Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2025 – 04:05 am BST

PDB ID	:	9H5O / pdb_00009h5o
Title	:	NNMT-SAM IN COMPLEX WITH 20s
Authors	:	Johansson, P.
Deposited on	:	2024-10-23
Resolution	:	1.90 Å(reported)

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

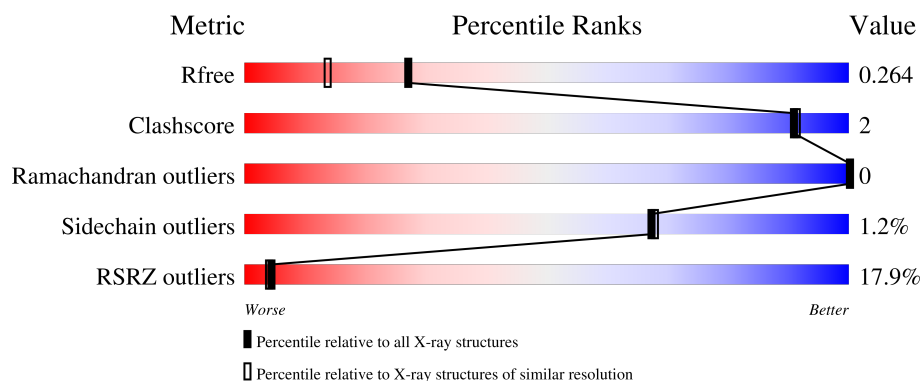|		
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 1.90 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	Percentile Ranks	Value
Rfree		0.264
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		1.2%
RSRZ outliers		17.9%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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	B	280	19% / 85% · 12%
1	D	280	12% / 84% · · 11%

WORLDWIDE
wwPDB
PROTEIN DATA BANK

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 4342 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 Nicotinamide N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	247	Total	C	N	O	S	0	2	0
			1949	1255	313	369	12			
1	D	249	Total	C	N	O	S	0	2	0
			1969	1270	316	371	12			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	HIS	-	expression tag	UNP P40261
B	-17	ASN	-	expression tag	UNP P40261
B	-16	HIS	-	expression tag	UNP P40261
B	-15	ASN	-	expression tag	UNP P40261
B	-14	HIS	-	expression tag	UNP P40261
B	-13	ASN	-	expression tag	UNP P40261
B	-12	HIS	-	expression tag	UNP P40261
B	-11	ASN	-	expression tag	UNP P40261
B	-10	HIS	-	expression tag	UNP P40261
B	-9	ASN	-	expression tag	UNP P40261
B	-8	HIS	-	expression tag	UNP P40261
B	-7	ASN	-	expression tag	UNP P40261
B	-6	ALA	-	expression tag	UNP P40261
B	-5	ALA	-	expression tag	UNP P40261
B	-4	ALA	-	expression tag	UNP P40261
B	-3	GLU	-	expression tag	UNP P40261
B	-2	ASN	-	expression tag	UNP P40261
B	-1	LEU	-	expression tag	UNP P40261
B	0	TYR	-	expression tag	UNP P40261
B	1	PHE	-	expression tag	UNP P40261
B	2	GLN	-	expression tag	UNP P40261
B	100	ALA	LYS	engineered mutation	UNP P40261
B	101	ALA	GLU	engineered mutation	UNP P40261
B	103	ALA	GLU	engineered mutation	UNP P40261
D	-18	HIS	-	expression tag	UNP P40261

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	ASN	-	expression tag	UNP P40261
D	-16	HIS	-	expression tag	UNP P40261
D	-15	ASN	-	expression tag	UNP P40261
D	-14	HIS	-	expression tag	UNP P40261
D	-13	ASN	-	expression tag	UNP P40261
D	-12	HIS	-	expression tag	UNP P40261
D	-11	ASN	-	expression tag	UNP P40261
D	-10	HIS	-	expression tag	UNP P40261
D	-9	ASN	-	expression tag	UNP P40261
D	-8	HIS	-	expression tag	UNP P40261
D	-7	ASN	-	expression tag	UNP P40261
D	-6	ALA	-	expression tag	UNP P40261
D	-5	ALA	-	expression tag	UNP P40261
D	-4	ALA	-	expression tag	UNP P40261
D	-3	GLU	-	expression tag	UNP P40261
D	-2	ASN	-	expression tag	UNP P40261
D	-1	LEU	-	expression tag	UNP P40261
D	0	TYR	-	expression tag	UNP P40261
D	1	PHE	-	expression tag	UNP P40261
D	2	GLN	-	expression tag	UNP P40261
D	100	ALA	LYS	engineered mutation	UNP P40261
D	101	ALA	GLU	engineered mutation	UNP P40261
D	103	ALA	GLU	engineered mutation	UNP P40261

