



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:37 pm BST

PDB ID : 5KPC
Title : Pavine N-methyltransferase H206A mutant in complex with S-adenosylmethionine pH 6
Authors : Torres, M.A.; Hoffarth, E.; Eugenio, L.; Savtchouk, J.; Chen, X.; Morris, J.; Facchini, P.J.; Ng, K.K.S.
Deposited on : 2016-07-03
Resolution : 2.50 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 ⓘ symbol.

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

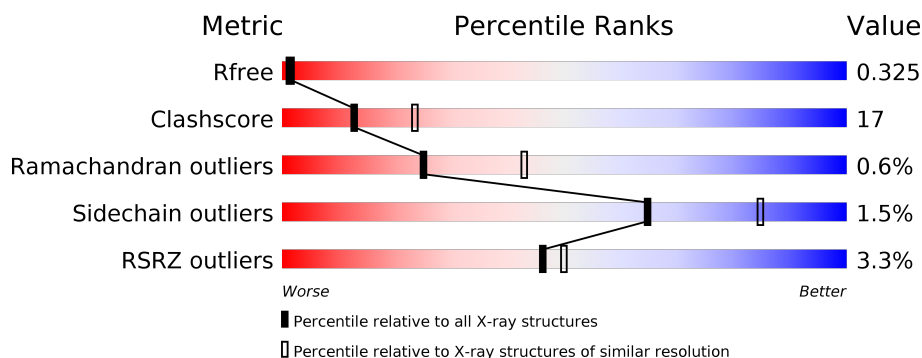
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 ≥ 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	397	<div> <div>3%</div> <div>55%</div> <div>28%</div> <div>16%</div> </div>
1	B	397	<div> <div>3%</div> <div>50%</div> <div>29%</div> <div>19%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5479 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 Pavine N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2745	1769	443	513	20			
1	B	322	Total	C	N	O	S	0	0	0
			2643	1706	423	494	20			

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-40	MET	-	expression tag	UNP C3SBW0
A	-39	ARG	-	expression tag	UNP C3SBW0
A	-38	GLY	-	expression tag	UNP C3SBW0
A	-37	SER	-	expression tag	UNP C3SBW0
A	-36	HIS	-	expression tag	UNP C3SBW0
A	-35	HIS	-	expression tag	UNP C3SBW0
A	-34	HIS	-	expression tag	UNP C3SBW0
A	-33	HIS	-	expression tag	UNP C3SBW0
A	-32	HIS	-	expression tag	UNP C3SBW0
A	-31	HIS	-	expression tag	UNP C3SBW0
A	-30	GLY	-	expression tag	UNP C3SBW0
A	-29	MET	-	expression tag	UNP C3SBW0
A	-28	ALA	-	expression tag	UNP C3SBW0
A	-27	SER	-	expression tag	UNP C3SBW0
A	-26	MET	-	expression tag	UNP C3SBW0
A	-25	THR	-	expression tag	UNP C3SBW0
A	-24	GLY	-	expression tag	UNP C3SBW0
A	-23	GLY	-	expression tag	UNP C3SBW0
A	-22	GLN	-	expression tag	UNP C3SBW0
A	-21	GLN	-	expression tag	UNP C3SBW0
A	-20	MET	-	expression tag	UNP C3SBW0
A	-19	GLY	-	expression tag	UNP C3SBW0
A	-18	ARG	-	expression tag	UNP C3SBW0
A	-17	ASP	-	expression tag	UNP C3SBW0
A	-16	LEU	-	expression tag	UNP C3SBW0

