



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:57 PM GMT

PDB ID : 4QG4  
Title : Crystal structure of the tetrameric GTP/dATP/ATP-bound SAMHD1 (H210A) mutant catalytic core  
Authors : Koharudin, L.M.I.; Wu, Y.; DeLucia, M.; Mehrens, J.; Gronenborn, A.M.; Ahn, J.  
Deposited on : 2014-05-22  
Resolution : 2.10 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.

---

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

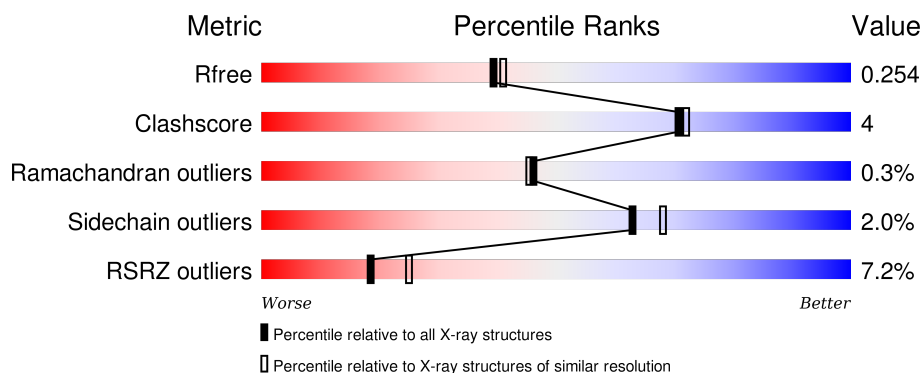
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	550	<div> <div>7%</div> <div>78% 9% 13%</div> </div>
1	B	550	<div> <div>7%</div> <div>78% 9% 13%</div> </div>
1	C	550	<div> <div>7%</div> <div>75% 11% 13%</div> </div>
1	D	550	<div> <div>4%</div> <div>79% 7% 13%</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 16631 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	3	0
			3952	2527	685	720	20			
1	B	481	Total	C	N	O	S	0	2	0
			3946	2525	685	716	20			
1	C	481	Total	C	N	O	S	0	2	0
			3946	2525	685	716	20			
1	D	481	Total	C	N	O	S	0	4	0
			3962	2533	688	721	20			

There are 148 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
A	78	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
A	79	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
A	80	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
A	81	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
A	82	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
A	83	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
A	84	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
A	85	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
A	86	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
A	87	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
A	88	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
A	89	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
A	90	LEU	-	EXPRESSION TAG	UNP Q9Y3Z3
A	91	VAL	-	EXPRESSION TAG	UNP Q9Y3Z3
A	92	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
A	93	ARG	-	EXPRESSION TAG	UNP Q9Y3Z3
A	94	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
A	95	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
A	96	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
A	97	MET	-	EXPRESSION TAG	UNP Q9Y3Z3

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	ALA	-	EXPRESSION TAG	UNP Q9Y3Z3
A	99	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
A	100	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
A	101	THR	-	EXPRESSION TAG	UNP Q9Y3Z3
A	102	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
A	103	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
A	104	GLN	-	EXPRESSION TAG	UNP Q9Y3Z3
A	105	GLN	-	EXPRESSION TAG	UNP Q9Y3Z3
A	106	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
A	107	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
A	108	ARG	-	EXPRESSION TAG	UNP Q9Y3Z3
A	109	ASP	-	EXPRESSION TAG	UNP Q9Y3Z3
A	110	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
A	111	ASN	-	EXPRESSION TAG	UNP Q9Y3Z3
A	112	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
A	210	ALA	HIS	ENGINEERED MUTATION	UNP Q9Y3Z3
B	77	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
B	78	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
B	79	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
B	80	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
B	81	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
B	82	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
B	83	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
B	84	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
B	85	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
B	86	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
B	87	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
B	88	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
B	89	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
B	90	LEU	-	EXPRESSION TAG	UNP Q9Y3Z3
B	91	VAL	-	EXPRESSION TAG	UNP Q9Y3Z3
B	92	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
B	93	ARG	-	EXPRESSION TAG	UNP Q9Y3Z3
B	94	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
B	95	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
B	96	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
B	97	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
B	98	ALA	-	EXPRESSION TAG	UNP Q9Y3Z3
B	99	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
B	100	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
B	101	THR	-	EXPRESSION TAG	UNP Q9Y3Z3
B	102	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	103	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
B	104	GLN	-	EXPRESSION TAG	UNP Q9Y3Z3
B	105	GLN	-	EXPRESSION TAG	UNP Q9Y3Z3
B	106	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
B	107	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
B	108	ARG	-	EXPRESSION TAG	UNP Q9Y3Z3
B	109	ASP	-	EXPRESSION TAG	UNP Q9Y3Z3
B	110	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
B	111	ASN	-	EXPRESSION TAG	UNP Q9Y3Z3
B	112	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
B	210	ALA	HIS	ENGINEERED MUTATION	UNP Q9Y3Z3
C	77	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
C	78	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
C	79	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
C	80	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
C	81	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
C	82	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
C	83	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
C	84	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
C	85	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
C	86	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
C	87	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
C	88	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
C	89	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
C	90	LEU	-	EXPRESSION TAG	UNP Q9Y3Z3
C	91	VAL	-	EXPRESSION TAG	UNP Q9Y3Z3
C	92	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
C	93	ARG	-	EXPRESSION TAG	UNP Q9Y3Z3
C	94	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
C	95	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
C	96	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
C	97	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
C	98	ALA	-	EXPRESSION TAG	UNP Q9Y3Z3
C	99	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
C	100	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
C	101	THR	-	EXPRESSION TAG	UNP Q9Y3Z3
C	102	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
C	103	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
C	104	GLN	-	EXPRESSION TAG	UNP Q9Y3Z3
C	105	GLN	-	EXPRESSION TAG	UNP Q9Y3Z3
C	106	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
C	107	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3

