



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:31 PM UTC

PDB ID : 2E0N / pdb_00002e0n
Title : Crystal structure of CbiL in complex with S-adenosylhomocysteine, a methyl-transferase involved in anaerobic vitamin B12 biosynthesis
Authors : Wada, K.; Fukuyama, K.
Deposited on : 2006-10-10
Resolution : 2.00 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

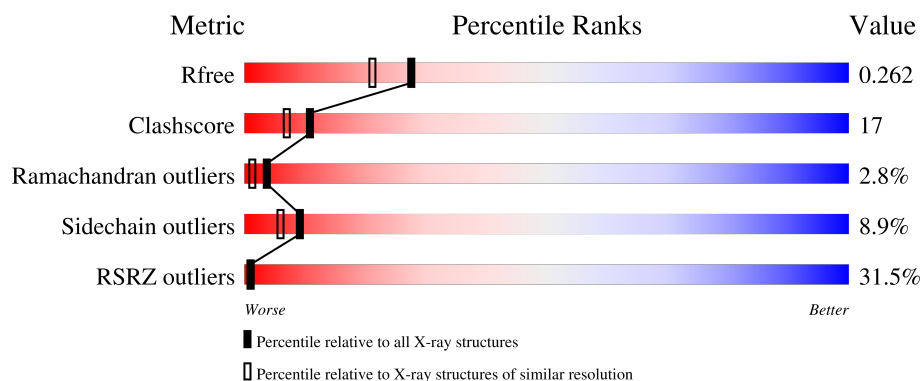
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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	259	34% 62% 22% 12%
1	B	259	22% 59% 19% 11% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3688 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 Precorrin-2 C20-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1691	1070	284	326	11			
1	B	238	Total	C	N	O	S	0	0	0
			1761	1115	296	339	11			

There are 26 discrepancies between the modelled and reference sequences:

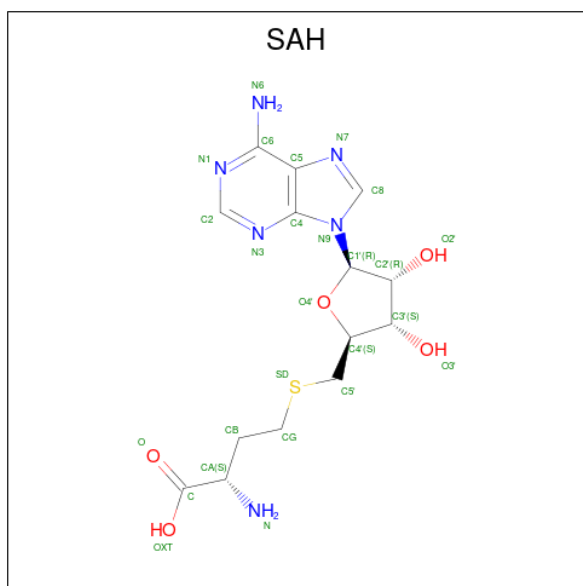
Chain	Residue	Modelled	Actual	Comment	Reference
A	247	LYS	-	cloning artifact	UNP Q8KFD9
A	248	LEU	-	cloning artifact	UNP Q8KFD9
A	249	ALA	-	cloning artifact	UNP Q8KFD9
A	250	ALA	-	cloning artifact	UNP Q8KFD9
A	251	ALA	-	cloning artifact	UNP Q8KFD9
A	252	LEU	-	cloning artifact	UNP Q8KFD9
A	253	GLU	-	cloning artifact	UNP Q8KFD9
A	254	HIS	-	expression tag	UNP Q8KFD9
A	255	HIS	-	expression tag	UNP Q8KFD9
A	256	HIS	-	expression tag	UNP Q8KFD9
A	257	HIS	-	expression tag	UNP Q8KFD9
A	258	HIS	-	expression tag	UNP Q8KFD9
A	259	HIS	-	expression tag	UNP Q8KFD9
B	247	LYS	-	cloning artifact	UNP Q8KFD9
B	248	LEU	-	cloning artifact	UNP Q8KFD9
B	249	ALA	-	cloning artifact	UNP Q8KFD9
B	250	ALA	-	cloning artifact	UNP Q8KFD9
B	251	ALA	-	cloning artifact	UNP Q8KFD9
B	252	LEU	-	cloning artifact	UNP Q8KFD9
B	253	GLU	-	cloning artifact	UNP Q8KFD9
B	254	HIS	-	expression tag	UNP Q8KFD9
B	255	HIS	-	expression tag	UNP Q8KFD9
B	256	HIS	-	expression tag	UNP Q8KFD9
B	257	HIS	-	expression tag	UNP Q8KFD9
B	258	HIS	-	expression tag	UNP Q8KFD9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	259	HIS	-	expression tag	UNP Q8KFD9

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: 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		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

