



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 11:23 AM UTC

PDB ID : 5GM1 / pdb_00005gm1
Title : Crystal structure of methyltransferase TleD complexed with SAH
Authors : Yu, F.; Li, M.J.; Xu, C.Y.; Zhou, H.; Sun, B.; Wang, Z.J.; Xu, Q.; Xie, M.Y.;
Zuo, G.; Huang, P.; Wang, Q.S.; He, J.H.
Deposited on : 2016-07-12
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:

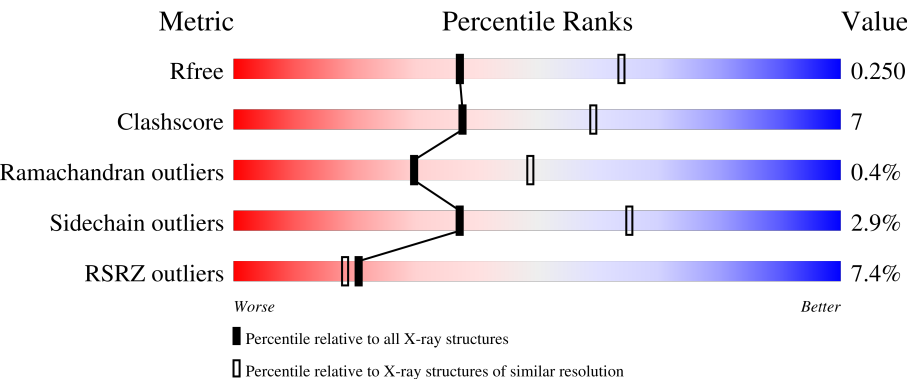
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 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.



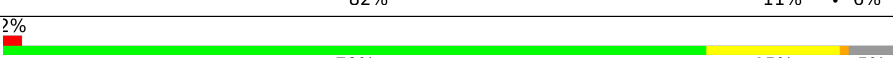
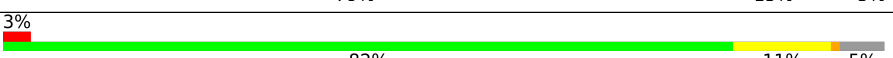
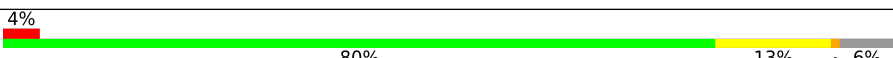
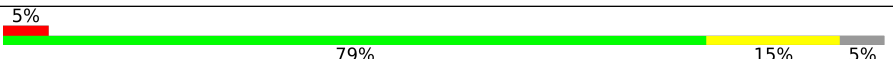
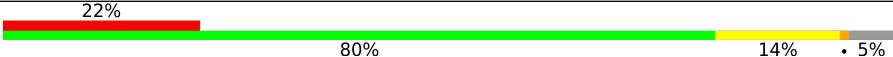
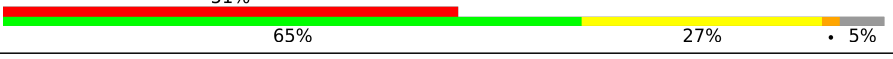
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. 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	297	% 79%14%• 5%
1	B	297	79%14%• 6%
1	C	297	2% 75%17%• 6%
1	D	297	% 80%13%• 6%
1	E	297	80%13%• 6%

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Mol	Chain	Length	Quality of chain
1	F	297	 80% 14% 6%
1	G	297	 5% 77% 15% 6%
1	H	297	 12% 75% 17% 6%
1	I	297	 82% 11% 6%
1	J	297	 2% 79% 15% 5%
1	K	297	 3% 82% 11% 5%
1	L	297	 4% 80% 13% 6%
1	M	297	 5% 79% 15% 5%
1	N	297	 22% 80% 14% 5%
1	O	297	 2% 77% 16% 6%
1	P	297	 0% 80% 13% 6%
1	Q	297	 13% 81% 13% 5%
1	R	297	 51% 65% 27% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 40182 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 O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	2	0
			2184	1384	371	417	12			
1	B	280	Total	C	N	O	S	0	1	0
			2164	1372	367	414	11			
1	C	280	Total	C	N	O	S	0	0	0
			2157	1370	365	411	11			
1	D	280	Total	C	N	O	S	0	1	0
			2169	1375	370	413	11			
1	E	279	Total	C	N	O	S	0	0	0
			2149	1364	364	410	11			
1	F	280	Total	C	N	O	S	0	0	0
			2158	1369	366	412	11			
1	G	280	Total	C	N	O	S	0	0	0
			2158	1369	366	412	11			
1	H	279	Total	C	N	O	S	0	0	0
			2149	1364	364	410	11			
1	I	280	Total	C	N	O	S	3	1	0
			2169	1375	370	413	11			
1	J	281	Total	C	N	O	S	0	0	0
			2167	1374	368	414	11			
1	K	281	Total	C	N	O	S	0	0	0
			2166	1375	367	413	11			
1	L	280	Total	C	N	O	S	0	0	0
			2158	1369	366	412	11			
1	M	281	Total	C	N	O	S	0	2	0
			2184	1384	371	417	12			
1	N	281	Total	C	N	O	S	0	2	0
			2184	1384	371	417	12			
1	O	280	Total	C	N	O	S	0	0	0
			2158	1369	366	412	11			
1	P	280	Total	C	N	O	S	0	0	0
			2158	1369	366	412	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	281	Total	C	N	O	S	0	2	0
			2184	1384	371	417	12			
1	R	281	Total	C	N	O	S	0	1	0
			2176	1379	370	416	11			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	LEU	-	expression tag	UNP A0A077K7L1
A	291	GLU	-	expression tag	UNP A0A077K7L1
A	292	HIS	-	expression tag	UNP A0A077K7L1
A	293	HIS	-	expression tag	UNP A0A077K7L1
A	294	HIS	-	expression tag	UNP A0A077K7L1
A	295	HIS	-	expression tag	UNP A0A077K7L1
A	296	HIS	-	expression tag	UNP A0A077K7L1
A	297	HIS	-	expression tag	UNP A0A077K7L1
B	290	LEU	-	expression tag	UNP A0A077K7L1
B	291	GLU	-	expression tag	UNP A0A077K7L1
B	292	HIS	-	expression tag	UNP A0A077K7L1
B	293	HIS	-	expression tag	UNP A0A077K7L1
B	294	HIS	-	expression tag	UNP A0A077K7L1
B	295	HIS	-	expression tag	UNP A0A077K7L1
B	296	HIS	-	expression tag	UNP A0A077K7L1
B	297	HIS	-	expression tag	UNP A0A077K7L1
C	290	LEU	-	expression tag	UNP A0A077K7L1
C	291	GLU	-	expression tag	UNP A0A077K7L1
C	292	HIS	-	expression tag	UNP A0A077K7L1
C	293	HIS	-	expression tag	UNP A0A077K7L1
C	294	HIS	-	expression tag	UNP A0A077K7L1
C	295	HIS	-	expression tag	UNP A0A077K7L1
C	296	HIS	-	expression tag	UNP A0A077K7L1
C	297	HIS	-	expression tag	UNP A0A077K7L1
D	290	LEU	-	expression tag	UNP A0A077K7L1
D	291	GLU	-	expression tag	UNP A0A077K7L1
D	292	HIS	-	expression tag	UNP A0A077K7L1
D	293	HIS	-	expression tag	UNP A0A077K7L1
D	294	HIS	-	expression tag	UNP A0A077K7L1
D	295	HIS	-	expression tag	UNP A0A077K7L1
D	296	HIS	-	expression tag	UNP A0A077K7L1
D	297	HIS	-	expression tag	UNP A0A077K7L1
E	290	LEU	-	expression tag	UNP A0A077K7L1
E	291	GLU	-	expression tag	UNP A0A077K7L1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	292	HIS	-	expression tag	UNP A0A077K7L1
E	293	HIS	-	expression tag	UNP A0A077K7L1
E	294	HIS	-	expression tag	UNP A0A077K7L1
E	295	HIS	-	expression tag	UNP A0A077K7L1
E	296	HIS	-	expression tag	UNP A0A077K7L1
E	297	HIS	-	expression tag	UNP A0A077K7L1
F	290	LEU	-	expression tag	UNP A0A077K7L1
F	291	GLU	-	expression tag	UNP A0A077K7L1
F	292	HIS	-	expression tag	UNP A0A077K7L1
F	293	HIS	-	expression tag	UNP A0A077K7L1
F	294	HIS	-	expression tag	UNP A0A077K7L1
F	295	HIS	-	expression tag	UNP A0A077K7L1
F	296	HIS	-	expression tag	UNP A0A077K7L1
F	297	HIS	-	expression tag	UNP A0A077K7L1
G	290	LEU	-	expression tag	UNP A0A077K7L1
G	291	GLU	-	expression tag	UNP A0A077K7L1
G	292	HIS	-	expression tag	UNP A0A077K7L1
G	293	HIS	-	expression tag	UNP A0A077K7L1
G	294	HIS	-	expression tag	UNP A0A077K7L1
G	295	HIS	-	expression tag	UNP A0A077K7L1
G	296	HIS	-	expression tag	UNP A0A077K7L1
G	297	HIS	-	expression tag	UNP A0A077K7L1
H	290	LEU	-	expression tag	UNP A0A077K7L1
H	291	GLU	-	expression tag	UNP A0A077K7L1
H	292	HIS	-	expression tag	UNP A0A077K7L1
H	293	HIS	-	expression tag	UNP A0A077K7L1
H	294	HIS	-	expression tag	UNP A0A077K7L1
H	295	HIS	-	expression tag	UNP A0A077K7L1
H	296	HIS	-	expression tag	UNP A0A077K7L1
H	297	HIS	-	expression tag	UNP A0A077K7L1
I	290	LEU	-	expression tag	UNP A0A077K7L1
I	291	GLU	-	expression tag	UNP A0A077K7L1
I	292	HIS	-	expression tag	UNP A0A077K7L1
I	293	HIS	-	expression tag	UNP A0A077K7L1
I	294	HIS	-	expression tag	UNP A0A077K7L1
I	295	HIS	-	expression tag	UNP A0A077K7L1
I	296	HIS	-	expression tag	UNP A0A077K7L1
I	297	HIS	-	expression tag	UNP A0A077K7L1
J	290	LEU	-	expression tag	UNP A0A077K7L1
J	291	GLU	-	expression tag	UNP A0A077K7L1
J	292	HIS	-	expression tag	UNP A0A077K7L1
J	293	HIS	-	expression tag	UNP A0A077K7L1

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Chain	Residue	Modelled	Actual	Comment	Reference
J	294	HIS	-	expression tag	UNP A0A077K7L1
J	295	HIS	-	expression tag	UNP A0A077K7L1
J	296	HIS	-	expression tag	UNP A0A077K7L1
J	297	HIS	-	expression tag	UNP A0A077K7L1
K	290	LEU	-	expression tag	UNP A0A077K7L1
K	291	GLU	-	expression tag	UNP A0A077K7L1
K	292	HIS	-	expression tag	UNP A0A077K7L1
K	293	HIS	-	expression tag	UNP A0A077K7L1
K	294	HIS	-	expression tag	UNP A0A077K7L1
K	295	HIS	-	expression tag	UNP A0A077K7L1
K	296	HIS	-	expression tag	UNP A0A077K7L1
K	297	HIS	-	expression tag	UNP A0A077K7L1
L	290	LEU	-	expression tag	UNP A0A077K7L1
L	291	GLU	-	expression tag	UNP A0A077K7L1
L	292	HIS	-	expression tag	UNP A0A077K7L1
L	293	HIS	-	expression tag	UNP A0A077K7L1
L	294	HIS	-	expression tag	UNP A0A077K7L1
L	295	HIS	-	expression tag	UNP A0A077K7L1
L	296	HIS	-	expression tag	UNP A0A077K7L1
L	297	HIS	-	expression tag	UNP A0A077K7L1
M	290	LEU	-	expression tag	UNP A0A077K7L1
M	291	GLU	-	expression tag	UNP A0A077K7L1
M	292	HIS	-	expression tag	UNP A0A077K7L1
M	293	HIS	-	expression tag	UNP A0A077K7L1
M	294	HIS	-	expression tag	UNP A0A077K7L1
M	295	HIS	-	expression tag	UNP A0A077K7L1
M	296	HIS	-	expression tag	UNP A0A077K7L1
M	297	HIS	-	expression tag	UNP A0A077K7L1
N	290	LEU	-	expression tag	UNP A0A077K7L1
N	291	GLU	-	expression tag	UNP A0A077K7L1
N	292	HIS	-	expression tag	UNP A0A077K7L1
N	293	HIS	-	expression tag	UNP A0A077K7L1
N	294	HIS	-	expression tag	UNP A0A077K7L1
N	295	HIS	-	expression tag	UNP A0A077K7L1
N	296	HIS	-	expression tag	UNP A0A077K7L1
N	297	HIS	-	expression tag	UNP A0A077K7L1
O	290	LEU	-	expression tag	UNP A0A077K7L1
O	291	GLU	-	expression tag	UNP A0A077K7L1
O	292	HIS	-	expression tag	UNP A0A077K7L1
O	293	HIS	-	expression tag	UNP A0A077K7L1
O	294	HIS	-	expression tag	UNP A0A077K7L1
O	295	HIS	-	expression tag	UNP A0A077K7L1

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Chain	Residue	Modelled	Actual	Comment	Reference
O	296	HIS	-	expression tag	UNP A0A077K7L1
O	297	HIS	-	expression tag	UNP A0A077K7L1
P	290	LEU	-	expression tag	UNP A0A077K7L1
P	291	GLU	-	expression tag	UNP A0A077K7L1
P	292	HIS	-	expression tag	UNP A0A077K7L1
P	293	HIS	-	expression tag	UNP A0A077K7L1
P	294	HIS	-	expression tag	UNP A0A077K7L1
P	295	HIS	-	expression tag	UNP A0A077K7L1
P	296	HIS	-	expression tag	UNP A0A077K7L1
P	297	HIS	-	expression tag	UNP A0A077K7L1
Q	290	LEU	-	expression tag	UNP A0A077K7L1
Q	291	GLU	-	expression tag	UNP A0A077K7L1
Q	292	HIS	-	expression tag	UNP A0A077K7L1
Q	293	HIS	-	expression tag	UNP A0A077K7L1
Q	294	HIS	-	expression tag	UNP A0A077K7L1
Q	295	HIS	-	expression tag	UNP A0A077K7L1
Q	296	HIS	-	expression tag	UNP A0A077K7L1
Q	297	HIS	-	expression tag	UNP A0A077K7L1
R	290	LEU	-	expression tag	UNP A0A077K7L1
R	291	GLU	-	expression tag	UNP A0A077K7L1
R	292	HIS	-	expression tag	UNP A0A077K7L1
R	293	HIS	-	expression tag	UNP A0A077K7L1
R	294	HIS	-	expression tag	UNP A0A077K7L1
R	295	HIS	-	expression tag	UNP A0A077K7L1
R	296	HIS	-	expression tag	UNP A0A077K7L1
R	297	HIS	-	expression tag	UNP A0A077K7L1

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	N	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	O	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	P	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	Q	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	R	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	81	Total	O	0	0
			81	81		
3	B	90	Total	O	0	0
			90	90		
3	C	51	Total	O	0	0
			51	51		
3	D	35	Total	O	0	0
			35	35		
3	E	48	Total	O	0	0
			48	48		
3	F	72	Total	O	0	0
			72	72		
3	G	22	Total	O	0	0
			22	22		
3	H	19	Total	O	0	0
			19	19		
3	I	46	Total	O	0	0
			46	46		
3	J	21	Total	O	0	0
			21	21		
3	K	11	Total	O	0	0
			11	11		
3	L	21	Total	O	0	0
			21	21		
3	M	28	Total	O	0	0
			28	28		
3	N	19	Total	O	0	0
			19	19		

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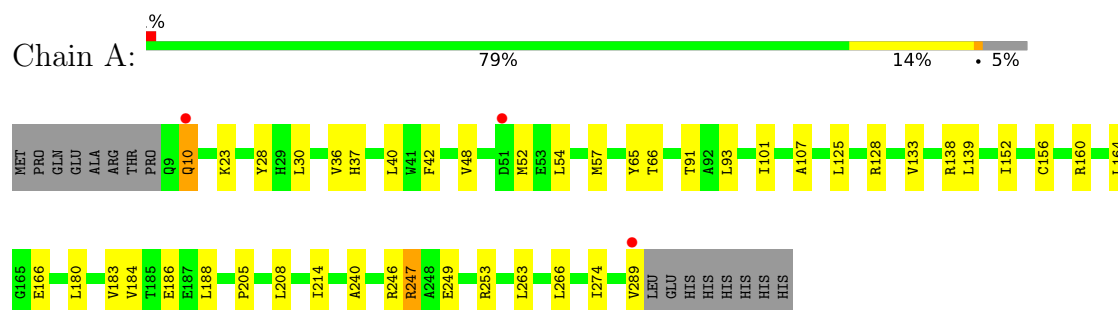
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	38	Total 38	O 38	0	0
3	P	25	Total 25	O 25	0	0
3	Q	24	Total 24	O 24	0	0
3	R	45	Total 45	O 45	0	0

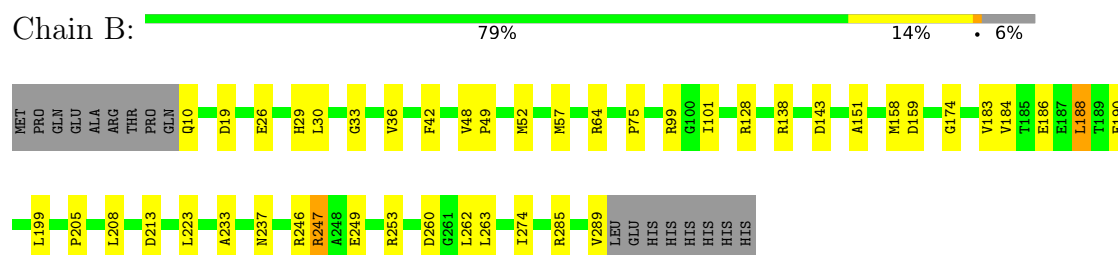
3 Residue-property plots [i](#)

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 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.

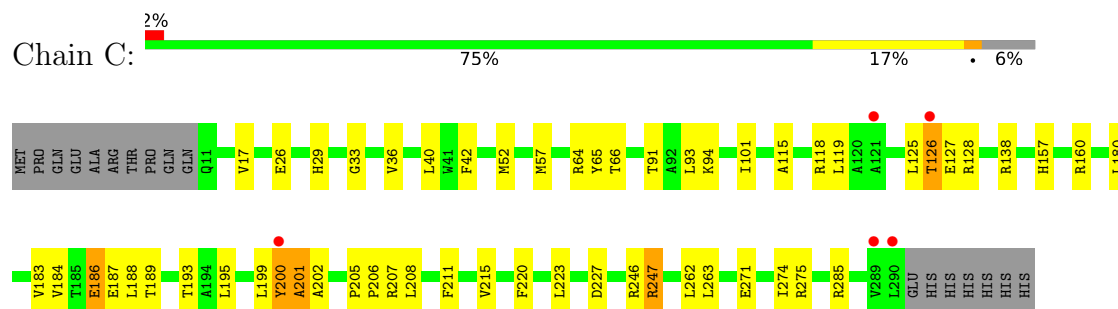
• Molecule 1: O-methyltransferase



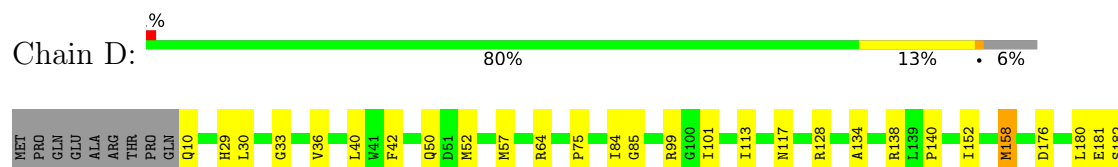
• Molecule 1: O-methyltransferase



• Molecule 1: O-methyltransferase



• Molecule 1: O-methyltransferase





• Molecule 1: O-methyltransferase

Chain E: 80% 13% • 6%



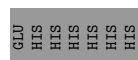
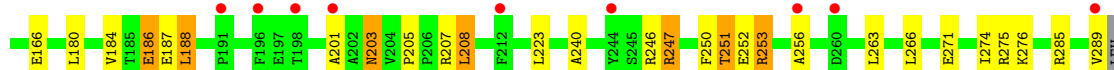
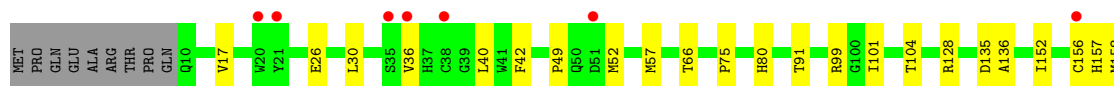
• Molecule 1: O-methyltransferase

Chain F: 80% 14% 6%



• Molecule 1: O-methyltransferase

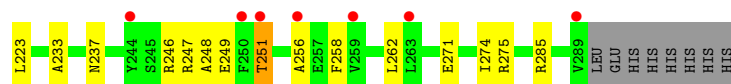
Chain G: 5% 77% 15% • 6%



• Molecule 1: O-methyltransferase

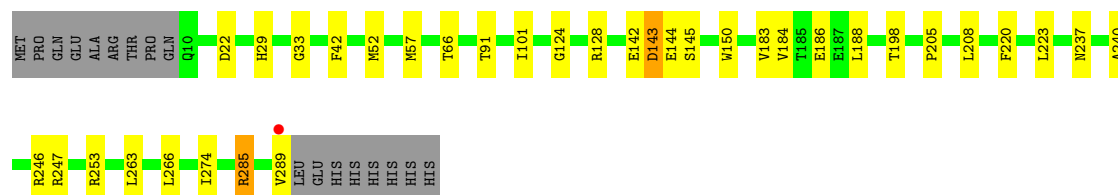
Chain H: 12% 75% 17% • 6%





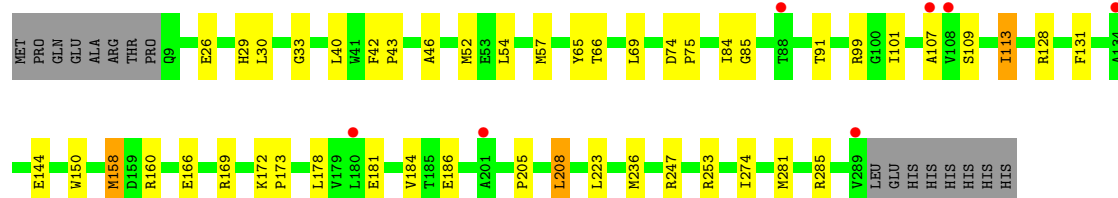
• Molecule 1: O-methyltransferase

Chain I: 82% 11% • 6%



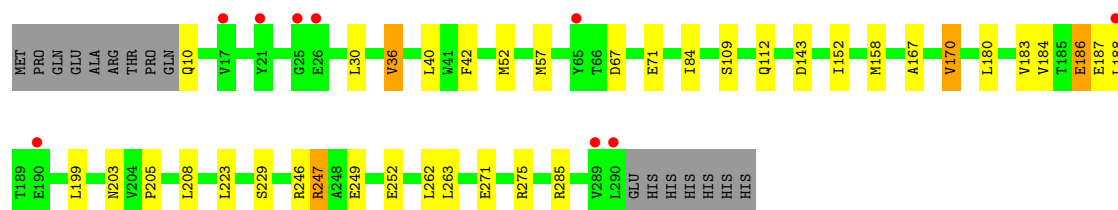
• Molecule 1: O-methyltransferase

Chain J: 79% 15% • 5%



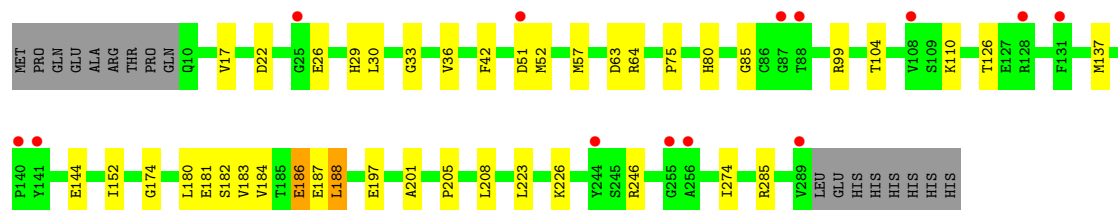
• Molecule 1: O-methyltransferase

Chain K: 82% 11% • 5%



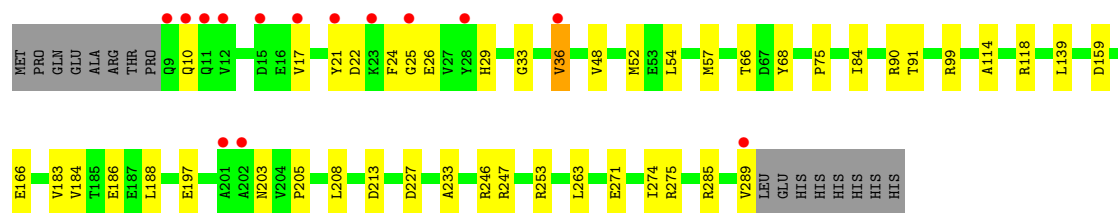
• Molecule 1: O-methyltransferase

Chain L: 80% 13% • 6%

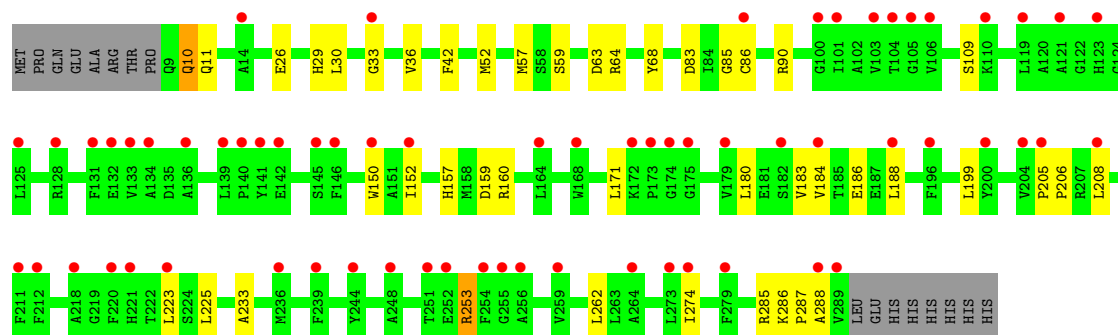
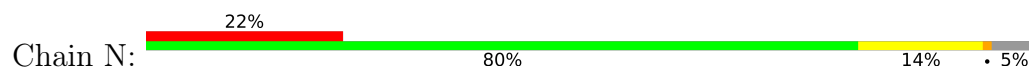


