Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 07:28 PM EDT

PDB ID	:	6W8D
Title	:	Structure of DNMT3A (R882H) in complex with CGT DNA
Authors	:	Anteneh, H.; Song, J.
Deposited on	:	2020-03-20
Resolution	:	2.60 Å(reported)

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

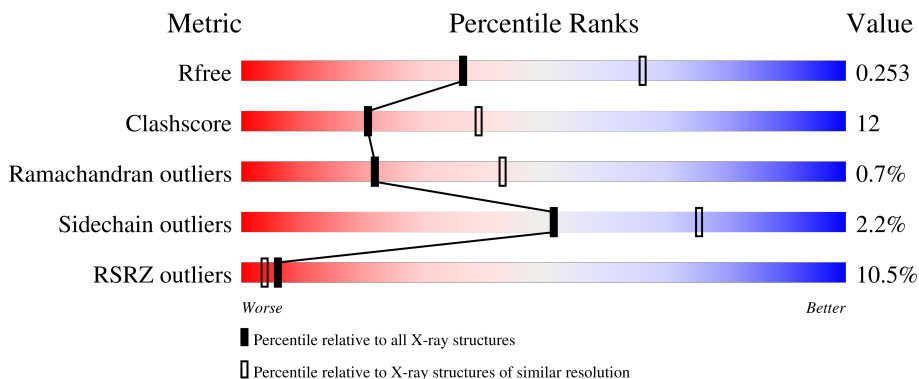|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.60 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.
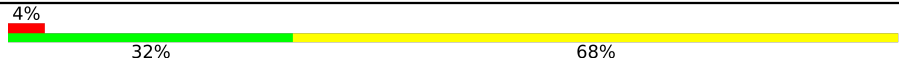
Metric	Percentile Ranks	Value
Rfree		0.253
Clashscore		12
Ramachandran outliers		0.7%
Sidechain outliers		2.2%
RSRZ outliers		10.5%

Worse ← → *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	285	9% / 77% / 22% / •
1	D	285	3% / 76% / 23% / •
2	B	209	16% / 65% / 23% / • / 11%
2	C	209	15% / 59% / 25% / 15%
3	E	25	12% / 48% / 48% / •

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Mol	Chain	Length	Quality of chain
3	F	25	

4%
32%
68%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 8368 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	284	Total	C	N	O	S	0	0	0
			2256	1440	403	400	13			
1	D	285	Total	C	N	O	S	0	0	0
			2268	1449	401	405	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	882	HIS	ARG	engineered mutation	UNP Q9Y6K1
D	882	HIS	ARG	engineered mutation	UNP Q9Y6K1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	187	Total	C	N	O	S	0	0	0
			1415	925	239	248	3			
2	C	177	Total	C	N	O	S	0	0	0
			1261	819	215	225	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	25	Total	C	N	O	P	0	0	0
			510	245	93	148	24			
3	F	25	Total	C	N	O	P	0	0	0
			510	245	93	148	24			

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

SAH

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

• Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	39	Total	O	0	0
			39	39		
5	B	6	Total	O	0	0
			6	6		
5	D	39	Total	O	0	0
			39	39		
5	C	5	Total	O	0	0
			5	5		
5	E	5	Total	O	0	0
			5	5		
5	F	2	Total	O	0	0
			2	2		

