2.51	0.44
1:B:428:LEU:HD13	1:C:425:ASN:HB2	2.00	0.44
1:B:327:ASN:O	1:D:326:GLN:CB	2.63	0.44
1:D:120:ASP:OD2	1:D:121:PRO:HD2	2.17	0.44
1:B:115:MET:HE3	1:B:115:MET:C	2.33	0.43
1:A:598:TRP:O	1:A:599:ASN:HB2	2.18	0.43
1:C:244:LEU:HD23	1:C:244:LEU:C	2.39	0.43
1:A:291:PRO:HG2	1:A:293:ASN:OD1	2.17	0.43
1:A:118:ILE:HD13	1:A:118:ILE:HG21	1.80	0.43
1:D:291:PRO:HG2	1:D:293:ASN:OD1	2.19	0.43
1:C:437:LYS:HE2	1:C:437:LYS:HB3	1.82	0.43
1:B:175:ALA:HB1	1:B:199:VAL:HG12	2.00	0.43
1:C:291:PRO:HG2	1:C:293:ASN:OD1	2.19	0.43
1:C:120:ASP:OD2	1:C:121:PRO:HD2	2.17	0.43
1:A:351:ALA:O	1:A:520:PHE:HA	2.19	0.43
1:C:119:ASN:HB2	2:D:702:DCP:H1'	2.00	0.43
2:A:701:DCP:O2G	2:A:701:DCP:O2B	2.36	0.43
1:A:158:PRO:HG3	1:D:118:ILE:HG21	2.00	0.42
1:B:291:PRO:HG2	1:B:293:ASN:OD1	2.18	0.42
1:A:120:ASP:OD2	1:A:121:PRO:HD2	2.18	0.42
1:B:381:ILE:HD12	1:B:381:ILE:HA	1.92	0.42
1:A:326:GLN:CG	1:C:327:ASN:O	2.68	0.42
1:C:320:CYS:HB3	1:C:325:ILE:O	2.19	0.42
1:A:455:LYS:CB	1:A:562:LEU:HD21	2.50	0.42
1:C:175:ALA:HB1	1:C:199:VAL:HG12	2.02	0.42
1:D:244:LEU:HD23	1:D:244:LEU:C	2.39	0.42
1:B:425:ASN:HB2	1:C:428:LEU:HD13	2.01	0.42
1:A:118:ILE:HG21	1:D:158:PRO:HG3	2.02	0.42
1:D:467:LYS:HD3	1:D:467:LYS:HA	1.91	0.41
1:A:244:LEU:HD23	1:A:244:LEU:C	2.40	0.41
2:C:705:DCP:H5'1	6:C:816:HOH:O	2.20	0.41
1:D:143:ARG:HD2	1:D:420:THR:HA	2.03	0.41
1:B:244:LEU:C	1:B:244:LEU:HD23	2.41	0.41
3:B:702:DTP:N6	1:D:372:ARG:HG2	2.36	0.41
1:D:320:CYS:HB3	1:D:325:ILE:O	2.21	0.41
1:B:115:MET:CE	1:B:116:LYS:CA	2.75	0.41
1:C:467:LYS:HG2	1:C:469:LYS:CD	2.52	0.40
1:A:331:TYR:CD1	1:A:332:LYS:N	2.89	0.40
1:D:175:ALA:HB1	1:D:199:VAL:HG12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ALA:HB1	1:A:199:VAL:HG12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	476/514 (93%)	469 (98%)	7 (2%)	0	100	100
1	B	476/514 (93%)	465 (98%)	11 (2%)	0	100	100
1	C	479/514 (93%)	467 (98%)	11 (2%)	1 (0%)	52	73
1	D	481/514 (94%)	470 (98%)	11 (2%)	0	100	100
All	All	1912/2056 (93%)	1871 (98%)	40 (2%)	1 (0%)	56	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	486	LYS

5.3.2 Protein sidechains [i](#)

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	426/459 (93%)	415 (97%)	11 (3%)	54 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	426/459 (93%)	414 (97%)	12 (3%)	51	76
