



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 09:45 PM UTC

PDB ID : 3WST / pdb_00003wst
Title : Crystal structure of C.elegans PRMT7 in complex with SAH(P31)
Authors : Hasegawa, M.; Toma-fukai, S.; Shimizu, T.
Deposited on : 2014-03-21
Resolution : 2.39 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

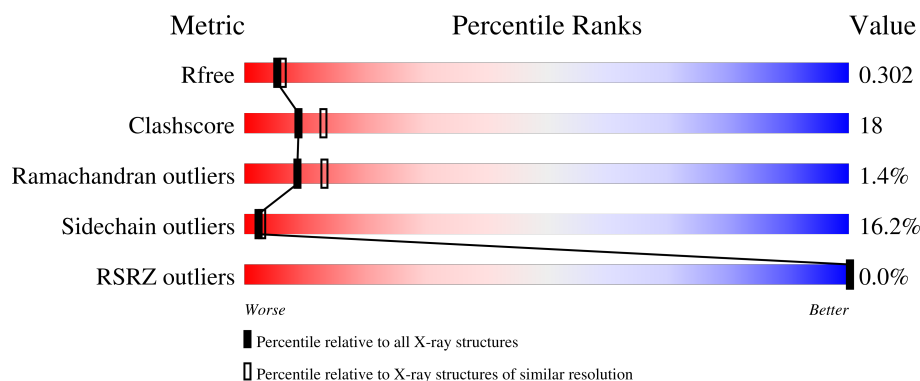
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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.



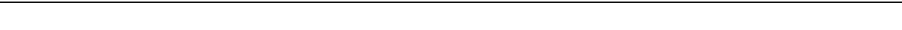
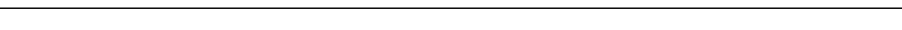
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	655	 67% 25% 6% ..
1	B	655	 58% 31% 8% .
1	C	655	 58% 34% 5% .
1	D	655	 65% 27% 5% .
1	E	655	 60% 28% 9% .

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Mol	Chain	Length	Quality of chain
1	F	655	 59% 31% 7% . .
1	G	655	 60% 31% 7% .
1	H	655	 62% 30% 5% .
1	I	655	 59% 31% 8% . .
1	J	655	 56% 33% 8% . .
1	K	655	 50% 38% 9% . .
1	L	655	 64% 28% 6% .
1	M	655	 49% 37% 9% . .
1	N	655	 51% 37% 8% . .
1	O	655	 52% 38% 8% . .
1	P	655	 59% 31% 6% . .
1	Q	655	 49% 38% 8% . .
1	R	655	 52% 37% 8% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 92645 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 Protein arginine N-methyltransferase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	641	Total	C	N	O	S	0	0	0
			5106	3247	857	975	27			
1	D	637	Total	C	N	O	S	0	0	0
			5078	3231	852	968	27			
1	B	638	Total	C	N	O	S	0	0	0
			5084	3234	853	970	27			
1	C	639	Total	C	N	O	S	0	0	0
			5091	3239	854	971	27			
1	F	638	Total	C	N	O	S	0	0	0
			5084	3234	853	970	27			
1	E	636	Total	C	N	O	S	0	0	0
			5069	3226	850	966	27			
1	G	636	Total	C	N	O	S	0	0	0
			5070	3227	850	966	27			
1	H	639	Total	C	N	O	S	0	0	0
			5091	3239	854	971	27			
1	I	644	Total	C	N	O	S	0	0	0
			5122	3257	860	978	27			
1	M	633	Total	C	N	O	S	0	0	0
			5049	3216	844	962	27			
1	N	638	Total	C	N	O	S	0	0	0
			5084	3234	853	970	27			
1	O	641	Total	C	N	O	S	0	0	0
			5106	3247	857	975	27			
1	P	636	Total	C	N	O	S	0	0	0
			5069	3226	850	966	27			
1	Q	632	Total	C	N	O	S	0	0	0
			5039	3209	845	958	27			
1	R	638	Total	C	N	O	S	0	0	0
			5084	3234	853	970	27			
1	J	644	Total	C	N	O	S	0	0	0
			5122	3257	860	978	27			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	K	641	Total	C	N	O	S	0	0	0
			5106	3247	857	975	27			
1	L	644	Total	C	N	O	S	0	0	0
			5122	3257	860	978	27			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP Q9XW42
A	-6	PRO	-	expression tag	UNP Q9XW42
A	-5	LEU	-	expression tag	UNP Q9XW42
A	-4	GLY	-	expression tag	UNP Q9XW42
A	-3	SER	-	expression tag	UNP Q9XW42
A	-2	GLY	-	expression tag	UNP Q9XW42
A	-1	ILE	-	expression tag	UNP Q9XW42
A	0	PRO	-	expression tag	UNP Q9XW42
D	-7	GLY	-	expression tag	UNP Q9XW42
D	-6	PRO	-	expression tag	UNP Q9XW42
D	-5	LEU	-	expression tag	UNP Q9XW42
D	-4	GLY	-	expression tag	UNP Q9XW42
D	-3	SER	-	expression tag	UNP Q9XW42
D	-2	GLY	-	expression tag	UNP Q9XW42
D	-1	ILE	-	expression tag	UNP Q9XW42
D	0	PRO	-	expression tag	UNP Q9XW42
B	-7	GLY	-	expression tag	UNP Q9XW42
B	-6	PRO	-	expression tag	UNP Q9XW42
B	-5	LEU	-	expression tag	UNP Q9XW42
B	-4	GLY	-	expression tag	UNP Q9XW42
B	-3	SER	-	expression tag	UNP Q9XW42
B	-2	GLY	-	expression tag	UNP Q9XW42
B	-1	ILE	-	expression tag	UNP Q9XW42
B	0	PRO	-	expression tag	UNP Q9XW42
C	-7	GLY	-	expression tag	UNP Q9XW42
C	-6	PRO	-	expression tag	UNP Q9XW42
C	-5	LEU	-	expression tag	UNP Q9XW42
C	-4	GLY	-	expression tag	UNP Q9XW42
C	-3	SER	-	expression tag	UNP Q9XW42
C	-2	GLY	-	expression tag	UNP Q9XW42
C	-1	ILE	-	expression tag	UNP Q9XW42
C	0	PRO	-	expression tag	UNP Q9XW42
F	-7	GLY	-	expression tag	UNP Q9XW42
F	-6	PRO	-	expression tag	UNP Q9XW42

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	LEU	-	expression tag	UNP Q9XW42
F	-4	GLY	-	expression tag	UNP Q9XW42
F	-3	SER	-	expression tag	UNP Q9XW42
F	-2	GLY	-	expression tag	UNP Q9XW42
F	-1	ILE	-	expression tag	UNP Q9XW42
F	0	PRO	-	expression tag	UNP Q9XW42
E	-7	GLY	-	expression tag	UNP Q9XW42
E	-6	PRO	-	expression tag	UNP Q9XW42
E	-5	LEU	-	expression tag	UNP Q9XW42
E	-4	GLY	-	expression tag	UNP Q9XW42
E	-3	SER	-	expression tag	UNP Q9XW42
E	-2	GLY	-	expression tag	UNP Q9XW42
E	-1	ILE	-	expression tag	UNP Q9XW42
E	0	PRO	-	expression tag	UNP Q9XW42
G	-7	GLY	-	expression tag	UNP Q9XW42
G	-6	PRO	-	expression tag	UNP Q9XW42
G	-5	LEU	-	expression tag	UNP Q9XW42
G	-4	GLY	-	expression tag	UNP Q9XW42
G	-3	SER	-	expression tag	UNP Q9XW42
G	-2	GLY	-	expression tag	UNP Q9XW42
G	-1	ILE	-	expression tag	UNP Q9XW42
G	0	PRO	-	expression tag	UNP Q9XW42
H	-7	GLY	-	expression tag	UNP Q9XW42
H	-6	PRO	-	expression tag	UNP Q9XW42
H	-5	LEU	-	expression tag	UNP Q9XW42
H	-4	GLY	-	expression tag	UNP Q9XW42
H	-3	SER	-	expression tag	UNP Q9XW42
H	-2	GLY	-	expression tag	UNP Q9XW42
H	-1	ILE	-	expression tag	UNP Q9XW42
H	0	PRO	-	expression tag	UNP Q9XW42
I	-7	GLY	-	expression tag	UNP Q9XW42
I	-6	PRO	-	expression tag	UNP Q9XW42
I	-5	LEU	-	expression tag	UNP Q9XW42
I	-4	GLY	-	expression tag	UNP Q9XW42
I	-3	SER	-	expression tag	UNP Q9XW42
I	-2	GLY	-	expression tag	UNP Q9XW42
I	-1	ILE	-	expression tag	UNP Q9XW42
I	0	PRO	-	expression tag	UNP Q9XW42
M	-7	GLY	-	expression tag	UNP Q9XW42
M	-6	PRO	-	expression tag	UNP Q9XW42
M	-5	LEU	-	expression tag	UNP Q9XW42
M	-4	GLY	-	expression tag	UNP Q9XW42

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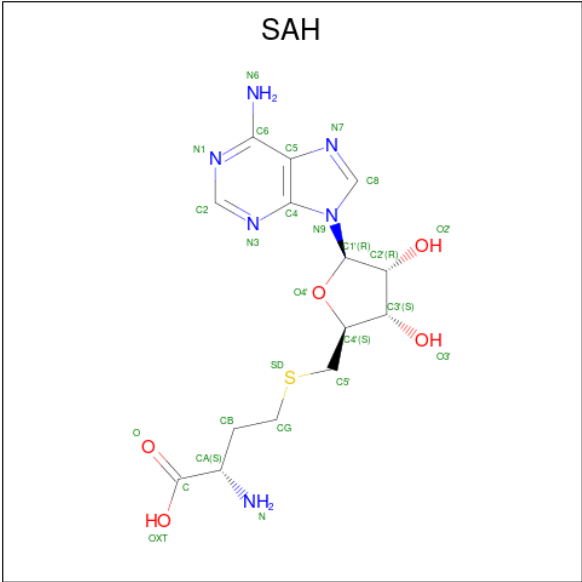
Chain	Residue	Modelled	Actual	Comment	Reference
M	-3	SER	-	expression tag	UNP Q9XW42
M	-2	GLY	-	expression tag	UNP Q9XW42
M	-1	ILE	-	expression tag	UNP Q9XW42
M	0	PRO	-	expression tag	UNP Q9XW42
N	-7	GLY	-	expression tag	UNP Q9XW42
N	-6	PRO	-	expression tag	UNP Q9XW42
N	-5	LEU	-	expression tag	UNP Q9XW42
N	-4	GLY	-	expression tag	UNP Q9XW42
N	-3	SER	-	expression tag	UNP Q9XW42
N	-2	GLY	-	expression tag	UNP Q9XW42
N	-1	ILE	-	expression tag	UNP Q9XW42
N	0	PRO	-	expression tag	UNP Q9XW42
O	-7	GLY	-	expression tag	UNP Q9XW42
O	-6	PRO	-	expression tag	UNP Q9XW42
O	-5	LEU	-	expression tag	UNP Q9XW42
O	-4	GLY	-	expression tag	UNP Q9XW42
O	-3	SER	-	expression tag	UNP Q9XW42
O	-2	GLY	-	expression tag	UNP Q9XW42
O	-1	ILE	-	expression tag	UNP Q9XW42
O	0	PRO	-	expression tag	UNP Q9XW42
P	-7	GLY	-	expression tag	UNP Q9XW42
P	-6	PRO	-	expression tag	UNP Q9XW42
P	-5	LEU	-	expression tag	UNP Q9XW42
P	-4	GLY	-	expression tag	UNP Q9XW42
P	-3	SER	-	expression tag	UNP Q9XW42
P	-2	GLY	-	expression tag	UNP Q9XW42
P	-1	ILE	-	expression tag	UNP Q9XW42
P	0	PRO	-	expression tag	UNP Q9XW42
Q	-7	GLY	-	expression tag	UNP Q9XW42
Q	-6	PRO	-	expression tag	UNP Q9XW42
Q	-5	LEU	-	expression tag	UNP Q9XW42
Q	-4	GLY	-	expression tag	UNP Q9XW42
Q	-3	SER	-	expression tag	UNP Q9XW42
Q	-2	GLY	-	expression tag	UNP Q9XW42
Q	-1	ILE	-	expression tag	UNP Q9XW42
Q	0	PRO	-	expression tag	UNP Q9XW42
R	-7	GLY	-	expression tag	UNP Q9XW42
R	-6	PRO	-	expression tag	UNP Q9XW42
R	-5	LEU	-	expression tag	UNP Q9XW42
R	-4	GLY	-	expression tag	UNP Q9XW42
R	-3	SER	-	expression tag	UNP Q9XW42
R	-2	GLY	-	expression tag	UNP Q9XW42

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-1	ILE	-	expression tag	UNP Q9XW42
R	0	PRO	-	expression tag	UNP Q9XW42
J	-7	GLY	-	expression tag	UNP Q9XW42
J	-6	PRO	-	expression tag	UNP Q9XW42
J	-5	LEU	-	expression tag	UNP Q9XW42
J	-4	GLY	-	expression tag	UNP Q9XW42
J	-3	SER	-	expression tag	UNP Q9XW42
J	-2	GLY	-	expression tag	UNP Q9XW42
J	-1	ILE	-	expression tag	UNP Q9XW42
J	0	PRO	-	expression tag	UNP Q9XW42
K	-7	GLY	-	expression tag	UNP Q9XW42
K	-6	PRO	-	expression tag	UNP Q9XW42
K	-5	LEU	-	expression tag	UNP Q9XW42
K	-4	GLY	-	expression tag	UNP Q9XW42
K	-3	SER	-	expression tag	UNP Q9XW42
K	-2	GLY	-	expression tag	UNP Q9XW42
K	-1	ILE	-	expression tag	UNP Q9XW42
K	0	PRO	-	expression tag	UNP Q9XW42
L	-7	GLY	-	expression tag	UNP Q9XW42
L	-6	PRO	-	expression tag	UNP Q9XW42
L	-5	LEU	-	expression tag	UNP Q9XW42
L	-4	GLY	-	expression tag	UNP Q9XW42
L	-3	SER	-	expression tag	UNP Q9XW42
L	-2	GLY	-	expression tag	UNP Q9XW42
L	-1	ILE	-	expression tag	UNP Q9XW42
L	0	PRO	-	expression tag	UNP Q9XW42

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



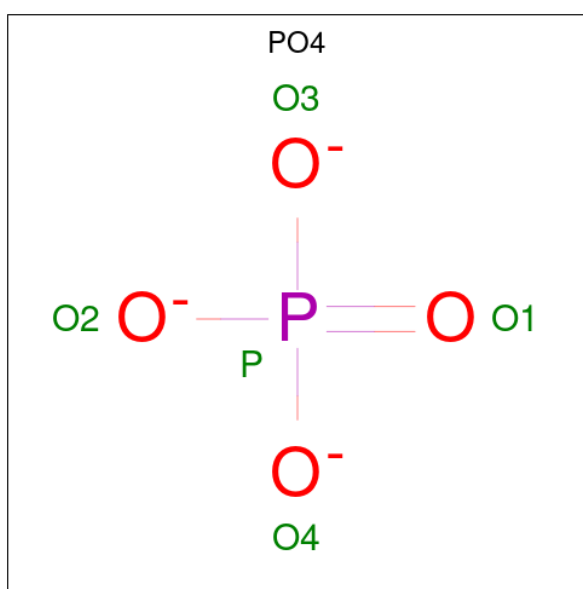
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	F	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	E	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	G	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	H	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	I	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	M	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
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		

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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	O	P	0	0
			5	4	1		
3	I	1	Total	O	P	0	0
			5	4	1		
3	M	1	Total	O	P	0	0
			5	4	1		
3	N	1	Total	O	P	0	0
			5	4	1		
3	O	1	Total	O	P	0	0
			5	4	1		
3	P	1	Total	O	P	0	0
			5	4	1		
3	Q	1	Total	O	P	0	0
			5	4	1		
3	R	1	Total	O	P	0	0
			5	4	1		
3	J	1	Total	O	P	0	0
			5	4	1		
3	K	1	Total	O	P	0	0
			5	4	1		
3	L	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	105	Total	O	0	0
			105	105		
4	D	93	Total	O	0	0
			93	93		
4	B	26	Total	O	0	0
			26	26		
4	C	16	Total	O	0	0
			16	16		
4	F	12	Total	O	0	0
			12	12		
4	E	41	Total	O	0	0
			41	41		
4	G	19	Total	O	0	0
			19	19		
4	H	59	Total	O	0	0
			59	59		

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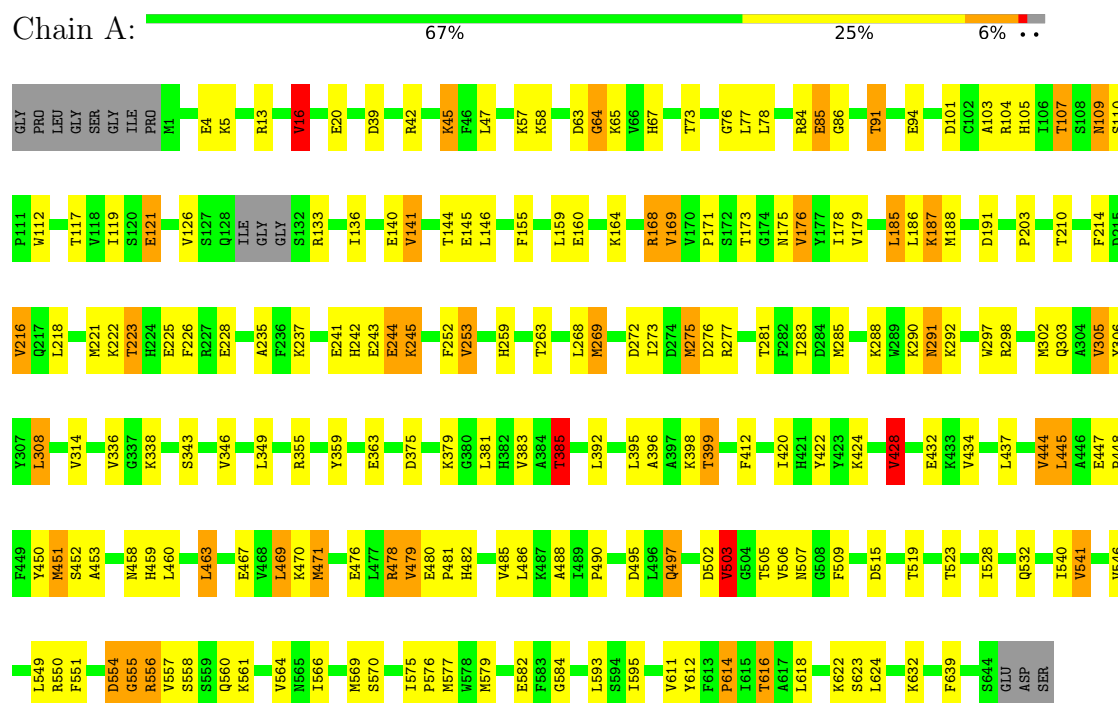
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	21	Total 21	O 21	0	0
4	M	2	Total 2	O 2	0	0
4	P	10	Total 10	O 10	0	0
4	Q	2	Total 2	O 2	0	0
4	R	2	Total 2	O 2	0	0
4	J	12	Total 12	O 12	0	0
4	K	6	Total 6	O 6	0	0
4	L	85	Total 85	O 85	0	0

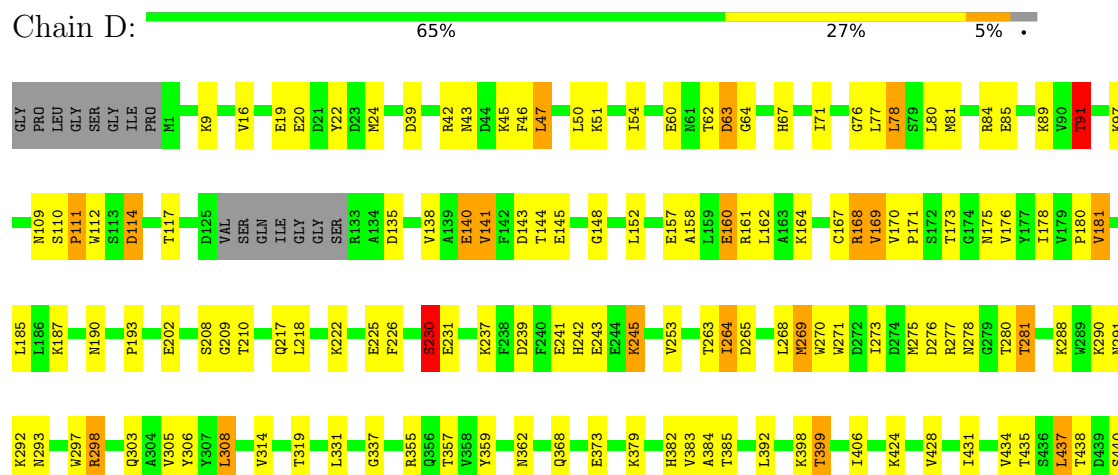
3 Residue-property plots [i](#)

