

# wwPDB X-ray Structure Validation Summary Report (i)

#### Sep 23, 2023 – 10:03 PM EDT

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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

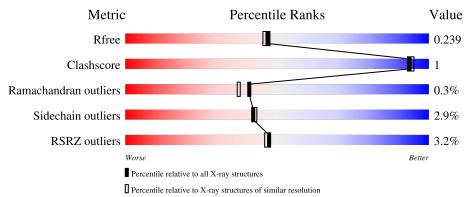
MolProbity	:	4.02b-467 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)		
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	А	416	4% 92%	5% •
1	В	416	2% 92%	6% ·
1	С	416	87%	7% 5%
1	D	416	85%	8% • 6%



# 2 Entry composition (i)

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	402	Total	С	Ν	0	S	0	4	0
	A	403	3164	1998	566	583	17	0	4	0
1	В	406	Total	С	Ν	0	S	0	1	0
	D	400	3167	2001	560	589	17	0		
1	С	394	Total	С	Ν	0	S	0	2	0
	C	394	3085	1953	546	569	17	0	3	0
1	П	393	Total	С	Ν	0	S	0	1	0
		აჟა	3064	1937	543	567	17	0		0

• Molecule 1 is a protein called Sugar 3-C-methyl transferase.

There are 48 discrepancies between the modelled and reference sequences:

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



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

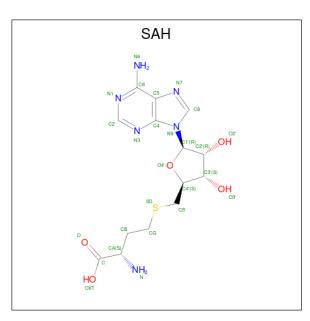
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• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Zn 1 1	0	0
2	В	1	Total Zn 1 1	0	0
2	С	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

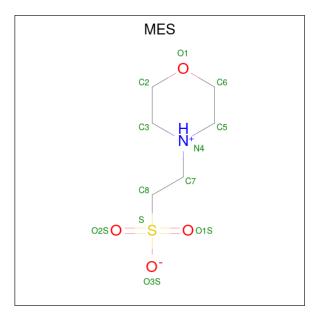
• Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	Δ	1	Total	С	Ν	0	S	0	0
5	Π	T	26	14	6	5	1	0	0
3	B	1	Total	С	Ν	Ο	$\mathbf{S}$	0	0
5	D	DI	26	14	6	5	1	0	0
3	С	1	Total	С	Ν	Ο	$\mathbf{S}$	0	0
5	U	T	26	14	6	5	1	0	0
3	Л	1	Total	С	N	0	$\mathbf{S}$	0	0
5	D	L	26	14	6	5	1	0	U

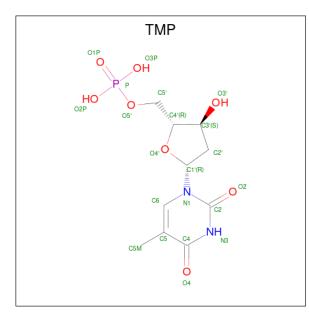
• Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	А	1	Total 12					0	0
4	В	1	Total 12		N 1		S 1	0	0

• 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	А	1	Total	0	N	0	P	0	0	
			21 Total		$\frac{2}{N}$	$\frac{8}{0}$	1 P			
5	В	1	21	•	1N 2	8	1	0	0	
5	С	1	Total	С		0	Р	0	0	
0	0	1	21	10	2	8	1	0	0	
5	D	1	Total	~	Ν	Ο	Р	0	0	
0	D	1	21	10	2	8	1	0	0	

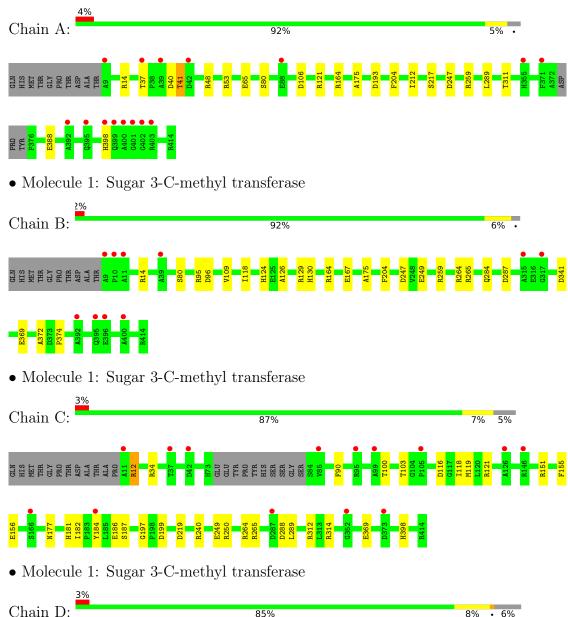
• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	187	Total O 187 187	0	0
6	В	182	Total         O           182         182	0	0
6	С	175	Total O 175 175	0	0
6	D	193	Total O 193 193	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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