1	C	429/459 (94%)	410 (96%)	19 (4%)	35	58
1	D	431/459 (94%)	416 (96%)	15 (4%)	43	68
All	All	1712/1836 (93%)	1655 (97%)	57 (3%)	46	71

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	MET
1	A	185	LYS
1	A	229	VAL
1	A	240	MET
1	A	315	TYR
1	A	354	LYS
1	A	368	SER
1	A	478	LYS
1	A	486	LYS
1	A	534	LYS
1	A	539	GLN
1	B	115	MET
1	B	229	VAL
1	B	240	MET
1	B	284	LEU
1	B	302	SER
1	B	315	TYR
1	B	326	GLN
1	B	354	LYS
1	B	368	SER
1	B	388	ASP
1	B	577	ASN
1	B	594	GLN
1	C	115	MET
1	C	134	ARG
1	C	184	GLU
1	C	229	VAL
1	C	240	MET
1	C	273	VAL
1	C	282	ASP
1	C	283	SER
1	C	315	TYR
1	C	328	ASN

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Mol	Chain	Res	Type
1	C	368[A]	SER
1	C	368[B]	SER
1	C	437	LYS
1	C	469	LYS
1	C	474	GLU
1	C	486	LYS
1	C	535[A]	ASN
1	C	535[B]	ASN
1	C	596	LYS
1	D	130	PRO
1	D	185	LYS
1	D	229	VAL
1	D	240	MET
1	D	273	VAL
1	D	277	GLU
1	D	315	TYR
1	D	326	GLN
1	D	359	LEU
1	D	368	SER
1	D	486	LYS
1	D	490	ASP
1	D	543	GLU
1	D	577	ASN
1	D	596	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	HIS
1	A	326	GLN
1	A	328	ASN
1	B	322	HIS
1	B	425	ASN
1	B	527	ASN
1	B	599	ASN
1	C	322	HIS
1	C	326	GLN
1	C	328	ASN
1	D	162	HIS
1	D	322	HIS
1	D	328	ASN
1	D	425	ASN

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Mol	Chain	Res	Type
1	D	535	ASN
1	D	594	GLN
1	D	599	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 [i](#)

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	0.67	0	33,45,45	1.46	4 (12%)
3	DTP	A	702	4	24,32,32	1.51	5 (20%)	32,50,50	1.63	4 (12%)
2	DCP	B	701	-	21,29,29	0.56	0	33,45,45	1.56	6 (18%)
3	DTP	B	702	4	24,32,32	1.28	2 (8%)	32,50,50	1.89	5 (15%)
2	DCP	C	701	4	21,29,29	1.01	1 (4%)	33,45,45	1.40	7 (21%)
5	GTP	C	704	4	25,34,34	0.99	2 (8%)	34,54,54	1.68	6 (17%)
2	DCP	C	705	-	21,29,29	0.78	0	33,45,45	1.54	5 (15%)
5	GTP	C	706	4	25,34,34	1.27	3 (12%)	34,54,54	1.85	7 (20%)
5	GTP	D	701	4	25,34,34	1.23	3 (12%)	34,54,54	1.85	12 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DCP	D	702	4	21,29,29	0.75	0	33,45,45	1.54	5 (15%)
2	DCP	D	703	-	21,29,29	0.72	0	33,45,45	1.41	5 (15%)
5	GTP	D	704	4	25,34,34	1.18	2 (8%)	34,54,54	1.78	7 (20%)

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	DTP	A	702	4	-	0/18/34/34	0/3/3/3
