



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 09:32 PM EDT

PDB ID : 6W8B  
Title : Structure of DNMT3A in complex with CGA DNA  
Authors : Anteneh, H.; Song, J.  
Deposited on : 2020-03-20  
Resolution : 2.40 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
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

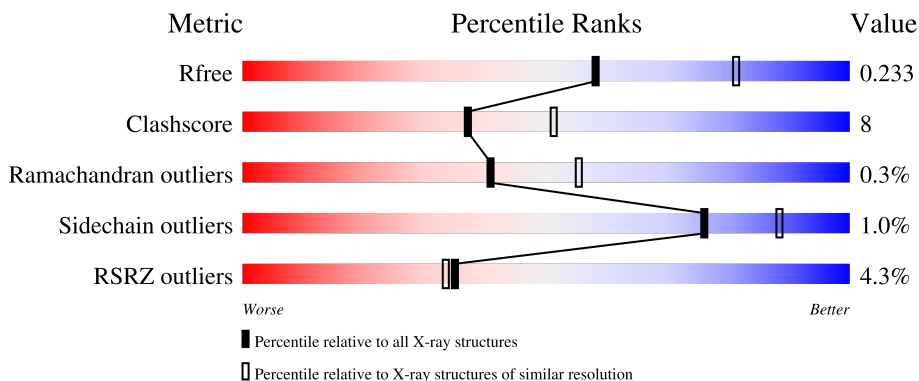
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	285	
1	D	285	
1	H	285	
1	K	285	
2	B	209	

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Mol	Chain	Length	Quality of chain
2	C	209	<p>11% 67% 21% 13%</p>
2	I	209	<p>7% 67% 25% 7%</p>
2	J	209	<p>12% 66% 20% 14%</p>
3	E	25	<p>68% 28% .</p>
3	F	25	<p>60% 36% .</p>
3	L	25	<p>64% 36%</p>
3	M	25	<p>60% 36% .</p>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 17091 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA (cytosine-5)-methyltransferase 3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	285	Total 2277	C 1453	N 404	O 407	S 13	0	1	0
1	D	285	Total 2299	C 1466	N 412	O 408	S 13	0	2	0
1	H	285	Total 2292	C 1461	N 403	O 415	S 13	0	2	0
1	K	285	Total 2289	C 1461	N 410	O 405	S 13	0	2	0

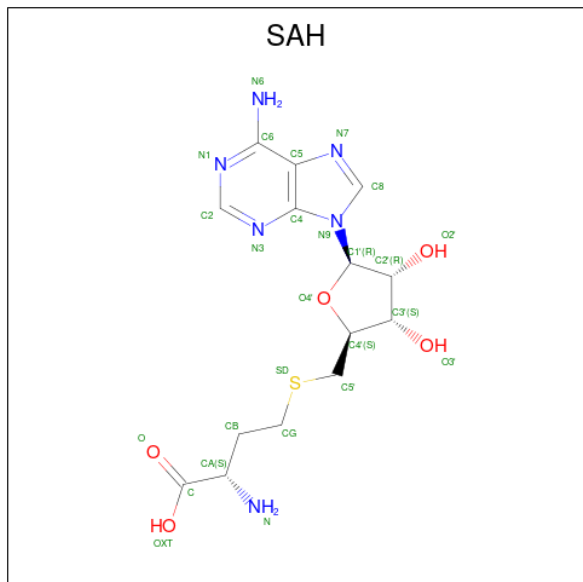
- Molecule 2 is a protein called DNA (cytosine-5)-methyltransferase 3-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	194	Total 1474	C 964	N 240	O 266	S 4	0	0	0
2	C	182	Total 1283	C 829	N 215	O 237	S 2	0	0	0
2	I	195	Total 1480	C 968	N 244	O 265	S 3	0	0	0
2	J	180	Total 1299	C 843	N 217	O 237	S 2	0	0	0

- Molecule 3 is a DNA chain called CGA DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	E	25	Total 493	C 235	N 88	O 146	P 24	0	0	0
3	F	25	Total 510	C 245	N 93	O 148	P 24	0	0	0
3	L	25	Total 493	C 235	N 88	O 146	P 24	0	0	0
3	M	25	Total 510	C 245	N 93	O 148	P 24	0	0	0

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	68	Total 68	68	0	0
5	B	6	Total 6	6	0	0
5	C	2	Total 2	2	0	0
5	D	65	Total 65	65	0	0
5	E	3	Total 3	3	0	0
5	F	3	Total 3	3	0	0

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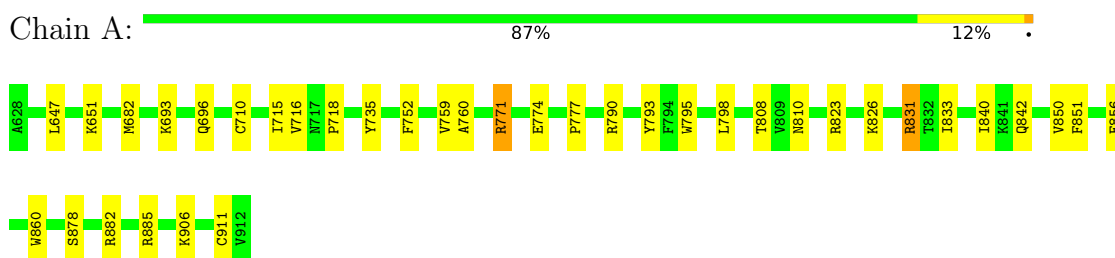
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
5	H	69	Total O 69 69	0	0
5	I	7	Total O 7 7	0	0
5	J	2	Total O 2 2	0	0
5	K	58	Total O 58 58	0	0
5	L	3	Total O 3 3	0	0
5	M	2	Total O 2 2	0	0

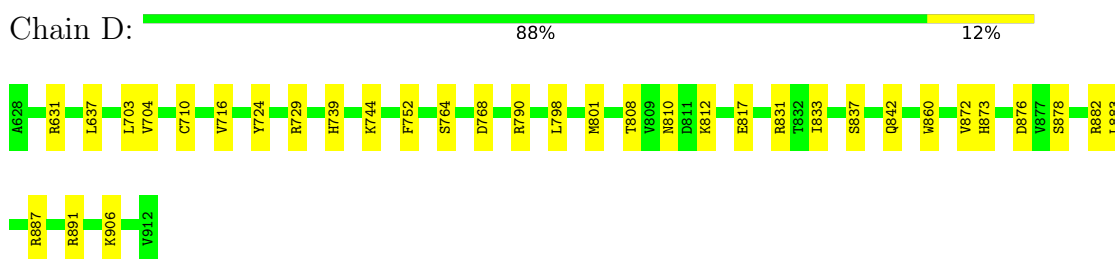
### 3 Residue-property plots [i](#)

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.

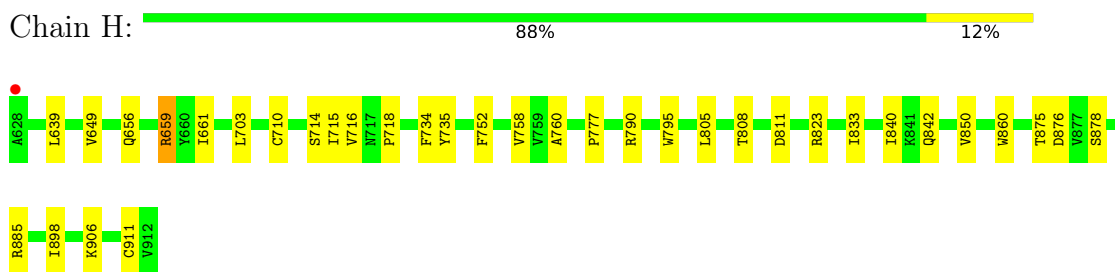
- Molecule 1: DNA (cytosine-5)-methyltransferase 3A



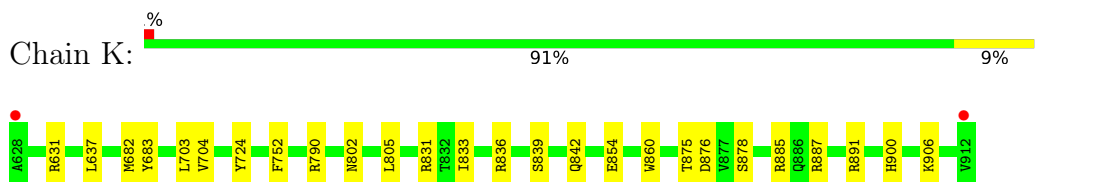
- Molecule 1: DNA (cytosine-5)-methyltransferase 3A