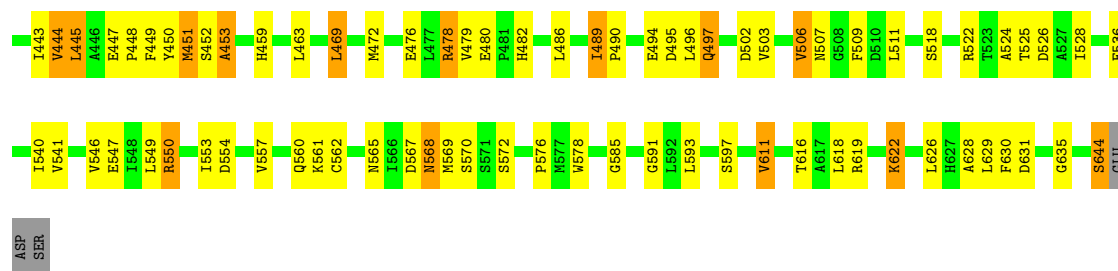
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Protein arginine N-methyltransferase 7



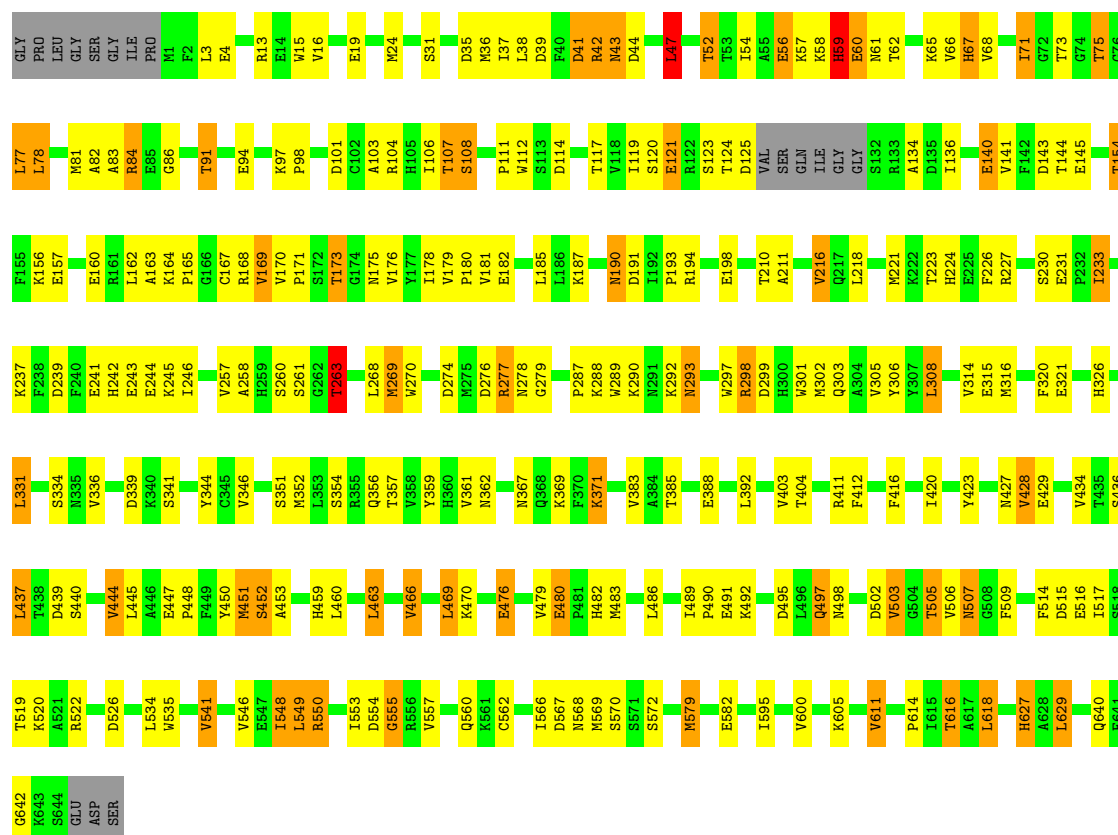
• Molecule 1: Protein arginine N-methyltransferase 7





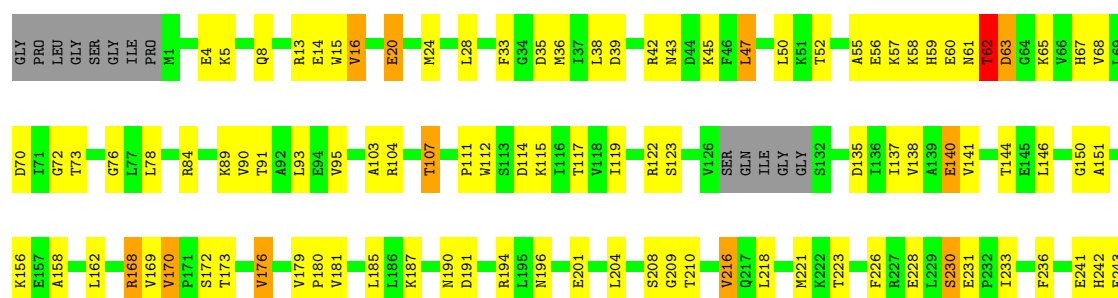
• Molecule 1: Protein arginine N-methyltransferase 7

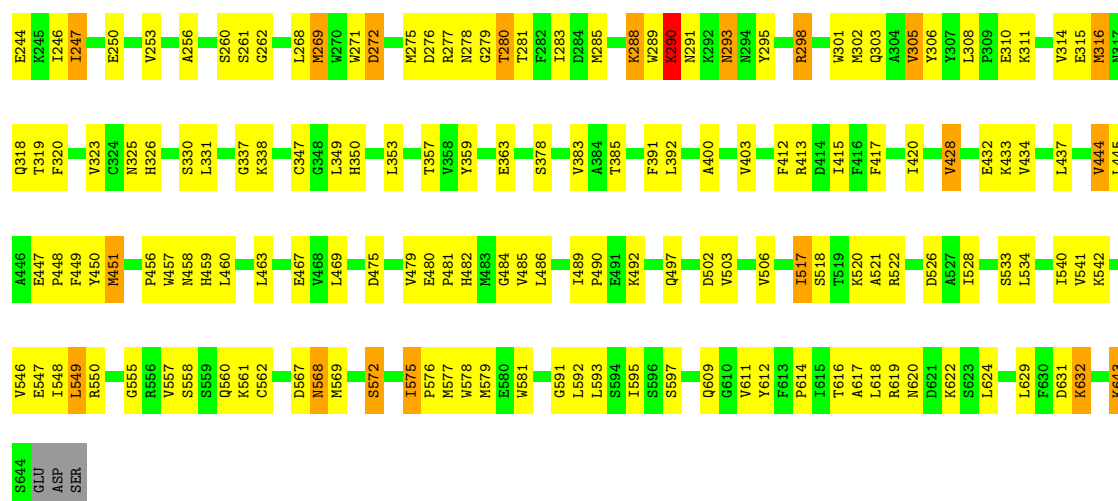
Chain B: 58% 31% 8% .



• Molecule 1: Protein arginine N-methyltransferase 7

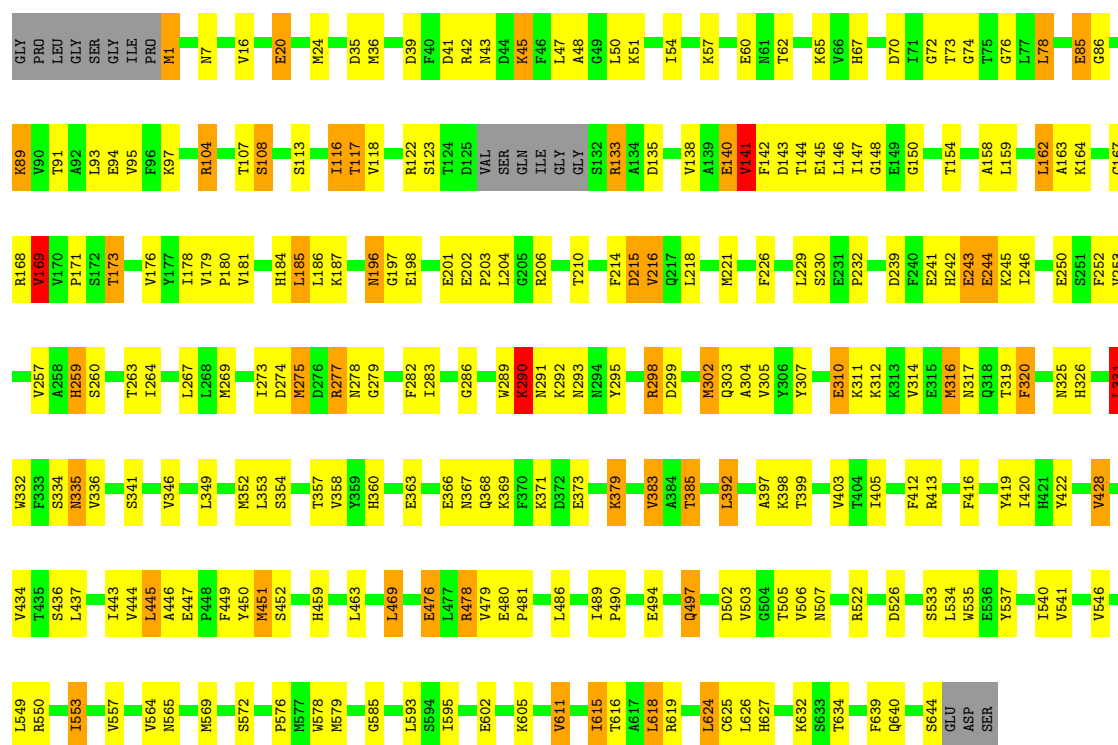
Chain C: 58% 34% 5% .





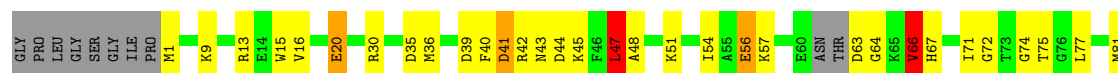
• Molecule 1: Protein arginine N-methyltransferase 7

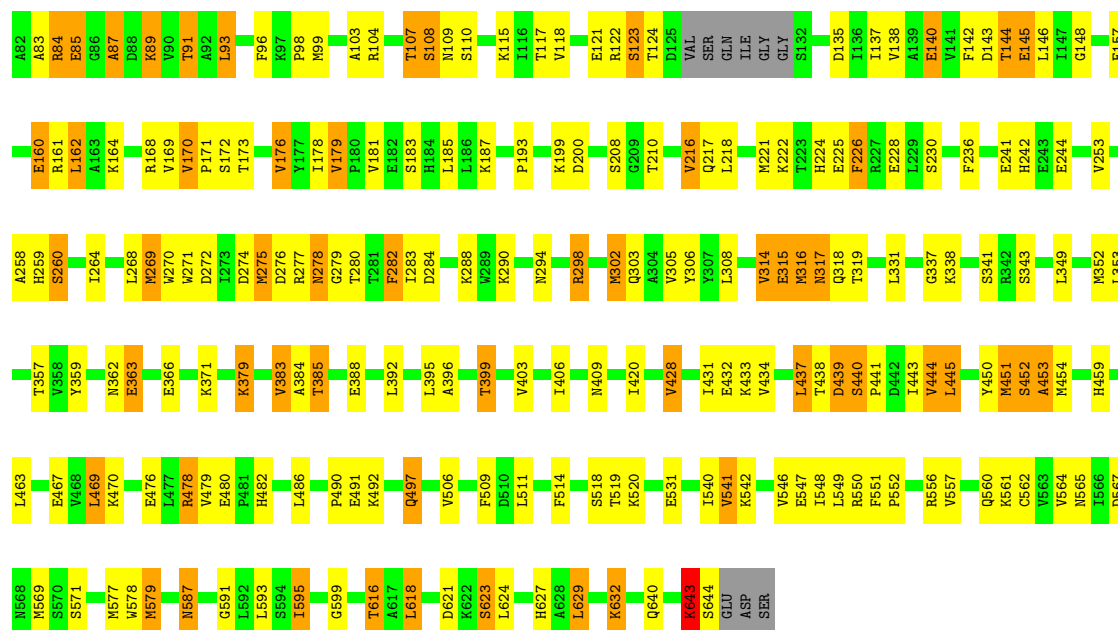
Chain F: 59% 31% 7% ..



• Molecule 1: Protein arginine N-methyltransferase 7

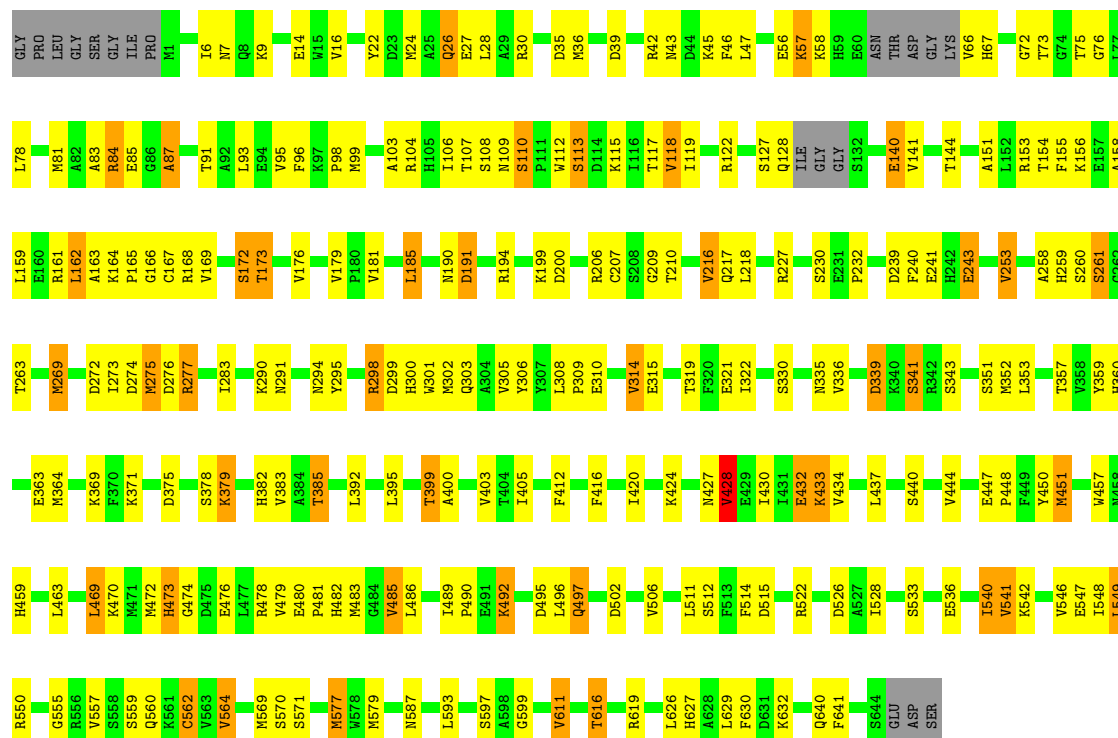
Chain E: 60% 28% 9% .





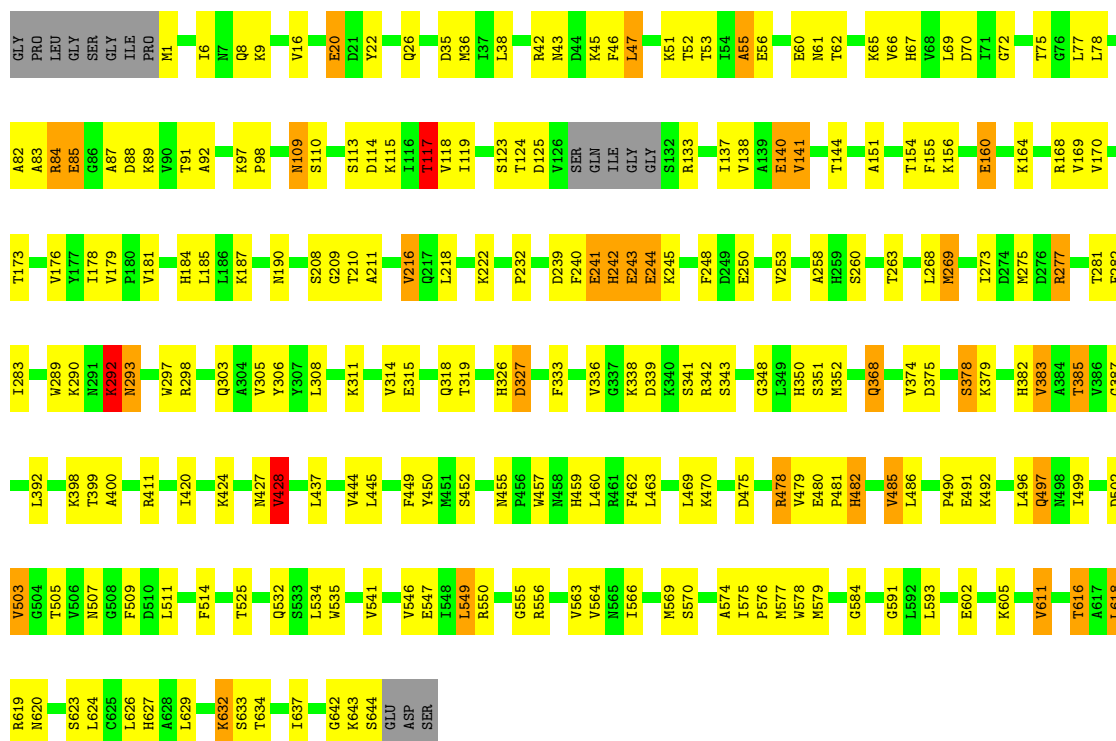
• Molecule 1: Protein arginine N-methyltransferase 7

Chain G: 60% 31% 7% .



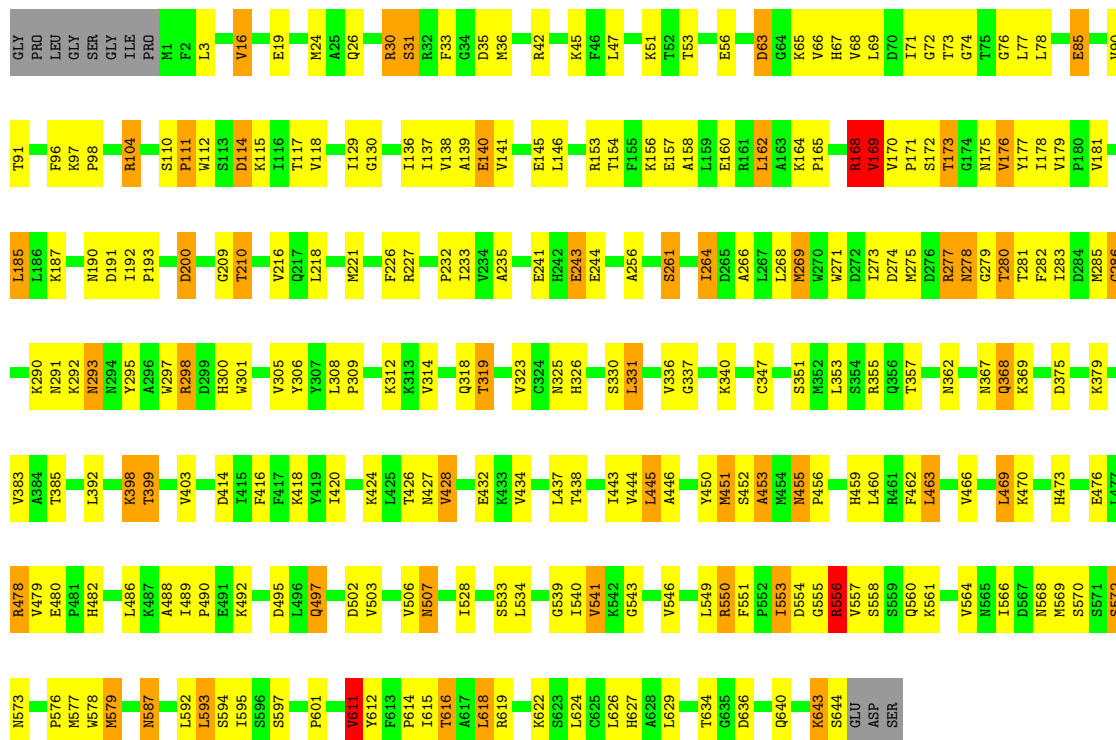
• Molecule 1: Protein arginine N-methyltransferase 7

Chain H: 62% 30% 5% .

