



Full wwPDB X-ray Structure Validation Report

Oct 22, 2014 – 06:32 AM EDT

PDB ID : 4TNZ
Title : Structure basis of cellular dNTP regulation, SAMHD1-GTP-dATP-dTTP complex
Authors : Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.
Deposited on : 2014-06-05
Resolution : 2.38 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

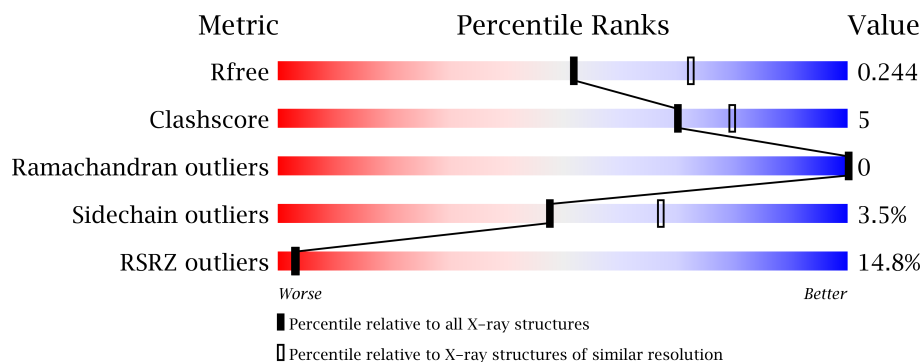
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.38 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2963 (2.40-2.36)
Clashscore	79885	3668 (2.40-2.36)
Ramachandran outliers	78287	3600 (2.40-2.36)
Sidechain outliers	78261	3602 (2.40-2.36)
RSRZ outliers	66119	2966 (2.40-2.36)

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
3	MG	A	704	-	X
3	MG	B	703	-	X
3	MG	C	702	-	X
3	MG	D	703	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16280 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.

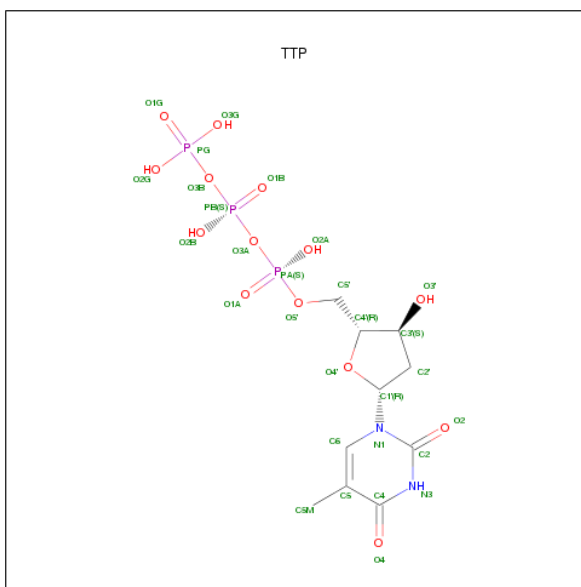
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	481	Total	C	N	O	S	0	2	0
			3948	2525	687	715	21			
1	A	480	Total	C	N	O	S	0	2	0
			3940	2521	686	712	21			
1	D	480	Total	C	N	O	S	0	1	0
			3934	2518	684	712	20			
1	B	481	Total	C	N	O	S	0	1	0
			3939	2520	686	712	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	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 THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).

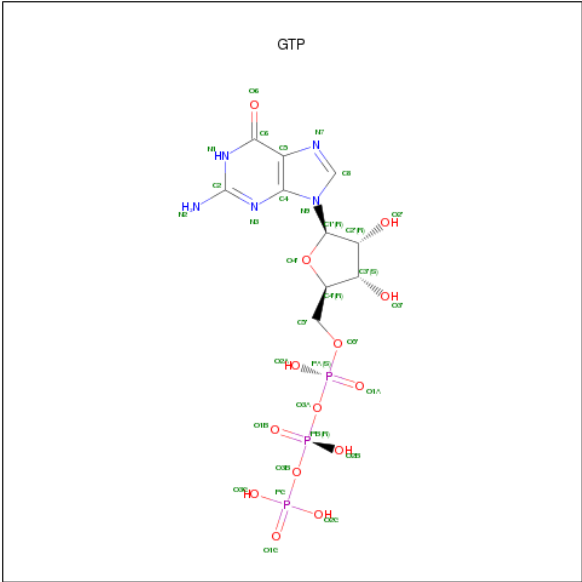


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	D	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

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

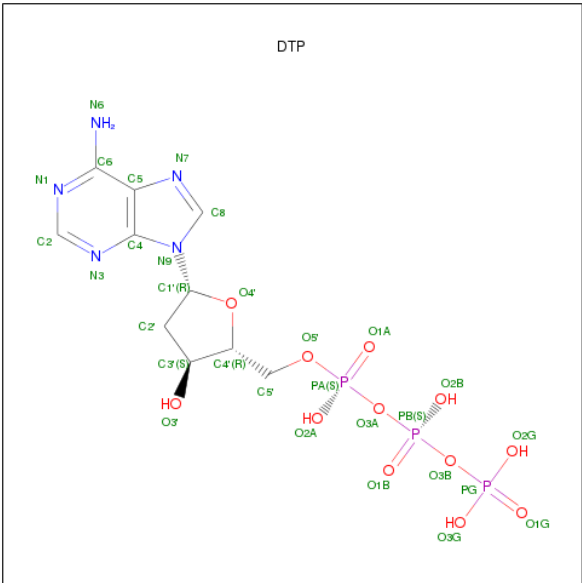
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	3	Total	Mg	0	0
			3	3		
3	D	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

- Molecule 5 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



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

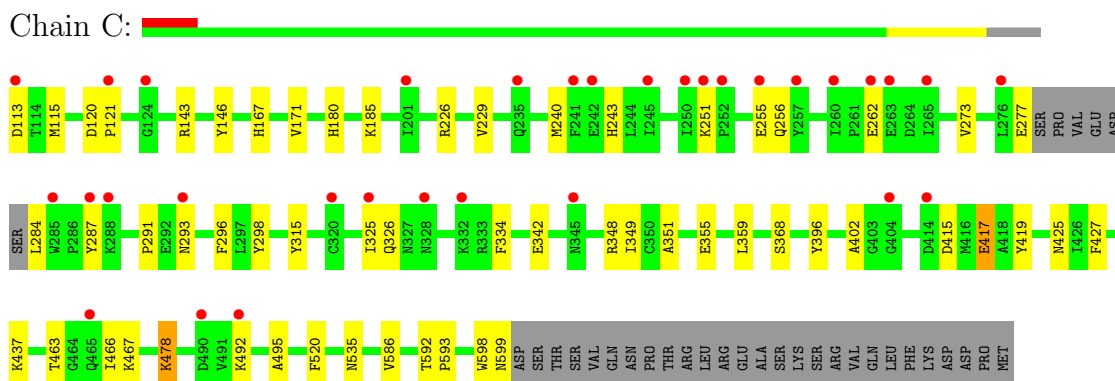
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	53	Total	O	0	0
			53	53		
6	A	47	Total	O	0	0
			47	47		
6	D	32	Total	O	0	0
			32	32		
6	B	15	Total	O	0	0
			15	15		