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# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	62.71Å 82.45Å 82.83Å	Deneiten
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$96.05^{\circ}$ $110.70^{\circ}$ $112.09^{\circ}$	Depositor
Resolution (Å)	30.00 - 2.00	Depositor
Resolution (A)	29.85 - 2.00	EDS
% Data completeness	96.6 (30.00-2.00)	Depositor
(in resolution range)	96.6 (29.85-2.00)	EDS
R <sub>merge</sub>	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$< I/\sigma(I) > 1$	$1.75 (at 2.00 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
D D	0.176 , $0.234$	Depositor
$R, R_{free}$	0.184 , $0.239$	DCC
$R_{free}$ test set	4528 reflections $(5.01%)$	wwPDB-VP
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 , $40.6$	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.48, < L^2 > = 0.31$	Xtriage
	0.028 for h,-h-k,-h-l	
Estimated twinning fraction	0.018 for -h,-l,-k	Xtriage
	0.014 for -h,h+l,h+k	
$F_o, F_c$ correlation	0.96	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.

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



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: MES, SAH, ZN, TMP

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	Mal Chain		nd lengths	Bond angles		
	Mol Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.73	0/3252	0.87	5/4410~(0.1%)	
1	В	0.73	2/3249~(0.1%)	0.89	9/4413~(0.2%)	
1	С	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	Ζ	Observed(Å)	Ideal(Å)
1	D	249	GLU	CD-OE2	7.23	1.33	1.25
1	С	249	GLU	CD-OE2	6.82	1.33	1.25
1	В	249	GLU	CD-OE2	6.30	1.32	1.25
1	С	156	GLU	CD-OE2	5.56	1.31	1.25
1	В	287	ASP	CB-CG	5.02	1.62	1.51

The worst 5 of 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	В	109	VAL	CB-CA-C	-8.23	95.77	111.40
1	А	106	ASP	CB-CG-OD2	6.80	124.42	118.30
1	А	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

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	А	3164	0	3069	9	0
1	В	3167	0	3050	5	0
1	С	3085	0	2986	9	0
1	D	3064	0	2968	12	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
3	А	26	0	19	2	0
3	В	26	0	19	1	0
3	С	26	0	19	0	0
3	D	26	0	19	1	0
4	А	12	0	13	0	0
4	В	12	0	13	0	0
5	А	21	0	13	0	0
5	В	21	0	13	0	0
5	С	21	0	13	0	0
5	D	21	0	13	0	0
6	А	187	0	0	2	0
6	В	182	0	0	0	0
6	С	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.

The worst 5 of 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

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	Perce	ntiles
1	А	403/416~(97%)	389~(96%)	13 (3%)	1 (0%)	47	44
1	В	405/416~(97%)	390~(96%)	14 (4%)	1 (0%)	47	44
1	С	393/416~(94%)	383~(98%)	9(2%)	1 (0%)	41	37
1	D	390/416~(94%)	381 (98%)	8 (2%)	1 (0%)	41	37
All	All	1591/1664~(96%)	1543 (97%)	44 (3%)	4 (0%)	41	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	41	THR
1	С	103	THR
1	D	145	SER
1	В	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	А	327/334~(98%)	321~(98%)	6(2%)	59	63
1	В	327/334~(98%)	321~(98%)	6 (2%)	59	63
1	С	318/334~(95%)	306 (96%)	12 (4%)	33	31
1	D	316/334~(95%)	303~(96%)	13 (4%)	30	28
All	All	1288/1336~(96%)	1251~(97%)	37 (3%)	42	43

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	D	92	MET
1	D	240	ARG
1	D	98	LEU
1	D	121	ARG
1	С	12	ARG

