



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:58 PM UTC

PDB ID : 8TDR / pdb_00008tdr
Title : Crystal structure of the methyltransferase domain of DNMT3A homotetramer
Authors : Lu, J.W.; Song, J.K.
Deposited on : 2023-07-04
Resolution : 3.32 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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

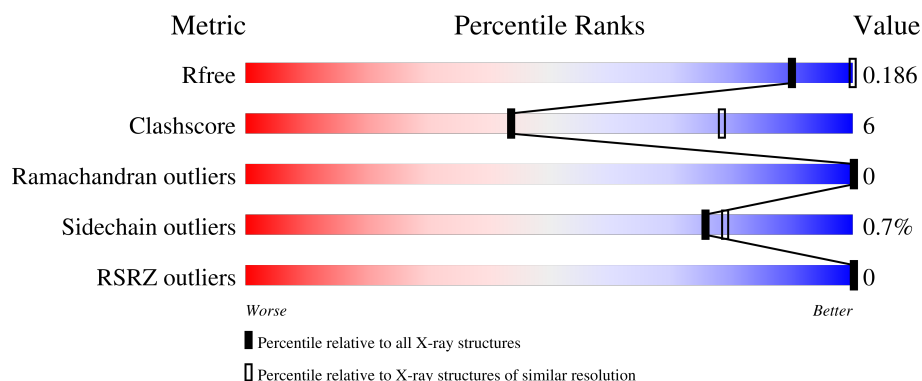
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.32 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}	180053	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	287	
1	B	287	
1	C	287	
1	D	287	
1	E	287	

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Mol	Chain	Length	Quality of chain
1	F	287	 51%10%38%
1	G	287	 54%8%38%
1	H	287	 54%11%34%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14431 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
1	A	273	Total	C	N	O	S	0	3	0
			2193	1403	390	387	13			
1	B	274	Total	C	N	O	S	0	2	0
			2195	1406	390	386	13			
1	C	274	Total	C	N	O	S	0	2	0
			2195	1406	391	385	13			
1	E	180	Total	C	N	O	S	0	0	0
			1349	873	231	238	7			
1	H	188	Total	C	N	O	S	0	0	0
			1426	921	248	250	7			
1	F	178	Total	C	N	O	S	0	0	0
			1373	891	233	242	7			
1	D	275	Total	C	N	O	S	0	2	0
			2208	1412	394	389	13			
1	G	178	Total	C	N	O	S	0	1	0
			1388	903	240	237	8			

There are 16 discrepancies between the modelled and reference sequences:

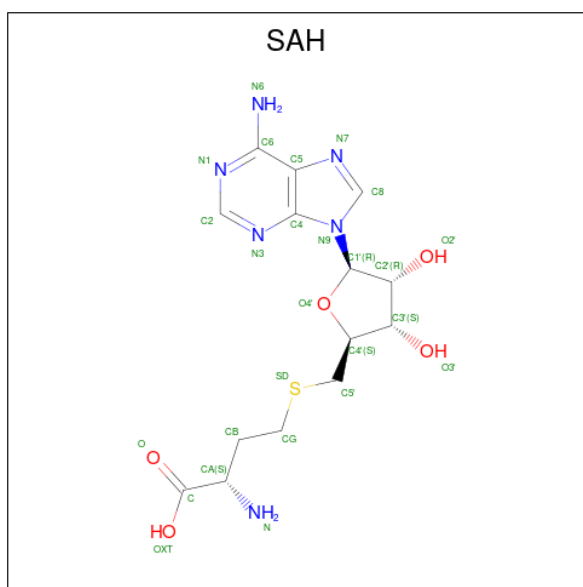
Chain	Residue	Modelled	Actual	Comment	Reference
A	626	GLY	-	expression tag	UNP Q9Y6K1
A	627	SER	-	expression tag	UNP Q9Y6K1
B	626	GLY	-	expression tag	UNP Q9Y6K1
B	627	SER	-	expression tag	UNP Q9Y6K1
C	626	GLY	-	expression tag	UNP Q9Y6K1
C	627	SER	-	expression tag	UNP Q9Y6K1
E	626	GLY	-	expression tag	UNP Q9Y6K1
E	627	SER	-	expression tag	UNP Q9Y6K1
H	626	GLY	-	expression tag	UNP Q9Y6K1
H	627	SER	-	expression tag	UNP Q9Y6K1
F	626	GLY	-	expression tag	UNP Q9Y6K1
F	627	SER	-	expression tag	UNP Q9Y6K1
D	626	GLY	-	expression tag	UNP Q9Y6K1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	627	SER	-	expression tag	UNP Q9Y6K1
G	626	GLY	-	expression tag	UNP Q9Y6K1
G	627	SER	-	expression tag	UNP Q9Y6K1

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).

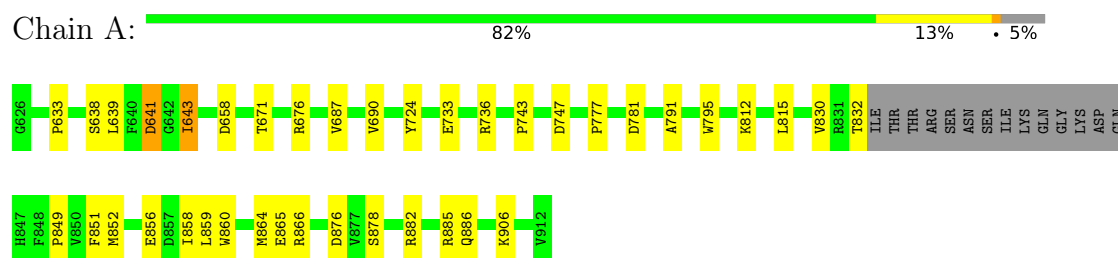


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

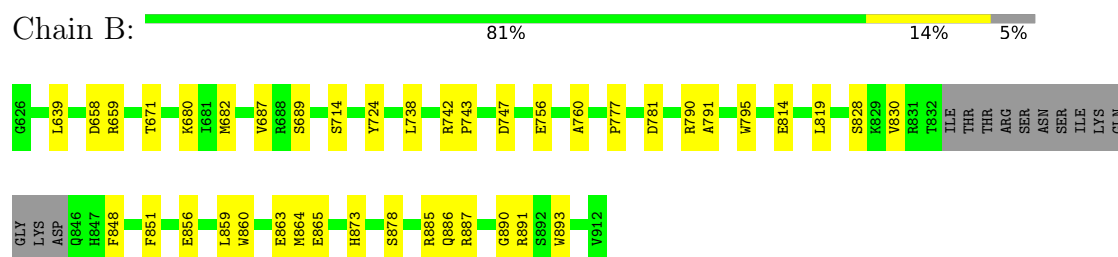
3 Residue-property plots [i](#)

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.

