



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:32 PM GMT

PDB ID : 1U2Z  
Title : Crystal structure of histone K79 methyltransferase Dot1p from yeast  
Authors : Sawada, K.; Yang, Z.; Horton, J.R.; Collins, R.E.; Zhang, X.; Cheng, X.  
Deposited on : 2004-07-20  
Resolution : 2.20 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

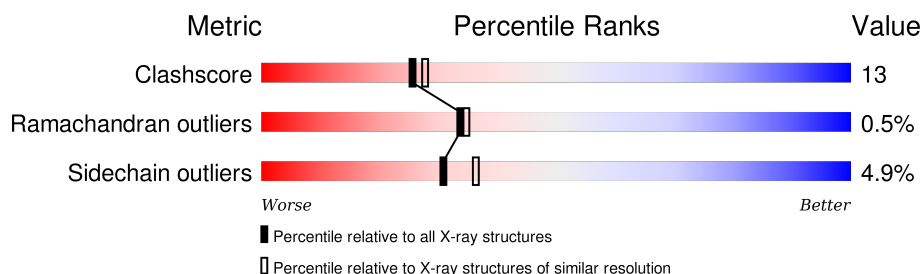
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	433	
1	B	433	
1	C	433	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9909 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-79 specific.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			3082	1976	508	581	17			
1	B	379	Total	C	N	O	S	0	0	0
			3085	1979	508	581	17			
1	C	385	Total	C	N	O	S	0	0	0
			3131	2004	520	590	17			

There are 24 discrepancies between the modelled and reference sequences:

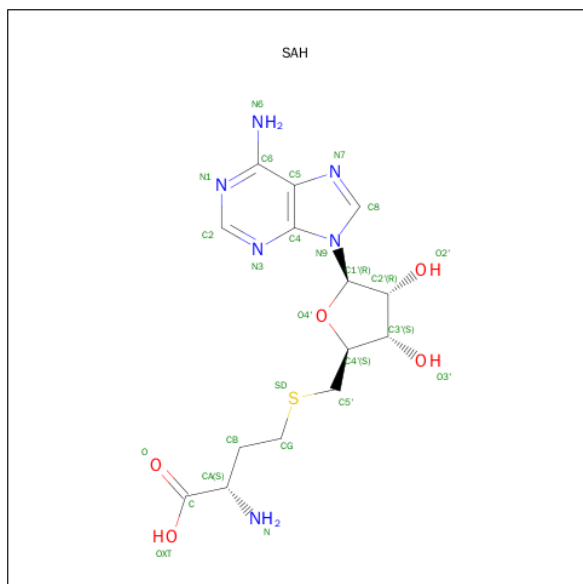
Chain	Residue	Modelled	Actual	Comment	Reference
A	150	MET	-	EXPRESSION TAG	UNP Q04089
A	151	GLY	-	EXPRESSION TAG	UNP Q04089
A	152	HIS	-	EXPRESSION TAG	UNP Q04089
A	153	HIS	-	EXPRESSION TAG	UNP Q04089
A	154	HIS	-	EXPRESSION TAG	UNP Q04089
A	155	HIS	-	EXPRESSION TAG	UNP Q04089
A	156	HIS	-	EXPRESSION TAG	UNP Q04089
A	157	HIS	-	EXPRESSION TAG	UNP Q04089
B	150	MET	-	EXPRESSION TAG	UNP Q04089
B	151	GLY	-	EXPRESSION TAG	UNP Q04089
B	152	HIS	-	EXPRESSION TAG	UNP Q04089
B	153	HIS	-	EXPRESSION TAG	UNP Q04089
B	154	HIS	-	EXPRESSION TAG	UNP Q04089
B	155	HIS	-	EXPRESSION TAG	UNP Q04089
B	156	HIS	-	EXPRESSION TAG	UNP Q04089
B	157	HIS	-	EXPRESSION TAG	UNP Q04089
C	150	MET	-	EXPRESSION TAG	UNP Q04089
C	151	GLY	-	EXPRESSION TAG	UNP Q04089
C	152	HIS	-	EXPRESSION TAG	UNP Q04089
C	153	HIS	-	EXPRESSION TAG	UNP Q04089
C	154	HIS	-	EXPRESSION TAG	UNP Q04089
C	155	HIS	-	EXPRESSION TAG	UNP Q04089
C	156	HIS	-	EXPRESSION TAG	UNP Q04089

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Chain	Residue	Modelled	Actual	Comment	Reference
C	157	HIS	-	EXPRESSION TAG	UNP Q04089

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ).



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

- Molecule 3 is water.