- Molecule 2 is 1,4-dimethyl-6-(methylamino)pyridine-3-carboxamide (CCD ID: A1IPM) (formula: $C_9H_{14}N_3O$) (labeled as "Ligand of Interest" by depositor).
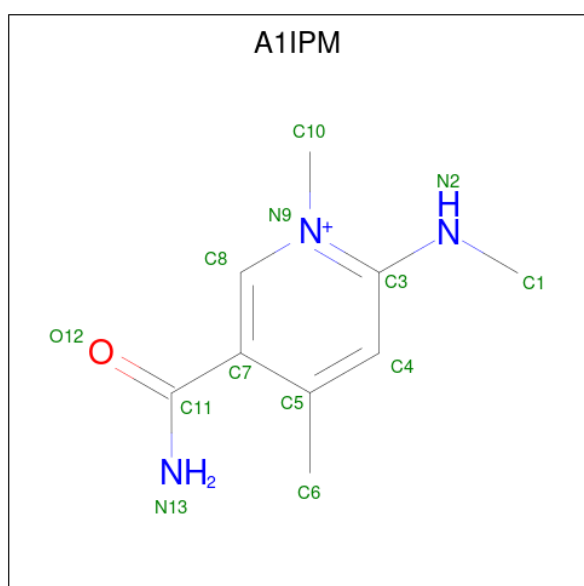
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total C N O 13 9 3 1				0	0
2	D	1	Total C N O 13 9 3 1				0	0

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).
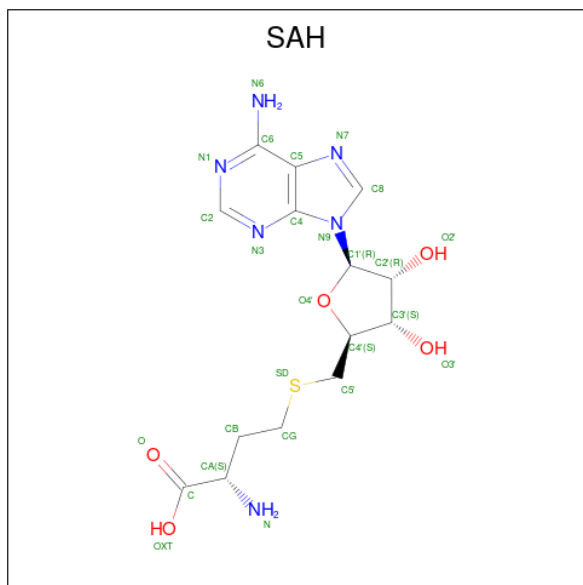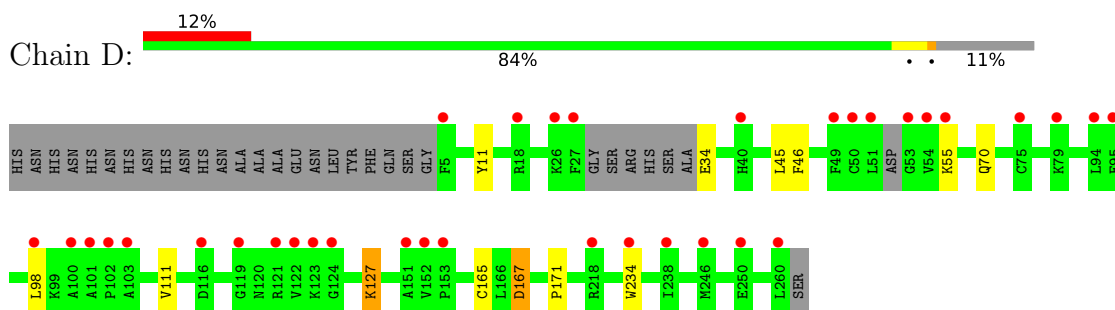

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total C N O S 26 14 6 5 1					0	0
3	D	1	Total C N O S 26 14 6 5 1					0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	150	Total O 150 150		0	0
4	D	196	Total O 196 196		0	0

3 Residue-property plots ⓘ

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: Nicotinamide N-methyltransferase

Chain B:

• Molecule 1: Nicotinamide N-methyltransferase

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.28Å 69.71Å 114.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.04 – 1.90 43.04 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.04-1.90) 100.0 (43.04-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 1.89Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.254 , 0.283 0.232 , 0.264	Depositor DCC
R_{free} test set	2022 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	-4.8	Xtriage
Anisotropy	-12.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.9	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4342	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 63.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.8545e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: A1IPM, 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	B	0.81	0/1989	1.03	1/2693 (0.0%)
1	D	0.83	0/2010	1.04	1/2720 (0.0%)
All	All	0.82	0/3999	1.04	2/5413 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	167	ASP	CA-CB-CG	5.75	118.35	112.60
1	B	167	ASP	CA-CB-CG	5.45	118.05	112.60

There are no chirality outliers.

