



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:19 AM UTC

PDB ID : 5UTU / pdb\_00005utu  
Title : 2.65 Angstrom Resolution Crystal Structure of S-adenosylhomocysteinase from *Cryptosporidium parvum* in Complex with SAH and NAD  
Authors : Minasov, G.; Shuvalova, L.; Dubrovskaya, I.; Winsor, J.; Stam, J.; Kwon, K.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CS-GID)  
Deposited on : 2017-02-15  
Resolution : 2.65 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](mailto: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>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

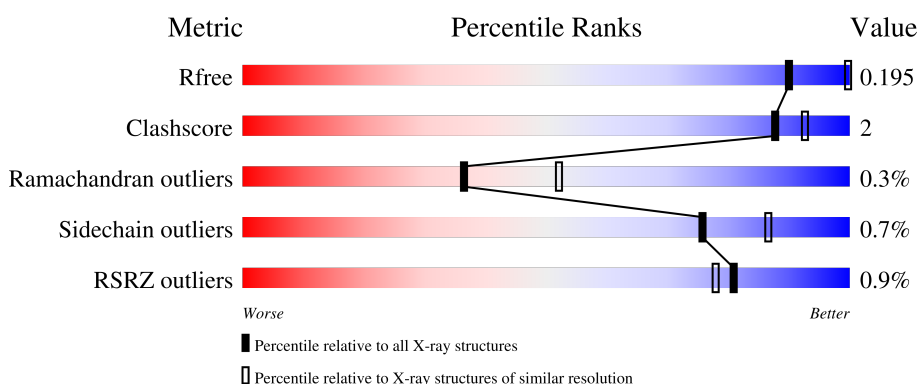
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

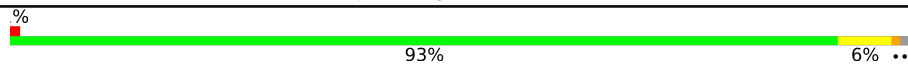
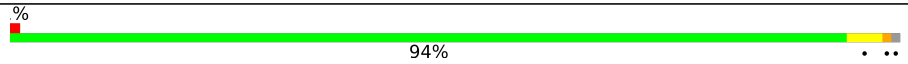
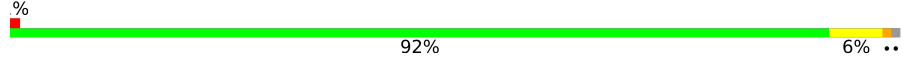
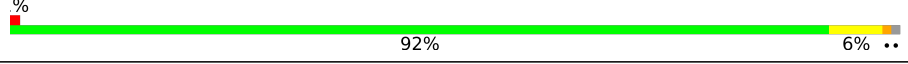
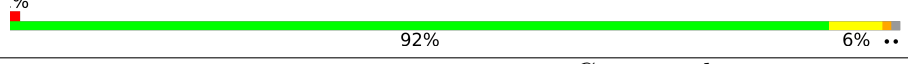
The reported resolution of this entry is 2.65 Å.

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.



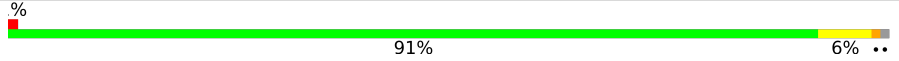
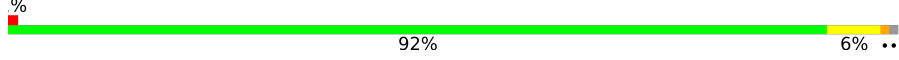
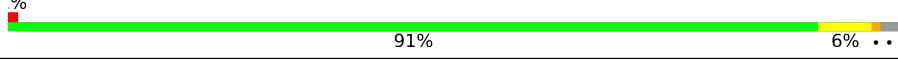
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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  $\geq 3$ , 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	498	 93% 6% ..
1	B	498	 94% ..
1	C	498	 92% 6% ..
1	D	498	 92% 6% ..
1	E	498	 92% 6% ..

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Mol	Chain	Length	Quality of chain
1	F	498	 <p>% 91% 6% ..</p>
1	G	498	 <p>% 92% 6% ..</p>
1	H	498	 <p>% 91% 6% ..</p>

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 33201 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 Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	494	Total 3979	C 2528	N 666	O 756	S 29	0	8	0
1	B	494	Total 3902	C 2478	N 654	O 742	S 28	0	0	0
1	C	491	Total 3877	C 2464	N 650	O 735	S 28	0	0	0
1	D	493	Total 3901	C 2477	N 653	O 742	S 29	0	1	0
1	E	494	Total 3950	C 2507	N 665	O 749	S 29	0	5	0
1	F	493	Total 3943	C 2503	N 660	O 751	S 29	0	6	0
1	G	495	Total 3949	C 2511	N 660	O 749	S 29	0	4	0
1	H	487	Total 3922	C 2495	N 654	O 744	S 29	0	9	0

There are 24 discrepancies between the modelled and reference sequences:

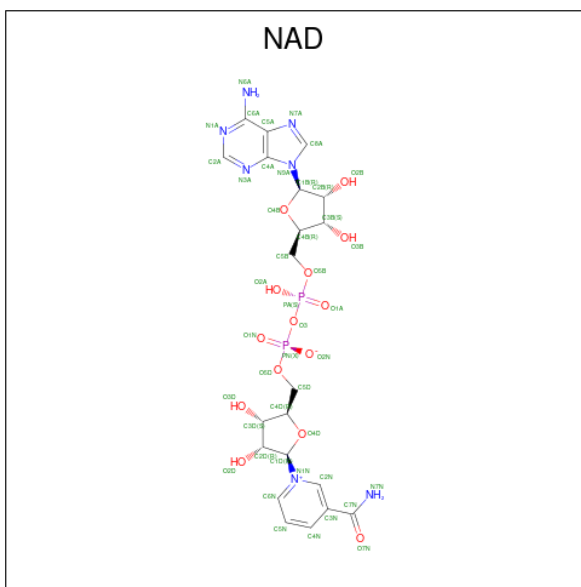
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q5CPH1
A	-1	ASN	-	expression tag	UNP Q5CPH1
A	0	ALA	-	expression tag	UNP Q5CPH1
B	-2	SER	-	expression tag	UNP Q5CPH1
B	-1	ASN	-	expression tag	UNP Q5CPH1
B	0	ALA	-	expression tag	UNP Q5CPH1
C	-2	SER	-	expression tag	UNP Q5CPH1
C	-1	ASN	-	expression tag	UNP Q5CPH1
C	0	ALA	-	expression tag	UNP Q5CPH1
D	-2	SER	-	expression tag	UNP Q5CPH1
D	-1	ASN	-	expression tag	UNP Q5CPH1
D	0	ALA	-	expression tag	UNP Q5CPH1
E	-2	SER	-	expression tag	UNP Q5CPH1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	expression tag	UNP Q5CPH1
E	0	ALA	-	expression tag	UNP Q5CPH1
F	-2	SER	-	expression tag	UNP Q5CPH1
F	-1	ASN	-	expression tag	UNP Q5CPH1
F	0	ALA	-	expression tag	UNP Q5CPH1
G	-2	SER	-	expression tag	UNP Q5CPH1
G	-1	ASN	-	expression tag	UNP Q5CPH1
G	0	ALA	-	expression tag	UNP Q5CPH1
H	-2	SER	-	expression tag	UNP Q5CPH1
H	-1	ASN	-	expression tag	UNP Q5CPH1
H	0	ALA	-	expression tag	UNP Q5CPH1

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



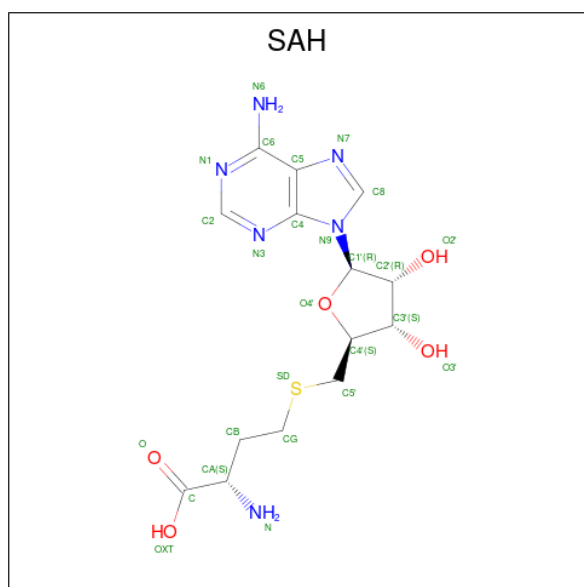
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ).

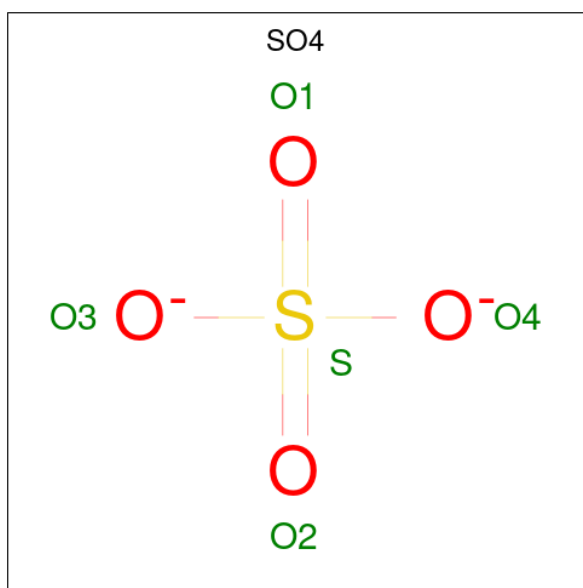


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	E	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	F	1	Total	C	N	O	S	0	1
			26	14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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	2	Total Cl 2 2	0	0
4	C	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0
4	E	2	Total Cl 2 2	0	0
4	F	1	Total Cl 1 1	0	0
4	G	2	Total Cl 2 2	0	0
4	H	1	Total Cl 1 1	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



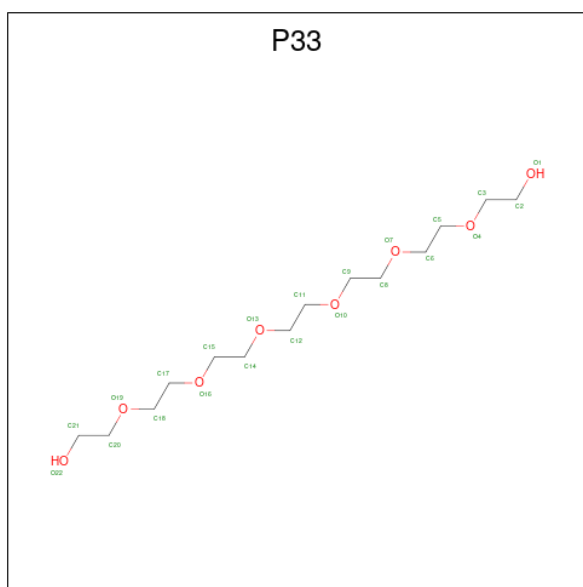
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0

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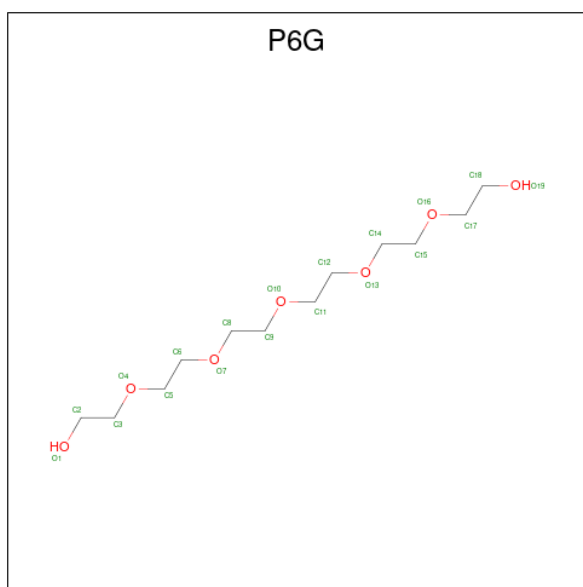
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total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

- Molecule 6 is 3,6,9,12,15,18-HEXAOXAICOSANE-1,20-DIOL (CCD ID: P33) (formula:  $C_{14}H_{30}O_8$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	C O	0	0
			22	14 8		
6	B	1	Total	C O	0	0
			22	14 8		
6	H	1	Total	C O	0	0
			22	14 8		

- Molecule 7 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C<sub>12</sub>H<sub>26</sub>O<sub>7</sub>).



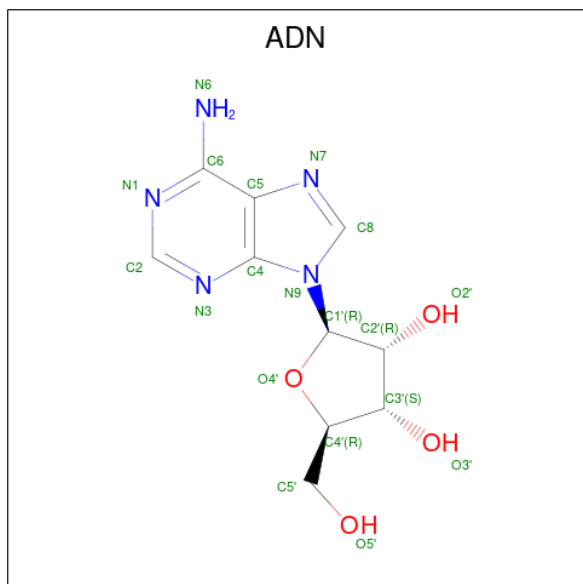
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	C O	0	0
			19	12 7		

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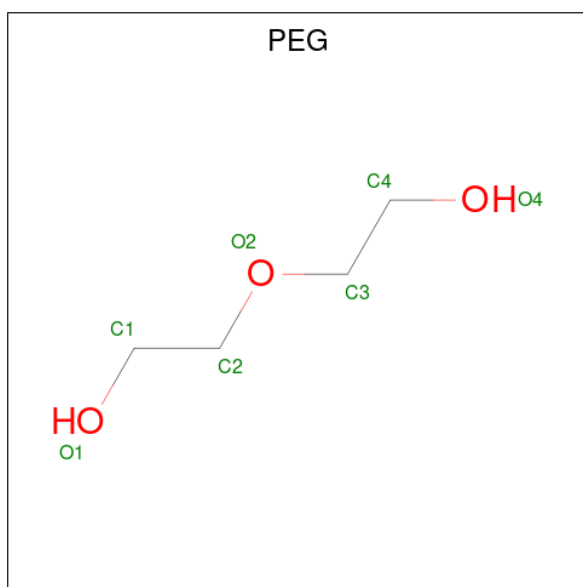
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	F	1	19	12	7	0	0

- Molecule 8 is ADENOSINE (CCD ID: ADN) (formula:  $C_{10}H_{13}N_5O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	F	1	19	10	5	4	0	1
8	H	1	19	10	5	4	0	1

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	G	1	Total C O 7 4 3	0	0
9	G	1	Total C O 7 4 3	0	0

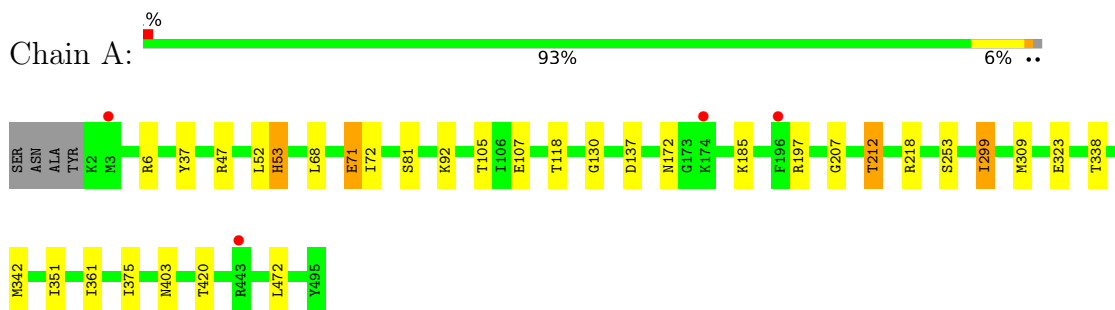
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	157	Total O 159 159	0	2
10	B	84	Total O 85 85	0	1
10	C	128	Total O 130 130	0	2
10	D	103	Total O 104 104	0	1
10	E	146	Total O 148 148	0	2
10	F	90	Total O 91 91	0	1
10	G	123	Total O 123 123	0	0
10	H	100	Total O 101 101	0	2

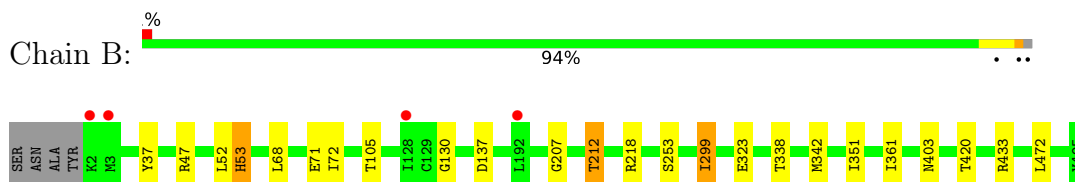
### 3 Residue-property plots [i](#)

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.

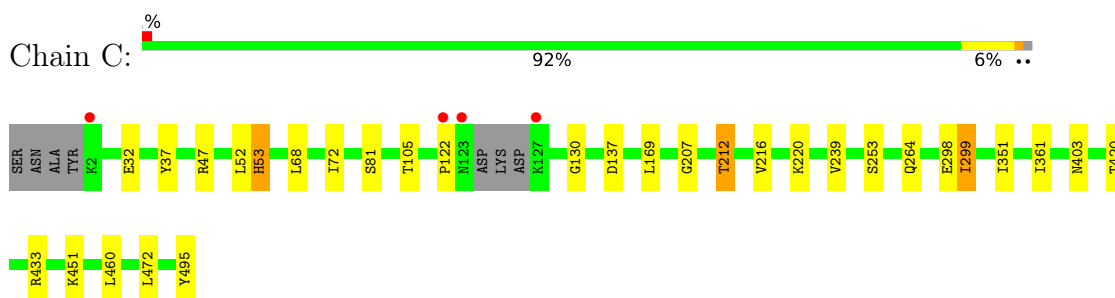
- Molecule 1: Adenosylhomocysteinase



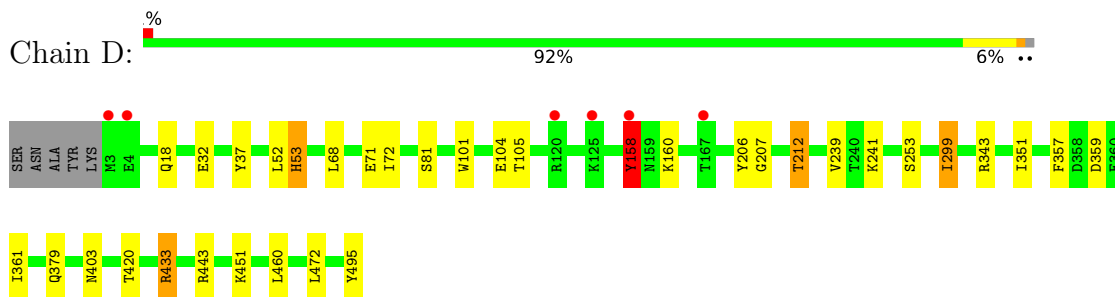
- Molecule 1: Adenosylhomocysteinase



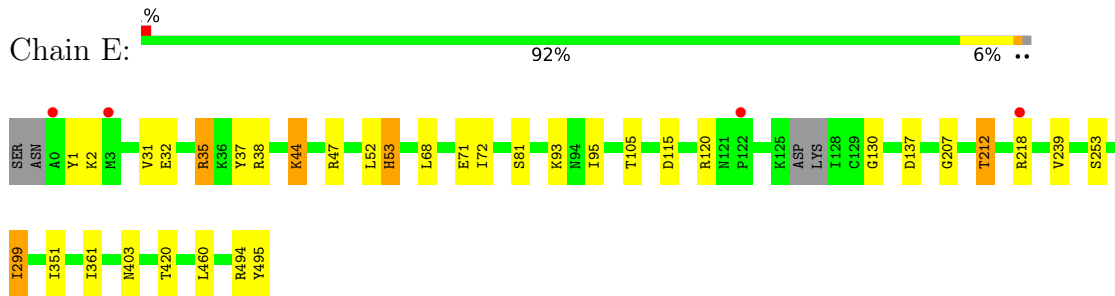
- Molecule 1: Adenosylhomocysteinase



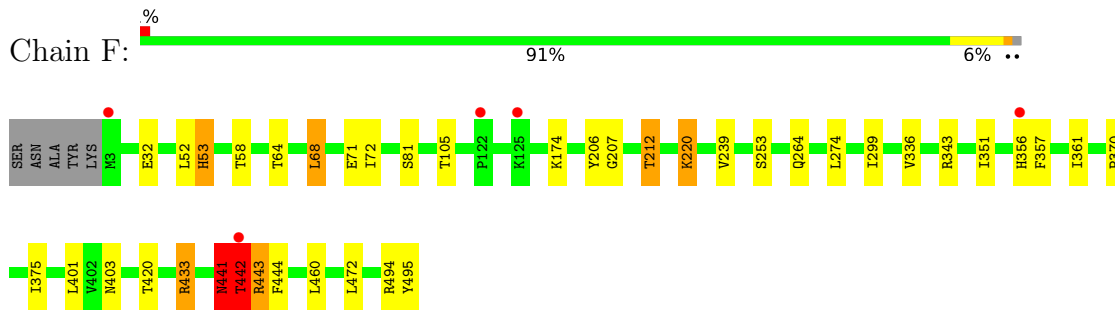
- Molecule 1: Adenosylhomocysteinase



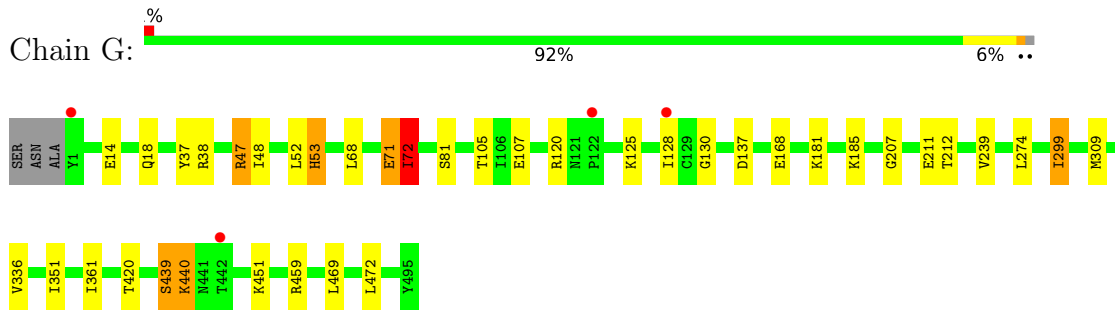
• Molecule 1: Adenosylhomocysteinase



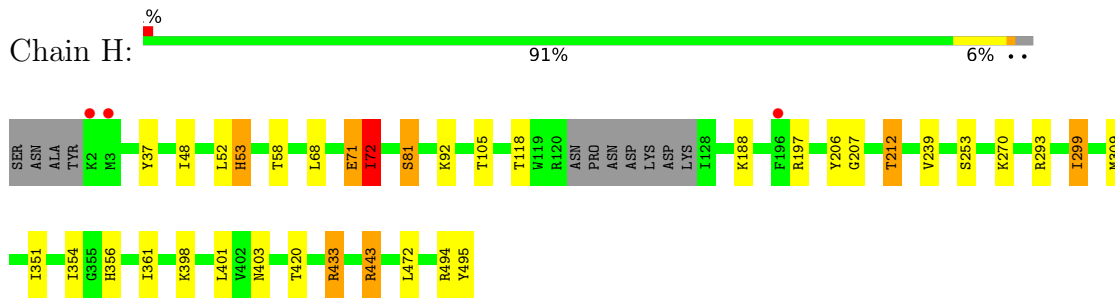
• Molecule 1: Adenosylhomocysteinase



• Molecule 1: Adenosylhomocysteinase



• Molecule 1: Adenosylhomocysteinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.91Å 185.83Å 121.62Å 90.00° 97.98° 90.00°	Depositor
Resolution (Å)	30.00 – 2.65 30.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.65) 99.9 (30.00-2.65)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.13 (at 2.64Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.170 , 0.202 (Not available) , 0.195	Depositor DCC
$R_{free}$ test set	6930 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.4	Xtrriage
Anisotropy	0.032	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 45.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	33201	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CL, PEG, SAH, NAD, P6G, ADN, SO4, P33

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	0.61	0/4045	0.96	13/5451 (0.2%)
1	B	0.59	1/3966 (0.0%)	0.94	11/5348 (0.2%)
1	C	0.64	1/3940 (0.0%)	0.94	10/5312 (0.2%)
1	D	0.62	1/3965 (0.0%)	0.97	15/5347 (0.3%)
1	E	0.63	0/4014	0.94	12/5410 (0.2%)
1	F	0.63	2/4009 (0.0%)	0.94	15/5406 (0.3%)
1	G	0.63	0/4015	0.98	14/5414 (0.3%)
1	H	0.59	0/3987	0.93	11/5374 (0.2%)
All	All	0.62	5/31941 (0.0%)	0.95	101/43062 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	443	ARG	C-O	-7.98	1.14	1.24
1	F	442	THR	N-CA	-5.98	1.38	1.46
1	D	359	ASP	CB-CG	-5.58	1.38	1.52
1	C	122	PRO	CA-C	5.28	1.58	1.52
1	B	323	GLU	C-O	-5.09	1.17	1.23

