



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:39 PM UTC

PDB ID : 5I7F / pdb_00005i7f
Title : Crystal structure of B. pseudomallei FabI in complex with NAD and PT405
Authors : Eltschkner, S.; Tonge, P.J.; Kisker, C.
Deposited on : 2016-02-17
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

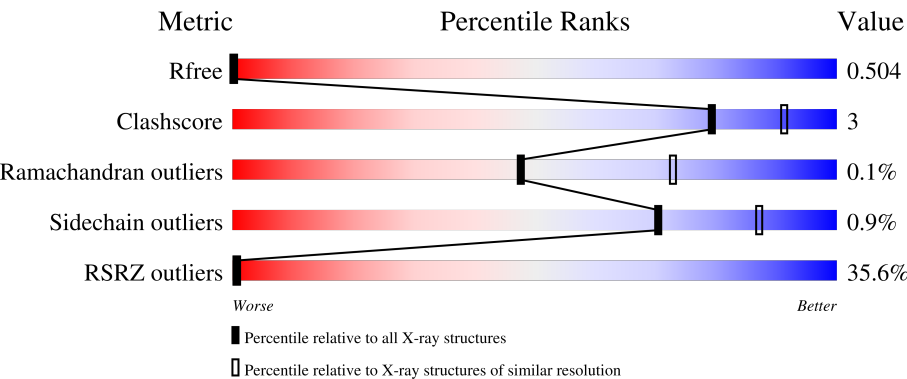
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	276	28% 86%7%7%
1	B	276	32% 86%8%7%
1	C	276	45% 88%5%7%
1	D	276	36% 86%7%7%
1	E	276	50% 89%.7%

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Mol	Chain	Length	Quality of chain
1	F	276	29%89% 7%
1	G	276	26%85% 8%7%
1	H	276	40%83% 10%7%
1	I	276	22%90% 7%
1	J	276	26%88% 5%7%
1	K	276	30%89% 7%
1	L	276	34%86% 7%7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 46664 atoms, of which 22715 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 Enoyl-[acyl-carrier-protein] reductase [NADH].

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	257	Total	C	H	N	O	S	0	0	0
			3754	1218	1842	325	363	6			
1	E	257	Total	C	H	N	O	S	0	1	0
			3765	1221	1848	325	365	6			
1	H	257	Total	C	H	N	O	S	0	0	0
			3759	1218	1847	325	363	6			
1	C	257	Total	C	H	N	O	S	0	0	0
			3754	1218	1842	325	363	6			
1	A	257	Total	C	H	N	O	S	0	0	0
			3759	1218	1847	325	363	6			
1	F	257	Total	C	H	N	O	S	19	1	0
			3777	1223	1859	326	363	6			
1	G	257	Total	C	H	N	O	S	0	1	0
			3766	1221	1849	325	365	6			
1	D	257	Total	C	H	N	O	S	0	0	0
			3759	1218	1847	325	363	6			
1	I	257	Total	C	H	N	O	S	0	0	0
			3772	1218	1860	325	363	6			
1	K	257	Total	C	H	N	O	S	0	1	0
			3771	1223	1853	326	363	6			
1	L	257	Total	C	H	N	O	S	0	0	0
			3774	1218	1862	325	363	6			
1	J	257	Total	C	H	N	O	S	19	1	0
			3809	1223	1891	326	363	6			

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	264	LYS	-	expression tag	UNP A0A069B9A4
B	265	LEU	-	expression tag	UNP A0A069B9A4
B	266	ALA	-	expression tag	UNP A0A069B9A4
B	267	ALA	-	expression tag	UNP A0A069B9A4
B	268	ALA	-	expression tag	UNP A0A069B9A4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	269	LEU	-	expression tag	UNP A0A069B9A4
B	270	GLU	-	expression tag	UNP A0A069B9A4
B	271	HIS	-	expression tag	UNP A0A069B9A4
B	272	HIS	-	expression tag	UNP A0A069B9A4
B	273	HIS	-	expression tag	UNP A0A069B9A4
B	274	HIS	-	expression tag	UNP A0A069B9A4
B	275	HIS	-	expression tag	UNP A0A069B9A4
B	276	HIS	-	expression tag	UNP A0A069B9A4
E	264	LYS	-	expression tag	UNP A0A069B9A4
E	265	LEU	-	expression tag	UNP A0A069B9A4
E	266	ALA	-	expression tag	UNP A0A069B9A4
E	267	ALA	-	expression tag	UNP A0A069B9A4
E	268	ALA	-	expression tag	UNP A0A069B9A4
E	269	LEU	-	expression tag	UNP A0A069B9A4
E	270	GLU	-	expression tag	UNP A0A069B9A4
E	271	HIS	-	expression tag	UNP A0A069B9A4
E	272	HIS	-	expression tag	UNP A0A069B9A4
E	273	HIS	-	expression tag	UNP A0A069B9A4
E	274	HIS	-	expression tag	UNP A0A069B9A4
E	275	HIS	-	expression tag	UNP A0A069B9A4
E	276	HIS	-	expression tag	UNP A0A069B9A4
H	264	LYS	-	expression tag	UNP A0A069B9A4
H	265	LEU	-	expression tag	UNP A0A069B9A4
H	266	ALA	-	expression tag	UNP A0A069B9A4
H	267	ALA	-	expression tag	UNP A0A069B9A4
H	268	ALA	-	expression tag	UNP A0A069B9A4
H	269	LEU	-	expression tag	UNP A0A069B9A4
H	270	GLU	-	expression tag	UNP A0A069B9A4
H	271	HIS	-	expression tag	UNP A0A069B9A4
H	272	HIS	-	expression tag	UNP A0A069B9A4
H	273	HIS	-	expression tag	UNP A0A069B9A4
H	274	HIS	-	expression tag	UNP A0A069B9A4
H	275	HIS	-	expression tag	UNP A0A069B9A4
H	276	HIS	-	expression tag	UNP A0A069B9A4
C	264	LYS	-	expression tag	UNP A0A069B9A4
C	265	LEU	-	expression tag	UNP A0A069B9A4
C	266	ALA	-	expression tag	UNP A0A069B9A4
C	267	ALA	-	expression tag	UNP A0A069B9A4
C	268	ALA	-	expression tag	UNP A0A069B9A4
C	269	LEU	-	expression tag	UNP A0A069B9A4
C	270	GLU	-	expression tag	UNP A0A069B9A4
C	271	HIS	-	expression tag	UNP A0A069B9A4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	272	HIS	-	expression tag	UNP A0A069B9A4
C	273	HIS	-	expression tag	UNP A0A069B9A4
C	274	HIS	-	expression tag	UNP A0A069B9A4
C	275	HIS	-	expression tag	UNP A0A069B9A4
C	276	HIS	-	expression tag	UNP A0A069B9A4
A	264	LYS	-	expression tag	UNP A0A069B9A4
A	265	LEU	-	expression tag	UNP A0A069B9A4
A	266	ALA	-	expression tag	UNP A0A069B9A4
A	267	ALA	-	expression tag	UNP A0A069B9A4
A	268	ALA	-	expression tag	UNP A0A069B9A4
A	269	LEU	-	expression tag	UNP A0A069B9A4
A	270	GLU	-	expression tag	UNP A0A069B9A4
A	271	HIS	-	expression tag	UNP A0A069B9A4
A	272	HIS	-	expression tag	UNP A0A069B9A4
A	273	HIS	-	expression tag	UNP A0A069B9A4
A	274	HIS	-	expression tag	UNP A0A069B9A4
A	275	HIS	-	expression tag	UNP A0A069B9A4
A	276	HIS	-	expression tag	UNP A0A069B9A4
F	264	LYS	-	expression tag	UNP A0A069B9A4
F	265	LEU	-	expression tag	UNP A0A069B9A4
F	266	ALA	-	expression tag	UNP A0A069B9A4
F	267	ALA	-	expression tag	UNP A0A069B9A4
F	268	ALA	-	expression tag	UNP A0A069B9A4
F	269	LEU	-	expression tag	UNP A0A069B9A4
F	270	GLU	-	expression tag	UNP A0A069B9A4
F	271	HIS	-	expression tag	UNP A0A069B9A4
F	272	HIS	-	expression tag	UNP A0A069B9A4
F	273	HIS	-	expression tag	UNP A0A069B9A4
F	274	HIS	-	expression tag	UNP A0A069B9A4
F	275	HIS	-	expression tag	UNP A0A069B9A4
F	276	HIS	-	expression tag	UNP A0A069B9A4
G	264	LYS	-	expression tag	UNP A0A069B9A4
G	265	LEU	-	expression tag	UNP A0A069B9A4
G	266	ALA	-	expression tag	UNP A0A069B9A4
G	267	ALA	-	expression tag	UNP A0A069B9A4
G	268	ALA	-	expression tag	UNP A0A069B9A4
G	269	LEU	-	expression tag	UNP A0A069B9A4
G	270	GLU	-	expression tag	UNP A0A069B9A4
G	271	HIS	-	expression tag	UNP A0A069B9A4
G	272	HIS	-	expression tag	UNP A0A069B9A4
G	273	HIS	-	expression tag	UNP A0A069B9A4
G	274	HIS	-	expression tag	UNP A0A069B9A4

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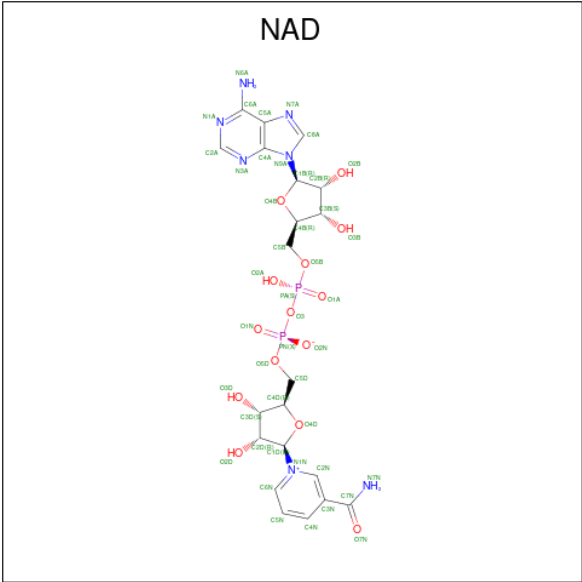
Chain	Residue	Modelled	Actual	Comment	Reference
G	275	HIS	-	expression tag	UNP A0A069B9A4
G	276	HIS	-	expression tag	UNP A0A069B9A4
D	264	LYS	-	expression tag	UNP A0A069B9A4
D	265	LEU	-	expression tag	UNP A0A069B9A4
D	266	ALA	-	expression tag	UNP A0A069B9A4
D	267	ALA	-	expression tag	UNP A0A069B9A4
D	268	ALA	-	expression tag	UNP A0A069B9A4
D	269	LEU	-	expression tag	UNP A0A069B9A4
D	270	GLU	-	expression tag	UNP A0A069B9A4
D	271	HIS	-	expression tag	UNP A0A069B9A4
D	272	HIS	-	expression tag	UNP A0A069B9A4
D	273	HIS	-	expression tag	UNP A0A069B9A4
D	274	HIS	-	expression tag	UNP A0A069B9A4
D	275	HIS	-	expression tag	UNP A0A069B9A4
D	276	HIS	-	expression tag	UNP A0A069B9A4
I	264	LYS	-	expression tag	UNP A0A069B9A4
I	265	LEU	-	expression tag	UNP A0A069B9A4
I	266	ALA	-	expression tag	UNP A0A069B9A4
I	267	ALA	-	expression tag	UNP A0A069B9A4
I	268	ALA	-	expression tag	UNP A0A069B9A4
I	269	LEU	-	expression tag	UNP A0A069B9A4
I	270	GLU	-	expression tag	UNP A0A069B9A4
I	271	HIS	-	expression tag	UNP A0A069B9A4
I	272	HIS	-	expression tag	UNP A0A069B9A4
I	273	HIS	-	expression tag	UNP A0A069B9A4
I	274	HIS	-	expression tag	UNP A0A069B9A4
I	275	HIS	-	expression tag	UNP A0A069B9A4
I	276	HIS	-	expression tag	UNP A0A069B9A4
K	264	LYS	-	expression tag	UNP A0A069B9A4
K	265	LEU	-	expression tag	UNP A0A069B9A4
K	266	ALA	-	expression tag	UNP A0A069B9A4
K	267	ALA	-	expression tag	UNP A0A069B9A4
K	268	ALA	-	expression tag	UNP A0A069B9A4
K	269	LEU	-	expression tag	UNP A0A069B9A4
K	270	GLU	-	expression tag	UNP A0A069B9A4
K	271	HIS	-	expression tag	UNP A0A069B9A4
K	272	HIS	-	expression tag	UNP A0A069B9A4
K	273	HIS	-	expression tag	UNP A0A069B9A4
K	274	HIS	-	expression tag	UNP A0A069B9A4
K	275	HIS	-	expression tag	UNP A0A069B9A4
K	276	HIS	-	expression tag	UNP A0A069B9A4
L	264	LYS	-	expression tag	UNP A0A069B9A4

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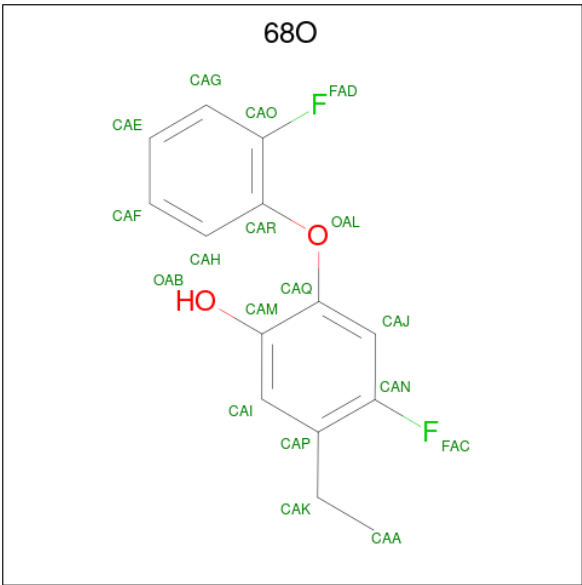
Chain	Residue	Modelled	Actual	Comment	Reference
L	265	LEU	-	expression tag	UNP A0A069B9A4
L	266	ALA	-	expression tag	UNP A0A069B9A4
L	267	ALA	-	expression tag	UNP A0A069B9A4
L	268	ALA	-	expression tag	UNP A0A069B9A4
L	269	LEU	-	expression tag	UNP A0A069B9A4
L	270	GLU	-	expression tag	UNP A0A069B9A4
L	271	HIS	-	expression tag	UNP A0A069B9A4
L	272	HIS	-	expression tag	UNP A0A069B9A4
L	273	HIS	-	expression tag	UNP A0A069B9A4
L	274	HIS	-	expression tag	UNP A0A069B9A4
L	275	HIS	-	expression tag	UNP A0A069B9A4
L	276	HIS	-	expression tag	UNP A0A069B9A4
J	264	LYS	-	expression tag	UNP A0A069B9A4
J	265	LEU	-	expression tag	UNP A0A069B9A4
J	266	ALA	-	expression tag	UNP A0A069B9A4
J	267	ALA	-	expression tag	UNP A0A069B9A4
J	268	ALA	-	expression tag	UNP A0A069B9A4
J	269	LEU	-	expression tag	UNP A0A069B9A4
J	270	GLU	-	expression tag	UNP A0A069B9A4
J	271	HIS	-	expression tag	UNP A0A069B9A4
J	272	HIS	-	expression tag	UNP A0A069B9A4
J	273	HIS	-	expression tag	UNP A0A069B9A4
J	274	HIS	-	expression tag	UNP A0A069B9A4
J	275	HIS	-	expression tag	UNP A0A069B9A4
J	276	HIS	-	expression tag	UNP A0A069B9A4

- 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	B	1	Total 71	C 21	H 27	N 7	O 14	P 2	0	0
2	E	1	Total 71	C 21	H 27	N 7	O 14	P 2	0	0
2	H	1	Total 71	C 21	H 27	N 7	O 14	P 2	0	0
2	C	1	Total 71	C 21	H 27	N 7	O 14	P 2	0	0
2	A	1	Total 71	C 21	H 27	N 7	O 14	P 2	0	0
2	F	1	Total 71	C 21	H 27	N 7	O 14	P 2	0	0
2	G	1	Total 71	C 21	H 27	N 7	O 14	P 2	0	0
2	D	1	Total 71	C 21	H 27	N 7	O 14	P 2	0	0
2	I	1	Total 71	C 21	H 27	N 7	O 14	P 2	0	0
2	K	1	Total 71	C 21	H 27	N 7	O 14	P 2	0	0
2	L	1	Total 71	C 21	H 27	N 7	O 14	P 2	0	0
2	J	1	Total 71	C 21	H 27	N 7	O 14	P 2	0	0

- Molecule 3 is 5-ethyl-4-fluoro-2-(2-fluorophenoxy)phenol (CCD ID: 68O) (formula: C₁₄H₁₂F₂O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	E	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	H	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	C	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	A	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	F	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	G	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	D	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	I	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	K	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	L	1	Total	C	F	H	O	0	0
			30	14	2	12	2		
3	J	1	Total	C	F	H	O	0	0
			30	14	2	12	2		

