



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:25 pm BST

PDB ID : 4M73  
Title : Mutant structure of methyltransferase from *Streptomyces hygrosopicus*  
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Deposited on : 2013-08-12  
Resolution : 2.00 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

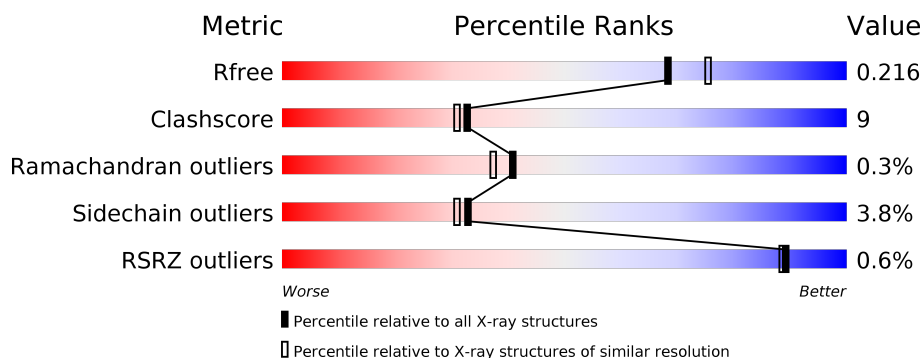
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	337	 83% 14% ...
1	B	337	 80% 16% ...

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6077 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.

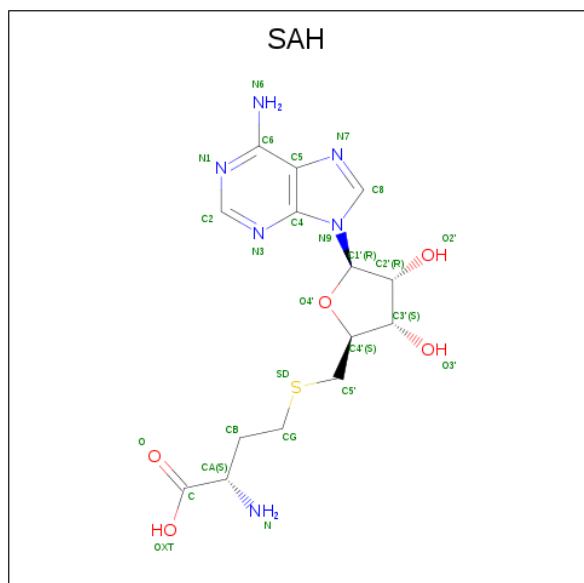
- Molecule 1 is a protein called Methyltransferase MppJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2581	1632	458	480	11			
1	B	333	Total	C	N	O	S	0	0	0
			2588	1637	459	481	11			

There are 6 discrepancies between the modelled and reference sequences:

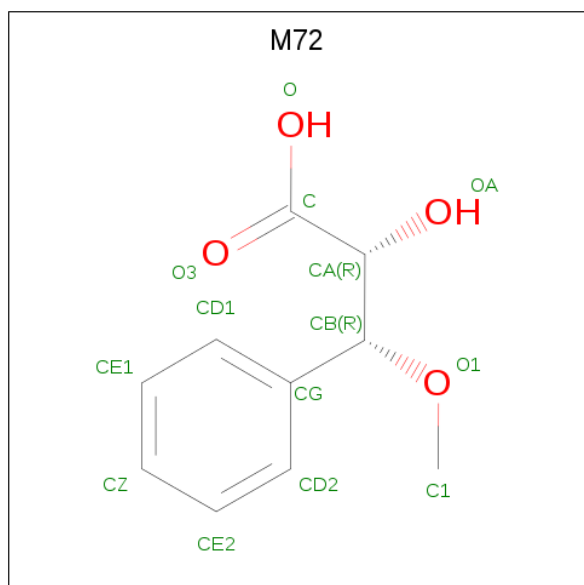
Chain	Residue	Modelled	Actual	Comment	Reference
A	127	LEU	ARG	ENGINEERED MUTATION	UNP Q643C8
A	244	ALA	ASP	ENGINEERED MUTATION	UNP Q643C8
A	300	GLU	VAL	ENGINEERED MUTATION	UNP Q643C8
B	127	LEU	ARG	ENGINEERED MUTATION	UNP Q643C8
B	244	ALA	ASP	ENGINEERED MUTATION	UNP Q643C8
B	300	GLU	VAL	ENGINEERED MUTATION	UNP Q643C8

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ).



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 (2R,3R)-2-hydroxy-3-methoxy-3-phenylpropanoic acid (three-letter code: M72) (formula: C<sub>10</sub>H<sub>12</sub>O<sub>4</sub>).