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

Mol	Chain	Res	Type
1	А	177	ASN
1	А	181	HIS
1	В	177	ASN
1	С	398	HIS
1	D	412	HIS

#### 5.3.3 RNA (i)

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 monosaccharides 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	Bo	ond leng	ths	B	Bond ang	gles
N101	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
5	TMP	С	503	-	22,22,22	1.66	5 (22%)	33,33,33	2.85	16 (48%)
4	MES	А	503	-	12,12,12	1.91	1 (8%)	14,16,16	1.64	3 (21%)
3	SAH	С	502	-	24,28,28	1.46	5 (20%)	25,40,40	2.02	10 (40%)
5	TMP	В	504	-	22,22,22	1.52	5 (22%)	33,33,33	2.23	13 (39%)
3	SAH	А	502	-	24,28,28	1.07	2 (8%)	25,40,40	2.46	8 (32%)
3	SAH	D	502	-	24,28,28	1.25	2 (8%)	25,40,40	1.92	8 (32%)
5	TMP	А	504	-	22,22,22	1.64	5 (22%)	33,33,33	2.66	16 (48%)
4	MES	В	503	-	12,12,12	1.48	1 (8%)	14,16,16	1.28	1 (7%)
5	TMP	D	503	-	22,22,22	1.19	2 (9%)	33,33,33	2.91	12 (36%)
3	SAH	В	502	-	24,28,28	1.12	2 (8%)	25,40,40	2.57	9 (36%)

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
5	TMP	С	503	-	-	1/10/22/22	0/2/2/2
4	MES	А	503	-	-	0/6/14/14	0/1/1/1
3	SAH	С	502	-	-	3/11/31/31	0/3/3/3
5	TMP	В	504	-	-	5/10/22/22	0/2/2/2
3	SAH	А	502	-	-	8/11/31/31	0/3/3/3
3	SAH	D	502	-	-	3/11/31/31	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TMP	А	504	-	-	1/10/22/22	0/2/2/2
4	MES	В	503	-	-	0/6/14/14	0/1/1/1
5	TMP	D	503	-	-	4/10/22/22	0/2/2/2
3	SAH	В	502	-	-	8/11/31/31	0/3/3/3

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The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	А	503	MES	C8-S	-6.27	1.68	1.77
5	А	504	TMP	C2-N1	4.13	1.45	1.38
5	С	503	TMP	C2-N1	4.11	1.45	1.38
4	В	503	MES	C8-S	-4.04	1.71	1.77
3	В	502	SAH	O4'-C1'	3.49	1.46	1.41

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
5	D	503	TMP	O2P-P-O5'	-8.43	84.31	106.73
3	А	502	SAH	CB-CA-N	7.07	128.71	110.17
3	В	502	SAH	CB-CA-N	7.00	128.53	110.17
5	D	503	TMP	O4-C4-C5	-6.61	117.23	124.90
5	С	503	TMP	O3P-P-O5'	-6.09	90.52	106.73

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	С	502	SAH	N-CA-CB-CG
3	С	502	SAH	C-CA-CB-CG
3	С	502	SAH	C4'-C5'-SD-CG
3	D	502	SAH	C4'-C5'-SD-CG
5	В	504	TMP	C5'-O5'-P-O2P

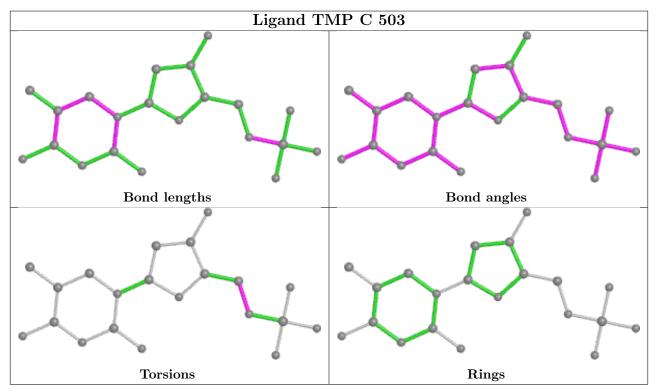
There are no ring outliers.

