



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:16 PM GMT

PDB ID : 4BZC  
Title : Crystal structure of the tetrameric dGTP-bound wild type SAMHD1 catalytic core  
Authors : Ji, X.; Yang, H.; Wu, Y.; Yan, J.; Mehrens, J.; DeLucia, M.; Hao, C.; Gronenborn, A.M.; Skowronski, J.; Ahn, J.; Xiong, Y.  
Deposited on : 2013-07-25  
Resolution : 2.88 Å(reported)

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

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

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

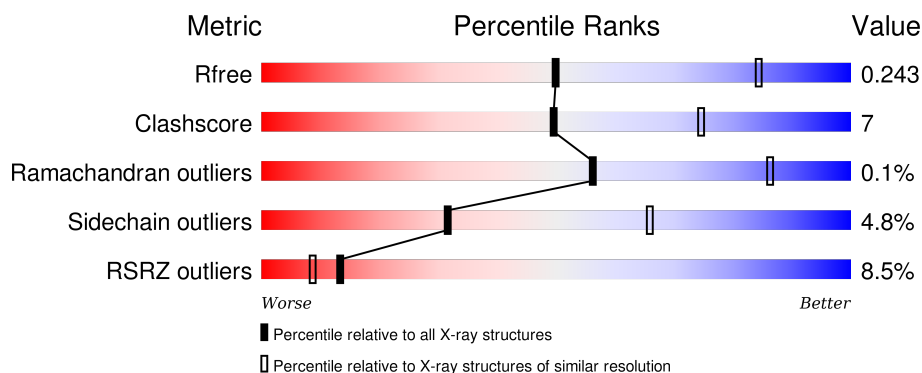
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.88 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	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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>4%</div> <div>70%</div> <div>15%</div> <div>•</div> <div>13%</div> </div>
1	B	550	<div> <div>11%</div> <div>73%</div> <div>11%</div> <div>•</div> <div>13%</div> </div>
1	C	550	<div> <div>6%</div> <div>72%</div> <div>14%</div> <div>•</div> <div>13%</div> </div>
1	D	550	<div> <div>8%</div> <div>70%</div> <div>13%</div> <div>•</div> <div>15%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15954 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 TRIPHOSPHO-HYDROLASE SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	0	0
			3880	2483	672	705	20			
1	B	477	Total	C	N	O	S	0	0	0
			3887	2489	678	700	20			
1	C	481	Total	C	N	O	S	0	0	0
			3932	2517	683	712	20			
1	D	470	Total	C	N	O	S	0	0	0
			3841	2462	666	693	20			

There are 144 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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	97	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
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
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

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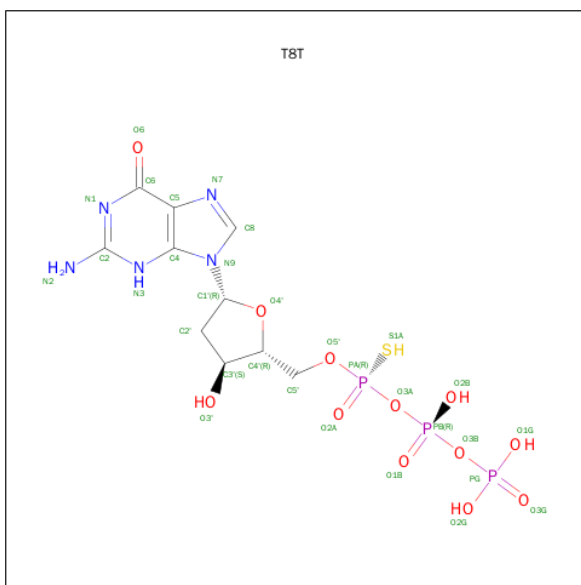
Chain	Residue	Modelled	Actual	Comment	Reference
B	103	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
B	104	GLN	-	EXPRESSION TAG	UNP Q9Y3Z3
B	105	GLN	-	EXPRESSION TAG	UNP Q9Y3Z3
B	106	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
B	107	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
B	108	ARG	-	EXPRESSION TAG	UNP Q9Y3Z3
B	109	ASP	-	EXPRESSION TAG	UNP Q9Y3Z3
B	110	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
B	111	ASN	-	EXPRESSION TAG	UNP Q9Y3Z3
B	112	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
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
C	108	ARG	-	EXPRESSION TAG	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

- Molecule 2 is 2'-DEOXYGUANOSINE-5'-O-(1-THIOTRIPHOSPHATE) (three-letter code: T8T) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
2	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

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

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

- Molecule 5 is water.

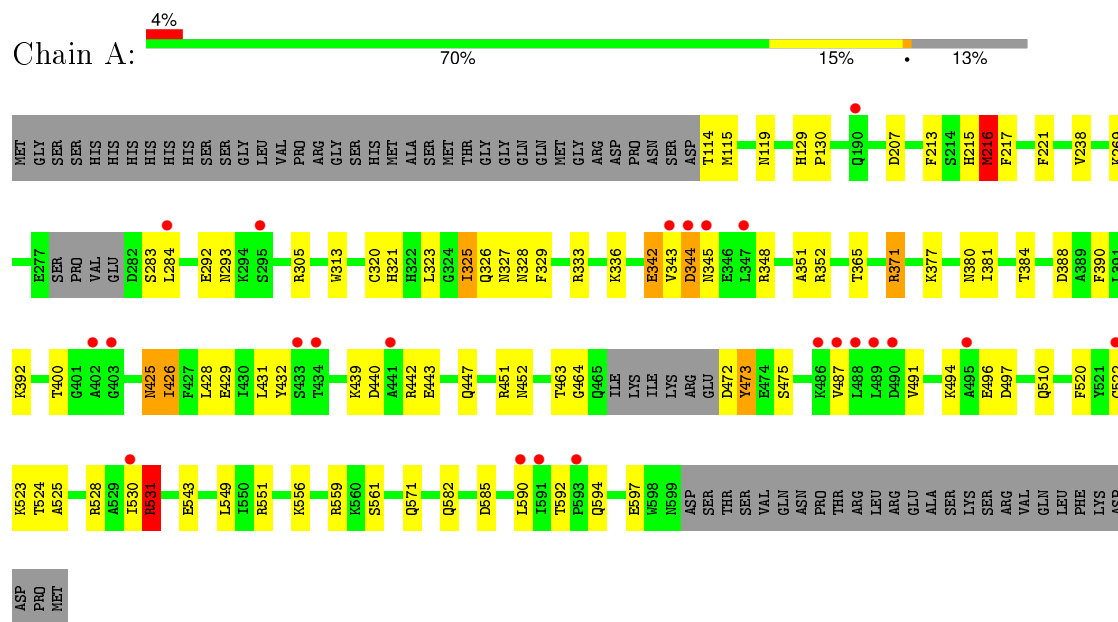
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	14	Total O 14 14	0	0
5	B	9	Total O 9 9	0	0
5	C	7	Total O 7 7	0	0
5	D	4	Total O 4 4	0	0



