



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:15 pm BST

PDB ID : 6MBJ  
Title : SETD3, a Histidine Methyltransferase, in Complex with an Actin Peptide and SAH, P21 Crystal Form  
Authors : Horton, J.R.; Dai, S.; Cheng, X.  
Deposited on : 2018-08-30  
Resolution : 1.78 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 : 2.11  
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) : 2.11

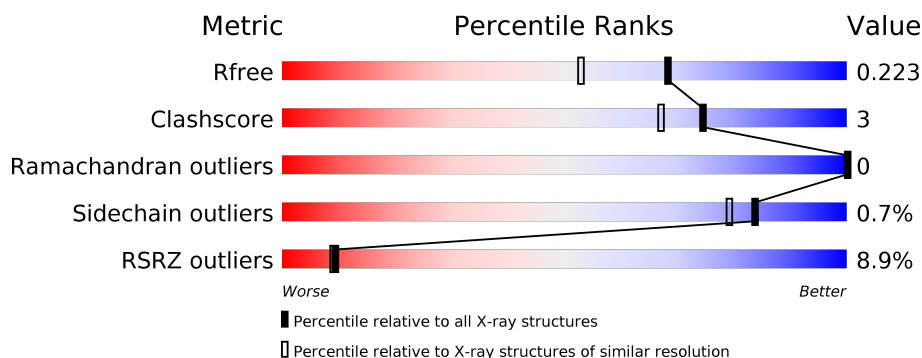
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	Y	15	<div> <div>33%</div> <div>100%</div> </div>
1	Z	15	<div> <div>27%</div> <div>80%</div> <div>20%</div> </div>
2	A	599	<div> <div>6%</div> <div>74%</div> <div>6%</div> <div>20%</div> </div>
2	B	599	<div> <div>7%</div> <div>75%</div> <div>6%</div> <div>19%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	605	-	-	-	X
3	EDO	A	613	-	-	-	X
3	EDO	B	1012	-	-	-	X
3	EDO	B	1016	-	-	X	X
5	GOL	A	622	-	-	-	X
6	ACT	A	624	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8891 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 Actin Peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	Y	15	Total	C	N	O	0	0	0
			124	82	20	22			
1	Z	15	Total	C	N	O	0	0	0
			124	82	20	22			

- Molecule 2 is a protein called Histone-lysine N-methyltransferase setd3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	481	Total	C	N	O	S	0	10	0
			3916	2505	663	729	19			
2	B	483	Total	C	N	O	S	0	5	0
			3898	2495	656	729	18			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q86TU7
A	-4	PRO	-	expression tag	UNP Q86TU7
A	-3	LEU	-	expression tag	UNP Q86TU7
A	-2	GLY	-	expression tag	UNP Q86TU7
A	-1	SER	-	expression tag	UNP Q86TU7
B	-5	GLY	-	expression tag	UNP Q86TU7
B	-4	PRO	-	expression tag	UNP Q86TU7
B	-3	LEU	-	expression tag	UNP Q86TU7
B	-2	GLY	-	expression tag	UNP Q86TU7
B	-1	SER	-	expression tag	UNP Q86TU7

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



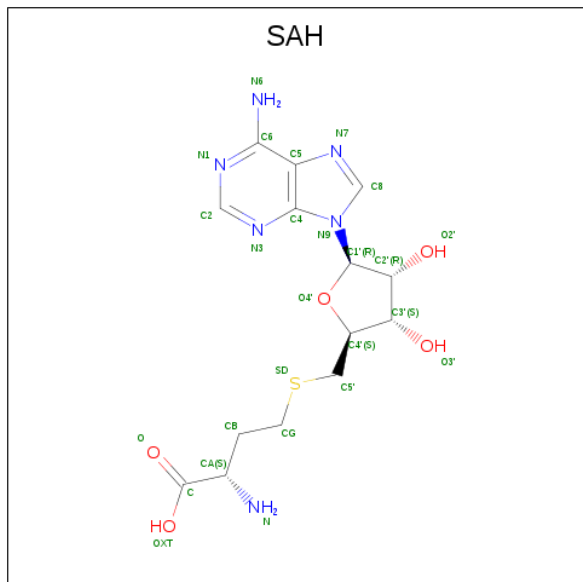
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	Y	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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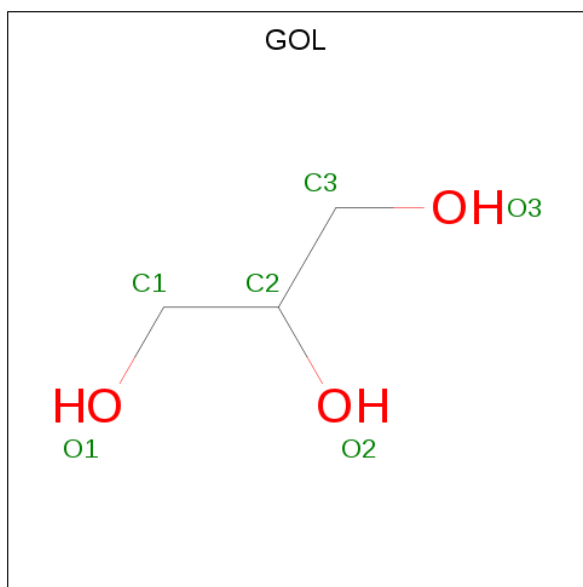
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0