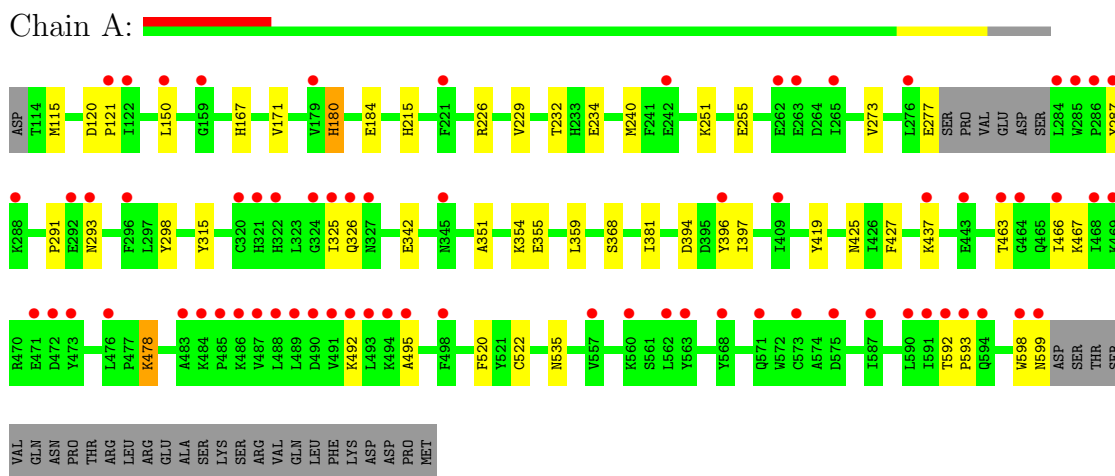
3 Residue-property plots

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.

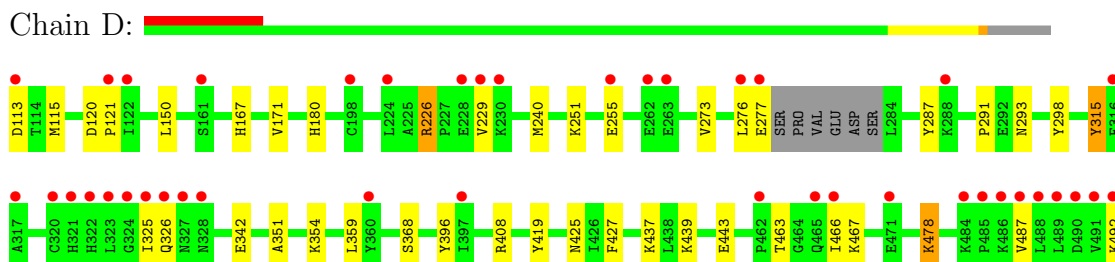
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