3 Residue-property plots ⓘ

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.
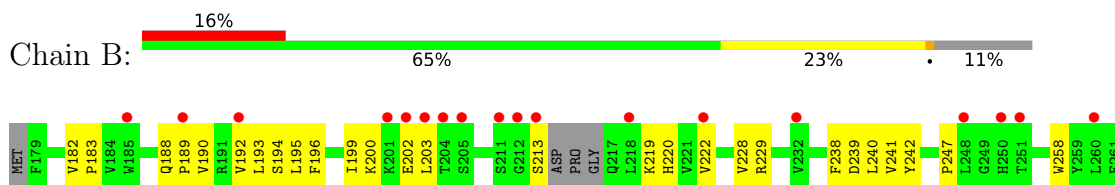
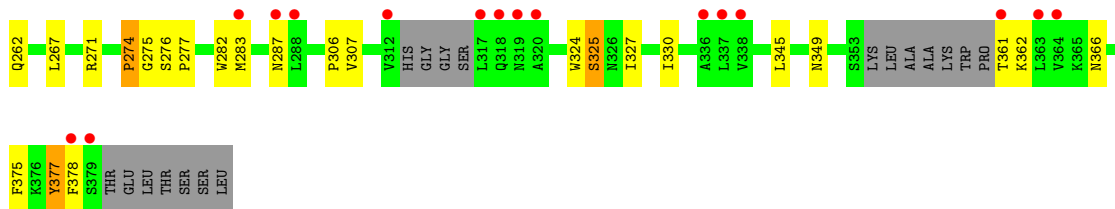- Molecule 1: DNA (cytosine-5)-methyltransferase 3A
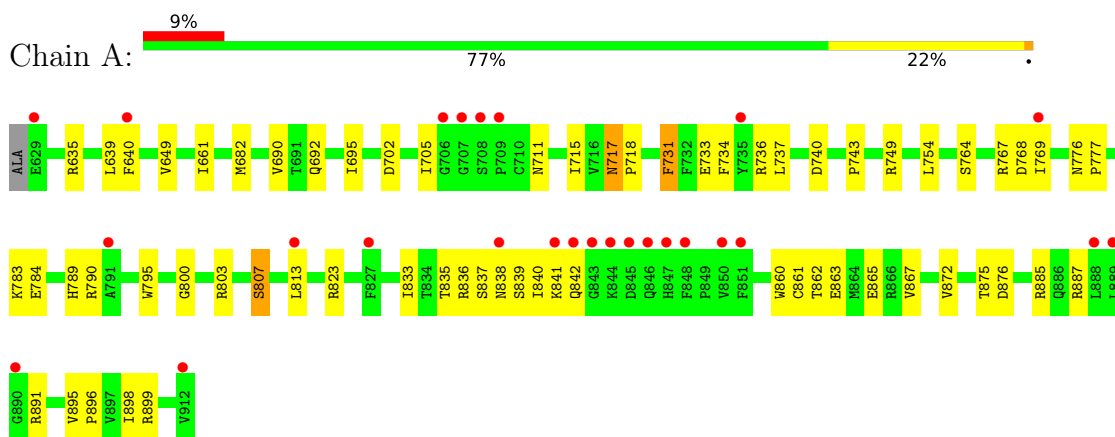
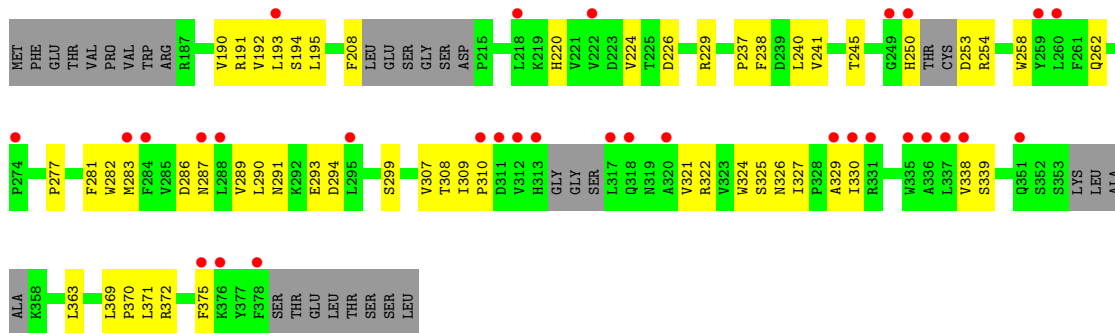- Molecule 1: DNA (cytosine-5)-methyltransferase 3A
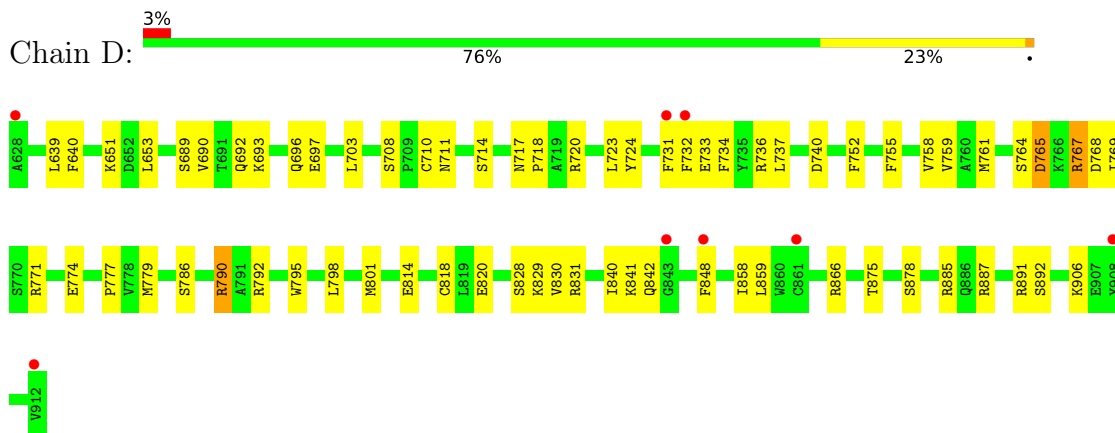
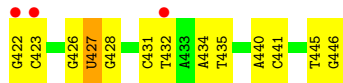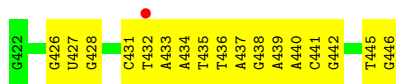- Molecule 2: DNA (cytosine-5)-methyltransferase 3-like

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

• Molecule 3: CGT DNA (25-MER)

• Molecule 3: CGT DNA (25-MER)

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	205.56Å 205.56Å 89.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.16 – 2.60 33.16 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (33.16-2.60) 99.9 (33.16-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.199 , 0.253 0.199 , 0.253	Depositor DCC
R_{free} test set	1989 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å^2)	81.3	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 76.2	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8368	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.26	0/2310	0.43	0/3124
1	D	0.27	0/2323	0.44	0/3142
2	B	0.28	0/1458	0.47	0/1997
2	C	0.32	0/1298	0.49	0/1780
3	E	0.55	0/550	0.95	0/846
3	F	0.60	0/550	0.97	0/846
All	All	0.33	0/8489	0.56	0/11735

There are no bond length outliers.

There are no bond angle outliers.

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	2256	0	2204	44	0
1	D	2268	0	2211	51	0
2	B	1415	0	1264	38	0
2	C	1261	0	1061	39	0
3	E	510	0	279	10	0
3	F	510	0	279	17	0
4	A	26	0	19	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	26	0	19	1	0
5	A	39	0	0	0	0
5	B	6	0	0	0	0
5	C	5	0	0	0	0
5	D	39	0	0	3	0
5	E	5	0	0	0	0
5	F	2	0	0	0	0
All	All	8368	0	7336	188	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 12.