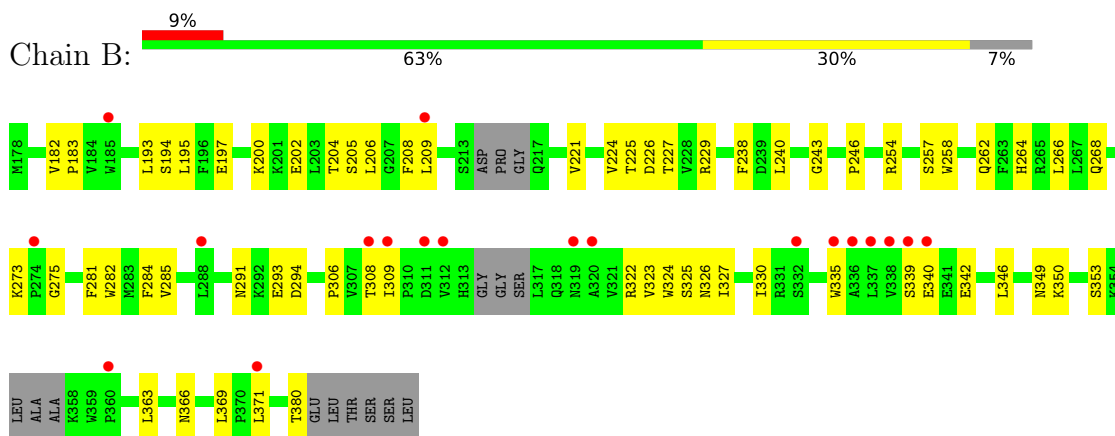
- Molecule 1: DNA (cytosine-5)-methyltransferase 3A



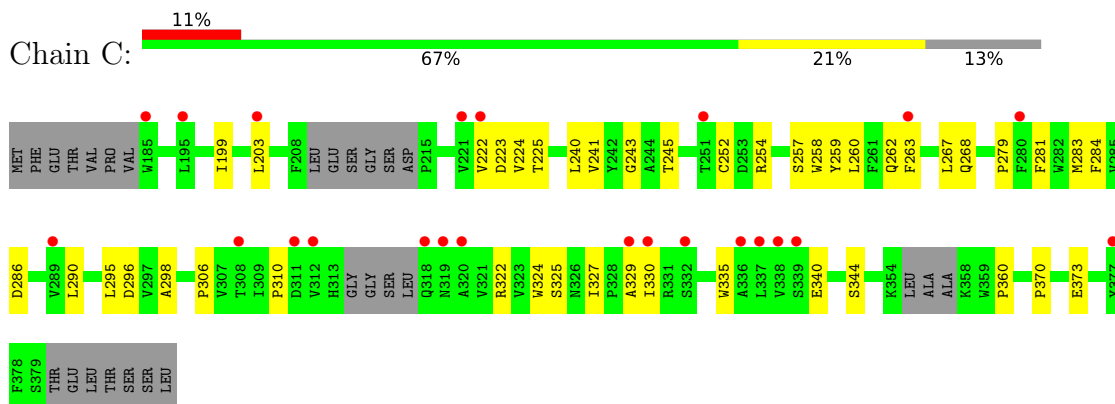
- Molecule 1: DNA (cytosine-5)-methyltransferase 3A



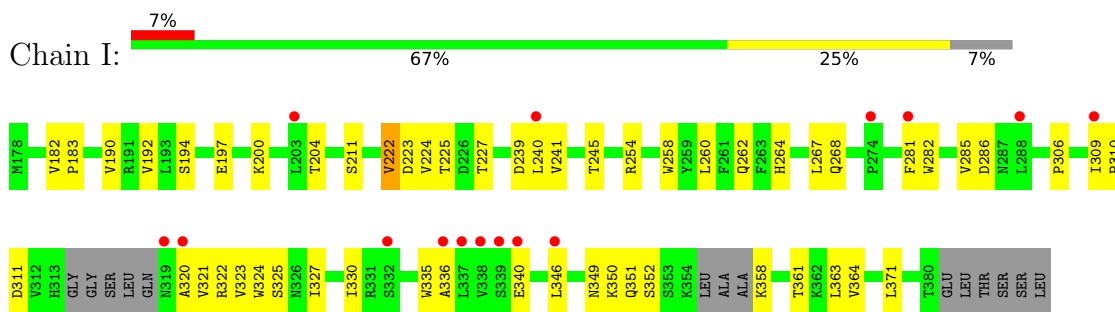
- Molecule 2: DNA (cytosine-5)-methyltransferase 3-like



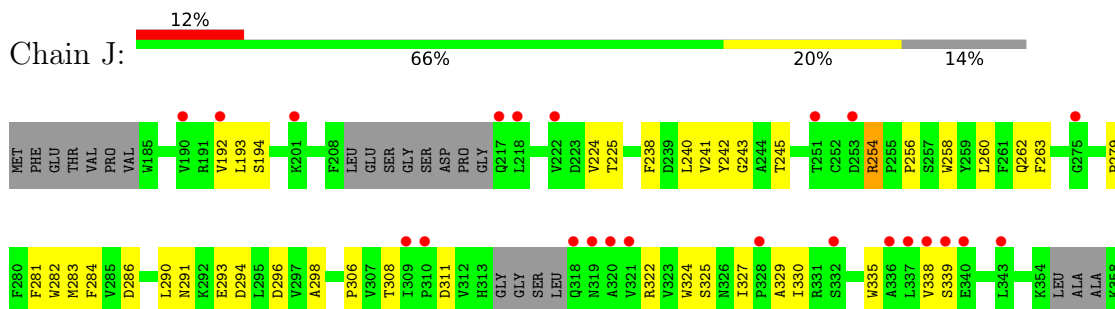
- Molecule 2: DNA (cytosine-5)-methyltransferase 3-like



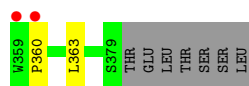
- Molecule 2: DNA (cytosine-5)-methyltransferase 3-like



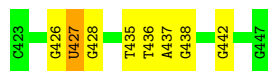
- Molecule 2: DNA (cytosine-5)-methyltransferase 3-like



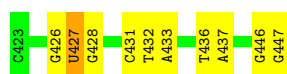




- Molecule 3: CGA DNA (25-MER)



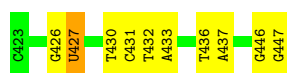
- Molecule 3: CGA DNA (25-MER)



- Molecule 3: CGA DNA (25-MER)



- Molecule 3: CGA DNA (25-MER)



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	186.35Å 186.35Å 81.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.87 – 2.40 48.87 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.87-2.40) 99.9 (48.87-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 2.39Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.212 , 0.233 0.212 , 0.233	Depositor DCC
$R_{free}$ test set	2012 reflections (1.62%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.2	Xtrriage
Anisotropy	0.605	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 61.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.488 for -h,-k,l 0.022 for h,-h-k,-l 0.022 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17091	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PYO, 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	0.27	0/2331	0.45	1/3153 (0.0%)
1	D	0.26	0/2356	0.42	0/3182
1	H	0.27	0/2346	0.43	0/3173
1	K	0.27	0/2349	0.44	1/3174 (0.0%)
2	B	0.28	0/1520	0.49	0/2089
2	C	0.28	0/1320	0.46	0/1817
2	I	0.27	0/1529	0.45	0/2101
2	J	0.31	0/1338	0.51	0/1842
3	E	0.53	0/530	0.95	0/815
3	F	0.55	0/550	0.91	0/846
3	L	0.55	0/530	0.96	0/815
3	M	0.56	0/550	0.95	0/846
All	All	0.32	0/17249	0.55	2/23853 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	682	MET	CA-CB-CG	-5.37	104.17	113.30
1	A	771	ARG	NE-CZ-NH1	5.16	122.88	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2277	0	2221	27	0
1	D	2299	0	2275	26	0
1	H	2292	0	2229	26	0
1	K	2289	0	2263	20	0
2	B	1474	0	1307	38	0
2	C	1283	0	1053	29	0
2	I	1480	0	1315	31	0
2	J	1299	0	1078	33	0
3	E	493	0	270	11	0
3	F	510	0	279	11	0
3	L	493	0	270	11	0
3	M	510	0	279	10	0
4	A	26	0	19	1	0
4	D	26	0	19	0	0
4	H	26	0	19	2	0
4	K	26	0	19	0	0
5	A	68	0	0	2	0
5	B	6	0	0	1	0
5	C	2	0	0	0	0
5	D	65	0	0	1	0
5	E	3	0	0	0	0
5	F	3	0	0	0	0
5	H	69	0	0	1	0
5	I	7	0	0	1	0
5	J	2	0	0	0	0
5	K	58	0	0	2	0
5	L	3	0	0	0	0
5	M	2	0	0	0	0
All	All	17091	0	14915	245	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 8.