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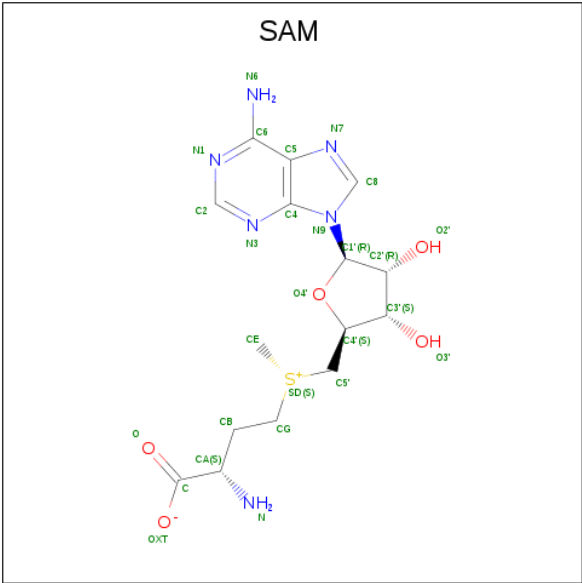
Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	TYR	-	expression tag	UNP C3SBW0
A	-14	ASP	-	expression tag	UNP C3SBW0
A	-13	ASP	-	expression tag	UNP C3SBW0
A	-12	ASP	-	expression tag	UNP C3SBW0
A	-11	ASP	-	expression tag	UNP C3SBW0
A	-10	LYS	-	expression tag	UNP C3SBW0
A	-9	ASP	-	expression tag	UNP C3SBW0
A	-8	ARG	-	expression tag	UNP C3SBW0
A	-7	TRP	-	expression tag	UNP C3SBW0
A	-6	ILE	-	expression tag	UNP C3SBW0
A	-5	ARG	-	expression tag	UNP C3SBW0
A	-4	PRO	-	expression tag	UNP C3SBW0
A	-3	ARG	-	expression tag	UNP C3SBW0
A	-2	ASP	-	expression tag	UNP C3SBW0
A	-1	LEU	-	expression tag	UNP C3SBW0
A	0	GLN	-	expression tag	UNP C3SBW0
A	206	ALA	HIS	engineered mutation	UNP C3SBW0
A	224	ASP	TYR	conflict	UNP C3SBW0
B	-40	MET	-	expression tag	UNP C3SBW0
B	-39	ARG	-	expression tag	UNP C3SBW0
B	-38	GLY	-	expression tag	UNP C3SBW0
B	-37	SER	-	expression tag	UNP C3SBW0
B	-36	HIS	-	expression tag	UNP C3SBW0
B	-35	HIS	-	expression tag	UNP C3SBW0
B	-34	HIS	-	expression tag	UNP C3SBW0
B	-33	HIS	-	expression tag	UNP C3SBW0
B	-32	HIS	-	expression tag	UNP C3SBW0
B	-31	HIS	-	expression tag	UNP C3SBW0
B	-30	GLY	-	expression tag	UNP C3SBW0
B	-29	MET	-	expression tag	UNP C3SBW0
B	-28	ALA	-	expression tag	UNP C3SBW0
B	-27	SER	-	expression tag	UNP C3SBW0
B	-26	MET	-	expression tag	UNP C3SBW0
B	-25	THR	-	expression tag	UNP C3SBW0
B	-24	GLY	-	expression tag	UNP C3SBW0
B	-23	GLY	-	expression tag	UNP C3SBW0
B	-22	GLN	-	expression tag	UNP C3SBW0
B	-21	GLN	-	expression tag	UNP C3SBW0
B	-20	MET	-	expression tag	UNP C3SBW0
B	-19	GLY	-	expression tag	UNP C3SBW0
B	-18	ARG	-	expression tag	UNP C3SBW0
B	-17	ASP	-	expression tag	UNP C3SBW0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	LEU	-	expression tag	UNP C3SBW0
B	-15	TYR	-	expression tag	UNP C3SBW0
B	-14	ASP	-	expression tag	UNP C3SBW0
B	-13	ASP	-	expression tag	UNP C3SBW0
B	-12	ASP	-	expression tag	UNP C3SBW0
B	-11	ASP	-	expression tag	UNP C3SBW0
B	-10	LYS	-	expression tag	UNP C3SBW0
B	-9	ASP	-	expression tag	UNP C3SBW0
B	-8	ARG	-	expression tag	UNP C3SBW0
B	-7	TRP	-	expression tag	UNP C3SBW0
B	-6	ILE	-	expression tag	UNP C3SBW0
B	-5	ARG	-	expression tag	UNP C3SBW0
B	-4	PRO	-	expression tag	UNP C3SBW0
B	-3	ARG	-	expression tag	UNP C3SBW0
B	-2	ASP	-	expression tag	UNP C3SBW0
B	-1	LEU	-	expression tag	UNP C3SBW0
B	0	GLN	-	expression tag	UNP C3SBW0
B	206	ALA	HIS	engineered mutation	UNP C3SBW0
B	224	ASP	TYR	conflict	UNP C3SBW0

- Molecule 2 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C₁₅H₂₂N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total 24	O 24	0	0
3	B	13	Total 13	O 13	0	0

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 ($\text{RSRZ} > 2$). 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.

[illegible]

Chain B:

3% 50% 29% 19%

MET ARG GLY SER HIS HIS HIS HIS HIS GLY MET ALA SER MET THR GLY GLN MET GLY ARG ASP LEU ASP LYS ASP ARG TRP ILE ARG PRO ARG ASP GLU LEU GLN MET GLU THR LYS GLN THR LYS THR LYS GLU VAL ASN ILE LYS ARG ARG ILE

K102 D103 E104 S105 L108 D109 E112 M115 M116 D117 L118 R122 K126 Q129 S130 I131 L132 D133 L134 H138 G139 S140 L141 T142 A146 V154 T158 F166 L174 D175 S177 N178 V179 L180 I181 L182 L183 D185 V186 T187 K188 F189 E190 R197 L198