• Molecule 1: O-methyltransferase

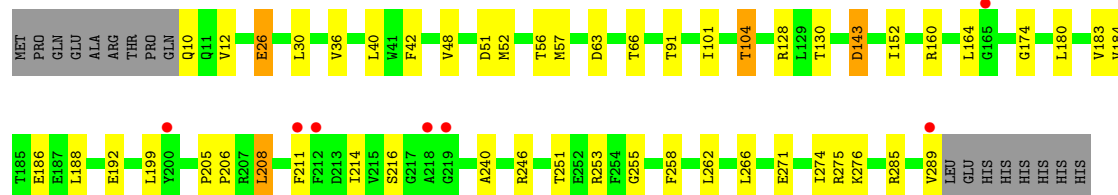
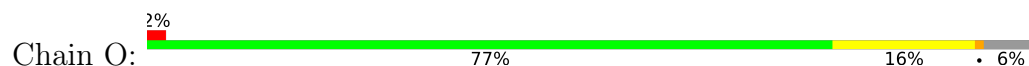
Chain M: 79% 15% • 5%



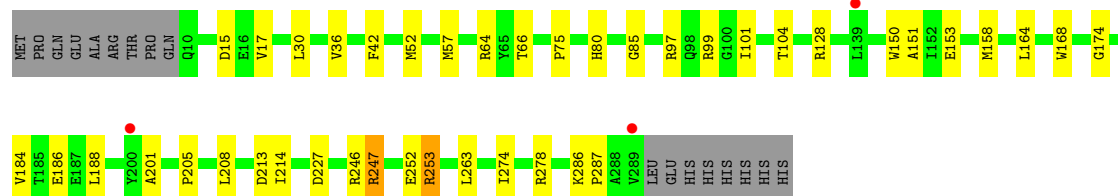
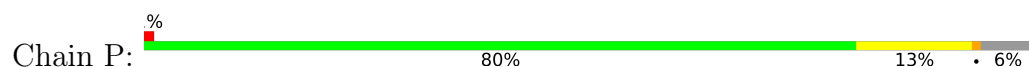
• Molecule 1: O-methyltransferase



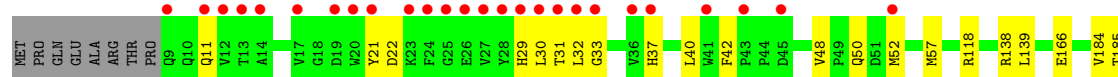
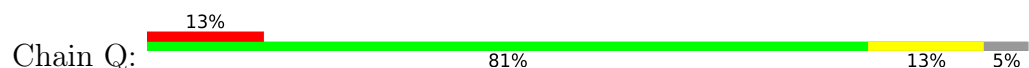
• Molecule 1: O-methyltransferase



• Molecule 1: O-methyltransferase

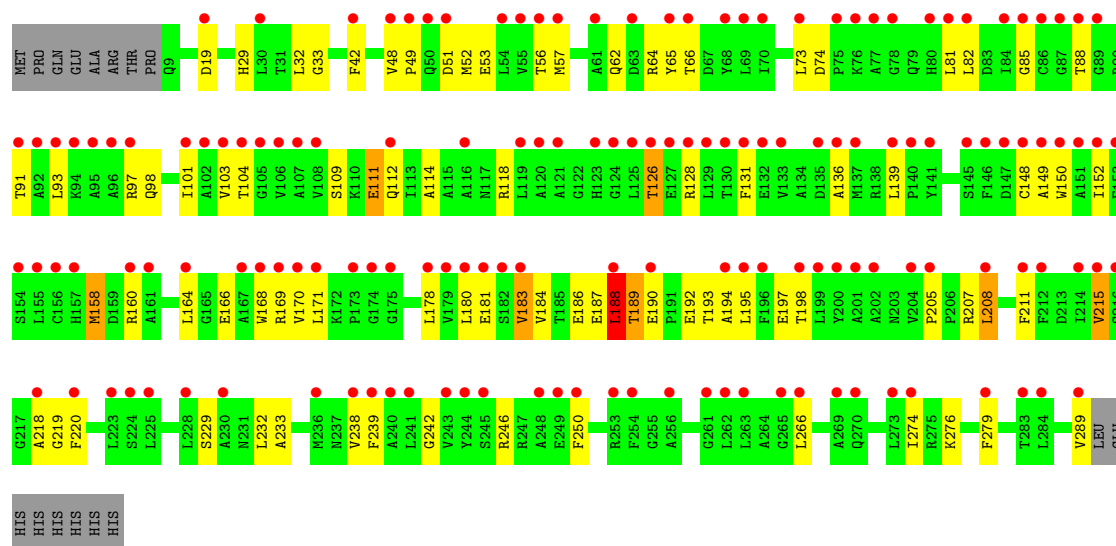


• Molecule 1: O-methyltransferase





• Molecule 1: O-methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	259.62Å 152.90Å 154.79Å 90.00° 93.33° 90.00°	Depositor
Resolution (Å)	102.27 – 2.50 102.27 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (102.27-2.50) 99.0 (102.27-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.52Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.207 , 0.248 0.211 , 0.250	Depositor DCC
R_{free} test set	10316 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 67.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	40182	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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	0.18	0/2229	0.38	0/3024
1	B	0.17	0/2209	0.36	0/2998
1	C	0.16	0/2202	0.35	0/2989
1	D	0.16	0/2214	0.33	0/3004
1	E	0.16	0/2194	0.36	0/2978
1	F	0.17	0/2203	0.36	0/2990
1	G	0.13	0/2203	0.32	0/2990
1	H	0.15	0/2194	0.31	0/2978
1	I	0.16	0/2214	0.36	0/3004
1	J	0.13	0/2212	0.31	0/3002
1	K	0.13	0/2211	0.31	0/3001
1	L	0.13	0/2203	0.30	0/2990
1	M	0.15	0/2229	0.33	0/3024
1	N	0.14	0/2229	0.31	0/3024
1	O	0.15	0/2203	0.35	0/2990
1	P	0.14	0/2203	0.33	0/2990
1	Q	0.18	0/2229	0.35	0/3024
1	R	0.16	0/2221	0.35	0/3014
All	All	0.15	0/39802	0.34	0/54014

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	2184	0	2139	31	0
1	B	2164	0	2120	33	0
1	C	2157	0	2119	34	0
1	D	2169	0	2128	27	0
1	E	2149	0	2108	27	0
1	F	2158	0	2116	31	0
1	G	2158	0	2116	33	0
1	H	2149	0	2108	43	0
1	I	2169	0	2128	24	0
1	J	2167	0	2124	33	0
1	K	2166	0	2127	27	0
1	L	2158	0	2116	28	0
1	M	2184	0	2139	39	0
1	N	2184	0	2139	38	0
1	O	2158	0	2116	34	0
1	P	2158	0	2116	33	0
1	Q	2184	0	2139	38	0
1	R	2176	0	2131	82	1
2	A	26	0	19	1	0
2	B	52	0	38	4	0
2	C	26	0	19	1	0
2	D	26	0	19	3	0
2	E	26	0	19	1	0
2	F	26	0	19	1	0
2	G	26	0	19	1	0
2	H	26	0	19	1	0
2	I	26	0	19	0	0
2	J	26	0	19	3	0
2	K	26	0	19	3	0
2	L	26	0	19	4	0
2	M	26	0	19	1	0
2	N	26	0	19	4	0
2	O	26	0	19	2	0
2	P	26	0	19	3	0
2	Q	26	0	19	0	0
2	R	26	0	19	1	0
3	A	81	0	0	2	0
3	B	90	0	0	8	0
3	C	51	0	0	7	0
3	D	35	0	0	3	0
3	E	48	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	72	0	0	6	0
3	G	22	0	0	6	0
3	H	19	0	0	10	0
3	I	46	0	0	8	0
3	J	21	0	0	3	0
3	K	11	0	0	5	0
3	L	21	0	0	7	0
3	M	28	0	0	10	0
3	N	19	0	0	7	0
3	O	38	0	0	4	0
3	P	25	0	0	13	0
3	Q	24	0	0	12	0
3	R	45	0	0	27	0
All	All	40182	0	38590	548	1

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 7.