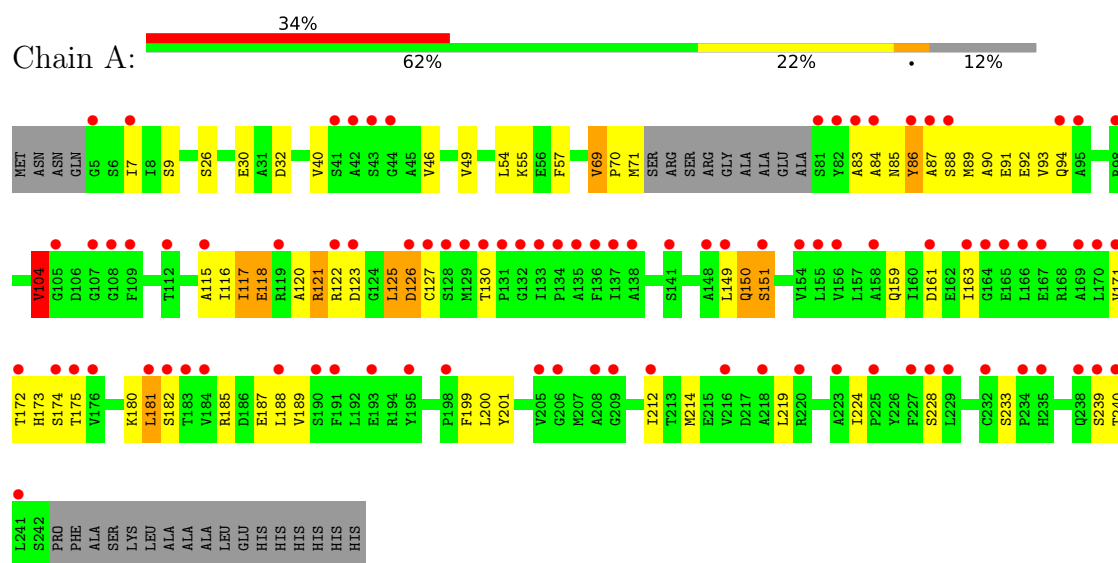
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total	O	0	0
			90	90		
3	B	94	Total	O	0	0
			94	94		

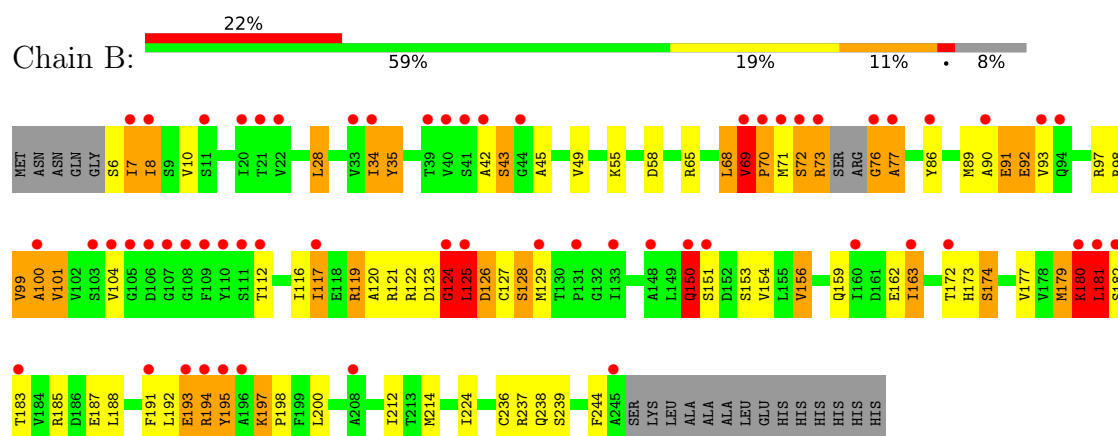
3 Residue-property plots [i](#)

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

• Molecule 1: Precorrin-2 C20-methyltransferase



• Molecule 1: Precorrin-2 C20-methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	87.82Å 87.82Å 123.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 50.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.00) 99.5 (50.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.223 , 0.266 0.218 , 0.262	Depositor DCC
R_{free} test set	1679 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3688	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: 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	0.99	3/1716 (0.2%)	1.11	7/2327 (0.3%)
1	B	1.17	9/1789 (0.5%)	1.54	29/2426 (1.2%)
All	All	1.09	12/3505 (0.3%)	1.35	36/4753 (0.8%)

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	2
1	B	0	10
All	All	0	12

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	192	LEU	C-N	8.06	1.43	1.33
1	B	100	ALA	N-CA	-7.14	1.37	1.45
1	B	69	VAL	CA-C	7.06	1.60	1.52
1	B	69	VAL	CA-CB	6.68	1.62	1.54
1	B	179	MET	C-N	-6.66	1.24	1.33
1	B	124	GLY	C-N	-6.29	1.24	1.33
1	B	194	ARG	C-N	-6.19	1.25	1.33
1	A	121	ARG	C-N	6.18	1.42	1.33
1	A	104	VAL	CA-CB	6.15	1.61	1.54
1	A	120	ALA	C-N	6.14	1.42	1.34
1	B	100	ALA	C-N	-5.65	1.26	1.33
1	B	180	LYS	N-CA	-5.58	1.39	1.46