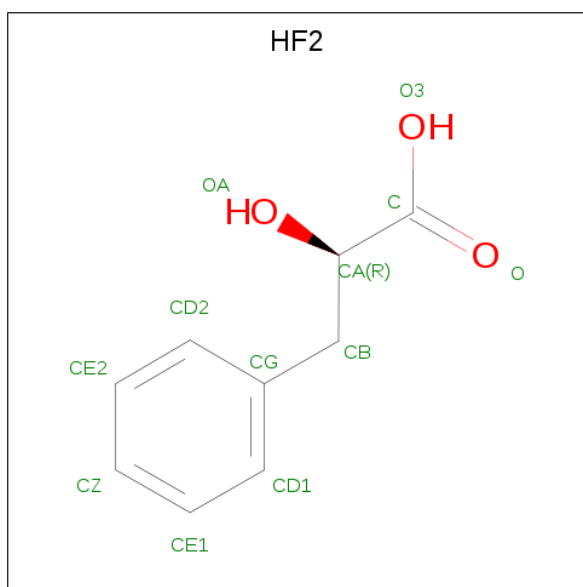


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			14	10	4		
3	B	1	Total	C	O	0	0
			14	10	4		

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Fe	0	0
			1	1		
4	A	1	Total	Fe	0	0
			1	1		

- Molecule 5 is (2R)-2-hydroxy-3-phenylpropanoic acid (three-letter code: HF2) (formula: C<sub>9</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 12 9 3	0	0
5	B	1	Total C O 12 9 3	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	7	Total Ca 7 7	0	0
6	A	6	Total Ca 6 6	0	0

- Molecule 7 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total I 1 1	0	0

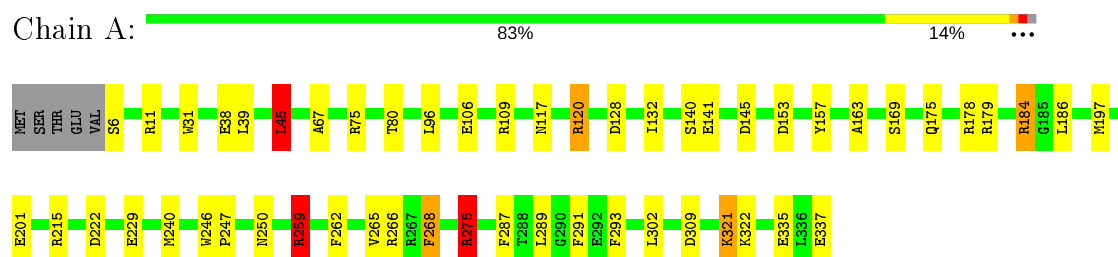
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	449	Total O 449 449	0	0
8	B	339	Total O 339 339	0	0

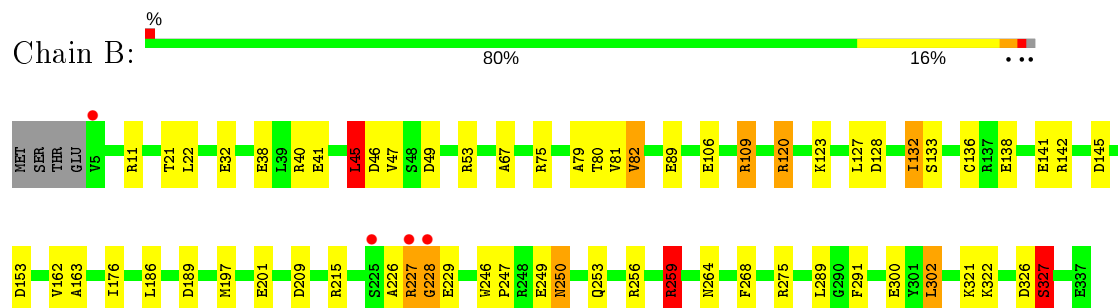
### 3 Residue-property plots [i](#)

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: Methyltransferase MppJ



#### • Molecule 1: Methyltransferase MppJ



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.99 Å 96.81 Å 135.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.05 – 2.00 28.52 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.0 (29.05-2.00) 93.0 (28.52-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.29 (at 2.00 Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.152 , 0.211 0.163 , 0.216	Depositor DCC
$R_{free}$ test set	2605 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.2	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6077	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: M72, SAH, CA, HF2, FE, IOD

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	1.07	6/2640 (0.2%)	1.32	17/3573 (0.5%)
1	B	0.96	6/2647 (0.2%)	1.20	16/3583 (0.4%)
All	All	1.01	12/5287 (0.2%)	1.26	33/7156 (0.5%)