All (245) 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)
2:J:327:ILE:HD11	2:J:330:ILE:HG13	1.44	0.97
2:J:281:PHE:HD2	2:J:327:ILE:HG22	1.31	0.95
2:J:281:PHE:CD2	2:J:327:ILE:HG22	2.08	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:808:THR:HG22	1:D:810:ASN:H	1.39	0.88
2:C:327:ILE:HD11	2:C:330:ILE:HG13	1.58	0.85
1:A:808:THR:HG22	1:A:810:ASN:H	1.43	0.84
2:J:327:ILE:HD12	2:J:329:ALA:H	1.43	0.83
2:C:327:ILE:HD12	2:C:329:ALA:H	1.46	0.79
2:J:279:PRO:HB2	2:J:281:PHE:HE1	1.51	0.76
4:H:1001:SAH:SD	5:H:1164:HOH:O	2.43	0.75
4:A:1001:SAH:SD	5:A:1163:HOH:O	2.45	0.74
2:I:327:ILE:HD12	2:I:371:LEU:HD11	1.71	0.73
2:I:285:VAL:HG12	2:I:323:VAL:HG23	1.73	0.69
2:I:309:ILE:HB	2:I:321:VAL:HG23	1.74	0.69
2:I:282:TRP:O	2:I:325:SER:HB2	1.93	0.69
2:I:222:VAL:HG23	2:I:223:ASP:H	1.56	0.68
2:B:291:ASN:ND2	2:B:294:ASP:OD1	2.26	0.68
2:C:222:VAL:HG13	2:C:223:ASP:H	1.58	0.67
1:D:744:LYS:HG2	1:K:854:GLU:HB3	1.75	0.67
2:C:199:ILE:HD13	2:C:203:LEU:HD22	1.78	0.65
2:J:256:PRO:HB2	2:J:290:LEU:HD23	1.79	0.65
1:H:718:PRO:HB3	3:L:442:DG:H2''	1.79	0.65
2:I:330:ILE:HA	2:I:335:TRP:HH2	1.61	0.65
1:A:718:PRO:HB3	3:E:442:DG:H2''	1.79	0.64
2:C:283:MET:HA	2:C:325:SER:OG	1.98	0.64
1:A:885:ARG:NH2	1:D:876:ASP:OD1	2.31	0.63
2:J:291:ASN:ND2	2:J:293:GLU:HG2	2.14	0.63
2:J:240:LEU:HD12	2:J:241:VAL:N	2.15	0.62
2:B:330:ILE:HA	2:B:335:TRP:HH2	1.65	0.62
2:B:322:ARG:NE	2:B:340:GLU:OE2	2.33	0.62
2:B:366:ASN:HA	2:B:369:LEU:HD12	1.81	0.61
3:L:437:DA:H61	3:M:431:DC:H42	1.48	0.60
2:J:283:MET:HA	2:J:325:SER:OG	2.02	0.60
2:B:306:PRO:HB2	2:B:322:ARG:HB3	1.83	0.60
2:B:309:ILE:HG22	2:B:363:LEU:HD13	1.82	0.60
1:D:790:ARG:NH2	1:D:833:ILE:O	2.35	0.59
2:C:254:ARG:HG2	2:C:258:TRP:CD2	2.38	0.59
3:L:436:DT:H2''	3:L:437:DA:C8	2.37	0.58
2:I:325:SER:OG	2:I:327:ILE:HG12	2.03	0.58
2:J:308:THR:HG22	2:J:322:ARG:HG2	1.87	0.57
1:D:831[B]:ARG:HD3	1:D:842:GLN:HA	1.86	0.57
2:J:327:ILE:HD11	2:J:330:ILE:CG1	2.27	0.56
2:J:193:LEU:HB3	2:J:241:VAL:HG12	1.87	0.56
1:K:805:LEU:HD13	1:K:900:HIS:CG	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:225:THR:HG22	2:I:258:TRP:HZ2	1.71	0.56
2:I:306:PRO:HB3	2:I:324:TRP:CE2	2.41	0.56
2:C:241:VAL:HG21	2:C:267:LEU:HD13	1.88	0.55
2:I:349:ASN:O	2:I:352:SER:OG	2.20	0.55
3:F:436:DT:H2''	3:F:437:DA:C8	2.40	0.55
2:J:254:ARG:HG2	2:J:258:TRP:CD2	2.42	0.55
1:H:876:ASP:OD1	1:K:885:ARG:NH2	2.37	0.54
3:F:446:DG:H2''	3:F:447:DG:O5'	2.07	0.54
1:H:885:ARG:HH22	1:K:876:ASP:CG	2.11	0.54
1:A:878:SER:HA	1:D:860:TRP:CE2	2.42	0.54
2:B:285:VAL:HG22	2:B:323:VAL:HG23	1.89	0.54
2:J:330:ILE:HA	2:J:335:TRP:HE1	1.72	0.54
1:A:860:TRP:CE2	1:D:878:SER:HA	2.43	0.54
1:H:710:CYS:N	3:M:427:PYO:HC5	2.23	0.54
2:J:245:THR:OG1	2:J:286:ASP:HA	2.08	0.54
2:B:306:PRO:HB3	2:B:324:TRP:CE2	2.43	0.53
3:L:437:DA:N6	3:M:431:DC:H42	2.06	0.53
1:H:860:TRP:CE2	1:K:878:SER:HA	2.44	0.53
1:H:878:SER:HA	1:K:860:TRP:CE2	2.43	0.53
3:M:446:DG:H2''	3:M:447:DG:O5'	2.08	0.53
2:C:263:PHE:CZ	2:C:284:PHE:HB2	2.44	0.53
2:I:310:PRO:HG3	2:I:336:ALA:O	2.09	0.52
1:D:724:TYR:OH	1:D:768:ASP:OD2	2.24	0.52
2:I:311:ASP:HB2	2:I:363:LEU:HD11	1.91	0.52
2:I:192:VAL:HG22	2:I:240:LEU:HB3	1.90	0.52
2:I:200:LYS:O	2:I:204:THR:HG23	2.09	0.52
3:L:437:DA:H2'	3:L:438:DG:C8	2.45	0.52
2:B:308:THR:HB	2:B:322:ARG:HG2	1.90	0.52
2:C:268:GLN:HG2	1:D:739:HIS:NE2	2.25	0.52
1:D:637:LEU:HB3	1:D:704:VAL:HG22	1.91	0.52
1:H:840:ILE:O	1:H:842:GLN:NE2	2.42	0.52
2:I:194:SER:OG	2:I:197:GLU:O	2.24	0.52
2:J:291:ASN:HD22	2:J:293:GLU:HG2	1.73	0.52
1:H:790:ARG:NH2	1:H:833:ILE:O	2.43	0.51
2:C:240:LEU:HA	2:C:281:PHE:O	2.11	0.51
1:H:885:ARG:NH2	1:K:876:ASP:OD1	2.38	0.51
2:J:282:TRP:O	2:J:325:SER:OG	2.29	0.51
2:J:240:LEU:HD12	2:J:241:VAL:H	1.75	0.51
2:B:246:PRO:HD2	5:B:406:HOH:O	2.10	0.51
2:J:279:PRO:HB2	2:J:281:PHE:CE1	2.38	0.51
3:M:436:DT:H2''	3:M:437:DA:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:260:LEU:HD11	2:C:298:ALA:HA	1.93	0.51
2:B:193:LEU:HD23	2:B:238:PHE:CZ	2.46	0.51
2:B:327:ILE:HD13	2:B:371:LEU:HD11	1.93	0.51
2:C:290:LEU:HB3	2:C:295:LEU:HG	1.93	0.51
2:C:281:PHE:CD2	2:C:327:ILE:HG22	2.46	0.50
2:I:241:VAL:HG21	2:I:267:LEU:HD13	1.92	0.50
3:L:428:DG:C8	3:L:428:DG:H5'	2.46	0.50
1:A:710:CYS:N	3:F:427:PYO:HC5	2.26	0.50
2:C:225:THR:HG22	2:C:258:TRP:HZ2	1.76	0.50
1:A:771:ARG:HH11	1:A:771:ARG:HG2	1.77	0.50
2:C:245:THR:OG1	2:C:286:ASP:HA	2.11	0.50
2:C:330:ILE:HA	2:C:335:TRP:HE1	1.77	0.50
1:A:840:ILE:O	1:A:842:GLN:NE2	2.44	0.50
3:E:437:DA:H61	3:F:431:DC:H42	1.58	0.50
2:I:224:VAL:HA	2:I:227:THR:HG23	1.94	0.50
3:E:428:DG:C8	3:E:428:DG:H5'	2.47	0.49
1:A:831[B]:ARG:HD3	1:A:842:GLN:HA	1.94	0.49
2:J:338:VAL:HG12	2:J:339:SER:H	1.78	0.49
2:B:200:LYS:O	2:B:204:THR:HG23	2.12	0.49
2:I:190:VAL:HG23	2:I:239:ASP:HB2	1.93	0.49
2:B:202:GLU:O	2:B:206:LEU:HD12	2.12	0.49
2:I:306:PRO:HB2	2:I:322:ARG:HB3	1.93	0.49
2:C:373:GLU:OE1	2:C:373:GLU:N	2.46	0.49
1:K:887:ARG:O	1:K:891:ARG:HG3	2.13	0.49
2:C:224:VAL:HG21	2:C:262:GLN:HB3	1.94	0.48
2:C:290:LEU:HD23	2:C:295:LEU:HD23	1.94	0.48
1:H:808:THR:HG22	1:H:811:ASP:CG	2.34	0.48
1:A:885:ARG:HH22	1:D:876:ASP:CG	2.14	0.48
1:H:906:LYS:HB2	1:H:911:CYS:SG	2.53	0.48
2:C:199:ILE:HB	2:C:203:LEU:HD13	1.94	0.48
1:K:875:THR:O	1:K:885:ARG:HD3	2.14	0.48
1:A:774:GLU:OE2	2:B:229:ARG:NH1	2.46	0.48
2:B:240:LEU:HA	2:B:281:PHE:O	2.13	0.48
2:B:349:ASN:O	2:B:353:SER:OG	2.27	0.48
1:A:716:VAL:HB	3:F:426:DG:H1'	1.96	0.47
2:C:279:PRO:HB2	2:C:281:PHE:CE1	2.49	0.47
2:C:322:ARG:NH2	2:C:340:GLU:OE2	2.47	0.47
1:A:790:ARG:NH2	1:A:833:ILE:O	2.47	0.47
1:H:777:PRO:HB3	1:H:795:TRP:CD2	2.50	0.47
3:E:437:DA:N6	3:F:431:DC:H42	2.13	0.47
3:L:437:DA:H61	3:M:431:DC:N4	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:VAL:HG12	2:B:183:PRO:O	2.15	0.47
