Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2024 – 11:49 PM EST

PDB ID	:	1P1C
Title	:	Guanidinoacetate Methyltransferase with Gd ion
Authors	:	Komoto, J.; Takusagawa, F.
Deposited on	:	2003-04-12
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 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:

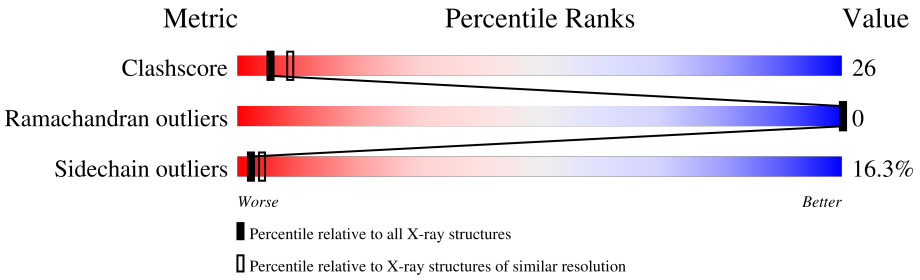
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	199	53% 36% 8% ·
1	B	199	53% 38% 7% ·

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3345 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.

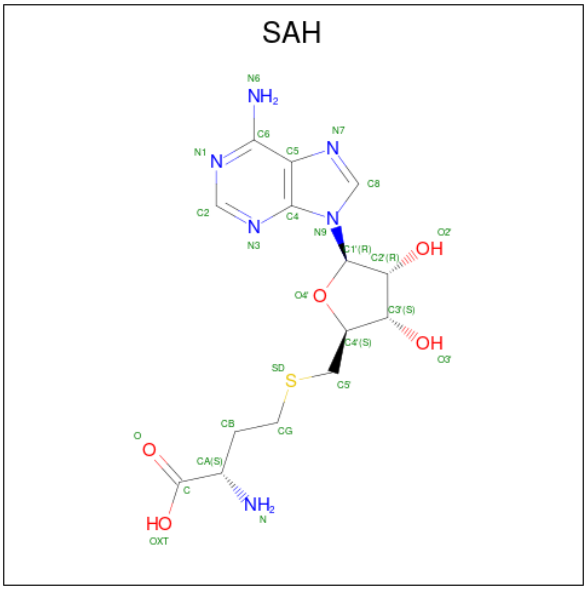
- Molecule 1 is a protein called Guanidinoacetate N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	0	0
			1548	1001	262	275	10			
1	B	193	Total	C	N	O	S	0	0	0
			1548	1001	262	275	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	VAL	GLU	SEE REMARK 999	UNP P10868
B	119	VAL	GLU	SEE REMARK 999	UNP P10868

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

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

- Molecule 3 is GADOLINIUM ION (three-letter code: GD3) (formula: Gd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Gd	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	113	Total	O	0	0
			113	113		
4	B	83	Total	O	0	0
			83	83		

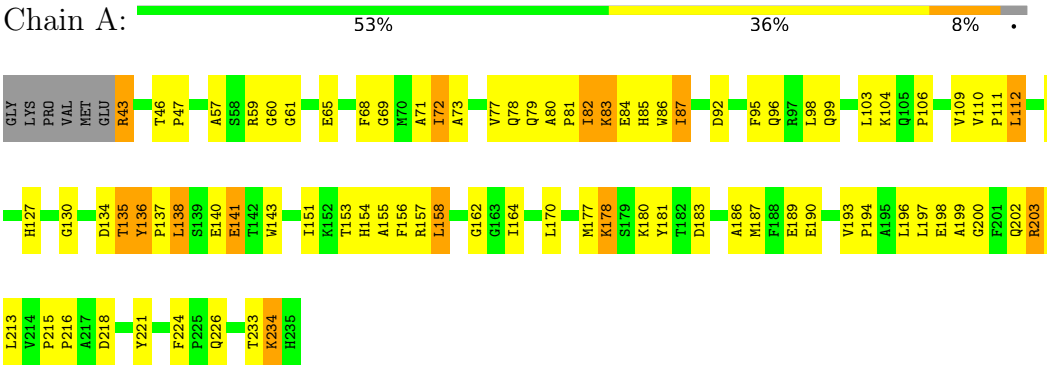
3 Residue-property plots (i)

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. 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.