*Continued on next page...*

*Continued from previous page...*

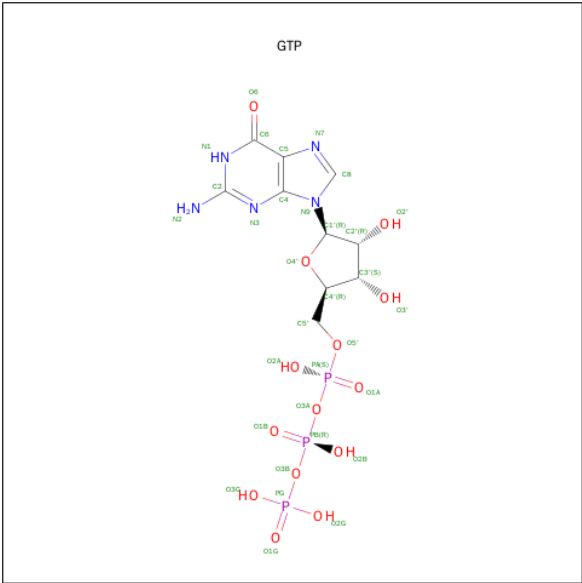
Chain	Residue	Modelled	Actual	Comment	Reference
C	108	ARG	-	EXPRESSION TAG	UNP Q9Y3Z3
C	109	ASP	-	EXPRESSION TAG	UNP Q9Y3Z3
C	110	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
C	111	ASN	-	EXPRESSION TAG	UNP Q9Y3Z3
C	112	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
C	210	ALA	HIS	ENGINEERED MUTATION	UNP Q9Y3Z3
D	77	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
D	78	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
D	79	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
D	80	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
D	81	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
D	82	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
D	83	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
D	84	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
D	85	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
D	86	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
D	87	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
D	88	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
D	89	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
D	90	LEU	-	EXPRESSION TAG	UNP Q9Y3Z3
D	91	VAL	-	EXPRESSION TAG	UNP Q9Y3Z3
D	92	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
D	93	ARG	-	EXPRESSION TAG	UNP Q9Y3Z3
D	94	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
D	95	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
D	96	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
D	97	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
D	98	ALA	-	EXPRESSION TAG	UNP Q9Y3Z3
D	99	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
D	100	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
D	101	THR	-	EXPRESSION TAG	UNP Q9Y3Z3
D	102	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
D	103	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
D	104	GLN	-	EXPRESSION TAG	UNP Q9Y3Z3
D	105	GLN	-	EXPRESSION TAG	UNP Q9Y3Z3
D	106	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
D	107	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
D	108	ARG	-	EXPRESSION TAG	UNP Q9Y3Z3
D	109	ASP	-	EXPRESSION TAG	UNP Q9Y3Z3
D	110	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
D	111	ASN	-	EXPRESSION TAG	UNP Q9Y3Z3
D	112	SER	-	EXPRESSION TAG	UNP Q9Y3Z3

*Continued on next page...*

Continued from previous page...

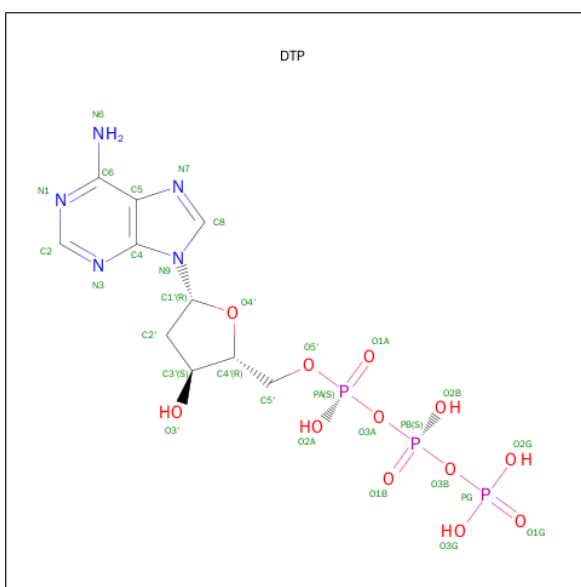
Chain	Residue	Modelled	Actual	Comment	Reference
D	210	ALA	HIS	ENGINEERED MUTATION	UNP Q9Y3Z3

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



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

- Molecule 3 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



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

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

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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		

*Continued on next page...*



*Continued from previous page...*

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

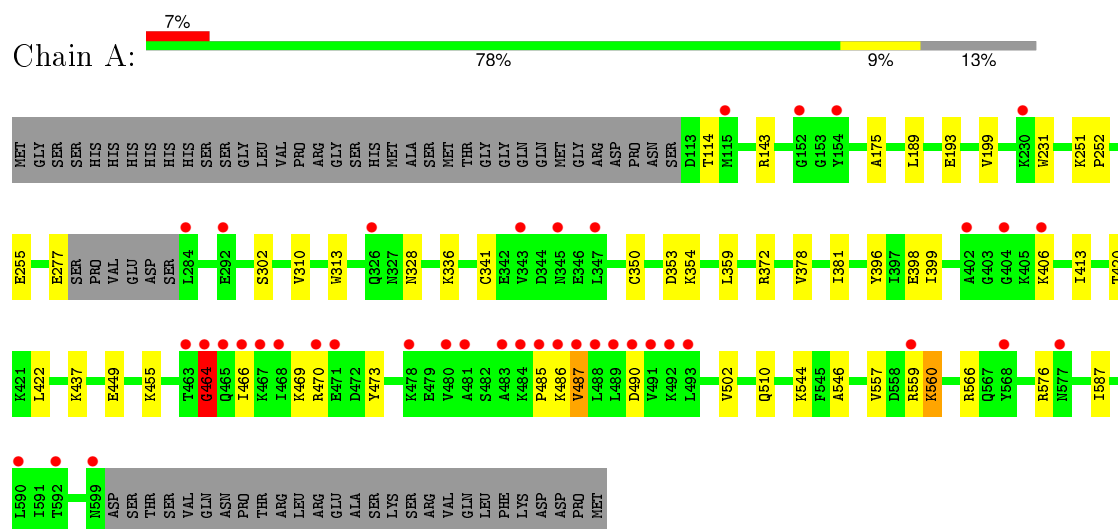
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	127	Total 127	O 127	0	0
6	B	173	Total 173	O 173	0	0
6	C	112	Total 112	O 112	0	0
6	D	157	Total 157	O 157	0	0

