



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2024 – 09:46 AM EST

PDB ID : 2H00
Title : Human methyltransferase 10 domain containing protein
Authors : Min, J.R.; Wu, H.; Zeng, H.; Loppnau, P.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Plotnikov, A.N.; Structural Genomics Consortium (SGC)
Deposited on : 2006-05-12
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

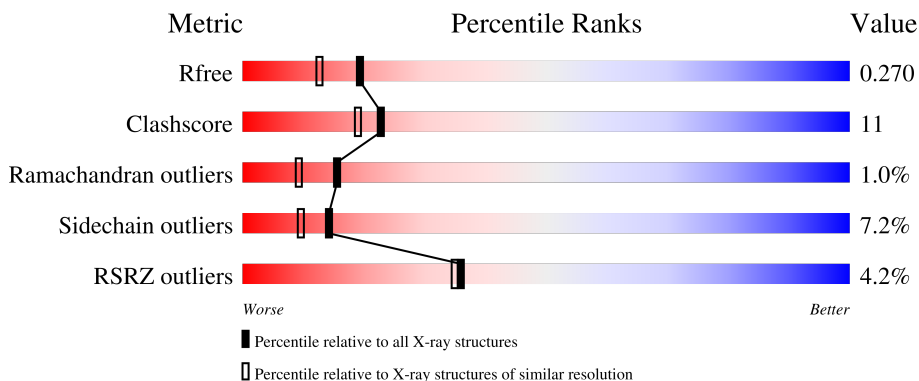
1 Overall quality at a glance

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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	254	4% 65% 20% 11%
1	B	254	6% 61% 18% 17%
1	C	254	% 63% 16% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DTU	A	2140	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5402 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 methyltransferase 10 domain containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	225	1812	1165	302	331	14	0	1	0
1	B	210	1682	1087	285	297	13	0	0	0
1	C	203	1621	1052	271	286	12	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

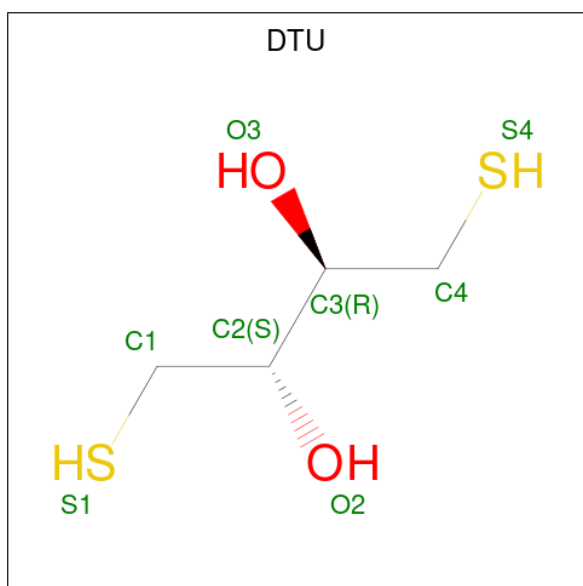
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	GB 29791720
A	2	SER	-	cloning artifact	GB 29791720
B	1	GLY	-	cloning artifact	GB 29791720
B	2	SER	-	cloning artifact	GB 29791720
C	1	GLY	-	cloning artifact	GB 29791720
C	2	SER	-	cloning artifact	GB 29791720

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S).



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

- Molecule 3 is (2R,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (three-letter code: DTU) (formula: C₄H₁₀O₂S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

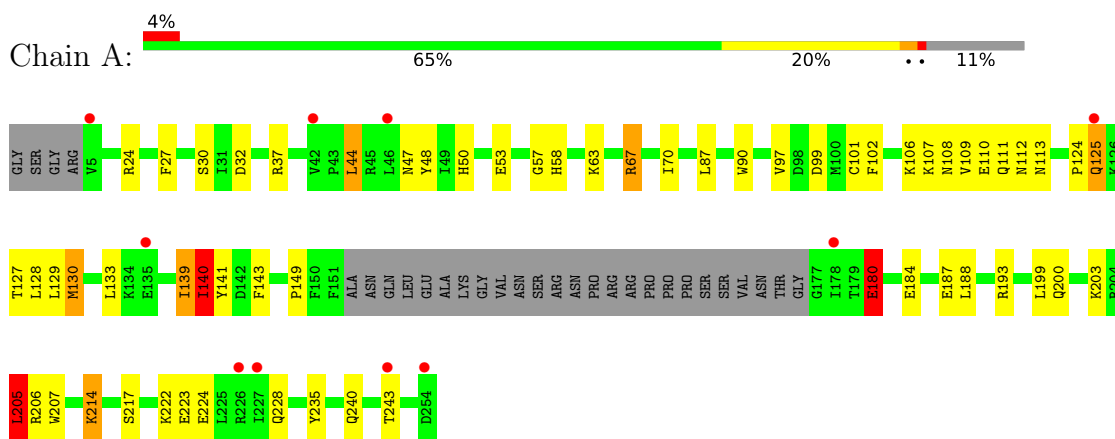
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	92	Total	O	0	0
			92	92		
5	B	47	Total	O	0	0
			47	47		
5	C	60	Total	O	0	0
			60	60		

