



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:57 PM GMT

PDB ID : 4QFX
Title : Crystal structure of the tetrameric dGTP/dATP-bound SAMHD1 (RN206) mutant catalytic core
Authors : Koharudin, L.M.I.; Wu, Y.; DeLucia, M.; Mehrens, J.; Gronenborn, A.M.; Ahn, J.
Deposited on : 2014-05-21
Resolution : 2.20 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

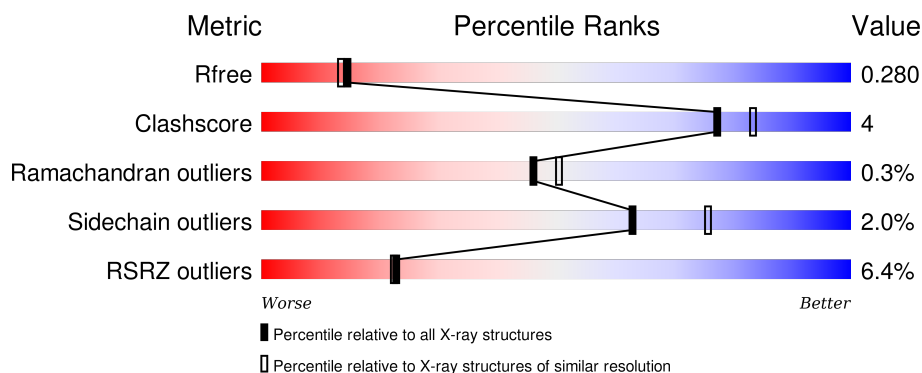
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	 7% 77% 10% • 13%
1	B	550	 5% 79% 8% 13%
1	C	550	 7% 76% 10% • 13%
1	D	550	 4% 81% 7% 13%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16513 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	3	0
			3946	2529	685	711	21			
1	B	481	Total	C	N	O	S	0	0	0
			3933	2517	685	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	1	0
			3941	2521	687	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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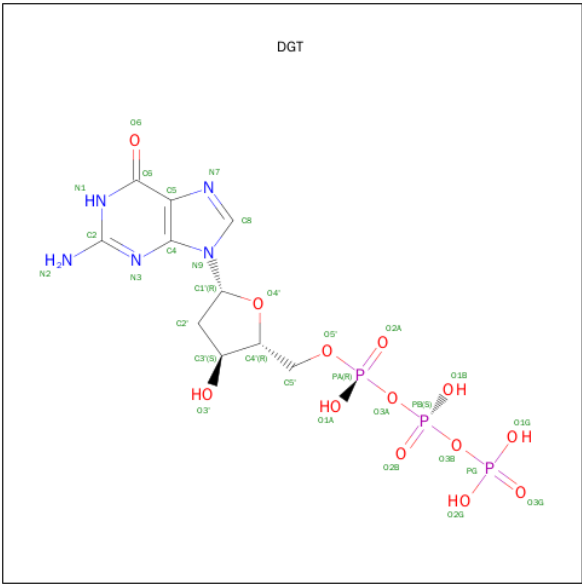
Chain	Residue	Modelled	Actual	Comment	Reference
C	106	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
C	107	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
C	108	ARG	-	EXPRESSION TAG	UNP Q9Y3Z3
C	109	ASP	-	EXPRESSION TAG	UNP Q9Y3Z3
C	110	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
C	111	ASN	-	EXPRESSION TAG	UNP Q9Y3Z3
C	112	SER	-	EXPRESSION TAG	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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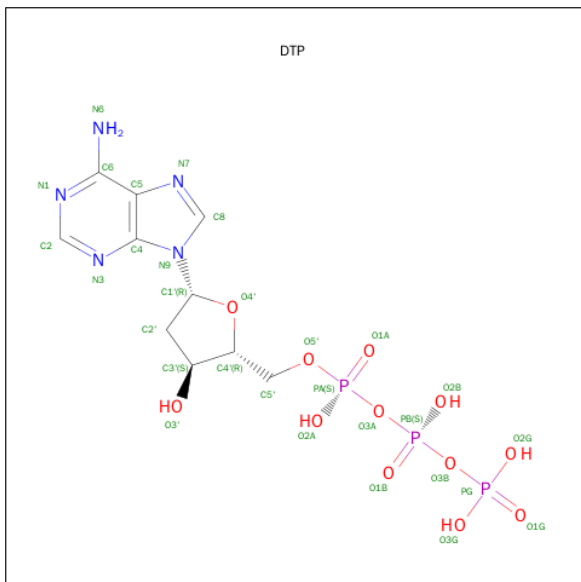
Chain	Residue	Modelled	Actual	Comment	Reference
D	110	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
D	111	ASN	-	EXPRESSION TAG	UNP Q9Y3Z3
D	112	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
D	206	ARG	HIS	ENGINEERED MUTATION	UNP Q9Y3Z3
D	207	ASN	ASP	ENGINEERED MUTATION	UNP Q9Y3Z3

- Molecule 2 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 3 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



