



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:57 AM UTC

PDB ID : 2BR5 / pdb_00002br5
Title : cmcI-N160 SAH
Authors : Oster, L.M.; Lester, D.R.; Terwisscha van Scheltinga, A.; svenda, M.;
Genereux, C.; Andersson, I.
Deposited on : 2005-05-01
Resolution : 2.83 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

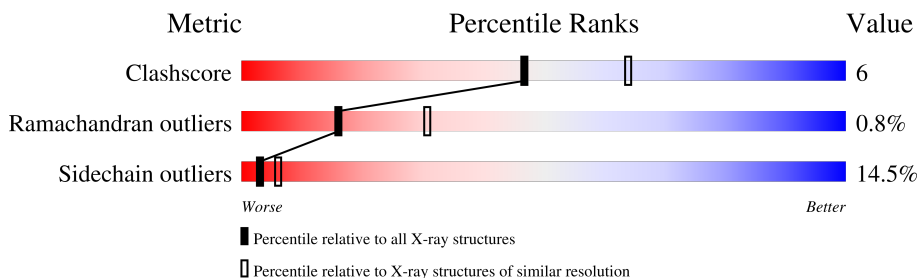
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 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	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	236	78% 17% . .
1	B	236	73% 20% 5% .
1	C	236	71% 21% . .
1	D	236	62% 17% . 18%
1	E	236	74% 21% . .
1	F	236	68% 18% . 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11055 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 CEPHALOSPORIN HYDROXYLASE CMCI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1861	1188	320	341	12			
1	B	232	Total	C	N	O	S	0	0	0
			1909	1216	328	353	12			
1	C	227	Total	C	N	O	S	0	0	0
			1860	1188	318	342	12			
1	D	194	Total	C	N	O	S	0	0	0
			1588	1009	274	293	12			
1	E	230	Total	C	N	O	S	0	0	0
			1896	1209	325	350	12			
1	F	206	Total	C	N	O	S	0	0	0
			1686	1079	288	307	12			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLN	LEU	engineered mutation	UNP O85726
A	160	ASN	ASP	engineered mutation	UNP O85726
A	200	PHE	LEU	engineered mutation	UNP O85726
B	10	GLN	LEU	engineered mutation	UNP O85726
B	160	ASN	ASP	engineered mutation	UNP O85726
B	200	PHE	LEU	engineered mutation	UNP O85726
C	10	GLN	LEU	engineered mutation	UNP O85726
C	160	ASN	ASP	engineered mutation	UNP O85726
C	200	PHE	LEU	engineered mutation	UNP O85726
D	160	ASN	ASP	engineered mutation	UNP O85726
E	10	GLN	LEU	engineered mutation	UNP O85726
E	160	ASN	ASP	engineered mutation	UNP O85726
E	200	PHE	LEU	engineered mutation	UNP O85726
F	160	ASN	ASP	engineered mutation	UNP O85726
F	200	PHE	LEU	engineered mutation	UNP O85726

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).



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
2	C	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	D	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	E	1	Total 26	C 14	N 6	O 5	S 1	0	0

- Molecule 3 is water.

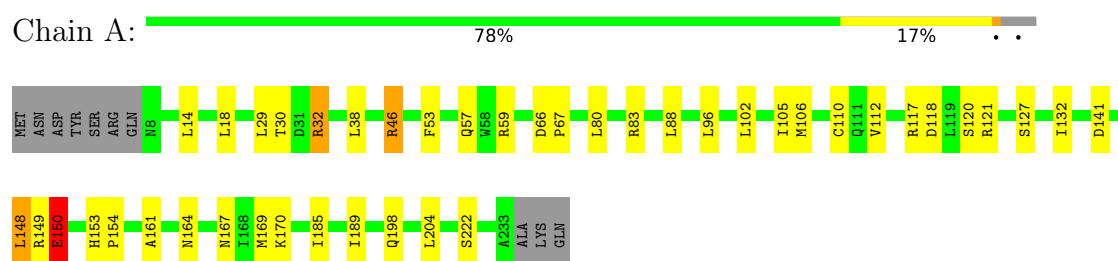
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	17	Total O 17 17	0	0
3	B	28	Total O 28 28	0	0
3	C	35	Total O 35 35	0	0
3	D	9	Total O 9 9	0	0
3	E	14	Total O 14 14	0	0
3	F	22	Total O 22 22	0	0

3 Residue-property plots [i](#)

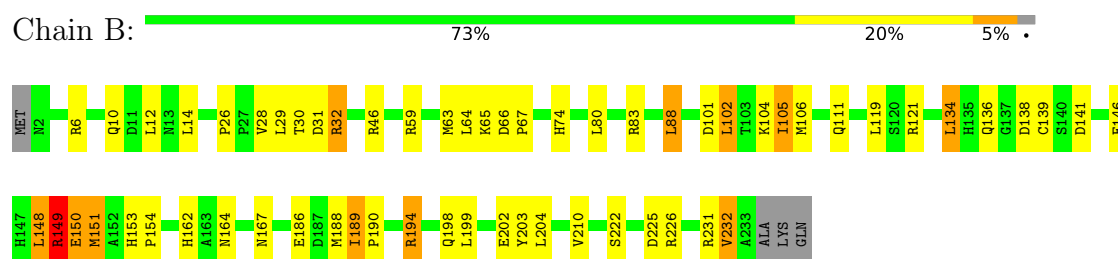
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

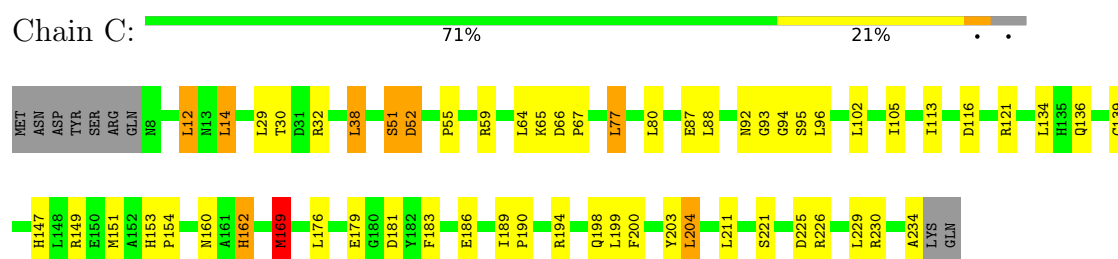
• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI