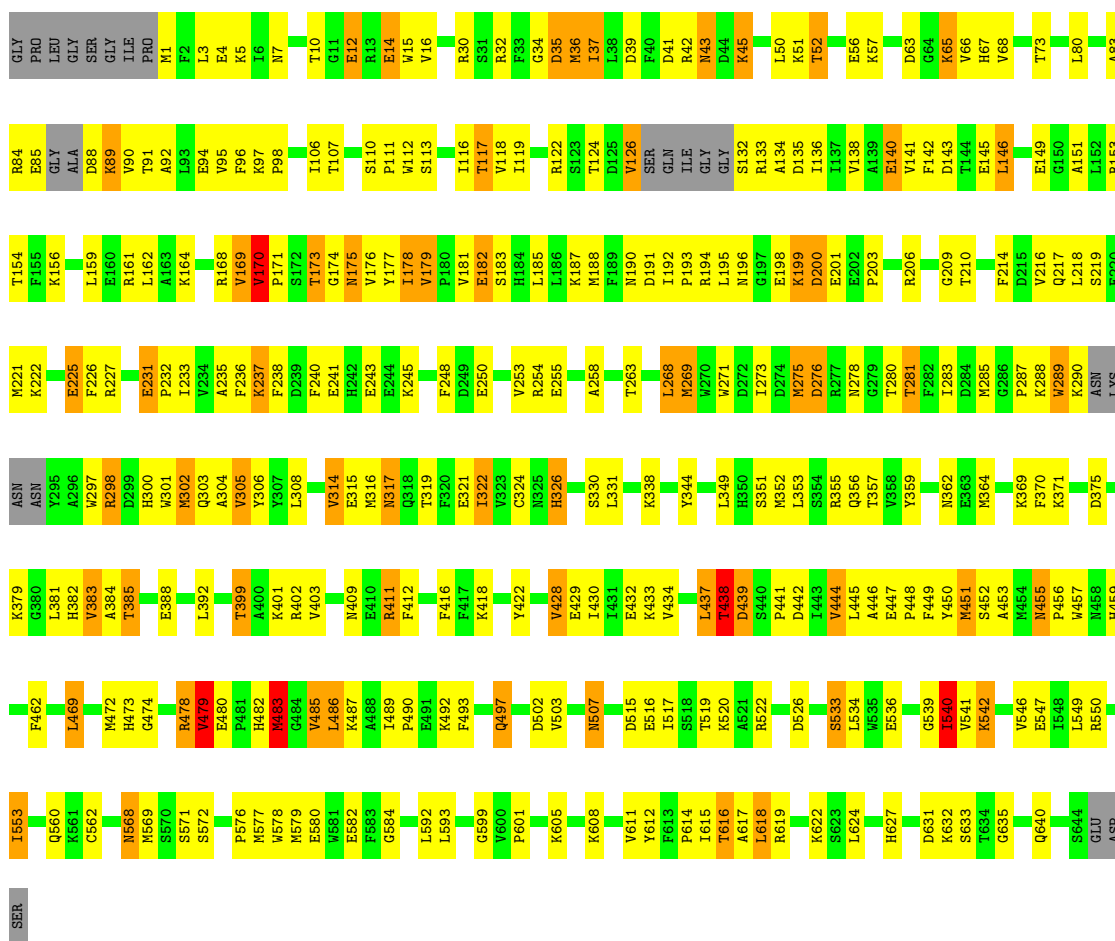


• Molecule 1: Protein arginine N-methyltransferase 7

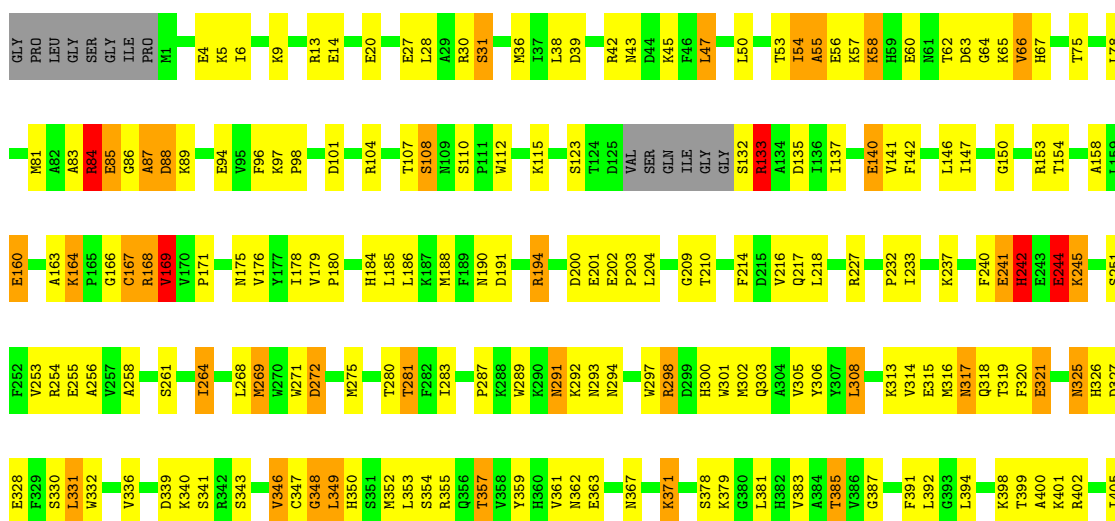
Chain I: 59% 31% 8% ..

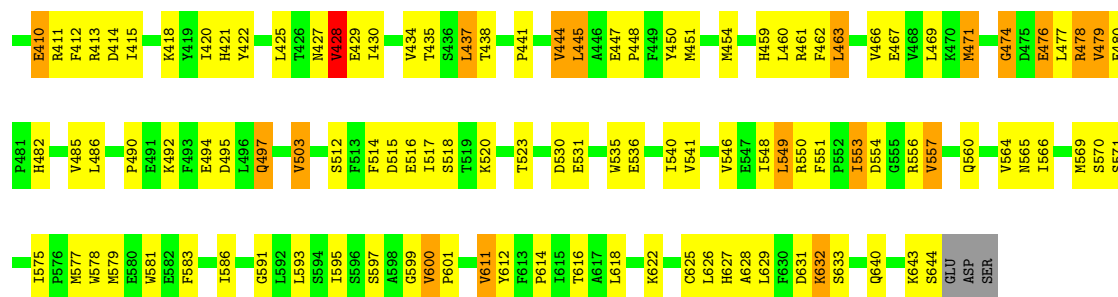


• Molecule 1: Protein arginine N-methyltransferase 7



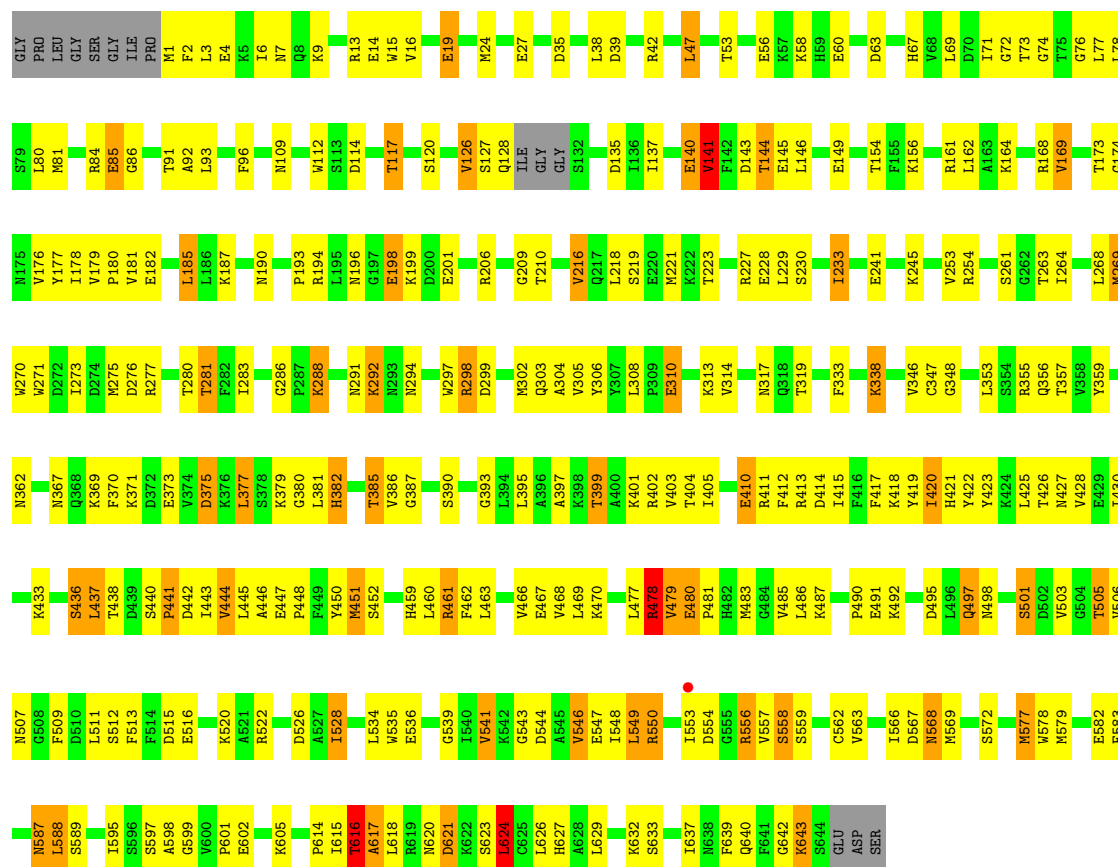
Chain N: 51% 37% 8% . .





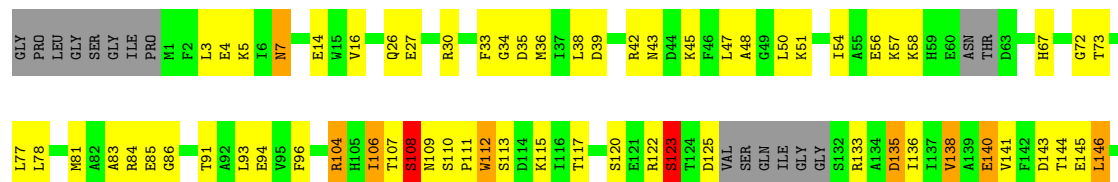
• Molecule 1: Protein arginine N-methyltransferase 7

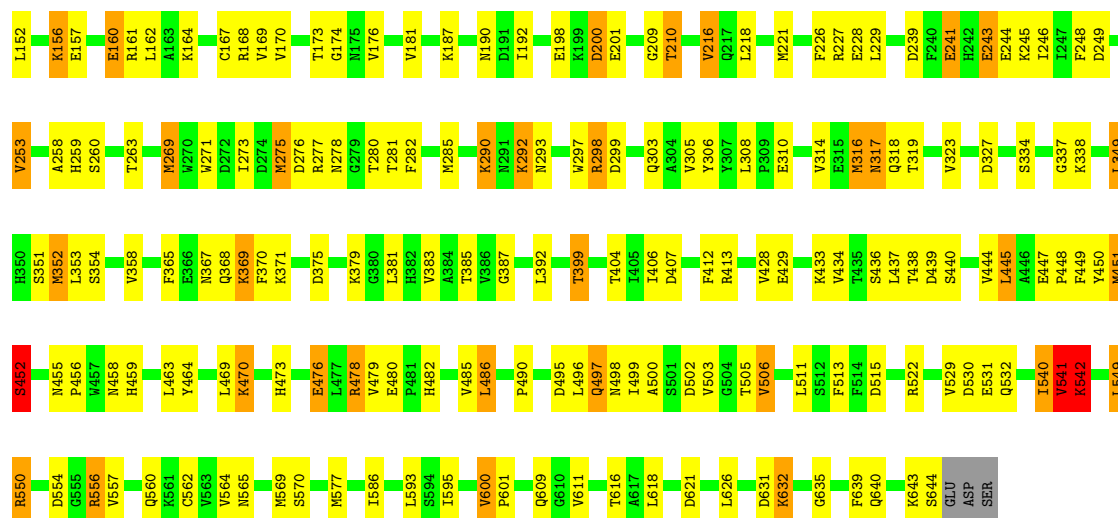
Chain O: 52% 38% 8% ..



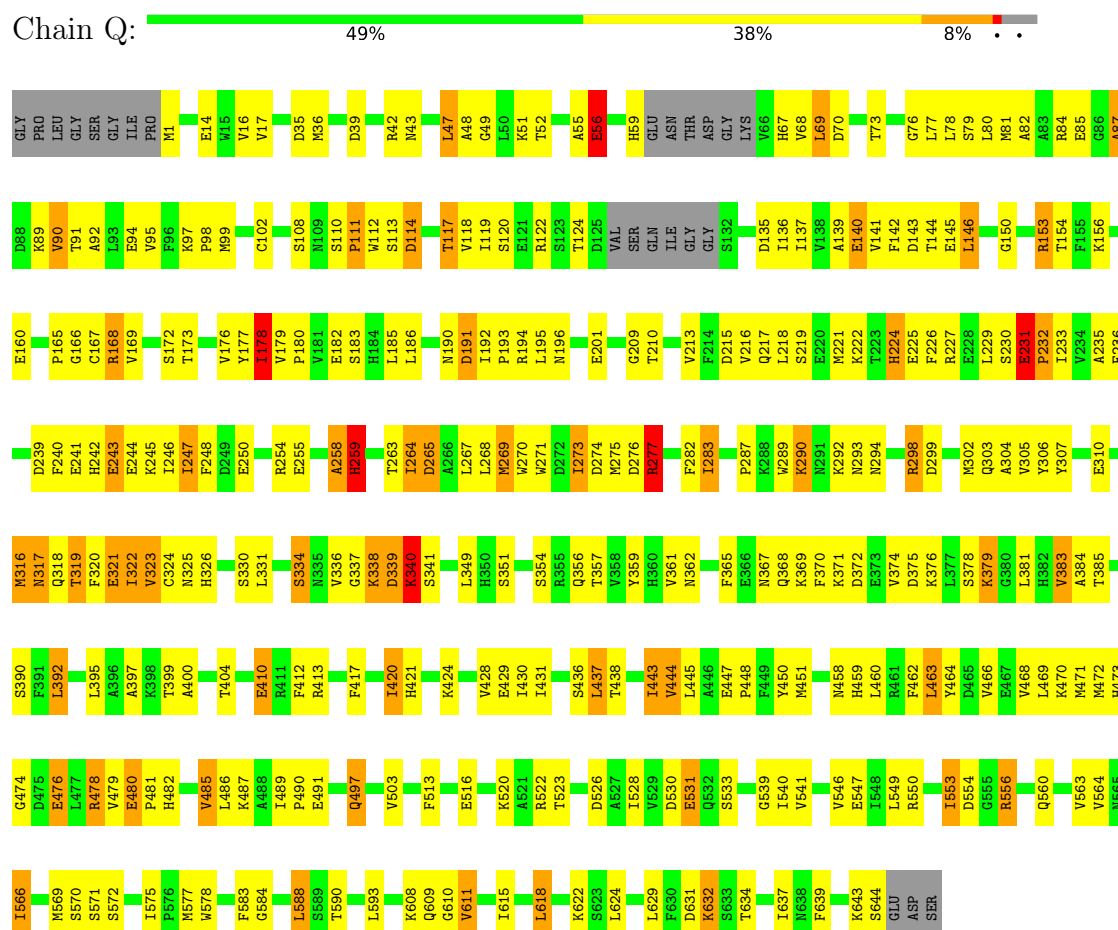
• Molecule 1: Protein arginine N-methyltransferase 7

Chain P: 59% 31% 6% ..



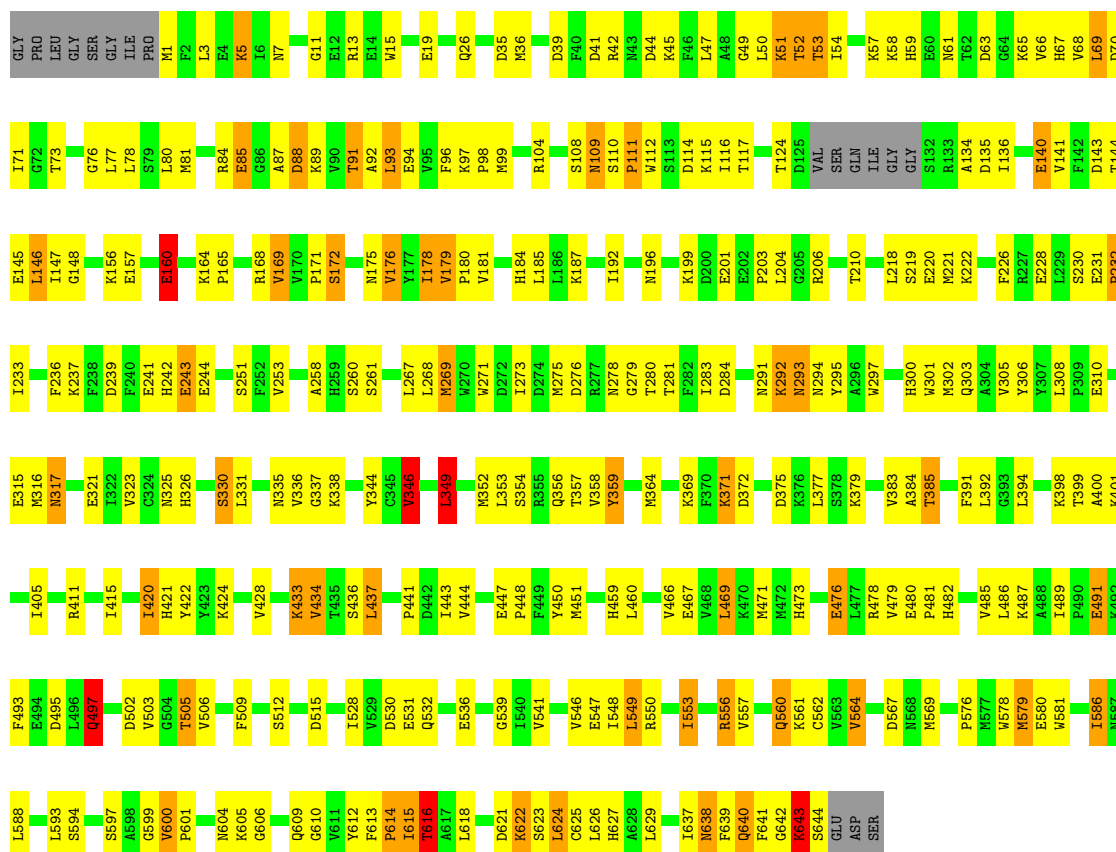


• Molecule 1: Protein arginine N-methyltransferase 7



• Molecule 1: Protein arginine N-methyltransferase 7

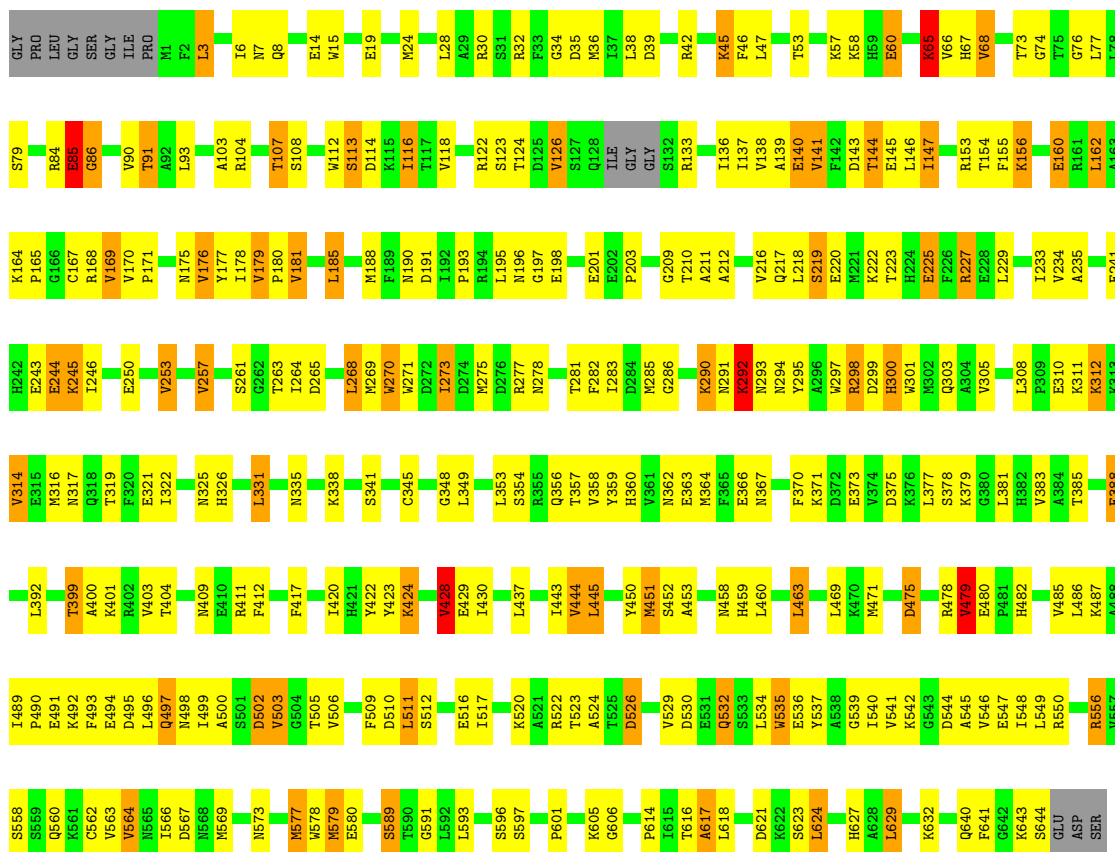






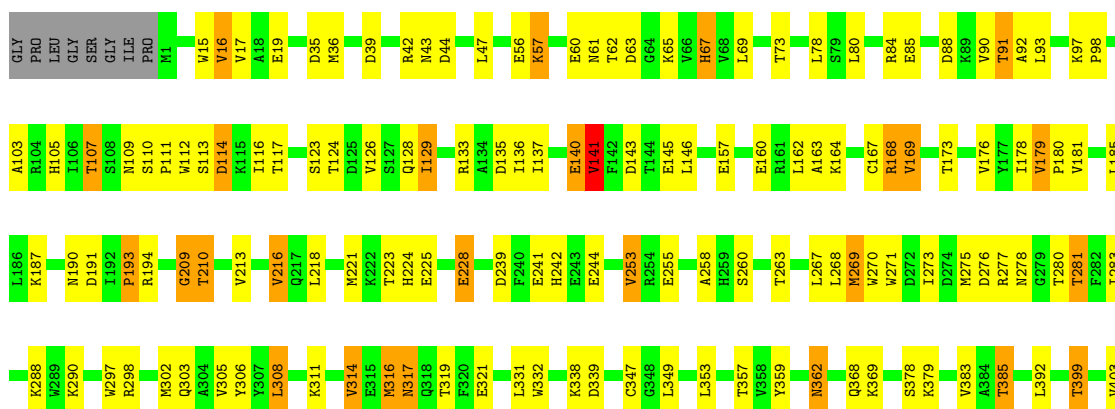
• Molecule 1: Protein arginine N-methyltransferase 7

Chain K: 50% 38% 9% ..