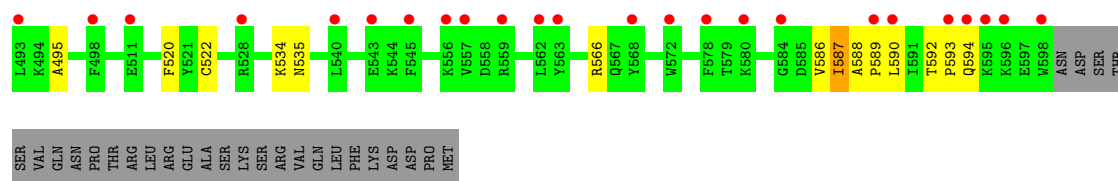


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



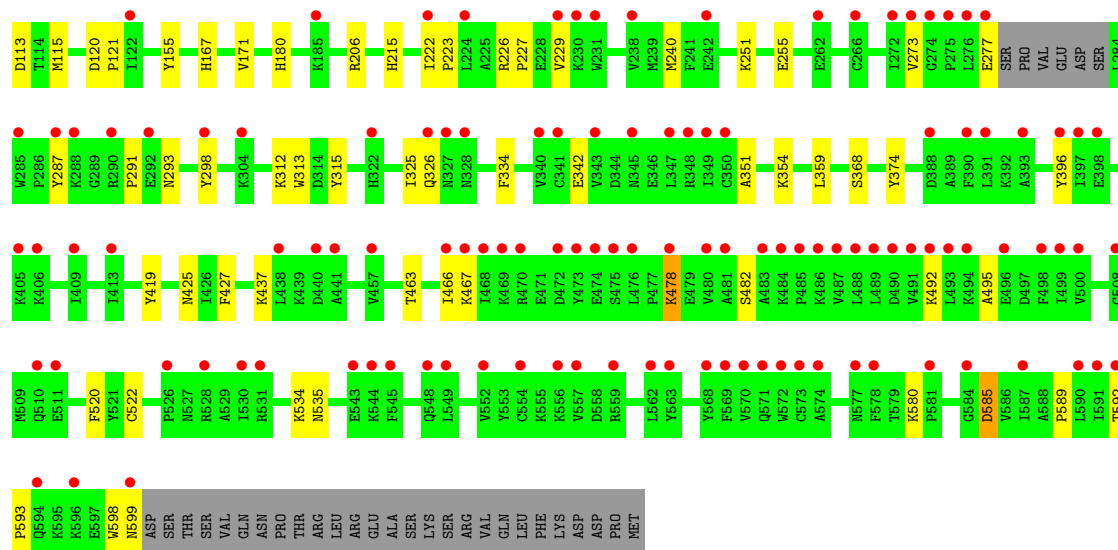
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.13Å 141.75Å 98.47Å 90.00° 116.29° 90.00°	Depositor
Resolution (Å)	88.29 – 2.38 48.74 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.4 (88.29-2.38) 98.5 (48.74-2.38)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.212 , 0.243 0.213 , 0.244	Depositor DCC
R_{free} test set	4158 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.6	EDS
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 83069 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16280	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.59	0/4032	0.69	0/5442
1	B	0.54	0/4031	0.68	1/5441 (0.0%)
1	C	0.62	0/4040	0.70	0/5453
1	D	0.58	0/4026	0.68	1/5434 (0.0%)
All	All	0.58	0/16129	0.69	2/21770 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	585	ASP	CB-CG-OD1	7.34	124.91	118.30
1	D	226	ARG	NE-CZ-NH2	5.10	122.85	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	3940	0	3926	31	0
1	B	3939	0	3925	37	0
1	C	3948	0	3930	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3934	0	3920	44	0
2	A	29	0	13	4	0
2	B	29	0	13	9	0
2	C	29	0	13	1	0
2	D	29	0	13	3	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	32	0	12	0	0
4	B	32	0	12	0	0
4	C	32	0	12	1	0
4	D	32	0	12	0	0
5	A	30	0	12	1	0
5	B	30	0	12	1	0
5	C	30	0	12	0	0
5	D	30	0	12	1	0
6	A	47	0	0	3	0
6	B	15	0	0	1	0
6	C	53	0	0	7	0
6	D	32	0	0	2	0
All	All	16280	0	15849	148	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 (148) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:566:ARG:CG	1:D:587:ILE:HD11	1.71	1.20
1:D:566:ARG:HG2	1:D:587:ILE:HD11	1.25	1.12
1:D:566:ARG:CB	1:D:587:ILE:HD11	1.82	1.10
1:D:566:ARG:HB3	1:D:587:ILE:CD1	1.88	1.04
1:D:566:ARG:HB3	1:D:587:ILE:HD11	1.45	0.95
1:D:588:ALA:O	1:D:592:THR:HG23	1.66	0.95
1:C:415:ASP:OD2	1:C:417:GLU:HG2	1.73	0.89
1:B:312:LYS:NZ	2:B:702:TTP:O1G	2.06	0.88
1:C:415:ASP:CG	1:C:417:GLU:HG2	1.97	0.84
1:D:408:ARG:HD2	6:D:831:HOH:O	1.86	0.75
1:D:566:ARG:HG2	1:D:587:ILE:CD1	2.11	0.74
1:D:589:PRO:O	1:D:593:PRO:HD3	1.88	0.73
1:A:355:GLU:OE1	6:A:822:HOH:O	2.09	0.70
1:C:415:ASP:OD1	1:C:417:GLU:HG2	1.90	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:402:ALA:HB2	1:C:417:GLU:HG3	1.72	0.70
1:A:226:ARG:O	1:A:229:VAL:HG12	1.93	0.69
1:D:226:ARG:O	1:D:229:VAL:HG12	1.93	0.68
1:B:226:ARG:O	1:B:229:VAL:HG12	1.93	0.68
1:B:291:PRO:HG2	1:B:293:ASN:OD1	1.94	0.68
1:C:326:GLN:HG2	1:A:326:GLN:HG2	1.76	0.68
1:A:150:LEU:CD2	2:A:703:TTP:H2'1	2.23	0.68
1:C:226:ARG:O	1:C:229:VAL:HG12	1.94	0.67
1:C:417:GLU:H	1:C:417:GLU:CD	1.97	0.67
1:D:326:GLN:HG2	1:B:326:GLN:HG2	1.76	0.67
1:C:291:PRO:HG2	1:C:293:ASN:OD1	1.94	0.66
1:A:291:PRO:HG2	1:A:293:ASN:OD1	1.96	0.66
1:D:291:PRO:HG2	1:D:293:ASN:OD1	1.96	0.66
1:C:120:ASP:OD1	1:C:121:PRO:HD2	1.96	0.65
1:D:590:LEU:O	1:D:593:PRO:HD2	1.95	0.65
1:D:592:THR:N	1:D:593:PRO:CD	2.61	0.64
1:C:415:ASP:OD1	1:C:417:GLU:CG	2.46	0.64
1:B:120:ASP:OD1	1:B:121:PRO:HD2	1.98	0.64
1:B:589:PRO:O	1:B:593:PRO:HD3	1.98	0.64
1:D:120:ASP:OD1	1:D:121:PRO:HD2	1.98	0.64
1:D:566:ARG:CG	1:D:587:ILE:CD1	2.63	0.63
1:A:120:ASP:OD1	1:A:121:PRO:HD2	1.99	0.63
1:C:417:GLU:N	1:C:417:GLU:OE2	2.31	0.62
1:C:586:VAL:HG11	1:A:522[A]:CYS:SG	2.39	0.62
1:B:312:LYS:CE	2:B:702:TTP:O1G	2.48	0.61
1:C:348:ARG:HD3	6:C:835:HOH:O	2.00	0.61
1:C:262:GLU:HG3	6:C:843:HOH:O	2.01	0.60
1:D:566:ARG:HD3	1:D:587:ILE:CG1	2.31	0.60
1:C:425:ASN:OD1	1:B:425:ASN:OD1	2.19	0.59
1:D:566:ARG:HB3	1:D:587:ILE:HD13	1.80	0.59
1:C:355:GLU:OE1	6:C:849:HOH:O	2.17	0.58
1:A:287:TYR:CD1	1:A:298:TYR:CE1	2.93	0.57
1:B:287:TYR:CD1	1:B:298:TYR:CE1	2.93	0.57
1:B:206:ARG:NH2	2:B:702:TTP:O2B	2.38	0.56
1:C:287:TYR:CD1	1:C:298:TYR:CE1	2.95	0.55
1:B:215:HIS:CE1	2:B:702:TTP:O2A	2.59	0.55
1:D:240:MET:CE	1:D:419:TYR:HD2	2.21	0.53
1:B:313:TRP:CZ2	1:B:334:PHE:HD1	2.27	0.53
1:D:589:PRO:O	1:D:593:PRO:CD	2.55	0.53
1:C:240:MET:CE	1:C:419:TYR:HD2	2.23	0.52
1:A:240:MET:CE	1:A:419:TYR:HD2	2.23	0.52
1:C:415:ASP:OD1	1:C:417:GLU:OE1	2.27	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:374:TYR:O	2:B:702:TTP:HM52	2.10	0.52
1:D:287:TYR:CD1	1:D:298:TYR:CE1	2.98	0.52
1:A:167:HIS:O	1:A:171:VAL:HG23	2.10	0.51
1:C:592:THR:N	1:C:593:PRO:CD	2.73	0.51