All (188) 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:840:ILE:HD12	1:A:841:LYS:HG2	1.50	0.94
2:B:267:LEU:CD2	2:B:271:ARG:HH21	1.86	0.88
2:C:309:ILE:HD13	2:C:363:LEU:HD22	1.66	0.78
2:B:267:LEU:HD21	2:B:271:ARG:NH2	1.99	0.78
1:A:840:ILE:CD1	1:A:841:LYS:HG2	2.14	0.77
2:B:267:LEU:HD22	2:B:271:ARG:HH21	1.50	0.76
1:A:715:ILE:HD12	3:F:426:DG:H21	1.52	0.75
2:B:193:LEU:HB3	2:B:241:VAL:HG12	1.67	0.74
2:C:308:THR:HG22	2:C:322:ARG:HG2	1.70	0.73
3:F:435:DT:H2'	3:F:436:DT:C6	2.24	0.73
1:D:759:VAL:HG11	1:D:779:MET:HG3	1.69	0.73
1:D:690:VAL:O	1:D:736:ARG:NH2	2.24	0.71
2:B:247:PRO:HA	2:B:287:ASN:HD22	1.54	0.70
2:C:283:MET:HB3	2:C:325:SER:CB	2.20	0.70
2:C:309:ILE:HD11	2:C:321:VAL:HB	1.73	0.70
1:D:820:GLU:OE2	1:D:866:ARG:NH2	2.25	0.69
2:B:267:LEU:CD2	2:B:271:ARG:NH2	2.56	0.68
2:C:338:VAL:HG12	2:C:339:SER:H	1.57	0.68
1:D:714:SER:HB2	1:D:758:VAL:HG21	1.74	0.68
1:A:840:ILE:HD12	1:A:841:LYS:N	2.07	0.68
2:B:193:LEU:HB2	2:B:238:PHE:CD2	2.28	0.68
1:D:718:PRO:HA	1:D:720:ARG:HH11	1.59	0.68
2:B:200:LYS:HA	2:B:203:LEU:HD12	1.76	0.67
2:B:327:ILE:HB	2:B:330:ILE:HG13	1.77	0.67
2:C:193:LEU:HB3	2:C:241:VAL:HG13	1.78	0.66
2:C:281:PHE:HA	2:C:326:ASN:HD21	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:283:MET:HB3	2:C:325:SER:HB3	1.78	0.65
2:C:291:ASN:ND2	2:C:293:GLU:OE1	2.26	0.65
1:A:840:ILE:O	1:A:842:GLN:NE2	2.30	0.64
1:A:837:SER:O	1:A:839:SER:N	2.30	0.64
1:D:736:ARG:HH21	1:D:737:LEU:HD21	1.62	0.64
1:D:818:CYS:HB3	1:D:866:ARG:HB3	1.80	0.64
1:A:767:ARG:NH1	1:A:768:ASP:OD1	2.31	0.63
2:B:182:VAL:HG22	2:B:183:PRO:HD2	1.80	0.63
1:D:818:CYS:HA	1:D:866:ARG:HD2	1.81	0.62
1:D:733:GLU:OE1	1:D:736:ARG:NH1	2.32	0.62
1:A:790:ARG:NH2	1:A:833:ILE:O	2.34	0.60
1:A:876:ASP:OD1	1:D:885:ARG:NH2	2.34	0.60
2:B:228:VAL:HG12	2:B:229:ARG:H	1.67	0.60
2:C:283:MET:HB3	2:C:325:SER:HB2	1.83	0.60
1:A:690:VAL:O	1:A:736:ARG:NH2	2.35	0.60
1:D:840:ILE:HD11	1:D:859:LEU:HD22	1.84	0.59
1:D:841:LYS:HG2	5:D:1138:HOH:O	2.02	0.59
1:D:774:GLU:OE2	2:C:229:ARG:NH1	2.36	0.58
3:F:434:DA:H2"	3:F:435:DT:OP1	2.03	0.58
1:A:705:ILE:HG22	1:A:754:LEU:HB3	1.84	0.58
1:A:860:TRP:CE2	1:D:878:SER:HA	2.37	0.58
1:A:695:ILE:HD11	1:A:737:LEU:HD22	1.86	0.58
1:D:840:ILE:O	1:D:842:GLN:NE2	2.36	0.58
2:C:240:LEU:HA	2:C:281:PHE:O	2.04	0.57
2:C:190:VAL:HG22	2:C:192:VAL:HG23	1.85	0.57
2:C:193:LEU:HG	2:C:195:LEU:HD21	1.86	0.57
1:D:786:SER:O	1:D:829:LYS:NZ	2.35	0.57
3:E:445:DT:H2"	3:E:446:DG:C8	2.40	0.56
1:D:792:ARG:NH2	3:E:427:PYO:O4'	2.40	0.55
2:B:193:LEU:HB2	2:B:238:PHE:CE2	2.41	0.55
2:B:202:GLU:N	2:B:202:GLU:OE2	2.39	0.55
1:A:717:ASN:HD22	1:A:718:PRO:HD2	1.71	0.55
1:A:862:THR:HB	1:A:872:VAL:HG23	1.88	0.55
2:C:245:THR:OG1	2:C:289:VAL:HG21	2.06	0.55
1:D:790:ARG:NH1	1:D:892:SER:O	2.40	0.55
2:C:208:PHE:HZ	2:C:372:ARG:HA	1.71	0.55
2:C:307:VAL:HG21	2:C:330:ILE:HG13	1.88	0.55
2:B:192:VAL:HG22	2:B:240:LEU:HB3	1.89	0.54
