



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2024 – 05:49 PM EST

PDB ID : 3KPY
Title : Crystal Structure of hPNMT in Complex AdoHcy and 6-Chlorooxindole
Authors : Drinkwater, N.; Martin, J.L.
Deposited on : 2009-11-17
Resolution : 2.40 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

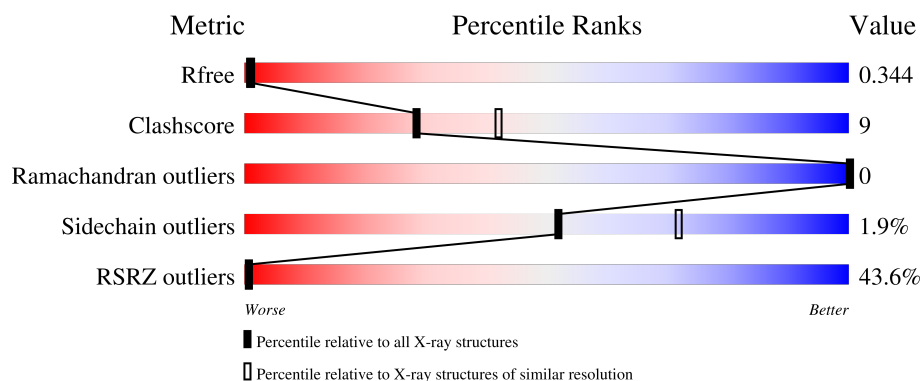
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	289	<div> <div>34%</div> <div>70%</div> <div>18%</div> <div>11%</div> </div>
1	B	289	<div> <div>46%</div> <div>78%</div> <div>14%</div> <div>• 7%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4441 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 Phenylethanolamine N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2016	1280	358	369	9			
1	B	268	Total	C	N	O	S	0	0	0
			2083	1320	370	384	9			

There are 14 discrepancies between the modelled and reference sequences:

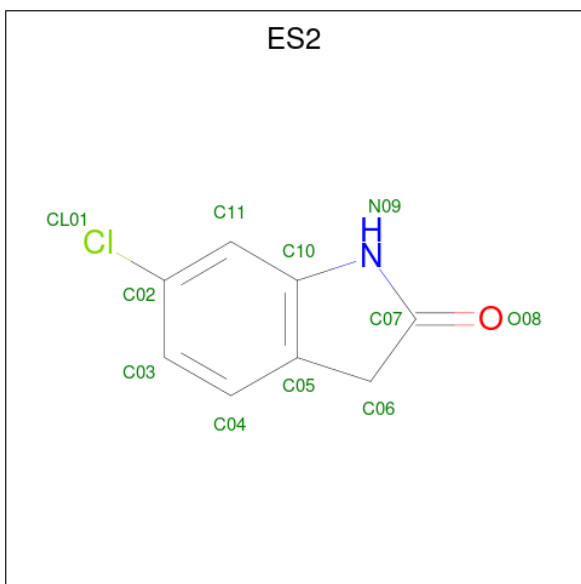
Chain	Residue	Modelled	Actual	Comment	Reference
A	283	GLU	-	expression tag	UNP P11086
A	284	HIS	-	expression tag	UNP P11086
A	285	HIS	-	expression tag	UNP P11086
A	286	HIS	-	expression tag	UNP P11086
A	287	HIS	-	expression tag	UNP P11086
A	288	HIS	-	expression tag	UNP P11086
A	289	HIS	-	expression tag	UNP P11086
B	283	GLU	-	expression tag	UNP P11086
B	284	HIS	-	expression tag	UNP P11086
B	285	HIS	-	expression tag	UNP P11086
B	286	HIS	-	expression tag	UNP P11086
B	287	HIS	-	expression tag	UNP P11086
B	288	HIS	-	expression tag	UNP P11086
B	289	HIS	-	expression tag	UNP P11086

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

- Molecule 3 is 6-chloro-1,3-dihydro-2H-indol-2-one (three-letter code: ES2) (formula: $\text{C}_8\text{H}_6\text{ClNO}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			11	8	1	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	Cl	N	O	0	0
			11	8	1	1	1		