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

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

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

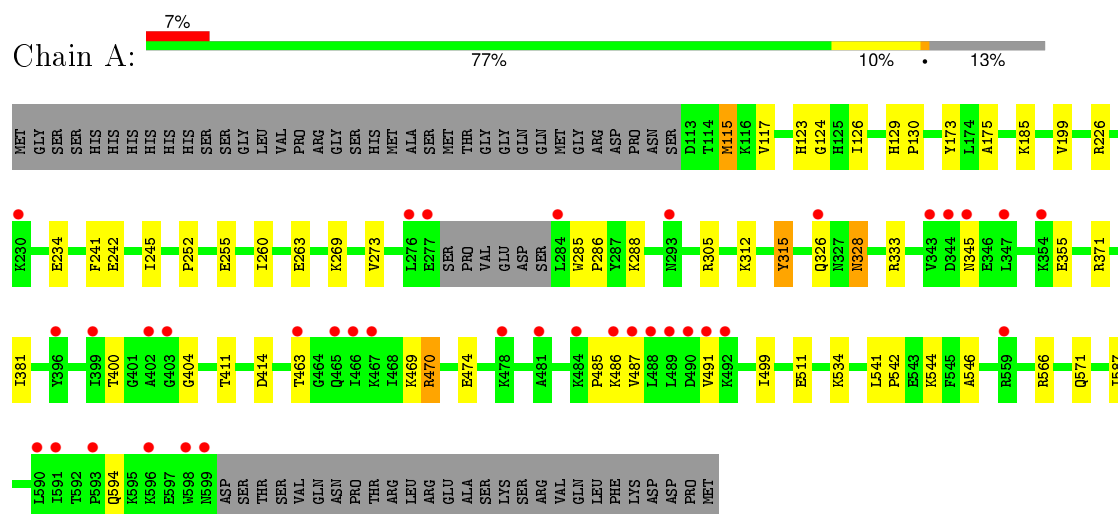
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	83	Total 83	O 83	0	0
5	B	114	Total 114	O 114	0	0
5	C	78	Total 78	O 78	0	0
5	D	109	Total 109	O 109	0	0

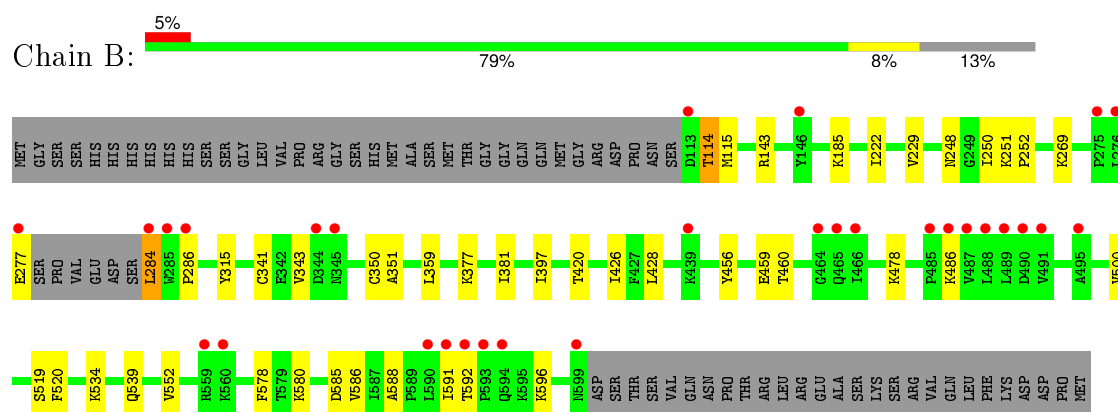
3 Residue-property plots

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.

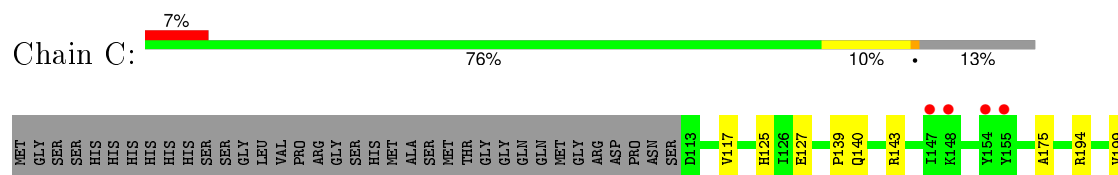
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

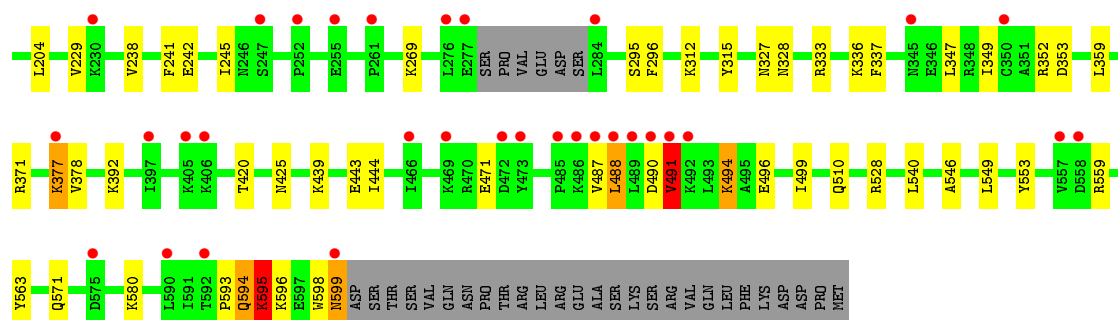


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

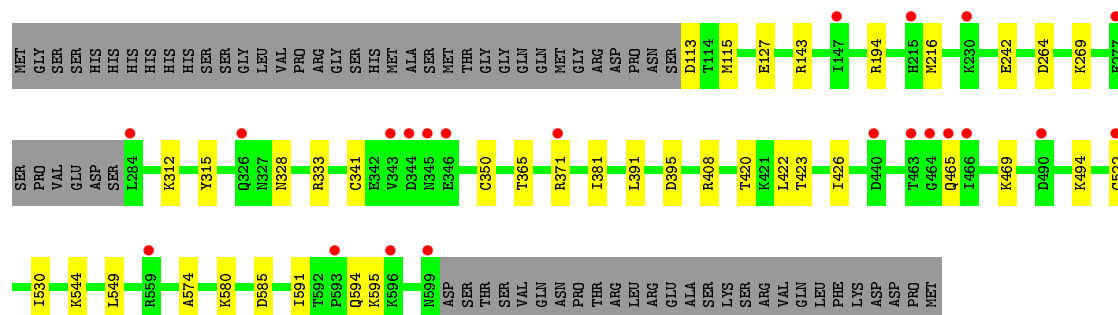
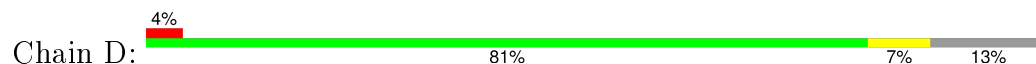