• Molecule 1: Protein arginine N-methyltransferase 7

Chain L: 64% 28% 6% ..



L629	F630	D631	K632	S633	L637	N638	F639	Q640	F641	D642	K643	S644	GLU	ASP	SER	V506	N507	G508	F509	E516	K520	T528	V541	V546	E547	L548	L549	R550	F551	P552	I553	D554	G555	R556	V557	Q560	K561	C562	V563	V564	M569	S572	M577	W578	M579	E580	W581	L583	S584	I595	V600	V611	T616	A617	L618	L624	G625	L626	H627	A628
F412	I420	V428	K433	V434	T435	S436	L437	S440	V444	L445	A446	E447	P448	F449	Y450	M451	S452	A453	M454	W457	N458	H459	L463	Y464	D465	V466	E467	V468	L469	K470	D475	E476	V479	E480	P481	H482	V485	L486	K487	P490	D495	L496	Q497	D502	V503															

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	190.70Å 190.70Å 373.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.41 – 2.39 47.41 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.41-2.39) 98.9 (47.41-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.234 , 0.303 0.233 , 0.302	Depositor DCC
R_{free} test set	29764 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 22.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l 0.069 for h,-h-k,-l 0.023 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	92645	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.30% 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, PO4

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	1.11	4/5217 (0.1%)	1.22	19/7044 (0.3%)
1	B	1.03	2/5195 (0.0%)	1.16	13/7014 (0.2%)
1	C	1.00	1/5202 (0.0%)	1.15	16/7024 (0.2%)
1	D	1.07	3/5189 (0.1%)	1.23	18/7006 (0.3%)
1	E	1.04	4/5179 (0.1%)	1.21	26/6990 (0.4%)
1	F	0.95	0/5195	1.15	20/7014 (0.3%)
1	G	1.00	2/5180 (0.0%)	1.13	14/6993 (0.2%)
1	H	1.07	5/5202 (0.1%)	1.21	17/7024 (0.2%)
1	I	1.00	0/5234	1.15	15/7068 (0.2%)
1	J	0.96	0/5234	1.16	23/7068 (0.3%)
1	K	0.95	1/5217 (0.0%)	1.13	20/7044 (0.3%)
1	L	1.11	7/5234 (0.1%)	1.23	22/7068 (0.3%)
1	M	0.89	0/5158	1.10	17/6962 (0.2%)
1	N	0.89	1/5195 (0.0%)	1.13	21/7014 (0.3%)
1	O	0.83	0/5217	1.05	9/7044 (0.1%)
1	P	0.94	0/5179	1.11	14/6990 (0.2%)
1	Q	0.86	0/5149	1.09	16/6951 (0.2%)
1	R	0.83	0/5195	1.06	17/7014 (0.2%)
All	All	0.98	30/93571 (0.0%)	1.15	317/126332 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	2
1	H	0	1
1	J	0	2
All	All	0	6

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	259	HIS	CG-CD2	6.26	1.42	1.35
1	D	270	TRP	CA-C	-6.21	1.45	1.52
1	H	184	HIS	CG-CD2	6.18	1.42	1.35
1	A	242	HIS	CA-C	-5.79	1.46	1.53
1	A	179	VAL	CA-C	-5.62	1.48	1.52

The worst 5 of 317 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	241	GLU	N-CA-C	13.44	130.36	113.43
1	F	346	VAL	N-CA-C	-12.93	100.86	113.53
1	N	346	VAL	N-CA-C	-12.16	101.52	113.20
1	C	62	THR	N-CA-C	9.77	121.92	111.28
1	L	643	LYS	N-CA-C	9.70	121.54	110.97

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	85	GLU	Peptide
1	E	282	PHE	Peptide
1	E	316	MET	Peptide
1	H	282	PHE	Peptide
1	J	291	ASN	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5106	0	4989	137	0
1	B	5084	0	4967	192	0
1	C	5091	0	4976	169	1
1	D	5078	0	4962	146	1
1	E	5069	0	4953	174	0
1	F	5084	0	4967	164	0
1	G	5070	0	4955	161	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	5091	0	4976	148	0
1	I	5122	0	5007	187	0
1	J	5122	0	5007	197	0
1	K	5106	0	4989	223	0
1	L	5122	0	5007	149	0
1	M	5049	0	4935	274	0
1	N	5084	0	4967	241	1
1	O	5106	0	4989	226	0
1	P	5069	0	4953	168	1
1	Q	5039	0	4927	242	0
1	R	5084	0	4967	212	0
2	A	26	0	19	0	0
2	B	26	0	19	2	0
2	C	26	0	19	1	0
2	D	26	0	19	0	0
2	E	26	0	19	3	0
2	F	26	0	19	2	0
2	G	26	0	19	2	0
2	H	26	0	19	1	0
2	I	26	0	19	1	0
2	J	26	0	19	0	0
2	K	26	0	19	3	0
2	L	26	0	19	0	0
2	M	26	0	19	2	0
2	N	26	0	19	2	0
2	O	26	0	19	0	0
2	P	26	0	19	3	0
2	Q	26	0	19	2	0
2	R	26	0	19	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
3	I	5	0	0	1	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
3	M	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	5	0	0	0	0
3	O	5	0	0	0	0
3	P	5	0	0	0	0
3	Q	5	0	0	1	0
3	R	5	0	0	0	0
4	A	105	0	0	0	0
4	B	26	0	0	0	0
4	C	16	0	0	1	0
4	D	93	0	0	3	0
4	E	41	0	0	0	0
4	F	12	0	0	1	0
4	G	19	0	0	1	0
4	H	59	0	0	1	0
4	I	21	0	0	3	0
4	J	12	0	0	1	0
4	K	6	0	0	0	0
4	L	85	0	0	4	0
4	M	2	0	0	2	0
4	P	10	0	0	2	0
4	Q	2	0	0	0	0
4	R	2	0	0	0	0
All	All	92645	0	89835	3367	2

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 18.

The worst 5 of 3367 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:490:PRO:HB3	1:L:569:MET:CE	1.55	1.36
1:G:490:PRO:HB3	1:G:569:MET:CE	1.58	1.32
1:F:490:PRO:HB3	1:F:569:MET:CE	1.60	1.28
1:M:569:MET:HG3	1:M:624:LEU:CD1	1.67	1.23
1:B:490:PRO:HB3	1:B:569:MET:CE	1.71	1.20

All (2) 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:D:554:ASP:OD1	1:C:550:ARG:NH2[3_554]	2.01	0.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:554:ASP:OD1	1:P:550:ARG:NH2[3_654]	2.09	0.11

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	637/655 (97%)	600 (94%)	34 (5%)	3 (0%)	24	37
1	B	634/655 (97%)	561 (88%)	62 (10%)	11 (2%)	7	10
1	C	635/655 (97%)	578 (91%)	47 (7%)	10 (2%)	7	11
1	D	633/655 (97%)	595 (94%)	34 (5%)	4 (1%)	21	32
1	E	630/655 (96%)	569 (90%)	53 (8%)	8 (1%)	9	14
1	F	634/655 (97%)	563 (89%)	62 (10%)	9 (1%)	9	13
1	G	630/655 (96%)	575 (91%)	50 (8%)	5 (1%)	16	25
1	H	635/655 (97%)	590 (93%)	39 (6%)	6 (1%)	14	22
1	I	642/655 (98%)	572 (89%)	58 (9%)	12 (2%)	6	8
1	J	642/655 (98%)	578 (90%)	54 (8%)	10 (2%)	7	11
1	K	637/655 (97%)	570 (90%)	53 (8%)	14 (2%)	5	6
1	L	642/655 (98%)	607 (94%)	34 (5%)	1 (0%)	43	58
1	M	625/655 (95%)	551 (88%)	65 (10%)	9 (1%)	9	13
1	N	634/655 (97%)	558 (88%)	67 (11%)	9 (1%)	9	13
1	O	637/655 (97%)	567 (89%)	61 (10%)	9 (1%)	9	13
1	P	630/655 (96%)	576 (91%)	48 (8%)	6 (1%)	12	20
1	Q	626/655 (96%)	526 (84%)	81 (13%)	19 (3%)	3	3
1	R	634/655 (97%)	567 (89%)	52 (8%)	15 (2%)	4	5
All	All	11417/11790 (97%)	10303 (90%)	954 (8%)	160 (1%)	9	13

5 of 160 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	63	ASP
1	B	59	HIS
1	B	60	GLU
1	B	278	ASN
1	F	290	LYS

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	556/569 (98%)	472 (85%)	84 (15%)	3	3
1	B	553/569 (97%)	466 (84%)	87 (16%)	2	3
1	C	554/569 (97%)	470 (85%)	84 (15%)	3	3
1	D	552/569 (97%)	472 (86%)	80 (14%)	3	4
1	E	551/569 (97%)	458 (83%)	93 (17%)	2	3
1	F	553/569 (97%)	462 (84%)	91 (16%)	2	3
1	G	552/569 (97%)	469 (85%)	83 (15%)	3	3
1	H	554/569 (97%)	471 (85%)	83 (15%)	3	3
1	I	557/569 (98%)	468 (84%)	89 (16%)	2	3
1	J	557/569 (98%)	469 (84%)	88 (16%)	2	3
1	K	556/569 (98%)	459 (83%)	97 (17%)	2	2
1	L	557/569 (98%)	473 (85%)	84 (15%)	3	3
1	M	550/569 (97%)	456 (83%)	94 (17%)	2	2
1	N	553/569 (97%)	448 (81%)	105 (19%)	1	2
1	O	556/569 (98%)	466 (84%)	90 (16%)	2	3
1	P	551/569 (97%)	457 (83%)	94 (17%)	2	2
1	Q	548/569 (96%)	456 (83%)	92 (17%)	2	3
1	R	553/569 (97%)	459 (83%)	94 (17%)	2	2
All	All	9963/10242 (97%)	8351 (84%)	1612 (16%)	2	3

5 of 1612 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	357	THR
1	P	564	VAL
1	L	546	VAL
1	N	503	VAL
1	N	355	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 326 such sidechains are listed below:

Mol	Chain	Res	Type
1	P	565	ASN
1	J	473	HIS
1	Q	105	HIS
1	R	259	HIS
1	K	362	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

36 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
3	PO4	I	702	-	4,4,4	1.18	0	6,6,6	1.51	2 (33%)
3	PO4	K	702	-	4,4,4	0.98	0	6,6,6	0.63	0
3	PO4	C	702	-	4,4,4	0.79	0	6,6,6	1.19	1 (16%)
3	PO4	O	702	-	4,4,4	0.86	0	6,6,6	0.42	0
3	PO4	D	702	-	4,4,4	1.10	0	6,6,6	1.75	2 (33%)
2	SAH	M	701	-	27,28,28	1.78	6 (22%)	36,40,40	2.35	12 (33%)
2	SAH	E	701	-	27,28,28	1.49	5 (18%)	36,40,40	2.16	14 (38%)
3	PO4	F	702	-	4,4,4	1.05	0	6,6,6	1.44	1 (16%)
3	PO4	P	702	-	4,4,4	0.90	0	6,6,6	1.02	0
2	SAH	B	701	-	27,28,28	1.41	5 (18%)	36,40,40	2.10	13 (36%)
3	PO4	M	702	-	4,4,4	0.80	0	6,6,6	0.83	0
3	PO4	J	702	-	4,4,4	1.07	0	6,6,6	0.79	0
3	PO4	G	702	-	4,4,4	1.10	0	6,6,6	1.00	0
2	SAH	F	701	-	27,28,28	1.36	4 (14%)	36,40,40	2.19	12 (33%)
3	PO4	L	702	-	4,4,4	1.11	0	6,6,6	0.93	0
3	PO4	E	702	-	4,4,4	0.71	0	6,6,6	0.95	0
3	PO4	B	702	-	4,4,4	0.87	0	6,6,6	1.12	0
2	SAH	A	701	-	27,28,28	1.61	5 (18%)	36,40,40	2.16	14 (38%)
2	SAH	K	701	-	27,28,28	1.40	5 (18%)	36,40,40	2.27	14 (38%)
2	SAH	C	701	-	27,28,28	1.35	4 (14%)	36,40,40	2.21	12 (33%)
3	PO4	Q	702	-	4,4,4	1.00	0	6,6,6	0.58	0
3	PO4	R	702	-	4,4,4	0.72	0	6,6,6	0.82	0
3	PO4	H	702	-	4,4,4	0.74	0	6,6,6	1.52	1 (16%)
2	SAH	R	701	-	27,28,28	1.51	6 (22%)	36,40,40	2.05	10 (27%)
2	SAH	N	701	-	27,28,28	1.47	5 (18%)	36,40,40	2.27	15 (41%)
3	PO4	A	702	-	4,4,4	0.67	0	6,6,6	1.36	1 (16%)
2	SAH	O	701	-	27,28,28	1.46	5 (18%)	36,40,40	2.25	14 (38%)
2	SAH	I	701	-	27,28,28	1.50	6 (22%)	36,40,40	2.32	17 (47%)
2	SAH	Q	701	-	27,28,28	1.39	4 (14%)	36,40,40	2.04	12 (33%)
3	PO4	N	702	-	4,4,4	1.01	0	6,6,6	0.75	0
2	SAH	L	701	-	27,28,28	1.55	6 (22%)	36,40,40	2.39	15 (41%)
2	SAH	H	701	-	27,28,28	1.59	5 (18%)	36,40,40	2.53	11 (30%)
2	SAH	J	701	-	27,28,28	1.37	4 (14%)	36,40,40	2.11	12 (33%)
2	SAH	D	701	-	27,28,28	1.54	5 (18%)	36,40,40	2.25	14 (38%)
2	SAH	G	701	-	27,28,28	1.60	4 (14%)	36,40,40	2.20	14 (38%)
2	SAH	P	701	-	27,28,28	1.58	5 (18%)	36,40,40	2.07	14 (38%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	A	701	-	-	0/15/31/31	0/3/3/3
2	SAH	I	701	-	-	1/15/31/31	0/3/3/3
2	SAH	C	701	-	-	1/15/31/31	0/3/3/3
2	SAH	O	701	-	-	0/15/31/31	0/3/3/3
2	SAH	M	701	-	-	3/15/31/31	0/3/3/3
2	SAH	K	701	-	-	0/15/31/31	0/3/3/3
2	SAH	D	701	-	-	0/15/31/31	0/3/3/3
2	SAH	G	701	-	-	4/15/31/31	0/3/3/3
2	SAH	Q	701	-	-	2/15/31/31	0/3/3/3
2	SAH	L	701	-	-	2/15/31/31	0/3/3/3
2	SAH	H	701	-	-	3/15/31/31	0/3/3/3
2	SAH	R	701	-	-	2/15/31/31	0/3/3/3
2	SAH	N	701	-	-	5/15/31/31	0/3/3/3
2	SAH	J	701	-	-	1/15/31/31	0/3/3/3
2	SAH	F	701	-	-	2/15/31/31	0/3/3/3
2	SAH	E	701	-	-	0/15/31/31	0/3/3/3
2	SAH	B	701	-	-	1/15/31/31	0/3/3/3
2	SAH	P	701	-	-	2/15/31/31	0/3/3/3

The worst 5 of 89 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	701	SAH	C5-C4	5.42	1.48	1.39
2	P	701	SAH	C5-C4	5.27	1.48	1.39
2	G	701	SAH	C5-C4	5.06	1.48	1.39
2	L	701	SAH	C5-C4	4.98	1.48	1.39
2	A	701	SAH	C5-C4	4.96	1.47	1.39

The worst 5 of 247 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	701	SAH	O4'-C1'-N9	-6.79	95.05	108.09
2	K	701	SAH	O4'-C1'-N9	-6.45	95.70	108.09
2	C	701	SAH	C5-C4-N3	-6.40	117.90	126.72
2	H	701	SAH	C5-C4-N3	-6.33	118.00	126.72
2	G	701	SAH	C5-C4-N3	-5.68	118.90	126.72

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

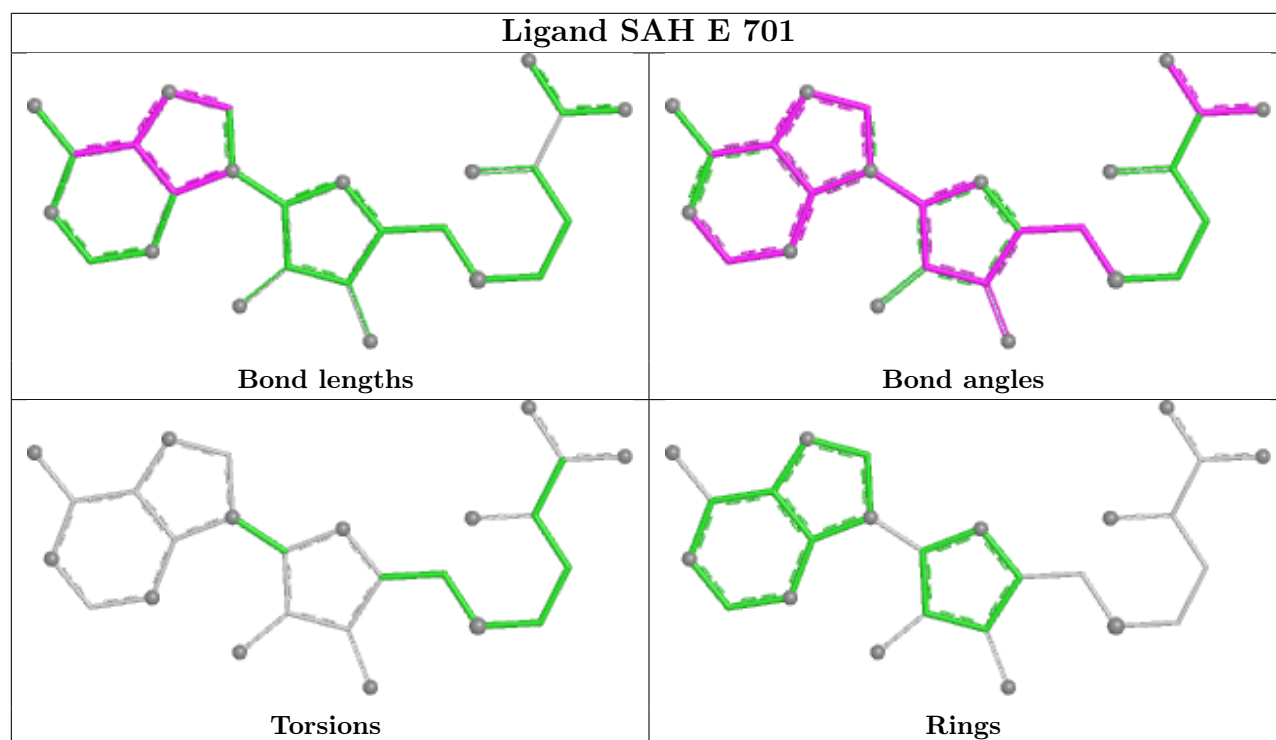
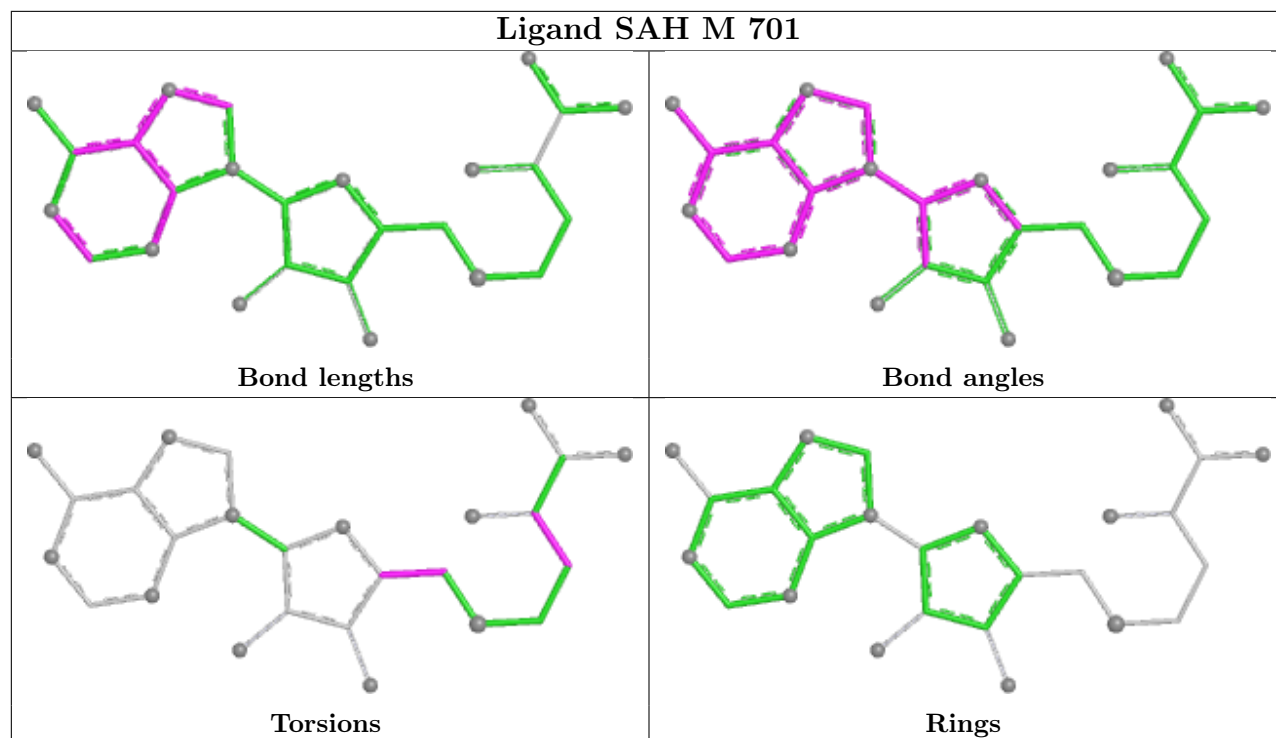
Mol	Chain	Res	Type	Atoms
2	F	701	SAH	O4'-C4'-C5'-SD
2	G	701	SAH	O4'-C4'-C5'-SD
2	G	701	SAH	C3'-C4'-C5'-SD
2	N	701	SAH	O-C-CA-N
2	N	701	SAH	O4'-C4'-C5'-SD

There are no ring outliers.