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	2
All	All	0	3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	ARG	CD-NE	-8.15	1.32	1.46
1	A	169	SER	CB-OG	8.12	1.52	1.42
1	B	138	GLU	CD-OE2	7.93	1.34	1.25
1	A	337	GLU	CD-OE2	-6.60	1.18	1.25
1	B	300	GLU	CD-OE1	6.50	1.32	1.25
1	A	31	TRP	CG-CD1	6.47	1.45	1.36
1	A	259	ARG	CD-NE	-6.26	1.35	1.46
1	A	120	ARG	CD-NE	-5.98	1.36	1.46
1	B	327	SER	N-CA	-5.51	1.35	1.46
1	B	120	ARG	CD-NE	-5.34	1.37	1.46
1	B	106	GLU	CD-OE2	5.22	1.31	1.25
1	B	32	GLU	CD-OE2	-5.17	1.20	1.25

All (33) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	ARG	NE-CZ-NH2	-26.91	106.84	120.30
1	B	120	ARG	NE-CZ-NH2	-20.12	110.24	120.30
1	A	120	ARG	NE-CZ-NH2	-20.10	110.25	120.30
1	A	259	ARG	NE-CZ-NH1	19.34	129.97	120.30
1	A	275	ARG	NE-CZ-NH1	18.69	129.65	120.30
1	A	259	ARG	NE-CZ-NH2	-18.45	111.07	120.30
1	B	40	ARG	NE-CZ-NH2	-17.35	111.62	120.30
1	A	120	ARG	NE-CZ-NH1	15.38	127.99	120.30
1	B	120	ARG	NE-CZ-NH1	15.16	127.88	120.30
1	B	40	ARG	NE-CZ-NH1	14.45	127.52	120.30
1	B	259	ARG	NE-CZ-NH2	-13.57	113.52	120.30
1	A	275	ARG	CD-NE-CZ	10.27	137.97	123.60
1	B	142	ARG	NE-CZ-NH1	9.63	125.11	120.30
1	B	259	ARG	NE-CZ-NH1	9.31	124.96	120.30
1	B	45	LEU	CA-CB-CG	7.36	132.23	115.30
1	B	142	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	A	259	ARG	CD-NE-CZ	6.54	132.76	123.60
1	B	275	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	A	309	ASP	CB-CG-OD1	6.12	123.81	118.30
1	B	11	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	B	109	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	B	327	SER	N-CA-C	-5.80	95.35	111.00
1	A	120	ARG	CG-CD-NE	-5.62	99.99	111.80
1	B	120	ARG	CG-CD-NE	-5.59	100.06	111.80
1	A	45	LEU	CA-CB-CG	5.51	127.96	115.30
1	A	321	LYS	CD-CE-NZ	5.33	123.96	111.70
1	A	275	ARG	CG-CD-NE	-5.26	100.76	111.80
1	A	120	ARG	CD-NE-CZ	5.21	130.89	123.60
1	A	222	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	268	PHE	CB-CG-CD2	-5.11	117.22	120.80
1	A	293	PHE	CB-CG-CD1	5.10	124.37	120.80
1	B	22	LEU	CA-CB-CG	-5.08	103.61	115.30
1	B	40	ARG	CD-NE-CZ	5.02	130.62	123.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	275	ARG	Sidechain
1	B	226	ALA	Peptide
1	B	326	ASP	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	2581	0	2495	40	0
1	B	2588	0	2504	47	0
2	A	26	0	19	0	0
2	B	26	0	19	0	0
3	A	14	0	11	3	0
3	B	14	0	11	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	12	0	7	2	0
5	B	12	0	7	1	0
6	A	6	0	0	0	0
6	B	7	0	0	0	0
7	A	1	0	0	0	0
8	A	449	0	0	16	1
8	B	339	0	0	19	0
All	All	6077	0	5073	90	1