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	359	ASP	CB-CA-C	-14.32	82.23	109.72
1	G	459	ARG	NE-CZ-NH2	9.56	127.80	119.20
1	G	47	ARG	NE-CZ-NH1	-9.35	112.15	121.50
1	C	433	ARG	CG-CD-NE	-8.85	92.53	112.00
1	B	433	ARG	CG-CD-NE	-8.54	93.22	112.00
1	G	439	SER	N-CA-C	-8.50	95.49	108.67
1	A	92	LYS	CB-CG-CD	8.44	130.70	111.30
1	G	451	LYS	CD-CE-NZ	-7.16	88.98	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	451	LYS	CD-CE-NZ	-7.09	89.20	111.90
1	D	451	LYS	CD-CE-NZ	-7.01	89.48	111.90
1	G	207	GLY	N-CA-C	6.82	120.16	111.09
1	G	72	ILE	N-CA-C	6.77	118.47	108.45
1	A	207	GLY	N-CA-C	6.71	120.02	111.09
1	H	207	GLY	N-CA-C	6.65	119.93	111.09
1	E	72	ILE	N-CA-C	6.63	118.27	108.45
1	C	207	GLY	N-CA-C	6.62	119.90	111.09
1	H	72	ILE	N-CA-C	6.62	118.24	108.45
1	E	207	GLY	N-CA-C	6.61	119.88	111.09
1	B	207	GLY	N-CA-C	6.52	119.76	111.09
1	D	212	THR	N-CA-C	6.51	120.14	109.85
1	F	443	ARG	CA-C-O	-6.47	113.54	120.46
1	A	72	ILE	N-CA-C	6.47	118.10	108.46
1	G	212	THR	N-CA-C	6.41	119.97	109.85
1	C	212	THR	N-CA-C	6.38	119.92	109.85
1	D	359	ASP	N-CA-C	6.37	121.05	113.28
1	F	212	THR	N-CA-C	6.34	119.87	109.85
1	D	72	ILE	N-CA-C	6.34	117.83	108.45
1	E	212	THR	N-CA-C	6.33	119.84	109.85
1	H	212	THR	N-CA-C	6.31	119.82	109.85
1	B	72	ILE	N-CA-C	6.31	117.79	108.45
1	A	212	THR	N-CA-C	6.23	119.69	109.85
1	C	72	ILE	N-CA-C	6.23	117.74	108.46
1	F	207	GLY	N-CA-C	6.21	119.35	111.09
1	F	72	ILE	N-CA-C	6.20	117.62	108.45
1	B	212	THR	N-CA-C	6.15	119.57	109.85
1	D	207	GLY	N-CA-C	6.08	119.18	111.09
1	D	343	ARG	CG-CD-NE	5.97	125.13	112.00
1	A	299	ILE	CB-CA-C	-5.95	104.39	110.88
1	H	443	ARG	CB-CG-CD	5.89	124.86	111.30
1	B	218	ARG	CB-CG-CD	5.87	124.80	111.30
1	C	105	THR	N-CA-C	-5.85	102.66	110.55
1	E	299	ILE	CB-CA-C	-5.83	104.53	110.88
1	H	299	ILE	CB-CA-C	-5.82	104.53	110.88
1	D	299	ILE	CB-CA-C	-5.82	104.54	110.88
1	B	299	ILE	CB-CA-C	-5.81	104.55	110.88
1	F	105	THR	N-CA-C	-5.80	102.72	110.55
1	D	71	GLU	N-CA-C	-5.80	100.25	109.76
1	C	299	ILE	CB-CA-C	-5.78	104.58	110.88
1	A	105	THR	N-CA-C	-5.76	102.77	110.55
1	F	299	ILE	CB-CA-C	-5.75	104.61	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	299	ILE	CB-CA-C	-5.74	104.62	110.88
1	D	105	THR	N-CA-C	-5.73	102.81	110.55
1	B	105	THR	N-CA-C	-5.72	102.82	110.55
1	H	433	ARG	CB-CA-C	-5.70	99.07	110.42
1	H	105	THR	N-CA-C	-5.66	102.90	110.55
1	B	218	ARG	NE-CZ-NH1	-5.66	115.84	121.50
1	E	105	THR	N-CA-C	-5.62	102.96	110.55
1	G	105	THR	N-CA-C	-5.60	102.99	110.55
1	D	433	ARG	CB-CA-C	-5.59	99.29	110.42
1	F	71	GLU	N-CA-C	-5.55	100.65	109.76
1	B	71	GLU	N-CA-C	-5.52	100.71	109.76
1	A	218	ARG	CB-CG-CD	5.51	123.98	111.30
1	D	443	ARG	CG-CD-NE	5.48	124.06	112.00
1	G	71	GLU	N-CA-C	-5.48	100.77	109.76
1	D	81	SER	N-CA-C	5.39	119.57	112.89
1	F	433	ARG	CB-CA-C	-5.37	99.73	110.42
1	A	81	SER	N-CA-C	5.37	119.55	112.89
1	C	420	THR	N-CA-C	-5.36	105.52	111.36
1	A	71[A]	GLU	N-CA-C	-5.34	101.00	109.76
1	A	71[B]	GLU	N-CA-C	-5.34	101.00	109.76
1	H	71	GLU	N-CA-C	-5.34	101.00	109.76
1	G	81	SER	N-CA-C	5.33	119.50	112.89
1	G	420	THR	N-CA-C	-5.32	105.56	111.36
1	H	420	THR	N-CA-C	-5.31	105.58	111.36
1	F	420	THR	N-CA-C	-5.30	105.58	111.36
1	A	420	THR	N-CA-C	-5.30	105.59	111.36
1	D	420	THR	N-CA-C	-5.28	105.61	111.36
1	B	420	THR	N-CA-C	-5.27	105.61	111.36
1	E	420	THR	N-CA-C	-5.26	105.63	111.36
1	E	44	LYS	CB-CG-CD	5.22	123.30	111.30
1	B	433	ARG	N-CA-C	5.20	117.62	111.33
1	G	47	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	A	218	ARG	NE-CZ-NH1	-5.17	116.33	121.50
1	D	158	TYR	CA-CB-CG	5.17	123.21	113.90
1	F	220	LYS	CA-CB-CG	5.17	124.44	114.10
1	F	343	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	A	6	ARG	CB-CG-CD	5.13	123.11	111.30
1	C	264	GLN	N-CA-C	5.13	117.30	110.53
1	E	71[A]	GLU	N-CA-C	-5.10	101.39	109.76
1	E	71[B]	GLU	N-CA-C	-5.10	101.39	109.76
1	E	218	ARG	NE-CZ-NH1	-5.10	116.40	121.50
1	E	218	ARG	CB-CG-CD	5.09	123.01	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	81	SER	N-CA-C	5.09	119.20	112.89
1	F	441	ASN	N-CA-C	5.09	121.64	110.80
1	G	459	ARG	NE-CZ-NH1	-5.07	116.43	121.50
1	E	81	SER	N-CA-C	5.06	119.17	112.89
1	C	81	SER	N-CA-C	5.06	119.16	112.89
1	F	264	GLN	N-CA-C	5.06	117.20	110.53
1	H	188	LYS	CA-CB-CG	5.04	124.17	114.10
1	F	220	LYS	CB-CG-CD	5.03	122.86	111.30
1	H	81	SER	N-CA-C	5.00	119.09	112.89

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	3979	0	4024	18	0
1	B	3902	0	3961	11	0
1	C	3877	0	3939	13	0
1	D	3901	0	3956	16	0
1	E	3950	0	4004	18	0
1	F	3943	0	3983	23	0
1	G	3949	0	4004	21	0
1	H	3922	0	3965	21	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	1	0
2	D	44	0	26	0	0
2	E	44	0	26	0	0
2	F	44	0	26	1	0
2	G	44	0	26	0	0
2	H	44	0	26	0	0
3	A	26	0	19	0	0
3	B	26	0	19	2	0
3	C	26	0	19	0	0
3	D	26	0	19	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	26	0	19	0	0
3	F	26	0	19	3	0
3	G	26	0	19	0	0
3	H	26	0	19	1	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
4	G	2	0	0	0	0
4	H	1	0	0	0	0
5	A	20	0	0	0	0
5	B	10	0	0	0	0
5	C	20	0	0	0	0
5	D	15	0	0	0	0
5	E	10	0	0	0	0
5	F	10	0	0	0	0
5	G	15	0	0	0	0
5	H	10	0	0	0	0
6	A	22	0	30	0	0
6	B	22	0	30	0	0
6	H	22	0	30	0	0
7	D	19	0	26	0	0
7	F	19	0	26	0	0
8	F	19	0	13	1	0
8	H	19	0	13	0	0
9	G	14	0	20	0	0
10	A	159	0	0	0	0
10	B	85	0	0	0	0
10	C	130	0	0	0	0
10	D	104	0	0	0	0
10	E	148	0	0	0	0
10	F	91	0	0	0	0
10	G	123	0	0	0	0
10	H	101	0	0	0	0
All	All	33201	0	32384	128	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (128) 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:H:118:THR:OG1	1:H:197:ARG:NH2	2.09	0.85
1:A:118:THR:OG1	1:A:197:ARG:NH1	2.09	0.84
1:E:2:LYS:HE2	1:E:115:ASP:OD2	1.81	0.79
1:E:35[B]:ARG:HG2	1:E:38[B]:ARG:HH21	1.52	0.74
1:E:47:ARG:NH1	1:E:130:GLY:O	2.21	0.73
1:A:47:ARG:NH1	1:A:130:GLY:O	2.21	0.73
1:B:47:ARG:NH1	1:B:130:GLY:O	2.21	0.73
1:C:47:ARG:NH1	1:C:130:GLY:O	2.21	0.72
1:E:35[B]:ARG:HG2	1:E:38[B]:ARG:NH2	2.04	0.71
1:G:48:ILE:HB	1:G:72:ILE:HD13	1.75	0.68
1:H:48:ILE:HB	1:H:72:ILE:HD13	1.75	0.68
1:G:47:ARG:NH1	1:G:130:GLY:O	2.27	0.66
1:F:442:THR:HG23	1:F:444:PHE:CE2	2.33	0.64
1:A:71[A]:GLU:HA	1:A:71[A]:GLU:OE1	1.99	0.61
1:E:93:LYS:HE3	1:E:95:ILE:HD11	1.83	0.61
1:A:107:GLU:HG3	1:A:185:LYS:HE3	1.84	0.59
1:G:137:ASP:OD1	1:G:211:GLU:HG2	2.03	0.59
1:D:158:TYR:CZ	1:D:160:LYS:HB2	2.38	0.58
1:F:442:THR:HG23	1:F:444:PHE:HE2	1.68	0.58
1:F:274:LEU:CD2	1:F:336:VAL:HG12	2.34	0.58
1:G:120:ARG:HD2	1:G:125:LYS:HG3	1.85	0.57
1:G:439:SER:O	1:G:440:LYS:CB	2.53	0.56
1:B:212:THR:HG21	3:B:502:SAH:HG1	1.87	0.56
1:A:172:ASN:HB3	1:F:370:PRO:HG2	1.87	0.56
1:H:92:LYS:O	1:H:92:LYS:HD3	2.06	0.56
1:D:158:TYR:CE2	1:D:160:LYS:HB2	2.42	0.55
1:E:31:VAL:O	1:E:35[B]:ARG:HG3	2.07	0.54
1:H:356[B]:HIS:HA	1:H:401:LEU:HD21	1.90	0.53
1:F:351:ILE:HG22	1:F:361:ILE:HD13	1.90	0.53
1:A:351:ILE:HG22	1:A:361:ILE:HD13	1.91	0.53
1:G:274:LEU:CD2	1:G:336[B]:VAL:HG12	2.38	0.52
1:F:274:LEU:HD22	1:F:336:VAL:HG12	1.92	0.52
1:H:351:ILE:HG22	1:H:361:ILE:HD13	1.92	0.51
1:D:351:ILE:HG22	1:D:361:ILE:HD13	1.92	0.51
1:G:168:GLU:HG3	1:G:181:LYS:HE2	1.93	0.51
1:A:299:ILE:HD13	1:B:472:LEU:HD21	1.91	0.51
1:C:351:ILE:HG22	1:C:361:ILE:HD13	1.92	0.51
1:E:351:ILE:HG22	1:E:361:ILE:HD13	1.92	0.51
1:G:351:ILE:HG22	1:G:361:ILE:HD13	1.92	0.51
1:H:71:GLU:C	1:H:72:ILE:HG12	2.36	0.51
1:C:472:LEU:HD21	1:D:299:ILE:HD13	1.93	0.51
1:F:64:THR:O	1:F:68:LEU:HD13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:71:GLU:C	1:G:72:ILE:HG12	2.36	0.50
1:D:37:TYR:HB2	1:D:68:LEU:HD22	1.94	0.50
1:G:299:ILE:HD13	1:H:472:LEU:HD21	1.93	0.50
1:B:351:ILE:HG22	1:B:361:ILE:HD13	1.92	0.50
1:B:37:TYR:HB2	1:B:68:LEU:HD22	1.94	0.50
1:C:37:TYR:HB2	1:C:68:LEU:HD22	1.93	0.50
1:C:299:ILE:HD13	1:D:472:LEU:HD21	1.94	0.49
1:F:174:LYS:N	1:F:174:LYS:HD2	2.27	0.49
1:A:37:TYR:HB2	1:A:68:LEU:HD22	1.94	0.49
1:A:323[B]:GLU:HA	1:A:323[B]:GLU:OE1	2.13	0.49
1:G:128:ILE:HD12	1:G:128:ILE:O	2.12	0.49
1:G:274:LEU:HD23	1:G:336[B]:VAL:HG12	1.95	0.49
1:H:53:HIS:HD1	1:H:81:SER:CB	2.26	0.49
1:C:169:LEU:HD12	1:C:169:LEU:N	2.28	0.49
1:G:107:GLU:HG3	1:G:185:LYS:HE2	1.94	0.49
1:C:137:ASP:OD1	1:C:212:THR:CG2	2.61	0.49
1:H:37:TYR:HB2	1:H:68:LEU:HD22	1.93	0.49
1:A:375:ILE:HD12	1:D:18:GLN:NE2	2.28	0.49
1:E:37:TYR:HB2	1:E:68:LEU:HD22	1.94	0.48
1:G:37:TYR:HB2	1:G:68:LEU:HD22	1.94	0.48
1:H:309:MET:HA	1:H:309:MET:HE2	1.94	0.48
1:E:137:ASP:OD1	1:E:212:THR:CG2	2.61	0.48
1:A:137:ASP:OD1	1:A:212:THR:CG2	2.61	0.48
1:B:137:ASP:OD1	1:B:212:THR:CG2	2.61	0.48
1:G:472:LEU:HD21	1:H:299:ILE:HD13	1.96	0.48
1:E:299:ILE:HD13	1:F:472:LEU:HD21	1.95	0.47
1:A:375:ILE:HD12	1:D:18:GLN:CD	2.39	0.47
1:B:137:ASP:OD1	3:B:502:SAH:HG1	2.15	0.47
1:D:52:LEU:O	1:D:53:HIS:C	2.59	0.46
3:F:502[A]:SAH:HN1	3:F:502[A]:SAH:HG1	1.42	0.46
1:H:354[B]:ILE:O	1:H:354[B]:ILE:HG12	2.16	0.46
1:C:32:GLU:HG2	1:C:460:LEU:HD22	1.98	0.46
1:G:309:MET:HA	1:G:309:MET:HE2	1.97	0.46
1:H:52:LEU:O	1:H:53:HIS:C	2.59	0.46
1:A:472:LEU:HD21	1:B:299:ILE:HD13	1.97	0.46
1:H:58:THR:OG1	3:H:502[A]:SAH:H2	2.17	0.45
1:A:52:LEU:O	1:A:53:HIS:C	2.59	0.45
1:B:52:LEU:O	1:B:53:HIS:C	2.59	0.45
1:E:1:TYR:CZ	1:E:120:ARG:HB2	2.51	0.45
1:E:52:LEU:O	1:E:53:HIS:C	2.59	0.45
1:F:52:LEU:O	1:F:53:HIS:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:LEU:O	1:C:53:HIS:C	2.59	0.45
1:E:239:VAL:HG22	1:F:494:ARG:CZ	2.46	0.45
1:A:172:ASN:CB	1:F:370:PRO:HG2	2.47	0.45
1:C:298:GLU:OE2	2:C:501:NAD:O2B	2.34	0.45
1:H:92:LYS:CD	1:H:92:LYS:C	2.90	0.45
1:F:356[B]:HIS:HA	1:F:401:LEU:HD21	1.99	0.44
1:G:52:LEU:O	1:G:53:HIS:C	2.59	0.44
1:D:241:LYS:NZ	3:D:502:SAH:O3'	2.46	0.44
1:F:274:LEU:HD23	1:F:336:VAL:HG12	1.99	0.44
1:F:441:ASN:O	1:F:443:ARG:N	2.50	0.44
1:F:375:ILE:HD12	1:G:18[B]:GLN:CD	2.42	0.44
1:F:32:GLU:HG2	1:F:460:LEU:HD22	1.99	0.43
1:E:32:GLU:HG2	1:E:460:LEU:HD22	2.00	0.43
1:H:206:TYR:CD2	1:H:433:ARG:HG2	2.53	0.43
1:F:239:VAL:HG21	1:F:495:TYR:CE1	2.53	0.43
1:G:439:SER:O	1:G:440:LYS:HB3	2.17	0.43
1:A:309:MET:HA	1:A:309:MET:HE2	2.01	0.43
1:C:253:SER:HB2	1:C:403:ASN:HB2	2.01	0.43
1:D:239:VAL:HG21	1:D:495:TYR:CE1	2.54	0.43
1:B:253:SER:HB2	1:B:403:ASN:HB2	2.01	0.43
1:H:253:SER:HB2	1:H:403:ASN:HB2	2.01	0.43
1:E:253:SER:HB2	1:E:403:ASN:HB2	2.01	0.42
1:D:206:TYR:CD2	1:D:433:ARG:HG2	2.55	0.42
1:C:239:VAL:HG21	1:C:495:TYR:CE1	2.55	0.42
1:H:92:LYS:HD3	1:H:92:LYS:C	2.45	0.42
1:G:239:VAL:HG22	1:H:494:ARG:CZ	2.50	0.42
1:F:58:THR:OG1	3:F:502[A]:SAH:H2	2.20	0.42
1:E:93:LYS:CE	1:E:95:ILE:HD11	2.49	0.41
1:F:357[A]:PHE:N	3:F:502[A]:SAH:OXT	2.53	0.41
1:C:216:VAL:HG12	1:C:220:LYS:HE2	2.02	0.41
1:D:32:GLU:HG2	1:D:460:LEU:HD22	2.03	0.41
1:E:239:VAL:HG21	1:E:495:TYR:CE1	2.55	0.41
1:A:253:SER:HB2	1:A:403:ASN:HB2	2.02	0.41
1:D:253:SER:HB2	1:D:403:ASN:HB2	2.02	0.41
1:F:206:TYR:CD2	1:F:433:ARG:HG2	2.56	0.41
1:F:253:SER:HB2	1:F:403:ASN:HB2	2.01	0.41
1:G:469:LEU:HD12	1:G:469:LEU:HA	1.92	0.41
1:H:239:VAL:HG21	1:H:495:TYR:CE1	2.56	0.41
1:D:357:PHE:N	3:D:502:SAH:OXT	2.52	0.40
2:F:501:NAD:C4N	8:F:503[B]:ADN:H3'	2.51	0.40
1:A:338:THR:O	1:A:342:MET:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:THR:O	1:B:342:MET:HG3	2.21	0.40
1:D:101:TRP:O	1:D:104:GLU:HG3	2.22	0.40
1:E:494:ARG:CZ	1:F:239:VAL:HG22	2.51	0.40
1:H:270:LYS:HD2	1:H:293:ARG:NH2	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	500/498 (100%)	486 (97%)	13 (3%)	1 (0%)	43 60
1	B	492/498 (99%)	477 (97%)	14 (3%)	1 (0%)	43 60
1	C	487/498 (98%)	473 (97%)	13 (3%)	1 (0%)	43 60
1	D	492/498 (99%)	478 (97%)	13 (3%)	1 (0%)	43 60
1	E	495/498 (99%)	480 (97%)	14 (3%)	1 (0%)	43 60
1	F	497/498 (100%)	484 (97%)	10 (2%)	3 (1%)	21 34
1	G	497/498 (100%)	482 (97%)	13 (3%)	2 (0%)	30 45
1	H	492/498 (99%)	479 (97%)	12 (2%)	1 (0%)	43 60
All	All	3952/3984 (99%)	3839 (97%)	102 (3%)	11 (0%)	36 52

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	440	LYS
1	F	442	THR
1	A	53	HIS
1	B	53	HIS
1	C	53	HIS
1	D	53	HIS

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Mol	Chain	Res	Type
1	E	53	HIS
1	F	53	HIS
1	G	53	HIS
1	H	53	HIS
1	F	441	ASN

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	334/435 (77%)	331 (99%)	3 (1%)	70	82
1	E	436/435 (100%)	433 (99%)	3 (1%)	76	86
1	F	436/435 (100%)	433 (99%)	3 (1%)	76	86
1	G	437/435 (100%)	434 (99%)	3 (1%)	76	86
1	H	433/435 (100%)	429 (99%)	4 (1%)	70	82
All	All	2076/2175 (95%)	2060 (99%)	16 (1%)	76	85

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	158	TYR
1	D	212	THR
1	D	379	GLN
1	E	35[A]	ARG
1	E	35[B]	ARG
1	E	44	LYS
1	F	68	LEU
1	F	212	THR
1	F	220	LYS
1	G	14	GLU
1	G	38	ARG
1	G	72	ILE
1	H	72	ILE
1	H	212	THR

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Mol	Chain	Res	Type
1	H	398	LYS
1	H	443	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	285	GLN
1	D	368	ASN
1	E	103	ASN
1	E	285	GLN
1	E	368	ASN
1	E	379	GLN
1	F	285	GLN
1	F	368	ASN
1	F	481	ASN
1	G	103	ASN
1	G	175	GLN
1	G	285	GLN
1	G	368	ASN
1	G	379	GLN
1	G	481	ASN
1	H	285	GLN
1	H	368	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](#)

