Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 11:37 AM EDT

PDB ID	:	3B5I
Title	:	Crystal structure of Indole-3-acetic Acid Methyltransferase
Authors	:	Ferrer, J.-L.; Noel, J.P.
Deposited on	:	2007-10-26
Resolution	:	2.75 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

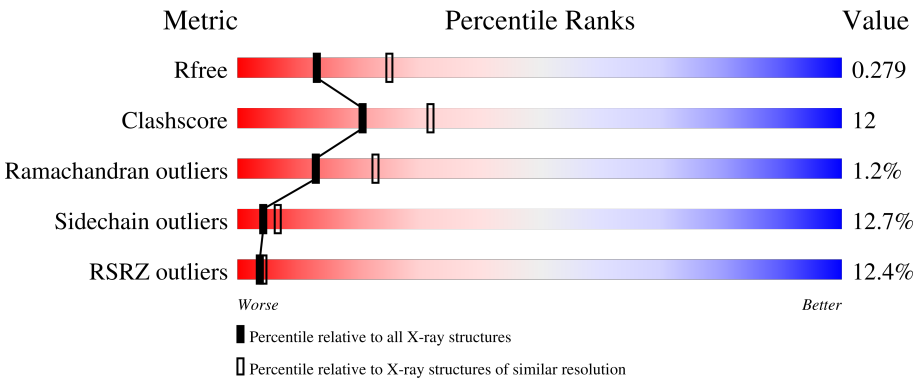
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	374	10% 60% 29% • 8%
1	B	374	13% 60% 29% • 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5468 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.

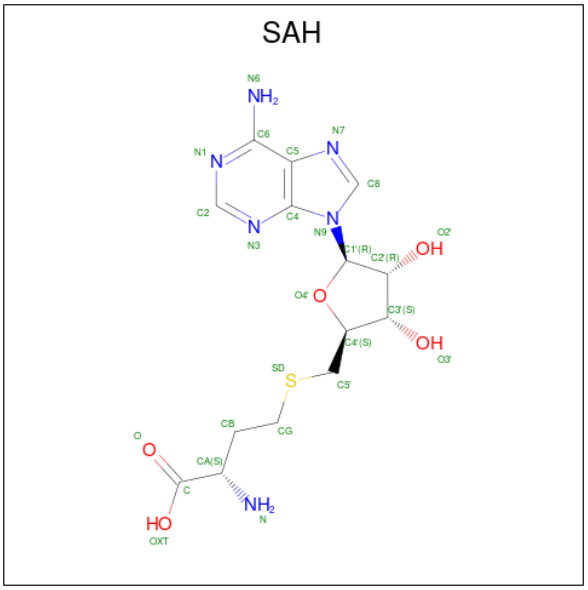
- Molecule 1 is a protein called S-adenosyl-L-methionine:salicylic acid carboxyl methyltransfe rase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	344	2657	1686	464	500	7	0	0	0
1	B	340	2621	1666	458	491	6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	LEU	GLN	engineered mutation	UNP Q9FLN8
B	23	LEU	GLN	engineered mutation	UNP Q9FLN8

- 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
			Total	C	N	O	S		
2	A	1	26	14	6	5	1	0	0
			Total	C	N	O	S		
2	B	1	26	14	6	5	1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

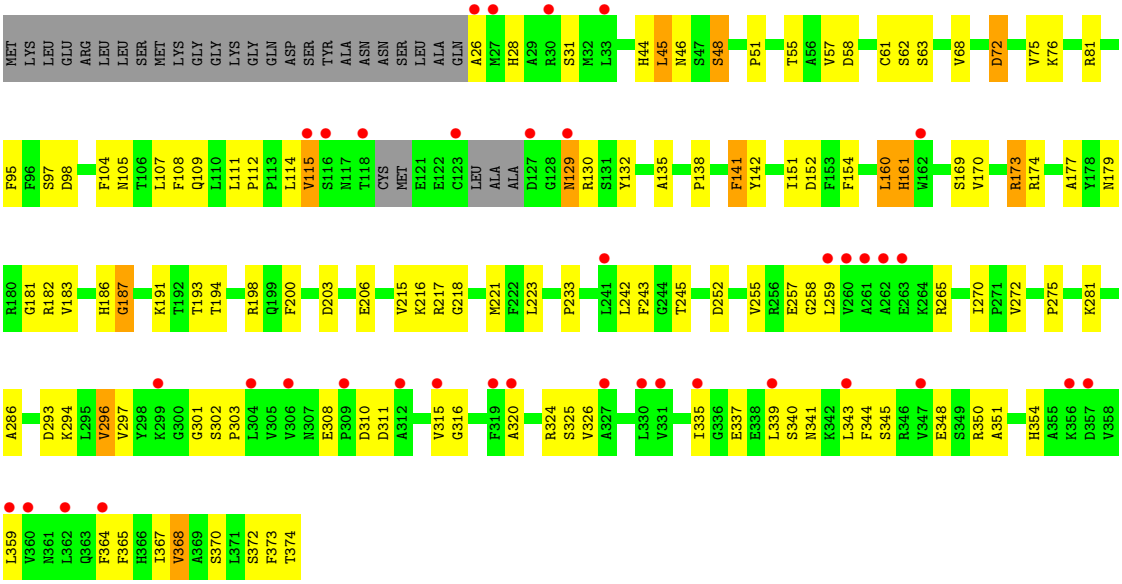
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	72	72	72	0	0
			Total	O		
4	B	64	64	64	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