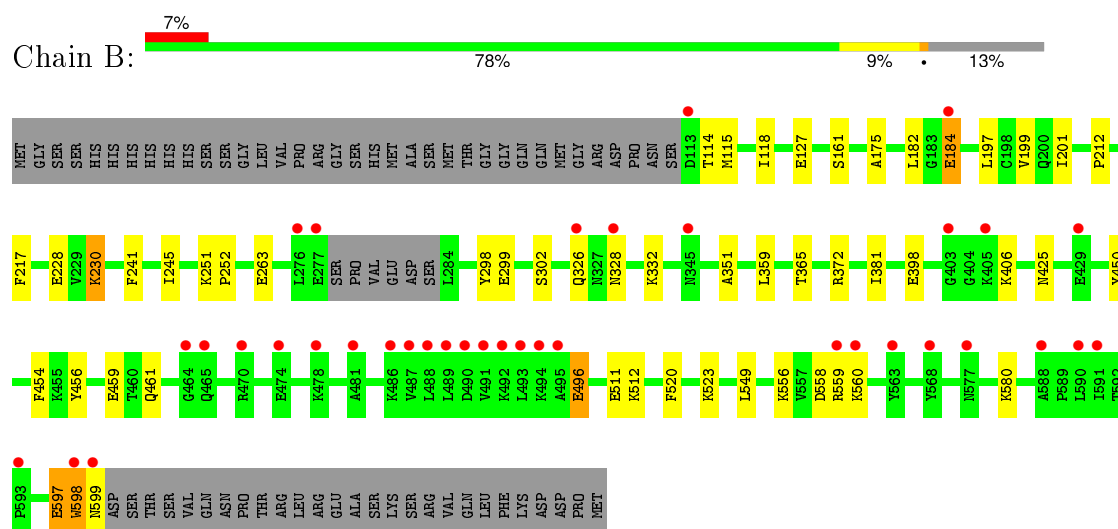
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

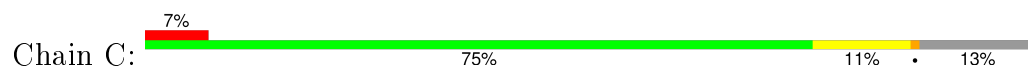
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

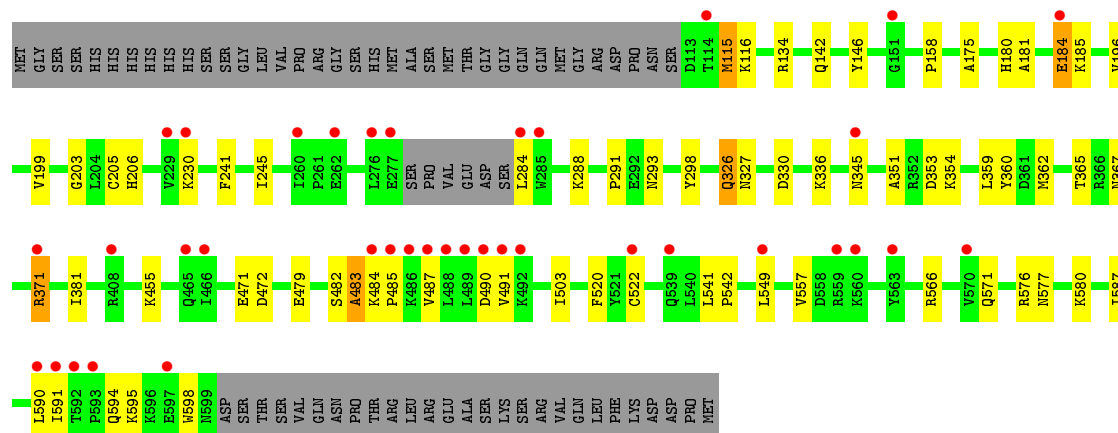


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

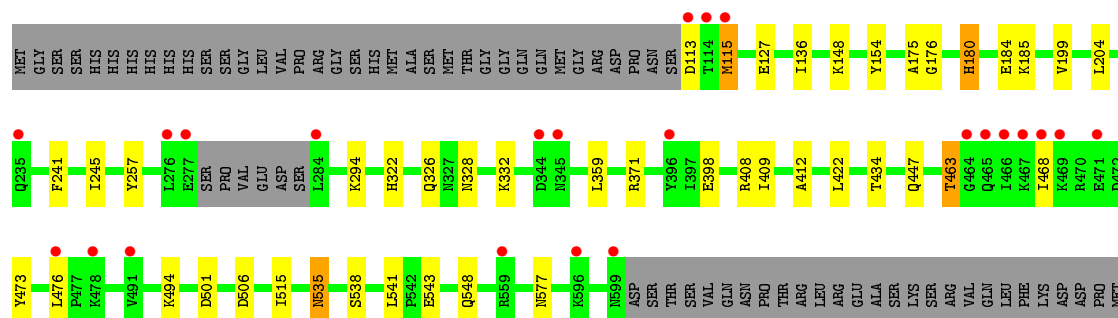
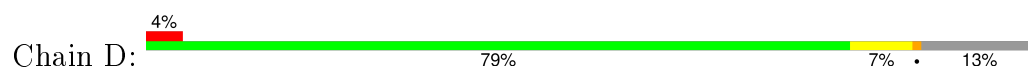


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.80Å 147.12Å 99.21Å 90.00° 114.00° 90.00°	Depositor
Resolution (Å)	41.74 – 2.10 41.74 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.74-2.10) 99.9 (41.74-2.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.223 , 0.245 0.237 , 0.254	Depositor DCC
$R_{free}$ test set	1999 reflections (1.52%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.9	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 43.7	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.38$	Xtriage
Outliers	0 of 133622 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16631	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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, ZN, DTP, MG

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	0.40	0/4044	0.57	1/5460 (0.0%)
1	B	0.41	0/4039	0.57	0/5453
1	C	0.38	0/4039	0.58	0/5453
1	D	0.42	0/4055	0.56	0/5475
All	All	0.40	0/16177	0.57	1/21841 (0.0%)