Note EDS was not executed.

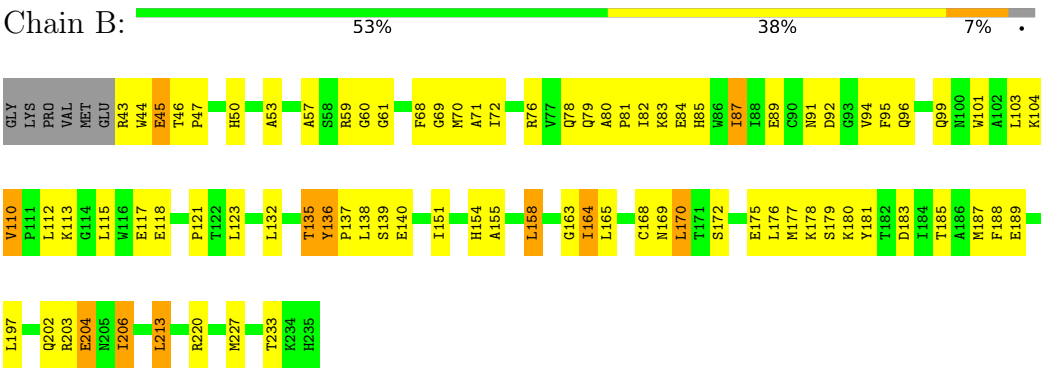
• Molecule 1: Guanidinoacetate N-methyltransferase

Chain A:



• Molecule 1: Guanidinoacetate N-methyltransferase

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	54.22Å 54.22Å 156.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.50)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.193 , 0.288	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3345	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GD3, 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	0.42	0/1596	0.61	0/2173
1	B	0.39	0/1596	0.62	0/2173
All	All	0.40	0/3192	0.62	0/4346

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	1548	0	1516	85	0
1	B	1548	0	1516	84	0
2	A	26	0	19	3	0
2	B	26	0	19	2	0
3	A	1	0	0	0	0
4	A	113	0	0	4	0
4	B	83	0	0	1	0
All	All	3345	0	3070	162	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 26.