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





- 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	88.56 Å 147.26 Å 98.80 Å 90.00° 114.63° 90.00°	Depositor
Resolution (Å)	38.34 – 2.20 38.34 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.34-2.20) 99.9 (38.34-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.20 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.228 , 0.270 0.239 , 0.280	Depositor DCC
R_{free} test set	2003 reflections (1.75%)	DCC
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 35.4	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Outliers	0 of 116315 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16513	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 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DTP, 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	0.29	0/4047	0.49	0/5463
1	B	0.29	0/4025	0.49	0/5433
1	C	0.29	0/4025	0.48	0/5433
1	D	0.30	0/4033	0.49	0/5444
All	All	0.29	0/16130	0.49	0/21773

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	3948	37	0
1	B	3933	0	3921	25	0
1	C	3933	0	3921	40	0
1	D	3941	0	3926	23	0
2	A	93	0	36	0	0
2	B	62	0	24	0	0
2	C	62	0	24	1	0
2	D	31	0	12	0	0
3	A	30	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	30	0	12	0	0
3	C	30	0	12	0	0
3	D	30	0	12	0	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	C	3	0	0	0	0
4	D	1	0	0	0	0
5	A	83	0	0	2	0
5	B	114	0	0	2	0
5	C	78	0	0	1	0
5	D	109	0	0	0	0
All	All	16513	0	15860	118	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 (118) 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:397:ILE:HG21	1:B:426:ILE:HD11	1.55	0.88
1:C:242:GLU:OE1	1:C:269:LYS:NZ	2.13	0.76
1:A:326:GLN:HG2	1:C:328:ASN:HA	1.69	0.74
1:B:534:LYS:NZ	5:B:886:HOH:O	2.24	0.70
1:A:226:ARG:NH2	1:A:414:ASP:OD2	2.27	0.68
1:B:248:ASN:HB2	1:B:250:ILE:HD11	1.77	0.65
1:B:539:GLN:OE1	1:D:544:LYS:NZ	2.26	0.65
1:C:377:LYS:HD3	1:C:378:VAL:HG23	1.80	0.64
1:A:333:ARG:NE	1:A:355:GLU:OE2	2.31	0.64
1:A:371:ARG:NH1	5:A:880:HOH:O	2.30	0.64
1:A:326:GLN:HG3	1:C:327:ASN:O	1.99	0.62
1:A:242:GLU:OE1	1:A:269:LYS:NZ	2.22	0.61
1:D:395:ASP:OD1	1:D:408:ARG:NH1	2.32	0.61
1:A:328:ASN:OD1	1:A:328:ASN:N	2.29	0.59
1:C:593:PRO:HA	1:C:599:ASN:HD21	1.67	0.59
1:A:571:GLN:HE22	1:A:594:GLN:HE22	1.51	0.59
1:D:465:GLN:O	1:D:465:GLN:HG3	2.05	0.57
1:A:234:GLU:HB3	1:A:273:VAL:HG23	1.86	0.57
1:C:336:LYS:HE2	1:D:127:GLU:HG3	1.88	0.56
1:C:494:LYS:HB2	1:C:496:GLU:HG2	1.88	0.55
1:D:423:THR:O	1:D:426:ILE:HD12	2.07	0.55
1:D:194:ARG:HH21	1:D:264:ASP:CG	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:371:ARG:HH22	1:D:549:LEU:HD21	1.72	0.55
1:A:485:PRO:O	1:A:487:VAL:N	2.38	0.55
1:C:392:LYS:HD2	1:C:444:ILE:HD11	1.89	0.55
1:B:428:LEU:HD13	1:C:425:ASN:HB2	1.89	0.53
1:A:534:LYS:HE3	1:A:542:PRO:O	2.08	0.53
1:A:566:ARG:HD3	1:A:587:ILE:HB	1.91	0.53
1:B:586:VAL:HG11	1:D:522:CYS:SG	2.50	0.52
1:D:328:ASN:OD1	1:D:365:THR:OG1	2.20	0.52
1:C:296:PHE:HB2	1:C:349:ILE:HG13	1.91	0.51
1:C:371:ARG:HH22	1:C:549:LEU:HD21	1.75	0.50
1:A:241:PHE:CE2	1:A:245[A]:ILE:HD11	2.47	0.50
1:C:352:ARG:NE	1:C:353:ASP:OD1	2.44	0.49
1:B:585:ASP:HA	1:B:592:THR:HG21	1.95	0.49
1:A:400:THR:HG23	1:A:404:GLY:HA2	1.95	0.49
1:C:117:VAL:HG22	1:C:127:GLU:HG2	1.95	0.49
1:D:580:LYS:NZ	1:D:585:ASP:OD2	2.31	0.48
1:D:591:ILE:O	1:D:594:GLN:HG2	2.13	0.48
1:D:422:LEU:HD12	1:D:426:ILE:HD11	1.94	0.48
1:A:260:ILE:HD11	1:A:263:GLU:CD	2.34	0.48
1:C:571:GLN:NE2	1:C:594:GLN:OE1	2.42	0.48
1:A:474:GLU:N	1:A:474:GLU:OE1	2.47	0.48
1:A:542:PRO:HB3	1:C:540:LEU:O	2.15	0.47
1:D:594:GLN:HG3	1:D:595:LYS:N	2.29	0.47
