



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:56 PM GMT

PDB ID : 4QFY
Title : Crystal structure of the tetrameric dGTP/dCTP-bound SAMHD1 (RN206) 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
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

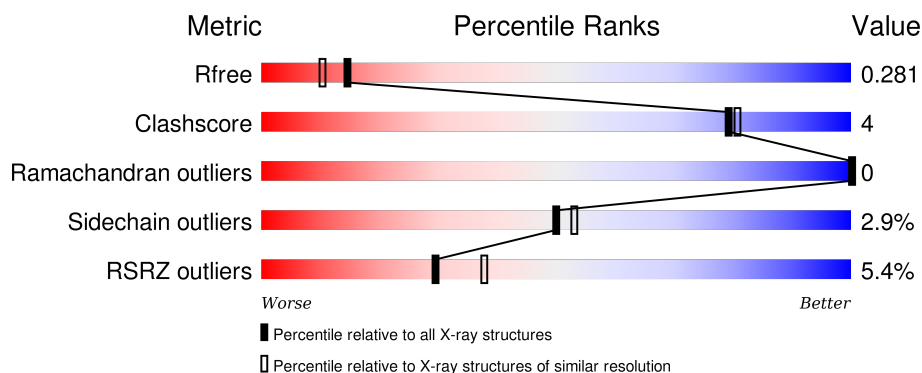
1 Overall quality at a glance

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 ≥ 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>6%</div> <div>76% 10% • 13%</div> </div>
1	B	550	<div> <div>3%</div> <div>79% 7% • 13%</div> </div>
1	C	550	<div> <div>7%</div> <div>78% 8% • 13%</div> </div>
1	D	550	<div> <div>3%</div> <div>80% 7% • 13%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16518 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	1	0
			3934	2518	685	711	20			
1	B	481	Total	C	N	O	S	0	1	0
			3940	2522	687	711	20			
1	C	481	Total	C	N	O	S	0	0	0
			3933	2517	685	711	20			
1	D	481	Total	C	N	O	S	0	2	0
			3949	2525	689	715	20			

There are 152 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

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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	206	ARG	HIS	ENGINEERED MUTATION	UNP Q9Y3Z3
A	207	ASN	ASP	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	102	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
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	206	ARG	HIS	ENGINEERED MUTATION	UNP Q9Y3Z3
B	207	ASN	ASP	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

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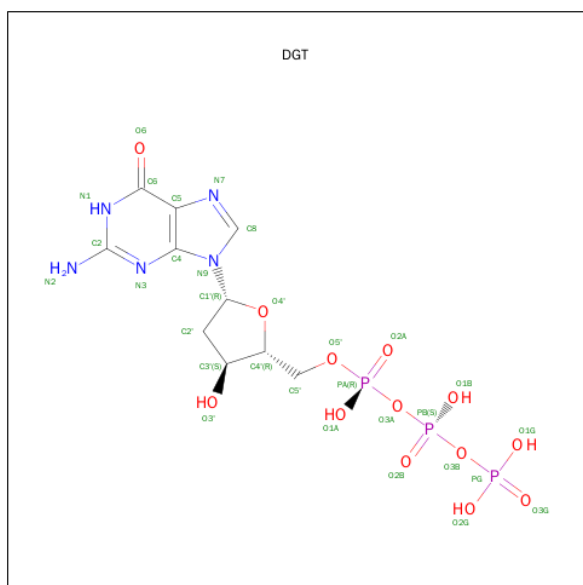
Chain	Residue	Modelled	Actual	Comment	Reference
C	106	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
C	107	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
C	108	ARG	-	EXPRESSION TAG	UNP Q9Y3Z3
C	109	ASP	-	EXPRESSION TAG	UNP Q9Y3Z3
C	110	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
C	111	ASN	-	EXPRESSION TAG	UNP Q9Y3Z3
C	112	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
C	206	ARG	HIS	ENGINEERED MUTATION	UNP Q9Y3Z3
C	207	ASN	ASP	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

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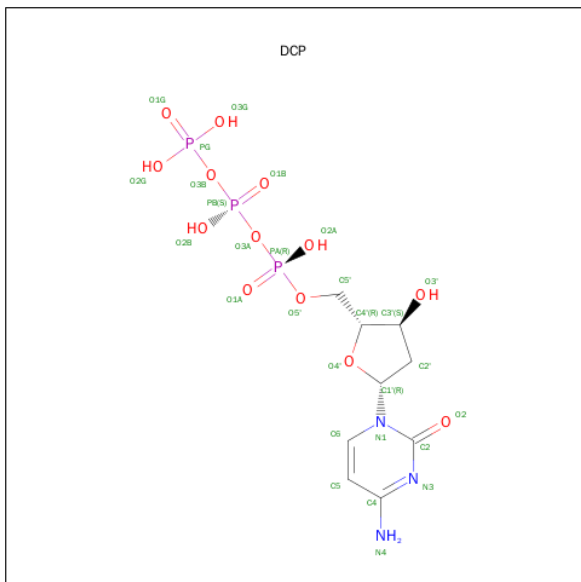
Chain	Residue	Modelled	Actual	Comment	Reference
D	110	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
D	111	ASN	-	EXPRESSION TAG	UNP Q9Y3Z3
D	112	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
D	206	ARG	HIS	ENGINEERED MUTATION	UNP Q9Y3Z3
D	207	ASN	ASP	ENGINEERED MUTATION	UNP Q9Y3Z3

- Molecule 2 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: $C_9H_{16}N_3O_{13}P_3$).