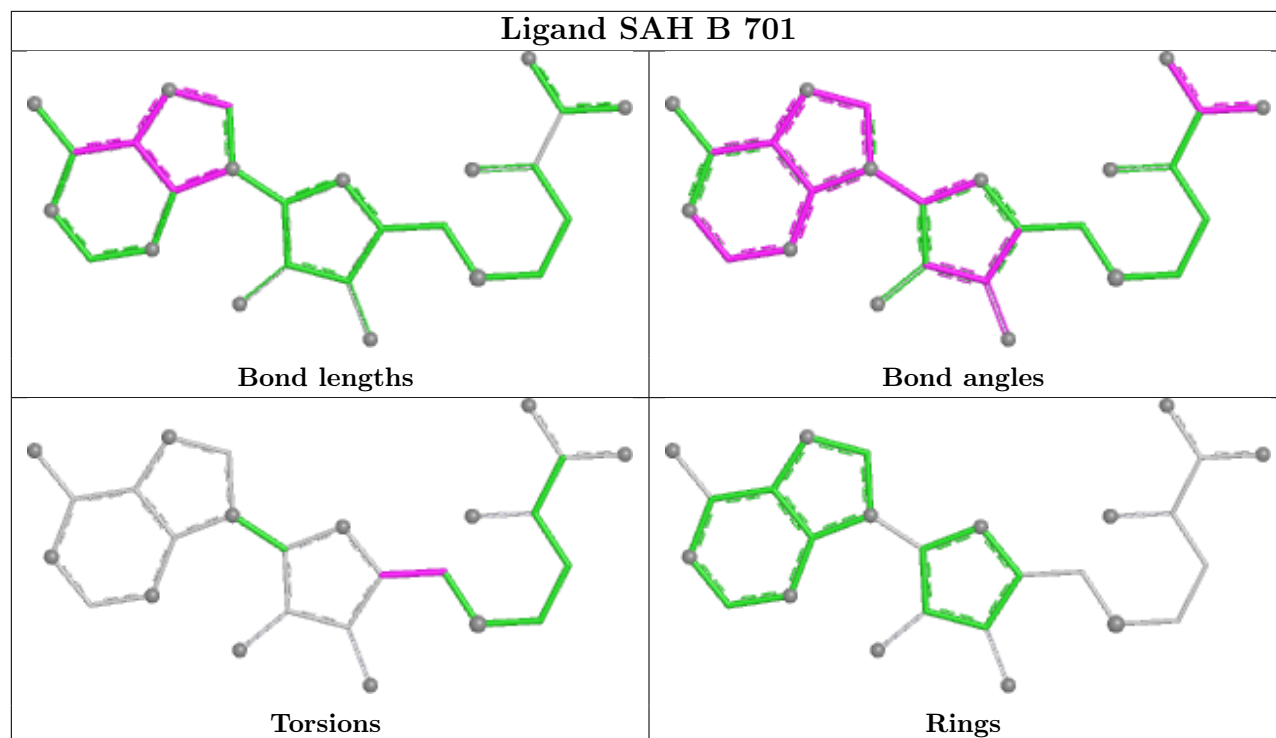
15 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	702	PO4	1	0
2	M	701	SAH	2	0
2	E	701	SAH	3	0
2	B	701	SAH	2	0
2	F	701	SAH	2	0
2	K	701	SAH	3	0
2	C	701	SAH	1	0
3	Q	702	PO4	1	0
2	R	701	SAH	2	0
2	N	701	SAH	2	0
2	I	701	SAH	1	0
2	Q	701	SAH	2	0
2	H	701	SAH	1	0
2	G	701	SAH	2	0
2	P	701	SAH	3	0

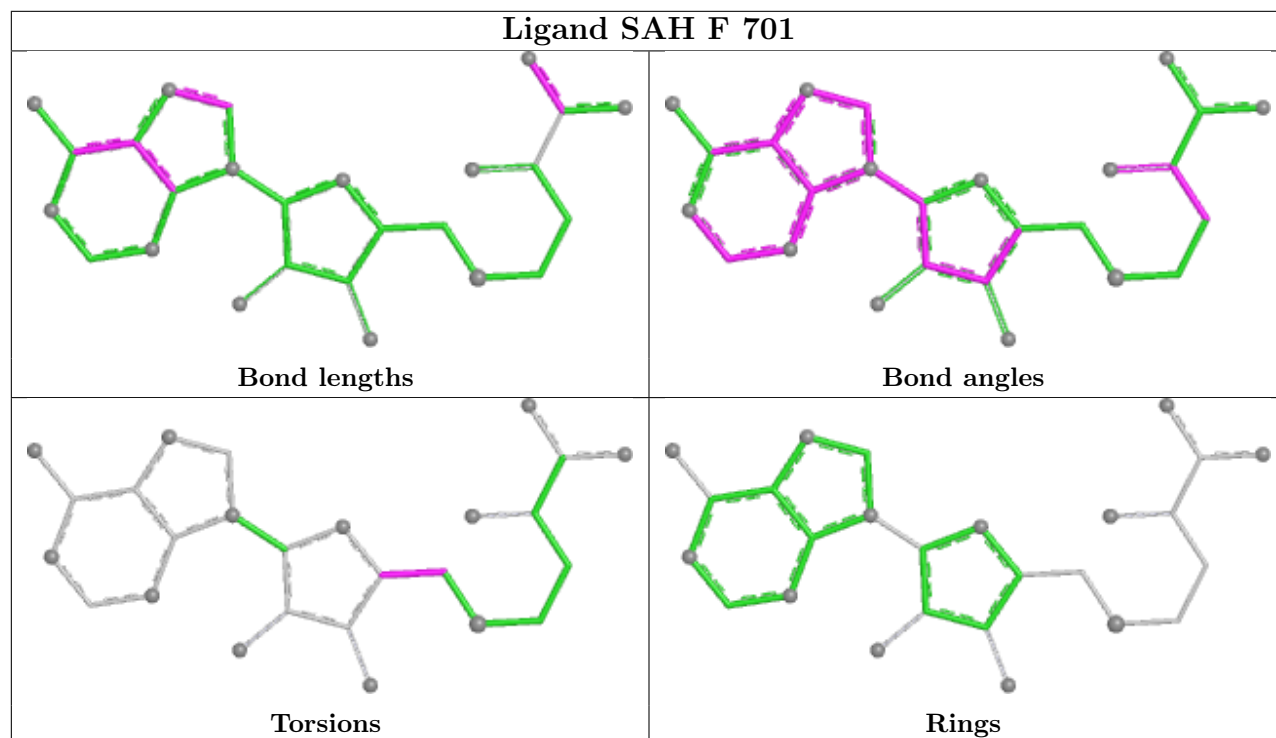
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

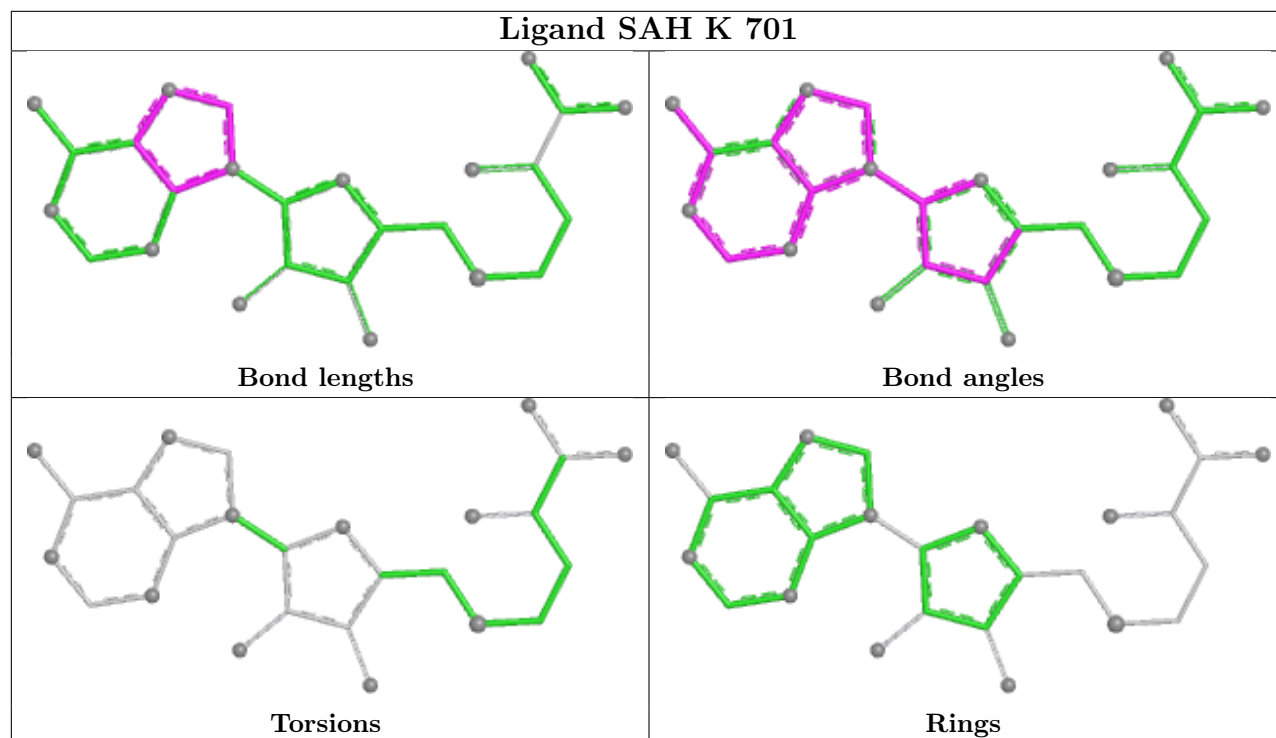
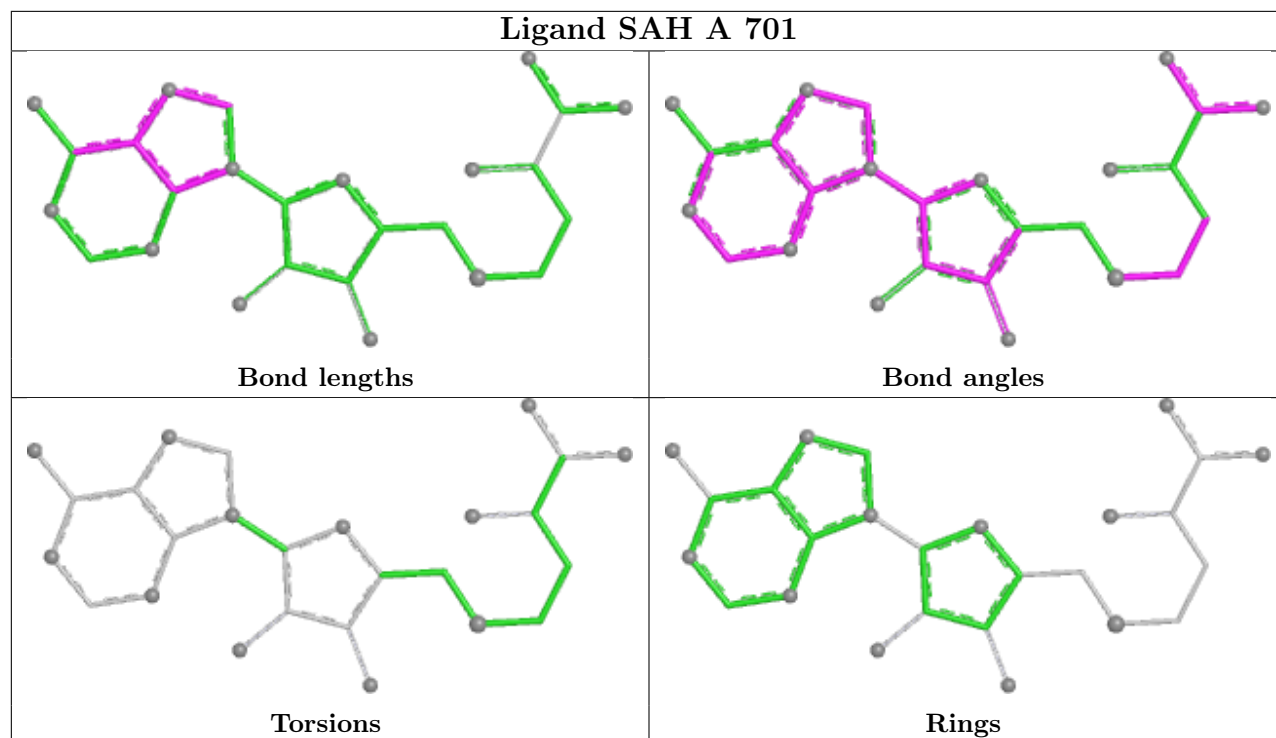


