



# Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 12:12 am BST

PDB ID : 6CX6  
Title : The structure of an As(III) S-adenosylmethionine methyltransferase with As(III) and S-adenosyl-L-homocysteine (SAH)  
Authors : Packianathan, C.; Kandavelu, P.; Rosen, B.P.  
Deposited on : 2018-04-02  
Resolution : 2.84 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

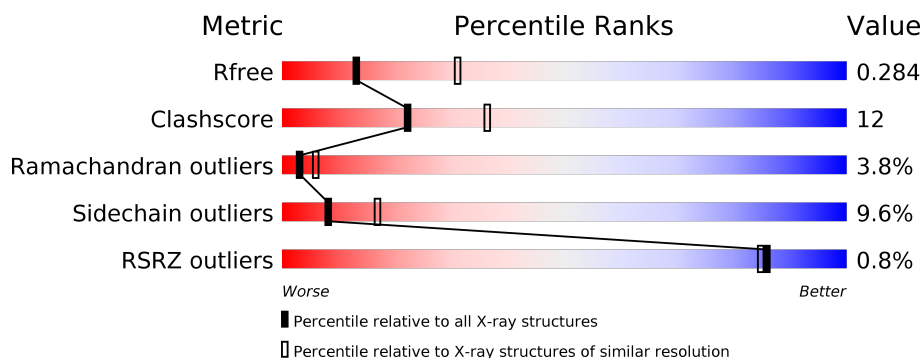
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.84 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	377	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 19%, green 62%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>62%</span> <span>20%</span> <span>5%</span> <span>12%</span> </div> </div>
1	B	377	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 61%, yellow 23%, orange 5%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>61%</span> <span>23%</span> <span>5%</span> <span>12%</span> </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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ARS	B	402	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5274 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.

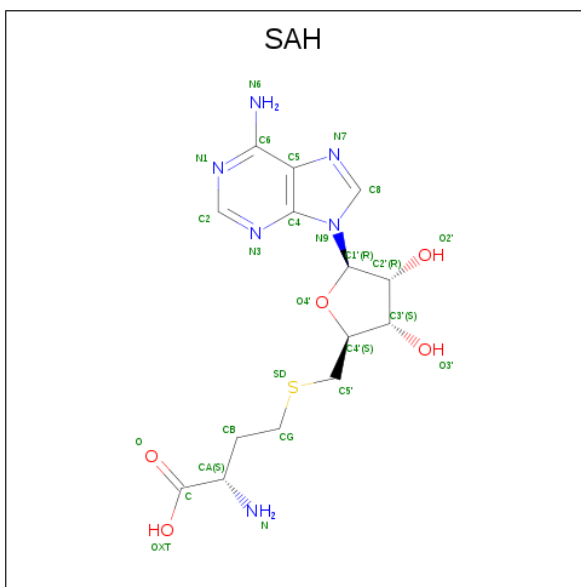
- Molecule 1 is a protein called Arsenic methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2569	1623	445	490	11			
1	B	333	Total	C	N	O	S	0	0	0
			2604	1648	451	494	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	371	SER	-	expression tag	UNP C0JV69
A	372	HIS	-	expression tag	UNP C0JV69
A	373	HIS	-	expression tag	UNP C0JV69
A	374	HIS	-	expression tag	UNP C0JV69
A	375	HIS	-	expression tag	UNP C0JV69
A	376	HIS	-	expression tag	UNP C0JV69
A	377	HIS	-	expression tag	UNP C0JV69
B	371	SER	-	expression tag	UNP C0JV69
B	372	HIS	-	expression tag	UNP C0JV69
B	373	HIS	-	expression tag	UNP C0JV69
B	374	HIS	-	expression tag	UNP C0JV69
B	375	HIS	-	expression tag	UNP C0JV69
B	376	HIS	-	expression tag	UNP C0JV69
B	377	HIS	-	expression tag	UNP C0JV69

- Molecule 2 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).