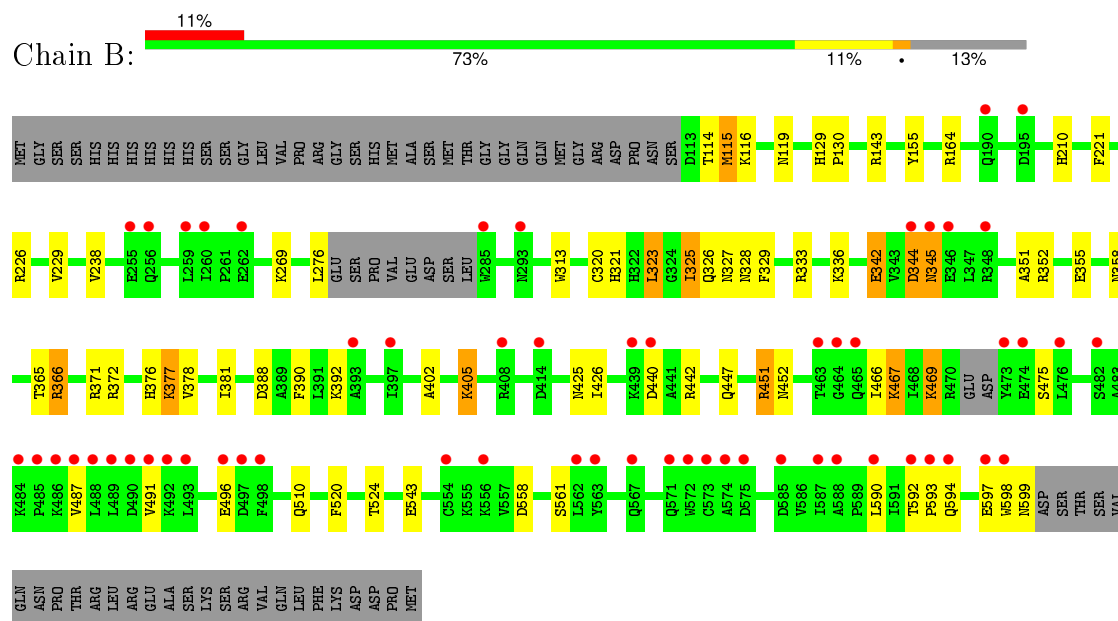
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: DEOXYNUCLEOSIDE TRIPHOSPHATE TRIPHOSPHOHYDROLASE SAMHD1

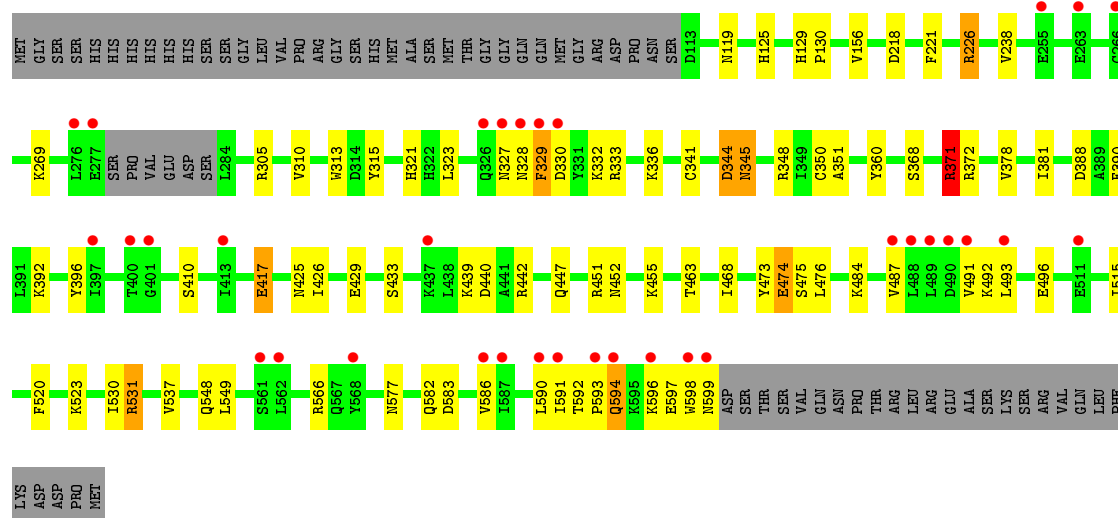


#### • Molecule 1: DEOXYNUCLEOSIDE TRIPHOSPHATE TRIPHOSPHOHYDROLASE SAMHD1



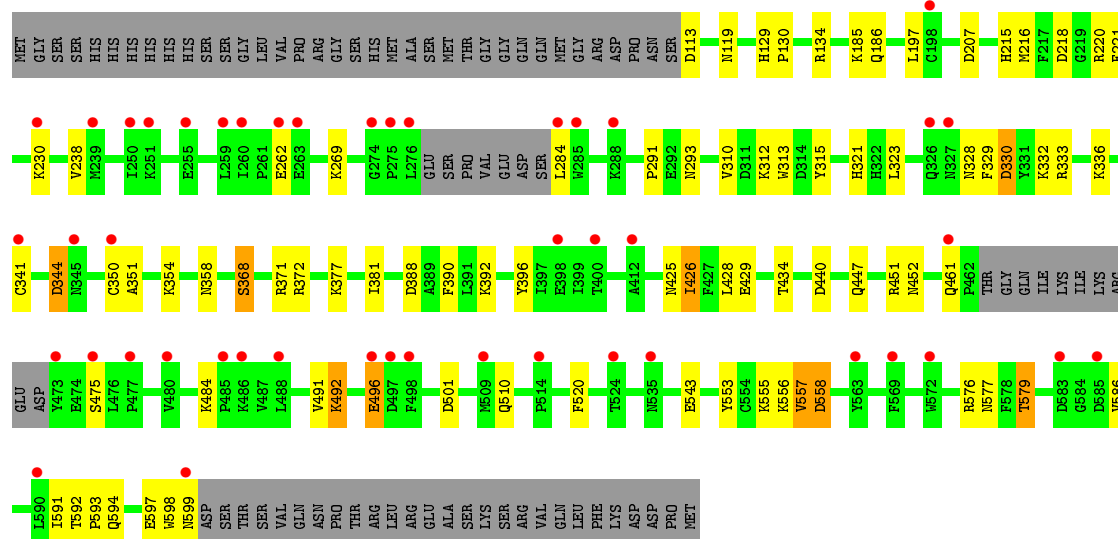
● Molecule 1: DEOXYNUCLEOSIDE TRIPHOSPHATE TRIPHOSPHOHYDROLASE SAMHD1

Chain C: 



● Molecule 1: DEOXYNUCLEOSIDE TRIPHOSPHATE TRIPHOSPHOHYDROLASE SAMHD1

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.00Å 138.73Å 93.72Å 90.00° 113.56° 90.00°	Depositor
Resolution (Å)	49.71 – 2.88 49.66 – 2.88	Depositor EDS
% Data completeness (in resolution range)	77.5 (49.71-2.88) 77.5 (49.66-2.88)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.80 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.190 , 0.245 0.193 , 0.243	Depositor DCC
$R_{free}$ test set	1662 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.8	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 68.4	EDS
Estimated twinning fraction	0.030 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 32677 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15954	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: MG, T8T, MN

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	0.66	0/3972	0.84	10/5364 (0.2%)
1	B	0.61	0/3978	0.85	9/5369 (0.2%)
1	C	0.65	0/4025	0.82	5/5434 (0.1%)
1	D	0.62	0/3933	0.78	2/5311 (0.0%)
All	All	0.63	0/15908	0.82	26/21478 (0.1%)