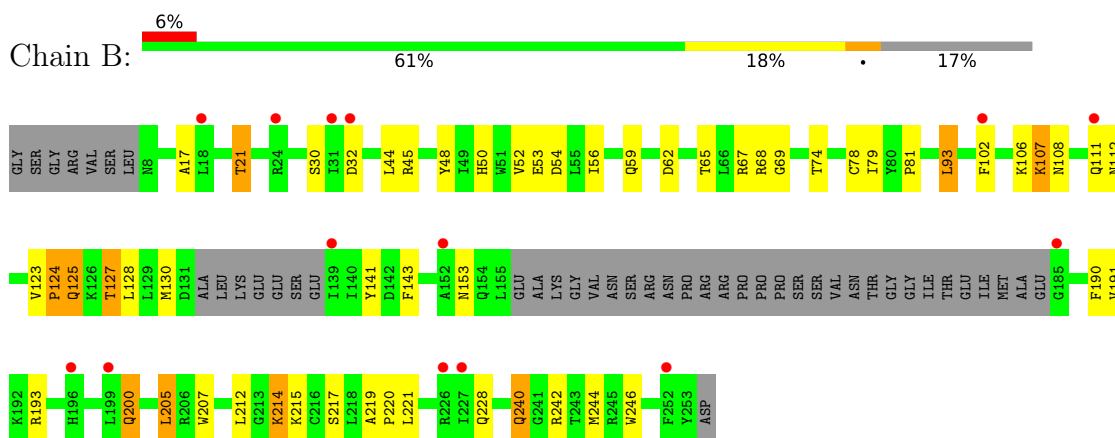
3 Residue-property plots [i](#)

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.

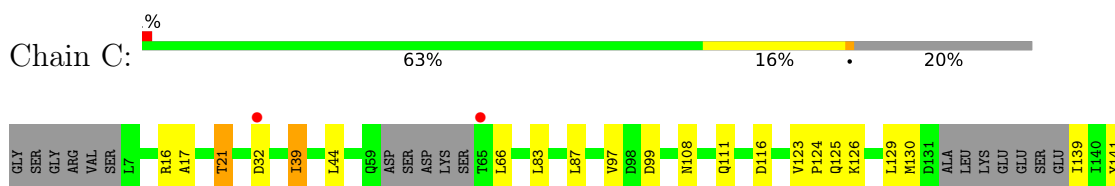
- Molecule 1: methyltransferase 10 domain containing protein

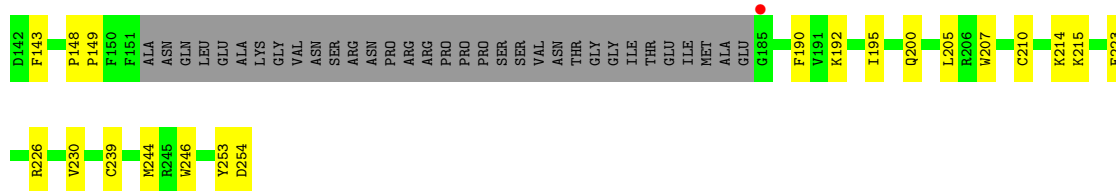


- Molecule 1: methyltransferase 10 domain containing protein



- Molecule 1: methyltransferase 10 domain containing protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	133.74Å 133.74Å 78.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	115.47 – 2.00 38.27 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (115.47-2.00) 98.0 (38.27-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.221 , 0.274 0.218 , 0.270	Depositor DCC
R_{free} test set	2751 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtrriage
Anisotropy	0.265	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5402	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, DTU, 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	0.96	1/1851 (0.1%)	0.89	4/2506 (0.2%)
1	B	0.75	0/1720	0.80	1/2328 (0.0%)
1	C	0.88	0/1658	0.89	0/2244
All	All	0.87	1/5229 (0.0%)	0.87	5/7078 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	109	VAL	CB-CG1	5.24	1.63	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	LEU	CA-CB-CG	6.82	130.99	115.30
1	A	67	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	B	93	LEU	CA-CB-CG	5.83	128.70	115.30
1	A	24	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	A	140	ILE	CB-CA-C	5.08	121.76	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	GLU	Peptide

5.2 Too-close contacts [i](#)

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	1812	0	1808	56	0
1	B	1682	0	1681	39	0
1	C	1621	0	1611	26	0
2	A	26	0	19	2	0
2	B	26	0	19	0	0
2	C	26	0	19	2	0
3	A	8	0	10	3	0
4	B	1	0	0	0	0
4	C	1	0	0	1	0
5	A	92	0	0	3	0
5	B	47	0	0	1	0
5	C	60	0	0	4	0
All	All	5402	0	5167	119	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 11.