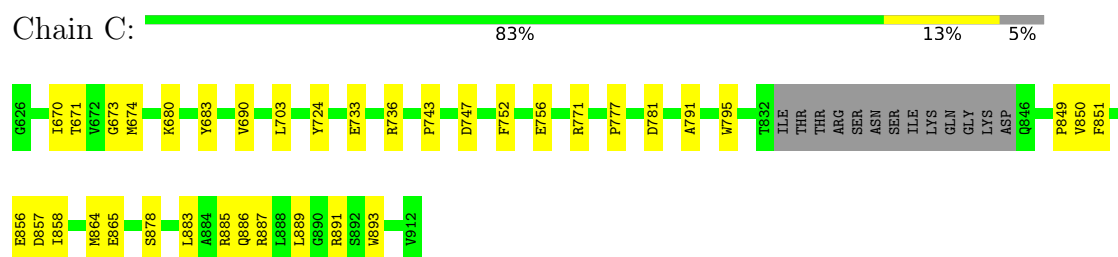
- Molecule 1: DNA (cytosine-5)-methyltransferase 3A



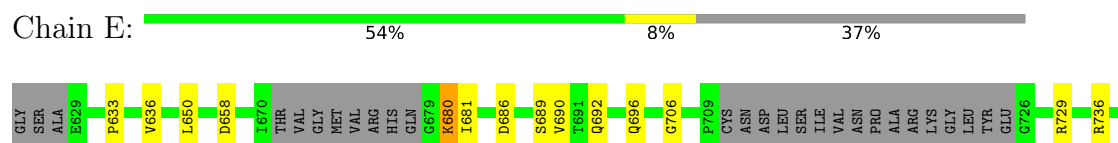
- Molecule 1: DNA (cytosine-5)-methyltransferase 3A

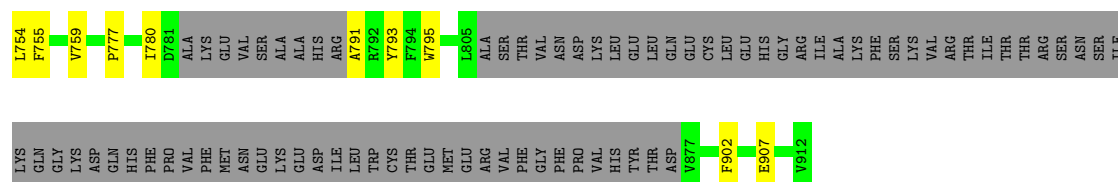


- Molecule 1: DNA (cytosine-5)-methyltransferase 3A

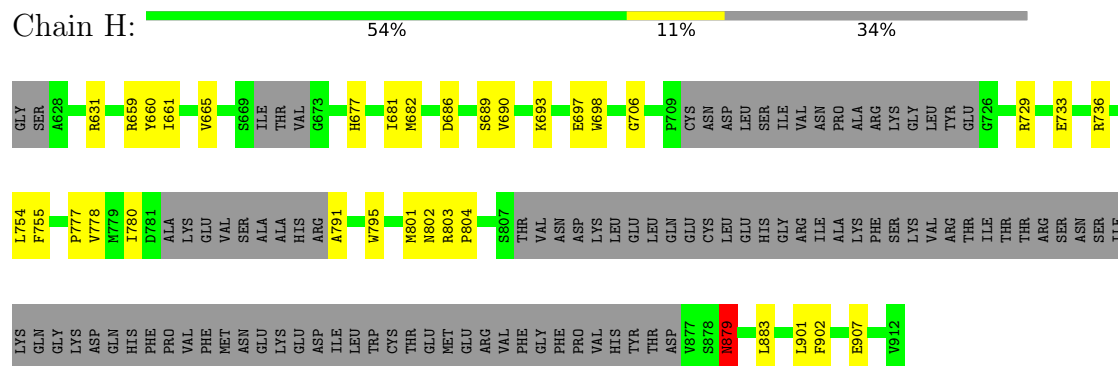


- Molecule 1: DNA (cytosine-5)-methyltransferase 3A

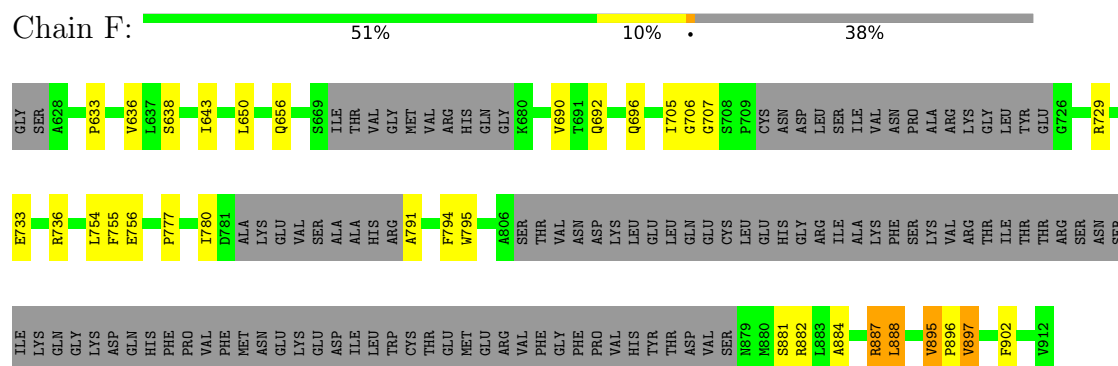




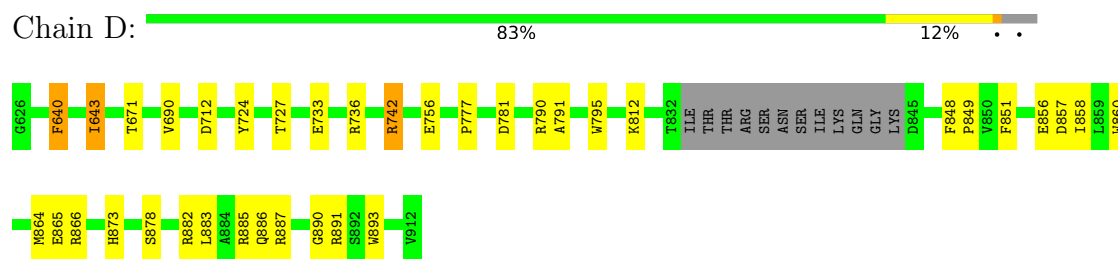
• Molecule 1: DNA (cytosine-5)-methyltransferase 3A



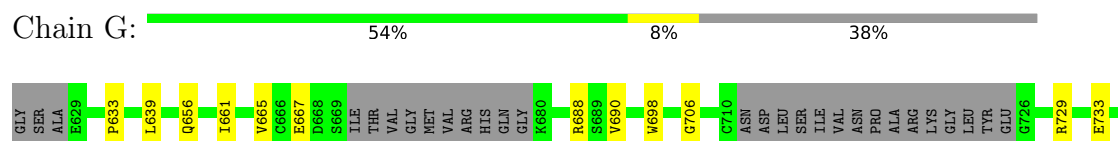
• Molecule 1: DNA (cytosine-5)-methyltransferase 3A



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



R736	L737	F755	V759	P777	I780	ASP	ALA	LYS	GLU	VAL	SER	ASN	ALA	ALA	HIS	ARG	A791	W795	G800	R803	P804	L805	ALA	SER	THR	THR	VAL	ASN	ASP	LYS	LEU	GLU	LEU	GLN	GLU	CYS	LEU	GLU	HIS	GLY	ARG	ILE	ALA	LYS	PHE	SER	LYS	VAL	ARG	THR	THR	THR	ARG
SER	ASN	SER	ILE	LYS	GLN	GLY	LYS	ASP	GLN	HIS	PHE	PRO	VAL	PHE	MET	ASN	GLU	LYS	GLU	ASP	ILE	LEU	TRP	CYS	THR	GLU	MET	GLU	ARG	VAL	PHE	GLY	PHE	PRO	VAL	HIS	TYR	THR	ASP	V877	A903	K906	V912										