3 monomers are involved in 4 short contacts:

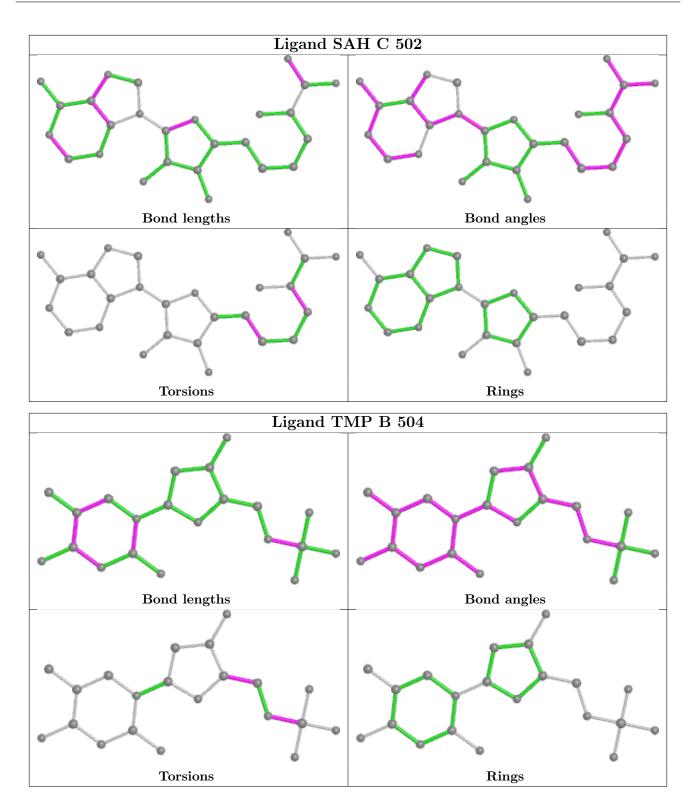
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	502	SAH	2	0
3	D	502	SAH	1	0
3	В	502	SAH	1	0



