



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 05:32 PM UTC

PDB ID : 8CFZ / pdb_00008cfz
Title : Crystal structure of S-adenosyl-L-homocysteine hydrolase from *P. aeruginosa* in complex with F2X-Entry library fragment H09
Authors : Malecki, P.H.; Gawel, M.; Stepniewska, M.; Brzezinski, K.
Deposited on : 2023-02-03
Resolution : 1.77 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

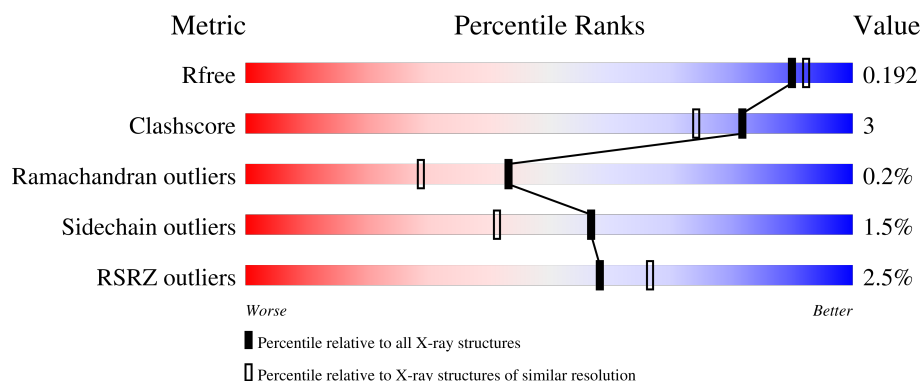
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	472	2% 91% 7%
1	B	472	91% 6%
1	C	472	3% 90% 7%
1	D	472	% 91% 6%
1	H	472	8% 92% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	472	% 92% 5% •
1	J	472	5% 90% 7% ••
1	K	472	91% 7% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	K	504	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 33061 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
1	A	464	Total	C	N	O	S	0	10	0
			3638	2294	629	692	23			
1	B	461	Total	C	N	O	S	0	7	0
			3598	2269	623	683	23			
1	C	461	Total	C	N	O	S	0	8	0
			3606	2273	625	685	23			
1	D	461	Total	C	N	O	S	0	9	0
			3610	2276	625	686	23			
1	H	461	Total	C	N	O	S	0	9	0
			3613	2277	625	688	23			
1	I	461	Total	C	N	O	S	0	9	0
			3608	2276	623	686	23			
1	J	461	Total	C	N	O	S	0	7	0
			3601	2271	624	683	23			
1	K	461	Total	C	N	O	S	0	10	0
			3616	2280	625	688	23			

There are 24 discrepancies between the modelled and reference sequences:

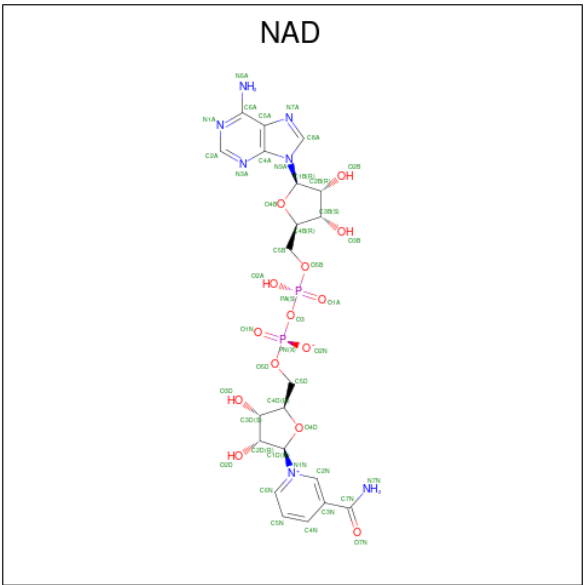
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9I685
A	-1	ASN	-	expression tag	UNP Q9I685
A	0	ALA	-	expression tag	UNP Q9I685
B	-2	SER	-	expression tag	UNP Q9I685
B	-1	ASN	-	expression tag	UNP Q9I685
B	0	ALA	-	expression tag	UNP Q9I685
C	-2	SER	-	expression tag	UNP Q9I685
C	-1	ASN	-	expression tag	UNP Q9I685
C	0	ALA	-	expression tag	UNP Q9I685
D	-2	SER	-	expression tag	UNP Q9I685
D	-1	ASN	-	expression tag	UNP Q9I685
D	0	ALA	-	expression tag	UNP Q9I685
H	-2	SER	-	expression tag	UNP Q9I685

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	ASN	-	expression tag	UNP Q9I685
H	0	ALA	-	expression tag	UNP Q9I685
I	-2	SER	-	expression tag	UNP Q9I685
I	-1	ASN	-	expression tag	UNP Q9I685
I	0	ALA	-	expression tag	UNP Q9I685
J	-2	SER	-	expression tag	UNP Q9I685
J	-1	ASN	-	expression tag	UNP Q9I685
J	0	ALA	-	expression tag	UNP Q9I685
K	-2	SER	-	expression tag	UNP Q9I685
K	-1	ASN	-	expression tag	UNP Q9I685
K	0	ALA	-	expression tag	UNP Q9I685

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



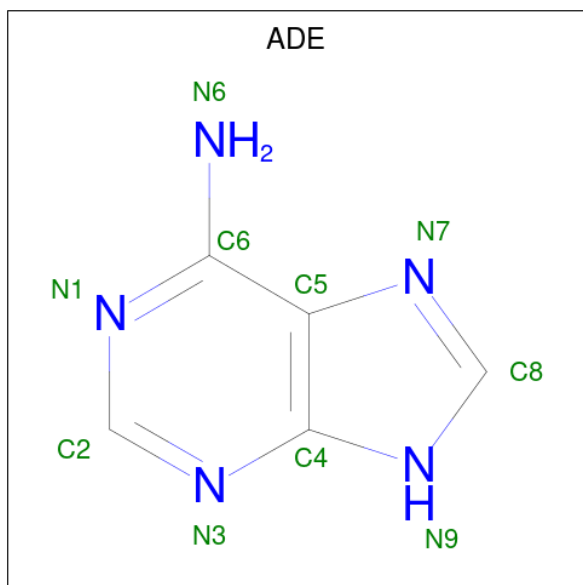
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

Continued on next page...

Continued from previous page...

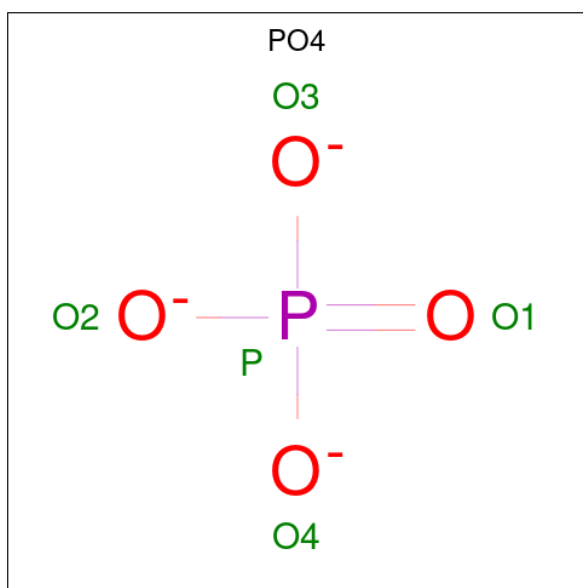
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	I	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	J	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	K	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is ADENINE (CCD ID: ADE) (formula: $C_5H_5N_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			10	5	5		
3	B	1	Total	C	N	0	0
			10	5	5		
3	C	1	Total	C	N	0	0
			10	5	5		
3	D	1	Total	C	N	0	0
			10	5	5		
3	H	1	Total	C	N	0	0
			10	5	5		
3	I	1	Total	C	N	0	0
			10	5	5		
3	J	1	Total	C	N	0	0
			10	5	5		
3	K	1	Total	C	N	0	0
			10	5	5		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	H	1	Total	O	P	0	0
			5	4	1		
4	H	1	Total	O	P	0	0
			5	4	1		
4	H	1	Total	O	P	0	0
			5	4	1		
4	H	1	Total	O	P	0	0
			5	4	1		
4	I	1	Total	O	P	0	0
			5	4	1		
4	I	1	Total	O	P	0	0
			5	4	1		
4	I	1	Total	O	P	0	0
			5	4	1		
4	J	1	Total	O	P	0	0
			5	4	1		
4	J	1	Total	O	P	0	0
			5	4	1		
4	J	1	Total	O	P	0	0
			5	4	1		
4	J	1	Total	O	P	0	0
			5	4	1		
4	K	1	Total	O	P	0	0
			5	4	1		
4	K	1	Total	O	P	0	0
			5	4	1		
4	K	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

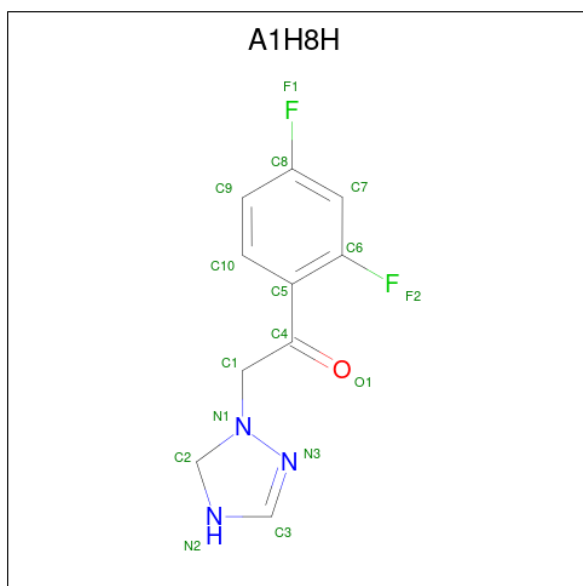
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	K	0	0
			1	1		
5	B	1	Total	K	0	0
			1	1		

Continued on next page...

Continued from previous page...

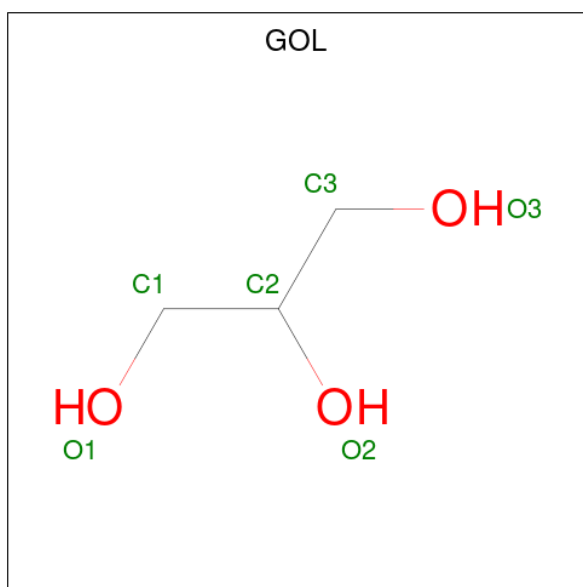
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total K 1 1	0	0
5	D	1	Total K 1 1	0	0
5	H	1	Total K 1 1	0	0
5	I	1	Total K 1 1	0	0
5	J	1	Total K 1 1	0	0
5	K	1	Total K 1 1	0	0

- Molecule 6 is 1-[2,4-bis(fluoranyl)phenyl]-2-(3,4-dihydro-1,2,4-triazol-2-yl)ethanone (CCD ID: A1H8H) (formula: C₁₀H₉F₂N₃O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C F N O 32 20 4 6 2	0	1
6	D	1	Total C F N O 32 20 4 6 2	0	1
6	I	1	Total C F N O 32 20 4 6 2	0	1
6	K	1	Total C F N O 32 20 4 6 2	0	1

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	J	1	Total	C	O	0	0
			6	3	3		
7	J	1	Total	C	O	0	0
			6	3	3		
7	J	1	Total	C	O	0	0
			6	3	3		
7	J	1	Total	C	O	0	0
			6	3	3		

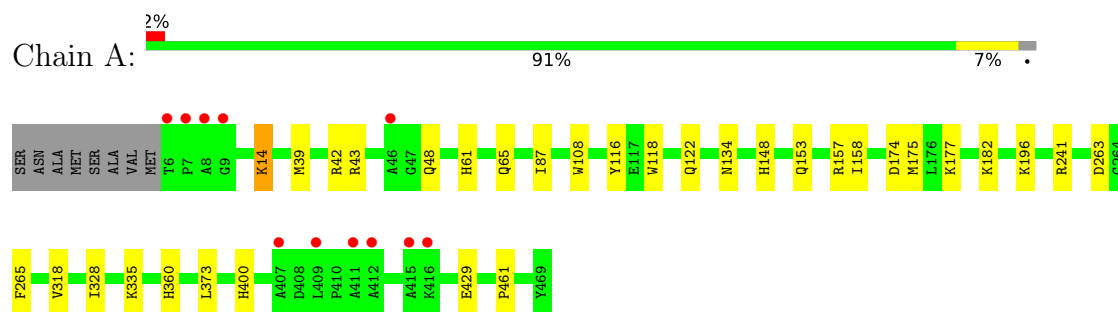
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	407	Total	O	0	16
			422	422		
8	B	456	Total	O	0	18
			474	474		
8	C	379	Total	O	0	15
			393	393		
8	D	444	Total	O	0	14
			459	459		
8	H	331	Total	O	0	18
			347	347		
8	I	437	Total	O	0	21
			456	456		
8	J	406	Total	O	0	21
			425	425		
8	K	438	Total	O	0	16
			453	453		

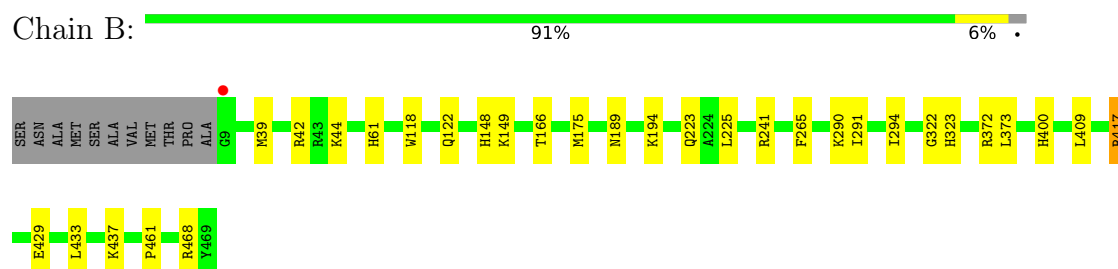
3 Residue-property plots [i](#)

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.

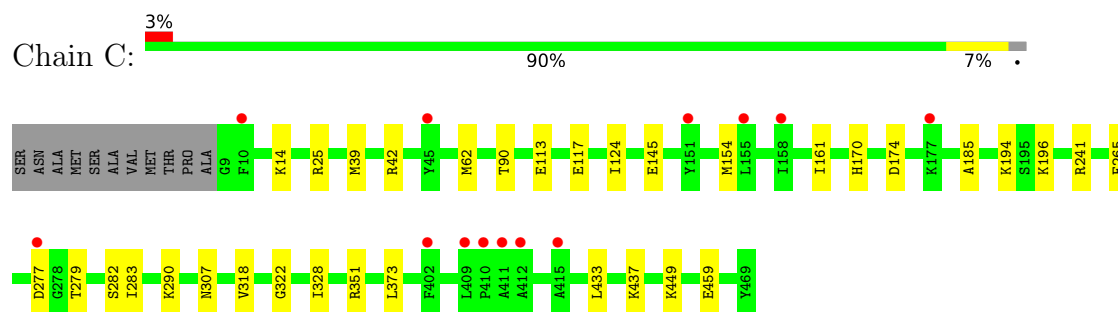
• Molecule 1: Adenosylhomocysteinase



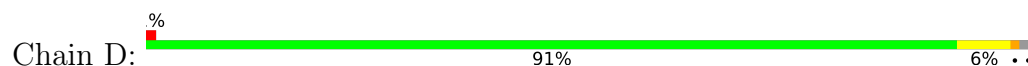
• Molecule 1: Adenosylhomocysteinase

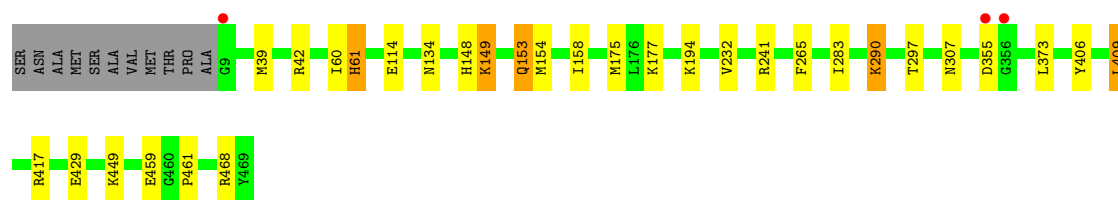


• Molecule 1: Adenosylhomocysteinase

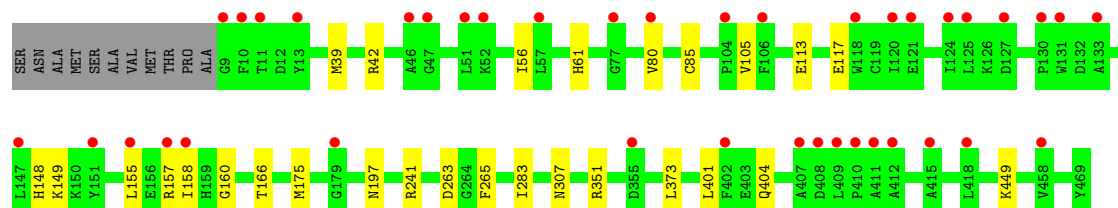


• Molecule 1: Adenosylhomocysteinase

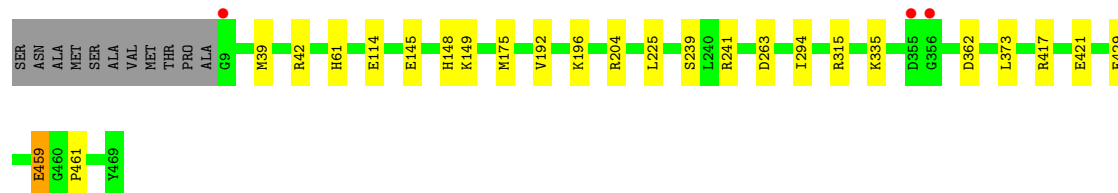
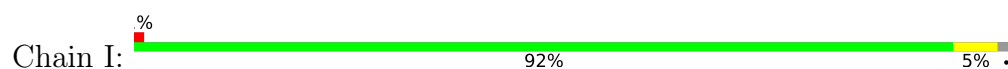