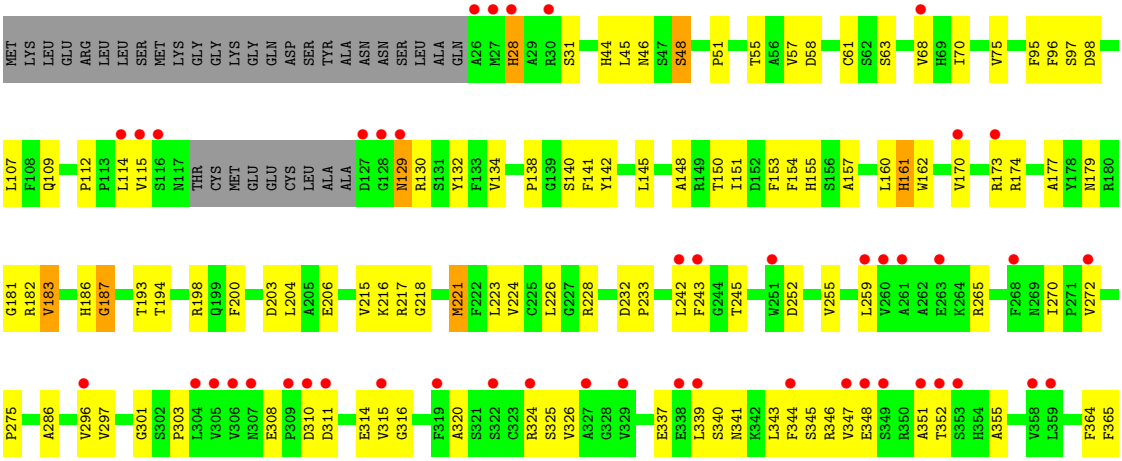
• Molecule 1: S-adenosyl-L-methionine:salicylic acid carboxyl methyltransferase-like protein

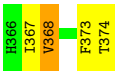
Chain A:



• Molecule 1: S-adenosyl-L-methionine:salicylic acid carboxyl methyltransferase-like protein

Chain B:




H366
I367
V368
F373
T374

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.27Å 129.40Å 68.33Å 90.00° 112.30° 90.00°	Depositor
Resolution (Å)	45.22 – 2.75 45.22 – 2.70	Depositor EDS
% Data completeness (in resolution range)	74.4 (45.22-2.75) 69.3 (45.22-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.257 , 0.282 0.252 , 0.279	Depositor DCC
R_{free} test set	1112 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	49.1	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.306 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5468	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, SAH

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	0.58	0/2720	0.71	3/3689 (0.1%)
1	B	0.56	0/2684	0.71	1/3642 (0.0%)
All	All	0.57	0/5404	0.71	4/7331 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	58	ASP	CB-CG-OD2	5.72	123.45	118.30
1	B	129	ASN	N-CA-CB	-5.30	101.06	110.60
1	A	58	ASP	OD1-CG-OD2	-5.04	113.73	123.30
1	A	58	ASP	CB-CG-OD1	5.01	122.81	118.30

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	A	2657	0	2566	65	0
1	B	2621	0	2538	67	0
2	A	26	0	19	0	0
2	B	26	0	19	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	72	0	0	3	0
4	B	64	0	0	9	0
All	All	5468	0	5142	129	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 12.