1:C:204:LEU:O	5:C:865:HOH:O	2.21	0.47
1:C:175:ALA:HB1	1:C:199:VAL:HG12	1.98	0.46
1:B:381:ILE:HD12	1:B:381:ILE:HA	1.82	0.46
1:B:114:THR:OG1	1:B:115:MET:N	2.49	0.45
1:B:588:ALA:HB1	1:B:591:ILE:HD13	1.98	0.45
1:A:252:PRO:HA	1:A:255:GLU:HG2	1.98	0.45
1:C:241:PHE:CZ	1:C:245:ILE:HD11	2.52	0.45
1:B:359:LEU:HA	1:B:359:LEU:HD23	1.79	0.45
1:D:544:LYS:HB3	1:D:544:LYS:HE2	1.78	0.45
1:C:238:VAL:HG23	1:C:269:LYS:HG2	1.98	0.45
1:C:499:ILE:HB	1:C:553:TYR:HB2	1.99	0.45
1:A:123:HIS:HB2	1:A:126[B]:ILE:HD11	1.99	0.45
1:B:460:THR:OG1	1:B:578:PHE:HB3	2.16	0.45
1:C:599:ASN:OD1	1:C:599:ASN:N	2.50	0.45
1:C:593:PRO:HA	1:C:599:ASN:ND2	2.31	0.44
1:C:490:ASP:O	1:C:491:VAL:HG22	2.16	0.44
1:D:312:LYS:HA	1:D:315:TYR:CE2	2.52	0.44
1:B:185:LYS:HA	1:B:185:LYS:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:LEU:HA	1:C:359:LEU:HD23	1.71	0.44
1:C:494:LYS:HB3	1:C:494:LYS:HE3	1.50	0.44
1:D:574:ALA:O	1:D:595:LYS:HE2	2.17	0.44
1:C:143:ARG:HD2	1:C:420:THR:HA	2.00	0.44
3:A:703:DTP:O1B	2:C:702:DGT:H5'A	2.17	0.44
1:A:544:LYS:NZ	1:A:546:ALA:O	2.49	0.44
1:D:341:CYS:HB2	1:D:350:CYS:SG	2.58	0.44
1:C:487:VAL:HG11	1:C:563:TYR:OH	2.18	0.43
1:B:222:ILE:HD13	1:B:222:ILE:HA	1.86	0.43
1:A:381:ILE:HA	1:A:381:ILE:HD12	1.82	0.43
1:A:226:ARG:HH21	1:A:411:THR:HA	1.83	0.43
1:A:226:ARG:HH22	1:A:414:ASP:CG	2.21	0.43
1:B:486:LYS:HD2	1:B:486:LYS:HA	1.68	0.43
1:C:312:LYS:HA	1:C:315:TYR:CE2	2.53	0.43
1:A:175:ALA:HB1	1:A:199:VAL:HG12	2.00	0.43
1:A:124:GLY:HA2	5:A:859:HOH:O	2.19	0.43
1:A:185:LYS:HD3	1:A:185:LYS:HA	1.81	0.43
1:A:126[B]:ILE:HD12	1:A:173:TYR:CD1	2.53	0.42
1:A:541:LEU:HB3	1:A:542:PRO:HD2	2.01	0.42
1:A:129:HIS:CG	1:A:130:PRO:HD2	2.54	0.42
1:A:326:GLN:N	1:A:326:GLN:OE1	2.52	0.42
1:B:456:TYR:OH	1:B:459:GLU:HB2	2.19	0.42
1:B:500:VAL:HG22	1:B:552:VAL:HG22	2.00	0.42
1:D:371:ARG:NH2	1:D:549:LEU:HD21	2.34	0.42
1:C:241:PHE:CE2	1:C:245:ILE:HD11	2.55	0.42
1:C:125:HIS:CE1	1:D:333:ARG:HB2	2.54	0.42
1:D:143:ARG:HD2	1:D:420:THR:HA	2.02	0.42
1:A:288:LYS:HA	1:A:288:LYS:HD3	1.79	0.42
1:B:143:ARG:HD2	1:B:420:THR:HA	2.02	0.42
1:C:510:GLN:O	1:C:546:ALA:HB2	2.20	0.42
1:B:351:ALA:O	1:B:520:PHE:HA	2.20	0.41
1:A:511:GLU:OE1	1:A:544:LYS:NZ	2.51	0.41
1:A:115:MET:HE1	1:A:117:VAL:HG22	2.01	0.41
1:B:596:LYS:HD2	1:B:596:LYS:HA	1.78	0.41
1:C:377:LYS:HG3	1:C:377:LYS:H	1.32	0.41
1:B:580:LYS:NZ	1:B:585:ASP:OD2	2.54	0.41
1:B:251:LYS:HB2	1:B:252:PRO:HD3	2.02	0.41
1:A:469:LYS:O	1:A:470:ARG:HB3	2.21	0.41
1:C:439:LYS:O	1:C:443:GLU:HG2	2.21	0.41
1:C:333:ARG:O	1:C:337:PHE:HD2	2.04	0.41
1:C:595:LYS:HG3	1:C:598:TRP:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:595:LYS:HG3	1:C:598:TRP:CE2	2.56	0.41
1:A:123:HIS:CB	1:A:126[B]:ILE:HD11	2.51	0.40
1:C:487:VAL:HG12	1:C:488:LEU:N	2.35	0.40
1:D:391:LEU:HA	1:D:391:LEU:HD23	1.91	0.40
1:C:580:LYS:HB2	1:C:598:TRP:CD2	2.56	0.40
1:C:139:PRO:HG2	1:C:140:GLN:NE2	2.36	0.40
1:B:269:LYS:NZ	5:B:901:HOH:O	2.34	0.40
1:C:295:SER:OG	1:C:347:LEU:O	2.35	0.40
1:D:381:ILE:HA	1:D:381:ILE:HD12	1.89	0.40
1:A:285:TRP:HA	1:A:286:PRO:HD3	1.95	0.40
1:B:284:LEU:O	1:B:286:PRO:HD3	2.20	0.40
1:A:312:LYS:HA	1:A:315:TYR:CE2	2.56	0.40
1:B:341:CYS:HB2	1:B:350:CYS:SG	2.62	0.40
1:D:242:GLU:OE1	1:D:269:LYS:NZ	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	480/550 (87%)	460 (96%)	18 (4%)	2 (0%)	39	42
1	B	477/550 (87%)	461 (97%)	16 (3%)	0	100	100
1	C	477/550 (87%)	457 (96%)	17 (4%)	3 (1%)	30	29
1	D	478/550 (87%)	465 (97%)	13 (3%)	0	100	100
All	All	1912/2200 (87%)	1843 (96%)	64 (3%)	5 (0%)	46	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	491	VAL

