



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 09:38 PM GMT

PDB ID : 5AO2  
Title : Crystal structure of human SAMHD1 (amino acid residues 115-583) R164A variant bound to dGTP  
Authors : Schwefel, D.; Taylor, I.A.  
Deposited on : 2015-09-09  
Resolution : 2.97 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

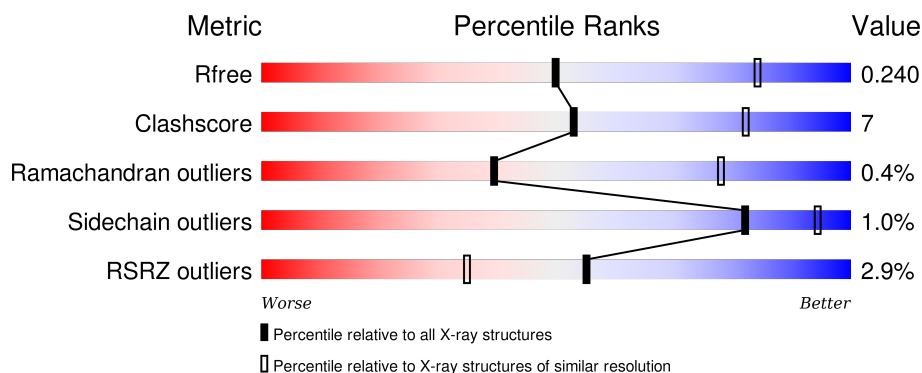
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.97 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	491	 2% 75% 13% 11%
1	B	491	 2% 72% 13% 15%
1	C	491	 3% 74% 14% 11%
1	D	491	 3% 73% 12% 15%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13606 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DEOXYNUCLEOSIDE TRIPHOSPHATE TRIPHOSPHO-HYDROLASE SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3433	2202	594	618	19			
1	B	419	Total	C	N	O	S	0	0	0
			3317	2130	568	601	18			
1	C	438	Total	C	N	O	S	0	0	1
			3452	2213	593	627	19			
1	D	419	Total	C	N	O	S	0	0	0
			3272	2099	560	595	18			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
A	94	ALA	-	EXPRESSION TAG	UNP Q9Y3Z3
A	95	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
A	96	TRP	-	EXPRESSION TAG	UNP Q9Y3Z3
A	97	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
A	98	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
A	99	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
A	100	GLN	-	EXPRESSION TAG	UNP Q9Y3Z3
A	101	PHE	-	EXPRESSION TAG	UNP Q9Y3Z3
A	102	GLU	-	EXPRESSION TAG	UNP Q9Y3Z3
A	103	LYS	-	EXPRESSION TAG	UNP Q9Y3Z3
A	104	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
A	105	ALA	-	EXPRESSION TAG	UNP Q9Y3Z3
A	106	LEU	-	EXPRESSION TAG	UNP Q9Y3Z3
A	107	GLU	-	EXPRESSION TAG	UNP Q9Y3Z3
A	108	VAL	-	EXPRESSION TAG	UNP Q9Y3Z3
A	109	LEU	-	EXPRESSION TAG	UNP Q9Y3Z3
A	110	PHE	-	EXPRESSION TAG	UNP Q9Y3Z3
A	111	GLN	-	EXPRESSION TAG	UNP Q9Y3Z3
A	112	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	113	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
A	114	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
A	164	ALA	ARG	ENGINEERED MUTATION	UNP Q9Y3Z3
B	93	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
B	94	ALA	-	EXPRESSION TAG	UNP Q9Y3Z3
B	95	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
B	96	TRP	-	EXPRESSION TAG	UNP Q9Y3Z3
B	97	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
B	98	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
B	99	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
B	100	GLN	-	EXPRESSION TAG	UNP Q9Y3Z3
B	101	PHE	-	EXPRESSION TAG	UNP Q9Y3Z3
B	102	GLU	-	EXPRESSION TAG	UNP Q9Y3Z3
B	103	LYS	-	EXPRESSION TAG	UNP Q9Y3Z3
B	104	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
B	105	ALA	-	EXPRESSION TAG	UNP Q9Y3Z3
B	106	LEU	-	EXPRESSION TAG	UNP Q9Y3Z3
B	107	GLU	-	EXPRESSION TAG	UNP Q9Y3Z3
B	108	VAL	-	EXPRESSION TAG	UNP Q9Y3Z3
B	109	LEU	-	EXPRESSION TAG	UNP Q9Y3Z3
B	110	PHE	-	EXPRESSION TAG	UNP Q9Y3Z3
B	111	GLN	-	EXPRESSION TAG	UNP Q9Y3Z3
B	112	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
B	113	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
B	114	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
B	164	ALA	ARG	ENGINEERED MUTATION	UNP Q9Y3Z3
C	93	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
C	94	ALA	-	EXPRESSION TAG	UNP Q9Y3Z3
C	95	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
C	96	TRP	-	EXPRESSION TAG	UNP Q9Y3Z3
C	97	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
C	98	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
C	99	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
C	100	GLN	-	EXPRESSION TAG	UNP Q9Y3Z3
C	101	PHE	-	EXPRESSION TAG	UNP Q9Y3Z3
C	102	GLU	-	EXPRESSION TAG	UNP Q9Y3Z3
C	103	LYS	-	EXPRESSION TAG	UNP Q9Y3Z3
C	104	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
C	105	ALA	-	EXPRESSION TAG	UNP Q9Y3Z3
C	106	LEU	-	EXPRESSION TAG	UNP Q9Y3Z3
C	107	GLU	-	EXPRESSION TAG	UNP Q9Y3Z3
C	108	VAL	-	EXPRESSION TAG	UNP Q9Y3Z3