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	124	GLY	O-C-N	-21.82	102.04	122.77
1	B	179	MET	CA-C-N	19.45	158.69	121.54
1	B	179	MET	C-N-CA	19.45	158.69	121.54
1	B	181	LEU	O-C-N	-15.00	102.64	122.59
1	B	124	GLY	CA-C-O	-10.62	109.01	122.61
1	B	182	SER	O-C-N	-9.29	110.24	122.59
1	B	34	ILE	O-C-N	-8.50	111.95	122.57
1	B	68	LEU	N-CA-C	8.46	123.73	112.13
1	B	101	VAL	CB-CA-C	7.70	119.89	110.73
1	B	182	SER	CA-C-O	7.68	131.50	120.51
1	B	126	ASP	O-C-N	6.62	131.39	122.59
1	B	99	VAL	CA-C-N	6.43	133.23	122.87
1	B	99	VAL	C-N-CA	6.43	133.23	122.87
1	B	125	LEU	O-C-N	6.41	131.11	122.59
1	B	194	ARG	O-C-N	-6.10	115.48	122.68
1	B	179	MET	CA-C-O	-6.07	113.53	121.73
1	B	192	LEU	N-CA-C	6.02	120.23	113.01
1	B	180	LYS	CA-C-O	-5.75	112.28	120.51
1	A	130	THR	CA-C-N	5.61	125.59	120.03
1	A	130	THR	C-N-CA	5.61	125.59	120.03
1	B	92	GLU	N-CA-C	-5.49	105.37	111.36
1	B	194	ARG	N-CA-C	-5.45	103.30	110.33
1	B	99	VAL	O-C-N	-5.42	117.48	123.18
1	A	57	PHE	N-CA-C	5.40	119.98	113.17
1	B	197	LYS	CA-C-N	5.36	125.28	119.76
1	B	197	LYS	C-N-CA	5.36	125.28	119.76
1	B	182	SER	N-CA-CB	-5.34	101.47	110.49
1	B	91	GLU	CB-CA-C	5.32	121.01	110.42
1	B	124	GLY	N-CA-C	-5.24	102.63	112.22
1	B	188	LEU	N-CA-C	5.21	116.64	111.07
1	A	83	ALA	N-CA-C	-5.16	106.93	113.18
1	B	193	GLU	CA-C-N	5.10	130.03	120.95
1	B	193	GLU	C-N-CA	5.10	130.03	120.95
1	A	87	ALA	N-CA-C	-5.09	100.43	108.73
1	A	32	ASP	N-CA-C	-5.05	106.28	112.90
1	A	125	LEU	N-CA-C	5.05	117.62	110.50