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 (90) 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:38:GLU:OE1	1:B:53:ARG:NH2	1.92	1.02
1:B:153:ASP:HB3	8:B:787:HOH:O	1.60	1.01
1:A:175:GLN:HG3	8:A:767:HOH:O	1.64	0.96
1:B:80:THR:HG22	8:B:790:HOH:O	1.66	0.95
1:B:41:GLU:OE2	8:B:767:HOH:O	1.85	0.94
1:B:109:ARG:NH2	8:B:805:HOH:O	2.13	0.82
1:B:253:GLN:OE1	8:B:639:HOH:O	1.97	0.79
1:A:259:ARG:O	1:A:259:ARG:HD3	1.83	0.79
1:B:136:CYS:SG	3:B:402:M72:O1	2.45	0.75
1:A:38:GLU:OE2	8:A:911:HOH:O	2.04	0.74
3:B:402:M72:O	3:B:402:M72:H12	1.87	0.74
1:B:209:ASP:HB3	8:B:721:HOH:O	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ARG:C	1:A:259:ARG:HD3	2.05	0.74
3:B:402:M72:OA	8:B:719:HOH:O	2.01	0.71
1:A:106:GLU:OE2	1:A:109:ARG:NH1	2.25	0.70
1:A:259:ARG:CD	1:A:259:ARG:O	2.41	0.69
1:A:120:ARG:HD3	8:A:569:HOH:O	1.92	0.69
1:A:153:ASP:OD1	1:A:179:ARG:NH2	2.26	0.68
1:A:184:ARG:NH1	8:A:900:HOH:O	2.27	0.67
1:B:322:LYS:HD3	5:B:404:HF2:HA	1.77	0.67
1:B:120:ARG:HD3	8:B:638:HOH:O	1.95	0.66
1:A:259:ARG:CD	1:A:259:ARG:C	2.64	0.65
1:A:6:SER:HB2	8:A:887:HOH:O	1.98	0.62
1:B:227:ARG:O	1:B:229:GLU:N	2.34	0.61
1:B:256:ARG:NH1	8:B:829:HOH:O	2.27	0.61
1:A:145:ASP:OD2	8:A:902:HOH:O	2.15	0.60
1:B:321:LYS:NZ	8:B:731:HOH:O	2.34	0.59
1:B:250:ASN:H	1:B:250:ASN:HD22	1.53	0.57
1:A:322:LYS:HD3	5:A:404:HF2:HA	1.87	0.56
1:A:275:ARG:HD2	1:A:302:LEU:O	2.06	0.55
1:A:140:SER:HB2	1:A:240:MET:HE2	1.88	0.54
1:B:291:PHE:CE2	1:B:302:LEU:HD11	2.43	0.53
1:B:327:SER:HB2	8:B:777:HOH:O	2.09	0.52
1:B:259:ARG:NH2	8:B:567:HOH:O	2.39	0.52
1:B:79:ALA:HB1	8:B:622:HOH:O	2.09	0.51
1:B:136:CYS:SG	3:B:402:M72:C1	2.99	0.51
1:A:201:GLU:HG2	8:A:708:HOH:O	2.10	0.50
1:A:215:ARG:NH1	8:A:501:HOH:O	2.43	0.49
1:A:175:GLN:HE22	1:A:178:ARG:HH11	1.60	0.49
1:B:227:ARG:C	1:B:229:GLU:H	2.16	0.49
1:A:6:SER:OG	8:A:730:HOH:O	1.79	0.49
1:A:215:ARG:NH2	8:A:501:HOH:O	2.44	0.48
1:B:38:GLU:CD	1:B:53:ARG:HH22	2.12	0.47
1:B:201:GLU:HA	1:B:201:GLU:OE1	2.14	0.47
3:A:402:M72:OA	8:A:896:HOH:O	2.14	0.47
1:B:264:ASN:ND2	8:B:704:HOH:O	2.46	0.47
1:B:246:TRP:HB3	1:B:247:PRO:HA	1.96	0.47
1:A:117:ASN:ND2	8:A:723:HOH:O	2.46	0.47
5:A:404:HF2:CD1	5:A:404:HF2:C	2.93	0.47
1:B:327:SER:HB3	8:B:619:HOH:O	2.14	0.47
1:A:11:ARG:HG2	1:B:89:GLU:OE2	2.14	0.46
1:B:227:ARG:O	1:B:228:GLY:C	2.54	0.46
1:A:250:ASN:H	1:A:250:ASN:HD22	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ALA:HA	1:B:186:LEU:O	2.16	0.46
1:B:259:ARG:CD	1:B:259:ARG:O	2.64	0.46
1:A:321:LYS:HE2	1:A:335:GLU:OE1	2.16	0.45
1:A:240:MET:HE3	1:A:240:MET:HB2	1.93	0.45
1:A:197:MET:HG2	8:A:921:HOH:O	2.17	0.45
1:A:321:LYS:HE2	1:A:335:GLU:CD	2.38	0.44
1:A:39:LEU:HG	1:A:45:LEU:HD13	1.99	0.44
1:B:141:GLU:O	1:B:145:ASP:HB2	2.18	0.44
1:B:46:ASP:HB3	1:B:49:ASP:HB3	1.99	0.44
1:B:75:ARG:HG2	8:B:791:HOH:O	2.18	0.44
1:A:128:ASP:O	1:A:132:ILE:HG12	2.18	0.43
1:A:157:TYR:CZ	1:A:266:ARG:HB2	2.53	0.43
1:B:162:VAL:HG11	1:B:176:ILE:HG21	2.00	0.43
1:A:291:PHE:CE2	1:A:302:LEU:HD21	2.54	0.43
1:B:259:ARG:HD3	1:B:259:ARG:O	2.19	0.42
1:A:321:LYS:CE	8:A:621:HOH:O	2.67	0.42
1:B:189:ASP:O	1:B:215:ARG:HA	2.19	0.42
1:B:82:VAL:HG13	8:B:556:HOH:O	2.19	0.42
1:A:67:ALA:HA	1:B:289:LEU:HD21	2.00	0.42
1:A:163:ALA:HA	1:A:186:LEU:O	2.19	0.42
3:A:402:M72:H5	3:A:402:M72:C	2.50	0.42
1:A:246:TRP:HB3	1:A:247:PRO:HA	2.01	0.42
1:B:256:ARG:NH2	8:B:666:HOH:O	2.53	0.42
1:B:291:PHE:CD2	1:B:302:LEU:HD11	2.55	0.41
1:A:96:LEU:HD13	1:A:287:PHE:HB2	2.01	0.41
1:A:289:LEU:HD21	1:B:67:ALA:HA	2.01	0.41
1:B:45:LEU:C	1:B:45:LEU:HD23	2.41	0.41
1:B:249:GLU:HG3	8:B:836:HOH:O	2.19	0.41
1:A:259:ARG:HA	1:A:259:ARG:HD3	1.51	0.41
3:A:402:M72:CD2	3:A:402:M72:C	2.99	0.41
1:B:128:ASP:O	1:B:132:ILE:HD12	2.21	0.41
1:A:175:GLN:CG	8:A:767:HOH:O	2.43	0.41
1:B:250:ASN:H	1:B:250:ASN:ND2	2.17	0.40
1:A:262:PHE:HB3	1:A:265:VAL:HG23	2.04	0.40
8:A:659:HOH:O	1:B:21:THR:HG23	2.21	0.40
1:B:259:ARG:CD	1:B:259:ARG:C	2.90	0.40
1:B:47:VAL:HG22	1:B:81:VAL:HG23	2.02	0.40