The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

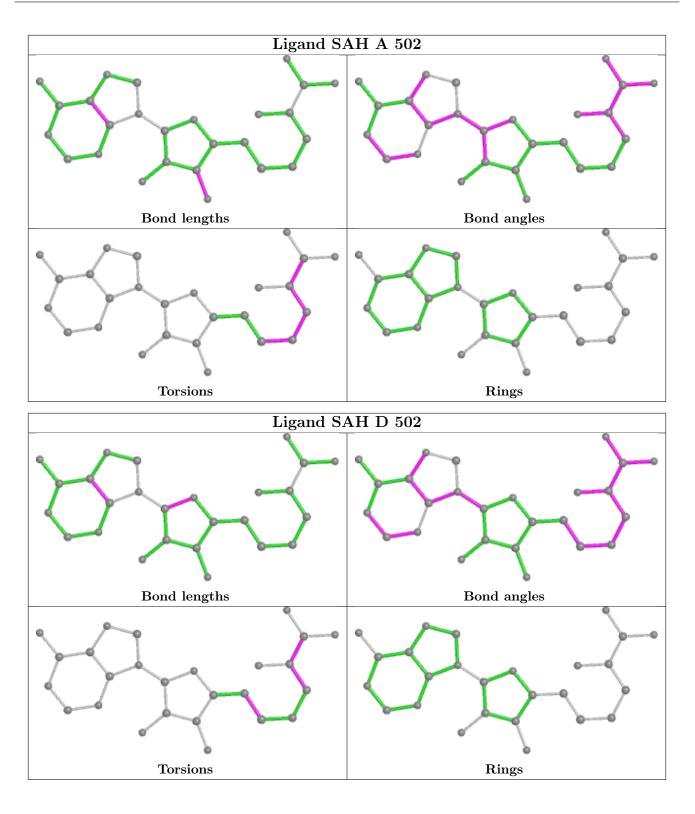




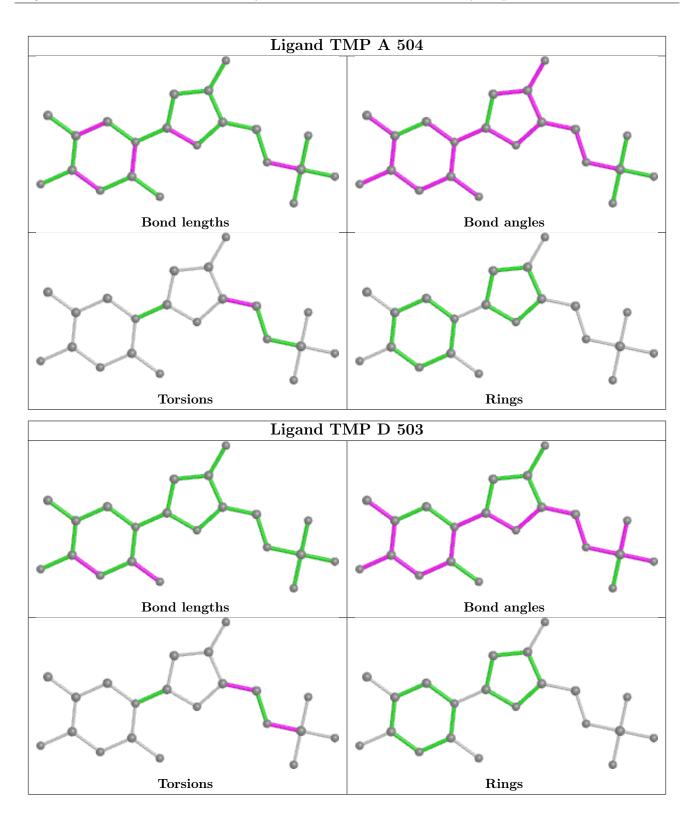




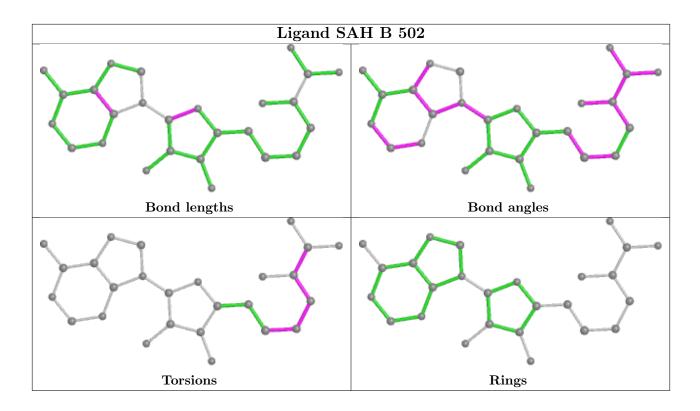












# 5.7 Other polymers (i)

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,  $95^{th}$  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		$OWAB(A^2)$	$\mathbf{Q}{<}0.9$
1	А	403/416~(96%)	-0.20	15 (3%) 4	41 41	13, 22, 51, 74	0
1	В	406/416~(97%)	-0.26	10 (2%) 5	57 56	11, 21, 47, 69	0
1	С	394/416~(94%)	-0.18	14 (3%)	42 42	11, 22, 48, 74	0
1	D	393/416~(94%)	-0.29	12 (3%) 4	49 48	11, 20, 47, 68	0
All	All	1596/1664~(95%)	-0.23	51 (3%) 4	47 46	11, 21, 48, 74	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	RSRZ
1	А	9	ALA	4.4
1	А	399	GLN	4.1
1	В	392	ALA	3.8
1	А	39	ALA	3.6
1	В	10	PRO	3.5

### 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 monosaccharides in this entry.

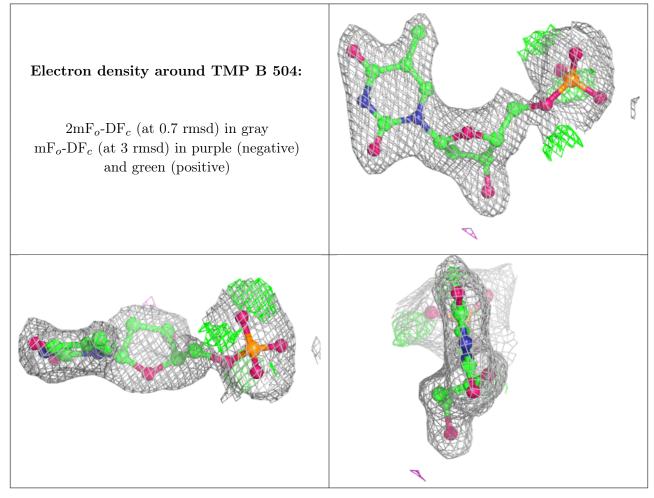
### 6.4 Ligands (i)

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. 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.