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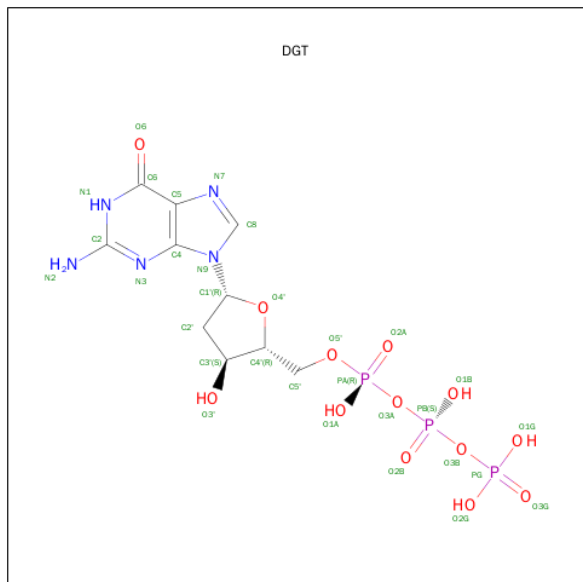
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Chain	Residue	Modelled	Actual	Comment	Reference
C	109	LEU	-	EXPRESSION TAG	UNP Q9Y3Z3
C	110	PHE	-	EXPRESSION TAG	UNP Q9Y3Z3
C	111	GLN	-	EXPRESSION TAG	UNP Q9Y3Z3
C	112	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
C	113	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
C	114	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
C	164	ALA	ARG	ENGINEERED MUTATION	UNP Q9Y3Z3
D	93	MET	-	EXPRESSION TAG	UNP Q9Y3Z3
D	94	ALA	-	EXPRESSION TAG	UNP Q9Y3Z3
D	95	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
D	96	TRP	-	EXPRESSION TAG	UNP Q9Y3Z3
D	97	SER	-	EXPRESSION TAG	UNP Q9Y3Z3
D	98	HIS	-	EXPRESSION TAG	UNP Q9Y3Z3
D	99	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
D	100	GLN	-	EXPRESSION TAG	UNP Q9Y3Z3
D	101	PHE	-	EXPRESSION TAG	UNP Q9Y3Z3
D	102	GLU	-	EXPRESSION TAG	UNP Q9Y3Z3
D	103	LYS	-	EXPRESSION TAG	UNP Q9Y3Z3
D	104	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
D	105	ALA	-	EXPRESSION TAG	UNP Q9Y3Z3
D	106	LEU	-	EXPRESSION TAG	UNP Q9Y3Z3
D	107	GLU	-	EXPRESSION TAG	UNP Q9Y3Z3
D	108	VAL	-	EXPRESSION TAG	UNP Q9Y3Z3
D	109	LEU	-	EXPRESSION TAG	UNP Q9Y3Z3
D	110	PHE	-	EXPRESSION TAG	UNP Q9Y3Z3
D	111	GLN	-	EXPRESSION TAG	UNP Q9Y3Z3
D	112	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
D	113	PRO	-	EXPRESSION TAG	UNP Q9Y3Z3
D	114	GLY	-	EXPRESSION TAG	UNP Q9Y3Z3
D	164	ALA	ARG	ENGINEERED MUTATION	UNP Q9Y3Z3