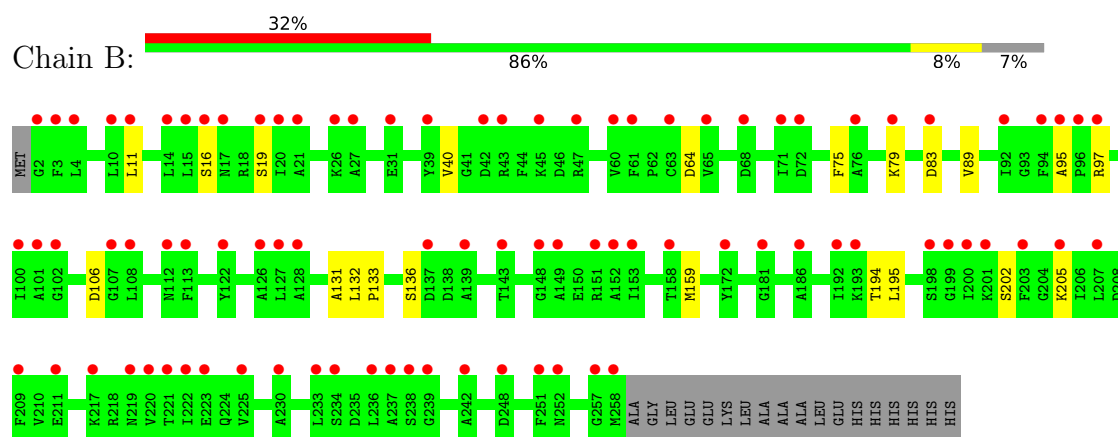
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	20	Total 20	O 20	0	0
4	E	22	Total 22	O 22	0	0
4	H	17	Total 17	O 17	0	0
4	C	13	Total 13	O 13	0	0
4	A	22	Total 22	O 22	0	0
4	F	24	Total 24	O 24	0	0
4	G	23	Total 23	O 23	0	0
4	D	32	Total 32	O 32	0	0
4	I	10	Total 10	O 10	0	0
4	K	18	Total 18	O 18	0	0
4	L	12	Total 12	O 12	0	0
4	J	20	Total 20	O 20	0	0

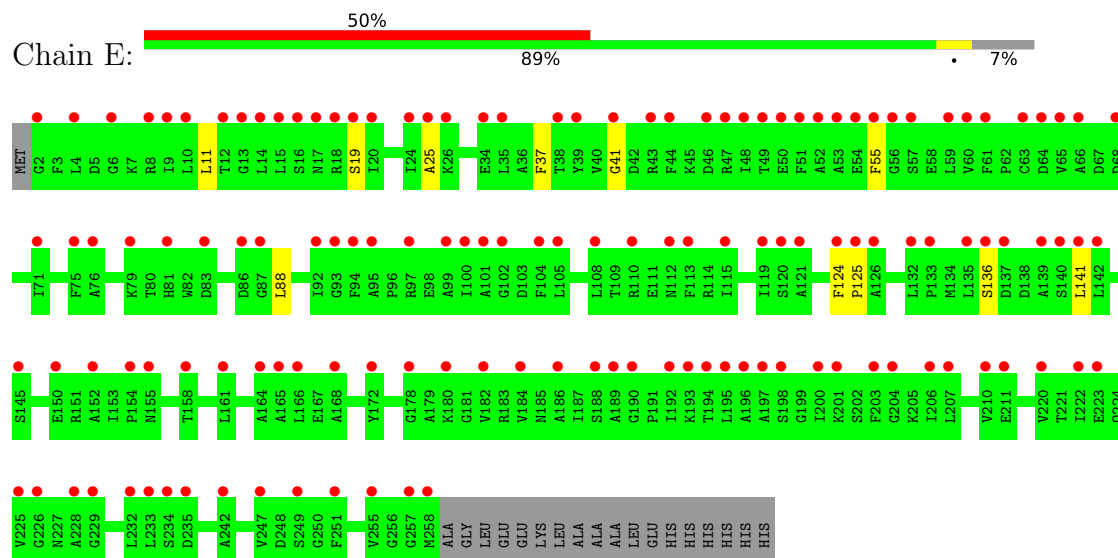
3 Residue-property plots

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.

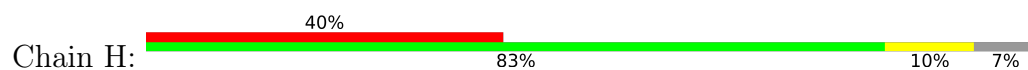
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

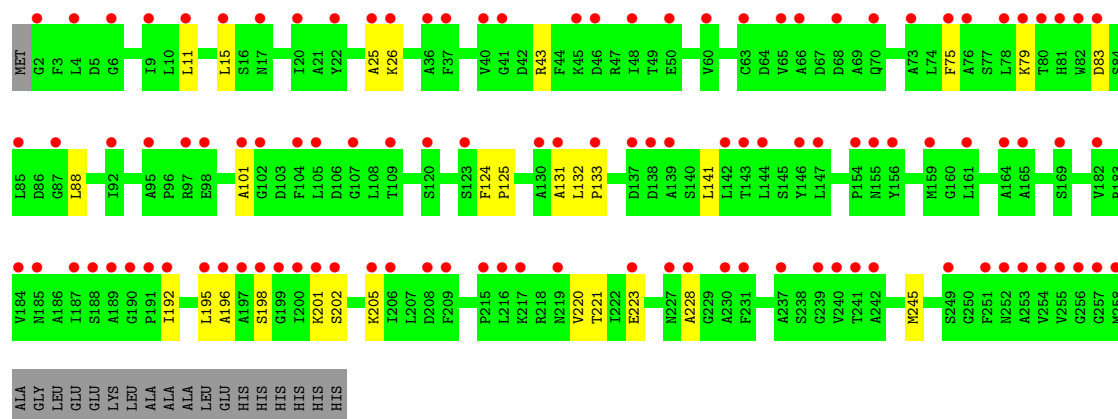


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

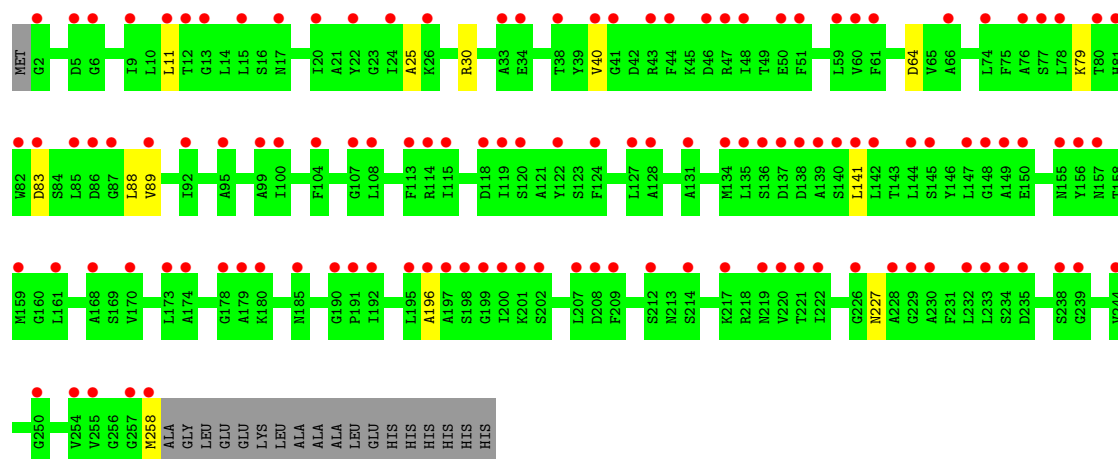
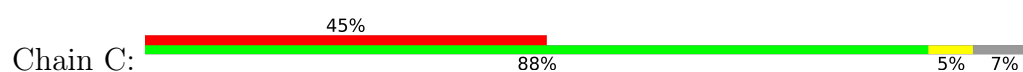


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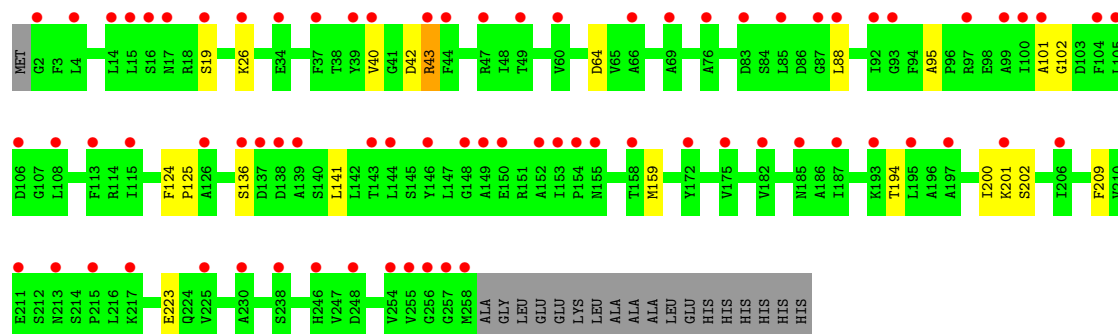
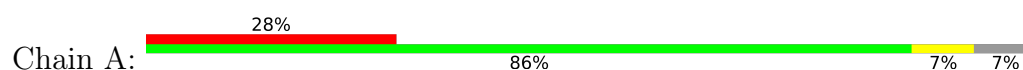




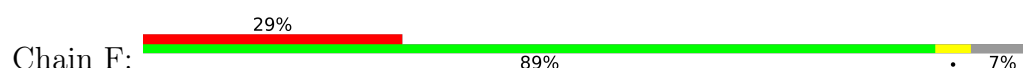
• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

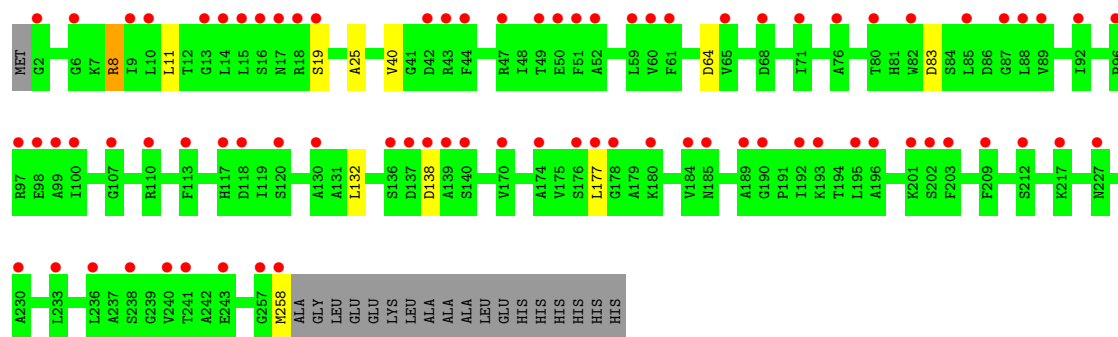


• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

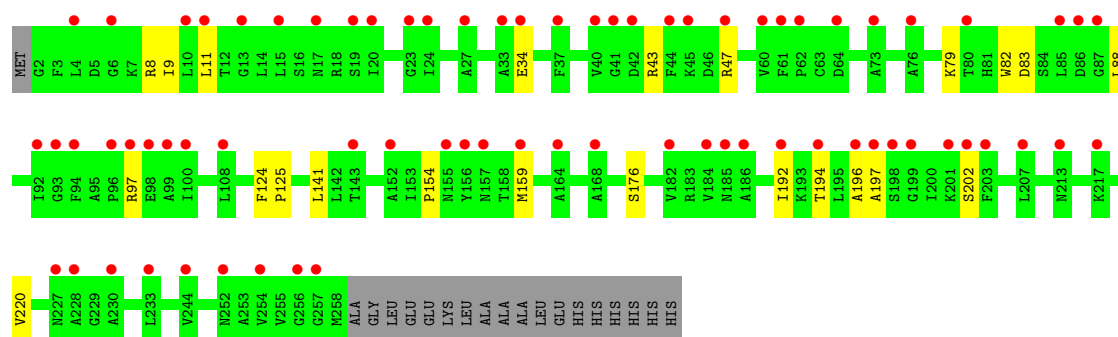
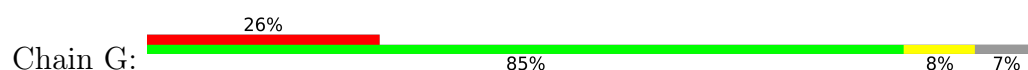


• Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

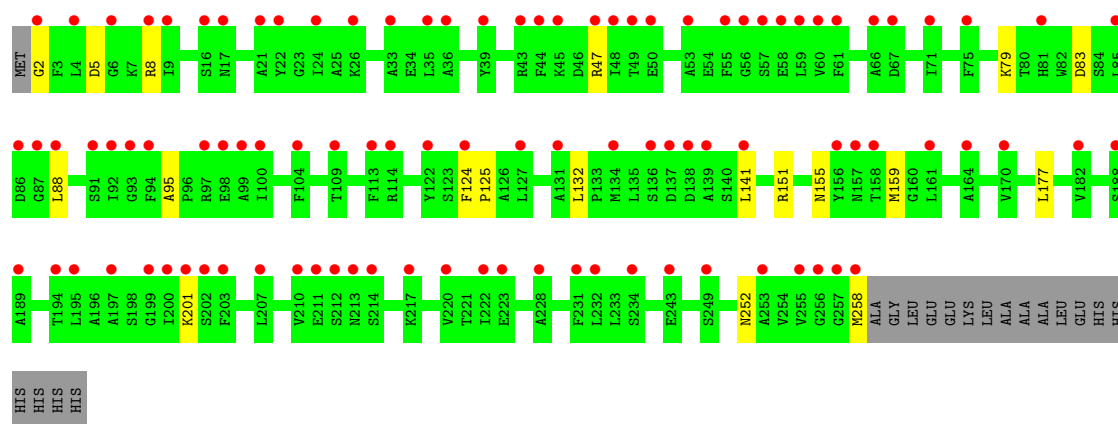
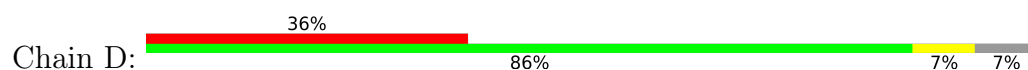




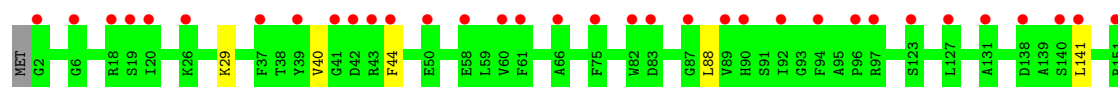
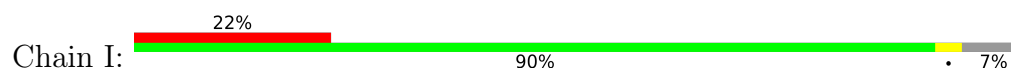
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

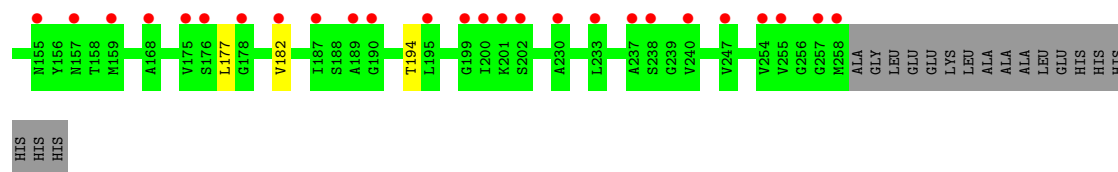


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



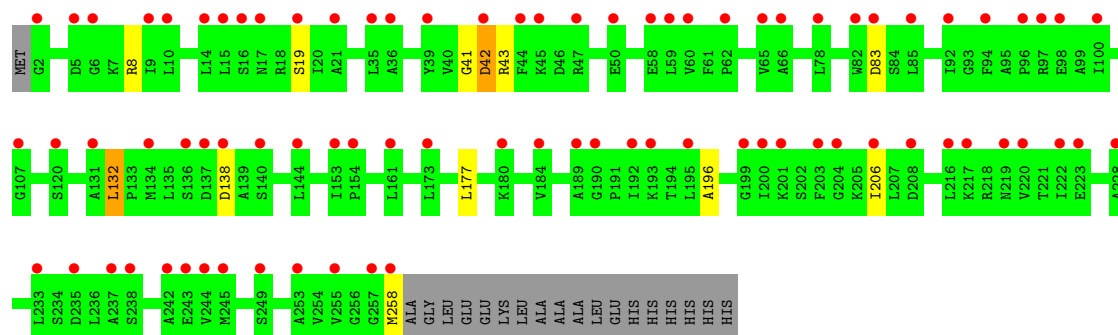
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]