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

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

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

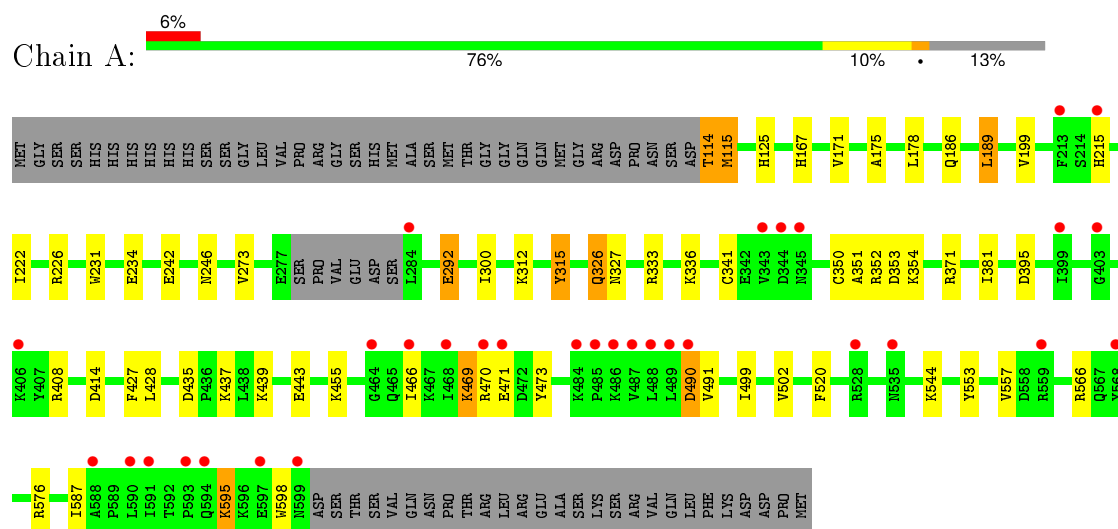
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	74	Total 74	O 74	0	0
5	B	124	Total 124	O 124	0	0
5	C	75	Total 75	O 75	0	0
5	D	121	Total 121	O 121	0	0

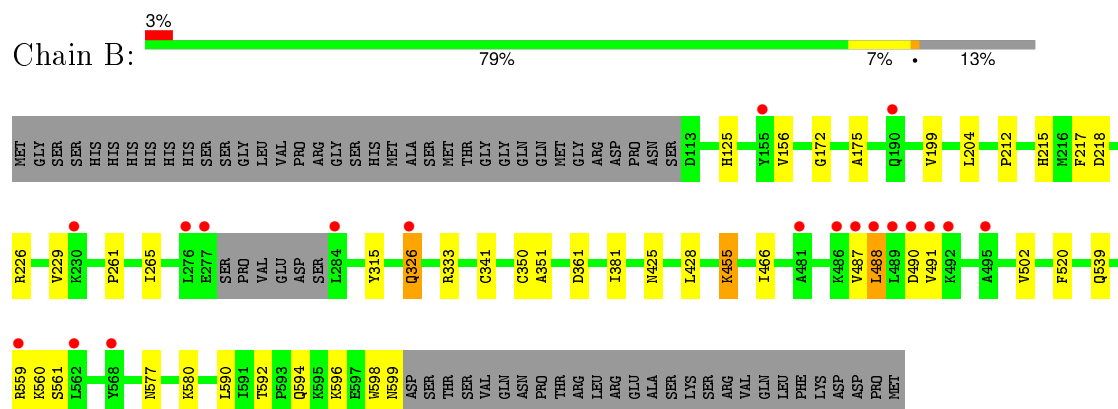
3 Residue-property plots [i](#)

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

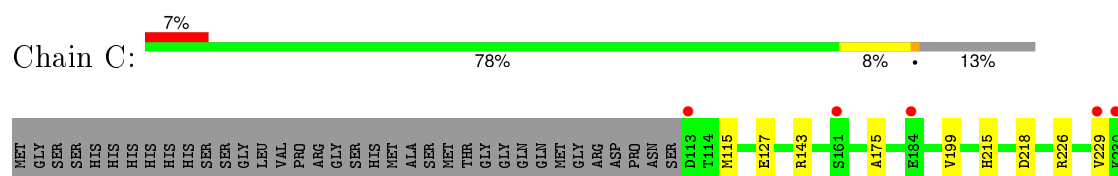
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

