



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:56 PM GMT

PDB ID : 4QG0
Title : Crystal structure of the tetrameric dGTP/dUTP-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 : 2.30 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

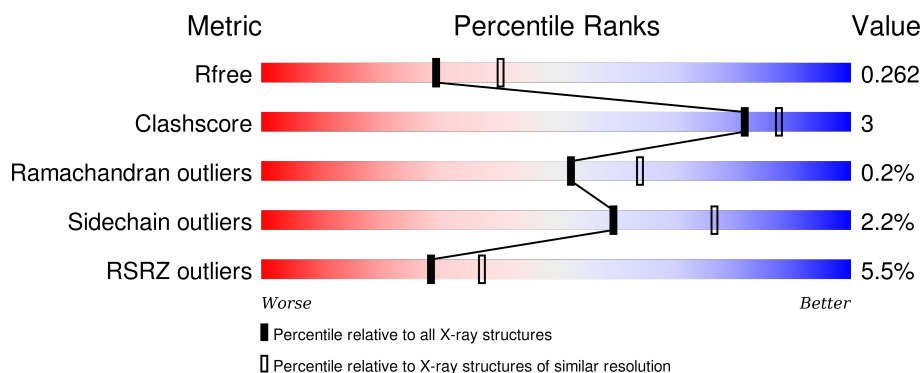
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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> <div></div> <div>80%</div> <div>7%</div> <div>13%</div> </div> </div>
1	B	550	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>8%</div> <div>13%</div> </div> </div>
1	C	550	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>10%</div> <div>13%</div> </div> </div>
1	D	550	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>7%</div> <div>13%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DUT	C	703	-	-	-	X
5	EDO	D	706	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16309 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	2	0
			3946	2527	688	711	20			
1	B	480	Total	C	N	O	S	0	2	0
			3938	2521	688	709	20			
1	C	481	Total	C	N	O	S	0	2	0
			3945	2525	686	714	20			
1	D	481	Total	C	N	O	S	0	1	0
			3939	2521	685	713	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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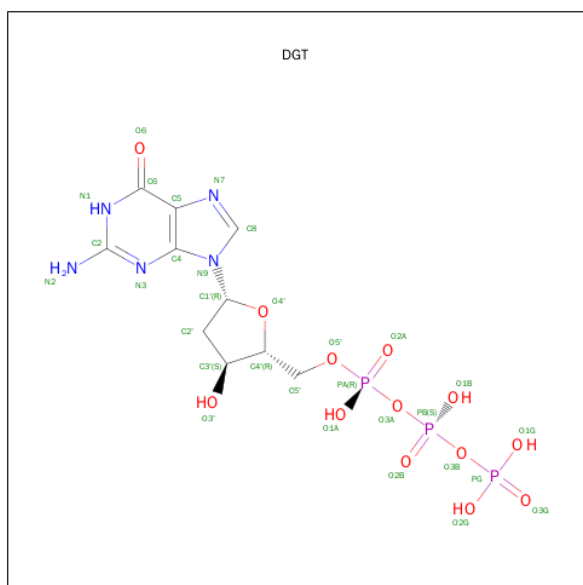
Chain	Residue	Modelled	Actual	Comment	Reference
C	106	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
C	107	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
C	108	ARG	-	EXPRESSION TAG	UNP Q9Y3Z3
C	109	ASP	-	EXPRESSION TAG	UNP Q9Y3Z3
C	110	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
C	111	ASN	-	EXPRESSION TAG	UNP Q9Y3Z3
C	112	SER	-	EXPRESSION TAG	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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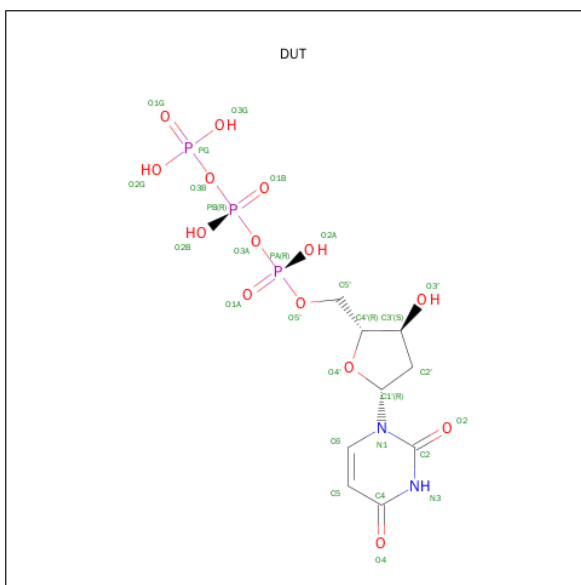
Chain	Residue	Modelled	Actual	Comment	Reference
D	110	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
D	111	ASN	-	EXPRESSION TAG	UNP Q9Y3Z3
D	112	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
D	206	ARG	HIS	ENGINEERED MUTATION	UNP Q9Y3Z3
D	207	ASN	ASP	ENGINEERED MUTATION	UNP Q9Y3Z3

- 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	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	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is DEOXYURIDINE-5'-TRIPHOSPHATE (three-letter code: DUT) (formula: $C_9H_{15}N_2O_{14}P_3$).