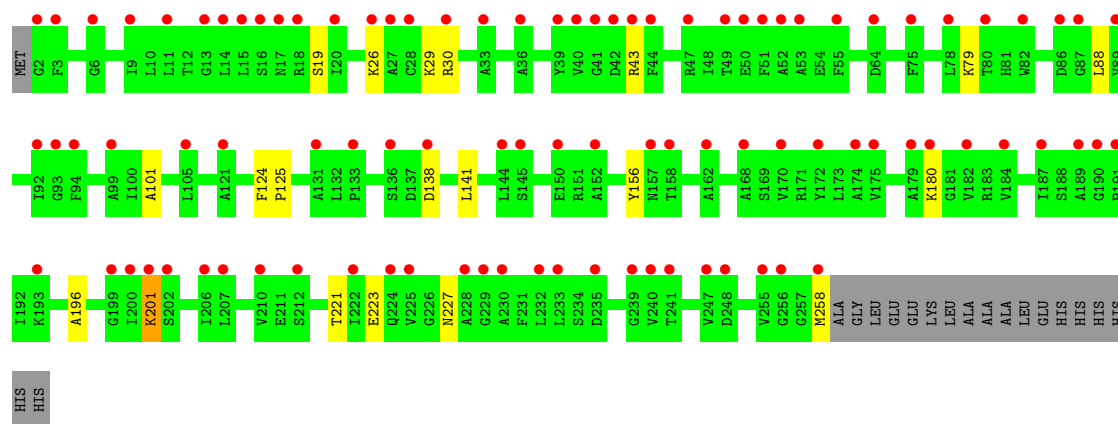
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain K:



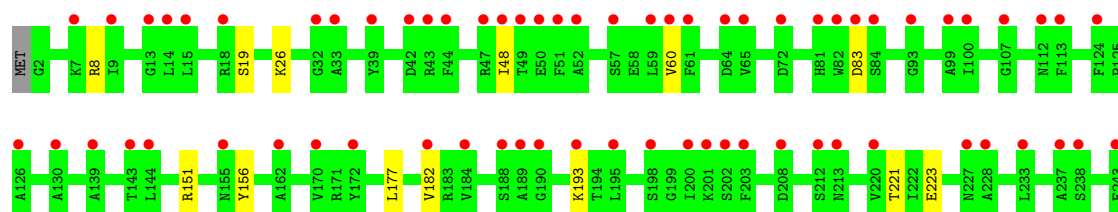
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain L:



- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

Chain J:



F251	N252	V253	V254	V255	C256	G257	F258	ALA	GLY	LEU	GLU	GLU	LYS	LEU	ALA	ALA	ALA	LEU	GLU	HIS	HIS	HIS	HIS
------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.43Å 109.78Å 269.80Å 90.00° 104.51° 90.00°	Depositor
Resolution (Å)	47.17 – 2.70 47.17 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.4 (47.17-2.70) 94.5 (47.17-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.192 , 0.223 0.479 , 0.504	Depositor DCC
R_{free} test set	4941 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	115.1	Xtrriage
Anisotropy	0.070	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.47$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	46664	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7678e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NAD, 68O

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	0.46	2/1945 (0.1%)	0.76	2/2631 (0.1%)
1	B	0.38	0/1945	0.70	0/2631
1	C	0.36	0/1945	0.71	0/2631
1	D	0.39	0/1945	0.70	0/2631
1	E	0.38	0/1953	0.69	1/2642 (0.0%)
1	F	0.39	0/1954	0.71	0/2642
1	G	0.38	0/1953	0.71	0/2642
1	H	0.38	0/1945	0.71	0/2631
1	I	0.38	0/1945	0.70	0/2631
1	J	0.38	0/1954	0.70	0/2642
1	K	0.40	0/1954	0.74	3/2642 (0.1%)
1	L	0.38	0/1945	0.71	1/2631 (0.0%)
All	All	0.39	2/23383 (0.0%)	0.71	7/31627 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	43	ARG	CZ-NH2	-6.74	1.24	1.33
1	A	43	ARG	CD-NE	-6.43	1.37	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	ARG	NE-CZ-NH2	-8.93	111.17	119.20
1	A	43	ARG	NE-CZ-NH1	6.98	128.48	121.50
1	K	132	LEU	CA-C-N	-6.04	113.39	119.56
1	K	132	LEU	C-N-CA	-6.04	113.39	119.56
1	K	41	GLY	N-CA-C	-5.30	106.00	112.68
1	E	41	GLY	N-CA-C	-5.27	105.01	112.81
1	L	201	LYS	N-CA-C	5.18	117.32	111.11

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	1912	1847	1919	15	0
1	B	1912	1842	1919	18	0
1	C	1912	1842	1919	7	0
1	D	1912	1847	1919	10	0
1	E	1917	1848	1923	7	0
1	F	1918	1859	1932	7	0
1	G	1917	1849	1923	12	0
1	H	1912	1847	1919	16	0
1	I	1912	1860	1919	4	0
1	J	1918	1891	1932	12	0
1	K	1918	1853	1932	7	0
1	L	1912	1862	1919	15	0
2	A	44	27	26	3	0
2	B	44	27	26	3	0
2	C	44	27	26	1	0
2	D	44	27	26	0	0
2	E	44	27	26	1	0
2	F	44	27	26	1	0
2	G	44	27	26	2	0
2	H	44	27	26	1	0
2	I	44	27	26	2	0
2	J	44	27	26	1	0
2	K	44	27	26	2	0
2	L	44	27	26	2	0
3	A	18	12	0	1	0
3	B	18	12	0	0	0
3	C	18	12	0	0	0
3	D	18	12	0	1	0
3	E	18	12	0	0	0
3	F	18	12	0	0	0
3	G	18	12	0	1	0
3	H	18	12	0	0	0
3	I	18	12	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	18	12	0	1	0
3	K	18	12	0	0	0
3	L	18	12	0	1	0
4	A	22	0	0	0	0
4	B	20	0	0	1	0
4	C	13	0	0	0	0
4	D	32	0	0	0	0
4	E	22	0	0	0	0
4	F	24	0	0	0	0
4	G	23	0	0	0	0
4	H	17	0	0	0	0
4	I	10	0	0	0	0
4	J	20	0	0	1	0
4	K	18	0	0	0	0
4	L	12	0	0	0	0
All	All	23949	22715	23387	125	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 (125) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:101:ALA:HB1	1:L:201:LYS:HD2	1.50	0.91
1:H:101:ALA:HB1	1:H:201:LYS:HD2	1.56	0.87
1:G:97:ARG:NH1	1:L:138:ASP:OD2	2.15	0.79
1:C:30:ARG:NH2	1:C:227:ASN:OD1	2.18	0.76
1:A:101:ALA:HB1	1:A:201:LYS:HD2	1.67	0.76
1:B:202:SER:HB3	1:B:205:LYS:HD2	1.68	0.75
1:H:79:LYS:NZ	1:H:83:ASP:O	2.23	0.72
1:C:79:LYS:NZ	1:C:83:ASP:O	2.25	0.69
1:G:79:LYS:NZ	1:G:83:ASP:O	2.27	0.67
1:L:101:ALA:CB	1:L:201:LYS:HD2	2.24	0.65
1:B:11:LEU:HD23	1:B:89:VAL:HB	1.80	0.63
1:D:79:LYS:NZ	1:D:83:ASP:O	2.32	0.63
1:D:155:ASN:ND2	1:D:201:LYS:O	2.32	0.62
2:I:301:NAD:O1N	2:I:301:NAD:H2N	1.99	0.62
1:J:19:SER:OG	2:J:301:NAD:O1A	2.18	0.61
1:B:97:ARG:NE	4:B:401:HOH:O	2.33	0.60
1:J:193:LYS:NZ	4:J:401:HOH:O	2.34	0.60
2:B:301:NAD:O1N	2:B:301:NAD:H2N	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:THR:HG21	2:B:301:NAD:O2N	2.04	0.58
1:A:194:THR:HG21	2:A:301:NAD:O2N	2.04	0.57
1:K:19:SER:OG	2:K:301:NAD:O1A	2.19	0.57
1:B:106:ASP:OD2	1:L:26:LYS:NZ	2.38	0.56
1:B:195:LEU:HG	1:J:83:ASP:OD2	2.06	0.56
1:C:11:LEU:HD23	1:C:89:VAL:HB	1.88	0.56
2:A:301:NAD:O1N	2:A:301:NAD:H2N	2.05	0.56
1:A:102:GLY:H	1:A:201:LYS:HD3	1.70	0.55
1:H:101:ALA:CB	1:H:201:LYS:HD2	2.33	0.55
1:F:19:SER:OG	2:F:301:NAD:O1A	2.21	0.55
1:H:202:SER:HB2	1:H:205:LYS:HD2	1.88	0.55
1:E:19:SER:OG	2:E:301:NAD:O1A	2.26	0.53
1:B:79:LYS:NZ	1:B:83:ASP:O	2.40	0.53
1:B:19:SER:OG	2:B:301:NAD:O1A	2.20	0.53
1:D:2:GLY:N	1:D:5:ASP:OD2	2.42	0.52
1:A:95:ALA:HB2	1:A:159:MET:CE	2.40	0.51
1:H:221:THR:HB	1:H:223:GLU:OE1	2.11	0.51
1:B:40:VAL:HG23	1:B:64:ASP:HB2	1.94	0.50
1:K:42:ASP:N	1:K:42:ASP:OD1	2.44	0.50
1:L:196:ALA:HB2	2:L:301:NAD:O2A	2.12	0.50
1:G:9:ILE:HG22	1:G:11:LEU:HD12	1.94	0.50
1:G:88:LEU:HB3	1:G:141:LEU:HD22	1.94	0.49
1:I:194:THR:HG21	2:I:301:NAD:O2N	2.12	0.49
1:J:156:TYR:OH	3:J:302:68O:OAB	2.23	0.49
1:K:138:ASP:OD1	1:K:138:ASP:N	2.45	0.49
1:L:88:LEU:HB3	1:L:141:LEU:HD22	1.94	0.49
1:J:8:ARG:HH12	1:J:83:ASP:HB3	1.76	0.49
1:L:221:THR:HB	1:L:223:GLU:OE1	2.14	0.48
1:C:11:LEU:HD13	1:C:25:ALA:HB2	1.96	0.47
1:G:47:ARG:CZ	1:L:79:LYS:HE2	2.44	0.47
1:F:11:LEU:CD2	1:F:25:ALA:HB2	2.45	0.47
1:J:151:ARG:NH2	1:J:252:ASN:O	2.47	0.47
1:H:88:LEU:HB3	1:H:141:LEU:HD22	1.96	0.47
1:F:8:ARG:HH22	1:F:83:ASP:H	1.63	0.47
1:G:192:ILE:HD11	1:G:220:VAL:HG23	1.97	0.47
1:B:16:SER:HB2	1:J:83:ASP:OD1	2.14	0.47
1:D:88:LEU:HB3	1:D:141:LEU:HD22	1.97	0.47
1:H:195:LEU:O	1:H:198:SER:OG	2.28	0.47
1:H:196:ALA:HB2	2:H:301:NAD:O2A	2.15	0.47
1:A:40:VAL:HG23	1:A:64:ASP:HB2	1.98	0.46
1:C:40:VAL:HG23	1:C:64:ASP:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:48:ILE:HG23	1:J:60:VAL:HG11	1.96	0.46
1:K:196:ALA:HB2	2:K:301:NAD:O2A	2.15	0.46
1:L:156:TYR:OH	3:L:302:68O:OAB	2.26	0.46
1:B:16:SER:CB	1:J:83:ASP:OD1	2.64	0.46
1:A:26:LYS:NZ	1:A:223:GLU:OE2	2.49	0.46
2:G:301:NAD:H2N	2:G:301:NAD:O1N	2.16	0.46
1:E:25:ALA:HB1	1:E:55:PHE:CE2	2.51	0.46
1:L:19:SER:OG	2:L:301:NAD:O1A	2.23	0.46
1:D:151:ARG:NH2	1:D:252:ASN:O	2.46	0.45
1:H:26:LYS:NZ	1:H:223:GLU:HG3	2.30	0.45
1:D:132:LEU:HD13	1:D:177:LEU:HD22	1.98	0.45
1:H:192:ILE:HD11	1:H:220:VAL:HG23	1.99	0.45
1:B:11:LEU:HD23	1:B:89:VAL:CB	2.46	0.45
1:G:34:GLU:HG2	1:G:82:TRP:HZ2	1.81	0.45
1:B:202:SER:HB3	1:B:205:LYS:CD	2.44	0.44
1:C:196:ALA:HB2	2:C:301:NAD:O2A	2.17	0.44
1:A:101:ALA:CB	1:A:201:LYS:HD2	2.43	0.44
1:A:42:ASP:O	1:A:43:ARG:HB3	2.18	0.44
1:G:196:ALA:HB2	2:G:301:NAD:O2A	2.17	0.44
1:I:88:LEU:HB3	1:I:141:LEU:HD22	1.99	0.44
1:F:40:VAL:HG23	1:F:64:ASP:HB2	1.99	0.44
1:F:132:LEU:HD13	1:F:177:LEU:HD22	2.01	0.43
1:D:95:ALA:HB2	1:D:159:MET:CE	2.49	0.43
1:E:88:LEU:HB3	1:E:141:LEU:HD22	1.99	0.43
1:F:258:MET:HE3	1:G:154:PRO:HD2	2.00	0.43
1:B:11:LEU:HD23	1:B:89:VAL:CG2	2.48	0.43
1:A:26:LYS:NZ	1:A:223:GLU:HG3	2.34	0.43
1:J:221:THR:HB	1:J:223:GLU:OE1	2.19	0.43
1:H:11:LEU:CD2	1:H:25:ALA:HB2	2.49	0.42
1:A:64:ASP:OD1	2:A:301:NAD:N6A	2.49	0.42
1:D:159:MET:HE3	3:D:302:68O:CAE	2.48	0.42
1:G:159:MET:HE3	3:G:302:68O:CAE	2.50	0.42
1:L:30:ARG:NH2	1:L:227:ASN:OD1	2.46	0.42
1:A:201:LYS:HB3	1:A:201:LYS:HE3	1.86	0.42
1:B:11:LEU:CD2	1:B:89:VAL:HG21	2.49	0.42
1:C:88:LEU:HB3	1:C:141:LEU:HD22	2.00	0.42
1:A:88:LEU:HB3	1:A:141:LEU:HD22	2.02	0.42
1:H:75:PHE:CZ	1:H:131:ALA:HB2	2.55	0.41
1:K:8:ARG:HH12	1:K:83:ASP:HB3	1.85	0.41
1:L:101:ALA:HA	1:L:201:LYS:HD3	2.01	0.41
1:E:37:PHE:HZ	1:E:55:PHE:HD2	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:PHE:HB3	1:E:125:PRO:CD	2.50	0.41
1:I:40:VAL:O	1:I:44:PHE:HD2	2.03	0.41
1:L:124:PHE:HB3	1:L:125:PRO:CD	2.49	0.41
1:H:228:ALA:HB1	1:H:245:MET:HE1	2.02	0.41
1:G:194:THR:O	1:G:197:ALA:HB3	2.20	0.41
1:K:132:LEU:HD13	1:K:177:LEU:HD22	2.01	0.41
1:K:206:ILE:HG12	1:L:258:MET:SD	2.61	0.41
1:H:15:LEU:HD23	1:H:195:LEU:HD12	2.02	0.41
1:B:132:LEU:N	1:B:133:PRO:CD	2.84	0.41
1:J:223:GLU:OE1	1:J:223:GLU:N	2.47	0.41
1:B:75:PHE:CZ	1:B:131:ALA:HB2	2.56	0.41
1:A:209:PHE:CG	1:D:258:MET:HG2	2.56	0.41
1:L:138:ASP:OD1	1:L:138:ASP:N	2.50	0.41
1:E:37:PHE:CZ	1:E:55:PHE:HD2	2.39	0.41
1:A:124:PHE:HB3	1:A:125:PRO:CD	2.51	0.41
1:A:200:ILE:HD12	3:A:302:68O:CAN	2.50	0.41
1:H:124:PHE:HB3	1:H:125:PRO:CD	2.51	0.41
1:D:124:PHE:HB3	1:D:125:PRO:CD	2.51	0.41
1:F:138:ASP:OD1	1:F:138:ASP:N	2.53	0.40
1:I:177:LEU:HB3	1:I:182:VAL:HB	2.03	0.40
1:B:95:ALA:HB2	1:B:159:MET:HE1	2.04	0.40
1:E:11:LEU:HD13	1:E:25:ALA:HB2	2.04	0.40
1:J:177:LEU:HB3	1:J:182:VAL:HB	2.03	0.40
1:H:132:LEU:HB3	1:H:133:PRO:HD3	2.04	0.40
1:G:124:PHE:HB3	1:G:125:PRO:CD	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	255/276 (92%)	241 (94%)	13 (5%)	1 (0%)	30 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	255/276 (92%)	243 (95%)	12 (5%)	0	100	100
1	C	255/276 (92%)	241 (94%)	14 (6%)	0	100	100
1	D	255/276 (92%)	244 (96%)	11 (4%)	0	100	100
1	E	256/276 (93%)	244 (95%)	12 (5%)	0	100	100
1	F	256/276 (93%)	243 (95%)	13 (5%)	0	100	100
1	G	256/276 (93%)	242 (94%)	13 (5%)	1 (0%)	30	54
1	H	255/276 (92%)	243 (95%)	12 (5%)	0	100	100
1	I	255/276 (92%)	243 (95%)	12 (5%)	0	100	100
1	J	256/276 (93%)	245 (96%)	11 (4%)	0	100	100
1	K	256/276 (93%)	245 (96%)	11 (4%)	0	100	100
1	L	255/276 (92%)	243 (95%)	12 (5%)	0	100	100
All	All	3065/3312 (92%)	2917 (95%)	146 (5%)	2 (0%)	48	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	202	SER
1	A	202	SER