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	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	464	GLY	N-CA-C	5.32	126.40	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	205	CYS	Mainchain

## 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	3952	0	3924	31	0
1	B	3946	0	3922	35	0
1	C	3946	0	3922	42	0
1	D	3962	0	3930	31	0
2	A	64	0	23	1	0
2	B	64	0	23	3	0
3	A	30	0	12	0	0
3	B	30	0	12	0	0
3	C	30	0	12	1	0
3	D	30	0	12	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	127	0	0	6	0
6	B	173	0	0	13	0
6	C	112	0	0	8	0
6	D	157	0	0	12	0
All	All	16631	0	15792	140	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 (140) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ARG:NH1	6:A:856:HOH:O	1.96	0.98
2:B:701:GTP:O3G	6:B:922:HOH:O	1.88	0.90
1:B:450:TYR:OH	6:B:886:HOH:O	1.89	0.88
6:B:922:HOH:O	3:D:701:DTP:O1G	1.93	0.85
1:A:328:ASN:HA	1:C:326:GLN:HG2	1.58	0.85

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:GLU:OE2	6:B:926:HOH:O	1.96	0.82
1:A:277:GLU:O	6:A:895:HOH:O	1.99	0.78
1:D:468:ILE:HD11	1:D:476:LEU:HD11	1.67	0.77
1:D:322:HIS:NE2	6:D:866:HOH:O	2.19	0.75
1:C:206:HIS:O	6:C:896:HOH:O	2.03	0.75
1:C:142:GLN:OE1	6:C:846:HOH:O	2.06	0.73
1:D:506:ASP:OD1	6:D:920:HOH:O	2.06	0.73
1:B:299:GLU:OE2	6:B:897:HOH:O	2.06	0.73
1:C:577:ASN:OD1	1:C:595:LYS:NZ	2.21	0.72
1:D:113:ASP:O	6:D:921:HOH:O	2.08	0.71
6:B:922:HOH:O	3:D:701:DTP:O2B	2.09	0.70
1:D:326:GLN:NE2	6:D:953:HOH:O	2.24	0.70
1:D:175:ALA:HB1	1:D:199:VAL:HG12	1.74	0.69
1:C:479:GLU:OE1	1:C:576:ARG:NH1	2.26	0.69
1:D:408:ARG:NH1	6:D:954:HOH:O	2.25	0.69
1:C:485:PRO:HA	1:C:571:GLN:HE21	1.59	0.68
1:D:473:TYR:OH	6:D:883:HOH:O	2.12	0.68
1:C:336:LYS:HE3	1:D:127:GLU:HG3	1.75	0.68
1:A:302:SER:O	6:A:843:HOH:O	2.13	0.67
1:D:257:TYR:OH	6:D:921:HOH:O	2.12	0.67
1:C:371:ARG:HH11	1:C:371:ARG:HB3	1.62	0.65
1:B:118:ILE:HD11	1:C:158:PRO:HG3	1.79	0.64
1:A:490:ASP:N	1:A:490:ASP:OD1	2.30	0.63
1:B:184:GLU:N	1:B:184:GLU:OE1	2.33	0.62
1:C:487:VAL:HG23	1:C:590:LEU:HD12	1.80	0.61
1:A:455:LYS:HG2	1:A:557:VAL:HG12	1.82	0.61
1:B:597:GLU:O	1:B:599:ASN:N	2.28	0.60
1:A:470:ARG:HD3	1:A:473:TYR:CE2	2.36	0.60
1:C:298:TYR:O	6:C:829:HOH:O	2.17	0.59
1:B:175:ALA:HB1	1:B:199:VAL:HG12	1.83	0.59
1:B:372:ARG:NH1	6:B:881:HOH:O	2.34	0.59
1:B:161:SER:OG	6:B:900:HOH:O	2.17	0.59
1:C:175:ALA:HB1	1:C:199:VAL:HG12	1.85	0.58
1:B:398:GLU:CD	1:B:406:LYS:HD2	2.25	0.57
1:C:580:LYS:HD3	1:C:598:TRP:HB3	1.87	0.57
1:C:367:ASN:OD1	1:C:371:ARG:NH2	2.30	0.56
1:C:327:ASN:HA	6:C:891:HOH:O	2.04	0.56
1:C:181:ALA:HA	1:C:184:GLU:OE1	2.04	0.56
1:D:543:GLU:N	1:D:543:GLU:OE1	2.32	0.56
2:B:701:GTP:O2B	6:B:922:HOH:O	2.18	0.56
1:B:328:ASN:OD1	1:B:365:THR:OG1	2.16	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ALA:HB1	1:A:199:VAL:HG12	1.88	0.55
1:A:252:PRO:HA	1:A:255:GLU:HG2	1.89	0.55
1:C:360:TYR:OH	6:C:912:HOH:O	1.84	0.53
1:C:566:ARG:HD3	1:C:587:ILE:HB	1.91	0.53
1:D:535:ASN:OD1	1:D:535:ASN:N	2.32	0.52
1:C:455:LYS:HG2	1:C:557:VAL:HG12	1.92	0.52
1:D:332:LYS:HG3	6:D:907:HOH:O	2.11	0.51
1:A:464:GLY:O	1:A:544:LYS:NZ	2.43	0.51
1:A:566:ARG:HD3	1:A:587:ILE:HB	1.93	0.51
1:C:115:MET:HG2	1:C:116:LYS:N	2.25	0.51
1:D:468:ILE:HG22	1:D:548:GLN:OE1	2.11	0.51
1:A:341:CYS:SG	1:A:350:CYS:SG	3.04	0.51
1:B:425:ASN:OD1	6:B:865:HOH:O	2.19	0.50
1:A:510:GLN:O	1:A:546:ALA:HB2	2.12	0.50
1:C:134:ARG:HD2	6:C:869:HOH:O	2.10	0.50
1:C:482:SER:OG	1:C:483:ALA:N	2.44	0.49
1:A:490:ASP:OD2	1:A:560:LYS:HG2	2.13	0.49
1:C:146:TYR:OH	6:C:832:HOH:O	2.11	0.49
1:D:468:ILE:CD1	1:D:476:LEU:HD11	2.41	0.49
1:A:485:PRO:O	1:A:487:VAL:N	2.47	0.48