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	189	VAL	Mainchain
1	A	86	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	B	124	GLY	Mainchain
1	B	126	ASP	Mainchain
1	B	179	MET	Peptide
1	B	180	LYS	Mainchain
1	B	181	LEU	Mainchain,Peptide
1	B	193	GLU	Peptide
1	B	244	PHE	Peptide
1	B	69	VAL	Peptide
1	B	76	GLY	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	1691	0	1718	48	0
1	B	1761	0	1783	73	0
2	A	26	0	19	0	0
2	B	26	0	19	1	0
3	A	90	0	0	2	0
3	B	94	0	0	5	0
All	All	3688	0	3539	117	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 (117) 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:89:MET:HE1	1:B:116:ILE:HG23	1.28	1.14
1:B:89:MET:HE1	1:B:116:ILE:CG2	1.84	1.05
1:A:89:MET:HE1	1:A:116:ILE:HG23	1.51	0.91
1:A:181:LEU:HD21	1:A:228:SER:OG	1.71	0.90
1:A:70:PRO:O	1:A:71:MET:HB2	1.72	0.89
1:B:69:VAL:HG22	1:B:70:PRO:HD3	1.55	0.89
1:B:92:GLU:HB2	3:B:378:HOH:O	1.77	0.84
1:B:150:GLN:HG2	1:B:150:GLN:O	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:VAL:HG11	1:B:125:LEU:HD22	1.64	0.78
1:B:89:MET:CE	1:B:116:ILE:HG23	2.11	0.78
1:B:180:LYS:HA	2:B:301:SAH:O3'	1.85	0.77
1:B:90:ALA:HB2	1:B:119:ARG:HH22	1.52	0.74
1:B:93:VAL:CG1	1:B:125:LEU:HD22	2.19	0.72
1:B:150:GLN:O	1:B:151:SER:HB2	1.91	0.71
1:B:7:ILE:HA	1:B:99:VAL:O	1.92	0.70
1:A:181:LEU:O	1:A:181:LEU:HD23	1.94	0.68
1:B:42:ALA:O	1:B:43:SER:HB3	1.95	0.67
1:A:89:MET:HE1	1:A:116:ILE:CG2	2.24	0.66
1:A:86:TYR:HA	1:A:89:MET:CE	2.26	0.64
1:B:8:ILE:O	1:B:100:ALA:HA	1.97	0.64
1:A:69:VAL:HG12	1:A:70:PRO:HD2	1.79	0.64
1:B:150:GLN:O	1:B:150:GLN:CG	2.45	0.64
1:A:86:TYR:HA	1:A:89:MET:HE2	1.80	0.63
1:B:35:TYR:HA	1:B:65:ARG:O	1.98	0.63
1:A:171:VAL:HG23	1:A:172:THR:HG23	1.79	0.63
1:B:89:MET:HE1	1:B:116:ILE:HG21	1.75	0.63
1:A:93:VAL:HG21	1:A:125:LEU:HD13	1.79	0.63
1:B:200:LEU:HD11	1:B:212:ILE:CG2	2.29	0.63
1:A:40:VAL:HG12	1:A:46:VAL:HG12	1.80	0.62
1:B:7:ILE:HD11	1:B:101:VAL:HG12	1.81	0.62
1:A:214:MET:HE1	1:A:239:SER:HB3	1.81	0.61
1:B:8:ILE:HG22	1:B:128:SER:HB2	1.83	0.60
1:B:10:VAL:HG23	1:B:100:ALA:HB1	1.84	0.60
1:B:195:TYR:CE1	1:B:197:LYS:HB2	2.37	0.59
1:B:76:GLY:O	1:B:77:ALA:CB	2.49	0.59
1:A:150:GLN:HE22	1:B:73:ARG:HH22	1.50	0.59
1:A:214:MET:HE1	1:A:239:SER:CB	2.32	0.59
1:B:90:ALA:HB2	1:B:119:ARG:NH2	2.17	0.58
1:A:121:ARG:O	1:A:123:ASP:O	2.22	0.57
1:B:7:ILE:O	1:B:127:CYS:HA	2.04	0.57
1:B:163:ILE:HG13	1:B:191:PHE:HB2	1.86	0.57
1:A:181:LEU:HD22	1:A:228:SER:O	2.04	0.57
1:B:159:GLN:NE2	1:B:180:LYS:NZ	2.53	0.57
1:B:181:LEU:O	1:B:183:THR:N	2.38	0.56
1:B:191:PHE:O	1:B:194:ARG:O	2.22	0.56
1:B:34:ILE:O	1:B:100:ALA:O	2.24	0.56
1:B:153:SER:O	1:B:174:SER:HB2	2.05	0.55
1:A:200:LEU:HD11	1:A:212:ILE:CG2	2.36	0.55
1:B:120:ALA:O	1:B:124:GLY:O	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ARG:O	1:B:122:ARG:HG2	2.07	0.55
1:B:89:MET:CE	1:B:116:ILE:CG2	2.74	0.54
1:B:6:SER:CA	3:B:322:HOH:O	2.56	0.54
1:A:159:GLN:HG3	1:A:180:LYS:HB2	1.90	0.53
1:A:93:VAL:HG21	1:A:125:LEU:CD1	2.39	0.53
1:A:88:SER:O	1:A:91:GLU:HB2	2.09	0.52
1:B:69:VAL:HG22	1:B:70:PRO:CD	2.36	0.52
1:B:159:GLN:HE21	1:B:180:LYS:NZ	2.08	0.52
1:A:149:LEU:O	1:A:150:GLN:C	2.53	0.52
1:B:198:PRO:HB2	1:B:236:CYS:HB2	1.91	0.51
1:B:10:VAL:HG11	1:B:28:LEU:HD13	1.93	0.51
1:B:10:VAL:CG2	1:B:100:ALA:HB1	2.41	0.51
1:B:117:ILE:HD13	1:B:129:MET:HG3	1.93	0.51
1:A:7:ILE:HG22	1:A:126:ASP:O	2.11	0.50
1:B:159:GLN:NE2	1:B:180:LYS:HZ2	2.10	0.50
1:A:150:GLN:O	1:A:151:SER:HB2	2.10	0.50
1:B:121:ARG:C	1:B:123:ASP:H	2.17	0.50
1:A:84:ALA:C	1:A:86:TYR:H	2.20	0.50
1:B:194:ARG:O	1:B:195:TYR:O	2.29	0.50
1:B:159:GLN:HG2	1:B:180:LYS:HD2	1.94	0.49
1:B:49:VAL:HG23	1:B:104:VAL:HG21	1.94	0.49
1:B:34:ILE:O	1:B:35:TYR:HB2	2.14	0.48
1:B:121:ARG:O	1:B:122:ARG:CG	2.62	0.48
1:A:86:TYR:HD1	1:A:89:MET:HE3	1.79	0.47
1:B:92:GLU:HB3	1:B:97:ARG:HB2	1.95	0.47
1:A:86:TYR:HA	1:A:89:MET:HE3	1.96	0.47
1:B:200:LEU:HD11	1:B:212:ILE:HG23	1.97	0.47
1:A:7:ILE:O	1:A:127:CYS:HA	2.14	0.47
1:A:115:ALA:O	1:A:118:GLU:HG3	2.14	0.47
1:B:76:GLY:O	1:B:77:ALA:HB3	2.15	0.47
1:A:199:PHE:O	1:A:214:MET:HG2	2.15	0.47
1:B:68:LEU:O	1:B:69:VAL:C	2.57	0.46
1:A:188:LEU:HD22	1:A:224:ILE:HD12	1.98	0.46
1:B:185:ARG:HB2	1:B:224:ILE:HB	1.97	0.46
1:A:26:SER:O	1:A:30:GLU:HG3	2.15	0.46
1:A:118:GLU:CD	1:A:122:ARG:HH22	2.24	0.45
1:B:172:THR:HB	1:B:173:HIS:CD2	2.52	0.45
1:B:72:SER:HB3	1:B:76:GLY:O	2.17	0.45
1:B:159:GLN:HE21	1:B:180:LYS:HZ3	1.63	0.45
1:B:34:ILE:O	1:B:35:TYR:CB	2.65	0.45
1:A:188:LEU:HD22	1:A:224:ILE:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:MET:HE1	1:B:239:SER:CB	2.48	0.44
1:A:150:GLN:NE2	1:B:73:ARG:HH12	2.16	0.44
1:B:8:ILE:HD11	3:B:341:HOH:O	2.16	0.44
1:A:173:HIS:HB3	3:A:362:HOH:O	2.18	0.43
1:B:8:ILE:HD13	1:B:98:ARG:HH21	1.84	0.43
1:B:86:TYR:CG	1:B:119:ARG:HD2	2.53	0.43
1:A:150:GLN:HE21	1:B:73:ARG:HH12	1.67	0.43
1:B:187:GLU:HG3	3:B:315:HOH:O	2.19	0.43
1:A:55:LYS:HA	1:A:55:LYS:HD2	1.62	0.43
1:B:69:VAL:CG2	1:B:70:PRO:HD3	2.37	0.42
1:B:163:ILE:HB	1:B:187:GLU:HG2	2.02	0.42
1:B:156:VAL:HB	1:B:177:VAL:HB	2.01	0.42
1:A:86:TYR:CD1	1:A:89:MET:HE3	2.54	0.42
1:B:42:ALA:O	1:B:43:SER:CB	2.67	0.41
1:A:85:ASN:HA	3:A:373:HOH:O	2.21	0.41
1:B:86:TYR:HA	1:B:89:MET:HE2	2.03	0.41
1:A:9:SER:HB2	1:A:117:ILE:HD11	2.02	0.41
1:A:117:ILE:N	1:A:117:ILE:HD13	2.36	0.41
1:A:175:THR:HG23	1:A:233:SER:HB2	2.03	0.41
1:A:185:ARG:HB2	1:A:224:ILE:CG1	2.50	0.41
1:A:121:ARG:NH1	1:B:238:GLN:O	2.43	0.40
1:A:70:PRO:O	1:A:71:MET:CB	2.56	0.40
1:B:35:TYR:H	1:B:65:ARG:H	1.68	0.40
1:A:49:VAL:HG23	1:A:104:VAL:HG11	2.02	0.40
1:A:201:TYR:CD2	1:A:219:LEU:HD21	2.56	0.40
1:A:90:ALA:O	1:A:94:GLN:HG2	2.21	0.40
1:B:159:GLN:NE2	3:B:381:HOH:O	2.45	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	225/259 (87%)	217 (96%)	6 (3%)	2 (1%)	14	9
1	B	234/259 (90%)	206 (88%)	17 (7%)	11 (5%)	2	0
All	All	459/518 (89%)	423 (92%)	23 (5%)	13 (3%)	4	1