All (119) 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:47:ASN:HD21	1:A:240:GLN:HE21	1.13	0.92
1:A:180:GLU:N	1:A:180:GLU:OE2	2.03	0.91
1:A:67:ARG:HH12	1:A:206[B]:ARG:HH12	1.14	0.89
1:A:140:ILE:C	1:A:140:ILE:HD13	1.94	0.87
1:A:30:SER:H	1:A:112:ASN:HD21	1.24	0.86
1:B:30:SER:H	1:B:112:ASN:HD21	1.23	0.85
4:C:402:CL:CL	5:C:451:HOH:O	2.32	0.83
1:B:32:ASP:H	1:B:108:ASN:HD21	1.27	0.83
1:B:44:LEU:HD13	1:B:240:GLN:HB2	1.58	0.83
1:B:17:ALA:O	1:B:21:THR:HG23	1.80	0.82
1:A:139:ILE:HD12	1:A:140:ILE:H	1.45	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:LYS:HD2	1:C:130:MET:CB	2.14	0.78
1:A:67:ARG:HH12	1:A:206[B]:ARG:NH1	1.82	0.77
1:C:17:ALA:O	1:C:21:THR:HG23	1.84	0.76
1:A:113:ASN:HB3	5:A:2182:HOH:O	1.86	0.75
1:C:32:ASP:H	1:C:108:ASN:HD21	1.33	0.75
1:C:223:GLU:OE1	1:C:226:ARG:NH1	2.20	0.75
1:A:32:ASP:H	1:A:108:ASN:HD21	1.33	0.75
1:A:44:LEU:HD23	1:A:240:GLN:HG2	1.70	0.74
1:B:141:TYR:HB2	1:B:205:LEU:HD22	1.70	0.72
1:A:140:ILE:HD11	1:A:206[A]:ARG:HG3	1.72	0.72
1:A:140:ILE:HD11	1:A:206[B]:ARG:HG3	1.70	0.72
1:C:116:ASP:HB2	5:C:418:HOH:O	1.91	0.70
1:A:222:LYS:HE2	1:A:235:TYR:CE2	2.26	0.70
1:A:44:LEU:CD2	1:A:240:GLN:HG2	2.22	0.69
1:C:126:LYS:HG3	5:C:419:HOH:O	1.93	0.69
1:B:128:LEU:HD12	1:B:193:ARG:HG2	1.76	0.67
1:A:50:HIS:HE1	1:B:54:ASP:OD1	1.79	0.65
1:C:16:ARG:HA	1:C:39:ILE:HD13	1.79	0.65
1:B:228:GLN:HA	1:B:228:GLN:OE1	1.98	0.63
1:A:44:LEU:HD23	1:A:240:GLN:CG	2.28	0.63
1:A:130:MET:HG3	1:A:200:GLN:HE21	1.63	0.62
3:A:2140:DTU:O2	3:A:2140:DTU:S4	2.56	0.61
1:A:140:ILE:C	1:A:140:ILE:CD1	2.67	0.61
1:B:53:GLU:OE1	5:B:440:HOH:O	2.16	0.60
1:A:67:ARG:NH1	1:A:206[B]:ARG:HH12	1.95	0.59
1:B:124:PRO:HD2	1:B:127:THR:HG21	1.83	0.59
1:A:47:ASN:ND2	1:A:240:GLN:HE21	1.92	0.59
1:B:242:ARG:HB3	1:C:214:LYS:HD3	1.85	0.57
1:A:67:ARG:NH1	1:A:206[B]:ARG:NH1	2.52	0.57
1:A:184:GLU:HB3	1:A:214:LYS:HE3	1.86	0.57
1:A:87:LEU:HD22	1:B:59:GLN:HB3	1.86	0.57
1:C:148:PRO:HB3	1:C:190:PHE:CD2	2.41	0.55
1:B:32:ASP:N	1:B:108:ASN:HD21	2.01	0.55
1:B:124:PRO:HB2	1:B:127:THR:HG22	1.87	0.55
1:A:139:ILE:CD1	1:A:140:ILE:H	2.18	0.55
1:C:108:ASN:HD22	1:C:111:GLN:HE21	1.53	0.54
1:C:148:PRO:HG3	1:C:210:CYS:SG	2.48	0.54
1:B:143:PHE:HA	1:B:207:TRP:O	2.09	0.53
1:A:32:ASP:H	1:A:108:ASN:ND2	2.03	0.53
1:B:45:ARG:HH11	1:B:45:ARG:HG3	1.73	0.53
1:B:44:LEU:HB2	1:B:240:GLN:HE21	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:GLU:HG3	3:A:2140:DTU:H4C2	1.91	0.52
1:A:106:LYS:HG2	3:A:2140:DTU:H3	1.91	0.52
1:A:149:PRO:HG3	2:A:300:SAH:C8	2.40	0.52
1:A:58:HIS:HD2	5:A:2213:HOH:O	1.93	0.51
1:A:107:LYS:HD2	5:A:2232:HOH:O	2.11	0.51
1:B:69:GLY:HA3	1:B:143:PHE:CZ	2.47	0.50
1:A:37:ARG:HD2	1:A:101:CYS:SG	2.51	0.50
1:C:253:TYR:O	1:C:254:ASP:HB2	2.11	0.49
1:C:129:LEU:HD11	1:C:200:GLN:OE1	2.12	0.49