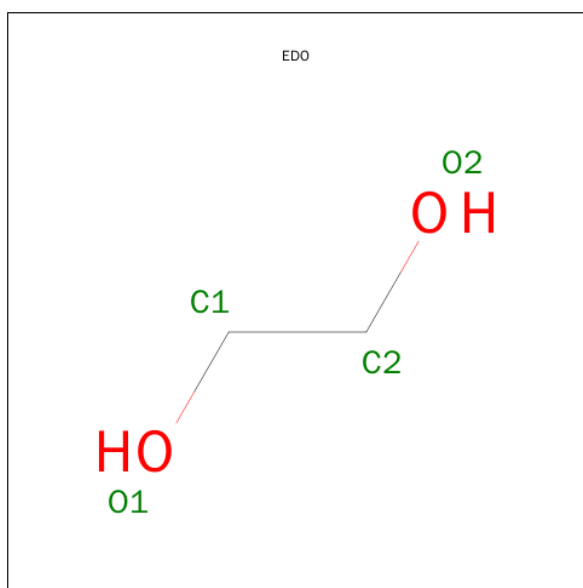


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 28	C 9	N 2	O 14	P 3	0	0
3	A	1	Total 28	C 9	N 2	O 14	P 3	0	0
3	B	1	Total 28	C 9	N 2	O 14	P 3	0	0
3	B	1	Total 28	C 9	N 2	O 14	P 3	0	0
3	C	1	Total 28	C 9	N 2	O 14	P 3	0	0
3	C	1	Total 28	C 9	N 2	O 14	P 3	0	0
3	D	1	Total 28	C 9	N 2	O 14	P 3	0	0
3	D	1	Total 28	C 9	N 2	O 14	P 3	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	3	Total Mg 3 3	0	0
4	D	2	Total Mg 2 2	0	0
4	C	1	Total Mg 1 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	2	2		

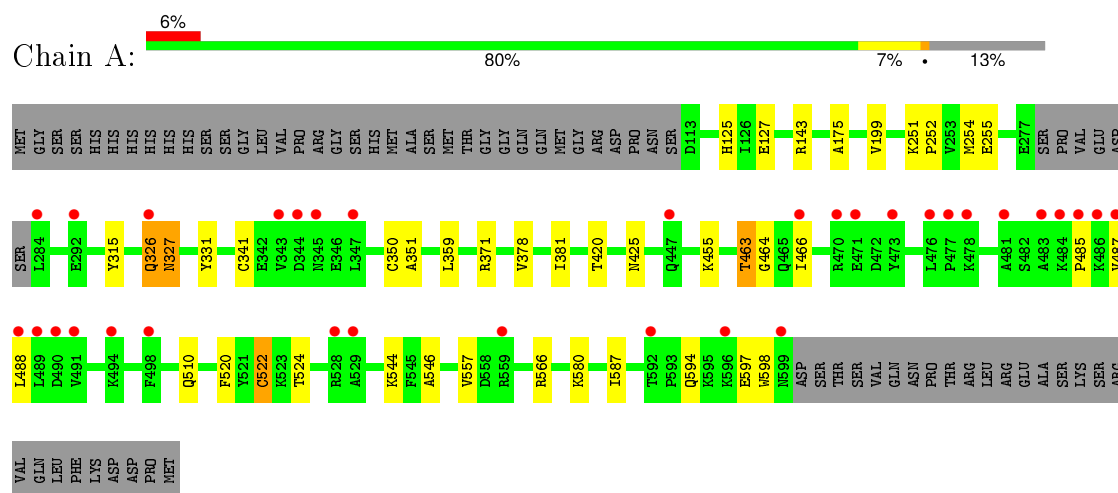
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	43	Total	O	0	0
			43	43		
6	B	45	Total	O	0	0
			45	45		
6	C	39	Total	O	0	0
			39	39		
6	D	55	Total	O	0	0
			55	55		

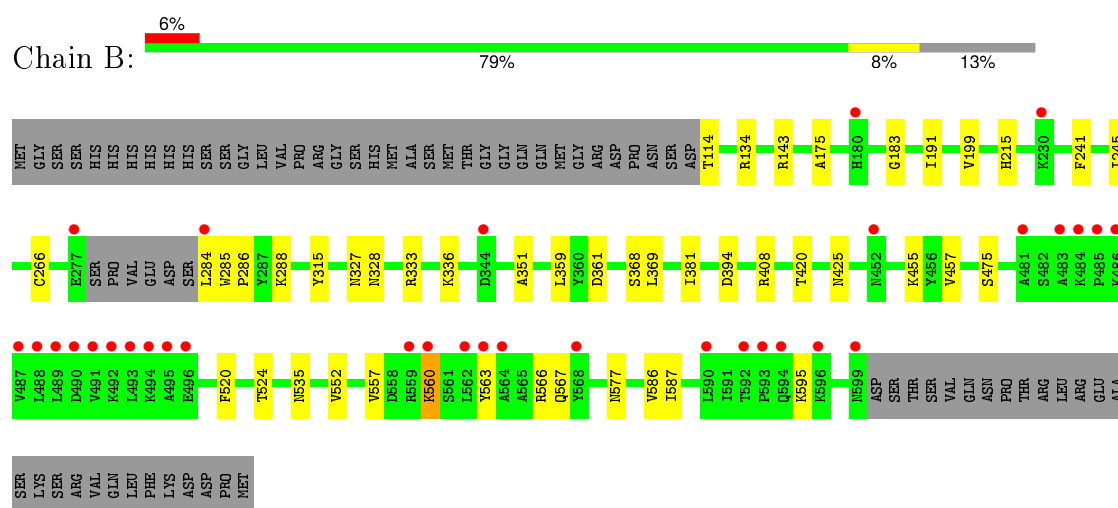
3 Residue-property plots

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

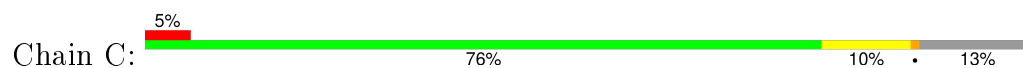
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