1:D:412:ALA:HB3	1:D:422:LEU:HD22	1.96	0.47
1:A:251:LYS:HB2	1:A:252:PRO:HD3	1.95	0.47
1:C:203:GLY:O	1:C:206:HIS:ND1	2.43	0.47
1:B:580:LYS:HB2	1:B:598:TRP:CG	2.49	0.47
1:A:576:ARG:NE	6:A:869:HOH:O	2.04	0.47
1:D:180[A]:HIS:O	1:D:184:GLU:OE1	2.33	0.46
1:B:456:TYR:OH	1:B:459:GLU:HB2	2.14	0.46
1:C:326:GLN:H	1:C:326:GLN:CD	2.19	0.46
1:B:461:GLN:HE21	1:B:549:LEU:CD2	2.28	0.46
1:C:503:ILE:HB	1:C:549:LEU:HB3	1.96	0.46
1:A:353:ASP:OD1	1:A:354:LYS:N	2.47	0.46
2:B:701:GTP:H5''	3:D:701:DTP:O2B	2.16	0.46
1:C:241:PHE:O	1:C:245:ILE:HG12	2.16	0.45
1:B:328:ASN:HB3	1:D:328:ASN:HB2	1.99	0.45
1:D:241:PHE:O	1:D:245:ILE:HG12	2.16	0.45
1:B:556:LYS:HG3	1:B:558:ASP:OD1	2.16	0.45
1:D:115:MET:O	1:D:115:MET:HG3	2.13	0.45
1:C:185:LYS:HD3	1:C:185:LYS:HA	1.82	0.45
1:C:471:GLU:HG2	1:C:472:ASP:OD1	2.16	0.45
1:A:310:VAL:HG12	1:A:313:TRP:CZ3	2.52	0.45
1:B:241:PHE:O	1:B:245:ILE:HG12	2.17	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:GLU:HB3	1:A:406:LYS:HD2	1.99	0.44
1:C:591:ILE:O	1:C:594:GLN:HG2	2.17	0.44
1:B:461:GLN:HE21	1:B:549:LEU:HD21	1.83	0.44
1:B:559:ARG:HH21	1:B:560:LYS:NZ	2.16	0.44
1:B:197:LEU:O	1:B:201:ILE:HG13	2.18	0.44
1:D:371:ARG:NH1	6:D:899:HOH:O	2.50	0.44
1:C:353:ASP:OD1	1:C:354:LYS:N	2.50	0.43
1:C:541:LEU:HB3	1:C:542:PRO:HD2	2.01	0.43
1:B:359:LEU:HA	1:B:359:LEU:HD23	1.81	0.43
1:B:230:LYS:HE3	1:B:230:LYS:HB2	1.76	0.43
1:B:351:ALA:O	1:B:520:PHE:HA	2.19	0.43
1:A:143:ARG:HD2	1:A:420:THR:HA	2.01	0.42
1:A:399:ILE:HD13	1:A:422:LEU:HD13	2.01	0.42
1:A:449:GLU:OE2	6:A:837:HOH:O	2.22	0.42
1:B:298:TYR:O	6:B:948:HOH:O	2.21	0.42
1:A:381:ILE:HA	1:A:381:ILE:HD12	1.89	0.42
1:D:136:ILE:HG13	1:D:204:LEU:HD21	1.99	0.42
1:B:332:LYS:NZ	6:B:883:HOH:O	2.42	0.42
1:B:251:LYS:HB2	1:B:252:PRO:HD3	2.00	0.42
1:D:176:GLY:O	1:D:180[A]:HIS:HB2	2.19	0.42
1:D:359:LEU:HB3	1:D:515:ILE:HD12	2.02	0.42
1:D:398:GLU:OE2	6:D:956:HOH:O	2.21	0.42
1:C:351:ALA:O	1:C:520:PHE:HA	2.20	0.42
1:C:381:ILE:HD12	1:C:381:ILE:HA	1.80	0.41
1:A:336:LYS:HE3	1:B:127:GLU:HG3	2.01	0.41
1:A:396:TYR:CE1	1:A:437:LYS:HD2	2.55	0.41
1:D:148:LYS:HE3	1:D:154:TYR:CD2	2.55	0.41
1:B:556:LYS:HD2	1:B:556:LYS:HA	1.86	0.41
1:D:409:ILE:HG13	6:D:848:HOH:O	2.20	0.41
1:C:484:LYS:O	1:C:484:LYS:HG3	2.20	0.41
1:B:381:ILE:HG12	1:B:454:PHE:HB2	2.03	0.41
1:C:230:LYS:HB2	1:C:230:LYS:HE3	1.84	0.41
1:B:182:LEU:HD23	1:B:182:LEU:HA	1.89	0.41
1:B:302:SER:O	6:B:948:HOH:O	2.21	0.41
1:D:185:LYS:HD2	1:D:185:LYS:HA	1.85	0.41
1:A:310:VAL:HG12	1:A:313:TRP:CE3	2.56	0.41
1:A:378:VAL:O	1:A:381:ILE:HG22	2.21	0.40
1:A:231:TRP:CZ3	1:A:413:ILE:HB	2.55	0.40
2:A:701:GTP:H5''	3:C:701:DTP:O2B	2.22	0.40
1:C:362:MET:O	1:C:365:THR:HB	2.21	0.40
1:A:372:ARG:CZ	6:A:856:HOH:O	2.58	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:ARG:HG3	1:A:560:LYS:N	2.37	0.40
1:C:359:LEU:HA	1:C:359:LEU:HD23	1.72	0.40
1:D:538:SER:HB3	1:D:541:LEU:HG	2.03	0.40
1:B:496:GLU:O	1:B:496:GLU:HG3	2.21	0.40
1:D:463:THR:OG1	1:D:577:ASN:O	2.40	0.40
1:B:212:PRO:HD2	1:B:217:PHE:CD1	2.56	0.40
1:D:294:LYS:NZ	6:D:942:HOH:O	2.26	0.40
1:C:330:ASP:OD2	6:C:830:HOH:O	2.22	0.40
1:C:291:PRO:HG2	1:C:293:ASN:OD1	2.21	0.40
1:C:180[A]:HIS:NE2	1:C:196:VAL:HG11	2.36	0.40
1:C:483:ALA:O	1:C:485:PRO:HD3	2.21	0.40
1:B:511[A]:GLU:OE2	1:B:512:LYS:NZ	2.45	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	480/550 (87%)	467 (97%)	11 (2%)	2 (0%)	39	37
1	B	479/550 (87%)	464 (97%)	13 (3%)	2 (0%)	39	37
1	C	479/550 (87%)	464 (97%)	13 (3%)	2 (0%)	39	37
1	D	481/550 (88%)	470 (98%)	11 (2%)	0	100	100
All	All	1919/2200 (87%)	1865 (97%)	48 (2%)	6 (0%)	46	45