1:D:651:LYS:NZ	5:D:1101:HOH:O	2.40	0.54
1:D:717:ASN:HB2	3:E:428:DG:O4'	2.08	0.54
1:D:841:LYS:HE3	1:D:848:PHE:CE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:GLU:OE1	1:A:736:ARG:NH1	2.42	0.53
1:A:764:SER:OG	1:A:767:ARG:NH2	2.42	0.52
1:D:875:THR:O	1:D:885:ARG:HD3	2.10	0.52
2:C:369:LEU:O	2:C:371:LEU:N	2.42	0.52
1:A:635:ARG:NH2	1:A:702:ASP:OD1	2.30	0.52
2:B:307:VAL:HG21	2:B:330:ILE:HG22	1.91	0.52
3:E:434:DA:H2"	3:E:435:DT:H5"	1.93	0.51
2:C:282:TRP:O	2:C:325:SER:HB2	2.10	0.51
1:D:764:SER:O	1:D:767:ARG:HG3	2.10	0.51
2:C:224:VAL:HG21	2:C:262:GLN:HB3	1.93	0.51
1:D:777:PRO:HB3	1:D:795:TRP:CE2	2.45	0.51
1:D:711:ASN:OD1	1:D:711:ASN:N	2.44	0.50
1:A:863:GLU:O	1:A:867:VAL:HG23	2.10	0.50
1:A:823:ARG:NH1	1:A:863:GLU:OE1	2.45	0.50
2:C:208:PHE:CE1	2:C:375:PHE:HB2	2.46	0.50
2:C:309:ILE:CD1	2:C:363:LEU:HD22	2.39	0.50
2:B:282:TRP:O	2:B:325:SER:HB2	2.12	0.50
1:A:695:ILE:HD12	1:A:740:ASP:HB2	1.93	0.49
2:B:377:TYR:HD1	2:B:378:PHE:N	2.09	0.49
1:D:723:LEU:CD2	1:D:732:PHE:CZ	2.96	0.49
3:F:437:DA:H2"	3:F:438:DG:C8	2.48	0.49
3:F:433:DA:H2"	3:F:434:DA:N7	2.27	0.49
3:F:439:DA:H4'	3:F:440:DA:OP1	2.13	0.49
3:F:441:DC:H2'	3:F:442:DG:C8	2.48	0.49
1:D:723:LEU:CD2	1:D:732:PHE:CE2	2.96	0.48
3:E:440:DA:H2"	3:E:441:DC:O5'	2.13	0.48
1:A:807:SER:HB2	1:A:813:LEU:HD21	1.95	0.48
1:D:693:LYS:O	1:D:697:GLU:HG3	2.13	0.48
1:D:723:LEU:HD23	1:D:723:LEU:O	2.13	0.48
2:C:193:LEU:HB2	2:C:238:PHE:CD2	2.49	0.48
1:D:653:LEU:O	1:D:906:LYS:NZ	2.40	0.48
2:C:290:LEU:HB3	2:C:294:ASP:HB2	1.96	0.48
1:D:761:MET:HE1	1:D:769:ILE:HD12	1.96	0.47
2:C:309:ILE:HD13	2:C:363:LEU:CD2	2.38	0.47
2:C:309:ILE:HG13	2:C:321:VAL:O	2.14	0.47
1:D:723:LEU:HB2	1:D:765:ASP:OD2	2.14	0.47
1:A:783:LYS:NZ	1:A:784:GLU:OE2	2.47	0.47
3:F:440:DA:H2"	3:F:441:DC:O5'	2.13	0.47
1:A:840:ILE:HD12	1:A:841:LYS:H	1.79	0.47
2:B:361:THR:HG22	2:B:362:LYS:H	1.79	0.47
2:C:208:PHE:HE1	2:C:375:PHE:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:237:PRO:C	2:C:238:PHE:HD1	2.17	0.47
1:D:718:PRO:HA	1:D:720:ARG:NH1	2.28	0.47
2:C:193:LEU:HD13	2:C:238:PHE:HE2	1.79	0.46
1:A:875:THR:O	1:A:885:ARG:HD3	2.16	0.46
2:B:274:PRO:O	2:B:276:SER:N	2.49	0.46
1:A:836:ARG:HE	1:A:836:ARG:HB3	1.64	0.46
1:A:837:SER:O	1:A:840:ILE:HG13	2.16	0.46
1:D:703:LEU:HA	1:D:752:PHE:O	2.16	0.46
1:D:798:LEU:HB2	1:D:801:MET:HB3	1.97	0.46
2:B:306:PRO:HB3	2:B:324:TRP:CE2	2.51	0.46
2:B:196:PHE:HA	2:B:222:VAL:HG23	1.97	0.45
1:A:800:GLY:HA3	1:A:803:ARG:HD3	1.99	0.45
3:E:422:DG:H2"	3:E:423:DC:O5'	2.16	0.45
3:E:434:DA:H4'	3:E:435:DT:OP1	2.14	0.45
2:B:366:ASN:OD1	2:B:366:ASN:N	2.49	0.45
2:B:242:TYR:HD1	2:B:283:MET:HG3	1.81	0.45
2:B:247:PRO:CA	2:B:287:ASN:HD22	2.25	0.45
1:D:724:TYR:OH	1:D:768:ASP:OD2	2.25	0.45
2:B:377:TYR:HD1	2:B:378:PHE:H	1.65	0.44
1:D:858:ILE:HG22	5:D:1138:HOH:O	2.16	0.44
3:E:431:DC:H2"	3:E:432:DT:C6	2.52	0.44
1:A:777:PRO:HB3	1:A:795:TRP:CE2	2.52	0.44
2:B:188:GLN:HB2	2:B:189:PRO:HD2	1.98	0.44