2:C:257:SER:OG	1:D:729:ARG:NH2	2.48	0.47
2:J:224:VAL:HG21	2:J:262:GLN:HB3	1.97	0.47
1:D:808:THR:HG22	1:D:810:ASN:N	2.20	0.46
4:H:1001:SAH:HN1	4:H:1001:SAH:HG1	1.56	0.46
2:J:306:PRO:HB3	2:J:324:TRP:CE2	2.50	0.46
2:I:240:LEU:HA	2:I:281:PHE:O	2.16	0.46
2:B:227:THR:HG21	2:B:266:LEU:HD21	1.97	0.46
1:A:715:ILE:HG12	1:A:760:ALA:HB1	1.98	0.46
1:A:777:PRO:HB3	1:A:795:TRP:CD2	2.51	0.46
2:C:279:PRO:HB2	2:C:281:PHE:HE1	1.81	0.46
1:D:887:ARG:O	1:D:891:ARG:HG3	2.15	0.46
1:H:875:THR:O	1:H:885:ARG:HD3	2.16	0.46
1:D:812:LYS:HB3	1:D:817:GLU:HB2	1.98	0.46
2:J:192:VAL:HA	2:J:240:LEU:O	2.15	0.46
1:K:891:ARG:HD3	5:K:1132:HOH:O	2.16	0.46
1:K:631:ARG:NH1	1:K:906:LYS:O	2.49	0.46
1:H:716:VAL:HB	3:M:426:DG:H1'	1.99	0.45
1:D:837:SER:HB3	1:D:882:ARG:NH1	2.31	0.45
2:I:346:LEU:O	2:I:350:LYS:N	2.49	0.45
3:L:428:DG:H5'	3:L:428:DG:H8	1.82	0.45
3:F:432:DT:H2'	3:F:433:DA:C8	2.51	0.45
1:K:831[B]:ARG:HD3	1:K:842:GLN:HA	1.97	0.45
2:C:243:GLY:O	2:C:284:PHE:HA	2.17	0.45
2:C:306:PRO:HB3	2:C:324:TRP:CE2	2.52	0.45
1:D:716:VAL:HB	3:E:426:DG:H1'	1.97	0.45
3:E:436:DT:H2''	3:E:437:DA:C8	2.52	0.45
2:I:361:THR:HA	2:I:364:VAL:HG12	1.97	0.45
1:K:637:LEU:HB3	1:K:704:VAL:HG22	1.99	0.45
1:D:883:LEU:HB2	3:F:437:DA:OP2	2.16	0.45
1:H:715:ILE:HG12	1:H:760:ALA:HB1	1.99	0.45
1:H:718:PRO:HG3	3:L:442:DG:H1'	1.99	0.45
2:J:260:LEU:HD21	2:J:298:ALA:HA	1.99	0.44
2:I:258:TRP:CE2	2:I:262:GLN:HG3	2.53	0.44
1:A:906:LYS:HB2	1:A:911:CYS:SG	2.58	0.44
1:H:805:LEU:HD23	1:H:805:LEU:HA	1.75	0.44
3:M:446:DG:H4'	3:M:447:DG:OP1	2.18	0.44
2:I:264:HIS:O	2:I:268:GLN:HG2	2.17	0.44
3:M:432:DT:H2'	3:M:433:DA:C8	2.53	0.44
2:J:243:GLY:O	2:J:284:PHE:HA	2.18	0.44
2:B:282:TRP:O	2:B:325:SER:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:435:DT:H4'	3:E:436:DT:OP1	2.18	0.44
1:H:714:SER:HB2	1:H:758:VAL:HG21	1.98	0.43
1:H:823:ARG:NH2	1:H:850:VAL:HG21	2.33	0.43
2:B:227:THR:CG2	2:B:266:LEU:HD21	2.48	0.43
1:D:872:VAL:HG12	1:D:873:HIS:CD2	2.54	0.43
2:I:322:ARG:HH21	2:I:340:GLU:CD	2.21	0.43
2:J:311:ASP:HB2	2:J:363:LEU:HD11	2.01	0.43
2:J:338:VAL:HG12	2:J:339:SER:N	2.33	0.43
1:K:836:ARG:O	1:K:839:SER:OG	2.25	0.43
2:J:258:TRP:HD1	1:K:724:TYR:CZ	2.36	0.43
2:J:327:ILE:HD12	2:J:327:ILE:C	2.39	0.43
3:M:430:DT:H2''	3:M:431:DC:H5''	1.99	0.43
2:B:195:LEU:HD23	2:B:224:VAL:HG11	2.00	0.43
2:B:264:HIS:O	2:B:268:GLN:HG2	2.17	0.43
1:D:798:LEU:O	1:D:801:MET:HG3	2.19	0.43
1:H:649:VAL:HG21	1:H:898:ILE:HB	2.01	0.43
2:B:258:TRP:CE2	2:B:262:GLN:HG3	2.53	0.43
1:D:837:SER:HB3	1:D:882:ARG:HH12	1.83	0.43
1:A:777:PRO:HB3	1:A:795:TRP:CE2	2.53	0.43
2:B:194:SER:HB2	2:B:197:GLU:O	2.18	0.43
1:A:826:LYS:NZ	1:A:856:GLU:OE2	2.48	0.43
2:B:281:PHE:HA	2:B:326:ASN:HD21	1.83	0.43
2:C:340:GLU:O	2:C:344:SER:OG	2.35	0.43
1:K:802:ASN:OD1	1:K:802:ASN:N	2.51	0.43
1:A:651:LYS:NZ	5:A:1109:HOH:O	2.48	0.43
1:H:703:LEU:HA	1:H:752:PHE:O	2.19	0.43
1:D:631:ARG:NH1	1:D:906:LYS:O	2.52	0.43
3:E:437:DA:H2'	3:E:438:DG:C8	2.54	0.43
2:B:257:SER:HB3	2:B:294:ASP:OD2	2.19	0.42
1:H:777:PRO:HB3	1:H:795:TRP:CE2	2.53	0.42
1:K:805:LEU:HD13	1:K:900:HIS:ND1	2.33	0.42
2:J:193:LEU:HB2	2:J:238:PHE:CE1	2.55	0.42
2:J:193:LEU:O	2:J:242:TYR:N	2.41	0.42
1:K:703:LEU:HA	1:K:752:PHE:O	2.20	0.42
1:A:693:LYS:O	1:A:696:GLN:HG3	2.20	0.42
2:C:252:CYS:HG	2:C:259:TYR:HE1	1.67	0.42
3:F:428:DG:H5'	3:F:428:DG:C8	2.54	0.42
2:B:208:PHE:O	2:B:209:LEU:HD13	2.19	0.42
1:D:703:LEU:HA	1:D:752:PHE:O	2.20	0.42
1:H:659:ARG:HG2	1:H:661:ILE:HG13	2.01	0.42
2:I:182:VAL:HG12	2:I:183:PRO:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:211:SER:O	2:I:211:SER:OG	2.34	0.42
3:L:432:DT:H2'	3:L:433:DA:O5'	2.19	0.42
1:A:759:VAL:HA	1:A:793:TYR:CE2	2.55	0.42
1:A:771:ARG:NE	2:B:226:ASP:HA	2.35	0.42
2:B:273:LYS:O	2:B:275:GLY:N	2.52	0.42
2:C:199:ILE:H	2:C:199:ILE:HG13	1.70	0.42
2:B:195:LEU:HD23	2:B:221:VAL:HG21	2.02	0.41
2:B:346:LEU:O	2:B:350:LYS:N	2.39	0.41
3:F:446:DG:H4'	3:F:447:DG:OP1	2.20	0.41
2:I:309:ILE:O	2:I:320:ALA:HA	2.20	0.41
1:A:752:PHE:HB3	1:A:798:LEU:HD23	2.03	0.41
2:B:330:ILE:HA	2:B:335:TRP:CH2	2.51	0.41
1:K:683:TYR:HB3	5:K:1127:HOH:O	2.20	0.41
1:D:891:ARG:HD3	5:D:1125:HOH:O	2.20	0.41
1:A:851:PHE:CE1	1:A:856:GLU:HG2	2.55	0.41
1:K:790:ARG:NH2	1:K:833:ILE:O	2.54	0.41
2:B:339:SER:O	2:B:342:GLU:N	2.53	0.41
1:H:656:GLN:HE21	1:H:911:CYS:N	2.18	0.41
2:I:351:GLN:CD	2:I:351:GLN:H	2.24	0.41
3:L:435:DT:H4'	3:L:436:DT:OP1	2.20	0.41
1:D:752:PHE:HB3	1:D:798:LEU:HD23	2.03	0.41
2:I:245:THR:OG1	2:I:286:ASP:HA	2.21	0.41
1:A:647:LEU:O	1:A:651:LYS:HG3	2.21	0.41
1:A:682:MET:HE2	1:A:682:MET:HB3	1.75	0.41
2:B:243:GLY:O	2:B:284:PHE:HA	2.21	0.41
2:B:291:ASN:OD1	2:B:293:GLU:HG2	2.20	0.41
1:A:823:ARG:NH2	1:A:850:VAL:HG21	2.36	0.41
2:B:225:THR:HG22	2:B:258:TRP:HZ2	1.86	0.41
3:E:437:DA:H61	3:F:431:DC:N4	2.18	0.41
2:J:263:PHE:CZ	2:J:284:PHE:HB2	2.56	0.41
2:B:380:THR:O	2:B:380:THR:OG1	2.31	0.40
1:D:710:CYS:N	3:E:427:PYO:HC5	2.35	0.40
2:J:225:THR:HG22	2:J:258:TRP:HZ2	1.86	0.40
3:E:428:DG:H5'	3:E:428:DG:H8	1.86	0.40
1:H:714:SER:HA	1:H:760:ALA:O	2.20	0.40
1:H:639:LEU:HD12	1:H:734:PHE:CD1	2.57	0.40
2:I:358:LYS:O	5:I:401:HOH:O	2.21	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	284/285 (100%)	275 (97%)	9 (3%)	0	100	100
1	D	285/285 (100%)	277 (97%)	8 (3%)	0	100	100
1	H	285/285 (100%)	277 (97%)	8 (3%)	0	100	100
1	K	285/285 (100%)	276 (97%)	9 (3%)	0	100	100
2	B	186/209 (89%)	172 (92%)	14 (8%)	0	100	100
2	C	174/209 (83%)	158 (91%)	13 (8%)	3 (2%)	9	11
2	I	189/209 (90%)	174 (92%)	14 (7%)	1 (0%)	29	41
2	J	172/209 (82%)	159 (92%)	12 (7%)	1 (1%)	25	36
All	All	1860/1976 (94%)	1768 (95%)	87 (5%)	5 (0%)	41	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	360	PRO
2	J	360	PRO
2	I	222	VAL
2	C	310	PRO
2	C	370	PRO