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

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

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	451	ARG	NE-CZ-NH1	12.89	126.74	120.30
1	B	451	ARG	NE-CZ-NH2	-12.80	113.90	120.30
1	C	226	ARG	CG-CD-NE	8.26	129.14	111.80
1	B	366	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	A	531	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	C	531	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	B	115	MET	CB-CG-SD	6.47	131.82	112.40
1	B	371	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	216	MET	CG-SD-CE	-6.22	90.25	100.20
1	B	405	LYS	CB-CA-C	-6.06	98.27	110.40
1	D	451	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	473	TYR	CB-CG-CD1	-5.76	117.55	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	551	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	D	368	SER	N-CA-CB	-5.74	101.89	110.50
1	A	333	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	451	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	C	451	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	C	371	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	B	325	ILE	CB-CA-C	-5.40	100.80	111.60
1	A	440	ASP	N-CA-CB	5.36	120.25	110.60
1	A	473	TYR	CB-CG-CD2	5.34	124.20	121.00
1	C	333	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	352	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	325	ILE	CB-CA-C	-5.15	101.30	111.60
1	B	442	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	559	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	330	ASP	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3880	0	3844	76	0
1	B	3887	0	3872	54	0
1	C	3932	0	3913	59	2
1	D	3841	0	3817	69	2
2	A	93	0	39	3	0
2	B	93	0	39	4	0
2	C	93	0	39	12	0
2	D	93	0	39	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	14	0	0	1	0
5	B	9	0	0	1	0
5	C	7	0	0	0	0
5	D	4	0	0	0	0
All	All	15954	0	15602	225	2

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 7.