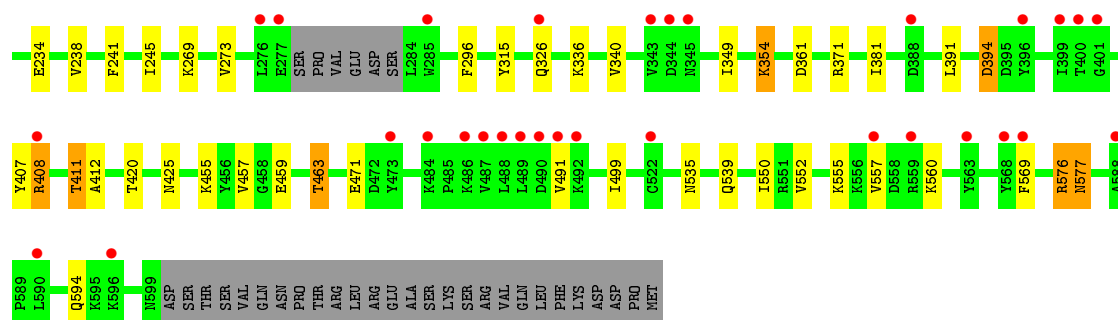


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

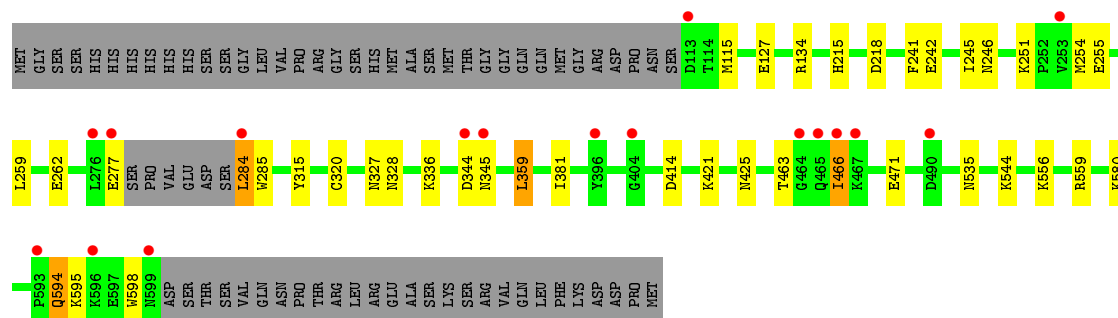
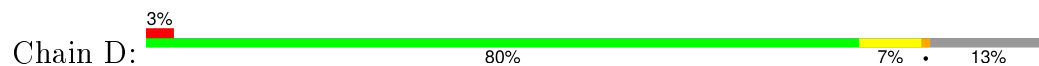


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.97Å 147.02Å 98.87Å 90.00° 114.31° 90.00°	Depositor
Resolution (Å)	38.67 – 2.10 38.67 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.67-2.10) 99.8 (38.67-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.226 , 0.269 0.237 , 0.281	Depositor DCC
R_{free} test set	2011 reflections (1.54%)	DCC
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 38.8	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.39$	Xtriage
Outliers	2 of 132853 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16518	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.29	0/4026	0.48	0/5434
1	B	0.31	0/4036	0.48	0/5448
1	C	0.29	0/4025	0.49	0/5433
1	D	0.31	0/4041	0.48	0/5455
All	All	0.30	0/16128	0.48	0/21770