F199 A200 V201 A202 L203 I204 E205 M206 M207 K208 I221 A222 Q223 D224 G225 F228 V229 E230 H231 H232 K235 A238 Y239 Q240 Y241 L244 D245 D248 I254 F255 P256 SER G258 T259 L260 V261 M262 S263 S264 S265 S266 L267 L268 L269 Q272 E273 D274 V275 W281 T282 L283



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.22Å 71.74Å 96.31Å 90.00° 98.96° 90.00°	Depositor
Resolution (Å)	47.57 – 2.50 47.57 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.57-2.50) 99.6 (47.57-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, R_{free}	0.235 , 0.326 0.236 , 0.325	Depositor DCC
R_{free} test set	1268 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.698	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5479	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: SAM

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	0.56	0/2807	0.69	1/3778 (0.0%)
1	B	0.54	1/2704 (0.0%)	0.66	0/3640
All	All	0.55	1/5511 (0.0%)	0.68	1/7418 (0.0%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	248	ASP	CA-CB	5.68	1.66	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	LEU	CA-CB-CG	5.74	128.51	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	346	TRP	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	2745	0	2705	92	0
1	B	2643	0	2599	89	0
2	A	27	0	22	5	0
2	B	27	0	22	3	0
3	A	24	0	0	2	0
3	B	13	0	0	3	0
All	All	5479	0	5348	179	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 17.