All (129) 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:259:LEU:HB3	1:B:339:LEU:HD21	1.42	1.02
1:A:259:LEU:HB3	1:A:339:LEU:HD21	1.41	1.00
1:A:296:VAL:HG13	1:A:368:VAL:HG13	1.54	0.88
1:A:179:ASN:OD1	1:A:182:ARG:HB2	1.79	0.82
1:A:359:LEU:HB3	4:A:671:HOH:O	1.81	0.80
1:A:194:THR:O	1:A:198:ARG:HG3	1.81	0.80
1:B:179:ASN:OD1	1:B:182:ARG:HB2	1.81	0.79
1:A:181:GLY:HA2	1:A:265:ARG:HE	1.47	0.79
1:B:181:GLY:HA2	1:B:265:ARG:HE	1.46	0.79
1:B:373:PHE:O	1:B:374:THR:HB	1.82	0.78
1:A:341:ASN:O	1:A:345:SER:HB2	1.83	0.78
1:B:296:VAL:HG13	1:B:368:VAL:HG13	1.67	0.76
1:B:301:GLY:HA2	1:B:364:PHE:H	1.49	0.75
1:B:112:PRO:HG2	1:B:130:ARG:HB2	1.65	0.75
1:B:341:ASN:O	1:B:345:SER:HB2	1.87	0.75
1:A:373:PHE:O	1:A:374:THR:HB	1.86	0.73
1:A:182:ARG:HD3	1:A:187:GLY:HA3	1.71	0.72
1:B:297:VAL:HG12	1:B:367:ILE:HG12	1.70	0.72
1:A:55:THR:HG21	1:A:151:ILE:HD13	1.74	0.69
1:A:108:PHE:CG	1:B:138:PRO:HG3	2.28	0.68
1:A:57:VAL:HG22	1:A:95:PHE:HB2	1.75	0.68
1:A:301:GLY:HA2	1:A:364:PHE:H	1.60	0.67
1:A:243:PHE:HZ	1:A:326:VAL:HG11	1.59	0.67
1:B:57:VAL:HG22	1:B:95:PHE:HB2	1.78	0.66
1:A:112:PRO:HG2	1:A:130:ARG:HB2	1.79	0.65
1:A:297:VAL:HG12	1:A:367:ILE:HG12	1.78	0.65
1:B:182:ARG:HD3	1:B:187:GLY:HA3	1.77	0.64
1:B:243:PHE:HZ	1:B:326:VAL:HG11	1.63	0.63
1:B:154:PHE:HB2	1:B:221:MET:HG3	1.80	0.62
1:A:130:ARG:HD3	1:A:132:TYR:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ARG:O	1:A:354:HIS:ND1	2.34	0.61
1:B:161:HIS:ND1	1:B:226:LEU:HG	2.17	0.59
1:B:55:THR:HG21	1:B:151:ILE:HD13	1.85	0.58
1:A:108:PHE:CD1	1:B:138:PRO:HG3	2.39	0.57
1:B:130:ARG:HD3	1:B:132:TYR:O	2.05	0.57
1:B:154:PHE:HB2	1:B:221:MET:CG	2.34	0.57
1:B:194:THR:O	1:B:198:ARG:HG3	2.03	0.57
1:A:181:GLY:HA2	1:A:265:ARG:NE	2.19	0.56
1:A:26:ALA:N	4:A:662:HOH:O	2.37	0.56
1:A:154:PHE:HB2	1:A:221:MET:HG3	1.88	0.56
1:A:115:VAL:HG23	1:A:129:ASN:HD21	1.71	0.55
1:A:243:PHE:CZ	1:A:326:VAL:HG11	2.42	0.54
1:A:193:THR:HB	1:A:233:PRO:HB2	1.88	0.54
1:B:181:GLY:HA2	1:B:265:ARG:NE	2.19	0.54
1:B:193:THR:HB	1:B:233:PRO:HB2	1.89	0.54
1:A:200:PHE:CZ	1:A:275:PRO:HG3	2.43	0.54
1:B:259:LEU:HB3	1:B:339:LEU:CD2	2.26	0.54
1:B:316:GLY:HA2	1:B:351:ALA:HB3	1.90	0.53
1:A:161:HIS:H	1:A:161:HIS:CD2	2.26	0.53
1:A:303:PRO:HG3	1:A:364:PHE:CE2	2.44	0.53
1:A:182:ARG:CD	1:A:187:GLY:HA3	2.38	0.53
1:B:200:PHE:CZ	1:B:275:PRO:HG3	2.44	0.52
1:B:345:SER:C	4:B:663:HOH:O	2.46	0.52
1:B:243:PHE:CZ	1:B:326:VAL:HG11	2.43	0.52
1:A:61:CYS:O	1:A:98:ASP:OD1	2.28	0.52
1:A:154:PHE:HB2	1:A:221:MET:CG	2.40	0.51
1:A:44:HIS:HB2	1:A:218:GLY:HA3	1.92	0.51
1:B:28:HIS:HB2	4:B:655:HOH:O	2.10	0.51
1:B:98:ASP:OD1	2:B:401:SAH:H1'	2.10	0.51
1:B:186:HIS:O	1:B:187:GLY:C	2.48	0.51
1:B:182:ARG:CD	1:B:187:GLY:HA3	2.41	0.50
1:B:142:TYR:CE1	1:B:203:ASP:HB3	2.47	0.50
1:B:347:VAL:N	4:B:663:HOH:O	2.45	0.50
1:B:70:ILE:HD11	4:B:671:HOH:O	2.12	0.49
1:B:303:PRO:HG3	1:B:364:PHE:CE2	2.47	0.49
1:A:259:LEU:HB3	1:A:339:LEU:CD2	2.28	0.49
1:A:320:ALA:HB2	1:A:348:GLU:HB3	1.95	0.49