All (162) 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:A:69:GLY:HA3	2:A:2001:SAH:HG2	1.48	0.94
1:A:60:GLY:HA2	1:A:82:ILE:HD12	1.50	0.93
1:A:198:GLU:C	4:A:4107:HOH:O	2.07	0.93
1:B:177:MET:HE1	1:B:187:MET:HB2	1.48	0.91
1:B:177:MET:CE	1:B:181:TYR:HB2	2.06	0.85
1:B:177:MET:HE2	1:B:181:TYR:HB2	1.57	0.85
1:A:177:MET:HE1	1:A:187:MET:HB2	1.59	0.83
1:A:177:MET:HE1	1:A:181:TYR:HB2	1.67	0.76
1:B:68:PHE:HB2	1:B:87:ILE:HD11	1.69	0.75
1:A:177:MET:CE	1:A:181:TYR:HB2	2.17	0.74
1:A:189:GLU:HA	1:A:193:VAL:HG13	1.71	0.72
1:B:43:ARG:NH1	1:B:70:MET:HG3	2.05	0.72
1:B:80:ALA:HB1	1:B:81:PRO:HD2	1.72	0.72
1:B:69:GLY:HA3	2:B:2002:SAH:HG2	1.74	0.68
1:B:50:HIS:CD2	1:B:76:ARG:HB2	2.30	0.67
1:B:83:LYS:HG3	1:B:84:GLU:HG3	1.75	0.67
1:A:59:ARG:HG2	1:A:164:ILE:HG22	1.76	0.67
1:B:95:PHE:CZ	1:B:113:LYS:HB2	2.30	0.67
1:B:43:ARG:HH12	1:B:70:MET:HG3	1.61	0.66
1:A:218:ASP:OD1	1:B:70:MET:HG2	1.95	0.66
1:A:199:ALA:N	4:A:4107:HOH:O	2.25	0.65
1:A:154:HIS:O	1:A:158:LEU:HB2	1.96	0.64
1:A:59:ARG:NH1	1:A:164:ILE:HB	2.12	0.64
1:A:123:LEU:O	1:A:157:ARG:NH2	2.31	0.64
1:A:177:MET:HA	1:A:177:MET:HE2	1.80	0.63
1:B:95:PHE:O	1:B:99:GLN:HG3	1.97	0.63
1:B:151:ILE:HA	1:B:155:ALA:CB	2.28	0.63
1:B:206:ILE:HG13	1:B:206:ILE:O	1.99	0.62
1:B:151:ILE:HA	1:B:155:ALA:HB3	1.82	0.61
1:A:83:LYS:HG3	1:A:84:GLU:HG3	1.83	0.60
1:A:85:HIS:O	1:A:109:VAL:HA	2.01	0.60
1:A:189:GLU:HA	1:A:193:VAL:CG1	2.31	0.60
1:A:136:TYR:HE2	1:A:138:LEU:HD21	1.67	0.60
1:A:177:MET:HE3	1:A:187:MET:HG3	1.84	0.60
1:B:177:MET:HE1	1:B:181:TYR:HB2	1.84	0.59
1:A:124:PRO:O	1:A:158:LEU:HD12	2.03	0.59
1:B:92:ASP:O	1:B:96:GLN:HG3	2.03	0.59
1:B:168:CYS:SG	1:B:170:LEU:HD22	2.43	0.59
1:A:92:ASP:O	1:A:96:GLN:HG3	2.03	0.58
1:A:189:GLU:OE1	1:A:203:ARG:NH1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:GLY:HA2	1:B:83:LYS:HD3	1.86	0.58
1:A:69:GLY:CA	2:A:2001:SAH:HG2	2.30	0.58
1:B:95:PHE:CE1	1:B:113:LYS:HB2	2.39	0.57
1:B:135:THR:CG2	1:B:136:TYR:N	2.67	0.57
1:A:178:LYS:HE2	1:B:137:PRO:O	2.03	0.57
1:A:80:ALA:C	1:A:82:ILE:H	2.09	0.56
1:B:163:GLY:O	1:B:233:THR:HA	2.07	0.55
1:A:46:THR:HB	1:A:47:PRO:HD3	1.89	0.55
1:B:203:ARG:HH21	1:B:206:ILE:HG13	1.72	0.54
1:A:143:TRP:CZ2	1:B:175:GLU:HG3	2.42	0.54
1:B:91:ASN:OD1	1:B:94:VAL:HG23	2.08	0.54
1:A:59:ARG:HG2	1:A:164:ILE:CG2	2.37	0.54
1:A:61:GLY:C	1:A:83:LYS:HG2	2.27	0.54
1:A:177:MET:HE1	1:A:187:MET:CB	2.34	0.54
1:B:177:MET:HE3	1:B:187:MET:HG3	1.90	0.54
1:A:157:ARG:HG3	1:A:158:LEU:N	2.22	0.54
