



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 09:39 PM BST

PDB ID : 6U8W  
Title : Crystal structure of DNMT3B(K777A)-DNMT3L in complex with CpGpT DNA  
Authors : Gao, L.; Zhang, Z.M.; Song, J.  
Deposited on : 2019-09-06  
Resolution : 2.95 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.

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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	:	2.13.1
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)	:	2.13.1

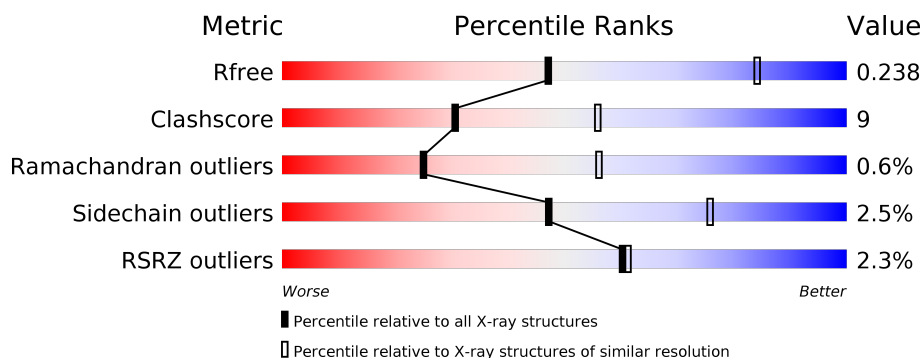
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	291	<div> <div>76%</div> <div>24%</div> </div>
1	D	291	<div> <div>77%</div> <div>22%</div> <div>.</div> </div>
2	B	209	<div> <div>4%</div> <div>73%</div> <div>18%</div> <div>8%</div> </div>
2	C	209	<div> <div>7%</div> <div>65%</div> <div>21%</div> <div>14%</div> <div>.</div> </div>
3	E	25	<div> <div>56%</div> <div>44%</div> </div>
3	F	25	<div> <div>64%</div> <div>32%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8431 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 3B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	1	0
			2298	1474	401	411	12			
1	D	291	Total	C	N	O	S	0	1	0
			2301	1479	401	409	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	777	ALA	LYS	engineered mutation	UNP Q9UBC3
D	777	ALA	LYS	engineered mutation	UNP Q9UBC3

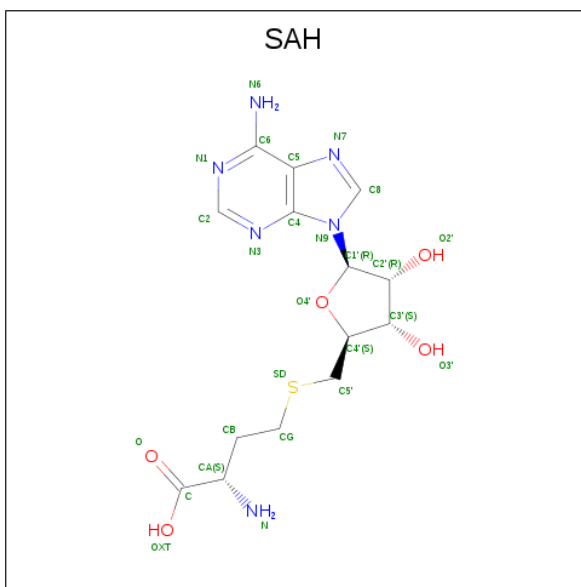
- Molecule 2 is a protein called DNA (cytosine-5)-methyltransferase 3-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	192	Total	C	N	O	S	0	0	0
			1404	920	239	242	3			
2	C	180	Total	C	N	O	S	0	0	0
			1343	878	230	232	3			

- Molecule 3 is a DNA chain called CpGpT 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<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S) (labeled as "Ligand of Interest" by author).



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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

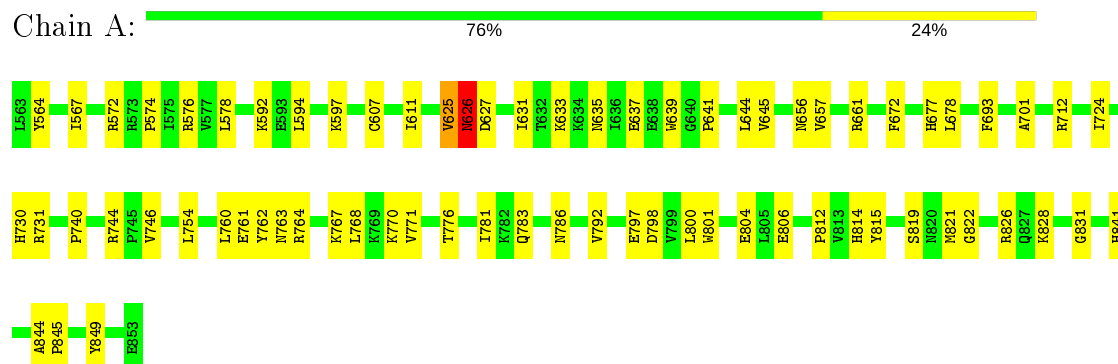
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total	O	0	0
			6	6		
6	D	4	Total	O	0	0
			4	4		
6	F	1	Total	O	0	0
			1	1		