All (225) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:556:LYS:O	1:D:557:VAL:HG22	1.44	1.17
1:D:215:HIS:NE2	2:D:700:T8T:O2A	1.84	1.09
1:A:325:ILE:C	1:C:328:ASN:HB2	1.77	1.04
1:B:402:ALA:O	1:B:405:LYS:HD2	1.60	0.99
1:D:368:SER:OG	1:D:372:ARG:NH1	1.97	0.97
1:A:328:ASN:HB2	1:A:365:THR:OG1	1.71	0.89
1:B:143:ARG:NH2	1:B:210:HIS:O	2.05	0.89
1:B:328:ASN:HB2	1:B:365:THR:OG1	1.73	0.88
1:B:325:ILE:C	1:D:328:ASN:HB2	1.93	0.88
1:D:207:ASP:OD1	2:D:700:T8T:S1A	2.32	0.88
1:C:474:GLU:HA	1:C:474:GLU:OE1	1.73	0.88
1:D:598:TRP:O	1:D:599:ASN:HB2	1.76	0.86
1:A:429:GLU:OE2	1:D:429:GLU:HG3	1.75	0.85
1:A:523:LYS:NZ	2:C:800:T8T:O3G	2.10	0.84
1:B:325:ILE:O	1:D:328:ASN:HB2	1.78	0.84
1:B:226:ARG:O	1:B:229:VAL:HG12	1.77	0.83
1:B:155:TYR:O	1:B:451:ARG:NH2	2.13	0.81
1:B:325:ILE:HG22	1:B:326:GLN:N	1.95	0.80
1:A:215:HIS:HB2	5:A:2007:HOH:O	1.82	0.79
1:A:325:ILE:HG22	1:A:326:GLN:N	1.97	0.78
1:D:113:ASP:HB3	1:D:130:PRO:HB3	1.67	0.75
1:A:325:ILE:O	1:C:328:ASN:HB2	1.86	0.74
1:D:556:LYS:O	1:D:557:VAL:CG2	2.30	0.74
1:B:325:ILE:CG2	1:B:326:GLN:N	2.50	0.74
1:A:325:ILE:CG2	1:A:326:GLN:N	2.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:LYS:HZ2	2:C:800:T8T:PG	2.13	0.70
1:A:597:GLU:OE1	1:A:597:GLU:N	2.21	0.70
2:A:700:T8T:H5'	2:A:700:T8T:H8	1.73	0.70
2:B:800:T8T:O3G	2:B:900:T8T:O2B	2.10	0.69
1:B:238:VAL:HG13	1:B:269:LYS:HG2	1.75	0.69
1:B:597:GLU:N	1:B:597:GLU:OE1	2.23	0.68
1:D:238:VAL:HG13	1:D:269:LYS:HG2	1.75	0.68
1:A:305:ARG:NE	1:A:348:ARG:HH11	1.89	0.68
1:D:461:GLN:H	1:D:579:THR:CG2	2.08	0.67
1:A:585:ASP:OD1	1:A:592:THR:HG21	1.95	0.67
1:A:238:VAL:HG13	1:A:269:LYS:HG2	1.75	0.67
1:D:597:GLU:N	1:D:597:GLU:OE1	2.22	0.67
1:C:238:VAL:HG13	1:C:269:LYS:HG2	1.77	0.66
1:A:524:THR:HG21	1:C:566:ARG:CZ	2.26	0.66
1:A:400:THR:HG21	1:D:434:THR:HG21	1.78	0.66
1:C:597:GLU:OE1	1:C:597:GLU:N	2.25	0.66
1:B:164:ARG:NH1	2:B:700:T8T:S1A	2.67	0.65
1:B:524:THR:OG1	1:D:586:VAL:HG11	1.96	0.65
1:B:543:GLU:HG3	1:D:543:GLU:HG3	1.79	0.65
1:B:558:ASP:OD1	1:B:561:SER:CB	2.46	0.64
1:D:558:ASP:N	1:D:558:ASP:OD1	2.30	0.63
1:B:372:ARG:NE	1:D:358:ASN:OD1	2.31	0.63
1:B:333:ARG:NH2	2:D:800:T8T:S1A	2.71	0.63
2:C:700:T8T:S1A	2:C:700:T8T:O2B	2.57	0.62
1:D:291:PRO:HG2	1:D:293:ASN:OD1	2.00	0.62
1:D:556:LYS:C	1:D:557:VAL:HG13	2.20	0.61
1:A:523:LYS:NZ	2:C:900:T8T:O1G	2.26	0.61
1:A:326:GLN:N	1:C:328:ASN:HB2	2.15	0.61
1:B:333:ARG:NH1	1:B:355:GLU:OE2	2.33	0.61
1:B:342:GLU:OE2	1:B:345:ASN:HA	2.01	0.61
1:B:342:GLU:OE2	1:B:345:ASN:N	2.35	0.60
1:B:469:LYS:CD	1:B:469:LYS:N	2.65	0.60
1:A:342:GLU:OE2	1:A:345:ASN:N	2.34	0.59
1:A:325:ILE:C	1:C:328:ASN:CB	2.65	0.58
1:D:592:THR:OG1	1:D:593:PRO:HD3	2.04	0.58
1:C:455:LYS:NZ	2:C:900:T8T:O3G	2.34	0.58
1:A:343:VAL:HB	1:A:348:ARG:HE	1.68	0.58
1:C:592:THR:OG1	1:C:593:PRO:HD3	2.03	0.58
1:A:531:ARG:NH1	1:A:531:ARG:HB3	2.20	0.57
1:C:473:TYR:HA	1:C:476:LEU:HD12	1.87	0.57
1:D:329:PHE:CG	1:D:330:ASP:N	2.74	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:CYS:SG	1:C:583:ASP:CB	2.94	0.56
1:D:555:LYS:O	1:D:557:VAL:HG13	2.05	0.56
1:A:325:ILE:O	1:C:328:ASN:CB	2.53	0.56
1:B:376:HIS:CD2	1:B:378:VAL:H	2.24	0.56
1:A:525:ALA:HB3	1:C:586:VAL:CG1	2.35	0.56
1:B:592:THR:OG1	1:B:593:PRO:HD3	2.06	0.55
1:B:358:ASN:OD1	1:D:372:ARG:NH2	2.40	0.54
1:B:323:LEU:O	1:C:119:ASN:ND2	2.41	0.53
1:D:461:GLN:H	1:D:579:THR:HG23	1.74	0.53
1:B:377:LYS:HE2	5:B:2007:HOH:O	2.08	0.53
1:B:325:ILE:O	1:D:328:ASN:CB	2.55	0.52
1:B:376:HIS:HD2	1:B:378:VAL:H	1.57	0.52
1:B:558:ASP:OD1	1:B:561:SER:OG	2.27	0.52
1:A:530:ILE:HD12	1:C:582:GLN:O	2.09	0.51
1:A:425:ASN:HB2	1:D:428:LEU:CD1	2.40	0.51
1:A:119:ASN:ND2	1:D:323:LEU:O	2.43	0.51
1:A:342:GLU:OE2	1:A:345:ASN:HA	2.10	0.51
1:A:352:ARG:HH22	2:C:800:T8T:PG	2.34	0.51
1:A:328:ASN:HB2	1:A:365:THR:HG1	1.75	0.51
1:A:305:ARG:NE	1:A:348:ARG:NH1	2.56	0.51
2:B:800:T8T:O2A	1:D:354:LYS:NZ	2.32	0.51
1:B:377:LYS:NZ	2:B:800:T8T:O1B	2.44	0.50
1:A:522:CYS:SG	1:C:583:ASP:HB3	2.51	0.50
1:C:372:ARG:NE	2:C:800:T8T:O6	2.39	0.50
1:A:524:THR:HG21	1:C:566:ARG:NH2	2.27	0.50
1:B:116:LYS:HE3	2:C:900:T8T:S1A	2.52	0.50
1:B:321:HIS:CE1	1:C:321:HIS:CE1	3.00	0.50
1:D:461:GLN:HB2	1:D:579:THR:CG2	2.42	0.50
1:B:558:ASP:OD1	1:B:561:SER:HB2	2.10	0.50
1:B:155:TYR:HB3	1:B:451:ARG:NH2	2.26	0.49
1:B:469:LYS:N	1:B:469:LYS:HD2	2.27	0.49
1:A:323:LEU:O	1:D:119:ASN:ND2	2.45	0.49
1:C:439:LYS:HA	1:C:442:ARG:NH1	2.28	0.49
1:D:461:GLN:O	1:D:579:THR:HG22	2.12	0.49
1:C:371:ARG:HG3	1:C:371:ARG:HH11	1.78	0.49
1:C:433:SER:C	1:C:442:ARG:HH21	2.16	0.49
1:A:524:THR:CG2	1:C:566:ARG:NH2	2.76	0.49
1:A:425:ASN:HB2	1:D:428:LEU:HD12	1.94	0.48
1:A:428:LEU:CD1	1:D:425:ASN:HB2	2.43	0.48
1:D:381:ILE:HD12	1:D:381:ILE:HA	1.67	0.48
1:A:571:GLN:HE22	1:A:594:GLN:HE22	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:ALA:HB3	1:C:586:VAL:HG11	1.96	0.48
1:D:576:ARG:O	1:D:577:ASN:HB2	2.14	0.48
1:A:380:ASN:O	1:A:384:THR:HG23	2.14	0.48
1:D:461:GLN:H	1:D:579:THR:HG22	1.78	0.48
1:B:469:LYS:H	1:B:469:LYS:HD3	1.78	0.48
1:D:591:ILE:O	1:D:594:GLN:HB2	2.13	0.48
1:A:207:ASP:OD1	2:A:700:T8T:S1A	2.71	0.48
1:B:469:LYS:CD	1:B:469:LYS:H	2.27	0.48
1:A:428:LEU:HD13	1:D:425:ASN:HB2	1.96	0.47
1:C:345:ASN:C	1:C:345:ASN:OD1	2.52	0.47
1:A:522:CYS:SG	1:C:583:ASP:HB2	2.54	0.47
1:D:134:ARG:NE	1:D:134:ARG:HA	2.28	0.47
1:D:330:ASP:HB3	1:D:332:LYS:HB2	1.97	0.47
1:A:351:ALA:O	1:A:520:PHE:HA	2.15	0.47
1:A:129:HIS:CG	1:A:130:PRO:HD2	2.50	0.47
1:A:216:MET:HG3	1:A:217:PHE:N	2.22	0.47
1:A:371:ARG:NH2	1:C:537:VAL:O	2.48	0.47
1:D:129:HIS:CG	1:D:130:PRO:HD2	2.50	0.47
1:D:492:LYS:CG	1:D:492:LYS:O	2.62	0.47
1:C:591:ILE:O	1:C:594:GLN:HB2	2.15	0.47
1:D:381:ILE:HD13	1:D:553:TYR:CG	2.50	0.47
1:C:327:ASN:ND2	1:C:329:PHE:CD1	2.82	0.47
1:A:472:ASP:OD2	1:A:473:TYR:CZ	2.68	0.47
1:C:371:ARG:HH11	1:C:371:ARG:CG	2.28	0.46
1:A:543:GLU:OE1	1:A:543:GLU:N	2.30	0.46
1:D:351:ALA:O	1:D:520:PHE:HA	2.15	0.46
1:A:320:CYS:SG	1:A:327:ASN:HB2	2.55	0.46
1:D:207:ASP:CG	2:D:700:T8T:S1A	2.93	0.46
1:C:125:HIS:CE1	1:D:333:ARG:HB2	2.50	0.46
1:C:330:ASP:HB3	1:C:332:LYS:HB2	1.97	0.46
1:C:351:ALA:O	1:C:520:PHE:HA	2.15	0.46
1:D:341:CYS:CB	1:D:350:CYS:HG	2.29	0.46
1:B:325:ILE:CG2	1:B:326:GLN:H	2.27	0.46
1:B:342:GLU:OE2	1:B:345:ASN:CA	2.64	0.46
1:D:496:GLU:O	1:D:555:LYS:HE3	2.15	0.45
1:C:548:GLN:O	1:C:549:LEU:HD23	2.16	0.45
1:A:325:ILE:CG2	1:A:326:GLN:H	2.27	0.45
1:A:497:ASP:OD2	1:A:556:LYS:CE	2.65	0.45
2:C:800:T8T:O3G	2:C:900:T8T:O2B	2.35	0.45
1:A:313:TRP:CD1	1:A:329:PHE:CE2	3.04	0.45
1:B:328:ASN:HB2	1:B:365:THR:HG1	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:GLU:O	1:C:417:GLU:OE1	2.34	0.45
1:A:305:ARG:CZ	1:A:348:ARG:HH11	2.30	0.45
1:B:351:ALA:O	1:B:520:PHE:HA	2.16	0.45
1:A:221:PHE:CE1	1:A:390:PHE:HB3	2.52	0.45
2:C:700:T8T:H8	2:C:700:T8T:H5'	1.99	0.44
1:D:312:LYS:HE3	2:D:700:T8T:O1G	2.17	0.44
1:C:417:GLU:HA	1:C:417:GLU:OE1	2.17	0.44
1:C:463:THR:HG21	1:C:577:ASN:O	2.17	0.44
1:B:129:HIS:CG	1:B:130:PRO:HD2	2.51	0.44
1:B:221:PHE:CE1	1:B:390:PHE:HB3	2.52	0.44
1:A:463:THR:OG1	1:A:464:GLY:N	2.50	0.44
1:B:320:CYS:SG	1:B:327:ASN:HB2	2.58	0.44
1:A:342:GLU:OE2	1:A:345:ASN:CA	2.66	0.44
1:C:315:TYR:CE2	2:C:700:T8T:H5'A	2.53	0.44
1:A:525:ALA:HB3	1:C:586:VAL:HG13	1.98	0.44
1:B:598:TRP:O	1:B:599:ASN:CB	2.65	0.44
1:D:344:ASP:N	1:D:344:ASP:OD1	2.50	0.43
1:D:221:PHE:CE1	1:D:390:PHE:HB3	2.53	0.43
1:B:114:THR:OG1	1:B:115:MET:N	2.51	0.43
1:A:114:THR:HG22	1:A:115:MET:N	2.33	0.43
1:A:381:ILE:HA	1:A:381:ILE:HD12	1.86	0.43
1:C:221:PHE:CE1	1:C:390:PHE:HB3	2.52	0.43
1:A:494:LYS:HB2	1:A:497:ASP:OD1	2.19	0.43
1:B:344:ASP:OD1	1:B:344:ASP:N	2.52	0.43
1:B:381:ILE:HD12	1:B:381:ILE:HA	1.86	0.43
2:A:900:T8T:O3G	1:C:523:LYS:NZ	2.47	0.43
1:D:341:CYS:HB2	1:D:350:CYS:HG	1.84	0.43
1:C:378:VAL:O	1:C:381:ILE:HG22	2.18	0.43
1:C:341:CYS:CB	1:C:350:CYS:HG	2.31	0.43
1:B:388:ASP:O	1:B:392:LYS:HG3	2.19	0.43
1:A:426:ILE:HA	1:A:426:ILE:HD13	1.88	0.43
1:B:119:ASN:ND2	1:C:323:LEU:O	2.52	0.43
1:C:426:ILE:HD13	1:C:426:ILE:HA	1.91	0.43
1:C:368:SER:O	1:C:372:ARG:HG2	2.19	0.42
1:A:582:GLN:O	1:C:530:ILE:HD12	2.19	0.42
1:C:388:ASP:O	1:C:392:LYS:HG3	2.20	0.42
1:B:313:TRP:CD1	1:B:329:PHE:CE2	3.08	0.42
1:A:371:ARG:CZ	1:A:549:LEU:HD11	2.50	0.42
1:D:492:LYS:HG2	1:D:492:LYS:O	2.20	0.42
1:B:598:TRP:O	1:B:599:ASN:CG	2.58	0.42
1:D:388:ASP:O	1:D:392:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LEU:HG	1:A:292:GLU:OE2	2.20	0.42
1:A:388:ASP:O	1:A:392:LYS:HG3	2.20	0.42
1:C:305:ARG:NE	1:C:348:ARG:HH11	2.17	0.42
1:D:310:VAL:HG12	1:D:313:TRP:CZ3	2.54	0.42
1:C:129:HIS:CG	1:C:130:PRO:HD2	2.55	0.41
1:A:425:ASN:OD1	1:D:425:ASN:OD1	2.37	0.41
1:D:426:ILE:HD13	1:D:426:ILE:HA	1.94	0.41
1:D:461:GLN:N	1:D:579:THR:CG2	2.81	0.41
1:B:467:LYS:O	1:B:469:LYS:NZ	2.38	0.41
1:D:197:LEU:HA	1:D:197:LEU:HD23	1.93	0.41
1:D:461:GLN:HB2	1:D:579:THR:HG22	2.03	0.41
1:C:226:ARG:NE	1:C:410:SER:O	2.53	0.41
1:D:461:GLN:HB2	1:D:579:THR:HG21	2.02	0.41
1:A:213:PHE:HB2	1:A:216:MET:HG2	2.03	0.41
1:A:487:VAL:HG13	1:A:590:LEU:HD12	2.03	0.41
1:D:215:HIS:HA	1:D:218:ASP:OD1	2.21	0.41
1:B:487:VAL:HG13	1:B:590:LEU:HD12	2.03	0.41
1:D:262:GLU:H	1:D:262:GLU:CD	2.23	0.41
1:C:310:VAL:HG12	1:C:313:TRP:CZ3	2.56	0.41
1:A:524:THR:HG21	1:C:566:ARG:NH1	2.36	0.41
1:A:531:ARG:HB3	1:A:531:ARG:HH11	1.83	0.41
1:A:321:HIS:CE1	1:D:321:HIS:CE1	3.09	0.41
1:D:185:LYS:HG3	1:D:186:GLN:HG3	2.02	0.40
1:A:431:LEU:HD23	1:A:432:TYR:CE1	2.56	0.40
2:D:800:T8T:O2B	2:D:900:T8T:H5'	2.21	0.40
1:A:556:LYS:HB3	1:A:561:SER:CB	2.52	0.40
1:A:439:LYS:HG3	1:A:442:ARG:NH2	2.36	0.40
1:C:360:TYR:CE2	1:C:515:ILE:HG21	2.56	0.40
1:C:156:VAL:O	2:C:900:T8T:H8	2.21	0.40
1:C:487:VAL:HG13	1:C:590:LEU:HD12	2.04	0.40
1:C:598:TRP:O	1:C:599:ASN:CB	2.69	0.40
1:D:291:PRO:CG	1:D:293:ASN:OD1	2.69	0.40
1:D:293:ASN:N	1:D:293:ASN:OD1	2.52	0.40
1:A:344:ASP:OD1	1:A:344:ASP:N	2.53	0.40
1:C:344:ASP:N	1:C:344:ASP:OD1	2.55	0.40
1:D:220:ARG:NH1	1:D:501:ASP:OD2	2.42	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:493:LEU:O	1:D:396:TYR:OH[1_454]	2.10	0.10
1:C:396:TYR:OH	1:D:230:LYS:NZ[1_454]	2.10	0.10

