



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:27 AM GMT

PDB ID : 2QRV  
Title : Structure of Dnmt3a-Dnmt3L C-terminal domain complex  
Authors : Jia, D.; Cheng, X.  
Deposited on : 2007-07-29  
Resolution : 2.89 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.

---

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

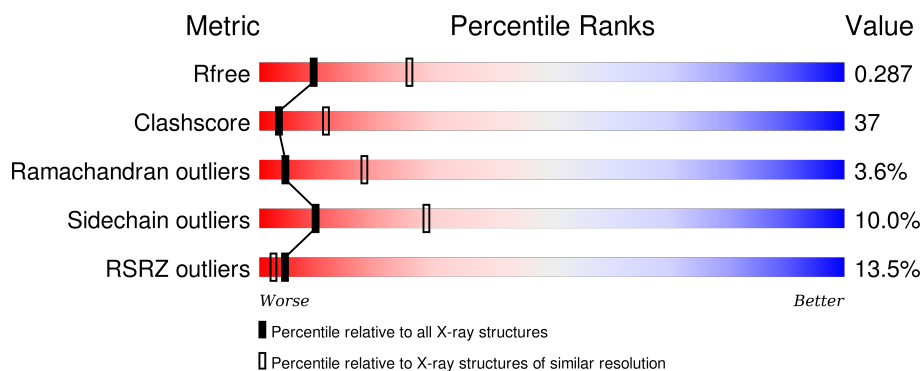
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.89 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	295	<div> <div>8%</div> <div>38% 45% 8% 8%</div> </div>
1	D	295	<div> <div>2%</div> <div>38% 44% 8% 9%</div> </div>
1	E	295	<div> <div>%</div> <div>38% 44% 8% 8%</div> </div>
1	H	295	<div> <div>8%</div> <div>35% 49% 7% 9%</div> </div>
2	B	230	<div> <div>16%</div> <div>40% 33% 8% 19%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	C	230	<div><div></div><div>17%</div><div>39%</div><div>38%</div><div>•</div><div>19%</div></div>
2	F	230	<div><div></div><div>17%</div><div>39%</div><div>37%</div><div>5%</div><div>19%</div></div>
2	G	230	<div><div></div><div>40%</div><div>40%</div><div>37%</div><div>•</div><div>19%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14657 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 DNA (cytosine-5)-methyltransferase 3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2143	1370	379	381	13			
1	D	267	Total	C	N	O	S	0	0	0
			2111	1350	372	376	13			
1	E	270	Total	C	N	O	S	0	0	0
			2128	1361	375	379	13			
1	H	267	Total	C	N	O	S	0	0	0
			2111	1350	372	376	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	614	MET	-	EXPRESSION TAG	UNP Q9Y6K1
A	615	GLY	-	EXPRESSION TAG	UNP Q9Y6K1
A	616	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
A	617	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
A	618	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
A	619	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
A	620	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
A	621	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
A	622	MET	-	EXPRESSION TAG	UNP Q9Y6K1
D	614	MET	-	EXPRESSION TAG	UNP Q9Y6K1
D	615	GLY	-	EXPRESSION TAG	UNP Q9Y6K1
D	616	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
D	617	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
D	618	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
D	619	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
D	620	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
D	621	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
D	622	MET	-	EXPRESSION TAG	UNP Q9Y6K1
E	614	MET	-	EXPRESSION TAG	UNP Q9Y6K1
E	615	GLY	-	EXPRESSION TAG	UNP Q9Y6K1
E	616	HIS	-	EXPRESSION TAG	UNP Q9Y6K1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	617	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
E	618	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
E	619	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
E	620	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
E	621	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
E	622	MET	-	EXPRESSION TAG	UNP Q9Y6K1
H	614	MET	-	EXPRESSION TAG	UNP Q9Y6K1
H	615	GLY	-	EXPRESSION TAG	UNP Q9Y6K1
H	616	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
H	617	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
H	618	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
H	619	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
H	620	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
H	621	HIS	-	EXPRESSION TAG	UNP Q9Y6K1
H	622	MET	-	EXPRESSION TAG	UNP Q9Y6K1