There are no planarity outliers.

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	B	1949	0	1958	6	0
1	D	1969	0	1980	9	0
2	B	13	0	0	0	0
2	D	13	0	0	0	0
3	B	26	0	19	1	0
3	D	26	0	19	1	0
4	B	150	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	196	0	0	4	0
All	All	4342	0	3976	13	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 2.

All (13) 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:238:ILE:HG22	1:D:234:TRP:HB3	1.82	0.61
1:B:53:GLY:HA3	4:B:538:HOH:O	2.02	0.59
1:D:165:CYS:HB2	4:D:402:HOH:O	2.03	0.57
1:B:11:TYR:CD2	3:B:302:SAH:H2'	2.46	0.50
1:D:111:VAL:HG13	1:D:127:LYS:HG2	1.94	0.49
1:B:111:VAL:HG13	1:B:127:LYS:HG2	1.95	0.48
1:D:171:PRO:HG3	4:D:556:HOH:O	2.16	0.45
1:D:34:GLU:N	4:D:401:HOH:O	2.50	0.45
1:D:11:TYR:CD2	3:D:302:SAH:H2'	2.53	0.44
1:B:46:PHE:HE2	1:D:46:PHE:HE2	1.66	0.43
1:D:45:LEU:HD13	1:D:70:GLN:HA	2.02	0.42
1:D:167:ASP:HB2	4:D:459:HOH:O	2.19	0.41
1:B:45:LEU:HD13	1:B:70:GLN:HA	2.02	0.41

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	B	243/280 (87%)	238 (98%)	5 (2%)	0	100	100
1	D	245/280 (88%)	240 (98%)	5 (2%)	0	100	100
All	All	488/560 (87%)	478 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	217/242 (90%)	215 (99%)	2 (1%)	75	77
1	D	219/242 (90%)	216 (99%)	3 (1%)	62	62
All	All	436/484 (90%)	431 (99%)	5 (1%)	67	71

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	98	LEU
1	B	127	LYS
1	D	55	LYS
1	D	98	LEU
1	D	127	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	120	ASN
1	B	145	GLN
1	B	240	GLN
1	D	36	GLN
1	D	240	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 oligosaccharides in this entry.

5.6   Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	SAH	D	302	-	24,28,28	0.67	0	25,40,40	1.19	2 (8%)
2	A1IPM	B	301	-	12,13,13	1.76	2 (16%)	14,18,18	2.67	4 (28%)
2	A1IPM	D	301	-	12,13,13	1.76	2 (16%)	14,18,18	2.86	4 (28%)
3	SAH	B	302	-	24,28,28	0.63	0	25,40,40	1.20	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
3	SAH	D	302	-	-	1/11/31/31	0/3/3/3
2	A1IPM	B	301	-	-	0/6/6/6	0/1/1/1
2	A1IPM	D	301	-	-	0/6/6/6	0/1/1/1
3	SAH	B	302	-	-	1/11/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	A1IPM	C3-N2	5.03	1.42	1.34
2	B	301	A1IPM	C3-N2	4.94	1.42	1.34
2	D	301	A1IPM	C11-N13	2.79	1.38	1.33
2	B	301	A1IPM	C11-N13	2.76	1.38	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	A1IPM	C1-N2-C3	-9.11	114.43	123.37
2	B	301	A1IPM	C1-N2-C3	-7.97	115.55	123.37
3	B	302	SAH	CB-CG-SD	-3.78	104.82	113.31
2	B	301	A1IPM	C5-C7-C11	3.53	123.24	120.58
3	D	302	SAH	CB-CG-SD	-3.31	105.88	113.31
2	B	301	A1IPM	C8-C7-C5	-3.26	118.85	120.00
2	D	301	A1IPM	C8-C7-C5	-3.15	118.89	120.00
2	D	301	A1IPM	C5-C7-C11	2.99	122.83	120.58
3	D	302	SAH	C5-C6-N6	2.37	123.95	120.35
2	D	301	A1IPM	C7-C11-N13	-2.35	114.68	118.29
3	B	302	SAH	C5-C6-N6	2.34	123.90	120.35
2	B	301	A1IPM	C7-C11-N13	-2.21	114.89	118.29
3	B	302	SAH	CB-CA-N	2.03	115.50	110.17