4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	179.43Å 179.43Å 108.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.29 – 3.32 46.29 – 3.32	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.29-3.32) 99.4 (46.29-3.32)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.210 , 0.240 (Not available) , 0.186	Depositor DCC
R_{free} test set	2005 reflections (3.49%)	wwPDB-VP
Wilson B-factor (Å ²)	84.8	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.398 for -h,-k,l 0.399 for h,-h-k,-l 0.397 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14431	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.26	0/2258	0.34	1/3051 (0.0%)
1	B	0.15	0/2254	0.33	1/3044 (0.0%)
1	C	0.10	0/2254	0.28	0/3045
1	D	0.24	0/2267	0.32	1/3062 (0.0%)
1	E	0.15	0/1380	0.37	1/1871 (0.1%)
1	F	0.25	0/1404	0.57	3/1898 (0.2%)
1	G	0.12	0/1422	0.33	0/1920
1	H	0.19	0/1458	0.48	1/1972 (0.1%)
All	All	0.19	0/14697	0.37	8/19863 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	881	SER	N-CA-C	11.33	123.63	111.28
1	F	884	ALA	N-CA-C	8.98	123.79	111.39
1	E	680	LYS	N-CA-C	6.20	117.83	111.14
1	A	641	ASP	N-CA-C	5.36	117.12	111.28
1	B	848	PHE	N-CA-C	-5.30	100.98	109.04
1	F	882	ARG	N-CA-C	5.30	117.36	109.25
1	D	640	PHE	N-CA-C	-5.17	104.11	111.24
1	H	879	ASN	N-CA-C	5.09	121.45	113.72

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	2193	0	2155	26	0
1	B	2195	0	2157	25	0
1	C	2195	0	2158	26	0
1	D	2208	0	2173	26	0
1	E	1349	0	1235	16	0
1	F	1373	0	1310	27	0
1	G	1388	0	1350	16	0
1	H	1426	0	1350	24	0
2	A	26	0	19	0	0
2	B	26	0	19	0	0
2	C	26	0	19	0	0
2	D	26	0	19	1	0
All	All	14431	0	13964	172	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 6.