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0

- Molecule 3 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
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

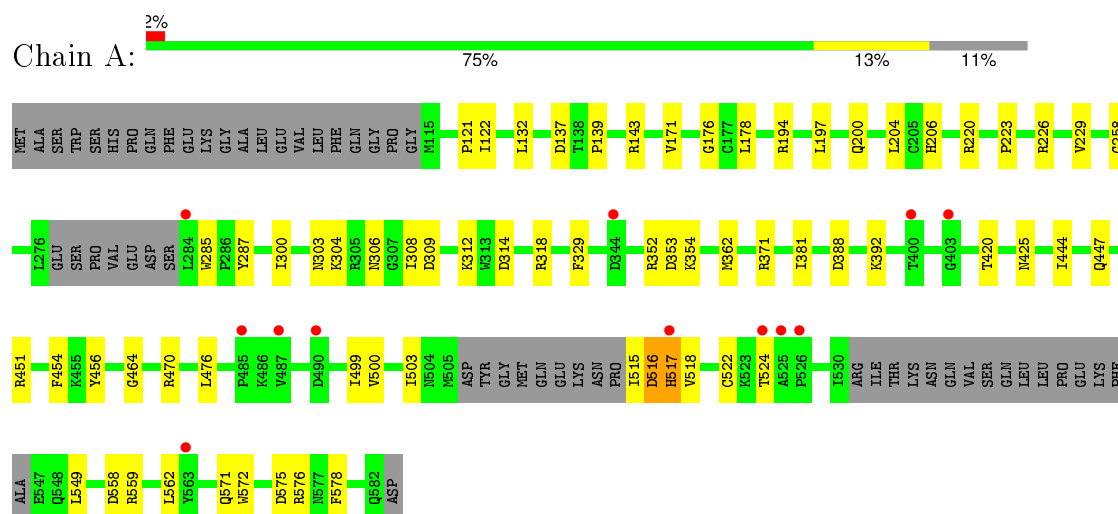
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	2	Total	O	0	0
			2	2		
4	C	1	Total	O	0	0
			1	1		