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



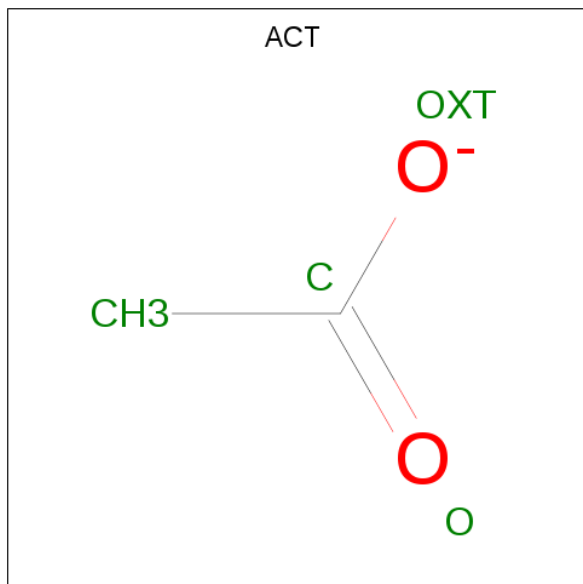
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
4	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0

- Molecule 7 is water.

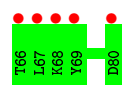
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	Y	11	Total O 11 11	0	0
7	A	304	Total O 304 304	0	0
7	Z	13	Total O 13 13	0	0
7	B	283	Total O 283 283	0	0



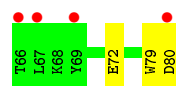
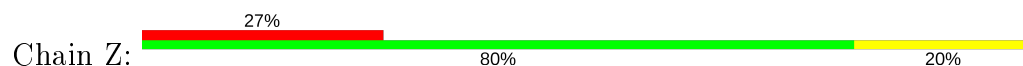
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

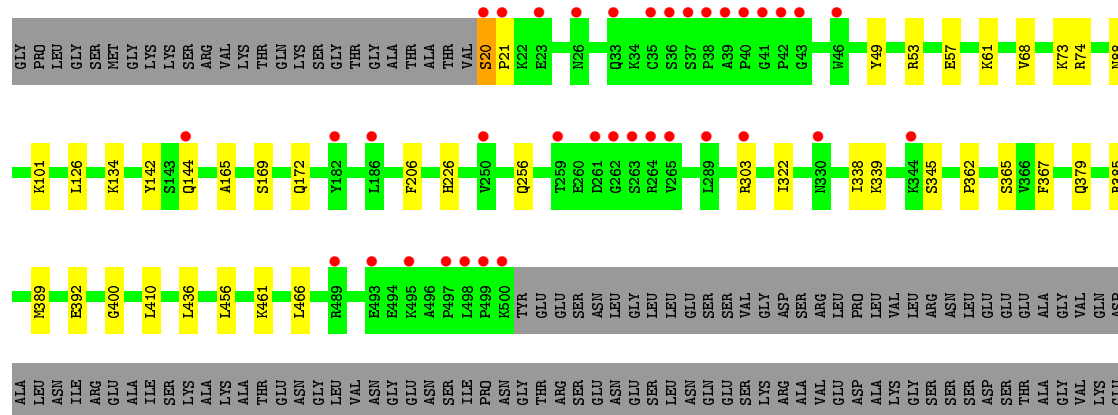
- Molecule 1: Actin Peptide



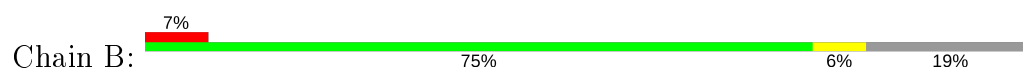
- Molecule 1: Actin Peptide

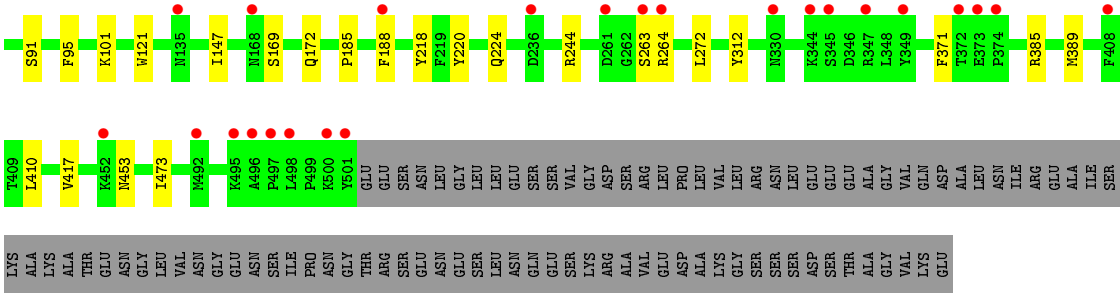


- Molecule 2: Histone-lysine N-methyltransferase setd3



- Molecule 2: Histone-lysine N-methyltransferase setd3





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.35Å 176.17Å 66.58Å 90.00° 92.86° 90.00°	Depositor
Resolution (Å)	39.07 – 1.78 39.07 – 1.78	Depositor EDS
% Data completeness (in resolution range)	93.5 (39.07-1.78) 93.5 (39.07-1.78)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 1.78Å)	Xtriage
Refinement program	PHENIX (1.13_2998)	Depositor
R, $R_{free}$	0.199 , 0.223 0.199 , 0.223	Depositor DCC
$R_{free}$ test set	1992 reflections (1.61%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.2	Xtriage
Anisotropy	0.657	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.047 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8891	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SAH, EDO, ACT

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	Y	0.26	0/128	0.50	0/175
1	Z	0.23	0/128	0.52	0/175
2	A	0.26	0/4033	0.42	0/5461
2	B	0.26	0/3996	0.42	0/5415
All	All	0.26	0/8285	0.42	0/11226

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Y	124	0	115	0	0
1	Z	124	0	115	2	0
2	A	3916	0	3846	33	0
2	B	3898	0	3802	22	0
3	A	72	0	108	7	0
3	B	64	0	96	5	0
3	Y	4	0	6	0	0
4	A	26	0	19	0	0
4	B	26	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	18	0	24	3	0
6	A	8	0	6	3	0
7	A	304	0	0	3	0
7	B	283	0	0	0	0
7	Y	11	0	0	0	0
7	Z	13	0	0	0	0
All	All	8891	0	8156	53	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 3.