1:D:710:CYS:N	3:E:427:PYO:HC5	2.31	0.44
2:B:194:SER:O	2:B:220:HIS:ND1	2.41	0.44
1:A:776:ASN:HD22	1:A:776:ASN:HA	1.59	0.44
3:F:428:DG:C8	3:F:428:DG:H5'	2.52	0.44
1:D:723:LEU:HD22	1:D:732:PHE:CZ	2.53	0.44
2:C:258:TRP:CE2	2:C:262:GLN:HG3	2.53	0.44
2:C:310:PRO:HB3	2:C:338:VAL:HG21	1.99	0.44
1:D:692:GLN:NE2	1:D:696:GLN:OE1	2.51	0.43
2:C:245:THR:CG2	2:C:287:ASN:H	2.30	0.43
2:C:286:ASP:O	2:C:321:VAL:HG13	2.18	0.43
1:A:887:ARG:O	1:A:891:ARG:HG3	2.18	0.43
1:A:649:VAL:HG21	1:A:898:ILE:HG22	1.99	0.43
2:C:250:HIS:O	2:C:253:ASP:N	2.52	0.43
2:C:299:SER:HB2	2:C:324:TRP:HE1	1.83	0.43
2:B:258:TRP:CE2	2:B:262:GLN:HG3	2.53	0.43
1:D:830:VAL:HG12	1:D:831:ARG:O	2.19	0.43
3:E:426:DG:O6	3:F:442:DG:N1	2.51	0.43
1:A:639:LEU:HD12	1:A:734:PHE:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:640:PHE:HB3	4:D:1001:SAH:O4'	2.19	0.43
1:D:708:SER:HG	1:D:755:PHE:HZ	1.63	0.43
3:F:431:DC:H2'	3:F:432:DT:C6	2.54	0.43
1:A:711:ASN:HB2	3:F:428:DG:O3'	2.19	0.42
2:B:182:VAL:CG2	2:B:183:PRO:HD2	2.47	0.42
1:D:887:ARG:O	1:D:891:ARG:HG3	2.19	0.42
1:A:837:SER:C	1:A:839:SER:H	2.21	0.42
1:A:661:ILE:HG12	1:A:682:MET:HB3	2.01	0.42
2:C:327:ILE:HG22	2:C:329:ALA:H	1.84	0.42
1:D:764:SER:HA	1:D:767:ARG:HG2	2.02	0.42
2:B:345:LEU:O	2:B:349:ASN:N	2.53	0.42
1:D:814:GLU:OE1	1:D:828:SER:HB2	2.19	0.42
3:F:433:DA:H2"	3:F:434:DA:C8	2.55	0.42
1:A:715:ILE:CD1	3:F:426:DG:H21	2.28	0.42
2:B:193:LEU:HB2	2:B:238:PHE:HD2	1.83	0.42
1:D:771:ARG:NH1	2:C:226:ASP:HA	2.35	0.42
3:F:435:DT:H2"	3:F:436:DT:O5'	2.18	0.42
1:A:783:LYS:HD3	1:A:789:HIS:CD2	2.55	0.42
2:B:193:LEU:HG	2:B:195:LEU:HD21	2.01	0.42
2:B:325:SER:OG	2:B:327:ILE:HG12	2.19	0.42
1:D:779:MET:HA	1:D:792:ARG:O	2.20	0.42
1:A:862:THR:HA	1:A:865:GLU:OE2	2.19	0.41
1:A:835:THR:HG22	1:A:887:ARG:HA	2.02	0.41
1:D:639:LEU:HD12	1:D:734:PHE:CD1	2.55	0.41
2:B:199:ILE:O	2:B:203:LEU:HG	2.20	0.41
2:C:369:LEU:C	2:C:371:LEU:H	2.22	0.41
3:F:445:DT:H2"	3:F:446:DG:C8	2.55	0.41
2:B:190:VAL:HG23	2:B:239:ASP:HB2	2.02	0.41
1:A:743:PRO:HB3	1:A:749:ARG:HH11	1.86	0.41
2:B:190:VAL:HB	2:B:375:PHE:CG	2.55	0.41
1:D:692:GLN:HG2	1:D:740:ASP:HB3	2.03	0.41
3:F:436:DT:C4	3:F:437:DA:C6	3.08	0.40
1:A:640:PHE:HB3	4:A:1001:SAH:O4'	2.22	0.40
1:A:731:PHE:CE1	1:A:769:ILE:HG23	2.56	0.40
2:B:219:LYS:HA	2:B:219:LYS:HD2	1.88	0.40
2:C:194:SER:O	2:C:220:HIS:HA	2.21	0.40
1:A:895:VAL:N	1:A:896:PRO:HD2	2.36	0.40
2:B:228:VAL:HG12	2:B:229:ARG:N	2.34	0.40
1:D:830:VAL:HG13	1:D:842:GLN:HE22	1.84	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	282/285 (99%)	271 (96%)	10 (4%)	1 (0%)	34	57
1	D	283/285 (99%)	266 (94%)	17 (6%)	0	100	100
2	B	179/209 (86%)	165 (92%)	11 (6%)	3 (2%)	9	18
2	C	167/209 (80%)	147 (88%)	18 (11%)	2 (1%)	13	27
All	All	911/988 (92%)	849 (93%)	56 (6%)	6 (1%)	22	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	838	ASN
2	B	275	GLY
2	C	370	PRO
2	B	277	PRO
2	C	277	PRO
2	B	274	PRO