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	464	GLY
1	A	486	LYS
1	B	598	TRP

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	483	ALA
1	B	597	GLU
1	C	490	ASP

### 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	429/487 (88%)	420 (98%)	9 (2%)	61	66
1	B	428/487 (88%)	420 (98%)	8 (2%)	65	70
1	C	428/487 (88%)	419 (98%)	9 (2%)	61	66
1	D	430/487 (88%)	421 (98%)	9 (2%)	61	66
All	All	1715/1948 (88%)	1680 (98%)	35 (2%)	63	68

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	THR
1	A	189	LEU
1	A	193	GLU
1	A	359	LEU
1	A	466	ILE
1	A	469	LYS
1	A	487	VAL
1	A	502	VAL
1	A	560	LYS
1	B	114	THR
1	B	115	MET
1	B	184	GLU
1	B	230	LYS
1	B	263	GLU
1	B	326	GLN
1	B	496	GLU
1	B	523	LYS
1	C	115	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	184	GLU
1	C	284	LEU
1	C	288	LYS
1	C	326	GLN
1	C	345	ASN
1	C	371	ARG
1	C	491	VAL
1	C	522	CYS
1	D	115	MET
1	D	180[A]	HIS
1	D	180[B]	HIS
1	D	434	THR
1	D	447	GLN
1	D	463	THR
1	D	494	LYS
1	D	501	ASP
1	D	535	ASN

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

Mol	Chain	Res	Type
1	A	321	HIS
1	A	322	HIS
1	B	233	HIS
1	B	326	GLN
1	B	461	GLN
1	C	321	HIS
1	C	322	HIS
1	C	571	GLN
1	C	594	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	GTP	A	701	4	25,34,34	2.26	8 (32%)	34,54,54	1.62	6 (17%)
3	DTP	A	702	4	24,32,32	1.28	3 (12%)	32,50,50	2.16	4 (12%)
2	GTP	A	703	4	25,34,34	2.25	7 (28%)	34,54,54	1.75	8 (23%)
2	GTP	B	701	4	25,34,34	2.27	7 (28%)	34,54,54	1.82	9 (26%)
2	GTP	B	702	4	25,34,34	2.26	6 (24%)	34,54,54	1.75	8 (23%)
3	DTP	B	703	4	24,32,32	1.25	5 (20%)	32,50,50	2.20	4 (12%)
3	DTP	C	701	4	24,32,32	1.17	4 (16%)	32,50,50	2.06	6 (18%)
3	DTP	D	701	4	24,32,32	1.30	4 (16%)	32,50,50	2.20	6 (18%)

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	GTP	A	701	4	-	0/18/38/38	0/3/3/3
3	DTP	A	702	4	-	0/18/34/34	0/3/3/3
2	GTP	A	703	4	-	0/18/38/38	0/3/3/3
2	GTP	B	701	4	-	0/18/38/38	0/3/3/3
2	GTP	B	702	4	-	0/18/38/38	0/3/3/3
3	DTP	B	703	4	-	0/18/34/34	0/3/3/3
3	DTP	C	701	4	-	0/18/34/34	0/3/3/3
3	DTP	D	701	4	-	0/18/34/34	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	GTP	O2'-C2'	-2.76	1.36	1.43
3	B	703	DTP	C5'-C4'	-2.62	1.43	1.51
2	B	702	GTP	O2'-C2'	-2.57	1.36	1.43
3	A	702	DTP	O3'-C3'	-2.55	1.37	1.43
3	B	703	DTP	O3'-C3'	-2.46	1.37	1.43
3	D	701	DTP	O3'-C3'	-2.46	1.37	1.43
2	A	703	GTP	O2'-C2'	-2.46	1.37	1.43
2	B	701	GTP	O2'-C2'	-2.42	1.37	1.43
2	B	701	GTP	C2'-C3'	-2.35	1.47	1.53
2	A	701	GTP	C3'-C4'	-2.31	1.46	1.53
3	D	701	DTP	C5'-C4'	-2.29	1.44	1.51
3	A	702	DTP	C5'-C4'	-2.29	1.44	1.51
2	B	702	GTP	C5'-C4'	-2.27	1.44	1.51
3	C	701	DTP	PG-O3G	-2.21	1.46	1.54
2	A	703	GTP	PG-O3G	-2.21	1.46	1.54
2	A	703	GTP	C5'-C4'	-2.21	1.44	1.51
2	A	701	GTP	PG-O3G	-2.21	1.46	1.54
2	B	701	GTP	C3'-C4'	-2.19	1.47	1.53
2	B	702	GTP	C2'-C3'	-2.18	1.47	1.53
3	C	701	DTP	O3'-C3'	-2.17	1.38	1.43
2	A	701	GTP	C5'-C4'	-2.15	1.44	1.51
3	D	701	DTP	PG-O3G	-2.13	1.47	1.54
3	B	703	DTP	PG-O3G	-2.13	1.47	1.54
3	C	701	DTP	C5'-C4'	-2.12	1.44	1.51
3	B	703	DTP	C2'-C3'	-2.11	1.47	1.52
2	A	703	GTP	PG-O2G	-2.09	1.47	1.54
2	B	702	GTP	PG-O2G	-2.08	1.47	1.54
2	A	701	GTP	C2'-C3'	-2.06	1.47	1.53
2	A	701	GTP	PG-O2G	-2.04	1.47	1.54
2	A	703	GTP	C2'-C3'	-2.02	1.47	1.53
2	B	701	GTP	C5'-C4'	-2.01	1.45	1.51
2	B	701	GTP	PG-O2G	-2.00	1.47	1.54
3	B	703	DTP	C6-N6	2.71	1.43	1.34
3	D	701	DTP	C6-N6	2.85	1.43	1.34
3	C	701	DTP	C6-N6	2.85	1.43	1.34
3	A	702	DTP	C6-N6	3.03	1.44	1.34
2	A	703	GTP	C2-N2	6.50	1.47	1.34
2	B	702	GTP	C2-N2	6.54	1.47	1.34
2	A	701	GTP	O6-C6	6.58	1.40	1.24
2	B	701	GTP	C2-N2	6.61	1.47	1.34
2	A	701	GTP	C2-N2	6.71	1.47	1.34
2	B	701	GTP	O6-C6	6.94	1.41	1.24
2	A	703	GTP	O6-C6	6.95	1.41	1.24