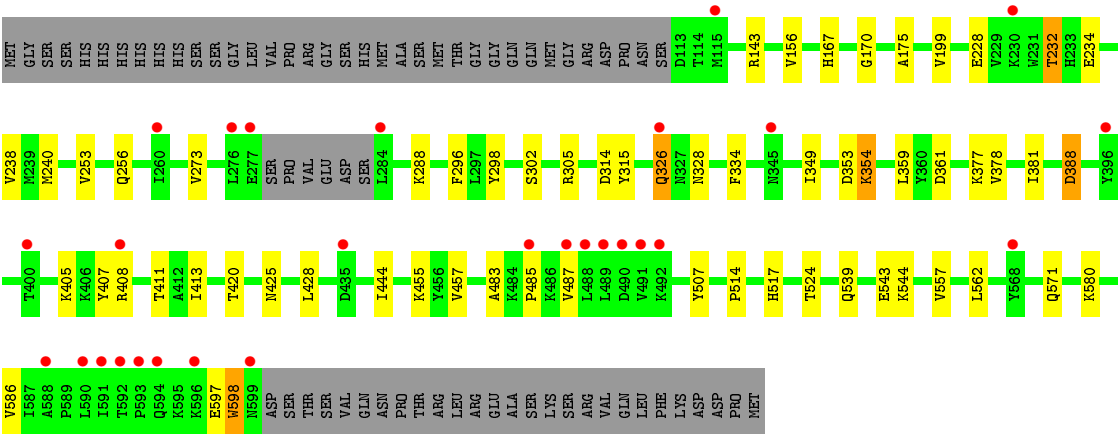


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

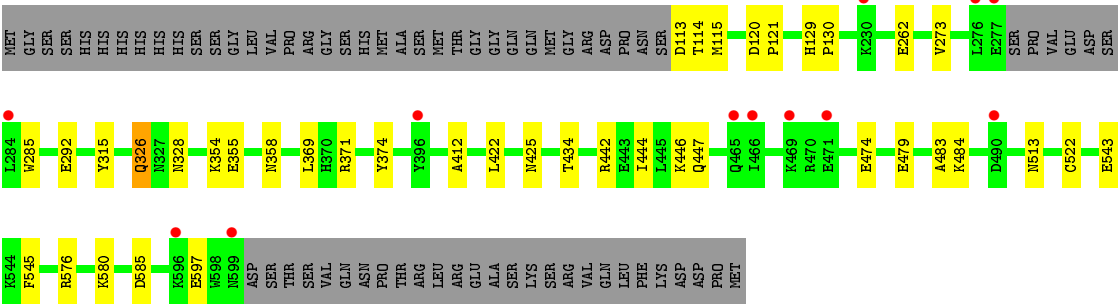
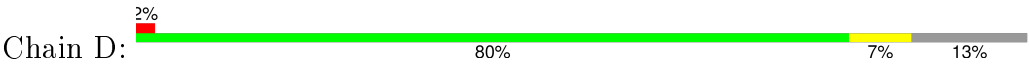


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.86Å 146.60Å 98.69Å 90.00° 114.62° 90.00°	Depositor
Resolution (Å)	42.91 – 2.30 42.91 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.91-2.30) 99.8 (42.91-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.197 , 0.250 0.209 , 0.262	Depositor DCC
R_{free} test set	2011 reflections (2.04%)	DCC
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.9	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	1 of 100413 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16309	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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, DUT, EDO, DGT

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	0.35	0/4045	0.53	0/5459
1	B	0.35	0/4036	0.51	0/5447
1	C	0.34	0/4043	0.52	0/5457
1	D	0.38	0/4034	0.54	0/5445
All	All	0.36	0/16158	0.52	0/21808

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3946	0	3941	28	0
1	B	3938	0	3936	28	0
1	C	3945	0	3935	36	0
1	D	3939	0	3927	24	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	1	0
2	D	31	0	12	0	0
3	A	56	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	56	0	21	2	0
3	C	56	0	21	2	0
3	D	56	0	20	0	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
5	D	4	0	6	1	0
6	A	43	0	0	1	0
6	B	45	0	0	2	0
6	C	39	0	0	3	0
6	D	55	0	0	1	0
All	All	16309	0	15875	101	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 3.

