Full wwPDB X-ray Structure Validation Report ⓘ

Nov 28, 2016 – 01:12 PM EST

PDB ID	:	5T6B
Title	:	X-ray structure of the KijD1 C3-methyltransfeerase, converted to monomeric form
Authors	:	Holden, H.M.; Thoden, J.B.; Dow, G.T.
Deposited on	:	2016-09-01
Resolution	:	2.00 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 ①) were used in the production of this report:

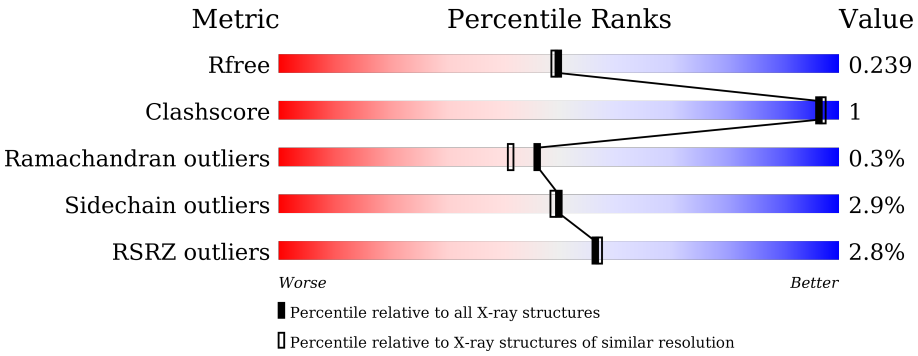
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 <=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	416	3% 92% 5% ·
1	B	416	2% 92% 6% ·
1	C	416	3% 87% 7% 5%
1	D	416	2% 85% 8% · 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13433 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 Sugar 3-C-methyl transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	4	0
			3164	1998	566	583	17			
1	B	406	Total	C	N	O	S	0	1	0
			3167	2001	560	589	17			
1	C	394	Total	C	N	O	S	0	3	0
			3085	1953	546	569	17			
1	D	393	Total	C	N	O	S	0	1	0
			3064	1937	543	567	17			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLN	-	expression tag	UNP B3TMQ9
A	0	HIS	-	expression tag	UNP B3TMQ9
A	92	MET	LYS	engineered mutation	UNP B3TMQ9
A	95	ARG	GLN	engineered mutation	UNP B3TMQ9
A	96	ASP	ARG	engineered mutation	UNP B3TMQ9
A	97	PHE	LEU	engineered mutation	UNP B3TMQ9
A	105	PRO	ALA	engineered mutation	UNP B3TMQ9
A	388	GLU	ASP	engineered mutation	UNP B3TMQ9
A	398	HIS	ARG	engineered mutation	UNP B3TMQ9
A	412	HIS	ARG	engineered mutation	UNP B3TMQ9
A	413	ILE	VAL	engineered mutation	UNP B3TMQ9
A	414	ARG	LEU	engineered mutation	UNP B3TMQ9
B	-1	GLN	-	expression tag	UNP B3TMQ9
B	0	HIS	-	expression tag	UNP B3TMQ9
B	92	MET	LYS	engineered mutation	UNP B3TMQ9
B	95	ARG	GLN	engineered mutation	UNP B3TMQ9
B	96	ASP	ARG	engineered mutation	UNP B3TMQ9
B	97	PHE	LEU	engineered mutation	UNP B3TMQ9
B	105	PRO	ALA	engineered mutation	UNP B3TMQ9
B	388	GLU	ASP	engineered mutation	UNP B3TMQ9
B	398	HIS	ARG	engineered mutation	UNP B3TMQ9