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	195/209 (93%)	193 (99%)	2 (1%)	68	86
1	B	195/209 (93%)	194 (100%)	1 (0%)	81	92
1	C	195/209 (93%)	194 (100%)	1 (0%)	81	92
1	D	195/209 (93%)	193 (99%)	2 (1%)	68	86
1	E	196/209 (94%)	195 (100%)	1 (0%)	81	92
1	F	196/209 (94%)	195 (100%)	1 (0%)	81	92
1	G	196/209 (94%)	193 (98%)	3 (2%)	57	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	195/209 (93%)	194 (100%)	1 (0%)	81	92
1	I	195/209 (93%)	194 (100%)	1 (0%)	81	92
1	J	196/209 (94%)	195 (100%)	1 (0%)	81	92
1	K	196/209 (94%)	193 (98%)	3 (2%)	57	81
1	L	195/209 (93%)	192 (98%)	3 (2%)	57	81
All	All	2345/2508 (94%)	2325 (99%)	20 (1%)	70	87

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	136	SER
1	E	136	SER
1	H	43	ARG
1	C	258	MET
1	A	19	SER
1	A	136	SER
1	F	8	ARG
1	G	8	ARG
1	G	43	ARG
1	G	176	SER
1	D	8	ARG
1	D	47	ARG
1	I	29	LYS
1	K	42	ASP
1	K	43	ARG
1	K	258	MET
1	L	29	LYS
1	L	43	ARG
1	L	180	LYS
1	J	26	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	219	ASN
1	H	117	HIS
1	H	155	ASN
1	H	252	ASN
1	C	81	HIS

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Mol	Chain	Res	Type
1	C	117	HIS
1	C	155	ASN
1	C	219	ASN
1	C	252	ASN
1	F	219	ASN
1	F	252	ASN
1	G	252	ASN
1	D	219	ASN
1	D	252	ASN
1	I	117	HIS
1	I	219	ASN
1	L	117	HIS
1	L	219	ASN
1	L	252	ASN
1	J	117	HIS
1	J	219	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](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	G	301	-	46,48,48	0.97	3 (6%)	64,73,73	0.70	1 (1%)
2	NAD	L	301	-	46,48,48	1.02	3 (6%)	64,73,73	0.71	1 (1%)
3	68O	D	302	-	19,19,19	1.38	2 (10%)	26,26,26	1.39	5 (19%)
3	68O	H	302	-	19,19,19	1.27	1 (5%)	26,26,26	1.30	3 (11%)
2	NAD	H	301	-	46,48,48	1.18	3 (6%)	64,73,73	0.81	3 (4%)
3	68O	J	302	-	19,19,19	1.25	1 (5%)	26,26,26	1.18	3 (11%)
3	68O	B	302	-	19,19,19	1.27	1 (5%)	26,26,26	1.24	3 (11%)
2	NAD	E	301	-	46,48,48	1.07	3 (6%)	64,73,73	0.71	1 (1%)
2	NAD	D	301	-	46,48,48	1.07	3 (6%)	64,73,73	0.73	1 (1%)
2	NAD	B	301	-	46,48,48	1.08	3 (6%)	64,73,73	0.73	2 (3%)
3	68O	C	302	-	19,19,19	1.34	2 (10%)	26,26,26	1.25	2 (7%)
3	68O	A	302	-	19,19,19	1.25	1 (5%)	26,26,26	1.28	3 (11%)
3	68O	K	302	-	19,19,19	1.24	1 (5%)	26,26,26	1.56	7 (26%)
3	68O	L	302	-	19,19,19	1.22	1 (5%)	26,26,26	1.29	3 (11%)
2	NAD	F	301	-	46,48,48	1.22	3 (6%)	64,73,73	0.68	1 (1%)
3	68O	F	302	-	19,19,19	1.24	1 (5%)	26,26,26	1.31	3 (11%)
3	68O	E	302	-	19,19,19	1.24	1 (5%)	26,26,26	1.29	3 (11%)
3	68O	I	302	-	19,19,19	1.23	1 (5%)	26,26,26	1.30	3 (11%)
2	NAD	C	301	-	46,48,48	1.12	3 (6%)	64,73,73	0.76	1 (1%)
2	NAD	J	301	-	46,48,48	1.23	3 (6%)	64,73,73	0.78	2 (3%)
2	NAD	I	301	-	46,48,48	1.13	3 (6%)	64,73,73	0.74	1 (1%)
2	NAD	K	301	-	46,48,48	1.18	3 (6%)	64,73,73	0.73	1 (1%)
3	68O	G	302	-	19,19,19	1.27	1 (5%)	26,26,26	1.33	3 (11%)
2	NAD	A	301	-	46,48,48	1.13	3 (6%)	64,73,73	0.78	2 (3%)

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	G	301	-	-	2/30/62/62	0/5/5/5
2	NAD	L	301	-	-	5/30/62/62	0/5/5/5
3	68O	D	302	-	-	0/6/6/6	0/2/2/2
3	68O	H	302	-	-	0/6/6/6	0/2/2/2
2	NAD	H	301	-	-	8/30/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	68O	J	302	-	-	0/6/6/6	0/2/2/2
3	68O	B	302	-	-	0/6/6/6	0/2/2/2
2	NAD	E	301	-	-	5/30/62/62	0/5/5/5
2	NAD	D	301	-	-	4/30/62/62	0/5/5/5
2	NAD	B	301	-	-	5/30/62/62	0/5/5/5
3	68O	C	302	-	-	0/6/6/6	0/2/2/2
3	68O	A	302	-	-	0/6/6/6	0/2/2/2
3	68O	K	302	-	-	2/6/6/6	0/2/2/2
3	68O	L	302	-	-	0/6/6/6	0/2/2/2
2	NAD	F	301	-	-	7/30/62/62	0/5/5/5
3	68O	F	302	-	-	0/6/6/6	0/2/2/2
3	68O	E	302	-	-	0/6/6/6	0/2/2/2
3	68O	I	302	-	-	0/6/6/6	0/2/2/2
2	NAD	C	301	-	-	7/30/62/62	0/5/5/5
2	NAD	J	301	-	-	14/30/62/62	0/5/5/5
2	NAD	I	301	-	-	3/30/62/62	0/5/5/5
2	NAD	K	301	-	-	7/30/62/62	0/5/5/5
3	68O	G	302	-	-	0/6/6/6	0/2/2/2
2	NAD	A	301	-	-	5/30/62/62	0/5/5/5

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	NAD	PA-O3	-6.02	1.53	1.59
2	J	301	NAD	PA-O3	-5.85	1.53	1.59
2	I	301	NAD	PA-O3	-5.63	1.53	1.59
2	K	301	NAD	PA-O3	-5.61	1.53	1.59
2	A	301	NAD	PA-O3	-5.47	1.53	1.59
2	H	301	NAD	PA-O3	-5.25	1.53	1.59
2	B	301	NAD	PA-O3	-4.99	1.54	1.59
2	D	301	NAD	PA-O3	-4.95	1.54	1.59
2	C	301	NAD	PA-O3	-4.91	1.54	1.59
2	L	301	NAD	PA-O3	-4.86	1.54	1.59
3	G	302	68O	CAK-CAP	-4.76	1.39	1.51
3	I	302	68O	CAK-CAP	-4.63	1.39	1.51
3	D	302	68O	CAK-CAP	-4.61	1.39	1.51
3	H	302	68O	CAK-CAP	-4.60	1.39	1.51
3	A	302	68O	CAK-CAP	-4.57	1.39	1.51
2	G	301	NAD	PA-O3	-4.56	1.54	1.59
3	B	302	68O	CAK-CAP	-4.53	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	302	68O	CAK-CAP	-4.52	1.39	1.51
2	E	301	NAD	PA-O3	-4.51	1.54	1.59
3	J	302	68O	CAK-CAP	-4.48	1.39	1.51
2	K	301	NAD	C2N-N1N	4.46	1.39	1.35
2	J	301	NAD	C2N-N1N	4.44	1.39	1.35
3	F	302	68O	CAK-CAP	-4.41	1.39	1.51
2	D	301	NAD	C2N-N1N	4.32	1.39	1.35
2	A	301	NAD	C2N-N1N	4.32	1.39	1.35
3	E	302	68O	CAK-CAP	-4.29	1.40	1.51
3	K	302	68O	CAK-CAP	-4.26	1.40	1.51
3	C	302	68O	CAK-CAP	-4.23	1.40	1.51
2	C	301	NAD	C2N-N1N	4.16	1.39	1.35
2	E	301	NAD	C2N-N1N	4.04	1.39	1.35
2	I	301	NAD	C2N-N1N	4.04	1.39	1.35
2	B	301	NAD	C2N-N1N	4.02	1.39	1.35
2	H	301	NAD	C2N-N1N	3.94	1.39	1.35
2	H	301	NAD	O4D-C1D	-3.93	1.35	1.40
2	L	301	NAD	C2N-N1N	3.82	1.39	1.35
2	F	301	NAD	C2N-N1N	3.80	1.39	1.35
2	F	301	NAD	O4D-C1D	-3.60	1.36	1.40
2	G	301	NAD	C2N-N1N	3.55	1.38	1.35
2	C	301	NAD	O4D-C1D	-3.36	1.36	1.40
2	E	301	NAD	O4D-C1D	-3.33	1.36	1.40
2	J	301	NAD	O4D-C1D	-3.08	1.36	1.40
2	K	301	NAD	O4D-C1D	-2.75	1.37	1.40
2	B	301	NAD	O4D-C1D	-2.69	1.37	1.40
3	C	302	68O	FAC-CAN	-2.69	1.28	1.35
3	D	302	68O	FAC-CAN	-2.52	1.28	1.35
2	A	301	NAD	O4D-C1D	-2.28	1.37	1.40
2	I	301	NAD	O4D-C1D	-2.26	1.37	1.40
2	G	301	NAD	O4D-C1D	-2.18	1.38	1.40
2	L	301	NAD	O4D-C1D	-2.16	1.38	1.40
2	D	301	NAD	O4D-C1D	-2.10	1.38	1.40

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	302	68O	CAI-CAP-CAN	3.23	120.10	116.54
2	C	301	NAD	O3-PA-O1A	3.19	120.30	110.70
3	K	302	68O	FAC-CAN-CAP	3.19	123.27	117.96
2	H	301	NAD	O3-PA-O1A	3.11	120.06	110.70
3	I	302	68O	CAI-CAP-CAN	3.11	119.96	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	NAD	O3-PA-O1A	3.08	119.96	110.70
3	B	302	68O	CAI-CAP-CAN	3.06	119.91	116.54
3	H	302	68O	CAI-CAP-CAN	3.06	119.90	116.54
3	L	302	68O	CAI-CAP-CAN	3.03	119.88	116.54
2	J	301	NAD	O2A-PA-O3	-3.03	99.09	107.27
2	I	301	NAD	O3-PA-O1A	3.01	119.75	110.70
3	A	302	68O	CAI-CAP-CAN	3.00	119.84	116.54
3	D	302	68O	CAI-CAP-CAN	2.99	119.83	116.54
3	F	302	68O	CAI-CAP-CAN	2.99	119.82	116.54
2	G	301	NAD	O3-PA-O1A	2.97	119.63	110.70
2	L	301	NAD	O3-PA-O1A	2.96	119.60	110.70
2	B	301	NAD	O3-PA-O1A	2.94	119.53	110.70
2	J	301	NAD	O3-PA-O1A	2.91	119.45	110.70
2	K	301	NAD	O3-PA-O1A	2.79	119.09	110.70
3	J	302	68O	CAI-CAP-CAN	2.78	119.60	116.54
3	K	302	68O	CAK-CAP-CAN	2.78	126.12	122.30
3	K	302	68O	CAQ-OAL-CAR	-2.77	111.48	118.09
2	D	301	NAD	O3-PA-O1A	2.69	118.81	110.70
2	A	301	NAD	O3-PA-O1A	2.68	118.76	110.70
2	F	301	NAD	O3-PA-O1A	2.63	118.61	110.70
3	C	302	68O	CAI-CAP-CAN	2.61	119.41	116.54
3	E	302	68O	CAI-CAP-CAN	2.50	119.29	116.54
3	A	302	68O	OAL-CAR-CAO	-2.48	114.22	119.33
3	K	302	68O	CAJ-CAN-CAP	-2.41	120.04	123.76
3	L	302	68O	OAL-CAR-CAO	-2.40	114.37	119.33
3	B	302	68O	OAL-CAR-CAO	-2.35	114.48	119.33
3	I	302	68O	OAL-CAR-CAO	-2.32	114.54	119.33
3	L	302	68O	CAJ-CAN-CAP	-2.29	120.23	123.76
3	K	302	68O	CAI-CAP-CAN	2.25	119.01	116.54
3	K	302	68O	CAK-CAP-CAI	-2.24	114.85	119.68
3	G	302	68O	OAL-CAR-CAO	-2.22	114.75	119.33
3	F	302	68O	OAL-CAR-CAO	-2.22	114.76	119.33
3	H	302	68O	OAL-CAR-CAO	-2.21	114.77	119.33
2	A	301	NAD	C4B-O4B-C1B	-2.20	104.60	109.47
3	C	302	68O	OAL-CAR-CAO	-2.19	114.81	119.33
3	B	302	68O	CAJ-CAN-CAP	-2.18	120.40	123.76
3	D	302	68O	OAL-CAR-CAO	-2.16	114.87	119.33
2	B	301	NAD	O2A-PA-O3	-2.16	101.43	107.27
3	I	302	68O	CAJ-CAN-CAP	-2.15	120.44	123.76
3	E	302	68O	OAL-CAR-CAO	-2.15	114.89	119.33
2	H	301	NAD	C4B-O4B-C1B	-2.15	104.72	109.47
3	H	302	68O	CAJ-CAN-CAP	-2.14	120.46	123.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	302	68O	CAJ-CAN-CAP	-2.14	120.46	123.76
2	H	301	NAD	O2A-PA-O3	-2.14	101.50	107.27
3	D	302	68O	CAG-CAO-CAR	-2.12	119.84	122.11
3	J	302	68O	CAJ-CAN-CAP	-2.11	120.51	123.76
3	D	302	68O	CAM-CAI-CAP	-2.08	118.52	121.52
3	A	302	68O	CAJ-CAN-CAP	-2.06	120.58	123.76
3	K	302	68O	OAL-CAR-CAO	-2.05	115.09	119.33
3	J	302	68O	OAL-CAR-CAO	-2.05	115.09	119.33
3	F	302	68O	CAJ-CAN-CAP	-2.05	120.61	123.76
3	E	302	68O	CAJ-CAN-CAP	-2.03	120.63	123.76
3	D	302	68O	FAD-CAO-CAR	2.00	120.87	118.01

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	NAD	C5B-O5B-PA-O2A
2	E	301	NAD	C5D-O5D-PN-O3
2	E	301	NAD	C5D-O5D-PN-O2N
2	H	301	NAD	PN-O3-PA-O5B
2	H	301	NAD	C5D-O5D-PN-O2N
2	C	301	NAD	C5B-O5B-PA-O2A
2	C	301	NAD	C5D-O5D-PN-O3
2	C	301	NAD	C5D-O5D-PN-O1N
2	C	301	NAD	C5D-O5D-PN-O2N
2	A	301	NAD	C5B-O5B-PA-O2A
2	F	301	NAD	PN-O3-PA-O5B
2	F	301	NAD	C5D-O5D-PN-O3
2	F	301	NAD	C5D-O5D-PN-O1N
2	F	301	NAD	C5D-O5D-PN-O2N
2	F	301	NAD	O4D-C1D-N1N-C2N
2	D	301	NAD	C5B-O5B-PA-O2A
2	K	301	NAD	C5D-O5D-PN-O2N
2	K	301	NAD	O4D-C1D-N1N-C2N
2	J	301	NAD	C5D-O5D-PN-O3
2	J	301	NAD	C5D-O5D-PN-O2N
2	J	301	NAD	O4D-C1D-N1N-C2N
2	J	301	NAD	O4D-C1D-N1N-C6N
3	K	302	68O	CAA-CAK-CAP-CAI
3	K	302	68O	CAA-CAK-CAP-CAN
2	B	301	NAD	O4D-C4D-C5D-O5D
2	J	301	NAD	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	B	301	NAD	C3D-C4D-C5D-O5D
2	I	301	NAD	O4D-C4D-C5D-O5D
2	I	301	NAD	C3D-C4D-C5D-O5D
2	J	301	NAD	O4B-C4B-C5B-O5B
2	G	301	NAD	C3D-C4D-C5D-O5D
2	L	301	NAD	C3D-C4D-C5D-O5D
2	B	301	NAD	PA-O3-PN-O5D
2	E	301	NAD	PN-O3-PA-O5B
2	C	301	NAD	PN-O3-PA-O5B
2	A	301	NAD	C3D-C4D-C5D-O5D
2	D	301	NAD	C3D-C4D-C5D-O5D
2	L	301	NAD	PA-O3-PN-O1N
2	G	301	NAD	O4D-C4D-C5D-O5D
2	B	301	NAD	C5B-O5B-PA-O1A
2	E	301	NAD	C5D-O5D-PN-O1N
2	H	301	NAD	C5B-O5B-PA-O1A
2	H	301	NAD	C5D-O5D-PN-O3
2	H	301	NAD	C5D-O5D-PN-O1N
2	C	301	NAD	C5B-O5B-PA-O1A
2	A	301	NAD	C5B-O5B-PA-O1A
2	D	301	NAD	C5B-O5B-PA-O1A
2	I	301	NAD	C5B-O5B-PA-O1A
2	K	301	NAD	C5D-O5D-PN-O3
2	K	301	NAD	C5D-O5D-PN-O1N
2	J	301	NAD	C5B-O5B-PA-O1A
2	J	301	NAD	C5B-O5B-PA-O2A
2	J	301	NAD	C5D-O5D-PN-O1N
2	L	301	NAD	O4D-C4D-C5D-O5D
2	J	301	NAD	C4B-C5B-O5B-PA
2	J	301	NAD	PA-O3-PN-O2N
2	J	301	NAD	C2D-C1D-N1N-C6N
2	E	301	NAD	O4D-C1D-N1N-C6N
2	H	301	NAD	O4D-C1D-N1N-C2N
2	H	301	NAD	O4D-C1D-N1N-C6N
2	A	301	NAD	O4D-C4D-C5D-O5D
2	F	301	NAD	O4D-C1D-N1N-C6N
2	K	301	NAD	O4D-C1D-N1N-C6N
2	L	301	NAD	PA-O3-PN-O2N
2	F	301	NAD	O4B-C4B-C5B-O5B
2	D	301	NAD	O4D-C4D-C5D-O5D
2	K	301	NAD	O4B-C4B-C5B-O5B
2	K	301	NAD	PA-O3-PN-O2N