2	DCP	B	701	-	-	0/18/34/34	0/2/2/2
3	DTP	B	702	4	-	0/18/34/34	0/3/3/3
2	DCP	C	701	4	-	0/18/34/34	0/2/2/2
5	GTP	C	704	4	-	0/18/38/38	0/3/3/3
2	DCP	C	705	-	-	0/18/34/34	0/2/2/2
5	GTP	C	706	4	-	0/18/38/38	0/3/3/3
5	GTP	D	701	4	-	0/18/38/38	0/3/3/3
2	DCP	D	702	4	-	0/18/34/34	0/2/2/2
2	DCP	D	703	-	-	0/18/34/34	0/2/2/2
5	GTP	D	704	4	-	0/18/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	DCP	O4'-C4'	-2.20	1.39	1.45
3	A	702	DTP	C5-N7	-2.16	1.32	1.39
3	A	702	DTP	C4-N3	-2.01	1.32	1.35
5	C	706	GTP	C6-C5	2.18	1.45	1.41
5	D	701	GTP	C6-C5	2.36	1.46	1.41
3	A	702	DTP	C2-N1	2.50	1.38	1.33
3	B	702	DTP	C2-N3	2.53	1.36	1.32
5	C	704	GTP	C5-C4	2.76	1.46	1.40
5	C	704	GTP	C6-C5	2.89	1.47	1.41
3	A	702	DTP	C2-N3	2.90	1.37	1.32
5	D	701	GTP	C5-C4	2.94	1.47	1.40
5	C	706	GTP	C5-C4	2.94	1.47	1.40
5	C	706	GTP	O4'-C1'	3.07	1.45	1.41
5	D	704	GTP	C5-C4	3.28	1.47	1.40
5	D	704	GTP	C6-C5	3.49	1.48	1.41
3	B	702	DTP	C5-C4	3.53	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	DTP	C5-C4	3.70	1.48	1.40
5	D	701	GTP	O4'-C1'	3.81	1.46	1.41

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	DTP	N3-C2-N1	-7.78	122.94	128.89
5	C	706	GTP	C5-C6-N1	-4.95	116.82	123.59
5	D	704	GTP	C5-C6-N1	-4.68	117.19	123.59
3	A	702	DTP	N3-C2-N1	-4.34	125.57	128.89
2	A	701	DCP	PB-O3B-PG	-3.86	119.71	132.67
2	D	702	DCP	PB-O3A-PA	-3.86	121.88	132.73
2	B	701	DCP	PB-O3B-PG	-3.83	119.83	132.67
5	D	701	GTP	C5-C6-N1	-3.76	118.44	123.59
5	D	701	GTP	PA-O3A-PB	-3.64	122.51	132.73
2	C	705	DCP	PB-O3A-PA	-3.58	122.66	132.73
5	C	706	GTP	PA-O3A-PB	-3.55	122.77	132.73
5	C	704	GTP	C6-C5-C4	-3.54	116.66	120.90
5	D	704	GTP	C6-C5-C4	-3.52	116.69	120.90
5	C	704	GTP	C5-C6-N1	-3.46	118.85	123.59
2	D	703	DCP	PB-O3A-PA	-3.40	123.19	132.73
5	D	704	GTP	PA-O3A-PB	-3.39	123.22	132.73
2	D	703	DCP	PB-O3B-PG	-3.31	121.57	132.67
2	B	701	DCP	PB-O3A-PA	-3.28	123.53	132.73
5	C	706	GTP	C4-C5-N7	-3.20	106.54	109.48
2	C	705	DCP	C5-C4-N4	-3.19	116.42	121.31
5	C	704	GTP	PA-O3A-PB	-3.08	124.08	132.73
2	D	702	DCP	PB-O3B-PG	-3.04	122.48	132.67
3	A	702	DTP	O4'-C1'-N9	-3.04	102.46	107.72
2	A	701	DCP	PB-O3A-PA	-3.02	124.24	132.73
5	D	701	GTP	C6-C5-C4	-2.99	117.32	120.90
2	C	701	DCP	PB-O3A-PA	-2.92	124.53	132.73