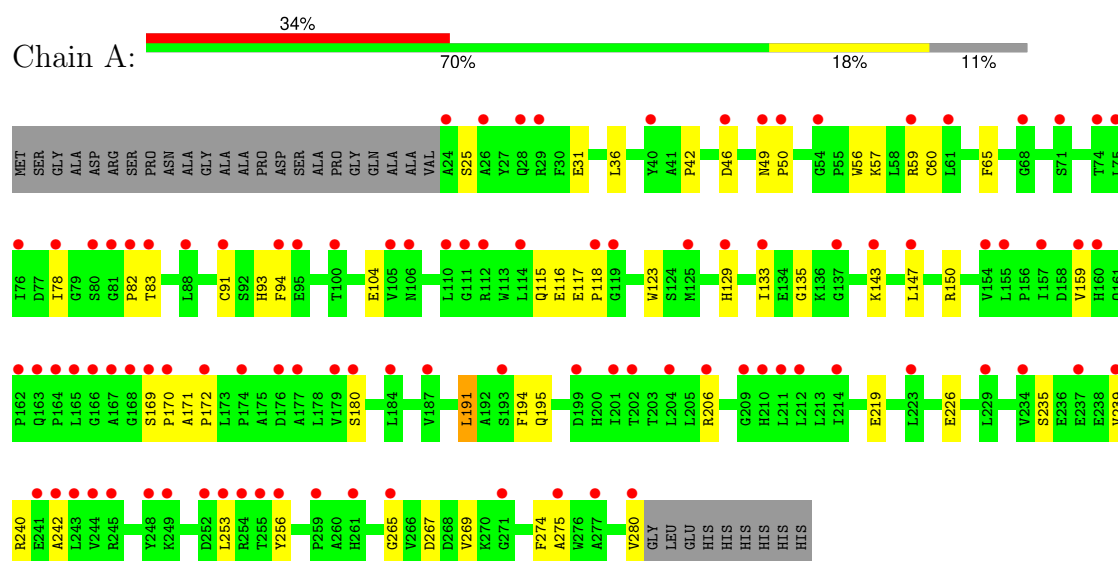
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	115	Total	O	0	0
			115	115		
4	B	153	Total	O	0	0
			153	153		

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. 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. 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: Phenylethanolamine N-methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	93.91Å 93.91Å 188.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.56 – 2.40 45.56 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.2 (45.56-2.40) 90.1 (45.56-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.39Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.206 , 0.271 0.309 , 0.344	Depositor DCC
R_{free} test set	1583 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4441	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 4.29% 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: ES2, 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	0.29	0/2067	0.46	0/2813
1	B	0.31	0/2136	0.47	0/2908
All	All	0.30	0/4203	0.46	0/5721

There are no bond length outliers.

There are no bond angle outliers.

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	A	2016	0	1983	38	0
1	B	2083	0	2045	32	0
2	A	26	0	20	2	0
2	B	26	0	20	3	0
3	A	11	0	6	3	0
3	B	11	0	6	3	0
4	A	115	0	0	9	0
4	B	153	0	0	8	0
All	All	4441	0	4080	72	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 9.