All (172) 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:F:895:VAL:HG22	1:F:896:PRO:CD	1.70	1.20
1:F:895:VAL:HG22	1:F:896:PRO:HD2	1.04	1.01
1:F:895:VAL:CG2	1:F:896:PRO:CD	2.54	0.84
1:F:895:VAL:CG2	1:F:896:PRO:HD2	2.00	0.81
1:A:849:PRO:HD2	1:A:858:ILE:HA	1.62	0.79
1:D:849:PRO:HD2	1:D:858:ILE:HA	1.67	0.76
1:H:780:ILE:O	1:H:791:ALA:HA	1.85	0.75
1:D:742[A]:ARG:HG2	1:D:742[A]:ARG:HH11	1.52	0.75
1:C:733:GLU:OE1	1:C:736:ARG:NH1	2.25	0.69
1:D:712:ASP:HB2	1:D:727:THR:HG22	1.73	0.69
1:D:733:GLU:OE1	1:D:736:ARG:NH1	2.25	0.69
1:C:690:VAL:O	1:C:736:ARG:NH2	2.26	0.69
1:H:660:TYR:HB3	1:H:681:ILE:HG13	1.73	0.68
1:A:733:GLU:OE1	1:A:736:ARG:NH1	2.27	0.67
1:G:780:ILE:O	1:G:791:ALA:HA	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:690:VAL:O	1:D:736:ARG:NH2	2.28	0.66
1:B:790:ARG:NH2	1:B:890:GLY:O	2.28	0.66
1:F:895:VAL:HG22	1:F:896:PRO:HD3	1.75	0.65
1:D:790:ARG:NH2	1:D:890:GLY:O	2.29	0.65
1:E:690:VAL:O	1:E:736:ARG:NH2	2.30	0.65
1:A:690:VAL:O	1:A:736:ARG:NH2	2.30	0.64
1:F:780:ILE:O	1:F:791:ALA:HA	1.99	0.63
1:C:849:PRO:HD2	1:C:858:ILE:HA	1.81	0.62
1:G:639:LEU:HD21	1:G:665:VAL:HG23	1.80	0.62
1:H:690:VAL:O	1:H:736:ARG:NH2	2.34	0.60
1:F:690:VAL:O	1:F:736:ARG:NH2	2.35	0.59
1:B:864:MET:HE1	1:B:886:GLN:HG2	1.85	0.59
1:C:771:ARG:NH2	1:H:733:GLU:OE1	2.36	0.59
1:A:639:LEU:HD22	1:A:687:VAL:HG23	1.85	0.58
1:G:690:VAL:O	1:G:736:ARG:NH2	2.36	0.58
1:B:743:PRO:HB2	1:B:747:ASP:HB3	1.85	0.58
1:F:895:VAL:CG2	1:F:896:PRO:HD3	2.33	0.58
1:A:633:PRO:HB2	1:A:658:ASP:HB2	1.84	0.58
1:H:778:VAL:HG22	1:H:803:ARG:HG3	1.85	0.57
1:B:814:GLU:OE1	1:B:828:SER:OG	2.24	0.56
1:G:661:ILE:HD13	1:G:698:TRP:HB3	1.88	0.56
1:C:671:THR:HG21	1:C:878:SER:HB2	1.88	0.55
1:H:693:LYS:O	1:H:697:GLU:HG3	2.06	0.55
1:G:667:GLU:HA	1:G:688:ARG:HH21	1.71	0.55
1:E:777:PRO:HB3	1:E:795:TRP:CE2	2.41	0.55
1:E:636:VAL:HG21	1:E:650:LEU:HD11	1.89	0.55
1:E:681:ILE:N	1:E:681:ILE:HD12	2.22	0.54
1:A:781:ASP:HA	1:A:791:ALA:HA	1.90	0.54
1:A:812:LYS:HE2	1:A:866[B]:ARG:HH11	1.73	0.54
1:G:777:PRO:HB3	1:G:795:TRP:CE2	2.43	0.54
1:B:658:ASP:O	1:H:631:ARG:NH2	2.40	0.54
1:D:781:ASP:HA	1:D:791:ALA:HA	1.91	0.53
1:C:781:ASP:HA	1:C:791:ALA:HA	1.90	0.53
1:H:706:GLY:O	1:H:755:PHE:HA	2.09	0.53
1:F:777:PRO:HB3	1:F:795:TRP:CE2	2.44	0.53
1:D:742[A]:ARG:HH11	1:D:742[A]:ARG:CG	2.20	0.52
1:C:864:MET:HE1	1:C:886:GLN:HG2	1.91	0.52
1:G:633:PRO:HB3	1:G:656:GLN:HB3	1.92	0.51
1:A:815:LEU:HD11	1:A:859:LEU:HD21	1.90	0.51
1:B:689:SER:HB2	1:H:804:PRO:HD2	1.93	0.51
1:G:639:LEU:HD12	1:G:737:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:640:PHE:HB3	2:D:1001:SAH:O4'	2.11	0.51
1:B:680:LYS:NZ	1:H:907:GLU:OE1	2.36	0.51
1:H:659:ARG:HH21	1:H:682:MET:HE1	1.76	0.51
1:C:743:PRO:HB2	1:C:747:ASP:HB3	1.92	0.50
1:D:812:LYS:HE2	1:D:866[B]:ARG:HH11	1.77	0.50
1:A:830:VAL:HG22	1:A:832:THR:H	1.77	0.50
1:B:671:THR:HG21	1:B:878:SER:HB2	1.93	0.50
1:E:686:ASP:O	1:E:689:SER:OG	2.30	0.50
1:G:688:ARG:CZ	1:G:729:ARG:HH21	2.25	0.50
1:F:887:ARG:O	1:F:887:ARG:HG2	2.11	0.49
1:E:754:LEU:HD13	1:E:902:PHE:CE1	2.47	0.49
1:B:756:GLU:OE1	1:B:893:TRP:NE1	2.39	0.49
1:F:636:VAL:HG21	1:F:650:LEU:HD11	1.94	0.49
1:A:743:PRO:HB2	1:A:747:ASP:HB3	1.96	0.48
1:H:777:PRO:HB3	1:H:795:TRP:CE2	2.49	0.48
1:E:759:VAL:HG23	1:E:793:TYR:CZ	2.48	0.48
1:E:633:PRO:HB2	1:E:658:ASP:HB2	1.95	0.48
1:F:633:PRO:HB3	1:F:656:GLN:HB3	1.95	0.48
1:D:756:GLU:OE1	1:D:893:TRP:NE1	2.38	0.48
1:G:706:GLY:O	1:G:755:PHE:HA	2.14	0.48
1:B:738:LEU:O	1:B:742[B]:ARG:HG2	2.14	0.47
1:F:706:GLY:O	1:F:755:PHE:HA	2.15	0.47
1:F:888:LEU:C	1:F:888:LEU:HD12	2.38	0.47
1:G:733:GLU:OE1	1:G:736:ARG:NH1	2.47	0.47
1:D:851:PHE:CE1	1:D:856:GLU:HG2	2.49	0.47
1:B:865:GLU:OE2	1:B:885:ARG:NH2	2.47	0.47
1:C:724:TYR:CD2	1:H:729:ARG:HA	2.48	0.47
1:B:878:SER:O	1:B:878:SER:OG	2.26	0.47
1:C:851:PHE:CE1	1:C:856:GLU:HG2	2.49	0.47
1:A:638:SER:OG	1:A:641:ASP:OD1	2.28	0.47
1:B:781:ASP:HA	1:B:791:ALA:HA	1.97	0.47
1:B:830:VAL:HG21	1:B:859:LEU:HD11	1.97	0.47
1:B:887:ARG:O	1:B:891:ARG:HG3	2.15	0.46
1:H:754:LEU:HD13	1:H:902:PHE:CE1	2.50	0.46
1:A:882:ARG:O	1:A:886:GLN:HG3	2.15	0.46
1:B:851:PHE:CE1	1:B:856:GLU:HG2	2.51	0.46
1:C:865:GLU:OE2	1:C:885:ARG:NH2	2.48	0.46
1:E:780:ILE:O	1:E:791:ALA:HA	2.16	0.46
1:A:643:ILE:HG13	1:A:643:ILE:O	2.16	0.46
1:A:724:TYR:CD1	1:F:729:ARG:HA	2.51	0.46
1:H:879:ASN:ND2	1:H:879:ASN:C	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:888:LEU:C	1:F:888:LEU:CD1	2.88	0.46
1:D:777:PRO:HB3	1:D:795:TRP:CE2	2.51	0.46
1:D:848:PHE:HB3	1:D:856:GLU:HB3	1.97	0.46
1:A:777:PRO:HB3	1:A:795:TRP:CE2	2.51	0.46
1:A:865:GLU:OE2	1:A:885:ARG:NH2	2.47	0.46
1:E:706:GLY:O	1:E:755:PHE:HA	2.16	0.46
1:D:671:THR:HG21	1:D:878:SER:HB2	1.98	0.45
1:D:864:MET:HE1	1:D:886:GLN:HG2	1.98	0.45
1:B:724:TYR:CD2	1:E:729:ARG:HA	2.51	0.45
1:C:851:PHE:HE1	1:C:856:GLU:HG2	1.81	0.45
1:C:864:MET:HB3	1:C:889:LEU:HD13	1.98	0.45
1:D:643:ILE:O	1:D:643:ILE:HG13	2.16	0.45
1:D:865:GLU:OE2	1:D:885:ARG:NH2	2.48	0.45
1:D:883:LEU:HD23	1:D:883:LEU:HA	1.86	0.45
1:B:777:PRO:HB3	1:B:795:TRP:CE2	2.52	0.45
1:A:671:THR:HG21	1:A:878:SER:HB2	1.98	0.45
1:A:864:MET:HE1	1:A:886:GLN:HA	1.99	0.45
1:F:692:GLN:NE2	1:F:696:GLN:OE1	2.42	0.45
1:C:777:PRO:HB3	1:C:795:TRP:CE2	2.52	0.44
1:H:665:VAL:HB	1:H:729:ARG:NH1	2.31	0.44
1:B:819:LEU:HA	1:B:863:GLU:HG2	1.98	0.44
1:D:882:ARG:O	1:D:886:GLN:HG3	2.18	0.44
1:E:680:LYS:HB2	1:E:681:ILE:HD12	1.98	0.44
1:F:895:VAL:HG13	1:F:897:VAL:H	1.82	0.44
1:D:878:SER:O	1:D:878:SER:OG	2.31	0.44
1:A:676:ARG:HD3	1:A:676:ARG:HA	1.80	0.44
1:G:903:ALA:O	1:G:906:LYS:HG2	2.18	0.44
1:F:754:LEU:HD13	1:F:902:PHE:CE1	2.53	0.44
1:F:895:VAL:HG13	1:F:897:VAL:N	2.33	0.44
1:A:852:MET:HE3	1:A:852:MET:HB2	1.77	0.43
1:C:878:SER:O	1:C:878:SER:OG	2.29	0.43
1:H:661:ILE:CD1	1:H:698:TRP:HB3	2.48	0.43
1:H:677:HIS:ND1	1:H:677:HIS:C	2.77	0.43
1:C:680:LYS:NZ	1:E:907:GLU:OE1	2.50	0.43
1:F:888:LEU:O	1:F:888:LEU:HD13	2.19	0.43
1:C:887:ARG:O	1:C:891:ARG:HG3	2.17	0.43
1:B:639:LEU:HD22	1:B:687:VAL:HG23	2.00	0.43
1:C:670:ILE:O	1:C:674:MET:HG3	2.19	0.43
1:A:851:PHE:CE1	1:A:856:GLU:HG2	2.54	0.42
1:C:703:LEU:HA	1:C:752:PHE:O	2.18	0.42
1:A:878:SER:HA	1:B:860:TRP:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:707:GLY:HA3	1:F:756:GLU:O	2.19	0.42
1:G:800:GLY:O	1:G:803:ARG:NH1	2.50	0.42
1:A:876:ASP:OD2	1:B:873:HIS:ND1	2.36	0.42
1:B:714:SER:HA	1:B:760:ALA:O	2.20	0.42
1:E:692:GLN:NE2	1:E:696:GLN:OE1	2.37	0.42
1:E:729:ARG:HH11	1:E:729:ARG:HG3	1.85	0.42
1:F:756:GLU:HB2	1:F:794:PHE:CE2	2.54	0.42
1:C:756:GLU:OE1	1:C:893:TRP:NE1	2.42	0.42
1:H:686:ASP:O	1:H:689:SER:OG	2.37	0.42
1:A:851:PHE:HE1	1:A:856:GLU:HG2	1.84	0.42
1:H:801:MET:HE3	1:H:901:LEU:HD13	2.02	0.42
1:D:887:ARG:O	1:D:891:ARG:HG3	2.20	0.42
1:C:771:ARG:HH22	1:H:733:GLU:CD	2.28	0.41
1:C:878:SER:HA	1:D:860:TRP:CE2	2.55	0.41
1:D:857:ASP:OD1	1:D:858:ILE:N	2.53	0.41
1:A:860:TRP:CE2	1:B:878:SER:HA	2.56	0.41
1:C:883:LEU:HD23	1:C:883:LEU:HA	1.87	0.41
1:H:803:ARG:N	1:H:804:PRO:HD3	2.36	0.41
1:A:906:LYS:HE2	1:A:906:LYS:HB2	1.83	0.41
1:B:659:ARG:HB2	1:B:682:MET:HE2	2.01	0.41
1:G:661:ILE:CD1	1:G:698:TRP:HB3	2.50	0.41
1:F:638:SER:HA	1:F:705:ILE:HG13	2.03	0.41
1:C:670:ILE:HG22	1:C:674:MET:HE3	2.02	0.41
1:C:673:GLY:HA3	1:C:683:TYR:OH	2.21	0.41
1:D:865:GLU:OE1	1:D:873:HIS:N	2.52	0.41
1:H:802:ASN:C	1:H:804:PRO:HD3	2.46	0.41
1:E:681:ILE:N	1:E:681:ILE:CD1	2.82	0.40
1:F:643:ILE:H	1:F:643:ILE:HD12	1.86	0.40
1:F:888:LEU:CD1	1:F:888:LEU:O	2.70	0.40
1:D:724:TYR:CD1	1:G:729:ARG:HA	2.57	0.40
1:H:659:ARG:HH21	1:H:682:MET:CE	2.34	0.40
1:G:759:VAL:HG11	1:G:791:ALA:HB3	2.03	0.40
1:C:850:VAL:HG22	1:C:857:ASP:O	2.21	0.40
1:F:729:ARG:NH1	1:F:733:GLU:OE2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	92/287 (32%)	89 (97%)	3 (3%)	0	100	100
1	B	135/287 (47%)	129 (96%)	6 (4%)	0	100	100
1	C	8/287 (3%)	8 (100%)	0	0	100	100
1	D	273/287 (95%)	265 (97%)	8 (3%)	0	100	100
1	E	48/287 (17%)	47 (98%)	1 (2%)	0	100	100
1	F	119/287 (42%)	116 (98%)	3 (2%)	0	100	100
1	G	168/287 (58%)	165 (98%)	3 (2%)	0	100	100
All	All	843/2009 (42%)	819 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	232/251 (92%)	231 (100%)	1 (0%)	84	83
1	B	229/251 (91%)	229 (100%)	0	100	100
1	C	124/251 (49%)	124 (100%)	0	100	100
1	D	233/251 (93%)	230 (99%)	3 (1%)	61	73
1	E	126/251 (50%)	126 (100%)	0	100	100
1	F	136/251 (54%)	132 (97%)	4 (3%)	37	62
1	G	140/251 (56%)	140 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	139/251 (55%)	137 (99%)	2 (1%)	59	72
All	All	1359/2008 (68%)	1349 (99%)	10 (1%)	76	79