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	B	43	SER
1	B	180	LYS
1	B	195	TYR
1	B	150	GLN
1	A	182	SER
1	B	45	ALA
1	B	125	LEU
1	B	174	SER
1	B	35	TYR
1	B	77	ALA
1	B	72	SER
1	B	70	PRO

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	182/206 (88%)	168 (92%)	14 (8%)	12	8
1	B	188/206 (91%)	169 (90%)	19 (10%)	7	4
All	All	370/412 (90%)	337 (91%)	33 (9%)	9	6

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	69	VAL
1	A	92	GLU

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Mol	Chain	Res	Type
1	A	104	VAL
1	A	117	ILE
1	A	118	GLU
1	A	126	ASP
1	A	151	SER
1	A	161	ASP
1	A	163	ILE
1	A	174	SER
1	A	181	LEU
1	A	187	GLU
1	A	240	THR
1	B	7	ILE
1	B	8	ILE
1	B	28	LEU
1	B	55	LYS
1	B	58	ASP
1	B	69	VAL
1	B	71	MET
1	B	73	ARG
1	B	91	GLU
1	B	112	THR
1	B	117	ILE
1	B	119	ARG
1	B	128	SER
1	B	150	GLN
1	B	154	VAL
1	B	156	VAL
1	B	162	GLU
1	B	163	ILE
1	B	237	ARG

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

Mol	Chain	Res	Type
1	A	85	ASN
1	A	150	GLN
1	B	159	GLN
1	B	173	HIS
1	B	238	GLN

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 oligosaccharides 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	SAH	B	301	-	27,28,28	1.11	2 (7%)	36,40,40	2.10	10 (27%)
2	SAH	A	300	-	27,28,28	1.13	2 (7%)	36,40,40	2.32	11 (30%)

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	301	-	-	0/15/31/31	0/3/3/3
2	SAH	A	300	-	-	0/15/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	SAH	C4-N3	2.53	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	SAH	C4-N3	2.39	1.38	1.34
2	A	300	SAH	O4'-C4'	-2.38	1.39	1.45
2	B	301	SAH	OXT-C	-2.15	1.23	1.30

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	SAH	N3-C2-N1	-7.50	117.23	128.58
2	B	301	SAH	N3-C2-N1	-7.49	117.25	128.58
2	A	300	SAH	N9-C8-N7	-4.94	106.93	113.94
2	A	300	SAH	C4-N9-C8	4.33	110.28	105.74
2	B	301	SAH	N9-C8-N7	-3.90	108.41	113.94
2	B	301	SAH	C2-N1-C6	3.60	124.64	118.73
2	B	301	SAH	OXT-C-O	-3.51	116.11	124.08
2	A	300	SAH	C5-N7-C8	3.35	108.71	103.45
2	A	300	SAH	C2-N3-C4	3.33	119.96	111.83
2	B	301	SAH	C2-N3-C4	3.18	119.60	111.83
2	B	301	SAH	C5-C4-N3	-3.07	122.49	126.72
2	A	300	SAH	C2-N1-C6	3.06	123.76	118.73
2	B	301	SAH	C5-N7-C8	2.86	107.94	103.45
2	A	300	SAH	C5'-SD-CG	-2.62	94.47	102.26
2	A	300	SAH	O4'-C4'-C3'	-2.56	100.07	105.15
2	B	301	SAH	C5'-SD-CG	-2.30	95.43	102.26
2	A	300	SAH	O4'-C1'-N9	-2.22	103.83	108.09
2	A	300	SAH	C4'-C5'-SD	2.18	121.55	113.78
2	B	301	SAH	C4-N9-C8	2.13	107.97	105.74
2	B	301	SAH	CB-CA-N	-2.08	104.70	110.12
2	A	300	SAH	C5-C4-N3	-2.01	123.95	126.72

There are no chirality outliers.

There are no torsion outliers.