1:D:167:HIS:O	1:D:171:VAL:HG23	2.10	0.51
1:C:167:HIS:O	1:C:171:VAL:HG23	2.10	0.51
1:A:592:THR:N	1:A:593:PRO:CD	2.73	0.51
1:B:592:THR:N	1:B:593:PRO:CD	2.73	0.51
1:B:240:MET:CE	1:B:419:TYR:HD2	2.24	0.51
1:B:167:HIS:O	1:B:171:VAL:HG23	2.11	0.51
1:A:397:ILE:HB	6:A:832:HOH:O	2.10	0.51
1:B:312:LYS:HE3	2:B:702:TTP:O1G	2.11	0.50
1:C:185:LYS:HD2	6:C:839:HOH:O	2.11	0.50
1:B:215:HIS:NE2	2:B:702:TTP:O5'	2.40	0.50
1:D:586:VAL:HG11	1:B:522[A]:CYS:SG	2.51	0.50
1:C:334:PHE:HA	6:C:849:HOH:O	2.12	0.50
1:C:256:GLN:HG3	6:C:801:HOH:O	2.12	0.49
1:A:598:TRP:O	1:A:599:ASN:HB2	2.12	0.49
2:B:702:TTP:O3G	2:B:702:TTP:O1B	2.29	0.49
1:B:589:PRO:O	1:B:593:PRO:CD	2.61	0.48
1:A:354:LYS:NZ	5:A:701:DTP:O1A	2.45	0.48
1:B:580:LYS:CE	1:B:585:ASP:OD2	2.62	0.48
1:C:415:ASP:OD1	1:C:417:GLU:CD	2.52	0.48
1:A:425:ASN:OD1	1:D:425:ASN:OD1	2.30	0.48
1:D:315:TYR:CE2	2:D:702:TTP:H5'1	2.49	0.47
1:C:417:GLU:N	1:C:417:GLU:CD	2.67	0.47
1:B:313:TRP:CZ2	1:B:334:PHE:CD1	3.02	0.47
2:D:702:TTP:O2B	2:D:702:TTP:O2G	2.32	0.47
1:A:396:TYR:CD1	1:A:437:LYS:HD2	2.50	0.47
1:D:354:LYS:NZ	5:D:705:DTP:O1A	2.48	0.47
1:B:478:LYS:HE2	1:B:495:ALA:HB1	1.98	0.46
1:B:463:THR:O	1:B:466:ILE:HG12	2.15	0.46
1:B:396:TYR:CD1	1:B:437:LYS:HD2	2.50	0.46
1:A:215:HIS:NE2	2:A:703:TTP:O5'	2.49	0.46
1:A:463:THR:O	1:A:466:ILE:HG12	2.16	0.46
1:D:478:LYS:HE2	1:D:495:ALA:HB1	1.98	0.46
1:D:592:THR:N	1:D:593:PRO:HD3	2.30	0.46
1:A:478:LYS:HE2	1:A:495:ALA:HB1	1.98	0.46
1:D:463:THR:O	1:D:466:ILE:HG12	2.16	0.46
1:C:251:LYS:O	1:C:255:GLU:HG3	2.16	0.45
1:D:396:TYR:CD1	1:D:437:LYS:HD2	2.51	0.45
1:C:478:LYS:HE2	1:C:495:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:C:703:GTP:O1B	4:C:703:GTP:O1A	2.33	0.45
1:A:287:TYR:HB3	1:A:298:TYR:OH	2.17	0.45
1:B:598:TRP:O	1:B:599:ASN:HB2	2.17	0.45
1:D:251:LYS:O	1:D:255:GLU:HG3	2.16	0.45
1:C:396:TYR:CD1	1:C:437:LYS:HD2	2.52	0.45
1:D:566:ARG:HD3	1:D:587:ILE:HG13	1.97	0.45
1:A:251:LYS:O	1:A:255:GLU:HG3	2.17	0.44
1:B:580:LYS:NZ	1:B:585:ASP:OD2	2.50	0.44
1:C:463:THR:O	1:C:466:ILE:HG12	2.17	0.44
1:B:251:LYS:O	1:B:255:GLU:HG3	2.17	0.44
1:D:487:VAL:HG22	1:D:590:LEU:CD1	2.48	0.44
1:B:215:HIS:HE1	2:B:702:TTP:O2A	2.01	0.44
1:D:276:LEU:C	6:D:830:HOH:O	2.56	0.44
1:D:287:TYR:HB3	1:D:298:TYR:OH	2.18	0.43
1:B:427:PHE:CD1	1:B:427:PHE:C	2.92	0.43
1:C:243:HIS:CE1	1:C:417:GLU:OE2	2.71	0.43
1:C:325:ILE:CG2	1:C:326:GLN:N	2.81	0.43
1:B:287:TYR:HB3	1:B:298:TYR:OH	2.17	0.43
1:D:566:ARG:CB	1:D:587:ILE:CD1	2.57	0.43
1:C:287:TYR:HB3	1:C:298:TYR:OH	2.18	0.43
1:A:215:HIS:HE2	2:A:703:TTP:PA	2.42	0.43
1:C:598:TRP:O	1:C:599:ASN:HB2	2.18	0.43
1:D:487:VAL:HG22	1:D:590:LEU:HD12	2.01	0.43
1:D:351:ALA:O	1:D:520:PHE:HA	2.18	0.43
1:A:351:ALA:O	1:A:520:PHE:HA	2.19	0.42
2:C:701:TTP:O2G	2:C:701:TTP:O1B	2.36	0.42
1:B:351:ALA:O	1:B:520:PHE:HA	2.19	0.42
1:D:150:LEU:CD2	2:D:702:TTP:H2'1	2.50	0.42
1:C:143:ARG:HD3	6:C:833:HOH:O	2.20	0.42
1:A:150:LEU:HD22	2:A:703:TTP:H2'1	1.99	0.42
1:B:354:LYS:NZ	5:B:701:DTP:O2A	2.53	0.42
1:A:232:THR:HB	1:A:234:GLU:OE1	2.19	0.42
1:A:381:ILE:HA	1:A:381:ILE:HD12	1.94	0.42
1:D:427:PHE:CD1	1:D:427:PHE:C	2.93	0.42
1:D:566:ARG:HD3	1:D:587:ILE:HG12	2.00	0.42
1:B:325:ILE:CG2	1:B:326:GLN:N	2.82	0.41
1:C:326:GLN:CG	1:A:326:GLN:HG2	2.48	0.41
1:C:351:ALA:O	1:C:520:PHE:HA	2.20	0.41
1:A:325:ILE:CG2	1:A:326:GLN:N	2.82	0.41
1:B:222:ILE:HB	1:B:223:PRO:HD3	2.02	0.41
1:D:439:LYS:O	1:D:443:GLU:HG2	2.20	0.41
1:D:325:ILE:CG2	1:D:326:GLN:N	2.83	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:427:PHE:C	1:A:427:PHE:CD1	2.94	0.41
1:A:394:ASP:HA	6:A:832:HOH:O	2.21	0.41
1:B:482:SER:C	6:B:814:HOH:O	2.59	0.41
1:C:146:TYR:HH	1:B:155:TYR:HH	1.69	0.41
1:C:427:PHE:CD1	1:C:427:PHE:C	2.94	0.41
1:A:180:HIS:O	1:A:184:GLU:HG2	2.20	0.40
1:D:592:THR:OG1	1:D:593:PRO:HD3	2.22	0.40
1:C:296:PHE:HB2	1:C:349:ILE:HG13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	478/514 (93%)	470 (98%)	8 (2%)	0	100	100
1	B	478/514 (93%)	469 (98%)	9 (2%)	0	100	100
1	C	479/514 (93%)	471 (98%)	8 (2%)	0	100	100
1	D	477/514 (93%)	468 (98%)	9 (2%)	0	100	100
All	All	1912/2056 (93%)	1878 (98%)	34 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	428/459 (93%)	416 (97%)	12 (3%)	56	76
1	B	428/459 (93%)	413 (96%)	15 (4%)	48	67
1	C	429/459 (94%)	414 (96%)	15 (4%)	48	67
1	D	427/459 (93%)	410 (96%)	17 (4%)	42	61
All	All	1712/1836 (93%)	1653 (97%)	59 (3%)	48	68