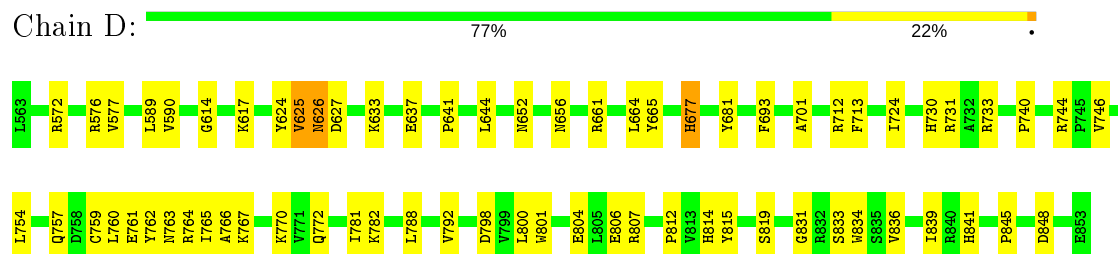
### 3 Residue-property plots [i](#)

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.

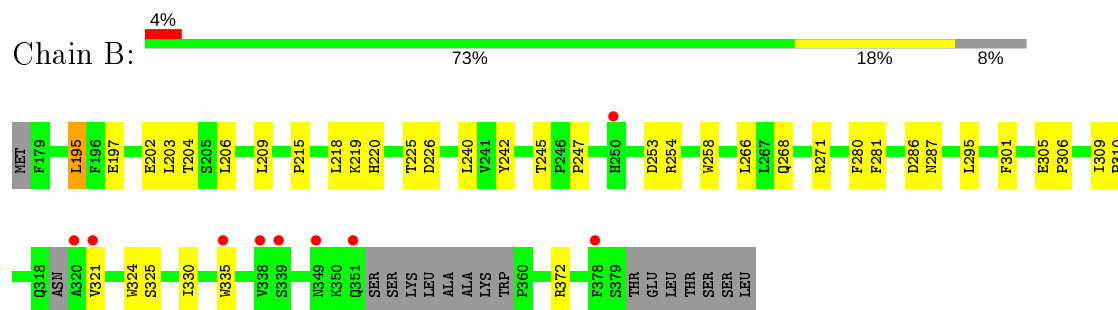
- Molecule 1: DNA (cytosine-5)-methyltransferase 3B



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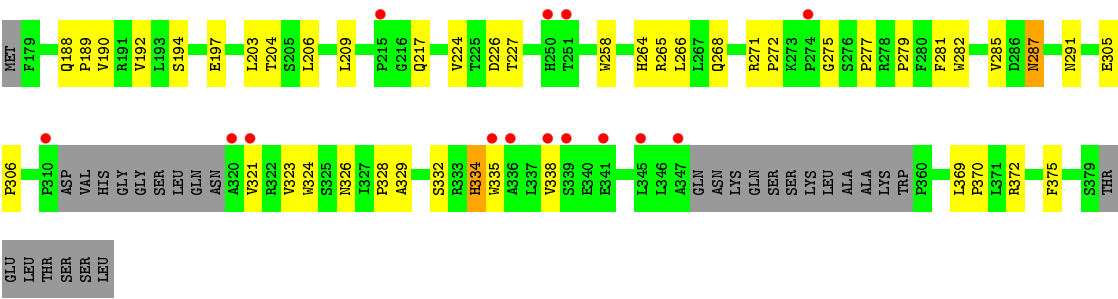


- Molecule 2: DNA (cytosine-5)-methyltransferase 3-like

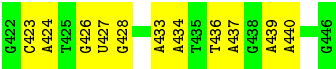


- Molecule 2: DNA (cytosine-5)-methyltransferase 3-like

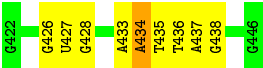




- Molecule 3: CpGpT DNA (25-MER)



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	193.51Å 193.51Å 49.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.38 – 2.95 48.38 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.38-2.95) 99.6 (48.38-2.95)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.216 , 0.236 0.216 , 0.238	Depositor DCC
$R_{free}$ test set	1977 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.7	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 38.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l 0.468 for h,-h-k,-l 0.032 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8431	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SAH, PYO

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	0/2353	0.46	0/3189
1	D	0.26	0/2356	0.44	0/3192
2	B	0.26	0/1450	0.45	0/1992
2	C	0.25	0/1389	0.45	0/1907
3	E	0.50	0/550	0.90	0/846
3	F	0.51	0/550	0.96	1/846 (0.1%)
All	All	0.30	0/8648	0.54	1/11972 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	434	DA	OP2-P-O3'	5.19	116.62	105.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	625	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	D	625	VAL	Peptide

## 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	2298	0	2248	42	0
1	D	2301	0	2264	45	0
2	B	1404	0	1216	27	0
2	C	1343	0	1183	30	0
3	E	510	0	279	6	0
3	F	510	0	279	6	0
4	A	26	0	19	0	0
4	D	26	0	19	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	6	0	0	0	0
6	D	4	0	0	0	0
6	F	1	0	0	0	0
All	All	8431	0	7507	147	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 9.