## 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	470/550 (86%)	464 (99%)	6 (1%)	0	100	100
1	B	471/550 (86%)	466 (99%)	5 (1%)	0	100	100
1	C	477/550 (87%)	471 (99%)	6 (1%)	0	100	100
1	D	464/550 (84%)	458 (99%)	5 (1%)	1 (0%)	52	83
All	All	1882/2200 (86%)	1859 (99%)	22 (1%)	1 (0%)	56	86

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	557	VAL

### 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	421/488 (86%)	402 (96%)	19 (4%)	34	68
1	B	421/488 (86%)	400 (95%)	21 (5%)	30	64
1	C	427/488 (88%)	405 (95%)	22 (5%)	29	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	417/488 (86%)	398 (95%)	19 (5%)	33	67
All	All	1686/1952 (86%)	1605 (95%)	81 (5%)	31	66

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	MET
1	A	283	SER
1	A	293	ASN
1	A	336	LYS
1	A	342	GLU
1	A	344	ASP
1	A	371	ARG
1	A	377	LYS
1	A	425	ASN
1	A	426	ILE
1	A	443	GLU
1	A	447	GLN
1	A	452	ASN
1	A	475	SER
1	A	491	VAL
1	A	496	GLU
1	A	510	GLN
1	A	528	ARG
1	A	531	ARG
1	B	276	LEU
1	B	323	LEU
1	B	336	LYS
1	B	342	GLU
1	B	344	ASP
1	B	345	ASN
1	B	366	ARG
1	B	377	LYS
1	B	425	ASN
1	B	426	ILE
1	B	440	ASP
1	B	447	GLN
1	B	452	ASN
1	B	466	ILE
1	B	467	LYS
1	B	469	LYS
1	B	475	SER