### 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	239/250 (96%)	235 (98%)	4 (2%)	60	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	246/250 (98%)	245 (100%)	1 (0%)	91	96
1	H	242/250 (97%)	240 (99%)	2 (1%)	81	91
1	K	244/250 (98%)	244 (100%)	0	100	100
2	B	142/191 (74%)	140 (99%)	2 (1%)	67	82
2	C	107/191 (56%)	106 (99%)	1 (1%)	78	90
2	I	142/191 (74%)	140 (99%)	2 (1%)	67	82
2	J	111/191 (58%)	107 (96%)	4 (4%)	35	54
All	All	1473/1764 (84%)	1457 (99%)	16 (1%)	76	87

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	735	TYR
1	A	831[A]	ARG
1	A	831[B]	ARG
1	A	882	ARG
2	B	205	SER
2	B	254	ARG
2	C	296	ASP
1	D	764	SER
1	H	659	ARG
1	H	735	TYR
2	I	254	ARG
2	I	260	LEU
2	J	194	SER
2	J	254	ARG
2	J	294	ASP
2	J	296	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	656	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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
3	PYO	L	427	1,3	16,20,21	2.03	4 (25%)	22,28,31	1.00	2 (9%)
3	PYO	F	427	1,3	16,20,21	2.03	4 (25%)	22,28,31	1.03	1 (4%)
3	PYO	E	427	1,3	16,20,21	2.04	4 (25%)	22,28,31	1.08	1 (4%)
3	PYO	M	427	1,3	16,20,21	2.03	4 (25%)	22,28,31	1.09	2 (9%)

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	PYO	L	427	1,3	-	4/7/25/26	0/2/2/2
3	PYO	F	427	1,3	-	4/7/25/26	0/2/2/2
3	PYO	E	427	1,3	-	4/7/25/26	0/2/2/2
3	PYO	M	427	1,3	-	4/7/25/26	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	427	PYO	C6-C5	6.24	1.49	1.35
3	E	427	PYO	C6-C5	6.21	1.49	1.35
3	L	427	PYO	C6-C5	6.19	1.49	1.35
3	M	427	PYO	C6-C5	6.16	1.49	1.35
3	E	427	PYO	C2-N1	2.99	1.46	1.40
3	L	427	PYO	C2-N1	2.93	1.46	1.40
3	M	427	PYO	C5-C4	2.93	1.46	1.40
3	F	427	PYO	C5-C4	2.90	1.46	1.40
3	E	427	PYO	C5-C4	2.89	1.46	1.40
3	L	427	PYO	C5-C4	2.83	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	427	PYO	C2-N1	2.82	1.46	1.40
3	F	427	PYO	C2-N1	2.72	1.45	1.40
3	M	427	PYO	C4-N3	2.39	1.42	1.33
3	E	427	PYO	C4-N3	2.37	1.42	1.33
3	F	427	PYO	C4-N3	2.37	1.42	1.33
3	L	427	PYO	C4-N3	2.37	1.42	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	427	PYO	C5-C4-N3	-3.90	119.51	124.29
3	M	427	PYO	C5-C4-N3	-3.81	119.62	124.29
3	F	427	PYO	C5-C4-N3	-3.78	119.65	124.29
3	L	427	PYO	C5-C4-N3	-3.47	120.03	124.29
3	M	427	PYO	C5-C6-N1	-2.15	119.01	121.19
3	L	427	PYO	C5-C6-N1	-2.11	119.05	121.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	427	PYO	C2'-C1'-N1-C6
3	E	427	PYO	C2'-C1'-N1-C2
3	L	427	PYO	C2'-C1'-N1-C6
3	L	427	PYO	C2'-C1'-N1-C2
3	M	427	PYO	C2'-C1'-N1-C6
3	F	427	PYO	C2'-C1'-N1-C6
3	M	427	PYO	C2'-C1'-N1-C2
3	F	427	PYO	C2'-C1'-N1-C2
3	F	427	PYO	O4'-C1'-N1-C6
3	F	427	PYO	O4'-C1'-N1-C2
3	M	427	PYO	O4'-C1'-N1-C2
3	E	427	PYO	O4'-C1'-N1-C6
3	L	427	PYO	O4'-C1'-N1-C6
3	M	427	PYO	O4'-C1'-N1-C6
3	E	427	PYO	O4'-C1'-N1-C2
3	L	427	PYO	O4'-C1'-N1-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	427	PYO	1	0
3	E	427	PYO	1	0
3	M	427	PYO	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	SAH	K	1001	-	24,28,28	1.21	3 (12%)	25,40,40	1.59	4 (16%)
4	SAH	A	1001	-	24,28,28	1.19	3 (12%)	25,40,40	1.74	4 (16%)
4	SAH	H	1001	-	24,28,28	1.20	3 (12%)	25,40,40	1.74	4 (16%)
4	SAH	D	1001	-	24,28,28	1.22	3 (12%)	25,40,40	1.65	4 (16%)

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
4	SAH	K	1001	-	-	4/11/31/31	0/3/3/3
4	SAH	A	1001	-	-	5/11/31/31	0/3/3/3
4	SAH	H	1001	-	-	5/11/31/31	0/3/3/3
4	SAH	D	1001	-	-	4/11/31/31	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1001	SAH	C2-N3	4.11	1.38	1.32
4	K	1001	SAH	C2-N3	4.06	1.38	1.32
4	H	1001	SAH	C2-N3	3.95	1.38	1.32
4	A	1001	SAH	C2-N3	3.88	1.38	1.32
4	D	1001	SAH	C2-N1	2.53	1.38	1.33
4	K	1001	SAH	C2-N1	2.49	1.38	1.33
4	H	1001	SAH	C2-N1	2.47	1.38	1.33
4	A	1001	SAH	C2-N1	2.45	1.38	1.33
4	D	1001	SAH	OXT-C	-2.10	1.23	1.30
4	H	1001	SAH	OXT-C	-2.09	1.23	1.30
4	A	1001	SAH	OXT-C	-2.08	1.23	1.30
4	K	1001	SAH	OXT-C	-2.05	1.23	1.30