All (179) 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:LYS:NZ	1:B:245:ASP:OD2	1.91	1.02
1:B:174:LEU:CD1	1:B:176:LEU:HG	2.01	0.91
1:A:314:TYR:O	1:A:319:LYS:HE3	1.74	0.88
1:A:279:ASN:HD22	1:A:280:HIS:H	1.21	0.85
1:A:26:GLU:OE1	1:A:29:ARG:NH1	2.12	0.82
1:A:218:SER:O	1:A:355:LYS:NZ	2.18	0.77
1:A:207:MET:O	3:A:501:HOH:O	2.03	0.76
1:A:18:ILE:HG12	1:A:23:VAL:HG11	1.68	0.75
1:B:112:GLU:O	1:B:116:MET:HG3	1.88	0.74
1:A:96:PHE:HB3	2:A:401:SAM:HE1	1.70	0.74
1:A:19:GLU:OE2	1:A:322:LYS:HG3	1.87	0.73
1:B:205:GLU:OE1	1:B:232:HIS:ND1	2.22	0.73
1:A:279:ASN:ND2	1:A:280:HIS:H	1.86	0.72
1:A:152:CYS:O	1:A:178:ASN:ND2	2.22	0.71
1:A:27:GLU:O	1:A:31:MET:HG3	1.90	0.71
1:A:279:ASN:HD22	1:A:280:HIS:N	1.91	0.68
1:A:310:PHE:HD2	1:A:324:ILE:HG13	1.57	0.68
1:A:125:ILE:HA	1:A:129:GLN:HE22	1.58	0.67
1:A:127:ASP:OD2	1:A:149:TYR:HB3	1.95	0.67
1:A:103:ASP:OD1	1:A:104:GLU:N	2.29	0.66
1:A:319:LYS:HA	1:A:322:LYS:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:PHE:HB2	1:B:335:SER:HB2	1.76	0.66
1:B:100:TYR:HB2	1:B:115:MET:HE2	1.77	0.65
1:A:304:ASP:HA	1:A:307:LYS:HD3	1.77	0.65
1:A:280:HIS:HD2	1:A:351:VAL:HG22	1.61	0.65
1:B:35:GLN:OE1	1:B:248:ASP:HB2	1.97	0.65
1:A:303:ILE:HG22	1:A:307:LYS:HD2	1.78	0.65
1:B:52:LEU:O	1:B:56:VAL:HG23	1.96	0.65
1:A:300:ASP:HA	1:A:303:ILE:HG13	1.79	0.64
1:A:60:GLN:OE1	3:A:502:HOH:O	2.15	0.64
1:A:131:ILE:HD13	1:A:197:ARG:HB2	1.79	0.64
1:B:53:ALA:O	1:B:57:THR:HG23	1.98	0.64
1:B:95:LYS:NZ	1:B:98:PRO:O	2.31	0.63
1:A:356:LYS:HE2	1:B:356:LYS:O	1.98	0.63
1:A:253:TYR:HE2	1:A:329:VAL:HG11	1.65	0.62
1:A:243:PRO:HD3	1:A:251:THR:HG21	1.80	0.61
1:A:63:LYS:HE3	1:A:211:GLU:OE2	2.01	0.60
1:B:305:GLU:O	1:B:309:ILE:HG13	2.01	0.60
1:B:25:ASP:OD2	1:B:328:ARG:NH2	2.34	0.60
1:B:81:ILE:HG12	1:B:86:LEU:HD21	1.83	0.60
1:A:96:PHE:HB3	2:A:401:SAM:CE	2.31	0.60
1:A:18:ILE:HA	1:A:23:VAL:HG12	1.84	0.59
1:A:95:LYS:NZ	1:A:98:PRO:O	2.29	0.59
1:A:67:MET:HE2	1:A:187:THR:HA	1.84	0.59
1:B:174:LEU:HD13	1:B:176:LEU:HG	1.82	0.59
1:A:156:GLY:N	1:A:180:GLU:O	2.30	0.58
1:B:174:LEU:HD12	1:B:176:LEU:HG	1.81	0.58
1:B:185:ASP:OD2	1:B:188:LYS:HG3	2.03	0.58
1:B:81:ILE:CD1	1:B:86:LEU:HD11	2.34	0.58
1:A:185:ASP:OD1	2:A:401:SAM:N6	2.30	0.57
1:B:100:TYR:HE2	1:B:102:LYS:HG3	1.70	0.57
1:B:131:ILE:CD1	1:B:197:ARG:HB2	2.35	0.57
1:B:97:SER:HB2	1:B:98:PRO:HD2	1.87	0.56
1:A:27:GLU:O	1:A:31:MET:N	2.33	0.56
1:B:186:VAL:HG23	2:B:401:SAM:C2	2.36	0.56
1:A:311:GLU:HG2	1:A:317:LYS:HA	1.87	0.55
1:B:230:GLU:HG3	1:B:350:GLN:HG2	1.87	0.55
1:B:25:ASP:CG	1:B:328:ARG:HH22	2.09	0.55
1:B:100:TYR:H	1:B:115:MET:HB2	1.70	0.55
1:A:296:LEU:HD11	1:A:328:ARG:HD2	1.88	0.55
1:A:108:LEU:O	1:A:111:SER:OG	2.25	0.55
1:A:255:PHE:HD2	1:A:260:LEU:HD12	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:PHE:CD2	1:B:86:LEU:HD13	2.42	0.55
1:A:300:ASP:OD1	1:A:328:ARG:HD3	2.07	0.54
1:A:52:LEU:HD23	1:B:282:THR:HG23	1.90	0.54
1:A:184:GLU:HG2	1:A:189:PHE:HD1	1.73	0.54
1:B:66:GLU:O	1:B:208:LYS:HB2	2.08	0.54
1:B:30:GLY:HA2	1:B:33:LYS:HG2	1.90	0.54
1:A:67:MET:HE3	1:A:213:PHE:HD1	1.73	0.53
1:B:297:LYS:HG3	1:B:298:ARG:N	2.22	0.53
1:A:92:LYS:HE2	1:A:109:ASP:OD2	2.09	0.53
1:B:108:LEU:O	1:B:112:GLU:HG3	2.09	0.53
1:B:202:ALA:HA	1:B:205:GLU:OE2	2.09	0.52
1:A:117:ASP:OD1	1:A:148:LYS:NZ	2.43	0.52
1:A:28:ILE:HD13	1:A:329:VAL:HG22	1.92	0.52
1:B:126:LYS:HB2	1:B:129:GLN:CD	2.30	0.52
1:A:13:ASN:OD1	1:A:16:LYS:NZ	2.19	0.52
1:B:261:VAL:HG23	3:B:510:HOH:O	2.10	0.52
1:A:67:MET:CE	1:A:187:THR:HA	2.40	0.51
1:B:232:HIS:HD2	1:B:338:TYR:OH	1.92	0.51
1:B:30:GLY:HA2	1:B:33:LYS:HE3	1.92	0.51
1:A:304:ASP:N	1:A:304:ASP:OD2	2.42	0.51
1:A:97:SER:HB2	1:A:98:PRO:HD2	1.92	0.51
2:B:401:SAM:HB1	2:B:401:SAM:H4'	1.91	0.51
1:B:133:ASP:OD2	1:B:142:THR:OG1	2.26	0.51
1:B:303:ILE:HD11	1:B:324:ILE:HD13	1.92	0.51
1:B:44:TYR:HA	1:B:51:GLN:HE22	1.76	0.51
1:B:92:LYS:HB2	1:B:109:ASP:OD1	2.11	0.51
1:A:18:ILE:HA	1:A:23:VAL:CG1	2.40	0.51