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

- Molecule 3 is ARSENIC (three-letter code: ARS) (formula: As).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	As	0	0
			1	1		
3	A	1	Total	As	0	0
			1	1		

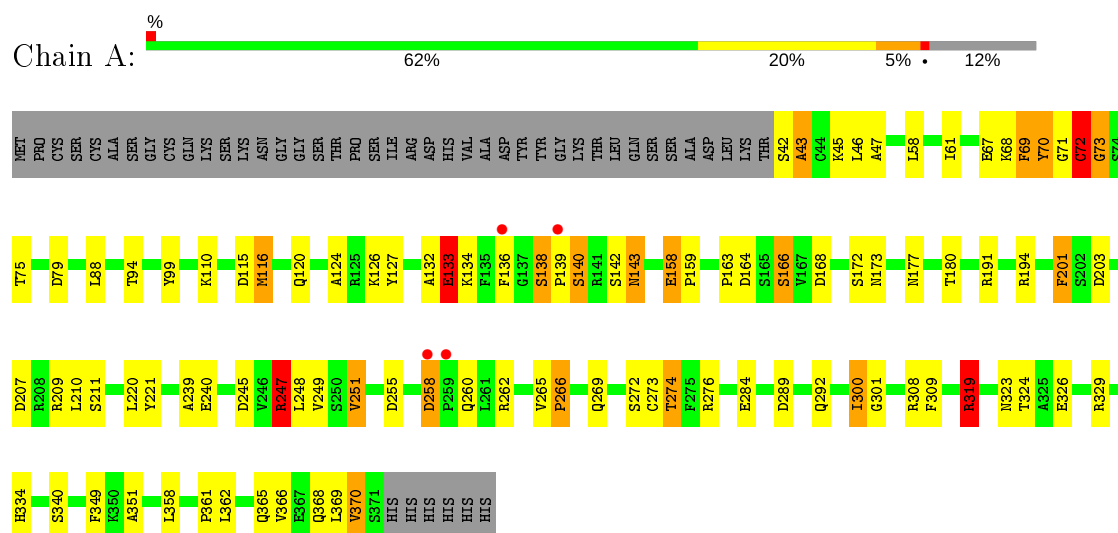
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		
4	B	23	Total	O	0	0
			23	23		

### 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: Arsenic methyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.80 Å   101.80 Å   175.01 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	48.87 – 2.84 48.87 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.87-2.84) 99.3 (48.87-2.84)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.26 (at 2.86 Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.215   ,   0.291 0.217   ,   0.284	Depositor DCC
$R_{free}$ test set	1128 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.8	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5274	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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: SAH, ARS

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	0.59	0/2620	0.85	5/3545 (0.1%)
1	B	0.56	0/2655	0.84	2/3589 (0.1%)
All	All	0.57	0/5275	0.84	7/7134 (0.1%)