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	643	ILE
1	H	879	ASN
1	H	883	LEU
1	F	887	ARG
1	F	888	LEU
1	F	895	VAL
1	F	897	VAL
1	D	643	ILE
1	D	742[A]	ARG
1	D	742[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	739	HIS
1	B	879	ASN
1	B	886	GLN
1	C	879	ASN
1	H	692	GLN
1	D	696	GLN
1	G	656	GLN
1	G	776	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 [i](#)

There are no oligosaccharides 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$
2	SAH	B	1001	-	27,28,28	1.10	4 (14%)	36,40,40	2.02	9 (25%)
2	SAH	C	1001	-	27,28,28	1.11	4 (14%)	36,40,40	2.03	9 (25%)
2	SAH	D	1001	-	27,28,28	1.10	4 (14%)	36,40,40	2.03	9 (25%)
2	SAH	A	1001	-	27,28,28	1.10	4 (14%)	36,40,40	2.02	9 (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	SAH	B	1001	-	-	4/15/31/31	0/3/3/3
2	SAH	C	1001	-	-	3/15/31/31	0/3/3/3
2	SAH	D	1001	-	-	3/15/31/31	0/3/3/3
2	SAH	A	1001	-	-	4/15/31/31	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1001	SAH	C2-N3	2.65	1.38	1.33
2	C	1001	SAH	C2-N3	2.60	1.38	1.33
2	A	1001	SAH	C2-N1	2.60	1.38	1.33
2	B	1001	SAH	C2-N3	2.59	1.38	1.33
2	A	1001	SAH	C2-N3	2.59	1.38	1.33
2	C	1001	SAH	C2-N1	2.56	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	SAH	C2-N1	2.53	1.38	1.33
2	D	1001	SAH	C2-N1	2.51	1.38	1.33
2	A	1001	SAH	OXT-C	-2.20	1.23	1.30
2	C	1001	SAH	OXT-C	-2.19	1.23	1.30
2	B	1001	SAH	OXT-C	-2.17	1.23	1.30
2	D	1001	SAH	OXT-C	-2.17	1.23	1.30
2	C	1001	SAH	C8-N7	2.16	1.35	1.31
2	B	1001	SAH	C8-N7	2.13	1.35	1.31
2	D	1001	SAH	C8-N7	2.11	1.35	1.31
2	A	1001	SAH	C8-N7	2.11	1.35	1.31