All (548) 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)
3:G:417:HOH:O	2:H:301:SAH:SD	1.97	1.23
1:F:22:ASP:O	3:F:401:HOH:O	1.67	1.09
1:R:57:MET:SD	3:R:442:HOH:O	2.14	1.03
1:N:86:CYS:SG	3:N:411:HOH:O	2.22	0.98
1:G:166:GLU:OE1	3:G:401:HOH:O	1.82	0.95
1:L:144:GLU:OE2	3:L:401:HOH:O	1.84	0.95
1:P:213:ASP:OD1	3:P:401:HOH:O	1.89	0.91
1:D:138:ARG:NH1	3:D:401:HOH:O	2.04	0.90
2:P:301:SAH:SD	3:P:425:HOH:O	2.30	0.89
1:R:238:VAL:O	3:R:401:HOH:O	1.90	0.88
1:P:151:ALA:O	3:P:402:HOH:O	1.91	0.88
1:O:63:ASP:OD2	3:O:401:HOH:O	1.89	0.87
1:M:24:PHE:N	3:M:401:HOH:O	2.06	0.86
1:R:148:CYS:SG	3:R:434:HOH:O	2.35	0.85
3:M:423:HOH:O	2:N:301:SAH:SD	2.35	0.84
1:R:19:ASP:OD1	3:R:402:HOH:O	1.95	0.84
3:Q:421:HOH:O	1:R:57:MET:SD	2.36	0.83
1:M:227:ASP:O	3:M:403:HOH:O	1.97	0.83
1:I:144:GLU:OE2	3:I:401:HOH:O	1.95	0.82
1:H:223:LEU:HD11	1:H:285:ARG:HE	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:74:ASP:OD1	3:R:403:HOH:O	1.96	0.82
1:M:57:MET:SD	3:N:414:HOH:O	2.38	0.82
1:M:197:GLU:O	3:M:404:HOH:O	1.97	0.81
1:P:52:MET:O	3:P:403:HOH:O	2.00	0.79
1:O:216:SER:OG	3:O:402:HOH:O	2.00	0.78
1:F:184:VAL:HG13	1:F:205:PRO:HG2	1.66	0.78
1:R:48:VAL:O	3:R:404:HOH:O	2.02	0.78
1:K:170:VAL:N	3:K:401:HOH:O	2.16	0.77
1:M:184:VAL:HG13	1:M:205:PRO:HG2	1.67	0.77
1:K:184:VAL:HG13	1:K:205:PRO:HG2	1.67	0.77
1:G:184:VAL:HG13	1:G:205:PRO:HG2	1.68	0.76
1:O:184:VAL:HG13	1:O:205:PRO:HG2	1.68	0.75
1:N:64:ARG:O	3:N:401:HOH:O	2.05	0.75
1:L:184:VAL:HG13	1:L:205:PRO:HG2	1.68	0.75
1:F:63:ASP:OD2	3:F:403:HOH:O	2.05	0.74
1:I:184:VAL:HG13	1:I:205:PRO:HG2	1.68	0.73
1:J:40:LEU:O	3:J:401:HOH:O	2.05	0.73
1:E:251:THR:HG22	1:E:256:ALA:HA	1.68	0.73
1:R:62:GLN:OE1	3:R:405:HOH:O	2.05	0.73
1:I:253:ARG:NH1	3:I:404:HOH:O	2.20	0.73
1:C:125:LEU:O	1:C:127:GLU:N	2.20	0.72
1:D:249:GLU:N	3:D:402:HOH:O	2.15	0.72
1:H:86:CYS:SG	3:H:402:HOH:O	2.46	0.72
1:J:184:VAL:HG13	1:J:205:PRO:HG2	1.71	0.72
1:O:101:ILE:O	1:O:128:ARG:NH1	2.23	0.72
1:E:184:VAL:HG13	1:E:205:PRO:HG2	1.72	0.71
1:N:287:PRO:O	3:N:402:HOH:O	2.08	0.71
1:P:184:VAL:HG13	1:P:205:PRO:HG2	1.72	0.71
1:I:124:GLY:O	3:I:402:HOH:O	2.06	0.71
1:O:285:ARG:HH21	1:Q:48:VAL:HB	1.55	0.71
1:N:68:TYR:N	3:N:401:HOH:O	2.24	0.71
1:B:247:ARG:HG3	1:B:263:LEU:HD11	1.72	0.71
1:E:64:ARG:HG2	1:F:40:LEU:HD23	1.72	0.71
1:A:23:LYS:O	1:Q:138:ARG:NH1	2.24	0.71
1:H:248:ALA:N	3:H:401:HOH:O	2.24	0.71
1:Q:185:THR:OG1	3:Q:403:HOH:O	2.10	0.70
1:B:19:ASP:OD1	3:B:401:HOH:O	2.09	0.70
1:G:52:MET:HB2	1:H:274:ILE:HG23	1.73	0.70
1:Q:252:GLU:O	3:Q:402:HOH:O	2.09	0.69
1:P:227:ASP:OD1	3:P:405:HOH:O	2.10	0.69
1:Q:274:ILE:HG23	1:R:52:MET:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:GLU:O	1:C:207:ARG:NH2	2.25	0.69
1:R:82:LEU:HA	3:R:410:HOH:O	1.91	0.69
1:H:184:VAL:HG13	1:H:205:PRO:HG2	1.73	0.69
1:P:66:THR:OG1	3:P:406:HOH:O	2.10	0.68
1:L:63:ASP:OD1	3:L:403:HOH:O	2.11	0.68
1:R:49:PRO:O	3:R:407:HOH:O	2.11	0.68
1:G:275:ARG:N	3:G:404:HOH:O	2.25	0.68
1:M:10:GLN:OE1	3:M:405:HOH:O	2.10	0.68
1:G:247:ARG:HG3	1:G:263:LEU:HD11	1.74	0.68
1:E:247:ARG:HG3	1:E:263:LEU:HD11	1.74	0.68
1:C:247:ARG:HG3	1:C:263:LEU:HD11	1.76	0.68
1:N:288:ALA:N	3:N:404:HOH:O	2.20	0.68
1:F:253:ARG:NH1	3:F:406:HOH:O	2.27	0.67
1:M:274:ILE:HG23	1:N:52[B]:MET:HB2	1.77	0.67
1:C:220:PHE:O	3:C:402:HOH:O	2.12	0.67
1:R:97:ARG:O	3:R:408:HOH:O	2.11	0.67
1:R:211:PHE:O	3:R:409:HOH:O	2.13	0.67
1:B:75:PRO:HG2	1:B:99:ARG:HG3	1.77	0.67
1:G:80:HIS:HE2	1:G:104:THR:HG1	1.41	0.67
1:A:30:LEU:O	1:B:246:ARG:NH2	2.27	0.67
1:K:36:VAL:HB	2:L:301:SAH:HB2	1.77	0.67
1:Q:31:THR:OG1	3:Q:404:HOH:O	2.13	0.66
1:G:101:ILE:O	1:G:128:ARG:NH1	2.28	0.66
1:D:184:VAL:HG13	1:D:205:PRO:HG2	1.77	0.66
1:I:220:PHE:O	3:I:403:HOH:O	2.13	0.66
1:M:90:ARG:NH1	3:M:402:HOH:O	1.96	0.66
1:B:10:GLN:OE1	3:B:402:HOH:O	2.14	0.66
1:N:285:ARG:NH2	3:R:404:HOH:O	2.27	0.66
1:K:247:ARG:HG3	1:K:263:LEU:HD11	1.76	0.66
1:O:30:LEU:O	1:P:246:ARG:NH2	2.28	0.66
1:M:52[B]:MET:HB2	1:N:274:ILE:HG23	1.77	0.65
1:Q:30:LEU:O	1:R:246:ARG:NH2	2.30	0.65
1:Q:275:ARG:O	3:Q:403:HOH:O	2.14	0.65
1:F:101:ILE:O	1:F:128:ARG:NH1	2.29	0.65
1:F:223:LEU:HD11	1:F:285:ARG:HE	1.60	0.65
1:M:213:ASP:OD1	3:M:406:HOH:O	2.13	0.65
1:B:184:VAL:HG11	1:B:188:LEU:HD11	1.79	0.65
1:D:199:LEU:HD22	1:D:262:LEU:HD23	1.79	0.65
1:N:184:VAL:HG13	1:N:205:PRO:HG2	1.78	0.65
1:C:184:VAL:HG13	1:C:205:PRO:HG2	1.78	0.64
1:Q:184:VAL:HG13	1:Q:205:PRO:HG2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:113:ILE:HD12	1:J:131:PHE:HB3	1.78	0.64
1:H:87:GLY:O	3:H:402:HOH:O	2.15	0.64
1:I:42:PHE:HZ	1:I:57:MET:HB3	1.62	0.64
1:C:274:ILE:HG23	1:D:52:MET:HB2	1.80	0.63
1:G:30:LEU:O	1:H:246:ARG:NH2	2.31	0.63
1:G:42:PHE:HZ	1:G:57:MET:HB3	1.62	0.63
1:N:152:ILE:HG23	1:N:180:LEU:HD22	1.79	0.63
1:O:199:LEU:HD22	1:O:262:LEU:HD23	1.79	0.63
1:C:227:ASP:OD1	3:C:403:HOH:O	2.16	0.62
1:N:85:GLY:O	2:N:301:SAH:N	2.33	0.62
1:H:115:ALA:HA	1:H:118:ARG:HH11	1.65	0.62
1:B:48:VAL:O	1:D:285[A]:ARG:NH2	2.33	0.62
1:F:247:ARG:NH1	3:F:409:HOH:O	2.32	0.62
1:K:246:ARG:NH2	1:L:30:LEU:O	2.32	0.62
1:B:101:ILE:O	1:B:128:ARG:NH1	2.33	0.62
1:O:26:GLU:OE1	1:P:253:ARG:NH2	2.33	0.61
1:B:184:VAL:HG13	1:B:205:PRO:HG2	1.82	0.61
1:K:52:MET:HB2	1:L:274:ILE:HG23	1.82	0.61
1:A:247:ARG:HG3	1:A:263:LEU:HD11	1.81	0.61
1:C:200:TYR:O	1:C:202:ALA:N	2.33	0.61
1:H:42:PHE:HZ	1:H:57:MET:HB3	1.66	0.61
1:Q:249:GLU:N	3:Q:410:HOH:O	2.33	0.61
1:A:253:ARG:NH1	1:B:26:GLU:OE1	2.33	0.61
1:E:42:PHE:HZ	1:E:57:MET:HB3	1.65	0.61
2:B:301:SAH:N	3:B:406:HOH:O	2.21	0.61
1:M:68:TYR:OH	3:M:407:HOH:O	2.14	0.60
1:H:186:GLU:O	1:H:207:ARG:NH2	2.34	0.60
1:P:247:ARG:NH2	3:P:404:HOH:O	2.08	0.60
1:R:74:ASP:CG	3:R:403:HOH:O	2.42	0.60
1:J:75:PRO:HG2	1:J:99:ARG:HG3	1.82	0.60
1:H:99:ARG:O	3:H:403:HOH:O	2.15	0.59
1:O:52:MET:HB2	1:P:274:ILE:HG23	1.84	0.59
1:H:199:LEU:HD22	1:H:262:LEU:HD23	1.84	0.59
1:L:126:THR:N	3:L:410:HOH:O	2.35	0.59
1:Q:42:PHE:HZ	1:Q:57:MET:HB3	1.67	0.59
1:R:131:PHE:N	3:R:406:HOH:O	2.08	0.59
1:O:42:PHE:HZ	1:O:57:MET:HB3	1.68	0.59
1:G:49:PRO:O	3:G:403:HOH:O	2.17	0.59
1:I:223:LEU:HD11	1:I:285:ARG:HG3	1.84	0.59
1:F:247:ARG:HG3	1:F:263:LEU:HD11	1.84	0.59
1:H:233:ALA:O	1:H:237:ASN:ND2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52[B]:MET:HE3	1:B:233:ALA:HB2	1.85	0.58
1:K:223:LEU:HD11	1:K:285:ARG:HE	1.66	0.58
1:R:81:LEU:O	3:R:410:HOH:O	2.17	0.58
1:R:101:ILE:O	1:R:128:ARG:NH1	2.37	0.58
1:Q:52[B]:MET:HB2	1:R:274:ILE:HG23	1.83	0.58
1:C:64:ARG:HG2	1:D:40:LEU:HD23	1.86	0.58
1:K:229:SER:HB2	1:L:52:MET:HE3	1.85	0.58
1:N:59:SER:OG	3:N:403:HOH:O	2.17	0.58
1:I:101:ILE:O	1:I:128:ARG:NH1	2.36	0.58
1:J:223:LEU:HD11	1:J:285:ARG:HE	1.67	0.58
1:P:174:GLY:N	3:P:407:HOH:O	2.36	0.58
1:D:152:ILE:HG23	1:D:180:LEU:HD22	1.84	0.57
1:P:42:PHE:HZ	1:P:57:MET:HB3	1.69	0.57
1:A:184:VAL:HG13	1:A:205:PRO:HG2	1.86	0.57
1:N:199:LEU:HD22	1:N:262:LEU:HD23	1.86	0.57
1:B:174:GLY:O	1:B:285:ARG:NH1	2.38	0.57
1:C:36:VAL:HB	2:D:301:SAH:HB2	1.86	0.57
1:Q:118:ARG:NH1	3:Q:401:HOH:O	2.03	0.57
1:P:97:ARG:NH2	3:P:411:HOH:O	2.34	0.57
1:R:232:LEU:HD22	1:R:279:PHE:CD1	2.40	0.57
1:B:260:ASP:OD1	3:B:403:HOH:O	2.18	0.57
1:G:274:ILE:HG23	1:H:52:MET:HB2	1.87	0.57
1:Q:22:ASP:OD1	1:R:109:SER:OG	2.20	0.57
1:Q:40:LEU:HD23	1:R:64:ARG:HG2	1.87	0.57
1:Q:52[A]:MET:HB2	1:R:274:ILE:HG23	1.85	0.57
1:R:166:GLU:OE2	1:R:169:ARG:NH2	2.31	0.57
1:F:251:THR:HG22	1:F:256:ALA:HA	1.87	0.56
1:D:85:GLY:O	2:D:301:SAH:N	2.39	0.56
1:K:30:LEU:O	1:L:246:ARG:NH2	2.37	0.56
1:R:152:ILE:HG23	1:R:180:LEU:HD22	1.87	0.56
1:D:42:PHE:HZ	1:D:57:MET:HB3	1.70	0.56
1:L:80:HIS:HE2	1:L:104:THR:HG1	1.45	0.56
1:L:223:LEU:HD11	1:L:285:ARG:HE	1.70	0.56
1:R:188:LEU:O	1:R:192:GLU:HB2	2.05	0.56
2:O:301:SAH:H8	1:P:17:VAL:HG11	1.86	0.56
1:M:253:ARG:NH1	1:N:26:GLU:OE1	2.39	0.56
1:P:286:LYS:O	3:P:407:HOH:O	2.18	0.56
1:R:66:THR:OG1	3:R:411:HOH:O	2.18	0.56
2:K:301:SAH:HB2	1:L:36:VAL:HB	1.88	0.56
1:E:74:ASP:OD1	1:E:99:ARG:NH1	2.36	0.56
1:I:247:ARG:HG3	1:I:263:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:104:THR:HB	3:R:410:HOH:O	2.05	0.56
1:R:250:PHE:HE1	3:R:422:HOH:O	1.88	0.56
1:E:30:LEU:O	1:F:246:ARG:NH2	2.39	0.56
2:L:301:SAH:N	3:L:404:HOH:O	2.15	0.56
1:K:40:LEU:HD23	1:L:64:ARG:HG2	1.89	0.55
1:H:223:LEU:HD11	1:H:285:ARG:NE	2.18	0.55
1:J:144:GLU:HG2	1:J:172:LYS:HA	1.88	0.55
1:L:152:ILE:HG23	1:L:180:LEU:HD22	1.88	0.55
1:G:157:HIS:CE1	3:H:405:HOH:O	2.60	0.55
1:O:255:GLY:O	3:O:403:HOH:O	2.17	0.55
1:E:75:PRO:HG2	1:E:99:ARG:HG3	1.88	0.55
1:A:52[B]:MET:HB2	1:B:274:ILE:HG23	1.89	0.55
1:G:66:THR:HG23	1:G:91:THR:HG23	1.87	0.55
1:A:246:ARG:HD2	1:A:249:GLU:OE1	2.07	0.55
1:B:10:GLN:N	3:B:414:HOH:O	2.38	0.55
1:H:258:PHE:HA	3:H:411:HOH:O	2.07	0.54
1:K:152:ILE:HG23	1:K:180:LEU:HD22	1.88	0.54
1:Q:52[B]:MET:HE3	1:R:233:ALA:HB2	1.89	0.54
1:A:42:PHE:HZ	1:A:57:MET:HB3	1.73	0.54
1:H:249:GLU:N	3:H:401:HOH:O	1.97	0.54
1:R:109:SER:HB3	1:R:112:GLN:HB2	1.88	0.54
1:R:91:THR:HG21	1:R:152:ILE:HD12	1.89	0.54
1:O:183:VAL:HG11	1:O:208:LEU:HD23	1.88	0.54
1:C:199:LEU:HD22	1:C:262:LEU:HD23	1.90	0.54
1:F:42:PHE:HZ	1:F:57:MET:HB3	1.73	0.54
1:G:253:ARG:NH1	1:H:26:GLU:OE1	2.35	0.54
1:M:26:GLU:OE1	1:N:253:ARG:NH1	2.41	0.54
1:Q:239:PHE:HB2	1:R:32:LEU:HD21	1.89	0.54
1:Q:32:LEU:HG	3:Q:404:HOH:O	2.07	0.54
1:A:152:ILE:HG23	1:A:180:LEU:HD22	1.90	0.54
1:F:49:PRO:O	3:F:404:HOH:O	2.18	0.53
1:M:271:GLU:OE2	1:M:275:ARG:NE	2.41	0.53
1:A:138:ARG:NH1	3:A:409:HOH:O	2.41	0.53
1:D:101:ILE:O	1:D:128:ARG:NH1	2.41	0.53
1:H:143:ASP:OD1	1:H:169:ARG:NH1	2.38	0.53
1:N:42:PHE:HZ	1:N:57:MET:HB3	1.74	0.53
1:Q:233:ALA:HB2	1:R:52:MET:HE3	1.90	0.53
1:C:115:ALA:O	1:C:118:ARG:HG2	2.08	0.53
1:H:77:ALA:HA	3:H:403:HOH:O	2.09	0.53
1:H:120:ALA:HB2	1:H:131:PHE:HE2	1.74	0.53
1:F:285:ARG:NH2	3:F:414:HOH:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:42:PHE:HZ	1:J:57:MET:HB3	1.74	0.53
1:L:42:PHE:HZ	1:L:57:MET:HB3	1.74	0.53
1:O:274:ILE:HG23	1:P:52:MET:HB2	1.91	0.52
1:R:88:THR:O	3:R:412:HOH:O	2.19	0.52
1:C:285:ARG:NH2	3:C:411:HOH:O	2.41	0.52
3:Q:404:HOH:O	1:R:239:PHE:HD1	1.92	0.52
1:E:52:MET:HB2	1:F:274:ILE:HG23	1.92	0.52
1:O:271:GLU:OE2	1:O:275:ARG:NE	2.43	0.52
1:G:158:MET:O	1:G:203:ASN:ND2	2.42	0.52
1:K:271:GLU:OE2	1:K:275:ARG:NE	2.42	0.52
1:R:184:VAL:HG13	1:R:205:PRO:HG2	1.92	0.52
1:A:246:ARG:NH2	1:B:30:LEU:O	2.41	0.52
1:I:22:ASP:OD1	1:J:109:SER:OG	2.19	0.52
1:I:247:ARG:NH1	3:I:407:HOH:O	2.42	0.52
1:M:22:ASP:OD1	1:N:109:SER:OG	2.24	0.52
1:C:93:LEU:HD22	1:C:119:LEU:HG	1.91	0.52
1:J:101:ILE:O	1:J:128:ARG:NH1	2.43	0.52
1:J:160:ARG:N	3:J:405:HOH:O	2.42	0.52
1:I:52:MET:HB2	1:J:274:ILE:HG23	1.91	0.51
1:G:246:ARG:HH21	1:G:250:PHE:HZ	1.57	0.51
1:K:71:GLU:OE1	3:K:402:HOH:O	2.19	0.51
1:M:54:LEU:HA	1:M:57:MET:HE2	1.93	0.51
1:Q:21:TYR:O	3:Q:406:HOH:O	2.19	0.51
1:R:42:PHE:HZ	1:R:57:MET:HB3	1.74	0.51
1:R:187:GLU:O	1:R:188:LEU:HB2	2.11	0.51
1:M:52[A]:MET:HB2	1:N:274:ILE:HG23	1.93	0.51
1:N:83:ASP:HB3	1:N:86:CYS:HB3	1.92	0.51
1:J:65:TYR:O	1:J:69:LEU:HG	2.11	0.51
1:F:143:ASP:OD1	1:F:169:ARG:NH1	2.38	0.51
1:J:166:GLU:OE2	1:J:169:ARG:NH2	2.33	0.51
1:F:138:ARG:NH1	3:I:404:HOH:O	2.44	0.51
1:A:274:ILE:HG23	1:B:52:MET:HB2	1.91	0.50
1:G:276:LYS:N	3:G:404:HOH:O	2.34	0.50
1:M:285:ARG:HH21	1:O:48:VAL:HB	1.76	0.50
1:R:246:ARG:NH1	3:R:423:HOH:O	2.43	0.50
1:Q:139:LEU:H	1:Q:166:GLU:HG2	1.76	0.50
1:G:40:LEU:HD23	1:H:64:ARG:HG2	1.93	0.50
1:M:52[B]:MET:HE3	1:N:233:ALA:HB2	1.92	0.50
1:C:101:ILE:O	1:C:128:ARG:NH1	2.44	0.50
1:E:152:ILE:HG23	1:E:180:LEU:HD22	1.94	0.50
1:H:74:ASP:OD1	1:H:99:ARG:NH1	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:229:SER:HA	1:R:279:PHE:HB3	1.93	0.50
1:D:113:ILE:O	1:D:117:ASN:ND2	2.44	0.50
1:I:274:ILE:HG23	1:J:52:MET:HB2	1.93	0.50
1:R:19:ASP:HA	3:R:402:HOH:O	2.10	0.50
1:D:188:LEU:N	3:D:408:HOH:O	2.36	0.50
1:M:29:HIS:HA	1:M:33:GLY:O	2.11	0.50
1:O:152:ILE:HG23	1:O:180:LEU:HD22	1.94	0.50
1:K:199:LEU:HD22	1:K:262:LEU:HD23	1.94	0.49
1:L:85:GLY:O	2:L:301:SAH:N	2.44	0.49
1:E:83:ASP:OD2	3:E:401:HOH:O	2.18	0.49
1:G:152:ILE:HG23	1:G:180:LEU:HD22	1.94	0.49
1:H:87:GLY:N	3:H:402:HOH:O	2.45	0.49
1:I:246:ARG:NH2	1:J:30:LEU:O	2.46	0.49
1:M:274:ILE:HG23	1:N:52[A]:MET:HB2	1.94	0.49
1:R:73:LEU:HB2	1:R:178:LEU:HD22	1.95	0.49
1:F:139:LEU:H	1:F:166:GLU:HG2	1.77	0.49
1:H:63:ASP:CG	1:H:90:ARG:HH21	2.19	0.49
1:K:109:SER:OG	1:L:22:ASP:OD1	2.26	0.49
2:M:301:SAH:HB2	1:N:36:VAL:HB	1.95	0.49
1:R:194:ALA:O	1:R:198:THR:OG1	2.28	0.49
1:R:242:GLY:HA2	3:R:441:HOH:O	2.12	0.49
1:K:223:LEU:HD11	1:K:285:ARG:NE	2.27	0.49
1:O:164:LEU:HD12	1:O:214:ILE:HG22	1.95	0.49
1:R:170:VAL:HG23	3:R:416:HOH:O	2.11	0.49
1:H:251:THR:HG22	1:H:256:ALA:HA	1.94	0.49
1:B:49:PRO:O	1:D:285[B]:ARG:NH1	2.40	0.48
1:E:42:PHE:CZ	1:E:57:MET:HB3	2.47	0.48
1:K:67:ASP:OD2	3:K:403:HOH:O	2.20	0.48
1:K:84:ILE:HG22	1:K:158:MET:HE1	1.94	0.48
1:L:223:LEU:HD11	1:L:285:ARG:NE	2.27	0.48
1:P:164:LEU:HD12	1:P:214:ILE:HG22	1.94	0.48
1:B:151:ALA:O	3:B:404:HOH:O	2.19	0.48
1:E:101:ILE:O	1:E:128:ARG:NH1	2.46	0.48
1:L:110:LYS:HD3	3:L:413:HOH:O	2.13	0.48
1:N:223:LEU:HD11	1:N:285:ARG:NE	2.28	0.48
1:O:104:THR:HA	1:O:130:THR:O	2.13	0.48
2:C:301:SAH:HB2	1:D:36:VAL:HB	1.95	0.48
1:M:75:PRO:HG2	1:M:99:ARG:HG3	1.96	0.48
1:G:188:LEU:N	3:G:407:HOH:O	2.38	0.48
1:E:36:VAL:HB	2:F:301:SAH:HB2	1.94	0.48
1:A:101:ILE:O	1:A:128:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:66:THR:HG23	1:M:91:THR:HG23	1.96	0.48
1:O:253:ARG:HH11	1:P:30:LEU:HD11	1.79	0.48
1:P:85:GLY:O	2:P:301:SAH:N	2.47	0.48
2:E:301:SAH:HB2	1:F:36:VAL:HB	1.95	0.48
1:R:85:GLY:O	2:R:301:SAH:N	2.47	0.48
1:R:88:THR:HB	3:R:412:HOH:O	2.13	0.48
1:R:183:VAL:HG11	1:R:208:LEU:HD23	1.96	0.48
1:P:287:PRO:C	3:P:407:HOH:O	2.57	0.48
1:M:246:ARG:NH2	1:N:30:LEU:O	2.47	0.47
1:R:98:GLN:HA	3:R:440:HOH:O	2.13	0.47
1:A:40:LEU:HD23	1:B:64:ARG:HG2	1.97	0.47
1:J:74:ASP:OD1	1:J:99:ARG:NH1	2.43	0.47
1:J:144:GLU:HG2	1:J:173:PRO:HD3	1.97	0.47
1:C:40:LEU:HD23	1:D:64:ARG:HG2	1.97	0.47
1:C:138:ARG:NH1	3:C:414:HOH:O	2.47	0.47
1:J:107:ALA:HA	2:J:301:SAH:N3	2.30	0.47
1:B:246:ARG:HD2	1:B:249:GLU:OE1	2.15	0.47
1:P:247:ARG:HG3	1:P:263:LEU:HD11	1.95	0.47
2:B:302:SAH:SD	2:B:302:SAH:N	2.87	0.47
1:D:223:LEU:HD11	1:D:285[B]:ARG:HD3	1.96	0.47
1:H:197:GLU:HA	1:H:201:ALA:HA	1.97	0.47
1:M:247:ARG:HG3	1:M:263:LEU:HD11	1.96	0.47
1:M:285:ARG:NH2	1:O:48:VAL:O	2.47	0.47
1:R:168:TRP:NE1	1:R:219:GLY:O	2.48	0.47
1:A:139:LEU:H	1:A:166:GLU:HG2	1.80	0.47
1:B:223:LEU:HD11	1:B:285:ARG:HE	1.78	0.47
1:H:142:GLU:O	1:H:145:SER:OG	2.26	0.47
1:K:246:ARG:HD2	1:K:249:GLU:OE1	2.14	0.47
1:L:75:PRO:HG2	1:L:99:ARG:HG3	1.96	0.47
1:M:159:ASP:HB2	1:N:10:GLN:CD	2.40	0.47
1:N:223:LEU:HD11	1:N:285:ARG:HE	1.79	0.47
1:P:75:PRO:HG2	1:P:99:ARG:HG3	1.97	0.47
1:B:42:PHE:HZ	1:B:57:MET:HB3	1.79	0.47
1:D:50:GLN:NE2	1:F:285:ARG:HH12	2.13	0.47
1:M:36:VAL:HB	2:N:301:SAH:HB2	1.96	0.47
1:G:201:ALA:HB1	1:H:17:VAL:HG22	1.97	0.47
1:O:40:LEU:HD23	1:P:64:ARG:HG2	1.97	0.47
1:J:236:MET:HE2	1:J:236:MET:HA	1.97	0.46
1:K:42:PHE:HZ	1:K:57:MET:HB3	1.80	0.46
1:R:91:THR:HG21	1:R:152:ILE:CD1	2.45	0.46
1:E:139:LEU:H	1:E:166:GLU:HG2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:CYS:HA	1:A:160:ARG:NH2	2.29	0.46
1:A:48:VAL:O	1:E:285:ARG:NH2	2.48	0.46
1:C:138:ARG:CZ	3:C:414:HOH:O	2.63	0.46
2:O:301:SAH:HB2	1:P:36:VAL:HB	1.98	0.46
1:R:239:PHE:HE2	1:R:266:LEU:HD21	1.80	0.46
1:C:246:ARG:HH22	1:D:30:LEU:HB3	1.81	0.46
1:M:48:VAL:HB	1:Q:285:ARG:HH21	1.81	0.46
1:R:82:LEU:HB3	1:R:149:ALA:HB2	1.96	0.46
1:C:94:LYS:NZ	3:C:409:HOH:O	2.36	0.46
1:I:237:ASN:HD22	1:J:54:LEU:HD13	1.80	0.46
1:E:19:ASP:HB3	1:E:23:LYS:NZ	2.30	0.46
1:H:152:ILE:HG23	1:H:180:LEU:HD22	1.97	0.46
1:M:233:ALA:HB2	1:N:52[B]:MET:HE3	1.98	0.46
1:R:114:ALA:O	1:R:118:ARG:HG3	2.16	0.46
1:A:107:ALA:O	1:A:133:VAL:HA	2.16	0.46
1:B:29:HIS:HA	1:B:33:GLY:O	2.16	0.46
1:G:135:ASP:OD1	1:G:136:ALA:N	2.49	0.46
1:I:143:ASP:N	1:I:143:ASP:OD1	2.49	0.46
1:K:186:GLU:HB3	1:K:187:GLU:H	1.60	0.46
1:A:23:LYS:HG2	1:Q:138:ARG:HH22	1.81	0.45
1:C:195:LEU:HD23	1:C:195:LEU:HA	1.84	0.45
1:J:84:ILE:HG22	1:J:158:MET:HE1	1.99	0.45
1:D:84:ILE:HG22	1:D:158:MET:HE1	1.97	0.45
1:E:239:PHE:HB2	1:F:32:LEU:HD21	1.98	0.45
1:M:25:GLY:N	3:M:401:HOH:O	1.94	0.45
1:M:203:ASN:OD1	1:N:11:GLN:N	2.47	0.45
1:D:176:ASP:OD1	1:D:285[B]:ARG:HG3	2.17	0.45
1:R:232:LEU:HD22	1:R:279:PHE:HD1	1.81	0.45
1:C:65:TYR:OH	1:C:180:LEU:HD23	2.16	0.45
1:R:139:LEU:H	1:R:166:GLU:HG2	1.81	0.45
1:O:258:PHE:N	3:O:403:HOH:O	2.49	0.45
1:O:143:ASP:OD1	1:O:143:ASP:N	2.50	0.45
1:R:150:TRP:HB3	1:R:178:LEU:HB3	1.98	0.45
1:R:189:THR:O	1:R:193:THR:HG23	2.17	0.45
1:D:75:PRO:HG2	1:D:99:ARG:HG3	1.99	0.45
1:M:17:VAL:HG11	2:N:301:SAH:H8	1.98	0.45
1:B:213:ASP:OD1	3:B:405:HOH:O	2.21	0.45
1:J:223:LEU:HD11	1:J:285:ARG:NE	2.31	0.45
1:R:114:ALA:HB3	1:R:118:ARG:HH21	1.82	0.45
1:C:52:MET:HE3	1:D:229:SER:HB2	1.98	0.45
1:C:215:VAL:HG12	3:C:402:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:62:GLN:O	1:R:65:TYR:HB3	2.17	0.45
1:C:17:VAL:HG11	2:D:301:SAH:H8	1.99	0.45
1:I:91:THR:HG22	1:I:150:TRP:CZ2	2.52	0.45
1:F:271:GLU:OE2	1:F:275:ARG:NE	2.50	0.44
1:M:84:ILE:O	3:M:408:HOH:O	2.20	0.44
1:R:103:VAL:O	3:R:413:HOH:O	2.21	0.44
1:C:66:THR:HG23	1:C:91:THR:HG23	1.98	0.44
1:H:33:GLY:C	1:H:35:SER:H	2.24	0.44
1:L:29:HIS:HA	1:L:33:GLY:O	2.16	0.44
1:O:51:ASP:H	1:O:56:THR:HG21	1.82	0.44
1:R:164:LEU:HD13	1:R:215:VAL:HG23	1.98	0.44
1:C:42:PHE:HZ	1:C:57:MET:HB3	1.82	0.44
1:C:223:LEU:HD11	1:C:285:ARG:HB2	1.98	0.44
1:D:134:ALA:HB1	1:D:140:PRO:HD3	2.00	0.44
1:E:168:TRP:CE2	1:E:286:LYS:HG3	2.52	0.44
1:F:223:LEU:HD11	1:F:285:ARG:NE	2.30	0.44
1:L:174:GLY:O	1:L:285:ARG:NH1	2.50	0.44
1:N:171:LEU:O	1:N:286:LYS:NZ	2.35	0.44
1:A:65:TYR:OH	1:A:180:LEU:HD23	2.17	0.44
1:J:66:THR:HG23	1:J:91:THR:HG23	2.00	0.44
1:Q:199:LEU:HD22	1:Q:262:LEU:HD23	1.99	0.44
1:H:87:GLY:O	1:H:112:GLN:HB3	2.17	0.44
1:L:137:MET:HE2	2:L:301:SAH:HN62	1.81	0.44
1:R:215:VAL:O	1:R:218:ALA:HB3	2.18	0.44
1:E:66:THR:HG23	1:E:91:THR:HG23	2.00	0.44
1:L:188:LEU:N	3:L:412:HOH:O	2.50	0.44
1:G:186:GLU:HB3	1:G:187:GLU:H	1.64	0.44
1:O:206:PRO:HG2	1:O:211:PHE:HB2	1.98	0.44
1:R:29:HIS:HA	1:R:33:GLY:O	2.18	0.44
1:R:93:LEU:O	1:R:97:ARG:HG3	2.17	0.44
1:B:199:LEU:HD22	1:B:262:LEU:HD23	2.00	0.44
1:I:142:GLU:O	1:I:145:SER:OG	2.31	0.44
1:Q:37:HIS:O	1:R:62:GLN:NE2	2.39	0.44
1:D:181:GLU:HG3	1:D:182:SER:O	2.18	0.43
1:I:198:THR:OG1	3:I:405:HOH:O	2.21	0.43
1:K:112:GLN:OE1	2:K:301:SAH:O3'	2.24	0.43
1:P:278:ARG:NH2	3:P:413:HOH:O	2.42	0.43
1:P:101:ILE:O	1:P:128:ARG:NH1	2.51	0.43
1:Q:223:LEU:HD11	1:Q:285:ARG:HE	1.83	0.43
1:Q:278:ARG:NH1	3:Q:413:HOH:O	2.48	0.43
1:B:253:ARG:O	1:Q:138:ARG:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:21:TYR:HB2	1:N:109:SER:HB2	2.01	0.43
1:O:160:ARG:CZ	1:O:206:PRO:HD3	2.49	0.43
1:Q:22:ASP:HA	1:R:111:GLU:HB3	2.01	0.43
1:R:207:ARG:O	1:R:211:PHE:N	2.42	0.43
1:R:215:VAL:HA	1:R:218:ALA:HB3	2.00	0.43
1:G:156:CYS:O	1:G:203:ASN:HB2	2.18	0.43
1:K:158:MET:O	1:K:203:ASN:ND2	2.52	0.43
1:M:114:ALA:O	1:M:118:ARG:HG3	2.19	0.43
1:O:192:GLU:OE1	1:O:276:LYS:NZ	2.41	0.43
1:Q:288:ALA:N	3:Q:405:HOH:O	2.19	0.43
1:B:188:LEU:HD12	1:B:188:LEU:H	1.84	0.43
1:G:186:GLU:O	1:G:207:ARG:NH2	2.52	0.43
1:P:80:HIS:NE2	1:P:104:THR:OG1	2.38	0.43
1:N:225:LEU:O	1:Q:224:SER:HA	2.19	0.43
1:A:48:VAL:HB	1:E:285:ARG:HH21	1.84	0.43
1:C:157:HIS:ND1	1:C:201:ALA:O	2.48	0.43
1:G:240:ALA:HA	1:G:266:LEU:HD13	1.99	0.43
1:L:226:LYS:NZ	3:L:405:HOH:O	2.21	0.43
1:A:37:HIS:HD2	2:B:301:SAH:OXT	2.01	0.43
1:A:164:LEU:HD12	1:A:214:ILE:HG22	2.01	0.43
1:G:208:LEU:HD22	1:G:208:LEU:HA	1.91	0.43
1:Q:31:THR:HG22	1:R:246:ARG:HH21	1.84	0.43
1:B:143:ASP:N	1:B:143:ASP:OD1	2.50	0.42
1:R:53:GLU:O	1:R:57:MET:HG3	2.18	0.42
2:G:301:SAH:HB2	1:H:36:VAL:HB	1.99	0.42
1:H:271:GLU:OE2	1:H:275:ARG:NE	2.52	0.42
1:J:144:GLU:HG3	3:J:404:HOH:O	2.18	0.42
1:N:286:LYS:HA	1:N:287:PRO:HD3	1.93	0.42
1:O:246:ARG:NH2	1:P:30:LEU:O	2.52	0.42
1:P:168:TRP:CZ2	1:P:286:LYS:HE3	2.53	0.42
1:F:66:THR:HG23	1:F:91:THR:HG23	2.01	0.42
1:J:43:PRO:HG2	1:J:46:ALA:HB2	2.01	0.42
1:J:150:TRP:HB3	1:J:178:LEU:HB3	2.02	0.42
1:K:170:VAL:HG22	3:K:401:HOH:O	2.18	0.42
1:A:93:LEU:HD12	1:A:125:LEU:HD12	2.01	0.42
1:A:240:ALA:HA	1:A:266:LEU:HD13	2.02	0.42
2:A:301:SAH:HB2	1:B:36:VAL:HB	2.01	0.42
1:I:66:THR:HG23	1:I:91:THR:HG23	2.01	0.42
1:N:63:ASP:CG	1:N:90:ARG:HH21	2.27	0.42
1:Q:29:HIS:HA	1:Q:33:GLY:O	2.20	0.42
1:R:215:VAL:HG13	1:R:220:PHE:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:166:GLU:OE2	1:H:169:ARG:NH2	2.39	0.42
1:K:143:ASP:OD1	1:K:143:ASP:N	2.50	0.42
1:Q:11:GLN:OE1	1:R:197:GLU:HB2	2.20	0.42
1:R:181:GLU:HG2	1:R:211:PHE:CE1	2.55	0.42
1:E:51:ASP:H	1:E:56:THR:HG21	1.85	0.42
1:G:274:ILE:HG12	1:H:52:MET:HB2	2.01	0.42
1:H:75:PRO:HG2	1:H:99:ARG:HG3	2.01	0.42
1:M:10:GLN:CD	1:N:159:ASP:HB2	2.44	0.42
1:P:153:GLU:N	3:P:402:HOH:O	2.53	0.42
1:R:171:LEU:HG	3:R:416:HOH:O	2.20	0.42
1:R:192:GLU:OE1	1:R:276:LYS:NZ	2.36	0.42
1:A:36:VAL:HB	2:B:301:SAH:HB2	2.02	0.42
1:C:29:HIS:HA	1:C:33:GLY:O	2.19	0.42
1:C:211:PHE:O	1:C:215:VAL:HG23	2.19	0.42
1:C:271:GLU:OE2	1:C:275:ARG:NE	2.53	0.42
1:I:198:THR:CB	3:I:405:HOH:O	2.68	0.42
1:J:107:ALA:HB1	2:J:301:SAH:O2'	2.20	0.42
1:C:189:THR:O	1:C:193:THR:HG23	2.20	0.42
1:G:271:GLU:OE2	1:G:275:ARG:NE	2.52	0.42
1:I:237:ASN:ND2	1:J:54:LEU:HD13	2.34	0.42
1:L:186:GLU:HB3	1:L:187:GLU:H	1.69	0.42
1:G:17:VAL:HG21	1:H:157:HIS:HB3	2.02	0.41
1:I:29:HIS:HA	1:I:33:GLY:O	2.20	0.41
1:I:240:ALA:HA	1:I:266:LEU:HD13	2.02	0.41
1:N:160:ARG:CZ	1:N:206:PRO:HD3	2.50	0.41
1:O:174:GLY:HA3	1:Q:50:GLN:OE1	2.20	0.41
1:D:50:GLN:HE22	1:F:285:ARG:HH12	1.68	0.41
1:E:19:ASP:HB3	1:E:23:LYS:HZ1	1.85	0.41
1:F:156:CYS:HA	1:F:160:ARG:NH2	2.35	0.41
1:L:181:GLU:HG3	1:L:182:SER:O	2.20	0.41
1:P:150:TRP:HD1	1:P:150:TRP:O	2.02	0.41
1:R:51:ASP:H	1:R:56:THR:HG21	1.85	0.41
1:F:171:LEU:O	1:F:286:LYS:NZ	2.47	0.41
1:G:75:PRO:HG2	1:G:99:ARG:HG3	2.03	0.41
1:P:158:MET:HG2	2:P:301:SAH:N6	2.36	0.41
1:C:160:ARG:CZ	1:C:206:PRO:HD3	2.51	0.41
1:E:273:LEU:HD12	1:E:277:THR:OG1	2.21	0.41
1:F:195:LEU:HD23	1:F:195:LEU:HA	1.94	0.41
1:O:285:ARG:NH2	1:Q:48:VAL:O	2.53	0.41
1:A:28:TYR:OH	3:A:401:HOH:O	2.00	0.41
1:E:241:LEU:HB2	1:F:241:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:37:HIS:HE1	1:R:62:GLN:O	2.02	0.41
1:A:66:THR:HG23	1:A:91:THR:HG23	2.01	0.41
1:H:42:PHE:CZ	1:H:57:MET:HB3	2.52	0.41
1:J:113:ILE:HD13	1:J:113:ILE:HA	1.76	0.41
1:J:160:ARG:HE	1:J:181:GLU:CD	2.28	0.41
1:J:208:LEU:HD22	1:J:208:LEU:HA	1.84	0.41
2:K:301:SAH:H8	1:L:17:VAL:HG11	2.03	0.41
1:M:139:LEU:H	1:M:166:GLU:HG2	1.86	0.41
1:E:29:HIS:HA	1:E:33:GLY:O	2.21	0.41
1:J:29:HIS:HA	1:J:33:GLY:O	2.21	0.41
1:R:160:ARG:HE	1:R:181:GLU:CD	2.28	0.41
1:A:54:LEU:HD13	1:B:237:ASN:ND2	2.36	0.41
1:K:152:ILE:HG23	1:K:180:LEU:CD2	2.51	0.41
1:N:83:ASP:CG	1:N:150:TRP:HE1	2.28	0.41
1:O:240:ALA:HA	1:O:266:LEU:HD13	2.02	0.41
1:R:215:VAL:HA	1:R:218:ALA:CB	2.49	0.41
1:J:85:GLY:O	2:J:301:SAH:N	2.54	0.41
1:G:223:LEU:HD11	1:G:285:ARG:HE	1.86	0.40
1:K:167:ALA:C	3:K:401:HOH:O	2.64	0.40
1:O:12:VAL:HG11	1:P:201:ALA:C	2.46	0.40
1:A:10:GLN:CD	1:B:159:ASP:HB2	2.46	0.40
1:D:29:HIS:HA	1:D:33:GLY:O	2.22	0.40
1:H:208:LEU:HD22	1:H:208:LEU:HA	1.89	0.40
1:E:40:LEU:HD23	1:F:64:ARG:HG2	2.03	0.40
1:L:197:GLU:HA	1:L:201:ALA:HA	2.02	0.40
1:N:29:HIS:HA	1:N:33:GLY:O	2.21	0.40
1:G:251:THR:HG22	1:G:256:ALA:HA	2.04	0.40
1:H:43:PRO:HG2	1:H:46:ALA:HB2	2.03	0.40
1:H:115:ALA:HA	1:H:118:ARG:HD2	2.03	0.40
1:M:17:VAL:HG21	1:N:157:HIS:HB3	2.03	0.40
1:O:66:THR:HG23	1:O:91:THR:HG23	2.03	0.40
1:R:136:ALA:HB3	1:R:158:MET:SD	2.60	0.40
1:B:138:ARG:HD2	3:B:473:HOH:O	2.21	0.40
1:F:24:PHE:O	1:F:27:VAL:HG12	2.21	0.40
1:H:188:LEU:N	3:H:406:HOH:O	2.46	0.40
1:O:251:THR:HA	1:O:255:GLY:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:126:THR:OG1	1:R:126:THR:OG1[2_555]	2.14	0.06