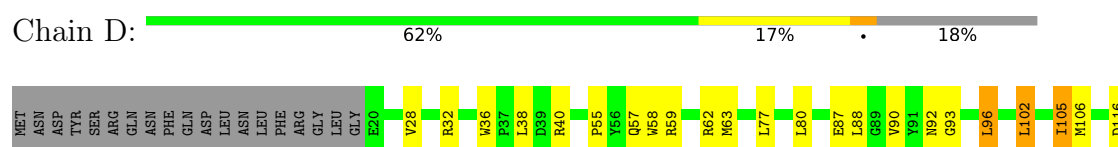
• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI

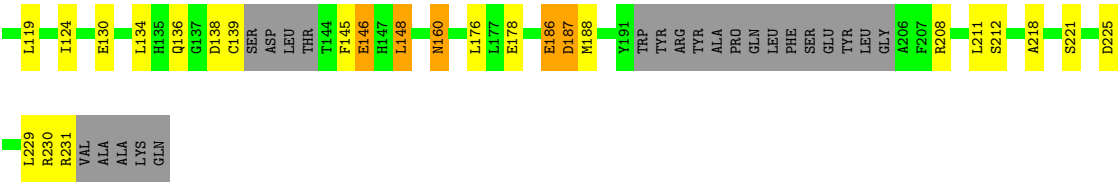


• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI

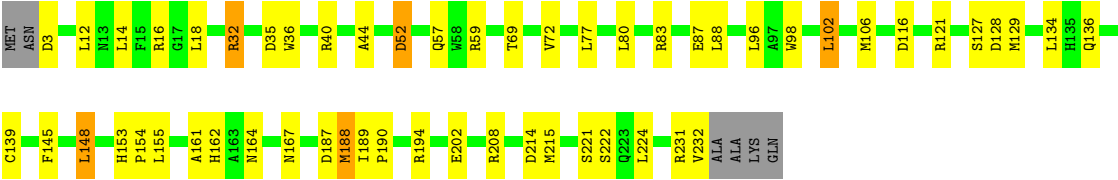


• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI

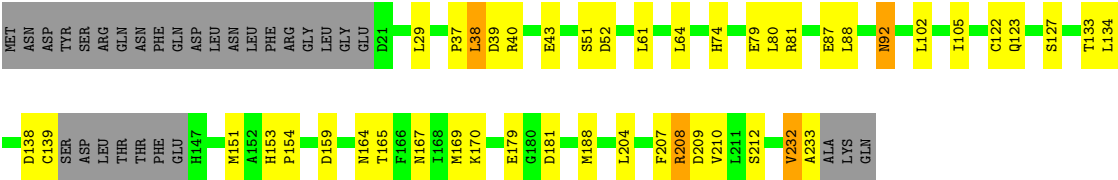




• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI



• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.91Å 102.52Å 181.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.83	Depositor
% Data completeness (in resolution range)	99.0 (49.39-2.83)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.231 , 0.301	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11055	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

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: 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	0.65	0/1915	0.91	2/2605 (0.1%)
1	B	0.73	0/1964	0.91	2/2672 (0.1%)
1	C	0.77	1/1914 (0.1%)	0.91	1/2605 (0.0%)
1	D	0.62	0/1631	0.84	1/2216 (0.0%)
1	E	0.69	0/1951	0.87	2/2654 (0.1%)
1	F	0.70	1/1736 (0.1%)	0.85	0/2364
All	All	0.70	2/11111 (0.0%)	0.89	8/15116 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	151	MET	SD-CE	6.56	1.96	1.79
1	C	169	MET	SD-CE	-5.97	1.64	1.79

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ALA	N-CA-C	-8.06	99.67	110.55
1	B	149	ARG	N-CA-C	6.73	116.94	108.45
1	E	32	ARG	N-CA-C	5.82	113.46	108.22
1	D	208	ARG	N-CA-C	5.60	119.59	112.87
1	E	188	MET	N-CA-C	5.33	117.83	111.71
1	C	162	HIS	N-CA-C	5.26	119.28	112.86
1	B	26	PRO	O-C-N	5.20	123.70	121.31
1	A	110	CYS	N-CA-C	5.18	117.34	108.90

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	1861	0	1771	19	0
1	B	1909	0	1805	29	0
1	C	1860	0	1765	30	0
1	D	1588	0	1508	18	0
1	E	1896	0	1794	20	0
1	F	1686	0	1599	16	0
2	A	26	0	19	1	0
2	B	26	0	19	0	0
2	C	26	0	19	1	0
2	D	26	0	19	1	0
2	E	26	0	19	3	0
3	A	17	0	0	0	0
3	B	28	0	0	0	0
3	C	35	0	0	3	0
3	D	9	0	0	0	0
3	E	14	0	0	3	0
3	F	22	0	0	0	0
All	All	11055	0	10337	121	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 6.