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	702	GTP	O6-C6	7.02	1.41	1.24

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	703	DTP	N3-C2-N1	-10.14	121.13	128.89
3	D	701	DTP	N3-C2-N1	-10.11	121.15	128.89
3	A	702	DTP	N3-C2-N1	-9.94	121.28	128.89
3	C	701	DTP	N3-C2-N1	-8.88	122.09	128.89
2	B	702	GTP	C4'-O4'-C1'	-4.71	104.54	109.72
2	B	702	GTP	C5-C6-N1	-4.41	117.56	123.59
2	A	703	GTP	C5-C6-N1	-4.18	117.87	123.59
2	B	701	GTP	C5-C6-N1	-4.12	117.96	123.59
2	A	703	GTP	C4'-O4'-C1'	-4.04	105.28	109.72
2	A	701	GTP	C5-C6-N1	-3.85	118.32	123.59
2	B	701	GTP	C4'-O4'-C1'	-3.74	105.61	109.72
2	B	701	GTP	PA-O3A-PB	-3.65	122.47	132.73
3	D	701	DTP	C4-C5-N7	-3.62	106.15	109.48
2	A	703	GTP	PA-O3A-PB	-3.60	122.62	132.73
3	A	702	DTP	C4-C5-N7	-3.41	106.34	109.48
3	C	701	DTP	C4-C5-N7	-3.37	106.38	109.48
2	A	701	GTP	C4'-O4'-C1'	-3.32	106.08	109.72
2	A	701	GTP	N3-C2-N1	-3.24	122.50	127.44
2	A	701	GTP	PA-O3A-PB	-3.24	123.63	132.73
2	B	702	GTP	PA-O3A-PB	-3.24	123.64	132.73
2	B	701	GTP	N3-C2-N1	-3.01	122.86	127.44
3	B	703	DTP	C4-C5-N7	-2.94	106.77	109.48
2	A	703	GTP	N3-C2-N1	-2.92	123.00	127.44
3	B	703	DTP	PA-O3A-PB	-2.73	125.06	132.73
3	B	703	DTP	C1'-N9-C4	-2.73	122.53	127.16
3	D	701	DTP	PA-O3A-PB	-2.66	125.26	132.73
2	B	701	GTP	C4-C5-N7	-2.58	107.11	109.48
3	A	702	DTP	PB-O3B-PG	-2.56	124.10	132.67
2	B	702	GTP	N3-C2-N1	-2.50	123.64	127.44
2	A	703	GTP	PB-O3B-PG	-2.39	124.65	132.67
3	C	701	DTP	PA-O3A-PB	-2.36	126.10	132.73
2	A	703	GTP	C4-C5-N7	-2.35	107.32	109.48
2	B	701	GTP	C1'-N9-C4	-2.34	123.41	126.94
2	B	702	GTP	PB-O3B-PG	-2.22	125.22	132.67
3	D	701	DTP	C1'-N9-C4	-2.14	123.53	127.16
3	A	702	DTP	C1'-N9-C4	-2.14	123.53	127.16
2	B	702	GTP	C4-C5-N7	-2.13	107.52	109.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	D	701	DTP	PB-O3B-PG	-2.05	125.81	132.67
2	B	702	GTP	O3A-PA-O5'	2.00	108.24	102.94
3	D	701	DTP	C2'-C1'-N9	2.06	119.16	114.16
2	B	701	GTP	O3G-PG-O3B	2.06	114.46	105.09
3	C	701	DTP	O5'-C5'-C4'	2.27	117.48	109.12
2	A	701	GTP	O3A-PA-O5'	2.36	109.19	102.94
3	C	701	DTP	O2B-PB-O3B	2.38	115.88	105.09
2	B	701	GTP	C2'-C1'-N9	2.48	118.08	114.29
3	C	701	DTP	O2A-PA-O3A	2.51	116.46	105.09
2	A	703	GTP	C2'-C1'-N9	3.00	118.87	114.29
2	B	702	GTP	C6-N1-C2	3.03	120.14	115.94
2	A	703	GTP	C6-N1-C2	3.20	120.38	115.94
2	B	701	GTP	C6-N1-C2	3.20	120.38	115.94
2	A	701	GTP	C6-N1-C2	3.44	120.72	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	GTP	1	0
2	B	701	GTP	3	0
3	C	701	DTP	1	0
3	D	701	DTP	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	481/550 (87%)	0.49	41 (8%)	13	18	28, 46, 67, 88	202 (41%)
1	B	481/550 (87%)	0.43	37 (7%)	16	22	26, 43, 67, 78	169 (35%)
1	C	481/550 (87%)	0.55	37 (7%)	16	22	28, 48, 74, 94	161 (33%)
1	D	481/550 (87%)	0.34	23 (4%)	34	43	26, 42, 61, 72	139 (28%)
All	All	1924/2200 (87%)	0.45	138 (7%)	18	25	26, 45, 68, 94	671 (34%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	464	GLY	12.4
1	B	488	LEU	9.2
1	B	489	LEU	6.3
1	A	489	LEU	6.1
1	C	590	LEU	5.4
1	C	276	LEU	5.4
1	A	488	LEU	5.3
1	C	491	VAL	5.3
1	C	489	LEU	5.2
1	B	113	ASP	5.1
1	C	488	LEU	5.1
1	D	276	LEU	5.0