All (53) 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:A:101:LYS:HD2	2:B:101:LYS:HE2	1.57	0.85
2:A:456:LEU:H	3:A:609:EDO:H22	1.51	0.74
2:A:461:LYS:NZ	7:A:703:HOH:O	2.27	0.67
2:A:20:SER:N	2:A:21:PRO:HD2	2.11	0.65
2:A:101:LYS:HE3	2:B:101:LYS:HG3	1.85	0.59
2:B:244:ARG:HH22	3:B:1016:EDO:H21	1.68	0.58
2:B:263:SER:OG	2:B:264:ARG:NH1	2.40	0.54
2:A:144:GLN:HG2	2:A:226:HIS:HD2	1.76	0.51
2:A:400:GLY:HA3	3:A:619:EDO:H12	1.93	0.50
2:A:20:SER:N	2:A:21:PRO:CD	2.74	0.50
2:B:244:ARG:NH2	3:B:1016:EDO:H21	2.27	0.50
2:A:379:GLN:NE2	7:A:717:HOH:O	2.45	0.50
2:A:461:LYS:NZ	3:A:609:EDO:H21	2.27	0.49
2:A:73:LYS:HD2	3:B:1016:EDO:H22	1.93	0.49
2:A:338:ILE:HA	5:A:622:GOL:H11	1.96	0.48
2:A:169:SER:HB3	2:A:172:GLN:HG2	1.94	0.48
2:B:147:ILE:HD12	2:B:218:TYR:CE2	2.49	0.48
2:B:60:ARG:CZ	3:B:1016:EDO:H11	2.44	0.48
2:B:30:GLU:HG2	2:B:55:LEU:HD11	1.96	0.48
2:A:339:LYS:HB3	5:A:622:GOL:H2	1.97	0.47
2:A:466:LEU:HD12	3:A:603:EDO:H21	1.96	0.47
2:B:417:VAL:HA	3:B:1015:EDO:H12	1.97	0.47
1:Z:72:GLU:HG3	2:B:312:TYR:O	2.17	0.45
2:A:303:ARG:NH2	2:B:453:ASN:HB3	2.32	0.45
2:A:68:VAL:HG21	2:A:165:ALA:HA	1.99	0.45
2:A:436:LEU:HD21	5:A:622:GOL:H31	1.98	0.44
2:A:206:PHE:HE2	6:A:624:ACT:H2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:256:GLN:NE2	7:A:705:HOH:O	2.33	0.44
2:A:410:LEU:HD12	2:A:410:LEU:HA	1.87	0.44
2:B:49:TYR:CZ	2:B:53:ARG:HD2	2.53	0.44
2:B:169:SER:HB3	2:B:172:GLN:HG2	2.00	0.43
2:A:392:GLU:H	2:A:392:GLU:CD	2.22	0.43
2:B:220:TYR:O	2:B:224:GLN:HG2	2.18	0.43
2:A:456:LEU:H	3:A:609:EDO:C2	2.26	0.43
2:B:371:PHE:HB2	2:B:473:ILE:HG12	2.01	0.42
2:A:101:LYS:CD	2:B:101:LYS:HE2	2.40	0.42
2:A:88:ASN:HB2	2:A:126:LEU:HD21	2.01	0.42
2:A:385:ARG:O	2:A:389:MET:HG3	2.18	0.42
2:A:367:PHE:HA	6:A:623:ACT:H1	2.00	0.42
2:B:57:GLU:O	2:B:61:LYS:HG3	2.19	0.42
2:A:134:LYS:NZ	2:A:142:TYR:OH	2.38	0.41
2:A:49:TYR:CZ	2:A:53:ARG:HD2	2.55	0.41
2:B:264:ARG:CZ	2:B:264:ARG:HB2	2.49	0.41
2:A:322:ILE:HD12	3:A:604:EDO:H11	2.02	0.41
2:A:362:PRO:HG2	2:A:365:SER:HB2	2.02	0.41
2:A:206:PHE:CE2	6:A:624:ACT:H2	2.55	0.41
2:B:185:PRO:HA	2:B:188:PHE:CD1	2.55	0.41
2:B:91:SER:HB3	2:B:121:TRP:CE2	2.56	0.41
2:A:57:GLU:O	2:A:61:LYS:HG2	2.21	0.40
2:B:95:PHE:CE1	2:B:272:LEU:HD21	2.56	0.40
2:B:385:ARG:O	2:B:389:MET:HG3	2.21	0.40
1:Z:79:TRP:O	1:Z:80:ASP:HB3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	13/15 (87%)	13 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	13/15 (87%)	13 (100%)	0	0	100	100
2	A	489/599 (82%)	483 (99%)	6 (1%)	0	100	100
2	B	486/599 (81%)	480 (99%)	6 (1%)	0	100	100
All	All	1001/1228 (82%)	989 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Y	13/14 (93%)	13 (100%)	0	100	100
1	Z	13/14 (93%)	13 (100%)	0	100	100
2	A	424/521 (81%)	421 (99%)	3 (1%)	84	79
2	B	418/521 (80%)	415 (99%)	3 (1%)	84	79
All	All	868/1070 (81%)	862 (99%)	6 (1%)	84	79