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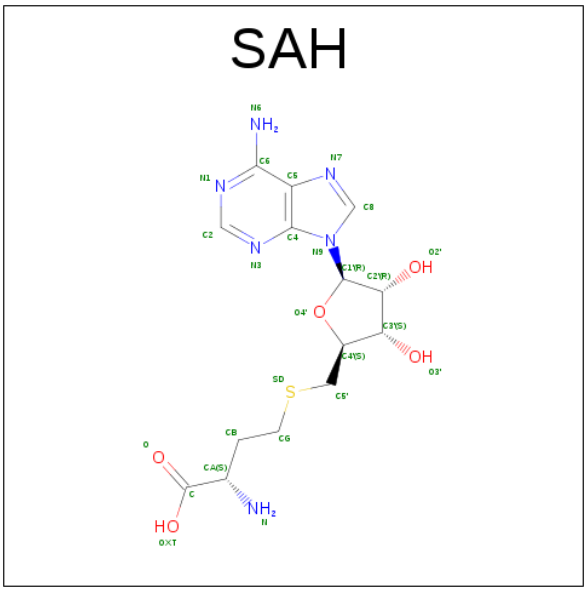
Chain	Residue	Modelled	Actual	Comment	Reference
B	412	HIS	ARG	engineered mutation	UNP B3TMQ9
B	413	ILE	VAL	engineered mutation	UNP B3TMQ9
B	414	ARG	LEU	engineered mutation	UNP B3TMQ9
C	-1	GLN	-	expression tag	UNP B3TMQ9
C	0	HIS	-	expression tag	UNP B3TMQ9
C	92	MET	LYS	engineered mutation	UNP B3TMQ9
C	95	ARG	GLN	engineered mutation	UNP B3TMQ9
C	96	ASP	ARG	engineered mutation	UNP B3TMQ9
C	97	PHE	LEU	engineered mutation	UNP B3TMQ9
C	105	PRO	ALA	engineered mutation	UNP B3TMQ9
C	388	GLU	ASP	engineered mutation	UNP B3TMQ9
C	398	HIS	ARG	engineered mutation	UNP B3TMQ9
C	412	HIS	ARG	engineered mutation	UNP B3TMQ9
C	413	ILE	VAL	engineered mutation	UNP B3TMQ9
C	414	ARG	LEU	engineered mutation	UNP B3TMQ9
D	-1	GLN	-	expression tag	UNP B3TMQ9
D	0	HIS	-	expression tag	UNP B3TMQ9
D	92	MET	LYS	engineered mutation	UNP B3TMQ9
D	95	ARG	GLN	engineered mutation	UNP B3TMQ9
D	96	ASP	ARG	engineered mutation	UNP B3TMQ9
D	97	PHE	LEU	engineered mutation	UNP B3TMQ9
D	105	PRO	ALA	engineered mutation	UNP B3TMQ9
D	388	GLU	ASP	engineered mutation	UNP B3TMQ9
D	398	HIS	ARG	engineered mutation	UNP B3TMQ9
D	412	HIS	ARG	engineered mutation	UNP B3TMQ9
D	413	ILE	VAL	engineered mutation	UNP B3TMQ9
D	414	ARG	LEU	engineered mutation	UNP B3TMQ9

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

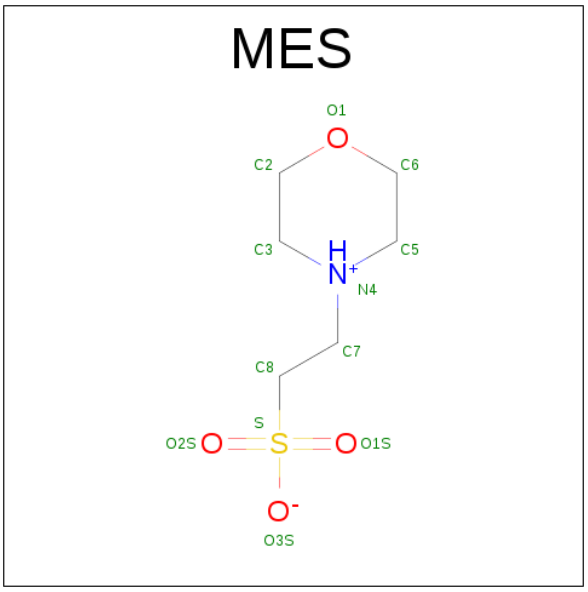
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