All (1) 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)
8:A:798:HOH:O	8:A:841:HOH:O[4_455]	2.08	0.12

## 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	330/337 (98%)	318 (96%)	12 (4%)	0	100	100
1	B	331/337 (98%)	318 (96%)	11 (3%)	2 (1%)	25	19
All	All	661/674 (98%)	636 (96%)	23 (4%)	2 (0%)	41	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	228	GLY
1	B	227	ARG

### 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	262/267 (98%)	254 (97%)	8 (3%)	40	40
1	B	263/267 (98%)	251 (95%)	12 (5%)	27	23
All	All	525/534 (98%)	505 (96%)	20 (4%)	33	31

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	75	ARG
1	A	80	THR
1	A	141	GLU
1	A	184	ARG
1	A	229	GLU
1	A	259	ARG
1	A	268	PHE
1	B	45	LEU
1	B	82	VAL
1	B	123	LYS
1	B	127	LEU
1	B	132	ILE
1	B	133	SER
1	B	197	MET
1	B	250	ASN
1	B	259	ARG
1	B	268	PHE
1	B	302	LEU
1	B	327	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	175	GLN
1	A	250	ASN
1	B	117	ASN
1	B	250	ASN
1	B	264	ASN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 16 are monoatomic - leaving 6 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	HF2	B	404	-	9,12,12	0.54	0	12,15,15	2.44	1 (8%)
5	HF2	A	404	-	9,12,12	0.62	0	12,15,15	1.86	2 (16%)
3	M72	B	402	4	10,14,14	1.25	1 (10%)	13,18,18	2.19	3 (23%)
2	SAH	A	401	-	21,28,28	1.26	4 (19%)	20,40,40	2.02	8 (40%)
2	SAH	B	401	-	21,28,28	1.07	2 (9%)	20,40,40	2.15	6 (30%)
3	M72	A	402	4	10,14,14	1.10	1 (10%)	13,18,18	1.57	2 (15%)