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	281/297 (95%)	275 (98%)	4 (1%)	2 (1%)	18	34
1	B	279/297 (94%)	275 (99%)	4 (1%)	0	100	100
1	C	278/297 (94%)	269 (97%)	5 (2%)	4 (1%)	9	17
1	D	279/297 (94%)	275 (99%)	3 (1%)	1 (0%)	30	49
1	E	277/297 (93%)	275 (99%)	2 (1%)	0	100	100
1	F	278/297 (94%)	274 (99%)	4 (1%)	0	100	100
1	G	278/297 (94%)	267 (96%)	9 (3%)	2 (1%)	18	34
1	H	277/297 (93%)	269 (97%)	7 (2%)	1 (0%)	30	49
1	I	279/297 (94%)	275 (99%)	3 (1%)	1 (0%)	30	49
1	J	279/297 (94%)	273 (98%)	6 (2%)	0	100	100
1	K	279/297 (94%)	271 (97%)	7 (2%)	1 (0%)	30	49
1	L	278/297 (94%)	272 (98%)	5 (2%)	1 (0%)	30	49
1	M	281/297 (95%)	273 (97%)	7 (2%)	1 (0%)	30	49
1	N	281/297 (95%)	273 (97%)	6 (2%)	2 (1%)	18	34
1	O	278/297 (94%)	270 (97%)	7 (2%)	1 (0%)	30	49
1	P	278/297 (94%)	271 (98%)	5 (2%)	2 (1%)	18	34
1	Q	281/297 (95%)	274 (98%)	6 (2%)	1 (0%)	30	49
1	R	280/297 (94%)	269 (96%)	9 (3%)	2 (1%)	18	34
All	All	5021/5346 (94%)	4900 (98%)	99 (2%)	22 (0%)	30	49

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	126	THR
1	C	201	ALA
1	K	188	LEU
1	O	188	LEU
1	P	188	LEU
1	Q	188	LEU
1	R	188	LEU
1	A	10	GLN
1	A	188	LEU
1	C	187	GLU
1	C	188	LEU
1	D	188	LEU
1	G	188	LEU
1	H	188	LEU
1	I	188	LEU
1	L	188	LEU
1	M	188	LEU
1	N	10	GLN
1	N	188	LEU
1	G	203	ASN
1	P	253	ARG
1	R	189	THR

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	226/239 (95%)	221 (98%)	5 (2%)	45	73
1	B	224/239 (94%)	216 (96%)	8 (4%)	31	58
1	C	223/239 (93%)	216 (97%)	7 (3%)	35	62
1	D	224/239 (94%)	215 (96%)	9 (4%)	28	54
1	E	222/239 (93%)	217 (98%)	5 (2%)	44	72
1	F	223/239 (93%)	218 (98%)	5 (2%)	45	73
1	G	223/239 (93%)	214 (96%)	9 (4%)	28	54
1	H	222/239 (93%)	214 (96%)	8 (4%)	31	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	224/239 (94%)	218 (97%)	6 (3%)	39	67
1	J	224/239 (94%)	216 (96%)	8 (4%)	31	58
1	K	224/239 (94%)	216 (96%)	8 (4%)	31	58
1	L	223/239 (93%)	218 (98%)	5 (2%)	45	73
1	M	226/239 (95%)	221 (98%)	5 (2%)	45	73
1	N	226/239 (95%)	222 (98%)	4 (2%)	51	77
1	O	223/239 (93%)	215 (96%)	8 (4%)	31	58
1	P	223/239 (93%)	218 (98%)	5 (2%)	45	73
1	Q	226/239 (95%)	223 (99%)	3 (1%)	61	82
1	R	225/239 (94%)	214 (95%)	11 (5%)	22	45
All	All	4031/4302 (94%)	3912 (97%)	119 (3%)	37	64

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	VAL
1	A	186	GLU
1	A	208	LEU
1	A	247	ARG
1	A	289	VAL
1	B	158	MET
1	B	183	VAL
1	B	186	GLU
1	B	188	LEU
1	B	190	GLU
1	B	208	LEU
1	B	247	ARG
1	B	289	VAL
1	C	26	GLU
1	C	126	THR
1	C	183	VAL
1	C	186	GLU
1	C	200	TYR
1	C	208	LEU
1	C	247	ARG
1	D	10	GLN
1	D	158	MET
1	D	183	VAL

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Mol	Chain	Res	Type
1	D	186	GLU
1	D	190	GLU
1	D	208	LEU
1	D	247	ARG
1	D	285[A]	ARG
1	D	285[B]	ARG
1	E	52	MET
1	E	183	VAL
1	E	188	LEU
1	E	208	LEU
1	E	251	THR
1	F	26	GLU
1	F	183	VAL
1	F	186	GLU
1	F	208	LEU
1	F	247	ARG
1	G	26	GLU
1	G	36	VAL
1	G	186	GLU
1	G	208	LEU
1	G	247	ARG
1	G	251	THR
1	G	252	GLU
1	G	253	ARG
1	G	289	VAL
1	H	26	GLU
1	H	118	ARG
1	H	142	GLU
1	H	183	VAL
1	H	186	GLU
1	H	208	LEU
1	H	247	ARG
1	H	251	THR
1	I	143	ASP
1	I	183	VAL
1	I	186	GLU
1	I	208	LEU
1	I	285	ARG
1	I	289	VAL
1	J	26	GLU
1	J	113	ILE
1	J	158	MET

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Mol	Chain	Res	Type
1	J	186	GLU
1	J	208	LEU
1	J	247	ARG
1	J	253	ARG
1	J	281	MET
1	K	10	GLN
1	K	36	VAL
1	K	170	VAL
1	K	183	VAL
1	K	186	GLU
1	K	208	LEU
1	K	247	ARG
1	K	252	GLU
1	L	26	GLU
1	L	51	ASP
1	L	183	VAL
1	L	186	GLU
1	L	208	LEU
1	M	36	VAL
1	M	183	VAL
1	M	186	GLU
1	M	208	LEU
1	M	289	VAL
1	N	183	VAL
1	N	186	GLU
1	N	208	LEU
1	N	253	ARG
1	O	10	GLN
1	O	26	GLU
1	O	36	VAL
1	O	104	THR
1	O	143	ASP
1	O	186	GLU
1	O	208	LEU
1	O	289	VAL
1	P	15	ASP
1	P	186	GLU
1	P	208	LEU
1	P	247	ARG
1	P	252	GLU
1	Q	186	GLU
1	Q	208	LEU

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Mol	Chain	Res	Type
1	Q	289	VAL
1	R	111	GLU
1	R	126	THR
1	R	158	MET
1	R	183	VAL
1	R	186	GLU
1	R	188	LEU
1	R	190	GLU
1	R	195	LEU
1	R	208	LEU
1	R	215	VAL
1	R	289	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	C	60	GLN
1	I	123	HIS
1	I	237	ASN
1	J	237	ASN
1	K	29	HIS
1	M	10	GLN
1	N	10	GLN
1	P	117	ASN
1	P	237	ASN
1	Q	10	GLN
1	R	112	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

19 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	F	301	-	27,28,28	1.09	4 (14%)	36,40,40	2.19	12 (33%)
2	SAH	A	301	-	27,28,28	1.06	4 (14%)	36,40,40	2.06	10 (27%)
2	SAH	O	301	-	27,28,28	1.10	4 (14%)	36,40,40	2.05	10 (27%)
2	SAH	L	301	-	27,28,28	1.10	4 (14%)	36,40,40	2.07	11 (30%)
2	SAH	E	301	-	27,28,28	1.11	5 (18%)	36,40,40	1.95	9 (25%)
2	SAH	C	301	-	27,28,28	1.08	5 (18%)	36,40,40	2.04	9 (25%)
2	SAH	R	301	-	27,28,28	1.10	4 (14%)	36,40,40	2.01	9 (25%)
2	SAH	D	301	-	27,28,28	1.11	4 (14%)	36,40,40	2.06	10 (27%)
2	SAH	Q	301	-	27,28,28	1.08	5 (18%)	36,40,40	1.97	9 (25%)
2	SAH	B	301	-	27,28,28	1.07	3 (11%)	36,40,40	2.04	10 (27%)
2	SAH	P	301	-	27,28,28	1.10	5 (18%)	36,40,40	1.98	11 (30%)
2	SAH	M	301	-	27,28,28	1.11	4 (14%)	36,40,40	2.03	10 (27%)
2	SAH	K	301	-	27,28,28	1.07	3 (11%)	36,40,40	2.06	10 (27%)
2	SAH	B	302	-	27,28,28	1.11	4 (14%)	36,40,40	2.14	12 (33%)
2	SAH	I	301	-	27,28,28	1.08	4 (14%)	36,40,40	2.01	10 (27%)
2	SAH	N	301	-	27,28,28	1.11	4 (14%)	36,40,40	2.04	9 (25%)
2	SAH	H	301	-	27,28,28	1.15	3 (11%)	36,40,40	2.29	11 (30%)
2	SAH	G	301	-	27,28,28	1.15	4 (14%)	36,40,40	2.01	9 (25%)
2	SAH	J	301	-	27,28,28	1.10	4 (14%)	36,40,40	2.07	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	F	301	-	-	1/15/31/31	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	A	301	-	-	1/15/31/31	0/3/3/3
2	SAH	O	301	-	-	5/15/31/31	0/3/3/3
2	SAH	L	301	-	-	2/15/31/31	0/3/3/3
2	SAH	E	301	-	-	2/15/31/31	0/3/3/3
2	SAH	C	301	-	-	1/15/31/31	0/3/3/3
2	SAH	R	301	-	-	3/15/31/31	0/3/3/3
2	SAH	D	301	-	-	3/15/31/31	0/3/3/3
2	SAH	Q	301	-	-	3/15/31/31	0/3/3/3
2	SAH	B	301	-	-	2/15/31/31	0/3/3/3
2	SAH	P	301	-	-	3/15/31/31	0/3/3/3
2	SAH	M	301	-	-	2/15/31/31	0/3/3/3
2	SAH	K	301	-	-	1/15/31/31	0/3/3/3
2	SAH	B	302	-	-	8/15/31/31	0/3/3/3
2	SAH	I	301	-	-	2/15/31/31	0/3/3/3
2	SAH	N	301	-	-	2/15/31/31	0/3/3/3
2	SAH	H	301	-	-	3/15/31/31	0/3/3/3
2	SAH	G	301	-	-	1/15/31/31	0/3/3/3
2	SAH	J	301	-	-	1/15/31/31	0/3/3/3

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	SAH	OXT-C	-2.74	1.21	1.30
2	A	301	SAH	C2-N1	2.65	1.38	1.33
2	F	301	SAH	C2-N3	2.65	1.38	1.33
2	B	302	SAH	C2-N3	2.65	1.38	1.33
2	H	301	SAH	C2-N1	2.64	1.38	1.33
2	H	301	SAH	C2-N3	2.63	1.38	1.33
2	R	301	SAH	C2-N1	2.62	1.38	1.33
2	E	301	SAH	C2-N1	2.62	1.38	1.33
2	L	301	SAH	C2-N1	2.61	1.38	1.33
2	D	301	SAH	C2-N1	2.61	1.38	1.33
2	B	302	SAH	C2-N1	2.61	1.38	1.33
2	N	301	SAH	C2-N1	2.59	1.38	1.33
2	G	301	SAH	C2-N1	2.58	1.38	1.33
2	D	301	SAH	C2-N3	2.58	1.38	1.33
2	M	301	SAH	C2-N3	2.57	1.38	1.33
2	B	301	SAH	C2-N1	2.57	1.38	1.33
2	P	301	SAH	C2-N3	2.56	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	301	SAH	C2-N1	2.55	1.38	1.33
2	J	301	SAH	C2-N3	2.54	1.38	1.33
2	I	301	SAH	C2-N1	2.54	1.38	1.33
2	L	301	SAH	C2-N3	2.54	1.38	1.33
2	P	301	SAH	C2-N1	2.53	1.38	1.33
2	N	301	SAH	C2-N3	2.52	1.38	1.33
2	O	301	SAH	C2-N1	2.51	1.38	1.33
2	R	301	SAH	C2-N3	2.50	1.38	1.33
2	G	301	SAH	C2-N3	2.50	1.38	1.33
2	M	301	SAH	C2-N1	2.49	1.38	1.33
2	F	301	SAH	C2-N1	2.49	1.38	1.33
2	J	301	SAH	C2-N1	2.48	1.38	1.33
2	C	301	SAH	C2-N1	2.47	1.38	1.33
2	K	301	SAH	C2-N3	2.47	1.38	1.33
2	O	301	SAH	C2-N3	2.46	1.38	1.33
2	C	301	SAH	C2-N3	2.42	1.38	1.33
2	Q	301	SAH	C2-N1	2.42	1.38	1.33
2	M	301	SAH	OXT-C	-2.42	1.22	1.30
2	E	301	SAH	C2-N3	2.40	1.38	1.33
2	A	301	SAH	C2-N3	2.36	1.38	1.33
2	O	301	SAH	OXT-C	-2.34	1.23	1.30
2	N	301	SAH	OXT-C	-2.34	1.23	1.30
2	B	301	SAH	C2-N3	2.31	1.38	1.33
2	H	301	SAH	OXT-C	-2.30	1.23	1.30
2	Q	301	SAH	C2-N3	2.29	1.38	1.33
2	A	301	SAH	OXT-C	-2.28	1.23	1.30
2	I	301	SAH	OXT-C	-2.27	1.23	1.30
2	I	301	SAH	C2-N3	2.27	1.38	1.33
2	E	301	SAH	OXT-C	-2.27	1.23	1.30
2	E	301	SAH	C8-N7	2.25	1.36	1.31
2	R	301	SAH	OXT-C	-2.24	1.23	1.30
2	B	302	SAH	OXT-C	-2.23	1.23	1.30
2	D	301	SAH	OXT-C	-2.23	1.23	1.30
2	K	301	SAH	OXT-C	-2.22	1.23	1.30
2	Q	301	SAH	OXT-C	-2.21	1.23	1.30
2	I	301	SAH	C5-N7	-2.21	1.35	1.39
2	P	301	SAH	OXT-C	-2.20	1.23	1.30
2	F	301	SAH	OXT-C	-2.19	1.23	1.30
2	C	301	SAH	OXT-C	-2.18	1.23	1.30
2	B	301	SAH	OXT-C	-2.17	1.23	1.30
2	J	301	SAH	OXT-C	-2.17	1.23	1.30
2	G	301	SAH	C8-N7	2.17	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	301	SAH	C8-N7	2.15	1.35	1.31
2	J	301	SAH	C8-N7	2.14	1.35	1.31
2	P	301	SAH	C8-N7	2.13	1.35	1.31
2	R	301	SAH	C8-N7	2.11	1.35	1.31
2	L	301	SAH	OXT-C	-2.11	1.23	1.30
2	Q	301	SAH	C5-N7	-2.11	1.35	1.39
2	M	301	SAH	C8-N7	2.09	1.35	1.31
2	B	302	SAH	C8-N7	2.08	1.35	1.31
2	L	301	SAH	C8-N7	2.08	1.35	1.31
2	C	301	SAH	C8-N7	2.07	1.35	1.31
2	O	301	SAH	C8-N7	2.07	1.35	1.31
2	C	301	SAH	C5-N7	-2.07	1.35	1.39
2	N	301	SAH	C8-N7	2.05	1.35	1.31
2	P	301	SAH	C5-N7	-2.04	1.35	1.39
2	E	301	SAH	C5-N7	-2.04	1.35	1.39
2	D	301	SAH	C8-N7	2.01	1.35	1.31
2	A	301	SAH	C8-N7	2.00	1.35	1.31
2	F	301	SAH	C8-N7	2.00	1.35	1.31

All (191) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	SAH	N3-C2-N1	-5.92	119.62	128.58
2	I	301	SAH	N3-C2-N1	-5.83	119.76	128.58
2	B	301	SAH	N3-C2-N1	-5.82	119.77	128.58
2	A	301	SAH	N3-C2-N1	-5.79	119.82	128.58
2	K	301	SAH	N3-C2-N1	-5.74	119.90	128.58
2	N	301	SAH	N3-C2-N1	-5.72	119.93	128.58
2	E	301	SAH	N3-C2-N1	-5.71	119.94	128.58
2	R	301	SAH	N3-C2-N1	-5.71	119.94	128.58
2	Q	301	SAH	N3-C2-N1	-5.65	120.03	128.58
2	J	301	SAH	N3-C2-N1	-5.65	120.03	128.58
2	H	301	SAH	N3-C2-N1	-5.58	120.13	128.58
2	M	301	SAH	N3-C2-N1	-5.57	120.15	128.58
2	D	301	SAH	N3-C2-N1	-5.57	120.15	128.58
2	G	301	SAH	N3-C2-N1	-5.53	120.21	128.58
2	O	301	SAH	N3-C2-N1	-5.46	120.31	128.58
2	F	301	SAH	N3-C2-N1	-5.42	120.38	128.58
2	L	301	SAH	N3-C2-N1	-5.40	120.41	128.58
2	B	302	SAH	N3-C2-N1	-5.38	120.43	128.58
2	H	301	SAH	O4'-C1'-N9	5.31	118.29	108.09
2	P	301	SAH	N3-C2-N1	-5.31	120.54	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	SAH	C5-C4-N3	-4.97	119.87	126.72
2	B	302	SAH	C5-C4-N3	-4.84	120.05	126.72
2	F	301	SAH	C5-C4-N3	-4.70	120.25	126.72
2	F	301	SAH	N9-C8-N7	-4.64	107.35	113.94
2	L	301	SAH	C5-C4-N3	-4.55	120.45	126.72
2	J	301	SAH	C5-C4-N3	-4.54	120.47	126.72
2	O	301	SAH	C5-C4-N3	-4.50	120.53	126.72
2	G	301	SAH	C5-C4-N3	-4.47	120.56	126.72
2	N	301	SAH	C5-C4-N3	-4.46	120.58	126.72
2	I	301	SAH	N9-C8-N7	-4.46	107.61	113.94
2	P	301	SAH	C5-C4-N3	-4.44	120.60	126.72
2	M	301	SAH	C5-C4-N3	-4.41	120.64	126.72
2	L	301	SAH	C5'-SD-CG	-4.38	89.25	102.26
2	A	301	SAH	N9-C8-N7	-4.36	107.75	113.94
2	C	301	SAH	C5-C4-N3	-4.35	120.73	126.72
2	D	301	SAH	C5-C4-N3	-4.33	120.75	126.72
2	K	301	SAH	C5-C4-N3	-4.27	120.84	126.72
2	B	301	SAH	C5'-SD-CG	-4.25	89.65	102.26
2	H	301	SAH	C5'-SD-CG	-4.23	89.69	102.26
2	R	301	SAH	C5-C4-N3	-4.22	120.91	126.72
2	F	301	SAH	C5-N7-C8	4.22	110.08	103.45
2	K	301	SAH	C5'-SD-CG	-4.17	89.88	102.26
2	Q	301	SAH	C5-C4-N3	-4.15	121.00	126.72
2	D	301	SAH	C5'-SD-CG	-4.12	90.05	102.26
2	B	301	SAH	N9-C8-N7	-4.07	108.16	113.94
2	D	301	SAH	N9-C8-N7	-4.06	108.18	113.94
2	O	301	SAH	C5'-SD-CG	-4.04	90.28	102.26
2	E	301	SAH	C5-C4-N3	-4.03	121.16	126.72
2	C	301	SAH	C5'-SD-CG	-4.02	90.34	102.26
2	J	301	SAH	N9-C8-N7	-4.00	108.25	113.94
2	B	301	SAH	C5-C4-N3	-4.00	121.20	126.72
2	J	301	SAH	C5'-SD-CG	-3.99	90.42	102.26
2	M	301	SAH	N9-C8-N7	-3.99	108.28	113.94
2	E	301	SAH	N9-C8-N7	-3.98	108.29	113.94
2	A	301	SAH	C5-C4-N3	-3.98	121.24	126.72
2	K	301	SAH	N9-C8-N7	-3.93	108.35	113.94
2	R	301	SAH	C5'-SD-CG	-3.93	90.61	102.26
2	F	301	SAH	C5'-SD-CG	-3.92	90.62	102.26
2	I	301	SAH	C5-C4-N3	-3.91	121.34	126.72
2	R	301	SAH	N9-C8-N7	-3.88	108.43	113.94
2	G	301	SAH	C5'-SD-CG	-3.87	90.77	102.26
2	Q	301	SAH	N9-C8-N7	-3.85	108.47	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	SAH	N9-C8-N7	-3.85	108.48	113.94
2	G	301	SAH	N9-C8-N7	-3.81	108.53	113.94
2	N	301	SAH	N9-C8-N7	-3.81	108.53	113.94
2	Q	301	SAH	C5'-SD-CG	-3.77	91.08	102.26
2	H	301	SAH	N9-C8-N7	-3.74	108.63	113.94
2	M	301	SAH	C5'-SD-CG	-3.73	91.18	102.26
2	N	301	SAH	C5'-SD-CG	-3.73	91.20	102.26
2	O	301	SAH	N9-C8-N7	-3.72	108.66	113.94
2	P	301	SAH	N9-C8-N7	-3.72	108.67	113.94
2	I	301	SAH	C5-N7-C8	3.72	109.29	103.45
2	H	301	SAH	C2-N3-C4	3.69	120.86	111.83
2	A	301	SAH	C5-N7-C8	3.68	109.23	103.45
2	B	302	SAH	O4'-C1'-N9	3.62	115.05	108.09
2	B	302	SAH	N9-C8-N7	-3.61	108.82	113.94
2	A	301	SAH	C5'-SD-CG	-3.59	91.61	102.26
2	L	301	SAH	N9-C8-N7	-3.56	108.88	113.94
2	H	301	SAH	N3-C4-N9	3.52	133.16	127.17
2	P	301	SAH	C5'-SD-CG	-3.52	91.82	102.26
2	D	301	SAH	C5-N7-C8	3.49	108.94	103.45
2	M	301	SAH	C5-N7-C8	3.48	108.91	103.45
2	J	301	SAH	C5-N7-C8	3.47	108.91	103.45
2	J	301	SAH	C2-N3-C4	3.47	120.30	111.83
2	F	301	SAH	C2-N3-C4	3.47	120.30	111.83
2	C	301	SAH	C2-N3-C4	3.43	120.21	111.83
2	B	302	SAH	C2-N3-C4	3.43	120.20	111.83
2	B	302	SAH	C5'-SD-CG	-3.42	92.11	102.26
2	B	301	SAH	C5-N7-C8	3.42	108.82	103.45
2	G	301	SAH	C2-N3-C4	3.40	120.12	111.83
2	O	301	SAH	C5-N7-C8	3.39	108.78	103.45
2	N	301	SAH	C2-N3-C4	3.39	120.12	111.83
2	M	301	SAH	C2-N3-C4	3.39	120.10	111.83
2	R	301	SAH	C2-N3-C4	3.37	120.05	111.83
2	K	301	SAH	C2-N3-C4	3.36	120.03	111.83
2	K	301	SAH	C5-N7-C8	3.35	108.72	103.45
2	E	301	SAH	C5'-SD-CG	-3.35	92.32	102.26
2	O	301	SAH	C2-N3-C4	3.35	120.01	111.83
2	Q	301	SAH	C5-N7-C8	3.34	108.71	103.45
2	B	301	SAH	C2-N3-C4	3.33	119.98	111.83
2	E	301	SAH	C5-N7-C8	3.33	108.69	103.45
2	B	302	SAH	C5-N7-C8	3.33	108.69	103.45
2	L	301	SAH	C2-N3-C4	3.33	119.97	111.83
2	G	301	SAH	C5-N7-C8	3.33	108.68	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	SAH	C2-N3-C4	3.32	119.94	111.83
2	R	301	SAH	C5-N7-C8	3.31	108.65	103.45
2	F	301	SAH	C4-C5-N7	-3.31	106.80	110.58
2	P	301	SAH	C5-N7-C8	3.30	108.64	103.45
2	N	301	SAH	C5-N7-C8	3.29	108.62	103.45
2	A	301	SAH	C2-N3-C4	3.28	119.84	111.83
2	Q	301	SAH	C2-N3-C4	3.28	119.83	111.83
2	I	301	SAH	C2-N3-C4	3.27	119.82	111.83
2	E	301	SAH	C2-N3-C4	3.24	119.74	111.83
2	B	302	SAH	N3-C4-N9	3.23	132.67	127.17
2	P	301	SAH	C2-N3-C4	3.20	119.65	111.83
2	L	301	SAH	C5-N7-C8	3.20	108.48	103.45
2	A	301	SAH	OXT-C-O	-3.14	116.96	124.08
2	C	301	SAH	C5-N7-C8	3.12	108.36	103.45
2	C	301	SAH	N3-C4-N9	3.09	132.43	127.17
2	N	301	SAH	N3-C4-N9	3.09	132.43	127.17
2	L	301	SAH	N3-C4-N9	3.09	132.42	127.17
2	J	301	SAH	N3-C4-N9	3.08	132.40	127.17
2	M	301	SAH	OXT-C-O	-3.07	117.11	124.08
2	D	301	SAH	N3-C4-N9	3.01	132.29	127.17
2	M	301	SAH	N3-C4-N9	2.98	132.23	127.17
2	K	301	SAH	N3-C4-N9	2.98	132.23	127.17
2	O	301	SAH	N3-C4-N9	2.94	132.17	127.17
2	B	301	SAH	N3-C4-N9	2.93	132.15	127.17
2	I	301	SAH	C5'-SD-CG	-2.92	93.60	102.26
2	F	301	SAH	N3-C4-N9	2.92	132.13	127.17
2	H	301	SAH	C5-N7-C8	2.90	108.00	103.45
2	G	301	SAH	N3-C4-N9	2.87	132.05	127.17
2	R	301	SAH	N3-C4-N9	2.83	131.99	127.17
2	P	301	SAH	N3-C4-N9	2.82	131.97	127.17
2	B	302	SAH	OXT-C-O	-2.82	117.69	124.08
2	K	301	SAH	OXT-C-O	-2.82	117.69	124.08
2	E	301	SAH	OXT-C-O	-2.81	117.70	124.08
2	L	301	SAH	OXT-C-O	-2.73	117.89	124.08
2	H	301	SAH	OXT-C-O	-2.72	117.91	124.08
2	A	301	SAH	N3-C4-N9	2.71	131.78	127.17
2	I	301	SAH	N3-C4-N9	2.71	131.77	127.17
2	O	301	SAH	OXT-C-O	-2.70	117.95	124.08
2	D	301	SAH	OXT-C-O	-2.69	117.97	124.08
2	G	301	SAH	OXT-C-O	-2.63	118.12	124.08
2	A	301	SAH	C4-C5-N7	-2.62	107.59	110.58
2	I	301	SAH	OXT-C-O	-2.60	118.19	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	301	SAH	OXT-C-O	-2.59	118.19	124.08
2	N	301	SAH	OXT-C-O	-2.59	118.21	124.08
2	A	301	SAH	C4-N9-C8	2.58	108.45	105.74
2	Q	301	SAH	N3-C4-N9	2.58	131.55	127.17
2	J	301	SAH	OXT-C-O	-2.51	118.38	124.08
2	E	301	SAH	N3-C4-N9	2.51	131.44	127.17
2	O	301	SAH	C4-C5-N7	-2.47	107.76	110.58
2	I	301	SAH	C4-N9-C8	2.46	108.32	105.74
2	Q	301	SAH	OXT-C-O	-2.44	118.53	124.08
2	Q	301	SAH	C4-C5-N7	-2.44	107.80	110.58
2	B	301	SAH	C4-N9-C8	2.42	108.28	105.74
2	C	301	SAH	OXT-C-O	-2.42	118.58	124.08
2	M	301	SAH	C4-C5-N7	-2.42	107.82	110.58
2	R	301	SAH	OXT-C-O	-2.42	118.59	124.08
2	P	301	SAH	C4-C5-N7	-2.42	107.82	110.58
2	G	301	SAH	C4-C5-N7	-2.41	107.83	110.58
2	E	301	SAH	C4-C5-N7	-2.41	107.83	110.58
2	J	301	SAH	C4-C5-N7	-2.38	107.86	110.58
2	D	301	SAH	C4-C5-N7	-2.37	107.87	110.58
2	I	301	SAH	C4-C5-N7	-2.36	107.89	110.58
2	B	302	SAH	C4-C5-N7	-2.33	107.92	110.58
2	F	301	SAH	C4-N9-C8	2.30	108.15	105.74
2	H	301	SAH	C5'-C4'-C3'	-2.29	109.34	115.06
2	O	301	SAH	O4'-C1'-N9	2.27	112.45	108.09
2	R	301	SAH	C4-C5-N7	-2.27	107.99	110.58
2	B	301	SAH	OXT-C-O	-2.22	119.05	124.08
2	H	301	SAH	C4-N9-C8	2.21	108.06	105.74
2	F	301	SAH	C6-C5-C4	2.21	120.19	117.18
2	D	301	SAH	C4-N9-C8	2.20	108.05	105.74
2	K	301	SAH	C4-C5-N7	-2.19	108.08	110.58
2	B	301	SAH	C4-C5-N7	-2.18	108.08	110.58
2	N	301	SAH	C4-C5-N7	-2.18	108.09	110.58
2	B	302	SAH	O4'-C4'-C5'	2.18	114.44	108.83
2	F	301	SAH	O4'-C1'-N9	2.15	112.22	108.09
2	L	301	SAH	C4-C5-N7	-2.13	108.14	110.58
2	B	302	SAH	C6-C5-C4	2.12	120.07	117.18
2	P	301	SAH	C3'-C2'-C1'	2.09	105.41	101.46
2	K	301	SAH	C4-N9-C8	2.07	107.91	105.74
2	C	301	SAH	C4-N9-C8	2.07	107.91	105.74
2	F	301	SAH	OXT-C-O	-2.06	119.41	124.08
2	L	301	SAH	C6-C5-C4	2.05	119.97	117.18
2	P	301	SAH	C6-C5-C4	2.04	119.97	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	301	SAH	C3'-C2'-C1'	2.03	105.30	101.46
2	M	301	SAH	C4-N9-C8	2.03	107.86	105.74
2	J	301	SAH	C4-N9-C8	2.01	107.85	105.74