All (101) 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:B:328:ASN:HA	1:D:326:GLN:HG3	1.42	1.01
3:B:702:DUT:O2G	6:B:830:HOH:O	1.80	0.98
1:A:331:TYR:OH	6:A:820:HOH:O	2.00	0.78
3:C:703:DUT:O2A	6:C:807:HOH:O	2.01	0.76
1:A:425:ASN:OD1	1:D:425:ASN:ND2	2.20	0.72
1:C:298:TYR:O	6:C:835:HOH:O	2.08	0.71
1:C:354:LYS:HE2	3:C:701:DUT:O2A	1.90	0.71
1:C:302:SER:O	6:C:835:HOH:O	2.09	0.70
1:B:328:ASN:HA	1:D:326:GLN:CG	2.20	0.69
1:C:234:GLU:HB3	1:C:273:VAL:HG12	1.76	0.68
1:B:455:LYS:HG2	1:B:557:VAL:HG12	1.75	0.68
1:C:232:THR:OG1	1:C:234:GLU:OE1	2.14	0.65
1:D:355:GLU:OE1	1:D:358:ASN:ND2	2.29	0.65
1:B:327:ASN:O	1:D:326:GLN:HG3	1.97	0.64
1:A:326:GLN:OE1	1:A:327:ASN:N	2.22	0.63
1:C:543:GLU:HG3	1:C:544:LYS:HG3	1.81	0.63
1:D:328:ASN:ND2	6:D:805:HOH:O	2.29	0.61
1:A:175:ALA:HB1	1:A:199:VAL:HG12	1.81	0.61
1:C:580:LYS:HD3	1:C:598:TRP:HB3	1.83	0.60
1:A:252:PRO:HA	1:A:255:GLU:HG2	1.86	0.58
1:A:127:GLU:HG3	1:B:336:LYS:HE3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:ARG:HD3	1:B:587:ILE:HB	1.87	0.56
1:A:566:ARG:HD3	1:A:587:ILE:HB	1.88	0.55
1:A:326:GLN:HG3	1:C:326[A]:GLN:HG2	1.88	0.55
1:A:544:LYS:HE2	1:C:539:GLN:HB3	1.91	0.52
1:A:326:GLN:HG3	1:C:326[A]:GLN:CG	2.39	0.52
1:B:175:ALA:HB1	1:B:199:VAL:HG12	1.91	0.51
1:C:353:ASP:OD1	1:C:354:LYS:N	2.43	0.51
1:B:425:ASN:HB2	1:C:428:LEU:HD13	1.93	0.51
1:A:341:CYS:HB2	1:A:350:CYS:SG	2.51	0.51
1:B:143:ARG:HD2	1:B:420:THR:HA	1.92	0.49
1:A:371:ARG:NH2	1:C:361:ASP:OD1	2.32	0.49
1:C:455:LYS:HG2	1:C:557:VAL:HG12	1.92	0.49
1:C:408:ARG:N	1:C:411:THR:OG1	2.39	0.49
1:D:597:GLU:OE1	1:D:597:GLU:N	2.44	0.49
1:B:586:VAL:HG21	1:D:522:CYS:SG	2.54	0.48
1:A:522:CYS:SG	1:A:524:THR:OG1	2.71	0.47
1:B:351:ALA:O	1:B:520:PHE:HA	2.14	0.47
1:B:359:LEU:HA	1:B:359:LEU:HD23	1.74	0.47
1:A:597:GLU:OE1	1:A:597:GLU:N	2.28	0.47
1:B:361:ASP:OD2	1:D:371:ARG:NH2	2.46	0.46
1:C:507:TYR:HB3	1:C:514:PRO:HG3	1.97	0.46
1:B:560:LYS:HD2	1:B:560:LYS:HA	1.48	0.46
1:B:381:ILE:HD12	1:B:381:ILE:HA	1.82	0.46
1:A:510:GLN:O	1:A:546:ALA:HB2	2.16	0.45
1:A:455:LYS:HG2	1:A:557:VAL:HG12	1.97	0.45
1:A:143:ARG:HD2	1:A:420:THR:HA	1.98	0.45
1:B:215:HIS:HE2	3:B:702:DUT:PA	2.40	0.45
1:C:485:PRO:HA	1:C:571:GLN:HE21	1.82	0.45
1:B:183:GLY:HA2	1:B:191:ILE:HD12	1.98	0.45
1:B:285:TRP:HA	1:B:286:PRO:HD3	1.80	0.45
1:B:586:VAL:HG11	1:D:522:CYS:SG	2.57	0.44
1:C:405:LYS:HD2	1:C:407:TYR:CZ	2.52	0.44
1:D:374:TYR:O	5:D:706:EDO:O2	2.36	0.44
1:A:351:ALA:O	1:A:520:PHE:HA	2.17	0.44
1:A:580:LYS:HD2	1:A:598:TRP:HB3	2.00	0.44
1:D:483:ALA:O	1:D:484:LYS:HD2	2.18	0.44
1:B:457:VAL:HG22	1:B:552:VAL:O	2.17	0.44
1:D:479:GLU:OE1	1:D:576:ARG:NH1	2.48	0.43
1:C:167:HIS:ND1	1:C:314:ASP:OD2	2.48	0.43
1:B:425:ASN:OD1	1:C:425:ASN:ND2	2.50	0.43
1:D:444:ILE:O	1:D:447:GLN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LYS:O	1:A:254:MET:HB2	2.19	0.43
1:A:463:THR:HG22	1:A:464:GLY:H	1.82	0.43
1:C:305:ARG:NH1	1:C:517:HIS:HD2	2.17	0.42
1:D:120:ASP:OD1	1:D:121:PRO:HD2	2.19	0.42
1:A:326:GLN:O	1:C:328:ASN:HB2	2.19	0.42
1:A:125:HIS:CE1	1:B:333:ARG:HB2	2.54	0.42
1:C:296:PHE:HB2	1:C:349:ILE:HG13	2.01	0.42
1:C:175:ALA:HB1	1:C:199:VAL:HG12	2.01	0.42
6:B:805:HOH:O	1:D:543:GLU:HG2	2.20	0.42
1:B:241:PHE:O	1:B:245:ILE:HG12	2.19	0.42
1:C:228:GLU:OE1	1:C:228:GLU:N	2.42	0.42
1:C:156:VAL:O	2:C:702:DGT:H8	2.20	0.42
1:B:266:CYS:SG	1:B:288:LYS:HE3	2.59	0.42
1:D:369:LEU:HD23	1:D:369:LEU:HA	1.90	0.42
1:B:369:LEU:HA	1:B:369:LEU:HD23	1.92	0.42
1:C:377:LYS:HG3	1:C:378:VAL:HG23	2.01	0.42
1:D:513:ASN:HB2	1:D:545:PHE:CE2	2.55	0.42
1:D:580:LYS:NZ	1:D:585:ASP:OD2	2.41	0.41
1:A:522:CYS:SG	1:C:586:VAL:HG11	2.60	0.41
1:A:381:ILE:HA	1:A:381:ILE:HD12	1.86	0.41
1:B:563:TYR:O	1:B:567:GLN:HG2	2.20	0.41
1:C:483:ALA:O	1:C:485:PRO:HD3	2.20	0.41
1:D:113:ASP:HB3	1:D:114:THR:H	1.74	0.41
1:C:359:LEU:HA	1:C:359:LEU:HD23	1.81	0.41
1:A:485:PRO:O	1:A:487:VAL:N	2.50	0.41
1:C:143:ARG:HD2	1:C:420:THR:HA	2.02	0.41
1:A:378:VAL:O	1:A:381:ILE:HG22	2.20	0.41
1:D:442:ARG:HG2	1:D:446:LYS:HE2	2.02	0.41
1:C:253:VAL:O	1:C:256:GLN:HB3	2.21	0.41
1:C:170:GLY:HA3	1:C:314:ASP:OD1	2.20	0.41
1:A:463:THR:O	1:A:466:ILE:HB	2.21	0.41
1:B:394:ASP:O	1:B:408:ARG:HD2	2.21	0.41
1:C:388:ASP:OD1	1:C:444:ILE:HD13	2.20	0.41
1:B:134:ARG:HD3	1:B:134:ARG:HA	1.91	0.41
1:D:129:HIS:CG	1:D:130:PRO:HD2	2.56	0.41
1:C:381:ILE:HD12	1:C:381:ILE:HA	1.75	0.41
1:C:334:PHE:CE2	1:C:359:LEU:HD21	2.57	0.40
1:D:285:TRP:CD2	1:D:292:GLU:HG2	2.57	0.40
1:D:412:ALA:HB3	1:D:422:LEU:HD22	2.04	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	479/550 (87%)	467 (98%)	12 (2%)	0	100	100
1	B	478/550 (87%)	465 (97%)	12 (2%)	1 (0%)	52	64
1	C	479/550 (87%)	460 (96%)	18 (4%)	1 (0%)	52	64
1	D	478/550 (87%)	467 (98%)	10 (2%)	1 (0%)	52	64
All	All	1914/2200 (87%)	1859 (97%)	52 (3%)	3 (0%)	52	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	595	LYS
1	C	598	TRP
1	D	262	GLU