1:A:153:THR:O	1:A:157:ARG:HD3	2.08	0.53
1:B:193:VAL:HG22	1:B:194:PRO:HD3	1.89	0.53
1:A:140:GLU:OE2	1:B:180:LYS:HE3	2.09	0.53
1:B:177:MET:HE1	1:B:187:MET:CB	2.31	0.53
1:A:80:ALA:HB3	1:A:82:ILE:HD13	1.89	0.53
1:A:59:ARG:NH2	1:A:162:GLY:O	2.42	0.52
1:B:60:GLY:HA2	1:B:82:ILE:HD12	1.92	0.52
1:B:87:ILE:HG13	1:B:87:ILE:O	2.04	0.52
1:A:86:TRP:CD1	1:A:110:VAL:HG13	2.45	0.52
1:B:118:GLU:C	1:B:121:PRO:HD2	2.30	0.52
1:B:151:ILE:HG21	1:B:196:LEU:HD12	1.90	0.52
1:A:98:LEU:HD12	1:A:98:LEU:O	2.10	0.52
1:B:213:LEU:HD12	1:B:227:MET:HG3	1.91	0.51
1:A:61:GLY:O	1:A:83:LYS:HG2	2.10	0.51
1:B:91:ASN:HB3	1:B:94:VAL:HB	1.91	0.51
1:B:164:ILE:HG13	1:B:165:LEU:N	2.24	0.50
1:B:115:LEU:HB3	1:B:117:GLU:OE2	2.13	0.49
1:B:172:SER:O	1:B:176:LEU:HG	2.12	0.49
1:A:68:PHE:CZ	1:A:71:ALA:HB2	2.48	0.49
1:A:206:ILE:O	1:A:206:ILE:HG13	2.11	0.49
1:A:43:ARG:HD2	1:A:72:ILE:CD1	2.42	0.49
1:B:44:TRP:CE3	1:B:213:LEU:HD22	2.48	0.49
1:A:183:ASP:HB3	1:A:186:ALA:CB	2.42	0.49
1:A:199:ALA:HA	4:A:4112:HOH:O	2.13	0.49
1:A:143:TRP:CH2	1:B:175:GLU:HG3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:THR:HB	1:B:47:PRO:HD3	1.95	0.48
1:B:110:VAL:HG22	1:B:110:VAL:O	2.12	0.48
1:A:224:PHE:HE2	1:A:226:GLN:HE21	1.61	0.48
1:B:69:GLY:CA	2:B:2002:SAH:HG2	2.42	0.48
1:B:188:PHE:HE1	1:B:206:ILE:HD13	1.78	0.48
1:A:80:ALA:HB1	1:A:81:PRO:HD2	1.95	0.48
1:B:57:ALA:HA	1:B:82:ILE:HD11	1.95	0.48
1:B:135:THR:HG23	1:B:136:TYR:H	1.79	0.48
1:B:169:ASN:OD1	1:B:172:SER:HB3	2.14	0.47
1:B:204:GLU:H	1:B:204:GLU:HG3	1.38	0.47
1:B:118:GLU:O	1:B:121:PRO:HD2	2.14	0.47
1:B:189:GLU:OE1	1:B:203:ARG:NH1	2.47	0.47
1:B:85:HIS:HB3	1:B:109:VAL:HB	1.97	0.47
1:A:57:ALA:HB1	1:A:82:ILE:CD1	2.45	0.47
1:A:151:ILE:HA	1:A:155:ALA:HB3	1.97	0.47
1:B:80:ALA:C	1:B:82:ILE:H	2.19	0.47
1:A:177:MET:HE2	1:A:181:TYR:HB2	1.96	0.46
1:A:110:VAL:HG22	1:A:110:VAL:O	2.16	0.46
1:B:177:MET:HE2	1:B:177:MET:HA	1.96	0.46
1:B:203:ARG:NH2	1:B:206:ILE:HG13	2.30	0.46
1:B:169:ASN:CG	1:B:172:SER:HB3	2.35	0.46
1:A:65:GLU:O	1:A:87:ILE:HA	2.15	0.46
1:A:154:HIS:ND1	1:A:157:ARG:NH1	2.64	0.46
1:B:154:HIS:O	1:B:158:LEU:HD22	2.15	0.46
1:B:76:ARG:O	1:B:76:ARG:HD2	2.16	0.46
1:B:43:ARG:HG3	1:B:72:ILE:HD11	1.98	0.46
1:A:59:ARG:CZ	1:A:162:GLY:O	2.64	0.45
1:A:135:THR:HG23	1:A:136:TYR:N	2.31	0.45
1:A:156:PHE:CD2	1:A:234:LYS:HE3	2.51	0.45
1:B:80:ALA:HB3	1:B:82:ILE:HD13	1.98	0.45
1:A:59:ARG:NE	1:A:162:GLY:O	2.49	0.45
1:A:73:ALA:O	1:A:77:VAL:HG23	2.17	0.45