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	302	SAH	N-CA-CB-CG
2	E	301	SAH	C-CA-CB-CG
2	I	301	SAH	C-CA-CB-CG
2	O	301	SAH	C-CA-CB-CG
2	P	301	SAH	N-CA-CB-CG
2	P	301	SAH	C-CA-CB-CG
2	R	301	SAH	N-CA-CB-CG
2	R	301	SAH	C-CA-CB-CG
2	B	302	SAH	C-CA-CB-CG
2	Q	301	SAH	C-CA-CB-CG
2	B	302	SAH	C2'-C1'-N9-C8
2	B	302	SAH	C2'-C1'-N9-C4
2	B	302	SAH	O-C-CA-CB
2	B	302	SAH	OXT-C-CA-CB
2	A	301	SAH	C-CA-CB-CG
2	D	301	SAH	C-CA-CB-CG
2	F	301	SAH	C-CA-CB-CG
2	G	301	SAH	C-CA-CB-CG
2	H	301	SAH	C-CA-CB-CG
2	K	301	SAH	C-CA-CB-CG
2	L	301	SAH	C-CA-CB-CG
2	M	301	SAH	C-CA-CB-CG
2	E	301	SAH	N-CA-CB-CG
2	I	301	SAH	N-CA-CB-CG
2	O	301	SAH	N-CA-CB-CG
2	Q	301	SAH	N-CA-CB-CG
2	H	301	SAH	CB-CG-SD-C5'
2	P	301	SAH	CB-CG-SD-C5'
2	B	302	SAH	O4'-C4'-C5'-SD
2	M	301	SAH	CB-CG-SD-C5'
2	B	301	SAH	C-CA-CB-CG
2	C	301	SAH	C-CA-CB-CG
2	J	301	SAH	C-CA-CB-CG
2	N	301	SAH	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	L	301	SAH	CB-CG-SD-C5'
2	B	301	SAH	O-C-CA-N
2	H	301	SAH	O-C-CA-N
2	O	301	SAH	O-C-CA-N
2	D	301	SAH	CB-CG-SD-C5'
2	N	301	SAH	CB-CG-SD-C5'
2	R	301	SAH	CB-CG-SD-C5'
2	O	301	SAH	CB-CG-SD-C5'
2	Q	301	SAH	CB-CG-SD-C5'
2	B	302	SAH	CB-CG-SD-C5'
2	O	301	SAH	C2'-C1'-N9-C8
2	D	301	SAH	O-C-CA-N

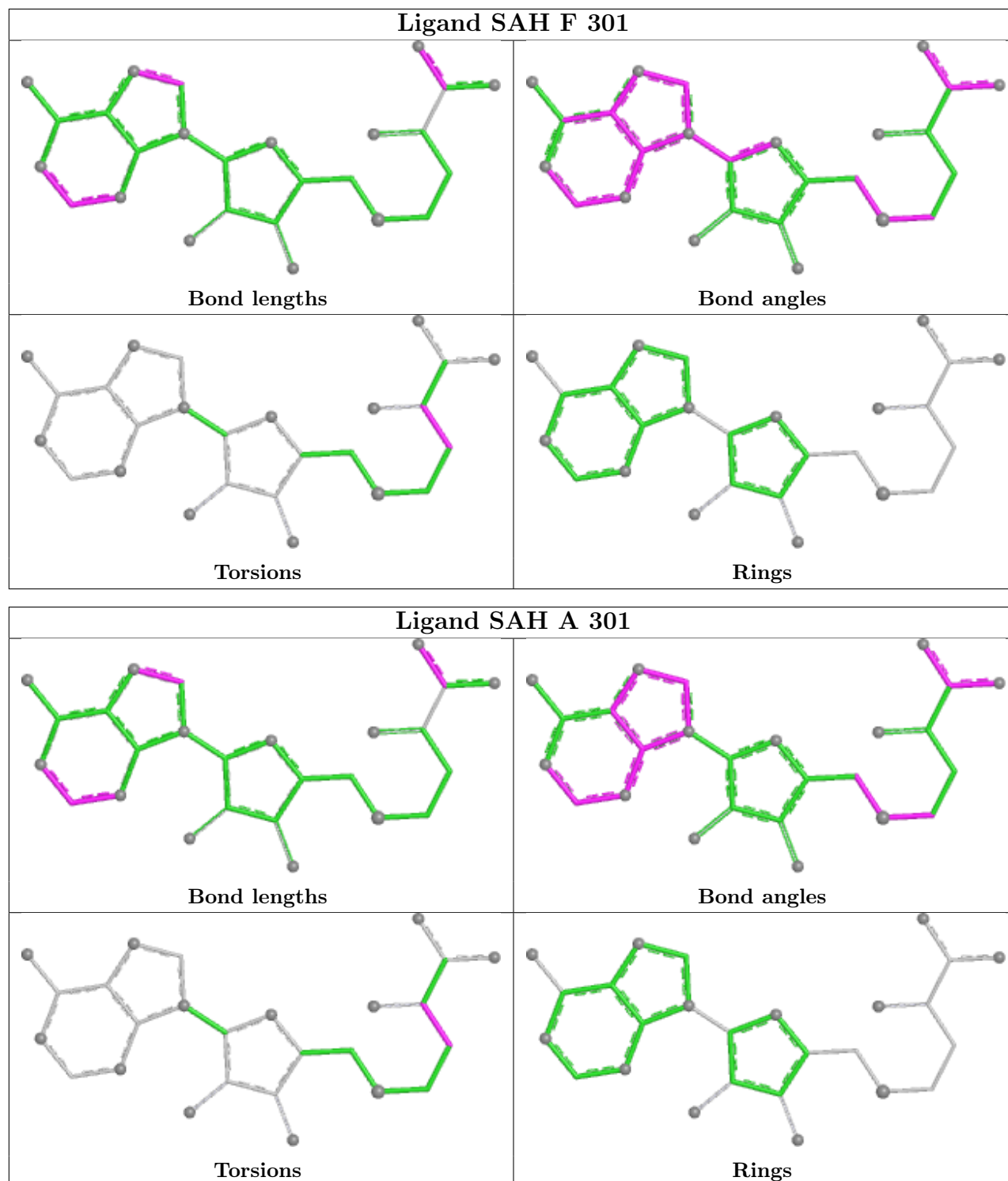
There are no ring outliers.

17 monomers are involved in 34 short contacts:

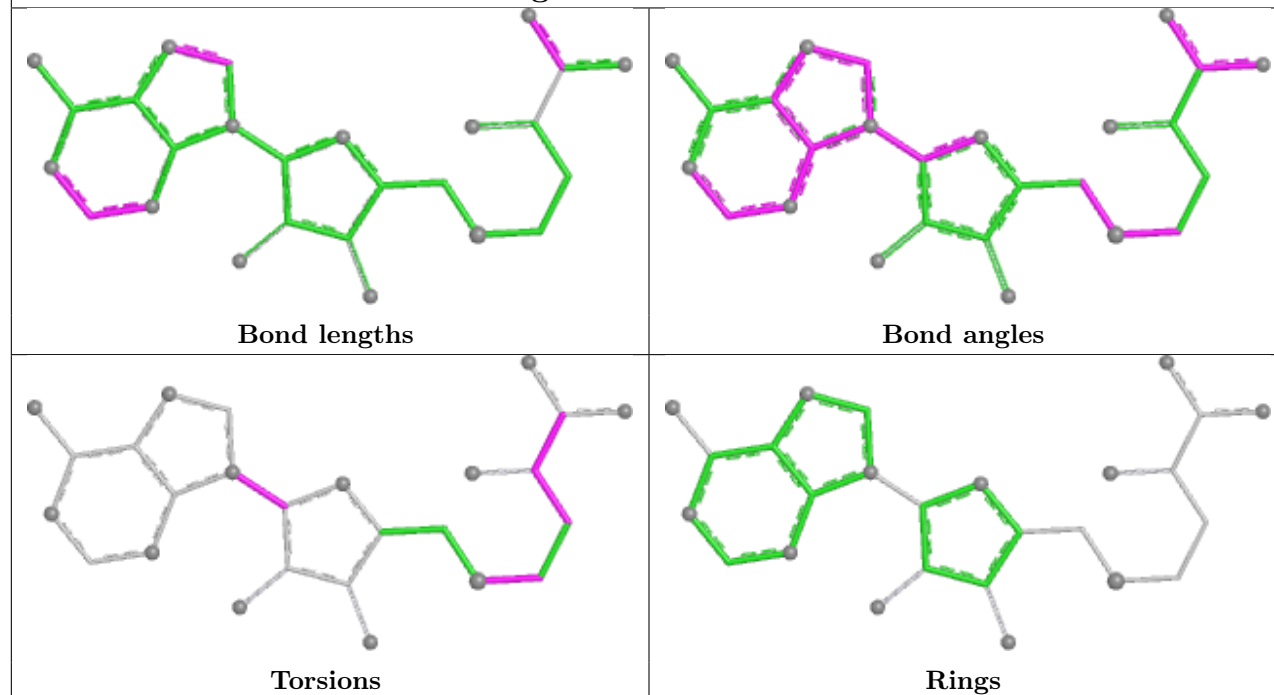
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	SAH	1	0
2	A	301	SAH	1	0
2	O	301	SAH	2	0
2	L	301	SAH	4	0
2	E	301	SAH	1	0
2	C	301	SAH	1	0
2	R	301	SAH	1	0
2	D	301	SAH	3	0
2	B	301	SAH	3	0
2	P	301	SAH	3	0
2	M	301	SAH	1	0
2	K	301	SAH	3	0
2	B	302	SAH	1	0
2	N	301	SAH	4	0
2	H	301	SAH	1	0
2	G	301	SAH	1	0
2	J	301	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 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

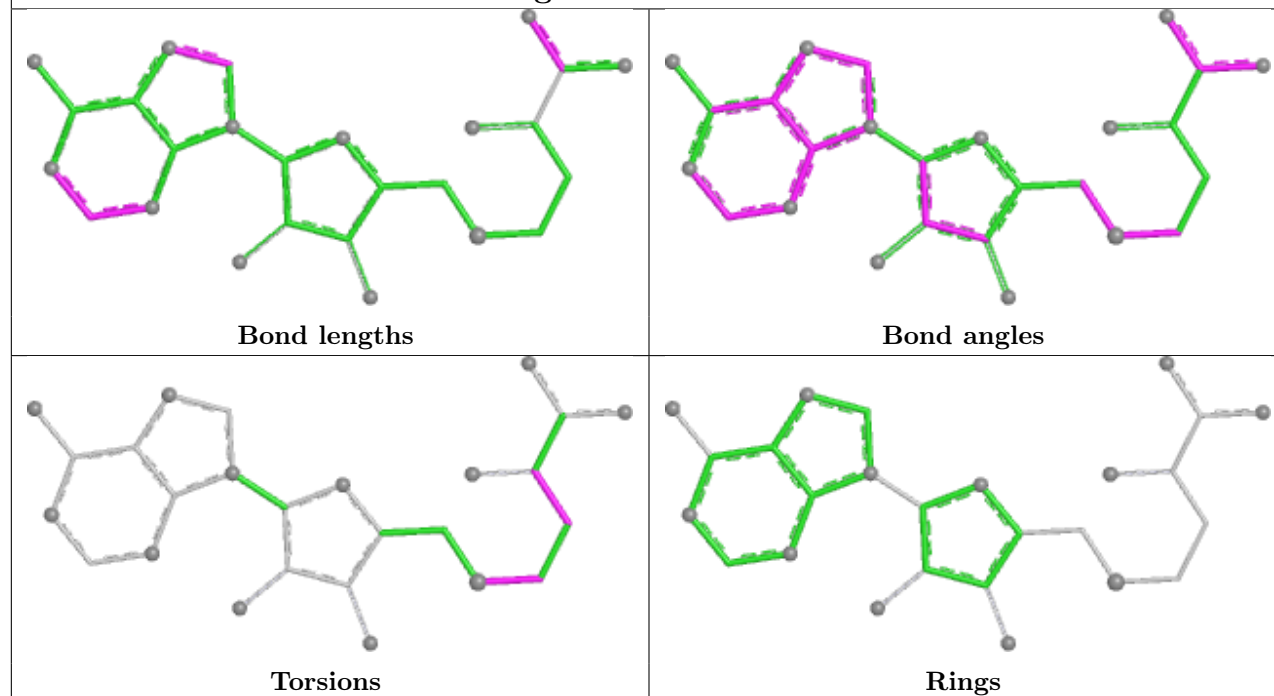
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