Ligand SAH B 701

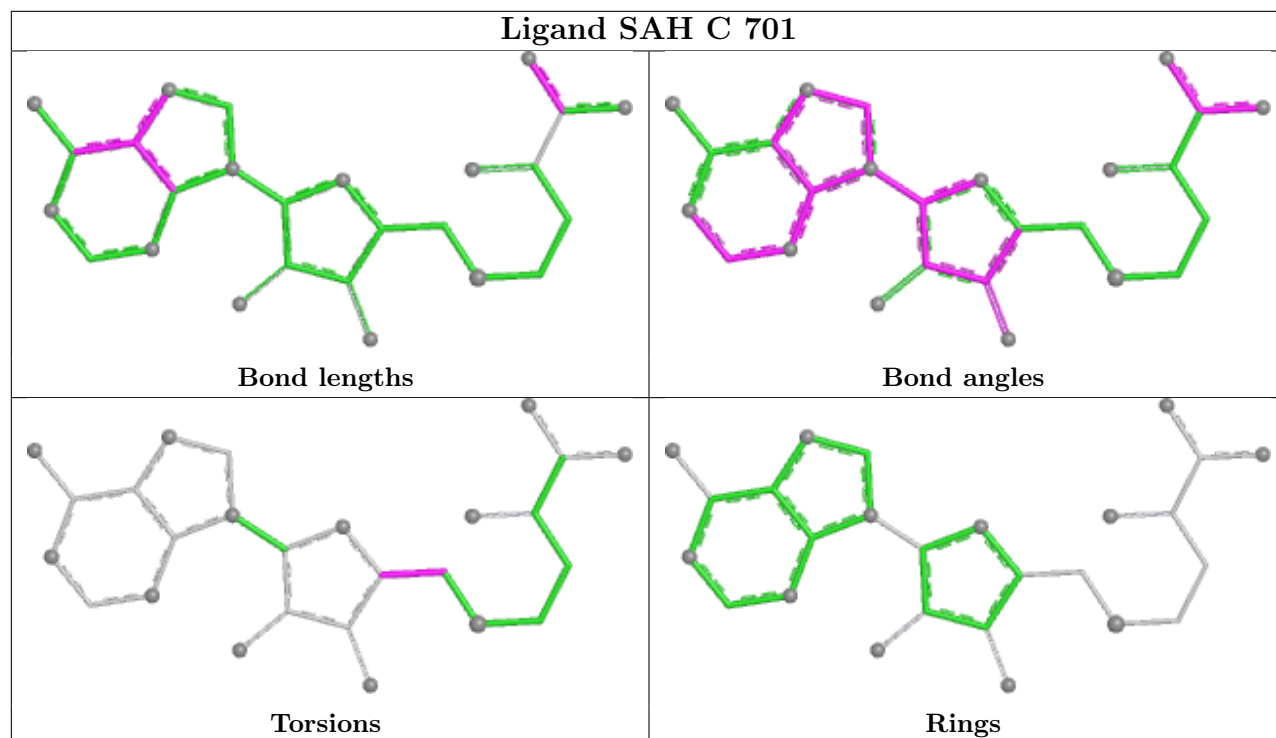


Ligand SAH F 701

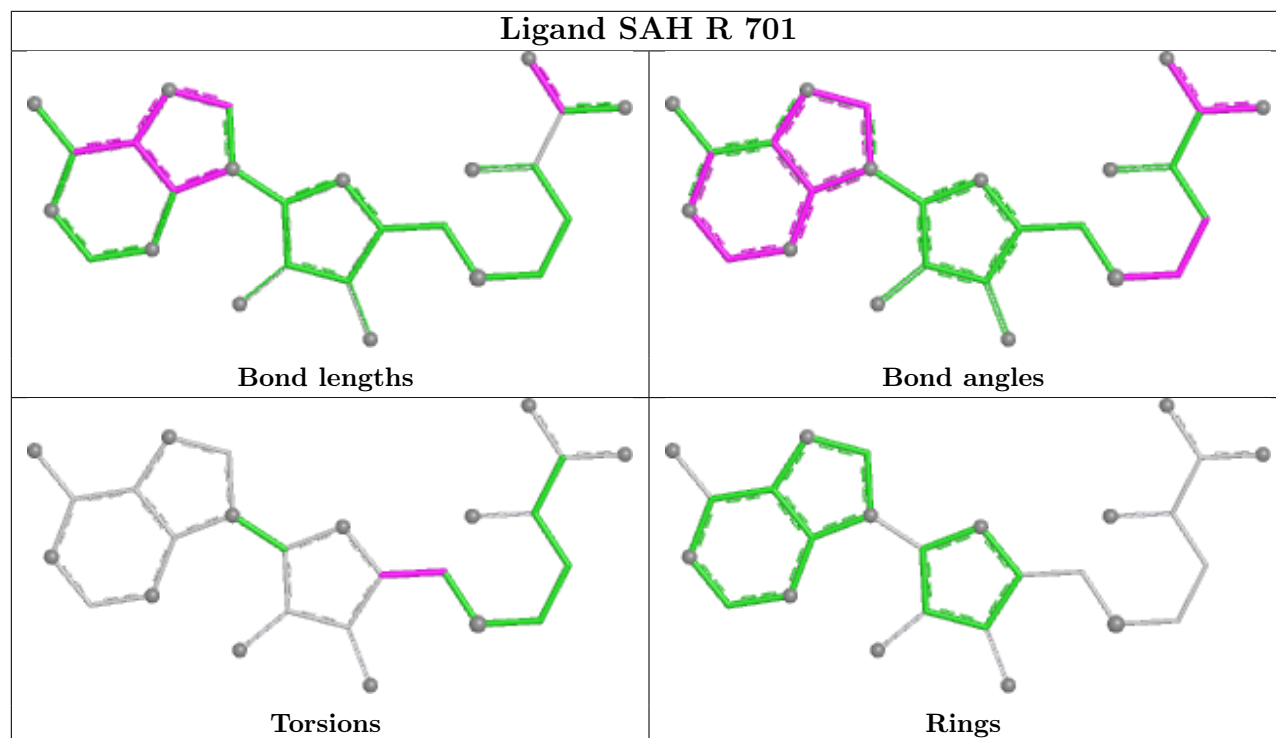


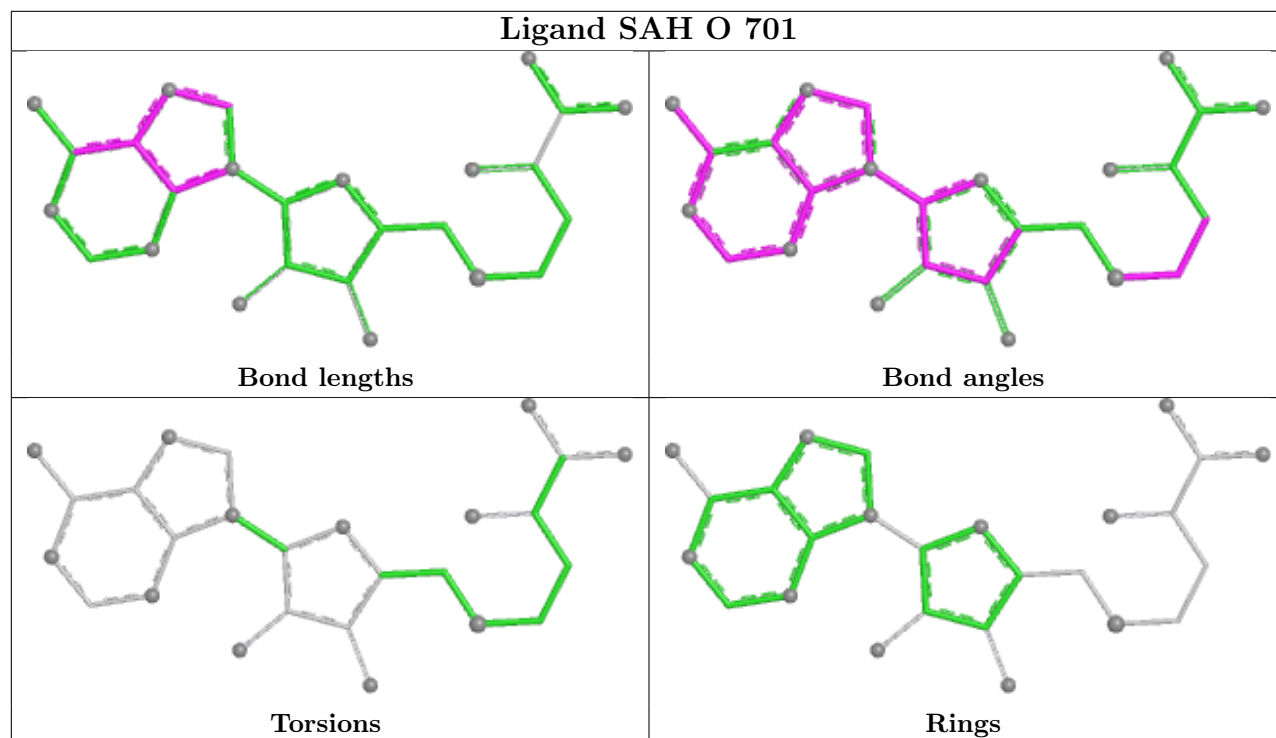
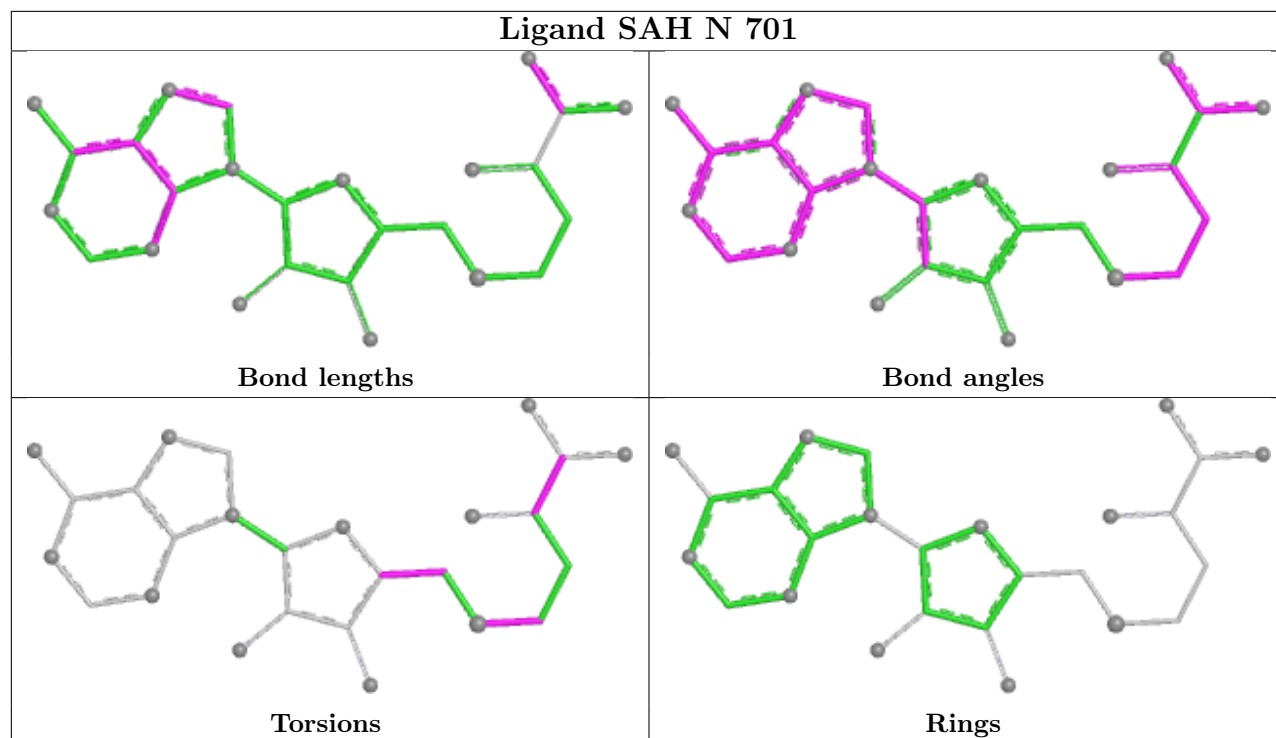