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	HF2	B	404	-	-	3/4/8/8	0/1/1/1
5	HF2	A	404	-	-	2/4/8/8	0/1/1/1
3	M72	B	402	4	-	6/10/14/14	0/1/1/1
2	SAH	A	401	-	-	0/7/31/31	0/3/3/3
2	SAH	B	401	-	-	2/7/31/31	0/3/3/3
3	M72	A	402	4	-	2/10/14/14	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	SAH	C2-N3	2.72	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	SAH	C2-N3	2.55	1.36	1.32
2	B	401	SAH	C4-N3	2.36	1.38	1.35
3	B	402	M72	O1-CB	2.30	1.47	1.42
2	A	401	SAH	C2-N1	2.30	1.38	1.33
3	A	402	M72	O1-CB	2.29	1.47	1.42
2	A	401	SAH	C5-C4	2.15	1.46	1.40
2	A	401	SAH	O3'-C3'	2.13	1.48	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	404	HF2	CB-CA-C	7.93	121.19	111.10
3	B	402	M72	CG-CB-CA	-5.85	99.95	112.18
2	B	401	SAH	N3-C2-N1	-5.14	120.65	128.68
2	A	401	SAH	CB-CG-SD	-4.95	102.20	113.31
5	A	404	HF2	CB-CA-C	4.81	117.21	111.10
3	A	402	M72	CG-CB-CA	-4.28	103.24	112.18
2	B	401	SAH	C5-C6-N6	-4.17	114.01	120.35
2	B	401	SAH	C1'-N9-C4	-4.04	119.55	126.64
3	B	402	M72	C1-O1-CB	3.46	123.58	113.60
2	A	401	SAH	N6-C6-N1	3.20	125.22	118.57
2	B	401	SAH	N6-C6-N1	3.14	125.09	118.57
3	B	402	M72	O1-CB-CA	3.07	122.74	107.41
2	A	401	SAH	C5-C6-N6	-2.74	116.19	120.35
3	A	402	M72	O1-CB-CA	2.64	120.59	107.41
2	B	401	SAH	CB-CG-SD	-2.51	107.68	113.31
2	A	401	SAH	O4'-C4'-C5'	-2.49	102.41	108.83
2	A	401	SAH	C1'-N9-C4	-2.47	122.30	126.64
2	A	401	SAH	N3-C2-N1	-2.29	125.09	128.68
2	A	401	SAH	O3'-C3'-C4'	2.22	117.47	111.05
5	A	404	HF2	CZ-CE1-CD1	2.15	123.46	120.19
2	B	401	SAH	C5'-SD-CG	-2.05	96.12	102.27
2	A	401	SAH	C4'-C5'-SD	-2.02	106.54	113.78

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	404	HF2	C-CA-CB-CG
5	A	404	HF2	OA-CA-CB-CG
3	A	402	M72	CA-CB-O1-C1
3	A	402	M72	CG-CB-O1-C1

