



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 04:47 am BST

PDB ID : 1O9S
Title : Crystal structure of a ternary complex of the human histone methyltransferase SET7/9
Authors : Xiao, B.; Jing, C.; Wilson, J.R.; Walker, P.A.; Vasisht, N.; Kelly, G.; Howell, S.; Taylor, I.A.; Blackburn, G.M.; Gamblin, S.J.
Deposited on : 2002-12-18
Resolution : 1.75 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

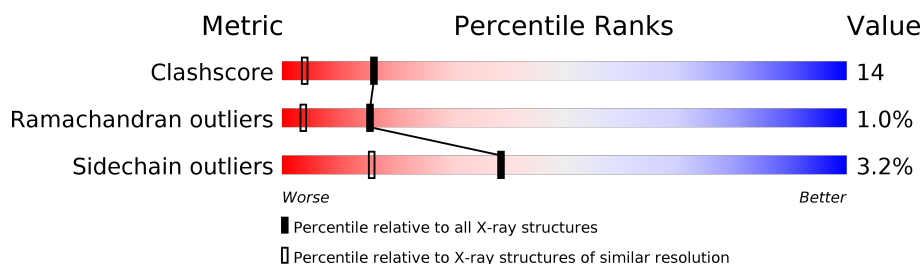
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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))
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	259	78% 16% . .
1	B	259	79% 15% . .
2	K	10	30% 60% 10%
2	L	10	10% 20% 30% 40%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4767 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 HISTONE-LYSINE N-METHYLTRANSFERASE, H3 LYSINE-4 SPECIFIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	3	0
			1959	1237	320	391	11			
1	B	250	Total	C	N	O	S	0	4	0
			1962	1238	321	391	12			

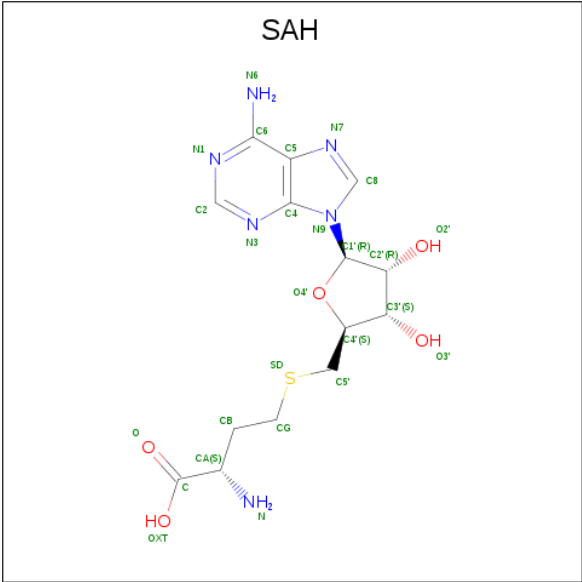
- Molecule 2 is a protein called GENE FRAGMENT FOR HISTONE H3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	10	Total	C	N	O	0	0	0
			87	53	19	15			
2	L	6	Total	C	N	O	0	0	0
			49	29	11	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	10	TYR	SER	conflict	UNP Q16776
L	10	TYR	SER	conflict	UNP Q16776

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			25	14	6	4	1		
3	B	1	Total	C	N	O	S	0	0
			25	14	6	4	1		

- Molecule 4 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	311	Total	O	0	0
			311	311		
4	B	328	Total	O	0	0
			328	328		
4	K	16	Total	O	0	0
			16	16		
4	L	5	Total	O	0	0
			5	5		

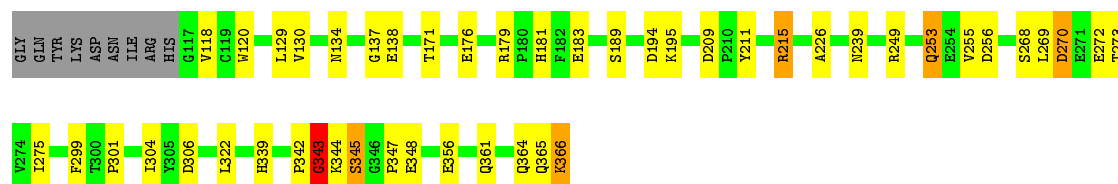
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.


Note EDS was not executed.