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	SAH	N3-C2-N1	-5.51	120.24	128.58
2	D	1001	SAH	N3-C2-N1	-5.50	120.25	128.58
2	C	1001	SAH	N3-C2-N1	-5.50	120.26	128.58
2	A	1001	SAH	N3-C2-N1	-5.43	120.36	128.58
2	C	1001	SAH	C5-C4-N3	-4.77	120.15	126.72
2	A	1001	SAH	C5-C4-N3	-4.77	120.15	126.72
2	D	1001	SAH	C5-C4-N3	-4.76	120.17	126.72
2	B	1001	SAH	C5-C4-N3	-4.68	120.27	126.72
2	C	1001	SAH	N9-C8-N7	-3.84	108.48	113.94
2	D	1001	SAH	N9-C8-N7	-3.82	108.51	113.94
2	A	1001	SAH	N9-C8-N7	-3.80	108.55	113.94
2	B	1001	SAH	N9-C8-N7	-3.79	108.56	113.94
2	C	1001	SAH	C2-N3-C4	3.49	120.36	111.83
2	D	1001	SAH	C2-N3-C4	3.49	120.35	111.83
2	A	1001	SAH	C2-N3-C4	3.48	120.33	111.83
2	B	1001	SAH	C2-N3-C4	3.47	120.30	111.83
2	C	1001	SAH	C5-N7-C8	3.47	108.90	103.45
2	D	1001	SAH	C5-N7-C8	3.44	108.86	103.45
2	A	1001	SAH	C5-N7-C8	3.44	108.85	103.45
2	B	1001	SAH	C5-N7-C8	3.40	108.79	103.45
2	B	1001	SAH	C5'-SD-CG	-3.33	92.38	102.26
2	C	1001	SAH	C5'-SD-CG	-3.24	92.65	102.26
2	A	1001	SAH	C5'-SD-CG	-3.24	92.66	102.26
2	D	1001	SAH	C5'-SD-CG	-3.23	92.67	102.26
2	D	1001	SAH	N3-C4-N9	3.17	132.55	127.17
2	A	1001	SAH	N3-C4-N9	3.16	132.54	127.17
2	C	1001	SAH	N3-C4-N9	3.14	132.50	127.17
2	B	1001	SAH	N3-C4-N9	3.12	132.47	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1001	SAH	OXT-C-O	-2.77	117.81	124.08
2	B	1001	SAH	OXT-C-O	-2.74	117.87	124.08
2	A	1001	SAH	OXT-C-O	-2.67	118.03	124.08
2	D	1001	SAH	OXT-C-O	-2.66	118.04	124.08
2	C	1001	SAH	C4-C5-N7	-2.47	107.76	110.58
2	A	1001	SAH	C4-C5-N7	-2.42	107.81	110.58
2	D	1001	SAH	C4-C5-N7	-2.39	107.84	110.58
2	B	1001	SAH	C4-C5-N7	-2.34	107.91	110.58

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	SAH	N-CA-CB-CG
2	A	1001	SAH	C-CA-CB-CG
2	B	1001	SAH	N-CA-CB-CG
2	B	1001	SAH	C-CA-CB-CG
2	C	1001	SAH	N-CA-CB-CG
2	C	1001	SAH	C-CA-CB-CG
2	D	1001	SAH	N-CA-CB-CG
2	D	1001	SAH	C-CA-CB-CG
2	A	1001	SAH	C2'-C1'-N9-C8
2	B	1001	SAH	C2'-C1'-N9-C8
2	D	1001	SAH	C2'-C1'-N9-C8
2	C	1001	SAH	C2'-C1'-N9-C8
2	A	1001	SAH	O4'-C1'-N9-C8
2	B	1001	SAH	O4'-C1'-N9-C8

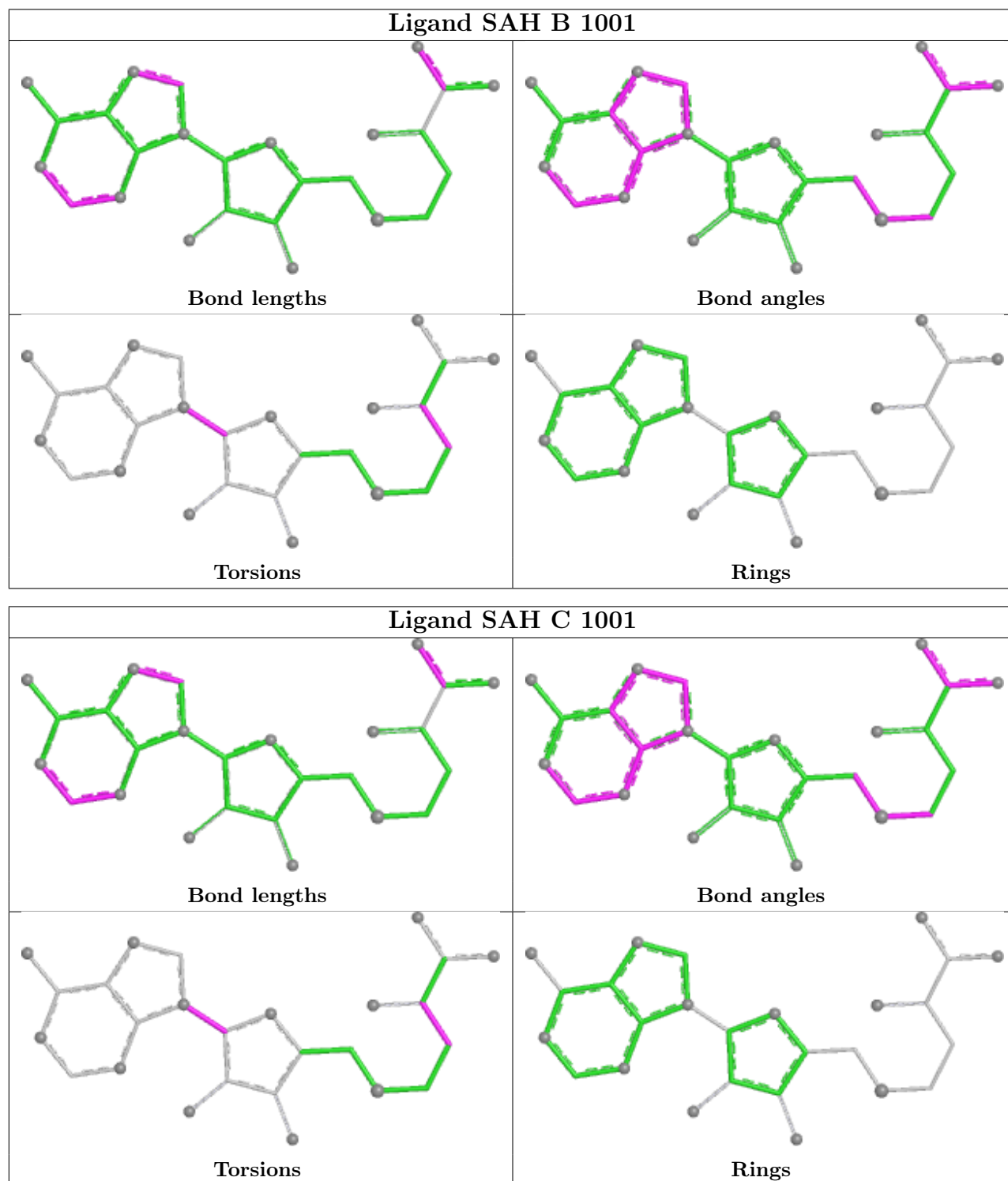
There are no ring outliers.