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	236/250 (94%)	230 (98%)	6 (2%)	47	73
1	D	238/250 (95%)	233 (98%)	5 (2%)	53	77
2	B	133/191 (70%)	130 (98%)	3 (2%)	50	75
2	C	108/191 (56%)	106 (98%)	2 (2%)	57	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	715/882 (81%)	699 (98%)	16 (2%)	52	76

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

Mol	Chain	Res	Type
1	A	692	GLN
1	A	717	ASN
1	A	731	PHE
1	A	807	SER
1	A	861	CYS
1	A	899	ARG
2	B	213	SER
2	B	325	SER
2	B	377	TYR
1	D	689	SER
1	D	731	PHE
1	D	765	ASP
1	D	767	ARG
1	D	790	ARG
2	C	191	ARG
2	C	254	ARG

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

Mol	Chain	Res	Type
1	A	717	ASN
1	A	776	ASN
2	B	287	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	PYO	E	427	3,1	16,20,21	2.07	4 (25%)	22,28,31	1.05	1 (4%)
3	PYO	F	427	3,1	16,20,21	2.07	4 (25%)	22,28,31	1.06	1 (4%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	427	PYO	C6-C5	6.35	1.49	1.35
3	F	427	PYO	C6-C5	6.34	1.49	1.35
3	F	427	PYO	C5-C4	2.97	1.46	1.40
3	E	427	PYO	C5-C4	2.95	1.46	1.40
3	E	427	PYO	C2-N1	2.80	1.46	1.40
3	F	427	PYO	C2-N1	2.64	1.45	1.40
3	F	427	PYO	C4-N3	2.44	1.43	1.33
3	E	427	PYO	C4-N3	2.44	1.43	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	427	PYO	C5-C4-N3	-4.07	119.30	124.29
3	F	427	PYO	C5-C4-N3	-3.99	119.39	124.29

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	427	PYO	C2'-C1'-N1-C6

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

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	427	PYO	2	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
4	SAH	A	1001	-	24,28,28	1.21	3 (12%)	25,40,40	1.59	4 (16%)
4	SAH	D	1001	-	24,28,28	1.21	3 (12%)	25,40,40	1.58	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	A	1001	-	-	3/11/31/31	0/3/3/3
4	SAH	D	1001	-	-	4/11/31/31	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	SAH	C2-N3	4.08	1.38	1.32
4	D	1001	SAH	C2-N3	4.04	1.38	1.32
4	D	1001	SAH	C2-N1	2.55	1.38	1.33
4	A	1001	SAH	C2-N1	2.51	1.38	1.33
4	D	1001	SAH	OXT-C	-2.07	1.23	1.30
4	A	1001	SAH	OXT-C	-2.04	1.23	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1001	SAH	N3-C2-N1	-5.36	120.30	128.68
4	A	1001	SAH	N3-C2-N1	-5.34	120.34	128.68
4	A	1001	SAH	C5'-SD-CG	-3.06	93.10	102.27
4	D	1001	SAH	C5'-SD-CG	-2.96	93.38	102.27
4	D	1001	SAH	OXT-C-O	-2.92	117.45	124.09
4	A	1001	SAH	OXT-C-O	-2.92	117.47	124.09
4	A	1001	SAH	OXT-C-CA	2.32	121.27	113.38
4	D	1001	SAH	OXT-C-CA	2.31	121.26	113.38

There are no chirality outliers.
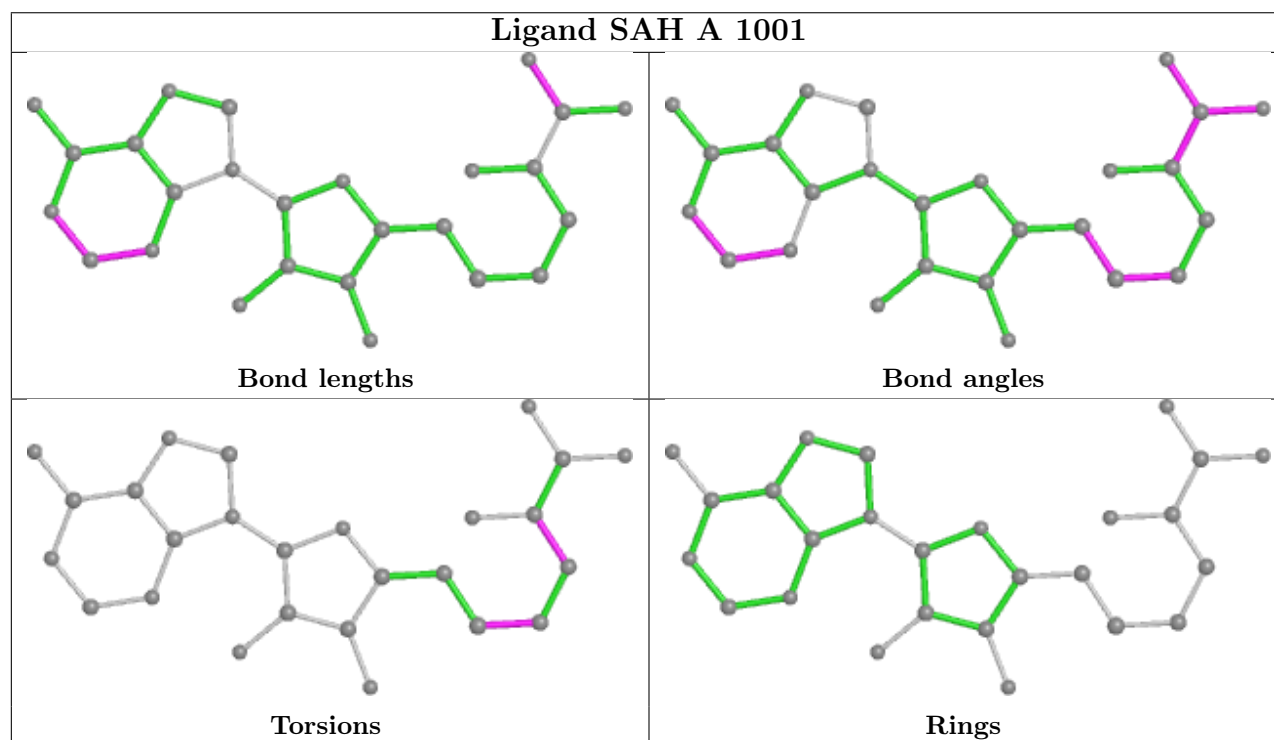
All (7) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	SAH	1	0
4	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SAH A 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand SAH D 1001

