



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 12:30 AM BST

PDB ID : 6U8X  
Title : Crystal structure of DNMT3B-DNMT3L in complex with CpApG DNA  
Authors : Gao, L.; 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

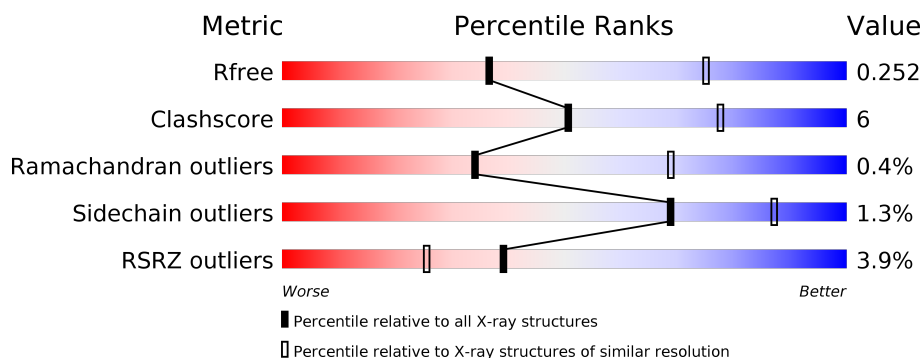
# 1 Overall quality at a glance

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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 style="width: 13%; background-color: red;"></div> <div style="width: 86%; background-color: green;"></div> <div style="width: 1%; background-color: yellow;"></div> <div style="width: 1%; background-color: orange;"></div> </div> <div> <div style="width: 13%; background-color: red;"></div> <div style="width: 86%; background-color: green;"></div> <div style="width: 1%; background-color: yellow;"></div> <div style="width: 1%; background-color: orange;"></div> </div>
1	D	291	<div> <div style="width: 15%; background-color: red;"></div> <div style="width: 84%; background-color: green;"></div> <div style="width: 1%; background-color: yellow;"></div> <div style="width: 1%; background-color: orange;"></div> </div> <div> <div style="width: 15%; background-color: red;"></div> <div style="width: 84%; background-color: green;"></div> <div style="width: 1%; background-color: yellow;"></div> <div style="width: 1%; background-color: orange;"></div> </div>
2	B	209	<div> <div style="width: 11%; background-color: red;"></div> <div style="width: 80%; background-color: green;"></div> <div style="width: 10%; background-color: yellow;"></div> <div style="width: 10%; background-color: orange;"></div> </div> <div> <div style="width: 11%; background-color: red;"></div> <div style="width: 80%; background-color: green;"></div> <div style="width: 10%; background-color: yellow;"></div> <div style="width: 10%; background-color: orange;"></div> </div>
2	C	209	<div> <div style="width: 7%; background-color: red;"></div> <div style="width: 73%; background-color: green;"></div> <div style="width: 15%; background-color: yellow;"></div> <div style="width: 11%; background-color: orange;"></div> </div> <div> <div style="width: 7%; background-color: red;"></div> <div style="width: 73%; background-color: green;"></div> <div style="width: 15%; background-color: yellow;"></div> <div style="width: 11%; background-color: orange;"></div> </div>
3	E	25	<div> <div style="width: 4%; background-color: red;"></div> <div style="width: 56%; background-color: green;"></div> <div style="width: 40%; background-color: yellow;"></div> <div style="width: 1%; background-color: orange;"></div> </div> <div> <div style="width: 4%; background-color: red;"></div> <div style="width: 56%; background-color: green;"></div> <div style="width: 40%; background-color: yellow;"></div> <div style="width: 1%; background-color: orange;"></div> </div>
3	F	25	<div> <div style="width: 72%; background-color: green;"></div> <div style="width: 24%; background-color: yellow;"></div> <div style="width: 1%; background-color: orange;"></div> </div> <div> <div style="width: 72%; background-color: green;"></div> <div style="width: 24%; background-color: yellow;"></div> <div style="width: 1%; background-color: orange;"></div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8598 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
			2311	1485	402	412	12			
1	D	291	Total	C	N	O	S	0	1	0
			2315	1488	403	412	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	189	Total	C	N	O	S	0	0	0
			1450	951	244	252	3			
2	C	186	Total	C	N	O	S	0	0	0
			1427	931	243	249	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	25	Total	C	N	O	P	0	0	0
			511	245	93	149	24			
3	F	25	Total	C	N	O	P	0	0	0
			511	245	93	149	24			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 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
5	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
5	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