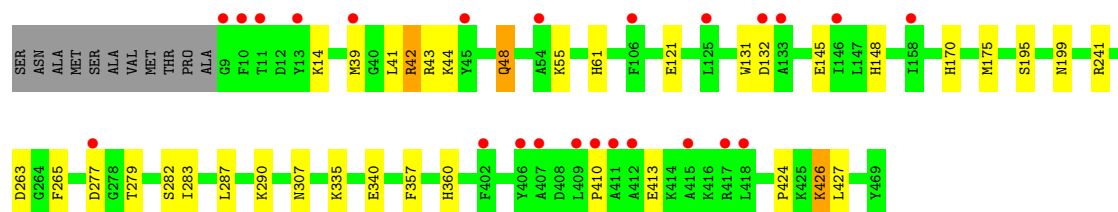
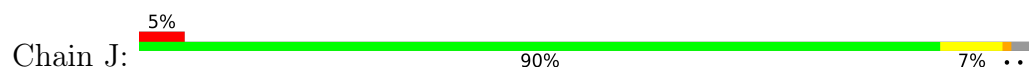
• Molecule 1: Adenosylhomocysteinase



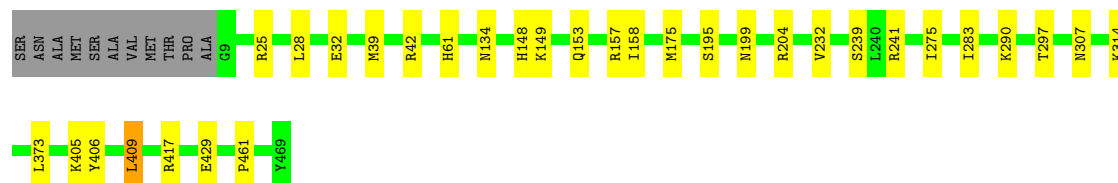
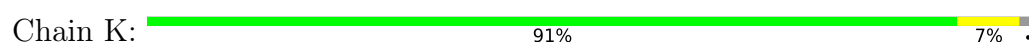
• Molecule 1: Adenosylhomocysteinase



• 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, α , β , γ	111.07Å 210.80Å 111.50Å 90.00° 105.83° 90.00°	Depositor
Resolution (Å)	43.42 – 1.77 43.42 – 1.77	Depositor EDS
% Data completeness (in resolution range)	98.2 (43.42-1.77) 98.4 (43.42-1.77)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 1.77Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.170 , 0.192 0.170 , 0.192	Depositor DCC
R_{free} test set	1082 reflections (0.23%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.105 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33061	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1H8H, GOL, ADE, NAD, K, 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	0.85	0/3717	0.79	0/5025
1	B	0.89	0/3673	0.78	1/4964 (0.0%)
1	C	0.80	0/3681	0.77	0/4975
1	D	0.87	0/3688	0.77	0/4985
1	H	0.76	0/3688	0.73	0/4985
1	I	0.84	0/3689	0.77	0/4986
1	J	0.83	0/3673	0.78	0/4963
1	K	0.85	0/3697	0.80	0/4997
All	All	0.84	0/29506	0.77	1/39880 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	372	ARG	CA-CB-CG	-5.25	103.60	114.10

There are no chirality outliers.

There are no planarity outliers.

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	3638	0	3656	21	0
1	B	3598	0	3615	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3606	0	3620	22	0
1	D	3610	0	3627	17	0
1	H	3613	0	3624	14	0
1	I	3608	0	3628	15	0
1	J	3601	0	3619	24	0
1	K	3616	0	3633	17	0
2	A	44	0	26	0	0
2	B	44	0	26	1	0
2	C	44	0	26	1	0
2	D	44	0	26	0	0
2	H	44	0	26	0	0
2	I	44	0	26	1	0
2	J	44	0	26	0	0
2	K	44	0	26	0	0
3	A	10	0	4	0	0
3	B	10	0	4	0	0
3	C	10	0	4	0	0
3	D	10	0	4	0	0
3	H	10	0	4	0	0
3	I	10	0	4	0	0
3	J	10	0	4	0	0
3	K	10	0	4	0	0
4	A	20	0	0	0	0
4	B	20	0	0	1	0
4	C	20	0	0	2	0
4	D	20	0	0	0	0
4	H	20	0	0	1	0
4	I	15	0	0	0	0
4	J	20	0	0	0	0
4	K	15	0	0	5	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
6	C	32	0	0	0	0
6	D	32	0	0	0	0
6	I	32	0	0	0	0
6	K	32	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	J	24	0	32	1	0
8	A	422	0	0	7	0
8	B	474	0	0	5	0
8	C	393	0	0	4	0
8	D	459	0	0	2	0
8	H	347	0	0	3	0
8	I	456	0	0	3	0
8	J	425	0	0	3	0
8	K	453	0	0	3	0
All	All	33061	0	29294	149	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 3.

All (149) 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:J:360:HIS:HE2	4:K:504:PO4:P	2.12	0.72
1:J:241[B]:ARG:HD2	8:J:829:HOH:O	1.92	0.68
1:D:406:TYR:HA	1:D:409:LEU:HD22	1.77	0.67
1:A:241[B]:ARG:HD2	8:A:847:HOH:O	1.96	0.65
1:A:182:LYS:NZ	8:A:601:HOH:O	2.30	0.64
1:K:241[B]:ARG:HD2	8:K:854:HOH:O	1.98	0.64
1:I:241[B]:ARG:HD2	8:I:855:HOH:O	1.97	0.64
1:C:459:GLU:OE2	1:J:43:ARG:NH1	2.31	0.64
1:D:241[B]:ARG:HD2	8:D:870:HOH:O	1.99	0.63
1:J:41:LEU:HG	7:J:504:GOL:H11	1.78	0.63
1:K:39[A]:MET:HE1	1:K:42:ARG:CZ	2.30	0.62
1:J:277:ASP:HB2	1:J:282:SER:HB3	1.82	0.61
1:B:241[B]:ARG:HD2	8:B:914:HOH:O	2.00	0.61
1:K:148:HIS:CG	1:K:175:MET:HE1	2.35	0.61
1:K:149:LYS:NZ	8:K:602:HOH:O	2.33	0.61
1:C:241[B]:ARG:HD2	8:C:746:HOH:O	1.98	0.61
1:K:148:HIS:CD2	1:K:175:MET:HE1	2.36	0.60
1:I:148:HIS:CG	1:I:175:MET:HE1	2.36	0.60
1:J:241[B]:ARG:NH2	1:J:263:ASP:O	2.31	0.60
1:J:360:HIS:NE2	4:K:504:PO4:O4	2.32	0.60
1:C:277:ASP:HB2	1:C:282:SER:HB3	1.82	0.60
1:D:283:ILE:HG13	1:D:307:ASN:HB3	1.85	0.59
1:C:433:LEU:HG	1:C:437:LYS:HE3	1.84	0.59
1:J:410:PRO:HG2	1:J:413:GLU:HG2	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:HIS:HA	1:B:373:LEU:HD21	1.85	0.59
1:B:223[B]:GLN:OE1	1:B:290:LYS:HE2	2.03	0.58
1:I:148:HIS:CD2	1:I:175:MET:HE1	2.38	0.58
1:A:400:HIS:HE1	8:A:876:HOH:O	1.87	0.57
1:B:417:ARG:NE	8:B:601:HOH:O	2.37	0.57
1:D:153:GLN:H	1:D:153:GLN:CD	2.12	0.56
1:H:113:GLU:O	1:H:117:GLU:HG2	2.05	0.56
1:I:225:LEU:HB3	1:I:294[B]:ILE:HG12	1.88	0.55
1:D:148:HIS:CG	1:D:175:MET:HE1	2.42	0.55
1:C:241[B]:ARG:HD3	1:C:265:PHE:CE1	2.42	0.54
8:I:908:HOH:O	1:J:170:HIS:HE1	1.89	0.54
1:J:426:LYS:HE3	8:J:618:HOH:O	2.08	0.53
1:C:373:LEU:HD22	2:C:502:NAD:N7N	2.23	0.53
1:A:39[A]:MET:HE1	1:A:42:ARG:CZ	2.37	0.53
1:D:149:LYS:NZ	8:D:604:HOH:O	2.41	0.53
1:B:148:HIS:CG	1:B:175:MET:HE1	2.44	0.53
1:I:39[A]:MET:HE1	1:I:42:ARG:CZ	2.39	0.53
1:B:39[A]:MET:HE1	1:B:42:ARG:CZ	2.39	0.53
1:H:373:LEU:HD12	8:H:785:HOH:O	2.09	0.53
1:H:404:GLN:NE2	8:H:603:HOH:O	2.42	0.52
1:B:44:LYS:NZ	8:B:602:HOH:O	2.42	0.52
1:H:39[A]:MET:HE1	1:H:42:ARG:CZ	2.39	0.52
1:A:14:LYS:HG2	1:A:108:TRP:CZ3	2.44	0.52
1:I:373:LEU:HD22	2:I:501:NAD:N7N	2.24	0.52
1:C:25:ARG:NH1	4:C:504:PO4:O2	2.41	0.52
1:A:196:LYS:HE3	1:D:468:ARG:HB2	1.90	0.51
1:K:283:ILE:HG13	1:K:307:ASN:HB3	1.93	0.51
1:K:157:ARG:NH1	8:K:604:HOH:O	2.39	0.50
1:C:39[A]:MET:HE1	1:C:42:ARG:CZ	2.41	0.50
1:D:39[A]:MET:HE1	1:D:42:ARG:CZ	2.42	0.50
1:A:429:GLU:OE1	1:A:461:PRO:HA	2.12	0.50
1:B:433:LEU:HG	1:B:437:LYS:HE2	1.93	0.50
1:A:43:ARG:NH2	8:A:607:HOH:O	2.46	0.49
1:C:283:ILE:HG13	1:C:307:ASN:HB3	1.94	0.49
1:H:241[B]:ARG:HD2	8:H:841:HOH:O	2.11	0.49
1:J:39[A]:MET:HE1	1:J:42:ARG:CZ	2.43	0.49
1:A:318:VAL:HG12	1:A:328:ILE:HD13	1.95	0.49
1:A:48:GLN:NE2	8:A:605:HOH:O	2.43	0.49
1:I:241[B]:ARG:NH1	1:I:263:ASP:O	2.36	0.48
1:C:113:GLU:O	1:C:117:GLU:HG2	2.13	0.48
1:I:149:LYS:NZ	8:I:605:HOH:O	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:340:GLU:HB2	1:J:357:PHE:CZ	2.48	0.48
1:K:406:TYR:HA	1:K:409:LEU:HD22	1.96	0.48
1:B:400:HIS:HE1	8:B:925:HOH:O	1.94	0.48
1:H:241[B]:ARG:NH1	1:H:263:ASP:O	2.38	0.48
1:I:204:ARG:HA	1:I:239:SER:HB2	1.96	0.47
1:B:468:ARG:HB2	1:C:196:LYS:HE3	1.96	0.47
1:C:277:ASP:HB3	1:C:279:THR:H	1.78	0.47
1:J:277:ASP:HB3	1:J:279:THR:H	1.78	0.47
1:A:241[B]:ARG:HD3	1:A:265:PHE:CE1	2.49	0.47
1:H:56:ILE:HB	1:H:80:VAL:HG12	1.96	0.46
1:B:118:TRP:O	1:B:122:GLN:HG2	2.16	0.46
1:A:148:HIS:CD2	1:A:175:MET:HE1	2.50	0.46
1:H:283:ILE:HG13	1:H:307:ASN:HB3	1.98	0.46
1:J:55:LYS:HB3	1:J:131:TRP:CH2	2.50	0.46
1:H:241[B]:ARG:HD3	1:H:265:PHE:CE1	2.51	0.46
1:A:360:HIS:HE2	4:B:503:PO4:P	2.39	0.46
1:J:287:LEU:O	1:J:290:LYS:HG2	2.16	0.46
1:B:225:LEU:HB3	1:B:294[B]:ILE:HG12	1.97	0.46
1:A:241[B]:ARG:NH1	1:A:263:ASP:O	2.48	0.45
1:D:114:GLU:H	1:D:114:GLU:CD	2.24	0.45
1:K:232:VAL:HG12	1:K:297:THR:HB	1.97	0.45
1:K:28:LEU:O	1:K:32:GLU:HG3	2.16	0.45
1:K:429:GLU:OE1	1:K:461:PRO:HA	2.16	0.45
1:H:61:HIS:CE1	1:H:85:CYS:SG	3.10	0.44
1:B:194:LYS:C	1:B:194:LYS:HD3	2.42	0.44
1:D:134:ASN:HA	1:D:158[A]:ILE:HD13	1.99	0.44
1:H:155:LEU:HD23	1:H:158[B]:ILE:HD12	2.00	0.44
1:H:351:ARG:NH2	4:H:504:PO4:O1	2.50	0.44
1:K:204:ARG:HA	1:K:239:SER:HB2	1.98	0.44
1:D:290:LYS:HB2	1:D:290:LYS:HE3	1.66	0.44
1:J:148:HIS:CD2	1:J:175:MET:HE1	2.53	0.44
1:J:426:LYS:HA	1:J:426:LYS:HD2	1.78	0.44
1:H:148:HIS:CE1	1:H:175:MET:HE1	2.52	0.44
1:D:241[B]:ARG:HD3	1:D:265:PHE:CE1	2.53	0.43
1:B:322:GLY:O	1:B:373:LEU:HD23	2.17	0.43
1:J:48:GLN:OE1	1:J:48:GLN:N	2.52	0.43
1:C:449:LYS:HD3	8:C:743:HOH:O	2.18	0.43
1:C:351:ARG:NH2	4:C:505:PO4:O3	2.52	0.43
1:C:318:VAL:HG12	1:C:328:ILE:HD13	2.01	0.42
1:K:314:LYS:HG3	4:K:505:PO4:O4	2.19	0.42
1:C:290:LYS:HB3	1:C:290:LYS:HE3	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:145:GLU:OE2	1:I:149:LYS:NZ	2.38	0.42
1:A:134:ASN:HA	1:A:158[A]:ILE:HD13	2.02	0.42
1:C:322:GLY:O	1:C:373:LEU:HD23	2.19	0.42
1:D:194:LYS:HD3	1:D:194:LYS:C	2.44	0.42
1:J:424:PRO:HD2	1:J:427:LEU:HD12	2.01	0.42
1:A:373:LEU:HD12	8:A:826:HOH:O	2.18	0.42
1:B:189:ASN:HA	1:B:194:LYS:HD2	2.01	0.42
1:K:195:SER:O	1:K:199:ASN:HB2	2.20	0.42
1:C:170:HIS:CE1	8:C:855:HOH:O	2.73	0.42
1:J:241[B]:ARG:HD3	1:J:265:PHE:CE1	2.55	0.42
1:D:232:VAL:HG12	1:D:297:THR:HB	2.01	0.42
1:I:114:GLU:H	1:I:114:GLU:CD	2.27	0.42
1:I:459[B]:GLU:H	1:I:459[B]:GLU:HG3	1.64	0.42
1:J:360:HIS:NE2	4:K:504:PO4:O2	2.53	0.42
1:B:373:LEU:HD22	2:B:501:NAD:N7N	2.35	0.42
1:H:160:GLY:HA3	1:H:401:LEU:HD13	2.01	0.42
1:K:405:LYS:O	1:K:409:LEU:HD13	2.20	0.42
1:A:65:GLN:CD	1:A:65:GLN:H	2.27	0.41
1:I:315:ARG:NH1	1:I:362:ASP:HB2	2.35	0.41
1:C:124:ILE:HG23	1:C:154:MET:SD	2.61	0.41
1:K:25:ARG:NH1	4:K:504:PO4:O3	2.48	0.41
1:C:170:HIS:HE1	8:C:855:HOH:O	2.02	0.41
1:B:291:ILE:HG21	1:B:294[B]:ILE:HG13	2.01	0.41
1:A:87:ILE:HG22	1:A:116:TYR:HB2	2.02	0.41
1:C:161:ILE:O	1:C:185:ALA:HA	2.20	0.41
1:I:192:VAL:HG13	1:I:196:LYS:HG3	2.03	0.41
1:A:118:TRP:O	1:A:122:GLN:HG2	2.21	0.41
1:A:153:GLN:O	1:A:157:ARG:NH1	2.54	0.41
1:B:241[B]:ARG:HD3	1:B:265:PHE:CE1	2.55	0.41
1:D:60:ILE:O	1:D:61:HIS:C	2.63	0.41
1:B:149:LYS:HE2	8:B:881:HOH:O	2.20	0.41
1:B:429:GLU:OE1	1:B:461:PRO:HA	2.21	0.41
1:D:154:MET:O	1:D:158[A]:ILE:HG12	2.21	0.41
1:I:429:GLU:OE1	1:I:461:PRO:HA	2.21	0.41
1:J:195:SER:O	1:J:199:ASN:HB2	2.21	0.40
1:A:335:LYS:HD2	8:A:801:HOH:O	2.21	0.40
1:K:134:ASN:HA	1:K:158[A]:ILE:HD13	2.04	0.40
1:B:223[B]:GLN:CD	1:B:290:LYS:HE2	2.46	0.40
1:B:409:LEU:HA	1:B:409:LEU:HD23	1.81	0.40
1:C:62:MET:HB3	1:C:90:THR:HG23	2.03	0.40
1:D:429:GLU:OE1	1:D:461:PRO:HA	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:426:LYS:NZ	8:J:614:HOH:O	2.54	0.40
1:J:283:ILE:HG13	1:J:307:ASN:HB3	2.03	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	472/472 (100%)	461 (98%)	10 (2%)	1 (0%)	43	29
1	B	466/472 (99%)	455 (98%)	10 (2%)	1 (0%)	43	29
1	C	467/472 (99%)	458 (98%)	9 (2%)	0	100	100
1	D	468/472 (99%)	457 (98%)	10 (2%)	1 (0%)	43	29
1	H	468/472 (99%)	456 (97%)	12 (3%)	0	100	100
1	I	468/472 (99%)	457 (98%)	10 (2%)	1 (0%)	43	29
1	J	466/472 (99%)	455 (98%)	10 (2%)	1 (0%)	43	29
1	K	469/472 (99%)	459 (98%)	9 (2%)	1 (0%)	43	29
All	All	3744/3776 (99%)	3658 (98%)	80 (2%)	6 (0%)	43	29