2	C	705	DCP	PB-O3B-PG	-2.88	123.01	132.67
5	D	701	GTP	O3A-PA-O5'	-2.88	95.31	102.94
2	C	701	DCP	C5-C4-N4	-2.69	117.18	121.31
5	C	704	GTP	C4-C5-N7	-2.68	107.02	109.48
5	D	704	GTP	C4-C5-N7	-2.65	107.04	109.48
5	C	704	GTP	N3-C2-N1	-2.64	123.43	127.44
5	D	704	GTP	N3-C2-N1	-2.63	123.44	127.44
2	C	701	DCP	PB-O3B-PG	-2.63	123.86	132.67
5	C	706	GTP	PB-O3B-PG	-2.58	124.03	132.67
5	C	706	GTP	N3-C2-N1	-2.56	123.54	127.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	701	GTP	C4'-O4'-C1'	-2.50	106.97	109.72
5	D	701	GTP	PB-O3B-PG	-2.47	124.40	132.67
5	C	706	GTP	C6-C5-C4	-2.41	118.01	120.90
5	D	701	GTP	N2-C2-N3	-2.36	113.28	117.80
5	D	704	GTP	PB-O3B-PG	-2.32	124.88	132.67
2	D	703	DCP	C5-C4-N4	-2.30	117.78	121.31
3	B	702	DTP	C1'-N9-C4	-2.28	123.29	127.16
3	B	702	DTP	PB-O3B-PG	-2.28	125.03	132.67
5	D	701	GTP	N3-C2-N1	-2.26	124.00	127.44
2	A	701	DCP	O4'-C1'-N1	2.17	111.48	107.72
3	B	702	DTP	O3G-PG-O1G	2.17	117.58	110.58
2	D	702	DCP	O2A-PA-O1A	2.19	124.41	112.53
5	D	701	GTP	O3G-PG-O2G	2.24	115.89	107.38
5	D	701	GTP	O2B-PB-O1B	2.25	124.70	112.53
2	B	701	DCP	O2G-PG-O1G	2.25	117.84	110.58
2	C	701	DCP	C2'-C3'-C4'	2.29	107.51	102.77
2	C	701	DCP	C2-N3-C4	2.47	119.10	115.61
2	C	701	DCP	N4-C4-N3	2.55	121.14	116.50
2	C	701	DCP	O3G-PG-O2G	2.61	117.31	107.38
3	B	702	DTP	N6-C6-N1	2.69	124.97	119.20
2	D	703	DCP	N4-C4-N3	2.73	121.48	116.50
2	B	701	DCP	O3G-PG-O2G	2.76	117.90	107.38
2	D	702	DCP	O4'-C1'-N1	2.89	112.72	107.72
2	D	703	DCP	C2-N3-C4	2.97	119.80	115.61
2	C	705	DCP	N4-C4-N3	3.15	122.25	116.50
3	A	702	DTP	O3G-PG-O1G	3.23	120.96	110.58
5	D	701	GTP	N2-C2-N1	3.33	122.72	117.20
2	D	702	DCP	C2-N3-C4	3.34	120.32	115.61
2	B	701	DCP	O4'-C1'-N1	3.34	113.50	107.72
2	B	701	DCP	C2-N3-C4	3.47	120.51	115.61
5	D	701	GTP	C6-N1-C2	3.65	121.01	115.94
2	C	705	DCP	C2-N3-C4	3.70	120.84	115.61
2	A	701	DCP	C2-N3-C4	3.83	121.01	115.61
3	A	702	DTP	N6-C6-N1	4.27	128.37	119.20
5	C	704	GTP	C6-N1-C2	4.30	121.90	115.94
5	C	706	GTP	C6-N1-C2	4.80	122.60	115.94
5	D	704	GTP	C6-N1-C2	4.95	122.80	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	DCP	1	0
2	B	701	DCP	1	0
3	B	702	DTP	1	0
2	C	705	DCP	1	0