Of 58 ligands modelled in this entry, 11 are monoatomic - leaving 47 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	D	504	-	4,4,4	0.49	0	6,6,6	0.07	0
5	SO4	A	504	-	4,4,4	0.44	0	6,6,6	0.09	0
3	SAH	A	502	-	27,28,28	1.46	6 (22%)	36,40,40	1.97	12 (33%)
5	SO4	C	504	-	4,4,4	0.45	0	6,6,6	0.10	0
3	SAH	H	502[A]	-	27,28,28	1.47	6 (22%)	36,40,40	1.98	11 (30%)
3	SAH	F	502[A]	-	27,28,28	1.48	5 (18%)	36,40,40	2.13	13 (36%)
3	SAH	E	502	-	27,28,28	1.43	6 (22%)	36,40,40	1.98	11 (30%)
5	SO4	H	506	-	4,4,4	0.44	0	6,6,6	0.12	0
3	SAH	C	502	-	27,28,28	1.39	6 (22%)	36,40,40	1.94	12 (33%)
8	ADN	F	503[B]	-	21,21,21	1.57	4 (19%)	31,31,31	2.26	12 (38%)
2	NAD	E	501	-	46,48,48	1.17	5 (10%)	64,73,73	1.62	9 (14%)
6	P33	B	507	-	21,21,21	0.55	0	20,20,20	0.26	0
3	SAH	B	502	-	27,28,28	1.51	5 (18%)	36,40,40	2.17	12 (33%)
5	SO4	A	507	-	4,4,4	0.44	0	6,6,6	0.27	0
6	P33	A	508	-	21,21,21	0.58	0	20,20,20	0.25	0
9	PEG	G	508	-	6,6,6	0.53	0	5,5,5	0.23	0
5	SO4	F	505	-	4,4,4	0.47	0	6,6,6	0.08	0
5	SO4	D	506	-	4,4,4	0.44	0	6,6,6	0.11	0
5	SO4	A	506	-	4,4,4	0.46	0	6,6,6	0.20	0
5	SO4	C	506	-	4,4,4	0.45	0	6,6,6	0.13	0
2	NAD	G	501	-	46,48,48	1.21	7 (15%)	64,73,73	1.62	11 (17%)
5	SO4	H	505	-	4,4,4	0.46	0	6,6,6	0.12	0
2	NAD	D	501	-	46,48,48	1.18	7 (15%)	64,73,73	1.61	10 (15%)
5	SO4	G	505	-	4,4,4	0.45	0	6,6,6	0.21	0
7	P6G	F	507	-	18,18,18	0.53	0	17,17,17	0.24	0
2	NAD	A	501	-	46,48,48	1.18	5 (10%)	64,73,73	1.57	10 (15%)
2	NAD	C	501	-	46,48,48	1.23	6 (13%)	64,73,73	1.70	13 (20%)
2	NAD	F	501	-	46,48,48	1.22	6 (13%)	64,73,73	1.67	12 (18%)
5	SO4	G	506	-	4,4,4	0.48	0	6,6,6	0.27	0
2	NAD	B	501	-	46,48,48	1.15	6 (13%)	64,73,73	1.57	11 (17%)
9	PEG	G	509	-	6,6,6	0.52	0	5,5,5	0.26	0
5	SO4	B	505	-	4,4,4	0.43	0	6,6,6	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	D	505	-	4,4,4	0.47	0	6,6,6	0.23	0
5	SO4	A	505	-	4,4,4	0.46	0	6,6,6	0.14	0
5	SO4	B	506	-	4,4,4	0.46	0	6,6,6	0.12	0
2	NAD	H	501	-	46,48,48	1.14	5 (10%)	64,73,73	1.60	11 (17%)
5	SO4	C	505	-	4,4,4	0.47	0	6,6,6	0.17	0
5	SO4	E	506	-	4,4,4	0.49	0	6,6,6	0.09	0
5	SO4	C	507	-	4,4,4	0.45	0	6,6,6	0.15	0
5	SO4	F	506	-	4,4,4	0.44	0	6,6,6	0.18	0
5	SO4	E	505	-	4,4,4	0.46	0	6,6,6	0.10	0
3	SAH	G	502	-	27,28,28	1.50	6 (22%)	36,40,40	1.88	11 (30%)
6	P33	H	507	-	21,21,21	0.52	0	20,20,20	0.31	0
5	SO4	G	507	-	4,4,4	0.48	0	6,6,6	0.14	0
3	SAH	D	502	-	27,28,28	1.51	5 (18%)	36,40,40	2.20	13 (36%)
8	ADN	H	503[B]	-	21,21,21	1.51	5 (23%)	31,31,31	2.12	11 (35%)
7	P6G	D	507	-	18,18,18	0.53	0	17,17,17	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAH	A	502	-	-	2/15/31/31	0/3/3/3
3	SAH	H	502[A]	-	-	6/15/31/31	0/3/3/3
3	SAH	F	502[A]	-	-	6/15/31/31	0/3/3/3
3	SAH	E	502	-	-	3/15/31/31	0/3/3/3
8	ADN	F	503[B]	-	-	2/6/22/22	0/3/3/3
3	SAH	C	502	-	-	2/15/31/31	0/3/3/3
2	NAD	E	501	-	-	4/30/62/62	0/5/5/5
6	P33	B	507	-	-	9/19/19/19	-
3	SAH	B	502	-	-	4/15/31/31	0/3/3/3
6	P33	A	508	-	-	8/19/19/19	-
9	PEG	G	508	-	-	1/4/4/4	-
2	NAD	G	501	-	-	5/30/62/62	0/5/5/5
2	NAD	D	501	-	-	5/30/62/62	0/5/5/5
7	P6G	F	507	-	-	7/16/16/16	-
2	NAD	A	501	-	-	5/30/62/62	0/5/5/5
2	NAD	C	501	-	-	4/30/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	F	501	-	-	4/30/62/62	0/5/5/5
2	NAD	B	501	-	-	5/30/62/62	0/5/5/5
9	PEG	G	509	-	-	3/4/4/4	-
2	NAD	H	501	-	-	5/30/62/62	0/5/5/5
3	SAH	G	502	-	-	3/15/31/31	0/3/3/3
6	P33	H	507	-	-	10/19/19/19	-
8	ADN	H	503[B]	-	-	1/6/22/22	0/3/3/3
3	SAH	D	502	-	-	6/15/31/31	0/3/3/3
7	P6G	D	507	-	-	7/16/16/16	-

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	502	SAH	C5-C4	4.60	1.47	1.39
8	F	503[B]	ADN	C5-C4	4.55	1.47	1.39
3	B	502	SAH	C5-C4	4.54	1.47	1.39
3	F	502[A]	SAH	C5-C4	4.45	1.47	1.39
3	H	502[A]	SAH	C5-C4	4.43	1.47	1.39
2	A	501	NAD	C5A-C4A	4.39	1.46	1.39
3	E	502	SAH	C5-C4	4.38	1.46	1.39
3	D	502	SAH	C5-C4	4.37	1.46	1.39
2	B	501	NAD	C5A-C4A	4.33	1.46	1.39
2	G	501	NAD	C5A-C4A	4.31	1.46	1.39
2	F	501	NAD	C5A-C4A	4.31	1.46	1.39
3	A	502	SAH	C5-C4	4.26	1.46	1.39
2	H	501	NAD	C5A-C4A	4.25	1.46	1.39
8	H	503[B]	ADN	C5-C4	4.23	1.46	1.39
2	E	501	NAD	C5A-C4A	4.21	1.46	1.39
2	C	501	NAD	C5A-C4A	4.10	1.46	1.39
3	C	502	SAH	C5-C4	4.03	1.46	1.39
2	D	501	NAD	C5A-C4A	3.75	1.45	1.39
2	C	501	NAD	C5A-C6A	3.02	1.49	1.41
2	C	501	NAD	O4D-C1D	2.92	1.44	1.40
8	F	503[B]	ADN	C5-C6	2.89	1.49	1.41
3	D	502	SAH	C5-N7	-2.88	1.33	1.39
8	H	503[B]	ADN	C8-N7	2.88	1.37	1.31
3	F	502[A]	SAH	C5-C6	2.83	1.48	1.41
3	D	502	SAH	C5-C6	2.82	1.48	1.41
2	F	501	NAD	O4D-C1D	2.81	1.44	1.40
3	B	502	SAH	C5-N7	-2.80	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	502[A]	SAH	C8-N7	2.78	1.37	1.31
8	F	503[B]	ADN	C8-N7	2.73	1.36	1.31
3	H	502[A]	SAH	C8-N7	2.72	1.36	1.31
3	B	502	SAH	C8-N7	2.72	1.36	1.31
2	D	501	NAD	PN-O3	2.72	1.62	1.59
3	H	502[A]	SAH	C5-C6	2.69	1.48	1.41
2	E	501	NAD	C5A-C6A	2.68	1.48	1.41
2	B	501	NAD	C5A-N7A	-2.67	1.34	1.39
3	C	502	SAH	C5-N7	-2.65	1.34	1.39
3	E	502	SAH	C5-C6	2.64	1.48	1.41
3	A	502	SAH	C4-N9	-2.63	1.32	1.37
2	C	501	NAD	C5A-N7A	-2.61	1.34	1.39
2	E	501	NAD	C8A-N7A	2.60	1.36	1.31
2	G	501	NAD	C5A-N7A	-2.58	1.34	1.39
2	H	501	NAD	C5A-C6A	2.58	1.48	1.41
2	A	501	NAD	C5A-N7A	-2.56	1.34	1.39
2	F	501	NAD	C5A-N7A	-2.55	1.34	1.39
8	H	503[B]	ADN	C5-C6	2.55	1.48	1.41
3	G	502	SAH	C5-C6	2.53	1.48	1.41
3	D	502	SAH	C8-N7	2.51	1.36	1.31
3	A	502	SAH	C5-C6	2.49	1.47	1.41
8	H	503[B]	ADN	C5-N7	-2.49	1.34	1.39
2	G	501	NAD	C5A-C6A	2.48	1.47	1.41
2	H	501	NAD	C5A-N7A	-2.47	1.34	1.39
2	F	501	NAD	C4A-N9A	-2.46	1.32	1.37
3	G	502	SAH	C4-N9	-2.46	1.32	1.37
3	G	502	SAH	C5-N7	-2.46	1.34	1.39
2	D	501	NAD	O4D-C1D	2.46	1.44	1.40
8	F	503[B]	ADN	C5-N7	-2.45	1.34	1.39
2	D	501	NAD	C5A-N7A	-2.44	1.34	1.39
2	G	501	NAD	C8A-N7A	2.43	1.36	1.31
3	A	502	SAH	C8-N7	2.43	1.36	1.31
2	F	501	NAD	C5A-C6A	2.43	1.47	1.41
2	A	501	NAD	C8A-N7A	2.43	1.36	1.31
2	H	501	NAD	C8A-N7A	2.43	1.36	1.31
3	E	502	SAH	C5-N7	-2.41	1.34	1.39
3	G	502	SAH	C8-N7	2.39	1.36	1.31
3	B	502	SAH	C5-C6	2.39	1.47	1.41
2	A	501	NAD	C5A-C6A	2.38	1.47	1.41
2	B	501	NAD	C5A-C6A	2.36	1.47	1.41
3	C	502	SAH	C8-N7	2.35	1.36	1.31
2	B	501	NAD	C8A-N7A	2.34	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	SAH	C5-C6	2.34	1.47	1.41
3	A	502	SAH	C5-N7	-2.32	1.34	1.39
3	H	502[A]	SAH	C5-N7	-2.30	1.34	1.39
3	E	502	SAH	C8-N7	2.30	1.36	1.31
3	B	502	SAH	OXT-C	-2.29	1.23	1.30
3	G	502	SAH	OXT-C	-2.29	1.23	1.30
2	D	501	NAD	C8A-N7A	2.29	1.36	1.31
2	G	501	NAD	PN-O3	2.28	1.62	1.59
3	H	502[A]	SAH	OXT-C	-2.27	1.23	1.30
2	D	501	NAD	C5A-C6A	2.25	1.47	1.41
2	G	501	NAD	PA-O3	2.25	1.61	1.59
2	E	501	NAD	C5A-N7A	-2.24	1.35	1.39
3	F	502[A]	SAH	C5-N7	-2.22	1.35	1.39
3	F	502[A]	SAH	OXT-C	-2.22	1.23	1.30
2	F	501	NAD	C8A-N7A	2.21	1.35	1.31
2	A	501	NAD	C4A-N9A	-2.20	1.33	1.37
2	B	501	NAD	C4A-N9A	-2.19	1.33	1.37
2	G	501	NAD	C4A-N9A	-2.15	1.33	1.37
2	E	501	NAD	O4D-C1D	2.14	1.43	1.40
2	D	501	NAD	C4A-N9A	-2.13	1.33	1.37
3	E	502	SAH	OXT-C	-2.13	1.23	1.30
2	H	501	NAD	C4A-N9A	-2.12	1.33	1.37
3	C	502	SAH	OXT-C	-2.11	1.23	1.30
2	C	501	NAD	C4A-N9A	-2.10	1.33	1.37
2	C	501	NAD	C8A-N9A	-2.10	1.34	1.37
3	A	502	SAH	OXT-C	-2.10	1.24	1.30
3	H	502[A]	SAH	C4-N9	-2.09	1.33	1.37
3	E	502	SAH	C4-N9	-2.08	1.33	1.37
8	H	503[B]	ADN	C4-N9	-2.06	1.33	1.37
3	D	502	SAH	OXT-C	-2.04	1.24	1.30
2	B	501	NAD	O4D-C1D	2.02	1.43	1.40
3	C	502	SAH	C4-N9	-2.02	1.33	1.37

All (205) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	503[B]	ADN	C5-C4-N3	-5.95	118.52	126.72
2	C	501	NAD	C5A-C4A-N3A	-5.88	118.62	126.72
3	D	502	SAH	C5-C4-N3	-5.82	118.71	126.72
3	B	502	SAH	C5-C4-N3	-5.78	118.76	126.72
8	H	503[B]	ADN	C5-C4-N3	-5.68	118.90	126.72
2	E	501	NAD	C5A-C4A-N3A	-5.63	118.97	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	501	NAD	C5A-C4A-N3A	-5.62	118.98	126.72
2	B	501	NAD	C5A-C4A-N3A	-5.54	119.09	126.72
2	G	501	NAD	C5A-C4A-N3A	-5.53	119.10	126.72
3	F	502[A]	SAH	C5-C4-N3	-5.51	119.12	126.72
3	H	502[A]	SAH	C5-C4-N3	-5.51	119.13	126.72
2	A	501	NAD	C5A-C4A-N3A	-5.38	119.31	126.72
2	D	501	NAD	C5A-C4A-N3A	-5.26	119.47	126.72
3	E	502	SAH	C5-C4-N3	-5.24	119.50	126.72
3	C	502	SAH	C5-C4-N3	-5.17	119.59	126.72
2	F	501	NAD	C5A-C4A-N3A	-5.10	119.69	126.72
3	A	502	SAH	C5-C4-N3	-4.91	119.96	126.72
3	G	502	SAH	C5-C4-N3	-4.67	120.28	126.72
2	C	501	NAD	N3A-C4A-N9A	4.59	134.97	127.17
3	B	502	SAH	O4'-C1'-N9	4.58	116.89	108.09
2	G	501	NAD	N3A-C4A-N9A	4.40	134.66	127.17
2	B	501	NAD	N3A-C4A-N9A	4.33	134.53	127.17
2	H	501	NAD	N3A-C4A-N9A	4.33	134.53	127.17
2	A	501	NAD	N3A-C4A-N9A	4.31	134.50	127.17
2	F	501	NAD	N3A-C4A-N9A	4.26	134.41	127.17
2	E	501	NAD	N3A-C4A-N9A	4.25	134.39	127.17
2	D	501	NAD	N3A-C4A-N9A	4.21	134.33	127.17
2	C	501	NAD	C4A-C5A-N7A	-4.21	105.77	110.58
2	F	501	NAD	N3A-C2A-N1A	-4.18	122.25	128.58
3	E	502	SAH	N3-C4-N9	4.16	134.25	127.17
8	F	503[B]	ADN	N3-C4-N9	4.13	134.20	127.17
8	F	503[B]	ADN	C4-C5-N7	-4.07	105.92	110.58
8	F	503[B]	ADN	O4'-C1'-N9	4.07	115.90	108.09
3	D	502	SAH	N3-C4-N9	4.04	134.03	127.17
3	B	502	SAH	N3-C4-N9	4.03	134.02	127.17
2	D	501	NAD	N3A-C2A-N1A	-3.99	122.54	128.58
3	F	502[A]	SAH	C4-C5-N7	-3.97	106.04	110.58
8	H	503[B]	ADN	C4-C5-N7	-3.94	106.08	110.58
2	A	501	NAD	N3A-C2A-N1A	-3.94	122.62	128.58
3	D	502	SAH	O4'-C1'-N9	3.92	115.61	108.09
3	F	502[A]	SAH	N3-C4-N9	3.91	133.82	127.17
3	H	502[A]	SAH	N3-C4-N9	3.91	133.81	127.17
3	C	502	SAH	N3-C4-N9	3.91	133.81	127.17
3	F	502[A]	SAH	O4'-C1'-N9	3.89	115.56	108.09
8	F	503[B]	ADN	C2-N3-C4	3.88	121.31	111.83
2	E	501	NAD	C4A-C5A-N7A	-3.87	106.16	110.58
3	H	502[A]	SAH	C4-C5-N7	-3.84	106.19	110.58
3	D	502	SAH	C2-N3-C4	3.82	121.17	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	NAD	C2A-N3A-C4A	3.82	121.16	111.83
2	D	501	NAD	C2A-N3A-C4A	3.81	121.14	111.83
3	D	502	SAH	C4-C5-N7	-3.81	106.22	110.58
3	A	502	SAH	N3-C4-N9	3.80	133.64	127.17
8	H	503[B]	ADN	N3-C4-N9	3.80	133.63	127.17
2	E	501	NAD	C2A-N3A-C4A	3.79	121.08	111.83
2	H	501	NAD	C2A-N3A-C4A	3.78	121.06	111.83
2	C	501	NAD	C2A-N3A-C4A	3.77	121.04	111.83
2	A	501	NAD	C2A-N3A-C4A	3.76	121.01	111.83
3	E	502	SAH	N3-C2-N1	-3.75	122.90	128.58
8	H	503[B]	ADN	C2-N3-C4	3.71	120.90	111.83
3	C	502	SAH	N3-C2-N1	-3.70	122.98	128.58
2	H	501	NAD	N3A-C2A-N1A	-3.70	122.98	128.58
3	B	502	SAH	C2-N3-C4	3.69	120.85	111.83
3	G	502	SAH	N3-C4-N9	3.69	133.44	127.17
3	E	502	SAH	C2-N3-C4	3.68	120.83	111.83
2	G	501	NAD	C2A-N3A-C4A	3.68	120.82	111.83
3	A	502	SAH	N3-C2-N1	-3.66	123.04	128.58
3	C	502	SAH	C2-N3-C4	3.65	120.75	111.83
2	B	501	NAD	C2A-N3A-C4A	3.65	120.74	111.83
3	B	502	SAH	C4-C5-N7	-3.64	106.42	110.58
2	G	501	NAD	N3A-C2A-N1A	-3.62	123.10	128.58
2	E	501	NAD	N3A-C2A-N1A	-3.62	123.11	128.58
3	A	502	SAH	C2-N3-C4	3.60	120.63	111.83
3	F	502[A]	SAH	C2-N3-C4	3.58	120.58	111.83
2	B	501	NAD	N3A-C2A-N1A	-3.57	123.17	128.58
3	B	502	SAH	N3-C2-N1	-3.56	123.19	128.58
3	G	502	SAH	N3-C2-N1	-3.55	123.20	128.58
3	H	502[A]	SAH	C2-N3-C4	3.55	120.51	111.83
8	F	503[B]	ADN	N3-C2-N1	-3.52	123.25	128.58
2	H	501	NAD	C4A-C5A-N7A	-3.49	106.59	110.58
3	D	502	SAH	N3-C2-N1	-3.47	123.32	128.58
2	C	501	NAD	N3A-C2A-N1A	-3.47	123.33	128.58
3	D	502	SAH	O4'-C4'-C5'	3.44	117.69	108.83
2	F	501	NAD	C4A-N9A-C8A	3.39	109.30	105.74
2	D	501	NAD	C4A-N9A-C8A	3.36	109.27	105.74
8	H	503[B]	ADN	N3-C2-N1	-3.34	123.52	128.58
3	E	502	SAH	C4-C5-N7	-3.34	106.76	110.58
2	G	501	NAD	C4A-C5A-N7A	-3.32	106.79	110.58
3	G	502	SAH	C2-N3-C4	3.31	119.93	111.83
2	C	501	NAD	C5A-N7A-C8A	3.31	108.65	103.45
2	D	501	NAD	C4A-C5A-N7A	-3.25	106.86	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	SAH	CB-CG-SD	-3.25	106.20	113.45
3	C	502	SAH	C4-C5-N7	-3.21	106.91	110.58
3	G	502	SAH	C4-C5-N7	-3.20	106.92	110.58
2	C	501	NAD	C4A-N9A-C8A	3.20	109.10	105.74
3	F	502[A]	SAH	N3-C2-N1	-3.15	123.81	128.58
3	H	502[A]	SAH	N3-C2-N1	-3.12	123.86	128.58
2	E	501	NAD	C4A-N9A-C8A	3.11	109.00	105.74
3	A	502	SAH	C4-C5-N7	-3.11	107.03	110.58
2	B	501	NAD	C4A-C5A-N7A	-3.09	107.05	110.58
2	G	501	NAD	C4A-N9A-C8A	3.08	108.97	105.74
3	A	502	SAH	C4-N9-C8	3.07	108.96	105.74
2	F	501	NAD	C4A-C5A-N7A	-3.05	107.09	110.58
2	D	501	NAD	N9A-C8A-N7A	-3.02	109.65	113.94
2	A	501	NAD	C4A-C5A-N7A	-3.01	107.14	110.58
3	E	502	SAH	C4-N9-C8	3.00	108.89	105.74
3	G	502	SAH	C4-N9-C8	3.00	108.88	105.74
2	E	501	NAD	C5A-N7A-C8A	3.00	108.16	103.45
8	F	503[B]	ADN	C5-N7-C8	2.98	108.14	103.45
3	D	502	SAH	C5-N7-C8	2.92	108.05	103.45
3	F	502[A]	SAH	C5-N7-C8	2.90	108.01	103.45
2	D	501	NAD	C5A-N7A-C8A	2.90	108.01	103.45
2	H	501	NAD	C4A-N9A-C8A	2.90	108.78	105.74
2	A	501	NAD	C4A-N9A-C8A	2.88	108.77	105.74
3	E	502	SAH	OXT-C-O	-2.88	117.56	124.08
3	B	502	SAH	O4'-C4'-C5'	2.83	116.11	108.83
8	H	503[B]	ADN	C5-N7-C8	2.78	107.82	103.45
3	H	502[A]	SAH	OXT-C-O	-2.78	117.77	124.08
3	E	502	SAH	C5-N7-C8	2.77	107.80	103.45
3	H	502[A]	SAH	C5-N7-C8	2.76	107.79	103.45
2	E	501	NAD	N9A-C8A-N7A	-2.75	110.03	113.94
2	F	501	NAD	C3N-C7N-N7N	2.75	121.13	117.74
2	H	501	NAD	C5A-N7A-C8A	2.75	107.77	103.45
2	G	501	NAD	C5A-N7A-C8A	2.73	107.74	103.45
3	C	502	SAH	C5-N7-C8	2.73	107.73	103.45
2	C	501	NAD	N9A-C8A-N7A	-2.72	110.07	113.94
3	F	502[A]	SAH	C4-N9-C8	2.66	108.53	105.74
3	F	502[A]	SAH	OXT-C-O	-2.65	118.06	124.08
2	F	501	NAD	N9A-C8A-N7A	-2.61	110.23	113.94
2	B	501	NAD	C6N-N1N-C1D	2.60	124.84	119.73
2	G	501	NAD	N9A-C8A-N7A	-2.60	110.25	113.94
3	B	502	SAH	C5-N7-C8	2.60	107.53	103.45
3	G	502	SAH	OXT-C-O	-2.60	118.19	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	503[B]	ADN	O4'-C1'-N9	2.58	113.04	108.09
2	B	501	NAD	C4A-N9A-C8A	2.57	108.44	105.74
3	B	502	SAH	OXT-C-O	-2.57	118.24	124.08
3	E	502	SAH	N9-C8-N7	-2.57	110.29	113.94
3	H	502[A]	SAH	C4-N9-C8	2.57	108.43	105.74
3	F	502[A]	SAH	C6-C5-N7	2.56	137.02	132.09
2	F	501	NAD	C5A-N7A-C8A	2.56	107.47	103.45
3	A	502	SAH	C6-C5-N7	2.52	136.95	132.09
3	F	502[A]	SAH	N9-C8-N7	-2.52	110.36	113.94
2	E	501	NAD	C6A-C5A-N7A	2.52	136.94	132.09
3	D	502	SAH	OXT-C-O	-2.52	118.37	124.08
2	H	501	NAD	N9A-C8A-N7A	-2.52	110.36	113.94
3	C	502	SAH	C4-N9-C8	2.51	108.37	105.74
3	C	502	SAH	N9-C8-N7	-2.50	110.39	113.94
2	A	501	NAD	C5A-N7A-C8A	2.47	107.33	103.45
3	G	502	SAH	C5-N7-C8	2.46	107.32	103.45
2	B	501	NAD	C6N-N1N-C2N	-2.45	119.80	121.88
2	B	501	NAD	C5A-N7A-C8A	2.44	107.28	103.45
3	H	502[A]	SAH	C6-C5-N7	2.43	136.77	132.09
3	C	502	SAH	OXT-C-O	-2.41	118.61	124.08
8	H	503[B]	ADN	C6-C5-N7	2.41	136.73	132.09
3	H	502[A]	SAH	N9-C8-N7	-2.40	110.53	113.94
3	A	502	SAH	OXT-C-O	-2.40	118.64	124.08
3	A	502	SAH	N9-C8-N7	-2.38	110.56	113.94
2	A	501	NAD	N9A-C8A-N7A	-2.36	110.58	113.94
8	H	503[B]	ADN	N9-C8-N7	-2.36	110.58	113.94
8	F	503[B]	ADN	C6-C5-N7	2.36	136.64	132.09
3	G	502	SAH	N9-C8-N7	-2.36	110.59	113.94
3	D	502	SAH	C4'-O4'-C1'	-2.35	104.28	109.47
3	G	502	SAH	C2-N1-C6	2.33	122.55	118.73
3	D	502	SAH	C6-C5-N7	2.32	136.57	132.09
2	F	501	NAD	C6N-N1N-C1D	2.31	124.27	119.73
2	C	501	NAD	C6A-C5A-N7A	2.30	136.53	132.09
3	B	502	SAH	C4'-O4'-C1'	-2.30	104.39	109.47
2	C	501	NAD	C3N-C7N-N7N	2.30	120.57	117.74
3	C	502	SAH	C6-C5-N7	2.29	136.51	132.09
2	G	501	NAD	C3N-C7N-N7N	2.29	120.56	117.74
3	A	502	SAH	C5-N7-C8	2.29	107.04	103.45
3	H	502[A]	SAH	C3'-C2'-C1'	2.27	105.77	101.46
3	G	502	SAH	C6-C5-N7	2.27	136.47	132.09
2	F	501	NAD	C6A-C5A-N7A	2.27	136.46	132.09
8	F	503[B]	ADN	C4'-O4'-C1'	-2.25	104.50	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	501	NAD	C3N-C7N-N7N	2.24	120.50	117.74
8	F	503[B]	ADN	N9-C8-N7	-2.23	110.78	113.94
3	E	502	SAH	C2-N1-C6	2.22	122.38	118.73
2	C	501	NAD	C6N-N1N-C1D	2.22	124.08	119.73
2	D	501	NAD	C6N-N1N-C1D	2.22	124.08	119.73
2	H	501	NAD	C6A-C5A-N7A	2.21	136.36	132.09
8	H	503[B]	ADN	C4-N9-C8	2.20	108.05	105.74
3	D	502	SAH	N9-C8-N7	-2.19	110.84	113.94
2	B	501	NAD	N9A-C8A-N7A	-2.17	110.85	113.94
2	D	501	NAD	C6A-C5A-N7A	2.17	136.27	132.09
3	C	502	SAH	C2-N1-C6	2.17	122.29	118.73
3	E	502	SAH	C6-C5-N7	2.16	136.25	132.09
3	B	502	SAH	C6-C5-N7	2.15	136.24	132.09
3	B	502	SAH	C2-N1-C6	2.15	122.26	118.73
3	D	502	SAH	C2-N1-C6	2.14	122.25	118.73
2	C	501	NAD	C6N-N1N-C2N	-2.13	120.07	121.88
2	A	501	NAD	C6N-N1N-C1D	2.12	123.89	119.73
8	H	503[B]	ADN	C4'-O4'-C1'	-2.12	104.78	109.47
3	F	502[A]	SAH	O4'-C4'-C5'	2.07	114.17	108.83
8	F	503[B]	ADN	C2-N1-C6	2.07	122.13	118.73
2	B	501	NAD	C3N-C7N-N7N	2.06	120.28	117.74
2	A	501	NAD	C6A-C5A-N7A	2.05	136.04	132.09
3	A	502	SAH	C2-N1-C6	2.05	122.10	118.73
2	G	501	NAD	C6A-C5A-N7A	2.05	136.04	132.09
8	F	503[B]	ADN	C4-N9-C8	2.04	107.89	105.74
3	F	502[A]	SAH	C2-N1-C6	2.04	122.08	118.73
2	H	501	NAD	C6N-N1N-C1D	2.03	123.72	119.73
3	C	502	SAH	O4'-C1'-N9	2.03	111.99	108.09
2	G	501	NAD	C5N-C4N-C3N	-2.03	118.37	120.36
2	F	501	NAD	C2A-N1A-C6A	2.01	122.03	118.73
2	C	501	NAD	O7N-C7N-N7N	-2.00	119.72	122.62

There are no chirality outliers.