All (72) 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:195:GLN:HE22	1:B:242:ALA:HA	1.46	0.79
1:B:263:GLN:HB2	4:B:2039:HOH:O	1.86	0.75
1:A:46:ASP:HB2	4:A:2217:HOH:O	1.91	0.69
1:A:195:GLN:HE22	1:A:242:ALA:HA	1.59	0.67
1:B:263:GLN:HG3	4:B:2159:HOH:O	1.98	0.63
1:A:253:LEU:HD13	1:A:275:ALA:HB2	1.81	0.63
1:B:207:PRO:HB3	1:B:281:GLY:HA3	1.80	0.61
1:A:159:VAL:HG13	2:A:2001:SAH:H2	1.82	0.60
1:A:115:GLN:HB2	1:A:117:GLU:HG3	1.84	0.59
1:B:267:ASP:OD2	1:B:269:VAL:HG12	2.04	0.58
1:A:280:VAL:HA	4:A:2258:HOH:O	2.03	0.57
1:A:135:GLY:HA2	4:B:2110:HOH:O	2.04	0.57
1:A:78:ILE:HB	1:A:180:SER:HB2	1.86	0.56
1:A:267:ASP:OD1	1:A:269:VAL:HG12	2.07	0.55
1:B:222:TYR:CZ	1:B:229:LEU:HD13	2.40	0.55
1:B:159:VAL:HG22	2:B:2002:SAH:N1	2.23	0.53
1:A:56:TRP:CE2	1:A:256:TYR:HB2	2.43	0.53
1:B:57:LYS:NZ	3:B:290:ES2:H06A	2.23	0.53
1:A:42:PRO:HG3	4:A:2217:HOH:O	2.08	0.53
1:B:95:GLU:HG2	4:B:2273:HOH:O	2.09	0.52
1:A:94:PHE:O	1:A:150:ARG:HD3	2.10	0.52
1:B:59:ARG:HG2	1:B:63:GLN:NE2	2.25	0.51
1:B:73:ARG:HG3	1:B:95:GLU:HG3	1.91	0.51
1:B:83:THR:HA	1:B:123:TRP:CZ2	2.46	0.51
1:A:83:THR:HA	1:A:123:TRP:CZ2	2.46	0.51
1:A:129:HIS:HE1	4:B:2109:HOH:O	1.93	0.51
3:B:290:ES2:H03	4:B:2309:HOH:O	2.10	0.50
1:B:146:GLN:HG2	1:B:150:ARG:HD2	1.93	0.49
1:A:265:GLY:N	4:A:2296:HOH:O	2.40	0.49
1:B:74:THR:HG22	1:B:96:ASP:HB3	1.95	0.49
3:A:290:ES2:H03	4:A:2311:HOH:O	2.13	0.49
4:A:2057:HOH:O	1:B:125:MET:HE2	2.12	0.48
1:A:56:TRP:CD2	1:A:256:TYR:HB2	2.48	0.48
1:A:31:GLU:OE2	1:A:226:GLU:HG2	2.15	0.47
1:B:104:GLU:O	1:B:108:GLN:HG3	2.14	0.47
1:A:50:PRO:O	1:A:59:ARG:NH2	2.44	0.47
1:A:219:GLU:OE1	1:A:269:VAL:HB	2.14	0.47
1:B:281:GLY:HA2	4:B:2199:HOH:O	2.13	0.47
1:B:88:LEU:O	1:B:143:LYS:HD2	2.15	0.47
1:A:57:LYS:NZ	3:A:290:ES2:H06A	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LYS:HZ3	3:B:290:ES2:H06A	1.79	0.46
1:B:95:GLU:HG2	1:B:95:GLU:H	1.61	0.46
1:B:159:VAL:HG13	2:B:2002:SAH:H2	1.95	0.46
1:A:116:GLU:HA	4:A:2269:HOH:O	2.15	0.45
1:A:143:LYS:HD3	4:A:2015:HOH:O	2.17	0.45
1:B:143:LYS:HD3	4:B:2009:HOH:O	2.15	0.45
1:A:117:GLU:HB3	1:A:118:PRO:CD	2.47	0.45
1:A:60:CYS:HB3	1:A:274:PHE:CD1	2.51	0.45
1:A:117:GLU:HB3	1:A:118:PRO:HD2	1.98	0.44
1:B:253:LEU:HD13	1:B:275:ALA:HB2	1.99	0.44
1:B:16:SER:HB2	1:B:20:GLN:NE2	2.32	0.44
1:B:258:MET:HA	1:B:259:PRO:HD3	1.89	0.43
1:A:36:LEU:HD11	1:A:82:PRO:HB2	2.01	0.43
1:A:169:SER:HA	1:A:170:PRO:HD3	1.85	0.43
1:A:82:PRO:HD2	1:A:83:THR:HG23	2.00	0.43
1:A:191:LEU:O	1:A:194:PHE:HB3	2.18	0.43
1:B:253:LEU:HA	1:B:274:PHE:O	2.19	0.43
1:B:78:ILE:HB	1:B:180:SER:HB2	2.01	0.42
1:A:240:ARG:NH2	4:A:2111:HOH:O	2.50	0.42
1:A:49:ASN:HA	1:A:50:PRO:HD3	1.87	0.41
1:A:171:ALA:HA	1:A:172:PRO:HD3	1.91	0.41
1:B:80:SER:O	2:B:2002:SAH:HA	2.20	0.41
1:A:159:VAL:HG22	2:A:2001:SAH:N1	2.36	0.41
1:A:91:CYS:HB3	1:A:147:LEU:HD13	2.03	0.41
1:B:33:ARG:HD3	1:B:33:ARG:HA	1.76	0.41
1:A:57:LYS:HZ3	3:A:290:ES2:H06A	1.84	0.41
1:A:235:SER:O	1:A:239:VAL:HG23	2.21	0.41
1:B:185:GLU:O	1:B:231:VAL:HG13	2.21	0.40
1:B:75:LEU:HD23	1:B:75:LEU:C	2.41	0.40
1:A:65:PHE:HB3	1:A:93:HIS:CE1	2.56	0.40
1:B:128:GLN:HE21	1:B:128:GLN:HA	1.85	0.40
1:A:129:HIS:O	1:A:133:ILE:HG13	2.21	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	255/289 (88%)	250 (98%)	5 (2%)	0	100	100
1	B	266/289 (92%)	261 (98%)	5 (2%)	0	100	100
All	All	521/578 (90%)	511 (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	A	212/233 (91%)	208 (98%)	4 (2%)	52	72
1	B	218/233 (94%)	214 (98%)	4 (2%)	54	73
All	All	430/466 (92%)	422 (98%)	8 (2%)	52	72