All (147) 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:C:224:VAL:HG21	2:C:266:LEU:HD11	1.51	0.91
1:A:754:LEU:O	1:A:770:LYS:NZ	2.17	0.78
1:D:781:ILE:HD11	1:D:800:LEU:HB2	1.71	0.73
1:A:576:ARG:HH21	1:A:641:PRO:HB2	1.53	0.72
1:D:576:ARG:HH21	1:D:641:PRO:HB2	1.56	0.71
2:C:204:THR:HG22	2:C:209:LEU:HB2	1.74	0.68
1:D:744:ARG:NH2	1:D:841:HIS:O	2.27	0.68
1:D:677:HIS:HE1	1:D:681:TYR:CZ	2.12	0.67
1:A:746:VAL:HG13	1:A:841:HIS:HD2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:764:ARG:NH2	1:D:798:ASP:OD2	2.29	0.66
1:D:760:LEU:HA	1:D:804:GLU:HG2	1.78	0.66
1:A:764:ARG:NH2	1:A:798:ASP:OD2	2.29	0.65
1:D:761:GLU:OE1	1:D:807:ARG:NH1	2.30	0.64
2:C:305:GLU:HG3	2:C:306:PRO:HD2	1.79	0.64
2:C:194:SER:OG	2:C:197:GLU:O	2.17	0.62
1:A:760:LEU:HA	1:A:804:GLU:HG2	1.82	0.61
1:D:757:GLN:HE21	1:D:766:ALA:H	1.47	0.61
2:C:206:LEU:O	2:C:372:ARG:NH2	2.33	0.60
1:D:731:ARG:NH2	1:D:831:GLY:O	2.31	0.60
2:C:334:HIS:ND1	2:C:334:HIS:O	2.34	0.60
2:B:309:ILE:HA	2:B:335:TRP:HE1	1.67	0.60
3:F:434:DA:H2"	3:F:435:DT:OP2	2.03	0.59
2:C:264:HIS:O	2:C:268:GLN:NE2	2.36	0.59
1:D:656:ASN:OD1	1:D:661:ARG:NH2	2.35	0.58
2:B:309:ILE:HG22	2:B:335:TRP:HZ2	1.68	0.58
1:A:625:VAL:O	1:A:625:VAL:HG12	2.04	0.58
1:D:757:GLN:HG2	1:D:766:ALA:HB3	1.85	0.58
1:D:767:LYS:HE2	1:D:792:VAL:HG23	1.86	0.57
2:B:268:GLN:HE21	2:B:271:ARG:HE	1.53	0.57
1:A:574:PRO:HB3	1:A:597:LYS:HG2	1.86	0.56
2:B:287:ASN:HA	2:B:321:VAL:HG22	1.87	0.56
1:D:833:SER:OG	1:D:834:TRP:N	2.39	0.56
2:C:285:VAL:HG13	2:C:321:VAL:HG11	1.88	0.54
1:D:757:GLN:HE21	1:D:766:ALA:N	2.05	0.54
1:D:767:LYS:NZ	1:D:788:LEU:HD21	2.22	0.54
2:C:209:LEU:HA	2:C:217:GLN:HE21	1.72	0.54
1:D:806:GLU:OE2	1:D:814:HIS:N	2.40	0.54
1:A:767:LYS:NZ	1:A:797:GLU:OE2	2.41	0.53
1:D:772:GLN:HB2	3:E:426:DG:OP2	2.08	0.53
2:B:206:LEU:O	2:B:372:ARG:NH1	2.42	0.53
1:D:572:ARG:NH1	1:D:848:ASP:O	2.41	0.53
2:C:287:ASN:HA	2:C:321:VAL:HG22	1.91	0.53
1:D:633:LYS:O	1:D:637:GLU:HG3	2.10	0.52
1:A:806:GLU:OE1	1:A:814:HIS:N	2.41	0.52
2:B:306:PRO:HB3	2:B:324:TRP:CE2	2.46	0.51
1:A:731:ARG:NH2	1:A:831:GLY:O	2.42	0.51
1:D:754:LEU:O	1:D:770:LYS:NZ	2.30	0.51
2:C:285:VAL:HG22	2:C:323:VAL:HG12	1.92	0.51
1:A:656:ASN:OD1	1:A:661:ARG:NH2	2.42	0.51
2:C:306:PRO:HB3	2:C:324:TRP:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:ILE:HG22	1:A:572:ARG:HG2	1.93	0.50
1:D:625:VAL:O	1:D:626:ASN:O	2.30	0.50
1:D:590:VAL:HG21	1:D:839:ILE:HG22	1.93	0.50
3:F:437:DA:H2''	3:F:438:DG:C8	2.47	0.50
3:F:433:DA:H1'	3:F:434:DA:H5'	1.93	0.50
1:A:625:VAL:CG1	1:A:625:VAL:O	2.60	0.50
2:C:275:GLY:O	2:C:277:PRO:HD3	2.11	0.50
2:C:190:VAL:HG12	2:C:375:PHE:CG	2.48	0.49
1:A:635:ASN:HB3	1:A:639:TRP:CZ3	2.47	0.49
2:B:271:ARG:HG2	2:B:280:PHE:HE2	1.78	0.49
2:C:271:ARG:HG3	2:C:272:PRO:HD2	1.94	0.49
2:B:268:GLN:NE2	2:B:271:ARG:HE	2.10	0.49
2:C:328:PRO:O	2:C:332:SER:HB3	2.13	0.49
3:E:436:DT:H2'	3:E:437:DA:C8	2.47	0.49
1:A:625:VAL:O	1:A:626:ASN:O	2.30	0.49
1:D:781:ILE:HD11	1:D:800:LEU:CB	2.42	0.48
2:C:227:THR:O	2:C:265:ARG:NH2	2.44	0.48
1:A:578:LEU:HB3	1:A:645:VAL:HG22	1.95	0.48
2:C:334:HIS:O	2:C:335:TRP:CG	2.67	0.48
2:B:225:THR:HG22	2:B:258:TRP:HZ2	1.78	0.48
1:A:812:PRO:O	1:A:815:TYR:HB2	2.14	0.48
2:C:209:LEU:HA	2:C:217:GLN:NE2	2.30	0.47
1:A:776:THR:HB	1:A:828:LYS:HG3	1.97	0.47
1:D:762:TYR:CD2	1:D:763:ASN:HB2	2.48	0.47
2:C:192:VAL:HG21	2:C:203:LEU:HD21	1.96	0.47
1:A:677:HIS:HB2	2:B:301:PHE:CE2	2.50	0.47