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	B	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	A	319	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	B	209	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	A	164	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	A	191	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	287	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	247	ARG	NE-CZ-NH2	-5.08	117.76	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	133	GLU	Peptide
1	B	157	ALA	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	2569	0	2506	60	0
1	B	2604	0	2569	64	2
2	A	26	0	19	0	0
2	B	26	0	19	2	0
3	A	1	0	0	0	0
3	B	1	0	0	2	0
4	A	24	0	0	0	0
4	B	23	0	0	1	0
All	All	5274	0	5113	121	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (121) 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:B:44:CYS:SG	3:B:402:ARS:AS	2.63	1.16
1:A:138:SER:O	1:A:140:SER:N	2.11	0.84
1:B:75:THR:HG22	1:B:201:PHE:HA	1.62	0.80
1:B:162:VAL:O	1:B:191:ARG:NH2	2.21	0.74
1:A:248:LEU:HD11	1:A:251:VAL:HG13	1.70	0.73
1:A:133:GLU:N	1:A:138:SER:OG	2.22	0.73
1:B:57:ILE:O	1:B:59:ALA:N	2.22	0.73
1:A:245:ASP:OD2	1:A:247:ARG:HD3	1.92	0.69
1:A:326:GLU:OE2	1:A:329:ARG:NH1	2.25	0.69
1:B:54:HIS:NE2	1:B:78:ALA:HB2	2.08	0.68
1:A:249:VAL:HB	1:A:274:THR:HG22	1.76	0.67
1:A:251:VAL:HG11	1:A:366:VAL:HB	1.75	0.67
1:B:132:ALA:HB2	1:B:142:SER:HB3	1.77	0.67
1:A:72:CYS:HB2	1:A:272:SER:OG	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:GLU:O	1:A:159:PRO:C	2.34	0.65
1:A:209:ARG:H	1:B:345:HIS:CD2	2.15	0.65
1:A:209:ARG:H	1:B:345:HIS:HD2	1.48	0.62
1:A:319:ARG:HH11	1:A:319:ARG:HG2	1.66	0.61
1:A:68:LYS:O	1:A:69:PHE:HB3	2.00	0.60
1:A:79:ASP:O	1:A:300:ILE:HG21	2.01	0.60
1:A:126:LYS:HD2	1:A:127:TYR:CE1	2.38	0.58
1:B:85:ALA:O	1:B:105:VAL:HG11	2.04	0.57
1:B:263:LYS:O	1:B:266:PRO:HD3	2.05	0.57
1:A:300:ILE:HG22	1:A:301:GLY:N	2.19	0.57
1:A:209:ARG:N	1:B:345:HIS:HD2	2.02	0.57
1:B:44:CYS:SG	1:B:224:CYS:SG	3.03	0.57
1:A:75:THR:OG1	1:A:201:PHE:HA	2.05	0.56
1:A:45:LYS:O	1:A:47:ALA:N	2.38	0.55
1:B:251:VAL:HG13	1:B:370:VAL:HA	1.87	0.55
1:B:350:LYS:HB3	1:B:355:TYR:CG	2.41	0.55
1:A:58:LEU:HA	1:A:61:ILE:HD13	1.89	0.55
1:B:188:GLU:OE2	1:B:191:ARG:NH1	2.39	0.55
1:A:72:CYS:CB	1:A:272:SER:OG	2.56	0.54
1:A:168:ASP:OD1	1:A:194:ARG:NH1	2.40	0.54
1:A:349:PHE:CZ	1:A:351:ALA:HB3	2.43	0.53
1:B:251:VAL:HG21	1:B:366:VAL:HG13	1.89	0.53
1:B:260:GLN:O	1:B:263:LYS:HB3	2.09	0.52
1:B:151:ILE:HG23	2:B:401:SAH:C2	2.38	0.52
1:B:339:VAL:O	1:B:340:SER:O	2.26	0.52
1:B:47:ALA:O	1:B:48:ALA:HB2	2.09	0.52
1:B:43:ALA:HB2	1:B:225:LEU:HD11	1.92	0.52
1:B:163:PRO:O	1:B:166:SER:OG	2.28	0.51
1:B:246:VAL:HG12	1:B:277:CYS:SG	2.51	0.51
1:B:41:THR:O	1:B:255:ASP:O	2.28	0.50
1:A:361:PRO:O	1:A:365:GLN:HG3	2.11	0.50
1:B:75:THR:HG21	1:B:172:SER:O	2.11	0.50
1:B:148:LYS:NZ	4:B:503:HOH:O	2.44	0.50
1:A:369:LEU:O	1:A:370:VAL:HB	2.12	0.50
1:B:40:LYS:O	1:B:42:SER:N	2.45	0.50
1:B:40:LYS:HE3	1:B:40:LYS:HA	1.94	0.49
1:A:251:VAL:HG12	1:A:273:CYS:SG	2.52	0.49
1:B:350:LYS:HB3	1:B:355:TYR:CD1	2.48	0.49