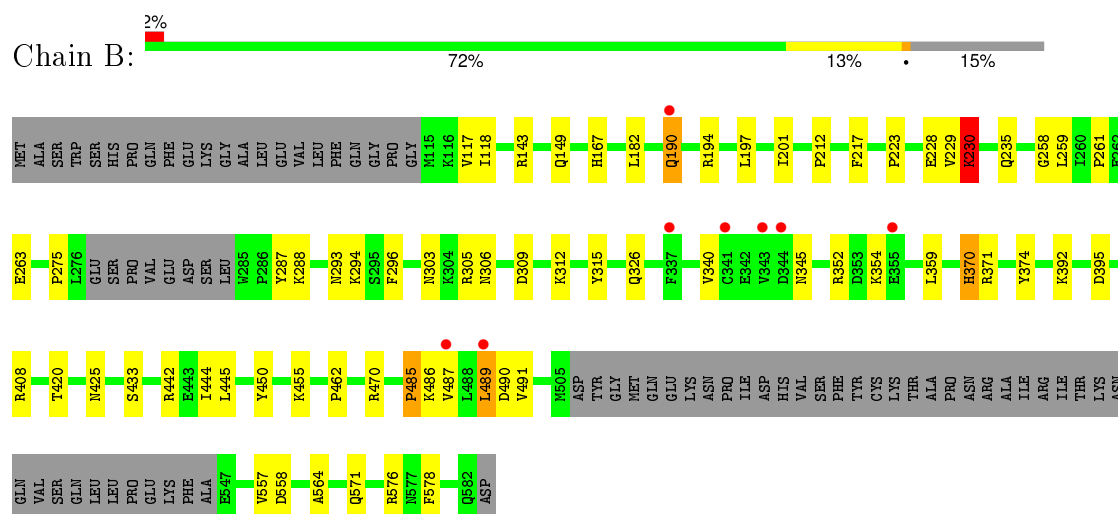
### 3 Residue-property plots

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

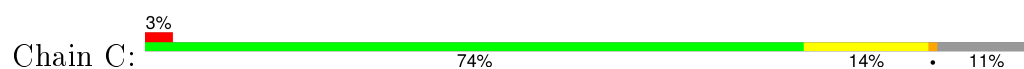
#### • Molecule 1: DEOXYNUCLEOSIDE TRIPHOSPHATE TRIPHOSPHOHYDROLASE SAMHD1