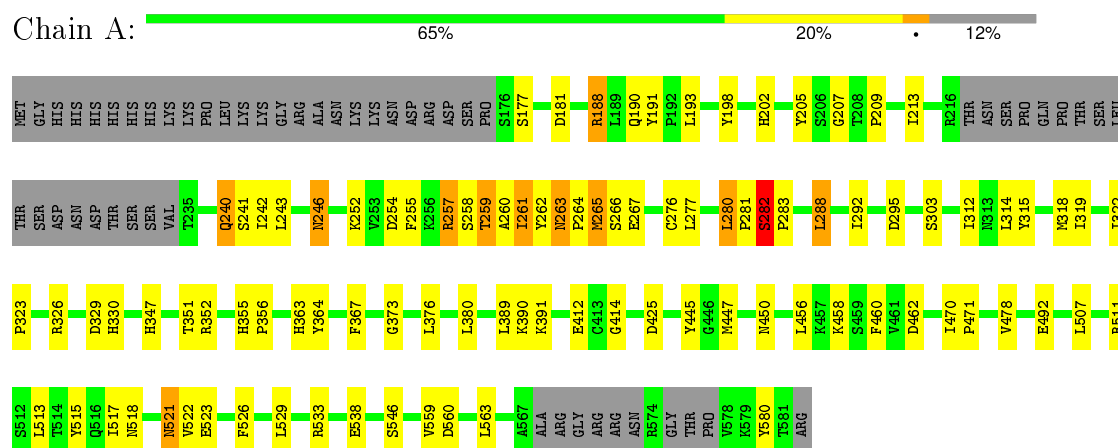
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	142	Total	O	0	0
			142	142		
3	B	203	Total	O	0	0
			203	203		
3	C	188	Total	O	0	0
			188	188		

### 3 Residue-property plots

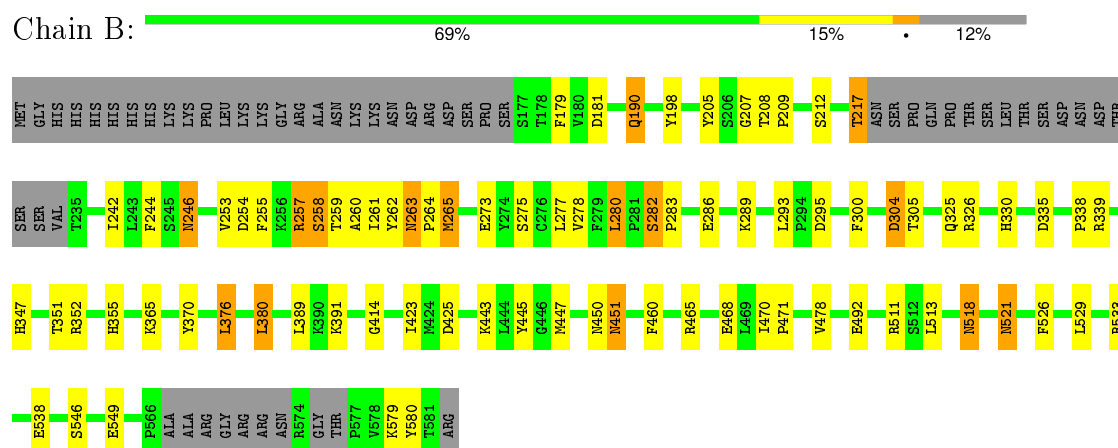
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

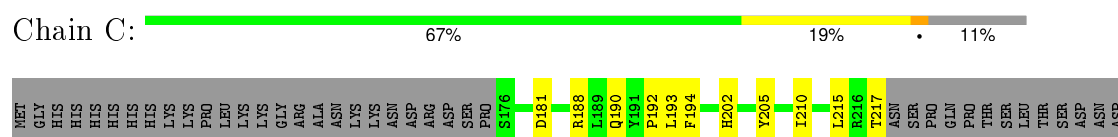
- Molecule 1: Histone-lysine N-methyltransferase, H3 lysine-79 specific