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	61	HIS
1	A	61	HIS
1	B	61	HIS
1	D	61	HIS
1	I	61	HIS
1	J	61	HIS

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	389/385 (101%)	386 (99%)	3 (1%)	73	63
1	B	384/385 (100%)	382 (100%)	2 (0%)	81	73
1	C	385/385 (100%)	381 (99%)	4 (1%)	68	55
1	D	386/385 (100%)	376 (97%)	10 (3%)	40	20
1	H	386/385 (100%)	379 (98%)	7 (2%)	51	33
1	I	386/385 (100%)	381 (99%)	5 (1%)	61	46
1	J	384/385 (100%)	375 (98%)	9 (2%)	44	25
1	K	387/385 (100%)	381 (98%)	6 (2%)	55	38
All	All	3087/3080 (100%)	3041 (98%)	46 (2%)	57	41

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	174	ASP
1	A	177	LYS
1	B	166	THR
1	B	417	ARG
1	C	14	LYS
1	C	145	GLU
1	C	174	ASP
1	C	194	LYS
1	D	149	LYS
1	D	153	GLN
1	D	177	LYS
1	D	290	LYS
1	D	355	ASP
1	D	373	LEU
1	D	409	LEU
1	D	417	ARG
1	D	449	LYS
1	D	459	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	105	VAL
1	H	149	LYS
1	H	157	ARG
1	H	166[A]	THR
1	H	166[B]	THR
1	H	197	ASN
1	H	449	LYS
1	I	335	LYS
1	I	417	ARG
1	I	421	GLU
1	I	459[A]	GLU
1	I	459[B]	GLU
1	J	14	LYS
1	J	42	ARG
1	J	44	LYS
1	J	48	GLN
1	J	121	GLU
1	J	132	ASP
1	J	145	GLU
1	J	335	LYS
1	J	426	LYS
1	K	153	GLN
1	K	275	ILE
1	K	290	LYS
1	K	373	LEU
1	K	409	LEU
1	K	417	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	129	GLN
1	B	197	ASN
1	B	345	GLN
1	B	400	HIS
1	C	170	HIS
1	D	129	GLN
1	H	336	ASN
1	H	345	GLN
1	H	400	HIS
1	I	170	HIS
1	J	170	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	170	HIS
1	K	404	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 66 ligands modelled in this entry, 8 are monoatomic - leaving 58 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
2	NAD	I	501	-	46,48,48	0.70	2 (4%)	64,73,73	0.70	2 (3%)
4	PO4	I	504	-	4,4,4	1.08	0	6,6,6	1.18	0
4	PO4	K	505	-	4,4,4	1.12	0	6,6,6	1.47	2 (33%)
7	GOL	J	504	-	5,5,5	0.78	0	5,5,5	1.18	0
4	PO4	I	503	-	4,4,4	0.89	0	6,6,6	1.48	1 (16%)
4	PO4	B	504	-	4,4,4	1.39	1 (25%)	6,6,6	1.77	2 (33%)
4	PO4	C	504	-	4,4,4	1.05	0	6,6,6	1.21	1 (16%)
3	ADE	J	502	-	11,11,11	1.31	2 (18%)	15,15,15	0.45	0
4	PO4	I	505	-	4,4,4	0.85	0	6,6,6	0.97	0
2	NAD	B	501	-	46,48,48	0.71	1 (2%)	64,73,73	0.68	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	A1H8H	D	508[B]	-	17,17,17	0.88	1 (5%)	20,23,23	1.57	2 (10%)
6	A1H8H	K	501[A]	-	17,17,17	0.89	1 (5%)	20,23,23	1.62	2 (10%)
3	ADE	H	502	-	11,11,11	1.07	1 (9%)	15,15,15	0.53	0
2	NAD	C	502	-	46,48,48	0.80	2 (4%)	64,73,73	0.74	1 (1%)
4	PO4	H	505	-	4,4,4	1.06	0	6,6,6	1.17	1 (16%)
3	ADE	A	502	-	11,11,11	1.55	1 (9%)	15,15,15	0.58	0
3	ADE	K	503	-	11,11,11	1.16	1 (9%)	15,15,15	0.64	0
4	PO4	C	506	-	4,4,4	1.39	0	6,6,6	0.89	0
6	A1H8H	I	507[B]	-	17,17,17	0.91	1 (5%)	20,23,23	1.65	3 (15%)
4	PO4	J	507	-	4,4,4	1.17	0	6,6,6	0.72	0
4	PO4	C	505	-	4,4,4	1.40	1 (25%)	6,6,6	1.34	1 (16%)
4	PO4	A	504	-	4,4,4	1.61	1 (25%)	6,6,6	1.10	0
7	GOL	J	506	-	5,5,5	0.67	0	5,5,5	0.92	0
4	PO4	B	506	-	4,4,4	0.90	0	6,6,6	1.03	0
4	PO4	D	504	-	4,4,4	0.42	0	6,6,6	2.26	3 (50%)
4	PO4	A	503	-	4,4,4	0.78	0	6,6,6	1.60	2 (33%)
6	A1H8H	C	501[A]	-	17,17,17	0.92	1 (5%)	20,23,23	1.63	2 (10%)
4	PO4	D	503	-	4,4,4	0.82	0	6,6,6	1.26	0
6	A1H8H	K	501[B]	-	17,17,17	0.92	1 (5%)	20,23,23	1.54	2 (10%)
4	PO4	D	505	-	4,4,4	1.23	1 (25%)	6,6,6	0.78	0
3	ADE	I	502	-	11,11,11	1.29	1 (9%)	15,15,15	0.60	0
4	PO4	J	508	-	4,4,4	1.35	1 (25%)	6,6,6	1.30	1 (16%)
4	PO4	H	504	-	4,4,4	0.76	0	6,6,6	1.27	0
2	NAD	A	501	-	46,48,48	0.84	2 (4%)	64,73,73	0.76	0
4	PO4	C	507	-	4,4,4	1.22	0	6,6,6	1.42	1 (16%)
2	NAD	H	501	-	46,48,48	0.64	1 (2%)	64,73,73	0.77	1 (1%)
4	PO4	J	510	-	4,4,4	1.00	0	6,6,6	1.10	0
4	PO4	A	506	-	4,4,4	0.87	0	6,6,6	1.08	1 (16%)
4	PO4	H	506	-	4,4,4	0.84	0	6,6,6	0.91	0
2	NAD	D	501	-	46,48,48	0.64	1 (2%)	64,73,73	0.61	0
4	PO4	J	509	-	4,4,4	0.58	0	6,6,6	1.66	1 (16%)
4	PO4	B	503	-	4,4,4	1.65	2 (50%)	6,6,6	1.23	1 (16%)
4	PO4	A	505	-	4,4,4	1.64	2 (50%)	6,6,6	1.04	0
4	PO4	K	504	-	4,4,4	1.47	1 (25%)	6,6,6	1.19	0
4	PO4	H	503	-	4,4,4	0.47	0	6,6,6	1.42	1 (16%)
6	A1H8H	C	501[B]	-	17,17,17	0.91	1 (5%)	20,23,23	1.59	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADE	C	503	-	11,11,11	1.44	2 (18%)	15,15,15	0.58	0
6	A1H8H	I	507[A]	-	17,17,17	0.96	1 (5%)	20,23,23	1.60	2 (10%)
2	NAD	K	502	-	46,48,48	0.57	0	64,73,73	0.76	2 (3%)
4	PO4	D	506	-	4,4,4	0.78	0	6,6,6	0.82	0
7	GOL	J	503	-	5,5,5	0.83	0	5,5,5	1.02	0
7	GOL	J	505	-	5,5,5	1.12	0	5,5,5	1.77	1 (20%)
3	ADE	B	502	-	11,11,11	1.47	1 (9%)	15,15,15	0.46	0
6	A1H8H	D	508[A]	-	17,17,17	0.89	1 (5%)	20,23,23	1.58	2 (10%)
4	PO4	B	505	-	4,4,4	1.36	1 (25%)	6,6,6	0.99	1 (16%)
3	ADE	D	502	-	11,11,11	0.95	1 (9%)	15,15,15	0.51	0
2	NAD	J	501	-	46,48,48	0.74	1 (2%)	64,73,73	0.80	3 (4%)
4	PO4	K	506	-	4,4,4	1.26	0	6,6,6	1.34	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	I	501	-	-	5/30/62/62	0/5/5/5
7	GOL	J	504	-	-	3/4/4/4	-
6	A1H8H	D	508[B]	-	-	0/7/15/15	0/2/2/2
3	ADE	J	502	-	-	-	0/2/2/2
2	NAD	B	501	-	-	4/30/62/62	0/5/5/5
6	A1H8H	K	501[A]	-	-	4/7/15/15	0/2/2/2
3	ADE	H	502	-	-	-	0/2/2/2
2	NAD	C	502	-	-	4/30/62/62	0/5/5/5
6	A1H8H	I	507[B]	-	-	6/7/15/15	0/2/2/2
3	ADE	A	502	-	-	-	0/2/2/2
3	ADE	K	503	-	-	-	0/2/2/2
7	GOL	J	506	-	-	2/4/4/4	-
6	A1H8H	C	501[A]	-	-	3/7/15/15	0/2/2/2
6	A1H8H	K	501[B]	-	-	0/7/15/15	0/2/2/2
3	ADE	I	502	-	-	-	0/2/2/2
2	NAD	A	501	-	-	4/30/62/62	0/5/5/5
2	NAD	H	501	-	-	4/30/62/62	0/5/5/5
2	NAD	D	501	-	-	4/30/62/62	0/5/5/5
6	A1H8H	C	501[B]	-	-	4/7/15/15	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADE	C	503	-	-	-	0/2/2/2
2	NAD	K	502	-	-	4/30/62/62	0/5/5/5
7	GOL	J	503	-	-	0/4/4/4	-
7	GOL	J	505	-	-	2/4/4/4	-
3	ADE	B	502	-	-	-	0/2/2/2
6	A1H8H	D	508[A]	-	-	0/7/15/15	0/2/2/2
3	ADE	D	502	-	-	-	0/2/2/2
2	NAD	J	501	-	-	4/30/62/62	0/5/5/5
6	A1H8H	I	507[A]	-	-	3/7/15/15	0/2/2/2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	ADE	C4-N9	3.43	1.41	1.36
6	I	507[A]	A1H8H	N1-N3	-3.43	1.36	1.41
6	K	501[B]	A1H8H	N1-N3	-3.31	1.36	1.41
6	C	501[A]	A1H8H	N1-N3	-3.29	1.36	1.41
6	I	507[B]	A1H8H	N1-N3	-3.24	1.36	1.41
6	C	501[B]	A1H8H	N1-N3	-3.19	1.36	1.41
6	K	501[A]	A1H8H	N1-N3	-3.16	1.36	1.41
6	D	508[B]	A1H8H	N1-N3	-3.09	1.36	1.41
3	B	502	ADE	C8-N9	3.05	1.42	1.35
6	D	508[A]	A1H8H	N1-N3	-3.02	1.36	1.41
4	A	504	PO4	P-O3	-2.77	1.46	1.54
4	K	504	PO4	P-O3	-2.60	1.47	1.54
2	H	501	NAD	PA-O3	2.58	1.62	1.59
3	I	502	ADE	C4-N9	2.54	1.40	1.36
2	C	502	NAD	PA-O3	2.51	1.62	1.59
2	C	502	NAD	PN-O3	2.45	1.62	1.59
4	B	504	PO4	P-O1	2.43	1.56	1.50
4	C	505	PO4	P-O3	-2.42	1.47	1.54
2	A	501	NAD	PN-O3	2.40	1.62	1.59
3	D	502	ADE	C8-N9	2.38	1.40	1.35
4	B	503	PO4	P-O2	-2.37	1.47	1.54
2	D	501	NAD	O7N-C7N	2.36	1.28	1.24
3	J	502	ADE	C8-N9	2.34	1.40	1.35
4	A	505	PO4	P-O2	-2.33	1.47	1.54
2	J	501	NAD	C7N-N7N	2.32	1.37	1.33
2	I	501	NAD	PA-O3	2.31	1.62	1.59
3	C	503	ADE	C4-N9	2.30	1.40	1.36
3	H	502	ADE	C8-N9	2.21	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	501	NAD	PN-O3	2.15	1.61	1.59
2	B	501	NAD	PN-O3	2.15	1.61	1.59
3	C	503	ADE	C8-N9	2.14	1.40	1.35
3	K	503	ADE	C8-N9	2.13	1.40	1.35
4	B	505	PO4	P-O2	-2.13	1.48	1.54
4	D	505	PO4	P-O4	-2.12	1.48	1.54
4	A	505	PO4	P-O1	2.11	1.55	1.50
3	J	502	ADE	C2-N3	2.10	1.37	1.33
4	J	508	PO4	P-O3	-2.07	1.48	1.54
2	A	501	NAD	PA-O3	2.04	1.61	1.59
4	B	503	PO4	P-O1	2.02	1.55	1.50

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	501[A]	A1H8H	C1-N1-C2	5.89	124.80	113.49
6	K	501[B]	A1H8H	C1-N1-C2	5.83	124.69	113.49
6	D	508[B]	A1H8H	C1-N1-C2	5.72	124.48	113.49
6	K	501[A]	A1H8H	C1-N1-C2	5.71	124.45	113.49
6	I	507[B]	A1H8H	C1-N1-C2	5.59	124.22	113.49
6	I	507[A]	A1H8H	C1-N1-C2	5.58	124.21	113.49
6	C	501[B]	A1H8H	C1-N1-C2	5.54	124.14	113.49
6	D	508[A]	A1H8H	C1-N1-C2	5.22	123.51	113.49
7	J	505	GOL	O3-C3-C2	-3.19	96.00	110.38
4	D	504	PO4	O4-P-O3	3.19	117.84	107.91
4	J	509	PO4	O2-P-O1	-3.01	100.32	110.95
4	B	504	PO4	O4-P-O2	-2.94	98.76	107.91
6	I	507[B]	A1H8H	N2-C2-N1	-2.87	96.46	103.53
6	K	501[A]	A1H8H	N2-C2-N1	-2.86	96.48	103.53
4	D	504	PO4	O2-P-O1	-2.79	101.09	110.95
2	J	501	NAD	O2A-PA-O1A	2.74	125.20	112.44
4	C	507	PO4	O4-P-O3	2.71	116.35	107.91
6	D	508[B]	A1H8H	N2-C2-N1	-2.71	96.85	103.53
6	K	501[B]	A1H8H	N2-C2-N1	-2.70	96.88	103.53
6	D	508[A]	A1H8H	N2-C2-N1	-2.68	96.92	103.53
6	C	501[B]	A1H8H	N2-C2-N1	-2.67	96.95	103.53
4	I	503	PO4	O2-P-O1	-2.65	101.60	110.95
4	K	505	PO4	O4-P-O2	-2.60	99.82	107.91
6	I	507[B]	A1H8H	C4-C1-N1	-2.60	108.97	112.00
6	C	501[A]	A1H8H	N2-C2-N1	-2.59	97.14	103.53
6	I	507[A]	A1H8H	N2-C2-N1	-2.59	97.15	103.53
4	D	504	PO4	O4-P-O1	-2.55	101.94	110.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	502	NAD	O3D-C3D-C4D	-2.50	103.90	111.08
4	B	504	PO4	O4-P-O3	2.47	115.58	107.91
4	H	503	PO4	O2-P-O1	-2.45	102.30	110.95
4	C	504	PO4	O4-P-O2	2.44	115.52	107.91
4	K	505	PO4	O4-P-O3	2.43	115.49	107.91
4	A	503	PO4	O2-P-O1	-2.34	102.66	110.95
4	A	503	PO4	O3-P-O2	2.31	115.11	107.91
2	K	502	NAD	O5B-C5B-C4B	-2.28	101.23	108.99
2	C	502	NAD	O2A-PA-O1A	2.26	122.96	112.44
2	H	501	NAD	O2A-PA-O1A	2.26	122.96	112.44
2	J	501	NAD	C2N-N1N-C1D	-2.26	114.16	119.13
4	B	503	PO4	O3-P-O2	2.21	114.80	107.91
4	J	508	PO4	O4-P-O1	-2.17	103.28	110.95
4	K	506	PO4	O3-P-O2	-2.08	101.45	107.91
2	I	501	NAD	O2N-PN-O1N	2.08	122.11	112.44
4	H	505	PO4	O4-P-O2	-2.07	101.47	107.91
2	J	501	NAD	O2N-PN-O3	2.06	112.85	107.27
4	B	505	PO4	O4-P-O3	2.06	114.31	107.91
4	C	505	PO4	O3-P-O2	2.05	114.28	107.91
2	B	501	NAD	O3D-C3D-C4D	-2.04	105.23	111.08
4	A	506	PO4	O4-P-O3	2.03	114.23	107.91
2	B	501	NAD	O2N-PN-O3	2.02	112.74	107.27
2	I	501	NAD	O3-PN-O1N	-2.00	104.68	110.70

There are no chirality outliers.