1:A:207:ASP:HB2	1:A:269:GLN:H	1.78	0.48
1:B:290:TYR:CZ	1:B:345:HIS:HB2	2.48	0.48
1:A:251:VAL:CG2	1:A:370:VAL:HG23	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:SER:O	1:A:43:ALA:HB3	2.15	0.47
1:B:40:LYS:HA	1:B:40:LYS:CE	2.44	0.47
1:A:239:ALA:O	1:A:240:GLU:C	2.52	0.47
1:A:284:GLU:H	1:A:323:ASN:HD21	1.62	0.47
1:A:68:LYS:O	1:A:69:PHE:CB	2.63	0.47
1:B:40:LYS:HD3	1:B:258:ASP:HB2	1.96	0.47
1:B:295:THR:HG23	1:B:316:LYS:C	2.35	0.47
1:B:91:GLY:O	1:B:93:GLY:N	2.47	0.47
1:A:329:ARG:O	1:A:334:HIS:HB3	2.14	0.46
1:B:91:GLY:HA3	1:B:175:VAL:HG21	1.97	0.46
1:A:221:TYR:C	1:A:221:TYR:CD1	2.89	0.46
1:B:79:ASP:C	1:B:79:ASP:OD1	2.54	0.46
1:A:251:VAL:HG23	1:A:370:VAL:HG23	1.98	0.46
1:A:349:PHE:CE1	1:A:351:ALA:HB3	2.51	0.46
1:B:173:ASN:HA	1:B:202:SER:O	2.16	0.46
1:B:83:GLU:HG3	1:B:83:GLU:O	2.15	0.46
1:A:110:LYS:HA	1:A:143:ASN:HB3	1.96	0.46
1:A:72:CYS:O	1:A:173:ASN:OD1	2.34	0.45
1:B:154:LEU:CD2	1:B:188:GLU:HG3	2.46	0.45
1:B:367:GLU:O	1:B:370:VAL:HG12	2.17	0.45
1:A:258:ASP:HB3	1:A:260:GLN:HE22	1.80	0.45
1:A:70:TYR:CD1	1:A:70:TYR:N	2.83	0.45
1:A:72:CYS:O	1:A:73:GLY:O	2.34	0.45
1:B:188:GLU:O	1:B:192:VAL:HG22	2.16	0.45
1:A:163:PRO:O	1:A:166:SER:OG	2.34	0.45
1:B:144:VAL:CG1	1:B:146:PHE:CE1	3.00	0.45
1:A:251:VAL:CG2	1:A:369:LEU:HD22	2.48	0.44
1:A:68:LYS:HB2	1:A:94:THR:HG21	1.98	0.44
1:A:71:GLY:C	1:A:72:CYS:O	2.55	0.44
2:B:401:SAH:H4'	2:B:401:SAH:HG2	1.90	0.44
1:B:41:THR:O	1:B:42:SER:CB	2.65	0.44
1:A:289:ASP:HB2	1:A:349:PHE:HA	2.00	0.43
1:B:154:LEU:HD23	1:B:188:GLU:HG3	1.99	0.43
1:A:94:THR:HG23	1:A:120:GLN:HE22	1.83	0.43
1:B:108:HIS:CG	1:B:109:GLY:N	2.86	0.43
1:B:98:VAL:HG13	1:B:111:VAL:HG11	2.00	0.43
1:B:119:ASN:OD1	1:B:119:ASN:N	2.50	0.43
1:A:300:ILE:HG22	1:A:301:GLY:H	1.82	0.43
1:A:61:ILE:HD12	1:A:61:ILE:N	2.33	0.43
1:B:152:GLU:N	1:B:152:GLU:OE1	2.44	0.43
1:B:198:GLU:OE2	1:B:276:ARG:NE	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:LEU:O	1:A:366:VAL:HG13	2.19	0.43
1:B:154:LEU:HB3	1:B:162:VAL:HB	2.00	0.43
1:B:108:HIS:CG	1:B:109:GLY:H	2.37	0.43
1:B:246:VAL:O	1:B:246:VAL:HG23	2.19	0.43
1:B:43:ALA:HB2	1:B:225:LEU:CD1	2.49	0.43
1:B:98:VAL:HG13	1:B:111:VAL:CG1	2.49	0.42
1:A:99:TYR:OH	1:A:124:ALA:O	2.32	0.42
1:B:174:CYS:O	3:B:402:ARS:AS	2.98	0.42
1:A:132:ALA:HB1	1:A:138:SER:HA	2.02	0.42
1:A:319:ARG:HH11	1:A:319:ARG:CG	2.32	0.42
1:B:105:VAL:CG1	1:B:109:GLY:HA3	2.50	0.42
1:B:173:ASN:HD22	1:B:173:ASN:H	1.68	0.41
1:B:211:SER:O	1:B:215:GLN:HG3	2.21	0.41
1:B:64:GLU:OE1	1:B:127:TYR:OH	2.22	0.41
1:B:247:ARG:HB2	1:B:276:ARG:HG2	2.02	0.41
1:B:41:THR:HA	1:B:256:VAL:HA	2.02	0.41
1:A:115:ASP:OD1	1:A:116:MET:N	2.54	0.40
1:A:177:ASN:N	1:A:203:ASP:OD2	2.45	0.40
1:A:309:PHE:CD2	1:A:358:LEU:HD12	2.55	0.40
1:A:88:LEU:C	1:A:88:LEU:HD23	2.42	0.40
1:B:318:VAL:O	1:B:320:VAL:HG13	2.21	0.40
1:A:265:VAL:N	1:A:266:PRO:HD3	2.37	0.40
1:A:324:THR:O	1:A:324:THR:HG22	2.22	0.40
1:A:211:SER:HB3	1:B:344:GLN:HE22	1.86	0.40
1:B:88:LEU:HG	1:B:90:LEU:HD13	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:GLN:OE1	1:B:269:GLN:OE1[6_545]	1.98	0.22
1:B:371:SER:OG	1:B:371:SER:OG[6_545]	2.05	0.15