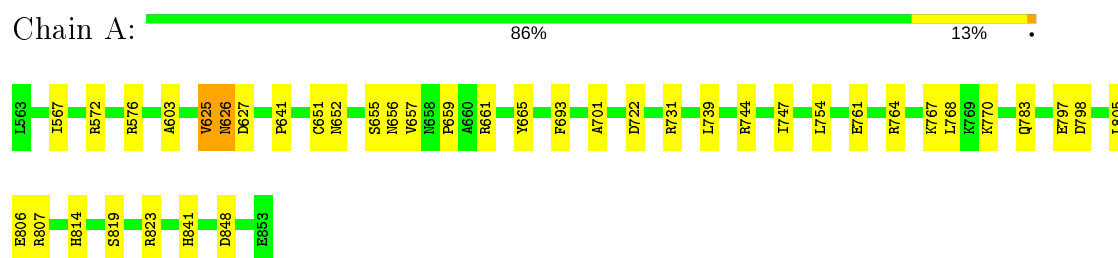
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total	O	0	0
			7	7		
6	B	1	Total	O	0	0
			1	1		
6	D	7	Total	O	0	0
			7	7		
6	E	2	Total	O	0	0
			2	2		
6	F	2	Total	O	0	0
			2	2		

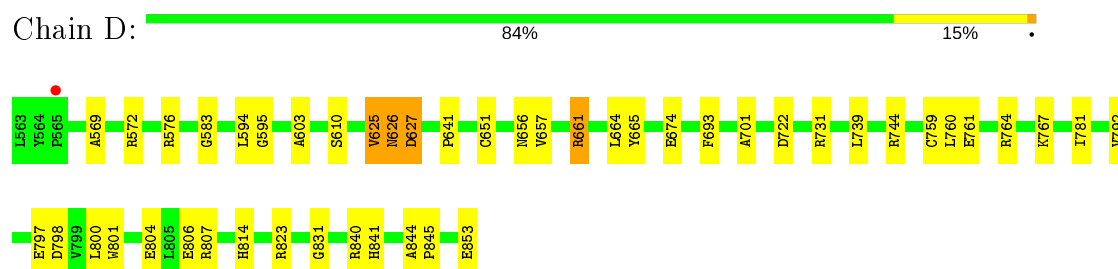
### 3 Residue-property plots

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.

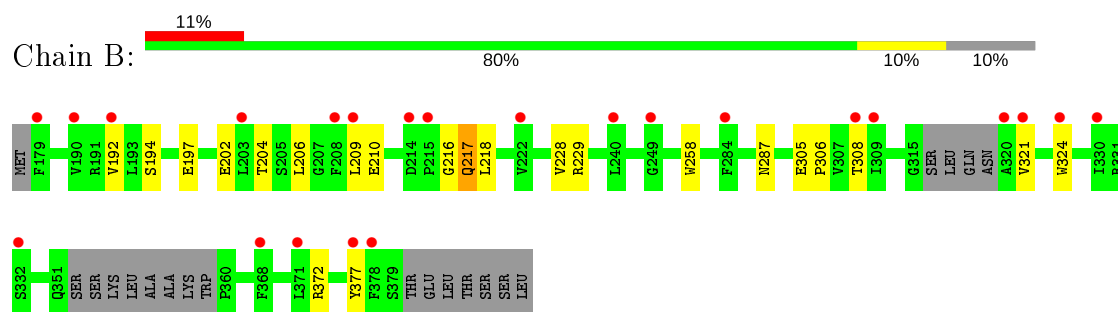
- Molecule 1: DNA (cytosine-5)-methyltransferase 3B



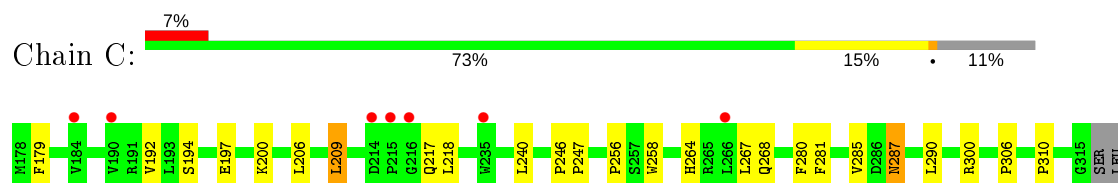
- Molecule 1: DNA (cytosine-5)-methyltransferase 3B

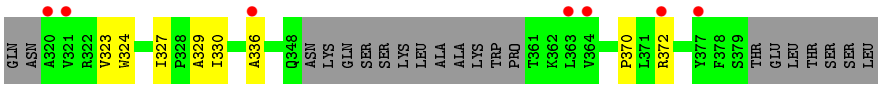


- Molecule 2: DNA (cytosine-5)-methyltransferase 3-like

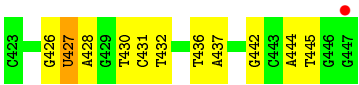


- Molecule 2: DNA (cytosine-5)-methyltransferase 3-like





• Molecule 3: CpApG DNA (25-MER)