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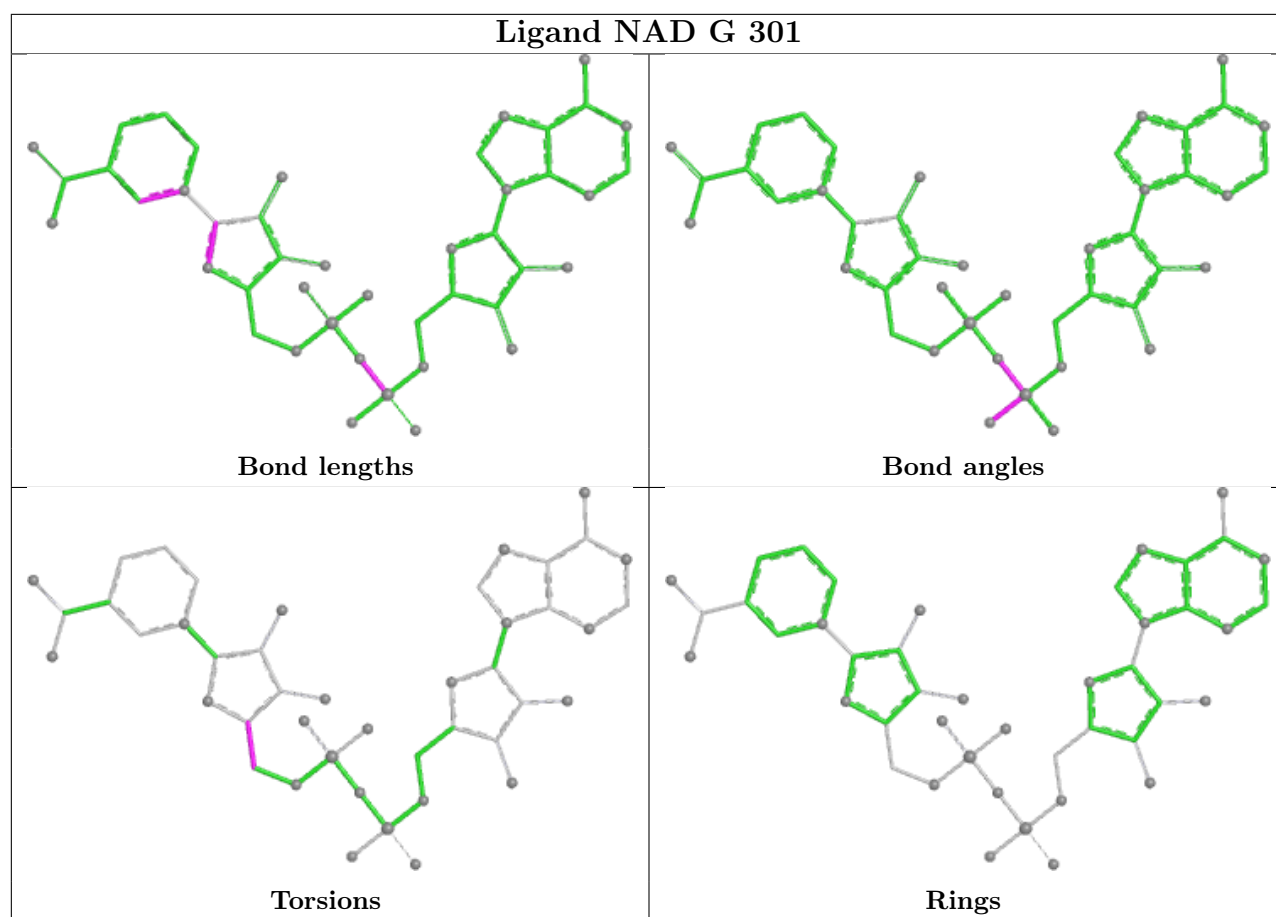
Mol	Chain	Res	Type	Atoms
2	J	301	NAD	PA-O3-PN-O1N
2	L	301	NAD	O4B-C4B-C5B-O5B
2	C	301	NAD	O4B-C4B-C5B-O5B
2	J	301	NAD	PN-O3-PA-O2A
2	H	301	NAD	O4B-C4B-C5B-O5B
2	A	301	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

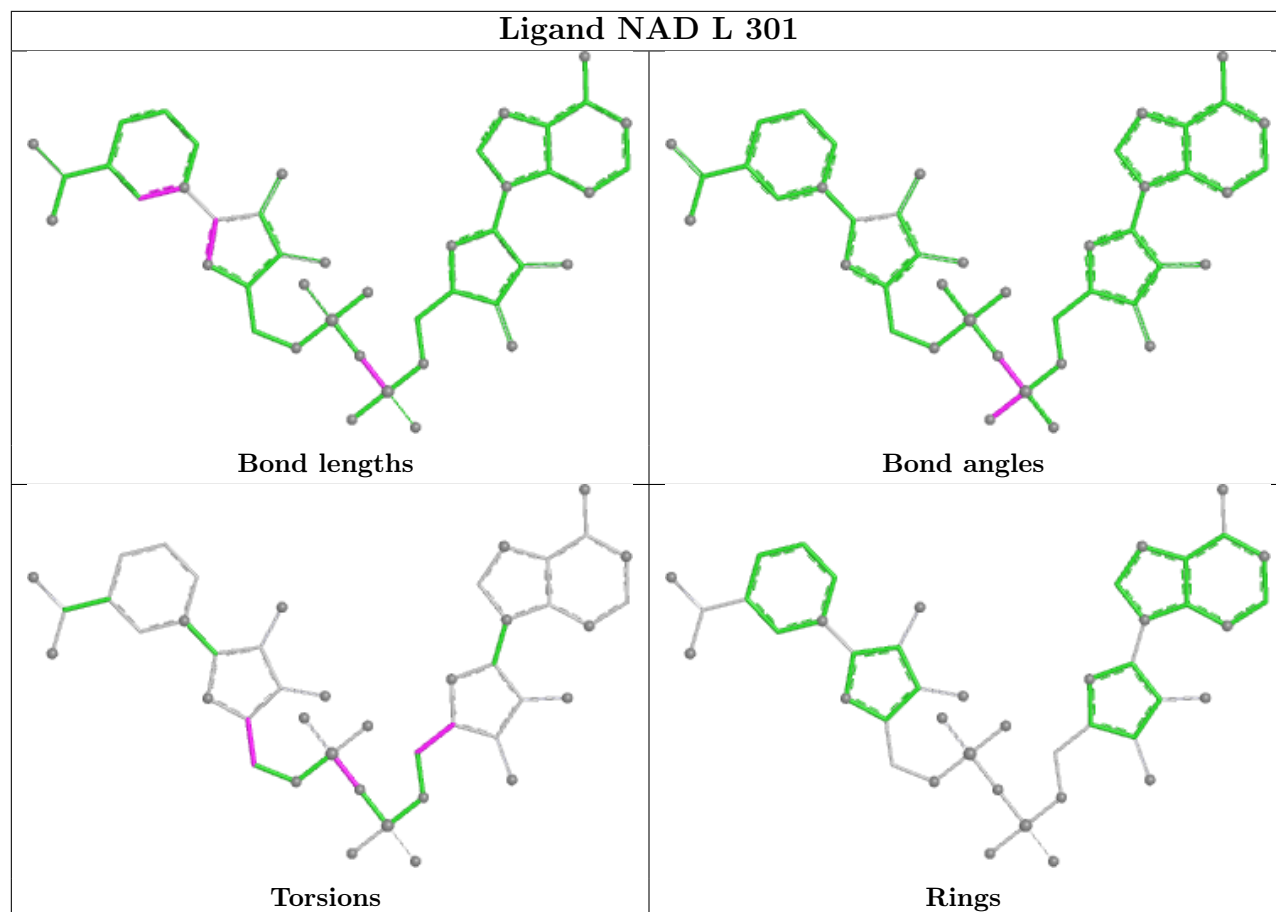
16 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	301	NAD	2	0
2	L	301	NAD	2	0
3	D	302	68O	1	0
2	H	301	NAD	1	0
3	J	302	68O	1	0
2	E	301	NAD	1	0
2	B	301	NAD	3	0
3	A	302	68O	1	0
3	L	302	68O	1	0
2	F	301	NAD	1	0
2	C	301	NAD	1	0
2	J	301	NAD	1	0
2	I	301	NAD	2	0
2	K	301	NAD	2	0
3	G	302	68O	1	0
2	A	301	NAD	3	0

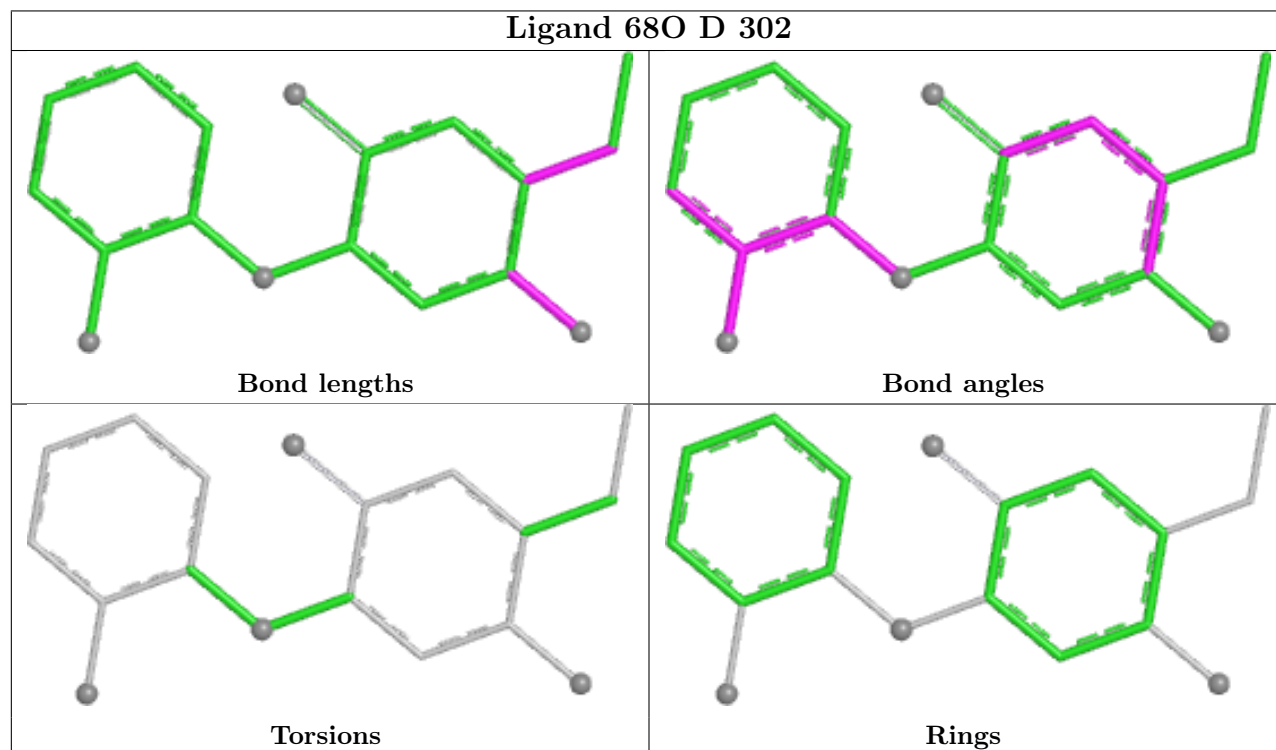
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