1:A:46:ASN:HB3	1:A:51:PRO:HB3	1.93	0.49
1:B:228:ARG:HB2	4:B:629:HOH:O	2.12	0.49
1:A:316:GLY:HA2	1:A:351:ALA:HB3	1.94	0.48
1:B:153:PHE:HE2	1:B:155:HIS:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ASP:OD2	1:A:372:SER:HB3	2.13	0.48
1:A:186:HIS:O	1:A:187:GLY:C	2.50	0.48
1:B:46:ASN:HB3	1:B:51:PRO:HB3	1.94	0.47
1:B:255:VAL:HG11	1:B:265:ARG:HH11	1.80	0.47
1:B:46:ASN:OD1	1:B:48:SER:HB3	2.14	0.47
1:B:140:SER:O	1:B:145:LEU:HD21	2.15	0.46
1:B:148:ALA:O	1:B:150:THR:HG23	2.16	0.46
1:B:182:ARG:NH1	1:B:187:GLY:HA3	2.30	0.46
1:A:46:ASN:OD1	1:A:48:SER:HB3	2.15	0.46
1:A:206:GLU:HG3	4:A:629:HOH:O	2.15	0.46
1:A:182:ARG:NH1	1:A:187:GLY:HA3	2.31	0.46
1:A:138:PRO:HD2	1:B:134:VAL:HG23	1.98	0.45
1:B:61:CYS:SG	1:B:96:PHE:HB3	2.57	0.45
1:A:142:TYR:CE1	1:A:203:ASP:HB3	2.51	0.45
1:A:255:VAL:HG11	1:A:265:ARG:HH11	1.82	0.45
1:B:223:LEU:O	1:B:368:VAL:HA	2.16	0.45
1:A:170:VAL:HG12	1:A:177:ALA:HB1	1.98	0.44
1:B:183:VAL:HG12	1:B:183:VAL:O	2.17	0.44
1:A:141:PHE:CD1	1:A:141:PHE:C	2.91	0.44
1:A:320:ALA:CB	1:A:348:GLU:HB3	2.48	0.44
1:B:311:ASP:O	1:B:315:VAL:HG23	2.18	0.44
1:B:157:ALA:HA	1:B:224:VAL:HG13	1.99	0.44
1:B:316:GLY:HA3	1:B:352:THR:CG2	2.48	0.44
1:B:311:ASP:OD1	1:B:314:GLU:HB2	2.18	0.44
1:A:45:LEU:HD22	1:A:81:ARG:NH1	2.33	0.43
1:B:270:ILE:HG22	1:B:272:VAL:HB	1.99	0.43
1:B:161:HIS:CD2	1:B:162:TRP:CD1	3.07	0.43
1:A:270:ILE:HG22	1:A:272:VAL:HB	1.99	0.43
1:B:297:VAL:CG1	1:B:367:ILE:HG12	2.43	0.43
1:A:72:ASP:O	1:A:76:LYS:HB2	2.18	0.43
1:A:161:HIS:H	1:A:161:HIS:HD2	1.65	0.43
1:B:232:ASP:HA	1:B:233:PRO:HD2	1.82	0.43
1:A:141:PHE:C	1:A:141:PHE:HD1	2.22	0.43
1:A:223:LEU:O	1:A:368:VAL:HA	2.18	0.43
1:A:152:ASP:OD1	1:A:216:LYS:HE2	2.19	0.42
1:A:173:ARG:HE	1:A:173:ARG:HB2	1.67	0.42
1:A:294:LYS:HB3	1:A:370:SER:HB3	2.01	0.42
1:A:160:LEU:HD21	1:A:223:LEU:HD22	2.01	0.42
1:A:257:GLU:HB3	1:A:258:GLY:H	1.69	0.42
1:A:373:PHE:O	1:A:374:THR:CB	2.64	0.42
1:A:129:ASN:HD22	1:A:130:ARG:N	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ALA:HB2	1:B:348:GLU:HB3	2.00	0.42
1:A:95:PHE:CD2	1:A:135:ALA:HB3	2.54	0.42
1:B:206:GLU:HG3	4:B:643:HOH:O	2.20	0.42
1:B:58:ASP:OD1	4:B:671:HOH:O	2.21	0.41
1:A:324:ARG:HG2	1:A:344:PHE:CD2	2.55	0.41
1:A:104:PHE:O	1:A:105:ASN:C	2.57	0.41
1:B:324:ARG:HG2	1:B:344:PHE:CD2	2.55	0.41
1:B:55:THR:HG21	1:B:151:ILE:CD1	2.51	0.41
1:A:111:LEU:HA	1:A:111:LEU:HD23	1.84	0.41
1:B:170:VAL:HG12	1:B:177:ALA:HB1	2.02	0.41
1:B:200:PHE:CZ	1:B:204:LEU:HD22	2.55	0.41
1:B:346:ARG:N	4:B:663:HOH:O	2.53	0.41
1:B:344:PHE:C	4:B:663:HOH:O	2.58	0.41
1:B:61:CYS:O	1:B:98:ASP:OD1	2.39	0.40
1:B:130:ARG:CD	1:B:132:TYR:O	2.69	0.40
1:A:311:ASP:O	1:A:315:VAL:HG23	2.20	0.40
1:B:44:HIS:HB2	1:B:218:GLY:HA3	2.02	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	338/374 (90%)	309 (91%)	25 (7%)	4 (1%)	13 23
1	B	336/374 (90%)	305 (91%)	27 (8%)	4 (1%)	13 23
All	All	674/748 (90%)	614 (91%)	52 (8%)	8 (1%)	13 23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	VAL