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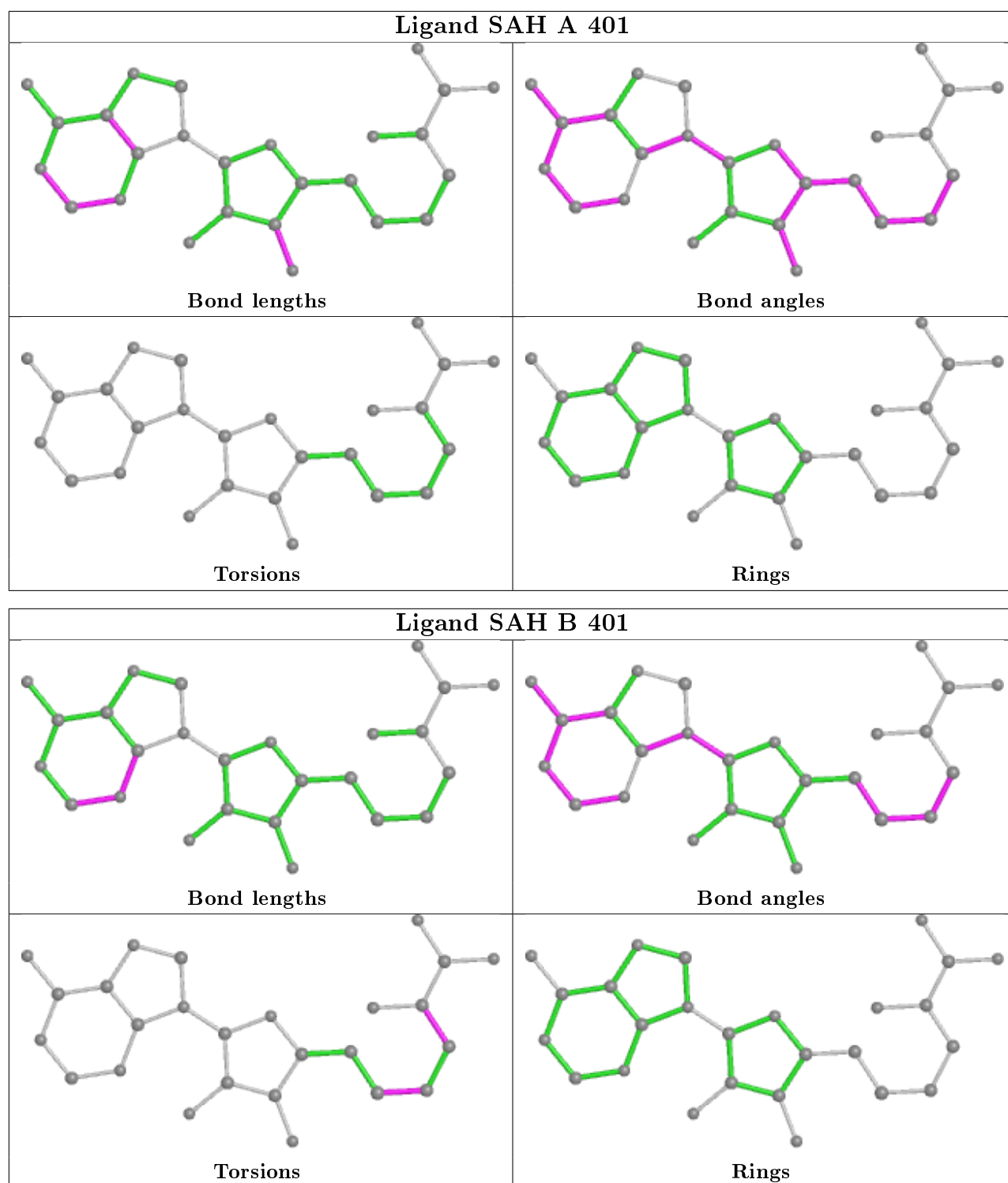
Mol	Chain	Res	Type	Atoms
3	B	402	M72	OA-CA-CB-CG
3	B	402	M72	CA-CB-O1-C1
3	B	402	M72	CG-CB-O1-C1
5	B	404	HF2	C-CA-CB-CG
5	B	404	HF2	OA-CA-CB-CG
3	B	402	M72	C-CA-CB-CG
3	B	402	M72	OA-CA-CB-O1
3	B	402	M72	C-CA-CB-O1
2	B	401	SAH	CB-CG-SD-C5'
2	B	401	SAH	N-CA-CB-CG
5	B	404	HF2	CA-CB-CG-CD2

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	404	HF2	1	0
5	A	404	HF2	2	0
3	B	402	M72	4	0
3	A	402	M72	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 ⓘ

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	332/337 (98%)	-0.57	0	100   100	13, 23, 43, 59	0
1	B	333/337 (98%)	-0.29	4 (1%)	79   78	17, 29, 53, 119	0
All	All	665/674 (98%)	-0.43	4 (0%)	89   88	13, 26, 49, 119	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	227	ARG	7.2
1	B	5	VAL	5.2
1	B	225	SER	2.9
1	B	228	GLY	2.7