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	113	ASP
1	C	115	MET
1	C	180	HIS
1	C	273	VAL
1	C	277	GLU
1	C	284	LEU
1	C	315	TYR
1	C	342	GLU
1	C	359	LEU
1	C	368	SER
1	C	417	GLU
1	C	467	LYS
1	C	478	LYS
1	C	492	LYS
1	C	535	ASN
1	A	115	MET
1	A	180	HIS
1	A	273	VAL
1	A	277	GLU
1	A	315	TYR
1	A	342	GLU
1	A	359	LEU
1	A	368	SER
1	A	467	LYS
1	A	478	LYS
1	A	492	LYS
1	A	535	ASN
1	D	113	ASP
1	D	115	MET
1	D	180	HIS
1	D	273	VAL
1	D	277	GLU
1	D	315	TYR

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Mol	Chain	Res	Type
1	D	342	GLU
1	D	359	LEU
1	D	368	SER
1	D	467	LYS
1	D	478	LYS
1	D	492	LYS
1	D	522	CYS
1	D	534	LYS
1	D	535	ASN
1	D	587	ILE
1	D	594	GLN
1	B	113	ASP
1	B	115	MET
1	B	180	HIS
1	B	227	PRO
1	B	273	VAL
1	B	277	GLU
1	B	315	TYR
1	B	342	GLU
1	B	359	LEU
1	B	368	SER
1	B	467	LYS
1	B	478	LYS
1	B	492	LYS
1	B	534	LYS
1	B	535	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	235	GLN
1	C	243	HIS
1	C	364	HIS
1	A	235	GLN
1	A	364	HIS
1	D	235	GLN
1	D	364	HIS
1	D	571	GLN
1	D	594	GLN
1	B	235	GLN
1	B	243	HIS
1	B	364	HIS

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 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	DTP	A	701	3	32,32,32	1.49	8 (25%)	50,50,50	1.65	9 (18%)
2	TTP	A	703	3	30,30,30	1.43	4 (13%)	42,47,47	2.01	7 (16%)
4	GTP	A	705	3	34,34,34	1.79	5 (14%)	52,54,54	2.19	16 (30%)
5	DTP	B	701	3	32,32,32	1.60	5 (15%)	50,50,50	1.53	9 (18%)
2	TTP	B	702	3	30,30,30	1.37	3 (10%)	42,47,47	2.20	7 (16%)
4	GTP	B	704	3	34,34,34	1.72	3 (8%)	52,54,54	2.61	12 (23%)
2	TTP	C	701	3	30,30,30	1.25	4 (13%)	42,47,47	2.21	8 (19%)
4	GTP	C	703	3	34,34,34	1.49	6 (17%)	52,54,54	2.86	11 (21%)
5	DTP	C	704	3	32,32,32	1.24	2 (6%)	50,50,50	1.76	6 (12%)
2	TTP	D	702	3	30,30,30	1.42	3 (10%)	42,47,47	1.82	7 (16%)
4	GTP	D	704	3	34,34,34	1.62	6 (17%)	52,54,54	2.62	17 (32%)
5	DTP	D	705	3	32,32,32	1.30	4 (12%)	50,50,50	1.86	10 (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
5	DTP	A	701	3	-	0/20/34/34	0/3/3/3
2	TTP	A	703	3	-	0/19/34/34	0/2/2/2
4	GTP	A	705	3	-	0/22/38/38	0/3/3/3
5	DTP	B	701	3	-	0/20/34/34	0/3/3/3
2	TTP	B	702	3	-	0/19/34/34	0/2/2/2
4	GTP	B	704	3	-	0/22/38/38	0/3/3/3
2	TTP	C	701	3	-	0/19/34/34	0/2/2/2
4	GTP	C	703	3	-	0/22/38/38	0/3/3/3
5	DTP	C	704	3	-	0/20/34/34	0/3/3/3
2	TTP	D	702	3	-	0/19/34/34	0/2/2/2
4	GTP	D	704	3	-	0/22/38/38	0/3/3/3
5	DTP	D	705	3	-	0/20/34/34	0/3/3/3

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	705	GTP	C5-N7	-5.65	1.31	1.38
4	A	705	GTP	C4-N9	-5.53	1.29	1.37
4	B	704	GTP	C4-N9	-5.31	1.30	1.37
4	B	704	GTP	C5-N7	-4.94	1.32	1.38
2	D	702	TTP	C2-N1	4.69	1.43	1.38
5	C	704	DTP	C4-N9	-4.42	1.31	1.37
2	B	702	TTP	C4-C5	4.30	1.51	1.40
5	B	701	DTP	C4-N9	-4.29	1.31	1.37
2	B	702	TTP	C2-N1	4.13	1.42	1.38
5	A	701	DTP	C4-N9	-3.95	1.32	1.37
2	A	703	TTP	C4-C5	3.82	1.49	1.40
4	D	704	GTP	C5-N7	-3.78	1.33	1.38
2	D	702	TTP	O2-C2	3.78	1.26	1.21
2	A	703	TTP	C2-N1	3.64	1.42	1.38
5	B	701	DTP	C5-C4	3.63	1.48	1.40
4	C	703	GTP	C6-N1	-3.58	1.31	1.36
2	C	701	TTP	C4-C5	3.55	1.49	1.40
4	D	704	GTP	C2-N2	3.55	1.37	1.32
2	B	702	TTP	O2-C2	3.46	1.26	1.21
5	B	701	DTP	PG-O3B	3.45	1.66	1.60
4	D	704	GTP	C4-N9	-3.34	1.32	1.37
4	C	703	GTP	C4-N9	-3.10	1.33	1.37
5	D	705	DTP	C5-C4	3.05	1.47	1.40
4	D	704	GTP	C2'-C1'	-3.00	1.49	1.53
4	A	705	GTP	O4'-C1'	2.99	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	704	GTP	C6-N1	-2.92	1.32	1.36
5	A	701	DTP	O4'-C4'	-2.92	1.38	1.45
4	B	704	GTP	C5-C4	2.87	1.47	1.40
5	D	705	DTP	PA-O3A	2.87	1.65	1.59
4	A	705	GTP	C8-N9	-2.86	1.32	1.36
4	C	703	GTP	O4'-C1'	2.86	1.44	1.41
4	C	703	GTP	C5-N7	-2.86	1.34	1.38
2	D	702	TTP	C4-C5	2.85	1.47	1.40
5	D	705	DTP	C4-N9	-2.74	1.33	1.37
4	D	704	GTP	C5-C4	2.73	1.46	1.40
5	D	705	DTP	C8-N9	-2.68	1.32	1.36
5	A	701	DTP	O4'-C1'	2.65	1.48	1.42
2	A	703	TTP	O2-C2	2.59	1.25	1.21
5	A	701	DTP	C8-N9	-2.56	1.32	1.36
4	C	703	GTP	C5-C4	2.48	1.46	1.40
5	A	701	DTP	PG-O3B	2.41	1.64	1.60
4	A	705	GTP	C5-C4	2.35	1.45	1.40
5	C	704	DTP	C5-C4	2.31	1.45	1.40
2	C	701	TTP	O2-C2	2.27	1.24	1.21
4	C	703	GTP	C2-N2	2.27	1.35	1.32
2	C	701	TTP	C4-N3	-2.22	1.33	1.36
2	A	703	TTP	PG-O2G	-2.22	1.46	1.54
5	A	701	DTP	PA-O2A	-2.22	1.45	1.55
5	B	701	DTP	PG-O2G	-2.21	1.46	1.54
5	B	701	DTP	PG-O3G	-2.13	1.47	1.54
2	C	701	TTP	PB-O3B	2.06	1.63	1.59
5	A	701	DTP	C2-N1	2.03	1.37	1.33
5	A	701	DTP	C5-C4	2.01	1.45	1.40