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Mol	Chain	Res	Type
1	B	183	VAL
1	A	187	GLY
1	A	286	ALA
1	B	187	GLY
1	B	286	ALA
1	A	62	SER
1	B	355	ALA

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	283/307 (92%)	245 (87%)	38 (13%)	4 5
1	B	278/307 (91%)	245 (88%)	33 (12%)	5 8
All	All	561/614 (91%)	490 (87%)	71 (13%)	4 7

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	31	SER
1	A	45	LEU
1	A	48	SER
1	A	63	SER
1	A	68	VAL
1	A	72	ASP
1	A	75	VAL
1	A	97	SER
1	A	107	LEU
1	A	109	GLN
1	A	114	LEU
1	A	115	VAL
1	A	129	ASN
1	A	141	PHE
1	A	160	LEU

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Mol	Chain	Res	Type
1	A	161	HIS
1	A	169	SER
1	A	173	ARG
1	A	174	ARG
1	A	191	LYS
1	A	215	VAL
1	A	217	ARG
1	A	242	LEU
1	A	245	THR
1	A	252	ASP
1	A	281	LYS
1	A	296	VAL
1	A	302	SER
1	A	308	GLU
1	A	310	ASP
1	A	325	SER
1	A	335	ILE
1	A	337	GLU
1	A	340	SER
1	A	343	LEU
1	A	365	PHE
1	A	368	VAL
1	B	28	HIS
1	B	31	SER
1	B	45	LEU
1	B	48	SER
1	B	63	SER
1	B	68	VAL
1	B	75	VAL
1	B	97	SER
1	B	107	LEU
1	B	109	GLN
1	B	114	LEU
1	B	115	VAL
1	B	129	ASN
1	B	141	PHE
1	B	160	LEU
1	B	161	HIS
1	B	173	ARG
1	B	174	ARG
1	B	215	VAL
1	B	216	LYS

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Mol	Chain	Res	Type
1	B	217	ARG
1	B	221	MET
1	B	242	LEU
1	B	245	THR
1	B	252	ASP
1	B	308	GLU
1	B	310	ASP
1	B	325	SER
1	B	337	GLU
1	B	340	SER
1	B	343	LEU
1	B	365	PHE
1	B	368	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	109	GLN
1	A	129	ASN
1	A	161	HIS
1	A	248	GLN
1	A	361	ASN
1	B	109	GLN
1	B	129	ASN
1	B	248	GLN
1	B	361	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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	$\#\|Z\| > 2$
2	SAH	A	401	-	24,28,28	1.05	2 (8%)	25,40,40	1.78	7 (28%)
2	SAH	B	401	-	24,28,28	1.32	3 (12%)	25,40,40	1.50	3 (12%)

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	-	-	3/11/31/31	0/3/3/3
2	SAH	B	401	-	-	2/11/31/31	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	SAH	C2-N3	4.18	1.38	1.32
2	B	401	SAH	C2-N1	3.17	1.39	1.33
2	A	401	SAH	C2-N3	2.91	1.36	1.32
2	B	401	SAH	C5'-C4'	2.11	1.60	1.52
2	A	401	SAH	OXT-C	-2.08	1.23	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	SAH	N3-C2-N1	-5.57	119.97	128.68
2	B	401	SAH	N3-C2-N1	-4.75	121.25	128.68
2	A	401	SAH	OXT-C-O	-2.77	117.80	124.09
2	A	401	SAH	O4'-C4'-C3'	2.60	110.26	105.11
2	B	401	SAH	C1'-N9-C4	-2.36	122.49	126.64
2	A	401	SAH	C5'-SD-CG	-2.30	95.35	102.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	SAH	C5'-SD-CG	-2.24	95.53	102.27
2	A	401	SAH	C2-N1-C6	2.21	122.54	118.75
2	A	401	SAH	OXT-C-CA	2.18	120.80	113.38
2	A	401	SAH	C1'-N9-C4	-2.01	123.11	126.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	SAH	N-CA-CB-CG
2	A	401	SAH	C-CA-CB-CG
2	B	401	SAH	N-CA-CB-CG
2	B	401	SAH	C-CA-CB-CG
2	A	401	SAH	CB-CG-SD-C5'