1:A:221:TYR:CE2	1:B:220:ARG:HD2	2.51	0.45
1:B:151:ILE:HA	1:B:155:ALA:HB2	1.97	0.45
1:A:134:ASP:OD2	2:A:2001:SAH:HB2	2.16	0.44
1:A:154:HIS:HB3	1:A:158:LEU:CD2	2.47	0.44
1:A:78:GLN:OE1	1:A:106:PRO:HD2	2.18	0.44
1:B:189:GLU:HA	1:B:193:VAL:HG13	1.99	0.44
1:A:124:PRO:O	1:A:127:HIS:HB2	2.17	0.44
1:A:156:PHE:CE2	1:A:234:LYS:HE3	2.52	0.44
1:B:99:GLN:NE2	4:B:4131:HOH:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:GLU:H	1:B:45:GLU:CD	2.14	0.43
1:A:183:ASP:HB3	1:A:186:ALA:HB3	2.01	0.43
1:A:193:VAL:N	1:A:194:PRO:CD	2.81	0.43
1:A:95:PHE:CE2	1:A:111:PRO:HB2	2.54	0.43
1:A:135:THR:CG2	1:A:136:TYR:N	2.81	0.43
1:B:68:PHE:CZ	1:B:71:ALA:HB2	2.54	0.43
1:B:154:HIS:HB3	1:B:158:LEU:HD22	2.01	0.43
1:B:193:VAL:N	1:B:194:PRO:CD	2.81	0.43
1:B:135:THR:HG23	1:B:136:TYR:N	2.32	0.43
1:B:70:MET:HB2	1:B:72:ILE:HD12	2.00	0.43
1:B:154:HIS:O	1:B:158:LEU:HB2	2.19	0.43
1:B:57:ALA:HB1	1:B:82:ILE:HD13	2.00	0.42
1:B:189:GLU:O	1:B:193:VAL:HG22	2.20	0.42
1:A:59:ARG:CG	1:A:164:ILE:HG22	2.47	0.42
1:A:95:PHE:O	1:A:99:GLN:HG3	2.20	0.42
1:A:140:GLU:HG2	1:A:141:GLU:OE2	2.20	0.42
1:A:200:GLY:N	4:A:4107:HOH:O	2.46	0.42
1:A:137:PRO:O	1:B:178:LYS:HE2	2.19	0.42
1:A:112:LEU:HB3	1:A:119:VAL:HG11	2.01	0.41
1:A:80:ALA:CB	1:A:82:ILE:HD13	2.50	0.41
1:B:107:HIS:O	1:B:109:VAL:HG12	2.20	0.41
1:A:87:ILE:O	1:A:87:ILE:HG13	2.19	0.41
1:B:59:ARG:CG	1:B:164:ILE:HG22	2.49	0.41
1:A:68:PHE:HB2	1:A:87:ILE:HD11	2.02	0.41
1:A:136:TYR:CD2	1:A:136:TYR:C	2.94	0.41
1:B:59:ARG:HG3	1:B:164:ILE:HG22	2.03	0.41
1:A:157:ARG:CG	1:A:158:LEU:N	2.83	0.41
1:A:177:MET:CE	1:A:177:MET:HA	2.45	0.41
1:A:177:MET:CE	1:A:187:MET:HB2	2.38	0.41
1:A:215:PRO:HA	1:A:216:PRO:HD3	1.86	0.41
1:B:78:GLN:HG3	1:B:101:TRP:CH2	2.55	0.41
1:A:80:ALA:O	1:A:82:ILE:N	2.53	0.41
1:A:136:TYR:HA	1:A:137:PRO:HD3	1.90	0.41
1:B:89:GLU:HG2	1:B:94:VAL:HG12	2.01	0.41
1:B:183:ASP:OD2	1:B:185:THR:N	2.53	0.41
1:A:130:GLY:HA2	1:A:164:ILE:O	2.21	0.40
1:A:224:PHE:CE2	1:A:226:GLN:HB2	2.56	0.40
1:B:50:HIS:HD2	1:B:76:ARG:HB2	1.83	0.40
1:B:53:ALA:HB3	1:B:76:ARG:HG3	2.04	0.40
1:B:80:ALA:HB1	1:B:81:PRO:CD	2.48	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	191/199 (96%)	185 (97%)	6 (3%)	0	100	100
1	B	191/199 (96%)	184 (96%)	7 (4%)	0	100	100
All	All	382/398 (96%)	369 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	163/168 (97%)	135 (83%)	28 (17%)	2	3
1	B	163/168 (97%)	138 (85%)	25 (15%)	2	5
All	All	326/336 (97%)	273 (84%)	53 (16%)	2	4