• Molecule 3: CpApG DNA (25-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	193.84 Å 193.84 Å 49.88 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.88 – 2.95 48.46 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.88-2.95) 99.8 (48.46-2.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 2.96 Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.227 , 0.252 0.227 , 0.252	Depositor DCC
$R_{free}$ test set	2002 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.3	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l 0.468 for h,-h-k,-l 0.027 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8598	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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	0.25	0/2369	0.42	0/3207
1	D	0.25	0/2373	0.42	0/3211
2	B	0.26	0/1498	0.44	0/2052
2	C	0.24	0/1474	0.43	0/2019
3	E	0.49	0/551	0.91	0/847
3	F	0.51	0/551	0.96	0/847
All	All	0.29	0/8816	0.53	0/12183

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
2	B	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	625	VAL	Peptide
2	B	216	GLY	Peptide
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	2311	0	2286	25	0
1	D	2315	0	2297	28	0
2	B	1450	0	1328	16	0
2	C	1427	0	1297	19	0
3	E	511	0	282	8	0
3	F	511	0	282	6	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	26	0	19	0	0
5	D	26	0	19	0	0
6	A	7	0	0	1	0
6	B	1	0	0	0	0
6	D	7	0	0	0	0
6	E	2	0	0	1	0
6	F	2	0	0	1	0
All	All	8598	0	7810	93	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 (93) 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:D:767:LYS:NZ	1:D:797:GLU:OE1	2.17	0.77
2:B:209:LEU:HA	2:B:217:GLN:HE21	1.49	0.76
2:C:194:SER:OG	2:C:197:GLU:O	2.10	0.68
1:A:754:LEU:O	1:A:770:LYS:NZ	2.30	0.65
1:A:744:ARG:NH2	1:A:841:HIS:O	2.31	0.64
1:A:761:GLU:OE1	1:A:807:ARG:NH2	2.31	0.62
2:C:179:PHE:HE2	2:C:280:PHE:H	1.46	0.62
1:A:807:ARG:NH1	6:A:1001:HOH:O	2.34	0.60
3:F:428:DA:N7	6:F:501:HOH:O	2.31	0.59
2:C:264:HIS:O	2:C:268:GLN:NE2	2.36	0.58
2:B:206:LEU:O	2:B:372:ARG:NH1	2.36	0.58
2:B:217:GLN:OE1	2:B:217:GLN:HA	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:GLU:HG3	2:B:306:PRO:HD2	1.87	0.57
2:C:300:ARG:NH1	1:D:674:GLU:OE1	2.36	0.57
3:E:436:DT:H2"	3:E:437:DA:C8	2.40	0.56
1:A:764:ARG:NH2	1:A:798:ASP:OD2	2.37	0.56
2:B:204:THR:HG23	2:B:209:LEU:HD12	1.88	0.56
2:B:194:SER:OG	2:B:197:GLU:O	2.23	0.56
1:D:594:LEU:HD21	1:D:840:ARG:HG3	1.88	0.55
1:A:656:ASN:HB2	1:A:701:ALA:HB1	1.88	0.55
1:D:569:ALA:HA	1:D:572:ARG:HD2	1.90	0.54
2:C:306:PRO:HB3	2:C:324:TRP:CE2	2.44	0.53
1:D:761:GLU:OE1	1:D:807:ARG:NH1	2.42	0.53
2:C:329:ALA:HB3	2:C:370:PRO:HB3	1.91	0.53
1:D:764:ARG:NH2	1:D:798:ASP:OD2	2.43	0.52
1:D:744:ARG:NH2	1:D:841:HIS:O	2.43	0.51
1:A:576:ARG:HH21	1:A:641:PRO:HB2	1.74	0.51
2:C:287:ASN:N	2:C:287:ASN:HD22	2.09	0.51
2:C:206:LEU:O	2:C:372:ARG:NH1	2.31	0.50
3:E:428:DA:N7	6:E:501:HOH:O	2.34	0.50
2:B:202:GLU:OE2	2:B:202:GLU:N	2.44	0.50