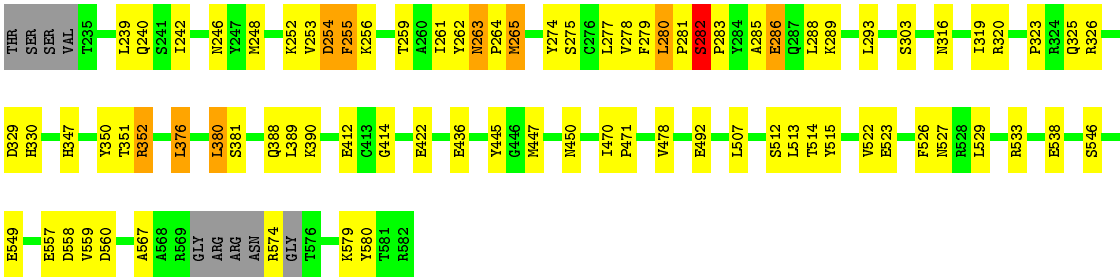


- Molecule 1: Histone-lysine N-methyltransferase, H3 lysine-79 specific



- Molecule 1: Histone-lysine N-methyltransferase, H3 lysine-79 specific





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.07 Å   146.28 Å   75.41 Å 90.00°   97.68°   90.00°	Depositor
Resolution (Å)	19.90 – 2.20	Depositor
% Data completeness (in resolution range)	98.9 (19.90-2.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.213 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9909	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	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: 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	0.40	1/3144 (0.0%)	0.67	3/4245 (0.1%)
1	B	0.46	1/3148 (0.0%)	0.70	4/4251 (0.1%)
1	C	0.45	1/3194 (0.0%)	0.73	6/4312 (0.1%)
All	All	0.44	3/9486 (0.0%)	0.70	13/12808 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	283	PRO	CA-C	-6.02	1.40	1.52
1	A	283	PRO	CA-C	-5.06	1.42	1.52
1	C	283	PRO	CA-C	-5.01	1.42	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	282	SER	C-N-CD	-13.69	90.49	120.60
1	A	282	SER	C-N-CD	-13.52	90.85	120.60
1	B	282	SER	C-N-CD	-8.76	101.34	120.60
1	C	255	PHE	CB-CG-CD2	-7.37	115.64	120.80
1	A	282	SER	C-N-CA	6.31	148.49	122.00
1	C	255	PHE	CB-CG-CD1	6.19	125.13	120.80
1	B	529	LEU	N-CA-CB	-5.33	99.74	110.40
1	C	529	LEU	N-CA-CB	-5.31	99.78	110.40
1	B	304	ASP	N-CA-CB	-5.22	101.20	110.60
1	A	529	LEU	N-CA-CB	-5.20	99.99	110.40
1	B	282	SER	N-CA-C	-5.02	97.44	111.00
1	C	254	ASP	CB-CG-OD1	5.02	122.82	118.30
1	C	282	SER	C-N-CA	5.01	143.04	122.00

There are no chirality outliers.



There are no planarity outliers.

## 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	3082	0	3064	87	0
1	B	3085	0	3069	68	0
1	C	3131	0	3116	84	0
2	A	26	0	19	2	0
2	B	26	0	19	0	0
2	C	26	0	19	1	0
3	A	142	0	0	0	0
3	B	203	0	0	0	0
3	C	188	0	0	0	0
All	All	9909	0	9306	234	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 13.