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	20	SER
2	A	74	ARG
2	A	345	SER
2	B	33	GLN
2	B	74	ARG
2	B	410	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

42 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	$\# Z  > 2$
3	EDO	B	1002	-	3,3,3	0.44	0	2,2,2	0.30	0
3	EDO	B	1014	-	3,3,3	0.47	0	2,2,2	0.24	0
3	EDO	B	1003	-	3,3,3	0.46	0	2,2,2	0.28	0
3	EDO	A	605	-	3,3,3	0.43	0	2,2,2	0.32	0
3	EDO	B	1016	-	3,3,3	0.48	0	2,2,2	0.40	0
3	EDO	A	615	-	3,3,3	0.46	0	2,2,2	0.30	0
6	ACT	A	623	-	1,3,3	1.27	0	0,3,3	0.00	-
3	EDO	Y	101	-	3,3,3	0.46	0	2,2,2	0.33	0
3	EDO	B	1015	-	3,3,3	0.46	0	2,2,2	0.27	0
3	EDO	B	1009	-	3,3,3	0.45	0	2,2,2	0.34	0
3	EDO	A	603	-	3,3,3	0.43	0	2,2,2	0.50	0
4	SAH	A	601	-	21,28,28	1.20	2 (9%)	20,40,40	1.63	3 (15%)
5	GOL	A	622	-	5,5,5	0.92	0	5,5,5	0.98	0
3	EDO	A	619	-	3,3,3	0.43	0	2,2,2	0.41	0
3	EDO	A	614	-	3,3,3	0.46	0	2,2,2	0.35	0
3	EDO	A	602	-	3,3,3	0.46	0	2,2,2	0.33	0
3	EDO	B	1017	-	3,3,3	0.46	0	2,2,2	0.31	0
3	EDO	B	1013	-	3,3,3	0.46	0	2,2,2	0.27	0
4	SAH	B	1001	-	21,28,28	1.18	2 (9%)	20,40,40	1.63	3 (15%)
3	EDO	A	613	-	3,3,3	0.46	0	2,2,2	0.33	0
3	EDO	A	616	-	3,3,3	0.46	0	2,2,2	0.32	0
3	EDO	A	618	-	3,3,3	0.44	0	2,2,2	0.37	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	A	608	-	3,3,3	0.44	0	2,2,2	0.37	0
3	EDO	B	1011	-	3,3,3	0.46	0	2,2,2	0.33	0
3	EDO	B	1007	-	3,3,3	0.45	0	2,2,2	0.43	0
5	GOL	A	621	-	5,5,5	0.82	0	5,5,5	1.08	0
6	ACT	A	624	-	1,3,3	1.36	0	0,3,3	0.00	-
3	EDO	B	1010	-	3,3,3	0.44	0	2,2,2	0.34	0
3	EDO	B	1005	-	3,3,3	0.45	0	2,2,2	0.41	0
3	EDO	B	1008	-	3,3,3	0.46	0	2,2,2	0.35	0
3	EDO	B	1006	-	3,3,3	0.46	0	2,2,2	0.31	0
3	EDO	A	610	-	3,3,3	0.43	0	2,2,2	0.32	0
3	EDO	A	606	-	3,3,3	0.45	0	2,2,2	0.34	0
3	EDO	B	1004	-	3,3,3	0.46	0	2,2,2	0.36	0
3	EDO	A	611	-	3,3,3	0.45	0	2,2,2	0.33	0
3	EDO	A	604	-	3,3,3	0.46	0	2,2,2	0.29	0
5	GOL	A	620	-	5,5,5	0.92	0	5,5,5	1.00	0
3	EDO	B	1012	-	3,3,3	0.44	0	2,2,2	0.34	0
3	EDO	A	612	-	3,3,3	0.45	0	2,2,2	0.34	0
3	EDO	A	609	-	3,3,3	0.44	0	2,2,2	0.26	0
3	EDO	A	607	-	3,3,3	0.45	0	2,2,2	0.35	0
3	EDO	A	617	-	3,3,3	0.45	0	2,2,2	0.31	0