2	D	702	DCP	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, 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(Å ²)	Q<0.9
1	A	479/514 (93%)	0.91	75 (15%) 3 3	32, 75, 123, 162	0
1	B	480/514 (93%)	1.48	120 (25%) 1 1	38, 99, 174, 214	0
1	C	481/514 (93%)	0.53	31 (6%) 23 26	28, 62, 104, 153	0
1	D	484/514 (94%)	0.97	77 (15%) 3 3	35, 76, 126, 181	0
All	All	1924/2056 (93%)	0.97	303 (15%) 3 3	28, 76, 143, 214	0

All (303) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	280	VAL	11.3
1	B	487	VAL	10.7
1	B	489	LEU	9.7
1	B	466	ILE	9.6
1	D	279	PRO	9.0
1	A	489	LEU	8.9
1	A	490	ASP	8.6
1	D	490	ASP	8.5
1	B	230	LYS	7.1
1	B	493	LEU	7.1
1	B	345	ASN	6.9
1	B	486	LYS	6.9
1	B	573	CYS	6.8
1	A	493	LEU	6.8
1	B	402	ALA	6.7
1	A	491	VAL	6.6
1	A	492	LYS	6.3
1	B	488	LEU	6.2
1	B	223	PRO	6.2
1	A	488	LEU	6.1
1	D	590	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
1	B	563	TYR	5.9
1	B	591	ILE	5.8
1	B	491	VAL	5.8
1	B	572	TRP	5.8
1	B	276	LEU	5.7
1	B	585	ASP	5.7
1	A	487	VAL	5.6
1	D	599	ASN	5.6
1	D	489	LEU	5.6
1	B	467	LYS	5.5
1	D	488	LEU	5.3
1	B	229	VAL	5.3
1	D	491	VAL	5.2
1	D	484	LYS	5.2
1	A	484	LYS	5.2
1	B	481	ALA	5.1
1	B	490	ASP	5.1
1	B	288	LYS	5.0
1	D	595	LYS	5.0
1	A	284	LEU	5.0
1	B	578	PHE	5.0
1	A	463	THR	4.9
1	B	554	CYS	4.9
1	B	484	LYS	4.9
1	B	287	TYR	4.9
1	D	557	VAL	4.9
1	B	592	THR	4.8
1	B	569	PHE	4.8
1	D	589	PRO	4.7
1	B	347	LEU	4.7
1	B	565	ALA	4.6
1	B	480	VAL	4.6
1	A	554	CYS	4.5
1	B	284	LEU	4.5
1	B	403	GLY	4.5
1	D	598	TRP	4.4
1	B	599	ASN	4.4
1	B	526	PRO	4.4
1	B	485	PRO	4.3
1	A	498	PHE	4.3
1	D	543	GLU	4.3
1	B	341	CYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	486	LYS	4.3
1	B	597	GLU	4.2
1	B	285	TRP	4.2
1	D	483	ALA	4.2
1	C	284	LEU	4.2
1	A	464	GLY	4.1
1	D	466	ILE	4.1
1	B	593	PRO	4.1
1	C	283	SER	4.1
1	B	556	LYS	4.0
1	B	275	PRO	4.0
1	A	276	LEU	4.0
1	A	568	TYR	4.0
1	C	464	GLY	4.0
1	B	574	ALA	3.9
1	B	570	VAL	3.9
1	B	476	LEU	3.9
1	B	492	LYS	3.9
1	C	113	ASP	3.9
1	D	596	LYS	3.9
1	D	326	GLN	3.9
1	B	326	GLN	3.9
1	D	568	TYR	3.8
1	C	490	ASP	3.8
1	B	465	GLN	3.8
1	C	327	ASN	3.8
1	D	230	LYS	3.8
1	B	557	VAL	3.8
1	B	562	LEU	3.8
1	D	229	VAL	3.7
1	D	563	TYR	3.7
1	B	472	ASP	3.7
1	A	480	VAL	3.7
1	D	540	LEU	3.6
1	C	594	GLN	3.6
1	C	255	GLU	3.6
1	B	221	PHE	3.6
1	B	413	ILE	3.5
1	D	597	GLU	3.5
1	D	482	SER	3.5
1	B	478	LYS	3.5