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Mol	Chain	Res	Type
1	C	595	LYS
1	C	596	LYS
1	A	470	ARG
1	A	486	LYS

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	430/488 (88%)	422 (98%)	8 (2%)	65	77
1	B	427/488 (88%)	418 (98%)	9 (2%)	61	74
1	C	427/488 (88%)	415 (97%)	12 (3%)	51	63
1	D	428/488 (88%)	422 (99%)	6 (1%)	74	85
All	All	1712/1952 (88%)	1677 (98%)	35 (2%)	63	76

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

Mol	Chain	Res	Type
1	A	115	MET
1	A	305	ARG
1	A	315	TYR
1	A	328	ASN
1	A	345	ASN
1	A	463	THR
1	A	491	VAL
1	A	499	ILE
1	B	114	THR
1	B	229	VAL
1	B	277	GLU
1	B	284	LEU
1	B	315	TYR
1	B	343	VAL
1	B	377	LYS
1	B	478	LYS
1	B	519	SER

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Mol	Chain	Res	Type
1	C	194	ARG
1	C	229	VAL
1	C	377	LYS
1	C	471	GLU
1	C	488	LEU
1	C	491	VAL
1	C	494	LYS
1	C	528	ARG
1	C	559	ARG
1	C	594	GLN
1	C	595	LYS
1	C	599	ASN
1	D	113	ASP
1	D	115	MET
1	D	216	MET
1	D	469	LYS
1	D	494	LYS
1	D	530	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	367	ASN
1	A	535	ASN
1	A	571	GLN
1	B	233	HIS
1	D	149	GLN
1	D	425	ASN

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	2.35	7 (28%)	35,52,52	1.63	9 (25%)
2	DGT	A	702	4	25,33,33	2.28	6 (24%)	35,52,52	1.66	10 (28%)
3	DTP	A	703	4	24,32,32	1.27	4 (16%)	32,50,50	2.19	5 (15%)
2	DGT	A	704	4	25,33,33	2.30	6 (24%)	35,52,52	1.50	7 (20%)
2	DGT	B	701	4	25,33,33	2.32	6 (24%)	35,52,52	1.65	9 (25%)
2	DGT	B	702	4	25,33,33	2.35	6 (24%)	35,52,52	1.70	10 (28%)
3	DTP	B	703	4	24,32,32	1.29	4 (16%)	32,50,50	2.21	5 (15%)
3	DTP	C	701	4	24,32,32	1.26	4 (16%)	32,50,50	2.17	4 (12%)
2	DGT	C	702	4	25,33,33	2.27	6 (24%)	35,52,52	1.68	9 (25%)
2	DGT	C	703	4	25,33,33	2.30	6 (24%)	35,52,52	1.61	9 (25%)
3	DTP	D	701	4	24,32,32	1.21	5 (20%)	32,50,50	2.23	6 (18%)
2	DGT	D	702	4	25,33,33	2.28	5 (20%)	35,52,52	1.62	9 (25%)

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
2	DGT	A	702	4	-	0/18/34/34	0/3/3/3
3	DTP	A	703	4	-	0/18/34/34	0/3/3/3
2	DGT	A	704	4	-	0/18/34/34	0/3/3/3
2	DGT	B	701	4	-	0/18/34/34	0/3/3/3
2	DGT	B	702	4	-	0/18/34/34	0/3/3/3
3	DTP	B	703	4	-	0/18/34/34	0/3/3/3
3	DTP	C	701	4	-	0/18/34/34	0/3/3/3
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DTP	D	701	4	-	0/18/34/34	0/3/3/3
2	DGT	D	702	4	-	0/18/34/34	0/3/3/3