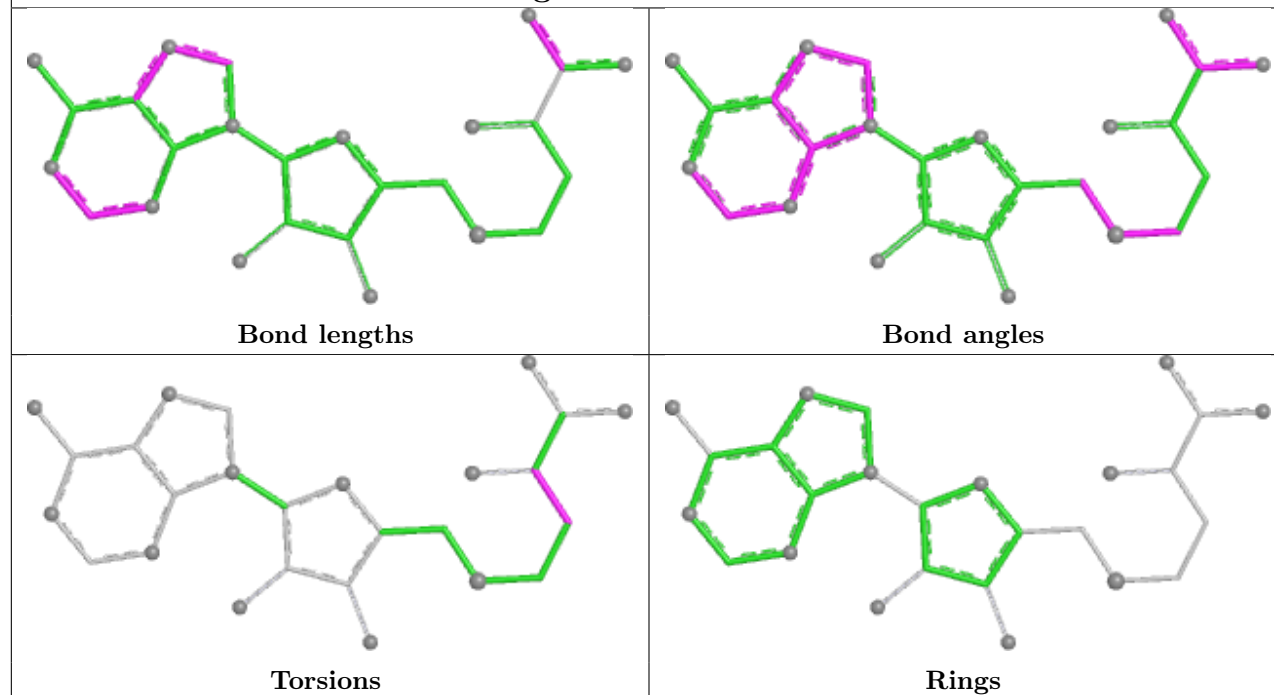
Ligand SAH O 301



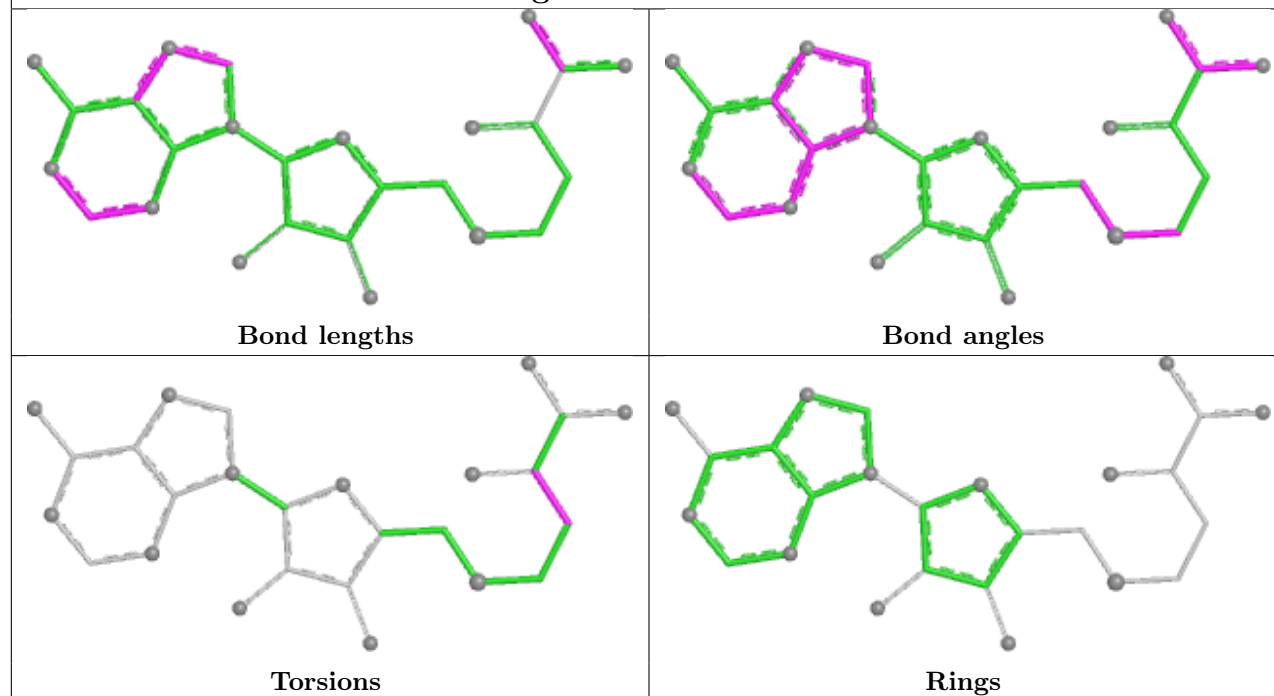
Ligand SAH L 301



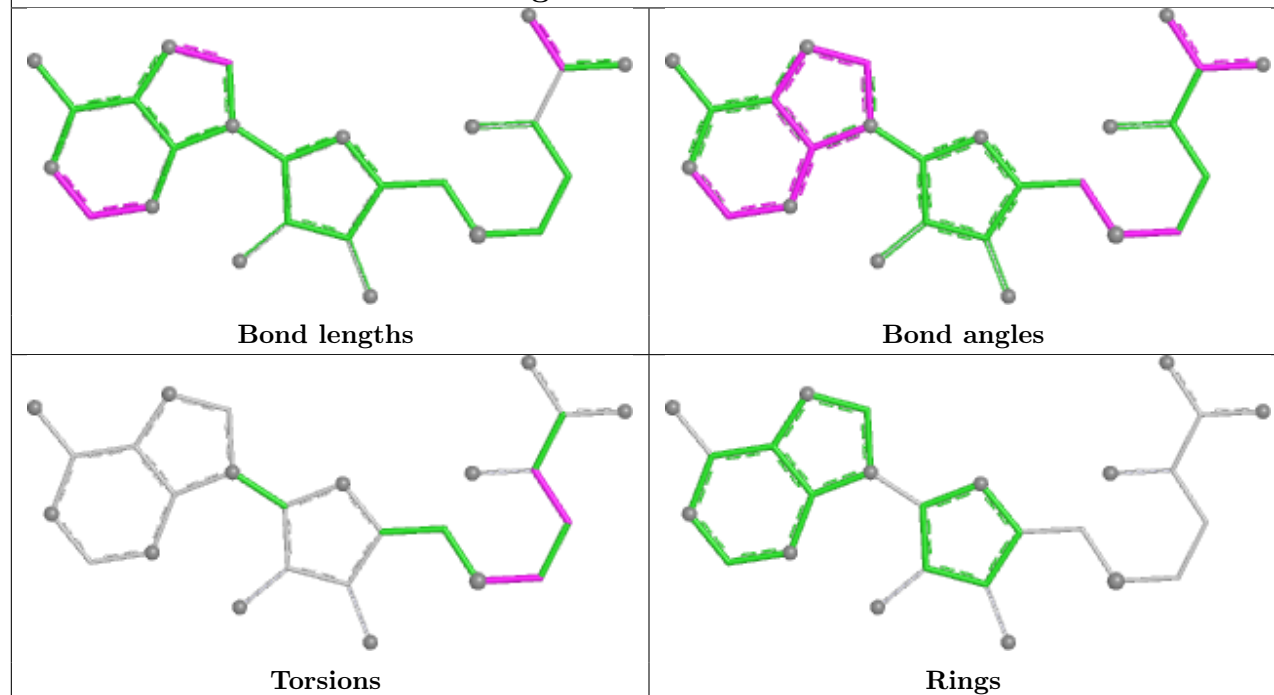
Ligand SAH E 301



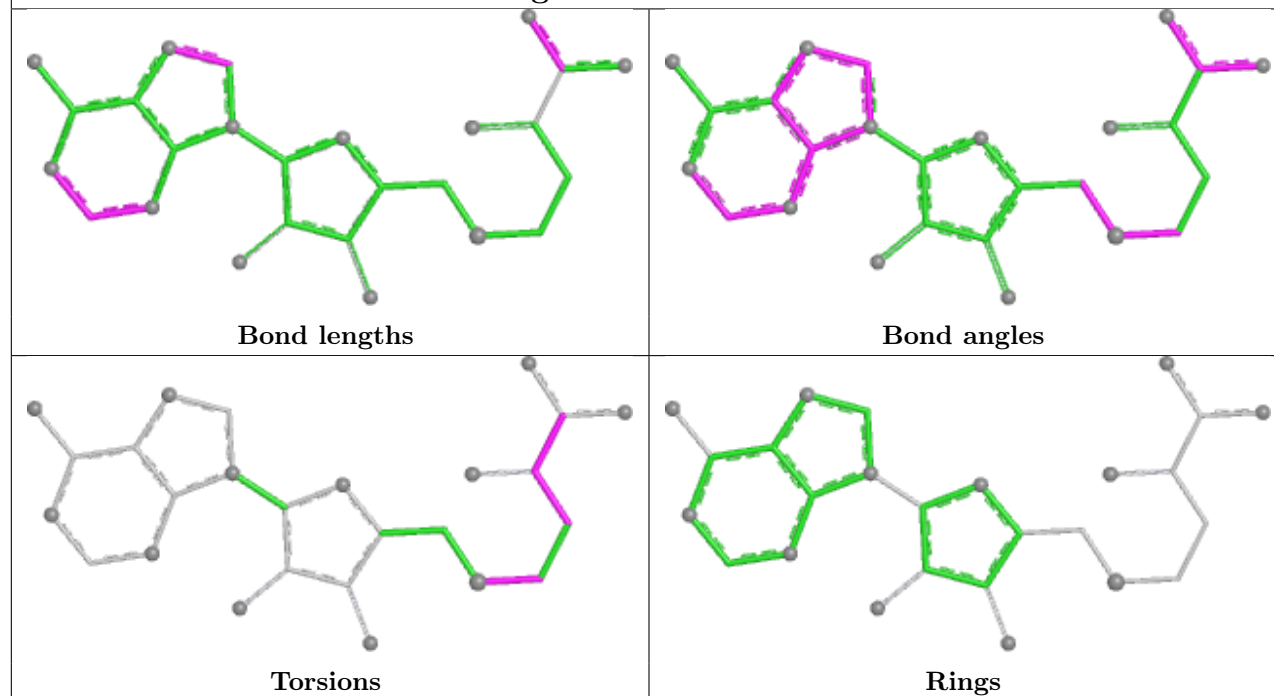
Ligand SAH C 301

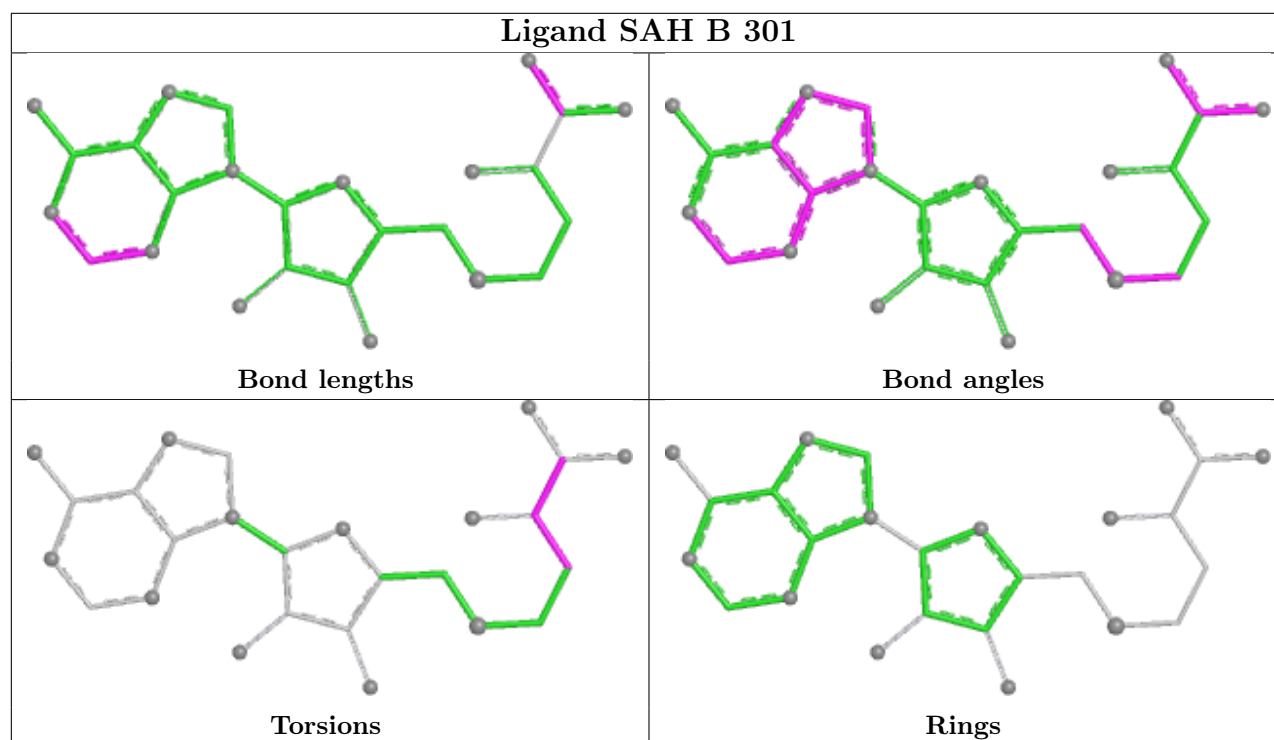
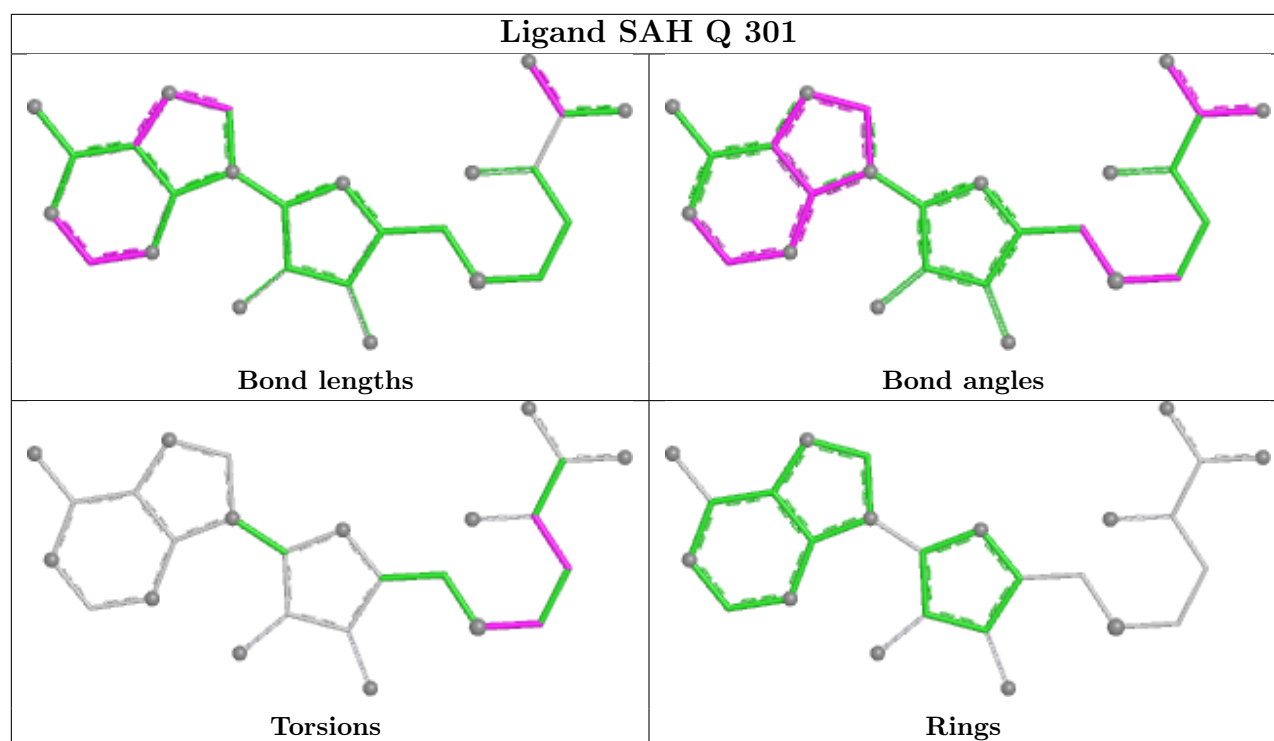


Ligand SAH R 301

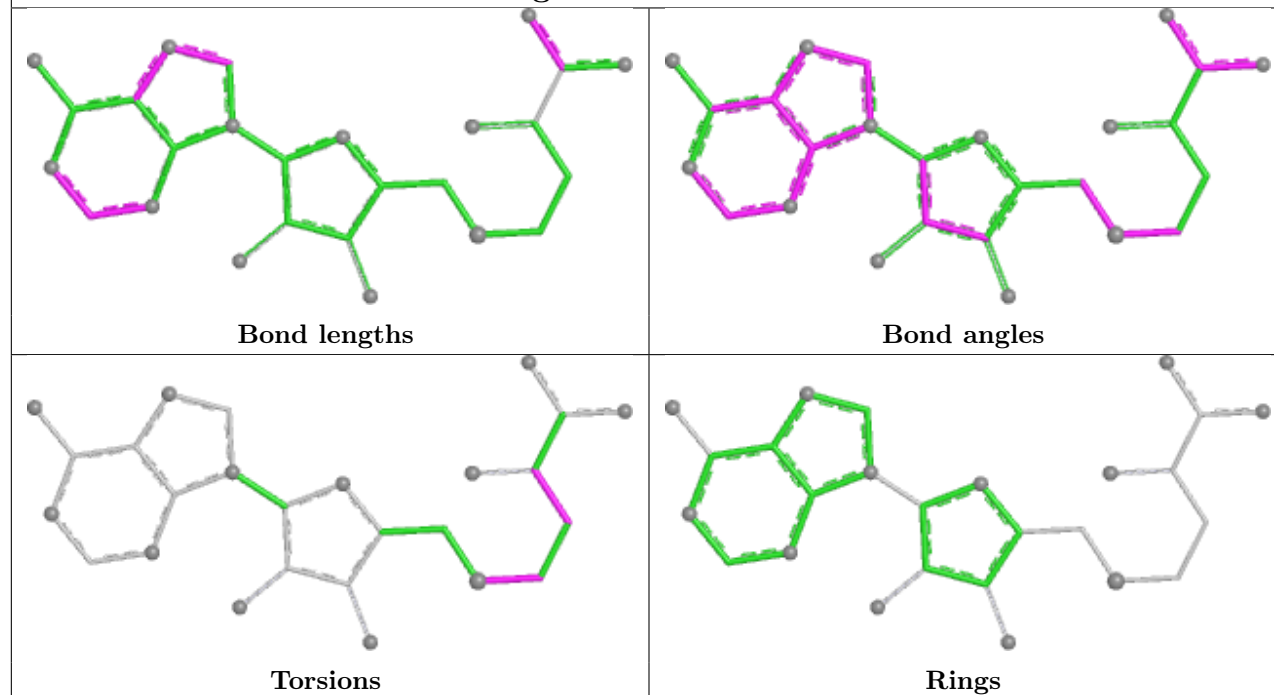


Ligand SAH D 301

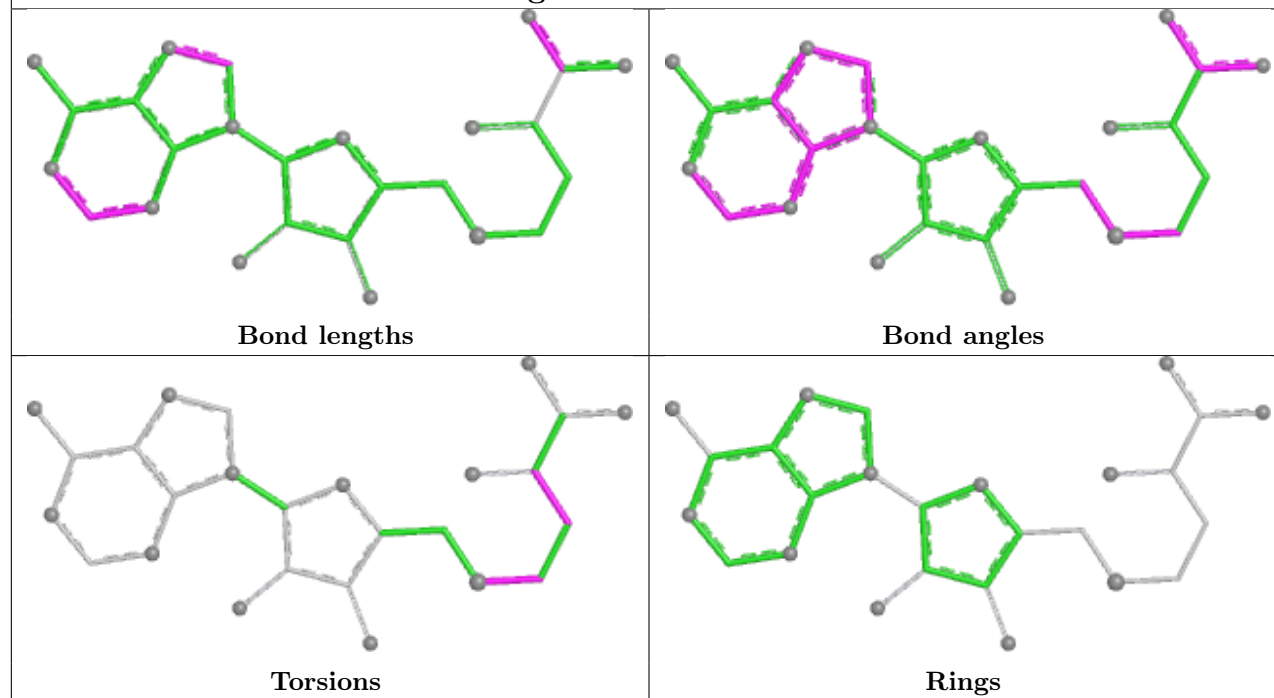


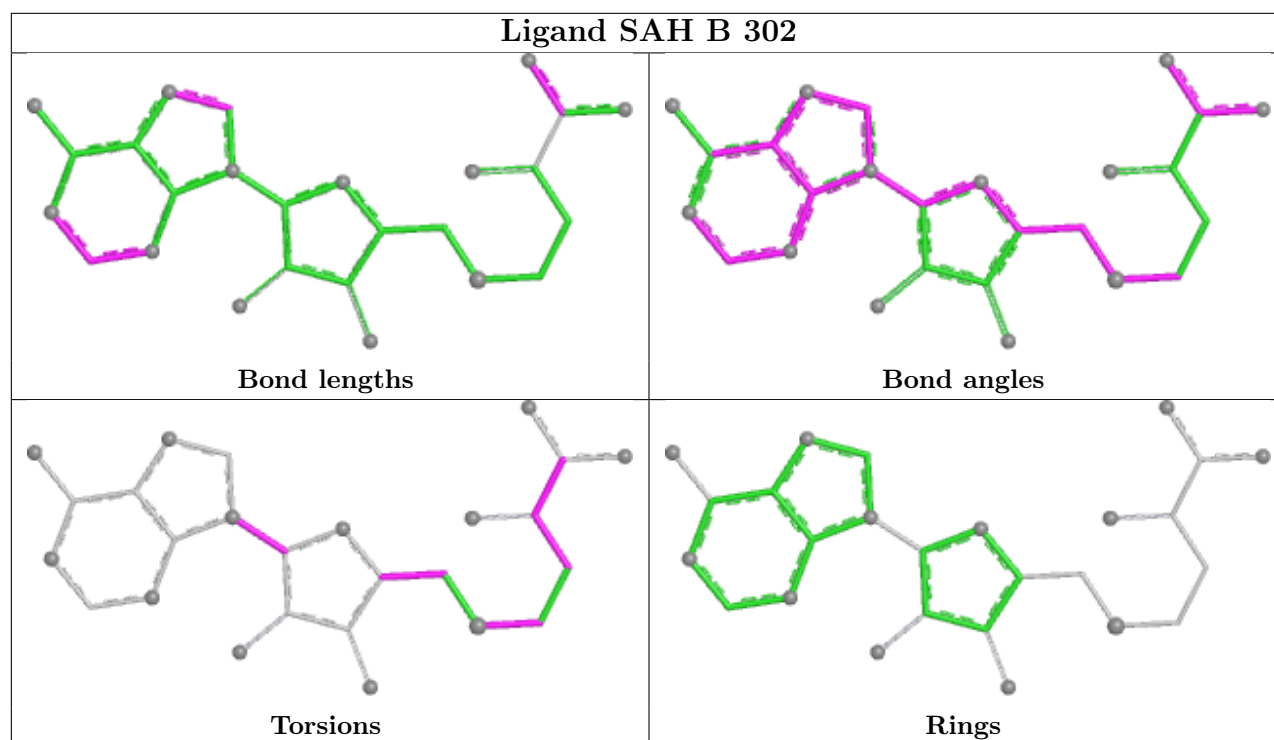
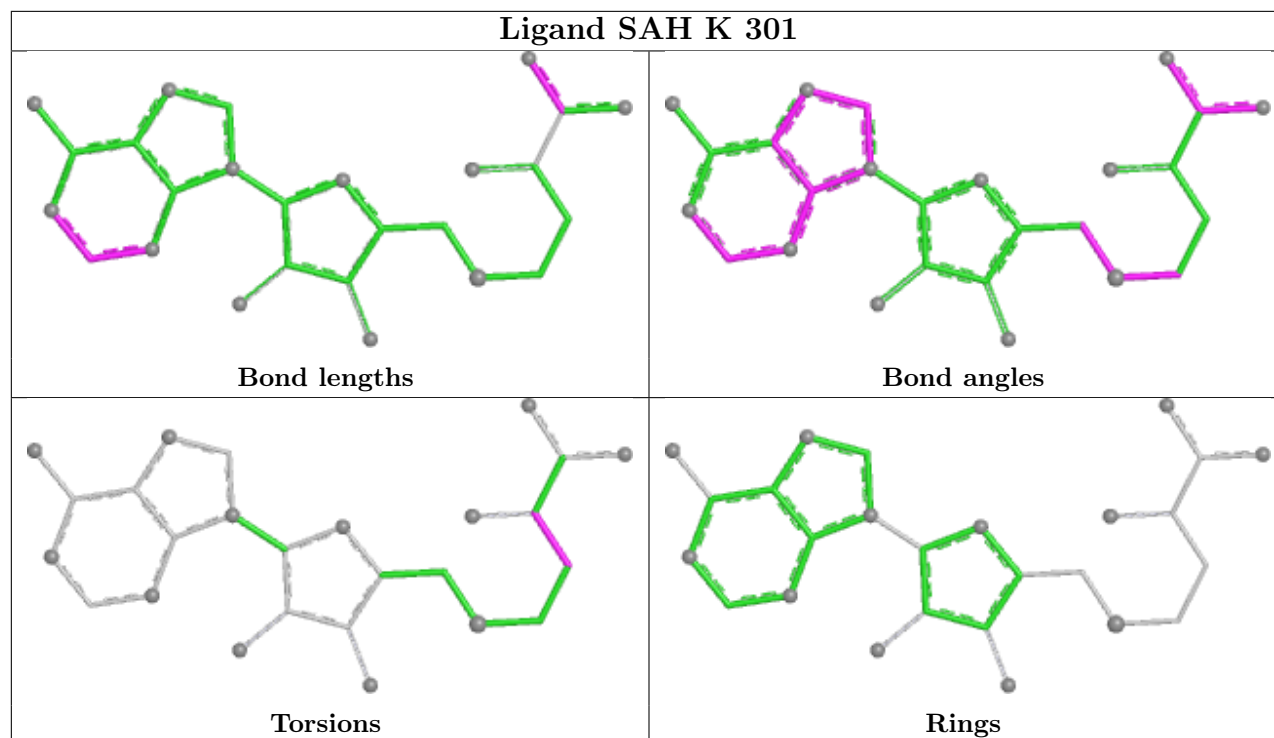