1:A:320:ALA:C	1:A:324:ILE:HD12	2.30	0.50
1:B:81:ILE:HD13	1:B:86:LEU:HD11	1.93	0.50
1:B:108:LEU:HB2	1:B:294:GLN:HG3	1.94	0.50
1:A:160:SER:HB3	1:A:163:GLN:HB2	1.94	0.49
1:B:26:GLU:HA	1:B:29:ARG:HH21	1.78	0.49
1:A:253:TYR:CE2	1:A:329:VAL:HG11	2.45	0.49
1:A:320:ALA:O	1:A:324:ILE:HD12	2.13	0.48
1:A:118:LEU:HD12	1:A:118:LEU:HA	1.65	0.48
1:B:175:ASP:O	1:B:176:LEU:HD23	2.13	0.48
1:A:300:ASP:OD2	1:A:328:ARG:NH1	2.47	0.48
1:A:290:LEU:O	1:A:294:GLN:HG2	2.13	0.48
1:B:146:ALA:O	1:B:178:ASN:ND2	2.47	0.48
1:A:132:LEU:O	1:A:198:ILE:HA	2.14	0.47
1:A:126:LYS:HG2	1:A:127:ASP:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:MET:HG2	1:A:333:ALA:HA	1.95	0.47
1:B:122:ARG:HG2	1:B:281:TRP:CZ2	2.49	0.47
1:B:230:GLU:OE2	1:B:348:LEU:HD13	2.14	0.47
1:B:84:PRO:HB2	1:B:309:ILE:HG21	1.96	0.47
1:A:303:ILE:HA	1:A:306:VAL:HG22	1.96	0.47
1:A:143:LEU:HD21	1:A:167:ILE:HG23	1.97	0.47
1:A:35:GLN:OE1	1:A:244:LEU:HD12	2.15	0.47
1:B:131:ILE:HD12	1:B:197:ARG:HB2	1.96	0.47
1:B:180:GLU:O	1:B:181:ILE:HD13	2.15	0.46
1:B:241:TYR:CE1	1:B:262:MET:HB2	2.49	0.46
1:A:264:SER:HB3	1:A:267:ILE:HB	1.98	0.46
1:A:280:HIS:CD2	1:A:351:VAL:HG22	2.47	0.46
1:B:232:HIS:H	1:B:232:HIS:HD1	1.61	0.46
1:B:232:HIS:CD2	1:B:338:TYR:OH	2.68	0.46
1:B:36:VAL:HG13	1:B:346:TRP:CH2	2.51	0.46
1:B:86:LEU:N	1:B:86:LEU:HD22	2.31	0.46
1:A:319:LYS:HB2	1:A:323:PHE:CE2	2.50	0.46
1:B:204:ILE:HD12	1:B:204:ILE:HA	1.82	0.46
1:B:93:THR:O	1:B:140:SER:HB2	2.16	0.46
1:A:164:LYS:HA	1:A:181:ILE:HG21	1.97	0.45
1:A:310:PHE:CD2	1:A:324:ILE:HG13	2.45	0.45
1:A:254:ILE:HD11	1:A:329:VAL:HG12	1.97	0.45
1:A:46:PRO:HD2	1:A:50:GLN:OE1	2.16	0.45
1:A:97:SER:HB2	1:A:98:PRO:CD	2.46	0.45
1:B:287:HIS:HB2	1:B:288:PRO:HD3	1.98	0.45
1:B:84:PRO:O	1:B:88:ILE:HD12	2.17	0.45
1:B:138:HIS:HB3	1:B:166:PHE:CE2	2.52	0.45
1:B:275:VAL:HG22	3:B:508:HOH:O	2.17	0.45
1:B:202:ALA:HB3	2:B:401:SAM:N	2.31	0.45
1:B:63:LYS:NZ	3:B:504:HOH:O	2.50	0.44
1:A:269:LEU:HB3	1:B:269:LEU:HB3	1.99	0.44
1:B:158:THR:O	1:B:183:LEU:HD12	2.17	0.44
1:B:187:THR:HG22	1:B:207:MET:HE1	1.98	0.44
1:B:134:LEU:HD12	1:B:200:ALA:HB2	1.99	0.44
1:B:239:TYR:HD1	1:B:240:GLN:O	2.01	0.44
1:A:103:ASP:OD2	1:A:105:SER:OG	2.34	0.44
1:A:205:GLU:OE2	1:A:231:HIS:HA	2.17	0.44
1:B:223:GLN:O	1:B:224:ASP:HB2	2.18	0.44
1:A:300:ASP:HA	1:A:303:ILE:CG1	2.47	0.43
1:A:97:SER:OG	2:A:401:SAM:OXT	2.30	0.43
1:B:255:PHE:HA	1:B:256:PRO:HD3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LEU:HA	1:A:272:GLN:HE21	1.84	0.43
1:A:204:ILE:HG12	1:A:231:HIS:HB3	1.99	0.43
1:B:238:ALA:O	1:B:239:TYR:HB3	2.19	0.43
1:B:130:SER:O	1:B:131:ILE:HD13	2.18	0.43
1:A:169:ASP:HA	1:A:172:LYS:HD3	2.01	0.43
2:A:401:SAM:HG2	2:A:401:SAM:H4'	1.92	0.43
1:A:126:LYS:H	1:A:129:GLN:NE2	2.16	0.42
1:B:199:PHE:CD1	1:B:228:PHE:HB3	2.54	0.42
1:A:356:LYS:HE3	1:B:272:GLN:O	2.19	0.42
1:B:319:LYS:HA	1:B:319:LYS:HD3	1.73	0.42
1:B:132:LEU:HD23	1:B:198:ILE:HG23	2.02	0.42
1:B:254:ILE:HD11	1:B:329:VAL:HG12	2.01	0.42
1:B:302:ASN:O	1:B:306:VAL:HG23	2.20	0.42
1:B:289:SER:OG	1:B:335:SER:O	2.31	0.42
1:B:118:LEU:HA	1:B:118:LEU:HD12	1.56	0.42
1:A:306:VAL:O	1:A:310:PHE:HB2	2.20	0.42
1:B:235:LYS:O	1:B:265:SER:OG	2.38	0.42
1:A:119:TYR:OH	1:A:230:GLU:OE1	2.38	0.41
1:B:26:GLU:OE2	1:B:29:ARG:NH2	2.54	0.41
1:A:303:ILE:HD13	1:A:303:ILE:HG21	1.85	0.41
1:A:240:GLN:HG2	1:A:261:VAL:HG22	2.01	0.41
1:A:52:LEU:O	1:A:56:VAL:HG23	2.20	0.41
1:B:221:ILE:HG21	1:B:221:ILE:HD13	1.82	0.41
1:B:264:SER:HB3	1:B:267:ILE:HB	2.03	0.41
1:A:18:ILE:HG22	1:A:325:THR:HG21	2.03	0.41
1:B:142:THR:HG23	1:B:154:VAL:HG12	2.02	0.41
1:A:286:LYS:HZ2	1:A:342:ASN:ND2	2.19	0.41
1:A:227:LEU:HG	1:A:228:PHE:N	2.36	0.41
1:A:45:LYS:HD3	1:A:45:LYS:HA	1.77	0.41
1:A:60:GLN:HA	1:A:63:LYS:HD2	2.02	0.40
1:B:260:LEU:HA	1:B:260:LEU:HD23	1.87	0.40
1:B:81:ILE:HD11	1:B:86:LEU:HD11	2.02	0.40
1:B:283:LEU:O	1:B:347:MET:HB2	2.21	0.40
1:B:35:GLN:NE2	1:B:244:LEU:HD12	2.36	0.40
1:A:158:THR:OG1	1:A:159:ASN:N	2.54	0.40