All (121) 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:E:164:ASN:HD21	1:E:167:ASN:HD22	1.22	0.85
1:B:66:ASP:HB2	1:B:67:PRO:HD2	1.66	0.76
1:E:88:LEU:HD22	1:E:139:CYS:SG	2.30	0.72
1:D:36:TRP:HB2	1:E:215:MET:HE3	1.72	0.71
1:A:105:ILE:HD11	1:B:105:ILE:CD1	2.21	0.70
1:C:87:GLU:OE1	1:C:160:ASN:ND2	2.23	0.67
1:D:186:GLU:O	1:D:187:ASP:HB2	1.95	0.67
1:C:52:ASP:HA	1:C:55:PRO:HG3	1.78	0.65
1:F:159:ASP:OD1	1:F:165:THR:HG23	1.98	0.64
1:C:234:ALA:C	3:C:2034:HOH:O	2.41	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:LEU:HA	1:B:105:ILE:HD12	1.79	0.62
1:C:151:MET:HE3	1:C:176:LEU:HD11	1.83	0.61
1:C:38:LEU:HG	1:F:204:LEU:HD22	1.84	0.59
1:C:162:HIS:HE1	1:C:186:GLU:O	1.86	0.58
1:F:164:ASN:HD21	1:F:167:ASN:HD22	1.51	0.58
1:C:204:LEU:HD13	1:F:38:LEU:HG	1.85	0.57
1:B:102:LEU:CD2	1:B:106:MET:HE3	2.35	0.56
1:E:77:LEU:HB3	1:E:106:MET:HE1	1.88	0.54
1:E:44:ALA:HA	3:E:2003:HOH:O	2.06	0.54
1:C:169:MET:HE3	1:C:229:LEU:HD23	1.90	0.54
1:C:189:ILE:HG23	1:C:200:PHE:CZ	2.43	0.54
1:D:160:ASN:HD21	1:D:186:GLU:CD	2.16	0.53
1:B:88:LEU:HD22	1:B:139:CYS:SG	2.48	0.53
1:E:18:LEU:HD21	2:E:301:SAH:CG	2.38	0.53
1:E:98:TRP:CE2	1:E:102:LEU:HD12	2.44	0.53
1:F:153:HIS:HD2	1:F:181:ASP:OD2	1.91	0.53
1:C:88:LEU:HD22	1:C:139:CYS:SG	2.49	0.53
1:F:232:VAL:O	1:F:233:ALA:HB2	2.10	0.52
1:E:116:ASP:O	1:E:136:GLN:HA	2.10	0.52
1:C:51:SER:O	1:C:51:SER:OG	2.27	0.51
1:D:186:GLU:O	1:D:187:ASP:CB	2.59	0.51
1:E:18:LEU:HD21	2:E:301:SAH:HG2	1.92	0.51
1:B:164:ASN:HD21	1:B:167:ASN:HD22	1.58	0.51
1:B:153:HIS:HA	1:B:154:PRO:C	2.36	0.51
1:C:199:LEU:HD22	1:C:203:TYR:CE2	2.46	0.51
1:A:59:ARG:HH11	1:A:59:ARG:HG2	1.76	0.50
1:A:164:ASN:HD21	1:A:167:ASN:HD22	1.59	0.50
1:F:208:ARG:HG2	1:F:209:ASP:N	2.26	0.50
1:F:37:PRO:HB2	1:F:39:ASP:OD1	2.13	0.49
1:A:118:ASP:OD1	1:A:120:SER:HB3	2.13	0.49
1:B:189:ILE:N	1:B:190:PRO:CD	2.76	0.49
2:C:301:SAH:H5'1	3:C:2035:HOH:O	2.13	0.48
1:B:102:LEU:HD22	1:B:106:MET:HE3	1.94	0.48
1:B:74:HIS:ND1	1:B:74:HIS:C	2.71	0.48
1:C:225:ASP:OD1	1:C:226:ARG:HG3	2.13	0.48
1:E:69:THR:HG23	1:E:224:LEU:HG	1.95	0.48
1:D:218:ALA:O	1:D:225:ASP:O	2.31	0.48
1:C:183:PHE:O	1:C:229:LEU:HB2	2.14	0.48
1:B:119:LEU:HD22	1:B:134:LEU:HG	1.95	0.47
1:D:116:ASP:OD1	2:D:301:SAH:H1'	2.15	0.47
1:A:53:PHE:CD2	1:A:53:PHE:C	2.92	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:LEU:HD13	1:B:151:MET:HE2	1.96	0.46
1:B:162:HIS:HE1	1:B:186:GLU:O	1.97	0.46
1:C:153:HIS:HA	1:C:154:PRO:C	2.40	0.46
1:C:194:ARG:NE	3:C:2029:HOH:O	2.34	0.46
1:D:62:ARG:H	1:D:92:ASN:HD21	1.62	0.46
1:A:153:HIS:HA	1:A:154:PRO:C	2.41	0.46
1:D:90:VAL:HG13	1:D:96:LEU:HD22	1.98	0.46
1:E:145:PHE:HA	1:E:148:LEU:HD23	1.96	0.46
1:A:32:ARG:HG2	1:A:32:ARG:HH11	1.81	0.45
1:A:105:ILE:HD11	1:B:105:ILE:HD11	1.96	0.45
1:A:66:ASP:HB2	1:A:67:PRO:CD	2.46	0.45
1:D:93:GLY:O	1:D:124:ILE:HD11	2.17	0.45
1:C:199:LEU:HD22	1:C:203:TYR:CZ	2.51	0.45