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	703	DTP	O3'-C3'	-2.89	1.36	1.43
3	C	701	DTP	O3'-C3'	-2.67	1.37	1.43
2	A	701	DGT	O3'-C3'	-2.67	1.37	1.43
3	A	703	DTP	O3'-C3'	-2.65	1.37	1.43
3	B	703	DTP	C5'-C4'	-2.63	1.43	1.51
2	D	702	DGT	O3'-C3'	-2.59	1.37	1.43
2	B	701	DGT	O3'-C3'	-2.55	1.37	1.43
2	B	702	DGT	O3'-C3'	-2.55	1.37	1.43
2	C	703	DGT	O3'-C3'	-2.54	1.37	1.43
2	C	702	DGT	O3'-C3'	-2.53	1.37	1.43
2	A	704	DGT	O3'-C3'	-2.52	1.37	1.43
2	A	702	DGT	O3'-C3'	-2.48	1.37	1.43
2	B	701	DGT	C2'-C3'	-2.45	1.46	1.52
2	A	702	DGT	C2'-C3'	-2.43	1.46	1.52
3	A	703	DTP	C5'-C4'	-2.42	1.43	1.51
3	D	701	DTP	O3'-C3'	-2.40	1.38	1.43
2	C	702	DGT	C2'-C3'	-2.36	1.46	1.52
2	D	702	DGT	C2'-C3'	-2.35	1.46	1.52
2	C	703	DGT	C2'-C3'	-2.35	1.46	1.52
3	D	701	DTP	C5'-C4'	-2.33	1.44	1.51
2	B	701	DGT	PG-O2G	-2.32	1.46	1.54
2	B	702	DGT	PG-O2G	-2.32	1.46	1.54
3	C	701	DTP	C5'-C4'	-2.31	1.44	1.51
2	B	701	DGT	O4'-C4'	-2.28	1.39	1.45
2	B	702	DGT	C2'-C3'	-2.27	1.46	1.52
2	A	702	DGT	PG-O2G	-2.27	1.46	1.54
3	A	703	DTP	PG-O3G	-2.25	1.46	1.54
2	A	701	DGT	C2'-C3'	-2.25	1.46	1.52
2	A	704	DGT	O4'-C4'	-2.23	1.39	1.45
2	D	702	DGT	PG-O2G	-2.23	1.46	1.54
2	A	701	DGT	PG-O2G	-2.22	1.46	1.54
2	A	704	DGT	PG-O2G	-2.21	1.46	1.54
2	C	702	DGT	PG-O2G	-2.18	1.46	1.54
2	A	702	DGT	O4'-C4'	-2.17	1.40	1.45
3	B	703	DTP	C2'-C3'	-2.16	1.47	1.52
3	C	701	DTP	C2'-C3'	-2.16	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	701	DTP	PG-O3G	-2.15	1.47	1.54
2	C	702	DGT	O4'-C4'	-2.14	1.40	1.45
2	C	703	DGT	PG-O2G	-2.14	1.47	1.54
2	B	702	DGT	O4'-C4'	-2.07	1.40	1.45
2	A	704	DGT	C2'-C3'	-2.07	1.47	1.52
2	A	701	DGT	O4'-C4'	-2.05	1.40	1.45
2	A	701	DGT	PG-O1G	-2.01	1.47	1.54
2	C	703	DGT	O4'-C4'	-2.01	1.40	1.45
3	D	701	DTP	C2'-C3'	-2.00	1.47	1.52
3	D	701	DTP	C6-N6	2.95	1.44	1.34
3	C	701	DTP	C6-N6	2.95	1.44	1.34
3	A	703	DTP	C6-N6	2.97	1.44	1.34
3	B	703	DTP	C6-N6	3.00	1.44	1.34
2	C	703	DGT	C2-N2	3.48	1.41	1.34
2	A	704	DGT	C2-N2	3.48	1.41	1.34
2	C	702	DGT	C2-N2	3.48	1.41	1.34
2	D	702	DGT	C2-N2	3.51	1.41	1.34
2	A	701	DGT	C2-N2	3.54	1.41	1.34
2	B	701	DGT	C2-N2	3.56	1.41	1.34
2	A	702	DGT	C2-N2	3.64	1.41	1.34
2	B	702	DGT	C2-N2	3.72	1.41	1.34
2	A	704	DGT	O6-C6	8.83	1.45	1.24
2	C	703	DGT	O6-C6	8.83	1.45	1.24
2	C	702	DGT	O6-C6	8.89	1.46	1.24
2	A	701	DGT	O6-C6	8.91	1.46	1.24
2	A	702	DGT	O6-C6	8.92	1.46	1.24
2	B	702	DGT	O6-C6	8.95	1.46	1.24
2	D	702	DGT	O6-C6	8.97	1.46	1.24
2	B	701	DGT	O6-C6	8.99	1.46	1.24