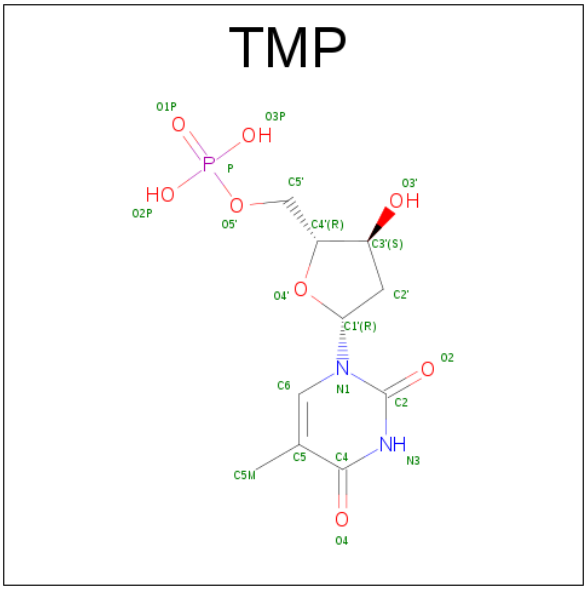
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is THYMIDINE-5'-PHOSPHATE (three-letter code: TMP) (formula: $C_{10}H_{15}N_2O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
5	B	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
5	C	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
5	D	1	Total	C	N	O	P	0	0
			21	10	2	8	1		

- Molecule 6 is water.

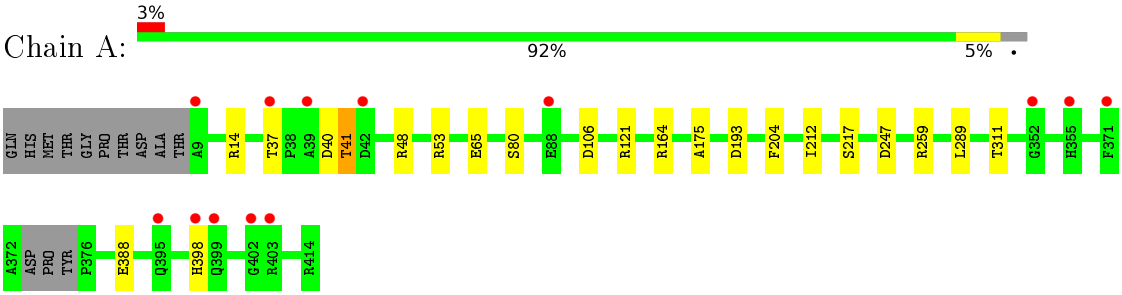
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	187	Total	O	0	0
			187	187		
6	B	182	Total	O	0	0
			182	182		
6	C	175	Total	O	0	0
			175	175		
6	D	193	Total	O	0	0
			193	193		

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.

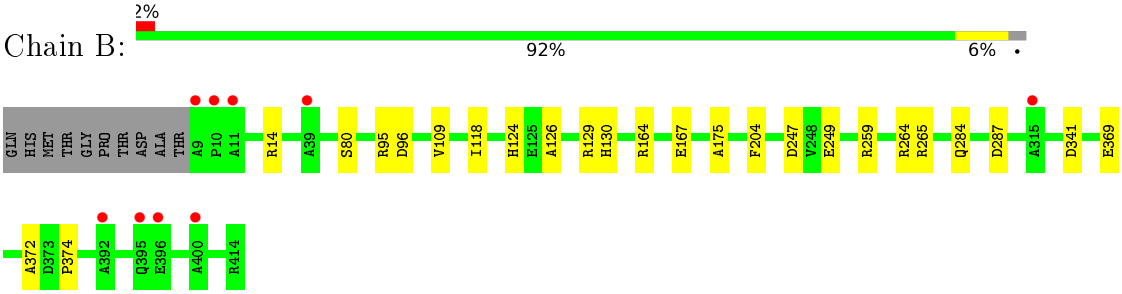
- Molecule 1: Sugar 3-C-methyl transferase

Chain A:



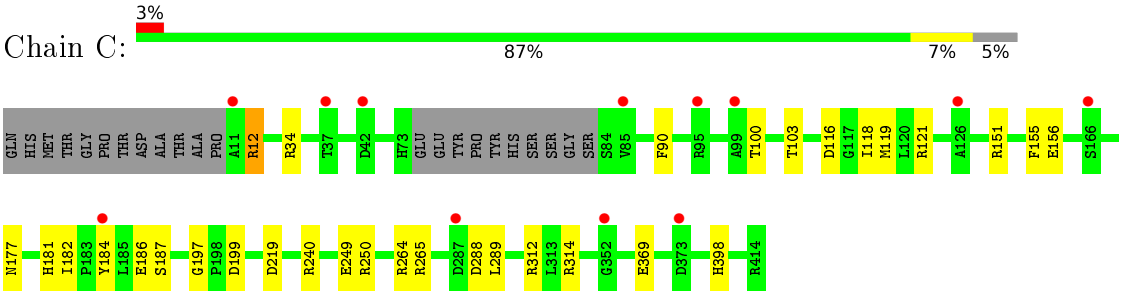
- Molecule 1: Sugar 3-C-methyl transferase