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	703	GTP	C6-C5-N7	14.73	136.12	134.14
4	B	704	GTP	C6-C5-N7	13.55	135.97	134.14
4	D	704	GTP	C6-C5-N7	10.64	135.57	134.14
2	B	702	TTP	PB-O3B-PG	-8.34	108.83	131.93
2	C	701	TTP	N3-C2-N1	7.92	122.58	115.97
4	D	704	GTP	C6-N1-C2	7.13	124.22	120.20
2	A	703	TTP	N3-C2-N1	6.83	121.68	115.97
5	C	704	DTP	N3-C2-N1	-6.52	123.15	128.89
5	D	705	DTP	C5-C4-N3	-6.42	119.72	125.98
2	B	702	TTP	PB-O3A-PA	-6.38	114.26	131.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	703	GTP	C5-C4-N3	-6.23	118.89	126.07
4	A	705	GTP	C6-C5-N7	6.16	134.97	134.14
2	A	703	TTP	PB-O3B-PG	-6.04	115.21	131.93
2	B	702	TTP	N3-C2-N1	6.03	121.01	115.97
2	C	701	TTP	C6-N1-C2	-5.69	120.79	122.41
4	C	703	GTP	PA-O3A-PB	-5.55	116.57	131.93
4	D	704	GTP	C5-C4-N3	-5.45	119.79	126.07
2	D	702	TTP	N3-C2-N1	5.39	120.47	115.97
5	B	701	DTP	C5-C4-N3	-5.30	120.81	125.98
4	C	703	GTP	N3-C4-N9	5.23	134.59	126.91
5	D	705	DTP	N3-C4-N9	5.19	134.29	125.39
2	C	701	TTP	PB-O3A-PA	-5.17	117.62	131.93
4	A	705	GTP	N2-C2-N3	-5.11	113.63	120.28
4	B	704	GTP	PA-O3A-PB	-5.09	117.84	131.93
4	A	705	GTP	PA-O3A-PB	-4.96	118.19	131.93
2	D	702	TTP	PB-O3B-PG	-4.90	118.37	131.93
5	A	701	DTP	N3-C4-N9	4.88	133.76	125.39
4	B	704	GTP	C6-N1-C2	4.84	122.94	120.20
2	D	702	TTP	PB-O3A-PA	-4.77	118.71	131.93
2	A	703	TTP	PB-O3A-PA	-4.74	118.80	131.93
5	C	704	DTP	N3-C4-N9	4.72	133.49	125.39
5	A	701	DTP	C5-C4-N3	-4.69	121.41	125.98
5	D	705	DTP	N3-C2-N1	-4.69	124.77	128.89
4	C	703	GTP	C2-N3-C4	4.68	120.91	115.30
4	A	705	GTP	N2-C2-N1	4.64	122.80	117.82
2	C	701	TTP	PB-O3B-PG	-4.63	119.10	131.93
4	D	704	GTP	C3'-C2'-C1'	4.63	108.18	100.92
4	A	705	GTP	C5-C4-N3	-4.58	120.79	126.07
4	B	704	GTP	C5-C4-N3	-4.56	120.81	126.07
2	D	702	TTP	C6-N1-C2	-4.52	121.12	122.41
5	B	701	DTP	N3-C4-N9	4.35	132.86	125.39
5	C	704	DTP	C5-C4-N3	-4.31	121.78	125.98
4	D	704	GTP	PA-O3A-PB	-4.04	120.75	131.93
5	C	704	DTP	C8-N9-C4	3.97	110.18	106.96
2	A	703	TTP	C5-C6-N1	-3.96	118.47	122.02
5	A	701	DTP	C8-N9-C4	3.94	110.16	106.96
2	B	702	TTP	C5-C6-N1	-3.78	118.62	122.02
4	C	703	GTP	O3G-PG-O2G	3.74	121.41	107.38
4	A	705	GTP	C6-N1-C2	3.63	122.25	120.20
5	D	705	DTP	PB-O3B-PG	-3.62	121.90	131.93
4	D	704	GTP	N3-C4-N9	3.55	132.12	126.91
4	D	704	GTP	C2-N3-C4	3.53	119.54	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	704	GTP	PB-O3B-PG	-3.43	122.43	131.93
4	B	704	GTP	N3-C4-N9	3.42	131.93	126.91
4	D	704	GTP	C4-C5-N7	-3.42	106.11	109.41
5	A	701	DTP	N3-C2-N1	-3.41	125.89	128.89
2	D	702	TTP	C5-C6-N1	-3.35	119.01	122.02
5	B	701	DTP	O3G-PG-O1G	3.33	121.24	110.36
2	C	701	TTP	C5-C6-N1	-3.31	119.05	122.02
4	A	705	GTP	N3-C4-N9	3.26	131.69	126.91
5	D	705	DTP	O3G-PG-O2G	3.25	119.58	107.38
4	A	705	GTP	O2'-C2'-C1'	-3.24	101.24	111.49
4	D	704	GTP	O4'-C1'-C2'	-3.20	102.03	106.69
4	C	703	GTP	PB-O3B-PG	-3.20	123.08	131.93
4	D	704	GTP	C4'-O4'-C1'	3.17	113.20	109.72
4	C	703	GTP	C6-N1-C2	3.16	121.98	120.20
4	C	703	GTP	C3'-C2'-C1'	3.15	105.87	100.92
4	B	704	GTP	C4-C5-N7	-3.14	106.37	109.41
5	A	701	DTP	PB-O3B-PG	-3.09	123.39	131.93
2	A	703	TTP	C4-N3-C2	-3.07	119.08	125.39
4	B	704	GTP	O3G-PG-O2G	3.03	118.76	107.38
4	B	704	GTP	C3'-C2'-C1'	3.00	105.63	100.92
4	D	704	GTP	O5'-PA-O1A	-2.98	97.71	109.37
4	A	705	GTP	C4-C5-N7	-2.96	106.55	109.41
4	B	704	GTP	C2-N3-C4	2.95	118.84	115.30
2	C	701	TTP	C4-N3-C2	-2.92	119.40	125.39
5	C	704	DTP	O3G-PG-O1G	2.90	119.85	110.36
4	A	705	GTP	C3'-C2'-C1'	2.89	105.46	100.92
4	B	704	GTP	N2-C2-N3	-2.85	116.57	120.28
4	D	704	GTP	PB-O3B-PG	-2.85	124.05	131.93
5	B	701	DTP	O4'-C1'-N9	-2.84	102.54	107.66
4	A	705	GTP	O3G-PG-O1G	2.84	119.64	110.36
4	C	703	GTP	O2'-C2'-C1'	-2.80	102.63	111.49
4	B	704	GTP	O2'-C2'-C1'	-2.75	102.79	111.49
5	A	701	DTP	O3G-PG-O2G	2.75	117.68	107.38
5	D	705	DTP	C4-C5-N7	-2.74	106.76	109.41
4	D	704	GTP	O3A-PB-O3B	-2.69	96.20	101.66
5	D	705	DTP	PA-O3A-PB	-2.64	124.63	131.93
2	B	702	TTP	C4-N3-C2	-2.63	120.00	125.39
5	B	701	DTP	PB-O3B-PG	-2.54	124.90	131.93
2	B	702	TTP	O4'-C1'-N1	2.52	112.19	107.66
2	C	701	TTP	O4'-C1'-N1	2.50	112.16	107.66
2	D	702	TTP	C4-N3-C2	-2.49	120.28	125.39
5	B	701	DTP	N3-C2-N1	-2.49	126.70	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	TTP	O3G-PG-O2G	2.46	116.62	107.38
4	A	705	GTP	O2B-PB-O1B	2.43	125.58	112.14
4	A	705	GTP	C2-N3-C4	2.40	118.18	115.30
5	B	701	DTP	O3A-PA-O5'	-2.39	96.59	102.91
5	A	701	DTP	N6-C6-N1	2.37	124.14	119.11
2	A	703	TTP	C6-N1-C2	-2.36	121.73	122.41
4	A	705	GTP	O5'-PA-O1A	-2.35	100.17	109.37
4	A	705	GTP	O2G-PG-O3B	2.33	116.19	105.14
5	D	705	DTP	C8-N9-C4	2.33	108.85	106.96
2	D	702	TTP	O3G-PG-O2G	2.31	116.03	107.38
5	D	705	DTP	O2A-PA-O3A	2.30	116.07	105.14
4	D	704	GTP	O2G-PG-O3B	2.30	116.06	105.14
5	A	701	DTP	C2'-C3'-C4'	2.29	107.82	102.73
4	A	705	GTP	O3B-PG-O1G	-2.27	94.89	110.43
5	C	704	DTP	C2-N3-C4	2.24	119.73	113.27
4	D	704	GTP	O3B-PG-O1G	-2.20	95.34	110.43
4	D	704	GTP	O4'-C4'-C3'	-2.19	100.70	105.16
2	C	701	TTP	O3G-PG-O2G	2.14	115.41	107.38
4	C	703	GTP	C4-C5-N7	-2.14	107.34	109.41
5	B	701	DTP	C4-C5-N7	-2.13	107.35	109.41
5	B	701	DTP	C2'-C3'-C4'	2.10	107.40	102.73
2	A	703	TTP	O3G-PG-O2G	2.07	115.16	107.38
5	A	701	DTP	O3B-PG-O1G	-2.02	96.57	110.43
4	D	704	GTP	O3G-PG-O1G	2.01	116.94	110.36
5	D	705	DTP	C2-N3-C4	2.00	119.04	113.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	480/514 (93%)	0.90	70 (14%) 3 3	31, 73, 120, 159	0
1	B	481/514 (93%)	1.52	117 (24%) 1 1	40, 94, 159, 200	0
1	C	481/514 (93%)	0.55	32 (6%) 17 19	33, 63, 106, 136	0
1	D	480/514 (93%)	0.86	65 (13%) 4 4	34, 74, 119, 155	0
All	All	1922/2056 (93%)	0.96	284 (14%) 3 3	31, 75, 134, 200	0