Bond lengths

Bond angles

Torsions

Rings
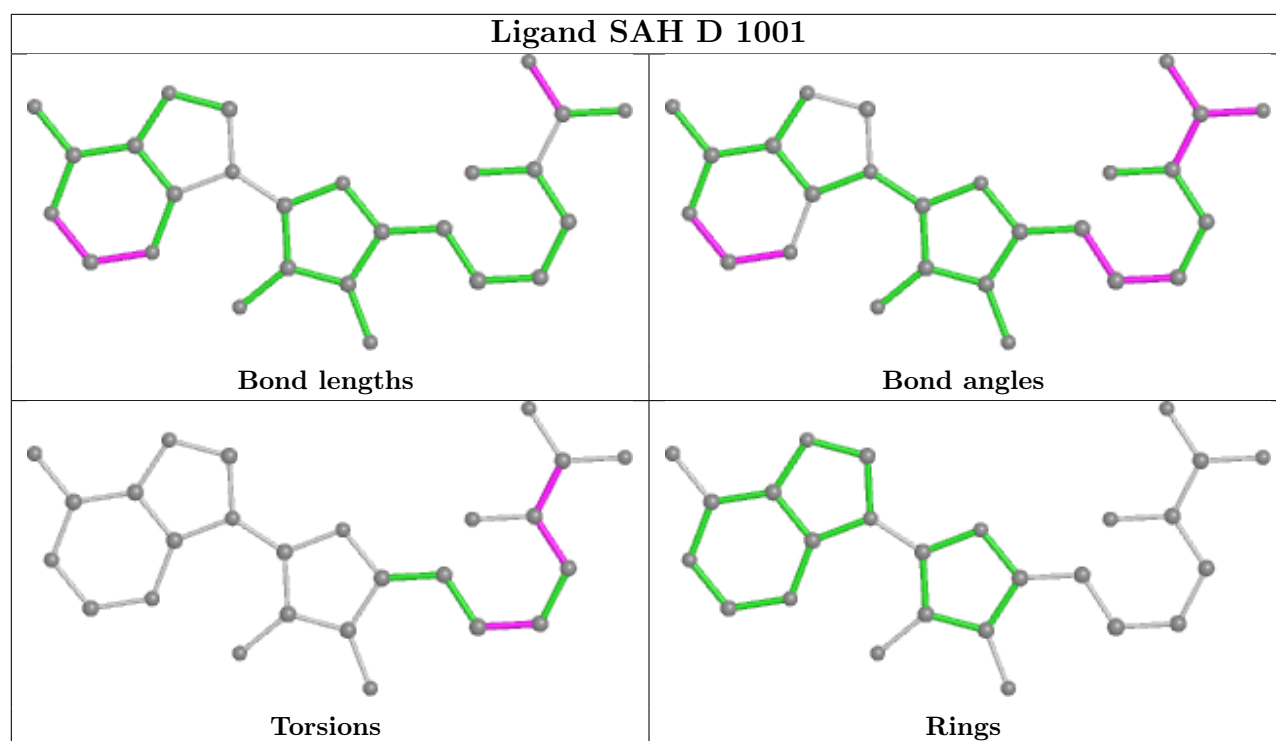
5.7 Other polymers ⓘ

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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(Å²)	Q<0.9
1	A	284/285 (99%)	0.49	26 (9%)	9	6	60, 88, 140, 195	0
1	D	285/285 (100%)	0.34	8 (2%)	53	46	54, 81, 125, 180	0
2	B	187/209 (89%)	0.81	34 (18%)	1	0	79, 135, 182, 205	0
2	C	177/209 (84%)	1.01	31 (17%)	1	0	95, 149, 195, 230	0
3	E	24/25 (96%)	0.58	3 (12%)	3	2	123, 151, 195, 226	0
3	F	24/25 (96%)	0.48	1 (4%)	36	29	96, 172, 199, 211	0
All	All	981/1038 (94%)	0.60	103 (10%)	6	4	54, 105, 181, 230	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	335	TRP	8.2
2	B	317	LEU	7.9
2	B	192	VAL	6.6
1	A	845	ASP	6.5
2	C	338	VAL	5.7
2	B	361	THR	5.2
2	C	313	HIS	5.1
2	B	320	ALA	5.0
2	C	310	PRO	4.8
2	C	329	ALA	4.7
1	A	707	GLY	4.5
2	C	288	LEU	4.5
2	B	379	SER	4.4
1	D	861	CYS	4.4
3	E	422	DG	4.3
2	B	218	LEU	4.0
2	C	337	LEU	4.0
2	C	318	GLN	3.9
2	C	320	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
2	C	331	ARG	3.9
3	E	423	DC	3.9
1	A	841	LYS	3.8
2	C	274	PRO	3.8
1	D	628	ALA	3.8
2	B	211	SER	3.7
1	D	912	VAL	3.7
2	B	319	ASN	3.7
2	B	318	GLN	3.5
1	A	850	VAL	3.4
2	B	283	MET	3.4
2	B	251	THR	3.4
2	B	364	VAL	3.3
3	F	432	DT	3.3
2	B	288	LEU	3.3
2	B	260	LEU	3.3
1	A	708	SER	3.3
2	C	317	LEU	3.2
1	D	843	GLY	3.2
2	C	259	TYR	3.2
2	C	222	VAL	3.2
2	B	338	VAL	3.2
2	C	295	LEU	3.1
2	B	378	PHE	3.1
2	B	205	SER	3.1
2	B	222	VAL	3.1
2	B	250	HIS	3.1
2	C	218	LEU	3.1
2	B	189	PRO	3.0
2	C	283	MET	3.0
1	A	706	GLY	3.0
2	C	249	GLY	3.0
1	A	912	VAL	3.0
1	A	827	PHE	3.0
2	B	202	GLU	2.9
2	C	336	ALA	2.9
1	A	843	GLY	2.9
1	A	709	PRO	2.9
1	A	848	PHE	2.9
1	A	640	PHE	2.8
2	C	312	VAL	2.8
2	C	311	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	735	TYR	2.7
2	C	376	LYS	2.7
2	B	213	SER	2.7
1	A	889	LEU	2.7
2	C	378	PHE	2.7
1	A	838	ASN	2.6
1	A	890	GLY	2.6
2	B	248	LEU	2.6
2	C	250	HIS	2.6
1	A	888	LEU	2.6
2	C	375	PHE	2.6
2	B	287	ASN	2.6
2	B	204	THR	2.5
1	A	846	GLN	2.5
2	C	284	PHE	2.5
2	C	260	LEU	2.5
1	A	847	HIS	2.5
2	B	212	GLY	2.5
2	B	203	LEU	2.5
2	C	330	ILE	2.5
1	D	908	TYR	2.4
2	C	287	ASN	2.4
1	A	844	LYS	2.4
2	B	337	LEU	2.4
2	B	312	VAL	2.3
2	B	185	TRP	2.3
1	D	732	PHE	2.3
3	E	432	DT	2.3
2	B	201	LYS	2.3
2	C	351	GLN	2.3
2	B	336	ALA	2.2
2	B	232	VAL	2.2
1	A	769	ILE	2.2
1	A	842	GLN	2.1
1	D	848	PHE	2.1
1	A	629	GLU	2.1
1	A	791	ALA	2.1
1	A	813	LEU	2.1
1	A	851	PHE	2.1
2	C	193	LEU	2.1
1	D	731	PHE	2.0
2	B	363	LEU	2.0