- Molecule 2 is a protein called DNA (cytosine-5)-methyltransferase 3-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	186	Total	C	N	O	S	0	0	0
			1515	991	254	266	4			
2	C	186	Total	C	N	O	S	0	0	0
			1515	991	254	266	4			
2	F	186	Total	C	N	O	S	0	0	0
			1515	991	254	266	4			
2	G	186	Total	C	N	O	S	0	0	0
			1515	991	254	266	4			

There are 12 discrepancies between the modelled and reference sequences:

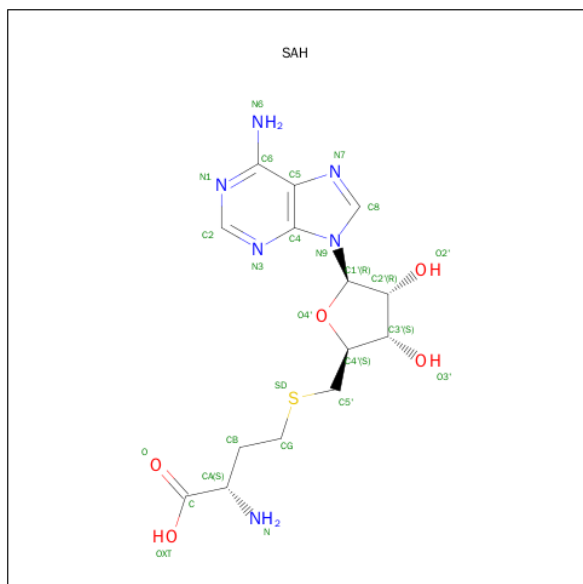
Chain	Residue	Modelled	Actual	Comment	Reference
B	157	GLY	-	EXPRESSION TAG	UNP Q9UJW3
B	158	SER	-	EXPRESSION TAG	UNP Q9UJW3
B	159	MET	-	EXPRESSION TAG	UNP Q9UJW3
C	157	GLY	-	EXPRESSION TAG	UNP Q9UJW3
C	158	SER	-	EXPRESSION TAG	UNP Q9UJW3
C	159	MET	-	EXPRESSION TAG	UNP Q9UJW3
F	157	GLY	-	EXPRESSION TAG	UNP Q9UJW3
F	158	SER	-	EXPRESSION TAG	UNP Q9UJW3
F	159	MET	-	EXPRESSION TAG	UNP Q9UJW3
G	157	GLY	-	EXPRESSION TAG	UNP Q9UJW3
G	158	SER	-	EXPRESSION TAG	UNP Q9UJW3

*Continued on next page...*

Continued from previous page...

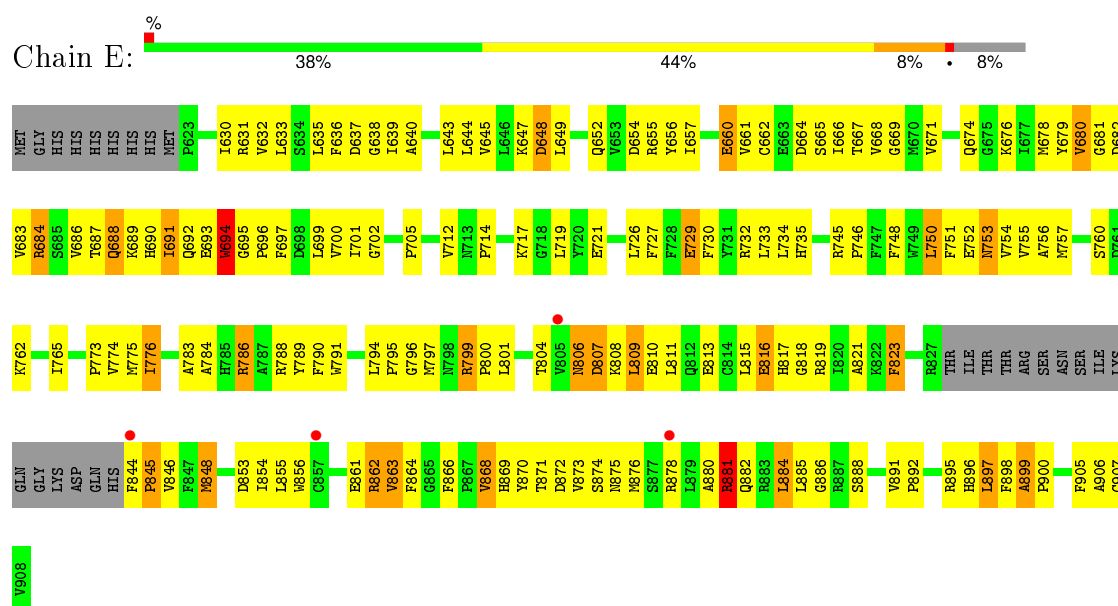
Chain	Residue	Modelled	Actual	Comment	Reference
G	159	MET	-	EXPRESSION TAG	UNP Q9UJW3