All (234) 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:188:ARG:HH11	1:A:188:ARG:HG2	1.17	1.04
1:C:286:GLU:OE1	1:C:286:GLU:N	1.90	1.04
1:C:253:VAL:HA	1:C:265:MET:HE2	1.38	1.02
1:B:217:THR:HG22	1:B:261:ILE:HD12	1.48	0.94
1:B:253:VAL:HA	1:B:265:MET:HE2	1.51	0.93
1:C:289:LYS:HG3	1:C:293:LEU:HD12	1.52	0.92
1:A:188:ARG:NH1	1:A:188:ARG:HG2	1.81	0.92
1:B:518:ASN:H	1:B:521:ASN:HD21	1.05	0.90
1:C:205:TYR:H	1:C:246:ASN:HD21	1.19	0.90
1:B:205:TYR:H	1:B:246:ASN:HD21	1.24	0.86
1:A:518:ASN:H	1:A:521:ASN:HD21	1.25	0.84
1:C:259:THR:HG21	1:C:263:ASN:HB2	1.60	0.83
1:C:217:THR:HA	1:C:261:ILE:HG12	1.61	0.83
1:B:518:ASN:H	1:B:521:ASN:ND2	1.75	0.82
1:C:282:SER:OG	1:C:286:GLU:OE2	1.97	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:ARG:HB3	1:B:326:ARG:NH1	1.95	0.81
1:C:533:ARG:NE	1:C:549:GLU:OE2	2.13	0.81
1:B:255:PHE:HD1	1:B:305:THR:HG22	1.45	0.80
1:B:538:GLU:OE1	1:B:546:SER:HB3	1.80	0.79
1:C:538:GLU:OE1	1:C:546:SER:HB3	1.83	0.79
1:A:513:LEU:O	1:A:513:LEU:HD13	1.84	0.78
1:A:259:THR:HG22	1:A:260:ALA:H	1.47	0.77
1:B:518:ASN:N	1:B:521:ASN:HD21	1.83	0.76
1:B:261:ILE:HG13	1:B:262:TYR:H	1.51	0.75
1:B:261:ILE:HG13	1:B:262:TYR:N	2.02	0.75
1:B:326:ARG:HB3	1:B:326:ARG:HH11	1.52	0.74
1:C:259:THR:O	1:C:259:THR:HG22	1.88	0.72
1:C:259:THR:HG23	1:C:262:TYR:O	1.90	0.71
1:C:217:THR:H	1:C:261:ILE:HD11	1.55	0.71
1:C:253:VAL:HA	1:C:265:MET:CE	2.18	0.71
1:A:538:GLU:OE1	1:A:546:SER:HB3	1.91	0.71
1:B:190:GLN:HG2	1:B:190:GLN:O	1.91	0.70
1:C:286:GLU:H	1:C:286:GLU:CD	1.95	0.70
1:A:538:GLU:OE1	1:A:546:SER:CB	2.40	0.69
1:B:242:ILE:HD11	1:B:280:LEU:HD11	1.74	0.69
1:A:181:ASP:HB2	1:A:580:TYR:CD2	2.27	0.69
1:A:188:ARG:CG	1:A:188:ARG:HH11	1.99	0.69
1:A:288:LEU:HD11	1:A:315:TYR:HD1	1.59	0.68
1:C:347:HIS:O	1:C:351:THR:HG23	1.93	0.68
1:C:538:GLU:OE1	1:C:546:SER:CB	2.42	0.68
1:A:511:ARG:HD2	1:A:515:TYR:CG	2.29	0.67
1:B:289:LYS:HG3	1:B:293:LEU:HD12	1.76	0.67
1:A:538:GLU:HA	1:A:538:GLU:OE1	1.93	0.67
1:C:242:ILE:HD11	1:C:280:LEU:HD11	1.74	0.67
1:B:263:ASN:C	1:B:263:ASN:HD22	1.96	0.67
1:B:242:ILE:HD11	1:B:280:LEU:CD1	2.25	0.67
1:C:252:LYS:O	1:C:265:MET:HE1	1.95	0.66
1:A:261:ILE:HG22	1:A:262:TYR:N	2.10	0.66
1:C:217:THR:HA	1:C:261:ILE:CG1	2.25	0.65
1:C:275:SER:O	1:C:280:LEU:HD22	1.96	0.65
1:A:470:ILE:HB	1:A:471:PRO:HD3	1.77	0.64
1:B:470:ILE:HB	1:B:471:PRO:HD3	1.80	0.64
1:C:242:ILE:HG13	1:C:319:ILE:HG23	1.78	0.64
1:A:205:TYR:H	1:A:246:ASN:HD21	1.45	0.64
1:B:533:ARG:NE	1:B:549:GLU:OE1	2.27	0.64
1:B:518:ASN:HD22	1:B:518:ASN:C	2.02	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:ILE:HB	1:C:471:PRO:HD3	1.79	0.63
1:A:281:PRO:HG3	1:A:330:HIS:HB2	1.79	0.63