There are no chirality outliers.
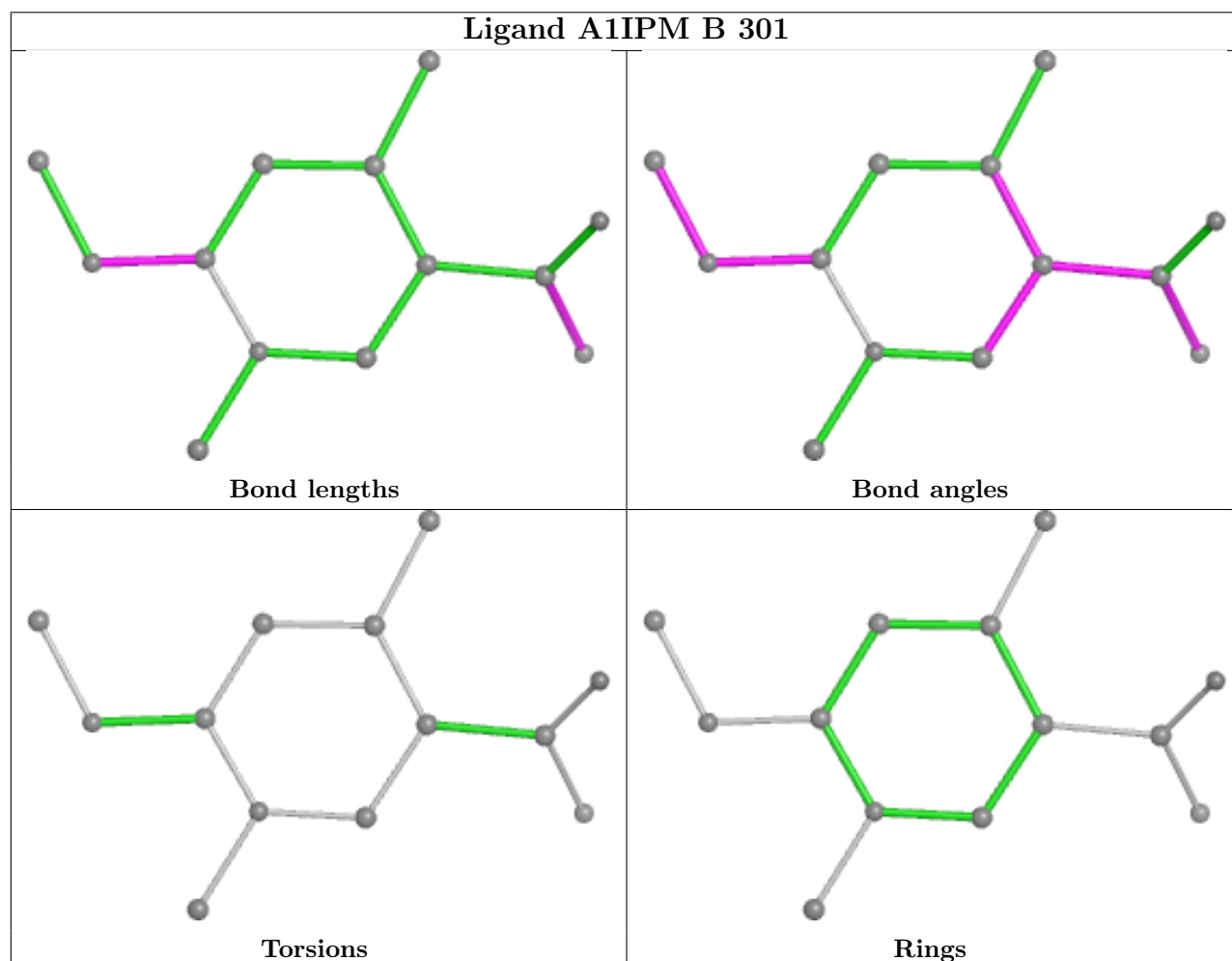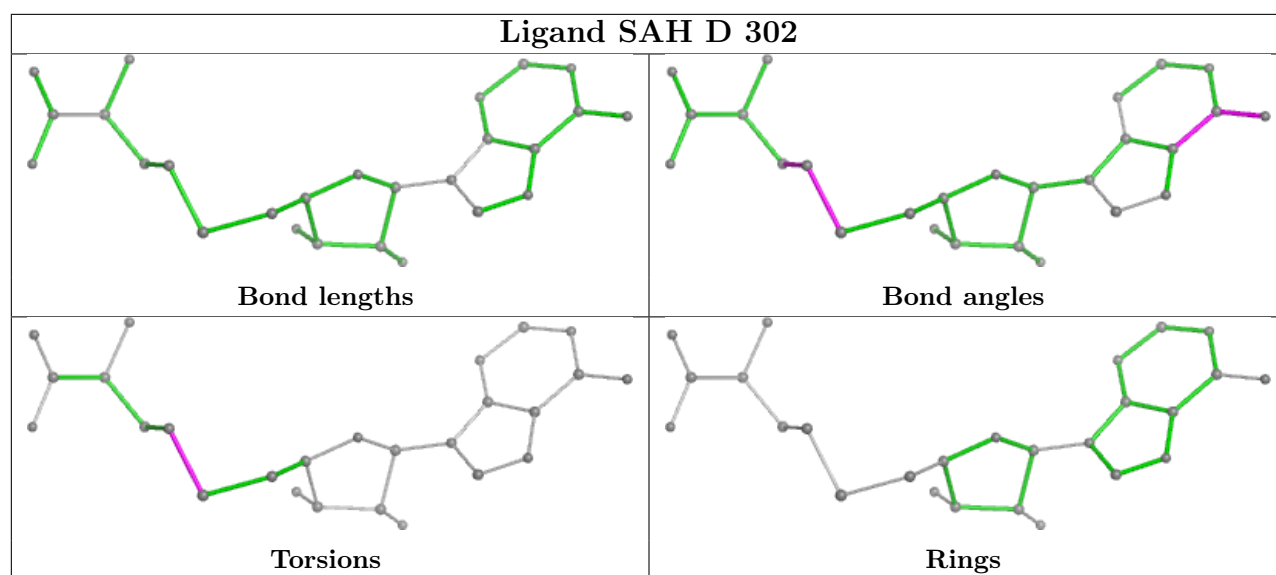
All (2) torsion outliers are listed below:

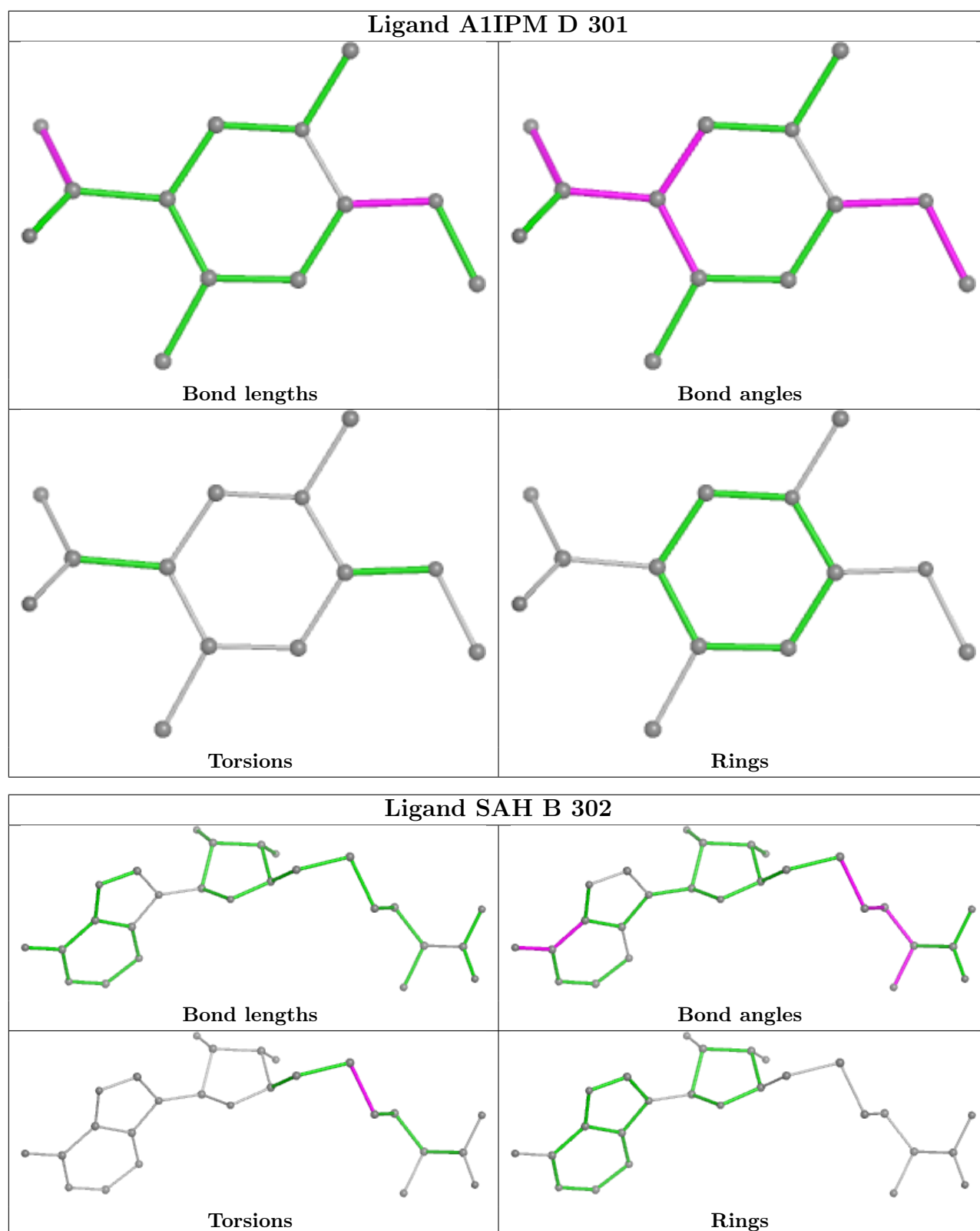| Mol	Chain	Res	Type	Atoms
3	B	302	SAH	CB-CG-SD-C5'
3	D	302	SAH	CB-CG-SD-C5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	302	SAH	1	0
3	B	302	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 D 302