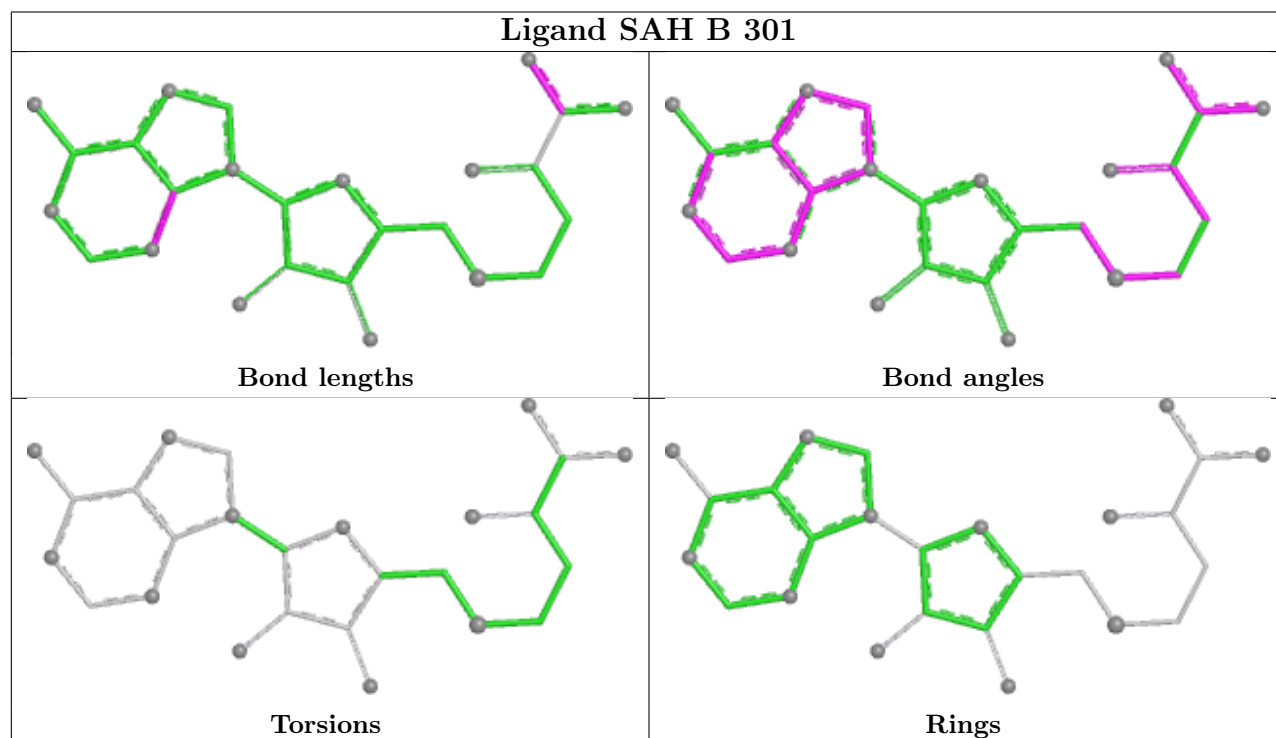
There are no ring outliers.