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	EDO	B	1002	-	-	0/1/1/1	-
3	EDO	B	1014	-	-	0/1/1/1	-
3	EDO	B	1003	-	-	0/1/1/1	-
3	EDO	A	605	-	-	0/1/1/1	-
3	EDO	B	1016	-	-	0/1/1/1	-
3	EDO	A	615	-	-	0/1/1/1	-
3	EDO	Y	101	-	-	0/1/1/1	-
3	EDO	B	1015	-	-	0/1/1/1	-
3	EDO	B	1009	-	-	1/1/1/1	-
3	EDO	A	603	-	-	1/1/1/1	-
4	SAH	A	601	-	-	3/7/31/31	0/3/3/3
5	GOL	A	622	-	-	2/4/4/4	-
3	EDO	A	619	-	-	1/1/1/1	-
3	EDO	A	614	-	-	0/1/1/1	-
3	EDO	A	602	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	1017	-	-	0/1/1/1	-
3	EDO	B	1013	-	-	0/1/1/1	-
4	SAH	B	1001	-	-	3/7/31/31	0/3/3/3
3	EDO	A	613	-	-	0/1/1/1	-
3	EDO	A	616	-	-	0/1/1/1	-
3	EDO	A	618	-	-	0/1/1/1	-
3	EDO	A	608	-	-	0/1/1/1	-
3	EDO	B	1011	-	-	0/1/1/1	-
3	EDO	B	1007	-	-	1/1/1/1	-
5	GOL	A	621	-	-	4/4/4/4	-
3	EDO	B	1010	-	-	0/1/1/1	-
3	EDO	B	1005	-	-	0/1/1/1	-
3	EDO	B	1008	-	-	0/1/1/1	-
3	EDO	B	1006	-	-	0/1/1/1	-
3	EDO	A	610	-	-	0/1/1/1	-
3	EDO	A	606	-	-	0/1/1/1	-
3	EDO	B	1004	-	-	0/1/1/1	-
3	EDO	A	611	-	-	0/1/1/1	-
3	EDO	A	604	-	-	0/1/1/1	-
5	GOL	A	620	-	-	0/4/4/4	-
3	EDO	B	1012	-	-	0/1/1/1	-
3	EDO	A	612	-	-	1/1/1/1	-
3	EDO	A	609	-	-	1/1/1/1	-
3	EDO	A	607	-	-	0/1/1/1	-
3	EDO	A	617	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	SAH	C2-N3	3.90	1.38	1.32
4	B	1001	SAH	C2-N3	3.89	1.38	1.32
4	A	601	SAH	C2-N1	2.48	1.38	1.33
4	B	1001	SAH	C2-N1	2.37	1.38	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	SAH	N3-C2-N1	-5.45	120.17	128.68
4	B	1001	SAH	N3-C2-N1	-5.37	120.29	128.68
4	B	1001	SAH	C5'-SD-CG	-3.04	93.13	102.27
4	A	601	SAH	C5'-SD-CG	-2.80	93.87	102.27
4	B	1001	SAH	C3'-C2'-C1'	2.48	104.71	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	SAH	C3'-C2'-C1'	2.37	104.54	100.98

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	621	GOL	O1-C1-C2-O2
5	A	621	GOL	O1-C1-C2-C3
5	A	622	GOL	O2-C2-C3-O3
5	A	622	GOL	C1-C2-C3-O3
5	A	621	GOL	C1-C2-C3-O3
3	A	619	EDO	O1-C1-C2-O2
3	B	1007	EDO	O1-C1-C2-O2
4	A	601	SAH	C3'-C4'-C5'-SD
4	B	1001	SAH	C3'-C4'-C5'-SD
4	A	601	SAH	O4'-C4'-C5'-SD
4	B	1001	SAH	O4'-C4'-C5'-SD
4	B	1001	SAH	CB-CG-SD-C5'
4	A	601	SAH	CB-CG-SD-C5'
5	A	621	GOL	O2-C2-C3-O3
3	A	609	EDO	O1-C1-C2-O2
3	B	1009	EDO	O1-C1-C2-O2
3	A	612	EDO	O1-C1-C2-O2
3	A	603	EDO	O1-C1-C2-O2

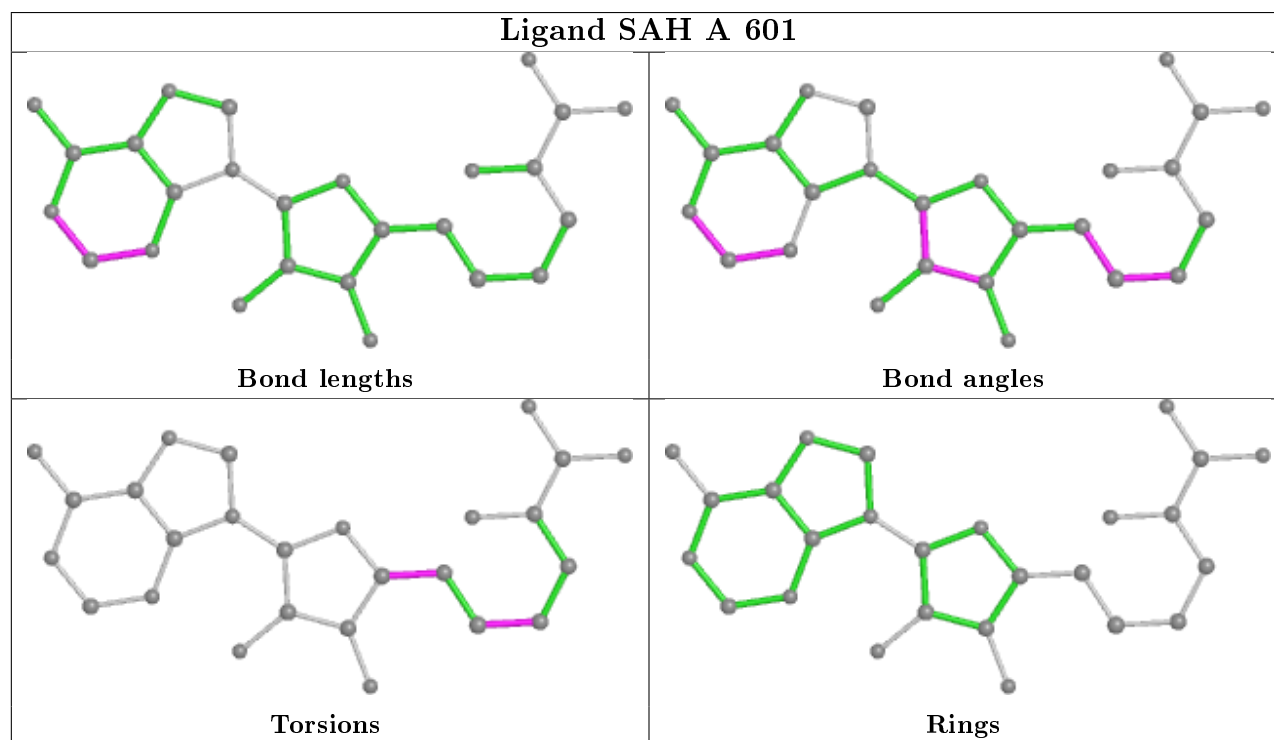
There are no ring outliers.