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	104	GLU
1	A	191	LEU
1	A	206	ARG
1	B	29	ARG
1	B	95	GLU
1	B	128	GLN
1	B	245	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS

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Mol	Chain	Res	Type
1	A	106	ASN
1	A	195	GLN
1	B	20	GLN
1	B	106	ASN
1	B	128	GLN
1	B	195	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	$\# Z > 2$
2	SAH	B	2002	-	23,28,28	4.07	10 (43%)	22,40,40	2.13	5 (22%)
2	SAH	A	2001	-	23,28,28	4.17	9 (39%)	22,40,40	2.08	5 (22%)
3	ES2	A	290	-	12,12,12	4.33	9 (75%)	17,17,17	4.17	3 (17%)
3	ES2	B	290	-	12,12,12	4.48	9 (75%)	17,17,17	4.06	3 (17%)

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	B	2002	-	-	1/11/31/31	0/3/3/3
2	SAH	A	2001	-	-	3/11/31/31	0/3/3/3
3	ES2	A	290	-	-	-	0/2/2/2
3	ES2	B	290	-	-	-	0/2/2/2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	SAH	C2-N3	11.11	1.49	1.32
2	B	2002	SAH	C2-N3	10.78	1.48	1.32
3	B	290	ES2	C10-C05	10.35	1.49	1.39
3	A	290	ES2	C10-C05	9.75	1.48	1.39
2	B	2002	SAH	C2-N1	9.50	1.50	1.33
2	A	2001	SAH	C2-N1	9.48	1.50	1.33
2	A	2001	SAH	C4-N3	9.23	1.48	1.35
2	B	2002	SAH	C4-N3	8.77	1.47	1.35
2	A	2001	SAH	C8-N7	6.36	1.46	1.34
2	B	2002	SAH	C8-N7	6.21	1.46	1.34
3	B	290	ES2	C03-C02	5.70	1.48	1.38
3	A	290	ES2	C03-C02	5.69	1.48	1.38
3	B	290	ES2	C10-N09	5.24	1.48	1.38
3	A	290	ES2	C10-N09	4.95	1.47	1.38
3	B	290	ES2	C07-N09	4.62	1.46	1.36
3	A	290	ES2	C07-N09	4.49	1.46	1.36
2	A	2001	SAH	O4'-C1'	4.35	1.46	1.40
3	A	290	ES2	C11-C02	4.27	1.45	1.38
3	B	290	ES2	C11-C02	4.22	1.45	1.38
2	B	2002	SAH	O4'-C1'	3.91	1.46	1.40
2	A	2001	SAH	C6-N6	3.41	1.46	1.34
2	B	2002	SAH	C6-N6	3.39	1.46	1.34
2	B	2002	SAH	OXT-C	3.17	1.40	1.30
3	B	290	ES2	C04-C05	3.08	1.44	1.39
3	A	290	ES2	C04-C03	3.01	1.43	1.38
2	A	2001	SAH	OXT-C	2.97	1.40	1.30
3	B	290	ES2	C04-C03	2.96	1.43	1.38
3	A	290	ES2	C04-C05	2.86	1.44	1.39
3	A	290	ES2	O08-C07	-2.51	1.18	1.23
2	A	2001	SAH	C6-N1	2.51	1.46	1.36
3	B	290	ES2	O08-C07	-2.40	1.18	1.23
3	A	290	ES2	C11-C10	2.38	1.43	1.39
2	B	2002	SAH	C6-N1	2.36	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	290	ES2	C11-C10	2.31	1.43	1.39
2	A	2001	SAH	C5-N7	2.11	1.47	1.39
2	B	2002	SAH	C1'-N9	-2.02	1.44	1.49
2	B	2002	SAH	C5-N7	2.01	1.47	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	290	ES2	O08-C07-C06	-15.04	119.29	126.97
3	B	290	ES2	O08-C07-C06	-13.72	119.96	126.97
3	B	290	ES2	C10-N09-C07	-7.90	108.35	111.70
2	A	2001	SAH	N3-C2-N1	-6.55	119.79	128.67
2	B	2002	SAH	N3-C2-N1	-6.37	120.02	128.67
3	A	290	ES2	C10-N09-C07	-6.33	109.02	111.70
2	B	2002	SAH	C4'-O4'-C1'	-5.79	104.62	109.92
2	A	2001	SAH	C4'-O4'-C1'	-4.72	105.60	109.92
3	A	290	ES2	C05-C06-C07	4.05	105.08	103.13
3	B	290	ES2	C05-C06-C07	3.72	104.92	103.13
2	B	2002	SAH	C5'-SD-CG	2.78	110.50	102.26
2	A	2001	SAH	C5'-SD-CG	2.61	110.02	102.26
2	A	2001	SAH	CB-CG-SD	-2.49	107.90	113.45
2	A	2001	SAH	OXT-C-O	-2.21	119.07	124.08
2	B	2002	SAH	CB-CG-SD	-2.04	108.90	113.45
2	B	2002	SAH	OXT-C-O	-2.02	119.49	124.08