Chain B:



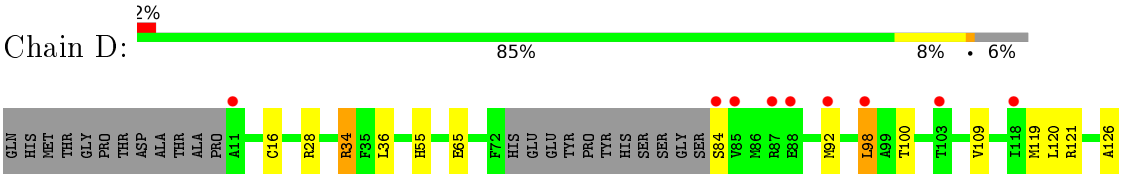
- Molecule 1: Sugar 3-C-methyl transferase

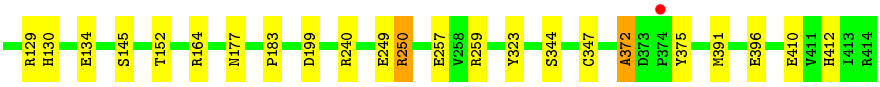
Chain C:



- Molecule 1: Sugar 3-C-methyl transferase

Chain D:




R129
H130
E134
S145
T152
R164
N177
P183
D199
R240
E249
R250
E257
Y258
R259
Y323
S344
C347
A372
D373
P374
Y375
M391
E396
E410
Y411
H412
I413
R414

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	62.71Å 82.45Å 82.83Å 96.05° 110.70° 112.09°	Depositor
Resolution (Å)	30.00 – 2.00 29.85 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.6 (30.00-2.00) 87.3 (29.85-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.176 , 0.234 0.184 , 0.239	Depositor DCC
R_{free} test set	4528 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	20.3	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.028 for h,-h-k,-h-l 0.018 for -h,-l,-k 0.014 for -h,h+l,h+k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13433	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.81 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2385e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TMP, ZN, SAH, MES

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	0.73	0/3252	0.87	5/4410 (0.1%)
1	B	0.73	2/3249 (0.1%)	0.89	9/4413 (0.2%)
1	C	0.77	2/3168 (0.1%)	0.88	6/4300 (0.1%)
1	D	0.77	1/3139 (0.0%)	0.91	9/4260 (0.2%)
All	All	0.75	5/12808 (0.0%)	0.89	29/17383 (0.2%)

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	D	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	249	GLU	CD-OE2	7.23	1.33	1.25
1	C	249	GLU	CD-OE2	6.82	1.33	1.25
1	B	249	GLU	CD-OE2	6.30	1.32	1.25
1	C	156	GLU	CD-OE2	5.56	1.31	1.25
1	B	287	ASP	CB-CG	5.02	1.62	1.51

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	259	ARG	NE-CZ-NH2	8.79	124.70	120.30
1	B	109	VAL	CB-CA-C	-8.23	95.77	111.40
1	A	106	ASP	CB-CG-OD2	6.80	124.42	118.30
1	A	48	ARG	NE-CZ-NH1	6.43	123.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	34	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	247	ASP	CB-CG-OD1	6.19	123.87	118.30
1	C	250	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	C	219	ASP	CB-CG-OD1	5.76	123.48	118.30
1	D	34	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	D	164	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	C	12	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	95	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	B	259	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	B	164	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	129	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	D	250	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	D	164	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	D	259	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	D	28	ARG	NE-CZ-NH2	5.15	122.88	120.30
1	B	95	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	A	259	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	96	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	B	247	ASP	CB-CG-OD1	5.08	122.87	118.30
1	C	199	ASP	CB-CG-OD1	5.08	122.87	118.30
1	B	265	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	D	391	MET	CA-CB-CG	-5.06	104.70	113.30
1	C	151	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	C	250	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	48	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	372	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3164	0	3069	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3167	0	3050	5	0
1	C	3085	0	2986	9	0
1	D	3064	0	2968	12	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	26	0	19	2	0
3	B	26	0	19	1	0
3	C	26	0	19	0	0
3	D	26	0	19	1	0
4	A	12	0	13	0	0
4	B	12	0	13	0	0
5	A	21	0	13	0	0
5	B	21	0	13	0	0
5	C	21	0	13	0	0
5	D	21	0	13	0	0
6	A	187	0	0	2	0
6	B	182	0	0	0	0
6	C	175	0	0	3	0
6	D	193	0	0	0	0
All	All	13433	0	12227	34	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 1.