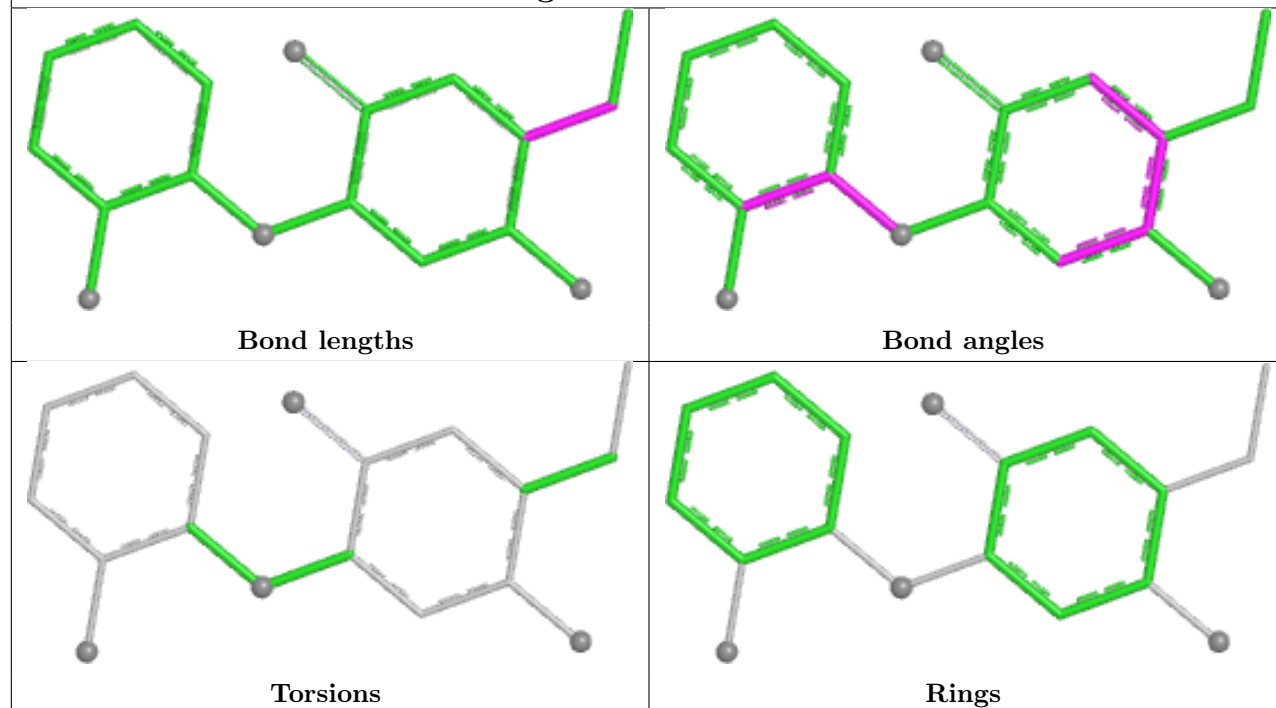
Ligand NAD L 301



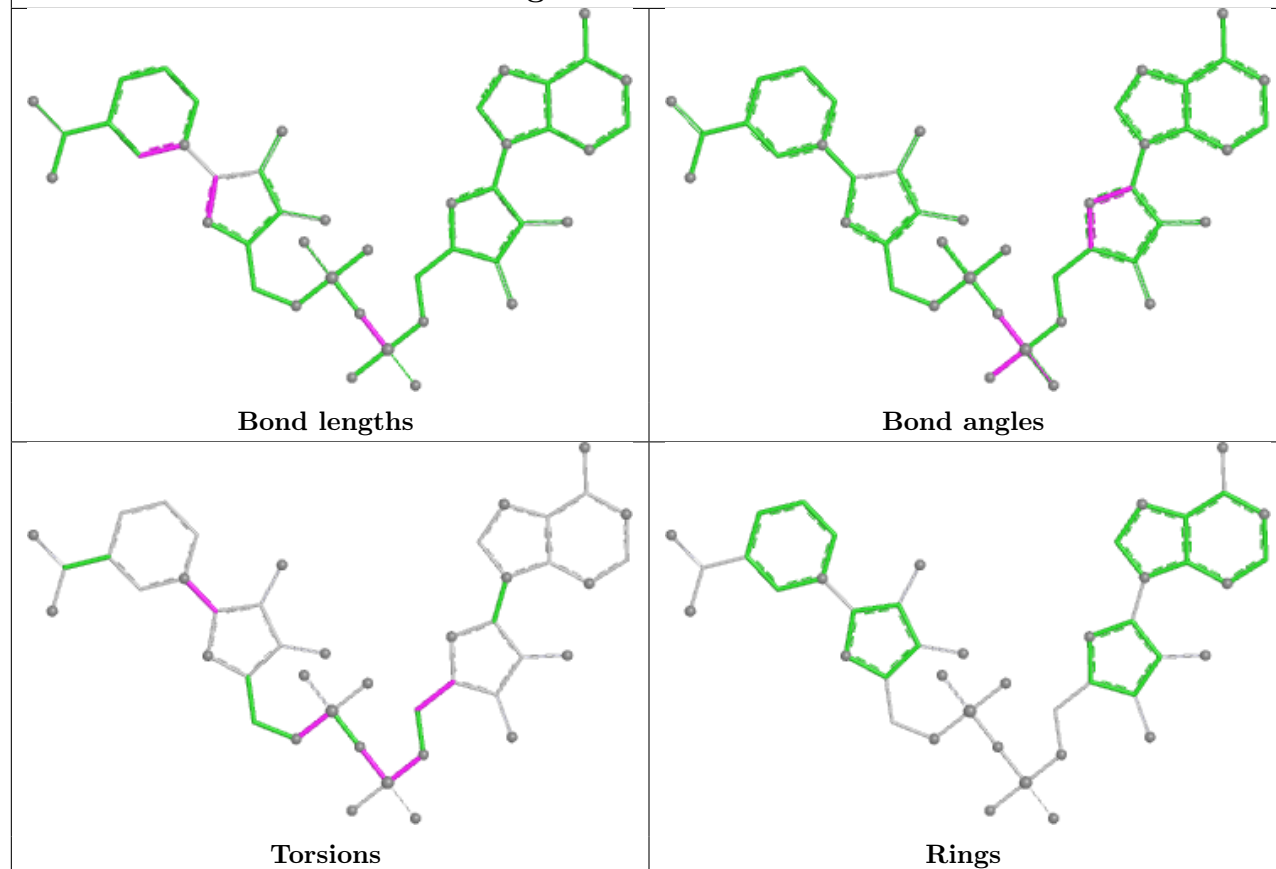
Ligand 68O D 302



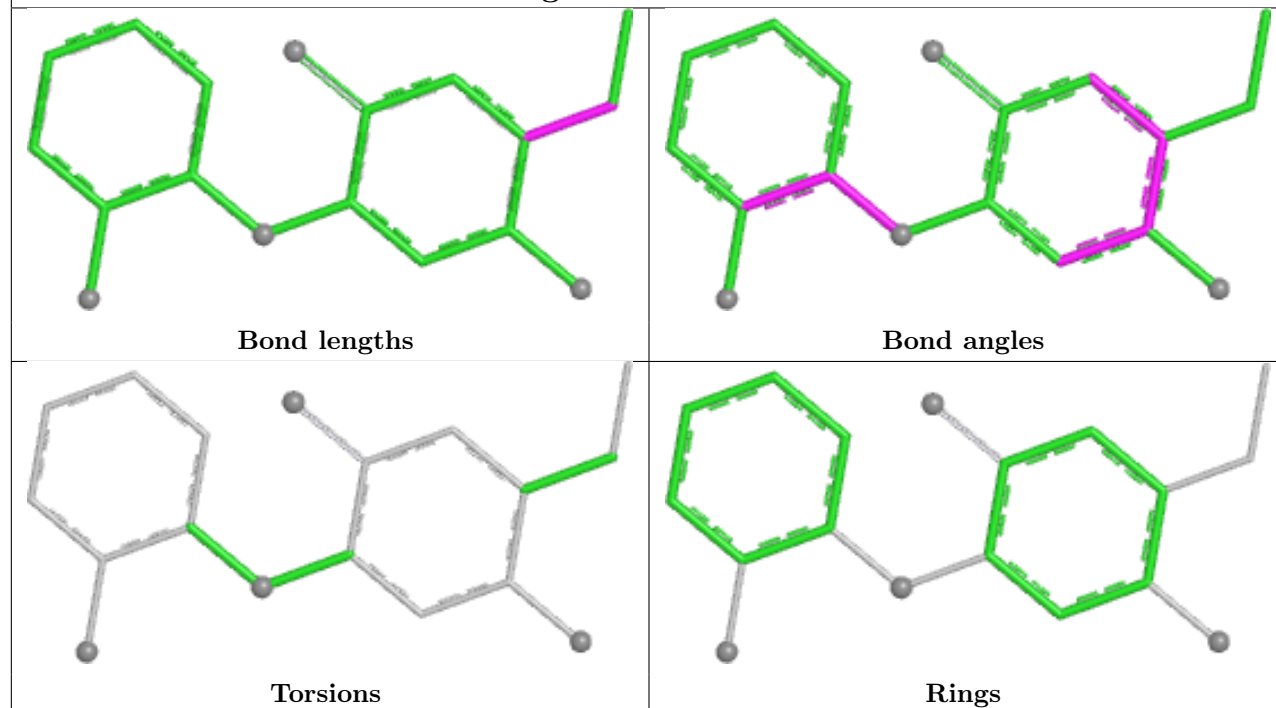
Ligand 68O H 302



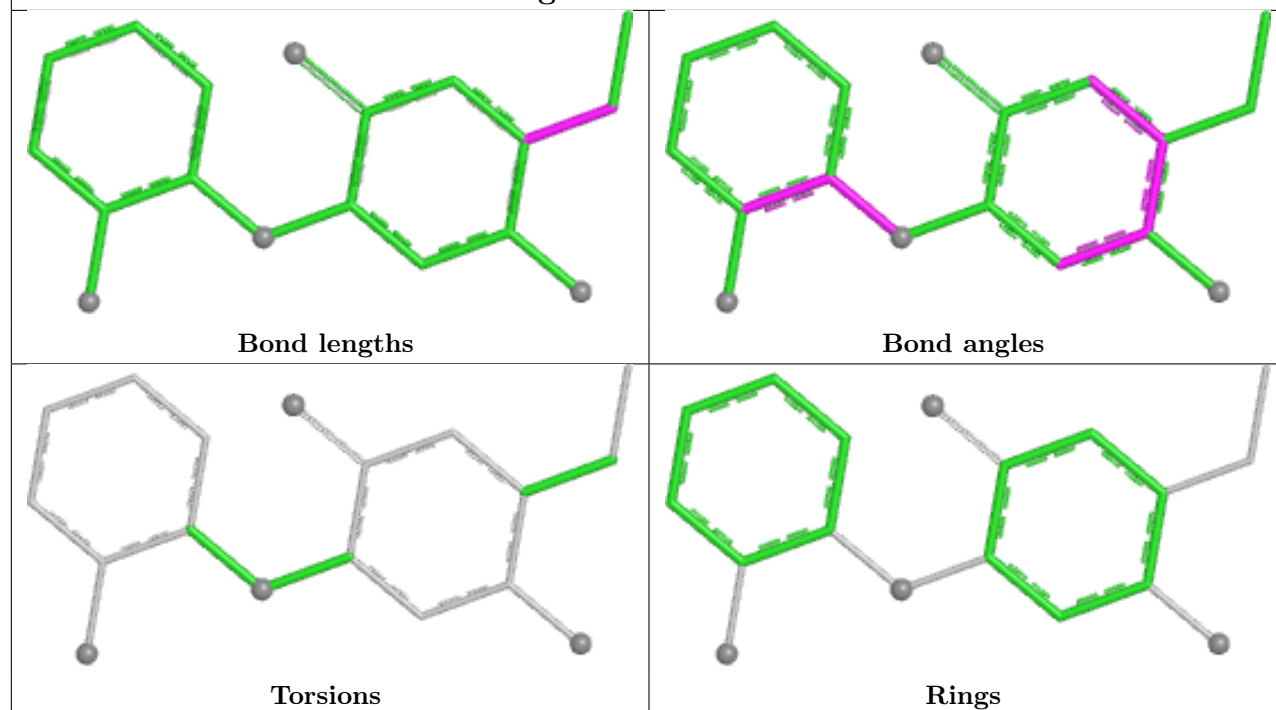
Ligand NAD H 301

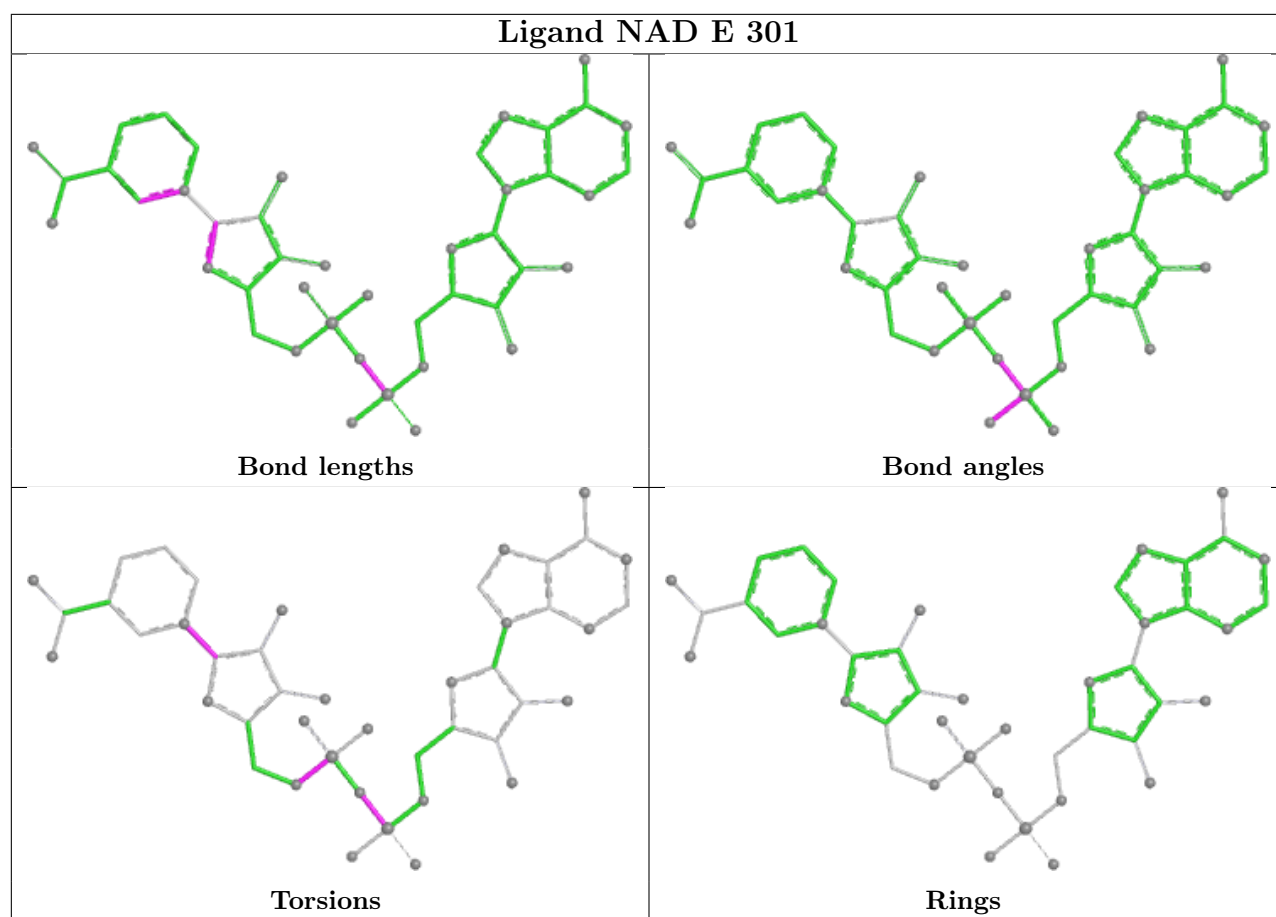


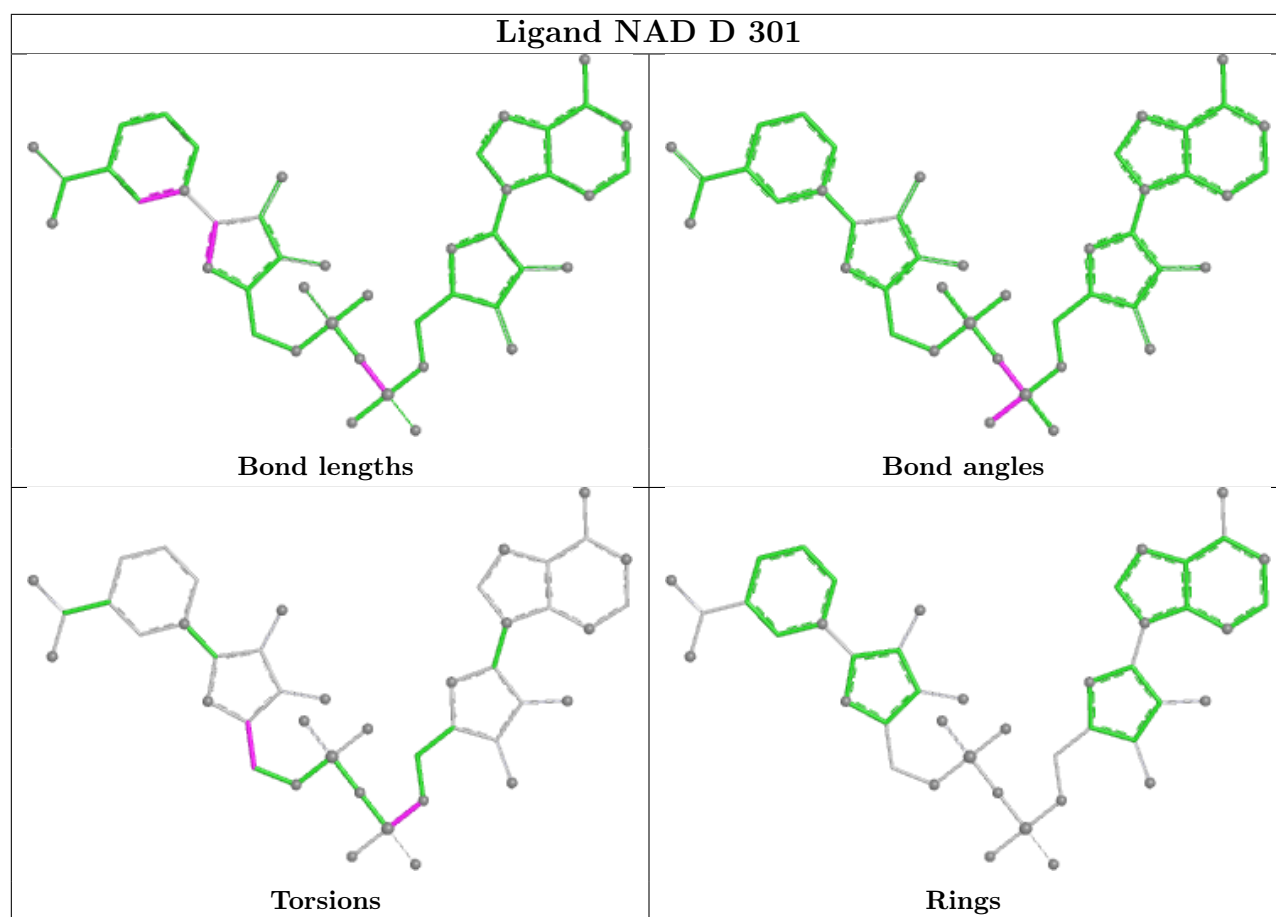
Ligand 68O J 302

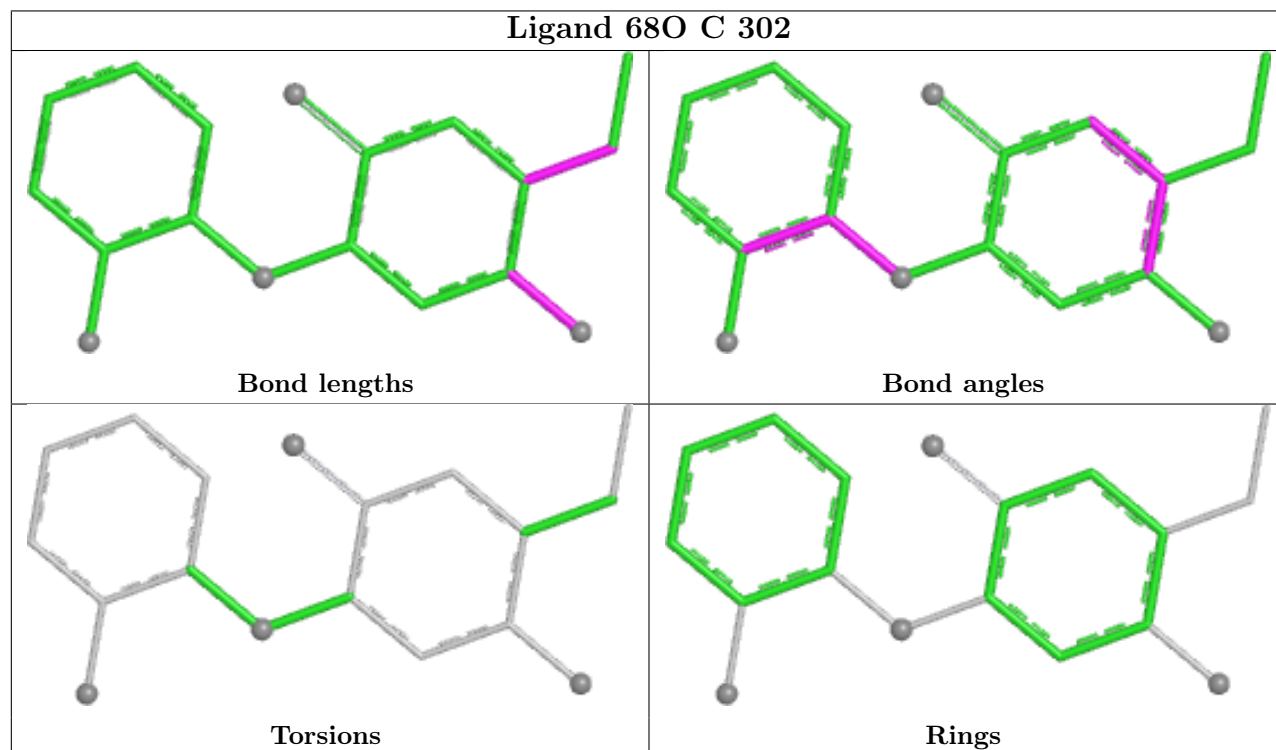
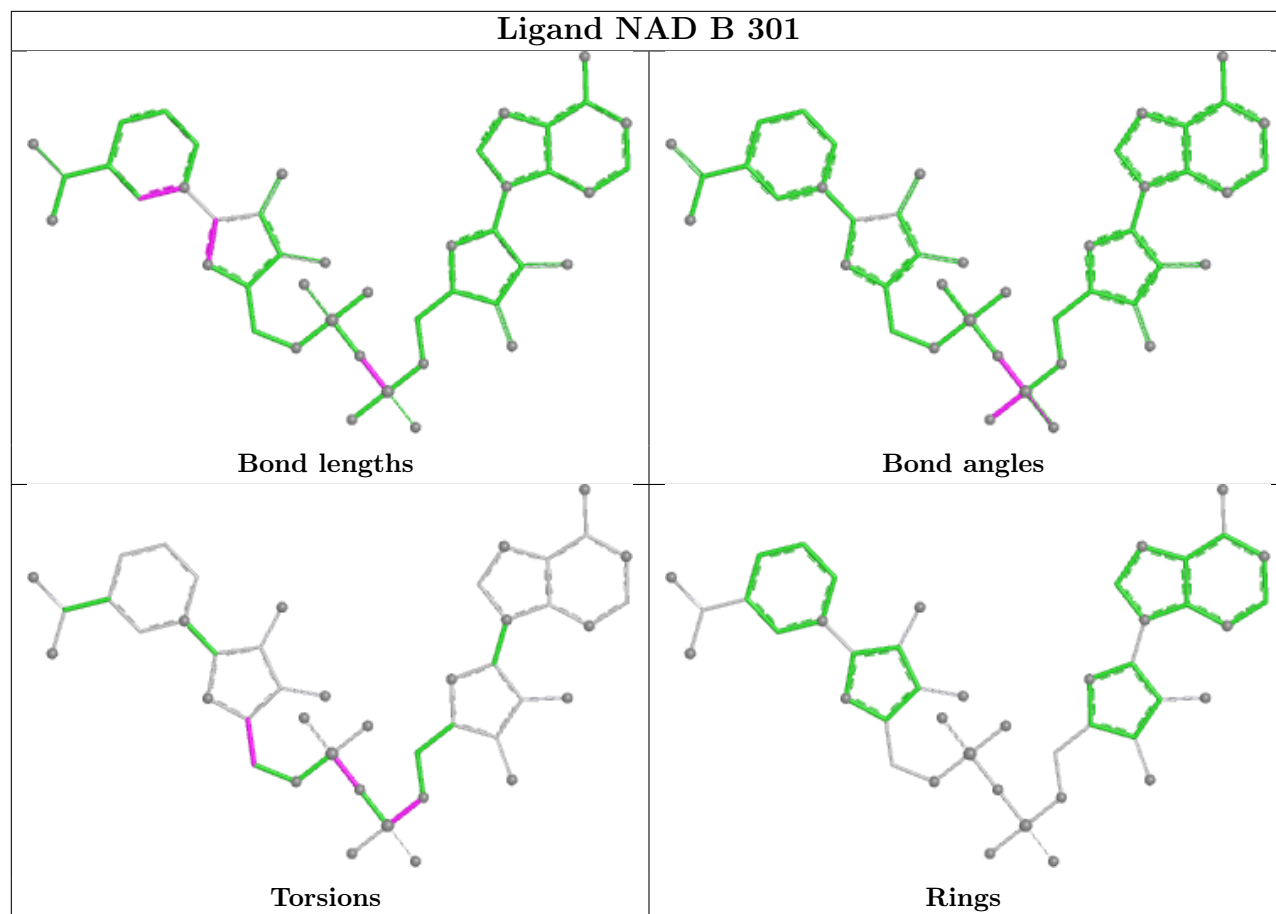