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1001	SAH	N3-C2-N1	-5.63	119.88	128.68
4	A	1001	SAH	N3-C2-N1	-5.60	119.93	128.68
4	K	1001	SAH	N3-C2-N1	-5.52	120.05	128.68
4	D	1001	SAH	N3-C2-N1	-5.49	120.09	128.68
4	H	1001	SAH	C5'-SD-CG	-3.59	91.50	102.27
4	A	1001	SAH	C5'-SD-CG	-3.46	91.90	102.27
4	D	1001	SAH	OXT-C-O	-3.20	116.82	124.09
4	A	1001	SAH	OXT-C-O	-3.19	116.86	124.09
4	K	1001	SAH	OXT-C-O	-3.17	116.89	124.09
4	D	1001	SAH	C5'-SD-CG	-3.02	93.20	102.27
4	H	1001	SAH	OXT-C-O	-3.01	117.25	124.09
4	A	1001	SAH	OXT-C-CA	2.51	121.94	113.38
4	K	1001	SAH	C5'-SD-CG	-2.47	94.87	102.27
4	H	1001	SAH	OXT-C-CA	2.44	121.68	113.38
4	D	1001	SAH	OXT-C-CA	2.21	120.90	113.38
4	K	1001	SAH	OXT-C-CA	2.20	120.87	113.38

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	SAH	N-CA-CB-CG
4	D	1001	SAH	N-CA-CB-CG
4	H	1001	SAH	N-CA-CB-CG
4	K	1001	SAH	N-CA-CB-CG
4	D	1001	SAH	CB-CG-SD-C5'

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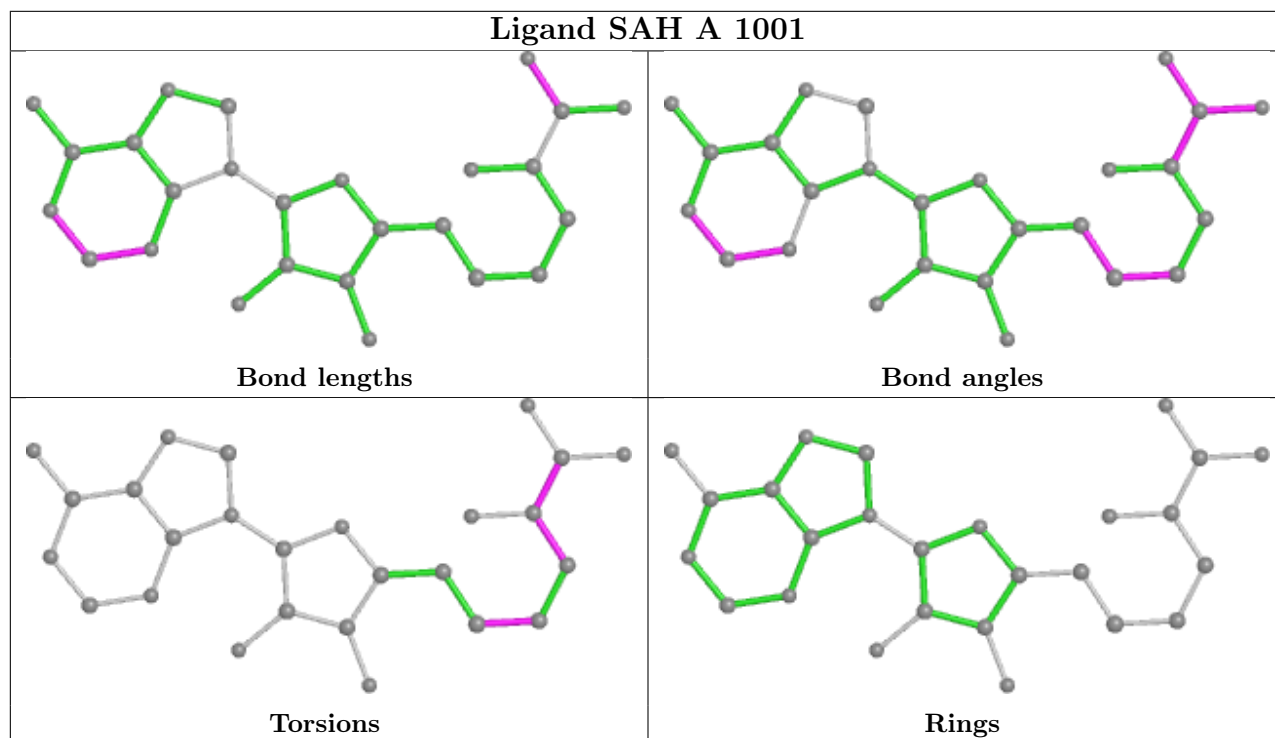
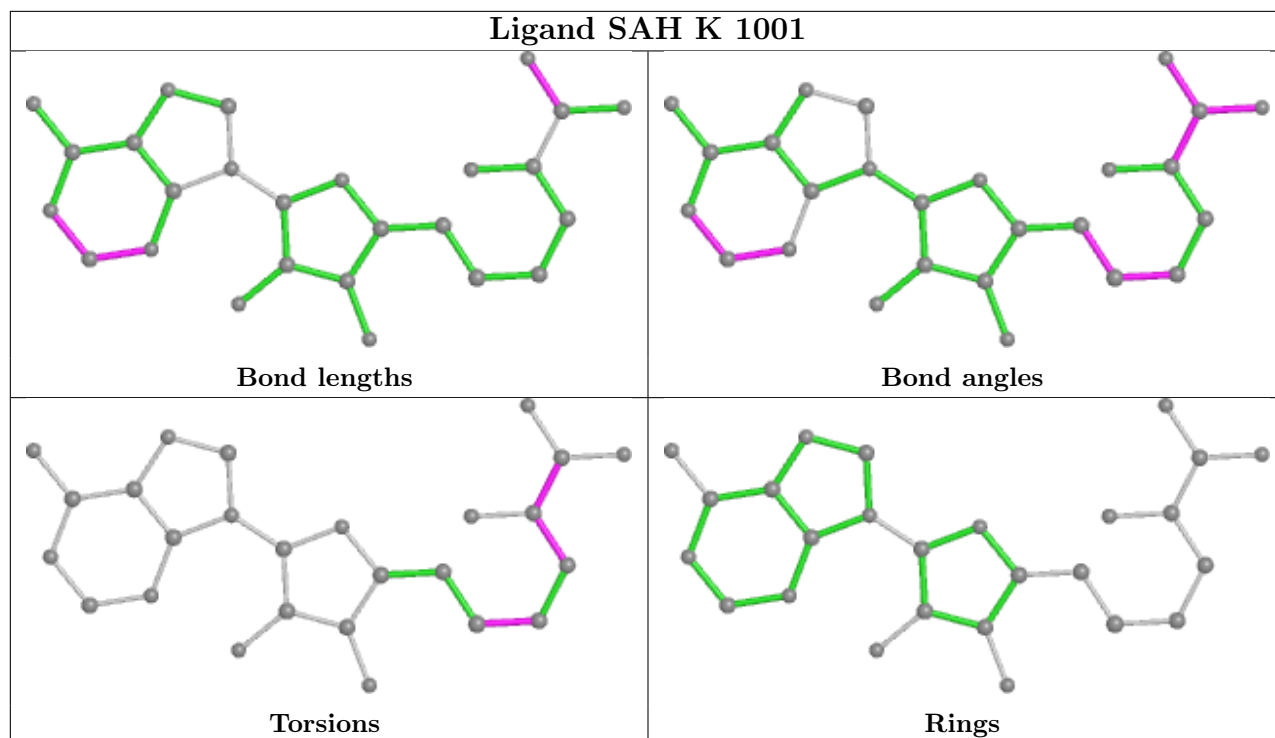
Mol	Chain	Res	Type	Atoms
4	K	1001	SAH	OXT-C-CA-CB
4	H	1001	SAH	CB-CG-SD-C5'
4	D	1001	SAH	OXT-C-CA-CB
4	H	1001	SAH	O-C-CA-CB
4	H	1001	SAH	OXT-C-CA-CB
4	K	1001	SAH	O-C-CA-CB
4	K	1001	SAH	CB-CG-SD-C5'
4	D	1001	SAH	O-C-CA-CB
4	A	1001	SAH	C-CA-CB-CG
4	H	1001	SAH	C-CA-CB-CG
4	A	1001	SAH	CB-CG-SD-C5'
4	A	1001	SAH	OXT-C-CA-CB
4	A	1001	SAH	O-C-CA-CB