Ligand SAH C 701

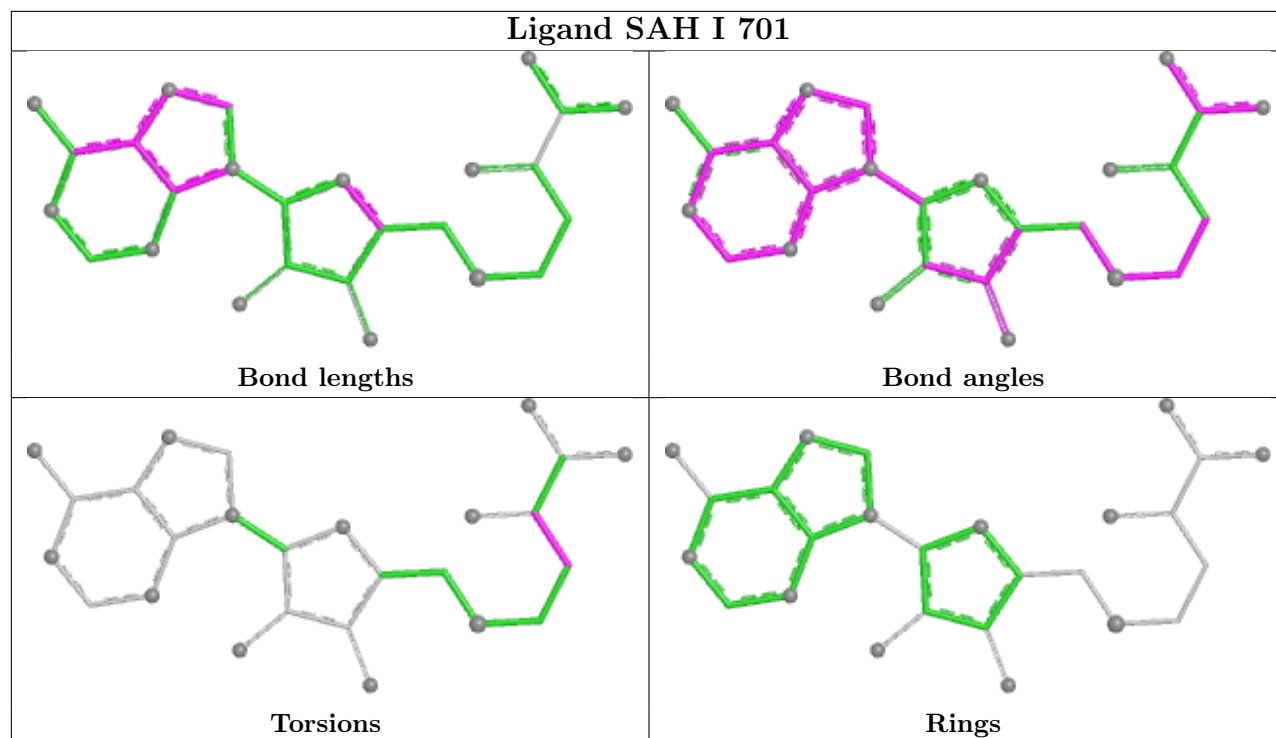


Ligand SAH R 701

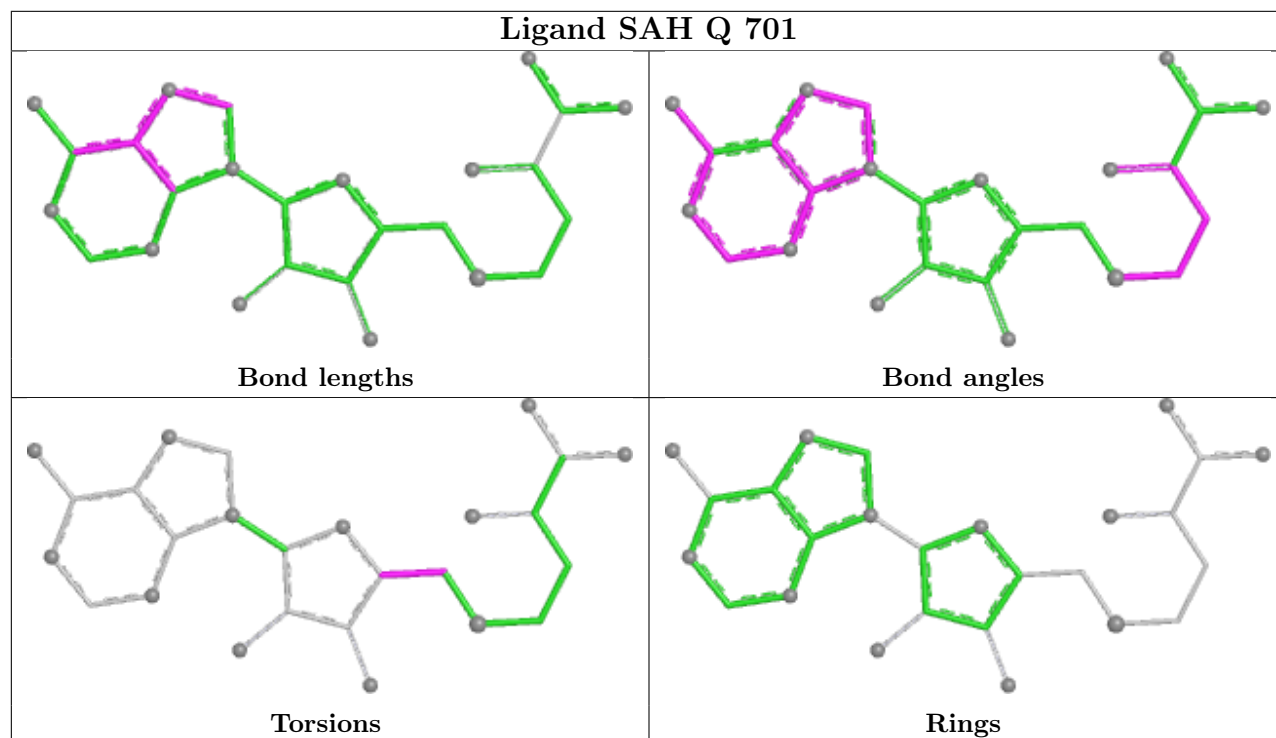




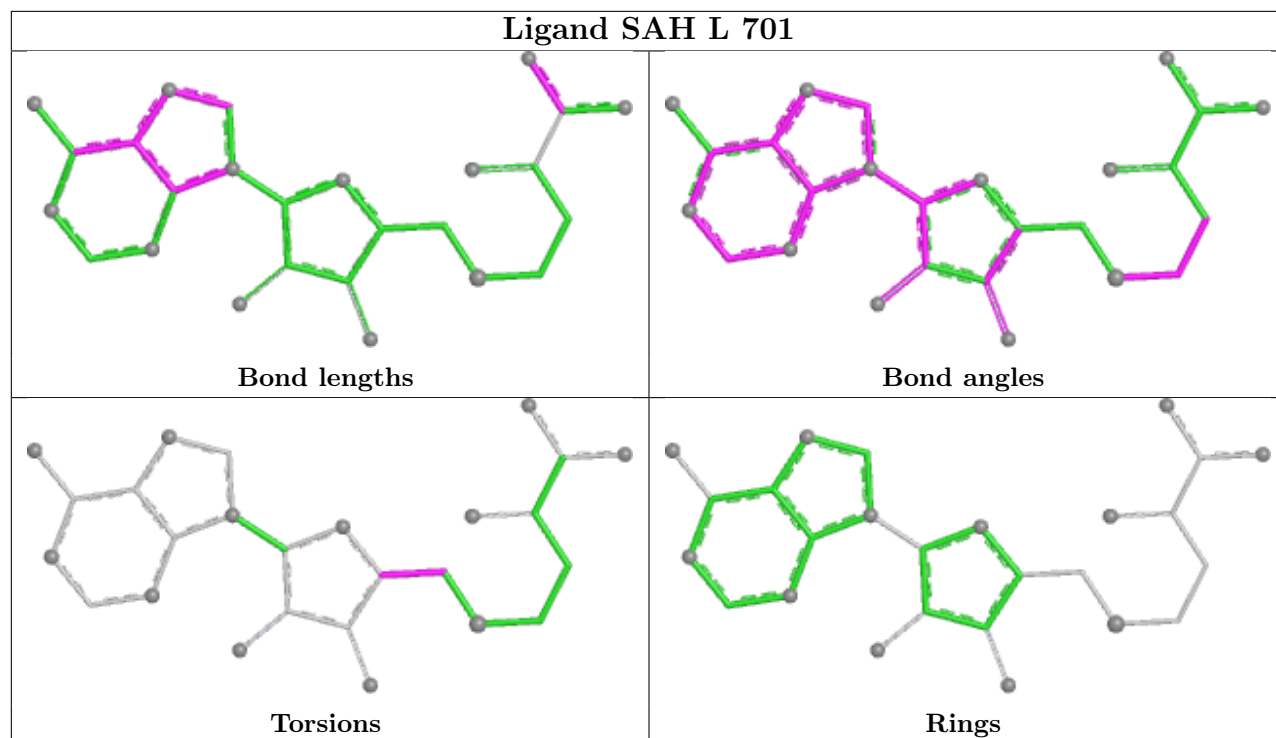
Ligand SAH I 701



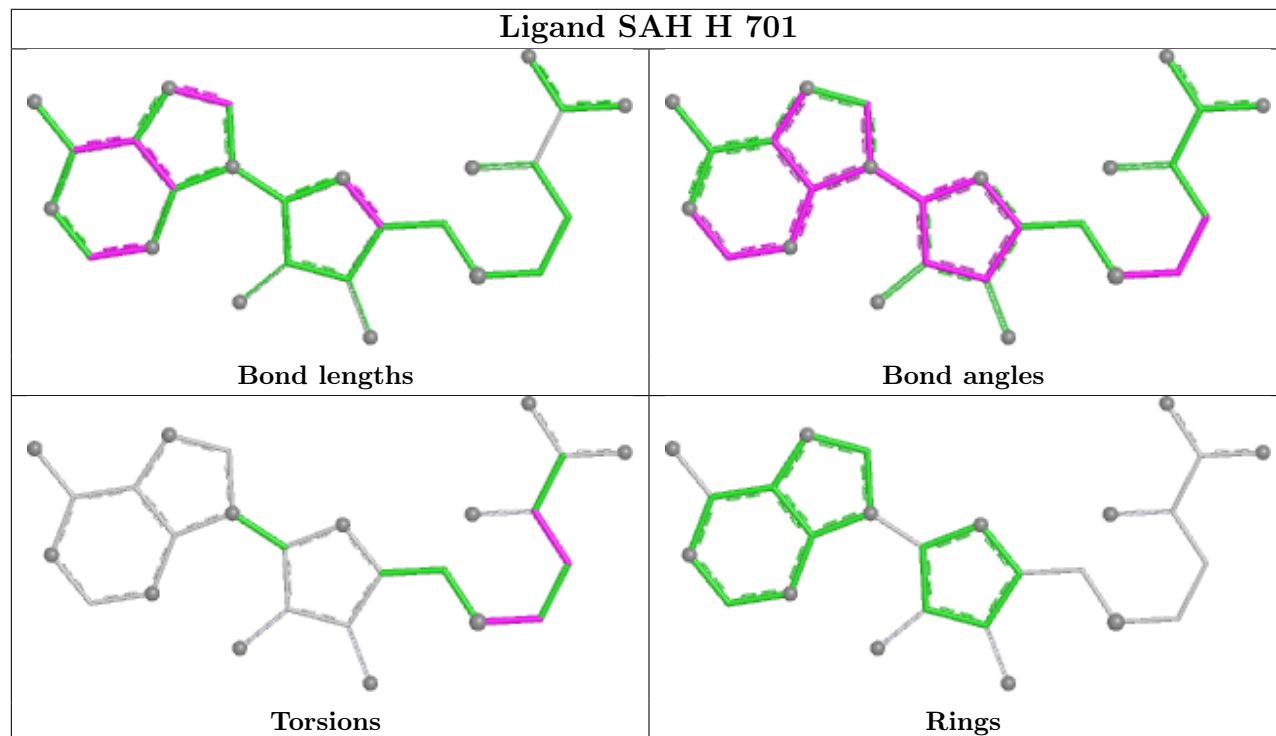
Ligand SAH Q 701



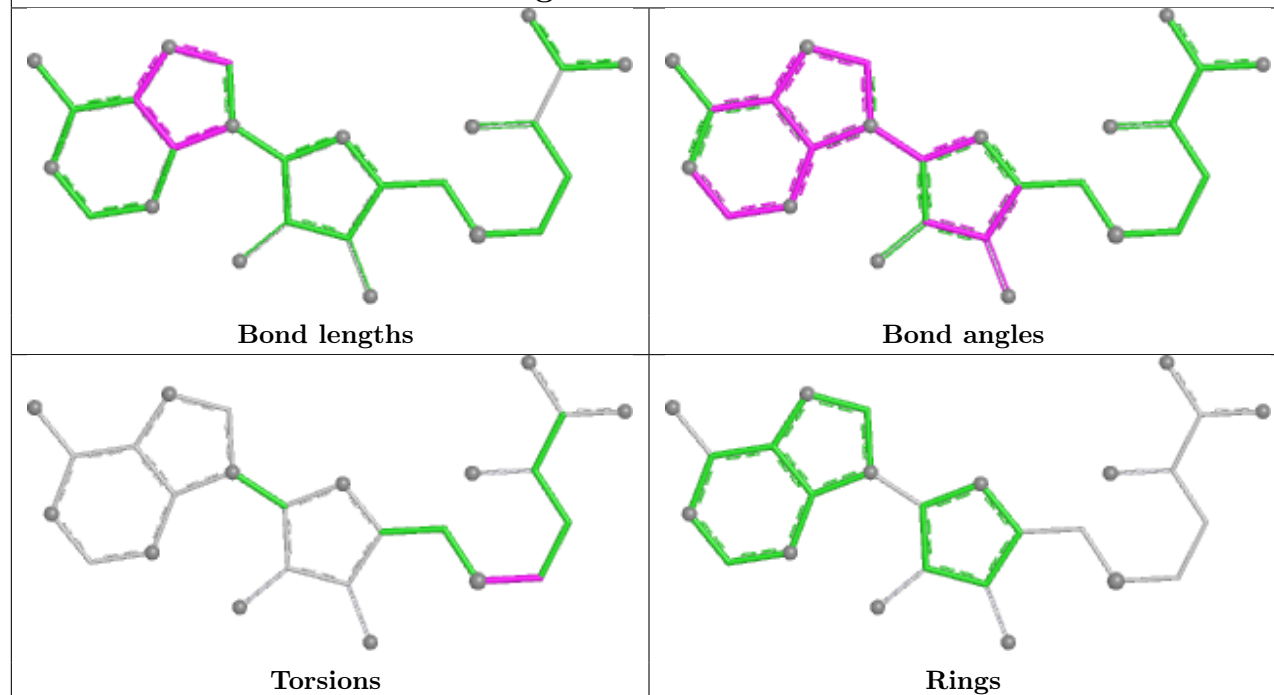
Ligand SAH L 701



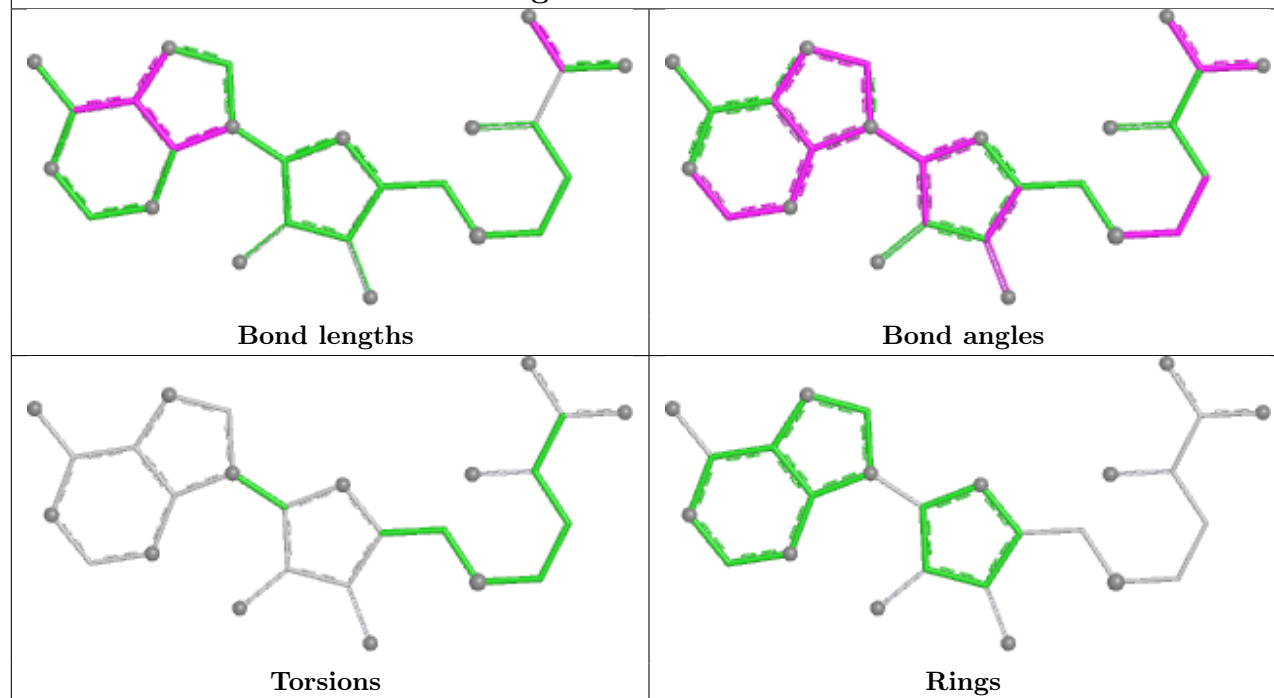
Ligand SAH H 701

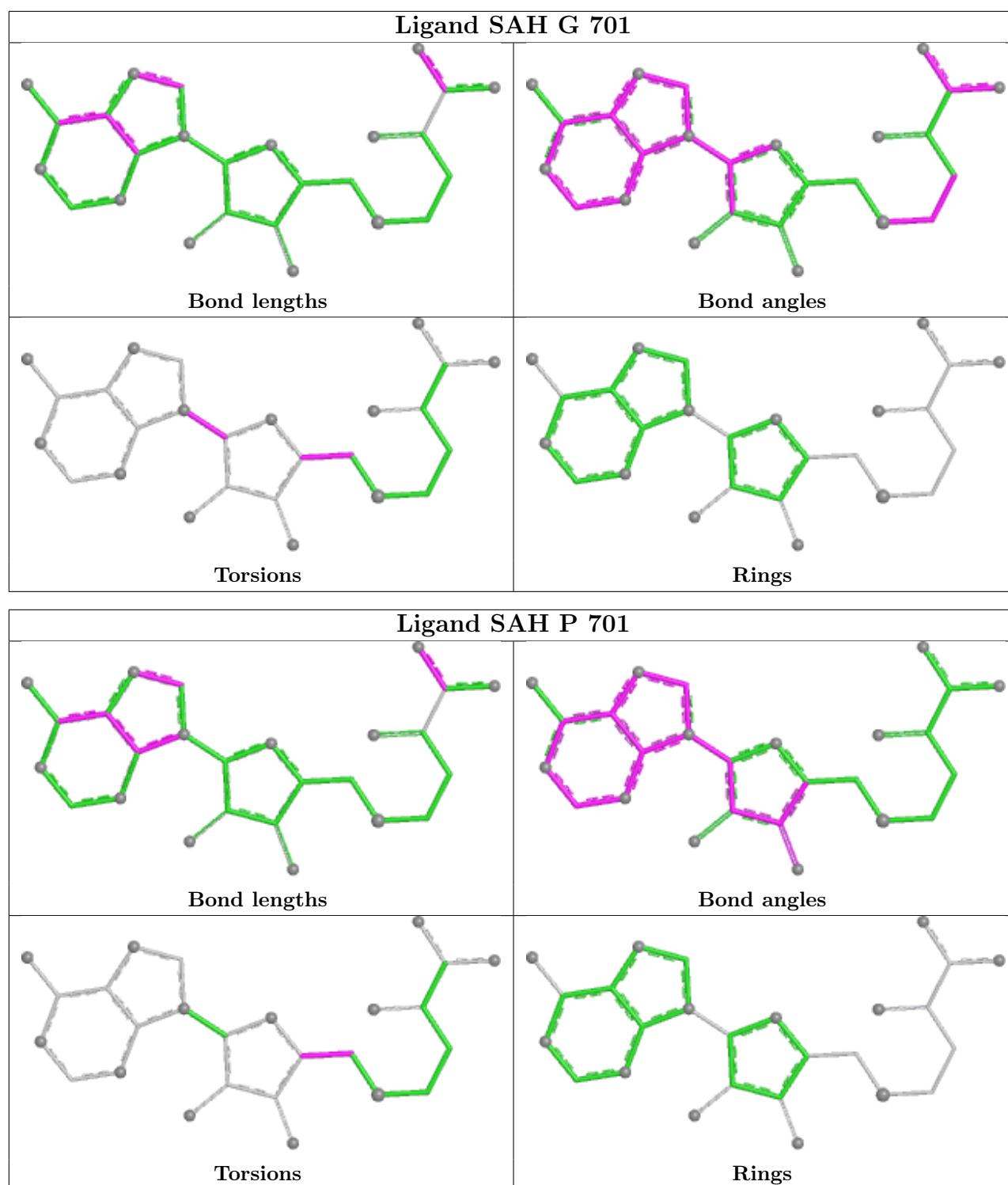


Ligand SAH J 701



Ligand SAH D 701





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	641/655 (97%)	-1.27	0 100 100	16, 33, 57, 83	0
1	B	638/655 (97%)	-1.14	0 100 100	24, 43, 74, 103	0
1	C	639/655 (97%)	-1.13	0 100 100	26, 44, 68, 100	0
1	D	637/655 (97%)	-1.26	0 100 100	19, 34, 56, 101	0
1	E	636/655 (97%)	-1.12	0 100 100	21, 41, 80, 124	0
1	F	638/655 (97%)	-1.06	0 100 100	27, 48, 75, 120	0
1	G	636/655 (97%)	-1.12	0 100 100	23, 43, 81, 129	0
1	H	639/655 (97%)	-1.22	0 100 100	18, 38, 60, 91	0
1	I	644/655 (98%)	-1.15	0 100 100	28, 44, 68, 94	0
1	J	644/655 (98%)	-1.08	0 100 100	29, 47, 69, 92	0
1	K	641/655 (97%)	-1.04	0 100 100	26, 52, 77, 99	0
1	L	644/655 (98%)	-1.29	0 100 100	19, 33, 55, 78	0
1	M	633/655 (96%)	-0.91	0 100 100	38, 61, 84, 110	0
1	N	638/655 (97%)	-1.01	0 100 100	36, 55, 75, 93	0
1	O	641/655 (97%)	-0.88	1 (0%) 91 89	39, 64, 96, 127	0
1	P	636/655 (97%)	-1.03	0 100 100	30, 51, 82, 105	0
1	Q	632/655 (96%)	-0.86	0 100 100	37, 62, 99, 124	0
1	R	638/655 (97%)	-0.80	0 100 100	44, 69, 99, 131	0
All	All	11495/11790 (97%)	-1.08	1 (0%) 100 100	16, 48, 82, 131	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	553	ILE	2.4

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

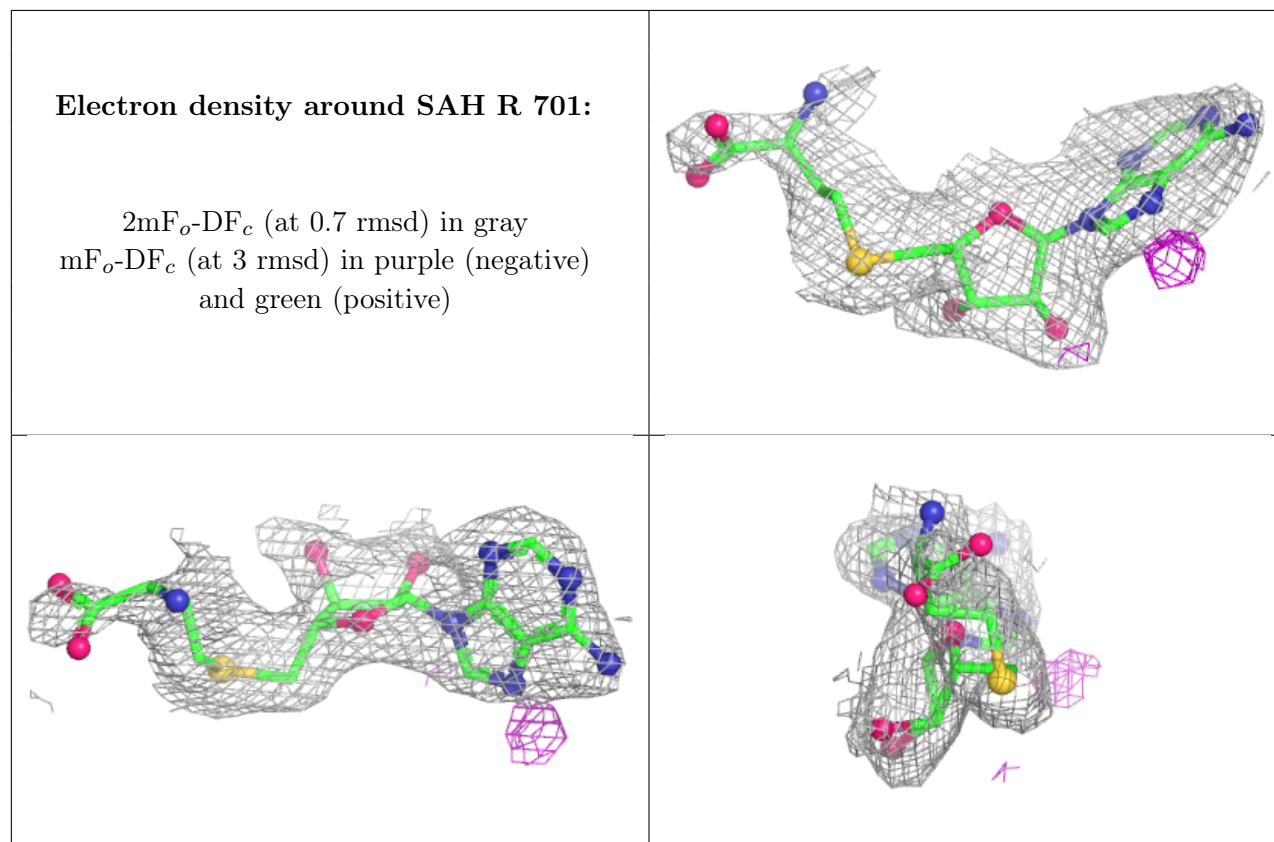
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SAH	R	701	26/26	0.98	0.06	47,56,92,99	0
3	PO4	M	702	5/5	0.98	0.05	70,71,74,78	0
3	PO4	N	702	5/5	0.98	0.03	52,57,62,66	0
3	PO4	O	702	5/5	0.98	0.04	57,58,70,72	0
3	PO4	R	702	5/5	0.98	0.05	52,55,59,61	0
2	SAH	E	701	26/26	0.99	0.04	43,53,63,65	0
2	SAH	G	701	26/26	0.99	0.04	46,63,72,72	0
2	SAH	H	701	26/26	0.99	0.03	24,29,33,34	0
2	SAH	I	701	26/26	0.99	0.03	35,38,45,47	0
2	SAH	M	701	26/26	0.99	0.04	36,61,74,79	0
2	SAH	N	701	26/26	0.99	0.04	40,53,58,58	0
2	SAH	O	701	26/26	0.99	0.03	37,41,47,52	0
2	SAH	P	701	26/26	0.99	0.04	43,53,63,65	0
2	SAH	Q	701	26/26	0.99	0.05	48,64,75,76	0
2	SAH	A	701	26/26	0.99	0.04	27,33,38,38	0
2	SAH	J	701	26/26	0.99	0.04	34,38,44,46	0
2	SAH	K	701	26/26	0.99	0.04	37,41,47,51	0
2	SAH	L	701	26/26	0.99	0.03	27,33,36,39	0
3	PO4	A	702	5/5	0.99	0.03	31,32,37,39	0
3	PO4	B	702	5/5	0.99	0.04	36,39,45,48	0
3	PO4	C	702	5/5	0.99	0.04	37,41,44,44	0
3	PO4	F	702	5/5	0.99	0.04	38,42,49,56	0
3	PO4	E	702	5/5	0.99	0.03	36,40,43,47	0
3	PO4	G	702	5/5	0.99	0.03	42,42,49,50	0
3	PO4	H	702	5/5	0.99	0.02	28,34,36,37	0
3	PO4	I	702	5/5	0.99	0.04	36,37,44,49	0
2	SAH	D	701	26/26	0.99	0.05	32,37,45,46	0

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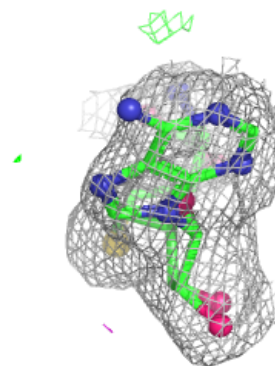
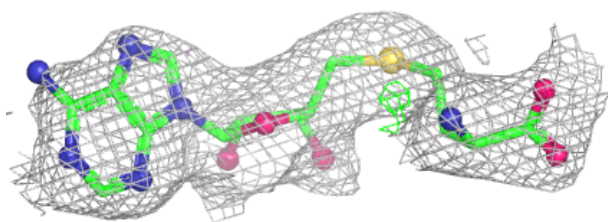
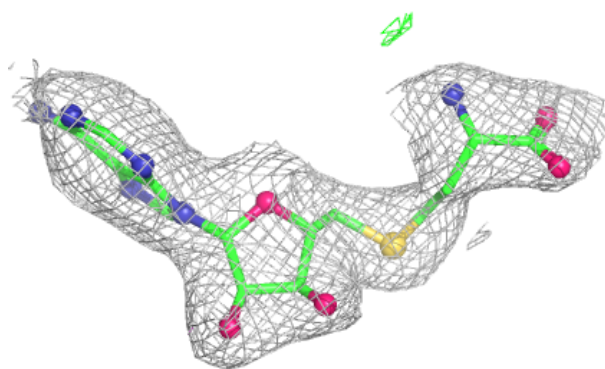
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SAH	B	701	26/26	0.99	0.04	36,43,57,58	0
2	SAH	C	701	26/26	0.99	0.03	36,48,57,59	0
3	PO4	P	702	5/5	0.99	0.03	43,43,45,47	0
3	PO4	Q	702	5/5	0.99	0.04	59,63,72,72	0
2	SAH	F	701	26/26	0.99	0.04	35,46,61,64	0
3	PO4	J	702	5/5	0.99	0.03	45,46,49,51	0
3	PO4	K	702	5/5	0.99	0.03	43,45,46,51	0
3	PO4	D	702	5/5	1.00	0.03	31,35,36,37	0
3	PO4	L	702	5/5	1.00	0.03	32,32,35,37	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.

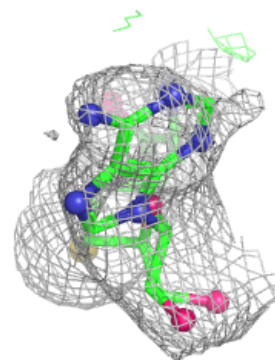
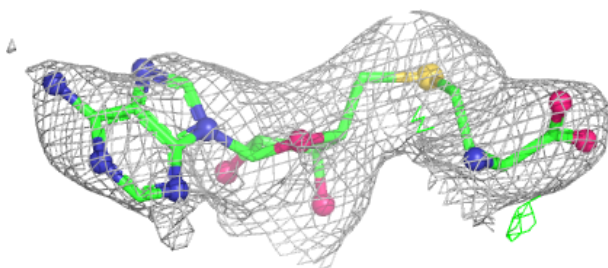
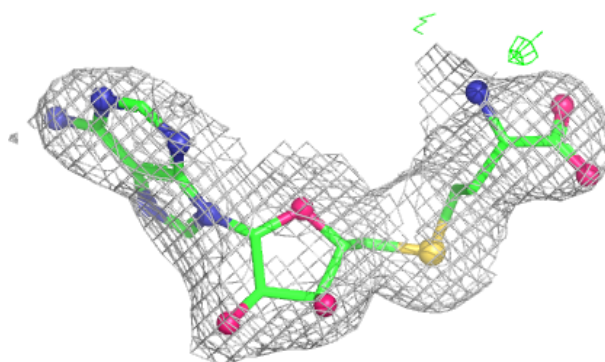


Electron density around SAH E 701:

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

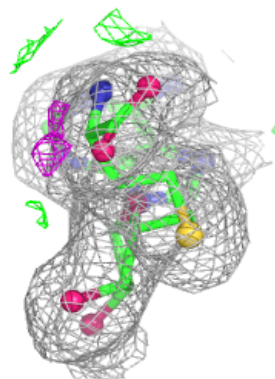
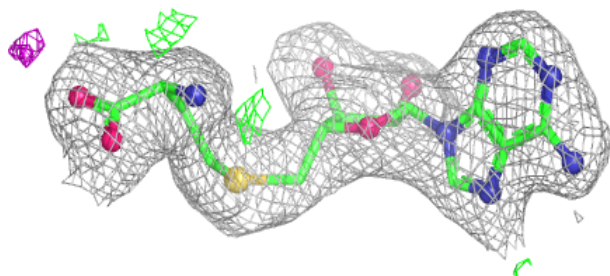
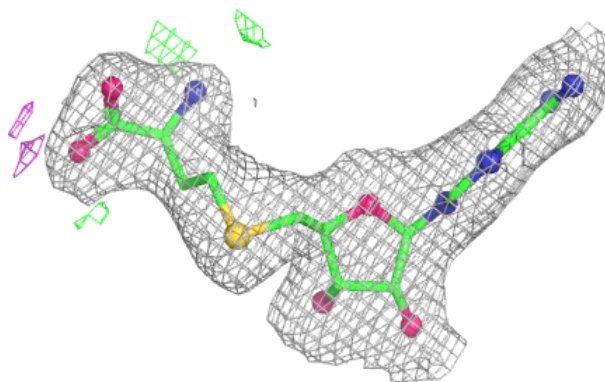
**Electron density around SAH G 701:**

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and green (positive)

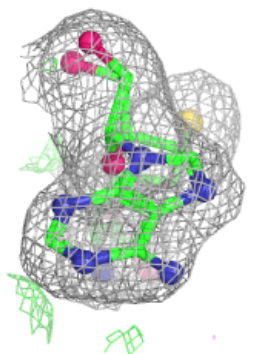
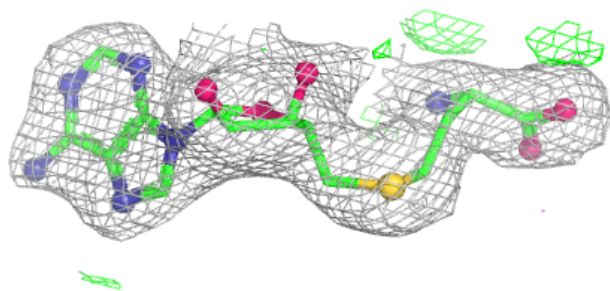
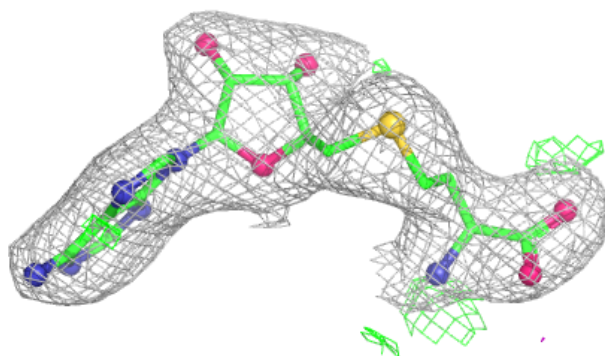


Electron density around SAH H 701:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