2:C:209:LEU:CB	2:C:217:GLN:HG2	2.42	0.50
1:D:603:ALA:O	1:D:625:VAL:HG22	2.12	0.50
1:A:656:ASN:HA	1:A:661:ARG:NH2	2.28	0.49
2:C:327:ILE:HB	2:C:330:ILE:HD12	1.93	0.49
1:A:657:VAL:HB	3:F:426:DG:H1'	1.93	0.49
2:B:306:PRO:HB3	2:B:324:TRP:CE2	2.47	0.49
1:A:767:LYS:NZ	1:A:797:GLU:OE2	2.44	0.49
2:B:372:ARG:HD3	2:B:377:TYR:CD1	2.48	0.48
1:A:603:ALA:O	1:A:625:VAL:HG22	2.13	0.48
1:A:651:CYS:N	3:F:427:PYO:HC5	2.29	0.48
2:C:310:PRO:HG3	2:C:336:ALA:HB3	1.95	0.48
2:C:209:LEU:HB2	2:C:217:GLN:HG2	1.96	0.48
2:C:200:LYS:HE3	2:C:218:LEU:HD22	1.95	0.47
1:A:567:ILE:O	1:A:572:ARG:NH1	2.47	0.47
2:C:192:VAL:HG12	2:C:240:LEU:HB3	1.97	0.47
1:A:806:GLU:OE1	1:A:814:HIS:N	2.47	0.47
3:F:433:DA:H2"	3:F:434:DA:H5"	1.96	0.47
2:B:192:VAL:HB	2:B:218:LEU:HB3	1.96	0.47
2:C:285:VAL:HG12	2:C:323:VAL:HG22	1.96	0.47
1:D:656:ASN:HB2	1:D:701:ALA:HB1	1.97	0.47
2:B:228:VAL:HG12	2:B:229:ARG:H	1.81	0.46
2:B:192:VAL:O	2:B:218:LEU:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:819:SER:HA	1:D:801:TRP:CE2	2.50	0.46
2:B:204:THR:HG22	2:B:209:LEU:HB2	1.98	0.46
1:A:722:ASP:HA	1:A:731:ARG:O	2.16	0.45
2:B:209:LEU:HA	2:B:217:GLN:NE2	2.26	0.45
1:A:572:ARG:NH1	1:A:848:ASP:O	2.50	0.45
2:C:246:PRO:HA	2:C:247:PRO:HD3	1.88	0.45
1:D:576:ARG:HH21	1:D:641:PRO:HB2	1.80	0.45
1:D:657:VAL:HB	3:E:426:DG:H1'	1.99	0.45
3:E:444:DA:H1'	3:E:445:DT:H5'	1.99	0.45
1:D:806:GLU:OE1	1:D:814:HIS:N	2.49	0.44
3:F:435:DT:H2''	3:F:436:DT:C6	2.53	0.44
1:D:626:ASN:HB3	1:D:627:ASP:H	1.62	0.44
1:D:651:CYS:N	3:E:427:PYO:HC5	2.32	0.44
1:D:781:ILE:HD12	1:D:800:LEU:HD12	1.99	0.44
1:A:665:TYR:CZ	2:B:258:TRP:HD1	2.36	0.44
1:A:659:PRO:HB3	3:E:442:DG:H4'	1.99	0.44
1:D:760:LEU:HA	1:D:804:GLU:HG2	2.00	0.43
1:A:652:ASN:OD1	1:A:652:ASN:N	2.49	0.43
1:D:722:ASP:HA	1:D:731:ARG:O	2.18	0.43
1:A:625:VAL:O	1:A:626:ASN:O	2.37	0.43
1:D:583:GLY:O	1:D:610:SER:HB3	2.19	0.43
2:C:258:TRP:HD1	1:D:665:TYR:CZ	2.37	0.43
1:A:693:PHE:HB3	1:A:739:LEU:HD23	2.01	0.43
1:D:693:PHE:HB3	1:D:739:LEU:HD23	2.01	0.42
1:D:731:ARG:NH2	1:D:831:GLY:O	2.39	0.42
3:E:430:DT:H2''	3:E:431:DC:H5''	2.00	0.42
1:D:595:GLY:O	1:D:853:GLU:N	2.50	0.42
1:A:805:LEU:HD11	1:A:823[B]:ARG:HH22	1.84	0.42
1:D:759:CYS:HA	1:D:807:ARG:HD2	2.00	0.42
1:A:768:LEU:HD13	1:A:783:GLN:HG3	2.02	0.41
1:D:661:ARG:HG3	1:D:661:ARG:H	1.67	0.41
2:B:287:ASN:HA	2:B:321:VAL:HG12	2.01	0.41
2:C:281:PHE:CD1	2:C:327:ILE:HG12	2.56	0.41
1:D:625:VAL:O	1:D:626:ASN:O	2.39	0.41
1:D:767:LYS:HE3	1:D:792:VAL:HG23	2.02	0.41
1:D:844:ALA:N	1:D:845:PRO:HD2	2.36	0.41
1:A:655:SER:O	1:A:661:ARG:HD3	2.20	0.40
2:C:256:PRO:HB2	2:C:290:LEU:HD23	2.03	0.40
3:E:431:DC:H2''	3:E:432:DT:C6	2.57	0.40
3:F:433:DA:H2''	3:F:434:DA:C8	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	290/291 (100%)	284 (98%)	4 (1%)	2 (1%)	22	56
1	D	290/291 (100%)	283 (98%)	5 (2%)	2 (1%)	22	56
2	B	183/209 (88%)	170 (93%)	13 (7%)	0	100	100
2	C	180/209 (86%)	170 (94%)	10 (6%)	0	100	100
All	All	943/1000 (94%)	907 (96%)	32 (3%)	4 (0%)	34	69