## 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	328/377 (87%)	285 (87%)	29 (9%)	14 (4%)	2	5
1	B	331/377 (88%)	288 (87%)	32 (10%)	11 (3%)	4	8
All	All	659/754 (87%)	573 (87%)	61 (9%)	25 (4%)	3	6

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	ALA
1	A	46	LEU
1	A	73	GLY
1	A	138	SER
1	A	300	ILE
1	A	370	VAL
1	B	58	LEU
1	B	340	SER
1	A	72	CYS
1	A	134	LYS
1	A	140	SER
1	A	340	SER
1	B	57	ILE
1	B	165	SER
1	B	172	SER
1	B	300	ILE
1	B	335	GLN
1	A	69	PHE
1	A	136	PHE
1	B	41	THR
1	A	139	PRO
1	B	48	ALA
1	A	266	PRO
1	B	77	PRO
1	B	298	GLY

### 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	274/317 (86%)	249 (91%)	25 (9%)	9	19
1	B	280/317 (88%)	252 (90%)	28 (10%)	7	16
All	All	554/634 (87%)	501 (90%)	53 (10%)	8	17

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	GLU
1	A	70	TYR
1	A	72	CYS
1	A	116	MET
1	A	133	GLU
1	A	142	SER
1	A	143	ASN
1	A	158	GLU
1	A	166	SER
1	A	172	SER
1	A	180	THR
1	A	201	PHE
1	A	210	LEU
1	A	220	LEU
1	A	247	ARG
1	A	251	VAL
1	A	255	ASP
1	A	258	ASP
1	A	262	ARG
1	A	274	THR
1	A	276	ARG
1	A	292	GLN
1	A	308	ARG
1	A	319	ARG
1	A	368	GLN
1	B	66	LEU
1	B	68	LYS
1	B	69	PHE
1	B	77	PRO
1	B	82	LEU
1	B	83	GLU
1	B	90	LEU
1	B	96	ARG
1	B	100	LEU

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Mol	Chain	Res	Type
1	B	119	ASN
1	B	121	LEU
1	B	122	GLU
1	B	133	GLU
1	B	140	SER
1	B	141	ARG
1	B	147	LEU
1	B	173	ASN
1	B	180	THR
1	B	191	ARG
1	B	193	LEU
1	B	202	SER
1	B	215	GLN
1	B	256	VAL
1	B	339	VAL
1	B	342	GLU
1	B	350	LYS
1	B	369	LEU
1	B	371	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	120	GLN
1	A	269	GLN
1	A	323	ASN
1	A	365	GLN
1	B	120	GLN
1	B	131	HIS
1	B	173	ASN
1	B	269	GLN
1	B	344	GLN
1	B	345	HIS
1	B	365	GLN

### 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 ⓘ

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$
2	SAH	A	401	-	21,28,28	1.03	1 (4%)	20,40,40	1.47	5 (25%)
2	SAH	B	401	-	21,28,28	1.08	1 (4%)	20,40,40	1.53	4 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	A	401	-	-	0/7/31/31	0/3/3/3
2	SAH	B	401	-	-	2/7/31/31	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	SAH	C5-C4	2.41	1.47	1.40
2	A	401	SAH	C5-C4	2.01	1.46	1.40

All (9) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	SAH	N3-C2-N1	-3.65	122.97	128.68
2	A	401	SAH	O4'-C1'-C2'	-3.31	102.08	106.93
2	A	401	SAH	N6-C6-N1	2.67	124.12	118.57
2	B	401	SAH	C2-N1-C6	2.63	123.26	118.75
2	B	401	SAH	CB-CG-SD	-2.54	107.62	113.31
2	A	401	SAH	C4'-C5'-SD	-2.39	105.19	113.78
2	B	401	SAH	N6-C6-N1	2.16	123.06	118.57
2	A	401	SAH	C4-C5-N7	-2.11	107.20	109.40
2	A	401	SAH	C3'-C2'-C1'	2.04	104.05	100.98

There are no chirality outliers.