Ligand SAH P 301

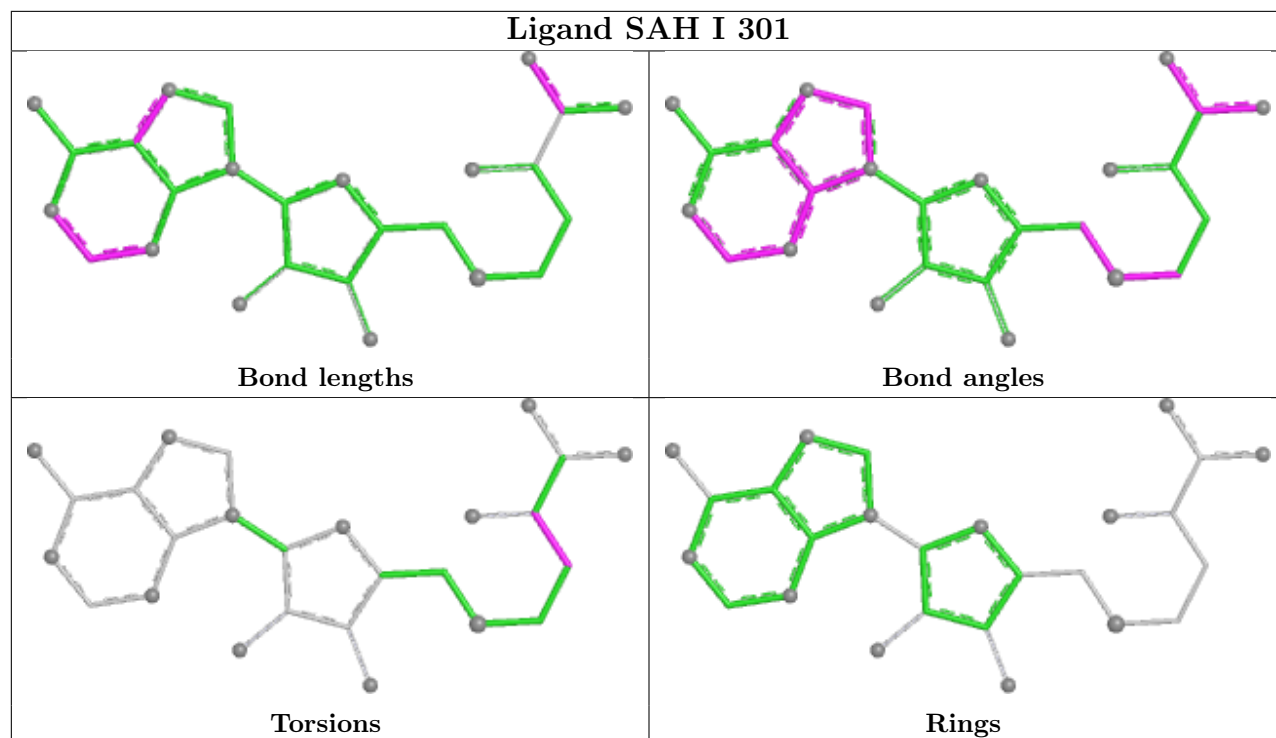


Ligand SAH M 301

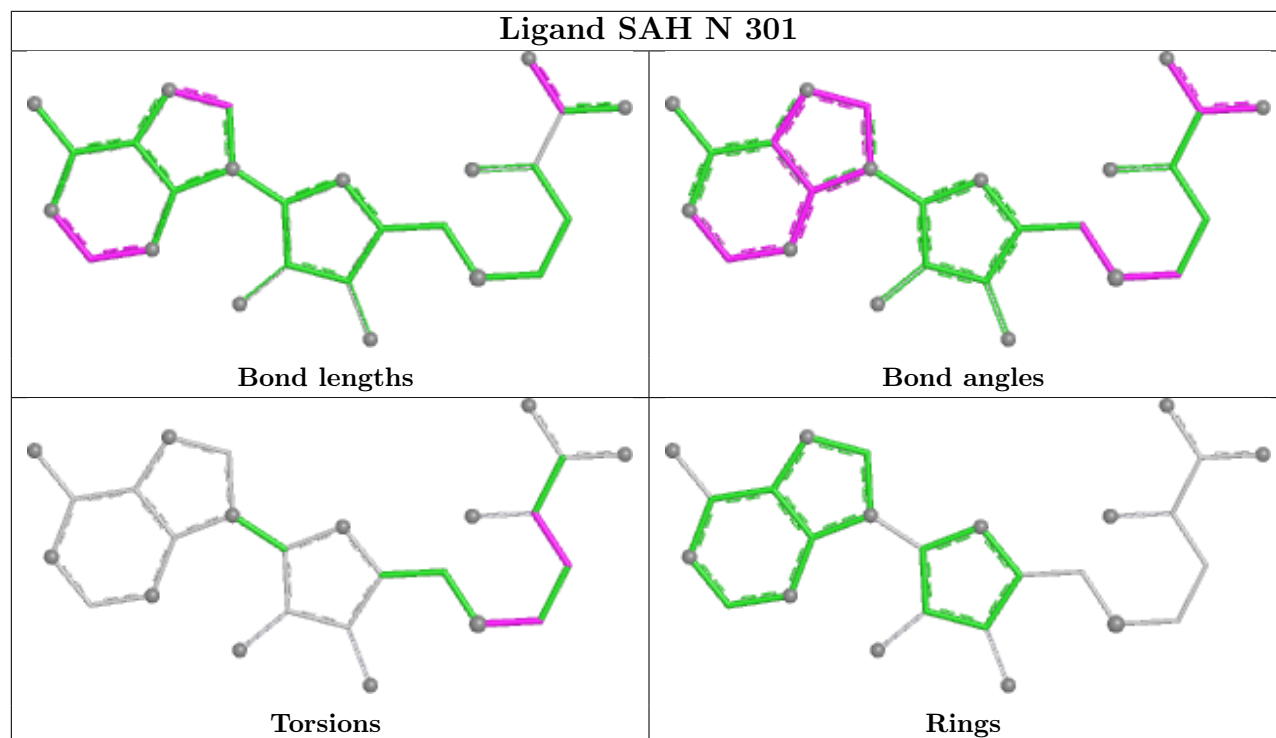


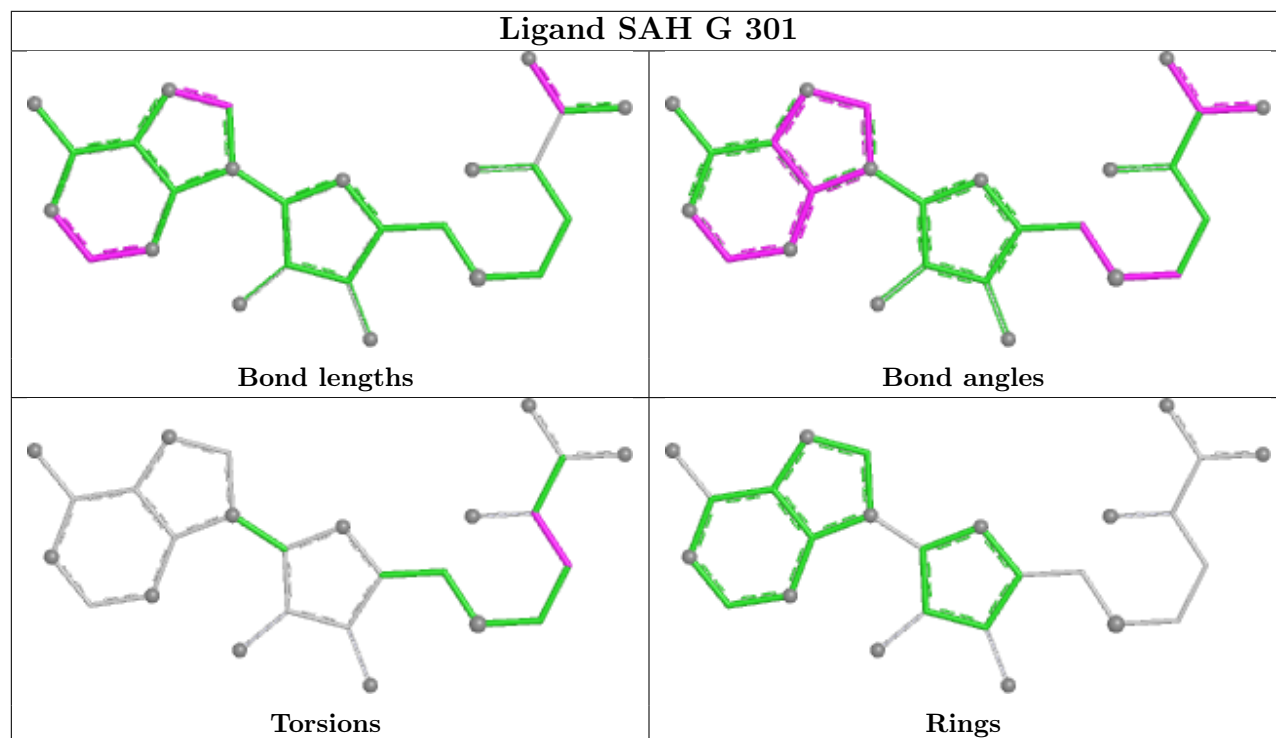
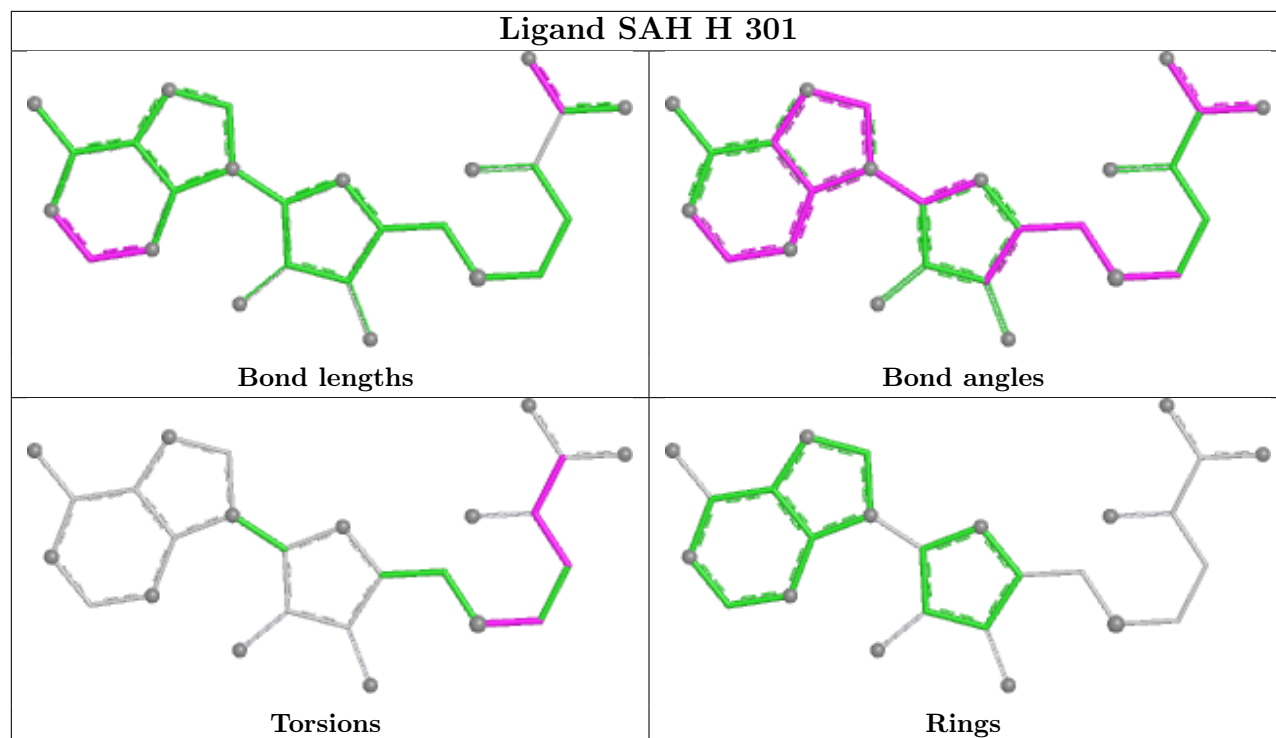


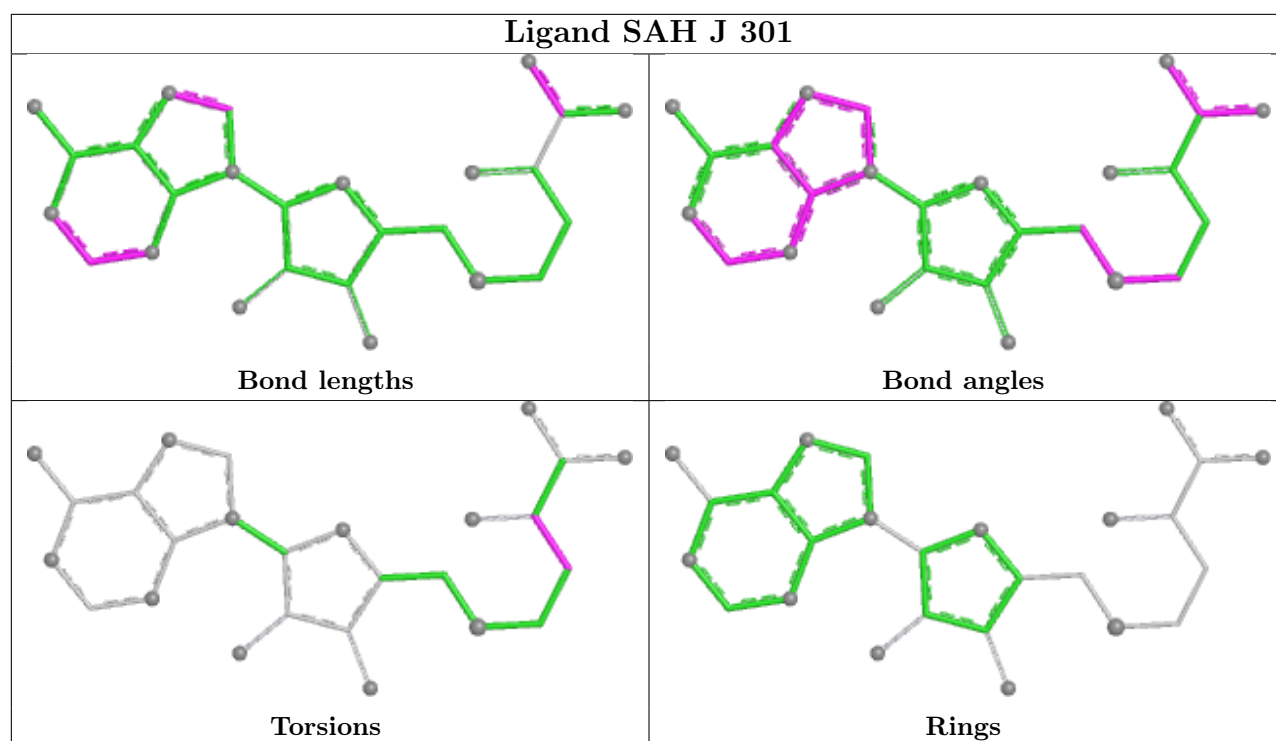
Ligand SAH I 301



Ligand SAH N 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 ⓘ

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	281/297 (94%)	-0.34	3 (1%) 78 75	24, 45, 71, 105	2 (0%)
1	B	280/297 (94%)	-0.07	0 100 100	26, 49, 77, 95	1 (0%)
1	C	280/297 (94%)	0.10	5 (1%) 67 64	38, 61, 87, 101	0
1	D	280/297 (94%)	0.02	2 (0%) 84 81	26, 60, 86, 101	1 (0%)
1	E	279/297 (93%)	-0.01	1 (0%) 88 86	30, 56, 77, 94	0
1	F	280/297 (94%)	-0.26	1 (0%) 88 86	28, 49, 75, 102	0
1	G	280/297 (94%)	0.65	16 (5%) 29 26	53, 85, 122, 138	0
1	H	279/297 (93%)	1.05	35 (12%) 8 6	64, 99, 123, 137	0
1	I	280/297 (94%)	-0.27	1 (0%) 88 86	19, 47, 96, 132	2 (0%)
1	J	281/297 (94%)	0.46	7 (2%) 58 54	35, 85, 113, 133	0
1	K	281/297 (94%)	0.42	9 (3%) 50 46	46, 76, 117, 127	0
1	L	280/297 (94%)	0.64	13 (4%) 37 33	51, 88, 120, 147	0
1	M	281/297 (94%)	0.31	14 (4%) 34 30	35, 63, 141, 169	2 (0%)
1	N	281/297 (94%)	1.39	65 (23%) 2 1	37, 107, 137, 152	2 (0%)
1	O	280/297 (94%)	0.26	7 (2%) 58 54	36, 70, 100, 124	0
1	P	280/297 (94%)	0.41	3 (1%) 78 75	42, 78, 105, 116	0
1	Q	281/297 (94%)	0.78	38 (13%) 7 5	36, 76, 159, 191	2 (0%)
1	R	281/297 (94%)	2.17	151 (53%) 0 0	62, 115, 149, 173	1 (0%)
All	All	5045/5346 (94%)	0.43	371 (7%) 20 18	19, 70, 124, 191	13 (0%)

All (371) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	104	THR	5.8
1	R	151	ALA	5.4
1	R	289	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
1	R	102	ALA	4.9
1	R	149	ALA	4.8
1	Q	11	GLN	4.6
1	R	164	LEU	4.6
1	N	289	VAL	4.5
1	R	106	VAL	4.5
1	P	289	VAL	4.5
1	R	148	CYS	4.4
1	R	136	ALA	4.3
1	M	17	VAL	4.3
1	Q	25	GLY	4.3
1	R	141	TYR	4.1
1	H	289	VAL	4.1
1	R	42	PHE	4.1
1	N	175	GLY	4.1
1	R	84	ILE	4.0
1	R	168	TRP	4.0
1	R	179	VAL	3.9
1	J	289	VAL	3.9
1	Q	20	TRP	3.9
1	Q	36	VAL	3.9
1	M	25	GLY	3.8
1	Q	14	ALA	3.8
1	F	289	VAL	3.8
1	Q	12	VAL	3.8
1	R	85	GLY	3.8
1	N	121	ALA	3.8
1	N	211	PHE	3.8
1	R	155	LEU	3.8
1	Q	289	VAL	3.7
1	R	116	ALA	3.7
1	R	77	ALA	3.7
1	H	125	LEU	3.7
1	R	49	PRO	3.7
1	Q	21	TYR	3.7
1	R	55	VAL	3.7
1	R	243	VAL	3.6
1	R	212	PHE	3.6
1	R	82	LEU	3.6
1	M	21	TYR	3.6
1	Q	27	VAL	3.6
1	R	139	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	R	200	TYR	3.6
1	N	133	VAL	3.6
1	C	290	LEU	3.6
1	E	289	VAL	3.5
1	N	218	ALA	3.5
1	R	171	LEU	3.5
1	R	121	ALA	3.5
1	R	70	ILE	3.5
1	R	218	ALA	3.4
1	N	141	TYR	3.4
1	R	108	VAL	3.4
1	Q	248	ALA	3.4
1	R	152	ILE	3.4
1	D	289	VAL	3.4
1	N	106	VAL	3.4
1	R	208	LEU	3.4
1	Q	24	PHE	3.3
1	Q	30	LEU	3.3
1	R	75	PRO	3.3
1	R	146	PHE	3.3
1	G	289	VAL	3.3
1	N	146	PHE	3.3
1	M	28	TYR	3.3
1	R	204	VAL	3.3
1	N	104	THR	3.3
1	R	211	PHE	3.3
1	R	125	LEU	3.3
1	R	241	LEU	3.3
1	R	273	LEU	3.3
1	R	154	SER	3.2
1	N	128	ARG	3.2
1	I	289	VAL	3.2
1	R	73	LEU	3.2
1	Q	17	VAL	3.2
1	H	124	GLY	3.2
1	N	134	ALA	3.2
1	R	236	MET	3.2
1	R	124	GLY	3.2
1	R	175	GLY	3.2
1	R	101	ILE	3.2
1	N	200	TYR	3.2
1	M	289	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	R	170	VAL	3.2
1	R	188	LEU	3.1
1	R	266	LEU	3.1
1	R	214	ILE	3.1
1	R	107	ALA	3.1
1	R	156	CYS	3.1
1	R	63	ASP	3.1
1	R	129	LEU	3.1
1	R	97	ARG	3.1
1	H	114	ALA	3.1
1	M	9	GLN	3.1
1	R	147	ASP	3.1
1	C	289	VAL	3.1
1	H	126	THR	3.1
1	R	95	ALA	3.1
1	R	180	LEU	3.1
1	R	103	VAL	3.1
1	L	244	TYR	3.0
1	R	160	ARG	3.0
1	O	289	VAL	3.0
1	R	215	VAL	3.0
1	N	212	PHE	3.0
1	R	131	PHE	3.0
1	R	250	PHE	3.0
1	N	174	GLY	3.0
1	Q	13	THR	3.0
1	N	220	PHE	3.0
1	H	133	VAL	3.0
1	R	150	TRP	3.0
1	K	21	TYR	3.0
1	N	119	LEU	3.0
1	Q	32	LEU	3.0
1	N	131	PHE	3.0
1	Q	274	ILE	2.9
1	Q	45	ASP	2.9
1	R	51	ASP	2.9
1	R	167	ALA	2.9
1	L	108	VAL	2.9
1	R	133	VAL	2.9
1	G	256	ALA	2.9
1	R	78	GLY	2.9
1	R	181	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	R	120	ALA	2.9
1	R	161	ALA	2.9
1	R	269	ALA	2.9
1	K	290	LEU	2.9
1	G	51	ASP	2.9
1	Q	33	GLY	2.9
1	R	216	SER	2.8
1	N	86	CYS	2.8
1	R	198	THR	2.8
1	R	178	LEU	2.8
1	R	262	LEU	2.8
1	H	131	PHE	2.8
1	A	289	VAL	2.8
1	G	36	VAL	2.8
1	N	140	PRO	2.8
1	R	130	THR	2.8
1	M	10	GLN	2.8
1	R	94	LYS	2.8
1	H	87	GLY	2.8
1	R	105	GLY	2.8
1	J	107	ALA	2.8
1	N	239	PHE	2.8
1	R	145	SER	2.8
1	R	66	THR	2.8
1	R	126	THR	2.8
1	R	194	ALA	2.8
1	R	195	LEU	2.8
1	Q	236	MET	2.8
1	K	289	VAL	2.7
1	R	48	VAL	2.7
1	R	153	GLU	2.7
1	R	80	HIS	2.7
1	N	204	VAL	2.7
1	Q	31	THR	2.7
1	R	157	HIS	2.7
1	L	51	ASP	2.7
1	G	21	TYR	2.7
1	R	93	LEU	2.7
1	R	137	MET	2.7
1	H	120	ALA	2.7
1	N	208	LEU	2.7
1	R	57	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	20	TRP	2.7
1	H	121	ALA	2.7
1	L	87	GLY	2.6
1	Q	23	LYS	2.6
1	R	274	ILE	2.6
1	N	259	VAL	2.6
1	R	96	ALA	2.6
1	R	256	ALA	2.6
1	N	184	VAL	2.6
1	Q	26	GLU	2.6
1	H	88	THR	2.6
1	N	136	ALA	2.6
1	R	50	GLN	2.6
1	R	201	ALA	2.6
1	R	248	ALA	2.6
1	G	244	TYR	2.6
1	N	244	TYR	2.6
1	G	191	PRO	2.6
1	J	108	VAL	2.6
1	H	256	ALA	2.6
1	C	200	TYR	2.6
1	Q	28	TYR	2.6
1	R	65	TYR	2.6
1	R	87	GLY	2.6
1	H	263	LEU	2.6
1	R	30	LEU	2.6
1	N	182	SER	2.6
1	Q	52[A]	MET	2.5
1	R	205	PRO	2.5
1	K	25	GLY	2.5
1	R	127	GLU	2.5
1	R	279	PHE	2.5
1	R	270[A]	GLN	2.5
1	Q	41	TRP	2.5
1	M	36	VAL	2.5
1	J	88	THR	2.5
1	R	56	THR	2.5
1	K	190	GLU	2.5
1	L	289	VAL	2.5
1	M	12	VAL	2.5
1	G	38	CYS	2.4
1	H	105	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	R	132	GLU	2.4
1	R	190	GLU	2.4
1	N	274	ILE	2.4
1	H	119	LEU	2.4
1	N	223	LEU	2.4
1	R	220	PHE	2.4
1	H	117	ASN	2.4
1	N	103	VAL	2.4
1	R	183	VAL	2.4
1	R	88	THR	2.4
1	R	140	PRO	2.4
1	M	23	LYS	2.4
1	A	51	ASP	2.4
1	H	129	LEU	2.4
1	R	68	TYR	2.4
1	R	123	HIS	2.4
1	H	118	ARG	2.4
1	N	254	PHE	2.4
1	M	201	ALA	2.4
1	R	249	GLU	2.4
1	N	255	GLY	2.4
1	A	10	GLN	2.4
1	M	11	GLN	2.4
1	N	188	LEU	2.4
1	Q	266	LEU	2.4
1	R	119	LEU	2.4
1	Q	37	HIS	2.4
1	N	279	PHE	2.4
1	H	137	MET	2.4
1	K	17	VAL	2.4
1	R	112	GLN	2.4
1	R	135	ASP	2.4
1	H	250	PHE	2.4
1	N	196	PHE	2.4
1	Q	258	PHE	2.4
1	Q	204	VAL	2.4
1	H	110	LYS	2.4
1	L	256	ALA	2.4
1	N	132	GLU	2.4
1	C	126	THR	2.3
1	N	164	LEU	2.3
1	N	273	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	R	199	LEU	2.3
1	R	254	PHE	2.3
1	N	179	VAL	2.3
1	H	134	ALA	2.3
1	N	252	GLU	2.3
1	N	173	PRO	2.3
1	N	105	GLY	2.3
1	R	239	PHE	2.3
1	Q	200	TYR	2.3
1	K	26	GLU	2.3
1	N	288	ALA	2.3
1	R	61	ALA	2.3
1	R	202	ALA	2.3
1	G	35	SER	2.3
1	N	168	TRP	2.3
1	H	123	HIS	2.3
1	R	81	LEU	2.3
1	R	196	PHE	2.3
1	N	14	ALA	2.3
1	R	128	ARG	2.3
1	H	122	GLY	2.3
1	R	224	SER	2.3
1	N	101	ILE	2.3
1	N	139	LEU	2.3
1	G	260	ASP	2.3
1	G	196	PHE	2.3
1	H	259	VAL	2.3
1	R	169	ARG	2.3
1	R	173	PRO	2.3
1	N	110	LYS	2.2
1	R	54	LEU	2.2
1	R	223	LEU	2.2
1	O	212	PHE	2.2
1	Q	43	PRO	2.2
1	J	201	ALA	2.2
1	N	256	ALA	2.2
1	N	264	ALA	2.2
1	R	86	CYS	2.2
1	Q	189	THR	2.2
1	L	255	GLY	2.2
1	R	174	GLY	2.2
1	P	139	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	R	253	ARG	2.2
1	Q	243	VAL	2.2
1	J	134	ALA	2.2
1	H	251	THR	2.2
1	O	200	TYR	2.2
1	Q	9	GLN	2.2
1	R	91	THR	2.2
1	N	125	LEU	2.2
1	R	261	GLY	2.2
1	R	263	LEU	2.2
1	N	205	PRO	2.2
1	N	172	LYS	2.2
1	N	248	ALA	2.2
1	O	218	ALA	2.2
1	O	165	GLY	2.2
1	M	15	ASP	2.2
1	Q	19	ASP	2.2
1	N	150	TRP	2.2
1	Q	254	PHE	2.2
1	R	92	ALA	2.1
1	R	230	ALA	2.1
1	R	19	ASP	2.1
1	R	245	SER	2.1
1	O	211	PHE	2.1
1	H	136	ALA	2.1
1	H	93	LEU	2.1
1	R	69	LEU	2.1
1	R	182	SER	2.1
1	G	212	PHE	2.1
1	N	123	HIS	2.1
1	H	20	TRP	2.1
1	R	240	ALA	2.1
1	R	89	GLY	2.1
1	R	284	LEU	2.1
1	L	88	THR	2.1
1	L	141	TYR	2.1
1	P	200	TYR	2.1
1	H	23	LYS	2.1
1	D	236	MET	2.1
1	Q	29	HIS	2.1
1	Q	196	PHE	2.1
1	G	201	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	202	ALA	2.1
1	R	76	LYS	2.1
1	G	156	CYS	2.1
1	L	140	PRO	2.1
1	L	131	PHE	2.0
1	R	238	VAL	2.0
1	C	121	ALA	2.0
1	R	225	LEU	2.0
1	R	228	LEU	2.0
1	H	100	GLY	2.0
1	H	127	GLU	2.0
1	N	142	GLU	2.0
1	G	198	THR	2.0
1	N	152	ILE	2.0
1	H	173	PRO	2.0
1	H	244	TYR	2.0
1	R	244	TYR	2.0
1	N	145	SER	2.0
1	L	128	ARG	2.0
1	J	180	LEU	2.0
1	K	188	LEU	2.0
1	H	25	GLY	2.0
1	L	25	GLY	2.0
1	N	33	GLY	2.0
1	N	100	GLY	2.0
1	O	219	GLY	2.0
1	R	265	GLY	2.0
1	N	251	THR	2.0
1	R	283	THR	2.0
1	N	236	MET	2.0
1	K	65	TYR	2.0
1	N	221	HIS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

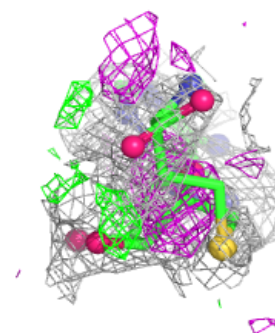
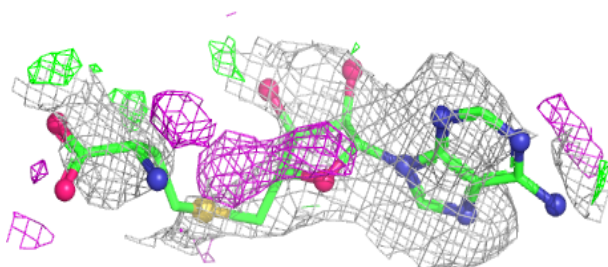
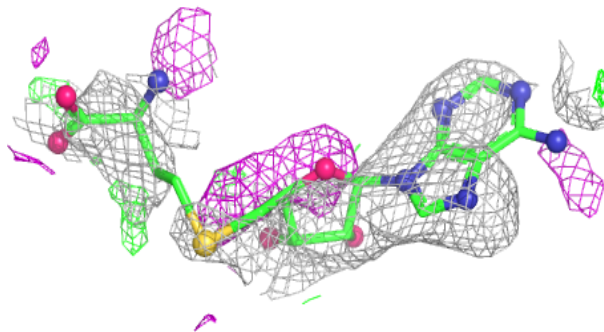
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SAH	R	301	26/26	0.64	0.20	118,121,122,123	0
2	SAH	B	302	26/26	0.73	0.18	105,107,108,108	0
2	SAH	N	301	26/26	0.77	0.18	105,107,108,108	0
2	SAH	H	301	26/26	0.77	0.21	98,102,105,106	0
2	SAH	J	301	26/26	0.87	0.15	88,89,91,91	0
2	SAH	P	301	26/26	0.88	0.14	72,74,75,75	0
2	SAH	K	301	26/26	0.90	0.13	75,79,80,81	0
2	SAH	L	301	26/26	0.91	0.12	85,87,89,89	0
2	SAH	G	301	26/26	0.92	0.11	74,75,77,77	0
2	SAH	Q	301	26/26	0.92	0.10	61,62,64,65	0
2	SAH	O	301	26/26	0.92	0.15	80,82,83,83	0
2	SAH	B	301	26/26	0.93	0.10	49,51,52,53	0
2	SAH	C	301	26/26	0.93	0.11	61,63,64,64	0
2	SAH	M	301	26/26	0.95	0.09	57,61,62,62	0
2	SAH	E	301	26/26	0.95	0.08	48,49,50,50	0
2	SAH	D	301	26/26	0.95	0.09	57,58,59,59	0
2	SAH	A	301	26/26	0.97	0.06	36,38,39,39	0
2	SAH	F	301	26/26	0.97	0.07	34,35,36,37	0
2	SAH	I	301	26/26	0.97	0.05	34,36,37,38	0