Ligand 68O B 302

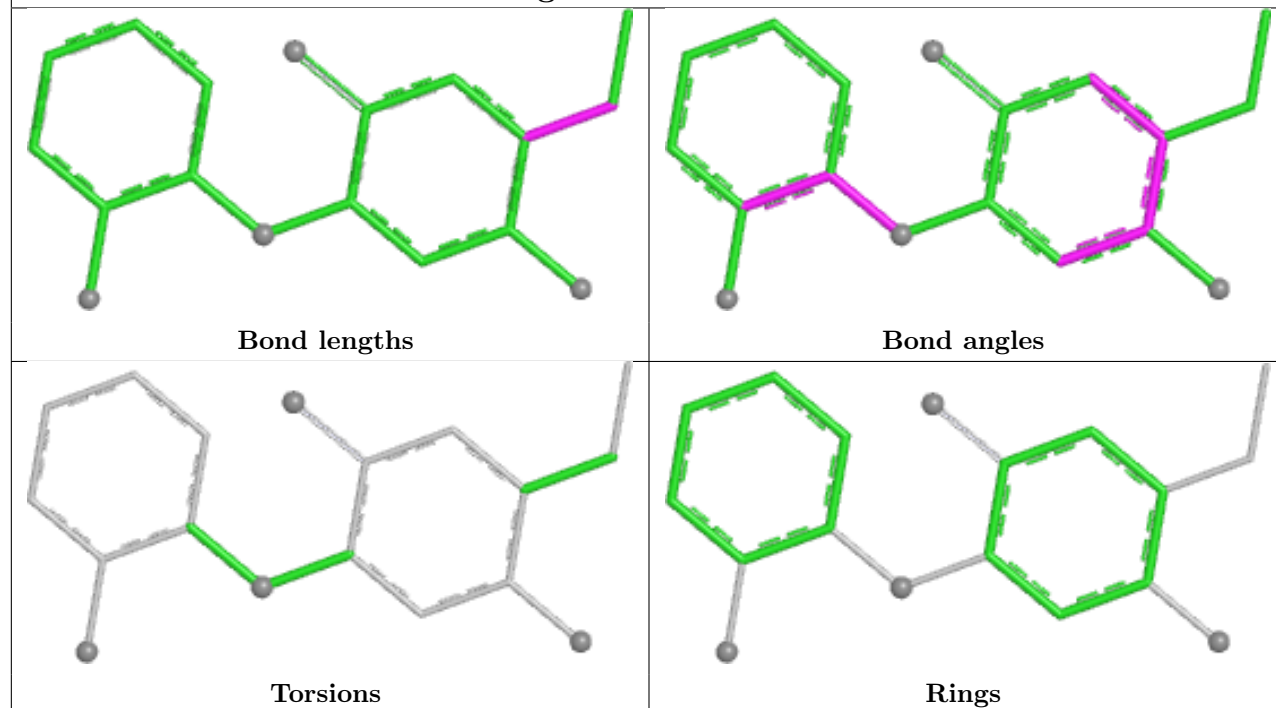




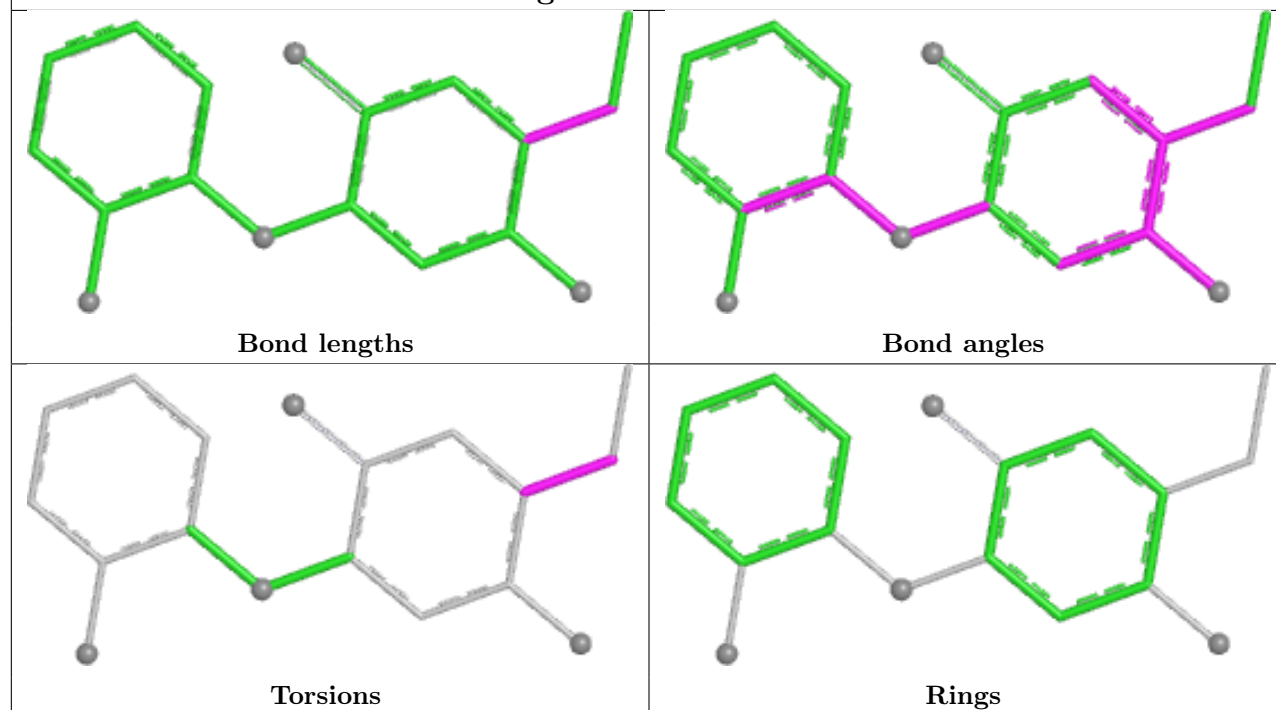




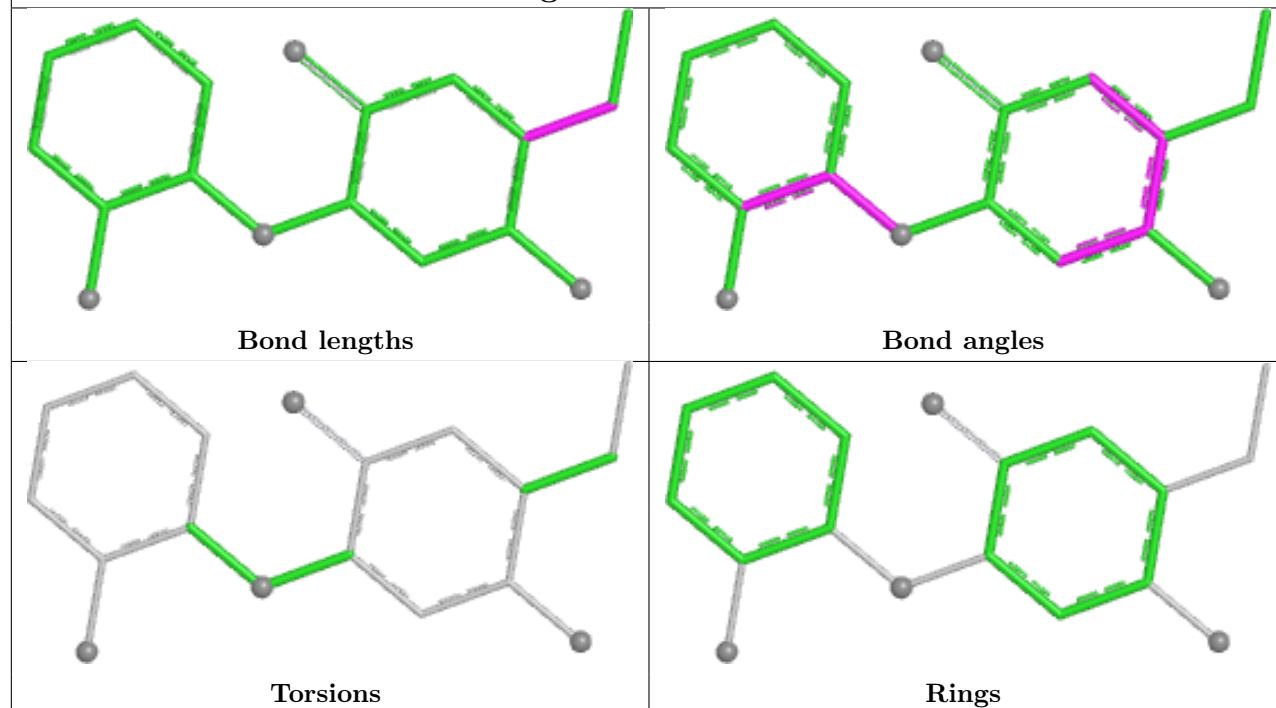
Ligand 68O A 302



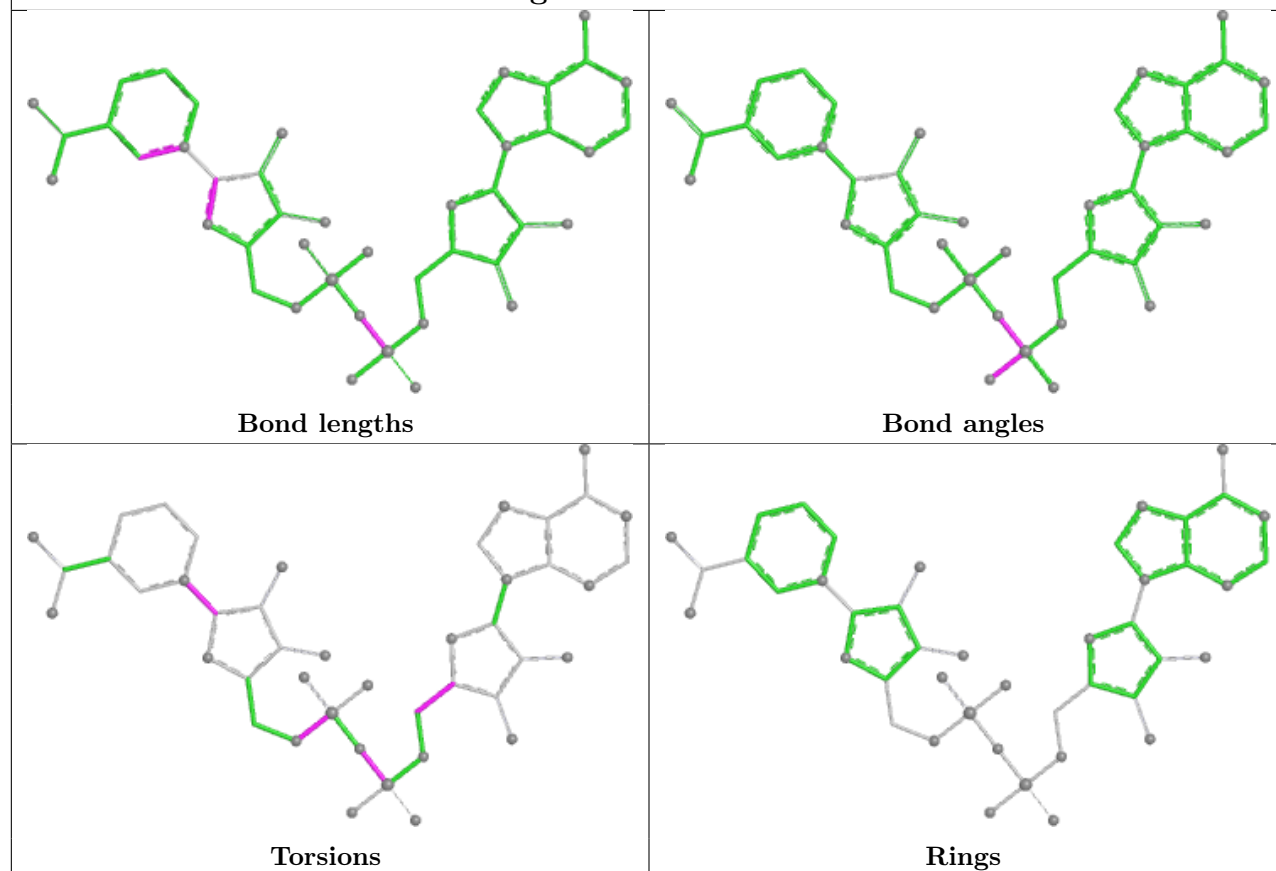
Ligand 68O K 302



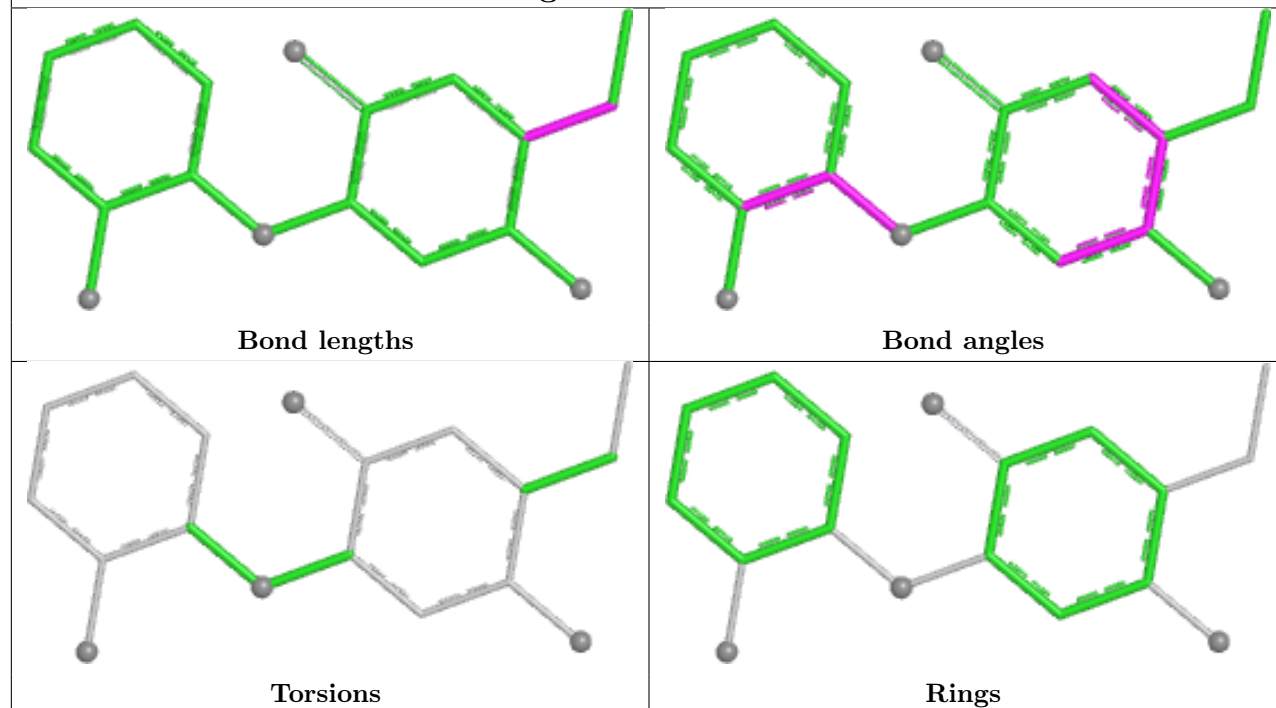