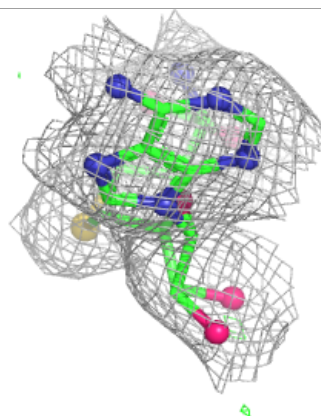
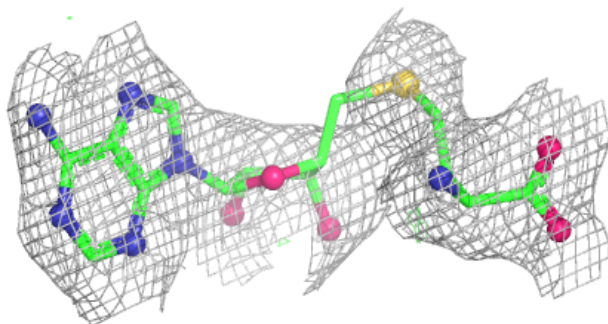
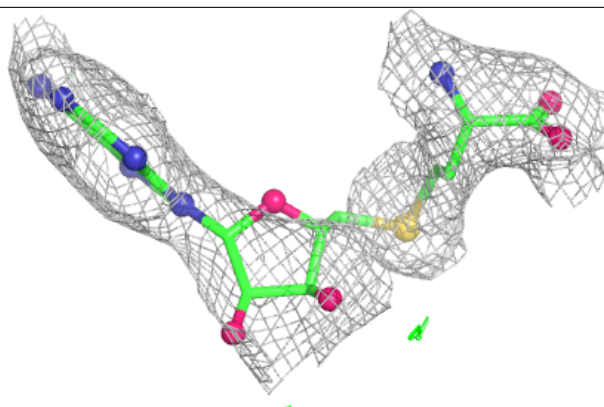
**Electron density around SAH I 701:**

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

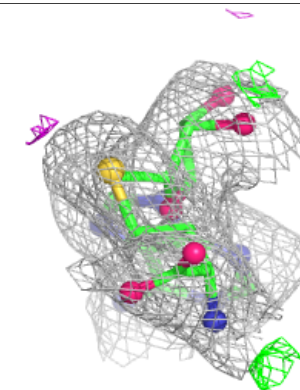
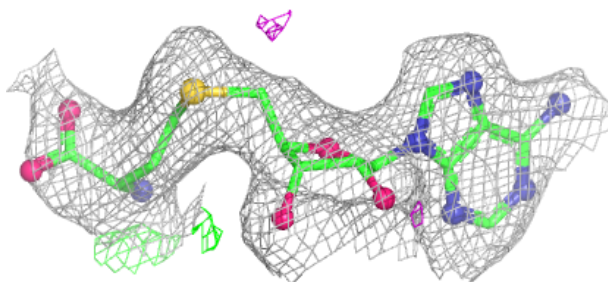
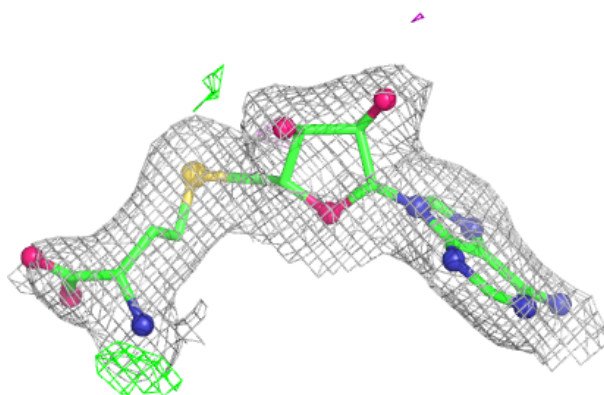


Electron density around SAH M 701:

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

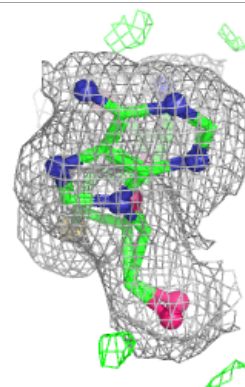
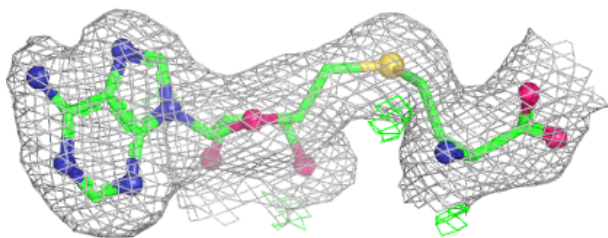
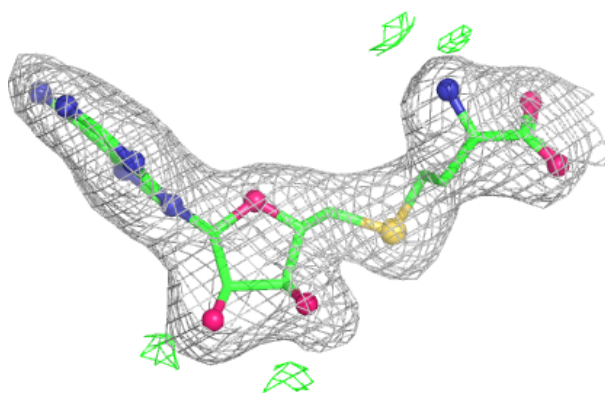
**Electron density around SAH N 701:**

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

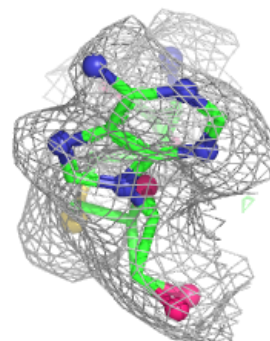
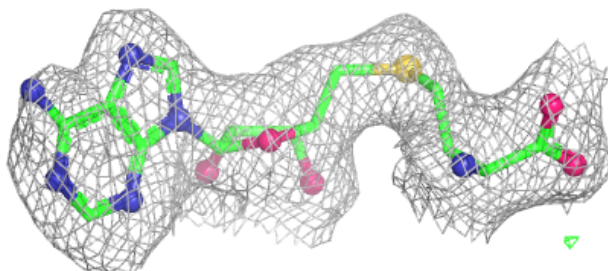
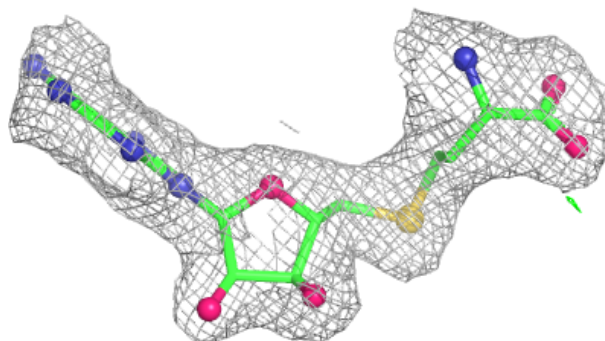


Electron density around SAH O 701:

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

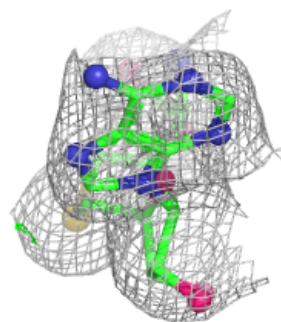
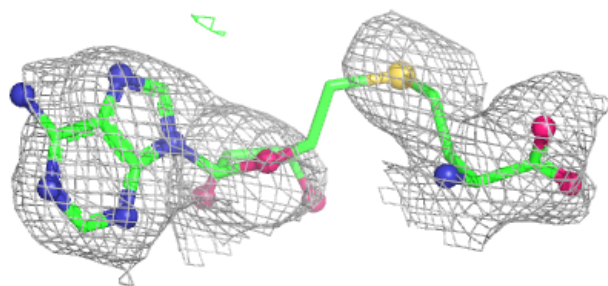
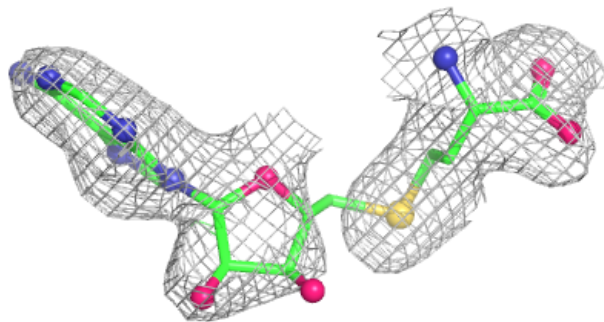
**Electron density around SAH P 701:**

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

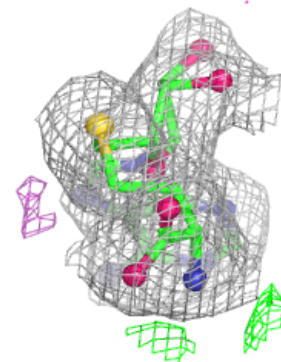
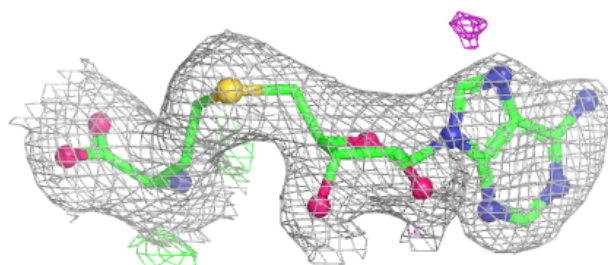
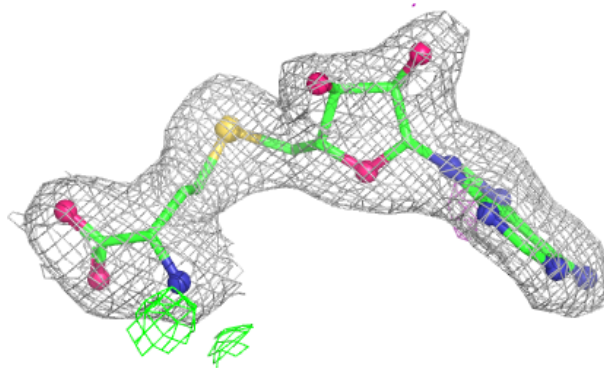


Electron density around SAH Q 701:

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

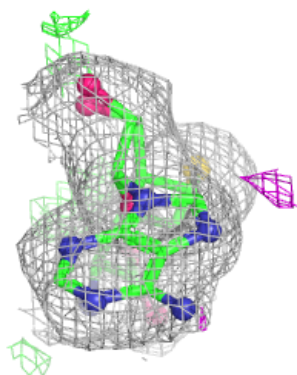
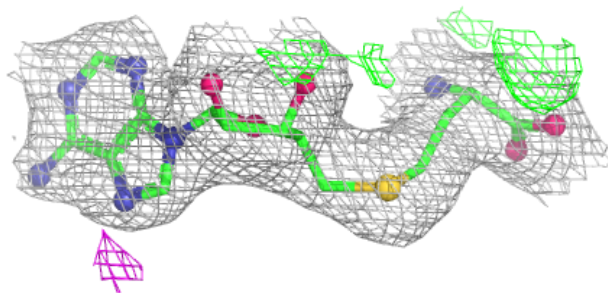
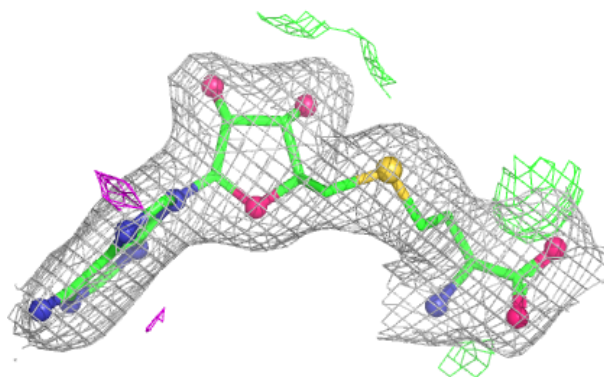
**Electron density around SAH A 701:**

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

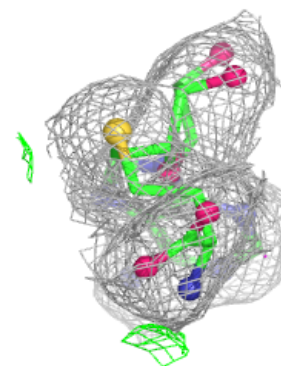
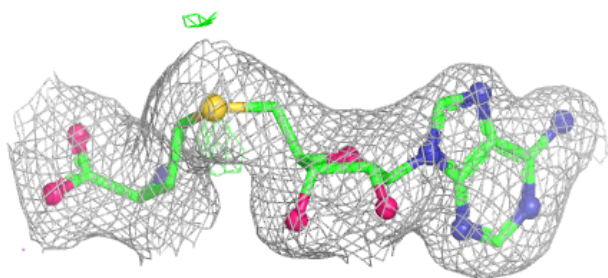
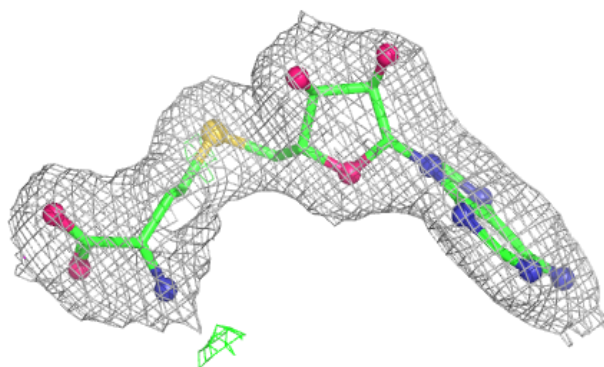


Electron density around SAH J 701:

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

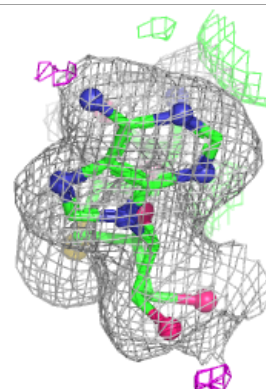
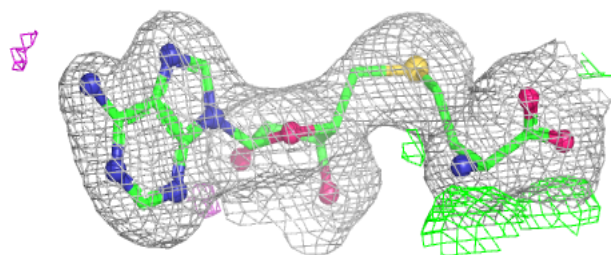
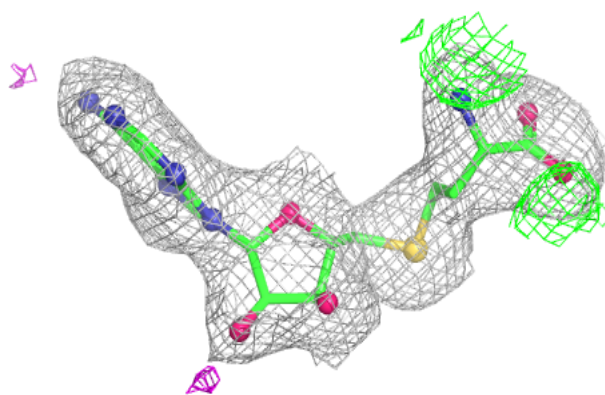
**Electron density around SAH K 701:**

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

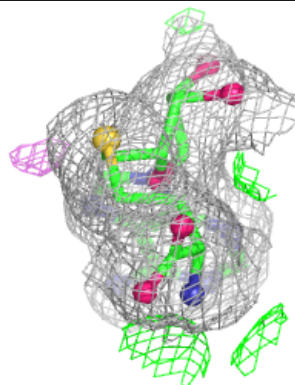
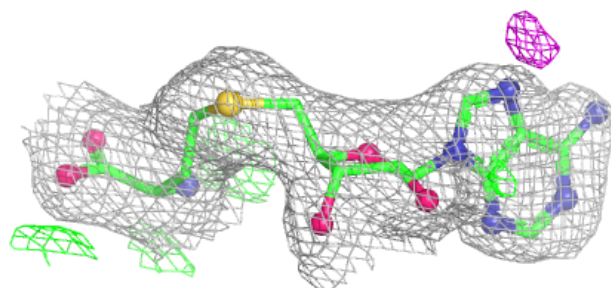
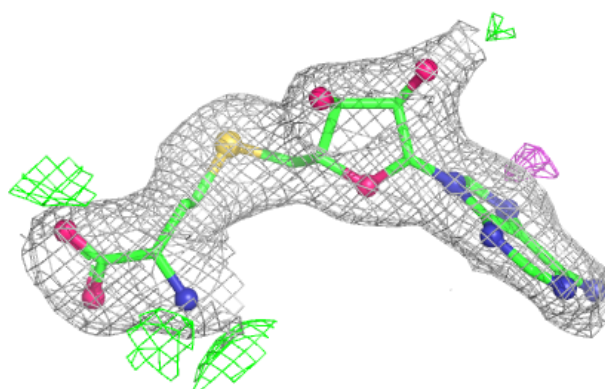


Electron density around SAH L 701:

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

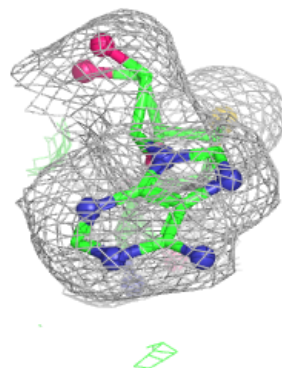
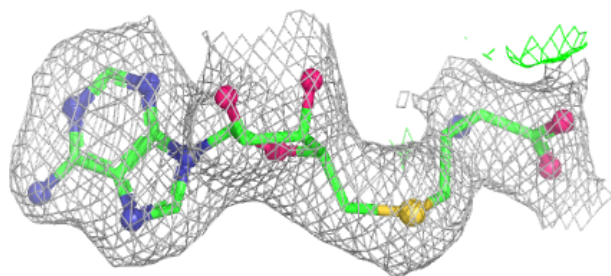
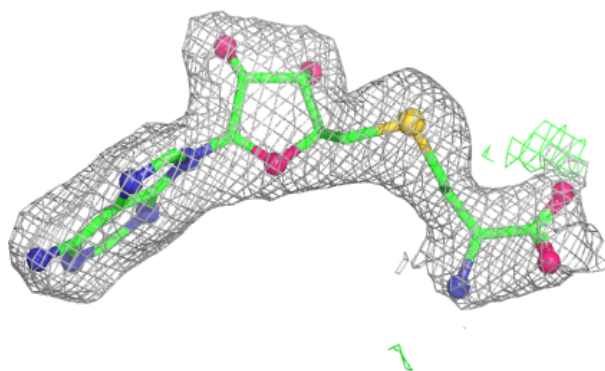
**Electron density around SAH D 701:**

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

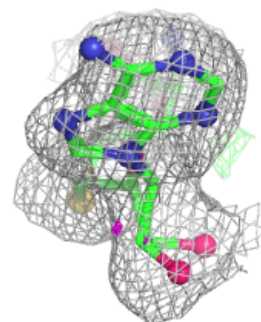
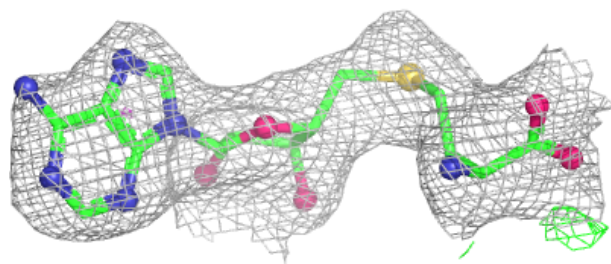
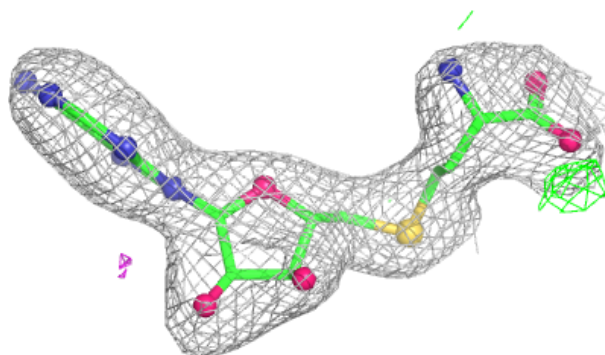


Electron density around SAH B 701:

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

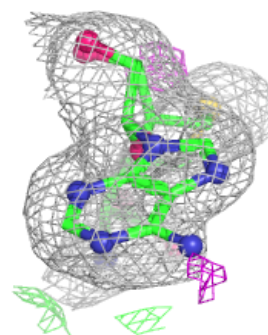
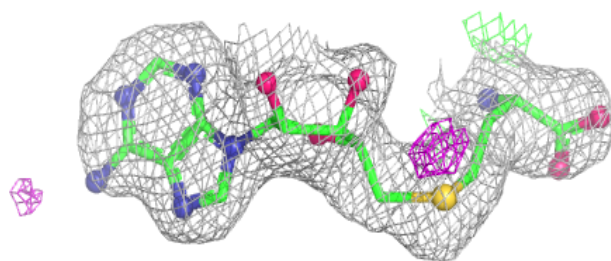
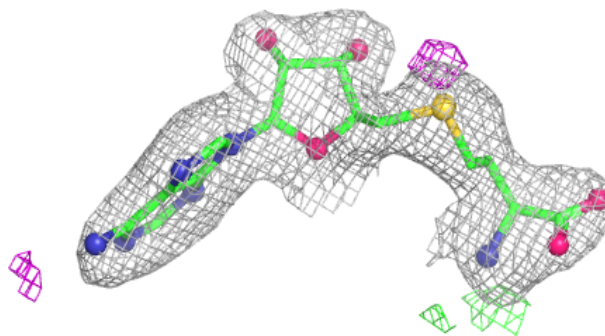
**Electron density around SAH C 701:**

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



Electron density around SAH F 701:

$2mF_o - DF_c$ (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.