1:C:192:LYS:HA	1:C:195:ILE:HD12	1.94	0.49
1:A:57:GLY:O	1:A:67:ARG:NH2	2.46	0.48
1:B:32:ASP:H	1:B:108:ASN:ND2	2.02	0.48
1:A:133:LEU:CD1	1:A:205:LEU:HD21	2.44	0.48
1:B:130:MET:CE	1:B:200:GLN:HG3	2.44	0.48
1:C:141:TYR:HB2	1:C:205:LEU:HG	1.96	0.48
1:C:83:LEU:O	1:C:87:LEU:HG	2.13	0.47
1:B:62:ASP:HB3	1:B:65:THR:OG1	2.14	0.47
1:B:102:PHE:CZ	1:B:106:LYS:HD3	2.49	0.47
1:A:149:PRO:HG3	2:A:300:SAH:H8	1.97	0.47
1:A:199:LEU:HD11	1:A:228:GLN:HG3	1.98	0.46
1:C:215:LYS:HD3	1:C:246:TRP:CE2	2.50	0.46
1:B:130:MET:SD	1:B:200:GLN:HG3	2.55	0.46
1:C:124:PRO:HD2	1:C:126:LYS:HE2	1.98	0.46
1:A:27:PHE:CE1	1:A:87:LEU:HD21	2.51	0.45
1:B:78:CYS:O	1:B:81:PRO:HD2	2.16	0.45
1:A:124:PRO:HG2	1:A:127:THR:CG2	2.46	0.45
1:B:219:ALA:HB3	1:B:220:PRO:HD3	1.98	0.45
1:B:56:ILE:O	1:B:67:ARG:NH1	2.50	0.45
1:B:130:MET:HE2	1:B:200:GLN:HG3	1.99	0.45
1:A:128:LEU:HD22	1:A:193:ARG:HB3	1.99	0.45
1:B:214:LYS:HZ3	1:B:214:LYS:HB2	1.82	0.45
1:C:124:PRO:HG2	1:C:126:LYS:HD3	1.99	0.45
1:A:143:PHE:HA	1:A:207:TRP:O	2.17	0.44
1:C:143:PHE:HA	1:C:207:TRP:O	2.17	0.44
1:B:128:LEU:CD1	1:B:193:ARG:HG2	2.45	0.44
1:A:130:MET:HE3	1:A:130:MET:HA	1.99	0.44
1:A:130:MET:SD	1:A:200:GLN:HG3	2.58	0.43
1:B:191:VAL:HG11	1:B:221:LEU:HD13	1.99	0.43
1:B:212:LEU:HB2	1:B:246:TRP:HB2	2.01	0.43
1:A:50:HIS:HD2	1:A:53:GLU:OE2	2.02	0.43
1:A:124:PRO:HG2	1:A:127:THR:HG23	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ASP:OD2	1:B:107:LYS:NZ	2.47	0.43
1:A:97:VAL:HG21	1:A:125:GLN:HG2	2.01	0.43
1:A:228:GLN:NE2	1:A:228:GLN:HA	2.34	0.43
1:B:128:LEU:HD23	1:B:128:LEU:HA	1.80	0.43
1:A:228:GLN:HA	1:A:228:GLN:HE21	1.84	0.42
1:A:102:PHE:CZ	1:A:106:LYS:HD2	2.55	0.42
1:C:129:LEU:CD1	1:C:200:GLN:OE1	2.68	0.42
1:B:48:TYR:O	1:B:52:VAL:HG13	2.20	0.42
1:C:149:PRO:HG3	2:C:302:SAH:H8	2.01	0.42
1:A:50:HIS:HB3	1:B:50:HIS:CG	2.56	0.41
1:C:139:ILE:N	5:C:416:HOH:O	2.53	0.41
1:C:149:PRO:HG3	2:C:302:SAH:C8	2.50	0.41
1:A:70:ILE:CD1	1:A:133:LEU:HD11	2.50	0.41
1:B:214:LYS:HB2	1:B:214:LYS:NZ	2.35	0.41
1:C:97:VAL:HG12	1:C:123:VAL:HG23	2.02	0.41
1:A:67:ARG:HB2	1:A:90:TRP:CD1	2.56	0.41
1:A:70:ILE:HD12	1:A:205:LEU:HD11	2.01	0.41
1:A:128:LEU:HB3	1:A:129:LEU:H	1.72	0.41
1:A:140:ILE:HD13	1:A:141:TYR:O	2.20	0.41
1:A:222:LYS:HE2	1:A:235:TYR:CD2	2.56	0.41
1:C:16:ARG:HA	1:C:39:ILE:CD1	2.47	0.41
1:B:128:LEU:HD21	1:B:190:PHE:CZ	2.55	0.41
1:B:215:LYS:HB2	1:B:246:TRP:CZ2	2.56	0.40
1:A:47:ASN:HD21	1:A:240:GLN:NE2	1.96	0.40
1:A:200:GLN:H	1:A:200:GLN:HG2	1.76	0.40
1:B:123:VAL:HB	1:B:127:THR:HG21	2.02	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	222/254 (87%)	217 (98%)	5 (2%)	0	100	100
1	B	204/254 (80%)	186 (91%)	13 (6%)	5 (2%)	5	2
1	C	195/254 (77%)	188 (96%)	6 (3%)	1 (0%)	29	23
All	All	621/762 (82%)	591 (95%)	24 (4%)	6 (1%)	15	9