All (284) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	493	LEU	10.1
1	D	488	LEU	9.9
1	A	488	LEU	9.7
1	B	480	VAL	9.1
1	B	485	PRO	9.0
1	B	573	CYS	8.7
1	B	488	LEU	8.1
1	A	487	VAL	8.0
1	B	484	LYS	7.8
1	A	491	VAL	7.5
1	B	498	PHE	7.4
1	B	276	LEU	7.2
1	B	592	THR	7.1
1	B	230	LYS	7.1
1	B	562	LEU	7.1
1	B	563	TYR	7.0
1	A	489	LEU	6.9
1	B	481	ALA	6.8
1	D	540	LEU	6.8
1	B	345	ASN	6.6
1	A	490	ASP	6.5

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Mol	Chain	Res	Type	RSRZ
1	B	578	PHE	6.4
1	D	466	ILE	6.4
1	B	489	LEU	6.4
1	B	347	LEU	6.2
1	D	590	LEU	6.2
1	B	478	LYS	6.1
1	D	490	ASP	6.0
1	A	284	LEU	5.8
1	D	491	VAL	5.8
1	B	591	ILE	5.6
1	B	569	PHE	5.5
1	A	493	LEU	5.5
1	B	396	TYR	5.5
1	B	476	LEU	5.4
1	B	554	CYS	5.4
1	B	492	LYS	5.4
1	B	596	LYS	5.4
1	A	286	PRO	5.3
1	D	489	LEU	5.3
1	D	493	LEU	5.3
1	B	288	LYS	5.2
1	B	572	TRP	5.0
1	A	486	LYS	5.0
1	D	543	GLU	5.0
1	B	469	LYS	5.0
1	B	491	VAL	4.9
1	B	590	LEU	4.9
1	B	570	VAL	4.8
1	B	341	CYS	4.7
1	A	492	LYS	4.6
1	B	486	LYS	4.6
1	B	467	LYS	4.6
1	A	568	TYR	4.5
1	B	568	TYR	4.4
1	A	562	LEU	4.3
1	B	487	VAL	4.3
1	D	598	TRP	4.3
1	B	397	ILE	4.3
1	B	457	VAL	4.2
1	D	556	LYS	4.2
1	A	484	LYS	4.1
1	B	274	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	486	LYS	4.1
1	B	511	GLU	4.1
1	B	285	TRP	4.0
1	A	563	TYR	4.0
1	B	350	CYS	4.0
1	D	492	LYS	4.0
1	D	557	VAL	3.9
1	B	266	CYS	3.9
1	C	113	ASP	3.9
1	B	277	GLU	3.8
1	D	465	GLN	3.8
1	D	559	ARG	3.8
1	A	345	ASN	3.7
1	D	596	LYS	3.7
1	D	589	PRO	3.7
1	B	328	ASN	3.6
1	C	265	ILE	3.5
1	C	201	ILE	3.5
1	A	466	ILE	3.5
1	B	557	VAL	3.5
1	A	575	ASP	3.4
1	B	577	ASN	3.4
1	B	528	ARG	3.4
1	B	287	TYR	3.4
1	B	545	PHE	3.4
1	C	492	LYS	3.4
1	B	413	ILE	3.4
1	A	285	TRP	3.3
1	B	470	ARG	3.3
1	B	526	PRO	3.3
1	B	275	PRO	3.3
1	A	494	LYS	3.3
1	A	593	PRO	3.3
1	D	320	CYS	3.3
1	D	317	ALA	3.3
1	B	231	TRP	3.2
1	A	473	TYR	3.2
1	B	584	GLY	3.2
1	D	563	TYR	3.2
1	C	404	GLY	3.2
1	B	543	GLU	3.2
1	B	292	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	472	ASP	3.2
1	D	288	LYS	3.2
1	B	473	TYR	3.2
1	A	571	GLN	3.1
1	D	276	LEU	3.1
1	D	485	PRO	3.1
1	B	440	ASP	3.1
1	A	221	PHE	3.1
1	D	229	VAL	3.1
1	A	276	LEU	3.1
1	D	498	PHE	3.1
1	C	262	GLU	3.1
1	A	263	GLU	3.0
1	D	325	ILE	3.0
1	A	592	THR	3.0
1	A	265	ILE	3.0
1	D	545	PHE	3.0
1	A	320	CYS	3.0
1	D	263	GLU	3.0
1	A	463	THR	3.0
1	A	594	GLN	3.0
1	A	468	ILE	2.9
1	A	437	LYS	2.9
1	D	568	TYR	2.9
1	D	594	GLN	2.9
1	B	496	GLU	2.9
1	D	484	LYS	2.9
1	A	287	TYR	2.9
1	B	273	VAL	2.9
1	C	263	GLU	2.8
1	B	548	GLN	2.8
1	C	241	PHE	2.8
1	B	326	GLN	2.8
1	D	121	PRO	2.8
1	A	464	GLY	2.8
1	B	475	SER	2.8
1	A	322	HIS	2.8
1	D	322	HIS	2.8
1	B	348	ARG	2.8
1	D	572	TRP	2.8
1	C	293	ASN	2.8
1	D	230	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	494	LYS	2.8
1	B	599	ASN	2.7
1	A	483	ALA	2.7
1	B	500	VAL	2.7
1	B	224	LEU	2.7
1	B	549	LEU	2.7
1	A	296	PHE	2.7
1	A	288	LYS	2.7
1	D	323	LEU	2.7
1	D	471	GLU	2.7
1	B	327	ASN	2.7
1	D	487	VAL	2.7
1	A	476	LEU	2.7
1	A	599	ASN	2.7
1	D	327	ASN	2.7
1	D	122	ILE	2.7
1	C	235	GLN	2.6
1	B	242	GLU	2.6
1	A	325	ILE	2.6
1	A	590	LEU	2.6
1	D	224	LEU	2.6
1	D	262	GLU	2.6