All (2) torsion outliers are listed below:

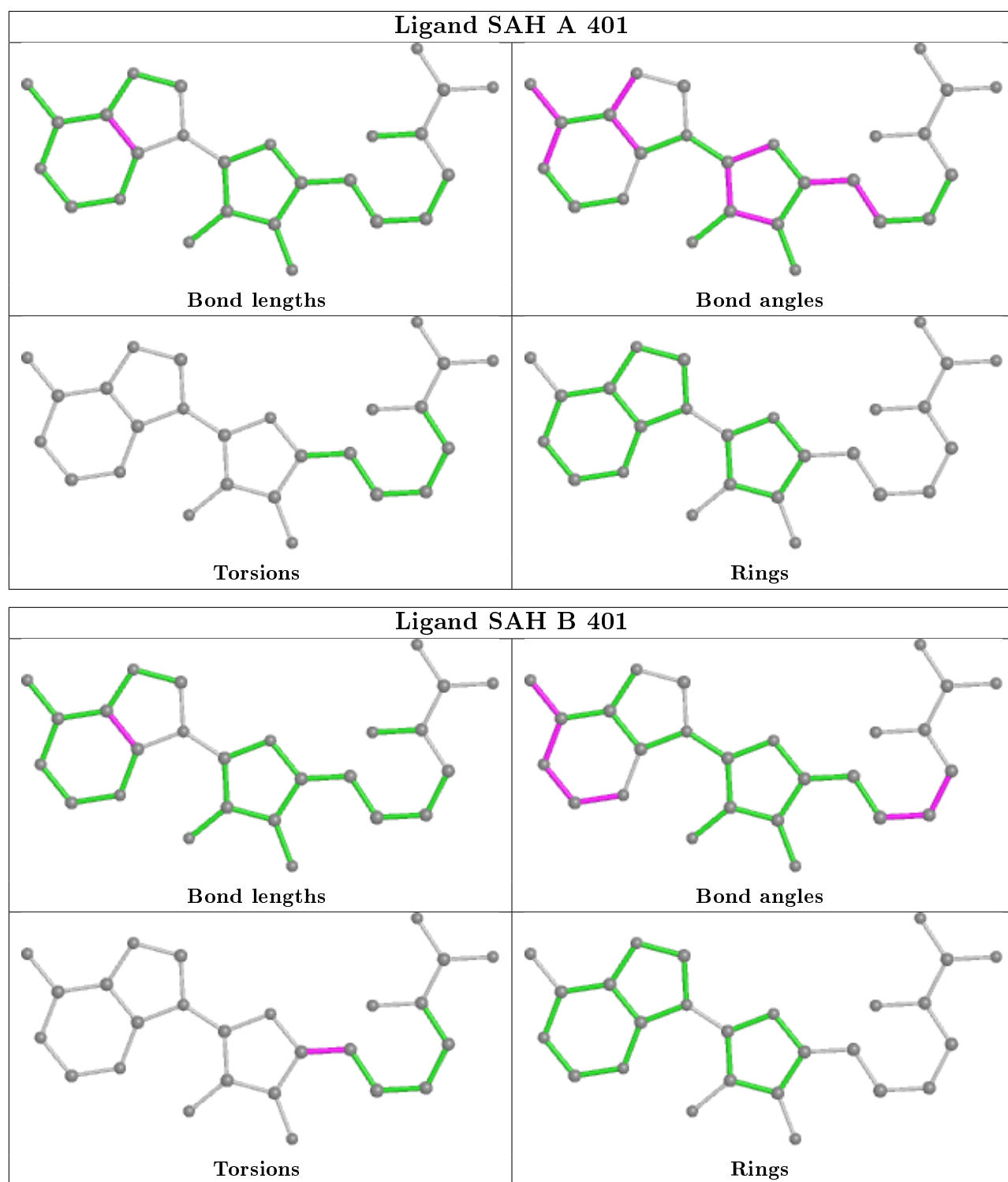
Mol	Chain	Res	Type	Atoms
2	B	401	SAH	O4'-C4'-C5'-SD
2	B	401	SAH	C3'-C4'-C5'-SD