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula:  $\text{C}_{14}\text{H}_{20}\text{N}_6\text{O}_5\text{S}$ ).

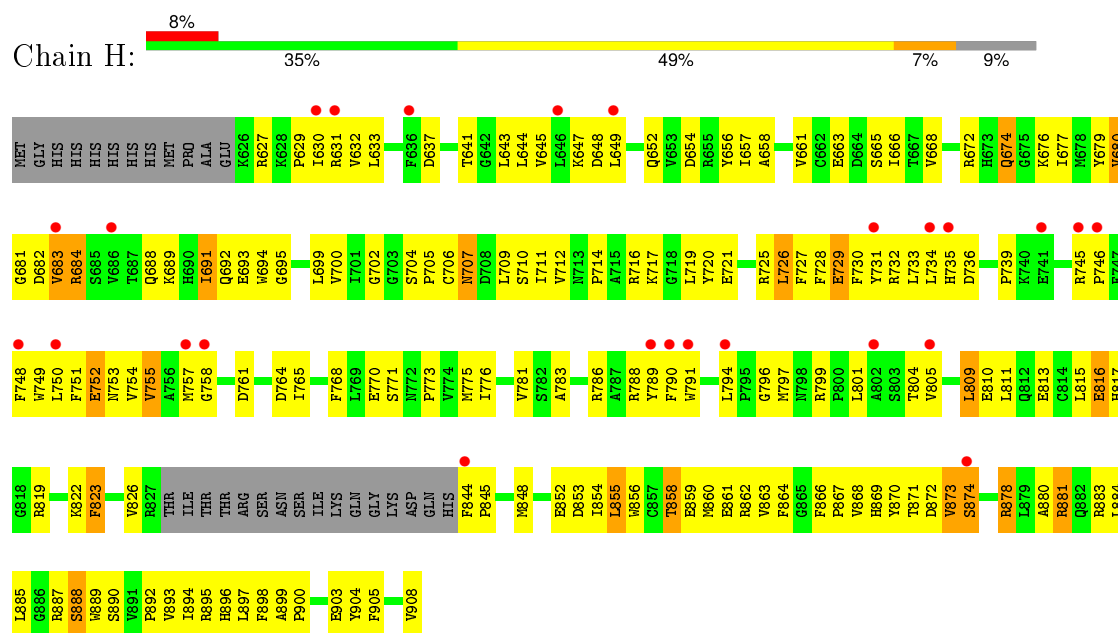


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 26	C 14	N 6	O 5	S 1	0	0
3	D	1	Total 26	C 14	N 6	O 5	S 1	0	0
3	E	1	Total 26	C 14	N 6	O 5	S 1	0	0
3	H	1	Total 26	C 14	N 6	O 5	S 1	0	0