All (34) 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:14:ARG:NE	1:A:65:GLU:OE2	2.25	0.67
1:D:98:LEU:HD11	1:D:126:ALA:CB	2.26	0.65
1:C:184[B]:TYR:CE2	1:C:187:SER:HB2	2.34	0.63
1:A:40:ASP:OD1	1:A:41:THR:N	2.38	0.56
1:D:410:GLU:O	1:D:412:HIS:HD2	1.90	0.54
1:C:184[A]:TYR:HE2	6:C:601:HOH:O	1.90	0.54
1:C:90:PHE:CD1	1:C:119:MET:HG2	2.42	0.54
1:C:155:PHE:O	6:C:601:HOH:O	2.19	0.53
1:C:116:ASP:OD1	1:C:118:ILE:HD13	2.09	0.52
1:A:53:ARG:NE	6:A:602:HOH:O	2.43	0.52
1:A:164[B]:ARG:NH1	6:A:601:HOH:O	2.32	0.51
1:B:80:SER:CB	3:B:502:SAH:HN1	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:ALA:HA	1:D:375:TYR:CE1	2.46	0.50
1:A:80:SER:CB	3:A:502:SAH:HN1	2.25	0.50
1:B:175:ALA:O	1:B:204:PHE:HA	2.12	0.50
1:A:175:ALA:O	1:A:204:PHE:HA	2.12	0.49
1:D:177:ASN:ND2	1:D:257:GLU:OE2	2.44	0.49
1:C:398:HIS:HD2	6:C:709:HOH:O	1.96	0.48
1:C:197:GLY:O	1:C:264:ARG:NH1	2.41	0.48
1:B:126:ALA:HA	1:D:250:ARG:HD3	1.97	0.47
1:C:177:ASN:O	1:C:181[A]:HIS:CE1	2.69	0.45
1:B:372:ALA:O	1:B:374:PRO:HA	2.17	0.45
1:A:212:ILE:HA	1:A:217:SER:OG	2.16	0.44
1:D:65:GLU:HG2	1:D:183:PRO:HG2	1.98	0.44
1:B:124:HIS:HB2	1:B:130:HIS:CE1	2.53	0.44
1:A:193:ASP:O	1:D:55:HIS:NE2	2.51	0.43
1:D:323:TYR:CD2	1:D:347[B]:CYS:SG	3.12	0.43
1:A:80:SER:OG	3:A:502:SAH:N	2.41	0.43
1:D:375:TYR:OH	1:D:396:GLU:HG3	2.19	0.42
1:D:134:GLU:O	1:D:152:THR:HA	2.18	0.42
1:D:120:LEU:HA	1:D:120:LEU:HD23	1.88	0.42
1:C:182:ILE:HG23	1:C:184[A]:TYR:CZ	2.55	0.41
1:D:109:VAL:O	1:D:130:HIS:HA	2.19	0.41
3:D:502:SAH:HB2	3:D:502:SAH:H4'	2.02	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	403/416 (97%)	389 (96%)	13 (3%)	1 (0%)	52	48
1	B	405/416 (97%)	390 (96%)	14 (4%)	1 (0%)	52	48
1	C	393/416 (94%)	383 (98%)	9 (2%)	1 (0%)	46	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	390/416 (94%)	381 (98%)	8 (2%)	1 (0%)	46 41
All	All	1591/1664 (96%)	1543 (97%)	44 (3%)	4 (0%)	46 41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	C	103	THR
1	D	145	SER
1	B	118	ILE