All (4) 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

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	243/252 (96%)	242 (100%)	1 (0%)	91	96
1	D	244/252 (97%)	240 (98%)	4 (2%)	62	84
2	B	142/191 (74%)	139 (98%)	3 (2%)	53	80
2	C	140/191 (73%)	137 (98%)	3 (2%)	53	80
All	All	769/886 (87%)	758 (99%)	11 (1%)	69	86

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	747	ILE
2	B	210	GLU
2	B	217	GLN
2	B	308	THR
2	C	209	LEU
2	C	267	LEU
2	C	287	ASN
1	D	661	ARG
1	D	664	LEU
1	D	823[A]	ARG
1	D	823[B]	ARG

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

Mol	Chain	Res	Type
1	A	772	GLN
2	B	217	GLN
2	C	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	1,3	14,20,21	5.73	12 (85%)	16,28,31	3.36	4 (25%)
3	PYO	F	427	1,3	14,20,21	3.67	5 (35%)	16,28,31	3.15	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	E	427	1,3	-	2/5/25/26	0/2/2/2
3	PYO	F	427	1,3	-	2/5/25/26	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	427	PYO	C2'-C3'	-10.30	1.25	1.53
3	F	427	PYO	C6-N1	8.93	1.46	1.35
3	E	427	PYO	C6-N1	8.92	1.46	1.35
3	E	427	PYO	O4'-C1'	7.12	1.51	1.41
3	E	427	PYO	O4'-C4'	-6.64	1.30	1.45
3	F	427	PYO	C2-N3	6.37	1.50	1.38
3	E	427	PYO	C2-N3	6.05	1.50	1.38
3	E	427	PYO	C3'-C4'	5.26	1.66	1.53
3	F	427	PYO	C6-C5	5.17	1.50	1.38
3	E	427	PYO	C6-C5	4.96	1.49	1.38
3	E	427	PYO	C2'-C1'	4.94	1.61	1.53
3	F	427	PYO	C4-N3	4.83	1.44	1.34
3	E	427	PYO	C4-N3	4.76	1.44	1.34
3	E	427	PYO	O2'-C2'	4.25	1.53	1.43
3	F	427	PYO	C5-C4	4.03	1.49	1.37
3	E	427	PYO	C5-C4	4.03	1.49	1.37
3	E	427	PYO	O3'-C3'	3.04	1.50	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	427	PYO	C4-N3-C2	12.52	120.59	114.42
3	F	427	PYO	C4-N3-C2	11.93	120.30	114.42
3	E	427	PYO	C3'-C2'-C1'	3.18	105.77	100.98
3	F	427	PYO	C6-C5-C4	2.34	120.24	117.27
3	F	427	PYO	C5-C4-N3	-2.29	119.69	123.43
3	E	427	PYO	C5-C4-N3	-2.25	119.75	123.43
3	E	427	PYO	C6-C5-C4	2.12	119.97	117.27

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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
5	SAH	A	902	-	21,28,28	1.20	2 (9%)	20,40,40	1.69	2 (10%)
5	SAH	D	902	-	21,28,28	1.20	2 (9%)	20,40,40	1.70	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
5	SAH	A	902	-	-	2/7/31/31	0/3/3/3
5	SAH	D	902	-	-	2/7/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	902	SAH	C2-N3	3.98	1.38	1.32
5	D	902	SAH	C2-N3	3.94	1.38	1.32
5	A	902	SAH	C2-N1	2.50	1.38	1.33
5	D	902	SAH	C2-N1	2.49	1.38	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	902	SAH	N3-C2-N1	-5.48	120.11	128.68
5	A	902	SAH	N3-C2-N1	-5.47	120.13	128.68
5	D	902	SAH	C5'-SD-CG	-3.68	91.22	102.27
5	A	902	SAH	C5'-SD-CG	-3.57	91.55	102.27

There are no chirality outliers.