All (60) 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
2	B	501	NAD	C2D-C1D-N1N-C2N
2	B	501	NAD	C2D-C1D-N1N-C6N
2	C	502	NAD	O4D-C1D-N1N-C2N
2	C	502	NAD	O4D-C1D-N1N-C6N
2	C	502	NAD	C2D-C1D-N1N-C2N
2	C	502	NAD	C2D-C1D-N1N-C6N
2	D	501	NAD	O4D-C1D-N1N-C2N
2	D	501	NAD	O4D-C1D-N1N-C6N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	501	NAD	C2D-C1D-N1N-C2N
2	D	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
2	I	501	NAD	O4D-C1D-N1N-C2N
2	I	501	NAD	O4D-C1D-N1N-C6N
2	I	501	NAD	C2D-C1D-N1N-C2N
2	I	501	NAD	C2D-C1D-N1N-C6N
2	J	501	NAD	O4D-C1D-N1N-C2N
2	J	501	NAD	O4D-C1D-N1N-C6N
2	J	501	NAD	C2D-C1D-N1N-C2N
2	J	501	NAD	C2D-C1D-N1N-C6N
2	K	502	NAD	O4D-C1D-N1N-C2N
2	K	502	NAD	O4D-C1D-N1N-C6N
2	K	502	NAD	C2D-C1D-N1N-C2N
2	K	502	NAD	C2D-C1D-N1N-C6N
6	C	501[A]	A1H8H	C1-C4-C5-C10
6	C	501[A]	A1H8H	C1-C4-C5-C6
6	C	501[B]	A1H8H	C4-C1-N1-N3
6	I	507[A]	A1H8H	C1-C4-C5-C10
6	I	507[B]	A1H8H	O1-C4-C5-C6
6	K	501[A]	A1H8H	O1-C4-C5-C6
7	J	504	GOL	C1-C2-C3-O3
7	J	505	GOL	C1-C2-C3-O3
7	J	506	GOL	C1-C2-C3-O3
7	J	506	GOL	O2-C2-C3-O3
7	J	504	GOL	O2-C2-C3-O3
6	I	507[B]	A1H8H	N1-C1-C4-O1
6	C	501[A]	A1H8H	O1-C4-C5-C6
6	C	501[B]	A1H8H	O1-C4-C5-C6
6	I	507[A]	A1H8H	O1-C4-C5-C6
6	C	501[B]	A1H8H	C1-C4-C5-C10
6	I	507[B]	A1H8H	C1-C4-C5-C10
6	K	501[A]	A1H8H	C1-C4-C5-C10
6	C	501[B]	A1H8H	C1-C4-C5-C6
6	I	507[A]	A1H8H	C1-C4-C5-C6
6	I	507[B]	A1H8H	C1-C4-C5-C6
6	K	501[A]	A1H8H	C1-C4-C5-C6
7	J	504	GOL	O1-C1-C2-O2
6	I	507[B]	A1H8H	N1-C1-C4-C5

Continued on next page...

Continued from previous page...

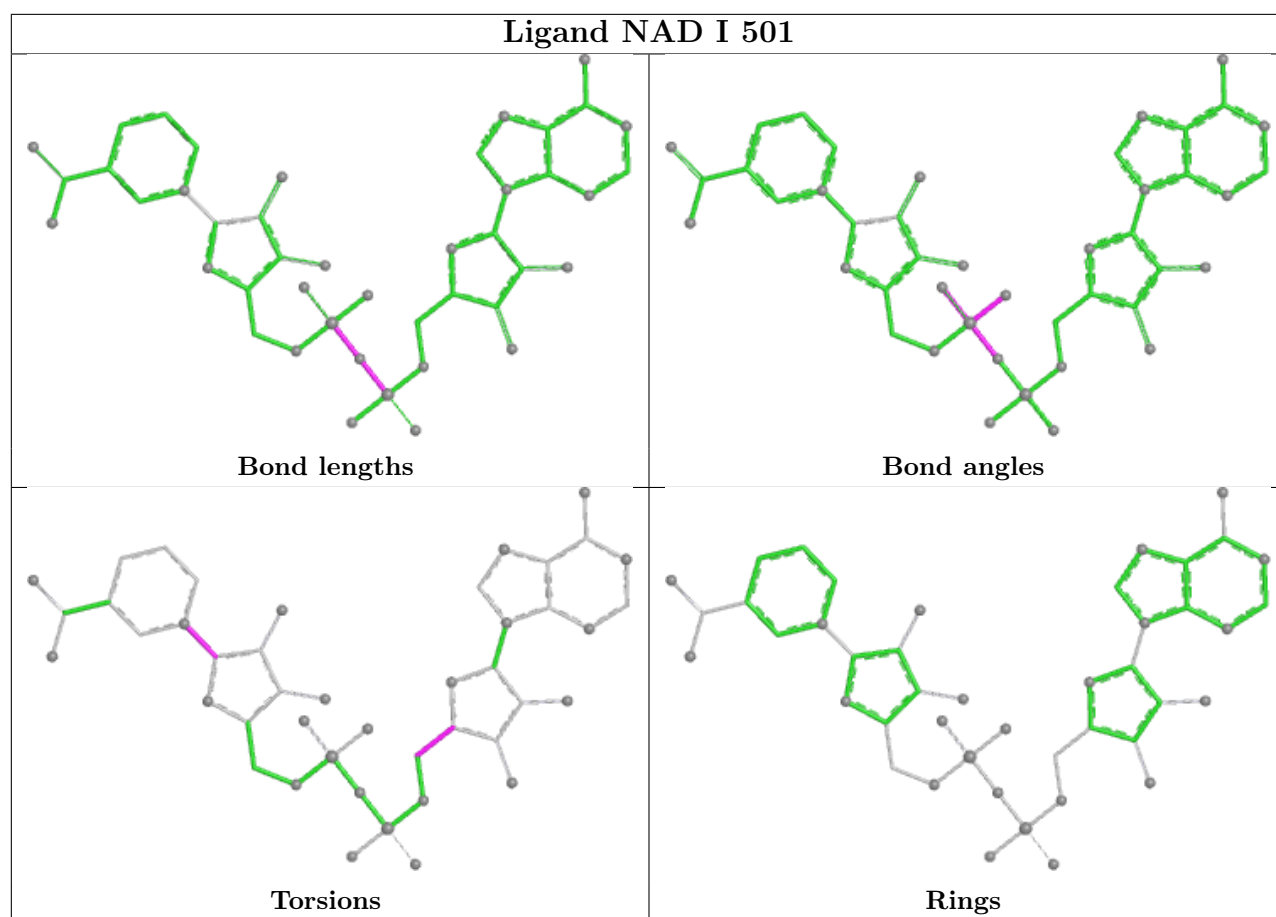
Mol	Chain	Res	Type	Atoms
7	J	505	GOL	O2-C2-C3-O3
6	I	507[B]	A1H8H	O1-C4-C5-C10
6	K	501[A]	A1H8H	O1-C4-C5-C10
2	I	501	NAD	O4B-C4B-C5B-O5B

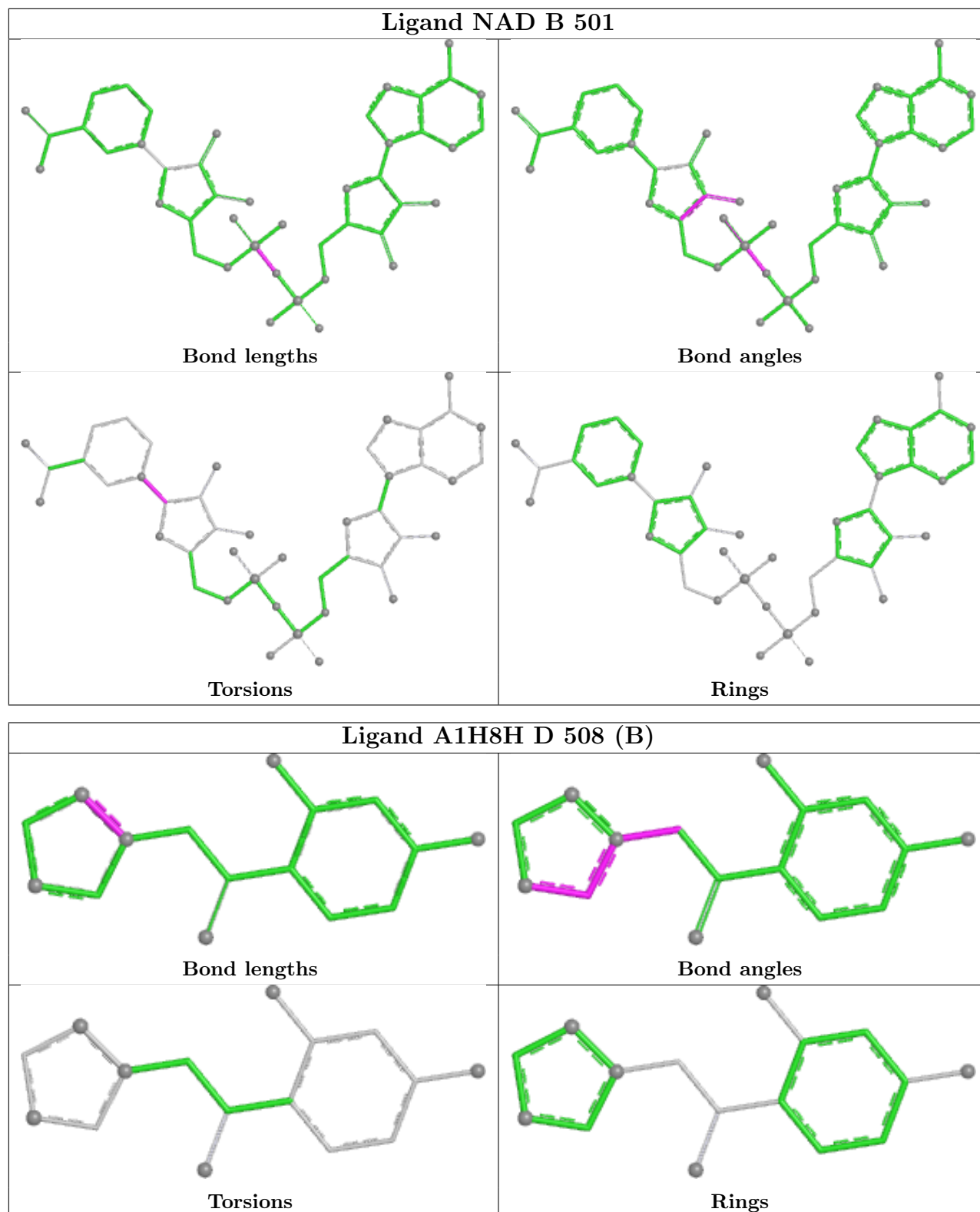
There are no ring outliers.

10 monomers are involved in 13 short contacts:

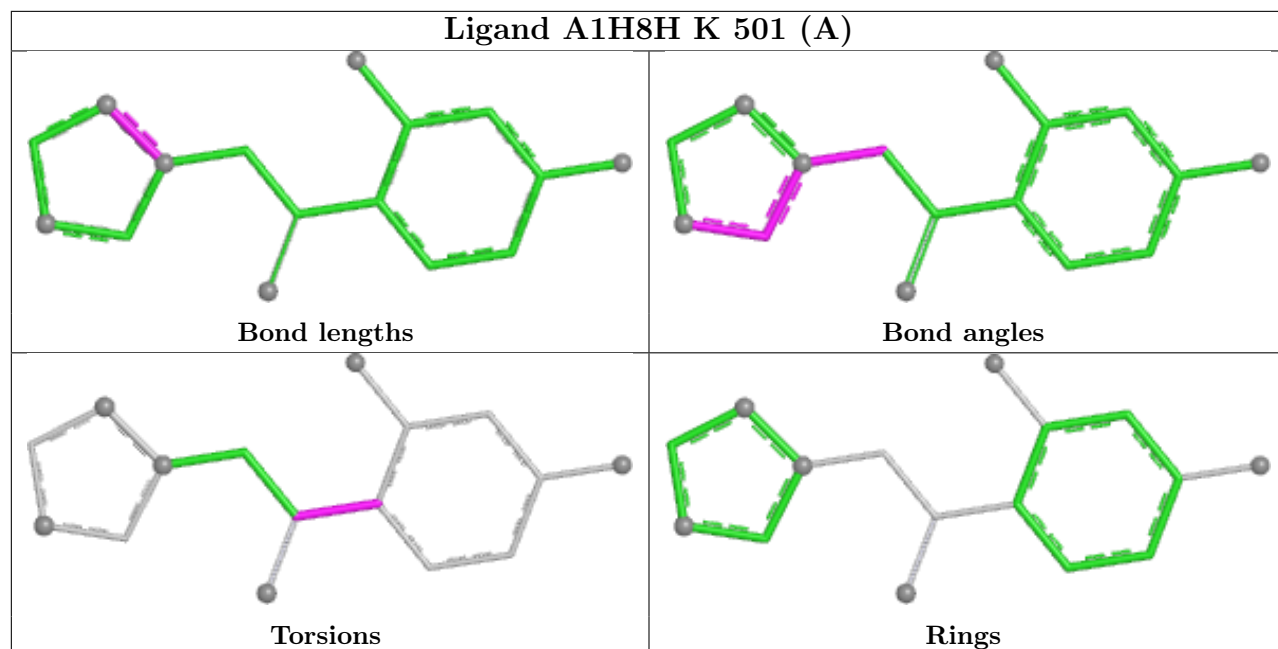
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	501	NAD	1	0
4	K	505	PO4	1	0
7	J	504	GOL	1	0
4	C	504	PO4	1	0
2	B	501	NAD	1	0
2	C	502	NAD	1	0
4	C	505	PO4	1	0
4	H	504	PO4	1	0
4	B	503	PO4	1	0
4	K	504	PO4	4	0

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.