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	407	TYR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3934	0	3922	39	0
1	B	3940	0	3928	27	0
1	C	3933	0	3921	34	0
1	D	3949	0	3932	23	0
2	A	93	0	36	1	0
2	B	31	0	12	0	0
2	C	93	0	36	3	0
2	D	31	0	12	1	0
3	A	28	0	12	2	0
3	B	28	0	12	1	0
3	C	28	0	12	2	0
3	D	28	0	12	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	3	0	0	0	0
4	D	1	0	0	0	0
5	A	74	0	0	0	0
5	B	124	0	0	0	0
5	C	75	0	0	0	0
5	D	121	0	0	1	0
All	All	16518	0	15847	112	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 (112) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:LYS:HE3	1:D:127:GLU:HG3	1.63	0.79
1:B:425:ASN:OD1	1:C:425:ASN:ND2	2.14	0.78
1:A:544:LYS:NZ	1:C:539:GLN:OE1	2.19	0.75
1:A:242:GLU:OE2	1:A:246:ASN:ND2	2.24	0.70
1:C:455:LYS:HG2	1:C:557:VAL:HG12	1.75	0.68
1:A:439:LYS:HD2	1:A:443:GLU:HG2	1.77	0.66
1:C:127:GLU:HG3	1:D:336:LYS:HE3	1.75	0.66
1:A:215:HIS:NE2	3:A:702:DCP:O2A	2.31	0.64
1:B:490:ASP:OD2	1:B:560:LYS:NZ	2.32	0.63
1:A:371:ARG:NH2	1:C:361:ASP:OD2	2.31	0.62
1:C:234:GLU:HB3	1:C:273:VAL:HG23	1.84	0.59
1:A:326:GLN:OE1	1:C:326:GLN:NE2	2.27	0.58
1:B:215[A]:HIS:NE2	3:B:701:DCP:O1A	2.28	0.57
1:B:326:GLN:HG3	1:D:328[A]:ASN:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:457:VAL:HB	1:C:552:VAL:HG13	1.87	0.56
1:D:535:ASN:OD1	1:D:535:ASN:N	2.38	0.56
1:C:552:VAL:HG11	1:C:569:PHE:CD1	2.42	0.55
1:A:490:ASP:N	1:A:490:ASP:OD1	2.30	0.54
1:C:296:PHE:HB2	1:C:349:ILE:HG13	1.89	0.54
1:C:215:HIS:HA	1:C:218:ASP:OD1	2.08	0.54
1:A:125:HIS:CE1	1:B:333:ARG:HB2	2.43	0.53
1:D:284:LEU:HD22	1:D:285:TRP:H	1.75	0.52
1:B:596:LYS:NZ	1:B:599:ASN:O	2.34	0.52
1:C:215:HIS:NE2	3:C:704:DCP:O1A	2.42	0.52
1:A:215:HIS:HE2	3:A:702:DCP:PA	2.32	0.52
1:A:435:ASP:OD2	1:A:437:LYS:HB2	2.10	0.51
1:C:391:LEU:O	1:C:394:ASP:HB2	2.10	0.51
1:D:215:HIS:NE2	3:D:702:DCP:O2A	2.43	0.51
1:A:326:GLN:HG3	1:A:327:ASN:N	2.26	0.50
1:C:408:ARG:HB2	1:C:411:THR:OG1	2.11	0.50
1:D:242:GLU:OE2	1:D:246:ASN:ND2	2.33	0.50
1:B:487:VAL:HG13	1:B:590:LEU:HD12	1.93	0.49
1:A:234:GLU:HB3	1:A:273:VAL:HG23	1.94	0.49
1:B:491:VAL:HG11	1:B:561:SER:HA	1.95	0.48
1:C:491:VAL:HG12	1:C:560:LYS:HG2	1.94	0.48
1:C:463:THR:OG1	1:C:577:ASN:O	2.30	0.47
1:A:175:ALA:HB1	1:A:199:VAL:HG12	1.95	0.47
1:D:327[A]:ASN:OD1	1:D:328[A]:ASN:N	2.47	0.47
1:D:215:HIS:HE2	3:D:702:DCP:PA	2.38	0.47
1:C:535:ASN:OD1	1:C:535:ASN:N	2.40	0.46
1:A:469:LYS:HG2	1:A:469:LYS:H	1.43	0.46
1:B:455:LYS:HA	1:B:455:LYS:HE3	1.98	0.46
1:A:186:GLN:HB2	1:A:189:LEU:HD22	1.96	0.46
1:B:175:ALA:HB1	1:B:199:VAL:HG12	1.97	0.46
1:A:470:ARG:HG3	1:A:473:TYR:CE2	2.51	0.46
1:D:215:HIS:HA	1:D:218:ASP:OD1	2.16	0.45
1:D:594:GLN:HG3	1:D:595:LYS:N	2.30	0.45
1:A:395:ASP:OD1	1:A:408:ARG:NH1	2.48	0.45
1:B:341:CYS:HB2	1:B:350:CYS:SG	2.56	0.45
1:A:455:LYS:HG2	1:A:557:VAL:HG12	1.98	0.45
1:A:473:TYR:CE1	1:A:502:VAL:HG11	2.52	0.45
1:C:499:ILE:HD11	1:C:555:LYS:HE2	1.97	0.45
1:A:167:HIS:O	1:A:171:VAL:HG23	2.17	0.45
1:A:292:GLU:HG3	1:A:292:GLU:H	1.54	0.45
1:B:539:GLN:OE1	1:D:544:LYS:NZ	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:CYS:HB2	1:A:350:CYS:SG	2.56	0.44
1:B:381:ILE:HD12	1:B:381:ILE:HA	1.75	0.44
1:C:560:LYS:HB3	1:C:560:LYS:HE3	1.53	0.44
1:A:428:LEU:HD12	1:D:425:ASN:HB2	1.98	0.44
1:B:172:GLY:HA3	1:B:204:LEU:HD13	2.00	0.44
1:A:595:LYS:HG2	1:A:598:TRP:CE2	2.53	0.44
1:B:156:VAL:O	2:C:702:DGT:H8	2.18	0.43
1:D:241:PHE:O	1:D:245:ILE:HG12	2.18	0.43
1:B:351:ALA:O	1:B:520:PHE:HA	2.18	0.43
1:C:238:VAL:HG13	1:C:269:LYS:HD3	2.00	0.43
1:A:352:ARG:CZ	1:A:354:LYS:HD2	2.49	0.43
1:B:212:PRO:HD2	1:B:217:PHE:CD1	2.53	0.43
1:D:359:LEU:HD12	1:D:359:LEU:HA	1.80	0.43
1:C:394:ASP:O	1:C:408:ARG:CZ	2.66	0.43
1:C:175:ALA:HB1	1:C:199:VAL:HG12	2.00	0.42
1:B:428:LEU:HD13	1:C:425:ASN:HB2	2.01	0.42
1:A:226:ARG:NH1	1:A:414:ASP:OD2	2.51	0.42
1:C:226:ARG:O	1:C:229:VAL:HG22	2.19	0.42
1:A:114:THR:HG22	1:A:115:MET:H	1.84	0.42
1:D:381:ILE:HA	1:D:381:ILE:HD12	1.85	0.42
1:D:320:CYS:SG	1:D:327[B]:ASN:HB2	2.60	0.42
2:C:702:DGT:H5'A	2:D:701:DGT:O1B	2.20	0.42
1:C:408:ARG:O	1:C:412:ALA:N	2.51	0.42
1:A:427:PHE:HD1	1:A:428:LEU:HD23	1.84	0.42
1:D:580:LYS:HB2	1:D:598:TRP:CG	2.55	0.42
1:D:134:ARG:HD2	5:D:900:HOH:O	2.19	0.42
1:A:222:ILE:HG21	1:A:231:TRP:HB3	2.01	0.42
1:A:499:ILE:HB	1:A:553:TYR:HB2	2.02	0.42
1:D:463:THR:O	1:D:466:ILE:HG22	2.20	0.42
2:A:701:DGT:H5'A	2:C:701:DGT:O1B	2.20	0.42
1:A:576:ARG:HB3	1:A:576:ARG:HE	1.71	0.42
1:A:333:ARG:HB2	1:B:125:HIS:CE1	2.54	0.42
1:A:381:ILE:HA	1:A:381:ILE:HD12	1.91	0.42
1:B:580:LYS:HB2	1:B:598:TRP:CG	2.55	0.42
1:C:576:ARG:HB3	1:C:576:ARG:HE	1.62	0.41
1:A:351:ALA:O	1:A:520:PHE:HA	2.19	0.41
1:B:488:LEU:H	1:B:488:LEU:HG	1.53	0.41
1:C:241:PHE:O	1:C:245:ILE:HG12	2.20	0.41
1:A:178:LEU:HD23	1:A:300:ILE:HG23	2.02	0.41
1:B:466:ILE:HD12	1:B:466:ILE:H	1.85	0.41
1:A:353:ASP:OD1	1:A:354:LYS:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ARG:HB3	1:B:229:VAL:HG12	2.01	0.41
1:C:143:ARG:HD2	1:C:420:THR:HA	2.01	0.41
1:D:251:LYS:O	1:D:255:GLU:HG3	2.21	0.41
1:B:261:PRO:O	1:B:265:ILE:HB	2.20	0.41
1:C:381:ILE:HD12	1:C:381:ILE:HA	1.81	0.41
1:B:215[A]:HIS:HA	1:B:218:ASP:OD1	2.21	0.41
1:A:312:LYS:HA	1:A:315:TYR:CE2	2.56	0.41
1:C:354:LYS:HE2	1:C:354:LYS:HB3	1.78	0.41
1:C:215:HIS:HE2	3:C:704:DCP:PA	2.43	0.40
1:D:254:MET:HE3	1:D:259:LEU:HD23	2.03	0.40
1:A:566:ARG:HD3	1:A:587:ILE:HB	2.03	0.40
1:B:596:LYS:HA	1:B:596:LYS:HD2	1.82	0.40
1:A:336:LYS:HD2	1:B:125:HIS:HB3	2.04	0.40
1:C:459:GLU:HA	1:C:550:ILE:O	2.21	0.40
1:C:394:ASP:CG	1:C:408:ARG:HH22	2.25	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	477/550 (87%)	466 (98%)	11 (2%)	0	100	100
1	B	478/550 (87%)	462 (97%)	16 (3%)	0	100	100
1	C	477/550 (87%)	458 (96%)	19 (4%)	0	100	100
1	D	479/550 (87%)	468 (98%)	11 (2%)	0	100	100
All	All	1911/2200 (87%)	1854 (97%)	57 (3%)	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	427/488 (88%)	415 (97%)	12 (3%)	51	55
1	B	428/488 (88%)	418 (98%)	10 (2%)	58	62
1	C	427/488 (88%)	414 (97%)	13 (3%)	48	51
1	D	429/488 (88%)	414 (96%)	15 (4%)	43	44
All	All	1711/1952 (88%)	1661 (97%)	50 (3%)	50	53