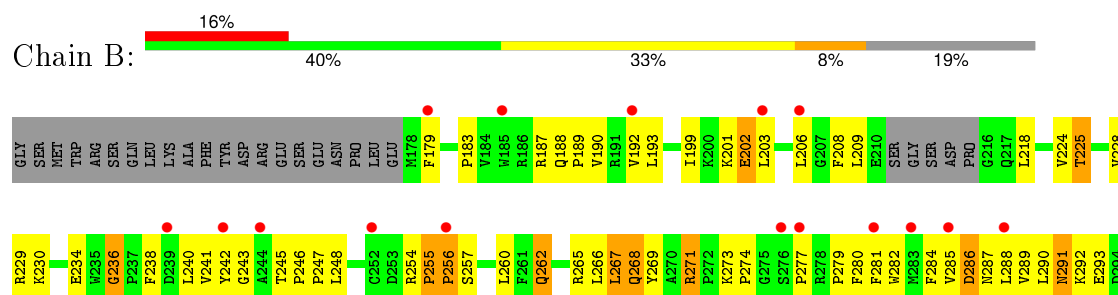




• Molecule 1: DNA (cytosine-5)-methyltransferase 3A

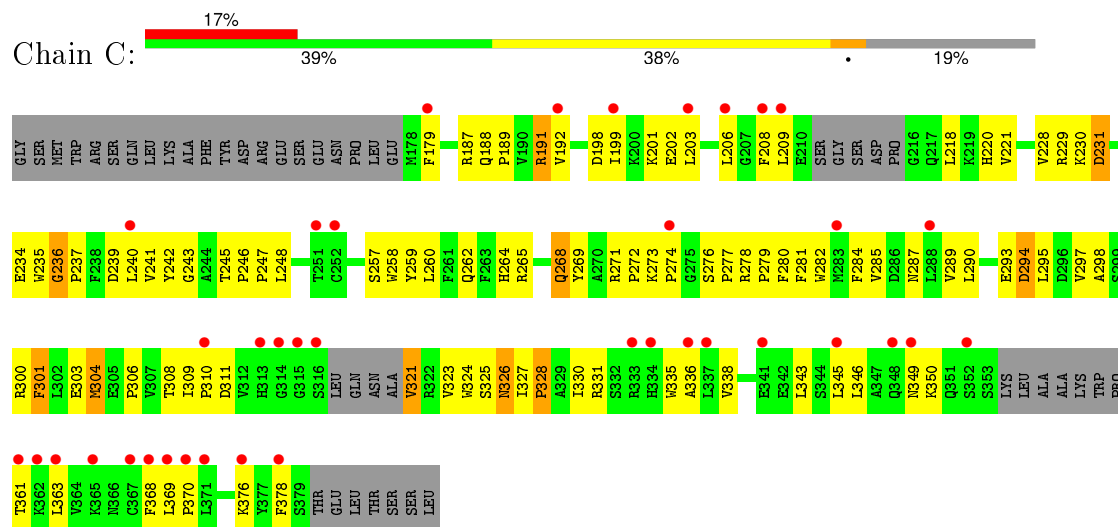


• Molecule 2: DNA (cytosine-5)-methyltransferase 3-like

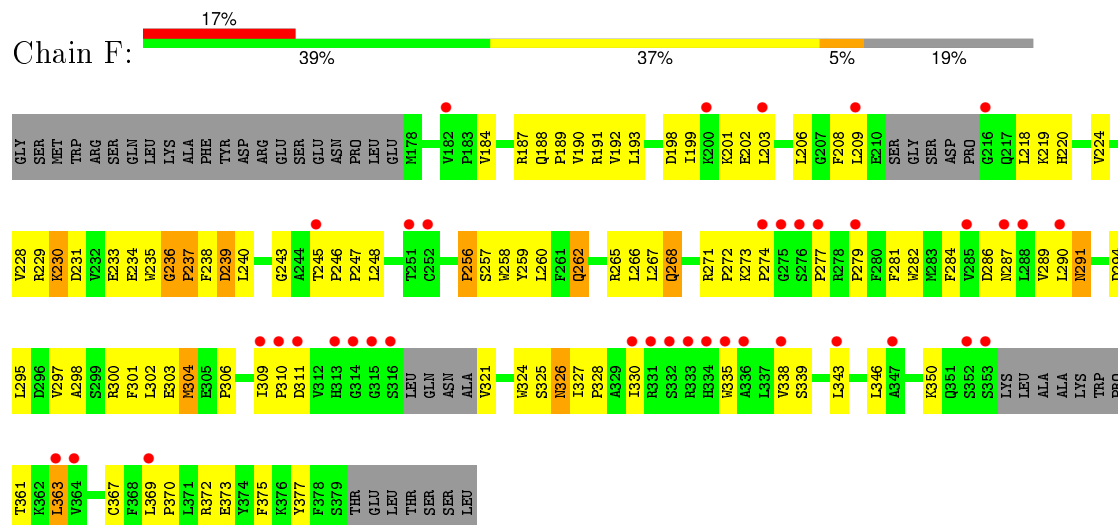




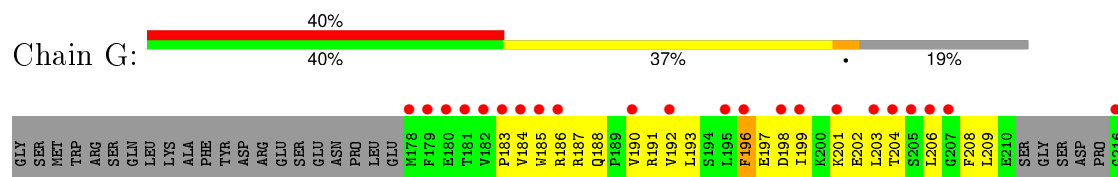
- Molecule 2: DNA (cytosine-5)-methyltransferase 3-like



- Molecule 2: DNA (cytosine-5)-methyltransferase 3-like



- Molecule 2: DNA (cytosine-5)-methyltransferase 3-like





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	401.88 Å   401.88 Å   49.69 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	38.90 – 2.89 43.85 – 2.90	Depositor EDS
% Data completeness (in resolution range)	81.9 (38.90-2.89) 92.7 (43.85-2.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.32 (at 2.90 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.259 , 0.281 0.271 , 0.287	Depositor DCC
$R_{free}$ test set	3124 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	77.8	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 79.4	EDS
Estimated twinning fraction	0.014 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 65264 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	14657	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: SAH

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	0.55	0/2196	0.83	2/2973 (0.1%)
1	D	0.52	0/2162	0.76	2/2926 (0.1%)
1	E	0.58	0/2180	0.78	1/2951 (0.0%)
1	H	0.44	0/2162	0.65	0/2926
2	B	0.41	0/1560	0.61	0/2120
2	C	0.37	0/1560	0.59	0/2120
2	F	0.35	0/1560	0.58	0/2120
2	G	0.36	0/1560	0.54	0/2120