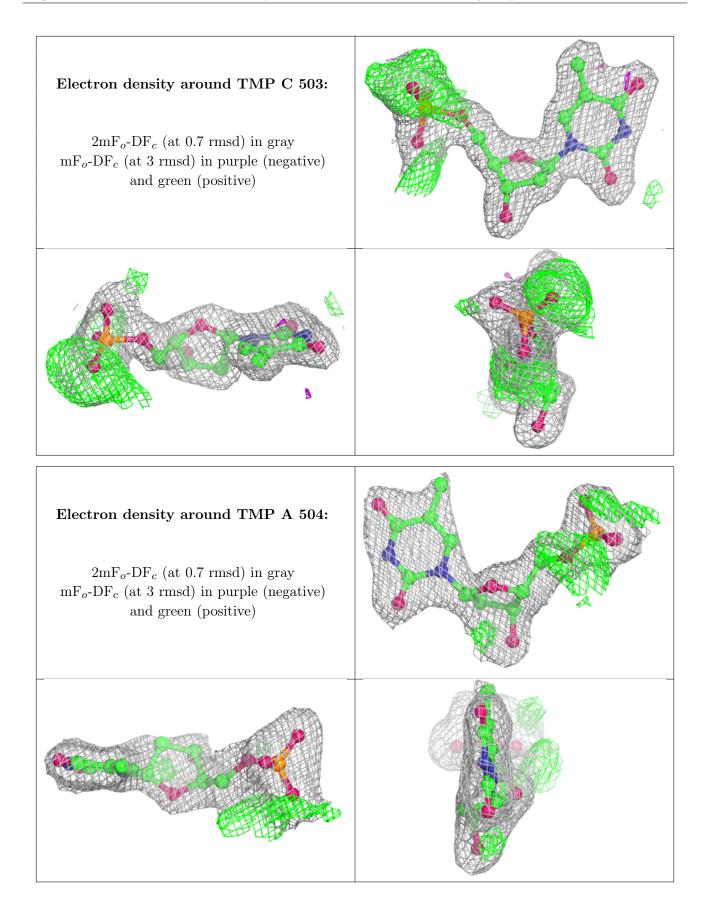


Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q < 0.9
5	TMP	В	504	21/21	0.83	0.13	$32,\!36,\!49,\!52$	0
5	TMP	С	503	21/21	0.83	0.12	18,23,31,37	0
5	TMP	А	504	21/21	0.84	0.13	42,44,49,50	0
5	TMP	D	503	21/21	0.85	0.10	17,19,32,39	0
3	SAH	А	502	26/26	0.94	0.13	13,15,23,25	0
3	SAH	В	502	26/26	0.95	0.11	10,11,18,20	0
3	SAH	D	502	26/26	0.95	0.09	16,19,20,22	0
3	SAH	С	502	26/26	0.96	0.09	12,16,19,20	0
4	MES	А	503	12/12	0.97	0.08	18,19,29,29	0
4	MES	В	503	12/12	0.97	0.07	19,20,20,21	0
2	ZN	D	501	1/1	0.99	0.04	34,34,34,34	0
2	ZN	С	501	1/1	1.00	0.02	21,21,21,21	0
2	ZN	А	501	1/1	1.00	0.03	25,25,25,25	0
2	ZN	В	501	1/1	1.00	0.03	22,22,22,22	0

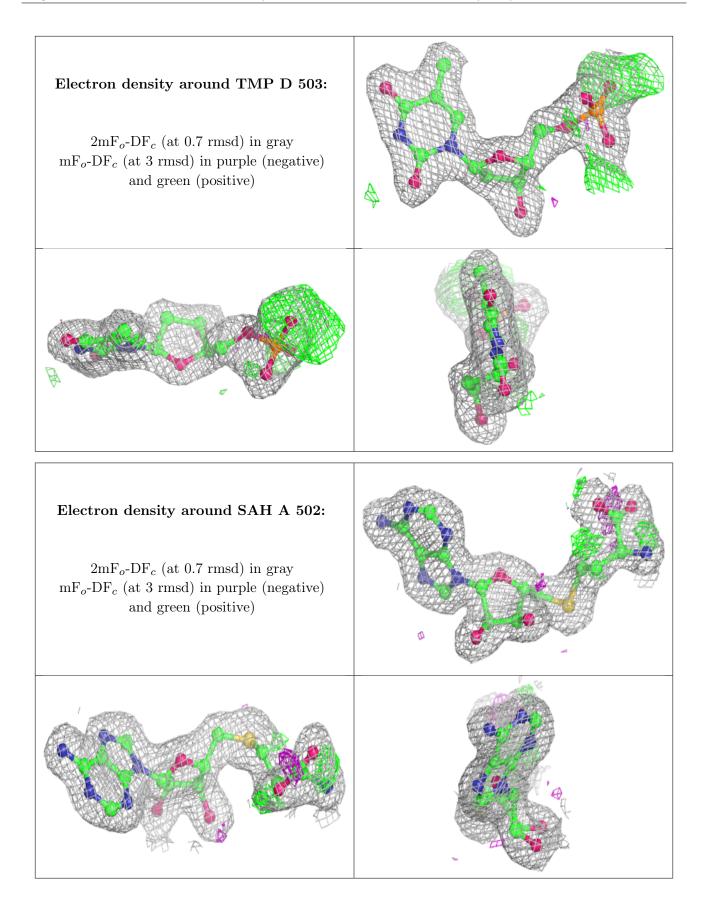
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