### 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(Å <sup>2</sup> )	Q<0.9
6	CA	A	409	1/1	0.79	0.11	73,73,73,73	0

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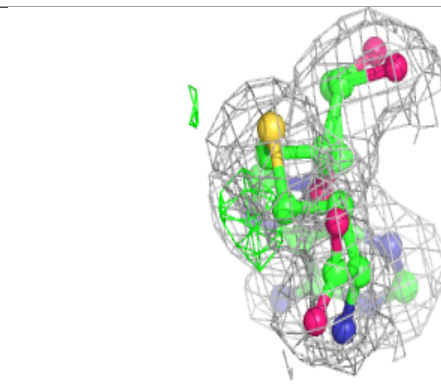
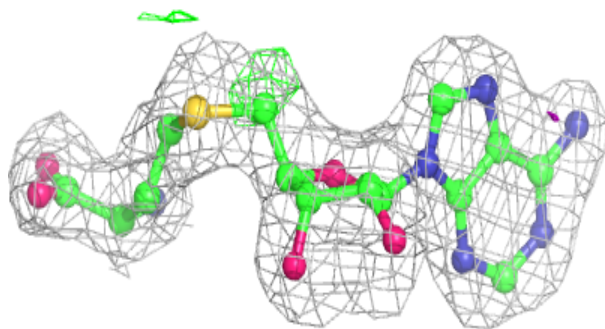
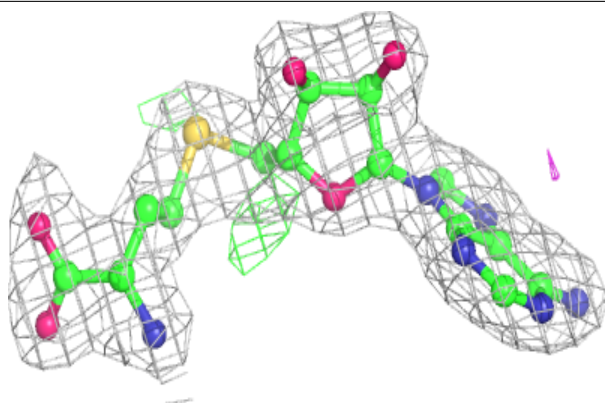
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	CA	B	406	1/1	0.91	0.08	70,70,70,70	0
3	M72	B	402	14/14	0.92	0.15	38,45,60,64	0
6	CA	B	408	1/1	0.93	0.07	39,39,39,39	0
2	SAH	B	401	26/26	0.94	0.09	29,36,45,48	0
5	HF2	A	404	12/12	0.95	0.08	24,26,31,34	0
3	M72	A	402	14/14	0.96	0.10	24,38,53,57	0
6	CA	A	407	1/1	0.97	0.07	35,35,35,35	0
6	CA	A	406	1/1	0.97	0.07	40,40,40,40	0
6	CA	B	411	1/1	0.97	0.04	41,41,41,41	0
5	HF2	B	404	12/12	0.97	0.07	25,27,36,41	0
6	CA	B	407	1/1	0.97	0.06	34,34,34,34	0
2	SAH	A	401	26/26	0.97	0.07	16,20,36,44	0
6	CA	B	405	1/1	0.98	0.05	33,33,33,33	0
6	CA	B	410	1/1	0.98	0.04	49,49,49,49	0
6	CA	A	405	1/1	0.98	0.03	35,35,35,35	0
6	CA	A	410	1/1	0.98	0.09	46,46,46,46	0
4	FE	B	403	1/1	0.99	0.07	23,23,23,23	0
6	CA	B	409	1/1	0.99	0.03	35,35,35,35	0
7	IOD	A	411	1/1	0.99	0.04	32,32,32,32	0
6	CA	A	408	1/1	0.99	0.04	35,35,35,35	0
4	FE	A	403	1/1	1.00	0.07	18,18,18,18	0

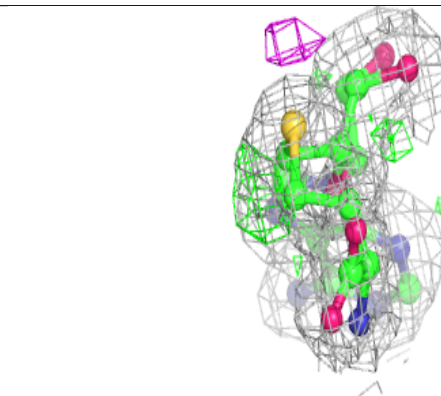
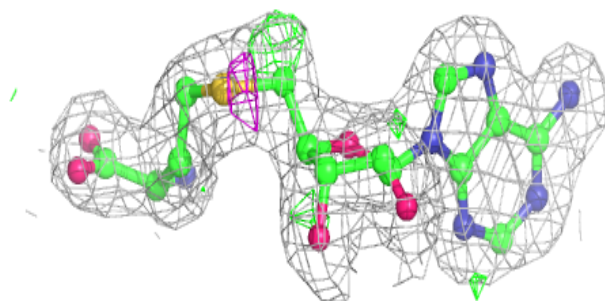
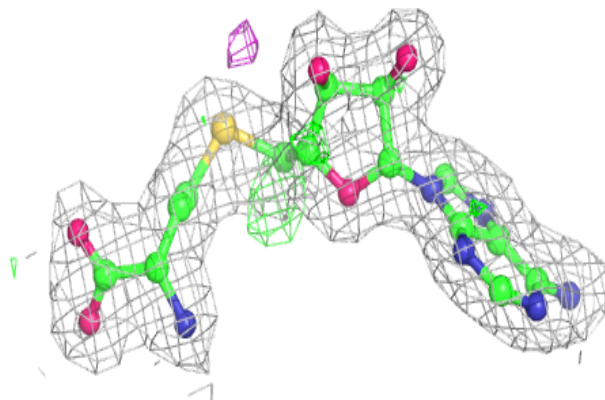
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around SAH B 401:**

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

**Electron density around SAH A 401:**

$2mF_o-DF_c$  (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.