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	125	GLN
1	B	153	ASN
1	B	107	LYS
1	B	124	PRO
1	C	125	GLN
1	B	111	GLN

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	199/224 (89%)	180 (90%)	19 (10%)	8	5
1	B	182/224 (81%)	169 (93%)	13 (7%)	14	10
1	C	174/224 (78%)	166 (95%)	8 (5%)	27	23
All	All	555/672 (83%)	515 (93%)	40 (7%)	14	9

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	48	TYR
1	A	63	LYS
1	A	99	ASP
1	A	111	GLN
1	A	125	GLN
1	A	130	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	139	ILE
1	A	140	ILE
1	A	180	GLU
1	A	187	GLU
1	A	188	LEU
1	A	203	LYS
1	A	205	LEU
1	A	214	LYS
1	A	217	SER
1	A	223	GLU
1	A	224	GLU
1	A	243	THR
1	B	21	THR
1	B	68	ARG
1	B	74	THR
1	B	79	ILE
1	B	93	LEU
1	B	125	GLN
1	B	127	THR
1	B	200	GLN
1	B	205	LEU
1	B	214	LYS
1	B	217	SER
1	B	240	GLN
1	B	244	MET
1	C	21	THR
1	C	39	ILE
1	C	44	LEU
1	C	66	LEU
1	C	99	ASP
1	C	230	VAL
1	C	239	CYS
1	C	244	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	47	ASN
1	A	50	HIS
1	A	103	ASN
1	A	108	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	111	GLN
1	A	112	ASN
1	A	125	GLN
1	A	200	GLN
1	A	228	GLN
1	B	59	GLN
1	B	103	ASN
1	B	108	ASN
1	B	112	ASN
1	B	240	GLN
1	C	108	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
3	DTU	A	2140	-	7,7,7	0.45	0	4,8,8	3.74	2 (50%)
2	SAH	C	302	-	24,28,28	1.35	4 (16%)	25,40,40	1.75	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SAH	A	300	-	24,28,28	1.24	2 (8%)	25,40,40	1.73	6 (24%)
2	SAH	B	301	-	24,28,28	1.35	2 (8%)	25,40,40	1.73	4 (16%)

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	DTU	A	2140	-	2/2/2/2	4/8/8/8	-
2	SAH	C	302	-	-	0/11/31/31	0/3/3/3
2	SAH	A	300	-	-	0/11/31/31	0/3/3/3
2	SAH	B	301	-	-	0/11/31/31	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	SAH	C2-N3	4.52	1.39	1.32
2	C	302	SAH	C2-N3	4.00	1.38	1.32
2	A	300	SAH	C2-N3	3.27	1.37	1.32
2	B	301	SAH	C2-N1	3.18	1.39	1.33
2	A	300	SAH	C2-N1	2.82	1.39	1.33
2	C	302	SAH	O4'-C1'	2.82	1.45	1.41
2	C	302	SAH	C2-N1	2.50	1.38	1.33
2	C	302	SAH	OXT-C	-2.09	1.23	1.30

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	302	SAH	N3-C2-N1	-5.55	120.00	128.68
2	B	301	SAH	N3-C2-N1	-5.47	120.12	128.68
2	A	300	SAH	N3-C2-N1	-5.45	120.16	128.68
3	A	2140	DTU	C3-C4-S4	-5.21	99.31	114.47
3	A	2140	DTU	C2-C1-S1	-4.99	99.96	114.47
2	C	302	SAH	O4'-C1'-C2'	-3.31	102.09	106.93
2	B	301	SAH	OXT-C-CA	3.20	124.27	113.38
2	C	302	SAH	OXT-C-O	-3.08	117.09	124.09
2	B	301	SAH	O4'-C1'-C2'	-2.95	102.61	106.93
2	B	301	SAH	OXT-C-O	-2.78	117.77	124.09
2	A	300	SAH	C5'-SD-CG	-2.60	94.45	102.27
2	A	300	SAH	OXT-C-O	-2.52	118.38	124.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	SAH	C2'-C3'-C4'	2.42	107.35	102.64
2	C	302	SAH	OXT-C-CA	2.11	120.59	113.38
2	A	300	SAH	C2-N1-C6	2.08	122.31	118.75
2	A	300	SAH	O4'-C1'-C2'	-2.03	103.96	106.93

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	2140	DTU	C2
3	A	2140	DTU	C3

All (4) torsion outliers are listed below:

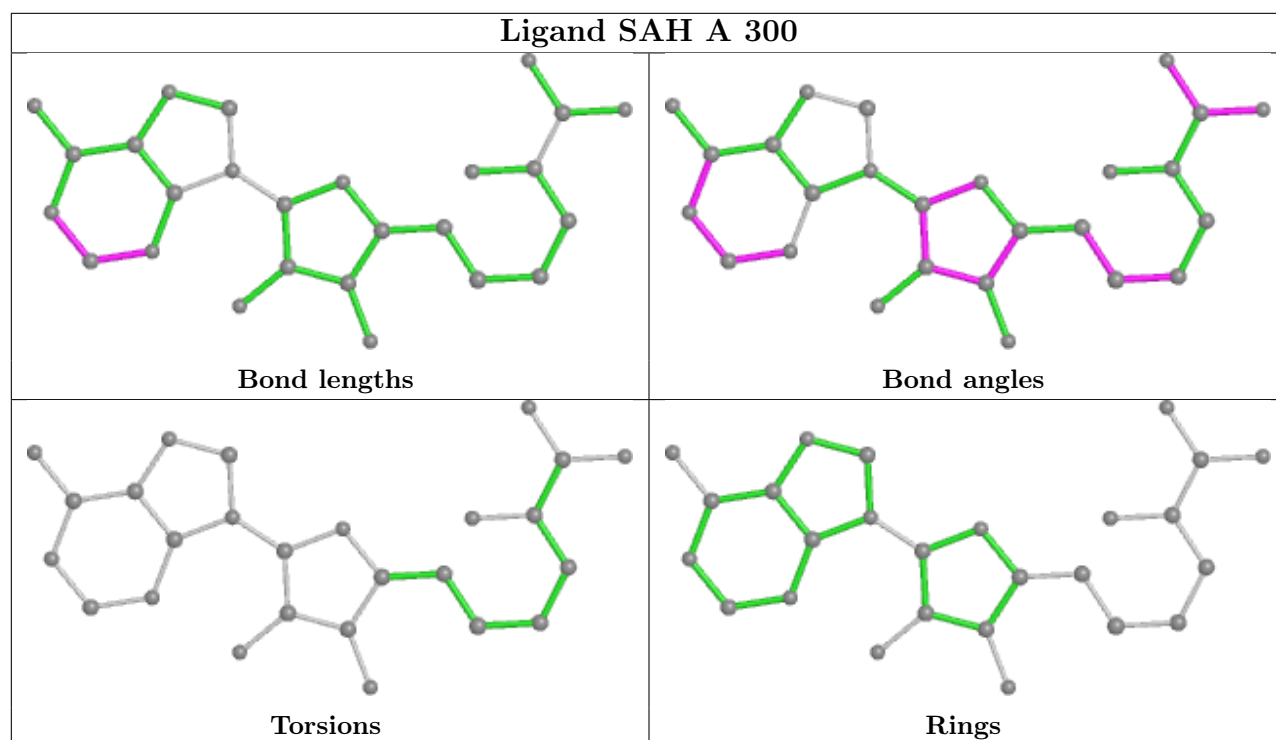
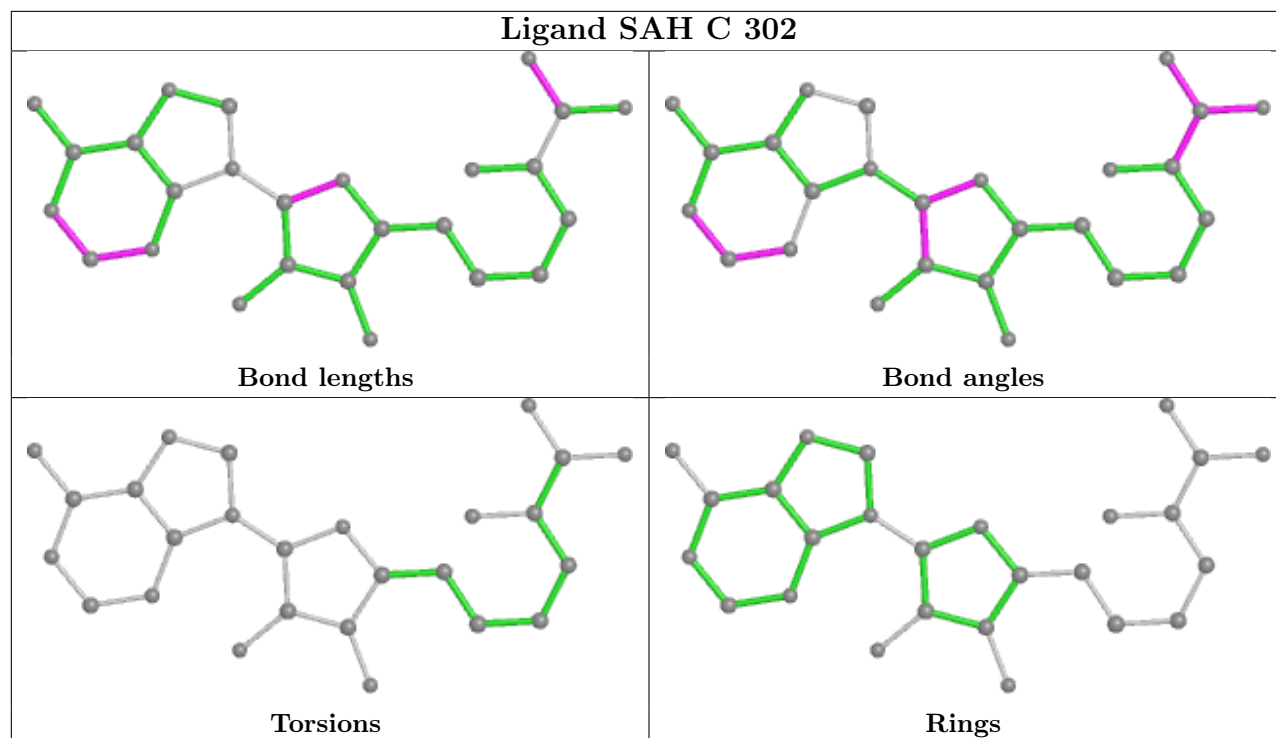
Mol	Chain	Res	Type	Atoms
3	A	2140	DTU	C1-C2-C3-O3
3	A	2140	DTU	O2-C2-C3-O3
3	A	2140	DTU	O2-C2-C3-C4
3	A	2140	DTU	S1-C1-C2-O2