All (4) torsion outliers are listed below:

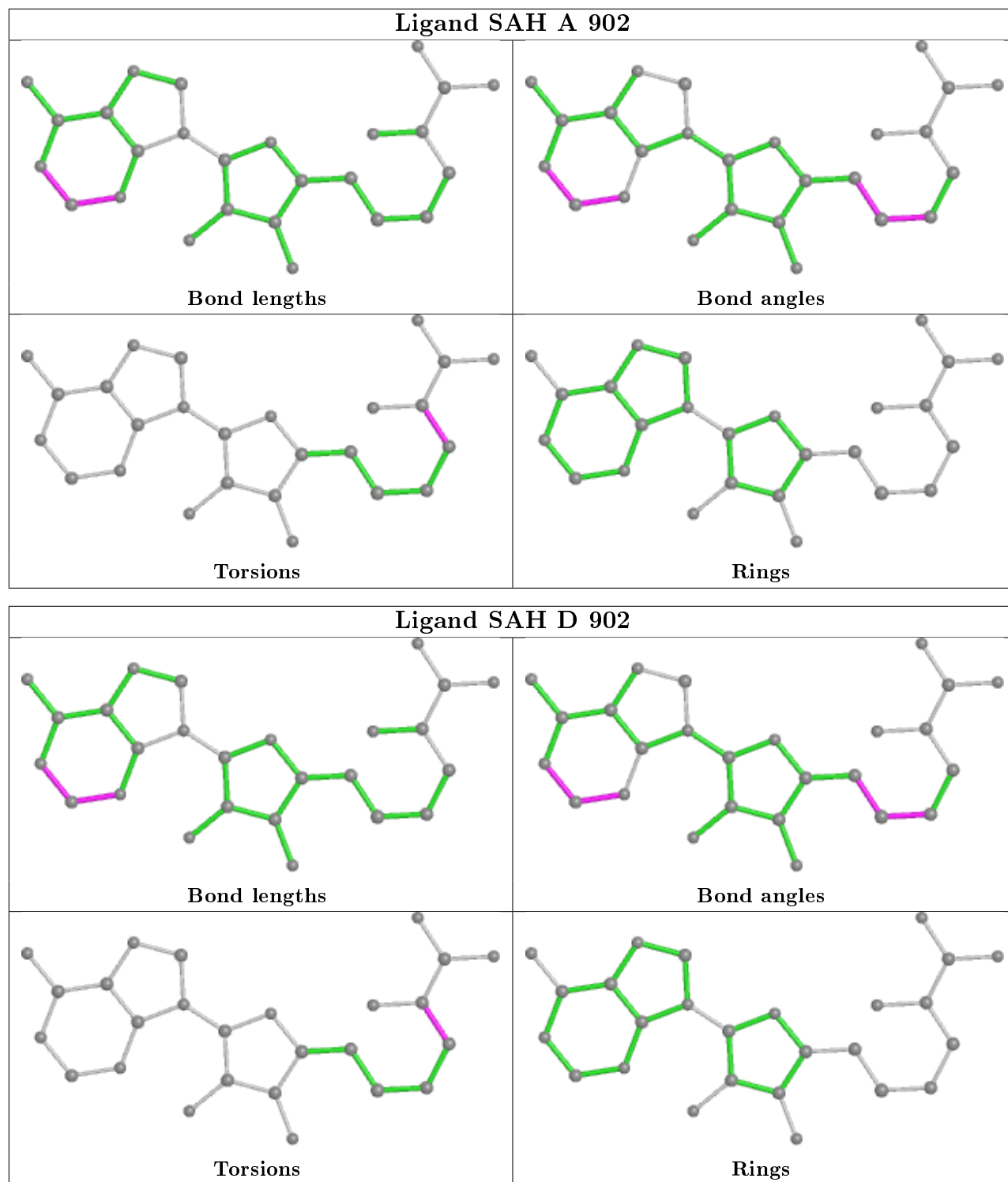
Mol	Chain	Res	Type	Atoms
5	A	902	SAH	N-CA-CB-CG
5	A	902	SAH	C-CA-CB-CG
5	D	902	SAH	N-CA-CB-CG
5	D	902	SAH	C-CA-CB-CG