Bond lengths

Bond angles

Torsions

Rings

Ligand A1IPM B 301

Bond lengths

Bond angles

Torsions

Rings

Ligand A1IPM D 301

Bond lengths

Bond angles

Torsions

Rings

Ligand SAH B 302

Bond lengths

Bond angles

Torsions

Rings

5.7　Other polymers ⓘ

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(Å²)	Q<0.9
1	B	247/280 (88%)	1.28	54 (21%)	3	2	2, 7, 40, 59	2 (0%)
1	D	249/280 (88%)	1.05	35 (14%)	7	7	2, 5, 30, 51	2 (0%)
All	All	496/560 (88%)	1.17	89 (17%)	4	4	2, 6, 34, 59	4 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	51	LEU	10.5
1	D	260	LEU	7.0
1	B	102	PRO	7.0
1	B	100	ALA	6.7
1	D	53	GLY	6.6
1	B	99	LYS	6.3
1	B	103	ALA	6.0
1	B	101	ALA	5.5
1	B	104	ALA	5.4
1	B	53	GLY	5.2
1	B	123	LYS	4.8
1	D	234	TRP	4.6
1	B	51	LEU	4.4
1	D	50	CYS	4.3
1	B	122	VAL	4.2
1	B	125	PRO	4.1
1	D	40	HIS	4.1
1	B	98	LEU	4.1
1	D	55	LYS	4.0
1	B	260	LEU	3.9
1	D	27	PHE	3.9
1	D	101	ALA	3.8
1	B	120	ASN	3.7
1	D	102	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	94	LEU	3.5
1	B	18	ARG	3.5
1	B	79	LYS	3.5
1	B	95	GLU	3.5
1	D	121	ARG	3.5
1	B	129	GLU	3.4
1	B	119	GLY	3.4
1	B	55	LYS	3.4
1	B	136	LYS	3.4
1	B	97	TRP	3.4
1	D	123	LYS	3.3
1	D	18	ARG	3.2
1	B	133	GLN	3.2
1	D	103	ALA	3.1
1	B	116	ASP	3.1
1	B	121	ARG	3.1
1	B	50	CYS	3.0
1	D	26	LYS	3.0