There are no symmetry-related clashes.

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	329/397 (83%)	304 (92%)	23 (7%)	2 (1%)	25	43
1	B	316/397 (80%)	287 (91%)	27 (8%)	2 (1%)	25	43
All	All	645/794 (81%)	591 (92%)	50 (8%)	4 (1%)	25	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	223	GLN
1	A	175	ASP
1	A	320	ALA
1	B	224	ASP

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	304/358 (85%)	300 (99%)	4 (1%)	69	87
1	B	293/358 (82%)	288 (98%)	5 (2%)	60	82
All	All	597/716 (83%)	588 (98%)	9 (2%)	65	85

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	SER
1	A	227	LEU

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Mol	Chain	Res	Type
1	A	279	ASN
1	A	319	LYS
1	B	174	LEU
1	B	187	THR
1	B	190	GLU
1	B	274	ASP
1	B	297	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	87	HIS
1	A	129	GLN
1	A	272	GLN
1	A	279	ASN
1	A	341	ASN
1	B	51	GLN
1	B	232	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 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
2	SAM	B	401	-	21,29,29	0.68	0	18,42,42	1.81	4 (22%)
2	SAM	A	401	-	21,29,29	0.66	0	18,42,42	1.68	2 (11%)

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	SAM	B	401	-	-	5/8/33/33	0/3/3/3
2	SAM	A	401	-	-	5/8/33/33	0/3/3/3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	SAM	C5'-SD-CG	6.21	119.23	103.40
2	B	401	SAM	C5'-SD-CG	5.06	116.30	103.40
2	B	401	SAM	C3'-C2'-C1'	3.05	105.57	100.98
2	B	401	SAM	C5-C6-N6	2.32	123.88	120.35
2	B	401	SAM	O2'-C2'-C3'	2.25	119.09	111.82
2	A	401	SAM	C5-C6-N6	2.16	123.63	120.35

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	SAM	N-CA-CB-CG
2	B	401	SAM	C-CA-CB-CG
2	B	401	SAM	CB-CG-SD-CE
2	B	401	SAM	CB-CG-SD-C5'
2	A	401	SAM	CB-CG-SD-CE
2	A	401	SAM	C4'-C5'-SD-CG
2	A	401	SAM	O4'-C4'-C5'-SD
2	A	401	SAM	C3'-C4'-C5'-SD