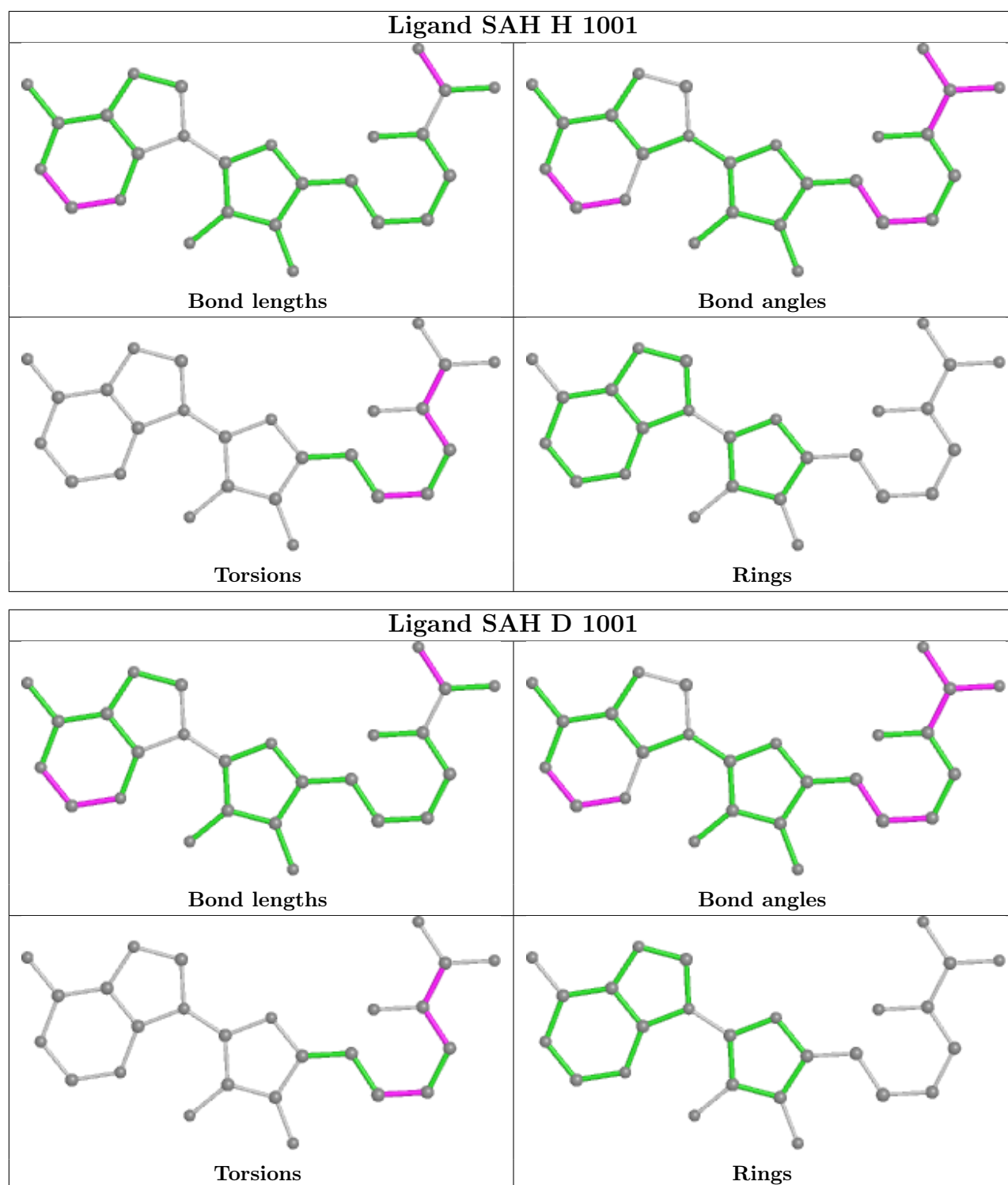
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	SAH	1	0
4	H	1001	SAH	2	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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	285/285 (100%)	-0.21	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	50, 69, 99, 152	0
1	D	285/285 (100%)	-0.24	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	47, 67, 99, 155	0
1	H	285/285 (100%)	-0.20	1 (0%) <span style="border: 1px solid blue; padding: 2px;">92</span> <span style="border: 1px solid blue; padding: 2px;">91</span>	49, 69, 98, 154	0
1	K	285/285 (100%)	-0.23	2 (0%) <span style="border: 1px solid blue; padding: 2px;">87</span> <span style="border: 1px solid blue; padding: 2px;">86</span>	49, 67, 95, 165	0
2	B	194/209 (92%)	0.45	19 (9%) <span style="border: 1px solid red; padding: 2px;">7</span> <span style="border: 1px solid red; padding: 2px;">7</span>	69, 118, 194, 217	0
2	C	182/209 (87%)	0.67	23 (12%) <span style="border: 1px solid red; padding: 2px;">3</span> <span style="border: 1px solid red; padding: 2px;">3</span>	78, 147, 203, 230	0
2	I	195/209 (93%)	0.38	15 (7%) <span style="border: 1px solid red; padding: 2px;">13</span> <span style="border: 1px solid red; padding: 2px;">12</span>	69, 118, 186, 211	0
2	J	180/209 (86%)	0.71	25 (13%) <span style="border: 1px solid red; padding: 2px;">2</span> <span style="border: 1px solid red; padding: 2px;">2</span>	79, 142, 201, 218	0
3	E	24/25 (96%)	-0.58	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	74, 121, 146, 184	0
3	F	24/25 (96%)	-0.57	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	87, 113, 148, 174	0
3	L	24/25 (96%)	-0.57	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	73, 120, 145, 201	0
3	M	24/25 (96%)	-0.59	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	84, 114, 148, 184	0
All	All	1987/2076 (95%)	0.05	85 (4%) <span style="border: 1px solid red; padding: 2px;">35</span> <span style="border: 1px solid red; padding: 2px;">33</span>	47, 84, 181, 230	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	338	VAL	11.6
2	B	338	VAL	10.8
2	C	337	LEU	10.7
2	B	336	ALA	10.3
2	C	336	ALA	8.8
2	B	337	LEU	7.9
1	K	628	ALA	7.2
2	J	217	GLN	7.0
2	J	332	SER	6.7
2	J	320	ALA	6.7
2	J	340	GLU	6.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	J	337	LEU	6.1
2	I	338	VAL	5.7
2	I	336	ALA	5.6
2	J	338	VAL	5.6
2	I	337	LEU	5.5
2	C	332	SER	5.5
2	J	309	ILE	5.4
2	I	339	SER	5.2
2	B	312	VAL	5.2
2	C	320	ALA	5.1
2	C	339	SER	4.9
2	J	310	PRO	4.9
2	B	311	ASP	4.7
2	C	319	ASN	4.6
2	C	318	GLN	4.5
2	J	336	ALA	4.4
2	J	319	ASN	4.2
2	B	339	SER	4.2
2	I	274	PRO	4.1
2	J	251	THR	4.1
2	J	318	GLN	4.1
2	J	190	VAL	4.1
2	B	320	ALA	4.0
2	J	275	GLY	3.7
2	J	339	SER	3.7
2	B	288	LEU	3.6
2	C	330	ILE	3.5
2	J	201	LYS	3.5
2	I	288	LEU	3.4
2	I	332	SER	3.3
2	C	222	VAL	3.3
2	B	340	GLU	3.3
2	J	343	LEU	3.2
2	B	274	PRO	3.1
2	J	359	TRP	3.1
2	J	321	VAL	3.1
2	C	289	VAL	2.9
2	I	319	ASN	2.9
2	I	309	ILE	2.9
2	I	340	GLU	2.9
2	J	192	VAL	2.8
2	J	222	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	319	ASN	2.7
2	C	311	ASP	2.7
2	C	280	PHE	2.7
2	B	185	TRP	2.5
2	C	308	THR	2.5
2	I	320	ALA	2.5
2	C	251	THR	2.4
2	C	203	LEU	2.4
2	C	377	TYR	2.4
2	B	209	LEU	2.4
2	J	360	PRO	2.4
2	B	335	TRP	2.4
2	B	332	SER	2.4
2	I	240	LEU	2.4
2	J	328	PRO	2.3
2	B	308	THR	2.3
2	C	221	VAL	2.2
1	H	628	ALA	2.2
1	K	912	VAL	2.2
2	B	371	LEU	2.2
2	C	195	LEU	2.2
2	J	253	ASP	2.1
2	C	312	VAL	2.1
2	C	185	TRP	2.1
2	I	203	LEU	2.1
2	C	329	ALA	2.1
2	C	263	PHE	2.1
2	I	346	LEU	2.1
2	J	218	LEU	2.1
2	B	309	ILE	2.0
2	I	281	PHE	2.0
2	B	360	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	PYO	E	427	19/20	0.98	0.15	62,71,79,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PYO	F	427	19/20	0.98	0.12	72,76,86,91	0
3	PYO	L	427	19/20	0.98	0.15	61,67,80,81	0
3	PYO	M	427	19/20	0.98	0.12	69,78,90,95	0