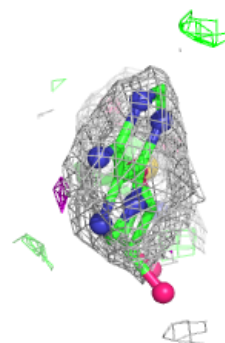
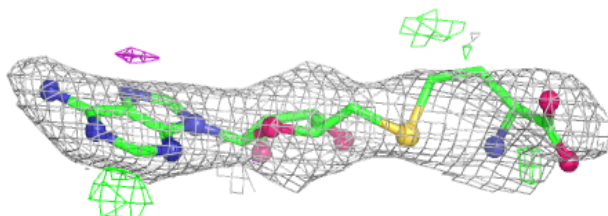
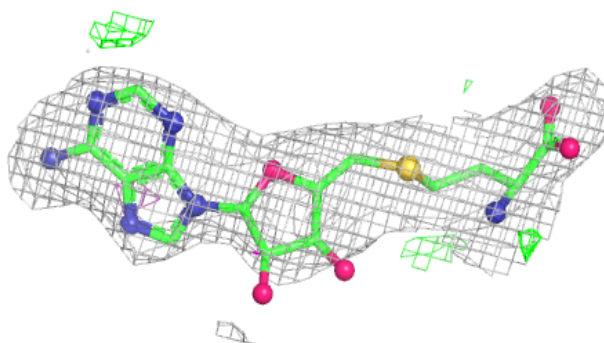
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH R 301:

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

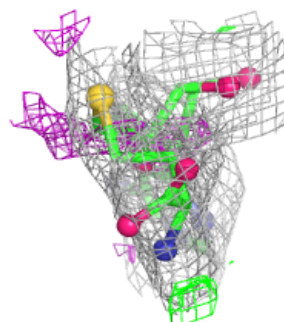
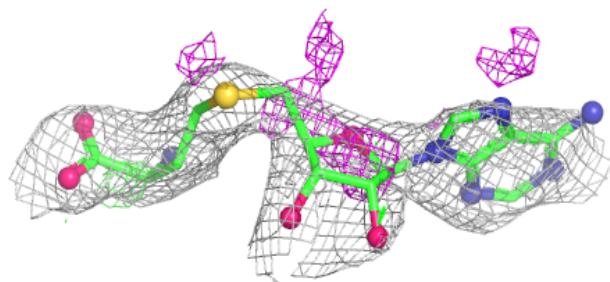
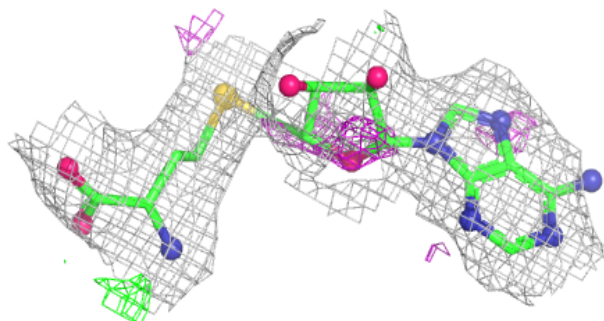
**Electron density around SAH B 302:**

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

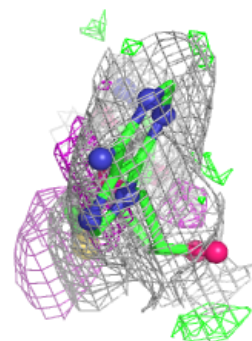
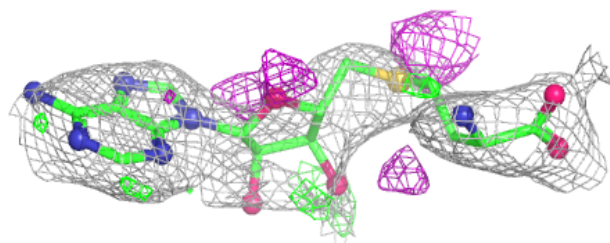
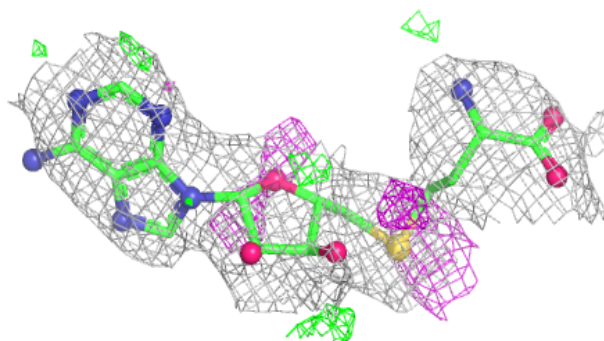


Electron density around SAH N 301:

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

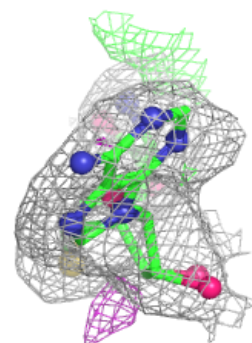
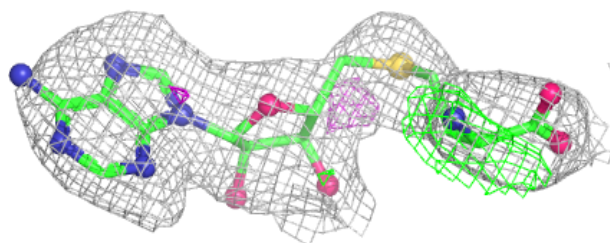
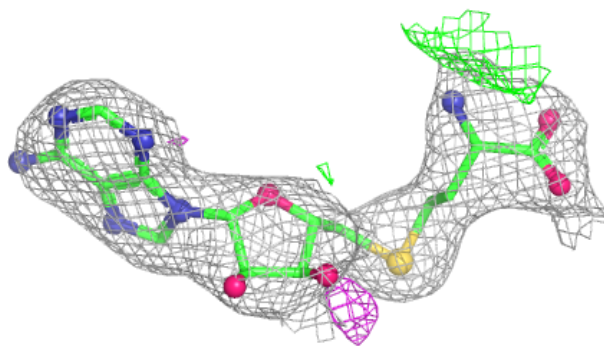
**Electron density around SAH H 301:**

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

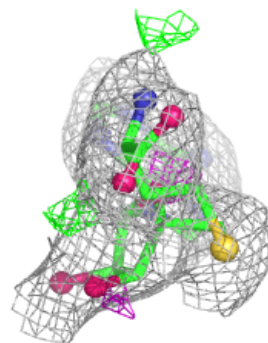
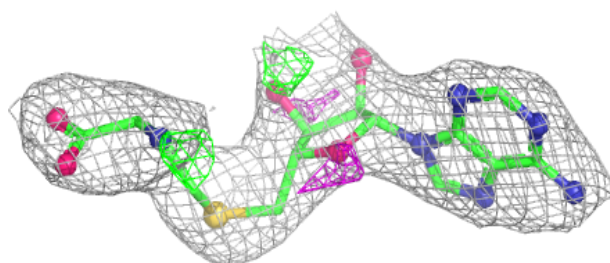
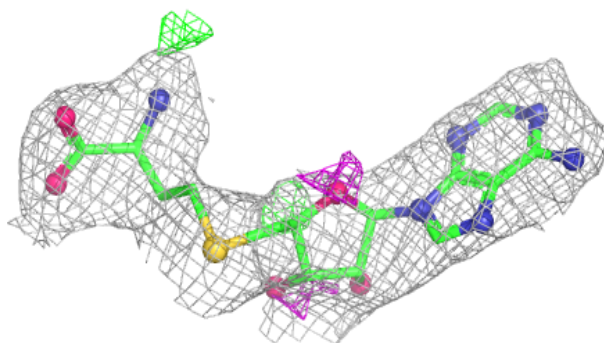


Electron density around SAH J 301:

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

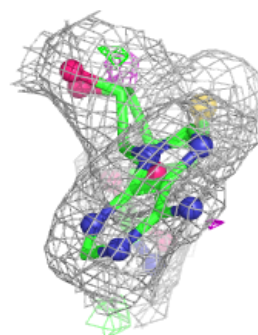
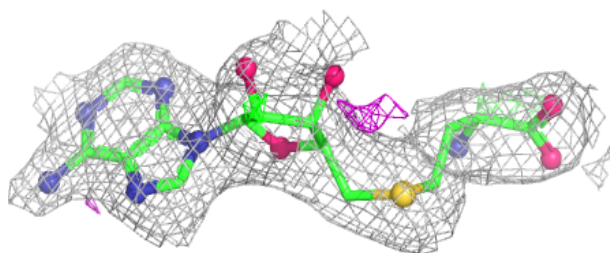
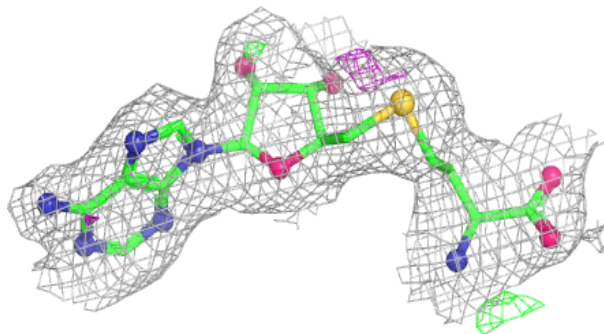
**Electron density around SAH P 301:**

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

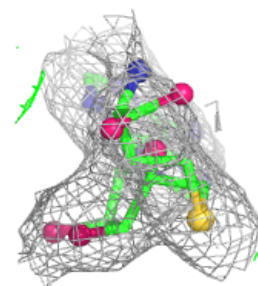
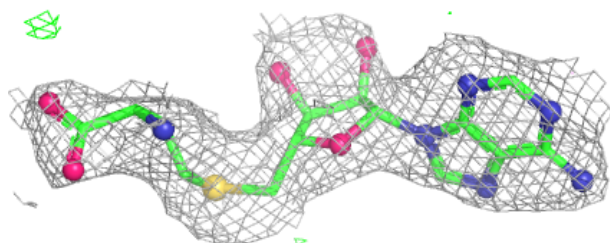
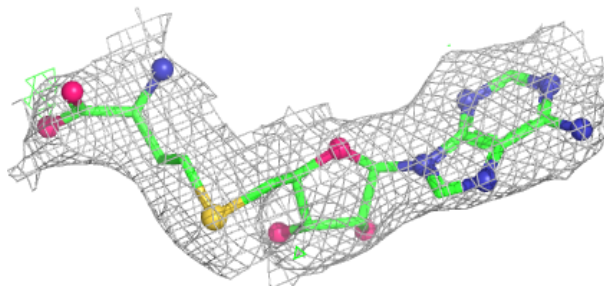


Electron density around SAH K 301:

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

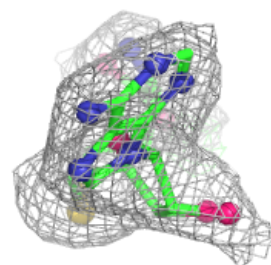
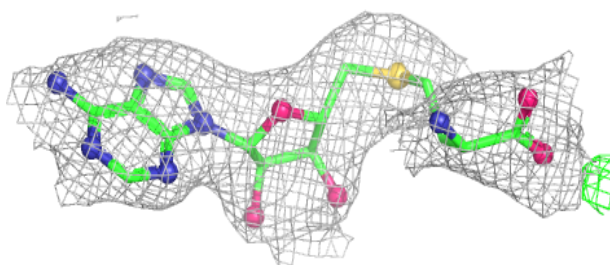
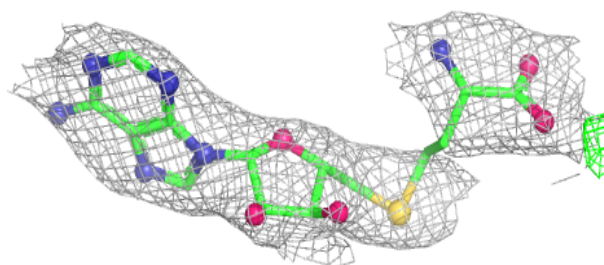
**Electron density around SAH L 301:**

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

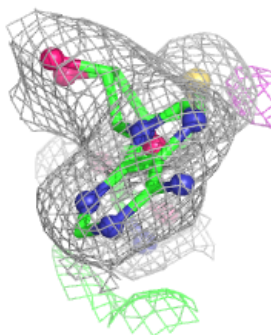
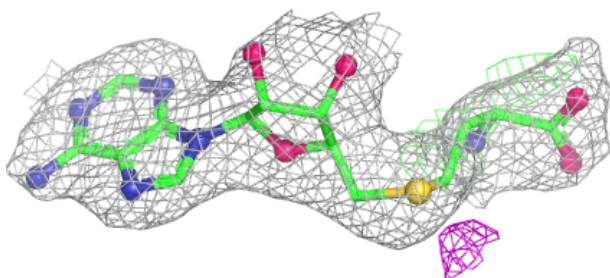
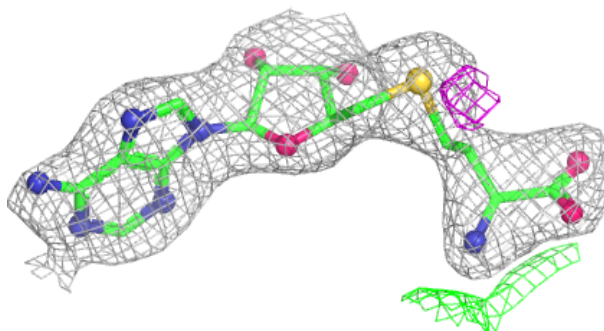


Electron density around SAH G 301:

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

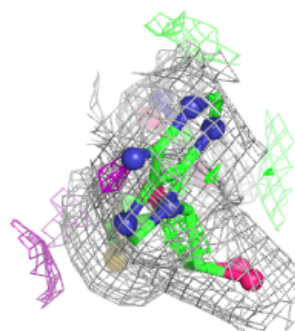
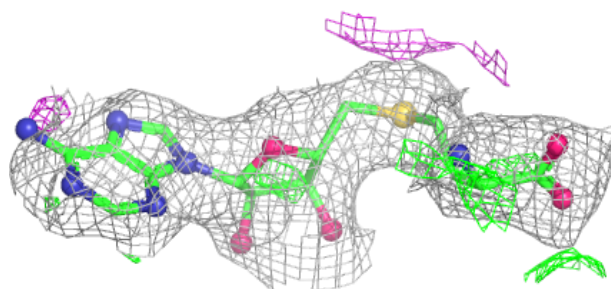
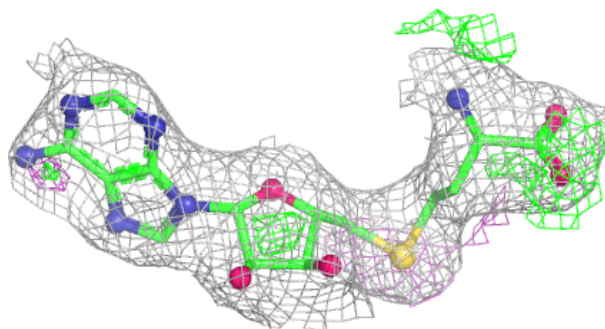
**Electron density around SAH Q 301:**

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

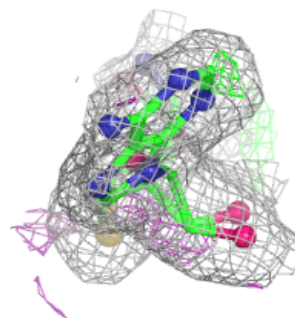
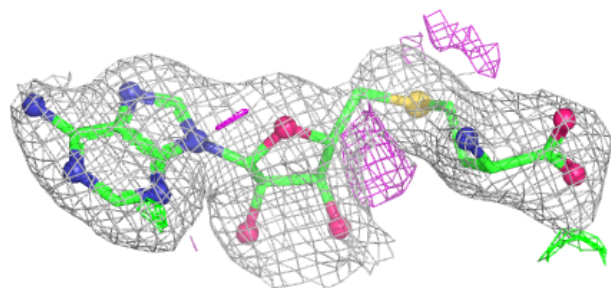
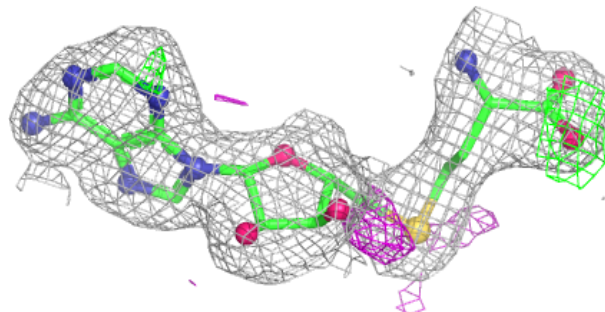


Electron density around SAH O 301:

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

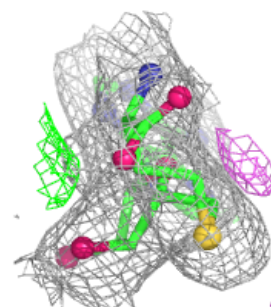
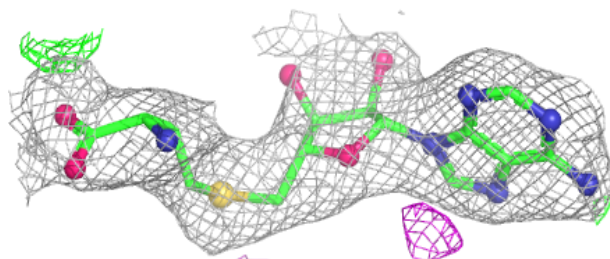
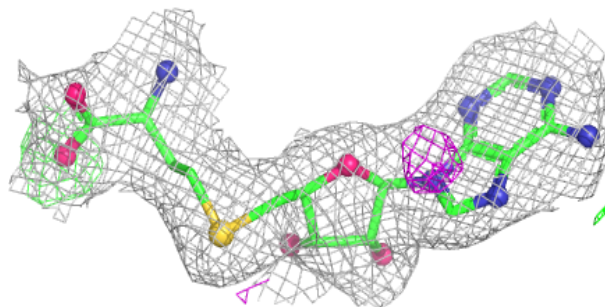
**Electron density around SAH B 301:**

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

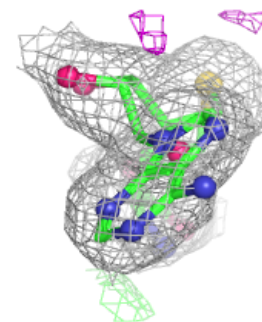
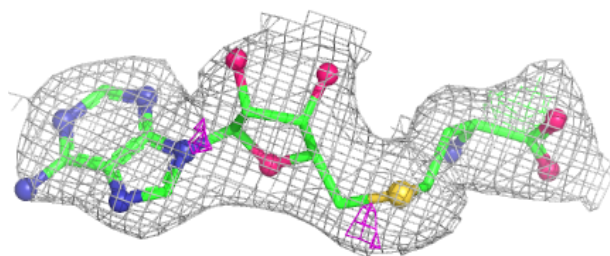


Electron density around SAH C 301:

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

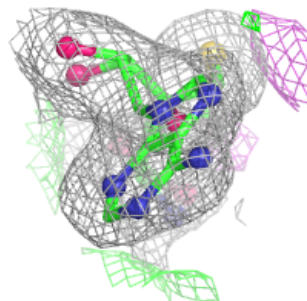
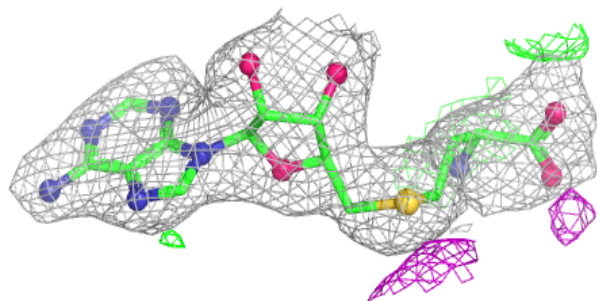
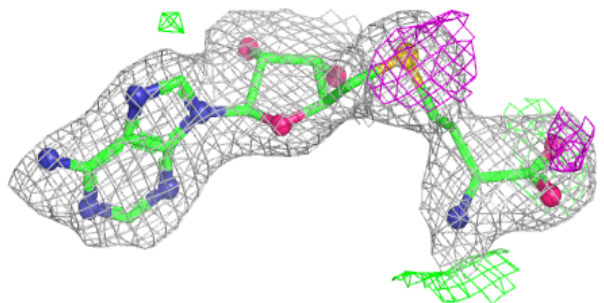
**Electron density around SAH M 301:**

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

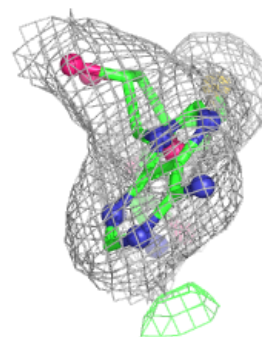
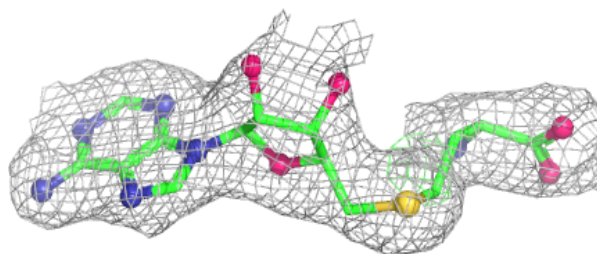
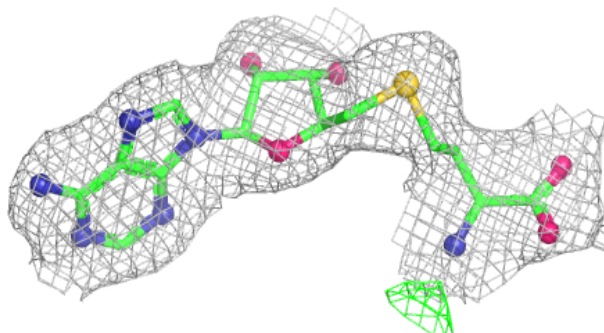


Electron density around SAH E 301:

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

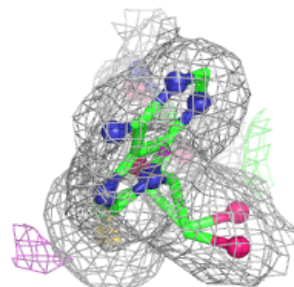
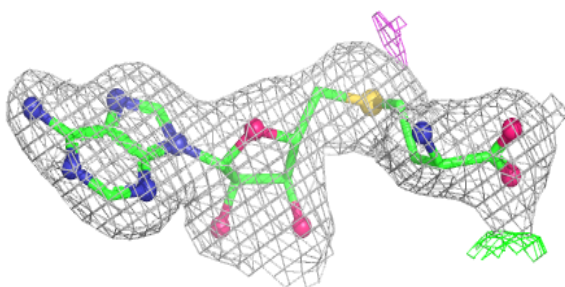
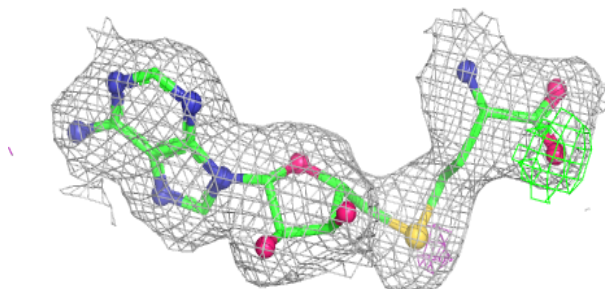
**Electron density around SAH D 301:**

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

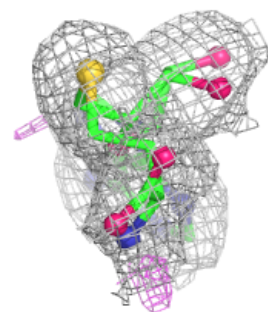
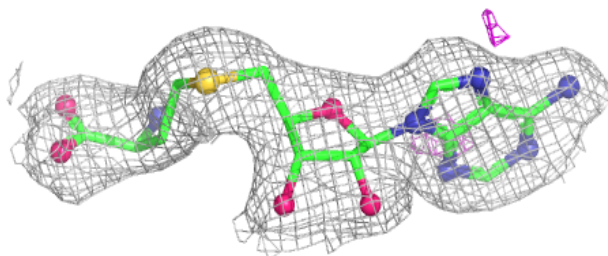
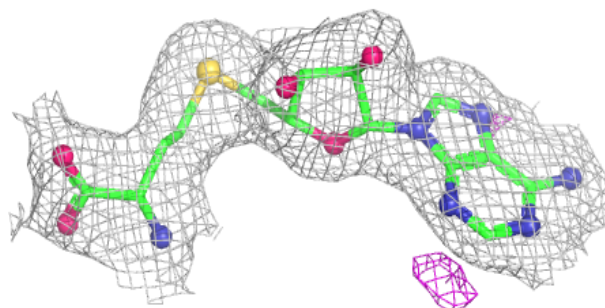


Electron density around SAH A 301:

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

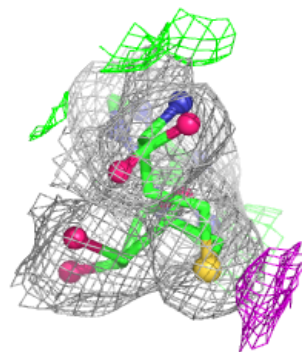
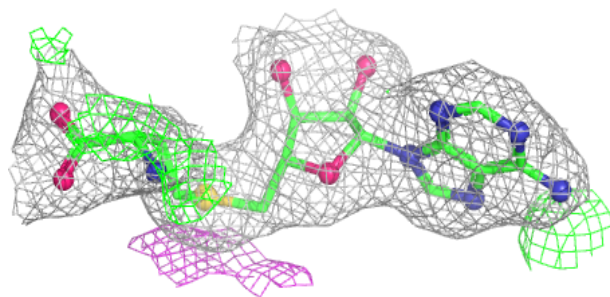
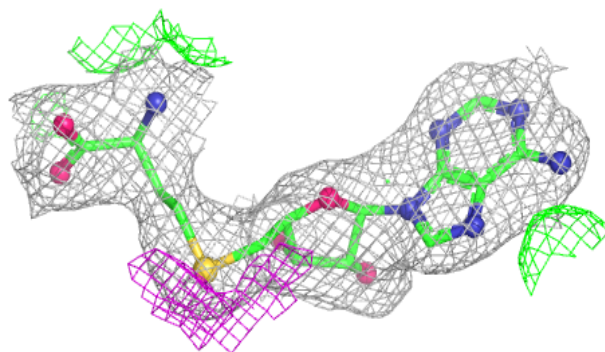
**Electron density around SAH F 301:**

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



Electron density around SAH I 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 [i](#)

There are no such residues in this entry.