2:C:329:ALA:HA	2:C:332:SER:HB3	1.96	0.47
1:D:590:VAL:HG12	1:D:836:VAL:HG13	1.96	0.46
3:F:436:DT:H2''	3:F:437:DA:C8	2.51	0.46
1:D:614:GLY:HA3	1:D:624:TYR:OH	2.15	0.46
1:A:819:SER:HA	1:D:801:TRP:CE2	2.50	0.46
1:D:759:CYS:HA	1:D:807:ARG:HD2	1.97	0.46
1:A:567:ILE:HD13	1:A:849:TYR:HD1	1.81	0.46
3:E:428:DG:H5'	3:E:428:DG:C8	2.51	0.46
1:A:633:LYS:O	1:A:637:GLU:HG2	2.14	0.46
2:C:282:TRP:NE1	2:C:326:ASN:HB2	2.30	0.46
1:D:589:LEU:HD21	1:D:812:PRO:HD3	1.96	0.46
3:E:433:DA:H2''	3:E:434:DA:H5''	1.98	0.46
3:E:439:DA:H2''	3:E:440:DA:C8	2.51	0.46
1:A:767:LYS:HD2	1:A:792:VAL:HG23	1.98	0.46
2:B:245:THR:HG22	2:B:286:ASP:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:764:ARG:NH1	1:D:804:GLU:OE1	2.50	0.45
2:B:204:THR:HG22	2:B:209:LEU:HB3	1.99	0.45
1:A:822:GLY:O	1:A:826:ARG:HG2	2.17	0.45
1:D:757:GLN:NE2	1:D:765:ILE:HA	2.31	0.45
1:A:768:LEU:HD11	1:A:783:GLN:HG3	1.99	0.45
2:B:245:THR:CG2	2:B:287:ASN:H	2.30	0.45
2:C:258:TRP:HD1	1:D:665:TYR:CZ	2.35	0.45
1:D:652:ASN:OD1	1:D:652:ASN:N	2.42	0.45
1:A:776:THR:HG22	1:A:828:LYS:HA	1.99	0.44
1:A:592:LYS:HA	1:A:592:LYS:HD3	1.87	0.44
2:C:226:ASP:HA	1:D:712:ARG:HE	1.81	0.44
1:A:656:ASN:N	1:A:701:ALA:O	2.50	0.44
2:B:240:LEU:HA	2:B:281:PHE:O	2.17	0.44
1:D:740:PRO:O	1:D:845:PRO:HG3	2.17	0.44
1:A:594:LEU:HD21	1:A:844:ALA:HA	2.00	0.44
2:B:202:GLU:N	2:B:202:GLU:OE2	2.50	0.44
1:A:762:TYR:CD1	1:A:763:ASN:HB2	2.53	0.43
1:A:764:ARG:NH1	1:A:804:GLU:OE1	2.51	0.43
2:B:203:LEU:HD12	2:B:218:LEU:HD12	2.00	0.43
2:B:195:LEU:CD2	2:B:266:LEU:HD12	2.48	0.43
1:A:657:VAL:HB	3:F:426:DG:H1'	1.99	0.43
1:A:781:ILE:HG23	1:A:800:LEU:HD12	2.00	0.43
2:B:309:ILE:HG22	2:B:335:TRP:CZ2	2.50	0.43
1:A:801:TRP:CE2	1:D:819:SER:HA	2.54	0.43
1:A:771:VAL:HG23	1:A:783:GLN:NE2	2.34	0.43
1:D:812:PRO:O	1:D:815:TYR:HB2	2.19	0.42
1:A:712:ARG:NH1	2:B:226:ASP:HA	2.35	0.42
2:B:309:ILE:HG13	2:B:309:ILE:O	2.18	0.42
2:C:265:ARG:HB2	1:D:713:PHE:CE2	2.55	0.42
2:B:253:ASP:OD1	2:B:253:ASP:N	2.49	0.42
2:C:279:PRO:HB2	2:C:281:PHE:CE2	2.54	0.42
2:C:329:ALA:HB3	2:C:370:PRO:CB	2.49	0.42
1:A:607:CYS:O	1:A:611:ILE:HG13	2.19	0.41
1:A:740:PRO:O	1:A:845:PRO:HG3	2.20	0.41
2:C:282:TRP:CE2	2:C:326:ASN:HB2	2.55	0.41
1:D:724:ILE:HD13	1:D:730:HIS:ND1	2.34	0.41
1:A:631:ILE:HB	1:A:678:LEU:HD21	2.02	0.41
2:C:188:GLN:HB3	2:C:189:PRO:HD2	2.02	0.41
1:D:656:ASN:N	1:D:701:ALA:O	2.53	0.41
1:D:767:LYS:CE	1:D:792:VAL:HG23	2.48	0.41
3:F:428:DG:H5'	3:F:428:DG:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:SER:HB3	2:B:330:ILE:HG21	2.01	0.41
1:A:644:LEU:HA	1:A:693:PHE:O	2.21	0.41
1:A:724:ILE:HD12	1:A:730:HIS:CE1	2.56	0.41
2:B:254:ARG:HD2	2:B:258:TRP:CD2	2.55	0.41
2:B:219:LYS:HD2	2:B:220:HIS:H	1.86	0.41
2:C:369:LEU:N	2:C:370:PRO:HD2	2.36	0.41
3:E:423:DC:H2"	3:E:424:DA:C8	2.56	0.41
2:B:195:LEU:HD21	2:B:266:LEU:HD12	2.04	0.40
2:B:197:GLU:OE2	2:B:247:PRO:HD3	2.21	0.40
1:D:617:LYS:HE3	1:D:815:TYR:HA	2.03	0.40
1:D:677:HIS:HE1	1:D:681:TYR:CE2	2.39	0.40
1:D:746:VAL:HG12	1:D:841:HIS:NE2	2.36	0.40
2:B:195:LEU:HD12	2:B:242:TYR:O	2.21	0.40
1:A:821:MET:HB3	1:A:821:MET:HE2	1.92	0.40
1:D:644:LEU:HA	1:D:693:PHE:O	2.21	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	290/291 (100%)	281 (97%)	7 (2%)	2 (1%)	22	52
1	D	290/291 (100%)	284 (98%)	4 (1%)	2 (1%)	22	52
2	B	186/209 (89%)	176 (95%)	8 (4%)	2 (1%)	14	40
2	C	174/209 (83%)	164 (94%)	10 (6%)	0	100	100
All	All	940/1000 (94%)	905 (96%)	29 (3%)	6 (1%)	25	56