All (117) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAD	O4D-C1D-N1N-C2N
2	A	501	NAD	O4D-C1D-N1N-C6N
2	A	501	NAD	C2D-C1D-N1N-C2N
2	A	501	NAD	C2D-C1D-N1N-C6N
2	B	501	NAD	O4D-C1D-N1N-C2N
2	B	501	NAD	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
2	B	501	NAD	C2D-C1D-N1N-C2N
2	B	501	NAD	C2D-C1D-N1N-C6N
2	C	501	NAD	O4D-C1D-N1N-C2N
2	C	501	NAD	O4D-C1D-N1N-C6N
2	C	501	NAD	C2D-C1D-N1N-C2N
2	C	501	NAD	C2D-C1D-N1N-C6N
2	D	501	NAD	O4D-C1D-N1N-C2N
2	D	501	NAD	O4D-C1D-N1N-C6N
2	D	501	NAD	C2D-C1D-N1N-C2N
2	D	501	NAD	C2D-C1D-N1N-C6N
2	E	501	NAD	O4D-C1D-N1N-C2N
2	E	501	NAD	O4D-C1D-N1N-C6N
2	E	501	NAD	C2D-C1D-N1N-C2N
2	E	501	NAD	C2D-C1D-N1N-C6N
2	F	501	NAD	O4D-C1D-N1N-C2N
2	F	501	NAD	O4D-C1D-N1N-C6N
2	F	501	NAD	C2D-C1D-N1N-C2N
2	F	501	NAD	C2D-C1D-N1N-C6N
2	G	501	NAD	O4D-C1D-N1N-C2N
2	G	501	NAD	O4D-C1D-N1N-C6N
2	G	501	NAD	C2D-C1D-N1N-C2N
2	G	501	NAD	C2D-C1D-N1N-C6N
2	H	501	NAD	O4D-C1D-N1N-C2N
2	H	501	NAD	O4D-C1D-N1N-C6N
2	H	501	NAD	C2D-C1D-N1N-C2N
2	H	501	NAD	C2D-C1D-N1N-C6N
3	A	502	SAH	O4'-C4'-C5'-SD
3	A	502	SAH	C3'-C4'-C5'-SD
3	C	502	SAH	C3'-C4'-C5'-SD
3	D	502	SAH	O4'-C4'-C5'-SD
3	D	502	SAH	C3'-C4'-C5'-SD
3	F	502[A]	SAH	N-CA-CB-CG
3	F	502[A]	SAH	C-CA-CB-CG
3	F	502[A]	SAH	O4'-C4'-C5'-SD
3	F	502[A]	SAH	C3'-C4'-C5'-SD
3	G	502	SAH	O4'-C4'-C5'-SD
3	G	502	SAH	C3'-C4'-C5'-SD
3	H	502[A]	SAH	N-CA-CB-CG
3	H	502[A]	SAH	C-CA-CB-CG
8	F	503[B]	ADN	O4'-C4'-C5'-O5'
8	F	503[B]	ADN	C3'-C4'-C5'-O5'
6	B	507	P33	O7-C8-C9-O10

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Mol	Chain	Res	Type	Atoms
7	D	507	P6G	O7-C8-C9-O10
6	B	507	P33	O16-C17-C18-O19
6	H	507	P33	O7-C8-C9-O10
7	F	507	P6G	O13-C14-C15-O16
6	H	507	P33	O10-C11-C12-O13
6	A	508	P33	O10-C11-C12-O13
6	A	508	P33	O4-C5-C6-O7
7	F	507	P6G	O4-C5-C6-O7
3	B	502	SAH	OXT-C-CA-N
7	F	507	P6G	O16-C17-C18-O19
6	H	507	P33	O13-C14-C15-O16
3	D	502	SAH	CA-CB-CG-SD
6	A	508	P33	O19-C20-C21-O22
7	D	507	P6G	O16-C17-C18-O19
3	F	502[A]	SAH	CA-CB-CG-SD
9	G	509	PEG	O2-C3-C4-O4
7	D	507	P6G	O4-C5-C6-O7
9	G	508	PEG	O2-C3-C4-O4
6	B	507	P33	O13-C14-C15-O16
6	B	507	P33	O19-C20-C21-O22
6	B	507	P33	O1-C2-C3-O4
7	F	507	P6G	O1-C2-C3-O4
3	B	502	SAH	CA-CB-CG-SD
6	H	507	P33	O4-C5-C6-O7
6	B	507	P33	O4-C5-C6-O7
3	B	502	SAH	O-C-CA-N
7	F	507	P6G	C2-C3-O4-C5
6	A	508	P33	C12-C11-O10-C9
7	F	507	P6G	C11-C12-O13-C14
6	B	507	P33	C12-C11-O10-C9
7	D	507	P6G	C9-C8-O7-C6
6	B	507	P33	C14-C15-O16-C17
3	D	502	SAH	C-CA-CB-CG
6	H	507	P33	C11-C12-O13-C14
9	G	509	PEG	O1-C1-C2-O2
6	A	508	P33	C14-C15-O16-C17
9	G	509	PEG	C1-C2-O2-C3
3	E	502	SAH	C3'-C4'-C5'-SD
6	H	507	P33	C21-C20-O19-C18
7	F	507	P6G	O10-C11-C12-O13
6	A	508	P33	C11-C12-O13-C14
3	C	502	SAH	O4'-C4'-C5'-SD

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Mol	Chain	Res	Type	Atoms
3	E	502	SAH	O4'-C4'-C5'-SD
3	H	502[A]	SAH	O4'-C4'-C5'-SD
6	B	507	P33	C6-C5-O4-C3
3	F	502[A]	SAH	CB-CG-SD-C5'
7	D	507	P6G	C6-C5-O4-C3
3	H	502[A]	SAH	CB-CG-SD-C5'
6	H	507	P33	C2-C3-O4-C5
3	H	502[A]	SAH	C2'-C1'-N9-C8
7	D	507	P6G	C15-C14-O13-C12
3	G	502	SAH	C-CA-CB-CG
2	B	501	NAD	O4B-C4B-C5B-O5B
8	H	503[B]	ADN	C3'-C4'-C5'-O5'
3	D	502	SAH	CB-CG-SD-C5'
3	D	502	SAH	N-CA-CB-CG
6	H	507	P33	C5-C6-O7-C8
2	A	501	NAD	O4B-C4B-C5B-O5B
3	B	502	SAH	O-C-CA-CB
6	A	508	P33	C9-C8-O7-C6
2	D	501	NAD	O4B-C4B-C5B-O5B
2	G	501	NAD	O4B-C4B-C5B-O5B
2	H	501	NAD	O4B-C4B-C5B-O5B
7	D	507	P6G	C5-C6-O7-C8
3	H	502[A]	SAH	O4'-C1'-N9-C8
6	H	507	P33	O16-C17-C18-O19
3	E	502	SAH	C-CA-CB-CG
6	A	508	P33	O16-C17-C18-O19
6	H	507	P33	C14-C15-O16-C17

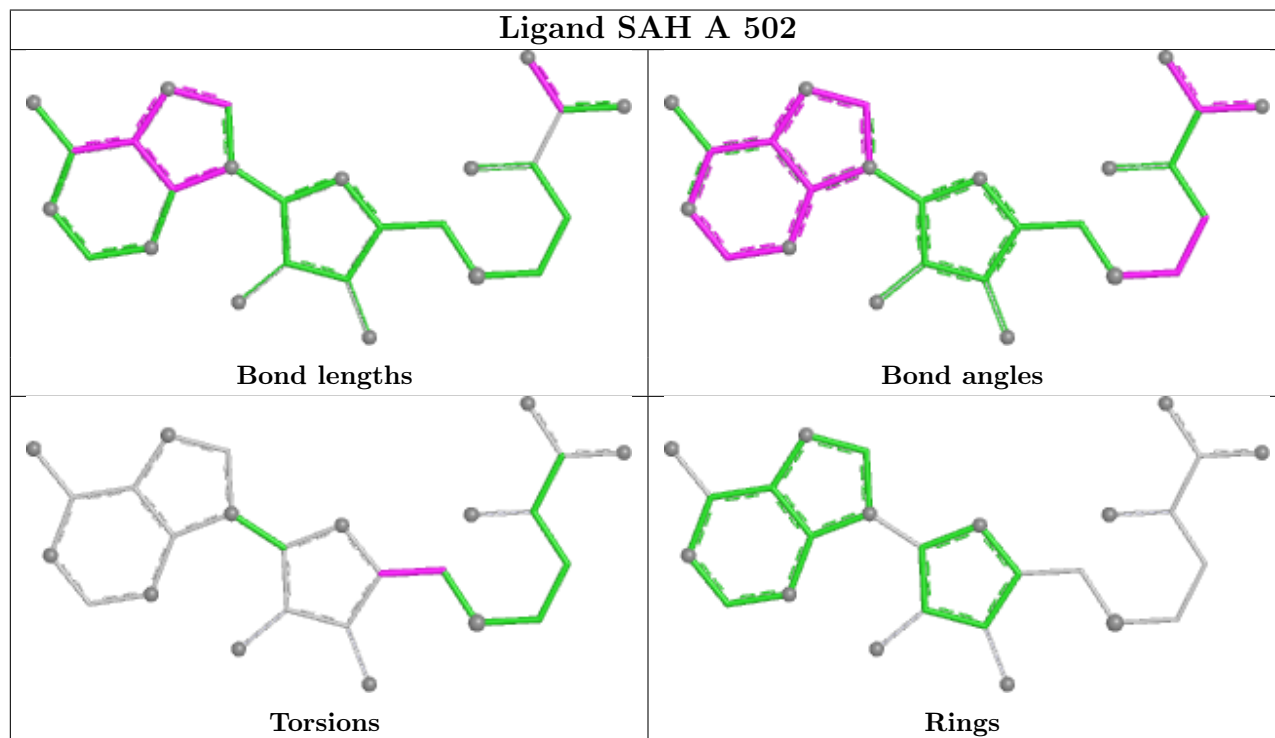
There are no ring outliers.

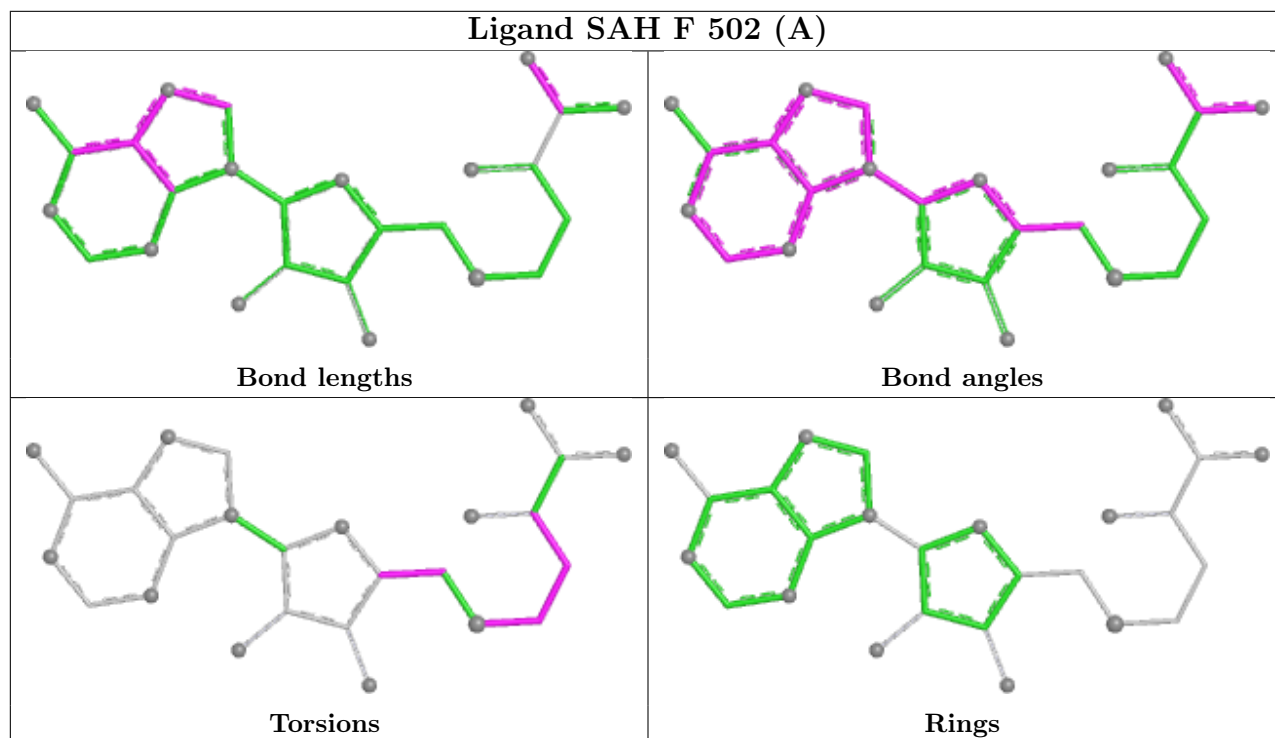
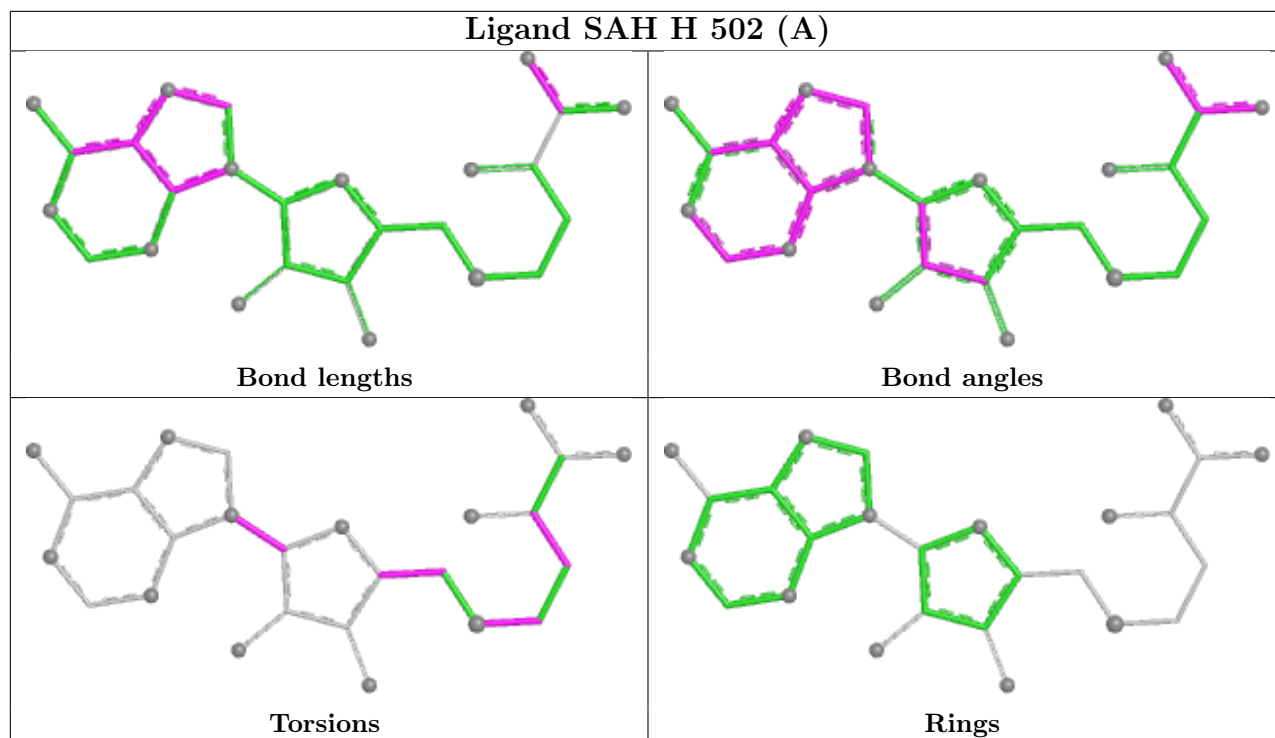
7 monomers are involved in 10 short contacts:

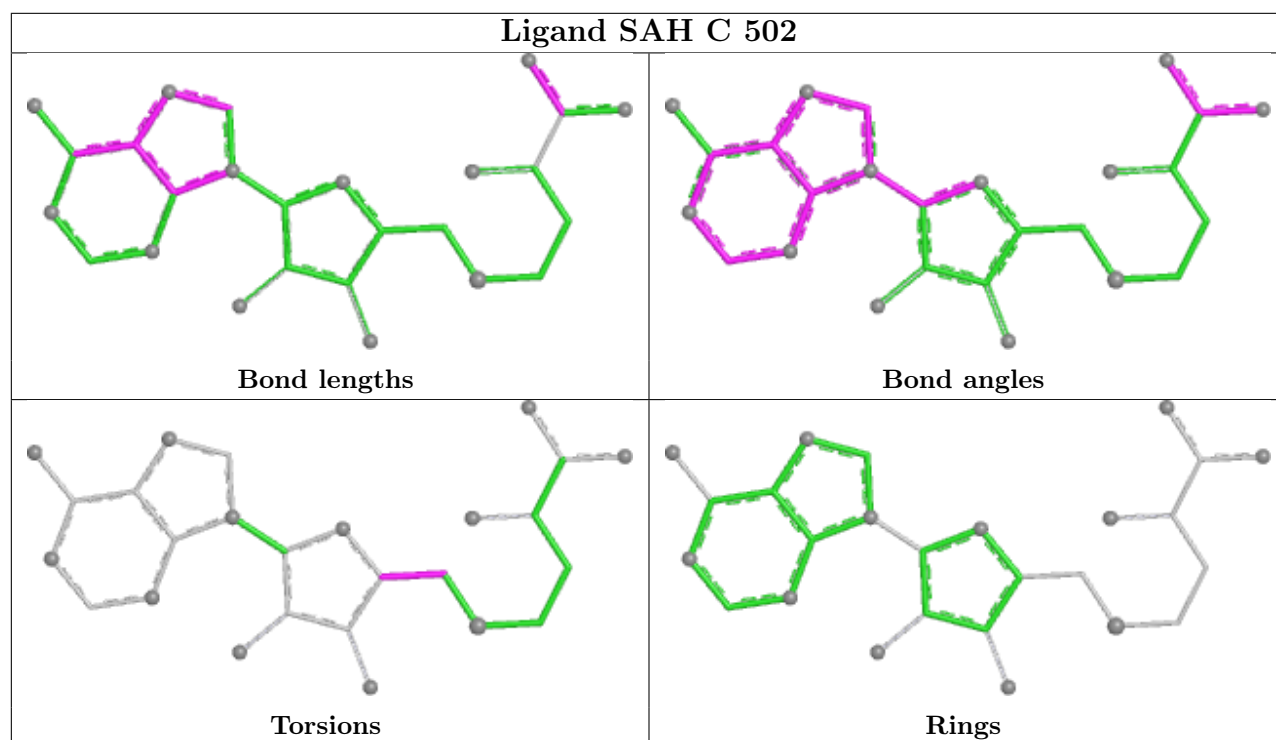
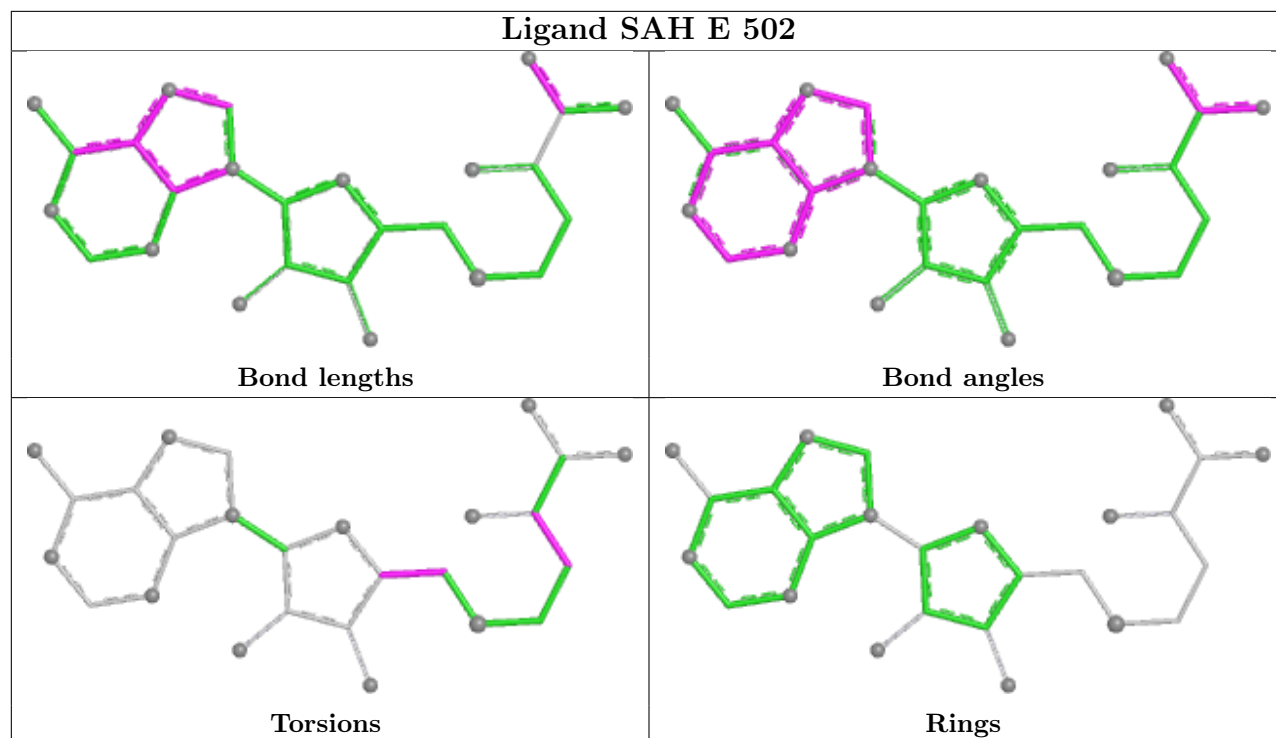
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	502[A]	SAH	1	0
3	F	502[A]	SAH	3	0
8	F	503[B]	ADN	1	0
3	B	502	SAH	2	0
2	C	501	NAD	1	0
2	F	501	NAD	1	0
3	D	502	SAH	2	0