1:E:153:HIS:HA	1:E:154:PRO:C	2.42	0.45
1:B:199:LEU:HD22	1:B:203:TYR:CE2	2.51	0.45
1:D:105:ILE:HG23	1:E:59:ARG:HD3	1.97	0.45
1:D:58:TRP:CD1	1:D:59:ARG:HG3	2.52	0.44
1:E:214:ASP:OD1	1:E:214:ASP:C	2.59	0.44
1:B:88:LEU:CD2	1:B:139:CYS:SG	3.06	0.44
1:B:162:HIS:CG	1:B:188:MET:HE3	2.52	0.44
1:A:112:VAL:O	1:A:132:ILE:HA	2.18	0.44
1:C:77:LEU:CD2	1:C:102:LEU:HD23	2.48	0.44
1:B:31:ASP:C	1:B:32:ARG:HG3	2.42	0.44
1:E:187:ASP:O	1:E:190:PRO:HD2	2.18	0.44
1:D:102:LEU:CD2	1:D:106:MET:HE3	2.48	0.44
1:C:153:HIS:ND1	1:C:181:ASP:OD2	2.51	0.43
1:C:59:ARG:H	1:F:74:HIS:CE1	2.37	0.43
1:B:199:LEU:HD23	1:B:199:LEU:HA	1.87	0.43
1:C:92:ASN:H	1:C:92:ASN:HD22	1.66	0.43
1:A:185:ILE:HD12	1:A:189:ILE:HD11	2.01	0.43
1:B:65:LYS:HZ2	1:B:186:GLU:CD	2.27	0.43
1:B:101:ASP:O	1:B:105:ILE:HG13	2.18	0.43
1:B:149:ARG:HD3	1:B:149:ARG:HA	1.80	0.43
1:F:92:ASN:HD22	1:F:92:ASN:H	1.66	0.43
1:B:210:VAL:O	1:B:232:VAL:HG23	2.19	0.43
1:D:211:LEU:HD23	1:D:230:ARG:O	2.19	0.43
1:F:153:HIS:HB3	1:F:154:PRO:HA	2.01	0.43
1:D:62:ARG:N	1:D:92:ASN:HD21	2.17	0.42
1:F:169:MET:HG2	1:F:207:PHE:CE2	2.54	0.42
1:C:189:ILE:HB	1:C:190:PRO:HD3	2.00	0.42
1:A:18:LEU:HD21	2:A:301:SAH:SD	2.60	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:TRP:CH2	1:E:102:LEU:HD21	2.53	0.42
1:A:149:ARG:O	1:A:150:GLU:C	2.62	0.42
1:A:164:ASN:ND2	1:A:167:ASN:HD22	2.17	0.42
1:A:102:LEU:HG	1:A:106:MET:HE3	2.01	0.42
1:C:66:ASP:HB2	1:C:67:PRO:CD	2.50	0.42
1:C:211:LEU:O	1:F:38:LEU:HD22	2.19	0.42
1:D:145:PHE:O	1:D:146:GLU:CB	2.68	0.42
1:E:3:ASP:N	3:E:2001:HOH:O	2.53	0.42
1:A:148:LEU:C	1:A:148:LEU:HD13	2.44	0.42
1:E:36:TRP:CE2	3:E:2003:HOH:O	2.72	0.42
1:A:32:ARG:HG2	1:A:32:ARG:NH1	2.35	0.42
1:C:93:GLY:O	1:C:94:GLY:C	2.60	0.42
1:D:145:PHE:O	1:D:146:GLU:HB2	2.20	0.41
1:C:77:LEU:HD22	1:C:102:LEU:HD23	2.02	0.41
1:A:105:ILE:HD11	1:B:105:ILE:HD13	2.00	0.41
1:B:194:ARG:HH11	1:B:194:ARG:HG3	1.86	0.41
1:A:46:ARG:NE	1:B:226:ARG:NH1	2.68	0.41
1:C:38:LEU:HD13	1:F:212:SER:HA	2.02	0.41
1:C:65:LYS:HZ2	1:C:186:GLU:CD	2.29	0.41
1:C:116:ASP:O	1:C:136:GLN:HA	2.21	0.41
1:B:162:HIS:CE1	1:B:186:GLU:O	2.74	0.41
1:B:204:LEU:HD23	1:B:204:LEU:HA	1.89	0.41
1:F:61:LEU:HD22	1:F:123:GLN:HB2	2.01	0.41
1:E:52:ASP:O	1:E:52:ASP:CG	2.63	0.41
1:C:169:MET:HE2	1:C:211:LEU:CD1	2.50	0.41
1:E:161:ALA:HA	2:E:301:SAH:H5'2	2.03	0.40
1:B:164:ASN:HD22	1:B:164:ASN:HA	1.74	0.40
1:D:148:LEU:HD22	1:D:148:LEU:HA	1.94	0.40
1:F:92:ASN:HA	1:F:122:CYS:HA	2.03	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	224/236 (95%)	215 (96%)	8 (4%)	1 (0%)	30	48
1	B	230/236 (98%)	218 (95%)	9 (4%)	3 (1%)	9	20
1	C	225/236 (95%)	217 (96%)	6 (3%)	2 (1%)	14	27
1	D	188/236 (80%)	170 (90%)	15 (8%)	3 (2%)	7	16
1	E	228/236 (97%)	211 (92%)	17 (8%)	0	100	100
1	F	202/236 (86%)	188 (93%)	13 (6%)	1 (0%)	24	43
All	All	1297/1416 (92%)	1219 (94%)	68 (5%)	10 (1%)	16	31