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	429/488 (88%)	421 (98%)	8 (2%)	65	81
1	B	428/488 (88%)	418 (98%)	10 (2%)	58	75
1	C	429/488 (88%)	413 (96%)	16 (4%)	41	55
1	D	428/488 (88%)	421 (98%)	7 (2%)	70	84
All	All	1714/1952 (88%)	1673 (98%)	41 (2%)	60	74

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	315	TYR
1	A	326	GLN
1	A	327	ASN
1	A	359	LEU
1	A	463	THR
1	A	488	LEU
1	A	522	CYS
1	A	594	GLN
1	B	114	THR
1	B	284	LEU
1	B	315	TYR
1	B	368	SER
1	B	475	SER
1	B	524	THR
1	B	535[A]	ASN
1	B	535[B]	ASN
1	B	560	LYS
1	B	577	ASN
1	C	232	THR
1	C	238	VAL
1	C	240	MET
1	C	288	LYS
1	C	315	TYR
1	C	326[A]	GLN
1	C	326[B]	GLN
1	C	354	LYS
1	C	388	ASP
1	C	413	ILE
1	C	457	VAL
1	C	487	VAL
1	C	524	THR
1	C	562	LEU
1	C	597[A]	GLU
1	C	597[B]	GLU
1	D	115	MET
1	D	273	VAL
1	D	315	TYR
1	D	326	GLN
1	D	354	LYS
1	D	434	THR
1	D	474	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	322	HIS
1	B	326	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 7 are monoatomic - leaving 13 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	2.30	5 (20%)	35,52,52	1.93	11 (31%)
3	DUT	A	702	4	20,29,29	2.01	4 (20%)	32,45,45	1.67	5 (15%)
3	DUT	A	703	4	20,29,29	2.06	3 (15%)	32,45,45	1.42	5 (15%)
2	DGT	B	701	4	25,33,33	2.20	4 (16%)	35,52,52	1.78	9 (25%)
3	DUT	B	702	4	20,29,29	2.01	3 (15%)	32,45,45	1.68	4 (12%)
3	DUT	B	703	4	20,29,29	2.04	3 (15%)	32,45,45	1.48	4 (12%)
3	DUT	C	701	4	20,29,29	2.00	3 (15%)	32,45,45	1.50	3 (9%)
2	DGT	C	702	4	25,33,33	2.37	5 (20%)	35,52,52	1.86	9 (25%)
3	DUT	C	703	-	20,29,29	2.03	4 (20%)	32,45,45	1.73	5 (15%)
3	DUT	D	701	4	20,29,29	2.03	3 (15%)	32,45,45	1.40	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DGT	D	702	4	25,33,33	2.26	5 (20%)	35,52,52	1.98	11 (31%)
3	DUT	D	703	4	20,29,29	2.00	4 (20%)	32,45,45	1.63	5 (15%)
5	EDO	D	706	-	3,3,3	0.57	0	2,2,2	0.30	0