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	SAH	N-CA-CB-CG
2	A	2001	SAH	C-CA-CB-CG
2	A	2001	SAH	C4'-C5'-SD-CG
2	B	2002	SAH	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 11 short contacts:

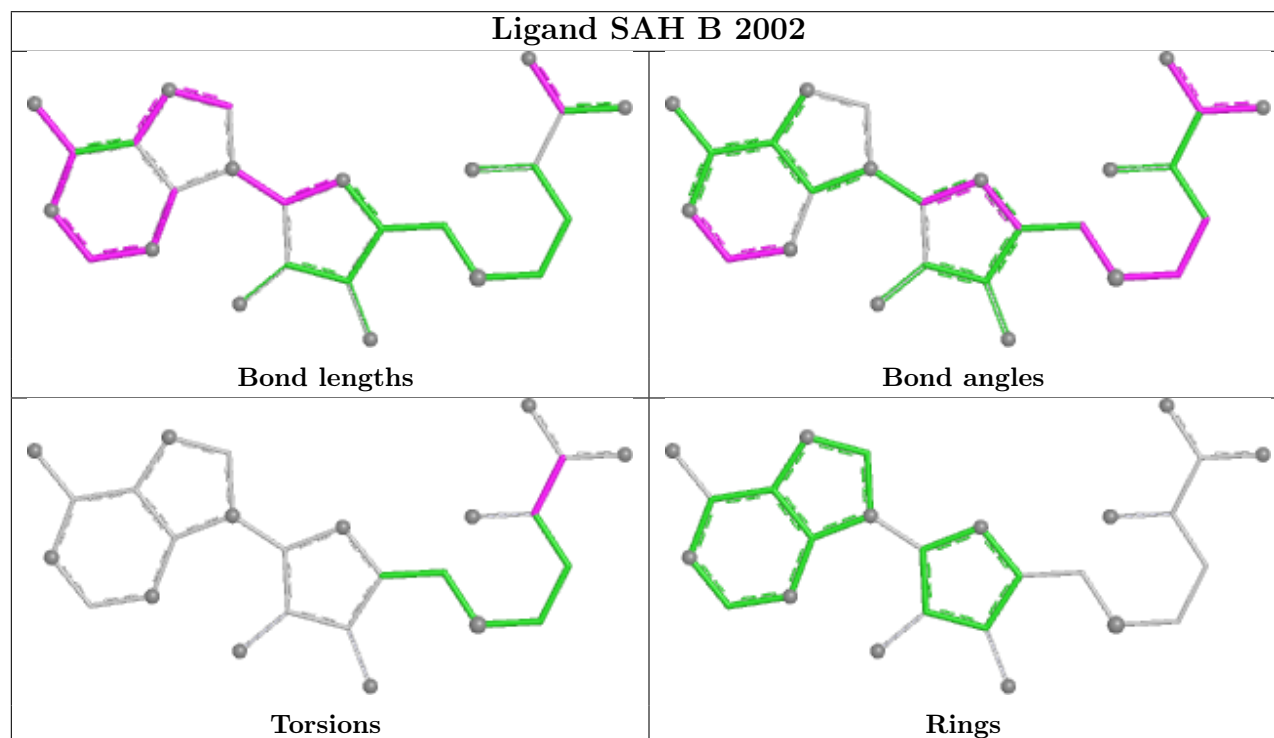
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2002	SAH	3	0
2	A	2001	SAH	2	0
3	A	290	ES2	3	0