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	72	ILE
1	A	79	GLN
1	A	82	ILE
1	A	83	LYS
1	A	87	ILE
1	A	103	LEU
1	A	104	LYS

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Mol	Chain	Res	Type
1	A	112	LEU
1	A	123	LEU
1	A	135	THR
1	A	136	TYR
1	A	138	LEU
1	A	141	GLU
1	A	158	LEU
1	A	170	LEU
1	A	178	LYS
1	A	180	LYS
1	A	190	GLU
1	A	196	LEU
1	A	197	LEU
1	A	202	GLN
1	A	203	ARG
1	A	204	GLU
1	A	206	ILE
1	A	213	LEU
1	A	233	THR
1	A	234	LYS
1	B	45	GLU
1	B	79	GLN
1	B	87	ILE
1	B	103	LEU
1	B	104	LYS
1	B	109	VAL
1	B	110	VAL
1	B	112	LEU
1	B	123	LEU
1	B	132	LEU
1	B	135	THR
1	B	136	TYR
1	B	138	LEU
1	B	139	SER
1	B	140	GLU
1	B	158	LEU
1	B	164	ILE
1	B	170	LEU
1	B	179	SER
1	B	196	LEU
1	B	197	LEU
1	B	202	GLN

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Mol	Chain	Res	Type
1	B	204	GLU
1	B	206	ILE
1	B	213	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	GLN
1	A	226	GLN
1	B	96	GLN
1	B	226	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is 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	B	2002	-	24,28,28	0.89	1 (4%)	25,40,40	1.41	2 (8%)
2	SAH	A	2001	-	24,28,28	0.87	1 (4%)	25,40,40	1.35	2 (8%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2002	SAH	C2-N3	2.57	1.36	1.32
2	A	2001	SAH	C2-N3	2.18	1.35	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2001	SAH	O4'-C1'-C2'	-3.72	101.50	106.93
2	B	2002	SAH	O4'-C1'-C2'	-3.55	101.73	106.93
2	A	2001	SAH	O2'-C2'-C3'	3.46	123.03	111.82
2	B	2002	SAH	O2'-C2'-C3'	3.39	122.78	111.82

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	B	2002	SAH	C-CA-CB-CG
2	A	2001	SAH	CB-CG-SD-C5'

There are no ring outliers.

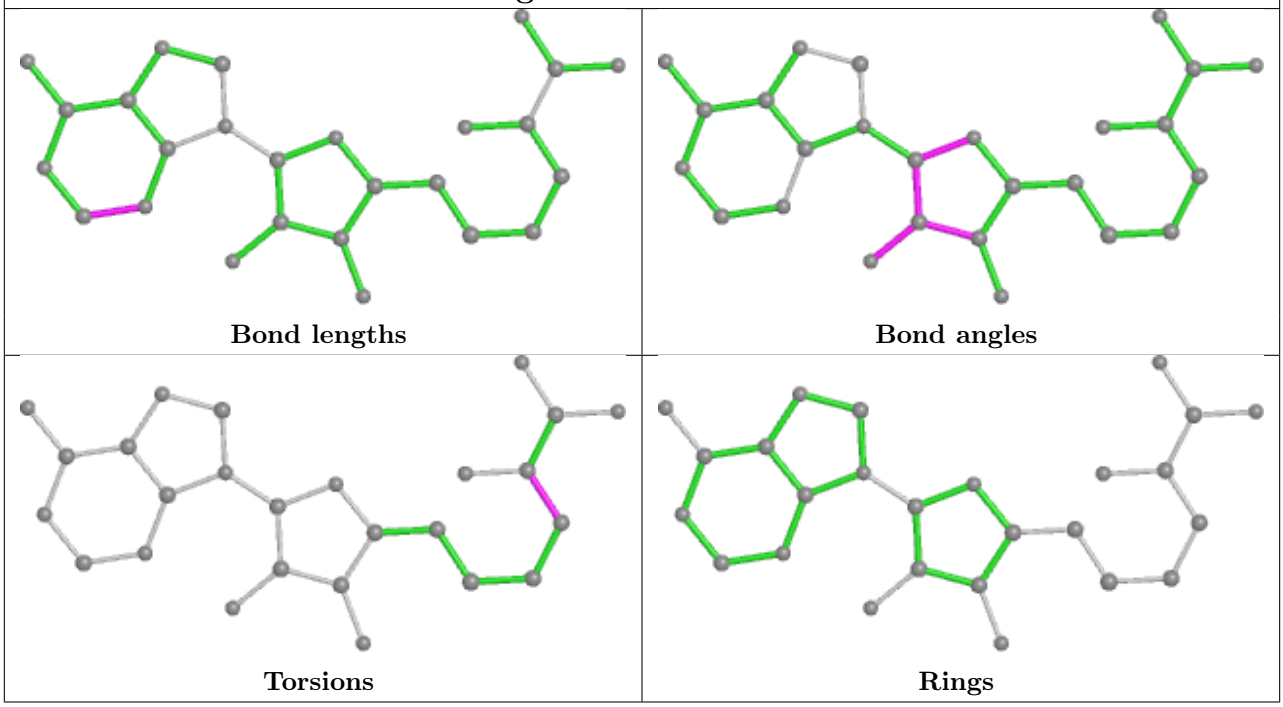
2 monomers are involved in 5 short contacts:

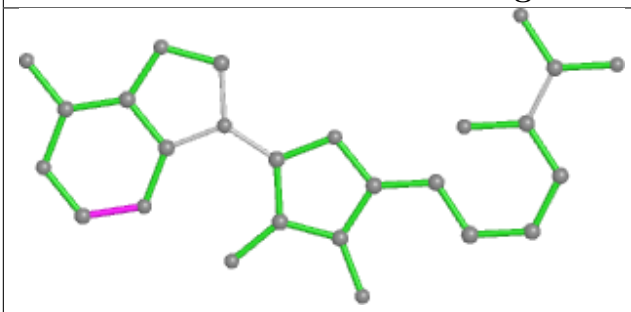
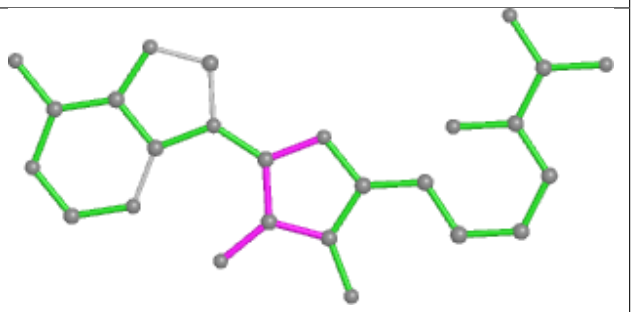
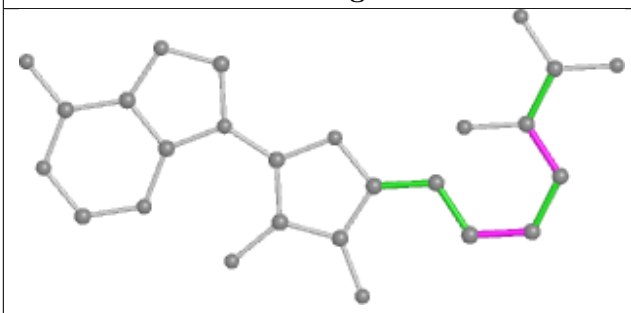
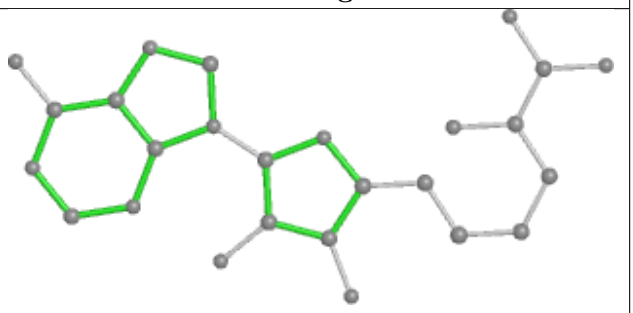
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2002	SAH	2	0
2	A	2001	SAH	3	0

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 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 B 2002



Ligand SAH A 2001	
 Bond lengths	 Bond angles
 Torsions	 Rings

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.