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	DUT	A	702	4	-	0/18/34/34	0/2/2/2
3	DUT	A	703	4	-	0/18/34/34	0/2/2/2
2	DGT	B	701	4	-	0/18/34/34	0/3/3/3
3	DUT	B	702	4	-	0/18/34/34	0/2/2/2
3	DUT	B	703	4	-	0/18/34/34	0/2/2/2
3	DUT	C	701	4	-	0/18/34/34	0/2/2/2
2	DGT	C	702	4	-	0/18/34/34	0/3/3/3
3	DUT	C	703	-	-	0/18/34/34	0/2/2/2
3	DUT	D	701	4	-	0/18/34/34	0/2/2/2
2	DGT	D	702	4	-	0/18/34/34	0/3/3/3
3	DUT	D	703	4	-	0/18/34/34	0/2/2/2
5	EDO	D	706	-	-	0/1/1/1	0/0/0/0

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	703	DUT	C6-N1	-3.47	1.30	1.35
3	D	701	DUT	O3'-C3'	-3.41	1.35	1.43
3	A	702	DUT	O3'-C3'	-3.21	1.36	1.43
3	A	703	DUT	O3'-C3'	-3.14	1.36	1.43
3	C	703	DUT	O3'-C3'	-3.13	1.36	1.43
3	B	702	DUT	O3'-C3'	-3.10	1.36	1.43
3	A	703	DUT	C6-N1	-3.06	1.31	1.35
3	D	703	DUT	C6-N1	-2.95	1.31	1.35
3	D	703	DUT	O3'-C3'	-2.93	1.36	1.43
3	C	703	DUT	C6-N1	-2.90	1.31	1.35
3	A	702	DUT	C6-N1	-2.85	1.31	1.35
3	D	701	DUT	C6-N1	-2.83	1.31	1.35
2	C	702	DGT	O3'-C3'	-2.75	1.37	1.43
3	B	702	DUT	C6-N1	-2.70	1.32	1.35
3	C	701	DUT	O3'-C3'	-2.70	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	701	DUT	C6-N1	-2.64	1.32	1.35
2	A	701	DGT	O3'-C3'	-2.63	1.37	1.43
3	B	703	DUT	O3'-C3'	-2.59	1.37	1.43
2	D	702	DGT	O3'-C3'	-2.31	1.38	1.43
3	C	703	DUT	C2'-C3'	-2.28	1.46	1.52
2	C	702	DGT	O4'-C4'	-2.27	1.39	1.45
2	B	701	DGT	O3'-C3'	-2.22	1.38	1.43
3	A	702	DUT	C2'-C3'	-2.13	1.47	1.52
3	D	703	DUT	C2'-C3'	-2.04	1.47	1.52
2	D	702	DGT	O4'-C4'	-2.00	1.40	1.45
2	A	701	DGT	O4'-C4'	-2.00	1.40	1.45
2	B	701	DGT	O4'-C1'	3.21	1.49	1.42
2	D	702	DGT	O4'-C1'	3.33	1.50	1.42
2	A	701	DGT	O4'-C1'	3.40	1.50	1.42
2	C	702	DGT	O4'-C1'	3.40	1.50	1.42
3	A	702	DUT	O4-C4	6.17	1.39	1.24
3	D	701	DUT	O4-C4	6.23	1.39	1.24
3	D	703	DUT	O4-C4	6.33	1.39	1.24
3	C	703	DUT	O4-C4	6.33	1.39	1.24
3	B	702	DUT	O4-C4	6.35	1.39	1.24
2	B	701	DGT	O6-C6	6.41	1.40	1.24
2	D	702	DGT	O6-C6	6.45	1.40	1.24
3	C	701	DUT	O4-C4	6.49	1.40	1.24
3	A	703	DUT	O4-C4	6.52	1.40	1.24
2	A	701	DGT	O6-C6	6.64	1.40	1.24
3	B	703	DUT	O4-C4	6.65	1.40	1.24
2	B	701	DGT	C2-N2	6.68	1.47	1.34
2	C	702	DGT	O6-C6	6.93	1.41	1.24
2	D	702	DGT	C2-N2	7.09	1.48	1.34
2	C	702	DGT	C2-N2	7.15	1.48	1.34
2	A	701	DGT	C2-N2	7.19	1.48	1.34