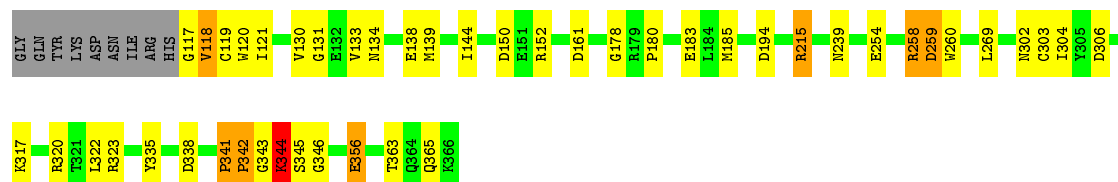
- Molecule 1: HISTONE-LYSINE N-METHYLTRANSFERASE, H3 LYSINE-4 SPECIFIC

Chain A: 

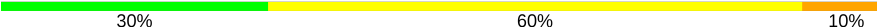


- Molecule 1: HISTONE-LYSINE N-METHYLTRANSFERASE, H3 LYSINE-4 SPECIFIC

Chain B: 



- Molecule 2: GENE FRAGMENT FOR HISTONE H3

Chain K: 



- Molecule 2: GENE FRAGMENT FOR HISTONE H3

Chain L: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.69 Å 75.44 Å 69.10 Å 90.00° 94.16° 90.00°	Depositor
Resolution (Å)	20.00 – 1.75	Depositor
% Data completeness (in resolution range)	89.9 (20.00-1.75)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.205 , 0.222	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4767	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MLZ, 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	0.49	0/2027	0.86	10/2757 (0.4%)
1	B	0.80	4/2039 (0.2%)	0.89	11/2772 (0.4%)
2	K	0.48	0/76	0.68	0/97
2	L	0.51	0/37	1.01	0/47
All	All	0.66	4/4179 (0.1%)	0.87	21/5673 (0.4%)

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
2	K	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	356[A]	GLU	CD-OE1	19.15	1.46	1.25
1	B	356[B]	GLU	CD-OE1	19.15	1.46	1.25
1	B	356[A]	GLU	CD-OE2	5.69	1.31	1.25
1	B	356[B]	GLU	CD-OE2	5.69	1.31	1.25

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	356[A]	GLU	OE1-CD-OE2	-10.66	110.51	123.30
1	B	356[B]	GLU	OE1-CD-OE2	-10.66	110.51	123.30
1	A	345	SER	N-CA-C	9.89	137.71	111.00
1	A	345	SER	N-CA-CB	-9.62	96.08	110.50
1	B	118	VAL	N-CA-CB	-7.13	95.82	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	306	ASP	CB-CG-OD2	6.81	124.43	118.30
1	A	343	GLY	N-CA-C	-6.76	96.21	113.10
1	A	256	ASP	CB-CG-OD2	6.29	123.96	118.30
1	A	306	ASP	CB-CG-OD2	6.20	123.88	118.30
1	B	194	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	345	SER	CB-CA-C	-6.09	98.52	110.10
1	A	270	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	194	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	215[A]	ARG	CD-NE-CZ	5.55	131.37	123.60
1	B	215[B]	ARG	CD-NE-CZ	5.55	131.37	123.60
1	A	215	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	117	GLY	CA-C-N	-5.25	105.66	117.20
1	B	117	GLY	C-N-CA	5.18	134.66	121.70
1	B	161	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	209	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	338	ASP	CB-CG-OD2	5.08	122.88	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	K	4	MLZ	Mainchain

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	1959	0	1848	49	0
1	B	1962	0	1841	55	1
2	K	87	0	96	11	0
2	L	49	0	55	12	0
3	A	25	0	19	1	0
3	B	25	0	19	1	0
4	A	311	0	0	12	0
4	B	328	0	0	10	0
4	K	16	0	0	1	0
4	L	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4767	0	3878	114	1

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 14.