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	THR
1	A	115	MET
1	A	189	LEU
1	A	292	GLU
1	A	315	TYR
1	A	326	GLN
1	A	466	ILE
1	A	469	LYS
1	A	471	GLU
1	A	490	ASP
1	A	491	VAL
1	A	595	LYS
1	B	315	TYR
1	B	326	GLN
1	B	361	ASP
1	B	455	LYS
1	B	488	LEU
1	B	502	VAL
1	B	559	ARG
1	B	577	ASN
1	B	592	THR
1	B	594	GLN
1	C	115	MET
1	C	315	TYR

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Mol	Chain	Res	Type
1	C	340	VAL
1	C	354	LYS
1	C	371	ARG
1	C	394	ASP
1	C	408	ARG
1	C	411	THR
1	C	463	THR
1	C	471	GLU
1	C	576	ARG
1	C	577	ASN
1	C	594	GLN
1	D	115	MET
1	D	262	GLU
1	D	277	GLU
1	D	284	LEU
1	D	315	TYR
1	D	344	ASP
1	D	345	ASN
1	D	359	LEU
1	D	414	ASP
1	D	421	LYS
1	D	466	ILE
1	D	471	GLU
1	D	556	LYS
1	D	559	ARG
1	D	594	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	321	HIS
1	A	425	ASN
1	B	235	GLN
1	C	243	HIS

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 ⓘ

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$
2	DGT	A	701	4	25,33,33	1.66	5 (20%)	35,52,52	1.73	7 (20%)
3	DCP	A	702	4	21,29,29	1.27	4 (19%)	33,45,45	1.50	6 (18%)
2	DGT	A	703	4	25,33,33	1.63	5 (20%)	35,52,52	1.78	9 (25%)
2	DGT	A	704	4	25,33,33	1.65	5 (20%)	35,52,52	1.75	7 (20%)
3	DCP	B	701	4	21,29,29	1.28	4 (19%)	33,45,45	1.50	6 (18%)
2	DGT	B	702	4	25,33,33	1.65	6 (24%)	35,52,52	1.76	8 (22%)
2	DGT	C	701	4	25,33,33	1.60	5 (20%)	35,52,52	1.70	8 (22%)
2	DGT	C	702	4	25,33,33	1.63	5 (20%)	35,52,52	1.74	6 (17%)
2	DGT	C	703	4	25,33,33	1.68	5 (20%)	35,52,52	1.80	6 (17%)
3	DCP	C	704	4	21,29,29	1.26	4 (19%)	33,45,45	1.53	8 (24%)
2	DGT	D	701	4	25,33,33	1.60	5 (20%)	35,52,52	1.76	9 (25%)
3	DCP	D	702	4	21,29,29	1.28	4 (19%)	33,45,45	1.50	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	DGT	A	701	4	-	0/18/34/34	0/3/3/3
3	DCP	A	702	4	-	0/18/34/34	0/2/2/2
2	DGT	A	703	4	-	0/18/34/34	0/3/3/3
2	DGT	A	704	4	-	0/18/34/34	0/3/3/3
3	DCP	B	701	4	-	0/18/34/34	0/2/2/2
2	DGT	B	702	4	-	0/18/34/34	0/3/3/3
2	DGT	C	701	4	-	0/18/34/34	0/3/3/3
2	DGT	C	702	4	-	0/18/34/34	0/3/3/3
2	DGT	C	703	4	-	0/18/34/34	0/3/3/3
3	DCP	C	704	4	-	0/18/34/34	0/2/2/2
2	DGT	D	701	4	-	0/18/34/34	0/3/3/3
3	DCP	D	702	4	-	0/18/34/34	0/2/2/2