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	327/334 (98%)	321 (98%)	6 (2%)	66 69
1	B	327/334 (98%)	321 (98%)	6 (2%)	66 69
1	C	318/334 (95%)	306 (96%)	12 (4%)	40 36
1	D	316/334 (95%)	303 (96%)	13 (4%)	37 32
All	All	1288/1336 (96%)	1251 (97%)	37 (3%)	50 49

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	121	ARG
1	A	289	LEU
1	A	311	THR
1	A	388	GLU
1	A	398	HIS
1	B	14	ARG
1	B	167	GLU
1	B	264	ARG
1	B	284	GLN

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Mol	Chain	Res	Type
1	B	341	ASP
1	B	369	GLU
1	C	12	ARG
1	C	34	ARG
1	C	100	THR
1	C	121	ARG
1	C	186	GLU
1	C	240	ARG
1	C	265	ARG
1	C	288	ASP
1	C	289	LEU
1	C	312	ARG
1	C	314	ARG
1	C	369	GLU
1	D	16	CYS
1	D	34	ARG
1	D	36	LEU
1	D	84	SER
1	D	92	MET
1	D	98	LEU
1	D	100	THR
1	D	119	MET
1	D	121	ARG
1	D	129	ARG
1	D	199	ASP
1	D	240	ARG
1	D	344	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	ASN
1	A	181	HIS
1	B	177	ASN
1	C	398	HIS
1	D	412	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	SAH	A	502	-	22,28,28	1.16	3 (13%)	18,40,40	2.68	4 (22%)
4	MES	A	503	-	12,12,12	1.82	1 (8%)	15,16,16	2.30	4 (26%)
5	TMP	A	504	-	17,22,22	1.19	2 (11%)	22,33,33	2.80	7 (31%)
3	SAH	B	502	-	22,28,28	1.15	2 (9%)	18,40,40	3.16	5 (27%)
4	MES	B	503	-	12,12,12	1.42	1 (8%)	15,16,16	1.75	3 (20%)
5	TMP	B	504	-	17,22,22	1.14	1 (5%)	22,33,33	2.77	7 (31%)
3	SAH	C	502	-	22,28,28	1.49	3 (13%)	18,40,40	2.34	5 (27%)
5	TMP	C	503	-	17,22,22	0.99	1 (5%)	22,33,33	3.22	9 (40%)
3	SAH	D	502	-	22,28,28	1.28	2 (9%)	18,40,40	2.20	5 (27%)
5	TMP	D	503	-	17,22,22	0.83	0	22,33,33	3.29	10 (45%)

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	502	-	-	0/7/31/31	0/3/3/3
4	MES	A	503	-	-	0/6/14/14	0/1/1/1
5	TMP	A	504	-	-	0/6/22/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAH	B	502	-	-	0/7/31/31	0/3/3/3
4	MES	B	503	-	-	0/6/14/14	0/1/1/1
5	TMP	B	504	-	-	0/6/22/22	0/2/2/2
3	SAH	C	502	-	-	0/7/31/31	0/3/3/3
5	TMP	C	503	-	-	0/6/22/22	0/2/2/2
3	SAH	D	502	-	-	0/7/31/31	0/3/3/3
5	TMP	D	503	-	-	0/6/22/22	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	MES	C8-S	-5.94	1.68	1.77
4	B	503	MES	C8-S	-3.81	1.71	1.77
3	A	502	SAH	C5'-SD	-2.56	1.76	1.81
3	C	502	SAH	C2-N1	2.09	1.37	1.33
3	A	502	SAH	O3'-C3'	2.15	1.48	1.43
3	C	502	SAH	O4'-C1'	2.41	1.44	1.41
5	A	504	TMP	O4'-C1'	2.48	1.48	1.42
3	B	502	SAH	C5-C4	2.61	1.46	1.40
5	B	504	TMP	P-O5'	2.76	1.67	1.59
5	C	503	TMP	P-O5'	2.79	1.67	1.59
5	A	504	TMP	P-O5'	2.82	1.68	1.59
3	D	502	SAH	O4'-C1'	2.94	1.45	1.41
3	A	502	SAH	C5-C4	2.99	1.47	1.40
3	B	502	SAH	O4'-C1'	3.30	1.46	1.41
3	D	502	SAH	C5-C4	3.31	1.48	1.40
3	C	502	SAH	C5-C4	4.17	1.49	1.40