All (114) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:PRO:HB2	1:B:342:PRO:CD	1.52	1.29
1:A:253:GLN:N	1:A:253:GLN:HE21	1.54	1.03
1:A:342:PRO:O	1:A:343:GLY:O	1.76	1.03
1:B:304:ILE:CG2	1:B:322:LEU:HD11	1.90	1.01
1:B:341:PRO:HB2	1:B:342:PRO:HD3	1.04	1.00
1:B:304:ILE:HG23	1:B:322:LEU:CD1	1.92	1.00
1:B:341:PRO:CB	1:B:342:PRO:HD3	1.93	0.98
1:B:304:ILE:HG23	1:B:322:LEU:HD11	0.99	0.96
1:B:341:PRO:CB	1:B:342:PRO:CD	2.44	0.96
1:A:342:PRO:C	1:A:343:GLY:O	2.00	0.94
1:A:253:GLN:H	1:A:253:GLN:NE2	1.67	0.91
2:L:4:MLZ:C	2:L:5:GLN:CA	2.52	0.88
1:B:259:ASP:N	1:B:259:ASP:OD1	2.08	0.86
1:A:344:LYS:CG	1:A:345:SER:N	2.41	0.84
1:B:343:GLY:HA2	2:K:9:LYS:HE2	1.61	0.83
1:B:317:LYS:NZ	2:L:6:THR:OG1	2.13	0.80
1:B:346:GLY:HA3	2:L:2:ARG:HH21	1.46	0.79
1:A:253:GLN:H	1:A:253:GLN:HE21	0.82	0.77
1:B:343:GLY:HA2	2:K:9:LYS:CE	2.17	0.75
1:B:343:GLY:CA	2:K:9:LYS:HE2	2.16	0.75
1:B:341:PRO:HB2	1:B:342:PRO:HD2	1.63	0.74
1:B:346:GLY:HA3	2:L:2:ARG:NH2	2.02	0.73
2:L:4:MLZ:CA	2:L:5:GLN:N	2.52	0.72
1:A:226:ALA:O	3:A:1367:SAH:N	2.24	0.71
1:A:211:TYR:CD1	1:A:215:ARG:NH2	2.59	0.70
1:B:260:TRP:CZ2	2:L:2:ARG:HG2	2.27	0.70
1:A:183:GLU:OE1	4:A:2067:HOH:O	2.08	0.70
1:A:344:LYS:HG2	1:A:345:SER:HB3	1.76	0.68
1:A:344:LYS:HG2	1:A:345:SER:N	2.09	0.68
2:L:3:THR:O	2:L:5:GLN:NE2	2.27	0.67
1:A:189:SER:HB2	4:A:2083:HOH:O	1.93	0.67
1:B:178:GLY:O	1:B:180:PRO:HD3	1.93	0.67
4:B:2231:HOH:O	2:L:2:ARG:NH1	2.28	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ARG:HD2	4:A:2107:HOH:O	1.94	0.66
1:A:342:PRO:O	1:A:343:GLY:C	2.34	0.65
1:B:302:ASN:HB3	1:B:323:ARG:NH2	2.12	0.65
1:A:134[B]:ASN:OD1	1:A:137:GLY:N	2.31	0.64
1:A:361:GLN:HB3	1:A:366:LYS:HD3	1.78	0.64
1:A:344:LYS:HG3	1:A:345:SER:N	2.14	0.63
1:B:118:VAL:HA	1:B:131:GLY:O	2.00	0.61
1:A:255:VAL:HG11	2:K:3:THR:HG22	1.82	0.61
1:A:361:GLN:HB3	1:A:366:LYS:CD	2.30	0.61
1:B:254:GLU:O	1:B:258:ARG:HG2	2.01	0.61
1:B:119[A]:CYS:SG	1:B:133:VAL:CG1	2.89	0.60
1:B:345:SER:O	2:L:2:ARG:NH2	2.34	0.60
1:A:253:GLN:N	1:A:253:GLN:NE2	2.34	0.60
1:B:335:TYR:CZ	2:L:4:MLZ:HCM3	2.37	0.60
1:A:120:TRP:CZ3	1:A:130:VAL:HG21	2.38	0.59
1:A:134[B]:ASN:ND2	1:A:138:GLU:HB2	2.17	0.59
1:A:183:GLU:CD	4:A:2067:HOH:O	2.40	0.59
1:A:249:ARG:HG3	1:A:275:ILE:CD1	2.33	0.59
1:B:139:MET:HE1	1:B:144:ILE:HG23	1.85	0.59
1:A:304:ILE:HB	1:A:322:LEU:HD11	1.84	0.59
1:A:344:LYS:HG2	1:A:345:SER:CB	2.33	0.58
2:K:1:ALA:HB3	2:K:6:THR:OG1	2.02	0.58
1:B:119[A]:CYS:SG	1:B:133:VAL:HG11	2.44	0.58
1:A:171:THR:HB	1:A:183:GLU:HG2	1.85	0.58
1:B:119[B]:CYS:SG	1:B:121:ILE:CG1	2.92	0.57