1	B	96	LYS	3.0
1	D	153	PRO	2.9
1	D	100	ALA	2.9
1	D	122	VAL	2.9
1	D	218	ARG	2.9
1	D	5	PHE	2.8
1	D	152	VAL	2.8
1	B	35	SER	2.7
1	D	250	GLU	2.7
1	B	105	PHE	2.6
1	B	126	GLU	2.6
1	B	178	ARG	2.6
1	B	137	GLN	2.6
1	D	119	GLY	2.6
1	B	218	ARG	2.6
1	D	116	ASP	2.6
1	B	234	TRP	2.5
1	D	94	LEU	2.5
1	B	8	LYS	2.5
1	B	151	ALA	2.5
1	B	111	VAL	2.5
1	D	79	LYS	2.5
1	B	47	LYS	2.5
1	B	124	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	112	THR	2.4
1	B	80	GLU	2.4
1	B	245	THR	2.4
1	D	151	ALA	2.4
1	B	54	VAL	2.4
1	D	54	VAL	2.3
1	D	49	PHE	2.3
1	B	57	ASP	2.2
1	B	46	PHE	2.2
1	B	117	LEU	2.2
1	D	98	LEU	2.2
1	B	78	PHE	2.2
1	B	130	LYS	2.2
1	D	238	ILE	2.2
1	B	138	VAL	2.1
1	D	246	MET	2.1
1	B	187	LEU	2.1
1	B	258	ARG	2.1
1	D	124	GLY	2.1
1	D	75	CYS	2.1
1	B	127	LYS	2.1
1	D	95	GLU	2.0
1	B	246	MET	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A1IPM	B	301	13/13	0.91	0.10	3,3,4,4	0
2	A1IPM	D	301	13/13	0.92	0.10	3,3,3,4	0
3	SAH	B	302	26/26	0.96	0.07	3,3,3,3	0
3	SAH	D	302	26/26	0.96	0.08	3,3,3,3	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.
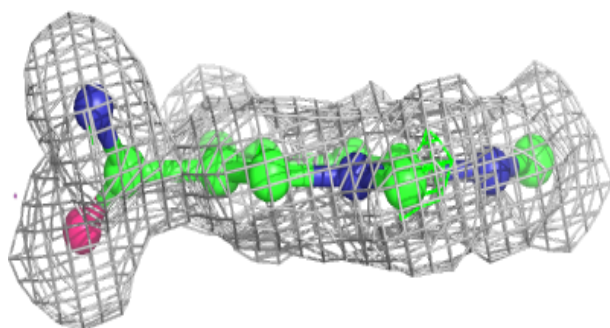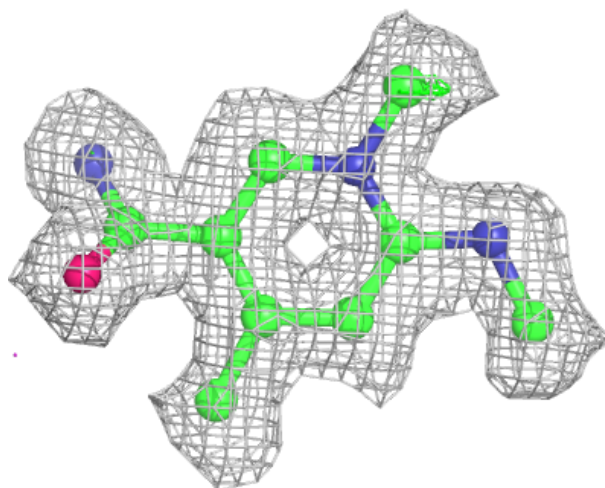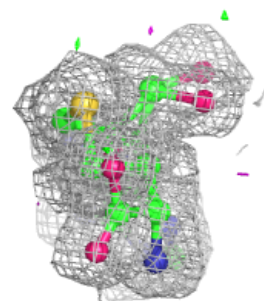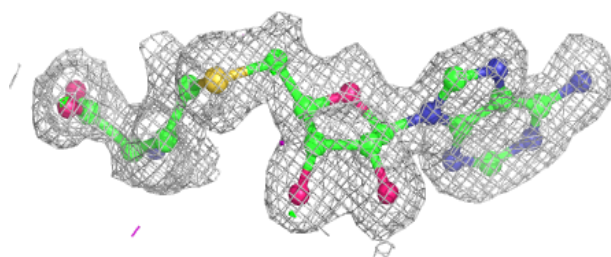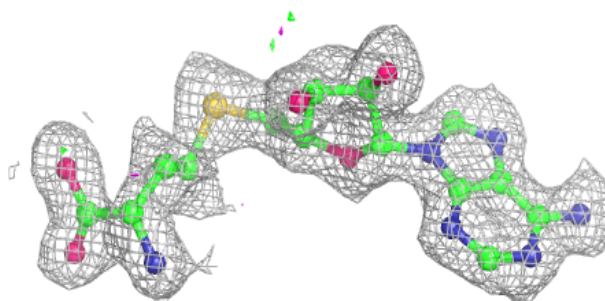