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	703	DUT	PB-O3A-PA	-5.26	117.95	132.73
2	D	702	DGT	N3-C2-N1	-5.17	119.58	127.44
2	C	702	DGT	N3-C2-N1	-4.89	120.00	127.44
2	A	701	DGT	N3-C2-N1	-4.87	120.02	127.44
3	B	702	DUT	PB-O3A-PA	-4.55	119.95	132.73
2	B	701	DGT	N3-C2-N1	-4.43	120.69	127.44
2	D	702	DGT	PA-O3A-PB	-3.92	121.73	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	DGT	PA-O3A-PB	-3.68	122.39	132.73
2	A	701	DGT	PA-O3A-PB	-3.60	122.63	132.73
3	A	702	DUT	PB-O3A-PA	-3.51	122.86	132.73
3	D	703	DUT	PB-O3B-PG	-3.42	121.19	132.67
2	C	702	DGT	PA-O3A-PB	-3.34	123.36	132.73
2	B	701	DGT	C4-C5-N7	-3.31	106.44	109.48
2	C	702	DGT	C5-C6-N1	-3.23	119.17	123.59
2	A	701	DGT	C4-C5-N7	-3.23	106.51	109.48
3	C	703	DUT	PB-O3B-PG	-3.19	121.96	132.67
3	B	702	DUT	PB-O3B-PG	-3.18	122.01	132.67
2	A	701	DGT	C5-C6-N1	-3.17	119.25	123.59
2	C	702	DGT	C4-C5-N7	-3.15	106.58	109.48
2	D	702	DGT	C4-C5-N7	-3.04	106.68	109.48
3	A	702	DUT	PB-O3B-PG	-2.98	122.66	132.67
3	D	703	DUT	PB-O3A-PA	-2.85	124.73	132.73
2	D	702	DGT	C5-C6-N1	-2.84	119.70	123.59
2	B	701	DGT	C5-C6-N1	-2.65	119.97	123.59
2	D	702	DGT	C6-C5-C4	-2.63	117.75	120.90
3	A	703	DUT	PB-O3B-PG	-2.46	124.41	132.67
3	C	701	DUT	PB-O3B-PG	-2.45	124.46	132.67
3	D	701	DUT	PB-O3B-PG	-2.45	124.47	132.67
2	B	701	DGT	C6-C5-C4	-2.42	118.00	120.90
2	A	701	DGT	C6-C5-C4	-2.20	118.27	120.90
3	B	703	DUT	PB-O3B-PG	-2.20	125.30	132.67
2	A	701	DGT	PB-O3B-PG	-2.10	125.62	132.67
3	A	703	DUT	PB-O3A-PA	-2.05	126.96	132.73
2	B	701	DGT	PB-O3B-PG	-2.04	125.81	132.67
3	A	703	DUT	O5'-C5'-C4'	2.02	116.56	109.12
2	C	702	DGT	N2-C2-N3	2.06	121.75	117.80
2	B	701	DGT	O1G-PG-O3B	2.08	114.52	105.09
3	B	703	DUT	O3A-PA-O5'	2.09	108.48	102.94
2	C	702	DGT	O5'-C5'-C4'	2.10	116.86	109.12
3	C	703	DUT	O3A-PA-O5'	2.11	108.53	102.94
2	A	701	DGT	C2'-C3'-C4'	2.15	107.24	102.77
3	C	703	DUT	O5'-C5'-C4'	2.16	117.07	109.12
2	D	702	DGT	O5'-C5'-C4'	2.17	117.12	109.12
2	B	701	DGT	O5'-C5'-C4'	2.18	117.17	109.12
3	B	703	DUT	O5'-C5'-C4'	2.18	117.17	109.12
3	C	701	DUT	O2A-PA-O3A	2.19	115.05	105.09
2	A	701	DGT	O3A-PA-O5'	2.20	108.77	102.94
2	A	701	DGT	O5'-C5'-C4'	2.22	117.31	109.12
3	A	702	DUT	O5'-C5'-C4'	2.28	117.53	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	702	DGT	O1G-PG-O3B	2.36	115.81	105.09
3	D	703	DUT	O4'-C1'-N1	2.36	111.81	107.72
2	D	702	DGT	O1G-PG-O3B	2.41	116.01	105.09
2	D	702	DGT	O3A-PA-O5'	2.51	109.59	102.94
3	D	701	DUT	O3A-PA-O5'	2.57	109.75	102.94
3	A	703	DUT	O3A-PA-O5'	2.58	109.78	102.94
3	B	702	DUT	O3A-PA-O5'	2.58	109.79	102.94
3	D	703	DUT	O3A-PA-O5'	2.63	109.92	102.94
2	C	702	DGT	O4'-C1'-N9	2.74	112.46	107.72
2	A	701	DGT	O4'-C1'-N9	2.90	112.73	107.72
2	D	702	DGT	O4'-C1'-N9	3.03	112.96	107.72
2	D	702	DGT	N2-C2-N1	3.08	122.31	117.20
2	B	701	DGT	C6-N1-C2	3.38	120.63	115.94
3	A	702	DUT	O3A-PA-O5'	3.54	112.32	102.94
2	D	702	DGT	C6-N1-C2	3.84	121.26	115.94
2	A	701	DGT	C6-N1-C2	4.13	121.67	115.94
2	C	702	DGT	C6-N1-C2	4.20	121.76	115.94
3	A	703	DUT	C4-N3-C2	5.04	119.13	114.14
3	D	701	DUT	C4-N3-C2	5.23	119.32	114.14
3	C	703	DUT	C4-N3-C2	5.51	119.60	114.14
3	B	702	DUT	C4-N3-C2	5.55	119.64	114.14
3	B	703	DUT	C4-N3-C2	5.56	119.65	114.14
3	A	702	DUT	C4-N3-C2	5.80	119.88	114.14
3	C	701	DUT	C4-N3-C2	5.87	119.96	114.14
3	D	703	DUT	C4-N3-C2	5.92	120.01	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	DUT	2	0
3	C	701	DUT	1	0
2	C	702	DGT	1	0
3	C	703	DUT	1	0