1:C:264:PRO:HB2	1:C:265:MET:HE1	1.79	0.63
1:B:521:ASN:C	1:B:521:ASN:HD22	2.02	0.62
1:A:191:TYR:HB2	1:A:391:LYS:HZ3	1.63	0.62
1:A:259:THR:HG22	1:A:260:ALA:N	2.14	0.61
1:B:451:ASN:N	1:B:451:ASN:OD1	2.24	0.61
1:C:261:ILE:HG13	1:C:262:TYR:N	2.16	0.61
1:B:275:SER:O	1:B:280:LEU:HD22	2.01	0.60
1:C:285:ALA:HB3	1:C:286:GLU:OE1	2.01	0.60
1:A:242:ILE:HG23	1:A:243:LEU:HG	1.84	0.59
1:C:263:ASN:HD21	1:C:265:MET:HB2	1.68	0.59
1:C:205:TYR:H	1:C:246:ASN:ND2	1.96	0.59
1:A:538:GLU:OE1	1:A:546:SER:HA	2.01	0.59
1:A:462:ASP:OD1	1:C:192:PRO:HG2	2.01	0.58
1:A:267:GLU:OE2	1:A:352:ARG:NH1	2.29	0.58
1:B:205:TYR:H	1:B:246:ASN:ND2	1.99	0.57
1:A:538:GLU:OE1	1:A:546:SER:CA	2.53	0.57
1:C:513:LEU:O	1:C:567:ALA:HB1	2.04	0.57
1:C:281:PRO:HG3	1:C:330:HIS:HB2	1.87	0.56
1:C:264:PRO:HB2	1:C:265:MET:CE	2.34	0.56
1:C:277:LEU:O	1:C:277:LEU:HD23	2.06	0.56
1:A:521:ASN:HD22	1:A:521:ASN:C	2.09	0.56
1:C:263:ASN:HD22	1:C:263:ASN:C	2.07	0.56
1:A:347:HIS:O	1:A:351:THR:HG23	2.05	0.56
1:C:259:THR:HG21	1:C:263:ASN:CB	2.35	0.56
1:B:538:GLU:OE1	1:B:546:SER:CB	2.50	0.56
1:C:422:GLU:OE2	2:C:803:SAH:O2'	2.24	0.55
1:C:514:THR:HA	1:C:567:ALA:O	2.06	0.55
1:B:492:GLU:HG3	1:B:526:PHE:CZ	2.41	0.55
1:A:367:PHE:HZ	1:C:325:GLN:OE1	1.90	0.55
1:B:347:HIS:O	1:B:351:THR:HG23	2.07	0.55
1:B:205:TYR:HB2	1:B:244:PHE:CG	2.42	0.55
1:A:326:ARG:HG3	1:A:326:ARG:HH11	1.71	0.54
1:A:492:GLU:HG3	1:A:526:PHE:CZ	2.42	0.54
1:A:414:GLY:HA2	1:A:450:ASN:HD22	1.72	0.54
1:B:414:GLY:HA2	1:B:450:ASN:HD22	1.72	0.54
1:A:288:LEU:HD11	1:A:315:TYR:CD1	2.40	0.54
1:C:492:GLU:HG3	1:C:526:PHE:CZ	2.43	0.54
1:C:278:VAL:O	1:C:330:HIS:HE1	1.89	0.54
1:B:326:ARG:HH11	1:B:326:ARG:CB	2.19	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:SER:HB2	1:B:352:ARG:NH2	2.23	0.54
1:C:255:PHE:CD2	1:C:303:SER:HA	2.42	0.54
1:A:202:HIS:HE1	1:B:425:ASP:OD1	1.91	0.53
1:B:181:ASP:HB2	1:B:580:TYR:CD2	2.43	0.53
1:C:478:VAL:HG13	1:C:478:VAL:O	2.08	0.53
1:A:261:ILE:HG21	1:A:355:HIS:CE1	2.44	0.53
1:A:276:CYS:SG	1:A:288:LEU:HB3	2.49	0.53
1:C:265:MET:N	1:C:265:MET:HE3	2.24	0.53
1:C:190:GLN:HE22	1:C:390:LYS:HA	1.74	0.53
1:B:278:VAL:O	1:B:330:HIS:HE1	1.91	0.53
1:C:259:THR:CG2	1:C:263:ASN:HB2	2.37	0.52
1:B:580:TYR:CD1	1:B:580:TYR:N	2.76	0.52
1:C:188:ARG:NH1	1:C:188:ARG:HB2	2.24	0.52
1:B:351:THR:HA	1:B:355:HIS:HD2	1.74	0.52
1:C:210:ILE:HB	1:C:352:ARG:HG3	1.91	0.52
1:A:260:ALA:O	1:A:261:ILE:C	2.48	0.52
1:A:207:GLY:C	1:A:209:PRO:HD3	2.29	0.52
1:A:425:ASP:OD1	1:C:202:HIS:HE1	1.92	0.52
1:A:246:ASN:HD22	1:A:246:ASN:H	1.57	0.52
1:A:276:CYS:SG	1:A:288:LEU:HD12	2.50	0.52
1:C:414:GLY:HA2	1:C:450:ASN:HD22	1.74	0.51
1:B:190:GLN:HE21	1:B:190:GLN:H	1.59	0.51
1:C:181:ASP:HB2	1:C:580:TYR:CD2	2.46	0.51