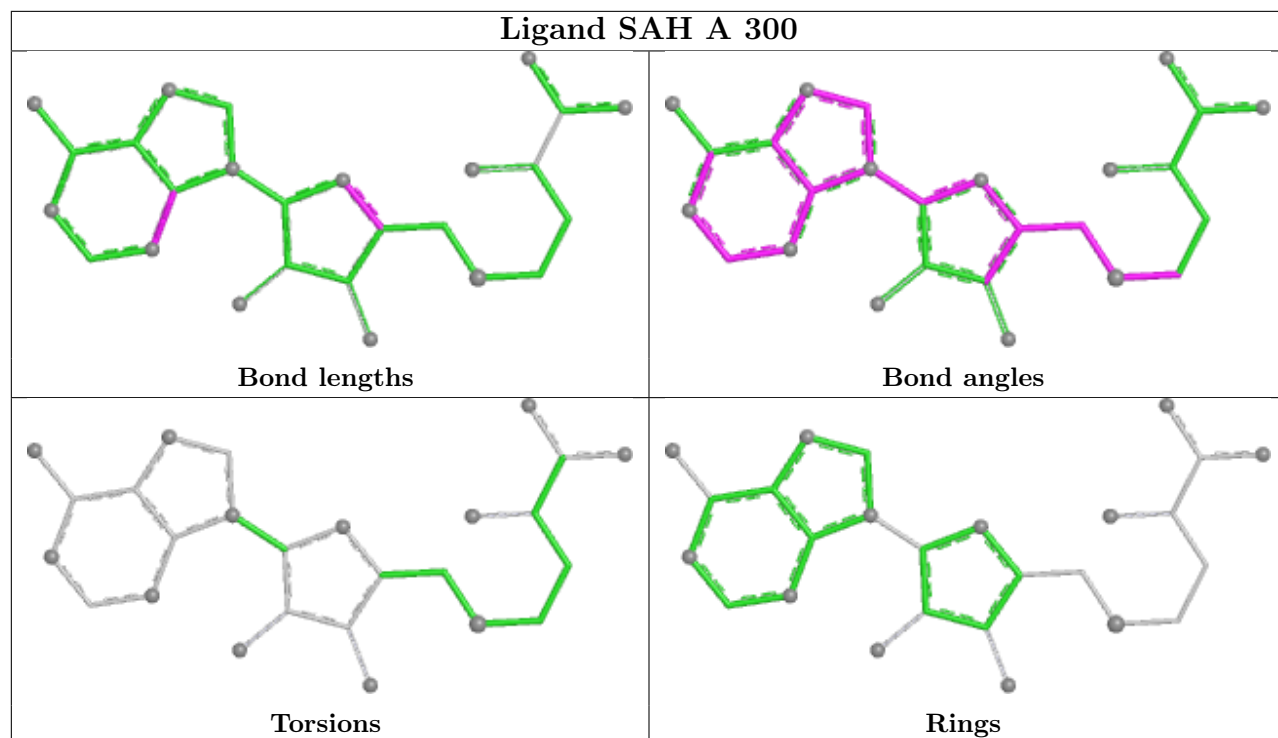
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	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 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	229/259 (88%)	1.79	89 (38%)  	16, 29, 43, 53	0
1	B	238/259 (91%)	1.38	58 (24%)  	17, 31, 44, 65	0
All	All	467/518 (90%)	1.58	147 (31%)  	16, 30, 44, 65	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	83	ALA	6.5
1	A	132	GLY	6.5
1	B	69	VAL	6.3
1	A	130	THR	5.2
1	A	128	SER	5.2
1	B	109	PHE	4.9
1	B	110	TYR	4.8
1	A	133	ILE	4.7
1	A	129	MET	4.7
1	A	87	ALA	4.6
1	A	188	LEU	4.5
1	A	195	TYR	4.5
1	A	131	PRO	4.3
1	B	93	VAL	4.3
1	A	240	THR	4.3
1	A	193	GLU	4.2
1	B	70	PRO	4.1
1	A	208	ALA	4.0
1	B	90	ALA	4.0
1	A	84	ALA	3.9
1	A	138	ALA	3.9
1	A	82	TYR	3.9
1	A	166	LEU	3.8
1	B	86	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	182	SER	3.7
1	B	181	LEU	3.7
1	A	112	THR	3.7
1	A	239	SER	3.6
1	A	127	CYS	3.6
1	A	137	ILE	3.5
1	B	73	ARG	3.5
1	B	117	ILE	3.5
1	A	123	ASP	3.4
1	A	161	ASP	3.4
1	B	124	GLY	3.4
1	B	125	LEU	3.3
1	B	7	ILE	3.3
1	A	228	SER	3.2
1	A	163	ILE	3.2
1	A	134	PRO	3.2
1	A	205	VAL	3.1
1	B	133	ILE	3.1
1	A	234	PRO	3.1
1	B	148	ALA	3.0
1	A	212	ILE	3.0
1	A	229	LEU	3.0
1	B	104	VAL	2.9
1	B	129	MET	2.9
1	A	126	ASP	2.9
1	A	182	SER	2.9
1	A	5	GLY	2.9
1	A	241	LEU	2.9
1	A	216	VAL	2.9
1	B	112	THR	2.9
1	B	105	GLY	2.9
1	A	172	THR	2.8
1	B	163	ILE	2.8
1	A	170	LEU	2.8
1	A	181	LEU	2.8
1	A	183	THR	2.8
1	B	111	SER	2.8
1	B	41	SER	2.7
1	A	136	PHE	2.7
1	A	169	ALA	2.7
1	A	7	ILE	2.7
1	B	20	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	88	SER	2.7
1	A	223	ALA	2.7
1	A	86	TYR	2.7
1	B	76	GLY	2.7
1	A	122	ARG	2.7
1	A	109	PHE	2.7
1	A	227	PHE	2.7
1	B	245	ALA	2.7
1	A	158	ALA	2.6
1	A	43	SER	2.6
1	B	72	SER	2.6
1	B	40	VAL	2.6
1	A	191	PHE	2.6
1	A	107	GLY	2.6
1	B	94	GLN	2.5
1	A	81	SER	2.5
1	B	11	SER	2.5
1	B	196	ALA	2.5
1	B	107	GLY	2.5
1	B	22	VAL	2.5
1	B	34	ILE	2.5
1	B	151	SER	2.4
1	B	100	ALA	2.4
1	A	218	ALA	2.4
1	B	180	LYS	2.4
1	B	191	PHE	2.4
1	A	154	VAL	2.4
1	A	156	VAL	2.4
1	B	8	ILE	2.4
1	A	184	VAL	2.4
1	B	33	VAL	2.4
1	B	183	THR	2.4
1	A	165	GLU	2.3
1	A	105	GLY	2.3
1	A	98	ARG	2.3
1	A	190	SER	2.3
1	A	175	THR	2.3
1	A	115	ALA	2.3
1	B	44	GLY	2.3
1	B	21	THR	2.3
1	B	150	GLN	2.3
1	B	108	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	77	ALA	2.3
1	A	174	SER	2.2
1	A	171	VAL	2.2
1	B	195	TYR	2.2
1	A	141	SER	2.2
1	A	198	PRO	2.2
1	A	108	GLY	2.2
1	A	209	GLY	2.2
1	A	155	LEU	2.2
1	A	94	GLN	2.2
1	A	95	ALA	2.2
1	A	151	SER	2.2
1	A	42	ALA	2.1
1	A	135	ALA	2.1
1	A	149	LEU	2.1
1	A	220	ARG	2.1
1	A	232	CYS	2.1
1	B	160	ILE	2.1
1	B	71	MET	2.1
1	A	44	GLY	2.1
1	A	148	ALA	2.1
1	B	106	ASP	2.1
1	A	238	GLN	2.1
1	B	39	THR	2.1
1	A	164	GLY	2.1
1	A	206	GLY	2.1
1	A	176	VAL	2.1
1	A	167	GLU	2.0
1	B	103	SER	2.1
1	B	194	ARG	2.0
1	B	131	PRO	2.0
1	B	193	GLU	2.0
1	A	41	SER	2.0
1	B	42	ALA	2.0
1	B	208	ALA	2.0
1	A	119	ARG	2.0
1	A	235	HIS	2.0
1	A	225	PRO	2.0
1	B	172	THR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