1	A	494	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	473	TYR	3.5
1	B	498	PHE	3.4
1	A	573	CYS	3.4
1	B	346	GLU	3.4
1	B	477	PRO	3.4
1	A	478	LYS	3.3
1	D	278	SER	3.3
1	D	498	PHE	3.3
1	B	560	LYS	3.3
1	B	500	VAL	3.2
1	A	565	ALA	3.2
1	C	288	LYS	3.2
1	D	485	PRO	3.2
1	A	326	GLN	3.2
1	D	528	ARG	3.2
1	B	470	ARG	3.2
1	A	285	TRP	3.2
1	B	348	ARG	3.1
1	A	286	PRO	3.1
1	A	238	VAL	3.1
1	B	531	ARG	3.1
1	D	493	LEU	3.1
1	A	496	GLU	3.1
1	A	245	ILE	3.1
1	A	481	ALA	3.0
1	B	185	LYS	3.0
1	D	531	ARG	3.0
1	B	222	ILE	3.0
1	A	342	GLU	3.0
1	B	471	GLU	3.0
1	A	562	LEU	3.0
1	B	576	ARG	3.0
1	D	327	ASN	3.0
1	D	328	ASN	3.0
1	D	470	ARG	3.0
1	D	492	LYS	3.0
1	B	587	ILE	3.0
1	D	277	GLU	3.0
1	A	560	LYS	2.9
1	A	591	ILE	2.9
1	B	548	GLN	2.9
1	B	454	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	477	PRO	2.9
1	B	464	GLY	2.9
1	A	476	LEU	2.9
1	D	487	VAL	2.9
1	C	465	GLN	2.8
1	D	346	GLU	2.8
1	B	328	ASN	2.8
1	D	288	LYS	2.8
1	C	596	LYS	2.8
1	A	321	HIS	2.8
1	D	343	VAL	2.8
1	D	594	GLN	2.8
1	B	400	THR	2.8
1	D	160	ALA	2.8
1	A	469	LYS	2.8
1	B	238	VAL	2.7
1	B	340	VAL	2.7
1	A	437	LYS	2.7
1	C	345	ASN	2.7
1	D	408	ARG	2.7
1	C	282	ASP	2.7
1	D	262	GLU	2.7
1	D	572	TRP	2.7
1	B	473	TYR	2.7
1	A	563	TYR	2.7
1	B	474	GLU	2.7
1	B	596	LYS	2.7
1	A	345	ASN	2.7
1	A	593	PRO	2.7
1	B	396	TYR	2.7
1	A	466	ILE	2.6
1	D	409	ILE	2.6
1	A	296	PHE	2.6
1	B	469	LYS	2.6
1	C	326	GLN	2.6
1	A	575	ASP	2.6
1	D	584	GLY	2.6
1	B	218	ASP	2.6
1	B	568	TYR	2.6
1	D	323	LEU	2.6
1	C	124	GLY	2.5
1	B	231	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	406	LYS	2.5
1	A	465	GLN	2.5
1	A	413	ILE	2.5
1	A	388	ASP	2.5
1	B	327	ASN	2.5
1	A	199	VAL	2.5
1	B	586	VAL	2.5
1	A	590	LEU	2.5
1	A	134	ARG	2.5
1	D	251	LYS	2.5
1	B	543	GLU	2.5
1	A	495	ALA	2.5
1	D	205	CYS	2.4
1	D	400	THR	2.4
1	B	325	ILE	2.4
1	B	419	TYR	2.4
1	D	581	PRO	2.4
1	A	190	GLN	2.4
1	B	504	ASN	2.4
1	A	230	LYS	2.4
1	B	388	ASP	2.4
1	B	158	PRO	2.4
1	B	468	ILE	2.4
1	A	122	ILE	2.4
1	A	126	ILE	2.4
1	B	590	LEU	2.4
1	A	598	TRP	2.4
1	D	285	TRP	2.4
1	D	320	CYS	2.4
1	C	252	PRO	2.4
1	A	583	ASP	2.4
1	D	122	ILE	2.4
1	C	285	TRP	2.3
1	B	266	CYS	2.3
1	B	545	PHE	2.3
1	C	251	LYS	2.3
1	B	343	VAL	2.3
1	B	561	SER	2.3
1	D	471	GLU	2.3
1	A	250	ILE	2.3
1	B	322	HIS	2.3