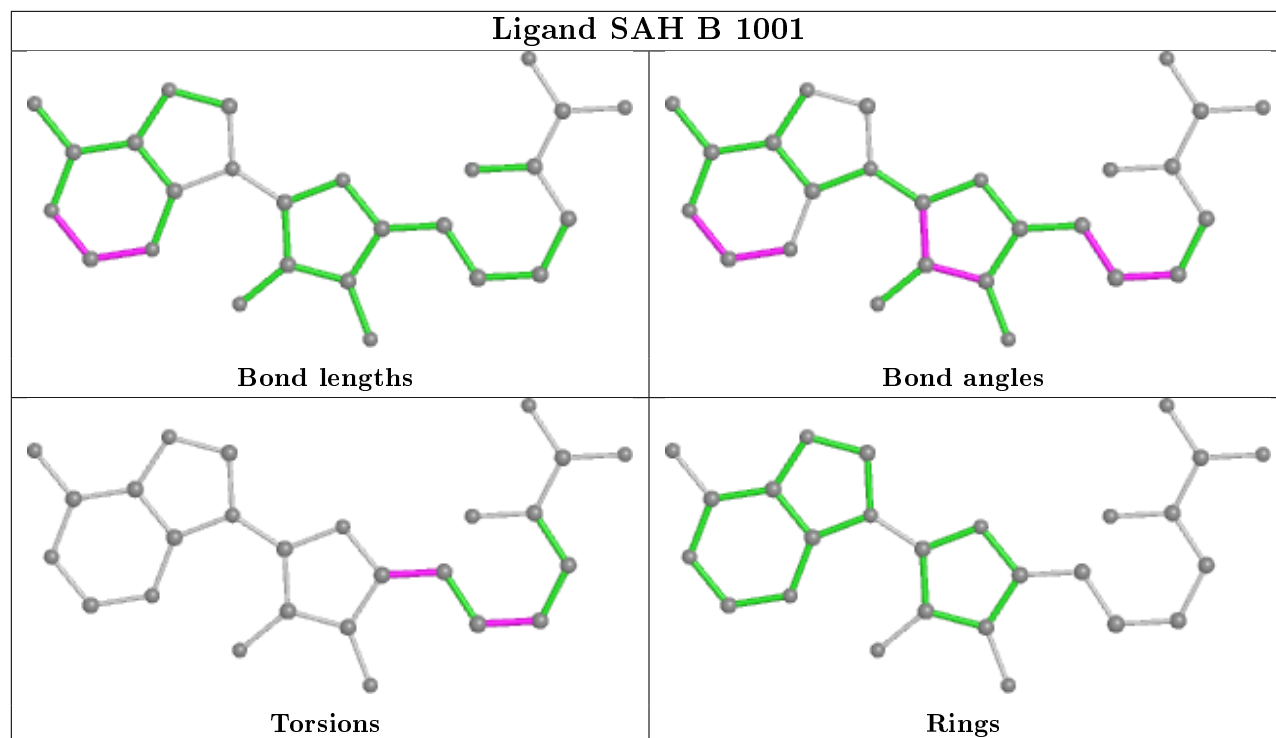
10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1016	EDO	4	0
6	A	623	ACT	1	0
3	B	1015	EDO	1	0
3	A	603	EDO	1	0
5	A	622	GOL	3	0
3	A	619	EDO	1	0
3	A	608	EDO	1	0
6	A	624	ACT	2	0
3	A	604	EDO	1	0
3	A	609	EDO	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [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	Y	15/15 (100%)	1.56	5 (33%) 0 0	18, 32, 64, 67	0
1	Z	15/15 (100%)	1.22	4 (26%) 0 0	26, 38, 66, 76	0
2	A	481/599 (80%)	0.53	36 (7%) 14 13	17, 30, 53, 74	0
2	B	483/599 (80%)	0.56	43 (8%) 9 9	18, 34, 62, 86	0
All	All	994/1228 (80%)	0.57	88 (8%) 9 9	17, 32, 59, 86	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	501	TYR	8.8
2	B	19	VAL	8.3
1	Y	66	THR	8.1
2	A	21	PRO	7.1
1	Z	66	THR	6.5
2	A	41	GLY	6.4
2	B	39	ALA	6.4
2	B	261	ASP	6.2
2	B	21	PRO	6.1
2	A	39	ALA	6.1
2	A	38	PRO	5.6
2	A	35	CYS	5.4
2	B	38	PRO	5.3
2	B	264	ARG	5.1
2	A	20	SER	5.1
2	B	408	PHE	4.8
2	A	37	SER	4.8
1	Z	80	ASP	4.7
2	B	20	SER	4.7
2	A	261	ASP	4.7
2	A	264	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
2	B	37	SER	4.3
2	B	33	GLN	4.2
2	A	263	SER	4.1
2	B	263	SER	4.0
1	Y	67	LEU	3.8
2	B	35	CYS	3.7
2	B	495	LYS	3.7
2	B	496	ALA	3.6
2	B	498	LEU	3.6
2	A	330	ASN	3.3
2	A	40	PRO	3.3
2	B	236	ASP	3.2
2	A	42	PRO	3.2
2	A	289	LEU	3.2
1	Y	69	TYR	3.0
2	A	33	GLN	3.0
2	B	41	GLY	3.0
2	B	373	GLU	3.0
2	B	345	SER	3.0
2	A	499	PRO	3.0
1	Y	80	ASP	3.0
2	B	40	PRO	3.0
2	A	495	LYS	2.9
1	Y	68	LYS	2.9
2	B	36	SER	2.9
2	B	30	GLU	2.9
2	A	36	SER	2.9
2	A	498	LEU	2.8
2	A	262	GLY	2.7
2	B	34	LYS	2.7
2	B	344	LYS	2.7
2	B	22	LYS	2.7
2	B	27	LEU	2.6
2	B	497	PRO	2.6
2	B	374	PRO	2.6
2	B	23	GLU	2.6
2	B	372	THR	2.5
1	Z	67	LEU	2.5
2	A	186	LEU	2.5
2	A	23	GLU	2.4
2	A	497	PRO	2.4
2	A	489	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	250	VAL	2.4
2	A	144	GLN	2.4
2	B	347	ARG	2.4
2	B	31	LEU	2.3
2	A	303	ARG	2.3
2	B	168	ASN	2.3
2	A	344	LYS	2.3
2	A	500	LYS	2.3
2	B	452	LYS	2.3
2	A	46	TRP	2.3
1	Z	69	TYR	2.3
2	B	29	SER	2.2
2	A	493	GLU	2.2
2	A	182	TYR	2.2
2	B	349	TYR	2.2
2	A	43	GLY	2.2
2	B	330	ASN	2.2
2	B	492	MET	2.2
2	B	25	LEU	2.1
2	A	265	VAL	2.1
2	B	500	LYS	2.1
2	A	26	ASN	2.0
2	B	188	PHE	2.0
2	A	259	THR	2.0
2	B	135	ASN	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