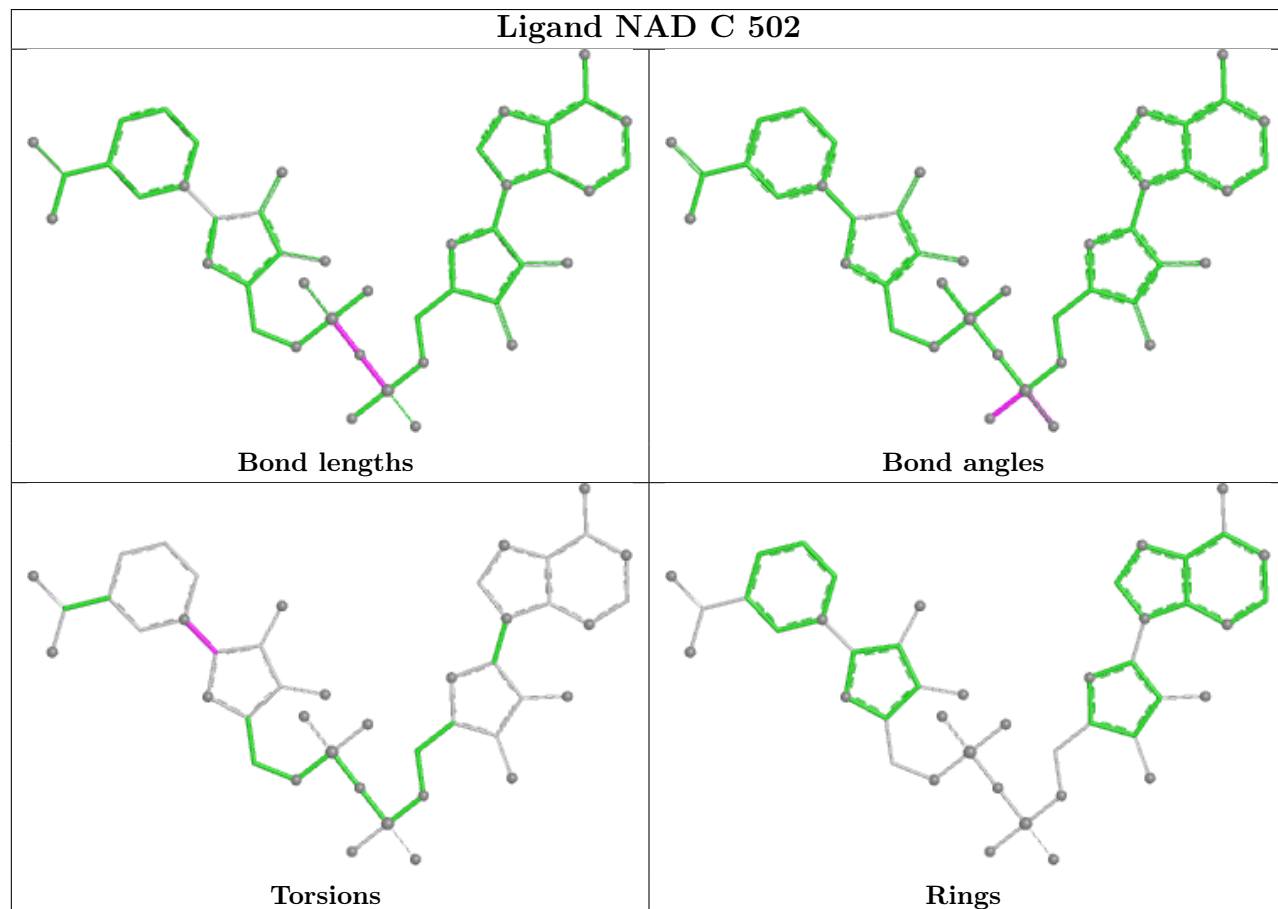




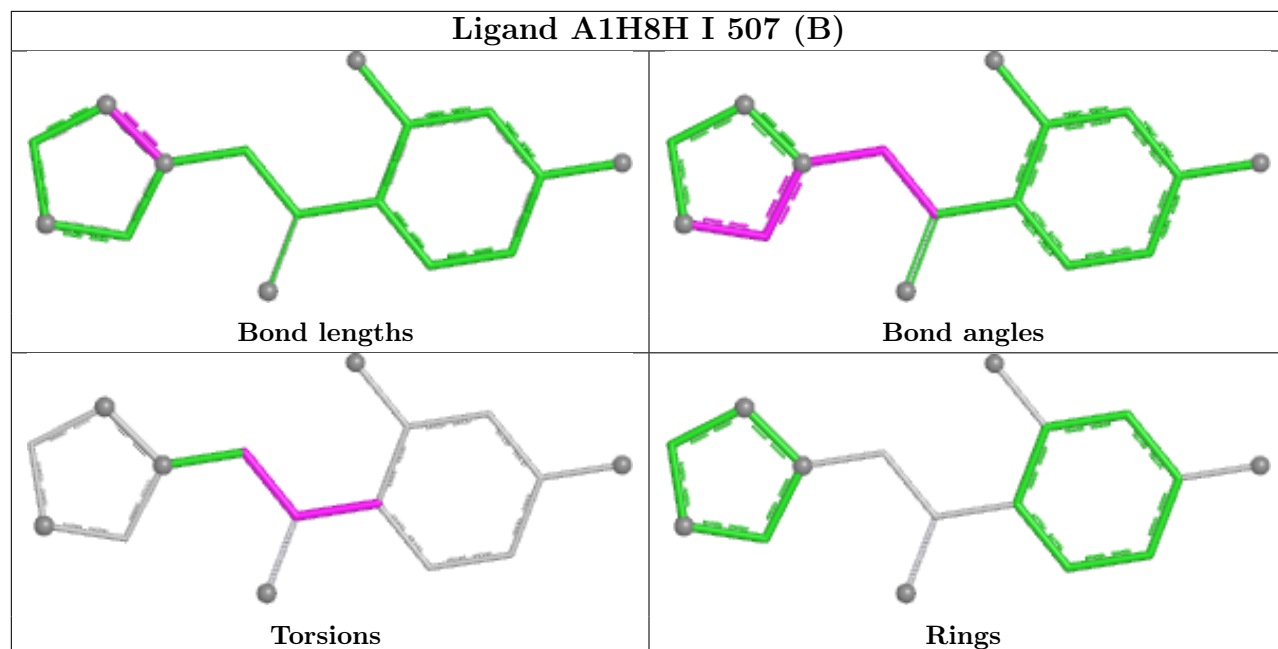
Ligand A1H8H K 501 (A)



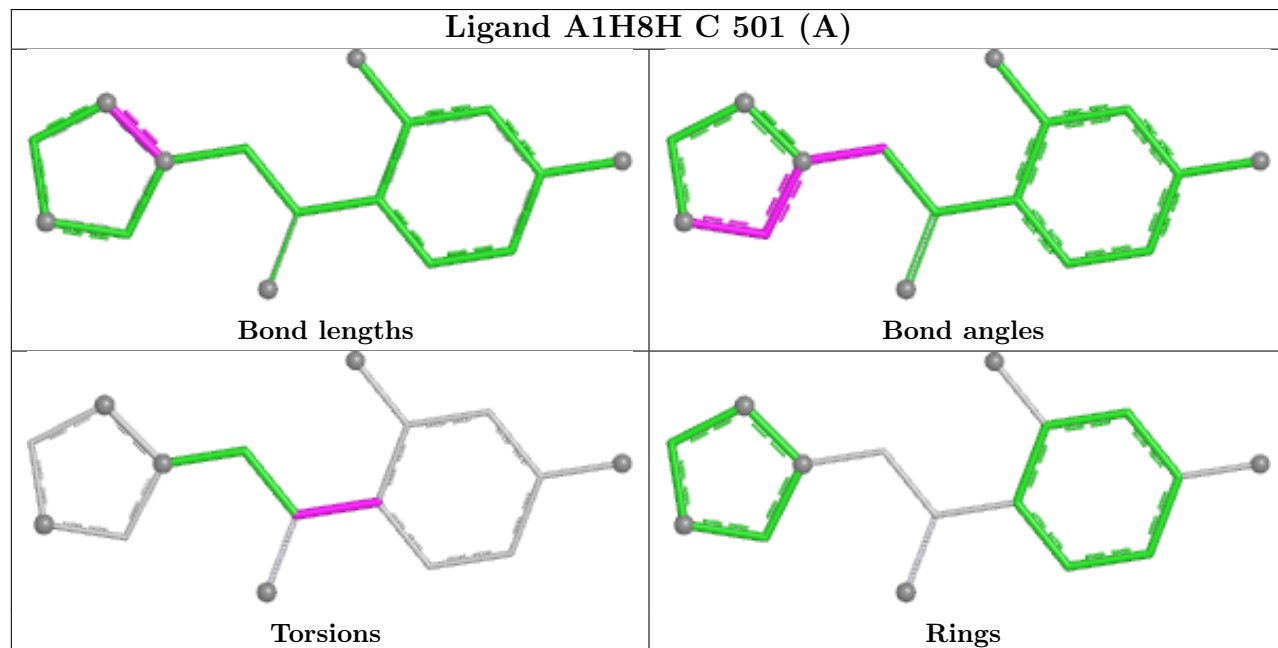
Ligand NAD C 502



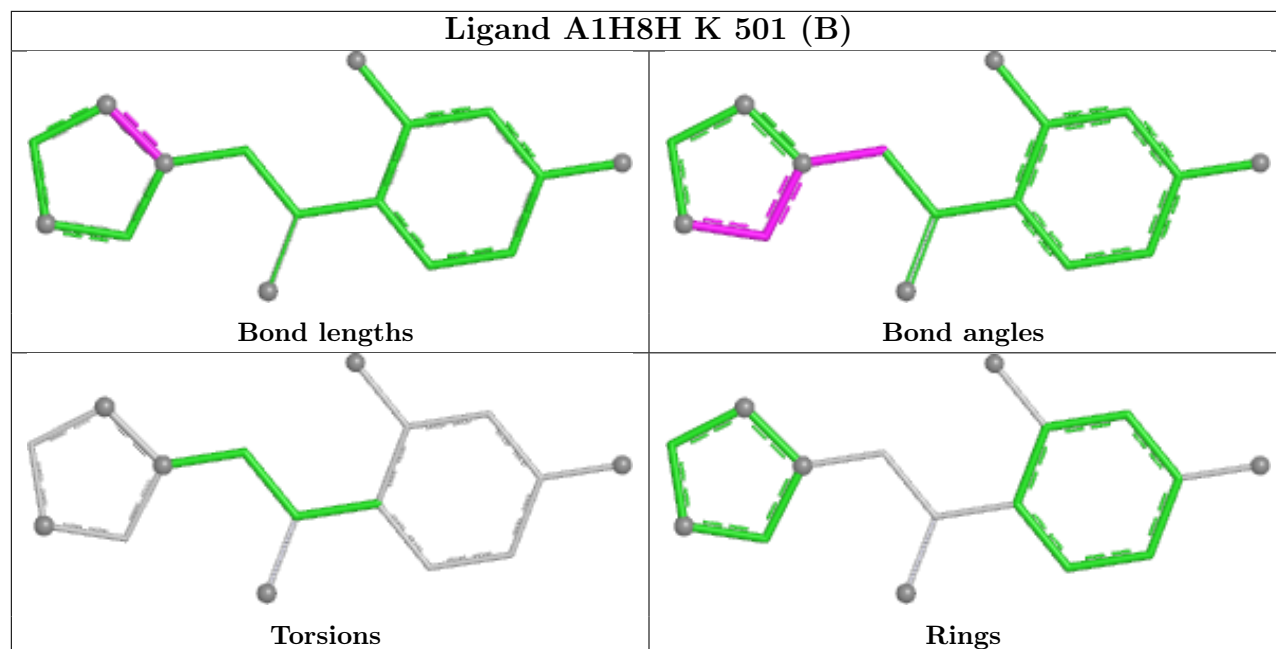
Ligand A1H8H I 507 (B)



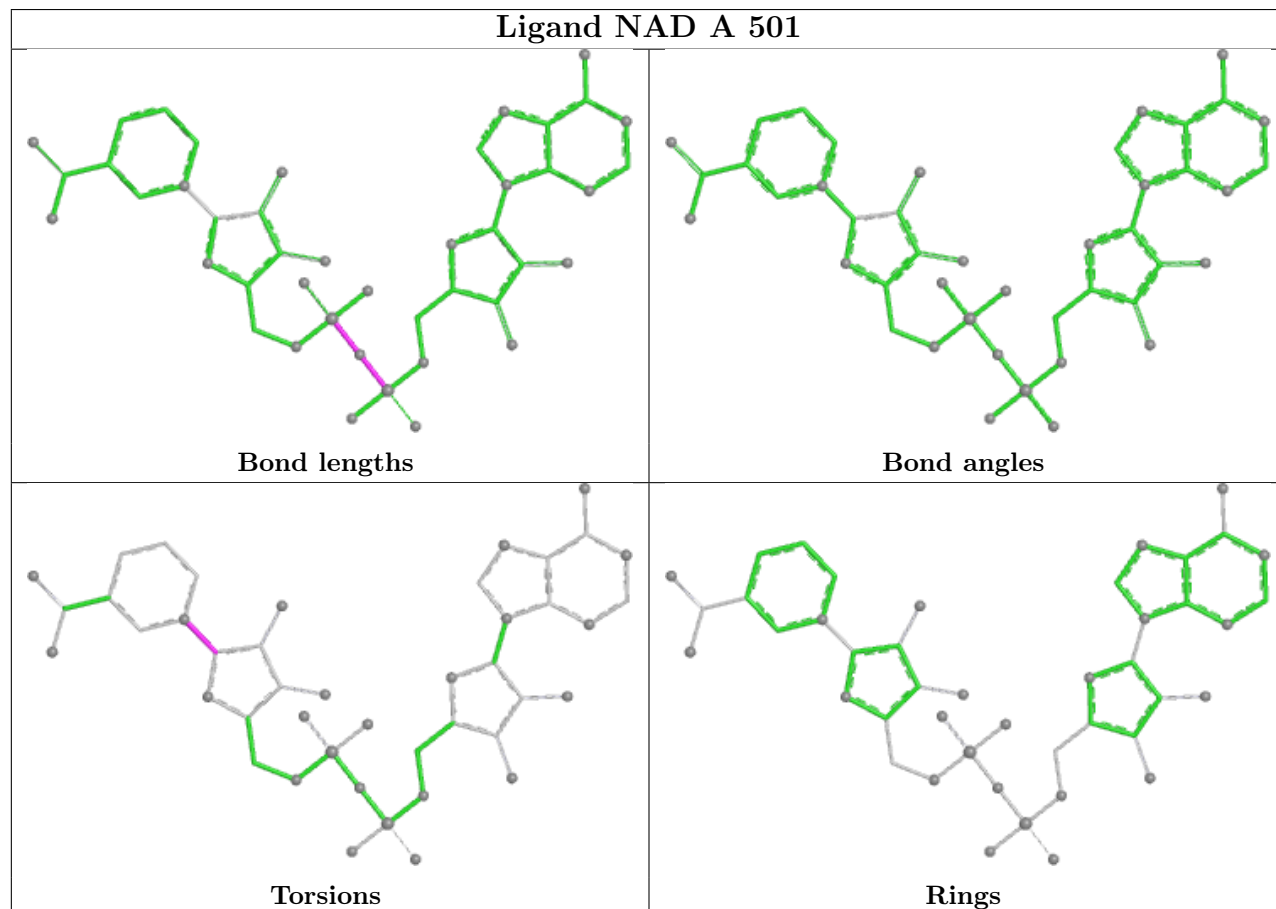
Ligand A1H8H C 501 (A)