1	A	486	LYS	4.9
1	A	463	THR	4.8
1	A	465	GLN	4.6
1	A	284	LEU	4.6
1	A	466	ILE	4.5
1	A	467	LYS	4.4
1	A	487	VAL	4.4
1	D	277	GLU	4.2
1	D	396	TYR	4.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	491	VAL	4.1
1	C	490	ASP	4.1
1	A	468	ILE	4.0
1	B	591	ILE	4.0
1	B	490	ASP	4.0
1	B	487	VAL	3.9
1	B	491	VAL	3.8
1	C	371	ARG	3.8
1	C	559	ARG	3.7
1	C	487	VAL	3.6
1	A	404	GLY	3.6
1	C	485	PRO	3.6
1	D	284	LEU	3.6
1	C	492	LYS	3.5
1	A	568	TYR	3.5
1	B	478	LYS	3.5
1	D	466	ILE	3.5
1	B	470	ARG	3.4
1	B	599	ASN	3.4
1	B	559	ARG	3.4
1	A	471	GLU	3.3
1	B	277	GLU	3.3
1	A	402	ALA	3.3
1	B	588	ALA	3.3
1	A	484	LYS	3.2
1	C	522	CYS	3.2
1	A	483	ALA	3.1
1	D	464	GLY	3.1
1	B	568	TYR	3.1
1	D	344	ASP	3.1
1	B	403	GLY	3.1
1	A	345	ASN	3.1
1	C	345	ASN	3.0
1	A	481	ALA	3.0
1	C	285	TRP	3.0
1	D	235	GLN	3.0
1	D	599	ASN	3.0
1	D	465	GLN	2.9
1	D	471	GLU	2.9
1	D	113	ASP	2.9
1	B	276	LEU	2.9
1	C	570	VAL	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	470	ARG	2.8
1	C	465	GLN	2.8
1	B	493	LEU	2.8
1	A	559	ARG	2.8
1	C	592	THR	2.8
1	A	490	ASP	2.8
1	C	230	LYS	2.8
1	D	491	VAL	2.8
1	B	465	GLN	2.8
1	C	593	PRO	2.7
1	C	486	LYS	2.7
1	B	492	LYS	2.7
1	C	277	GLU	2.7
1	D	114	THR	2.7
1	A	326	GLN	2.7
1	A	480	VAL	2.7
1	B	481	ALA	2.7
1	B	474	GLU	2.6
1	C	184	GLU	2.6
1	D	115	MET	2.6
1	B	598	TRP	2.6
1	B	326	GLN	2.6
1	B	495	ALA	2.6
1	A	115	MET	2.6
1	C	260	ILE	2.5
1	D	478	LYS	2.5
1	A	493	LEU	2.5
1	C	229	VAL	2.5
1	B	464	GLY	2.5
1	D	596	LYS	2.5
1	B	563	TYR	2.5
1	C	151	GLY	2.5
1	C	408	ARG	2.5
1	C	549	LEU	2.4
1	B	486	LYS	2.4
1	C	284	LEU	2.4
1	A	590	LEU	2.4
1	B	590	LEU	2.4
1	C	114	THR	2.4
1	B	593	PRO	2.4
1	A	347	LEU	2.3
1	C	466	ILE	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	328	ASN	2.3
1	A	292	GLU	2.3
1	B	429	GLU	2.3
1	A	577	ASN	2.3
1	C	262	GLU	2.3
1	D	467	LYS	2.3
1	B	560	LYS	2.3
1	C	484	LYS	2.3
1	C	560	LYS	2.3
1	C	539	GLN	2.2
1	D	559	ARG	2.2
1	B	184	GLU	2.2
1	B	577	ASN	2.2
1	D	476	LEU	2.2
1	A	406	LYS	2.2
1	A	485	PRO	2.2
1	B	405	LYS	2.2
1	C	563	TYR	2.2
1	A	230	LYS	2.1
1	A	478	LYS	2.1
1	B	345	ASN	2.1
1	A	154	TYR	2.1
1	A	152	GLY	2.1
1	C	597	GLU	2.1
1	D	468	ILE	2.1
1	A	592	THR	2.1
1	B	494	LYS	2.1
1	D	469	LYS	2.1
1	C	591	ILE	2.0
1	A	492	LYS	2.0
1	A	599	ASN	2.0
1	D	345	ASN	2.0
1	A	343	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 [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
5	ZN	A	705	1/1	0.96	0.15	0.76	42,42,42,42	0
5	ZN	D	703	1/1	0.98	0.15	0.29	40,40,40,40	0
3	DTP	C	701	30/30	0.98	0.15	0.07	30,35,38,42	11
3	DTP	B	703	30/30	0.98	0.15	-0.16	26,30,32,36	13
2	GTP	A	701	32/32	0.97	0.14	-0.27	28,34,43,45	0
3	DTP	D	701	30/30	0.98	0.15	-0.27	27,32,37,40	7
5	ZN	C	703	1/1	0.99	0.16	-0.31	42,42,42,42	0
2	GTP	B	702	32/32	0.96	0.13	-0.42	31,34,42,45	0
2	GTP	B	701	32/32	0.98	0.13	-0.55	28,33,39,43	0
3	DTP	A	702	30/30	0.98	0.13	-0.61	32,36,41,44	10
5	ZN	B	705	1/1	0.96	0.13	-0.74	39,39,39,39	0
2	GTP	A	703	32/32	0.98	0.11	-0.99	26,32,42,45	0
4	MG	C	702	1/1	0.97	0.11	-	42,42,42,42	0
4	MG	A	704	1/1	0.89	0.18	-	35,35,35,35	0
4	MG	B	704	1/1	0.84	0.13	-	39,39,39,39	0
4	MG	D	702	1/1	0.92	0.12	-	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.