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	626	ASN
1	D	626	ASN
1	A	627	ASP
1	D	627	ASP
2	B	215	PRO
2	B	310	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	238/251 (95%)	232 (98%)	6 (2%)	47	76
1	D	239/251 (95%)	234 (98%)	5 (2%)	53	79
2	B	123/191 (64%)	120 (98%)	3 (2%)	49	77
2	C	124/191 (65%)	120 (97%)	4 (3%)	39	70
All	All	724/884 (82%)	706 (98%)	18 (2%)	47	76

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	564	TYR
1	A	626	ASN
1	A	672	PHE
1	A	744	ARG
1	A	761	GLU
1	A	786	ASN
2	B	195	LEU
2	B	295	LEU
2	B	305	GLU
2	C	287	ASN
2	C	291	ASN
2	C	334	HIS
2	C	338	VAL
1	D	577	VAL
1	D	664	LEU
1	D	677	HIS

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Mol	Chain	Res	Type
1	D	733	ARG
1	D	782	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	626	ASN
1	D	677	HIS
1	D	698	ASN
1	D	757	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PYO	F	427	1,3	14,20,21	3.71	5 (35%)	16,28,31	3.29	3 (18%)
3	PYO	E	427	1,3	14,20,21	3.69	5 (35%)	16,28,31	3.18	3 (18%)