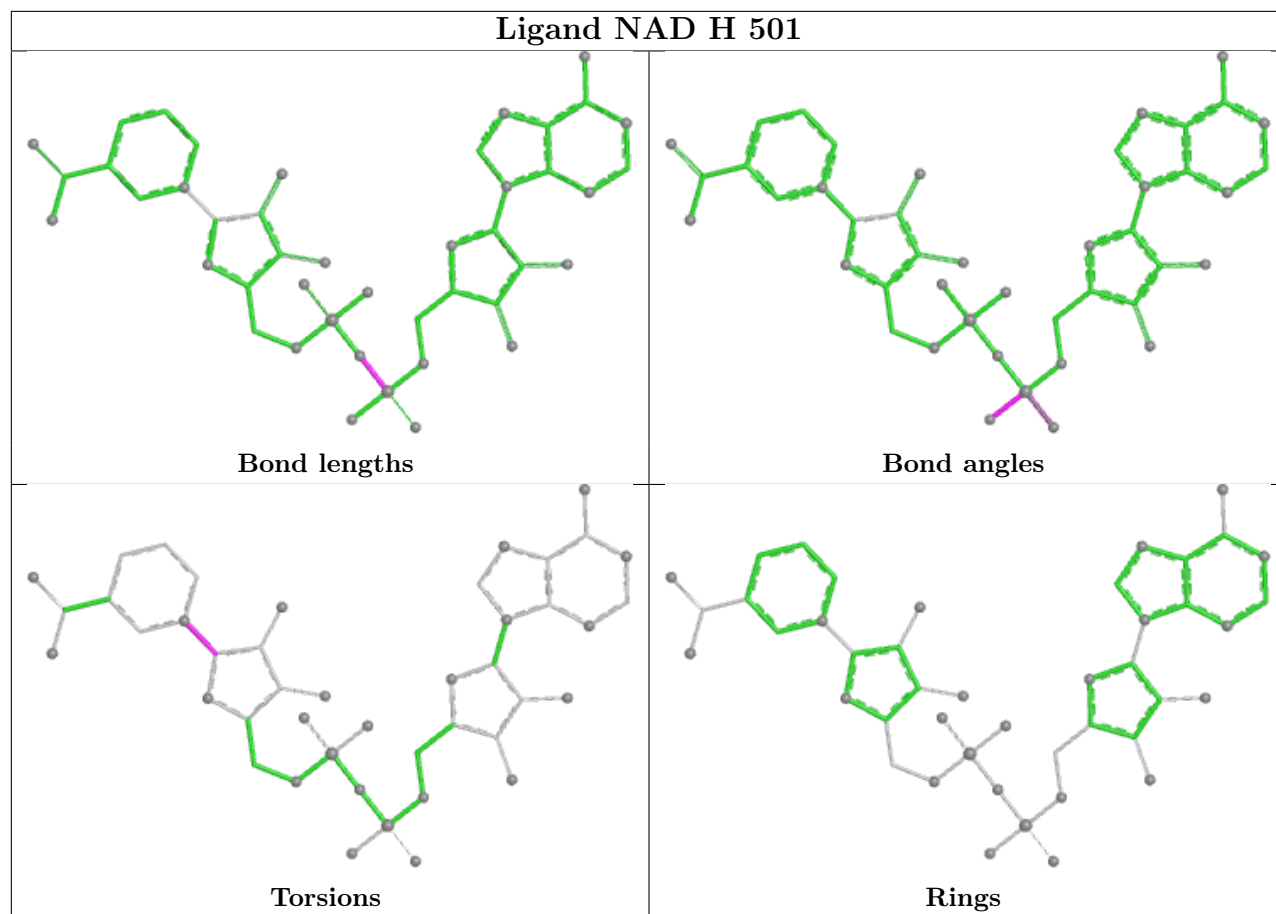


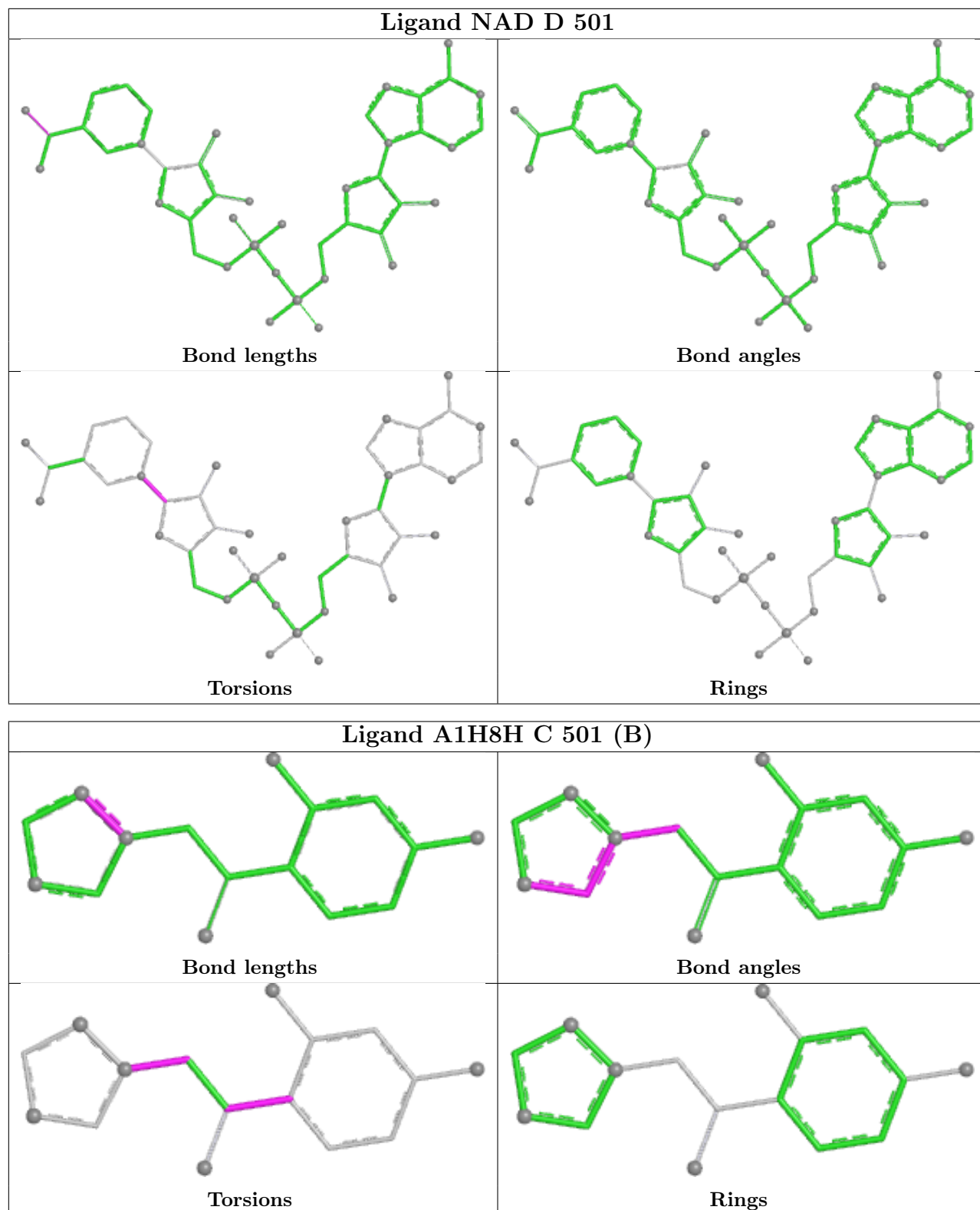
Ligand A1H8H K 501 (B)



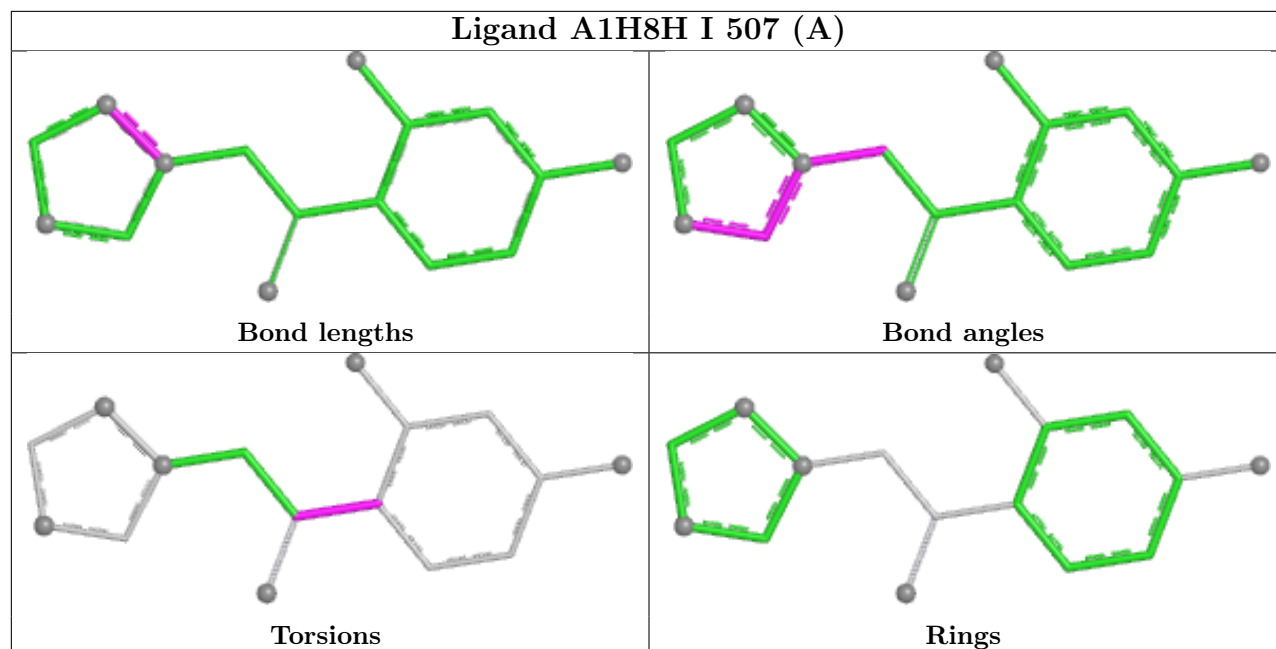
Ligand NAD A 501



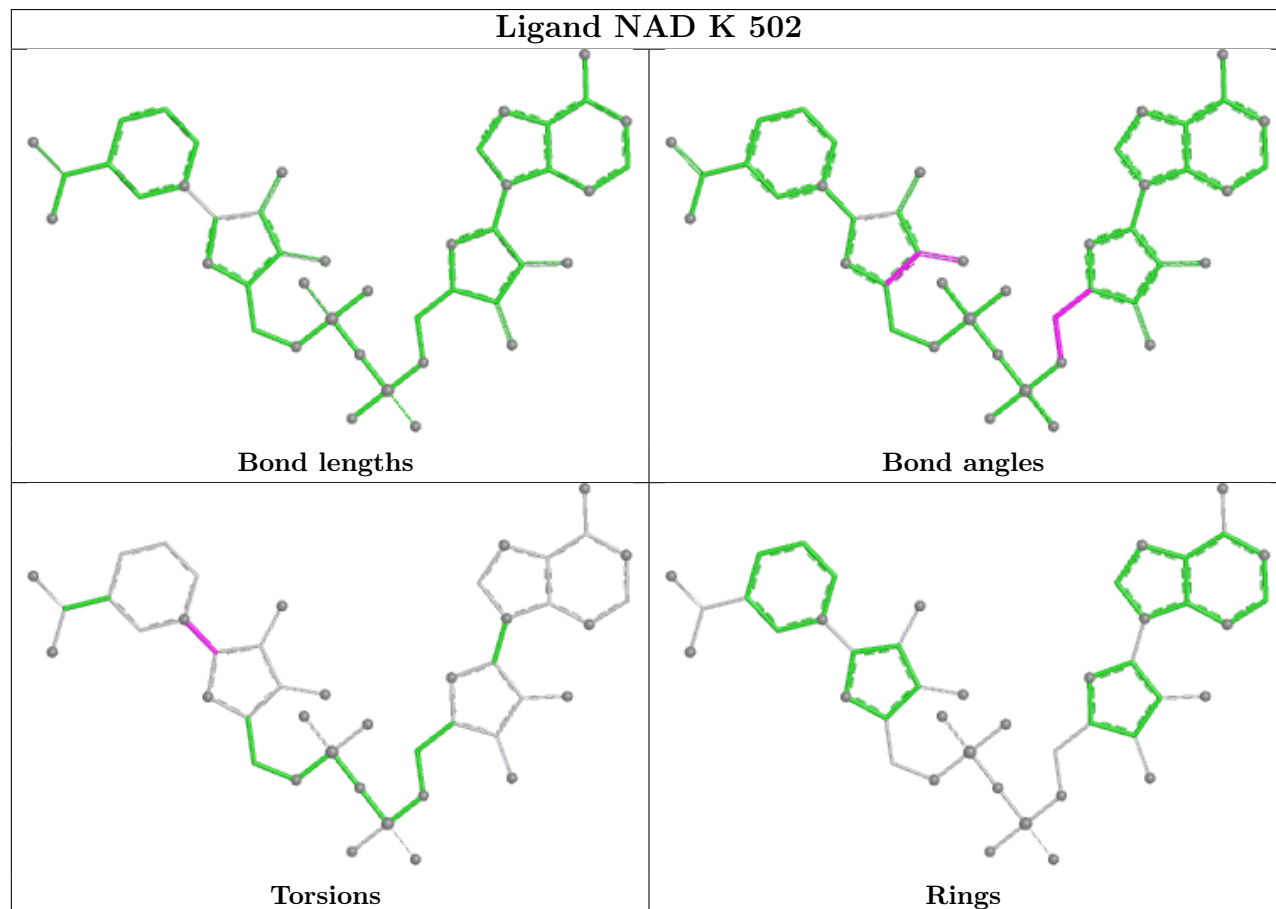


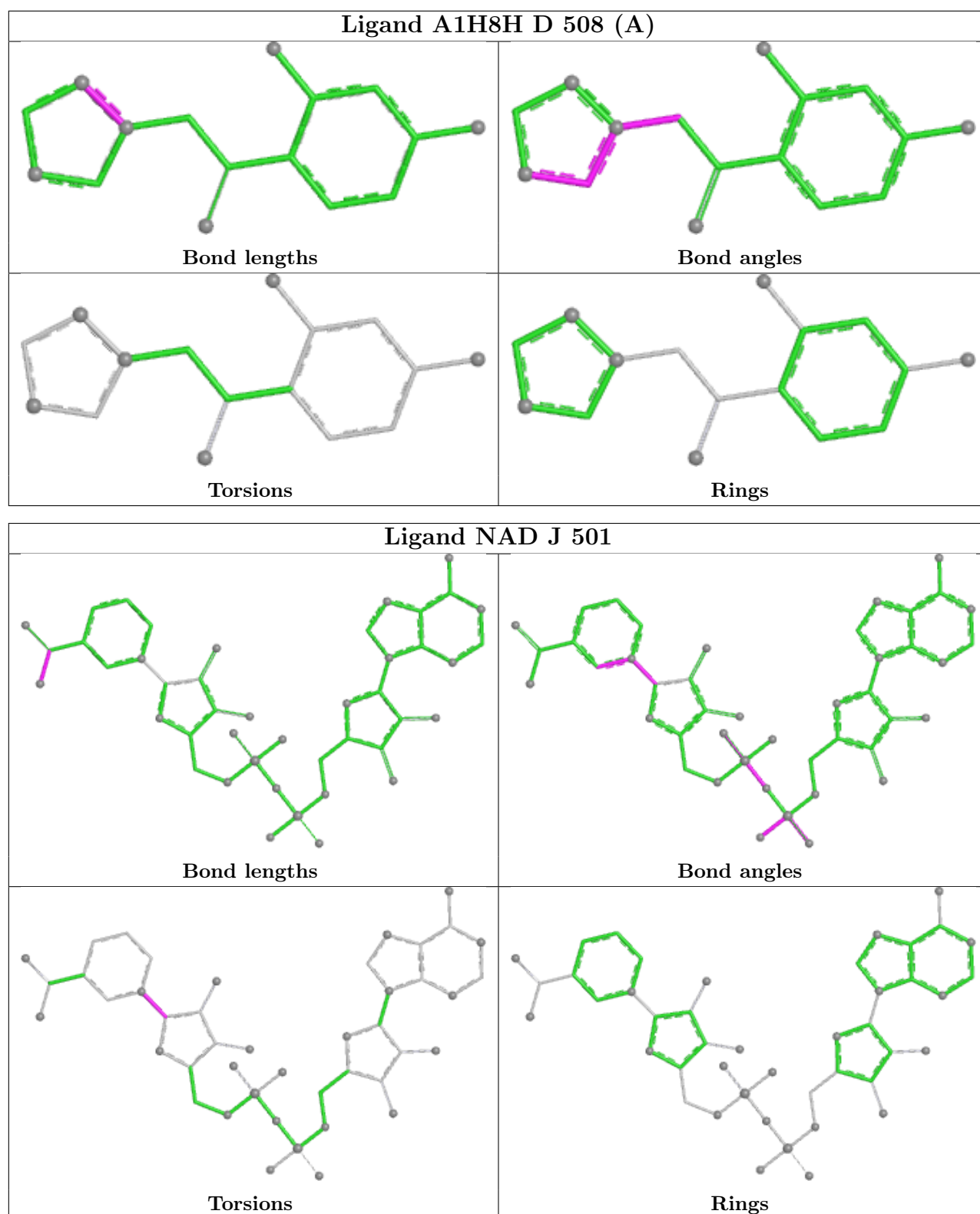


Ligand A1H8H I 507 (A)