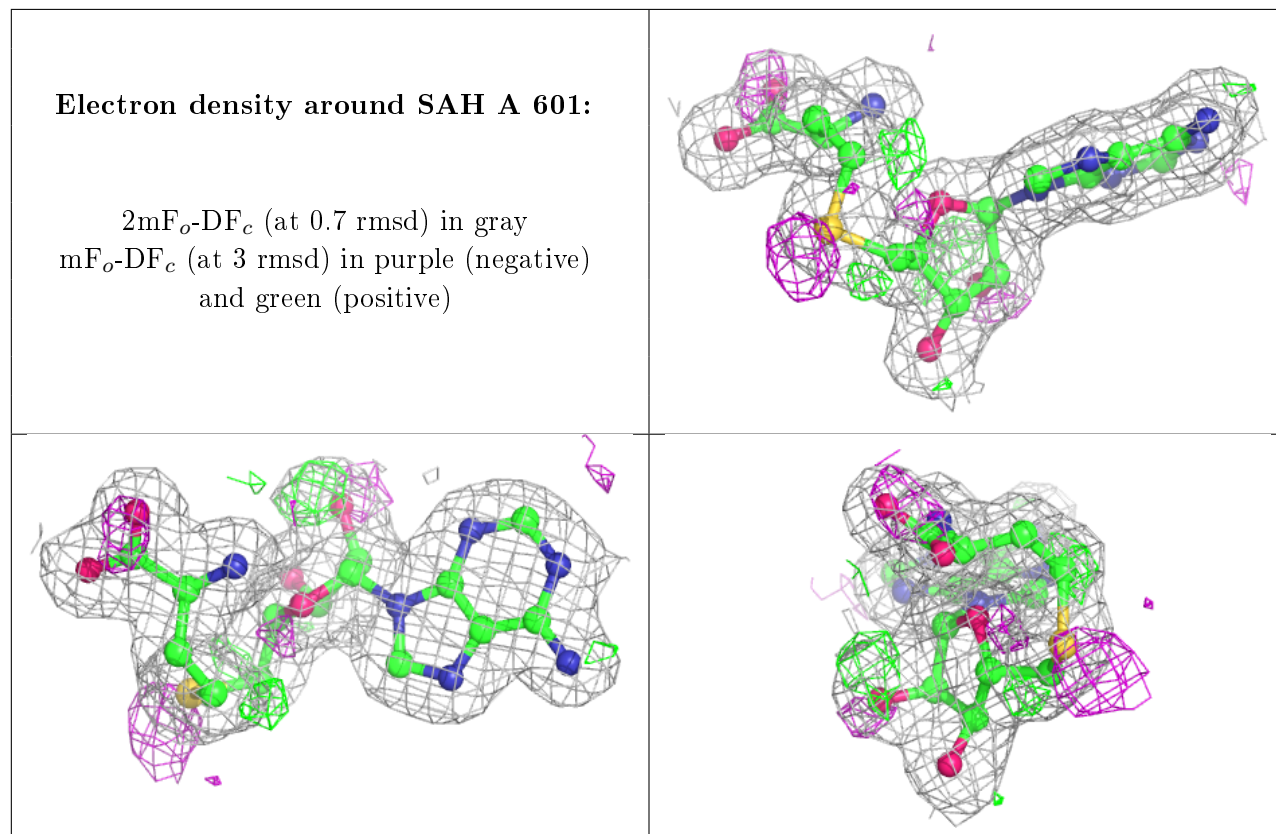
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	A	622	6/6	0.48	0.40	89,90,90,90	0
3	EDO	B	1012	4/4	0.48	0.59	78,78,79,79	0
3	EDO	B	1016	4/4	0.57	0.45	77,77,77,77	0
3	EDO	A	605	4/4	0.61	0.44	71,71,71,71	0
3	EDO	B	1006	4/4	0.63	0.37	70,70,70,71	0
5	GOL	A	620	6/6	0.63	0.25	73,73,73,73	0
3	EDO	A	613	4/4	0.63	0.49	88,88,88,89	0
3	EDO	A	609	4/4	0.65	0.22	62,62,62,62	0
3	EDO	A	607	4/4	0.66	0.28	63,63,63,63	0
3	EDO	A	612	4/4	0.68	0.28	81,81,81,82	0
3	EDO	B	1007	4/4	0.69	0.33	63,63,63,63	0
3	EDO	B	1002	4/4	0.71	0.23	52,52,52,52	0
3	EDO	A	619	4/4	0.71	0.20	59,59,59,59	0
5	GOL	A	621	6/6	0.73	0.35	58,58,59,59	0
3	EDO	A	617	4/4	0.73	0.32	82,82,82,82	0
3	EDO	B	1015	4/4	0.75	0.20	75,75,75,75	0
3	EDO	B	1009	4/4	0.77	0.16	62,62,63,63	0
3	EDO	Y	101	4/4	0.78	0.12	59,59,59,59	0
3	EDO	B	1013	4/4	0.80	0.22	53,53,53,53	0
3	EDO	A	608	4/4	0.81	0.33	67,67,67,67	0
3	EDO	A	610	4/4	0.81	0.28	64,64,64,64	0
3	EDO	B	1004	4/4	0.83	0.22	65,65,65,65	0
3	EDO	B	1017	4/4	0.84	0.27	63,63,63,63	0
6	ACT	A	623	4/4	0.84	0.15	47,47,47,48	0
3	EDO	B	1010	4/4	0.84	0.17	57,57,57,57	0
3	EDO	B	1011	4/4	0.85	0.17	73,73,73,73	0
3	EDO	B	1014	4/4	0.86	0.24	59,59,60,60	0
3	EDO	B	1005	4/4	0.86	0.14	52,52,52,52	0
3	EDO	B	1008	4/4	0.86	0.11	48,48,48,48	0
3	EDO	A	614	4/4	0.86	0.12	57,57,57,57	0
3	EDO	A	602	4/4	0.86	0.23	57,57,57,57	0
3	EDO	A	618	4/4	0.86	0.24	65,65,65,65	0
3	EDO	A	616	4/4	0.87	0.25	75,75,75,75	0
3	EDO	A	603	4/4	0.87	0.18	42,42,42,42	0
3	EDO	A	615	4/4	0.88	0.15	53,53,53,53	0
3	EDO	A	606	4/4	0.90	0.10	54,54,54,54	0
3	EDO	A	604	4/4	0.91	0.19	49,50,50,50	0
3	EDO	A	611	4/4	0.92	0.14	40,40,40,41	0
3	EDO	B	1003	4/4	0.92	0.17	56,56,56,56	0
6	ACT	A	624	4/4	0.93	0.27	71,71,71,71	0
4	SAH	A	601	26/26	0.95	0.11	15,17,20,21	0
4	SAH	B	1001	26/26	0.96	0.10	16,18,19,20	0