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Mol	Chain	Res	Type
1	B	491	VAL
1	B	496	GLU
1	B	510	GLN
1	B	594	GLN
1	C	218	ASP
1	C	329	PHE
1	C	336	LYS
1	C	344	ASP
1	C	345	ASN
1	C	371	ARG
1	C	417	GLU
1	C	425	ASN
1	C	429	GLU
1	C	440	ASP
1	C	447	GLN
1	C	452	ASN
1	C	468	ILE
1	C	474	GLU
1	C	475	SER
1	C	484	LYS
1	C	491	VAL
1	C	492	LYS
1	C	496	GLU
1	C	531	ARG
1	C	594	GLN
1	C	596	LYS
1	D	216	MET
1	D	284	LEU
1	D	315	TYR
1	D	336	LYS
1	D	344	ASP
1	D	371	ARG
1	D	377	LYS
1	D	426	ILE
1	D	440	ASP
1	D	447	GLN
1	D	452	ASN
1	D	475	SER
1	D	484	LYS
1	D	491	VAL
1	D	492	LYS
1	D	496	GLU

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Mol	Chain	Res	Type
1	D	510	GLN
1	D	558	ASP
1	D	579	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	HIS
1	A	293	ASN
1	A	425	ASN
1	A	594	GLN
1	A	599	ASN
1	B	215	HIS
1	B	243	HIS
1	B	376	HIS
1	B	425	ASN
1	C	235	GLN
1	C	243	HIS
1	C	328	ASN
1	C	425	ASN
1	D	235	GLN
1	D	243	HIS
1	D	364	HIS

### 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 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$
2	T8T	A	700	-	23,33,33	1.06	2 (8%)	33,52,52	2.04	10 (30%)
2	T8T	A	800	4	23,33,33	0.99	0	33,52,52	2.41	12 (36%)
2	T8T	A	900	4	23,33,33	0.94	1 (4%)	33,52,52	1.90	9 (27%)
2	T8T	B	700	-	23,33,33	1.54	3 (13%)	33,52,52	2.09	9 (27%)
2	T8T	B	800	4	23,33,33	1.39	3 (13%)	33,52,52	2.13	9 (27%)
2	T8T	B	900	4	23,33,33	0.88	1 (4%)	33,52,52	1.90	7 (21%)
2	T8T	C	700	-	23,33,33	0.98	2 (8%)	33,52,52	1.96	10 (30%)
2	T8T	C	800	4	23,33,33	1.25	3 (13%)	33,52,52	1.98	11 (33%)
2	T8T	C	900	4	23,33,33	1.14	2 (8%)	33,52,52	2.26	10 (30%)
2	T8T	D	700	-	23,33,33	1.21	3 (13%)	33,52,52	2.10	7 (21%)
2	T8T	D	800	4	23,33,33	1.01	1 (4%)	33,52,52	1.90	10 (30%)
2	T8T	D	900	4	23,33,33	1.11	3 (13%)	33,52,52	2.32	10 (30%)

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	T8T	A	700	-	-	0/13/34/34	0/3/3/3
2	T8T	A	800	4	-	0/13/34/34	0/3/3/3
2	T8T	A	900	4	-	0/13/34/34	0/3/3/3
2	T8T	B	700	-	-	0/13/34/34	0/3/3/3
2	T8T	B	800	4	-	0/13/34/34	0/3/3/3
2	T8T	B	900	4	-	0/13/34/34	0/3/3/3
2	T8T	C	700	-	-	0/13/34/34	0/3/3/3
2	T8T	C	800	4	-	0/13/34/34	0/3/3/3
2	T8T	C	900	4	-	0/13/34/34	0/3/3/3
2	T8T	D	700	-	-	0/13/34/34	0/3/3/3
2	T8T	D	800	4	-	0/13/34/34	0/3/3/3
2	T8T	D	900	4	-	0/13/34/34	0/3/3/3



All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	800	T8T	C4-N3	-2.26	1.32	1.35
2	D	900	T8T	C4-N3	-2.10	1.32	1.35
2	B	800	T8T	C4-N3	-2.07	1.32	1.35
2	D	700	T8T	PA-O5'	2.04	1.61	1.58
2	C	700	T8T	C5-C4	2.07	1.45	1.40
2	D	900	T8T	C5-C4	2.20	1.45	1.40
2	B	900	T8T	C6-C5	2.30	1.45	1.41
2	C	800	T8T	C6-C5	2.30	1.45	1.41
2	B	700	T8T	C5-C4	2.33	1.45	1.40
2	D	900	T8T	C6-C5	2.48	1.46	1.41
2	C	700	T8T	C6-C5	2.51	1.46	1.41
2	A	700	T8T	C5-C4	2.52	1.46	1.40
2	A	700	T8T	C6-C5	2.52	1.46	1.41
2	A	900	T8T	C6-C5	2.54	1.46	1.41
2	C	800	T8T	PA-O5'	2.73	1.62	1.58
2	B	800	T8T	C6-C5	2.79	1.46	1.41
2	D	700	T8T	C5-C4	2.90	1.47	1.40
2	C	800	T8T	C5-C4	2.93	1.47	1.40
2	C	900	T8T	C5-C4	3.18	1.47	1.40
2	C	900	T8T	C6-C5	3.27	1.47	1.41
2	D	700	T8T	C6-C5	3.31	1.47	1.41
2	B	800	T8T	PA-O5'	3.49	1.63	1.58
2	B	700	T8T	PA-O5'	4.21	1.64	1.58
2	B	700	T8T	C6-C5	4.42	1.50	1.41