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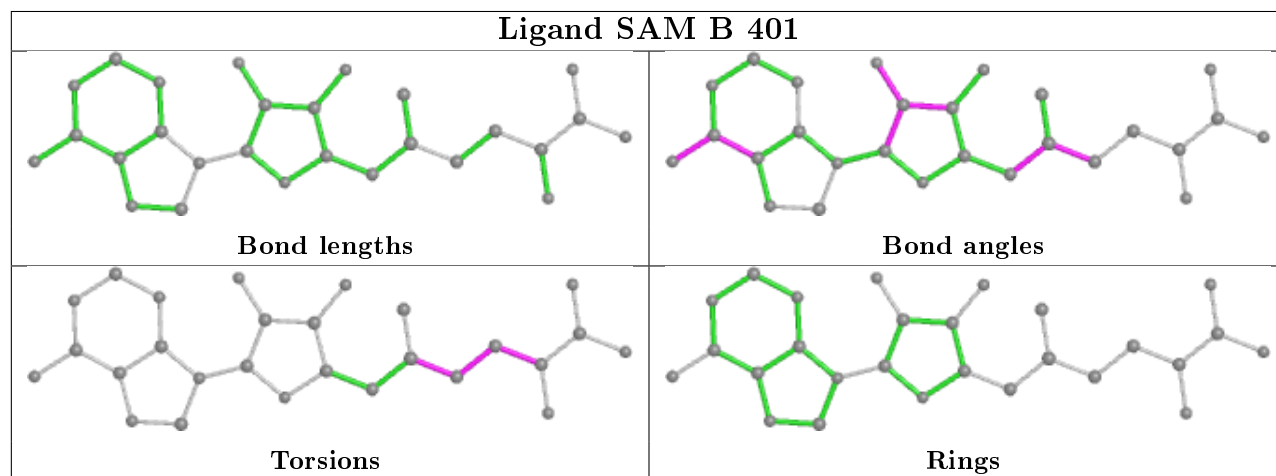
Mol	Chain	Res	Type	Atoms
2	A	401	SAM	CB-CG-SD-C5'
2	B	401	SAM	CA-CB-CG-SD

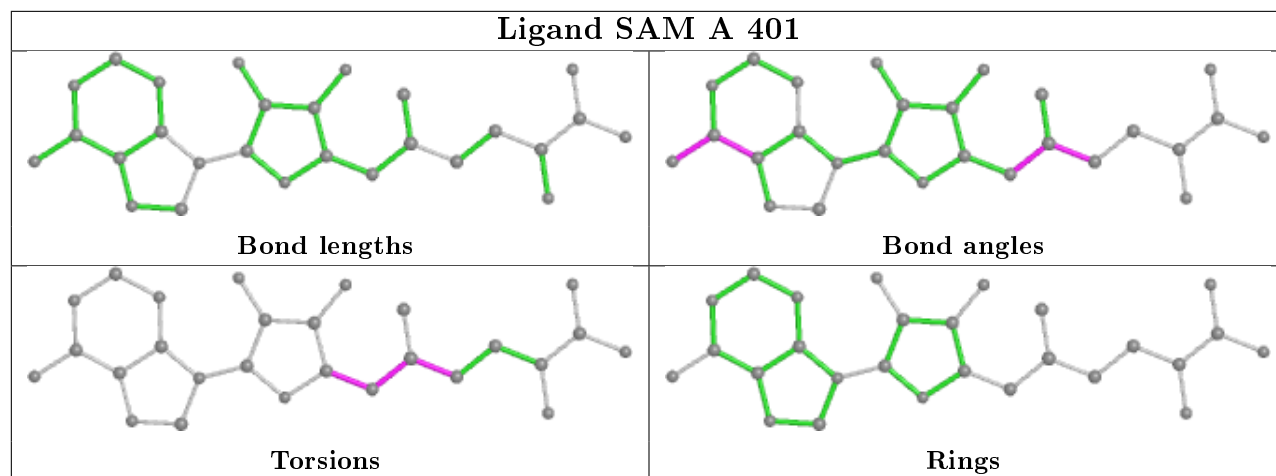
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	SAM	3	0
2	A	401	SAM	5	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, 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	335/397 (84%)	0.35	10 (2%) 50 53	20, 39, 64, 79	0
1	B	322/397 (81%)	0.39	12 (3%) 41 45	25, 43, 61, 74	0
All	All	657/794 (82%)	0.37	22 (3%) 46 50	20, 41, 62, 79	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	18	ILE	4.4
1	A	14	LEU	3.5
1	A	303	ILE	3.1
1	A	314	TYR	3.1
1	B	241	TYR	2.9
1	A	96	PHE	2.8
1	A	23	VAL	2.7
1	B	81	ILE	2.7
1	B	103	ASP	2.7
1	B	36	VAL	2.6
1	B	100	TYR	2.6
1	A	20	HIS	2.6
1	B	225	GLY	2.6
1	B	292	PHE	2.4
1	A	105	SER	2.4
1	B	88	ILE	2.3
1	B	105	SER	2.3
1	B	93	THR	2.2
1	A	324	ILE	2.2
1	A	320	ALA	2.1
1	B	248	ASP	2.1
1	B	255	PHE	2.1