Ligand NAD K 502





5.7 Other polymers ⓘ

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	464/472 (98%)	-0.08	11 (2%) 59 68	10, 28, 51, 88	10 (2%)
1	B	461/472 (97%)	-0.31	1 (0%) 91 93	11, 25, 42, 67	7 (1%)
1	C	461/472 (97%)	0.08	13 (2%) 55 62	10, 30, 55, 94	8 (1%)
1	D	461/472 (97%)	-0.19	3 (0%) 84 88	11, 27, 44, 76	9 (1%)
1	H	461/472 (97%)	0.40	39 (8%) 16 19	10, 33, 63, 98	9 (1%)
1	I	461/472 (97%)	-0.16	3 (0%) 84 88	11, 27, 44, 79	9 (1%)
1	J	461/472 (97%)	0.17	24 (5%) 33 39	10, 29, 53, 86	7 (1%)
1	K	461/472 (97%)	-0.08	0 100 100	12, 27, 43, 55	10 (2%)
All	All	3691/3776 (97%)	-0.02	94 (2%) 58 66	10, 28, 51, 98	69 (1%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	412	ALA	3.8
1	C	158[A]	ILE	3.8
1	I	9	GLY	3.8
1	J	410	PRO	3.8
1	J	411	ALA	3.7
1	J	158[A]	ILE	3.7
1	H	158[A]	ILE	3.6
1	H	410	PRO	3.6
1	J	409	LEU	3.6
1	A	8	ALA	3.5
1	H	409	LEU	3.5
1	A	411	ALA	3.4
1	H	125	LEU	3.3
1	J	10	PHE	3.3
1	J	45	TYR	3.3
1	H	10	PHE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	412	ALA	3.2
1	H	155	LEU	3.1
1	H	411	ALA	3.1
1	H	415	ALA	3.1
1	H	124	ILE	3.0
1	C	410	PRO	3.0
1	C	415	ALA	3.0
1	H	355	ASP	2.9
1	C	412	ALA	2.9
1	A	7	PRO	2.9
1	H	133	ALA	2.9
1	H	407	ALA	2.8
1	C	411	ALA	2.7
1	H	402	PHE	2.7
1	H	131	TRP	2.7
1	H	11	THR	2.6
1	A	9	GLY	2.6
1	B	9	GLY	2.6
1	H	118	TRP	2.6
1	A	46	ALA	2.6
1	A	415	ALA	2.6
1	H	9	GLY	2.5
1	J	402	PHE	2.5
1	A	409	LEU	2.5
1	H	52	LYS	2.5
1	H	13	TYR	2.5
1	H	412	ALA	2.5
1	J	407	ALA	2.5
1	I	355	ASP	2.5
1	H	106	PHE	2.5
1	D	356	GLY	2.5
1	H	179	GLY	2.5
1	H	147	LEU	2.4
1	J	54	ALA	2.4
1	D	355	ASP	2.3
1	A	6	THR	2.3
1	J	415	ALA	2.3
1	J	106	PHE	2.3
1	J	13	TYR	2.3
1	D	9	GLY	2.3
1	A	407	ALA	2.2
1	H	151	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	155	LEU	2.2
1	C	10	PHE	2.2
1	C	45	TYR	2.2
1	H	157	ARG	2.2
1	H	46	ALA	2.2
1	J	132	ASP	2.2
1	J	39[A]	MET	2.2
1	H	51	LEU	2.2
1	H	418	LEU	2.2
1	J	125	LEU	2.2
1	J	417	ARG	2.2
1	H	104	PRO	2.2
1	H	408	ASP	2.1
1	H	47	GLY	2.1
1	C	409	LEU	2.1
1	H	130	PRO	2.1
1	J	146	ILE	2.1
1	H	80	VAL	2.1
1	J	133	ALA	2.1
1	J	9	GLY	2.1
1	H	57	LEU	2.1
1	J	418	LEU	2.1
1	J	11	THR	2.1
1	C	151	TYR	2.1
1	C	402	PHE	2.1
1	H	120	ILE	2.1
1	J	406	TYR	2.1
1	H	77	GLY	2.0
1	I	356	GLY	2.0
1	C	277	ASP	2.0
1	J	277	ASP	2.0
1	A	416	LYS	2.0
1	H	121	GLU	2.0
1	H	127	ASP	2.0
1	H	458	VAL	2.0
1	C	177	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	A1H8H	C	501[A]	16/16	0.78	0.18	28,32,36,38	16
6	A1H8H	C	501[B]	16/16	0.78	0.18	28,32,35,35	16
6	A1H8H	I	507[A]	16/16	0.80	0.18	27,29,31,33	16
6	A1H8H	I	507[B]	16/16	0.80	0.18	29,30,42,42	16
6	A1H8H	D	508[A]	16/16	0.83	0.14	25,31,35,36	16
6	A1H8H	D	508[B]	16/16	0.83	0.14	29,33,37,37	16
6	A1H8H	K	501[A]	16/16	0.84	0.18	34,35,41,43	16
6	A1H8H	K	501[B]	16/16	0.84	0.18	32,35,40,41	16
4	PO4	A	505	5/5	0.88	0.12	27,29,36,42	5
4	PO4	A	506	5/5	0.89	0.12	44,45,50,53	5
4	PO4	C	507	5/5	0.89	0.12	29,30,39,45	5
4	PO4	D	506	5/5	0.89	0.12	40,40,48,49	5
4	PO4	H	505	5/5	0.89	0.12	32,33,42,45	5
7	GOL	J	504	6/6	0.89	0.12	44,46,53,53	0
4	PO4	K	505	5/5	0.90	0.12	41,43,45,49	5
4	PO4	H	506	5/5	0.90	0.10	54,55,61,66	0
7	GOL	J	506	6/6	0.90	0.13	32,34,41,55	0
4	PO4	I	505	5/5	0.91	0.10	51,52,65,66	0
4	PO4	B	506	5/5	0.91	0.09	46,52,60,63	0
4	PO4	C	505	5/5	0.91	0.14	35,37,41,48	5
4	PO4	H	504	5/5	0.92	0.12	36,40,44,46	5
7	GOL	J	505	6/6	0.92	0.11	32,33,38,39	0
4	PO4	K	506	5/5	0.92	0.10	25,27,30,39	0
7	GOL	J	503	6/6	0.93	0.10	35,40,50,53	0
4	PO4	H	503	5/5	0.93	0.09	45,45,48,50	0
4	PO4	A	504	5/5	0.94	0.13	32,34,39,43	5
4	PO4	D	504	5/5	0.94	0.09	23,25,33,35	0
4	PO4	D	505	5/5	0.94	0.10	38,42,46,49	5
4	PO4	B	505	5/5	0.94	0.12	34,34,47,50	5
4	PO4	I	504	5/5	0.94	0.09	25,26,35,36	5
4	PO4	J	510	5/5	0.95	0.09	41,41,46,47	5
4	PO4	K	504	5/5	0.95	0.09	24,31,37,40	5

Continued on next page...

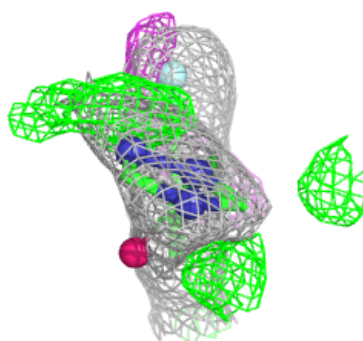
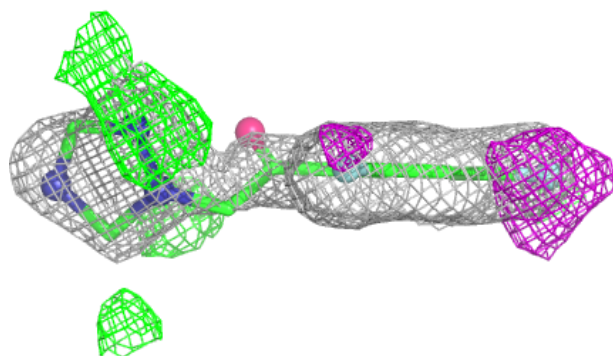
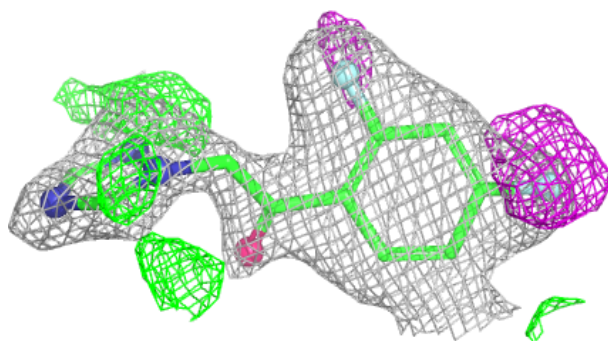
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PO4	B	504	5/5	0.95	0.09	21,21,25,31	5
3	ADE	H	502	10/10	0.95	0.07	28,31,34,35	0
3	ADE	A	502	10/10	0.95	0.06	20,24,25,25	0
4	PO4	B	503	5/5	0.95	0.09	24,33,36,38	5
4	PO4	C	506	5/5	0.95	0.09	37,46,49,49	5
4	PO4	J	507	5/5	0.95	0.09	29,36,38,39	0
4	PO4	J	508	5/5	0.96	0.09	32,34,35,43	5
4	PO4	J	509	5/5	0.96	0.08	26,26,30,33	5
3	ADE	C	503	10/10	0.96	0.06	23,24,27,28	0
3	ADE	I	502	10/10	0.97	0.05	20,22,24,24	0
3	ADE	J	502	10/10	0.97	0.05	22,23,26,26	0
3	ADE	K	503	10/10	0.97	0.05	18,21,22,23	0
4	PO4	C	504	5/5	0.97	0.06	36,41,45,45	0
4	PO4	A	503	5/5	0.97	0.12	33,37,40,40	0
3	ADE	B	502	10/10	0.98	0.04	18,21,22,23	0
2	NAD	H	501	44/44	0.98	0.04	19,24,28,31	0
3	ADE	D	502	10/10	0.98	0.04	21,22,24,24	0
2	NAD	K	502	44/44	0.98	0.05	21,26,30,32	0
4	PO4	D	503	5/5	0.98	0.09	28,29,34,38	0
2	NAD	D	501	44/44	0.98	0.04	20,24,28,30	0
4	PO4	I	503	5/5	0.98	0.05	23,25,30,32	5
2	NAD	B	501	44/44	0.99	0.04	19,22,24,26	0
2	NAD	I	501	44/44	0.99	0.04	20,24,27,29	0
5	K	C	508	1/1	0.99	0.06	24,24,24,24	0
5	K	D	507	1/1	0.99	0.03	22,22,22,22	0
5	K	H	507	1/1	0.99	0.06	27,27,27,27	0
5	K	J	511	1/1	0.99	0.04	22,22,22,22	0
2	NAD	J	501	44/44	0.99	0.04	17,22,25,27	0
2	NAD	C	502	44/44	0.99	0.04	19,23,26,29	0
2	NAD	A	501	44/44	0.99	0.04	16,21,25,28	0
5	K	A	507	1/1	1.00	0.03	22,22,22,22	0
5	K	I	506	1/1	1.00	0.03	21,21,21,21	0
5	K	B	507	1/1	1.00	0.03	20,20,20,20	0
5	K	K	507	1/1	1.00	0.05	21,21,21,21	0

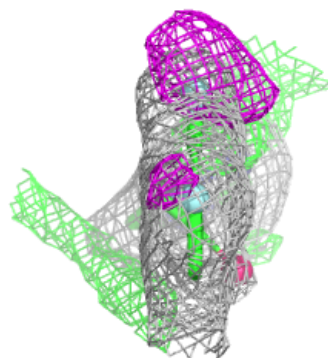
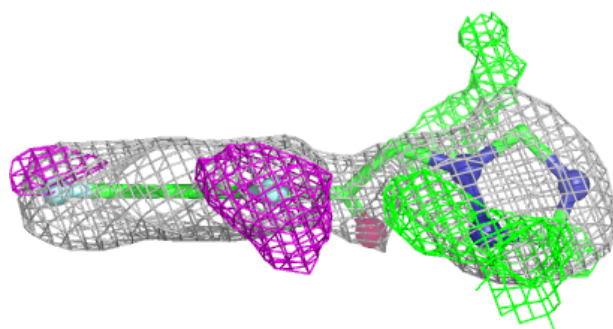
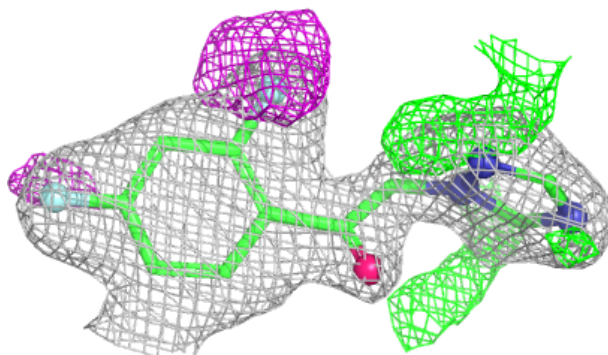
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1H8H C 501 (A):

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

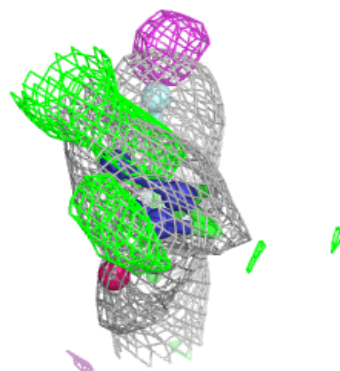
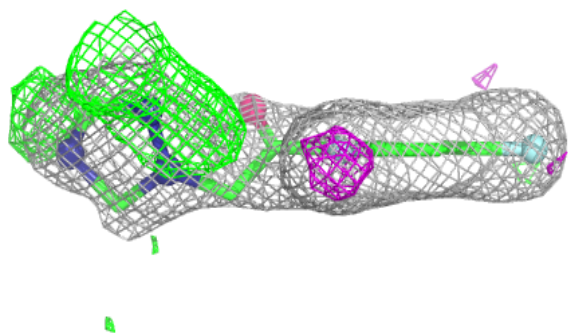
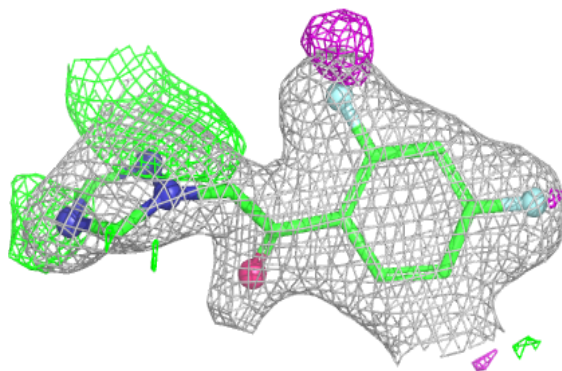
**Electron density around A1H8H C 501 (B):**

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

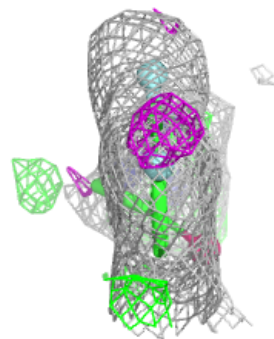
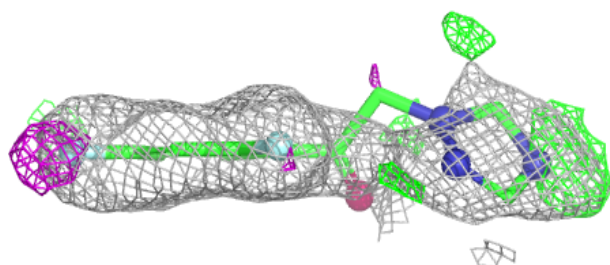
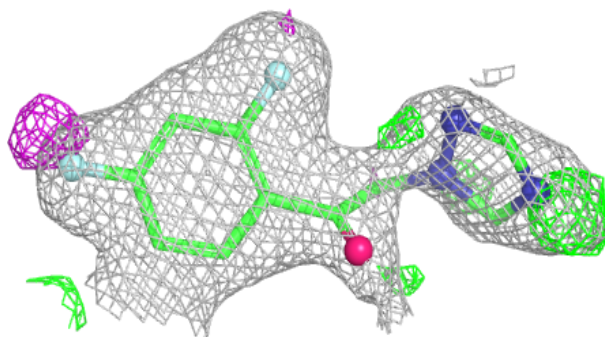


Electron density around A1H8H I 507 (A):

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

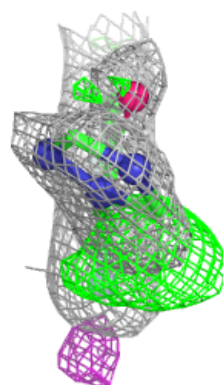
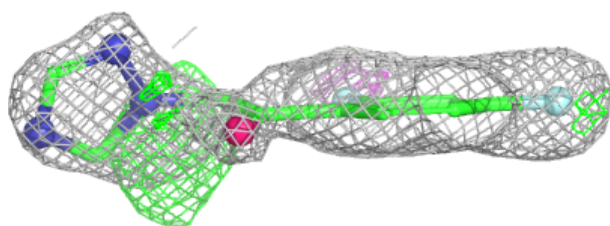
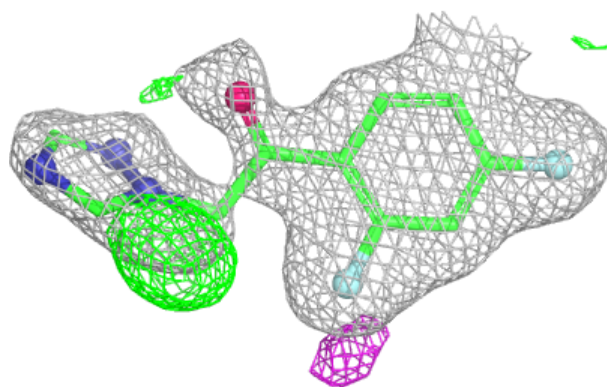
**Electron density around A1H8H I 507 (B):**