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 ⓘ

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%)	0.20	0 100 100	33, 63, 103, 154	0
1	D	291/291 (100%)	0.23	1 (0%) 94 87	30, 65, 105, 145	0
2	B	189/209 (90%)	0.57	23 (12%) 4 2	76, 122, 186, 199	0
2	C	186/209 (88%)	0.50	14 (7%) 14 8	74, 122, 173, 186	0
3	E	24/25 (96%)	0.03	1 (4%) 36 23	94, 130, 136, 137	0
3	F	24/25 (96%)	-0.31	0 100 100	98, 132, 136, 137	0
All	All	1005/1050 (95%)	0.32	39 (3%) 39 25	30, 83, 167, 199	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	215	PRO	12.7
2	C	216	GLY	9.1
2	C	320	ALA	6.6
2	B	320	ALA	6.0
2	B	321	VAL	4.5
2	C	321	VAL	4.5
1	D	565	PRO	3.4
2	B	371	LEU	3.3
2	C	363	LEU	3.2
2	B	208	PHE	3.1
3	E	447	DG	3.0
2	B	330	ILE	3.0
2	B	222	VAL	2.9
2	B	240	LEU	2.9
2	C	377	TYR	2.7
2	B	215	PRO	2.7
2	B	368	PHE	2.6
2	B	309	ILE	2.6
2	C	184	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	378	PHE	2.5
2	B	249	GLY	2.4
2	C	235	TRP	2.4
2	C	336	ALA	2.4
2	B	209	LEU	2.4
2	C	190	VAL	2.3
2	C	266	LEU	2.3
2	B	284	PHE	2.3
2	C	364	VAL	2.3
2	C	214	ASP	2.3
2	B	308	THR	2.2
2	C	372	ARG	2.2
2	B	190	VAL	2.2
2	B	179	PHE	2.2
2	B	332	SER	2.1
2	B	192	VAL	2.1
2	B	324	TRP	2.1
2	B	377	TYR	2.1
2	B	203	LEU	2.0
2	B	214	ASP	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	F	427	19/20	0.93	0.20	82,82,87,89	0
3	PYO	E	427	19/20	0.96	0.20	82,82,84,90	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

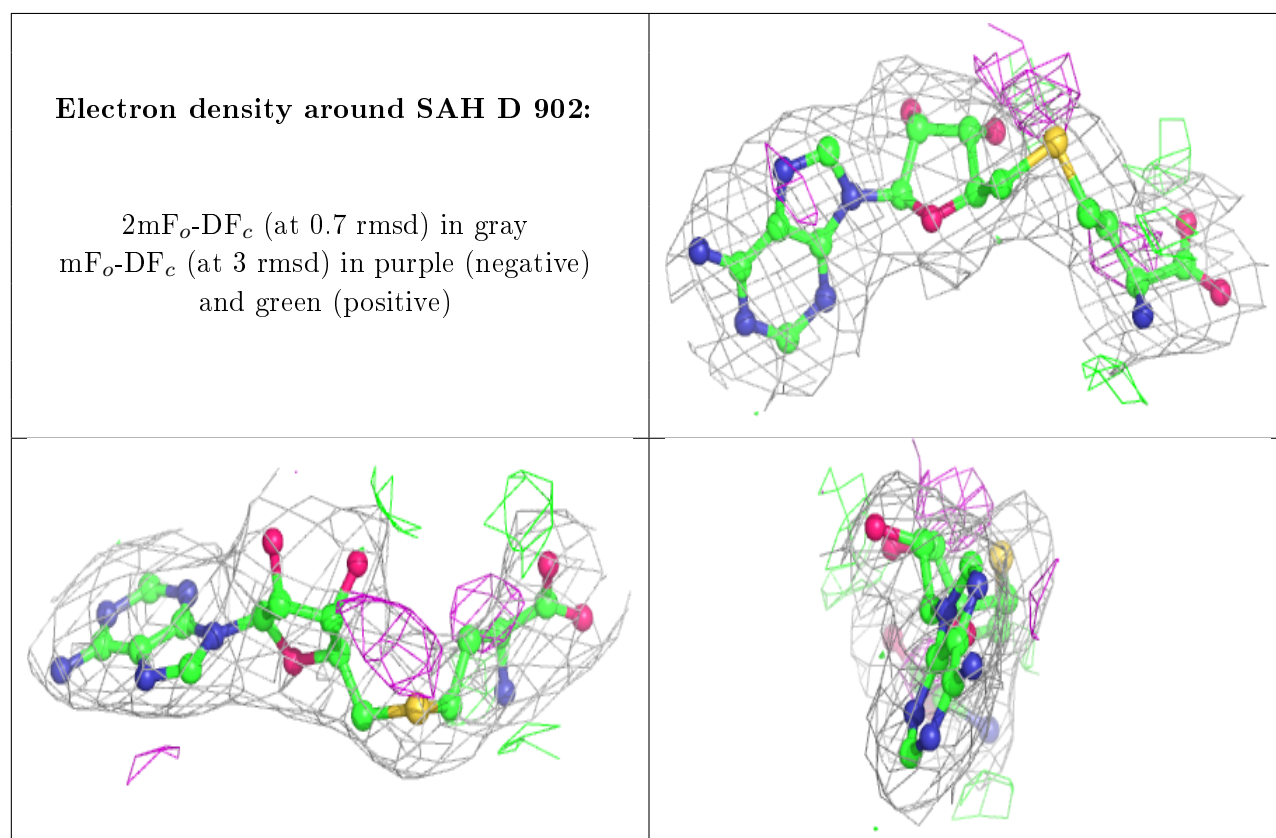
## 6.4 Ligands [i](#)