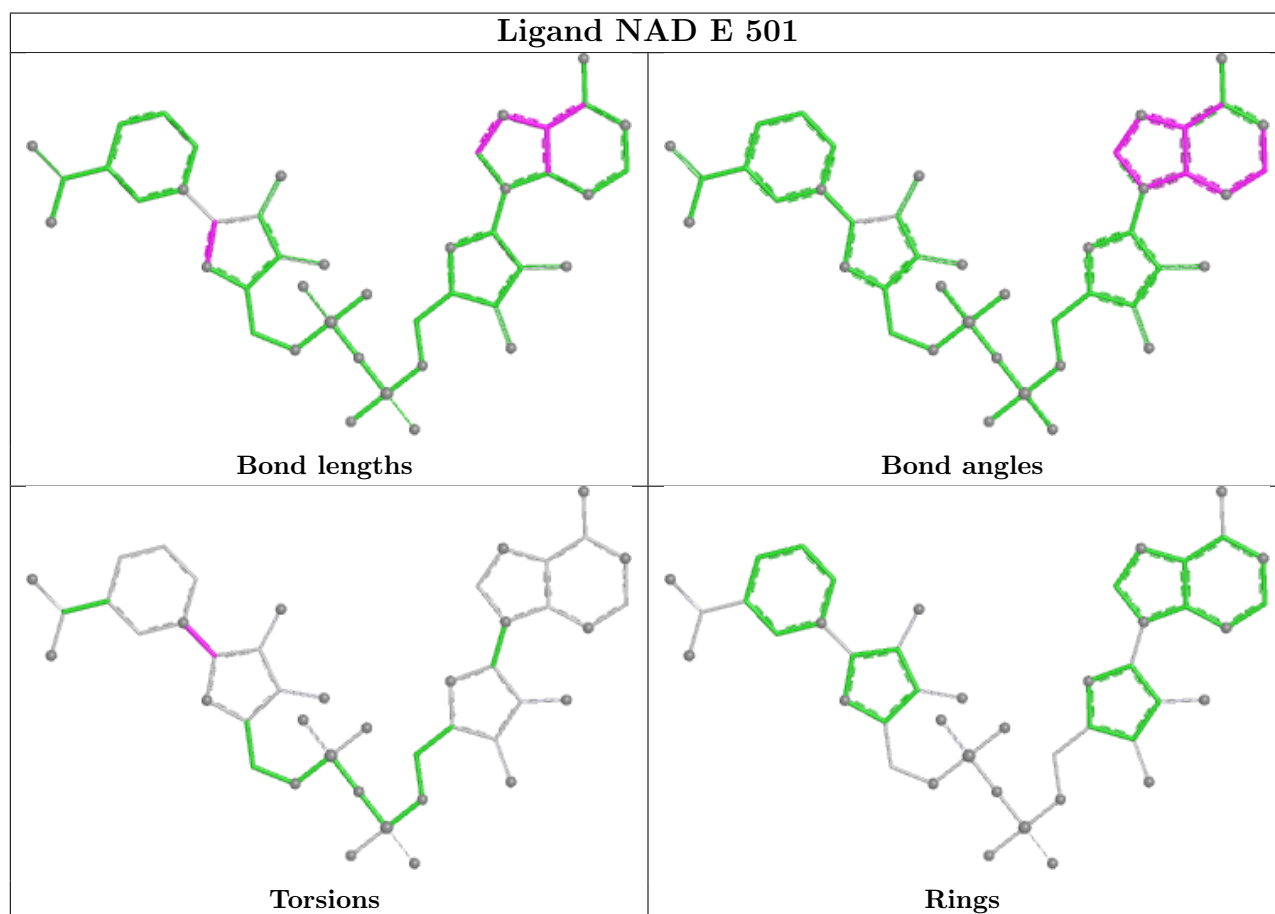
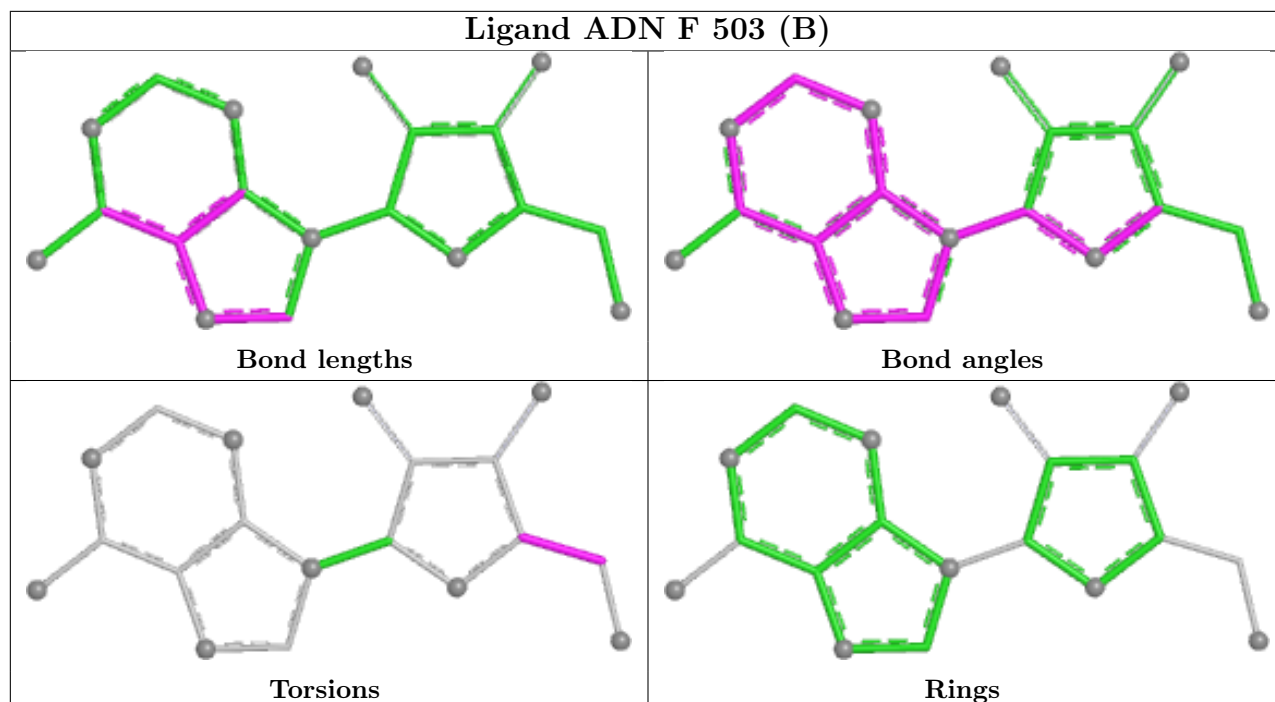
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

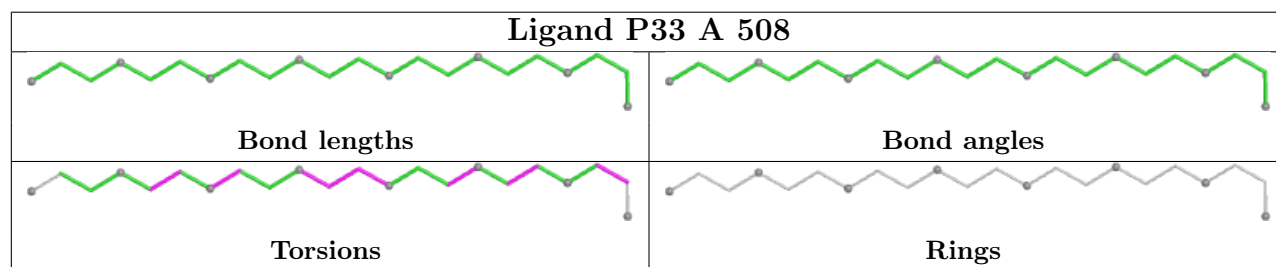
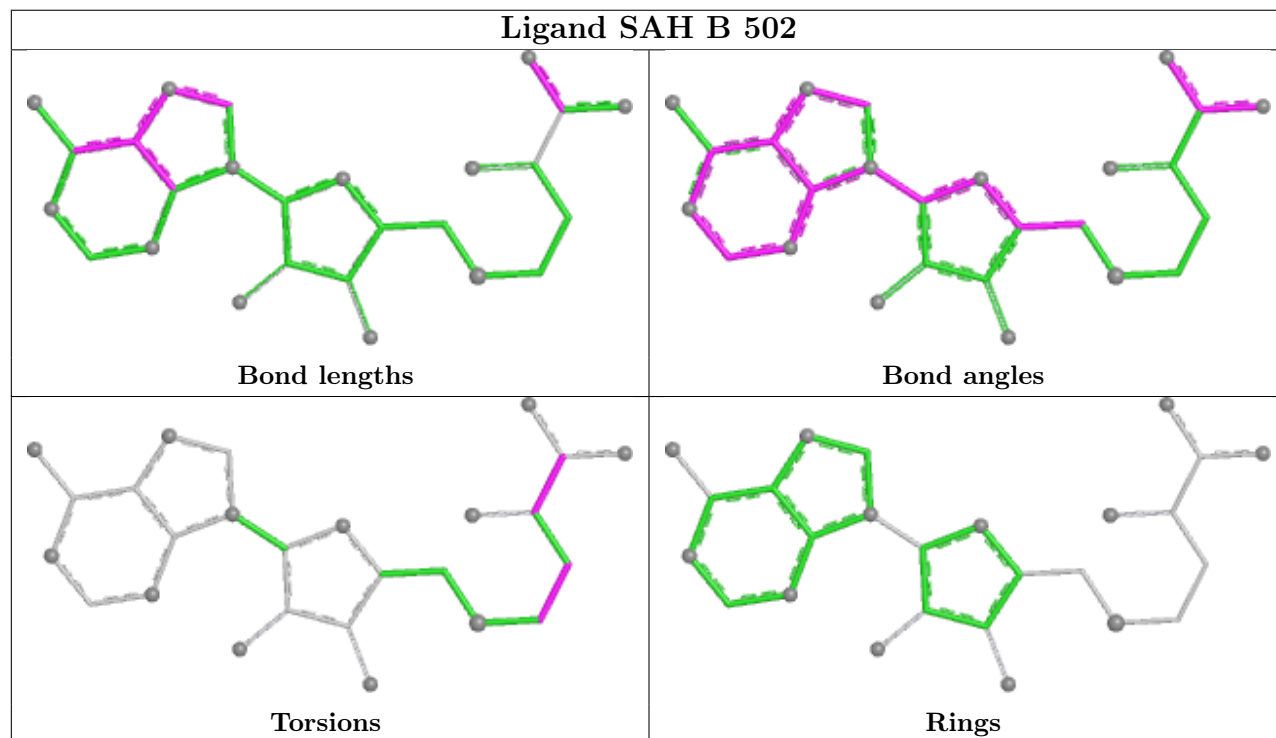
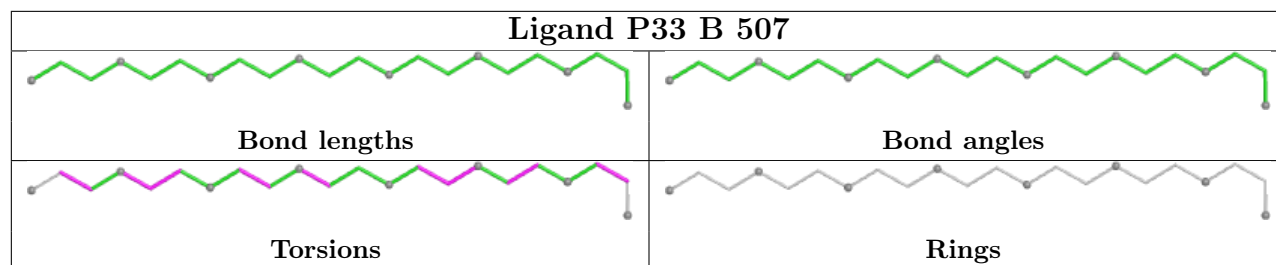
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