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	SAH	2	0

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	330/377 (87%)	-0.06	4 (1%) 79 76	35, 58, 90, 117	0
1	B	333/377 (88%)	-0.05	1 (0%) 94 93	37, 62, 90, 116	0
All	All	663/754 (87%)	-0.05	5 (0%) 86 85	35, 60, 90, 117	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	371	SER	3.8
1	A	139	PRO	3.0
1	A	258	ASP	2.6
1	A	259	PRO	2.6
1	A	136	PHE	2.3

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

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

### 6.3 Carbohydrates [i](#)

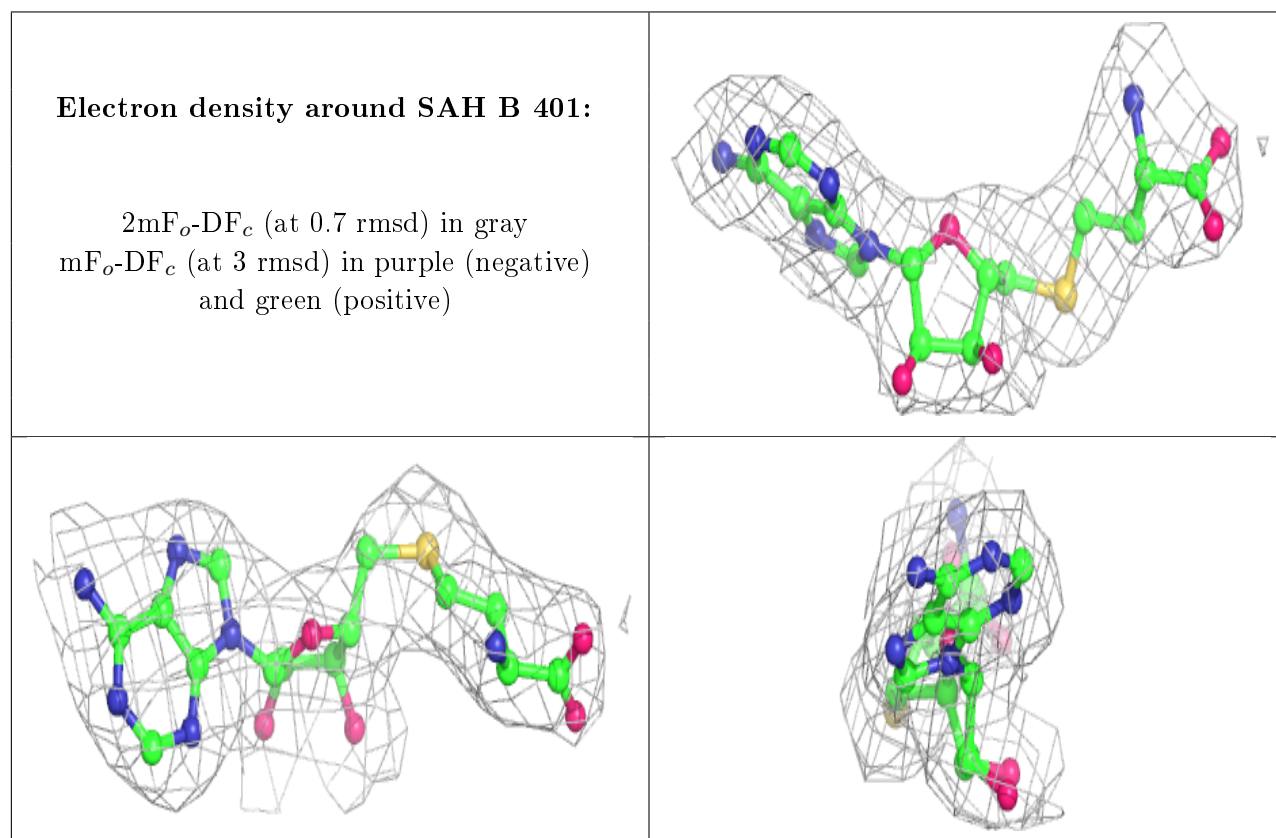
There are no carbohydrates in this entry.