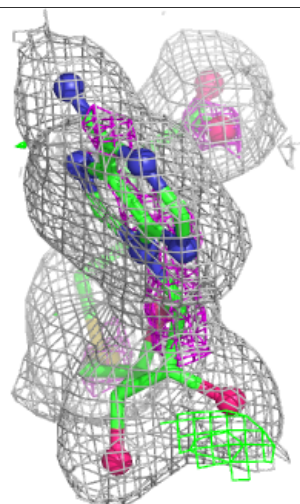
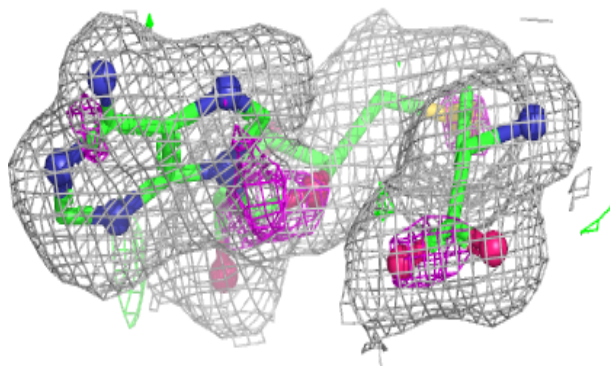
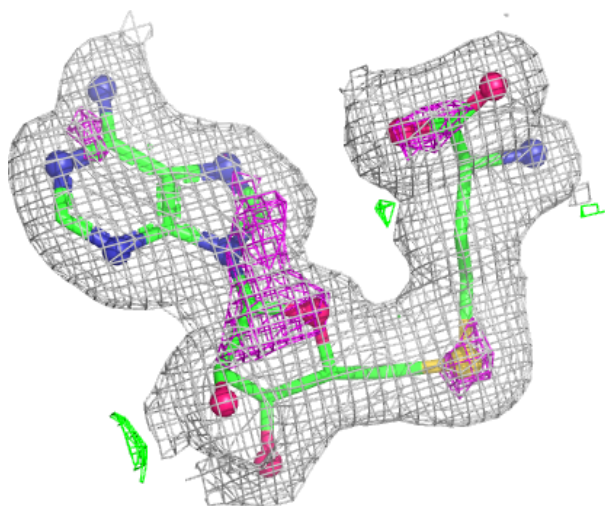
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SAH	A	300	26/26	0.92	0.09	18,24,28,31	0
2	SAH	B	301	26/26	0.95	0.08	14,19,24,25	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.

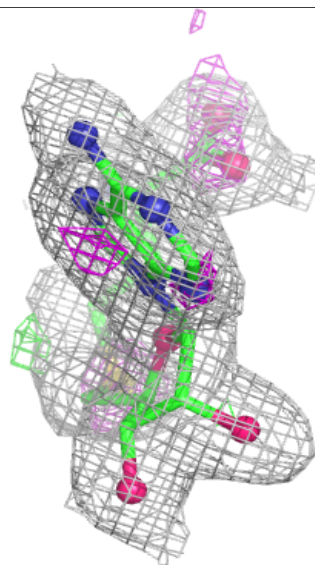
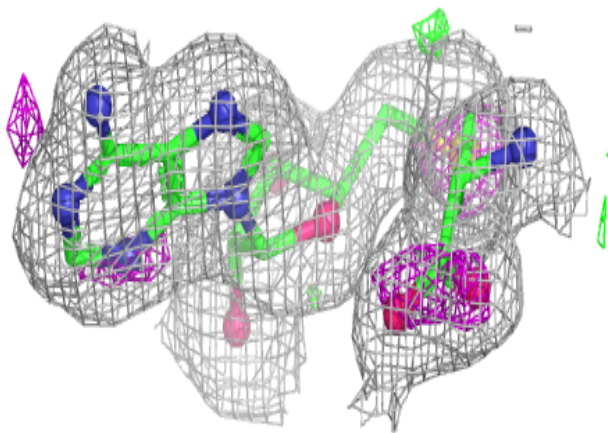
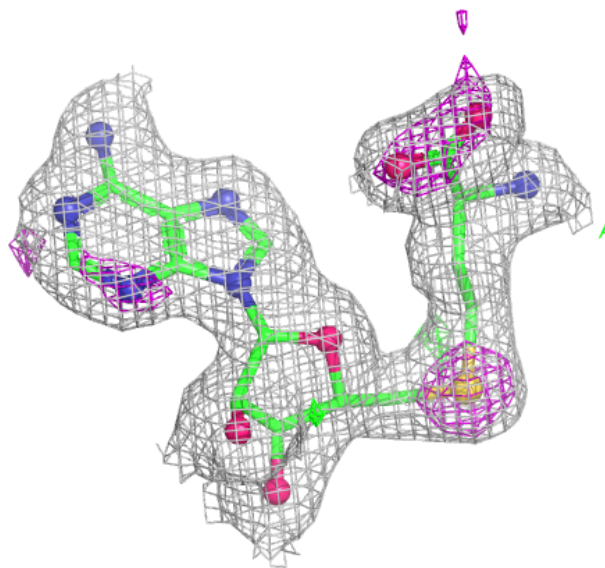
Electron density around SAH A 300:

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



Electron density around SAH 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.