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	146	GLU
1	A	150	GLU
1	C	14	LEU
1	D	187	ASP
1	F	138	ASP
1	B	10	GLN
1	B	150	GLU
1	B	225	ASP
1	C	12	LEU
1	D	55	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	198/207 (96%)	176 (89%)	22 (11%)	6	12
1	B	203/207 (98%)	168 (83%)	35 (17%)	2	3
1	C	197/207 (95%)	172 (87%)	25 (13%)	4	8
1	D	170/207 (82%)	141 (83%)	29 (17%)	2	3
1	E	202/207 (98%)	171 (85%)	31 (15%)	3	5
1	F	178/207 (86%)	153 (86%)	25 (14%)	3	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1148/1242 (92%)	981 (86%)	167 (14%)	3 6

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	29	LEU
1	A	30	THR
1	A	32	ARG
1	A	38	LEU
1	A	46	ARG
1	A	57	GLN
1	A	80	LEU
1	A	83	ARG
1	A	88	LEU
1	A	96	LEU
1	A	117	ARG
1	A	121	ARG
1	A	127	SER
1	A	141	ASP
1	A	148	LEU
1	A	150	GLU
1	A	169	MET
1	A	170	LYS
1	A	198	GLN
1	A	204	LEU
1	A	222	SER
1	B	6	ARG
1	B	12	LEU
1	B	14	LEU
1	B	28	VAL
1	B	29	LEU
1	B	30	THR
1	B	32	ARG
1	B	46	ARG
1	B	59	ARG
1	B	63	MET
1	B	64	LEU
1	B	80	LEU
1	B	83	ARG
1	B	88	LEU
1	B	102	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	104	LYS
1	B	105	ILE
1	B	111	GLN
1	B	121	ARG
1	B	134	LEU
1	B	136	GLN
1	B	138	ASP
1	B	141	ASP
1	B	146	GLU
1	B	148	LEU
1	B	149	ARG
1	B	150	GLU
1	B	151	MET
1	B	189	ILE
1	B	194	ARG
1	B	198	GLN
1	B	202	GLU
1	B	222	SER
1	B	231	ARG
1	B	232	VAL
1	C	12	LEU
1	C	14	LEU
1	C	29	LEU
1	C	30	THR
1	C	32	ARG
1	C	38	LEU
1	C	51	SER
1	C	52	ASP
1	C	64	LEU
1	C	77	LEU
1	C	80	LEU
1	C	95	SER
1	C	96	LEU
1	C	105	ILE
1	C	113	ILE
1	C	121	ARG
1	C	134	LEU
1	C	147	HIS
1	C	149	ARG
1	C	169	MET
1	C	179	GLU
1	C	198	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	204	LEU
1	C	221	SER
1	C	230	ARG
1	D	28	VAL
1	D	32	ARG
1	D	38	LEU
1	D	40	ARG
1	D	57	GLN
1	D	63	MET
1	D	77	LEU
1	D	80	LEU
1	D	87	GLU
1	D	88	LEU
1	D	96	LEU
1	D	102	LEU
1	D	105	ILE
1	D	119	LEU
1	D	130	GLU
1	D	134	LEU
1	D	136	GLN
1	D	138	ASP
1	D	139	CYS
1	D	148	LEU
1	D	160	ASN
1	D	176	LEU
1	D	178	GLU
1	D	186	GLU
1	D	188	MET
1	D	212	SER
1	D	221	SER
1	D	229	LEU
1	D	231	ARG
1	E	12	LEU
1	E	14	LEU
1	E	16	ARG
1	E	32	ARG
1	E	35	ASP
1	E	40	ARG
1	E	52	ASP
1	E	57	GLN
1	E	72	VAL
1	E	80	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	83	ARG
1	E	87	GLU
1	E	96	LEU
1	E	102	LEU
1	E	121	ARG
1	E	127	SER
1	E	128	ASP
1	E	129	MET
1	E	134	LEU
1	E	148	LEU
1	E	155	LEU
1	E	162	HIS
1	E	188	MET
1	E	189	ILE
1	E	194	ARG
1	E	202	GLU
1	E	208	ARG
1	E	221	SER
1	E	222	SER
1	E	231	ARG
1	E	232	VAL
1	F	29	LEU
1	F	38	LEU
1	F	40	ARG
1	F	43	GLU
1	F	51	SER
1	F	52	ASP
1	F	64	LEU
1	F	79	GLU
1	F	80	LEU
1	F	81	ARG
1	F	87	GLU
1	F	88	LEU
1	F	92	ASN
1	F	102	LEU
1	F	105	ILE
1	F	127	SER
1	F	133	THR
1	F	134	LEU
1	F	139	CYS
1	F	170	LYS
1	F	179	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	188	MET
1	F	208	ARG
1	F	210	VAL
1	F	232	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	25	HIS
1	A	135	HIS
1	A	160	ASN
1	A	162	HIS
1	A	164	ASN
1	B	2	ASN
1	B	111	GLN
1	B	153	HIS
1	B	162	HIS
1	B	164	ASN
1	C	92	ASN
1	C	111	GLN
1	C	135	HIS
1	C	160	ASN
1	C	162	HIS
1	D	57	GLN
1	D	92	ASN
1	D	136	GLN
1	D	162	HIS
1	E	8	ASN
1	E	74	HIS
1	E	131	ASN
1	E	160	ASN
1	E	164	ASN
1	E	167	ASN
1	F	25	HIS
1	F	153	HIS
1	F	164	ASN
1	F	175	HIS

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 ⓘ

5 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	A	301	-	27,28,28	1.13	5 (18%)	36,40,40	2.08	8 (22%)
2	SAH	B	301	-	27,28,28	1.09	3 (11%)	36,40,40	2.03	8 (22%)
2	SAH	D	301	-	27,28,28	1.10	4 (14%)	36,40,40	2.14	10 (27%)
2	SAH	E	301	-	27,28,28	1.09	5 (18%)	36,40,40	2.19	11 (30%)
2	SAH	C	301	-	27,28,28	1.08	3 (11%)	36,40,40	2.15	10 (27%)

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	A	301	-	-	4/15/31/31	0/3/3/3
2	SAH	B	301	-	-	3/15/31/31	0/3/3/3
2	SAH	D	301	-	-	0/15/31/31	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	E	301	-	-	7/15/31/31	0/3/3/3
2	SAH	C	301	-	-	3/15/31/31	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	SAH	C5-N7	-2.60	1.34	1.39
2	D	301	SAH	C2-N1	2.60	1.38	1.33
2	A	301	SAH	C2-N1	2.59	1.38	1.33
2	D	301	SAH	C2-N3	2.58	1.38	1.33
2	A	301	SAH	C2-N3	2.49	1.38	1.33
2	C	301	SAH	C2-N1	2.42	1.38	1.33
2	C	301	SAH	C8-N7	2.34	1.36	1.31
2	C	301	SAH	OXT-C	-2.27	1.23	1.30
2	B	301	SAH	C2-N1	2.25	1.37	1.33
2	A	301	SAH	OXT-C	-2.24	1.23	1.30
2	B	301	SAH	C2-N3	2.22	1.37	1.33
2	D	301	SAH	OXT-C	-2.22	1.23	1.30
2	E	301	SAH	C2-N1	2.16	1.37	1.33
2	E	301	SAH	C2-N3	2.11	1.37	1.33
2	A	301	SAH	C8-N7	2.10	1.35	1.31
2	E	301	SAH	C5-N7	-2.10	1.35	1.39
2	E	301	SAH	C8-N7	2.09	1.35	1.31
2	E	301	SAH	OXT-C	-2.08	1.24	1.30
2	D	301	SAH	C8-N7	2.06	1.35	1.31
2	A	301	SAH	C5-N7	-2.06	1.35	1.39