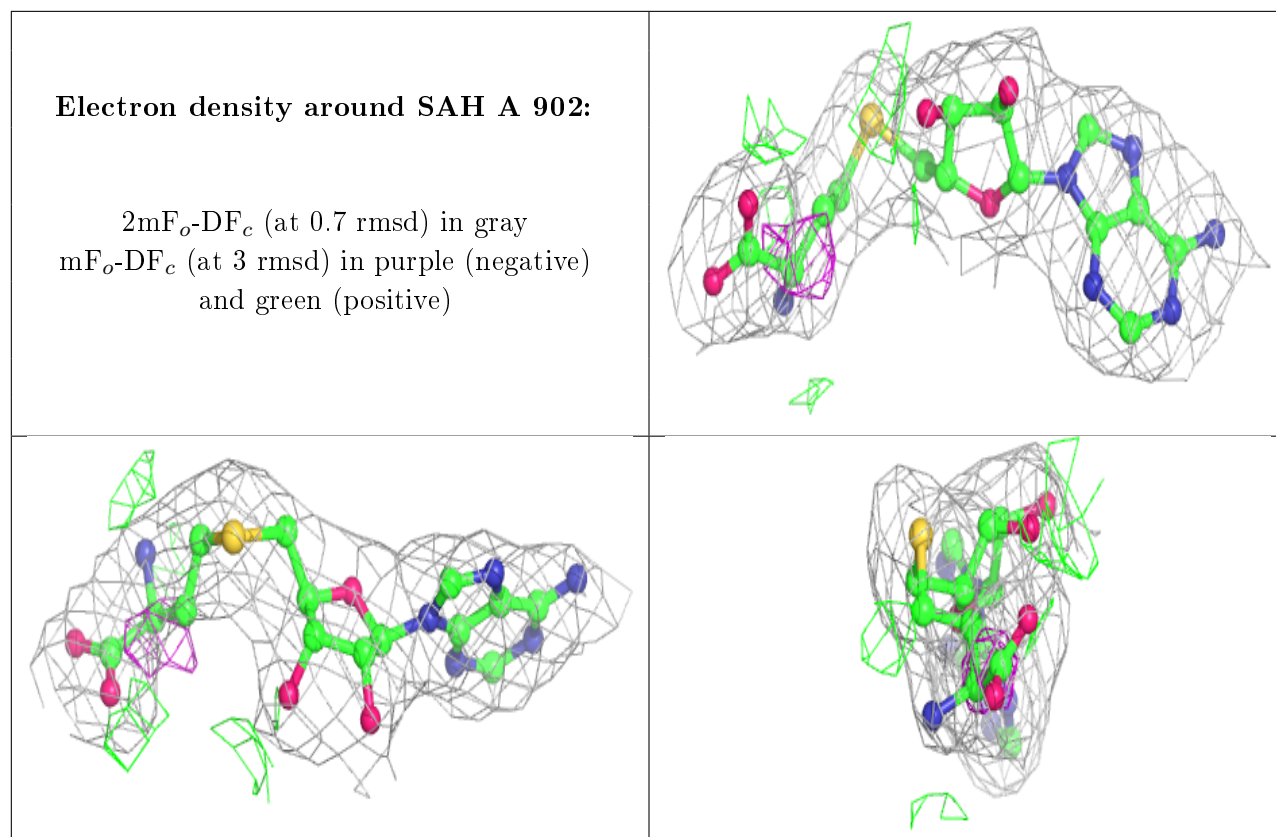
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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
4	MG	D	901	1/1	0.91	0.20	74,74,74,74	0
4	MG	A	901	1/1	0.92	0.22	69,69,69,69	0
5	SAH	D	902	26/26	0.95	0.20	33,52,55,57	0
5	SAH	A	902	26/26	0.96	0.22	30,52,56,59	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.