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	703	DTP	N3-C2-N1	-9.98	121.25	128.89
3	A	703	DTP	N3-C2-N1	-9.78	121.41	128.89
3	C	701	DTP	N3-C2-N1	-9.58	121.56	128.89
3	D	701	DTP	N3-C2-N1	-9.41	121.69	128.89
2	C	702	DGT	PA-O3A-PB	-4.37	120.45	132.73
3	D	701	DTP	C4-C5-N7	-4.04	105.77	109.48
2	C	703	DGT	PA-O3A-PB	-3.95	121.65	132.73
2	A	701	DGT	PA-O3A-PB	-3.82	122.00	132.73
2	D	702	DGT	PA-O3A-PB	-3.76	122.17	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	DGT	N3-C2-N1	-3.76	121.72	127.44
2	A	702	DGT	PA-O3A-PB	-3.73	122.24	132.73
2	A	701	DGT	N3-C2-N1	-3.73	121.76	127.44
3	D	701	DTP	PB-O3B-PG	-3.66	120.40	132.67
2	A	702	DGT	N3-C2-N1	-3.64	121.91	127.44
2	A	704	DGT	PA-O3A-PB	-3.63	122.53	132.73
2	A	704	DGT	N3-C2-N1	-3.59	121.98	127.44
2	B	701	DGT	C4-C5-N7	-3.54	106.23	109.48
2	B	701	DGT	N3-C2-N1	-3.53	122.07	127.44
2	C	702	DGT	N3-C2-N1	-3.51	122.10	127.44
3	A	703	DTP	C4-C5-N7	-3.49	106.26	109.48
3	B	703	DTP	C4-C5-N7	-3.49	106.27	109.48
3	D	701	DTP	PA-O3A-PB	-3.46	123.00	132.73
2	B	702	DGT	PA-O3A-PB	-3.46	123.01	132.73
2	D	702	DGT	N3-C2-N1	-3.40	122.26	127.44
3	C	701	DTP	C4-C5-N7	-3.38	106.37	109.48
2	C	703	DGT	N3-C2-N1	-3.38	122.30	127.44
2	B	701	DGT	PA-O3A-PB	-3.26	123.56	132.73
3	A	703	DTP	PA-O3A-PB	-3.15	123.87	132.73
3	C	701	DTP	PA-O3A-PB	-2.99	124.32	132.73
2	B	702	DGT	C4-C5-N7	-2.91	106.80	109.48
2	D	702	DGT	C4-C5-N7	-2.86	106.85	109.48
3	A	703	DTP	PB-O3B-PG	-2.84	123.16	132.67
2	B	702	DGT	C6-C5-C4	-2.82	117.53	120.90
2	C	702	DGT	C5-C6-N1	-2.79	119.78	123.59
2	A	704	DGT	C4-C5-N7	-2.75	106.95	109.48
3	B	703	DTP	PA-O3A-PB	-2.73	125.07	132.73
2	A	701	DGT	C6-C5-C4	-2.72	117.65	120.90
2	B	701	DGT	C5-C6-N1	-2.72	119.87	123.59
2	A	702	DGT	C4-C5-N7	-2.67	107.02	109.48
2	C	703	DGT	PB-O3B-PG	-2.65	123.80	132.67
2	A	701	DGT	C4-C5-N7	-2.64	107.05	109.48
2	B	701	DGT	C6-C5-C4	-2.56	117.84	120.90
2	C	702	DGT	C4-C5-N7	-2.55	107.13	109.48
2	C	703	DGT	C4-C5-N7	-2.52	107.16	109.48
3	C	701	DTP	PB-O3B-PG	-2.52	124.23	132.67
2	A	701	DGT	C5-C6-N1	-2.51	120.15	123.59
2	A	702	DGT	C6-C5-C4	-2.44	117.99	120.90
2	A	704	DGT	C5-C6-N1	-2.42	120.28	123.59
2	D	702	DGT	PB-O3B-PG	-2.39	124.66	132.67
2	C	703	DGT	C6-C5-C4	-2.39	118.04	120.90
2	B	702	DGT	C5-C6-N1	-2.37	120.34	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	704	DGT	C6-C5-C4	-2.37	118.07	120.90
2	D	702	DGT	C5-C6-N1	-2.34	120.38	123.59
2	A	702	DGT	C5-C6-N1	-2.34	120.39	123.59
2	C	702	DGT	C6-C5-C4	-2.28	118.18	120.90
3	D	701	DTP	C1'-N9-C4	-2.26	123.32	127.16
2	D	702	DGT	C6-C5-C4	-2.25	118.21	120.90
2	C	703	DGT	C5-C6-N1	-2.19	120.60	123.59
2	B	702	DGT	PB-O3B-PG	-2.16	125.42	132.67
2	A	702	DGT	PB-O3B-PG	-2.09	125.66	132.67
3	B	703	DTP	PB-O3B-PG	-2.06	125.77	132.67
2	B	701	DGT	O4'-C1'-N9	2.00	111.18	107.72
3	A	703	DTP	O5'-C5'-C4'	2.06	116.71	109.12
2	A	701	DGT	O5'-C5'-C4'	2.07	116.74	109.12
2	B	702	DGT	O5'-C5'-C4'	2.10	116.86	109.12
2	A	702	DGT	O5'-C5'-C4'	2.11	116.89	109.12
2	C	702	DGT	O4'-C1'-N9	2.13	111.40	107.72
3	D	701	DTP	O3A-PA-O5'	2.17	108.70	102.94
2	A	704	DGT	O5'-C5'-C4'	2.21	117.26	109.12
2	B	701	DGT	O5'-C5'-C4'	2.22	117.31	109.12
3	B	703	DTP	O3A-PA-O5'	2.35	109.16	102.94
2	A	701	DGT	O3A-PA-O5'	2.35	109.17	102.94
2	A	702	DGT	O4'-C1'-N9	2.37	111.82	107.72
2	C	703	DGT	O5'-C5'-C4'	2.38	117.88	109.12
2	C	702	DGT	O3A-PA-O5'	2.40	109.30	102.94
2	B	701	DGT	O3A-PA-O5'	2.42	109.37	102.94
2	C	703	DGT	C6-N1-C2	2.45	119.34	115.94
2	D	702	DGT	C6-N1-C2	2.45	119.34	115.94
2	A	702	DGT	C6-N1-C2	2.56	119.48	115.94
2	C	702	DGT	O5'-C5'-C4'	2.57	118.61	109.12
2	A	704	DGT	C6-N1-C2	2.66	119.62	115.94
2	D	702	DGT	O4'-C1'-N9	2.69	112.37	107.72
2	B	702	DGT	O4'-C1'-N9	2.75	112.47	107.72
2	B	702	DGT	C6-N1-C2	2.85	119.89	115.94
2	D	702	DGT	O3A-PA-O5'	2.88	110.57	102.94
2	B	701	DGT	C6-N1-C2	2.92	120.00	115.94
2	C	703	DGT	O3A-PA-O5'	2.96	110.78	102.94
2	C	702	DGT	C6-N1-C2	3.01	120.12	115.94
2	A	701	DGT	C6-N1-C2	3.06	120.19	115.94
2	A	701	DGT	O4'-C1'-N9	3.09	113.08	107.72
2	B	702	DGT	O3A-PA-O5'	3.13	111.23	102.94
2	A	702	DGT	O3A-PA-O5'	3.17	111.34	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	703	DTP	1	0
2	C	702	DGT	1	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	481/550 (87%)	0.52	36 (7%)	17	17	24, 42, 67, 85	389 (80%)
1	B	481/550 (87%)	0.49	30 (6%)	24	23	25, 39, 64, 84	396 (82%)
1	C	481/550 (87%)	0.57	36 (7%)	17	17	28, 45, 69, 91	389 (80%)
1	D	481/550 (87%)	0.33	22 (4%)	36	35	23, 37, 57, 74	384 (79%)
All	All	1924/2200 (87%)	0.48	124 (6%)	23	22	23, 41, 65, 91	1558 (80%)