1:A:267:GLU:CD	1:A:352:ARG:HH12	2.13	0.51
1:C:242:ILE:HD12	1:C:275:SER:OG	2.11	0.51
1:C:278:VAL:HG23	1:C:279:PHE:CD1	2.45	0.51
1:A:191:TYR:HB2	1:A:391:LYS:NZ	2.26	0.50
1:C:193:LEU:HD23	1:C:194:PHE:CE1	2.46	0.50
1:A:213:ILE:HD12	1:A:252:LYS:HB2	1.93	0.50
1:A:177:SER:HB2	1:A:580:TYR:O	2.11	0.50
1:B:414:GLY:HA2	1:B:450:ASN:ND2	2.26	0.49
1:A:264:PRO:HB2	1:A:265:MET:HE3	1.93	0.49
1:C:316:ASN:O	1:C:320:ARG:HG3	2.10	0.49
1:B:261:ILE:CG1	1:B:262:TYR:H	2.22	0.49
1:A:355:HIS:HB3	1:A:356:PRO:HD3	1.94	0.49
1:A:240:GLN:NE2	1:A:241:SER:O	2.46	0.49
1:C:288:LEU:HD21	1:C:319:ILE:HD11	1.92	0.49
1:C:188:ARG:HH11	1:C:188:ARG:CB	2.26	0.49
1:B:277:LEU:O	1:B:277:LEU:HD23	2.13	0.49
1:A:255:PHE:CD2	1:A:303:SER:HA	2.48	0.49
1:B:261:ILE:CG1	1:B:262:TYR:N	2.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ASP:H	1:A:265:MET:HE1	1.78	0.49
1:B:282:SER:OG	1:B:286:GLU:OE2	2.28	0.49
1:B:254:ASP:OD2	1:B:257:ARG:HG3	2.13	0.48
1:A:478:VAL:O	1:A:478:VAL:HG13	2.13	0.48
1:C:414:GLY:HA2	1:C:450:ASN:ND2	2.28	0.48
1:C:254:ASP:OD1	1:C:256:LYS:HB2	2.13	0.48
1:B:351:THR:HA	1:B:355:HIS:CD2	2.48	0.48
1:A:414:GLY:HA2	1:A:450:ASN:ND2	2.28	0.48
1:C:522:VAL:HG13	1:C:523:GLU:OE2	2.14	0.48
1:B:263:ASN:C	1:B:263:ASN:ND2	2.67	0.48
1:A:258:SER:O	1:A:259:THR:CB	2.62	0.48
1:B:198:TYR:OH	1:B:443:LYS:HE3	2.14	0.48
1:C:217:THR:N	1:C:261:ILE:HD11	2.27	0.48
1:C:190:GLN:NE2	1:C:390:LYS:HA	2.27	0.48
1:A:538:GLU:OE2	1:A:546:SER:HB2	2.14	0.48
1:A:511:ARG:HD2	1:A:515:TYR:CD1	2.48	0.48
1:C:515:TYR:HE1	1:C:527:ASN:OD1	1.97	0.47
1:B:208:THR:N	1:B:209:PRO:HD3	2.29	0.47
1:A:292:ILE:HD11	1:A:318:MET:SD	2.53	0.47
1:A:281:PRO:O	1:A:282:SER:C	2.50	0.47
1:A:559:VAL:HG12	1:A:560:ASP:N	2.29	0.47
1:B:255:PHE:CD1	1:B:305:THR:HG22	2.37	0.47
1:C:515:TYR:CE1	1:C:527:ASN:OD1	2.67	0.47
1:A:314:LEU:O	1:A:318:MET:HG3	2.15	0.47
1:C:259:THR:CG2	1:C:259:THR:O	2.60	0.47
1:A:254:ASP:CG	1:A:257:ARG:HB2	2.34	0.47
1:A:456:LEU:O	1:A:458:LYS:HG2	2.15	0.47
1:C:381:SER:HA	1:C:412:GLU:OE2	2.15	0.46
1:A:263:ASN:OD1	1:A:266:SER:HB2	2.15	0.46
1:A:522:VAL:HG13	1:A:523:GLU:HG3	1.98	0.46
1:C:253:VAL:CA	1:C:265:MET:HE2	2.28	0.46
1:A:213:ILE:CD1	1:A:252:LYS:HB2	2.45	0.46
1:C:350:TYR:CE2	1:C:574:ARG:HD2	2.51	0.46
1:B:277:LEU:HD22	1:B:338:PRO:CG	2.46	0.45
1:A:188:ARG:CG	1:A:188:ARG:NH1	2.61	0.45
1:A:280:LEU:HA	1:A:281:PRO:HD3	1.76	0.45
1:C:274:TYR:O	1:C:278:VAL:HG22	2.17	0.45
1:C:215:LEU:HD11	1:C:352:ARG:HD2	1.99	0.45
1:B:300:PHE:CE2	1:B:579:LYS:HD2	2.52	0.45
1:A:259:THR:O	1:A:260:ALA:HB3	2.17	0.45
1:A:517:ILE:HG13	1:A:563:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:TYR:CE2	1:C:264:PRO:HG3	2.52	0.44