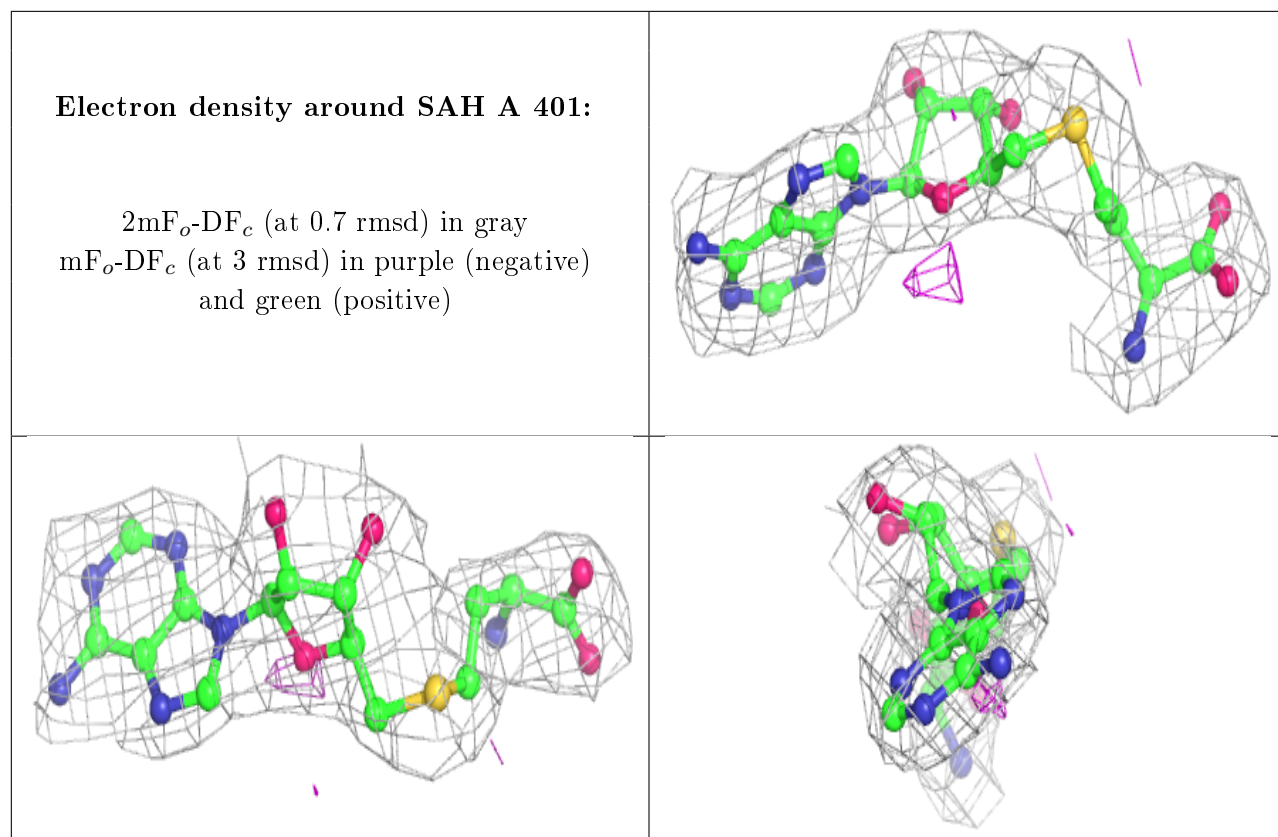
### 6.4 Ligands [i](#)

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( $\text{\AA}^2$ )	Q<0.9
2	SAH	B	401	26/26	0.94	0.18	47,54,66,69	0
2	SAH	A	401	26/26	0.96	0.19	39,48,63,64	0
3	ARS	A	402	1/1	0.99	0.09	69,69,69,69	0
3	ARS	B	402	1/1	1.00	0.12	60,60,60,60	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.