1:B:239:ASN:HB2	4:B:2210:HOH:O	2.04	0.57
1:B:323:ARG:HH11	1:B:323:ARG:HG3	1.70	0.56
1:A:120:TRP:CE3	1:A:130:VAL:HG21	2.41	0.55
1:B:363:THR:HB	4:B:2315:HOH:O	2.06	0.55
1:A:339:HIS:HA	1:A:347:PRO:HB3	1.89	0.55
1:B:303:CYS:CA	1:B:322:LEU:HD13	2.37	0.55
1:A:211:TYR:CE1	1:A:215:ARG:NH2	2.75	0.55
1:B:239:ASN:CB	4:B:2210:HOH:O	2.55	0.54
1:A:120:TRP:CE3	1:A:130:VAL:CG2	2.91	0.54
1:B:239:ASN:OD1	1:B:320:ARG:HD3	2.08	0.53
1:A:239:ASN:CB	4:A:2188:HOH:O	2.56	0.53
1:B:119[A]:CYS:SG	1:B:133:VAL:HG13	2.48	0.53
1:B:343:GLY:N	2:K:9:LYS:HE2	2.24	0.52
1:A:304:ILE:HG13	4:A:2257:HOH:O	2.09	0.52
1:A:356:GLU:HG3	4:A:2295:HOH:O	2.09	0.52
1:A:239:ASN:HB2	4:A:2188:HOH:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:GLU:CG	4:A:2295:HOH:O	2.57	0.52
1:B:363:THR:O	1:B:363:THR:HG22	2.10	0.52
1:A:342:PRO:CD	1:A:343:GLY:H	2.24	0.51
1:B:120:TRP:CZ2	1:B:180:PRO:HG3	2.46	0.51
1:B:258:ARG:N	4:B:2231:HOH:O	2.44	0.51
1:B:119[B]:CYS:SG	1:B:121:ILE:HG13	2.51	0.51
1:B:303:CYS:HA	1:B:322:LEU:HD13	1.92	0.51
2:L:4:MLZ:C	2:L:5:GLN:HA	2.39	0.50
1:B:356[A]:GLU:OE1	4:B:2311:HOH:O	2.19	0.50
2:K:8:ARG:HD3	2:K:10:TYR:OH	2.11	0.50
1:A:270:ASP:OD1	1:A:273:THR:N	2.43	0.49
1:A:268[A]:SER:OG	2:K:3:THR:OG1	2.19	0.48
1:A:176:GLU:HB2	1:A:181:HIS:NE2	2.29	0.47
1:B:254:GLU:HG3	4:B:2228:HOH:O	2.14	0.47
1:A:270:ASP:OD1	1:A:270:ASP:C	2.53	0.47
1:B:335:TYR:OH	2:L:4:MLZ:HCM3	2.15	0.46
1:B:303:CYS:C	1:B:322:LEU:HD13	2.36	0.46
1:B:120:TRP:CZ3	1:B:130:VAL:HG21	2.51	0.45
1:B:118:VAL:H	1:B:118:VAL:HG23	1.17	0.45
1:B:343:GLY:HA2	2:K:9:LYS:HE3	1.96	0.45
1:B:150:ASP:OD2	1:B:215[A]:ARG:NH2	2.50	0.44
1:B:120:TRP:CE3	1:B:130:VAL:HG21	2.53	0.44
1:A:134[B]:ASN:ND2	1:A:138:GLU:OE1	2.51	0.43
1:A:118:VAL:HG21	1:A:179:ARG:HG2	1.99	0.43
1:B:343:GLY:C	1:B:344:LYS:HG2	2.39	0.42
1:A:176:GLU:HG3	4:A:2060:HOH:O	2.19	0.42
1:B:120:TRP:CE3	1:B:130:VAL:CG2	3.03	0.42
1:B:134:ASN:CG	1:B:138:GLU:HB2	2.40	0.42
3:B:1367:SAH:O3'	4:B:2327:HOH:O	2.17	0.42
1:B:152:ARG:NH2	4:B:2032:HOH:O	2.53	0.42
1:A:195:LYS:NZ	4:A:2102:HOH:O	2.51	0.42
1:A:270:ASP:OD1	1:A:272:GLU:N	2.50	0.42
1:B:119[B]:CYS:SG	1:B:121:ILE:HG12	2.58	0.42
1:B:302:ASN:HB3	1:B:323:ARG:CZ	2.51	0.41
1:A:366:LYS:H	1:A:366:LYS:HG2	1.59	0.41
1:B:183:GLU:OE1	4:B:2078:HOH:O	2.22	0.41
4:A:2203:HOH:O	2:K:3:THR:CG2	2.69	0.41
2:K:8:ARG:HD2	4:K:2008:HOH:O	2.21	0.41
1:A:120:TRP:CE3	1:A:130:VAL:HG22	2.56	0.40
1:A:299:PHE:C	1:A:301:PRO:HD3	2.42	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:MET:SD	1:B:365:GLN:NE2[2_555]	2.18	0.02