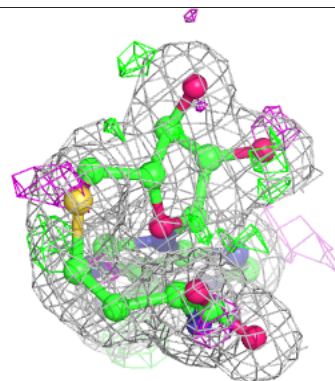
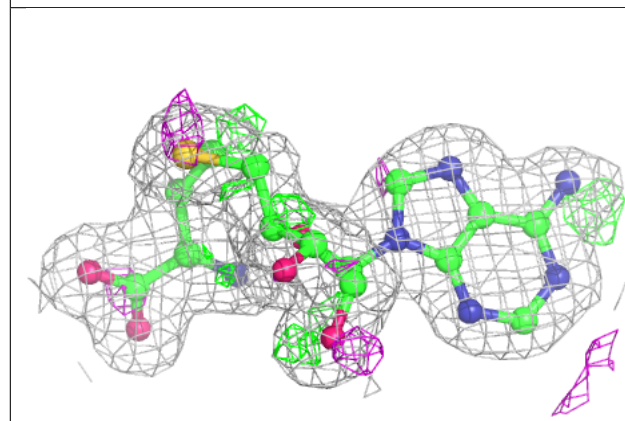
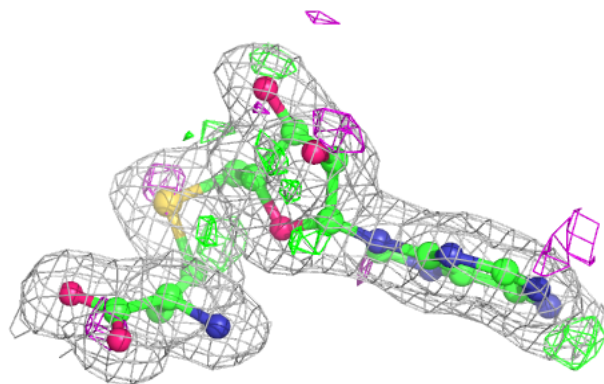
The following is a graphical depiction of the model fit to experimental electron density of all

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



**Electron density around SAH B 1001:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.