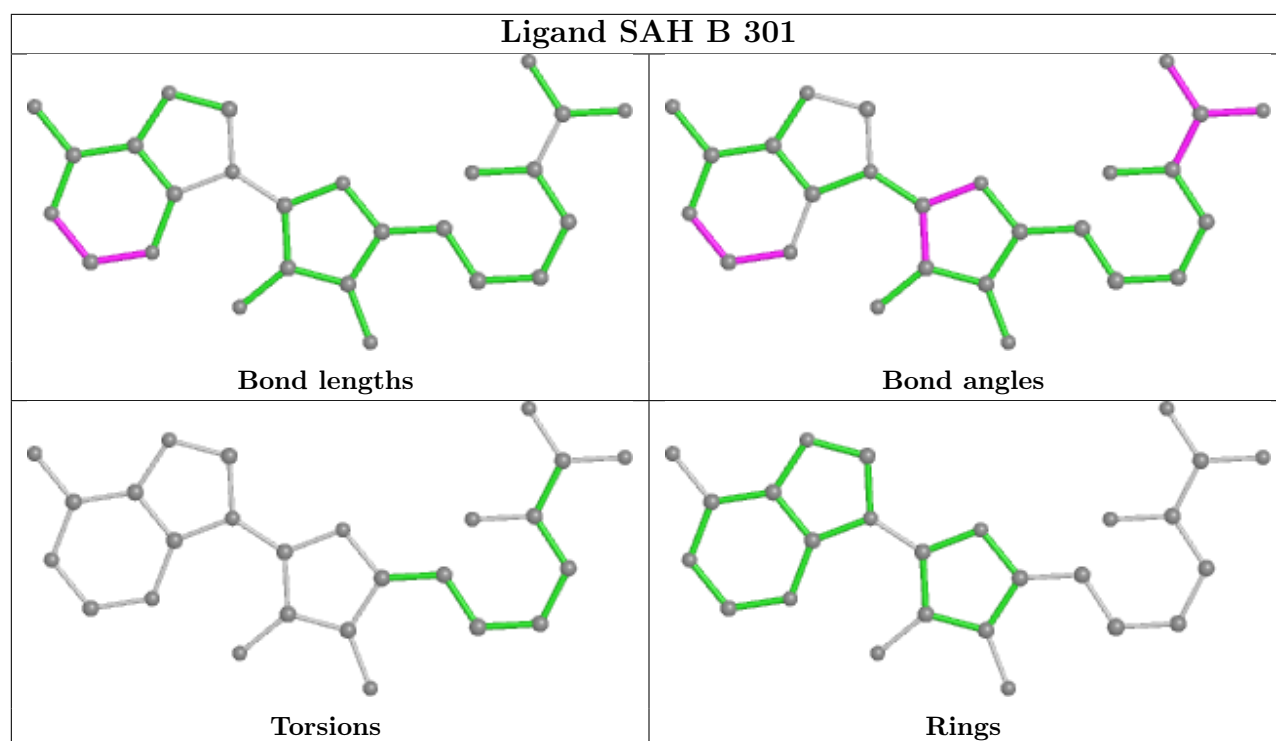
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2140	DTU	3	0
2	C	302	SAH	2	0
2	A	300	SAH	2	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	225/254 (88%)	0.31	10 (4%) 34 33	26, 36, 59, 68	0
1	B	210/254 (82%)	0.25	14 (6%) 17 17	34, 50, 65, 71	0
1	C	203/254 (79%)	0.16	3 (1%) 73 72	28, 42, 56, 65	0
All	All	638/762 (83%)	0.25	27 (4%) 36 35	26, 42, 61, 71	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	ILE	4.4
1	B	139	ILE	3.6
1	B	111	GLN	3.5
1	B	102	PHE	3.3
1	B	199	LEU	3.2
1	A	135	GLU	3.1
1	C	65	THR	2.8
1	A	125	GLN	2.7
1	B	185	GLY	2.7
1	B	227	ILE	2.6
1	A	46	LEU	2.6
1	A	254	ASP	2.6
1	C	185	GLY	2.6
1	B	252	PHE	2.6
1	A	42	VAL	2.6
1	B	226	ARG	2.6
1	C	32	ASP	2.4
1	B	31	ILE	2.4
1	A	227	ILE	2.3
1	A	226	ARG	2.3
1	B	18	LEU	2.3
1	B	24	ARG	2.3
1	B	196	HIS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	243	THR	2.2
1	B	32	ASP	2.1
1	B	152	ALA	2.1
1	A	5	VAL	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](#)

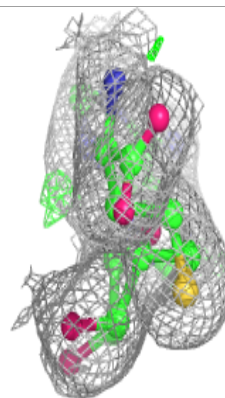
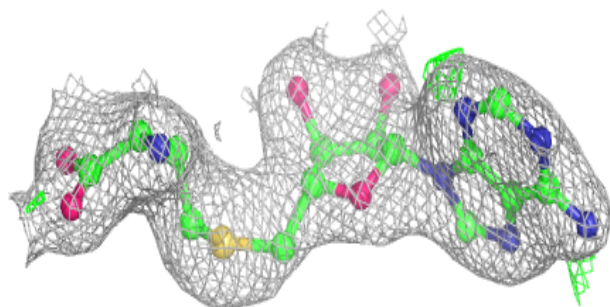
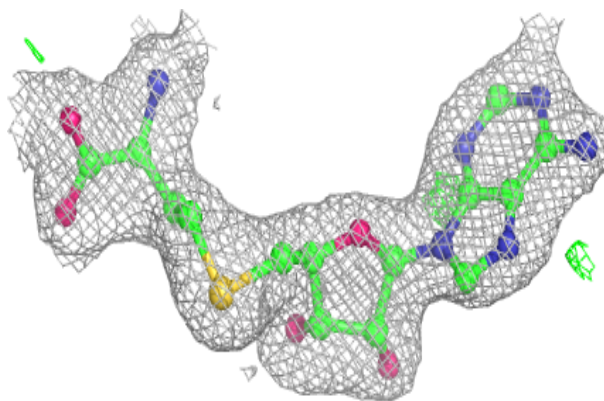
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	DTU	A	2140	8/8	0.84	0.18	47,56,63,64	0
2	SAH	C	302	26/26	0.89	0.12	40,43,46,47	0
2	SAH	A	300	26/26	0.91	0.12	26,32,36,37	0
4	CL	C	402	1/1	0.92	0.31	68,68,68,68	0
2	SAH	B	301	26/26	0.94	0.13	34,49,53,53	0
4	CL	B	401	1/1	0.95	0.35	58,58,58,58	0