1	D	462	PRO	2.6
1	D	397	ILE	2.6
1	D	584	GLY	2.6
1	B	490	ASP	2.6
1	B	406	LYS	2.6
1	C	325	ILE	2.6
1	C	285	TRP	2.6
1	C	490	ASP	2.6
1	C	276	LEU	2.6
1	C	242	GLU	2.5
1	D	595	LYS	2.5
1	D	328	ASN	2.5
1	B	438	LEU	2.5
1	C	251	LYS	2.5
1	A	598	TRP	2.5
1	B	391	LEU	2.5
1	A	469	LYS	2.5
1	A	293	ASN	2.5
1	B	581	PRO	2.5
1	B	262	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	511[A]	GLU	2.4
1	A	573	CYS	2.4
1	A	121	PRO	2.4
1	D	255	GLU	2.4
1	C	124	GLY	2.4
1	D	324	GLY	2.4
1	B	468	ILE	2.4
1	D	562	LEU	2.4
1	A	560	LYS	2.4
1	B	229	VAL	2.4
1	C	245	ILE	2.4
1	B	530	ILE	2.4
1	B	587	ILE	2.4
1	A	498	PHE	2.4
1	D	578	PHE	2.4
1	A	324	GLY	2.3
1	B	388	ASP	2.3
1	B	343	VAL	2.3
1	D	113	ASP	2.3
1	D	360	TYR	2.3
1	A	321	HIS	2.3
1	B	122	ILE	2.3
1	B	272	ILE	2.3
1	D	326	GLN	2.3
1	C	255	GLU	2.3
1	C	250	ILE	2.3
1	B	556	LYS	2.3
1	C	328	ASN	2.3
1	B	322	HIS	2.3
1	B	185	LYS	2.3
1	A	326	GLN	2.3
1	A	122	ILE	2.3
1	D	316	PHE	2.3
1	D	321	HIS	2.3
1	C	287	TYR	2.2
1	B	531	ARG	2.2
1	C	260	ILE	2.2
1	B	499	ILE	2.2
1	C	465	GLN	2.2
1	B	398	GLU	2.2
1	B	594	GLN	2.2
1	A	587	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	409	ILE	2.2
1	C	121	PRO	2.2
1	A	150	LEU	2.2
1	B	393	ALA	2.2
1	A	179	VAL	2.2
1	A	472	ASP	2.2
1	B	552	VAL	2.2
1	D	277	GLU	2.2
1	D	593	PRO	2.2
1	B	405	LYS	2.2
1	C	345	ASN	2.2
1	A	262	GLU	2.2
1	D	580	LYS	2.2
1	B	304	LYS	2.2
1	D	161	SER	2.2
1	A	292	GLU	2.1
1	B	290	ARG	2.1
1	C	414	ASP	2.1
1	C	332	LYS	2.1
1	D	528	ARG	2.1
1	C	320	CYS	2.1
1	A	159	GLY	2.1
1	A	409	ILE	2.1
1	A	485	PRO	2.1
1	A	591	ILE	2.1
1	D	228	GLU	2.1
1	C	257	TYR	2.1
1	B	349	ILE	2.1
1	D	198	CYS	2.1
1	B	559	ARG	2.1
1	B	571	GLN	2.1
1	B	574	ALA	2.1
1	B	238	VAL	2.1
1	A	242	GLU	2.1
1	B	544	LYS	2.1
1	A	396	TYR	2.1
1	B	298	TYR	2.1
1	B	390	PHE	2.1
1	B	441	ALA	2.1
1	A	443	GLU	2.1
1	C	252	PRO	2.1
1	B	222	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	557	VAL	2.0
1	A	495	ALA	2.0
1	B	483	ALA	2.0
1	B	508	GLY	2.0
1	B	510	GLN	2.0
1	C	288	LYS	2.0
1	B	466	ILE	2.0
1	A	471	GLU	2.0
1	B	474	GLU	2.0
1	A	327	ASN	2.0
1	B	340	VAL	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
3	MG	C	702	1/1	0.27	6.20	77,77,77,77	0
3	MG	D	703	1/1	0.33	6.17	85,85,85,85	0
3	MG	A	704	1/1	0.22	3.87	85,85,85,85	0
3	MG	B	703	1/1	0.28	3.47	92,92,92,92	0
2	TTP	B	702	29/29	0.17	0.43	77,86,112,129	0
4	GTP	B	704	32/32	0.17	-0.04	54,64,80,83	0
5	DTP	A	701	30/30	0.17	-0.06	31,35,41,44	0
2	TTP	D	702	29/29	0.16	-0.20	48,65,100,100	0
2	TTP	C	701	29/29	0.15	-0.20	40,56,96,101	0
4	GTP	C	703	32/32	0.15	-0.28	36,41,47,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	DTP	B	701	30/30	0.17	-0.30	43,49,60,61	0
5	DTP	D	705	30/30	0.18	-0.31	49,57,69,74	0
2	TTP	A	703	29/29	0.15	-0.41	50,66,100,108	0
4	GTP	D	704	32/32	0.14	-0.77	44,54,68,71	0
4	GTP	A	705	32/32	0.14	-0.80	38,45,53,54	0
5	DTP	C	704	30/30	0.15	-0.89	31,42,52,53	0
3	MG	C	705	1/1	0.16	-1.00	77,77,77,77	0
3	MG	A	702	1/1	0.12	-2.13	54,54,54,54	0
3	MG	D	701	1/1	0.15	-3.50	52,52,52,52	0
3	MG	A	706	1/1	0.12	-5.32	76,76,76,76	0

6.5 Other polymers ⓘ

There are no such residues in this entry.