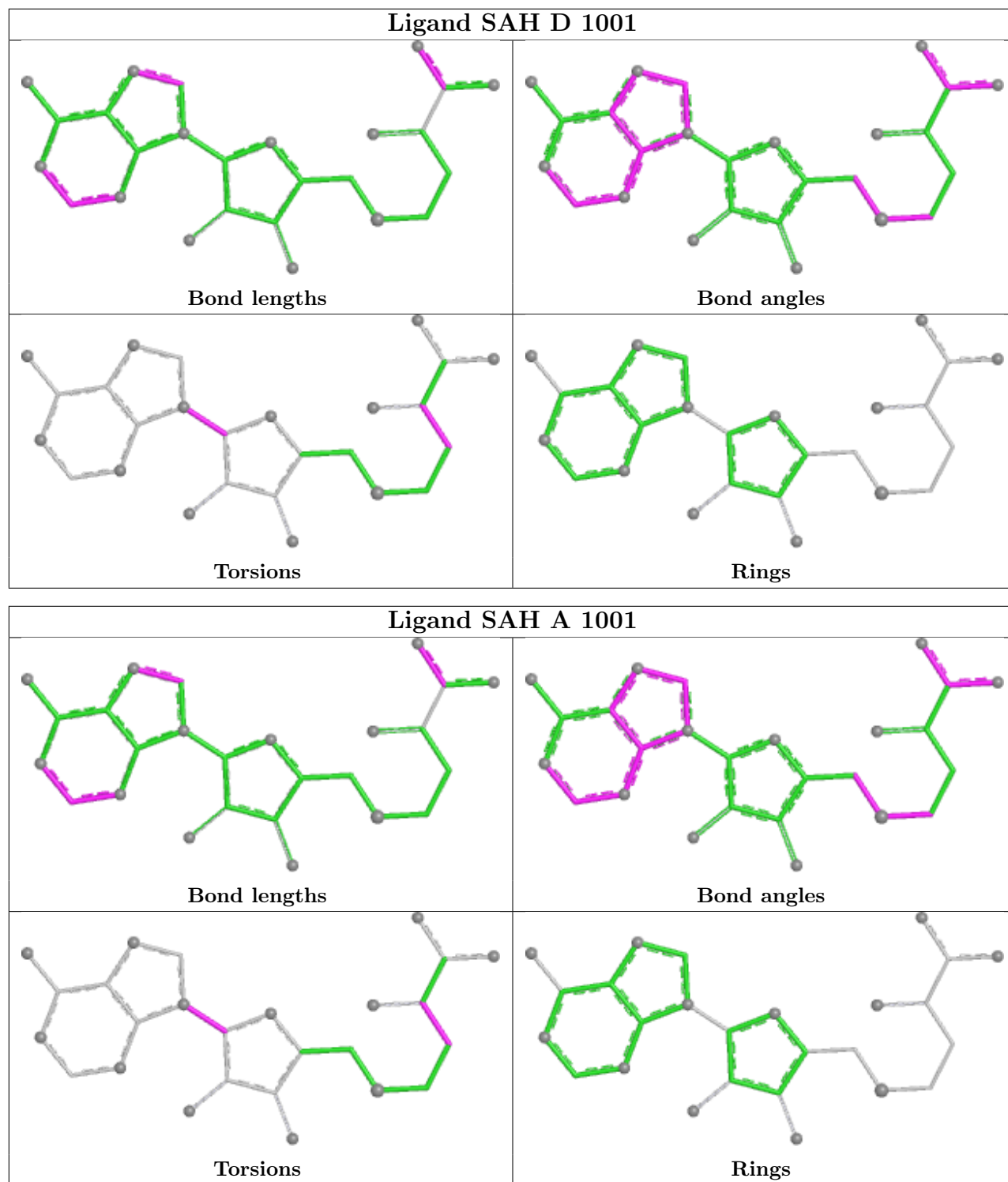
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1001	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 ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	273/287 (95%)	-1.30	0 100 100	33, 71, 107, 140	3 (1%)
1	B	274/287 (95%)	-1.31	0 100 100	36, 71, 112, 160	2 (0%)
1	C	274/287 (95%)	-1.31	0 100 100	35, 71, 110, 162	2 (0%)
1	D	275/287 (95%)	-1.30	0 100 100	36, 72, 112, 161	2 (0%)
1	E	180/287 (62%)	-1.10	0 100 100	54, 86, 145, 170	0
1	F	178/287 (62%)	-1.15	0 100 100	54, 89, 142, 177	0
1	G	178/287 (62%)	-1.13	0 100 100	58, 87, 142, 154	1 (0%)
1	H	188/287 (65%)	-1.11	0 100 100	50, 89, 146, 164	0
All	All	1820/2296 (79%)	-1.23	0 100 100	33, 76, 130, 177	10 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

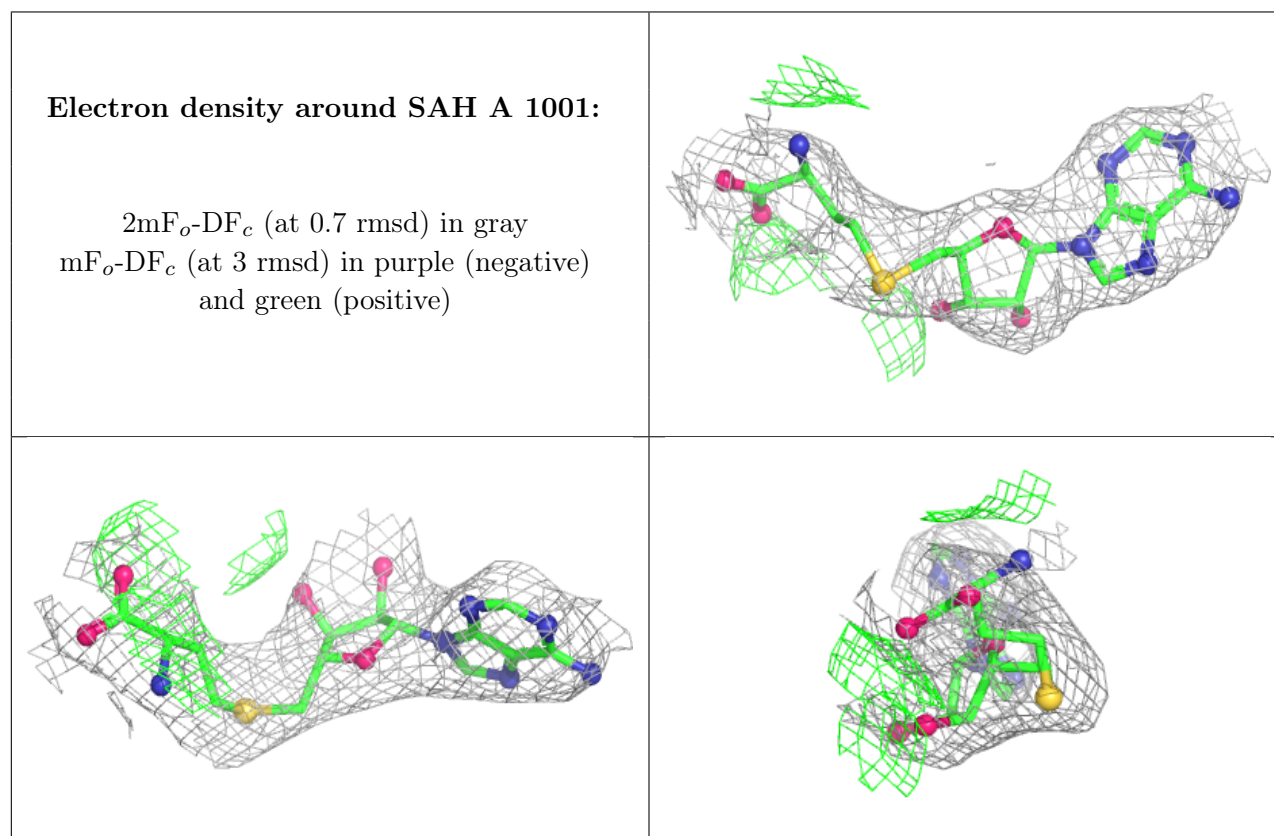
There are no oligosaccharides in this entry.