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	900	T8T	C5-C6-N1	-5.94	115.47	123.59
2	D	700	T8T	PB-O3A-PA	-5.85	112.85	133.44
2	A	800	T8T	C5-C6-N1	-5.57	115.98	123.59
2	B	900	T8T	PB-O3A-PA	-5.37	114.55	133.44
2	B	800	T8T	C5-C6-N1	-5.24	116.43	123.59
2	C	800	T8T	C5-C6-N1	-5.22	116.44	123.59
2	B	800	T8T	C4-C5-N7	-5.22	104.68	109.48
2	C	900	T8T	C6-C5-C4	-5.20	114.68	120.90
2	B	700	T8T	C4-C5-N7	-5.04	104.84	109.48
2	C	900	T8T	PB-O3A-PA	-4.92	116.12	133.44
2	A	700	T8T	C5-C6-N1	-4.80	117.03	123.59
2	D	800	T8T	C1'-N9-C4	-4.73	119.15	127.16
2	B	700	T8T	PB-O3B-PG	-4.72	116.83	132.67
2	D	900	T8T	PB-O3B-PG	-4.67	116.99	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	900	T8T	PB-O3A-PA	-4.61	117.21	133.44
2	B	700	T8T	C5-C6-N1	-4.46	117.49	123.59
2	D	700	T8T	C6-C5-C4	-4.40	115.64	120.90
2	A	900	T8T	N3-C2-N1	-4.40	120.75	127.44
2	A	800	T8T	N2-C2-N3	-4.34	109.47	117.80
2	C	700	T8T	C5-C6-N1	-4.25	117.78	123.59
2	D	800	T8T	C6-C5-C4	-3.97	116.16	120.90
2	C	700	T8T	C6-C5-C4	-3.95	116.17	120.90
2	A	800	T8T	C1'-N9-C4	-3.94	120.47	127.16
2	B	800	T8T	N2-C2-N3	-3.91	110.29	117.80
2	B	900	T8T	PB-O3B-PG	-3.83	119.82	132.67
2	B	900	T8T	C5-C6-N1	-3.77	118.44	123.59
2	D	700	T8T	C1'-N9-C4	-3.75	120.80	127.16
2	C	900	T8T	PB-O3B-PG	-3.74	120.11	132.67
2	A	900	T8T	C6-C5-C4	-3.74	116.43	120.90
2	D	700	T8T	C5-C6-N1	-3.66	118.58	123.59
2	C	800	T8T	C1'-N9-C4	-3.65	120.98	127.16
2	D	700	T8T	PB-O3B-PG	-3.64	120.45	132.67
2	B	700	T8T	C6-C5-C4	-3.57	116.63	120.90
2	A	800	T8T	O3'-C3'-C2'	-3.55	99.00	110.74
2	B	800	T8T	PB-O3B-PG	-3.46	121.08	132.67
2	A	700	T8T	PB-O3B-PG	-3.45	121.10	132.67
2	A	900	T8T	PB-O3A-PA	-3.44	121.35	133.44
2	C	700	T8T	C1'-N9-C4	-3.40	121.39	127.16
2	C	900	T8T	N3-C2-N1	-3.39	122.28	127.44
2	D	800	T8T	C4-C5-N7	-3.39	106.36	109.48
2	D	800	T8T	PB-O3A-PA	-3.38	121.55	133.44
2	D	900	T8T	N3-C2-N1	-3.36	122.32	127.44
2	A	700	T8T	C6-C5-C4	-3.27	116.98	120.90
2	D	900	T8T	C4-C5-N7	-3.27	106.47	109.48
2	C	900	T8T	C5-C6-N1	-3.23	119.17	123.59
2	C	900	T8T	O4'-C1'-N9	-3.20	102.18	107.72
2	C	800	T8T	C6-C5-C4	-3.14	117.14	120.90
2	C	700	T8T	PB-O3B-PG	-3.02	122.54	132.67
2	A	800	T8T	C4-C5-N7	-3.02	106.70	109.48
2	C	700	T8T	PB-O3A-PA	-3.01	122.86	133.44
2	A	700	T8T	N3-C2-N1	-3.00	122.88	127.44
2	A	900	T8T	C5-C6-N1	-2.99	119.49	123.59
2	D	800	T8T	PB-O3B-PG	-2.99	122.65	132.67
2	C	800	T8T	PB-O3B-PG	-2.88	123.00	132.67
2	D	700	T8T	N3-C2-N1	-2.87	123.07	127.44
2	B	900	T8T	C4-C5-N7	-2.85	106.85	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	700	T8T	C1'-N9-C4	-2.85	122.33	127.16
2	C	800	T8T	PB-O3A-PA	-2.76	123.75	133.44
2	A	800	T8T	N3-C2-N1	-2.72	123.30	127.44
2	B	900	T8T	O4'-C1'-N9	-2.71	103.02	107.72
2	B	800	T8T	PB-O3A-PA	-2.70	123.93	133.44
2	A	900	T8T	PB-O3B-PG	-2.69	123.64	132.67
2	A	700	T8T	C1'-N9-C4	-2.65	122.67	127.16
2	C	700	T8T	O5'-C5'-C4'	-2.40	100.28	109.12
2	A	800	T8T	PB-O3B-PG	-2.36	124.75	132.67
2	A	700	T8T	C2'-C1'-N9	-2.26	108.66	114.16
2	A	800	T8T	O2G-PG-O3B	-2.21	95.07	105.09
2	B	700	T8T	N3-C2-N1	-2.17	124.14	127.44
2	C	800	T8T	O3'-C3'-C2'	-2.15	103.63	110.74
2	D	900	T8T	C6-C5-C4	-2.15	118.33	120.90
2	C	700	T8T	O4'-C4'-C5'	-2.14	101.66	109.32
2	A	800	T8T	C6-C5-C4	-2.11	118.38	120.90
2	D	800	T8T	O5'-PA-O2A	-2.08	106.35	114.14
2	C	800	T8T	N3-C2-N1	-2.07	124.29	127.44
2	C	900	T8T	C1'-N9-C4	-2.04	123.70	127.16
2	B	800	T8T	O2G-PG-O3B	-2.04	95.83	105.09
2	B	800	T8T	C1'-N9-C4	-2.01	123.74	127.16
2	A	900	T8T	O4'-C1'-N9	-2.01	104.23	107.72
2	C	900	T8T	O3'-C3'-C2'	2.08	117.61	110.74
2	D	800	T8T	C6-N1-C2	2.08	118.83	115.94
2	D	800	T8T	O4'-C1'-C2'	2.11	110.47	106.27
2	D	900	T8T	O4'-C4'-C5'	2.13	116.94	109.32
2	A	700	T8T	C2'-C3'-C4'	2.13	107.19	102.77
2	D	800	T8T	O2G-PG-O1G	2.13	115.50	107.38
2	C	700	T8T	O1G-PG-O3G	2.17	117.55	110.58
2	A	900	T8T	C2'-C3'-C4'	2.17	107.27	102.77
2	C	800	T8T	O4'-C1'-C2'	2.28	110.81	106.27
2	A	800	T8T	O2G-PG-O1G	2.32	116.22	107.38
2	A	700	T8T	O2B-PB-O1B	2.33	125.14	112.53
2	C	800	T8T	C2'-C3'-C4'	2.35	107.66	102.77
2	D	800	T8T	O2G-PG-O3G	2.40	118.32	110.58
2	B	700	T8T	O3A-PA-O5'	2.42	110.52	101.47
2	B	700	T8T	O2B-PB-O1B	2.44	125.74	112.53
2	A	900	T8T	O2G-PG-O1G	2.49	116.86	107.38
2	B	900	T8T	O1G-PG-O3G	2.54	118.75	110.58
2	C	800	T8T	O2B-PB-O3B	2.62	116.96	105.09
2	B	800	T8T	C6-N1-C2	2.70	119.69	115.94
2	A	700	T8T	O4'-C1'-C2'	2.80	111.85	106.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	900	T8T	C2'-C3'-C4'	2.81	108.61	102.77
2	C	700	T8T	O2G-PG-O1G	2.96	118.65	107.38
2	D	900	T8T	N2-C2-N1	3.15	122.42	117.20
2	B	900	T8T	C6-N1-C2	3.33	120.55	115.94
2	C	900	T8T	O2G-PG-O3G	3.81	122.83	110.58
2	C	700	T8T	C6-N1-C2	3.82	121.23	115.94
2	A	800	T8T	C6-N1-C2	4.15	121.69	115.94
2	A	900	T8T	C6-N1-C2	4.20	121.77	115.94
2	B	700	T8T	C6-N1-C2	4.23	121.81	115.94
2	D	700	T8T	C6-N1-C2	4.33	121.95	115.94
2	B	800	T8T	N2-C2-N1	4.67	124.93	117.20
2	C	900	T8T	C6-N1-C2	4.89	122.73	115.94
2	C	800	T8T	C6-N1-C2	5.13	123.06	115.94
2	A	700	T8T	C6-N1-C2	5.16	123.10	115.94
2	D	900	T8T	C6-N1-C2	5.39	123.42	115.94
2	A	800	T8T	N2-C2-N1	6.05	127.22	117.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700	T8T	2	0
2	A	900	T8T	1	0
2	B	700	T8T	1	0
2	B	800	T8T	3	0
2	B	900	T8T	1	0
2	C	700	T8T	3	0
2	C	800	T8T	5	0
2	C	900	T8T	5	0
2	D	700	T8T	4	0
2	D	800	T8T	2	0
2	D	900	T8T	1	0