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	SAH	N3-C2-N1	-6.41	118.89	128.58
2	B	301	SAH	N3-C2-N1	-6.00	119.50	128.58
2	C	301	SAH	N3-C2-N1	-5.99	119.51	128.58
2	D	301	SAH	N3-C2-N1	-5.85	119.72	128.58
2	A	301	SAH	N3-C2-N1	-5.55	120.19	128.58
2	A	301	SAH	OXT-C-O	-4.83	113.12	124.08
2	B	301	SAH	C5-C4-N3	-4.79	120.12	126.72
2	D	301	SAH	C5-C4-N3	-4.66	120.30	126.72
2	A	301	SAH	C5-C4-N3	-4.59	120.40	126.72
2	C	301	SAH	N9-C8-N7	-4.20	107.97	113.94
2	E	301	SAH	C5-C4-N3	-4.20	120.94	126.72
2	D	301	SAH	N9-C8-N7	-4.17	108.02	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	SAH	OXT-C-O	-4.15	114.67	124.08
2	A	301	SAH	N9-C8-N7	-3.92	108.37	113.94
2	B	301	SAH	N9-C8-N7	-3.84	108.49	113.94
2	E	301	SAH	C5'-SD-CG	-3.79	91.01	102.26
2	E	301	SAH	OXT-C-O	-3.75	115.58	124.08
2	D	301	SAH	C2-N3-C4	3.69	120.84	111.83
2	E	301	SAH	N9-C8-N7	-3.68	108.71	113.94
2	A	301	SAH	C5-N7-C8	3.65	109.19	103.45
2	C	301	SAH	C5-C4-N3	-3.64	121.71	126.72
2	E	301	SAH	C2-N3-C4	3.63	120.70	111.83
2	D	301	SAH	C5-N7-C8	3.60	109.11	103.45
2	B	301	SAH	C2-N3-C4	3.59	120.59	111.83
2	C	301	SAH	OXT-C-O	-3.58	115.97	124.08
2	C	301	SAH	C5-N7-C8	3.54	109.02	103.45
2	B	301	SAH	C5-N7-C8	3.53	109.00	103.45
2	C	301	SAH	C5'-C4'-C3'	3.45	123.68	115.06
2	A	301	SAH	C2-N3-C4	3.44	120.23	111.83
2	C	301	SAH	C2-N3-C4	3.36	120.04	111.83
2	E	301	SAH	C5-N7-C8	3.19	108.47	103.45
2	D	301	SAH	N3-C4-N9	3.15	132.52	127.17
2	B	301	SAH	N3-C4-N9	3.11	132.45	127.17
2	C	301	SAH	C4-C5-N7	-2.94	107.22	110.58
2	A	301	SAH	N3-C4-N9	2.85	132.01	127.17
2	A	301	SAH	C4-C5-N7	-2.85	107.33	110.58
2	B	301	SAH	OXT-C-O	-2.82	117.69	124.08
2	D	301	SAH	C5'-SD-CG	-2.58	94.60	102.26
2	B	301	SAH	C4-C5-N7	-2.55	107.67	110.58
2	D	301	SAH	C4-C5-N7	-2.53	107.69	110.58
2	E	301	SAH	O4'-C4'-C5'	-2.45	102.52	108.83
2	E	301	SAH	N3-C4-N9	2.43	131.31	127.17
2	E	301	SAH	C4-C5-N7	-2.29	107.96	110.58
2	D	301	SAH	C4-N9-C8	2.15	108.00	105.74
2	C	301	SAH	O4'-C4'-C5'	-2.11	103.41	108.83
2	C	301	SAH	C4-N9-C8	2.11	107.95	105.74
2	E	301	SAH	O4'-C1'-N9	2.05	112.03	108.09

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	SAH	N-CA-CB-CG
2	E	301	SAH	N-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	301	SAH	C-CA-CB-CG
2	E	301	SAH	O4'-C4'-C5'-SD
2	E	301	SAH	C3'-C4'-C5'-SD
2	A	301	SAH	CA-CB-CG-SD
2	C	301	SAH	C-CA-CB-CG
2	B	301	SAH	OXT-C-CA-N
2	B	301	SAH	O-C-CA-N
2	A	301	SAH	O-C-CA-CB
2	E	301	SAH	C2'-C1'-N9-C8
2	B	301	SAH	CA-CB-CG-SD
2	A	301	SAH	OXT-C-CA-CB
2	C	301	SAH	CA-CB-CG-SD
2	E	301	SAH	O4'-C1'-N9-C8
2	A	301	SAH	CB-CG-SD-C5'
2	E	301	SAH	OXT-C-CA-N

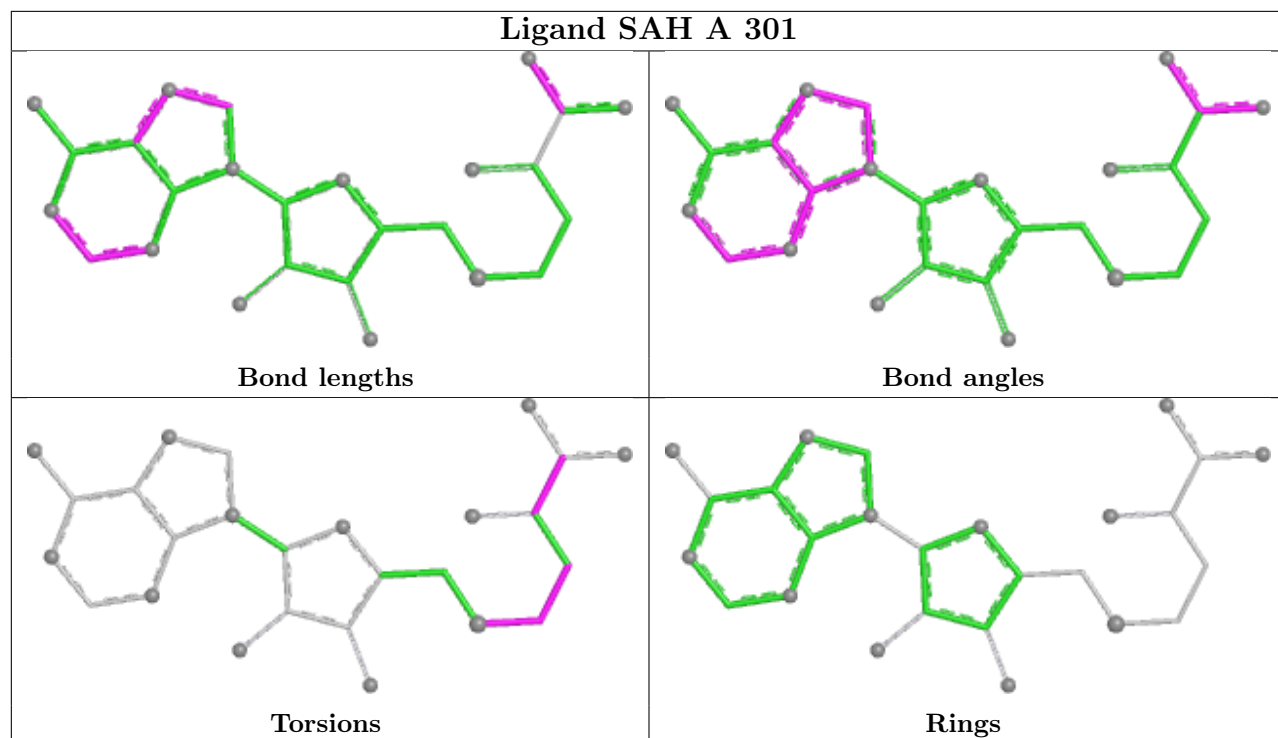
There are no ring outliers.