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	SAH	N3-C2-N1	-8.60	122.11	128.87
5	B	504	TMP	C5-C4-N3	-7.74	118.85	125.35
5	D	503	TMP	O2P-P-O5'	-7.68	84.31	106.72
5	C	503	TMP	C5-C4-N3	-7.30	119.22	125.35
3	A	502	SAH	N3-C2-N1	-7.29	123.14	128.87
5	A	504	TMP	C5-C4-N3	-6.91	119.55	125.35
3	B	502	SAH	C1'-N9-C4	-6.86	119.15	126.81
3	C	502	SAH	N3-C2-N1	-6.68	123.62	128.87
5	D	503	TMP	C5-C4-N3	-6.17	120.17	125.35
5	C	503	TMP	O5'-P-O1P	-5.81	92.47	107.08
3	D	502	SAH	N3-C2-N1	-5.64	124.44	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	503	TMP	O3P-P-O5'	-5.55	90.52	106.72
3	A	502	SAH	C1'-N9-C4	-4.31	122.00	126.81
3	C	502	SAH	C1'-N9-C4	-3.90	122.46	126.81
3	D	502	SAH	C1'-N9-C4	-3.51	122.89	126.81
4	A	503	MES	O2S-S-O1S	-2.76	106.16	113.96
3	D	502	SAH	CB-CA-N	-2.76	102.78	110.54
5	A	504	TMP	O3'-C3'-C2'	-2.75	101.45	110.74
4	B	503	MES	O2S-S-O1S	-2.43	107.09	113.96
5	D	503	TMP	O5'-P-O1P	-2.23	101.47	107.08
5	D	503	TMP	O4'-C4'-C5'	-2.23	101.31	109.29
3	B	502	SAH	C5'-SD-CG	-2.13	95.96	102.42
3	B	502	SAH	C4'-O4'-C1'	-2.06	107.46	109.64
5	B	504	TMP	O3P-P-O1P	2.00	117.17	110.63
4	A	503	MES	O3S-S-O2S	2.00	115.70	111.26
5	D	503	TMP	O3P-P-O1P	2.12	117.54	110.63
3	A	502	SAH	C2'-C1'-N9	2.13	119.16	113.47
3	D	502	SAH	N6-C6-N1	2.16	122.13	118.52
5	C	503	TMP	C2'-C3'-C4'	2.17	107.18	102.77
5	D	503	TMP	O3P-P-O5'	2.18	113.08	106.72
5	A	504	TMP	C4'-O4'-C1'	2.32	115.38	109.42
5	B	504	TMP	C2'-C3'-C4'	2.44	107.72	102.77
4	B	503	MES	O1S-S-C8	2.50	108.64	106.87
5	B	504	TMP	C5M-C5-C4	2.54	122.78	119.97
3	C	502	SAH	N6-C6-N1	2.82	123.25	118.52
5	B	504	TMP	O5'-C5'-C4'	2.83	119.31	109.09
5	C	503	TMP	O5'-C5'-C4'	2.84	119.32	109.09
3	C	502	SAH	C2-N1-C6	2.92	123.97	118.77
5	A	504	TMP	C2'-C3'-C4'	2.98	108.82	102.77
5	D	503	TMP	O5'-C5'-C4'	3.14	120.41	109.09
5	A	504	TMP	O5'-C5'-C4'	3.25	120.81	109.09
5	B	504	TMP	O4'-C1'-N1	3.27	113.43	107.71
5	D	503	TMP	O4'-C1'-N1	3.28	113.44	107.71
5	C	503	TMP	O3P-P-O2P	3.72	121.11	107.44
3	D	502	SAH	C5'-SD-CG	3.83	114.06	102.42
3	C	502	SAH	C5'-SD-CG	3.86	114.16	102.42
5	C	503	TMP	O2P-P-O5'	3.90	118.12	106.72
5	C	503	TMP	O4'-C1'-N1	3.94	114.59	107.71
4	A	503	MES	O2S-S-C8	4.35	109.94	106.87
5	D	503	TMP	O3P-P-O2P	4.74	124.83	107.44
4	B	503	MES	O2S-S-C8	4.98	110.39	106.87
5	A	504	TMP	O4'-C1'-N1	5.11	116.65	107.71
4	A	503	MES	O1S-S-C8	6.14	111.21	106.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	503	TMP	C4-N3-C2	6.19	120.32	115.16
3	B	502	SAH	CB-CA-N	6.40	128.53	110.54
3	A	502	SAH	CB-CA-N	6.46	128.71	110.54
5	A	504	TMP	C4-N3-C2	7.02	121.02	115.16
5	D	503	TMP	C4-N3-C2	7.79	121.66	115.16
5	B	504	TMP	C4-N3-C2	7.81	121.68	115.16