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	488	LEU	10.9
1	A	465	GLN	7.6
1	B	593	PRO	7.0
1	C	284	LEU	6.8
1	C	488	LEU	6.8
1	C	277	GLU	6.0
1	D	345	ASN	5.7
1	B	466	ILE	5.6
1	B	464	GLY	5.3
1	C	489	LEU	5.2
1	B	594	GLN	4.8
1	B	487	VAL	4.6
1	C	491	VAL	4.6
1	A	466	ILE	4.4
1	A	284	LEU	4.3
1	B	113	ASP	4.3
1	A	345	ASN	4.3
1	D	284	LEU	4.2
1	D	522	CYS	4.2
1	C	590	LEU	4.1
1	B	490	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	592	THR	4.0
1	C	487	VAL	4.0
1	A	277	GLU	3.9
1	A	590	LEU	3.9
1	C	490	ASP	3.9
1	A	467	LYS	3.9
1	B	495	ALA	3.8
1	B	559	ARG	3.8
1	B	599	ASN	3.6
1	C	276	LEU	3.6
1	D	466	ILE	3.5
1	A	344	ASP	3.4
1	A	490	ASP	3.3
1	A	347	LEU	3.3
1	A	599	ASN	3.2
1	B	465	GLN	3.1
1	A	486	LYS	3.1
1	B	277	GLU	3.1
1	A	487	VAL	3.1
1	D	277	GLU	3.0
1	A	488	LEU	3.0
1	D	465	GLN	3.0
1	C	557	VAL	3.0
1	A	399	ILE	3.0
1	C	492	LYS	2.9
1	A	478	LYS	2.9
1	C	147	ILE	2.9
1	A	293	ASN	2.9
1	C	469	LYS	2.8
1	C	345	ASN	2.8
1	C	486	LYS	2.8
1	D	215	HIS	2.8
1	C	252	PRO	2.8
1	C	575	ASP	2.8
1	C	599	ASN	2.8
1	B	590	LEU	2.7
1	A	598	TRP	2.7
1	A	559	ARG	2.7
1	B	284	LEU	2.6
1	D	599	ASN	2.6
1	A	593	PRO	2.6
1	D	490	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	559	ARG	2.6
1	D	593	PRO	2.6
1	A	354	LYS	2.6
1	A	276	LEU	2.5
1	B	345	ASN	2.5
1	D	596	LYS	2.5
1	C	350	CYS	2.5
1	A	402	ALA	2.5
1	C	592	THR	2.5
1	B	286	PRO	2.5
1	D	440	ASP	2.4
1	B	489	LEU	2.4
1	A	489	LEU	2.4
1	B	491	VAL	2.4
1	C	155	TYR	2.4
1	D	344	ASP	2.4
1	C	466	ILE	2.3
1	A	463	THR	2.3
1	D	326	GLN	2.3
1	D	464	GLY	2.3
1	C	405	LYS	2.3
1	C	473	TYR	2.3
1	A	403	GLY	2.3
1	A	326	GLN	2.3
1	A	396	TYR	2.3
1	B	146	TYR	2.3
1	C	261	PRO	2.3
1	B	485	PRO	2.3
1	C	485	PRO	2.3
1	C	154	TYR	2.3
1	A	230	LYS	2.3
1	D	371	ARG	2.3
1	B	591	ILE	2.2
1	C	406	LYS	2.2
1	C	230	LYS	2.2
1	D	147	ILE	2.2
1	D	346	GLU	2.2
1	A	481	ALA	2.2
1	B	285	TRP	2.2
1	A	492	LYS	2.2
1	B	560	LYS	2.2
1	B	276	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	255	GLU	2.2
1	A	596	LYS	2.1
1	C	148	LYS	2.1
1	D	230	LYS	2.1
1	A	484	LYS	2.1
1	B	486	LYS	2.1
1	C	472	ASP	2.1
1	A	343	VAL	2.1
1	C	377	LYS	2.1
1	B	439	LYS	2.1
1	A	591	ILE	2.1
1	A	491	VAL	2.1
1	D	343	VAL	2.1
1	C	558	ASP	2.1
1	D	463	THR	2.0
1	C	397	ILE	2.0
1	B	344	ASP	2.0
1	B	275	PRO	2.0
1	C	247	SER	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
2	DGT	B	702	31/31	0.94	0.14	-0.10	19,29,37,39	31
2	DGT	D	702	31/31	0.95	0.16	-0.35	21,28,37,41	31

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	DGT	C	702	31/31	0.94	0.16	-0.45	25,32,38,39	31
2	DGT	A	701	31/31	0.94	0.14	-0.59	24,31,35,39	31
2	DGT	B	701	31/31	0.96	0.15	-0.71	22,30,38,40	31
3	DTP	A	703	30/30	0.97	0.14	-0.73	28,32,39,43	20
3	DTP	D	701	30/30	0.97	0.15	-0.75	25,30,35,36	14
2	DGT	C	703	31/31	0.95	0.14	-0.95	28,36,45,49	31
3	DTP	C	701	30/30	0.96	0.12	-1.05	26,30,36,38	14
3	DTP	B	703	30/30	0.97	0.13	-1.05	22,27,30,30	22
2	DGT	A	704	31/31	0.96	0.12	-1.13	21,28,33,39	31
2	DGT	A	702	31/31	0.96	0.13	-1.30	27,36,43,47	31
4	MG	B	704	1/1	0.38	0.11	-	41,41,41,41	0
4	MG	C	706	1/1	0.96	0.08	-	41,41,41,41	0
4	MG	A	707	1/1	0.94	0.13	-	48,48,48,48	0
4	MG	C	704	1/1	0.72	0.12	-	33,33,33,33	0
4	MG	A	706	1/1	0.80	0.09	-	34,34,34,34	0
4	MG	A	705	1/1	0.72	0.09	-	41,41,41,41	0
4	MG	D	703	1/1	0.76	0.17	-	40,40,40,40	0
4	MG	C	705	1/1	0.71	0.13	-	37,37,37,37	1

6.5 Other polymers [i](#)

There are no such residues in this entry.