5	D	706	EDO	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, 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	481/550 (87%)	0.31	33 (6%)	20	27	23, 43, 69, 82	332 (69%)
1	B	480/550 (87%)	0.20	33 (6%)	20	27	24, 41, 65, 88	285 (59%)
1	C	481/550 (87%)	0.29	28 (5%)	26	35	26, 44, 66, 94	340 (70%)
1	D	481/550 (87%)	0.01	12 (2%)	61	70	21, 36, 57, 76	314 (65%)
All	All	1923/2200 (87%)	0.20	106 (5%)	29	37	21, 41, 64, 94	1271 (66%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	488	LEU	6.0
1	B	489	LEU	5.6
1	C	284	LEU	5.3
1	B	562	LEU	5.3
1	B	492	LYS	5.2
1	B	560	LYS	5.1
1	B	490	ASP	4.9
1	B	491	VAL	4.9
1	A	488	LEU	4.8
1	B	593	PRO	4.8
1	A	344	ASP	4.6
1	C	488	LEU	4.5
1	A	599	ASN	4.4
1	C	277	GLU	4.1
1	C	590	LEU	4.0
1	B	481	ALA	4.0
1	B	564	ALA	4.0
1	B	559	ARG	3.8
1	C	489	LEU	3.7
1	B	495	ALA	3.6
1	A	486	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	345	ASN	3.5
1	A	284	LEU	3.4
1	B	284	LEU	3.4
1	C	592	THR	3.3
1	B	485	PRO	3.2
1	B	484	LYS	3.2
1	C	599	ASN	3.2
1	B	568	TYR	3.2
1	A	485	PRO	3.1
1	D	466	ILE	3.1
1	C	485	PRO	3.1
1	D	396	TYR	3.1
1	A	343	VAL	3.1
1	B	592	THR	3.0
1	C	490	ASP	3.0
1	A	292	GLU	3.0
1	C	487	VAL	3.0
1	C	260	ILE	3.0
1	C	276	LEU	3.0
1	B	590	LEU	2.9
1	B	594	GLN	2.9
1	A	528	ARG	2.9
1	B	596	LYS	2.9
1	A	592	THR	2.8
1	A	529	ALA	2.8
1	B	599	ASN	2.8
1	C	345	ASN	2.8
1	A	498	PHE	2.7
1	D	465	GLN	2.7
1	B	452	ASN	2.7
1	D	599	ASN	2.7
1	C	408	ARG	2.7
1	B	493	LEU	2.7
1	A	466	ILE	2.7
1	B	487	VAL	2.7
1	D	276	LEU	2.6
1	B	483	ALA	2.6
1	D	490	ASP	2.6
1	C	326[A]	GLN	2.6
1	C	593	PRO	2.6
1	C	588	ALA	2.6
1	A	489	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	491	VAL	2.6
1	A	494	LYS	2.5
1	B	180	HIS	2.5
1	B	494	LYS	2.5
1	A	481	ALA	2.5
1	A	476	LEU	2.4
1	A	478	LYS	2.4
1	A	487	VAL	2.4
1	A	484	LYS	2.4
1	C	596	LYS	2.4
1	B	230	LYS	2.4
1	B	344	ASP	2.4
1	B	486	LYS	2.4
1	D	596	LYS	2.4
1	D	284	LEU	2.3
1	B	277	GLU	2.3
1	A	490	ASP	2.3
1	C	230	LYS	2.3
1	A	471	GLU	2.2
1	A	483	ALA	2.2
1	A	559	ARG	2.2
1	C	591	ILE	2.2
1	C	396	TYR	2.2
1	C	492	LYS	2.2
1	D	230	LYS	2.2
1	C	115	MET	2.2
1	D	471	GLU	2.2
1	B	563	TYR	2.2
1	A	347	LEU	2.2
1	A	326	GLN	2.1
1	D	469	LYS	2.1
1	A	473	TYR	2.1
1	A	477	PRO	2.1
1	C	435	ASP	2.1
1	C	491	VAL	2.1
1	B	496	GLU	2.1
1	C	568	TYR	2.1
1	D	277	GLU	2.0
1	C	400	THR	2.0
1	A	596	LYS	2.0
1	C	594	GLN	2.0
1	A	470	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	447	GLN	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
5	EDO	D	706	4/4	0.87	0.21	5.52	30,30,35,44	4
3	DUT	C	703	28/28	0.83	0.21	2.12	25,38,57,78	28
3	DUT	D	703	28/28	0.93	0.17	1.49	18,29,54,59	28
3	DUT	B	702	28/28	0.93	0.17	1.18	23,32,52,57	28
3	DUT	A	702	28/28	0.92	0.18	1.10	24,33,53,59	28
2	DGT	A	701	31/31	0.97	0.14	0.01	26,31,36,44	31
3	DUT	C	701	28/28	0.96	0.16	-0.09	22,31,39,43	0
3	DUT	B	703	28/28	0.97	0.14	-0.28	22,27,33,36	28
3	DUT	A	703	28/28	0.97	0.14	-0.34	26,33,43,44	0
2	DGT	C	702	31/31	0.97	0.13	-0.50	30,34,42,45	0
2	DGT	D	702	31/31	0.98	0.12	-0.60	20,27,31,35	0
3	DUT	D	701	28/28	0.97	0.13	-0.62	22,29,38,41	28
2	DGT	B	701	31/31	0.97	0.11	-1.11	25,30,39,40	31
4	MG	A	705	1/1	0.75	0.08	-	26,26,26,26	0
4	MG	D	704	1/1	0.93	0.11	-	31,31,31,31	0
4	MG	A	706	1/1	0.88	0.07	-	62,62,62,62	0
4	MG	D	705	1/1	0.65	0.14	-	58,58,58,58	0
4	MG	C	704	1/1	0.75	0.15	-	42,42,42,42	0
4	MG	B	704	1/1	0.91	0.23	-	61,61,61,61	0
4	MG	A	704	1/1	0.99	0.09	-	32,32,32,32	1

6.5 Other polymers

There are no such residues in this entry.