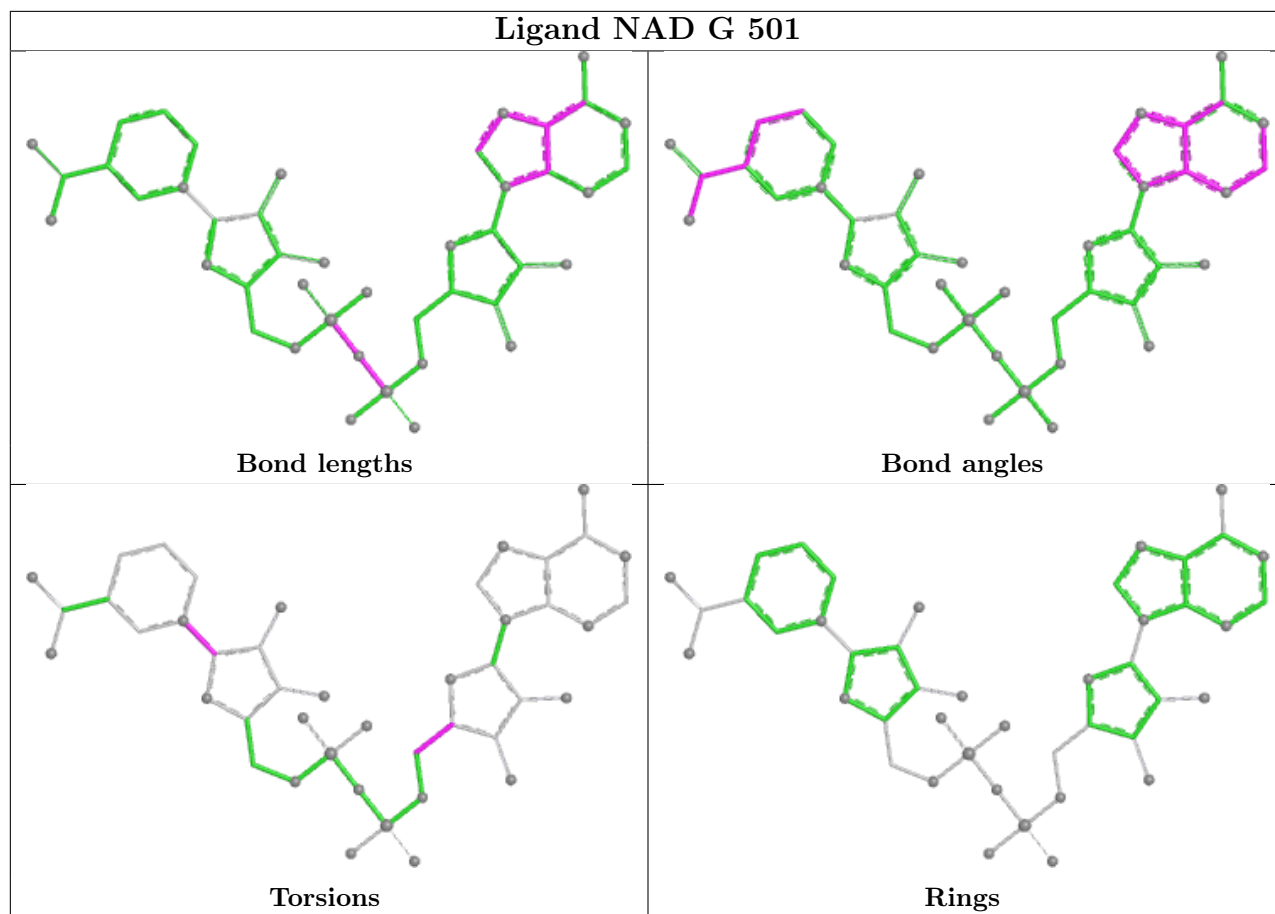


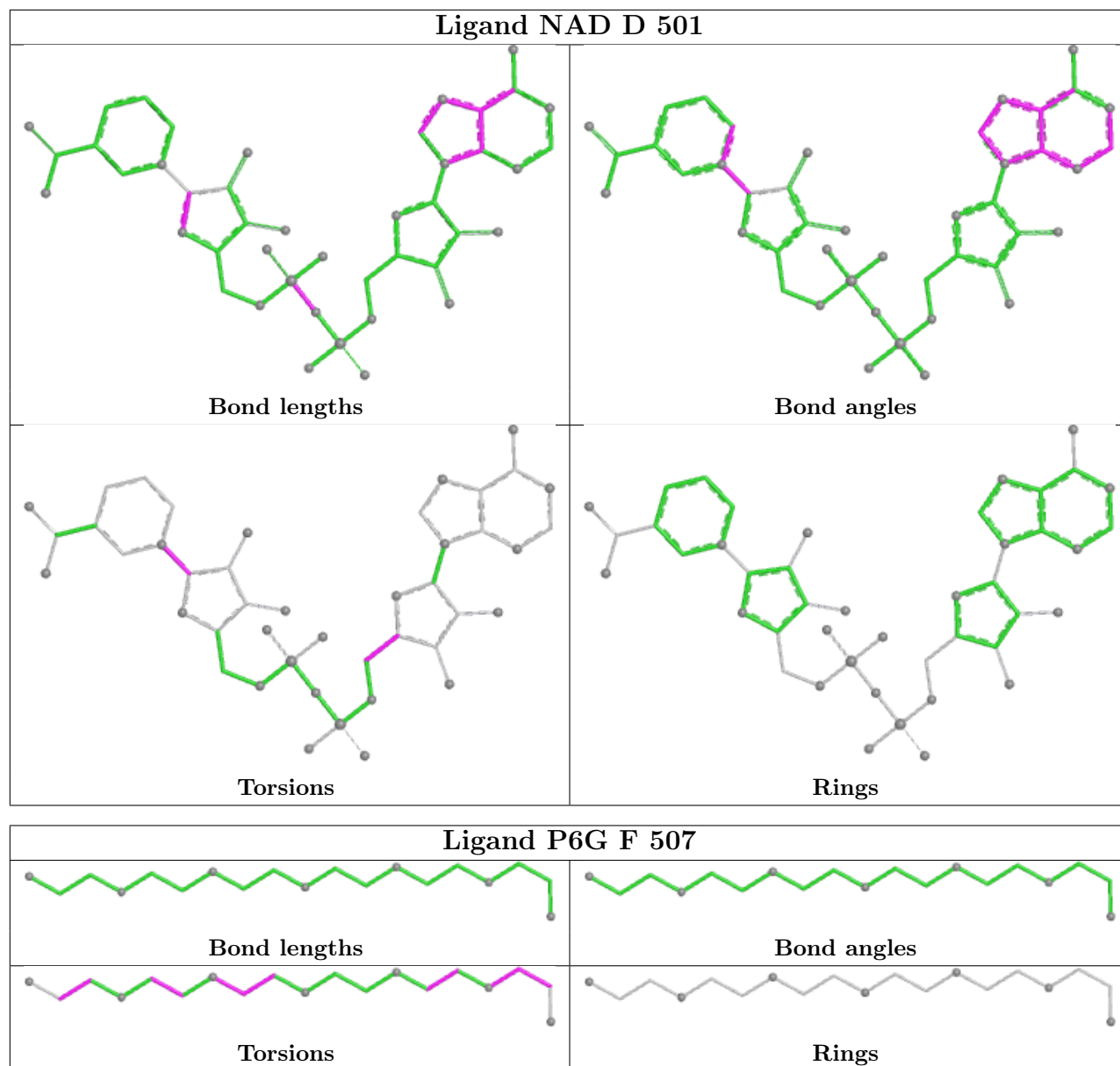


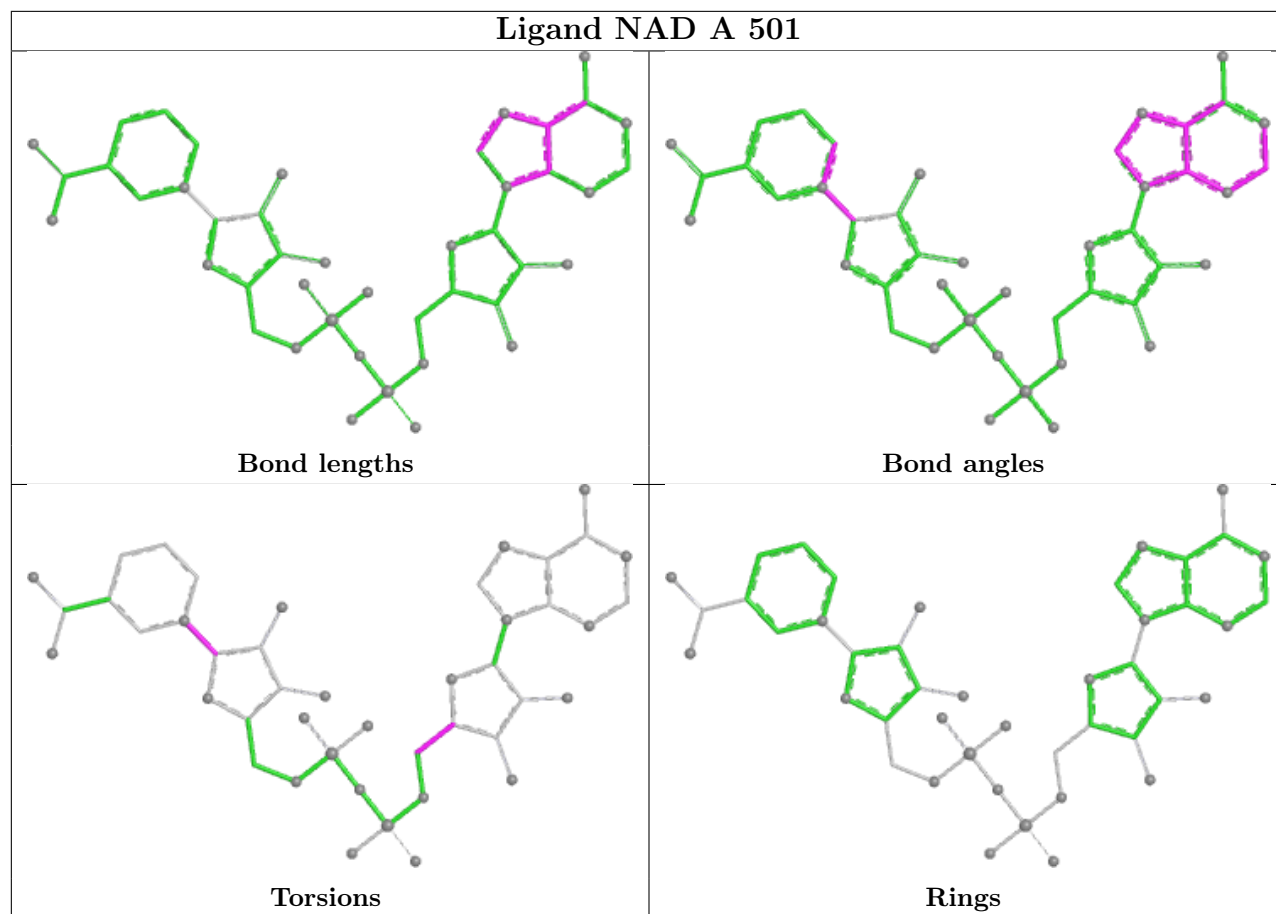


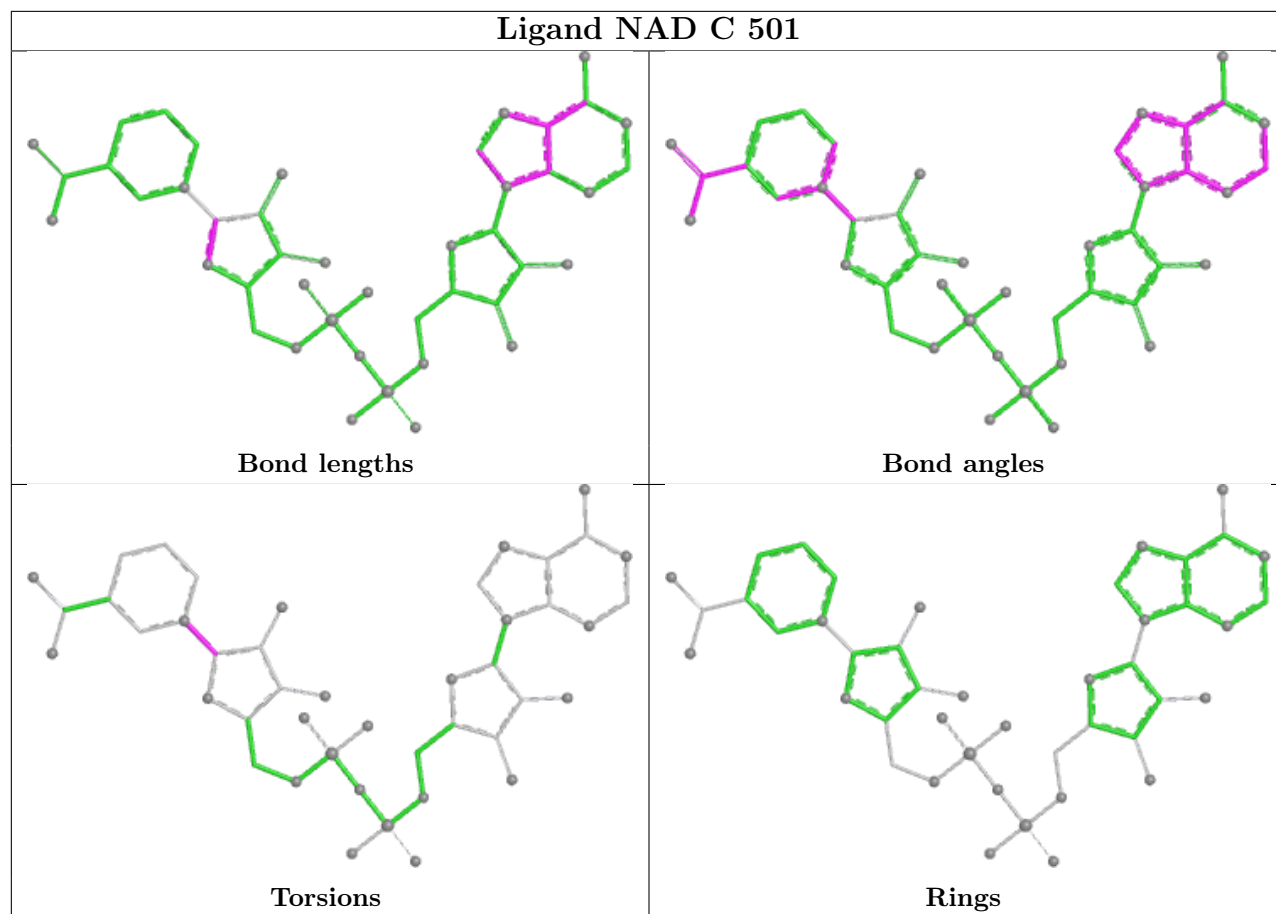


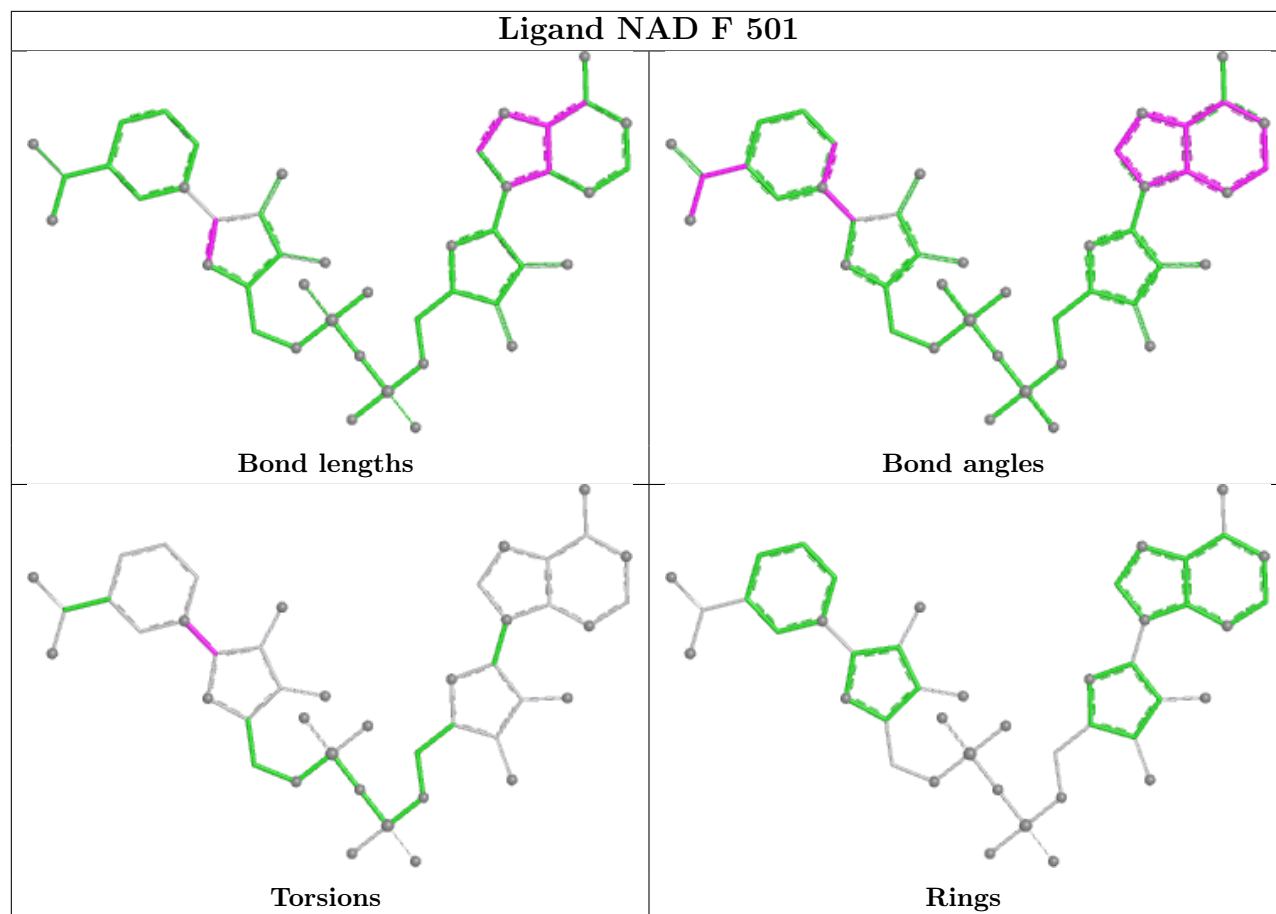


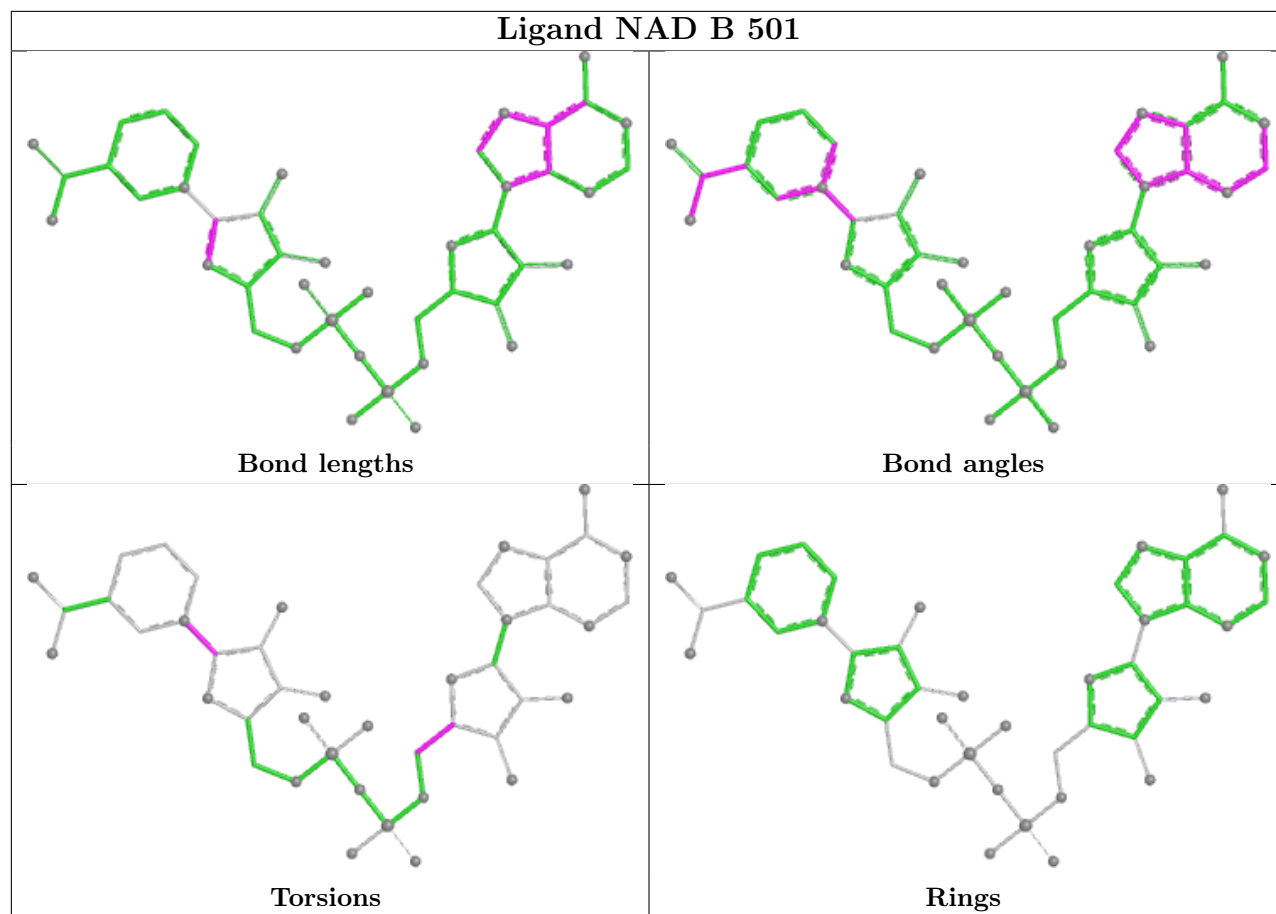


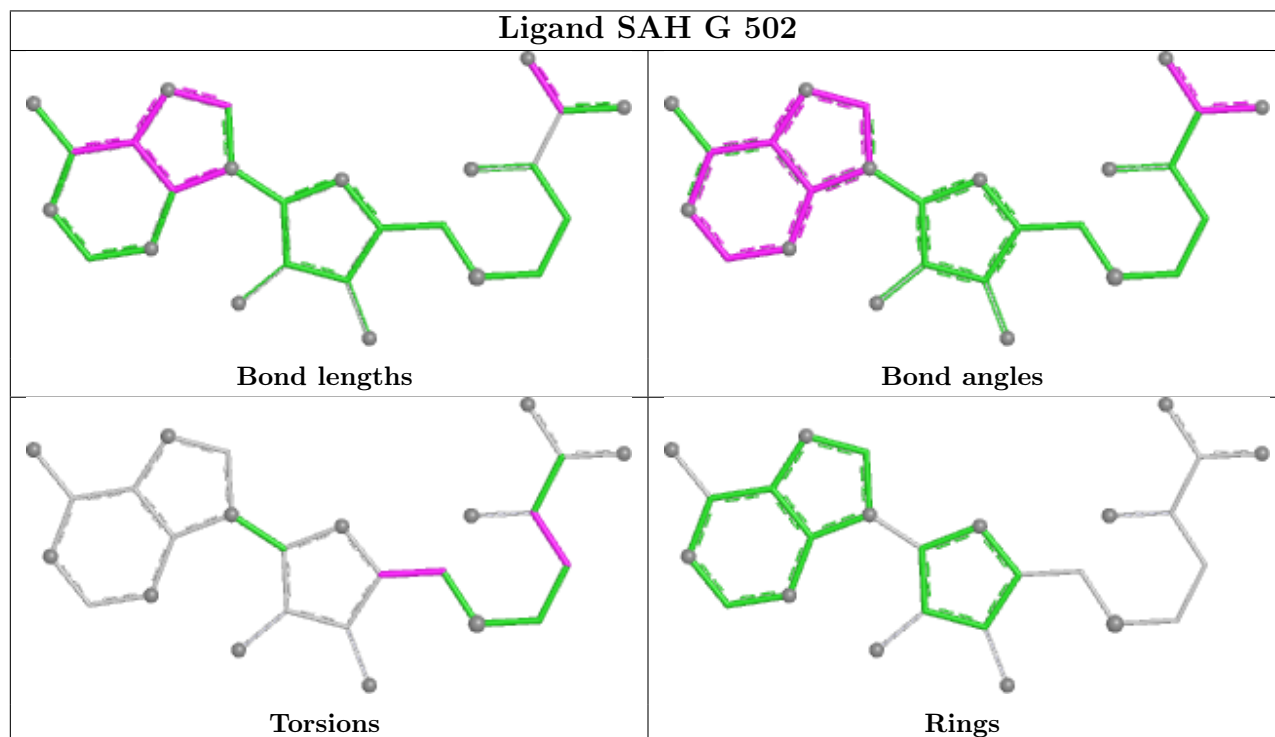
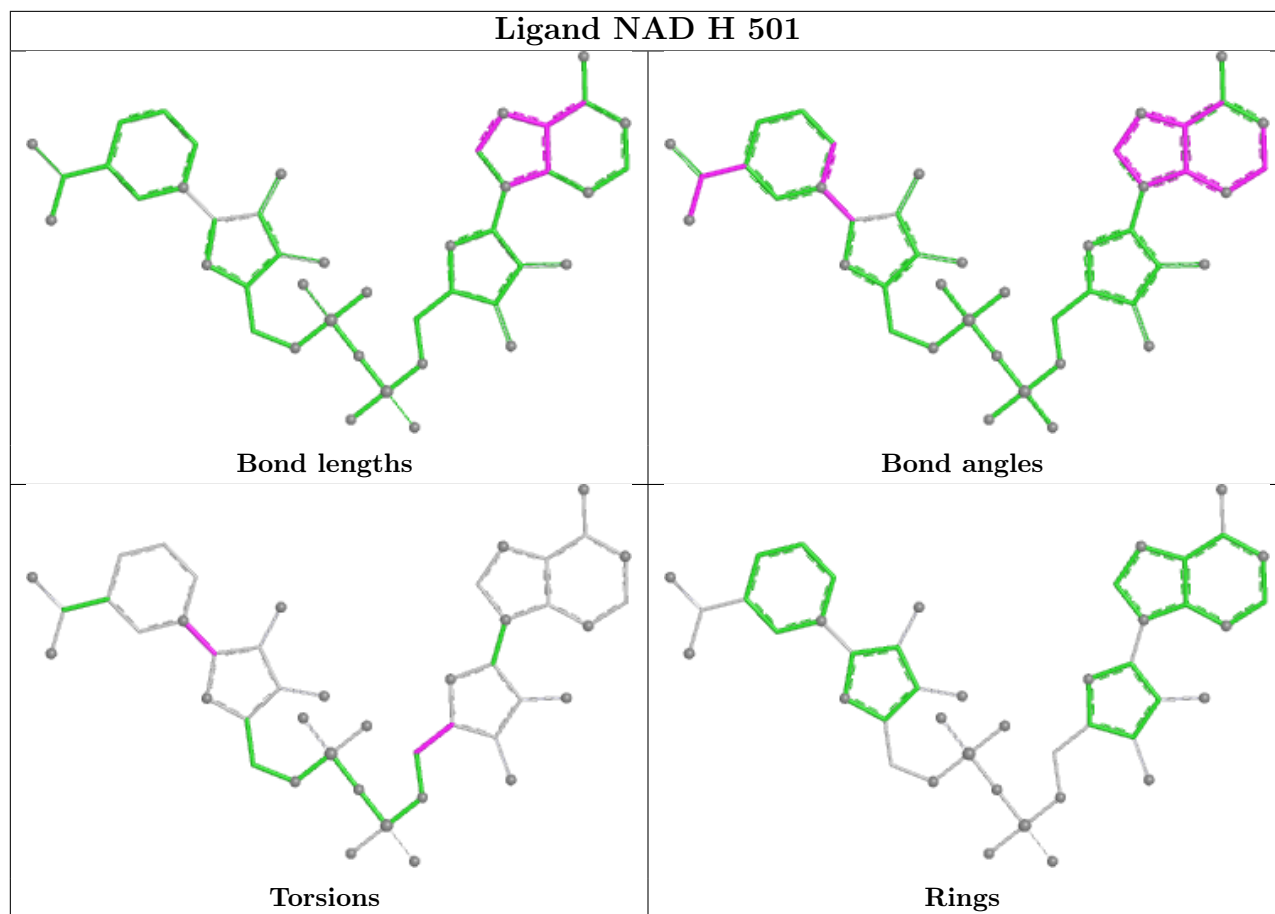


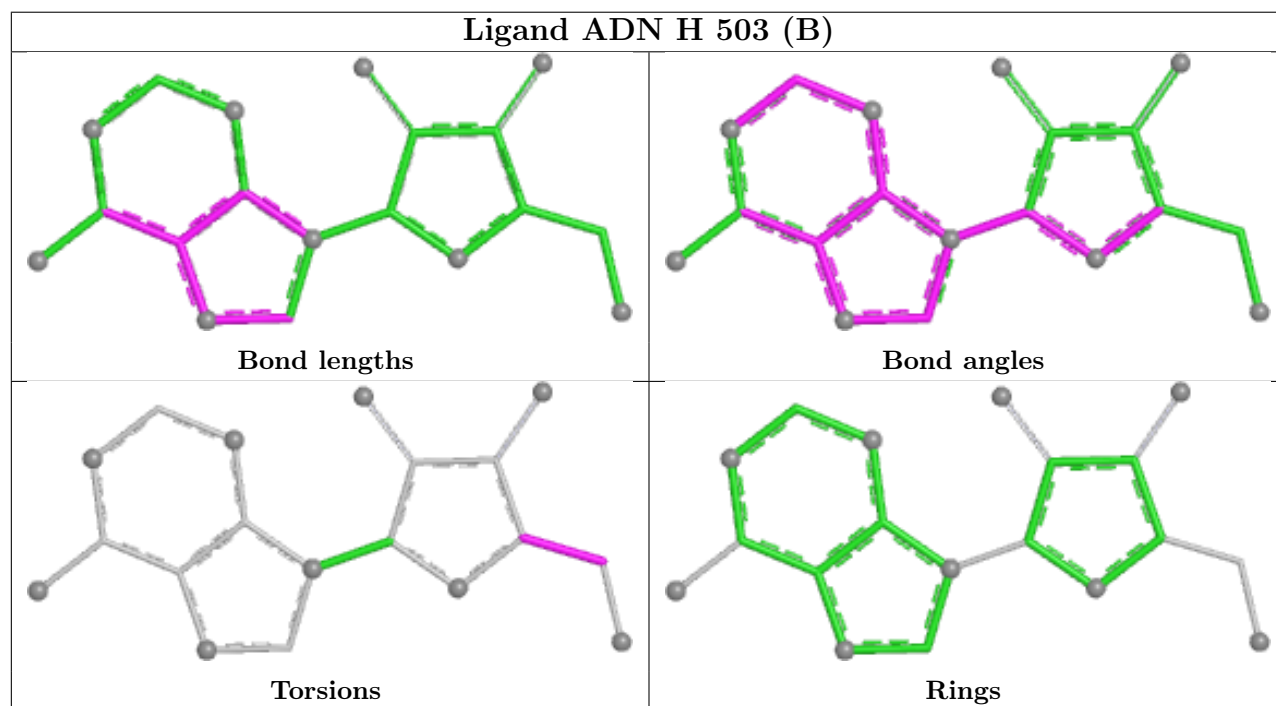
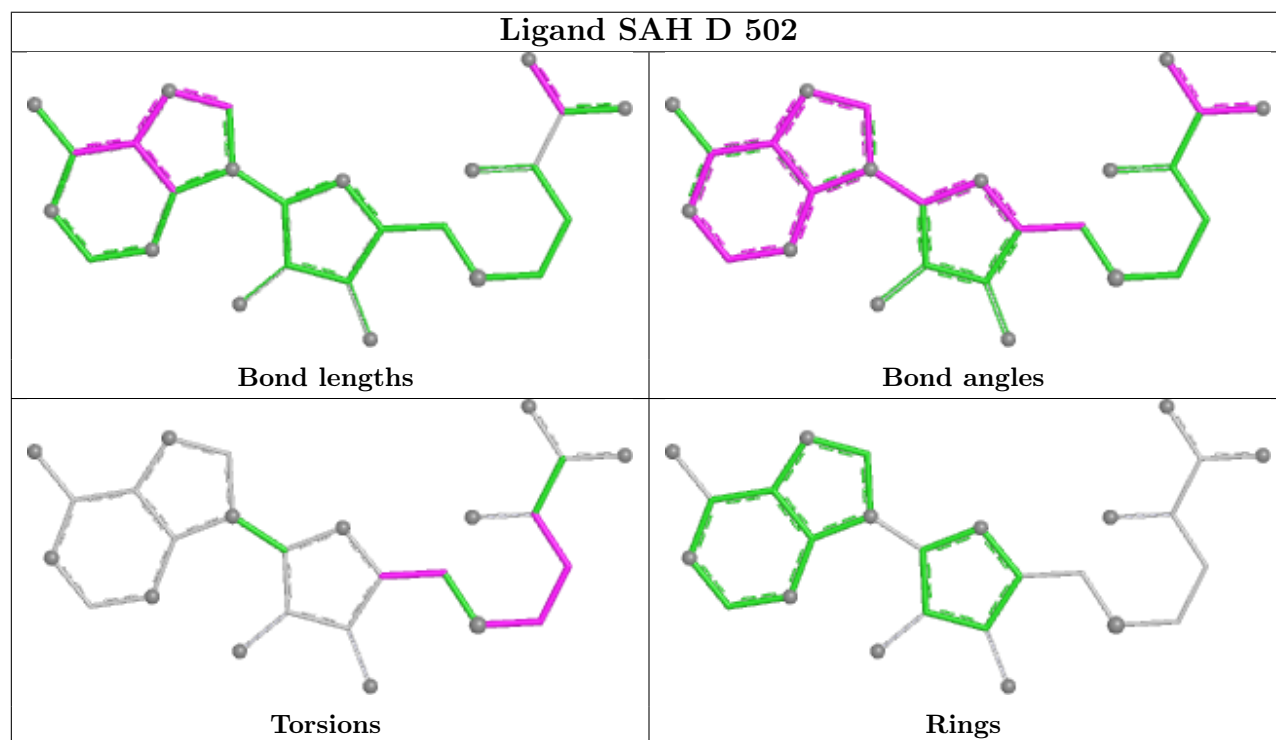
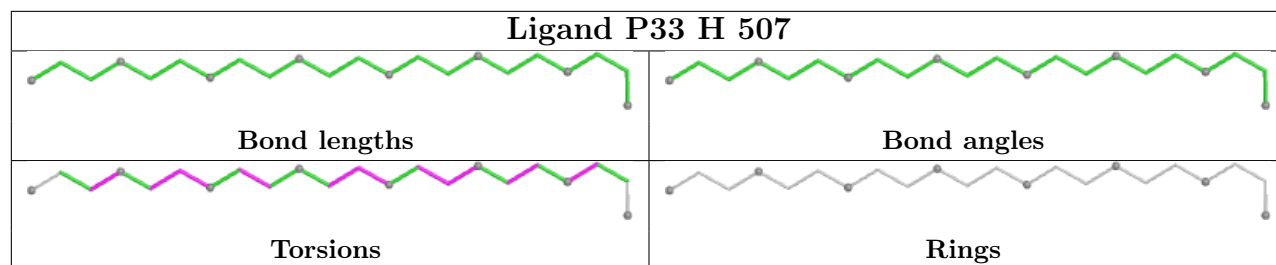


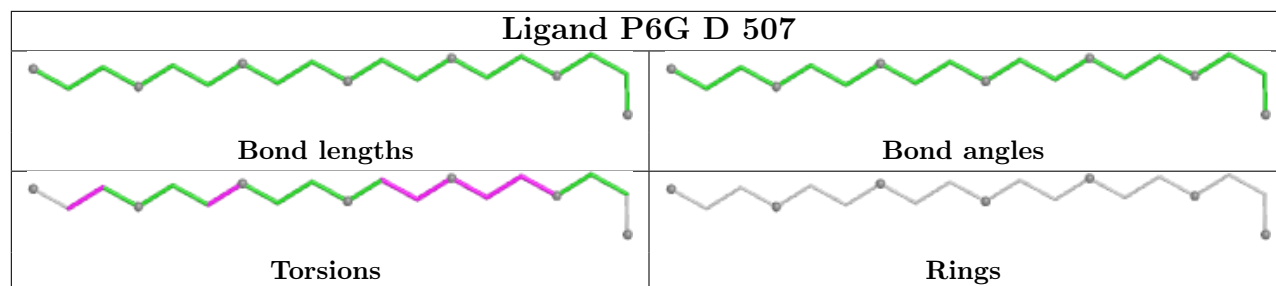












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	494/498 (99%)	-0.46	4 (0%) 82 79	19, 43, 84, 143	8 (1%)
1	B	494/498 (99%)	-0.31	4 (0%) 82 79	30, 54, 117, 170	0
1	C	491/498 (98%)	-0.44	4 (0%) 82 79	31, 45, 86, 151	0
1	D	493/498 (98%)	-0.37	6 (1%) 76 72	23, 50, 105, 157	1 (0%)
1	E	494/498 (99%)	-0.42	4 (0%) 82 79	19, 44, 85, 143	5 (1%)
1	F	493/498 (98%)	-0.39	5 (1%) 79 76	20, 49, 105, 128	6 (1%)
1	G	495/498 (99%)	-0.47	4 (0%) 82 79	19, 42, 85, 140	4 (0%)
1	H	487/498 (97%)	-0.34	3 (0%) 85 83	18, 51, 95, 136	9 (1%)
All	All	3941/3984 (98%)	-0.40	34 (0%) 81 78	18, 46, 97, 170	33 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	MET	4.0
1	F	356[A]	HIS	4.0
1	E	0	ALA	3.5
1	B	2	LYS	3.4
1	F	3	MET	3.4
1	D	125	LYS	3.2
1	H	196[A]	PHE	3.2
1	G	1	TYR	3.1
1	C	122	PRO	3.0
1	G	128	ILE	2.9
1	B	192	LEU	2.8
1	C	2	LYS	2.7
1	D	4	GLU	2.6
1	A	196[A]	PHE	2.5
1	C	123	ASN	2.5
1	H	3	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	122	PRO	2.4
1	B	3	MET	2.4
1	A	3	MET	2.3
1	A	174	LYS	2.3
1	E	3	MET	2.3
1	G	442	THR	2.2
1	E	122	PRO	2.2
1	E	218	ARG	2.2
1	D	158	TYR	2.2
1	F	122	PRO	2.2
1	F	125	LYS	2.2
1	B	128	ILE	2.2
1	D	167	THR	2.1
1	F	442	THR	2.1
1	C	127	LYS	2.1
1	H	2	LYS	2.1
1	A	443[A]	ARG	2.0
1	D	120	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	SO4	B	505	5/5	0.65	0.16	99,107,116,123	0
9	PEG	G	509	7/7	0.66	0.18	82,94,103,104	0
5	SO4	A	506	5/5	0.68	0.16	91,98,105,107	0
4	CL	D	503	1/1	0.75	0.12	80,80,80,80	0
5	SO4	C	507	5/5	0.76	0.11	94,99,104,106	0