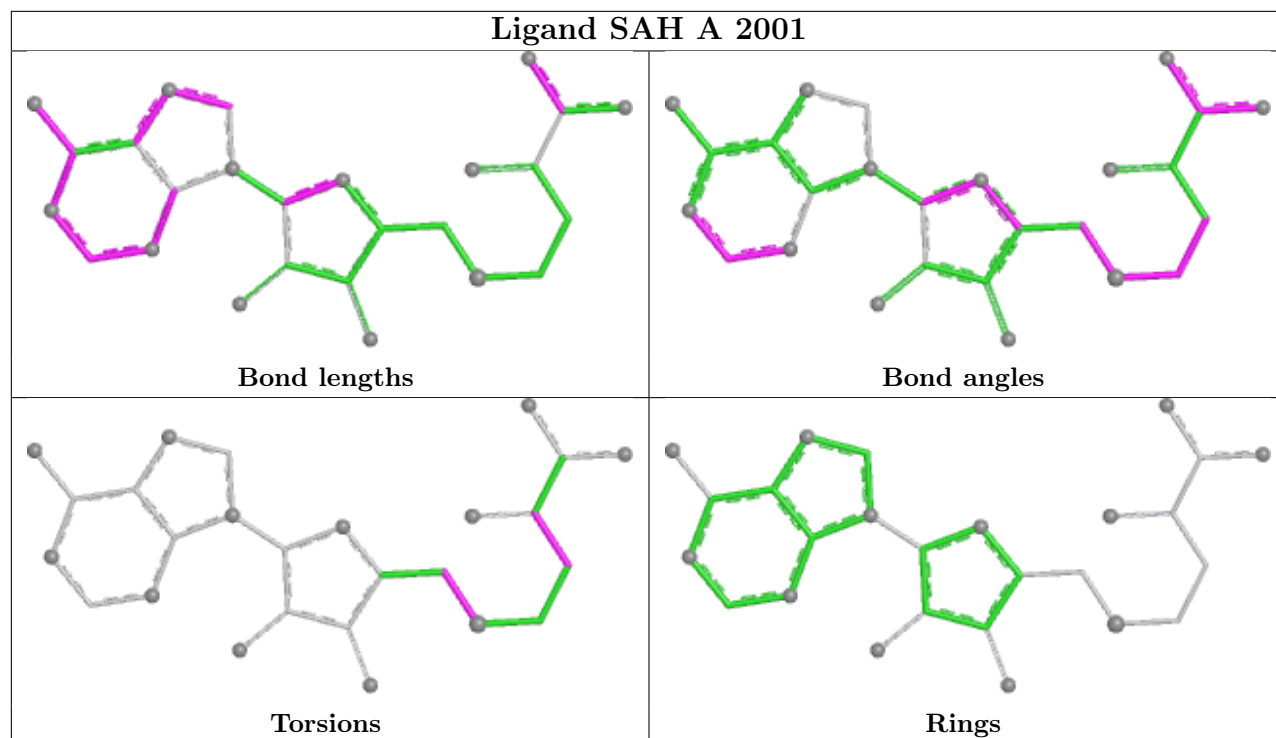
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	290	ES2	3	0

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Warning: The R factor obtained from EDS is 0.3137, which does not match the depositor's R factor of 0.206. Please interpret the results in this section carefully.

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	257/289 (88%)	1.75	97 (37%) 1 1	25, 41, 68, 90	5 (1%)
1	B	268/289 (92%)	2.13	132 (49%) 0 0	25, 37, 63, 122	1 (0%)
All	All	525/578 (90%)	1.94	229 (43%) 1 1	25, 39, 66, 122	6 (1%)