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	703	DGT	C5'-C4'	-2.83	1.42	1.51
2	A	701	DGT	C5'-C4'	-2.80	1.42	1.51
2	A	704	DGT	C5'-C4'	-2.66	1.43	1.51
2	B	702	DGT	C5'-C4'	-2.65	1.43	1.51
2	C	702	DGT	C5'-C4'	-2.63	1.43	1.51
2	C	703	DGT	O3'-C3'	-2.60	1.37	1.43
2	C	701	DGT	C5'-C4'	-2.60	1.43	1.51
2	D	701	DGT	O3'-C3'	-2.57	1.37	1.43
2	A	703	DGT	C5'-C4'	-2.56	1.43	1.51
2	A	703	DGT	O3'-C3'	-2.56	1.37	1.43
2	D	701	DGT	C5'-C4'	-2.54	1.43	1.51
2	C	702	DGT	O3'-C3'	-2.50	1.37	1.43
3	C	704	DCP	O3'-C3'	-2.48	1.37	1.43
2	A	701	DGT	O3'-C3'	-2.48	1.37	1.43
3	D	702	DCP	C5'-C4'	-2.47	1.43	1.51
2	A	704	DGT	O3'-C3'	-2.47	1.37	1.43
3	A	702	DCP	O3'-C3'	-2.44	1.37	1.43
3	B	701	DCP	O3'-C3'	-2.44	1.37	1.43
3	D	702	DCP	O3'-C3'	-2.39	1.38	1.43
2	B	702	DGT	O3'-C3'	-2.38	1.38	1.43
3	B	701	DCP	C5'-C4'	-2.36	1.44	1.51
2	C	703	DGT	C2'-C3'	-2.35	1.46	1.52
2	C	701	DGT	O3'-C3'	-2.34	1.38	1.43
2	A	701	DGT	C2'-C3'	-2.32	1.46	1.52
2	D	701	DGT	C2'-C3'	-2.30	1.46	1.52
3	A	702	DCP	C5'-C4'	-2.29	1.44	1.51
2	A	704	DGT	C2'-C3'	-2.28	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	704	DCP	C5'-C4'	-2.25	1.44	1.51
2	A	703	DGT	C2'-C3'	-2.24	1.46	1.52
3	B	701	DCP	C2'-C3'	-2.21	1.46	1.52
2	B	702	DGT	C2'-C3'	-2.21	1.46	1.52
3	C	704	DCP	C2'-C3'	-2.14	1.47	1.52
2	C	702	DGT	C2'-C3'	-2.13	1.47	1.52
3	A	702	DCP	C2'-C3'	-2.11	1.47	1.52
3	D	702	DCP	C2'-C3'	-2.03	1.47	1.52
2	C	701	DGT	C2'-C3'	-2.00	1.47	1.52
2	B	702	DGT	PG-O3G	2.45	1.59	1.51
3	C	704	DCP	C4-N4	2.72	1.43	1.35
3	D	702	DCP	C4-N4	2.73	1.43	1.35
3	A	702	DCP	C4-N4	2.75	1.43	1.35
3	B	701	DCP	C4-N4	2.83	1.43	1.35
2	C	702	DGT	C2-N2	2.95	1.40	1.34
2	D	701	DGT	C2-N2	3.14	1.40	1.34
2	A	704	DGT	C2-N2	3.15	1.40	1.34
2	C	703	DGT	C2-N2	3.21	1.40	1.34
2	B	702	DGT	C2-N2	3.22	1.40	1.34
2	C	701	DGT	C2-N2	3.24	1.40	1.34
2	A	701	DGT	C2-N2	3.31	1.40	1.34
2	A	703	DGT	C2-N2	3.37	1.40	1.34
2	B	702	DGT	O6-C6	4.67	1.35	1.24
2	A	701	DGT	O6-C6	4.84	1.36	1.24
2	C	701	DGT	O6-C6	4.84	1.36	1.24
2	A	704	DGT	O6-C6	4.86	1.36	1.24
2	C	703	DGT	O6-C6	4.92	1.36	1.24
2	C	702	DGT	O6-C6	4.96	1.36	1.24
2	D	701	DGT	O6-C6	4.98	1.36	1.24
2	A	703	DGT	O6-C6	5.05	1.36	1.24