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

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(Å^2)	Q<0.9
3	PYO	F	427	19/20	0.96	0.20	70,76,105,109	0
3	PYO	E	427	19/20	0.97	0.21	78,100,110,112	0

6.3　Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4　Ligands ⓘ

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.

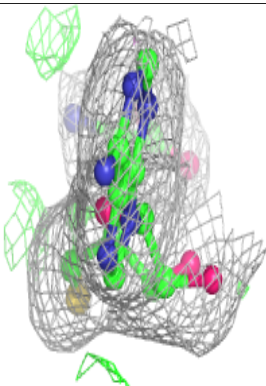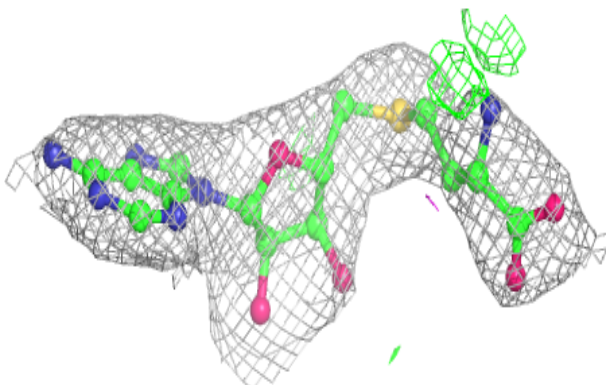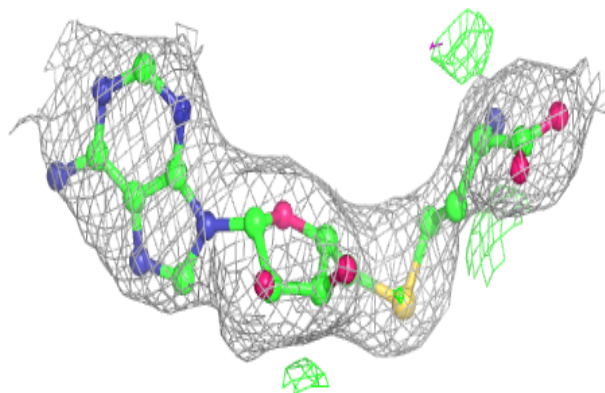| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SAH	A	1001	26/26	0.90	0.28	72,87,97,98	0
4	SAH	D	1001	26/26	0.95	0.20	79,92,96,99	0

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)
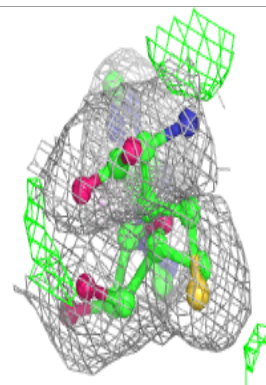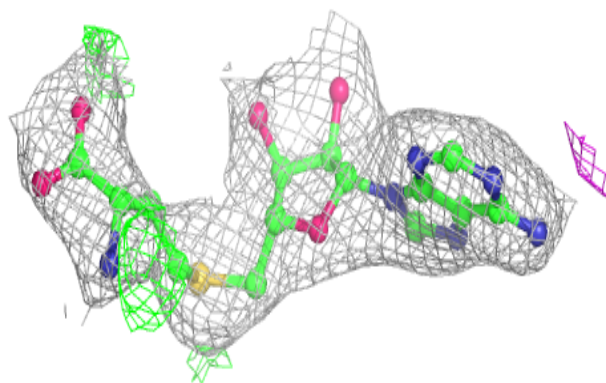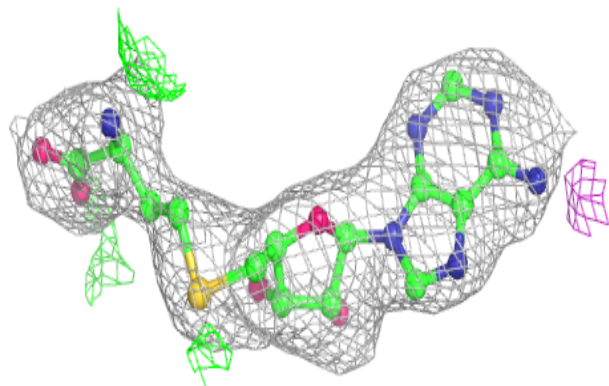
Electron density around SAH D 1001:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.