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	251/259 (97%)	240 (96%)	10 (4%)	1 (0%)	34	17
1	B	252/259 (97%)	237 (94%)	12 (5%)	3 (1%)	13	3
2	K	7/10 (70%)	5 (71%)	2 (29%)	0	100	100
2	L	3/10 (30%)	2 (67%)	0	1 (33%)	0	0
All	All	513/538 (95%)	484 (94%)	24 (5%)	5 (1%)	15	4

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	341	PRO
1	B	342	PRO
1	B	344	LYS
2	L	2	ARG
1	A	343	GLY

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	216/221 (98%)	209 (97%)	7 (3%)	39	16
1	B	217/221 (98%)	213 (98%)	4 (2%)	59	40
2	K	7/7 (100%)	6 (86%)	1 (14%)	3	0
2	L	4/7 (57%)	2 (50%)	2 (50%)	0	0
All	All	444/456 (97%)	430 (97%)	14 (3%)	39	16

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	LEU
1	A	253	GLN
1	A	269	LEU
1	A	348	GLU
1	A	364	GLN
1	A	365	GLN
1	A	366	LYS
1	B	258	ARG
1	B	259	ASP
1	B	269	LEU
1	B	344	LYS
2	K	3	THR
2	L	5	GLN
2	L	6	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	HIS
1	A	253	GLN
1	B	361	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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$
2	MLZ	L	4	2	8,9,10	0.75	0	4,9,11	1.60	1 (25%)
2	MLZ	K	4	2	8,9,10	0.68	0	4,9,11	1.44	1 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLZ	L	4	2	-	0/7/8/10	-
2	MLZ	K	4	2	-	0/7/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	4	MLZ	CM-NZ-CE	2.51	119.20	111.95
2	K	4	MLZ	CM-NZ-CE	2.46	119.06	111.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	4	MLZ	5	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 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	1367	-	23,27,28	1.20	2 (8%)	20,38,40	1.50	2 (10%)
3	SAH	B	1367	-	23,27,28	1.11	2 (8%)	20,38,40	1.60	4 (20%)

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	1367	-	-	3/8/29/31	0/3/3/3
3	SAH	B	1367	-	-	2/8/29/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1367	SAH	C2-N3	4.68	1.39	1.32
3	B	1367	SAH	C2-N3	3.27	1.37	1.32
3	A	1367	SAH	C2-N1	2.13	1.37	1.33
3	B	1367	SAH	C2-N1	2.00	1.37	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1367	SAH	N3-C2-N1	-5.36	120.30	128.68
3	B	1367	SAH	N3-C2-N1	-5.23	120.50	128.68
3	B	1367	SAH	CB-CG-SD	-2.71	107.23	113.31
3	B	1367	SAH	C3'-C2'-C1'	2.44	104.65	100.98
3	A	1367	SAH	C3'-C2'-C1'	2.31	104.45	100.98
3	B	1367	SAH	C5'-SD-CG	-2.01	96.23	102.27

There are no chirality outliers.