## 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, 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	476/550 (86%)	0.27	23 (4%) 34 29	29, 53, 94, 127	0
1	B	477/550 (86%)	0.76	58 (12%) 5 3	40, 76, 117, 137	0
1	C	481/550 (87%)	0.36	34 (7%) 19 13	28, 56, 102, 140	0
1	D	470/550 (85%)	0.62	46 (9%) 10 6	39, 73, 108, 140	0
All	All	1904/2200 (86%)	0.50	161 (8%) 13 9	28, 65, 107, 140	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	490	ASP	9.4
1	B	488	LEU	7.0
1	B	491	VAL	6.4
1	A	345	ASN	5.9
1	B	486	LYS	5.5
1	D	412	ALA	5.5
1	A	490	ASP	5.1
1	B	345	ASN	5.1
1	B	571	GLN	5.0
1	D	274	GLY	5.0
1	B	489	LEU	4.9
1	C	489	LEU	4.9
1	B	465	GLN	4.8
1	B	585	ASP	4.7
1	B	575	ASP	4.6
1	A	344	ASP	4.6
1	B	293	ASN	4.5
1	C	594	GLN	4.4
1	B	592	THR	4.1
1	A	190	GLN	4.1
1	D	262	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	590	LEU	4.1
1	B	493	LEU	4.0
1	D	480	VAL	4.0
1	D	198	CYS	4.0
1	D	263	GLU	4.0
1	D	285	TRP	3.9
1	B	593	PRO	3.9
1	B	464	GLY	3.8
1	D	276	LEU	3.8
1	B	393	ALA	3.7
1	A	590	LEU	3.7
1	B	492	LYS	3.7
1	B	285	TRP	3.7
1	D	488	LEU	3.6
1	C	593	PRO	3.6
1	C	413	ILE	3.6
1	C	326	GLN	3.6
1	D	288	LYS	3.6
1	B	573	CYS	3.5
1	C	568	TYR	3.5
1	B	255	GLU	3.5
1	B	482	SER	3.5
1	B	344	ASP	3.4
1	B	562	LEU	3.4
1	D	599	ASN	3.4
1	B	485	PRO	3.4
1	C	255	GLU	3.4
1	C	587	ILE	3.4
1	B	590	LEU	3.4
1	C	491	VAL	3.3
1	B	190	GLN	3.3
1	C	561	SER	3.3
1	A	488	LEU	3.3
1	D	255	GLU	3.3
1	B	414	ASP	3.3
1	B	463	THR	3.3
1	B	498	PHE	3.3
1	B	572	TRP	3.3
1	C	488	LEU	3.2
1	B	346	GLU	3.2
1	B	556	LYS	3.2
1	B	348	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	588	ALA	3.2
1	B	594	GLN	3.1
1	D	326	GLN	3.1
1	C	327	ASN	3.1
1	C	329	PHE	3.1
1	C	493	LEU	3.1
1	A	593	PRO	3.1
1	C	596	LYS	3.0
1	D	345	ASN	3.0
1	D	572	TRP	3.0
1	C	599	ASN	3.0
1	C	598	TRP	3.0
1	C	277	GLU	2.9
1	B	487	VAL	2.9
1	D	398	GLU	2.9
1	B	490	ASP	2.9
1	B	484	LYS	2.9
1	A	434	THR	2.9
1	B	259	LEU	2.9
1	B	397	ILE	2.9
1	D	485	PRO	2.9
1	D	585	ASP	2.8
1	D	327	ASN	2.8
1	C	276	LEU	2.8
1	B	408	ARG	2.8
1	C	401	GLY	2.7
1	A	522	CYS	2.7
1	B	260	ILE	2.7
1	D	230	LYS	2.7
1	D	486	LYS	2.7
1	D	583	ASP	2.7
1	D	477	PRO	2.7
1	D	461	GLN	2.7
1	B	473	TYR	2.7
1	B	256	GLN	2.6
1	C	487	VAL	2.6
1	B	587	ILE	2.6
1	A	487	VAL	2.6
1	B	440	ASP	2.6
1	C	562	LEU	2.5
1	D	563	TYR	2.5
1	D	260	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	563	TYR	2.5
1	A	441	ALA	2.5
1	C	397	ILE	2.5
1	B	496	GLU	2.5
1	B	554	CYS	2.5
1	A	486	LYS	2.5
1	B	262	GLU	2.4
1	C	586	VAL	2.4
1	D	475	SER	2.4
1	D	509	MET	2.4
1	B	574	ALA	2.4
1	C	400	THR	2.4
1	D	251	LYS	2.4
1	A	530	ILE	2.4
1	D	498	PHE	2.4
1	D	569	PHE	2.4
1	C	437	LYS	2.4
1	D	284	LEU	2.3
1	B	598	TRP	2.3
1	D	275	PRO	2.3
1	B	497	ASP	2.3
1	D	350	CYS	2.3
1	D	239	MET	2.3
1	D	524	THR	2.3
1	D	497	ASP	2.2
1	C	591	ILE	2.2
1	A	343	VAL	2.2
1	A	489	LEU	2.2
1	D	400	THR	2.2
1	C	266	CYS	2.2
1	D	590	LEU	2.2
1	D	496	GLU	2.2
1	D	535	ASN	2.2
1	A	347	LEU	2.2
1	D	259	LEU	2.2
1	B	567	GLN	2.1
1	D	473	TYR	2.1
1	B	439	LYS	2.1
1	A	495	ALA	2.1
1	B	195	ASP	2.1
1	D	514	PRO	2.1
1	B	474	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	328	ASN	2.1
1	C	330	ASP	2.1
1	A	591	ILE	2.1
1	D	341	CYS	2.1
1	A	403	GLY	2.1
1	A	295	SER	2.1
1	B	476	LEU	2.1
1	C	263	GLU	2.1
1	A	284	LEU	2.1
1	D	250	ILE	2.0
1	B	597	GLU	2.0
1	C	511	GLU	2.0
1	A	402	ALA	2.0
1	A	433	SER	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, 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
3	MN	A	750	1/1	1.00	0.16	0.09	25,25,25,25	0
2	T8T	B	700	31/31	0.93	0.18	-0.26	59,69,80,85	0
3	MN	C	750	1/1	0.99	0.16	-0.70	25,25,25,25	0
3	MN	B	750	1/1	0.99	0.15	-0.82	51,51,51,51	0
3	MN	D	750	1/1	1.00	0.15	-0.89	43,43,43,43	0
2	T8T	D	700	31/31	0.94	0.15	-0.90	63,72,80,88	0
2	T8T	C	700	31/31	0.97	0.12	-1.38	42,46,51,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	T8T	A	700	31/31	0.96	0.12	-1.48	36,41,62,73	0
2	T8T	C	900	31/31	0.99	0.10	-1.71	36,39,41,42	0
2	T8T	D	800	31/31	0.98	0.13	-1.90	39,43,49,55	0
2	T8T	A	900	31/31	0.97	0.13	-1.91	27,29,31,31	0
2	T8T	B	800	31/31	0.99	0.11	-2.01	37,40,48,48	0
2	T8T	A	800	31/31	0.99	0.13	-2.07	23,24,25,26	0
2	T8T	C	800	31/31	0.98	0.11	-2.12	30,32,36,37	0
2	T8T	B	900	31/31	0.98	0.11	-2.24	36,40,46,47	0
2	T8T	D	900	31/31	0.99	0.10	-2.73	36,38,42,43	0
4	MG	D	950	1/1	0.99	0.09	-	34,34,34,34	0
4	MG	A	950	1/1	0.99	0.10	-	25,25,25,25	0
4	MG	C	950	1/1	0.99	0.10	-	28,28,28,28	0
4	MG	B	950	1/1	0.97	0.11	-	36,36,36,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.