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	502	SAH	2	0
3	B	502	SAH	1	0
3	D	502	SAH	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, 95^{th} 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	403/416 (96%)	-0.24	13 (3%) 51 52	13, 22, 51, 74	0
1	B	406/416 (97%)	-0.30	9 (2%) 65 66	11, 21, 47, 69	0
1	C	394/416 (94%)	-0.20	12 (3%) 54 55	11, 22, 48, 74	0
1	D	393/416 (94%)	-0.31	10 (2%) 61 61	11, 20, 47, 68	0
All	All	1596/1664 (95%)	-0.26	44 (2%) 56 57	11, 21, 48, 74	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	ALA	4.2
1	A	399	GLN	3.9
1	B	392	ALA	3.9
1	A	39	ALA	3.5
1	B	10	PRO	3.4
1	B	395	GLN	3.1
1	C	99	ALA	3.0
1	D	98	LEU	3.0
1	C	11	ALA	3.0
1	A	403	ARG	3.0
1	B	39	ALA	3.0
1	D	11	ALA	2.8
1	C	95	ARG	2.7
1	A	42	ASP	2.7
1	C	184[A]	TYR	2.7
1	A	37	THR	2.6
1	B	9	ALA	2.6
1	C	126	ALA	2.6
1	D	92	MET	2.6
1	C	166	SER	2.5
1	A	355	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	395	GLN	2.5
1	A	402	GLY	2.5
1	C	37	THR	2.5
1	A	371	PHE	2.4
1	D	87	ARG	2.4
1	A	398	HIS	2.3
1	B	400	ALA	2.3
1	C	352	GLY	2.3
1	D	88	GLU	2.3
1	B	315	ALA	2.2
1	B	396	GLU	2.2
1	D	103	THR	2.2
1	C	42	ASP	2.2
1	D	374	PRO	2.2
1	D	118	ILE	2.1
1	A	88	GLU	2.1
1	A	352	GLY	2.1
1	D	84	SER	2.0
1	C	287	ASP	2.0
1	C	373	ASP	2.0
1	B	11	ALA	2.0
1	C	85	VAL	2.0
1	D	85	VAL	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SAH	A	502	26/26	0.94	0.13	0.96	13,15,23,25	0
3	SAH	B	502	26/26	0.95	0.11	0.89	10,11,18,20	0
5	TMP	D	503	21/21	0.85	0.10	0.50	17,19,32,39	0
5	TMP	C	503	21/21	0.82	0.12	0.49	18,23,31,37	0
5	TMP	B	504	21/21	0.83	0.13	0.20	32,36,49,52	0
5	TMP	A	504	21/21	0.85	0.12	-0.03	42,44,49,50	0
4	MES	A	503	12/12	0.97	0.08	-0.56	18,19,29,29	0
3	SAH	C	502	26/26	0.96	0.09	-0.57	12,16,19,20	0
3	SAH	D	502	26/26	0.95	0.08	-0.82	16,19,20,22	0
4	MES	B	503	12/12	0.98	0.07	-1.99	19,20,20,21	0
2	ZN	B	501	1/1	1.00	0.03	-2.13	22,22,22,22	0
2	ZN	D	501	1/1	0.99	0.03	-2.64	34,34,34,34	0
2	ZN	A	501	1/1	1.00	0.03	-2.77	25,25,25,25	0
2	ZN	C	501	1/1	1.00	0.02	-3.64	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.