1	B	119	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	525	ALA	2.3
1	B	584	GLY	2.3
1	A	398	GLU	2.3
1	B	323	LEU	2.3
1	B	455	LYS	2.3
1	B	399	ILE	2.3
1	A	288	LYS	2.3
1	B	386	ILE	2.3
1	B	443	GLU	2.3
1	D	465	GLN	2.3
1	B	564	ALA	2.3
1	D	468	ILE	2.3
1	A	586	VAL	2.3
1	A	485	PRO	2.3
1	A	327	ASN	2.3
1	D	276	LEU	2.3
1	D	325	ILE	2.3
1	D	587	ILE	2.3
1	B	267	PHE	2.3
1	C	403	GLY	2.3
1	C	241	PHE	2.2
1	D	558	ASP	2.2
1	A	317	ALA	2.2
1	A	574	ALA	2.2
1	B	122	ILE	2.2
1	B	499	ILE	2.2
1	B	291	PRO	2.2
1	C	543	GLU	2.2
1	D	159	GLY	2.2
1	C	260	ILE	2.2
1	B	228	GLU	2.2
1	B	321	HIS	2.2
1	D	348	ARG	2.2
1	C	325	ILE	2.2
1	D	547	GLU	2.2
1	C	126	ILE	2.1
1	C	205	CYS	2.1
1	C	422	LEU	2.1
1	D	569	PHE	2.1
1	B	577	ASN	2.1
1	D	321	HIS	2.1
1	D	559	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	263	GLU	2.1
1	D	480	VAL	2.1
1	A	115	MET	2.1
1	B	405	LYS	2.1
1	D	126	ILE	2.1
1	D	562	LEU	2.1
1	C	321	HIS	2.1
1	B	475	SER	2.1
1	D	396	TYR	2.1
1	A	320	CYS	2.1
1	B	157	PHE	2.1
1	A	599	ASN	2.0
1	C	328	ASN	2.0
1	B	115	MET	2.0
1	A	401	GLY	2.0
1	B	349	ILE	2.0
1	D	265	ILE	2.0
1	B	331	TYR	2.0
1	B	344	ASP	2.0
1	A	235	GLN	2.0
1	A	483	ALA	2.0
1	D	117	VAL	2.0
1	A	426	ILE	2.0
1	D	526	PRO	2.0
1	C	342	GLU	2.0
1	C	406	LYS	2.0
1	A	275	PRO	2.0
1	D	121	PRO	2.0
1	A	347	LEU	2.0
1	A	556	LYS	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 [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, 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	GTP	C	704	32/32	0.89	0.16	-1.30	20,23,28,31	0
2	DCP	B	701	28/28	0.89	0.15	-1.32	28,40,55,57	0
3	DTP	B	702	30/30	0.94	0.13	-1.39	16,20,33,36	0
3	DTP	A	702	30/30	0.97	0.14	-1.41	15,21,37,42	0
2	DCP	D	703	28/28	0.93	0.12	-1.51	32,39,58,64	0
5	GTP	D	704	32/32	0.94	0.12	-1.58	16,20,26,26	0
2	DCP	A	701	28/28	0.93	0.12	-2.09	38,46,67,75	0
2	DCP	C	705	28/28	0.95	0.11	-2.20	27,35,65,72	0
5	GTP	C	706	32/32	0.97	0.10	-2.26	16,22,25,26	0
2	DCP	D	702	28/28	0.94	0.13	-2.36	16,20,34,35	0
5	GTP	D	701	32/32	0.96	0.10	-2.39	22,26,29,30	0
2	DCP	C	701	28/28	0.96	0.12	-2.40	19,25,37,51	0
4	MG	C	703	1/1	0.77	0.12	-	15,15,15,15	0
4	MG	A	704	1/1	0.79	0.11	-	48,48,48,48	0
4	MG	C	702	1/1	0.87	0.12	-	32,32,32,32	0
4	MG	A	703	1/1	0.93	0.05	-	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.