All (229) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	24	ALA	6.0
1	B	14	PRO	6.0
1	B	227	ALA	5.0
1	B	261	HIS	4.9
1	B	95	GLU	4.7
1	B	182	PHE	4.7
1	B	231	VAL	4.6
1	A	275	ALA	4.5
1	B	159	VAL	4.4
1	B	188	SER	4.4
1	B	281	GLY	4.4
1	B	212	LEU	4.0
1	B	263	GLN	4.0
1	B	234	VAL	4.0
1	B	170	PRO	3.9
1	B	27	TYR	3.9
1	B	248	TYR	3.9
1	A	82	PRO	3.8
1	B	23	VAL	3.8
1	B	233	PRO	3.8
1	B	169	SER	3.8
1	A	167	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	30	PHE	3.7
1	B	246	SER	3.7
1	B	200	HIS	3.6
1	B	16	SER	3.6
1	A	254	ARG	3.6
1	B	181	ALA	3.6
1	B	15	ASP	3.6
1	B	235	SER	3.6
1	B	213	LEU	3.5
1	A	245	ARG	3.5
1	B	230	THR	3.5
1	A	81	GLY	3.4
1	A	157	ILE	3.4
1	B	194	PHE	3.4
1	A	170	PRO	3.3
1	A	177	ALA	3.3
1	B	22	ALA	3.3
1	A	280	VAL	3.2
1	B	272	VAL	3.2
1	A	172	PRO	3.2
1	A	80	SER	3.2
1	A	75	LEU	3.2
1	B	269	VAL	3.2
1	B	51	ASN	3.1
1	B	189	PRO	3.1
1	B	245	ARG	3.1
1	A	209	GLY	3.1
1	B	187	VAL	3.1
1	B	262	LEU	3.1
1	B	271	GLY	3.1
1	B	39	ASN	3.1
1	B	186	ALA	3.1
1	B	250	VAL	3.0
1	B	102	PHE	3.0
1	B	218	GLU	3.0
1	B	191	LEU	3.0
1	B	201	ILE	3.0
1	A	249	LYS	3.0
1	B	228	ARG	3.0
1	B	195	GLN	3.0
1	B	178	LEU	3.0
1	B	197	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	49	ASN	2.9
1	A	211	LEU	2.9
1	A	244	VAL	2.9
1	B	56	TRP	2.9
1	B	157	ILE	2.9
1	A	29	ARG	2.9
1	B	137	GLY	2.9
1	B	207	PRO	2.9
1	A	179	VAL	2.9
1	B	175	ALA	2.9
1	B	276	TRP	2.9
1	A	61	LEU	2.8
1	B	214	ILE	2.8
1	B	85	TYR	2.8
1	A	163	GLN	2.8
1	A	147	LEU	2.8
1	A	212	LEU	2.8
1	B	274	PHE	2.8
1	B	163	GLN	2.8
1	B	260	ALA	2.8
1	B	253	LEU	2.8
1	B	71	SER	2.8
1	A	159	VAL	2.8
1	B	198	LEU	2.7
1	B	199	ASP	2.7
1	B	237	GLU	2.7
1	A	229	LEU	2.7
1	B	41	ALA	2.7
1	B	254	ARG	2.7
1	B	49	ASN	2.7
1	A	168	GLY	2.7
1	B	215	GLY	2.7
1	A	26	ALA	2.7
1	B	192	ALA	2.7
1	B	196	ARG	2.7
1	A	164	PRO	2.7
1	A	71	SER	2.7
1	A	155	LEU	2.7
1	A	277	ALA	2.7
1	B	34	ALA	2.7
1	A	201	ILE	2.7
1	A	94	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	75	LEU	2.6
1	B	275	ALA	2.6
1	B	202	THR	2.6
1	B	164	PRO	2.6
1	B	206	ARG	2.6
1	A	271	GLY	2.6
1	B	108	GLN	2.6
1	B	273	PHE	2.6
1	B	73	ARG	2.6
1	A	184	LEU	2.6
1	A	187	VAL	2.6
1	B	256	TYR	2.6
1	A	78	ILE	2.6
1	A	110	LEU	2.6
1	A	180	SER	2.6
1	B	17	ALA	2.6
1	B	190	ASP	2.6
1	B	173	LEU	2.5
1	A	154	VAL	2.5
1	A	119	GLY	2.5
1	B	38	ASN	2.5
1	A	253	LEU	2.5
1	B	184	LEU	2.5
1	B	76	ILE	2.5
1	B	226	GLU	2.5
1	A	74	THR	2.5
1	B	252	ASP	2.5
1	B	45	GLY	2.5
1	A	237	GLU	2.5
1	A	68	GLY	2.5
1	B	72	GLY	2.5
1	A	88	LEU	2.5
1	B	229	LEU	2.5
1	B	280	VAL	2.5
1	A	242	ALA	2.5
1	A	241	GLU	2.5
1	B	24	ALA	2.4
1	B	240	ARG	2.4
1	B	267	ASP	2.4
1	A	40	TYR	2.4
1	A	204	LEU	2.4
1	A	243	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	261	HIS	2.4
1	B	216	ALA	2.4
1	A	166	GLY	2.4
1	B	217	LEU	2.4
1	A	162	PRO	2.4
1	A	54	GLY	2.4
1	A	100	THR	2.4
1	B	83	THR	2.4
1	A	176	ASP	2.4
1	B	103	LEU	2.4
1	A	129	HIS	2.4
1	A	210	HIS	2.4
1	A	259	PRO	2.4
1	A	83	THR	2.4
1	A	239	VAL	2.3
1	A	50	PRO	2.3
1	A	59	ARG	2.3
1	A	28	GLN	2.3
1	A	234	VAL	2.3
1	A	76	ILE	2.3
1	B	171	ALA	2.3
1	B	58	LEU	2.3
1	B	243	LEU	2.3
1	A	118	PRO	2.3
1	B	82	PRO	2.3
1	B	225	GLY	2.3
1	B	219	GLU	2.3
1	A	248	TYR	2.3
1	B	91	CYS	2.3
1	A	137	GLY	2.2
1	A	160	HIS	2.2
1	A	265	GLY	2.2
1	B	129	HIS	2.2
1	A	202	THR	2.2
1	A	214	ILE	2.2
1	A	223	LEU	2.2
1	B	220	SER	2.2
1	B	29	ARG	2.2
1	B	112	ARG	2.2
1	A	46	ASP	2.2
1	B	134	GLU	2.2
1	A	133	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	78	ILE	2.2
1	B	154	VAL	2.2
1	B	208	GLY	2.2
1	B	48	CYS	2.2
1	A	169	SER	2.2
1	A	193	SER	2.2
1	A	112	ARG	2.2
1	B	42	PRO	2.2
1	B	43	PRO	2.2
1	B	161	GLN	2.2
1	A	165	LEU	2.2
1	B	204	LEU	2.2
1	B	162	PRO	2.2
1	A	199	ASP	2.2
1	A	252	ASP	2.2
1	A	105	VAL	2.2
1	B	249	LYS	2.1
1	B	166	GLY	2.1
1	B	172	PRO	2.1
1	A	91	CYS	2.1
1	B	70	VAL	2.1
1	B	168	GLY	2.1
1	A	95	GLU	2.1
1	B	193	SER	2.1
1	A	106	ASN	2.1
1	A	125	MET	2.1
1	B	147	LEU	2.1
1	A	111	GLY	2.1
1	B	100	THR	2.1
1	A	114	LEU	2.0
1	A	206	ARG	2.0
1	B	277	ALA	2.0
1	B	81	GLY	2.0
1	A	143	LYS	2.0
1	A	174	PRO	2.0
1	A	255	THR	2.0
1	A	256	TYR	2.0
1	B	64	THR	2.0
1	B	257	ILE	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](#)