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](#)

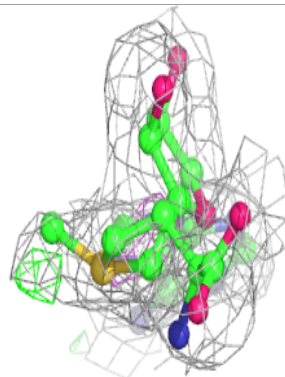
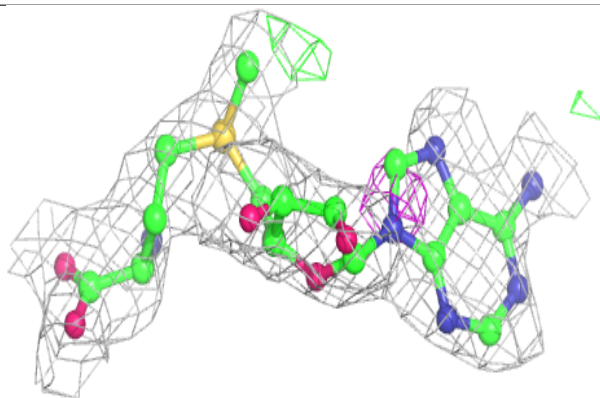
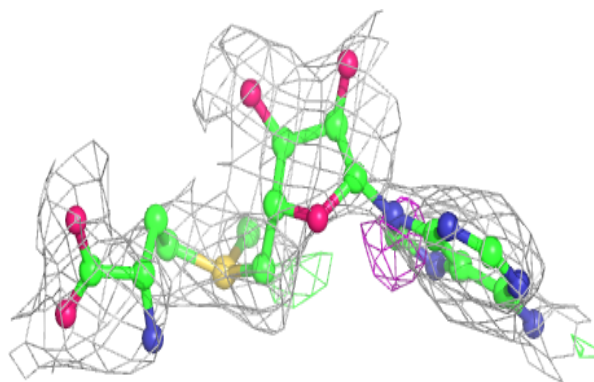
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SAM	B	401	27/27	0.66	0.27	46,61,69,88	0
2	SAM	A	401	27/27	0.80	0.24	38,56,63,80	0

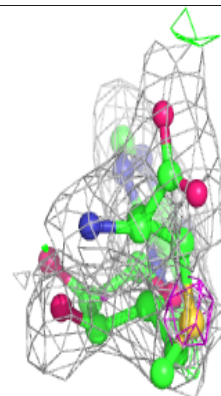
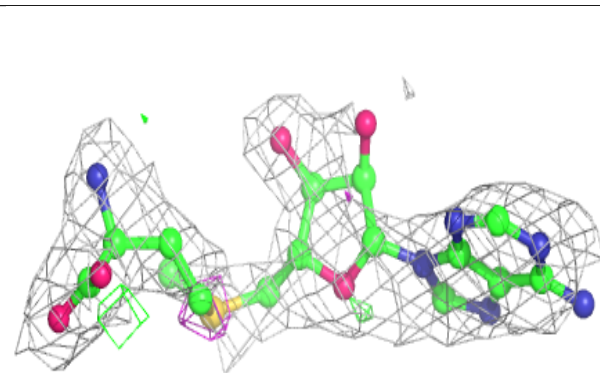
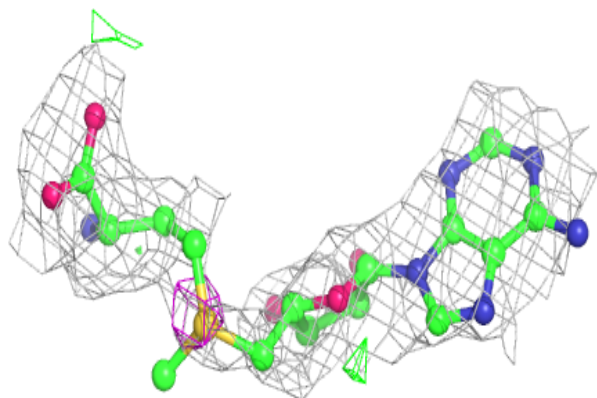
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAM 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 SAM 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.