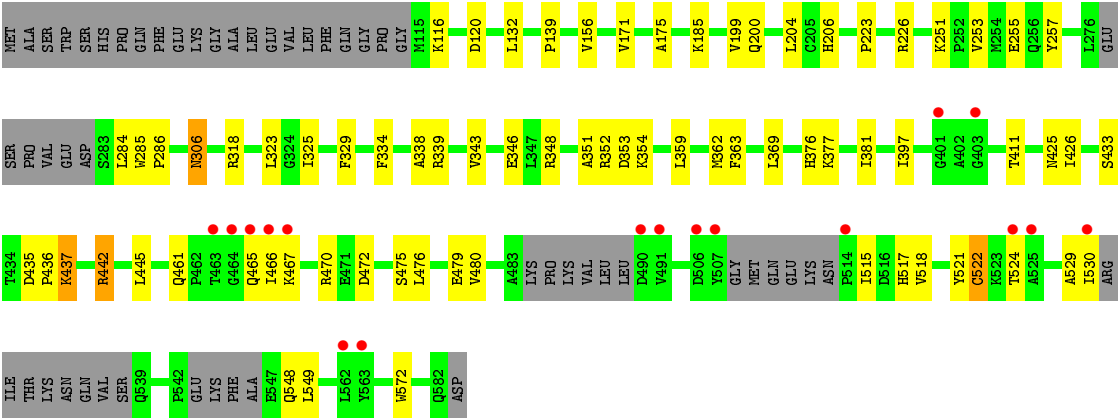


#### • Molecule 1: DEOXYNUCLEOSIDE TRIPHOSPHATE TRIPHOSPHOHYDROLASE SAMHD1

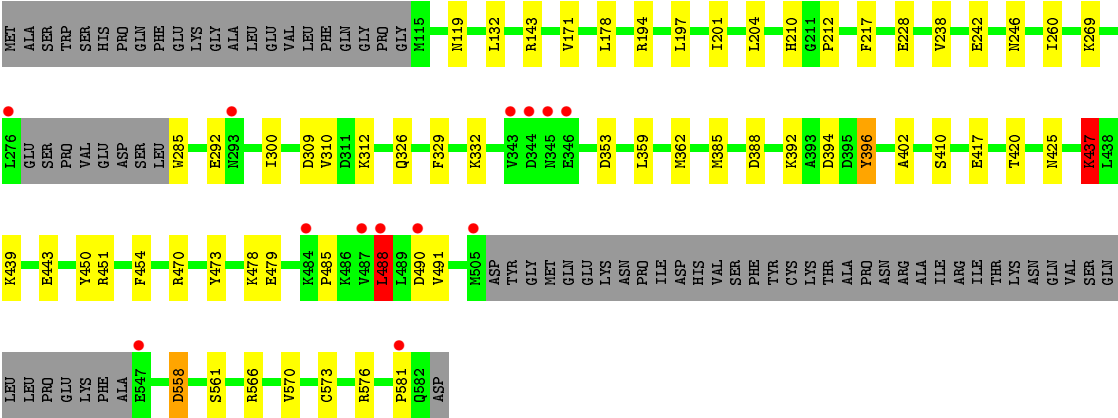


#### • Molecule 1: DEOXYNUCLEOSIDE TRIPHOSPHATE TRIPHOSPHOHYDROLASE SAMHD1





● Molecule 1: DEOXYNUCLEOSIDE TRIPHOSPHATE TRIPHOSPHOHYDROLASE SAMHD1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.71Å 199.32Å 81.80Å 90.00° 100.79° 90.00°	Depositor
Resolution (Å)	29.56 – 2.97 29.56 – 2.97	Depositor EDS
% Data completeness (in resolution range)	96.0 (29.56-2.97) 96.0 (29.56-2.97)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 2.95Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.156 , 0.234 0.171 , 0.240	Depositor DCC
$R_{free}$ test set	2197 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.0	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 81.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 43467 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13606	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, 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	0.50	0/3515	0.69	2/4758 (0.0%)
1	B	0.52	0/3397	0.73	3/4596 (0.1%)
1	C	0.48	0/3535	0.70	1/4783 (0.0%)
1	D	0.54	2/3352 (0.1%)	0.73	3/4539 (0.1%)
All	All	0.51	2/13799 (0.0%)	0.71	9/18676 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	573	CYS	CB-SG	-8.11	1.68	1.82
1	D	396	TYR	CE1-CZ	-8.11	1.28	1.38

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	437	LYS	CD-CE-NZ	-8.66	91.78	111.70
1	B	489	LEU	CA-CB-CG	8.60	135.09	115.30
1	D	488	LEU	CA-CB-CG	7.40	132.33	115.30
1	A	516	ASP	N-CA-C	-5.83	95.26	111.00
1	C	442	ARG	NE-CZ-NH2	5.77	123.19	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	230	LYS	Peptide
1	B	485	PRO	Peptide
1	C	284	LEU	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3433	0	3290	49	0
1	B	3317	0	3192	48	0
1	C	3452	0	3291	49	0
1	D	3272	0	3112	36	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	12	3	0
3	B	31	0	12	1	0
3	C	62	0	24	2	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
All	All	13606	0	12933	176	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 7.

The worst 5 of 176 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ASN:HB2	1:A:517:HIS:ND1	1.80	0.95
1:C:185:LYS:NZ	1:C:338:ALA:O	2.07	0.86
1:C:433:SER:OG	1:C:442:ARG:NH1	2.09	0.86
1:A:558:ASP:CA	1:A:559:ARG:N	2.39	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:HIS:HD1	1:B:374:TYR:HD2	1.32	0.76

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	426/491 (87%)	416 (98%)	7 (2%)	3 (1%)	26	67
1	B	413/491 (84%)	403 (98%)	7 (2%)	3 (1%)	26	67
1	C	426/491 (87%)	417 (98%)	9 (2%)	0	100	100
1	D	413/491 (84%)	405 (98%)	7 (2%)	1 (0%)	52	86
All	All	1678/1964 (85%)	1641 (98%)	30 (2%)	7 (0%)	39	78