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	F	427	1,3	-	2/5/25/26	0/2/2/2
3	PYO	E	427	1,3	-	2/5/25/26	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	427	PYO	C6-N1	9.17	1.47	1.35
3	E	427	PYO	C6-N1	9.01	1.46	1.35
3	E	427	PYO	C2-N3	6.21	1.50	1.38
3	F	427	PYO	C2-N3	6.19	1.50	1.38
3	F	427	PYO	C6-C5	5.28	1.50	1.38
3	E	427	PYO	C6-C5	5.27	1.50	1.38
3	E	427	PYO	C4-N3	5.05	1.45	1.34
3	F	427	PYO	C4-N3	4.98	1.45	1.34
3	E	427	PYO	C5-C4	4.06	1.49	1.37
3	F	427	PYO	C5-C4	4.05	1.49	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	427	PYO	C4-N3-C2	12.52	120.59	114.42
3	E	427	PYO	C4-N3-C2	12.04	120.36	114.42
3	E	427	PYO	C5-C4-N3	-2.36	119.58	123.43
3	F	427	PYO	C5-C4-N3	-2.31	119.66	123.43
3	E	427	PYO	C6-C5-C4	2.27	120.16	117.27
3	F	427	PYO	C6-C5-C4	2.21	120.08	117.27

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.



## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	901	-	21,28,28	1.17	2 (9%)	20,40,40	1.73	2 (10%)
4	SAH	D	901	-	21,28,28	1.16	2 (9%)	20,40,40	1.69	2 (10%)

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	901	-	-	2/7/31/31	0/3/3/3
4	SAH	D	901	-	-	3/7/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	SAH	C2-N3	3.89	1.38	1.32
4	D	901	SAH	C2-N3	3.89	1.38	1.32
4	D	901	SAH	C2-N1	2.42	1.38	1.33
4	A	901	SAH	C2-N1	2.41	1.38	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	901	SAH	N3-C2-N1	-5.44	120.18	128.68
4	A	901	SAH	N3-C2-N1	-5.42	120.20	128.68
4	A	901	SAH	C5'-SD-CG	-3.87	90.65	102.27
4	D	901	SAH	C5'-SD-CG	-3.44	91.96	102.27

There are no chirality outliers.

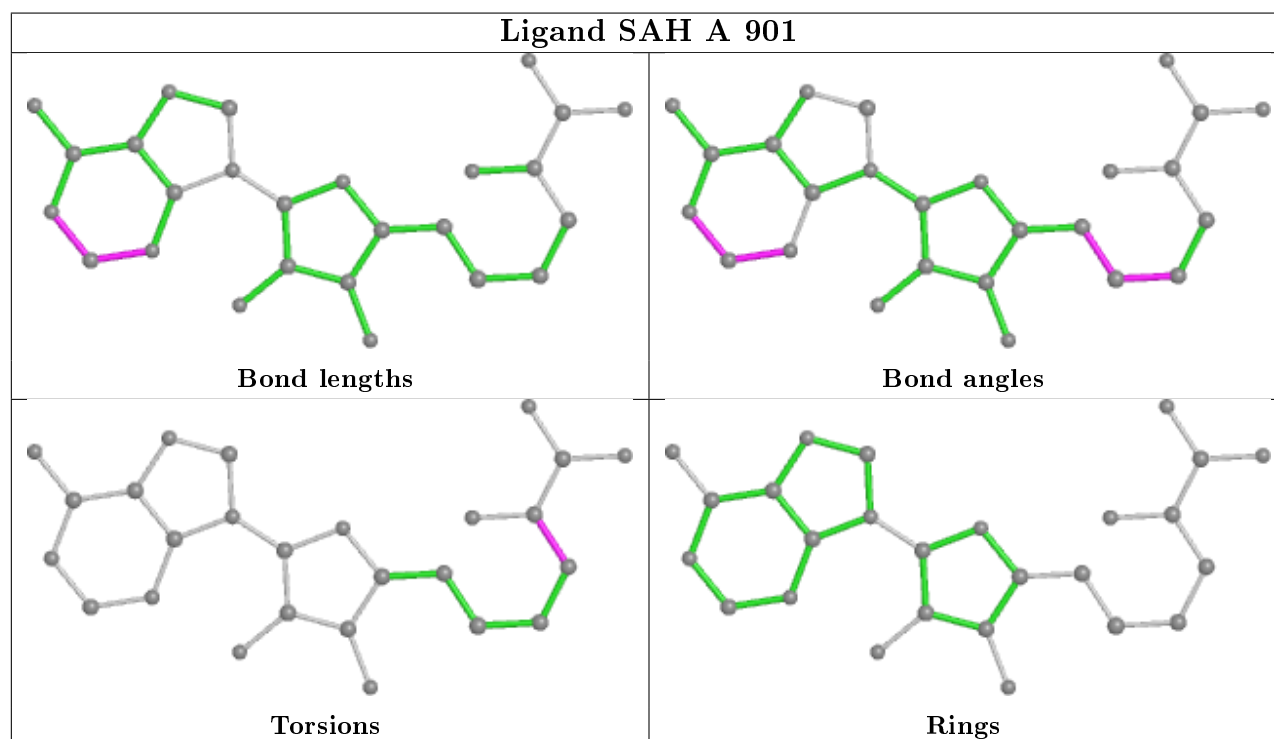
All (5) torsion outliers are listed below:

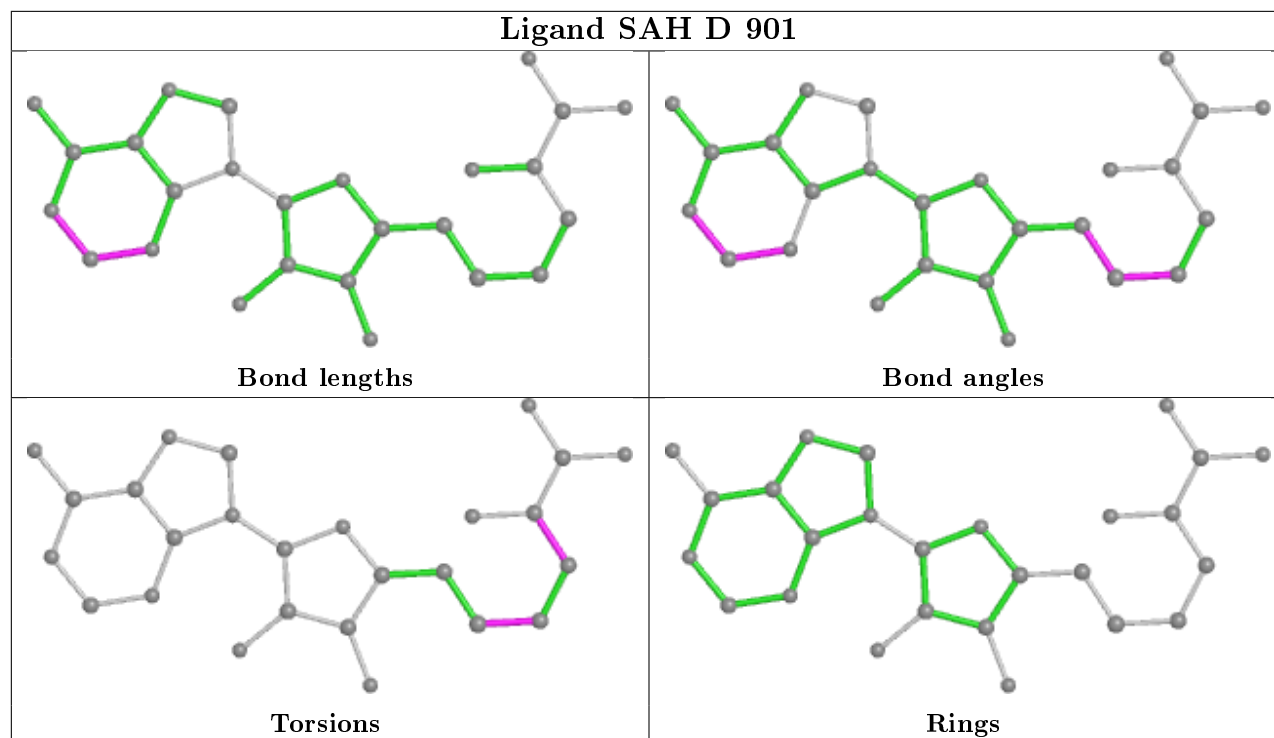
Mol	Chain	Res	Type	Atoms
4	A	901	SAH	N-CA-CB-CG
4	A	901	SAH	C-CA-CB-CG
4	D	901	SAH	N-CA-CB-CG
4	D	901	SAH	C-CA-CB-CG
4	D	901	SAH	CB-CG-SD-C5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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, 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	291/291 (100%)	-0.12	0 100 100	37, 69, 114, 140	0
1	D	291/291 (100%)	-0.16	0 100 100	38, 69, 115, 138	0
2	B	192/209 (91%)	0.18	9 (4%) 31 31	78, 127, 209, 230	0
2	C	180/209 (86%)	0.19	14 (7%) 13 11	76, 122, 197, 210	0
3	E	24/25 (96%)	-0.05	0 100 100	107, 160, 185, 187	0
3	F	24/25 (96%)	-0.06	0 100 100	108, 162, 182, 189	0
All	All	1002/1050 (95%)	-0.02	23 (2%) 60 61	37, 89, 186, 230	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	320	ALA	8.5
2	B	250	HIS	8.5
2	B	320	ALA	5.9
2	C	250	HIS	5.2
2	B	338	VAL	5.2
2	B	339	SER	4.9
2	C	338	VAL	3.8
2	C	310	PRO	3.6
2	C	345	LEU	3.6
2	C	321	VAL	3.5
2	B	321	VAL	3.3
2	C	347	ALA	3.1
2	C	251	THR	2.7
2	C	335	TRP	2.7
2	B	351	GLN	2.6
2	B	378	PHE	2.6
2	C	336	ALA	2.5
2	C	274	PRO	2.4
2	B	349	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	215	PRO	2.2
2	C	341	GLU	2.0
2	C	339	SER	2.0
2	B	335	TRP	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	0.95	0.12	78,85,95,99	0
3	PYO	F	427	19/20	0.96	0.14	78,84,95,101	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