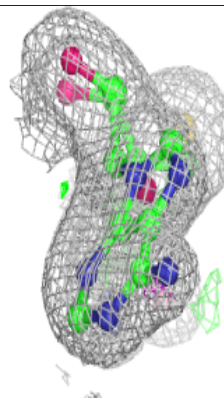
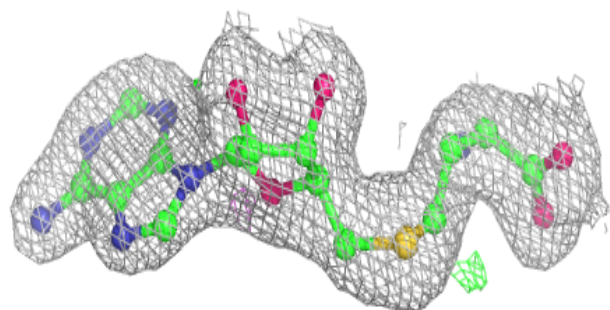
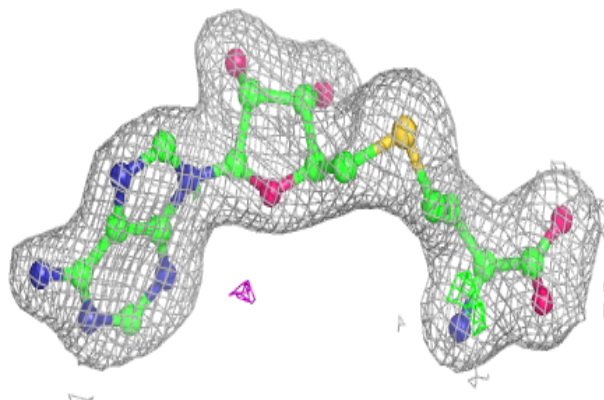
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

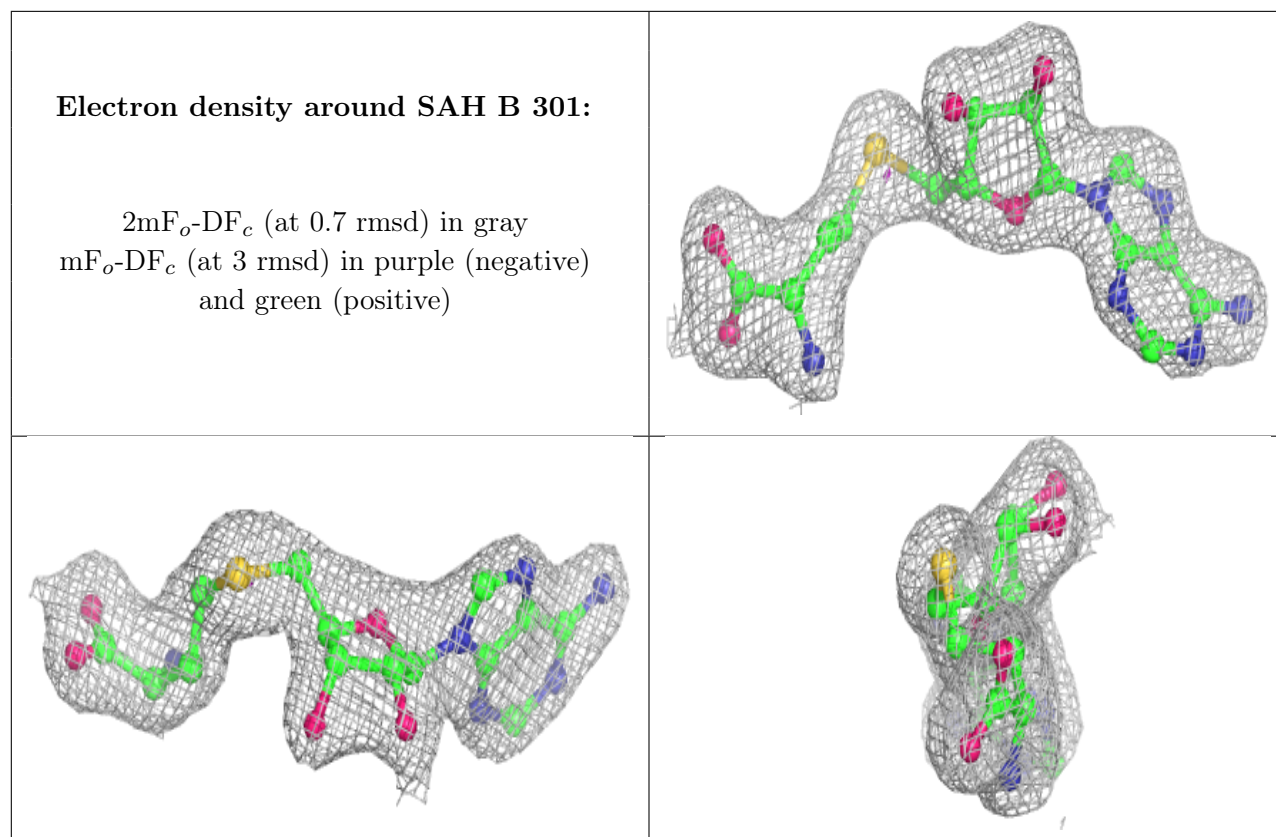
Electron density around SAH C 302:

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

**Electron density around SAH 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.