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	487	VAL
1	A	464	GLY
1	A	517	HIS
1	B	230	LYS
1	A	304	LYS

### 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	355/433 (82%)	354 (100%)	1 (0%)	94	98
1	B	344/433 (79%)	340 (99%)	4 (1%)	78	93
1	C	357/433 (82%)	353 (99%)	4 (1%)	80	93
1	D	336/433 (78%)	331 (98%)	5 (2%)	72	91
All	All	1392/1732 (80%)	1378 (99%)	14 (1%)	82	94

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	437	LYS
1	C	465	GLN
1	D	437	LYS
1	C	306	ASN
1	D	332	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	235	GLN
1	D	425	ASN
1	C	303	ASN
1	A	517	HIS
1	B	293	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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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$
3	DGT	A	1583	-	25,33,33	2.05	8 (32%)	29,52,52	1.60	2 (6%)
3	DGT	B	1583	-	25,33,33	2.04	9 (36%)	29,52,52	1.63	5 (17%)
3	DGT	C	1583	-	25,33,33	2.08	9 (36%)	29,52,52	1.76	6 (20%)
3	DGT	C	1584	-	25,33,33	2.13	9 (36%)	29,52,52	1.80	7 (24%)

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
3	DGT	A	1583	-	-	0/18/34/34	0/3/3/3
3	DGT	B	1583	-	-	0/18/34/34	0/3/3/3
3	DGT	C	1583	-	-	0/18/34/34	0/3/3/3
3	DGT	C	1584	-	-	0/18/34/34	0/3/3/3

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1583	DGT	C8-N7	-3.25	1.28	1.34
3	B	1583	DGT	C8-N7	-3.19	1.28	1.34
3	C	1584	DGT	C8-N7	-3.06	1.28	1.34
3	C	1583	DGT	C8-N7	-2.98	1.28	1.34
3	C	1583	DGT	C3'-C4'	-2.93	1.44	1.53

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1583	DGT	N3-C2-N1	-5.64	119.88	127.56
3	C	1584	DGT	N3-C2-N1	-5.63	119.90	127.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1583	DGT	N3-C2-N1	-5.61	119.92	127.56
3	B	1583	DGT	N3-C2-N1	-5.49	120.08	127.56
3	C	1583	DGT	C5-C6-N1	-2.90	119.73	123.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1583	DGT	3	0
3	B	1583	DGT	1	0
3	C	1583	DGT	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	436/491 (88%)	-0.20	12 (2%) 56 36	30, 58, 98, 176	1 (0%)
1	B	419/491 (85%)	-0.20	8 (1%) 70 50	29, 55, 108, 147	1 (0%)
1	C	438/491 (89%)	-0.02	17 (3%) 43 25	33, 65, 117, 151	0
1	D	419/491 (85%)	-0.10	13 (3%) 52 33	31, 65, 115, 163	0
All	All	1712/1964 (87%)	-0.13	50 (2%) 55 35	29, 61, 113, 176	2 (0%)

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	487	VAL	5.8
1	C	507	TYR	5.0
1	C	466	ILE	4.2
1	C	464	GLY	3.9
1	D	343	VAL	3.7

### 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, 95<sup>th</sup> percentile and maximum values of B factors



of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	DGT	C	1583	31/31	0.91	0.18	-0.05	47,81,125,186	0
2	FE	C	1001	1/1	0.99	0.22	-0.06	60,60,60,60	0
2	FE	D	1001	1/1	0.98	0.20	-0.52	69,69,69,69	0
3	DGT	B	1583	31/31	0.95	0.15	-0.75	41,76,129,146	0
3	DGT	C	1584	31/31	0.94	0.14	-0.75	54,83,131,161	0
3	DGT	A	1583	31/31	0.96	0.12	-1.36	46,76,107,114	0
2	FE	B	1001	1/1	0.99	0.17	-1.40	63,63,63,63	0
2	FE	A	1001	1/1	0.99	0.17	-1.44	58,58,58,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.