All	All	0.47	0/14940	0.69	5/20256 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	844	PHE	C-N-CD	-13.46	91.00	120.60
1	D	875	ASN	N-CA-C	-6.49	93.47	111.00
1	A	644	LEU	CA-CB-CG	6.20	129.55	115.30
1	D	872	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	E	881	ARG	NE-CZ-NH1	5.04	122.82	120.30

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	2143	0	2076	174	0
1	D	2111	0	2052	172	0
1	E	2128	0	2067	170	0
1	H	2111	0	2052	195	0
2	B	1515	0	1484	122	0
2	C	1515	0	1484	93	0
2	F	1515	0	1484	109	0
2	G	1515	0	1484	105	0
3	A	26	0	19	1	0
3	D	26	0	19	0	0
3	E	26	0	19	1	0
3	H	26	0	19	2	0
All	All	14657	0	14259	1076	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 37.

The worst 5 of 1076 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:E:786:ARG:HG3	1:E:786:ARG:HH11	1.19	1.06
1:E:655:ARG:HH12	1:E:695:GLY:HA3	1.20	1.05
2:B:271:ARG:HH11	2:B:271:ARG:HG3	1.13	1.05
1:E:854:ILE:HG22	1:E:855:LEU:H	1.18	1.05
1:A:843:HIS:O	1:A:845:PRO:HD3	1.59	1.02

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	268/295 (91%)	228 (85%)	30 (11%)	10 (4%)	4 17

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	263/295 (89%)	221 (84%)	35 (13%)	7 (3%)	6	25
1	E	266/295 (90%)	223 (84%)	34 (13%)	9 (3%)	5	19
1	H	263/295 (89%)	226 (86%)	29 (11%)	8 (3%)	5	22
2	B	178/230 (77%)	135 (76%)	34 (19%)	9 (5%)	2	9
2	C	178/230 (77%)	138 (78%)	32 (18%)	8 (4%)	3	12
2	F	178/230 (77%)	136 (76%)	36 (20%)	6 (3%)	5	19
2	G	178/230 (77%)	138 (78%)	33 (18%)	7 (4%)	4	15
All	All	1772/2100 (84%)	1445 (82%)	263 (15%)	64 (4%)	4	18