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	DGT	N3-C2-N1	-4.34	120.83	127.44
2	A	704	DGT	PA-O3A-PB	-4.32	120.59	132.73
2	C	703	DGT	N3-C2-N1	-4.24	120.98	127.44
2	B	702	DGT	N3-C2-N1	-4.18	121.08	127.44
3	C	704	DCP	PB-O3A-PA	-4.11	121.19	132.73
2	A	704	DGT	N3-C2-N1	-4.11	121.19	127.44
2	A	703	DGT	N3-C2-N1	-4.09	121.21	127.44
2	D	701	DGT	N3-C2-N1	-4.05	121.28	127.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	703	DGT	PA-O3A-PB	-4.03	121.42	132.73
2	C	702	DGT	N3-C2-N1	-4.02	121.31	127.44
3	A	702	DCP	PB-O3A-PA	-4.00	121.49	132.73
2	C	701	DGT	N3-C2-N1	-4.00	121.36	127.44
3	B	701	DCP	PB-O3A-PA	-3.93	121.69	132.73
3	D	702	DCP	PB-O3A-PA	-3.90	121.78	132.73
2	A	701	DGT	PA-O3A-PB	-3.86	121.88	132.73
2	C	702	DGT	PA-O3A-PB	-3.73	122.25	132.73
2	A	703	DGT	C5-C6-N1	-3.65	118.59	123.59
2	D	701	DGT	C5-C6-N1	-3.65	118.60	123.59
2	C	703	DGT	C5-C6-N1	-3.61	118.65	123.59
2	A	704	DGT	C5-C6-N1	-3.59	118.68	123.59
2	A	701	DGT	C5-C6-N1	-3.59	118.68	123.59
2	C	701	DGT	C5-C6-N1	-3.51	118.79	123.59
2	C	702	DGT	C5-C6-N1	-3.39	118.95	123.59
2	B	702	DGT	C5-C6-N1	-3.35	119.00	123.59
2	A	703	DGT	PA-O3A-PB	-3.21	123.72	132.73
2	D	701	DGT	C1'-N9-C4	-3.21	121.72	127.16
2	B	702	DGT	C1'-N9-C4	-3.12	121.87	127.16
2	D	701	DGT	C4-C5-N7	-2.73	106.97	109.48
2	C	701	DGT	PA-O3A-PB	-2.72	125.09	132.73
2	C	701	DGT	C4-C5-N7	-2.60	107.08	109.48
2	D	701	DGT	PA-O3A-PB	-2.57	125.50	132.73
2	C	702	DGT	C4-C5-N7	-2.56	107.12	109.48
2	D	701	DGT	PB-O3B-PG	-2.43	124.50	132.67
2	A	703	DGT	PB-O3B-PG	-2.43	124.51	132.67
2	B	702	DGT	C6-C5-C4	-2.42	118.01	120.90
2	A	703	DGT	C1'-N9-C4	-2.39	123.10	127.16
2	B	702	DGT	C4-C5-N7	-2.38	107.29	109.48
2	C	703	DGT	C4-C5-N7	-2.25	107.41	109.48
2	C	701	DGT	C1'-N9-C4	-2.22	123.39	127.16
2	A	704	DGT	C4-C5-N7	-2.22	107.44	109.48
3	D	702	DCP	PB-O3B-PG	-2.20	125.28	132.67
3	C	704	DCP	PB-O3B-PG	-2.20	125.31	132.67
2	D	701	DGT	C6-C5-C4	-2.19	118.28	120.90
3	C	704	DCP	C5-C4-N3	-2.18	119.05	121.80
2	A	703	DGT	C4-C5-N7	-2.17	107.48	109.48
2	A	701	DGT	C4-C5-N7	-2.17	107.49	109.48
3	A	702	DCP	C5-C4-N3	-2.16	119.08	121.80
3	B	701	DCP	C5-C4-N3	-2.08	119.17	121.80
3	D	702	DCP	C5-C4-N3	-2.05	119.22	121.80
2	C	701	DGT	C6-C5-C4	-2.04	118.46	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	DGT	C6-C5-C4	-2.00	118.51	120.90
3	B	701	DCP	O4'-C1'-N1	2.03	111.24	107.72
3	C	704	DCP	N4-C4-N3	2.04	120.21	116.50
2	A	704	DGT	O5'-C5'-C4'	2.04	116.66	109.12
3	B	701	DCP	N4-C4-N3	2.04	120.23	116.50
3	A	702	DCP	O5'-C5'-C4'	2.22	117.30	109.12
3	C	704	DCP	O5'-C5'-C4'	2.23	117.34	109.12
2	B	702	DGT	O5'-C5'-C4'	2.24	117.38	109.12
3	A	702	DCP	O4'-C1'-N1	2.36	111.81	107.72
2	A	703	DGT	O5'-C5'-C4'	2.38	117.89	109.12
2	C	701	DGT	O3A-PA-O5'	2.42	109.37	102.94
3	C	704	DCP	O3A-PA-O5'	2.45	109.45	102.94
2	D	701	DGT	O3A-PA-O5'	2.47	109.49	102.94
2	A	701	DGT	O3A-PA-O5'	2.49	109.55	102.94
2	C	702	DGT	O3A-PA-O5'	2.50	109.57	102.94
3	C	704	DCP	O4'-C1'-N1	2.55	112.13	107.72
3	D	702	DCP	O4'-C1'-N1	2.57	112.17	107.72
2	A	704	DGT	O3A-PA-O5'	2.65	109.97	102.94
2	C	703	DGT	O3A-PA-O5'	2.73	110.18	102.94
3	D	702	DCP	O3A-PA-O5'	2.78	110.32	102.94
3	A	702	DCP	O3A-PA-O5'	2.84	110.46	102.94
3	B	701	DCP	O3A-PA-O5'	3.03	110.97	102.94
3	C	704	DCP	C2-N3-C4	3.43	120.45	115.61
2	B	702	DGT	O3A-PA-O5'	3.48	112.17	102.94
2	A	703	DGT	O3A-PA-O5'	3.50	112.23	102.94
2	C	702	DGT	C6-N1-C2	3.63	120.98	115.94
3	D	702	DCP	C2-N3-C4	3.67	120.79	115.61
3	B	701	DCP	C2-N3-C4	3.96	121.20	115.61
2	C	701	DGT	C6-N1-C2	4.01	121.50	115.94
3	A	702	DCP	C2-N3-C4	4.02	121.28	115.61
2	A	704	DGT	C6-N1-C2	4.03	121.53	115.94
2	A	703	DGT	C6-N1-C2	4.08	121.60	115.94