1:B:376:LEU:O	1:B:380:LEU:HD22	2.18	0.44
1:C:514:THR:C	1:C:567:ALA:HB3	2.37	0.44
1:A:292:ILE:N	1:A:292:ILE:HD12	2.32	0.44
1:B:258:SER:O	1:B:259:THR:HB	2.17	0.44
1:A:580:TYR:N	1:A:580:TYR:CD1	2.85	0.44
1:A:373:GLY:O	2:A:801:SAH:HG2	2.17	0.44
1:B:190:GLN:OE1	1:B:391:LYS:N	2.50	0.44
1:A:326:ARG:HG3	1:A:326:ARG:NH1	2.31	0.44
1:B:264:PRO:HB2	1:B:265:MET:HE3	1.99	0.44
1:B:518:ASN:C	1:B:518:ASN:ND2	2.70	0.44
1:A:538:GLU:CD	1:A:546:SER:HB3	2.38	0.44
1:B:179:PHE:HD1	1:B:273:GLU:OE2	2.01	0.44
1:B:445:TYR:CB	1:B:447:MET:HE2	2.47	0.44
1:A:242:ILE:HD12	1:A:319:ILE:HG23	2.00	0.44
1:B:478:VAL:O	1:B:478:VAL:HG13	2.17	0.44
1:A:264:PRO:HB2	1:A:265:MET:CE	2.48	0.44
1:B:365:LYS:HE2	1:B:370:TYR:O	2.17	0.43
1:B:277:LEU:HD22	1:B:338:PRO:HG2	2.00	0.43
1:C:445:TYR:CB	1:C:447:MET:HE2	2.49	0.43
1:A:261:ILE:CG2	1:A:262:TYR:N	2.81	0.42
1:B:207:GLY:C	1:B:209:PRO:HD3	2.39	0.42
1:A:263:ASN:C	1:A:263:ASN:ND2	2.72	0.42
1:B:190:GLN:HE21	1:B:190:GLN:N	2.17	0.42
1:C:242:ILE:HG13	1:C:319:ILE:CG2	2.47	0.42
1:C:323:PRO:HB2	1:C:326:ARG:HG2	2.00	0.42
1:A:191:TYR:OH	1:A:193:LEU:HD13	2.20	0.42
1:B:465:ARG:HH11	1:B:468:GLU:CD	2.24	0.42
1:B:521:ASN:C	1:B:521:ASN:ND2	2.71	0.41
1:C:559:VAL:HG12	1:C:560:ASP:N	2.34	0.41
1:A:190:GLN:OE1	1:A:390:LYS:HB2	2.20	0.41
1:C:579:LYS:HB3	1:C:579:LYS:HE2	1.87	0.41
1:C:388:GLN:OE1	1:C:388:GLN:HA	2.20	0.41
2:A:801:SAH:H5'2	2:A:801:SAH:HB2	1.94	0.41
1:A:518:ASN:H	1:A:521:ASN:ND2	2.05	0.41
1:A:521:ASN:ND2	1:A:521:ASN:C	2.73	0.41
1:A:538:GLU:CD	1:A:546:SER:CB	2.88	0.41
1:C:239:LEU:O	1:C:248:MET:HA	2.20	0.41
1:A:322:ILE:HA	1:A:323:PRO:HD3	1.96	0.41
1:B:511:ARG:HG2	1:B:526:PHE:CD1	2.56	0.41
1:A:198:TYR:HA	1:B:423:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:THR:HG23	1:C:262:TYR:C	2.39	0.41
1:B:263:ASN:HD22	1:B:264:PRO:N	2.19	0.41
1:C:538:GLU:OE1	1:C:538:GLU:HA	2.20	0.41
1:A:511:ARG:HG2	1:A:526:PHE:CD1	2.55	0.41
1:C:188:ARG:HH11	1:C:188:ARG:HB2	1.83	0.41
1:B:445:TYR:HB2	1:B:447:MET:CE	2.51	0.41
1:A:363:HIS:O	1:A:364:TYR:C	2.60	0.41
1:A:213:ILE:O	1:A:213:ILE:HG13	2.21	0.41
1:A:312:ILE:O	1:A:315:TYR:HB3	2.21	0.40
1:A:367:PHE:CZ	1:C:325:GLN:OE1	2.72	0.40
1:C:557:GLU:HG3	1:C:558:ASP:OD2	2.21	0.40
1:C:376:LEU:O	1:C:380:LEU:HD22	2.22	0.40
1:C:445:TYR:HB2	1:C:447:MET:CE	2.51	0.40
1:A:445:TYR:CB	1:A:447:MET:HE2	2.52	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	372/433 (86%)	358 (96%)	11 (3%)	3 (1%)	24	22
1	B	372/433 (86%)	358 (96%)	11 (3%)	3 (1%)	24	22
1	C	378/433 (87%)	368 (97%)	10 (3%)	0	100	100
All	All	1122/1299 (86%)	1084 (97%)	32 (3%)	6 (0%)	34	35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	ARG
1	A	259	THR
1	A	261	ILE