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	845	PRO
1	D	849	ASN
1	E	845	PRO
1	H	874	SER
1	H	888	SER

### 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	224/259 (86%)	196 (88%)	28 (12%)	6	17
1	D	222/259 (86%)	194 (87%)	28 (13%)	5	16
1	E	223/259 (86%)	188 (84%)	35 (16%)	3	9
1	H	222/259 (86%)	203 (91%)	19 (9%)	13	36
2	B	166/210 (79%)	153 (92%)	13 (8%)	16	41
2	C	166/210 (79%)	154 (93%)	12 (7%)	18	46
2	F	166/210 (79%)	155 (93%)	11 (7%)	21	51
2	G	166/210 (79%)	157 (95%)	9 (5%)	27	62
All	All	1555/1876 (83%)	1400 (90%)	155 (10%)	9	28

5 of 155 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	807	ASP
1	E	665	SER
1	H	694	TRP
1	D	816	GLU
1	D	855	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	896	HIS
1	E	896	HIS
1	H	817	HIS
1	E	753	ASN
2	B	313	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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	SAH	A	1	-	20,28,28	1.96	6 (30%)	19,40,40	2.79	6 (31%)
3	SAH	D	4	-	20,28,28	1.72	5 (25%)	19,40,40	3.07	6 (31%)
3	SAH	E	5	-	20,28,28	1.97	6 (30%)	19,40,40	2.88	6 (31%)
3	SAH	H	8	-	20,28,28	1.91	4 (20%)	19,40,40	3.20	8 (42%)

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	SAH	A	1	-	-	0/7/31/31	0/3/3/3
3	SAH	D	4	-	-	0/7/31/31	0/3/3/3
3	SAH	E	5	-	-	0/7/31/31	0/3/3/3
3	SAH	H	8	-	-	0/7/31/31	0/3/3/3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	8	SAH	C5'-SD	-3.94	1.73	1.81
3	D	4	SAH	C5'-SD	-3.92	1.73	1.81
3	E	5	SAH	C5'-SD	-2.70	1.75	1.81
3	E	5	SAH	C8-N7	-2.54	1.29	1.34
3	A	1	SAH	C8-N7	-2.34	1.30	1.34

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5	SAH	N3-C2-N1	-9.38	121.71	128.89
3	A	1	SAH	N3-C2-N1	-8.59	122.31	128.89
3	H	8	SAH	N3-C2-N1	-8.49	122.39	128.89
3	D	4	SAH	N3-C2-N1	-7.93	122.82	128.89
3	H	8	SAH	CB-CG-SD	-6.52	100.99	113.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	SAH	1	0
3	E	5	SAH	1	0
3	H	8	SAH	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	272/295 (92%)	0.21	4 (1%) 76 74	30, 64, 106, 146	0
1	D	267/295 (90%)	0.16	5 (1%) 70 66	37, 75, 122, 157	0
1	E	270/295 (91%)	0.23	4 (1%) 76 74	27, 67, 111, 132	0
1	H	267/295 (90%)	0.57	25 (9%) 11 6	51, 101, 138, 170	0
2	B	186/230 (80%)	1.08	37 (19%) 1 1	55, 121, 187, 207	0
2	C	186/230 (80%)	1.06	38 (20%) 1 1	61, 118, 189, 206	0
2	F	186/230 (80%)	1.20	39 (20%) 1 1	66, 121, 189, 210	0
2	G	186/230 (80%)	2.83	93 (50%) 0 0	109, 163, 201, 210	0
All	All	1820/2100 (86%)	0.80	245 (13%) 4 2	27, 93, 181, 210	0

The worst 5 of 245 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	321	VAL	28.1
2	G	309	ILE	17.9
2	G	334	HIS	17.1
2	F	334	HIS	14.3
2	F	310	PRO	11.8

### 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	SAH	A	1	26/26	0.94	0.23	0.05	38,67,84,95	0
3	SAH	D	4	26/26	0.91	0.20	-0.32	40,59,71,73	0
3	SAH	E	5	26/26	0.96	0.19	-0.54	31,56,66,69	0
3	SAH	H	8	26/26	0.90	0.18	-0.59	49,104,112,114	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.