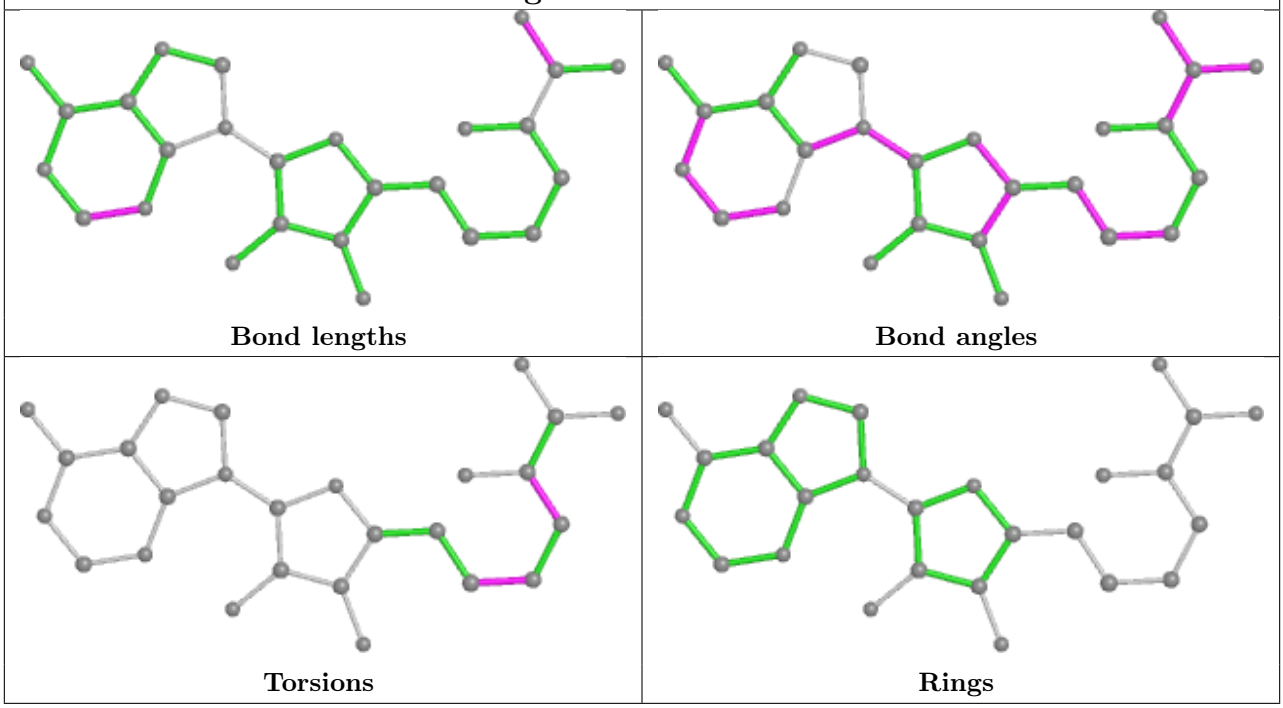
There are no ring outliers.

1 monomer is involved in 1 short contact:

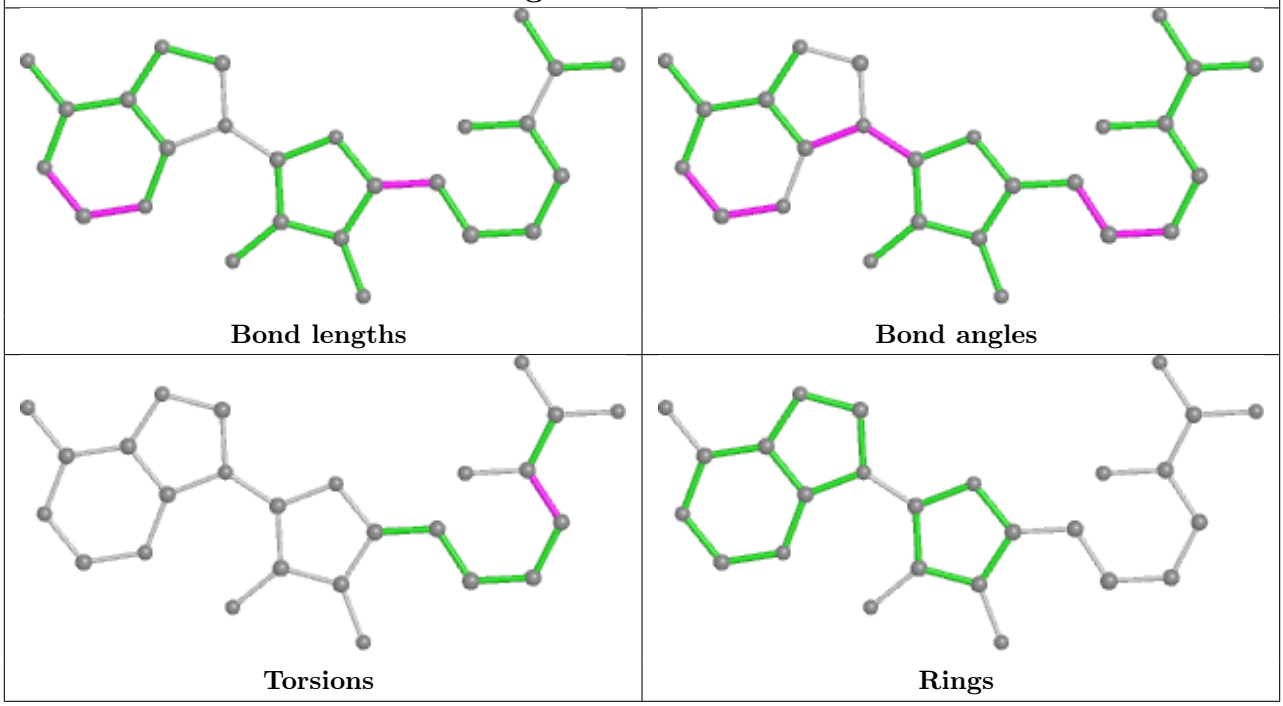
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	SAH	1	0

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 then 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.

Ligand SAH A 401



Ligand SAH B 401



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 (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, 95th 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^2)	Q<0.9
1	A	344/374 (91%)	0.84	38 (11%)	5	6	18, 44, 96, 116	0
1	B	340/374 (90%)	0.88	47 (13%)	2	3	18, 44, 94, 116	0
All	All	684/748 (91%)	0.86	85 (12%)	4	4	18, 44, 95, 116	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	311	ASP	9.4
1	B	344	PHE	8.6
1	B	259	LEU	6.2
1	B	127	ASP	6.2
1	A	26	ALA	5.8
1	A	259	LEU	5.6
1	B	351	ALA	5.5
1	A	343	LEU	5.1
1	A	263	GLU	4.8
1	A	118	THR	4.8
1	A	127	ASP	4.7
1	B	26	ALA	4.6
1	B	339	LEU	4.4
1	B	115	VAL	4.4
1	A	30	ARG	4.4
1	A	315	VAL	4.1
1	B	27	MET	4.1
1	B	359	LEU	4.1
1	A	123	CYS	3.9
1	B	30	ARG	3.9
1	A	347	VAL	3.9
1	B	305	VAL	3.8
1	A	306	VAL	3.8
1	A	262	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	327	ALA	3.7
1	B	349	SER	3.6
1	A	260	VAL	3.5
1	A	319	PHE	3.4
1	B	310	ASP	3.3
1	B	306	VAL	3.3
1	B	307	ASN	3.2
1	A	356	LYS	3.2
1	A	27	MET	3.2
1	B	348	GLU	3.2
1	B	329	VAL	3.1
1	B	268	PHE	3.0
1	A	331	VAL	2.9
1	A	129	ASN	2.8
1	A	115	VAL	2.8
1	A	327	ALA	2.8
1	B	170	VAL	2.7
1	A	357	ASP	2.7
1	B	309	PRO	2.7
1	B	68	VAL	2.7
1	A	162	TRP	2.7
1	A	362	LEU	2.7
1	B	263	GLU	2.6
1	B	358	VAL	2.6
1	B	242	LEU	2.6
1	A	335	ILE	2.5
1	B	260	VAL	2.5
1	A	33	LEU	2.5
1	B	319	PHE	2.5
1	A	241	LEU	2.5
1	A	116	SER	2.5
1	A	360	VAL	2.4
1	B	353	SER	2.4
1	A	261	ALA	2.4
1	B	114	LEU	2.4
1	B	116	SER	2.4
1	B	129	ASN	2.4
1	B	338	GLU	2.3
1	B	251	TRP	2.3
1	B	261	ALA	2.2
1	B	322	SER	2.2
1	A	330	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	324	ARG	2.2
1	B	272	VAL	2.2
1	B	352	THR	2.2
1	A	364	PHE	2.2
1	A	309	PRO	2.2
1	A	339	LEU	2.2
1	A	359	LEU	2.2
1	A	312	ALA	2.2
1	B	347	VAL	2.1
1	B	243	PHE	2.1
1	A	299	LYS	2.1
1	B	315	VAL	2.1
1	A	304	LEU	2.1
1	B	173	ARG	2.1
1	B	128	GLY	2.1
1	B	304	LEU	2.1
1	B	28	HIS	2.0
1	B	296	VAL	2.0
1	A	320	ALA	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