Electron density around A1IPM B 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
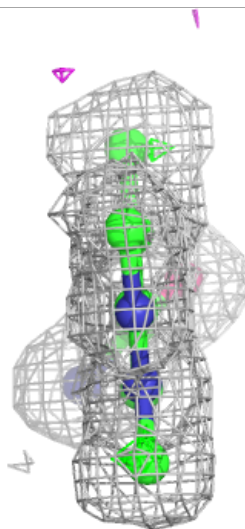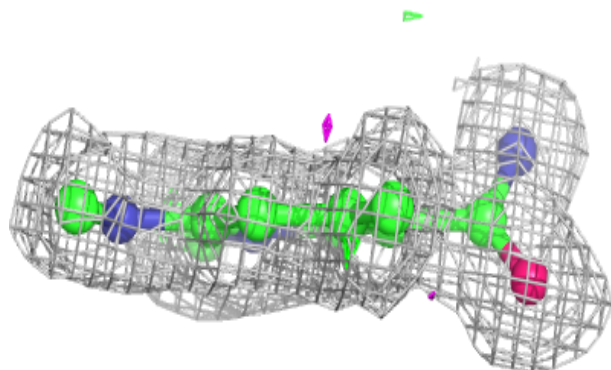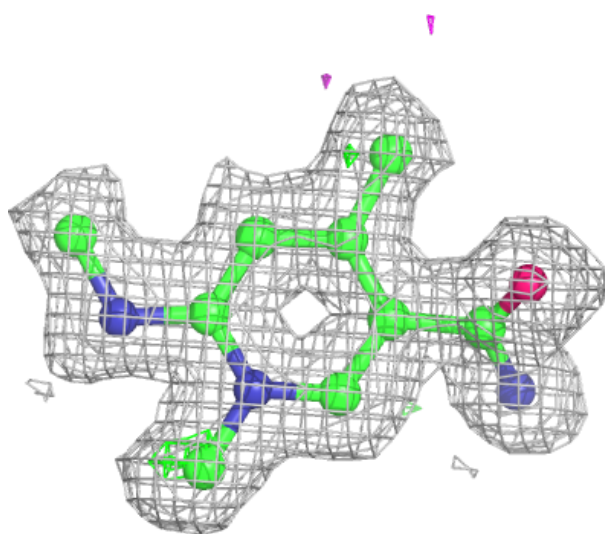
Electron density around A1IPM D 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
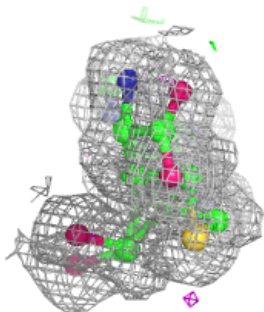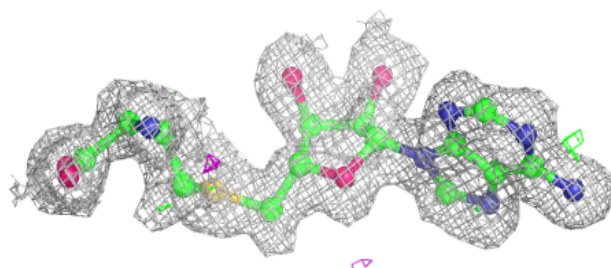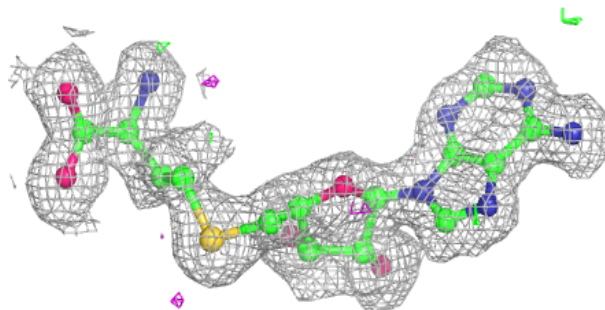and green (positive)
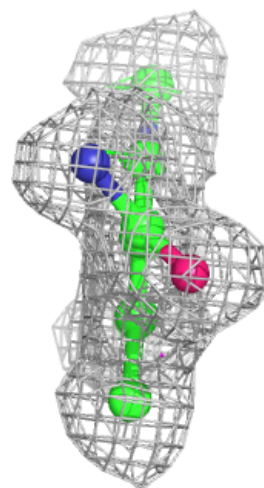
Electron density around SAH B 302:

$2mF_o$-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 D 302:

$2mF_o$-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.