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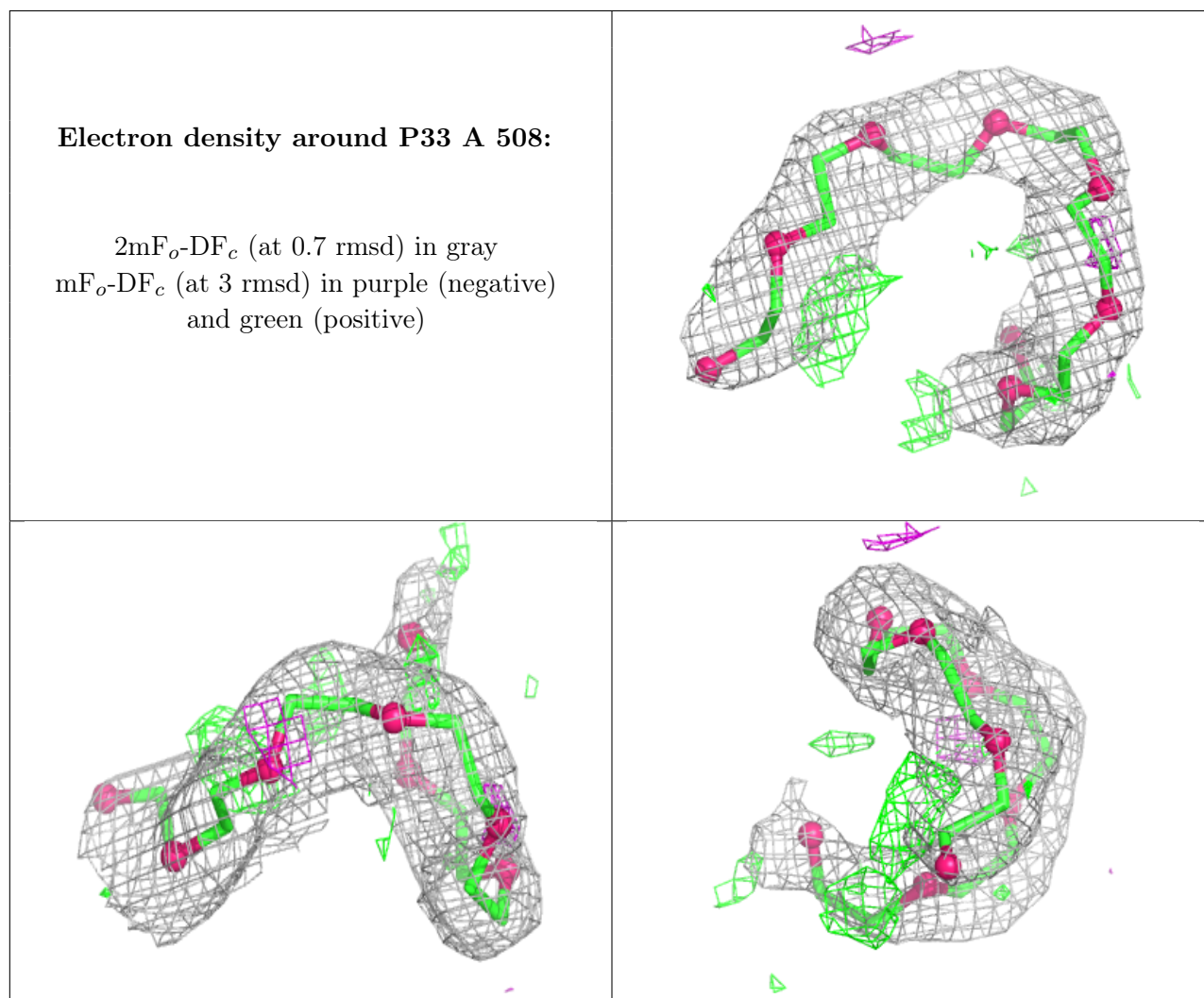
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	A	505	5/5	0.78	0.11	80,82,86,98	0
5	SO4	C	504	5/5	0.78	0.20	95,96,97,116	0
5	SO4	D	506	5/5	0.79	0.17	47,50,57,58	5
4	CL	H	504	1/1	0.79	0.12	67,67,67,67	0
4	CL	B	504	1/1	0.80	0.10	84,84,84,84	0
5	SO4	G	505	5/5	0.80	0.16	77,80,87,94	0
5	SO4	B	506	5/5	0.80	0.10	101,102,116,118	0
6	P33	A	508	22/22	0.82	0.14	62,77,84,90	0
5	SO4	E	505	5/5	0.82	0.16	86,91,96,101	0
5	SO4	H	505	5/5	0.83	0.11	93,101,109,119	0
4	CL	G	503	1/1	0.84	0.09	71,71,71,71	0
3	SAH	F	502[A]	26/26	0.84	0.22	37,65,72,73	26
5	SO4	A	504	5/5	0.84	0.18	80,83,94,98	0
4	CL	A	503	1/1	0.85	0.10	86,86,86,86	0
8	ADN	F	503[B]	19/19	0.85	0.14	40,52,58,60	19
5	SO4	H	506	5/5	0.85	0.12	81,94,99,101	0
5	SO4	G	507	5/5	0.87	0.09	74,81,87,95	0
5	SO4	F	505	5/5	0.87	0.11	85,91,97,106	0
5	SO4	D	504	5/5	0.87	0.09	85,86,90,100	0
5	SO4	C	506	5/5	0.88	0.11	102,108,115,119	0
6	P33	H	507	22/22	0.88	0.10	53,66,69,71	0
9	PEG	G	508	7/7	0.89	0.12	62,67,73,76	0
8	ADN	H	503[B]	19/19	0.89	0.11	29,35,37,37	19
3	SAH	B	502	26/26	0.90	0.13	42,52,80,96	0
6	P33	B	507	22/22	0.90	0.10	51,66,71,75	0
5	SO4	C	505	5/5	0.90	0.11	72,72,82,83	0
7	P6G	D	507	19/19	0.90	0.11	46,62,69,70	0
3	SAH	H	502[A]	26/26	0.91	0.18	47,93,98,100	26
4	CL	G	504	1/1	0.91	0.07	65,65,65,65	0
4	CL	F	504	1/1	0.91	0.06	80,80,80,80	0
7	P6G	F	507	19/19	0.91	0.10	48,59,70,71	0
4	CL	C	503	1/1	0.92	0.07	74,74,74,74	0
3	SAH	D	502	26/26	0.92	0.12	48,57,64,72	0
5	SO4	F	506	5/5	0.93	0.10	74,74,77,87	0
5	SO4	A	507	5/5	0.93	0.13	64,65,66,77	0
5	SO4	D	505	5/5	0.94	0.10	73,75,76,78	0
3	SAH	E	502	26/26	0.94	0.09	38,47,59,63	0
5	SO4	G	506	5/5	0.94	0.10	58,61,71,74	0
4	CL	E	503	1/1	0.94	0.08	66,66,66,66	0
4	CL	E	504	1/1	0.94	0.06	65,65,65,65	0
4	CL	B	503	1/1	0.95	0.09	52,52,52,52	0
3	SAH	C	502	26/26	0.95	0.08	29,41,63,66	0

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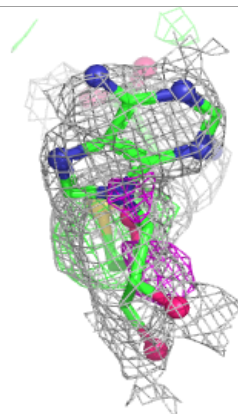
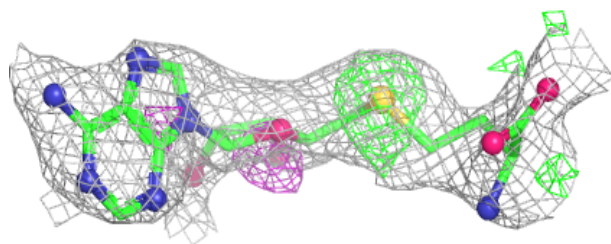
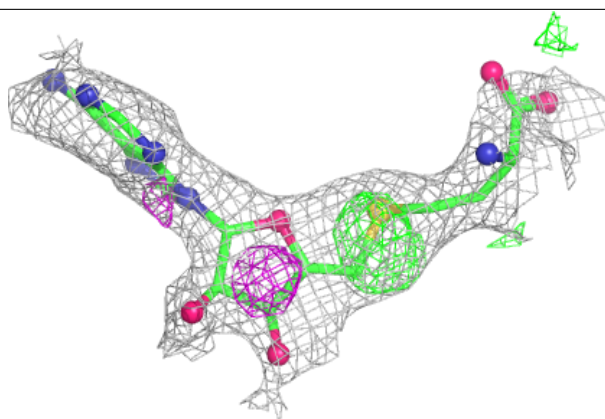
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SAH	A	502	26/26	0.95	0.07	32,38,45,54	0
5	SO4	E	506	5/5	0.95	0.07	62,70,71,75	0
3	SAH	G	502	26/26	0.96	0.07	29,41,56,60	0
2	NAD	C	501	44/44	0.97	0.06	31,36,40,43	0
2	NAD	A	501	44/44	0.98	0.06	29,32,36,37	0
2	NAD	D	501	44/44	0.98	0.06	27,31,35,37	0
2	NAD	E	501	44/44	0.98	0.06	29,35,39,42	0
2	NAD	F	501	44/44	0.98	0.05	26,30,34,36	0
2	NAD	G	501	44/44	0.98	0.04	27,31,34,39	0
2	NAD	H	501	44/44	0.98	0.05	33,36,38,40	0
2	NAD	B	501	44/44	0.98	0.05	30,35,40,43	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.

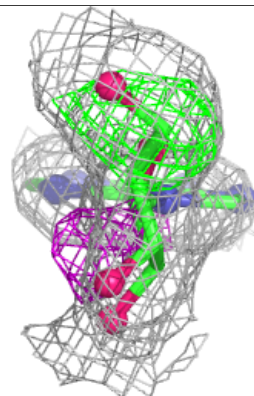
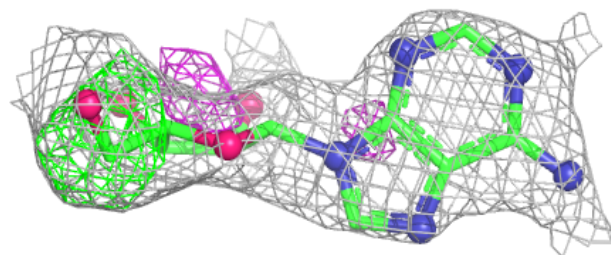
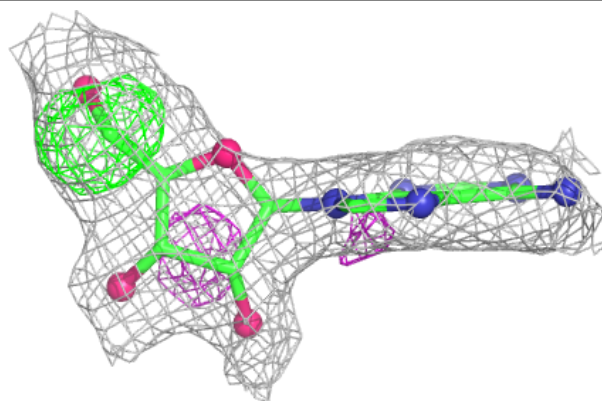


**Electron density around SAH F 502 (A):**

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

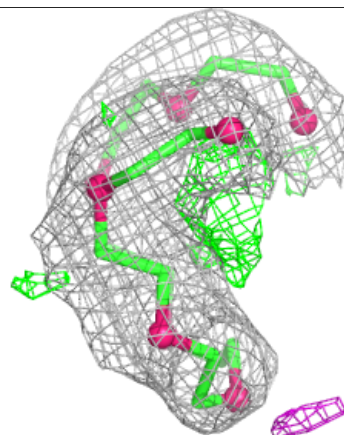
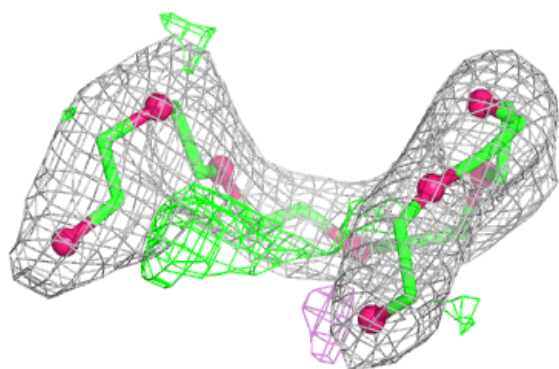
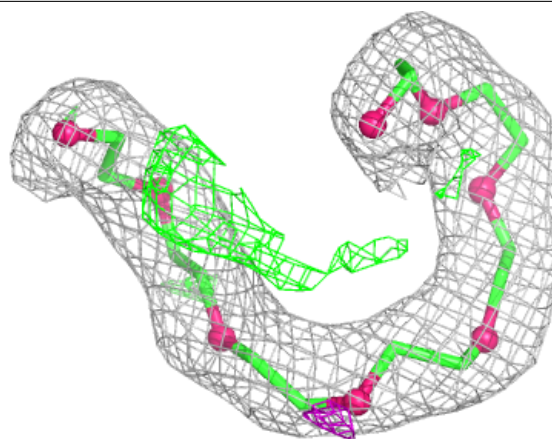
**Electron density around ADN F 503 (B):**

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

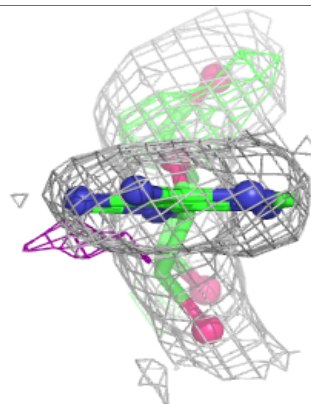
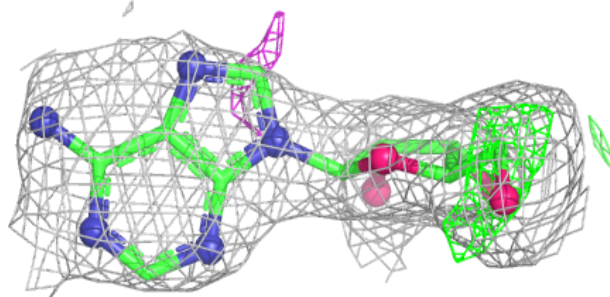
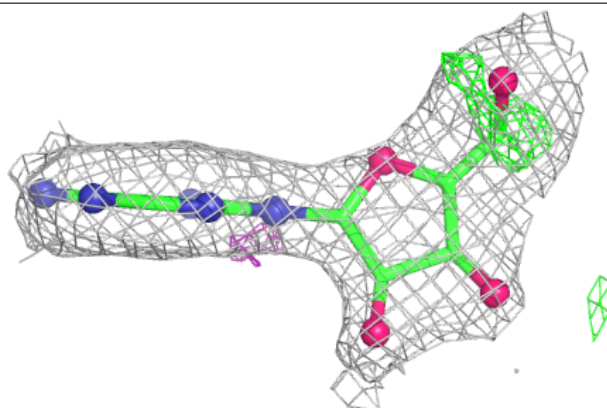


**Electron density around P33 H 507:**

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

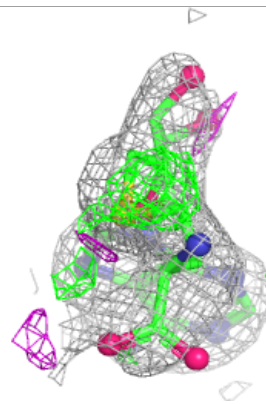
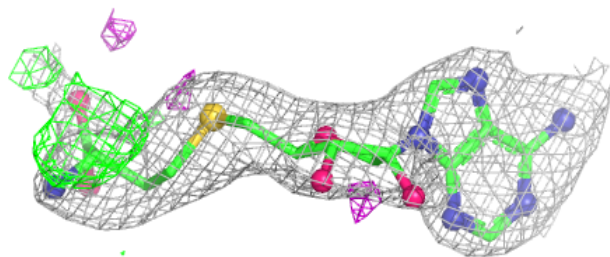
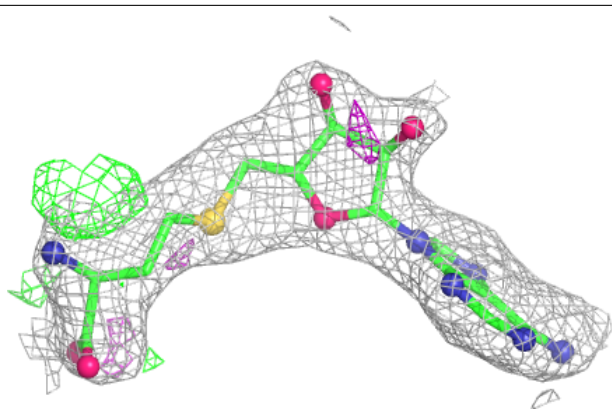
**Electron density around ADN H 503 (B):**

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



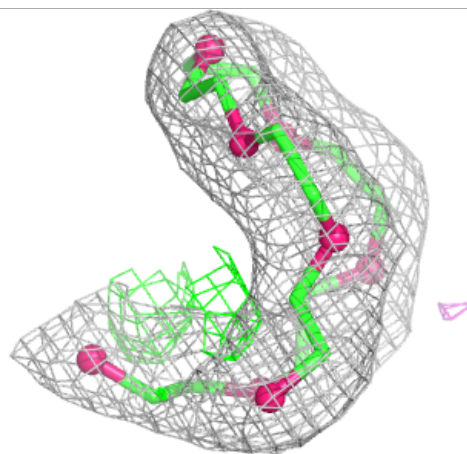
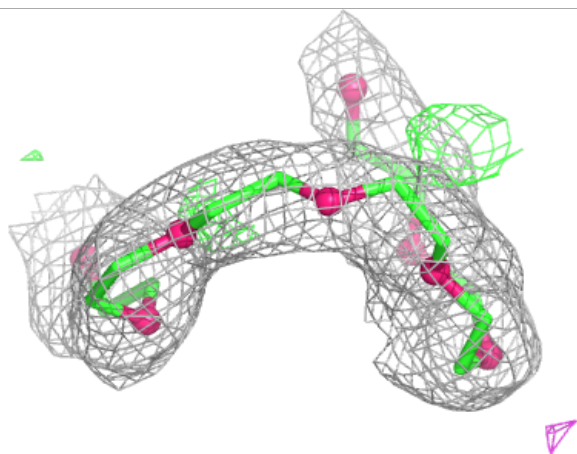
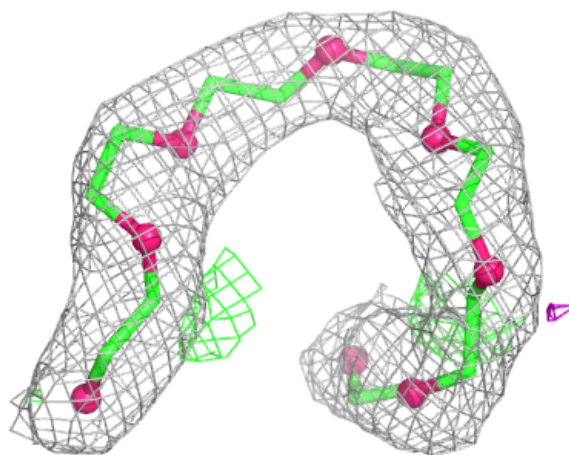
**Electron density around SAH B 502:**

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



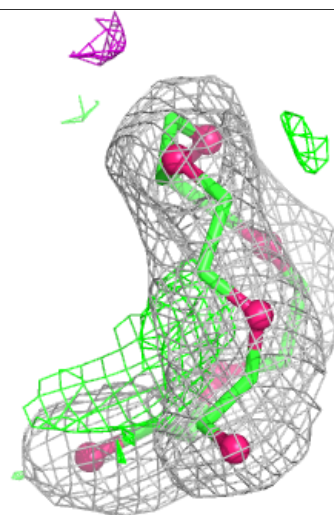
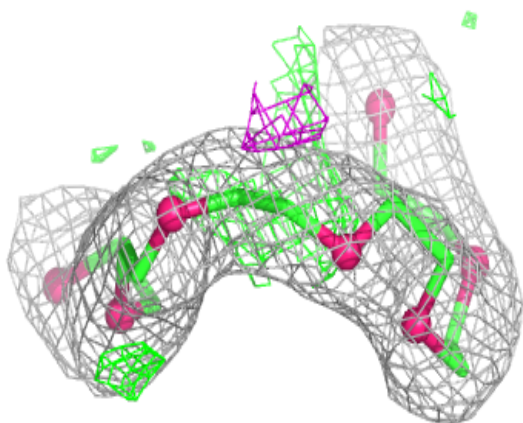
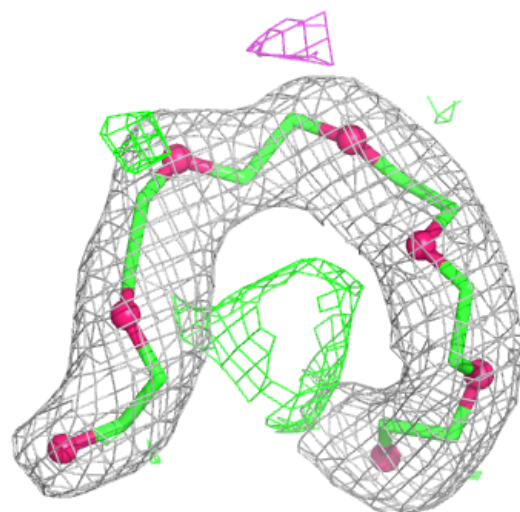
**Electron density around P33 B 507:**

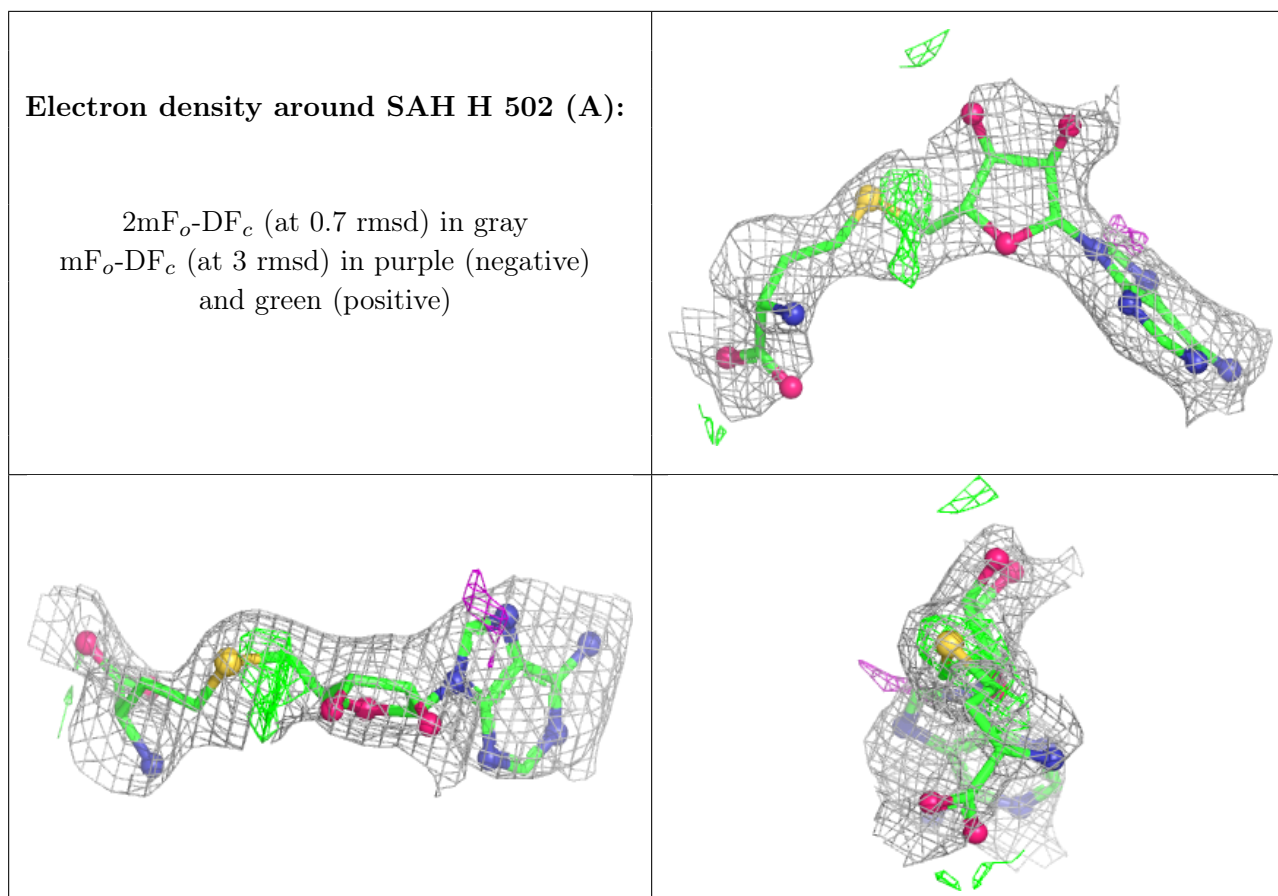
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around P6G D 507:**