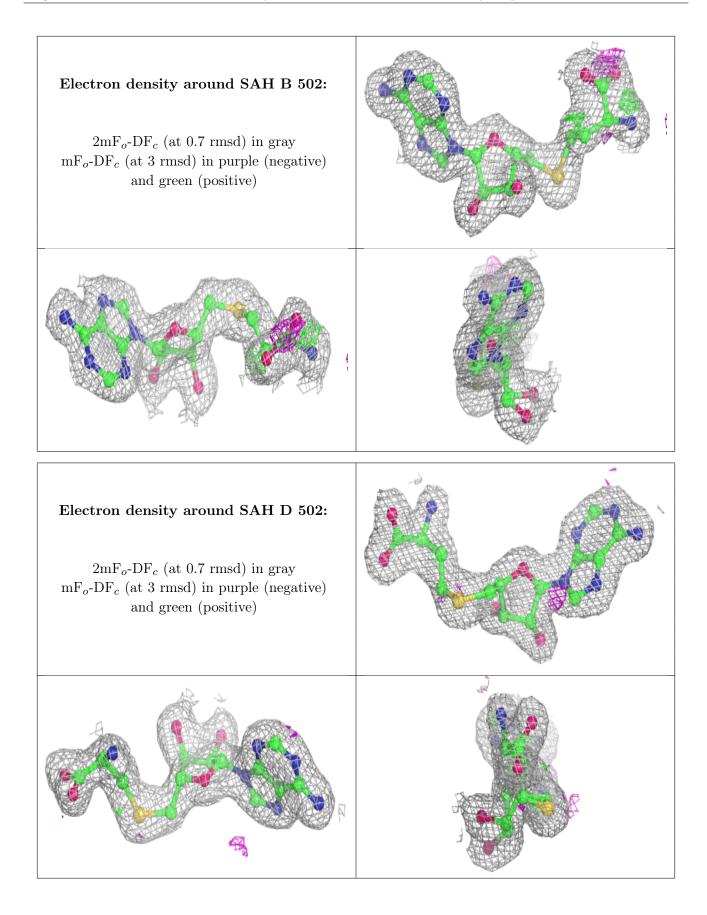




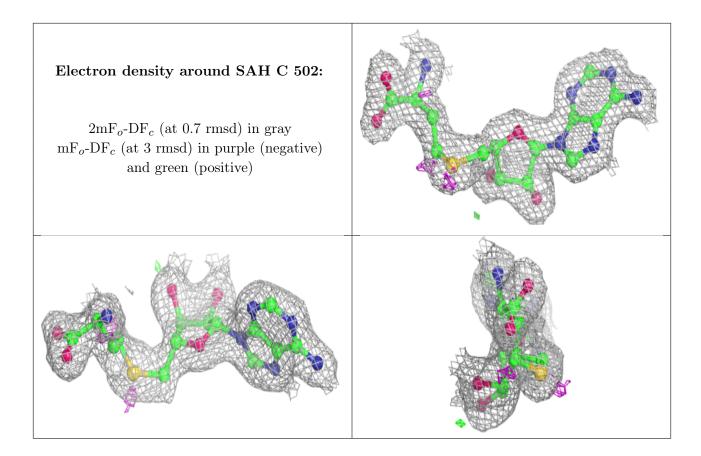












# 6.5 Other polymers (i)

There are no such residues in this entry.