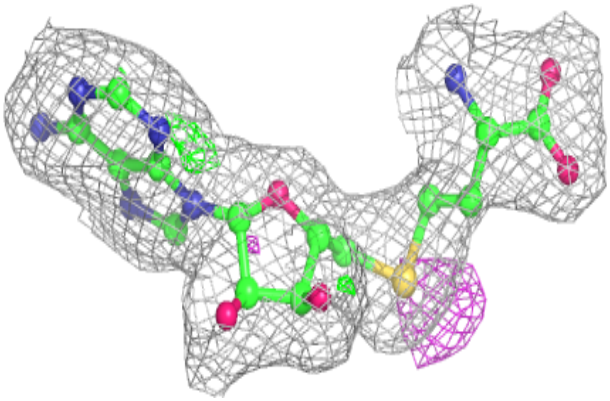
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

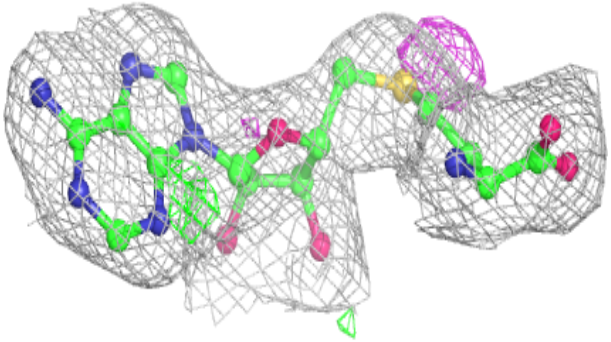
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	B	601	1/1	0.93	0.10	31,31,31,31	0
2	SAH	B	401	26/26	0.95	0.16	22,26,29,30	0
3	MG	A	601	1/1	0.96	0.13	34,34,34,34	0
2	SAH	A	401	26/26	0.97	0.17	23,26,29,30	0

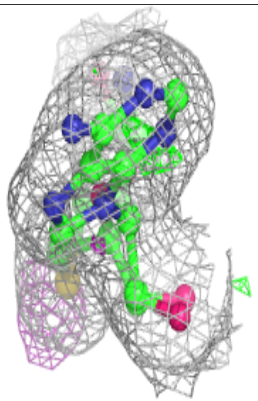
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

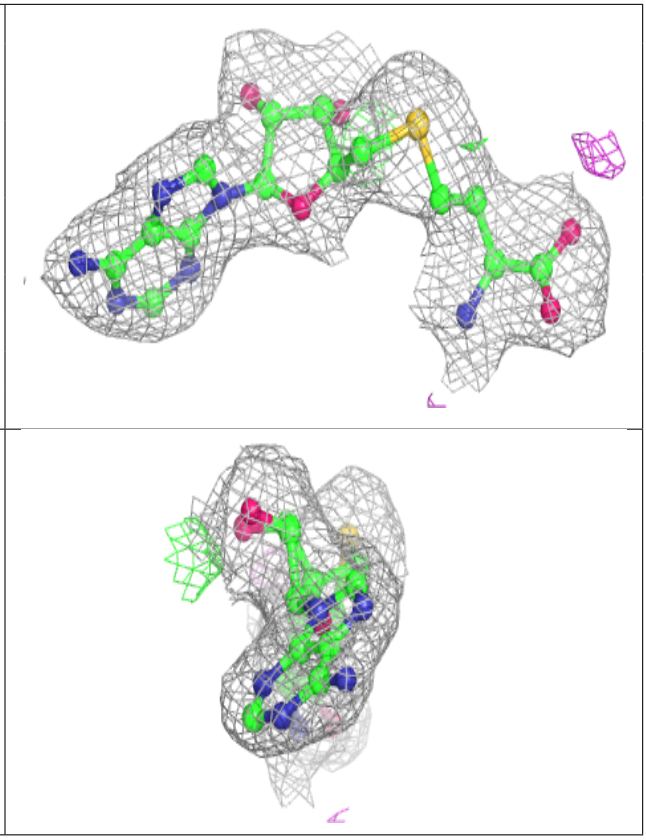






Electron density around SAH A 401:

$2mF_o$-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.