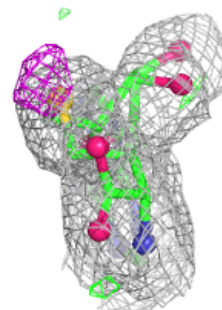
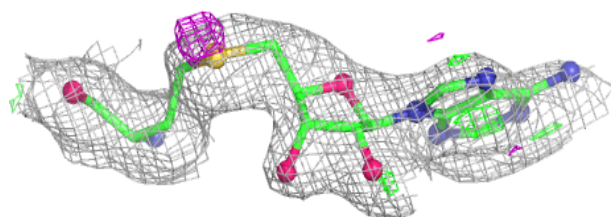
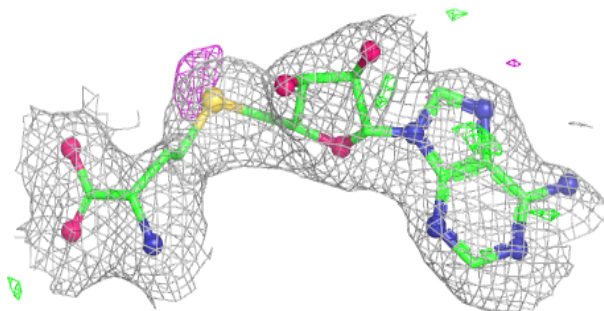
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ES2	A	290	11/11	0.71	0.31	54,63,75,81	0
3	ES2	B	290	11/11	0.72	0.30	58,71,88,89	0
2	SAH	B	2002	26/26	0.82	0.17	22,31,38,40	0
2	SAH	A	2001	26/26	0.87	0.15	30,39,44,58	0

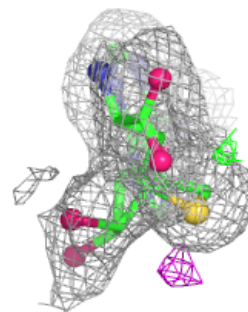
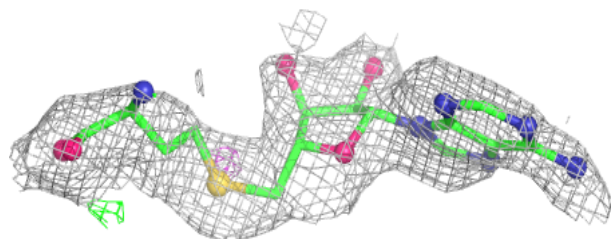
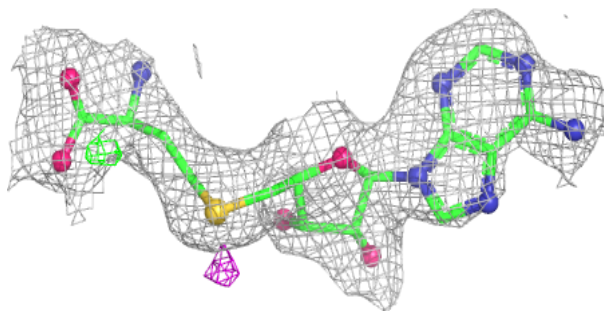
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH B 2002:

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

**Electron density around SAH A 2001:**

$2mF_o-DF_c$ (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.