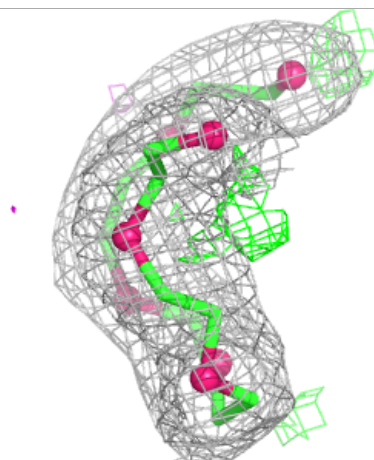
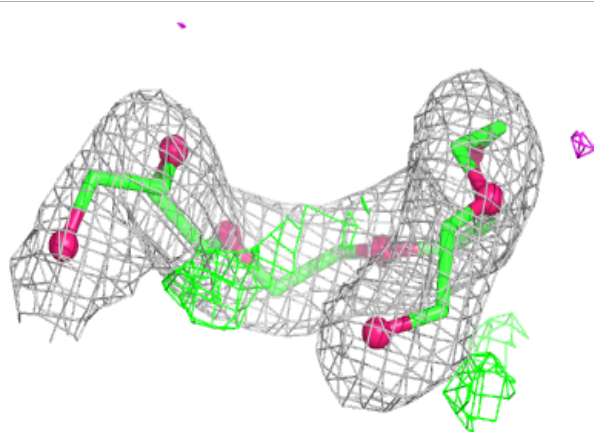
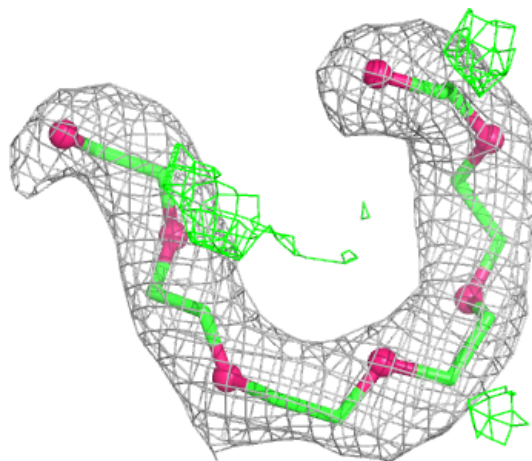
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

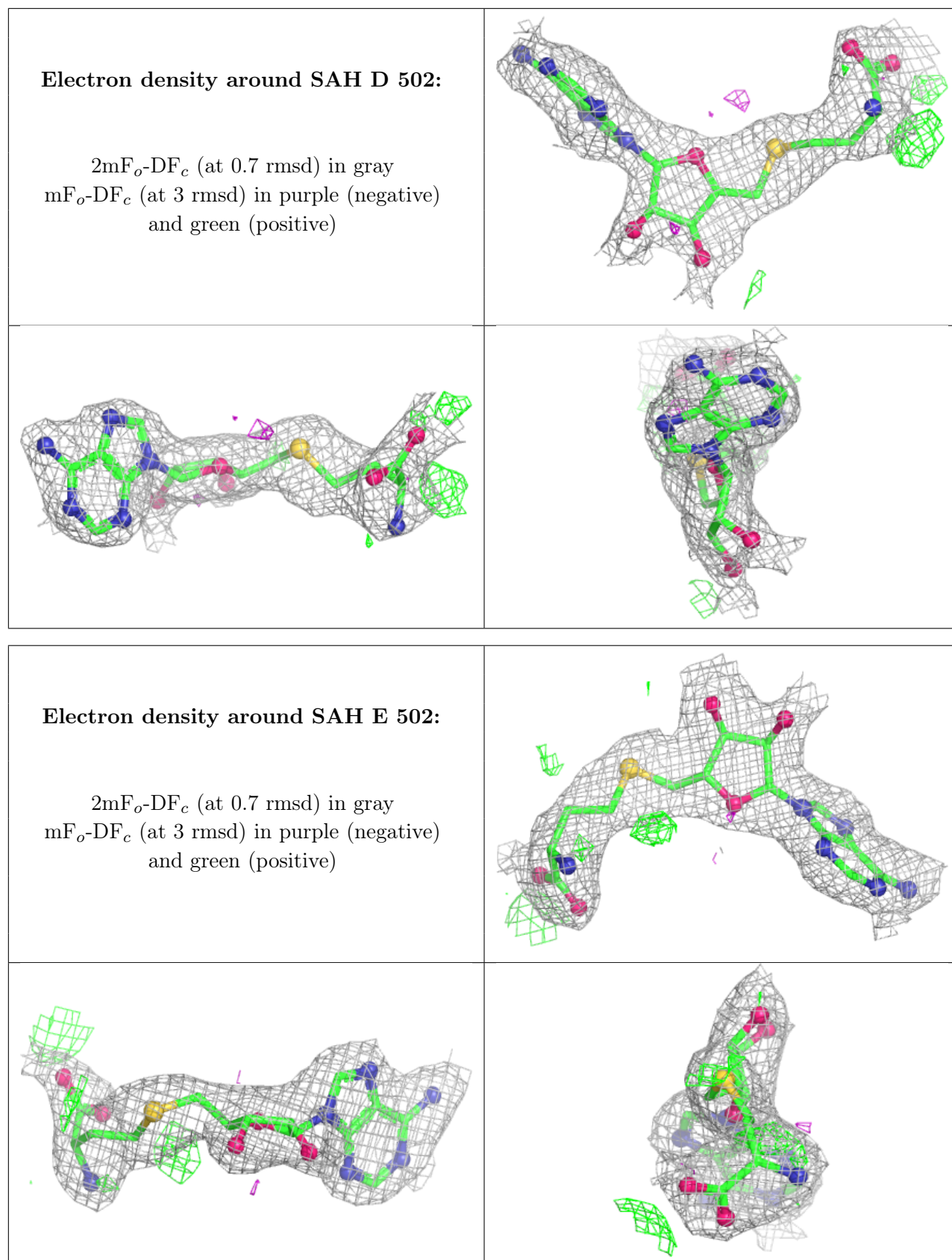




**Electron density around P6G F 507:**

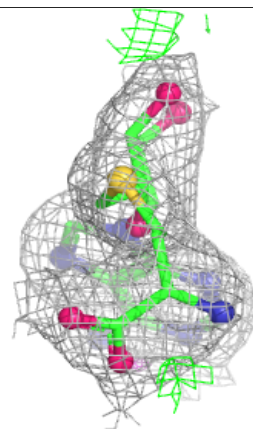
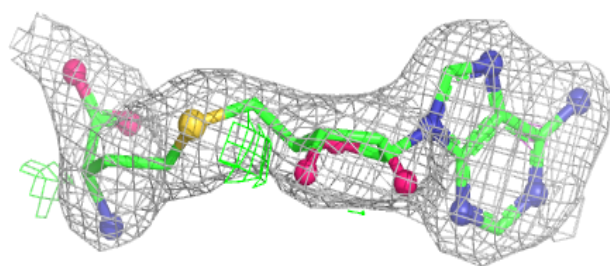
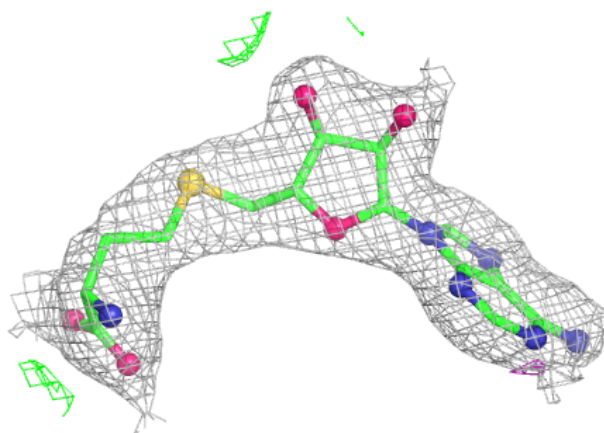
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



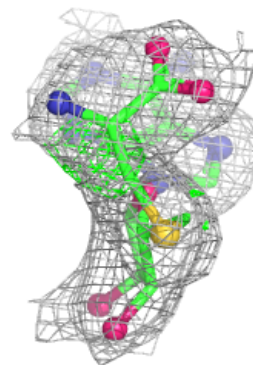
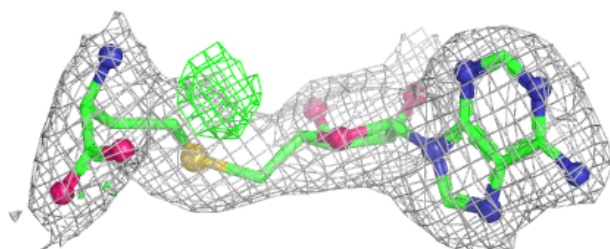
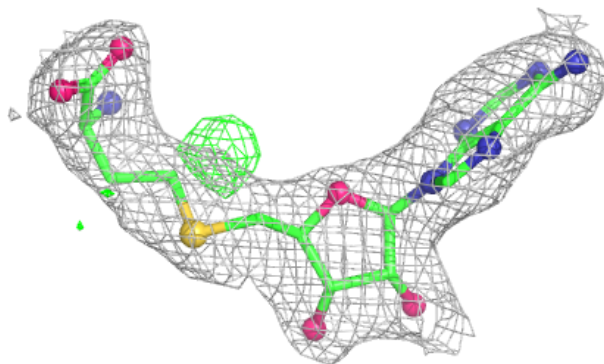


**Electron density around SAH C 502:**

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

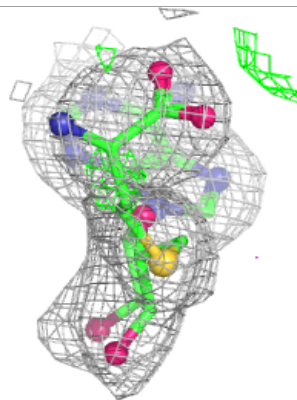
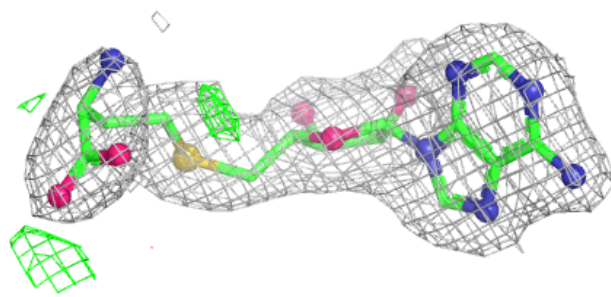
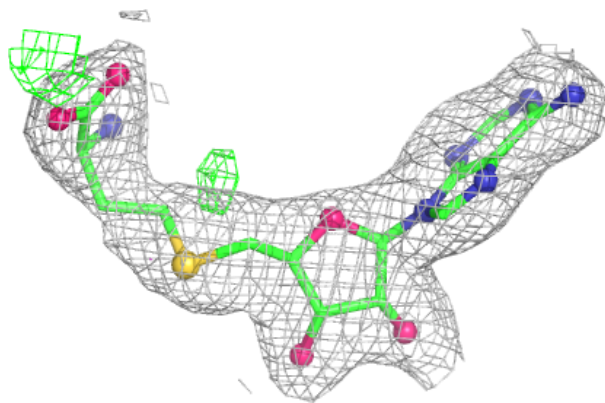
**Electron density around SAH A 502:**

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

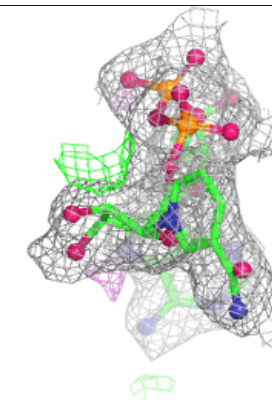
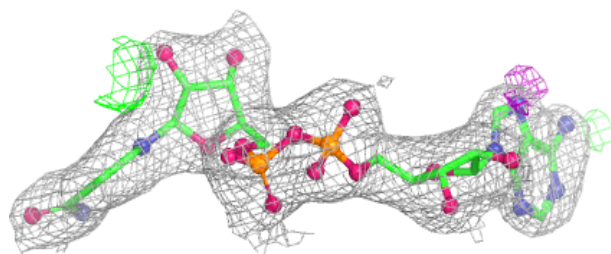
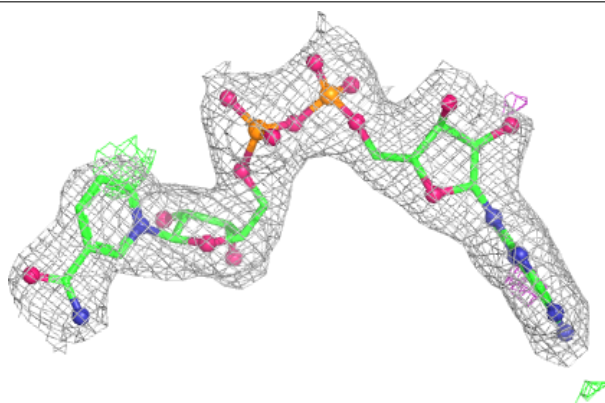


**Electron density around SAH G 502:**

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

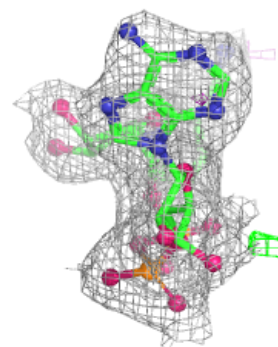
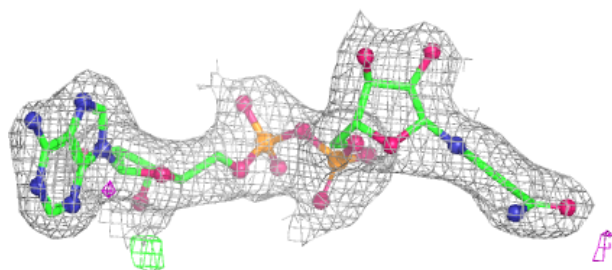
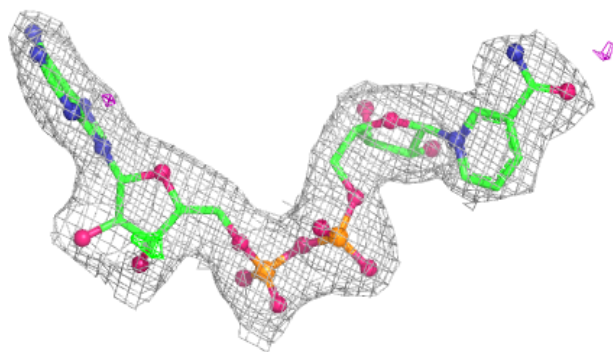
**Electron density around NAD C 501:**

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

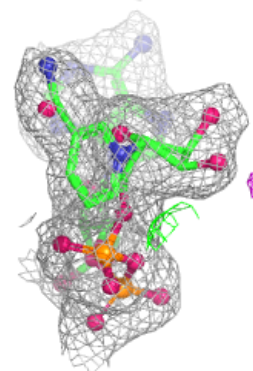
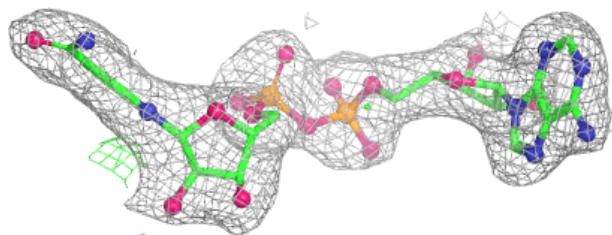
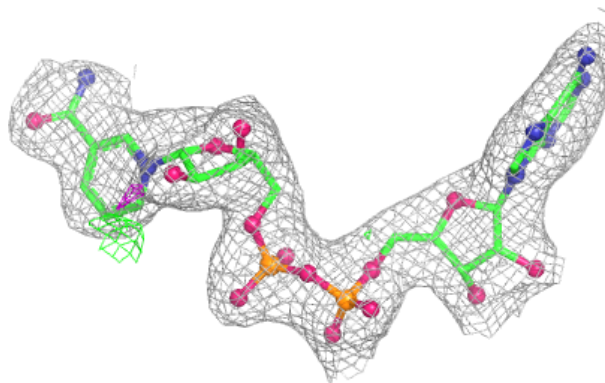


**Electron density around NAD A 501:**

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

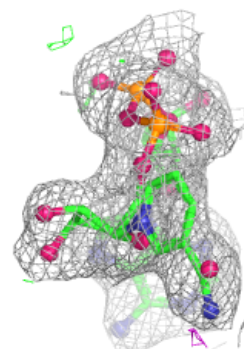
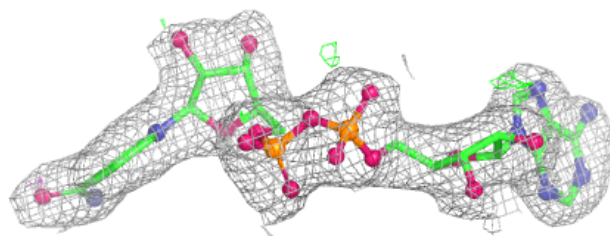
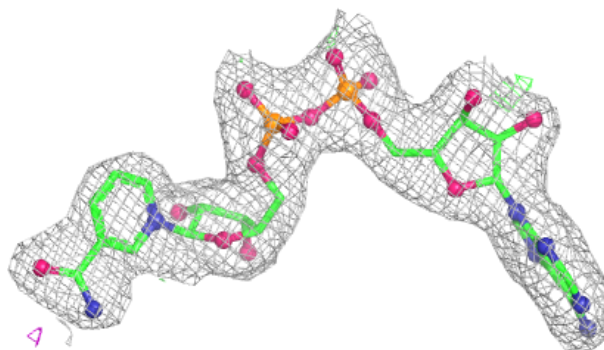
**Electron density around NAD D 501:**

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

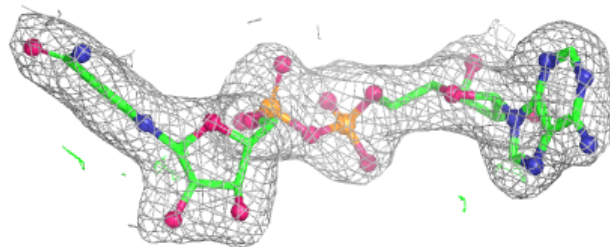
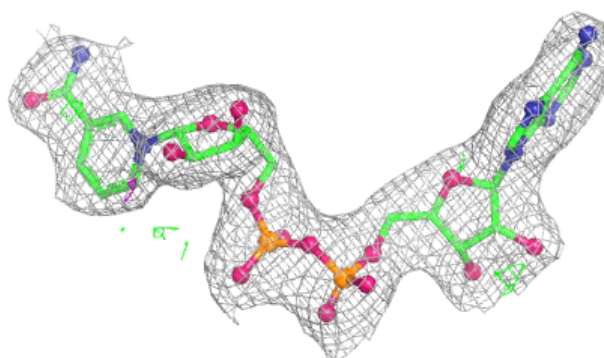


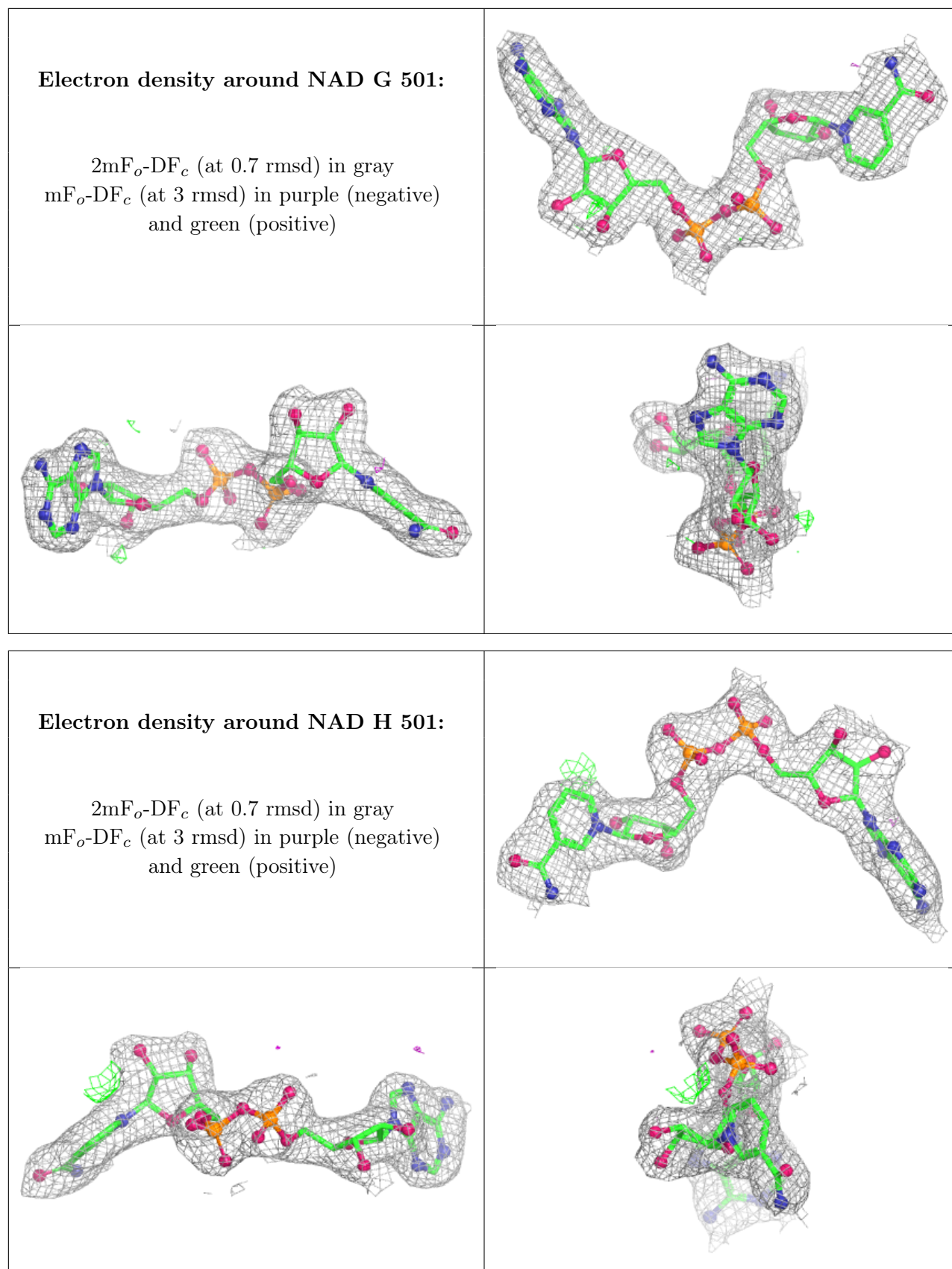
**Electron density around NAD E 501:**

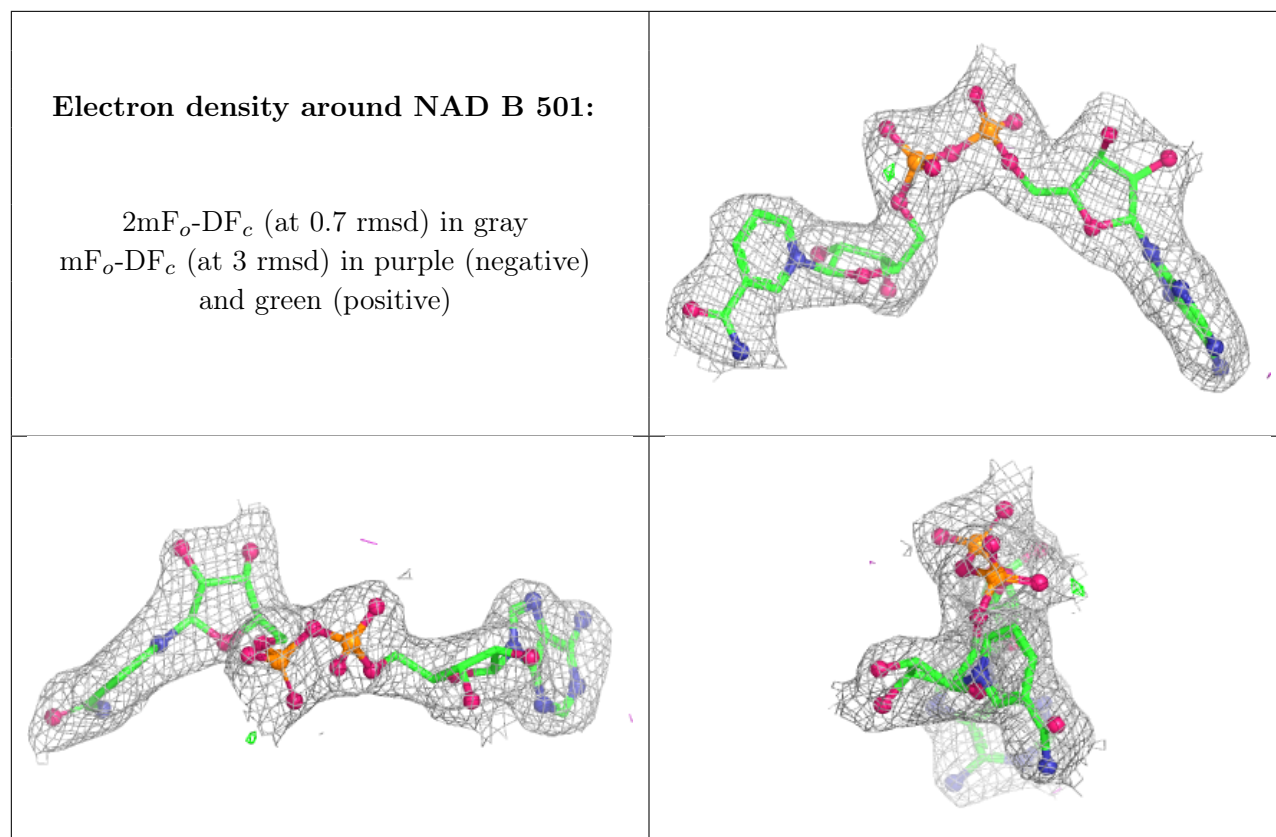
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around NAD F 501:**

$2mF_o-DF_c$  (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.