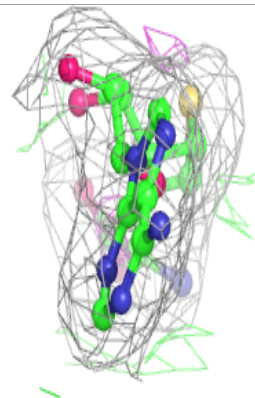
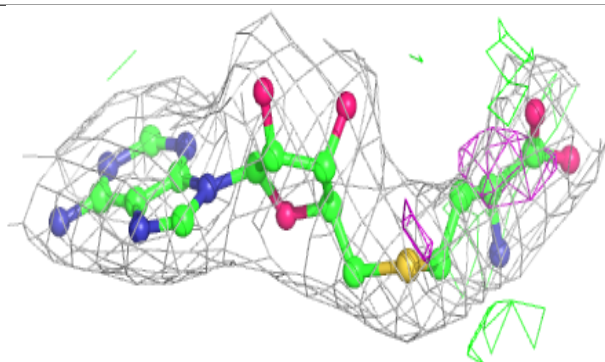
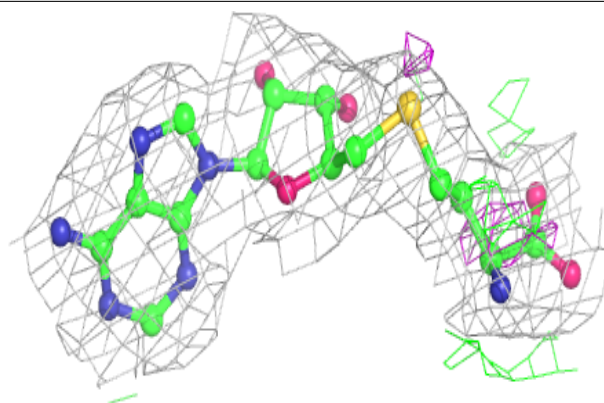
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	D	902	1/1	0.87	0.15	75,75,75,75	0
5	MG	A	902	1/1	0.91	0.21	81,81,81,81	0
4	SAH	A	901	26/26	0.96	0.17	42,52,59,64	0
4	SAH	D	901	26/26	0.97	0.16	43,53,61,67	0

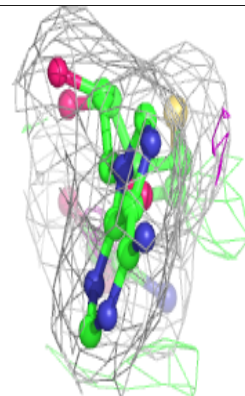
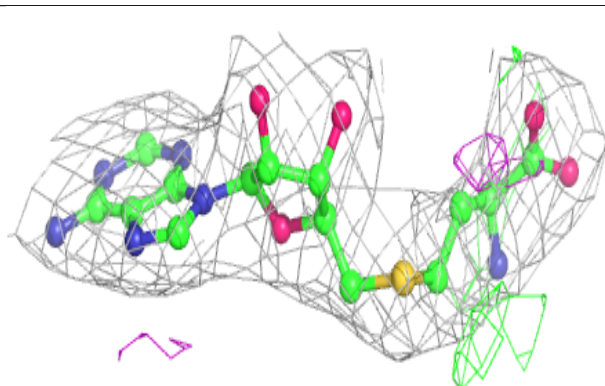
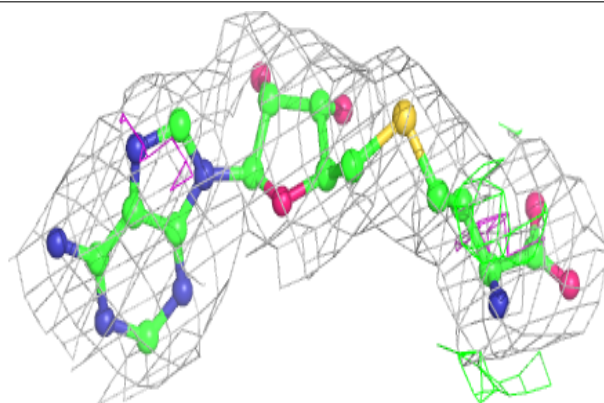
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around SAH A 901:**

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

**Electron density around SAH D 901:**

$2mF_o-DF_c$  (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.