All (5) torsion outliers are listed below:

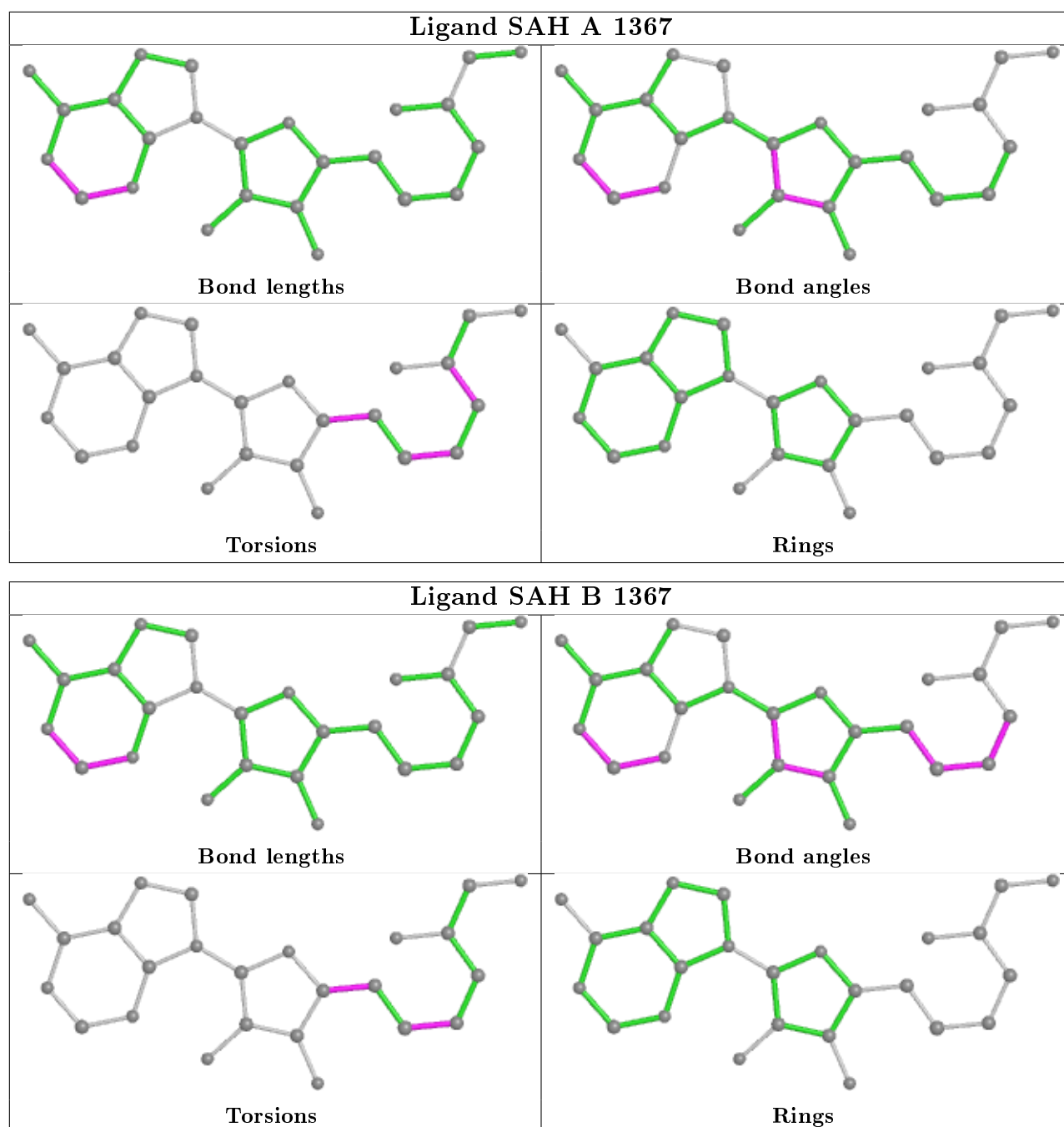
Mol	Chain	Res	Type	Atoms
3	A	1367	SAH	C-CA-CB-CG
3	A	1367	SAH	C3'-C4'-C5'-SD
3	A	1367	SAH	CB-CG-SD-C5'
3	B	1367	SAH	CB-CG-SD-C5'
3	B	1367	SAH	C3'-C4'-C5'-SD

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1367	SAH	1	0
3	B	1367	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 than 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	4:MLZ	C	5:GLN	N	1.76

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.