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

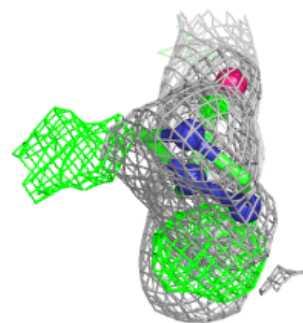
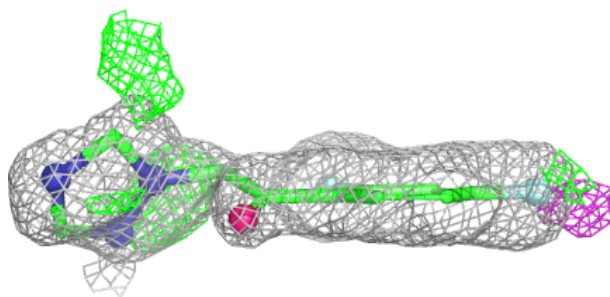
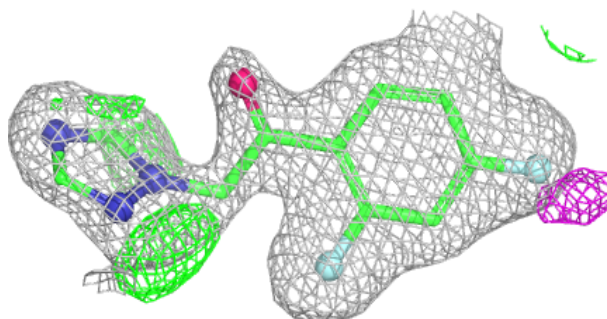


Electron density around A1H8H D 508 (A):

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

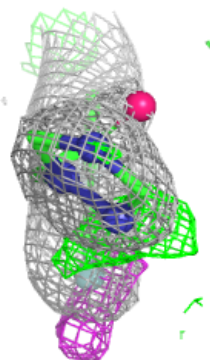
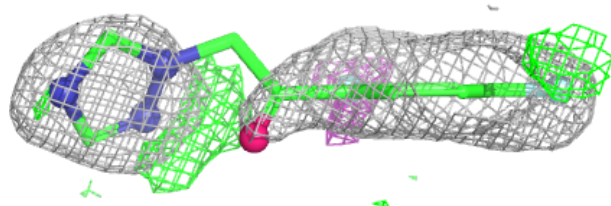
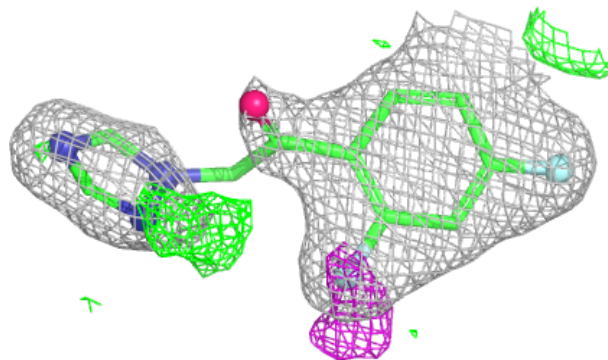
**Electron density around A1H8H D 508 (B):**

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

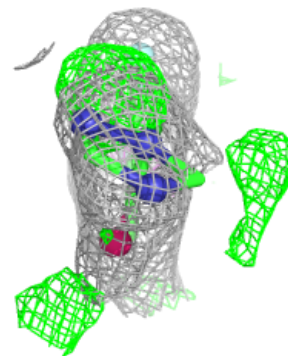
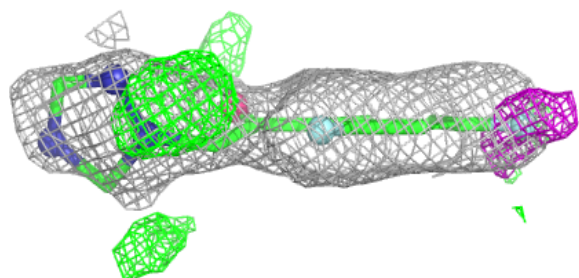
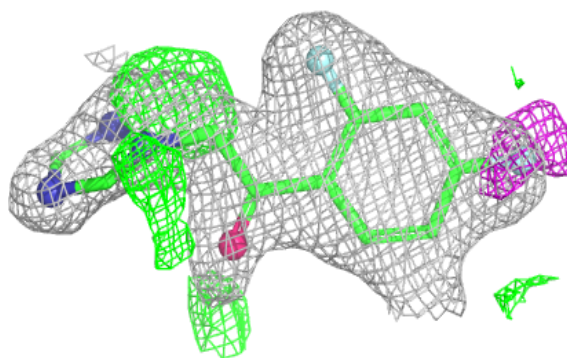


Electron density around A1H8H K 501 (A):

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

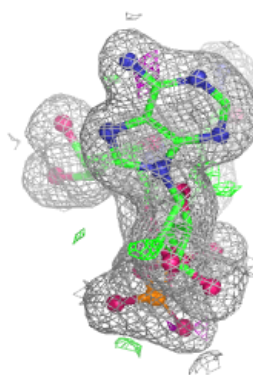
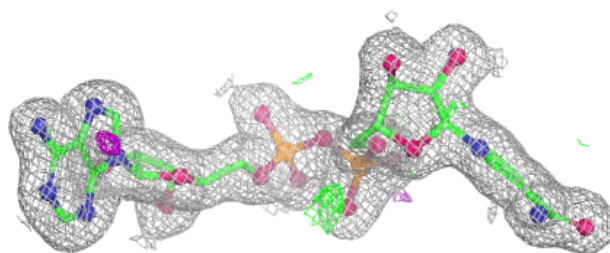
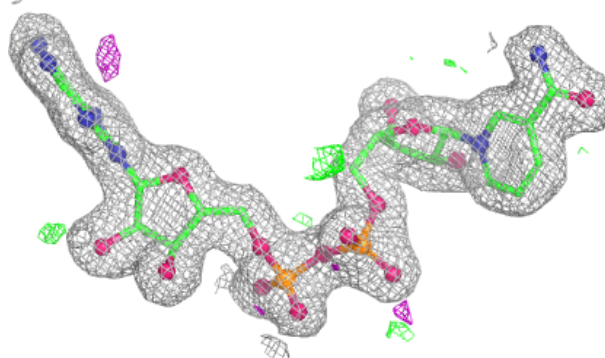
**Electron density around A1H8H K 501 (B):**

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

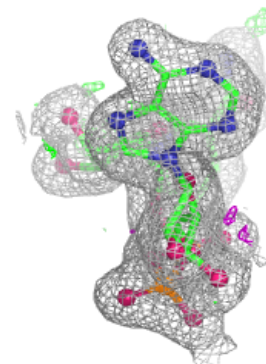
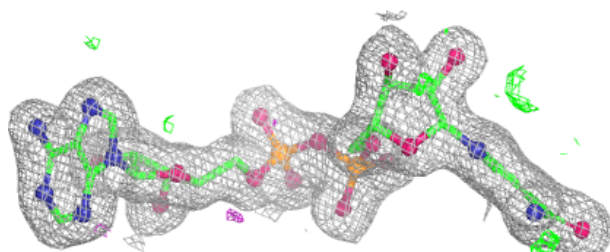
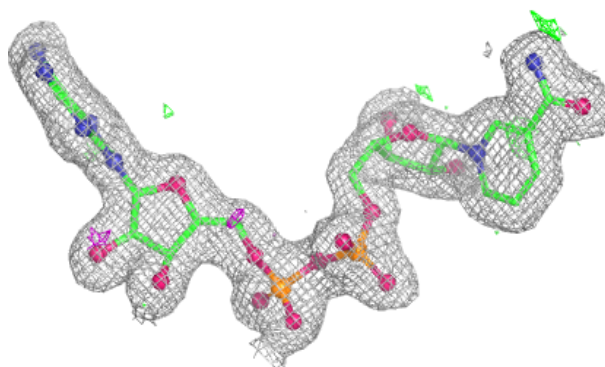


Electron density around NAD H 501:

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

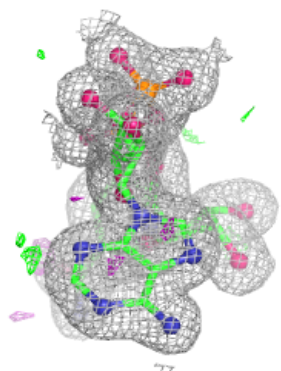
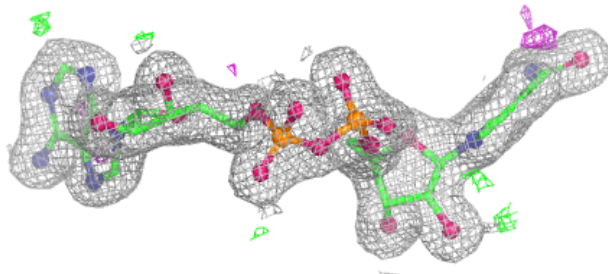
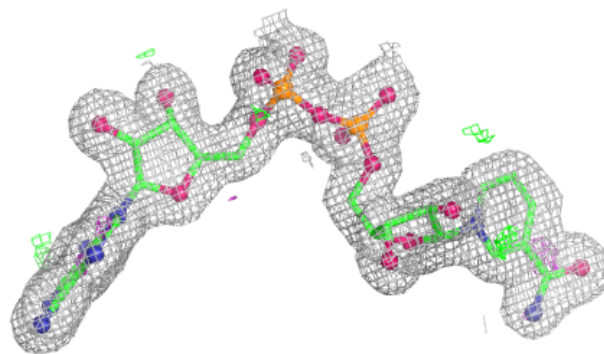
**Electron density around NAD K 502:**

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

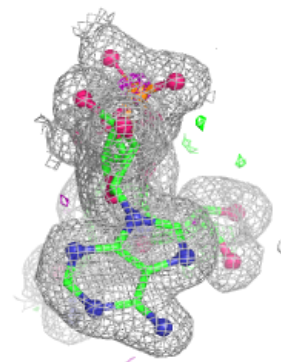
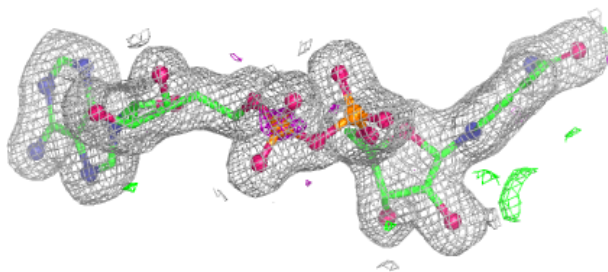
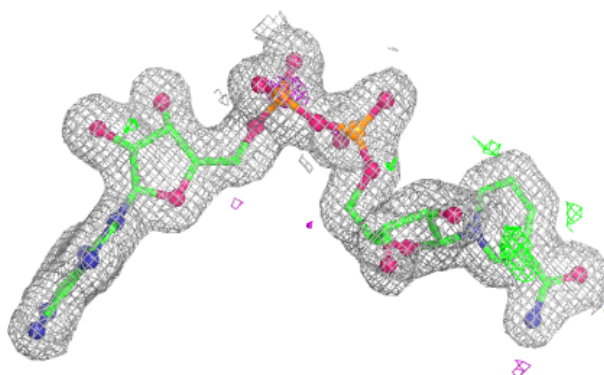


Electron density around NAD D 501:

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

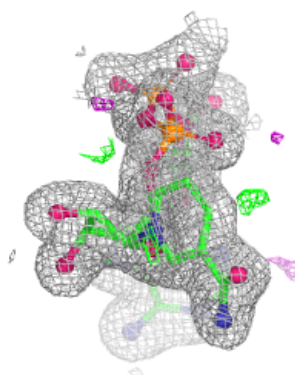
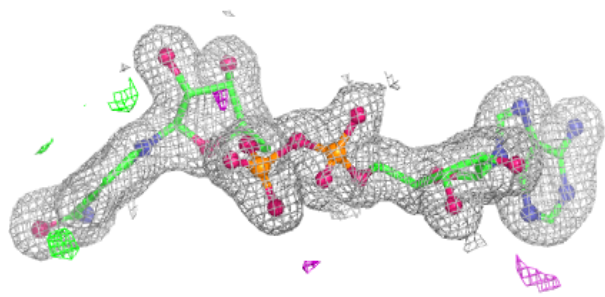
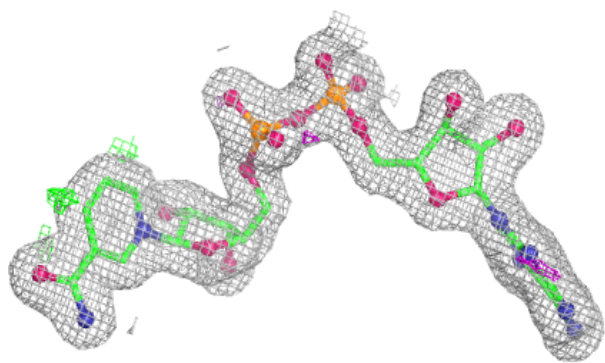
**Electron density around NAD B 501:**

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

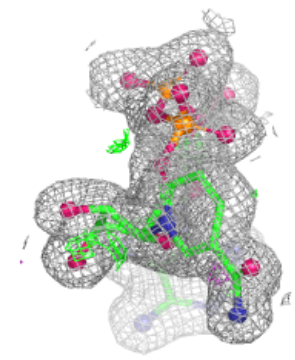
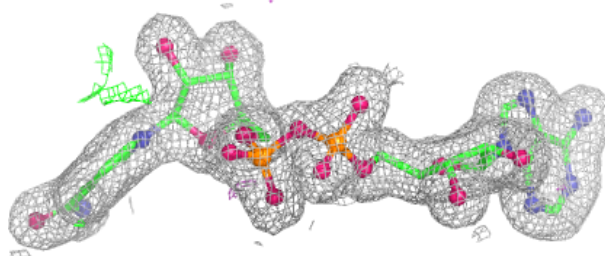
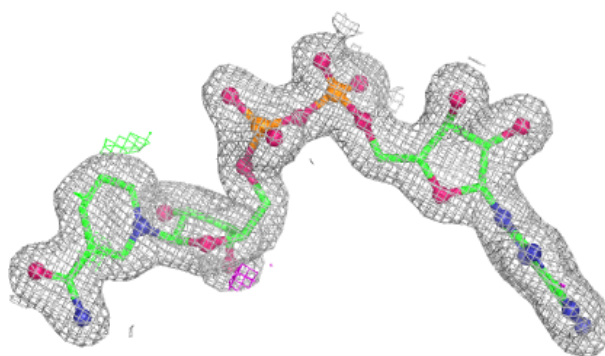


Electron density around NAD I 501:

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

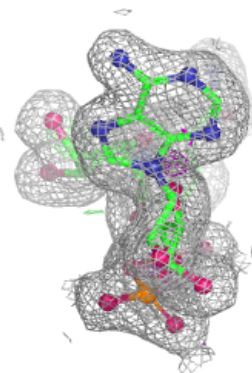
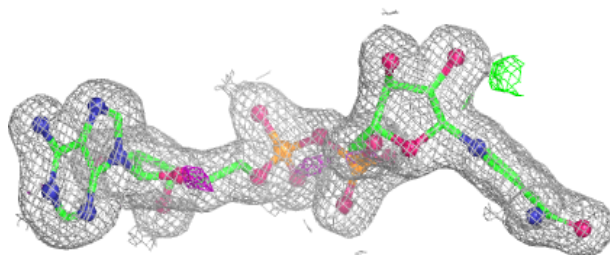
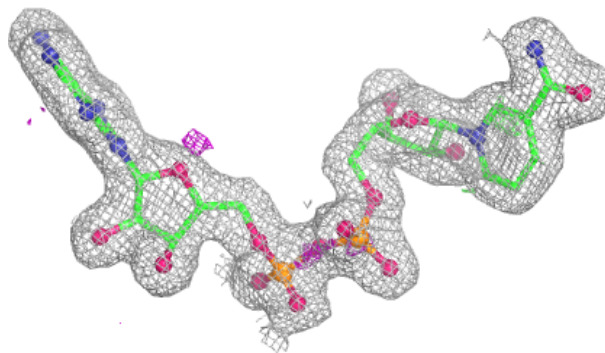
**Electron density around NAD J 501:**

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

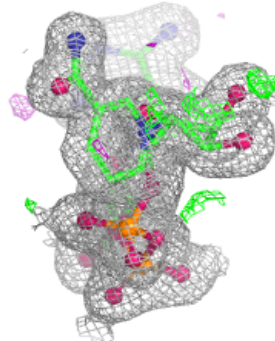
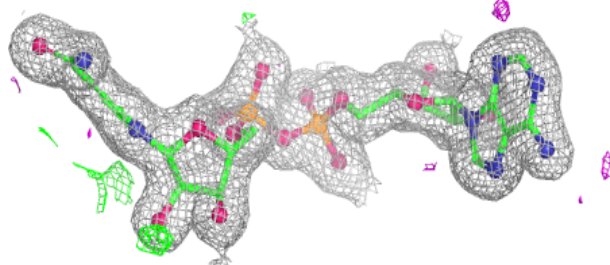
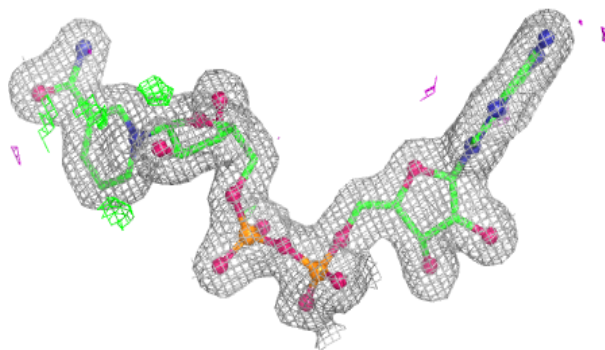


Electron density around NAD C 502:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.