2	B	702	DGT	C6-N1-C2	4.13	121.67	115.94
2	C	703	DGT	C6-N1-C2	4.17	121.73	115.94
2	D	701	DGT	C6-N1-C2	4.22	121.79	115.94
2	A	701	DGT	C6-N1-C2	4.29	121.89	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	DGT	1	0
3	A	702	DCP	2	0
3	B	701	DCP	1	0
2	C	701	DGT	1	0
2	C	702	DGT	2	0
3	C	704	DCP	2	0
2	D	701	DGT	1	0
3	D	702	DCP	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	480/550 (87%)	0.44	32 (6%) 21 28	17, 32, 52, 69	237 (49%)
1	B	481/550 (87%)	0.25	19 (3%) 42 51	16, 27, 48, 62	193 (40%)
1	C	481/550 (87%)	0.45	36 (7%) 17 23	18, 33, 57, 76	238 (49%)
1	D	481/550 (87%)	0.15	17 (3%) 48 57	14, 26, 42, 64	188 (39%)
All	All	1923/2200 (87%)	0.32	104 (5%) 29 38	14, 30, 52, 76	856 (44%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	489	LEU	8.5
1	B	488	LEU	8.0
1	A	488	LEU	6.8
1	C	488	LEU	6.5
1	D	345	ASN	5.2
1	A	599	ASN	5.1
1	A	284	LEU	4.8
1	D	466	ILE	4.7
1	D	465	GLN	4.7
1	D	284	LEU	4.7
1	A	489	LEU	4.6
1	C	276	LEU	4.6
1	D	396	TYR	4.5
1	D	113	ASP	4.3
1	A	487	VAL	4.3
1	B	490	ASP	4.2
1	A	345	ASN	4.2
1	D	599	ASN	4.1
1	C	489	LEU	4.1
1	B	284	LEU	4.1
1	C	590	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	596	LYS	4.0
1	C	596	LYS	3.7
1	A	490	ASP	3.5
1	A	535	ASN	3.5
1	B	487	VAL	3.4
1	A	466	ILE	3.3
1	B	495	ALA	3.3
1	A	470	ARG	3.2
1	C	490	ASP	3.2
1	B	562	LEU	3.2
1	D	277	GLU	3.1
1	A	593	PRO	3.1
1	C	487	VAL	3.1
1	B	486	LYS	3.1
1	D	404	GLY	2.9
1	C	408	ARG	2.9
1	B	491	VAL	2.9
1	A	344	ASP	2.9
1	D	464	GLY	2.8
1	B	492	LYS	2.8
1	C	400	THR	2.8
1	B	277	GLU	2.8
1	C	344	ASP	2.8
1	D	253	VAL	2.8
1	A	215	HIS	2.8
1	A	486	LYS	2.7
1	D	276	LEU	2.7
1	D	344	ASP	2.7
1	A	597	GLU	2.7
1	C	277	GLU	2.6
1	A	403	GLY	2.6
1	A	568	TYR	2.6
1	B	559	ARG	2.6
1	C	588	ALA	2.6
1	B	326	GLN	2.6
1	C	343	VAL	2.6
1	B	568	TYR	2.5
1	A	591	ILE	2.5
1	A	485	PRO	2.5
1	C	491	VAL	2.5
1	A	559	ARG	2.5
1	C	345	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	230	LYS	2.4
1	A	590	LEU	2.4
1	B	481	ALA	2.4
1	C	484	LYS	2.4
1	A	213	PHE	2.4
1	D	490	ASP	2.4
1	A	594	GLN	2.4
1	C	229	VAL	2.4
1	C	522	CYS	2.4
1	B	276	LEU	2.4
1	C	399	ILE	2.3
1	A	399	ILE	2.3
1	A	468	ILE	2.3
1	C	388	ASP	2.3
1	A	406	LYS	2.3
1	C	184	GLU	2.3
1	C	396	TYR	2.3
1	C	559	ARG	2.3
1	C	326	GLN	2.3
1	C	557	VAL	2.3
1	A	343	VAL	2.2
1	C	285	TRP	2.2
1	A	588	ALA	2.2
1	B	155	TYR	2.2
1	A	464	GLY	2.2
1	A	484	LYS	2.2
1	D	593	PRO	2.2
1	C	492	LYS	2.1
1	C	569	PHE	2.1
1	A	528	ARG	2.1
1	C	568	TYR	2.1
1	C	486	LYS	2.1
1	C	563	TYR	2.1
1	C	401	GLY	2.1
1	C	473	TYR	2.1
1	A	471	GLU	2.0
1	D	467	LYS	2.0
1	C	113	ASP	2.0
1	B	190	GLN	2.0
1	C	161	SER	2.0
1	B	230	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	DCP	D	702	28/28	0.94	0.15	0.31	13,18,22,24	28
2	DGT	A	703	31/31	0.96	0.13	-0.19	19,24,30,32	31
2	DGT	A	701	31/31	0.97	0.13	-0.32	17,21,28,30	0
2	DGT	C	703	31/31	0.96	0.13	-0.34	17,22,27,30	31
3	DCP	A	702	28/28	0.96	0.12	-0.40	19,25,31,33	28
3	DCP	C	704	28/28	0.96	0.12	-0.55	19,27,30,34	28
3	DCP	B	701	28/28	0.97	0.11	-0.58	14,19,23,28	28
2	DGT	C	701	31/31	0.96	0.12	-0.68	16,21,26,29	0
2	DGT	B	702	31/31	0.97	0.11	-0.83	15,17,21,22	0
2	DGT	C	702	31/31	0.97	0.12	-0.83	16,20,25,28	0
2	DGT	D	701	31/31	0.97	0.10	-0.95	15,19,26,27	0
2	DGT	A	704	31/31	0.97	0.10	-1.12	13,17,22,25	0
4	MG	C	707	1/1	0.92	0.07	-	22,22,22,22	0
4	MG	B	703	1/1	0.79	0.12	-	26,26,26,26	0
4	MG	C	706	1/1	0.95	0.07	-	35,35,35,35	0
4	MG	A	705	1/1	0.97	0.18	-	34,34,34,34	0
4	MG	D	703	1/1	0.96	0.04	-	17,17,17,17	1
4	MG	C	705	1/1	0.88	0.07	-	22,22,22,22	1
4	MG	A	706	1/1	0.80	0.14	-	19,19,19,19	0
4	MG	B	704	1/1	0.84	0.13	-	23,23,23,23	1

6.5 Other polymers [i](#)

There are no such residues in this entry.