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Mol	Chain	Res	Type
1	B	260	ALA
1	B	258	SER
1	B	257	ARG

### 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	350/398 (88%)	331 (95%)	19 (5%)	27	31
1	B	351/398 (88%)	332 (95%)	19 (5%)	27	31
1	C	355/398 (89%)	341 (96%)	14 (4%)	39	48
All	All	1056/1194 (88%)	1004 (95%)	52 (5%)	31	36

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	ARG
1	A	240	GLN
1	A	246	ASN
1	A	263	ASN
1	A	265	MET
1	A	277	LEU
1	A	280	LEU
1	A	282	SER
1	A	288	LEU
1	A	295	ASP
1	A	329	ASP
1	A	376	LEU
1	A	380	LEU
1	A	389	LEU
1	A	412	GLU
1	A	460	PHE
1	A	507	LEU
1	A	521	ASN
1	A	533	ARG

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Mol	Chain	Res	Type
1	B	190	GLN
1	B	217	THR
1	B	246	ASN
1	B	263	ASN
1	B	265	MET
1	B	280	LEU
1	B	295	ASP
1	B	304	ASP
1	B	325	GLN
1	B	335	ASP
1	B	339	ARG
1	B	376	LEU
1	B	380	LEU
1	B	389	LEU
1	B	451	ASN
1	B	460	PHE
1	B	513	LEU
1	B	518	ASN
1	B	521	ASN
1	C	240	GLN
1	C	263	ASN
1	C	265	MET
1	C	280	LEU
1	C	282	SER
1	C	286	GLU
1	C	329	ASP
1	C	352	ARG
1	C	376	LEU
1	C	380	LEU
1	C	389	LEU
1	C	436	GLU
1	C	507	LEU
1	C	512	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	HIS
1	A	246	ASN
1	A	263	ASN
1	A	302	ASN
1	A	310	ASN

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Mol	Chain	Res	Type
1	A	313	ASN
1	A	330	HIS
1	A	385	GLN
1	A	386	GLN
1	A	450	ASN
1	A	516	GLN
1	A	521	ASN
1	B	202	HIS
1	B	240	GLN
1	B	246	ASN
1	B	263	ASN
1	B	302	ASN
1	B	310	ASN
1	B	313	ASN
1	B	325	GLN
1	B	330	HIS
1	B	355	HIS
1	B	385	GLN
1	B	386	GLN
1	B	450	ASN
1	B	518	ASN
1	B	521	ASN
1	C	202	HIS
1	C	240	GLN
1	C	246	ASN
1	C	263	ASN
1	C	302	ASN
1	C	310	ASN
1	C	330	HIS
1	C	386	GLN
1	C	450	ASN
1	C	464	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

3 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$
2	SAH	A	801	-	20,28,28	1.00	1 (5%)	19,40,40	1.90	5 (26%)
2	SAH	B	802	-	20,28,28	0.66	0	19,40,40	1.42	4 (21%)
2	SAH	C	803	-	20,28,28	1.04	2 (10%)	19,40,40	1.50	3 (15%)

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	SAH	A	801	-	-	0/7/31/31	0/3/3/3
2	SAH	B	802	-	-	0/7/31/31	0/3/3/3
2	SAH	C	803	-	-	0/7/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	SAH	CB-CA	-2.72	1.39	1.53
2	C	803	SAH	CB-CA	-2.19	1.41	1.53
2	C	803	SAH	CG-SD	2.83	1.92	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	SAH	CB-CA-N	-5.63	94.51	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	803	SAH	CB-CA-N	-3.83	99.63	110.52
2	B	802	SAH	C4'-O4'-C1'	-3.02	106.40	109.72
2	A	801	SAH	C5'-SD-CG	-3.01	93.37	102.41
2	A	801	SAH	C4'-O4'-C1'	-2.37	107.11	109.72
2	B	802	SAH	C1'-N9-C4	-2.07	123.82	126.94
2	C	803	SAH	C1'-N9-C4	-2.00	123.92	126.94
2	B	802	SAH	O2'-C2'-C3'	2.02	118.40	111.83
2	B	802	SAH	O4'-C1'-N9	2.04	112.36	108.10
2	A	801	SAH	CB-CG-SD	2.15	117.71	113.57
2	A	801	SAH	C2'-C1'-N9	2.35	117.89	114.29
2	C	803	SAH	C2'-C1'-N9	2.72	118.44	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	SAH	2	0
2	C	803	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.