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, 95th 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.

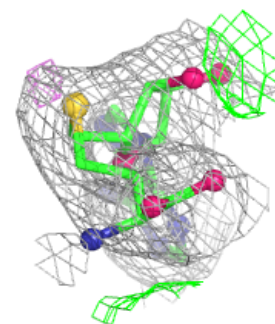
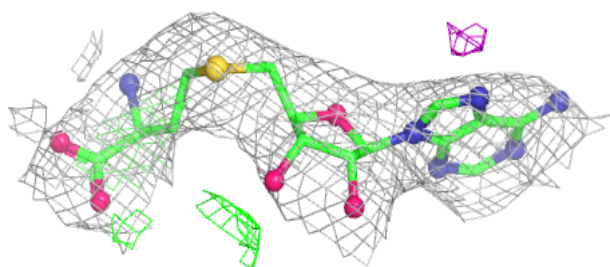
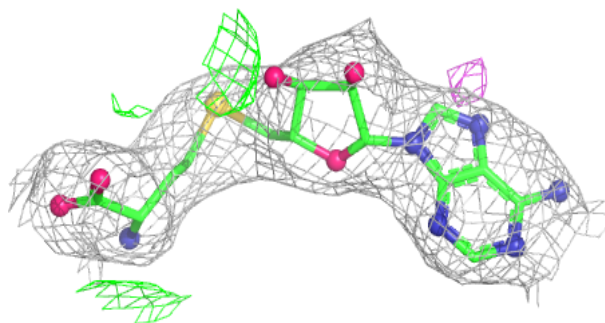
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SAH	A	1001	26/26	0.98	0.05	57,74,88,93	0
2	SAH	B	1001	26/26	0.99	0.05	61,74,88,96	0
2	SAH	C	1001	26/26	0.99	0.05	65,73,87,89	0
2	SAH	D	1001	26/26	0.99	0.05	61,73,86,88	0

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.

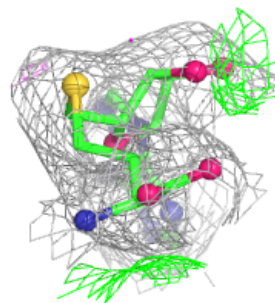
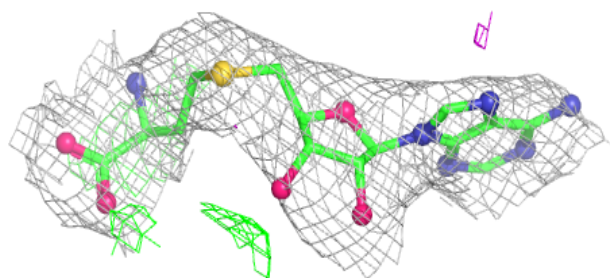
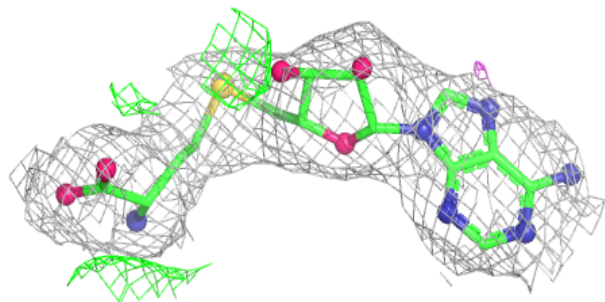


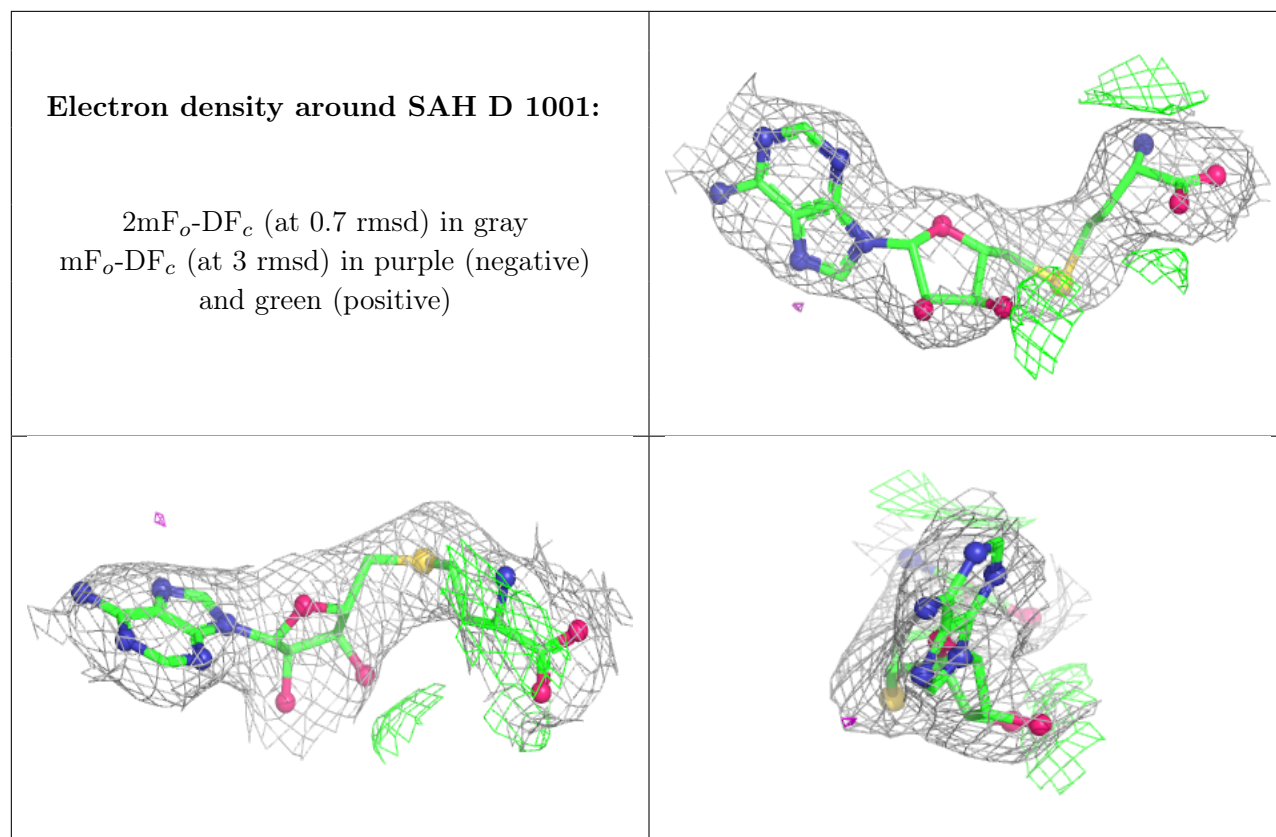
Electron density around SAH B 1001:

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

**Electron density around SAH C 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.