4 monomers are involved in 6 short contacts:

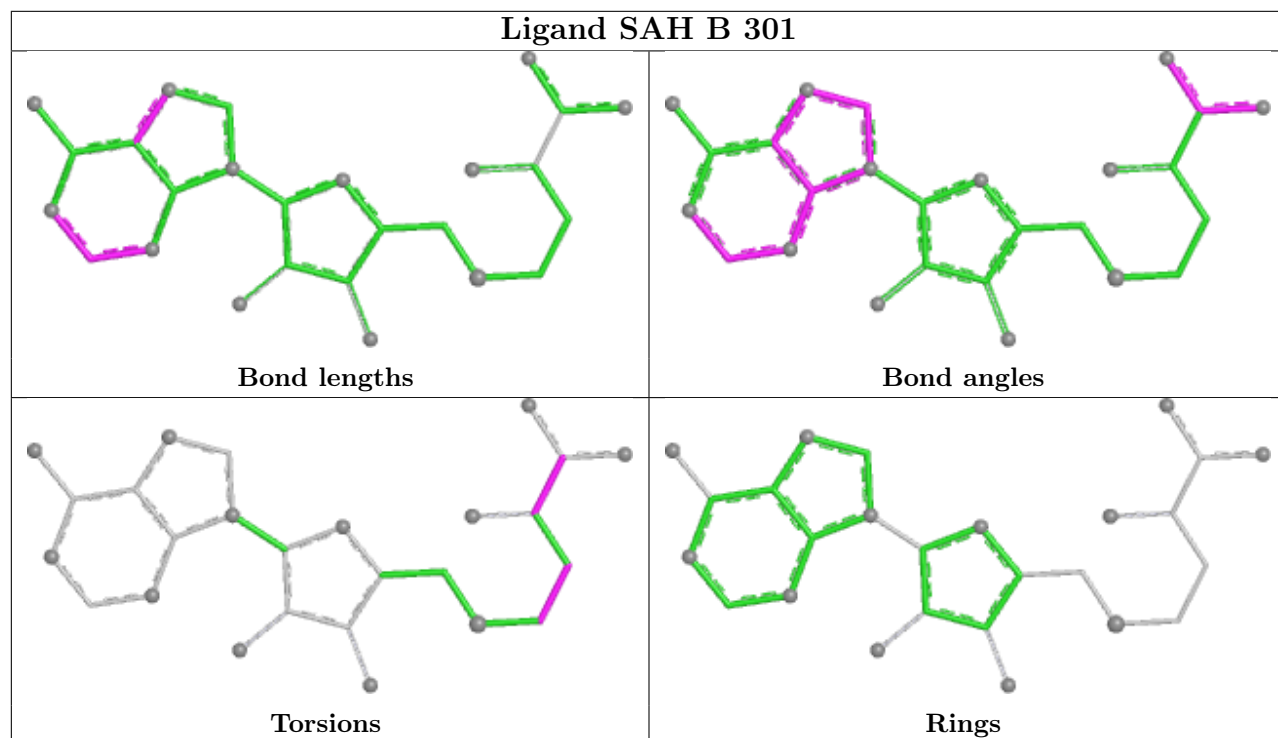
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	SAH	1	0
2	D	301	SAH	1	0
2	E	301	SAH	3	0
2	C	301	SAH	1	0