### 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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

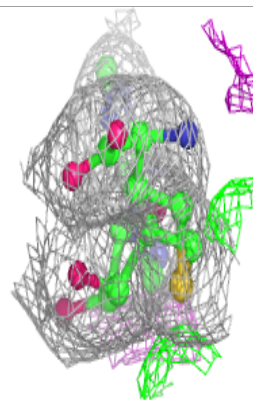
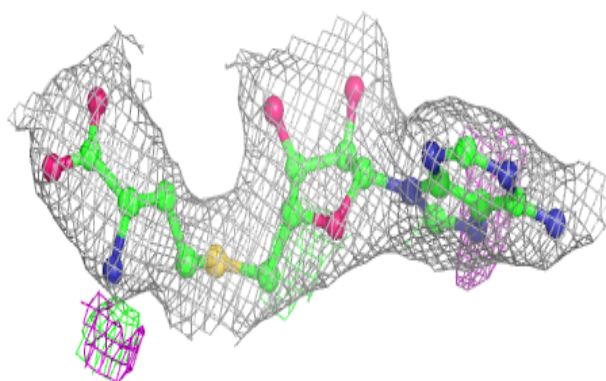
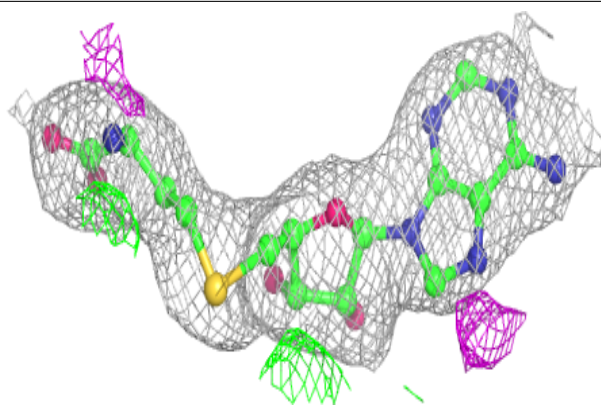
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SAH	A	1001	26/26	0.97	0.14	50,66,74,76	0
4	SAH	D	1001	26/26	0.97	0.15	53,68,98,119	0
4	SAH	H	1001	26/26	0.97	0.14	49,64,71,73	0
4	SAH	K	1001	26/26	0.97	0.16	48,64,74,78	0

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.

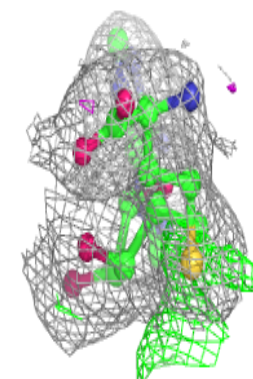
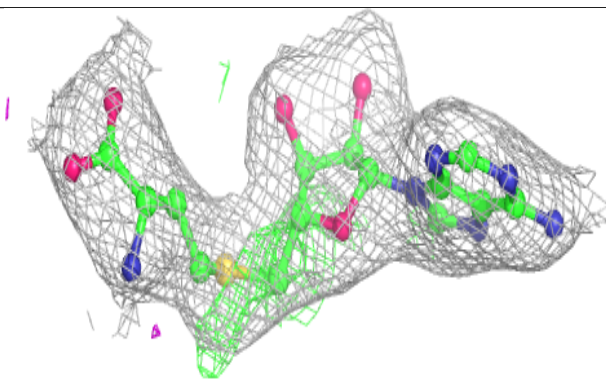
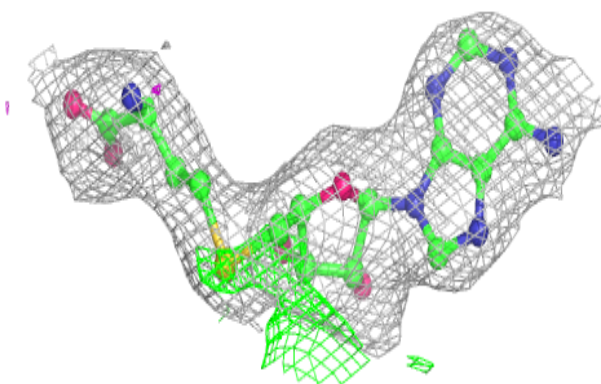


**Electron density around SAH A 1001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

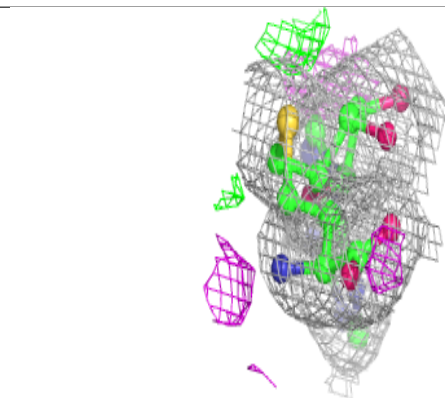
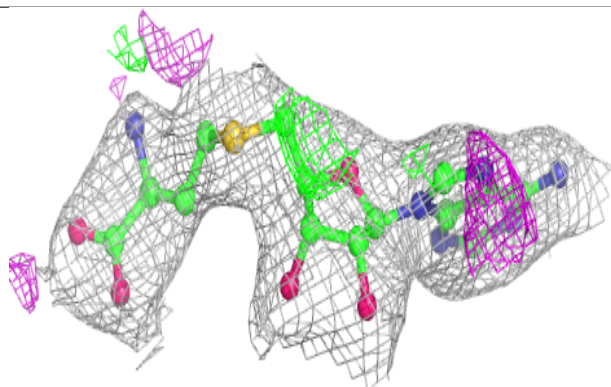
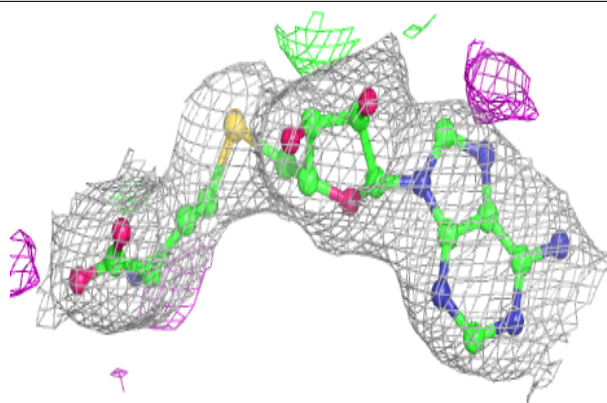
**Electron density around SAH D 1001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

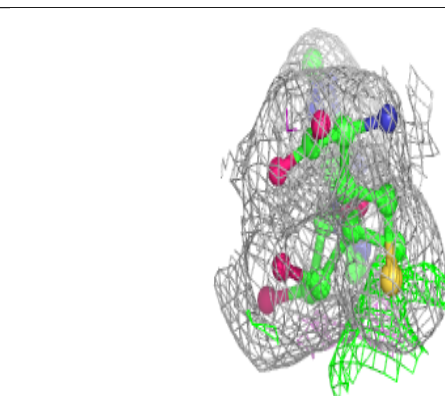
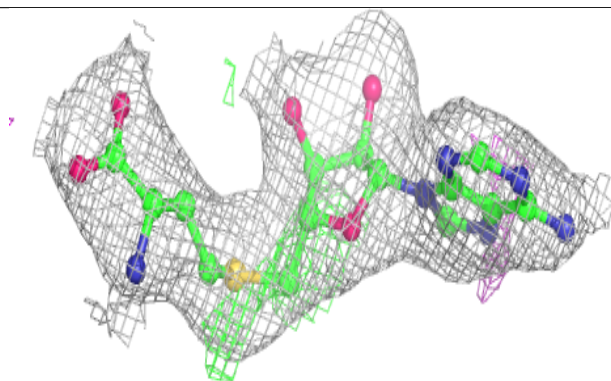
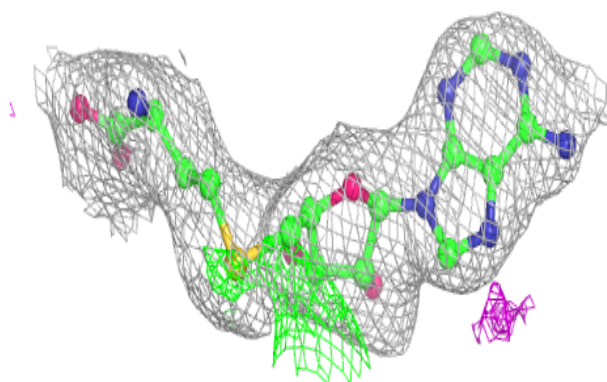


**Electron density around SAH H 1001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around SAH K 1001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.