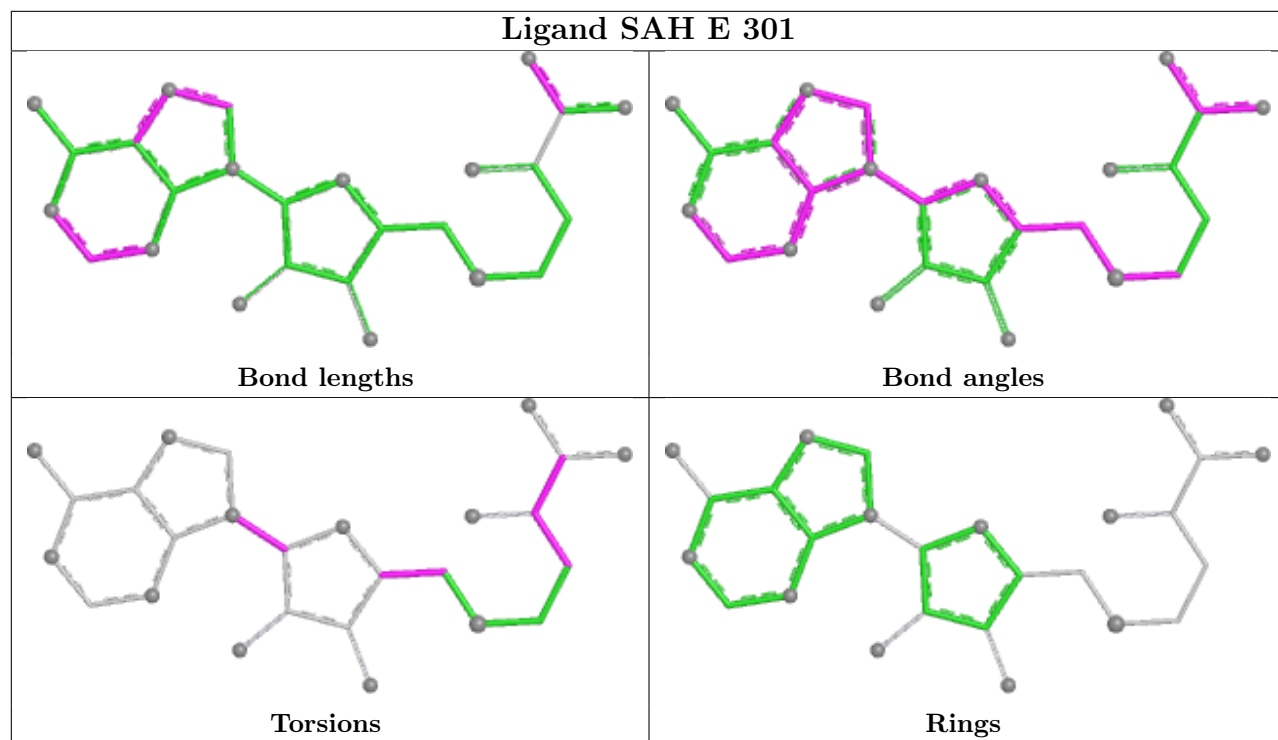
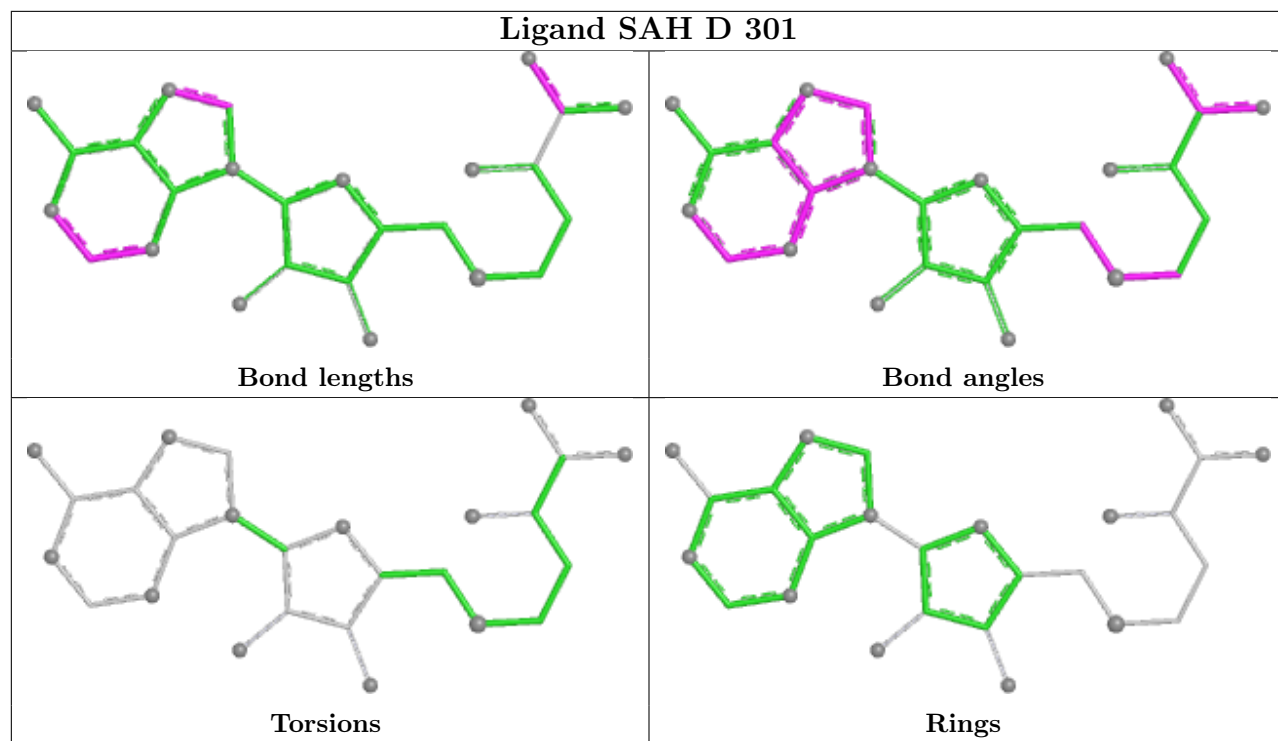
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

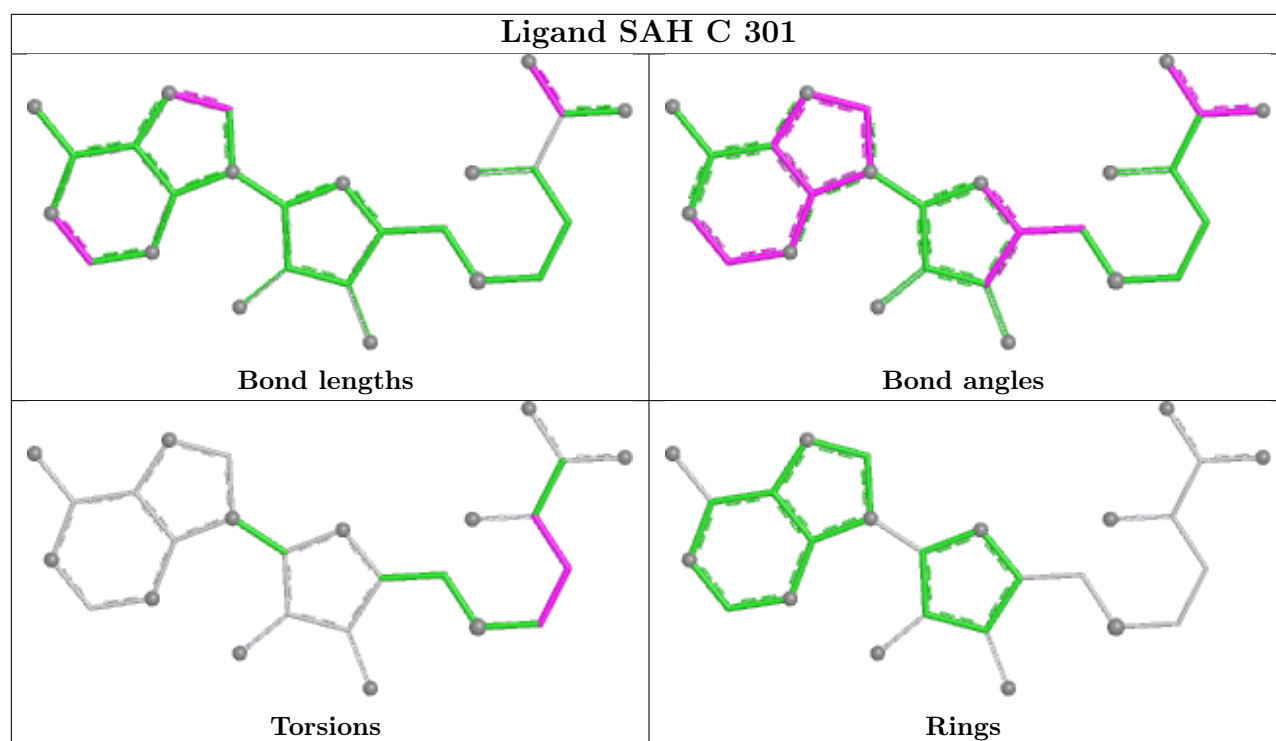
Ligand SAH A 301



Ligand SAH B 301







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.