Ligand 68O L 302



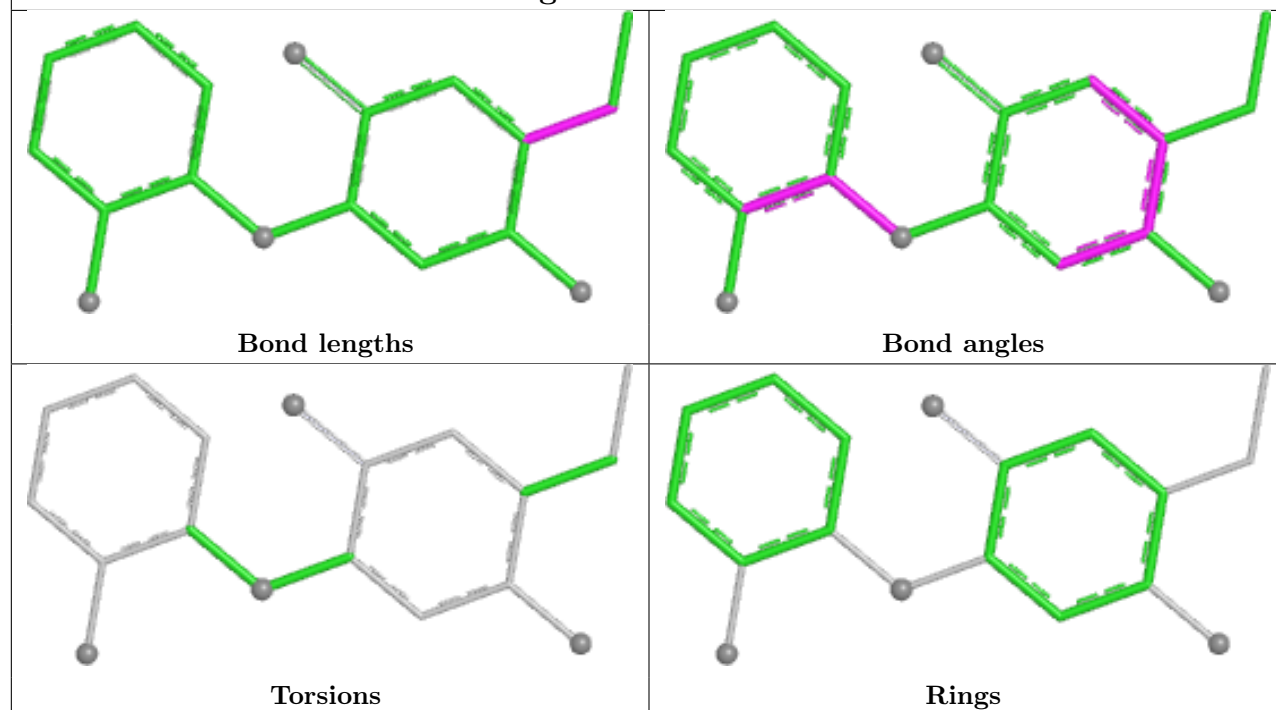
Ligand NAD F 301



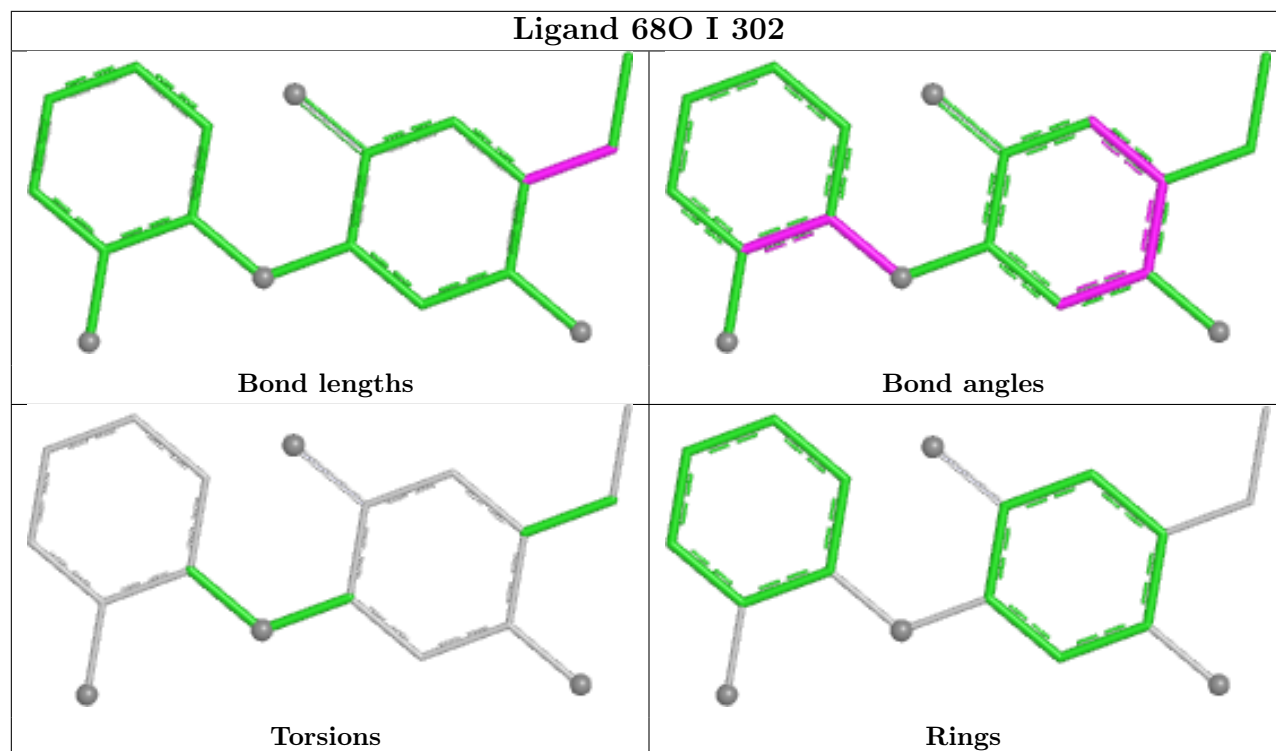
Ligand 68O F 302



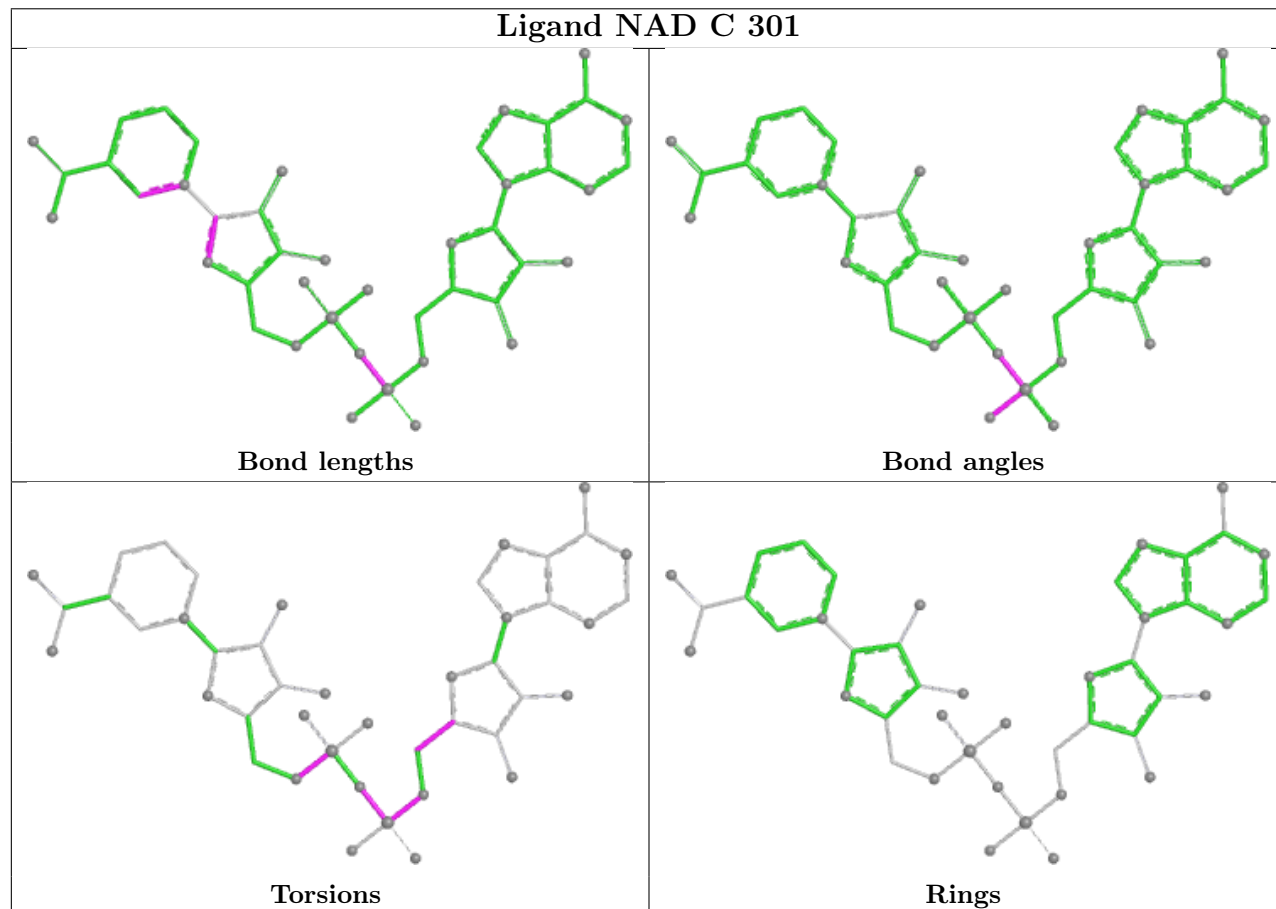
Ligand 68O E 302

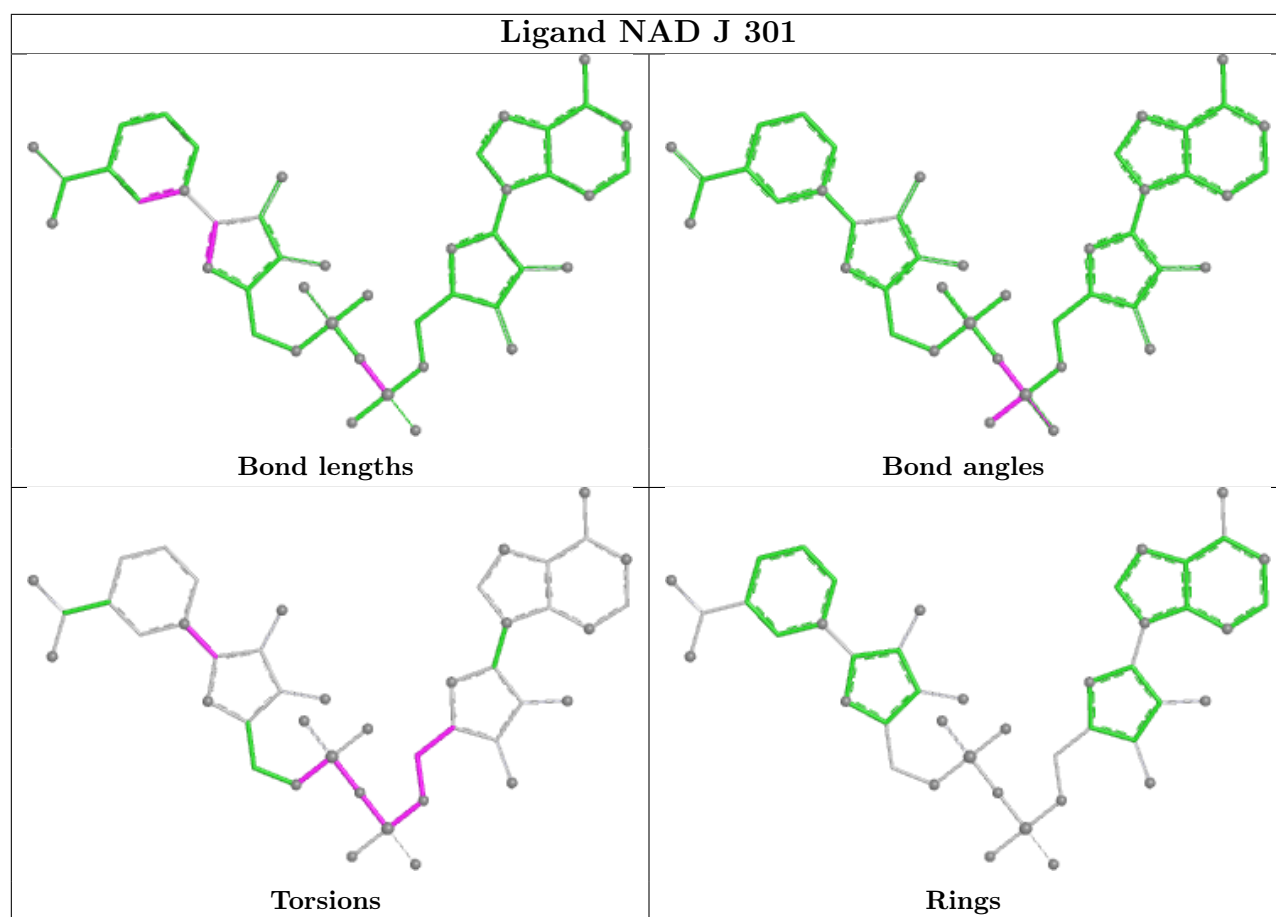


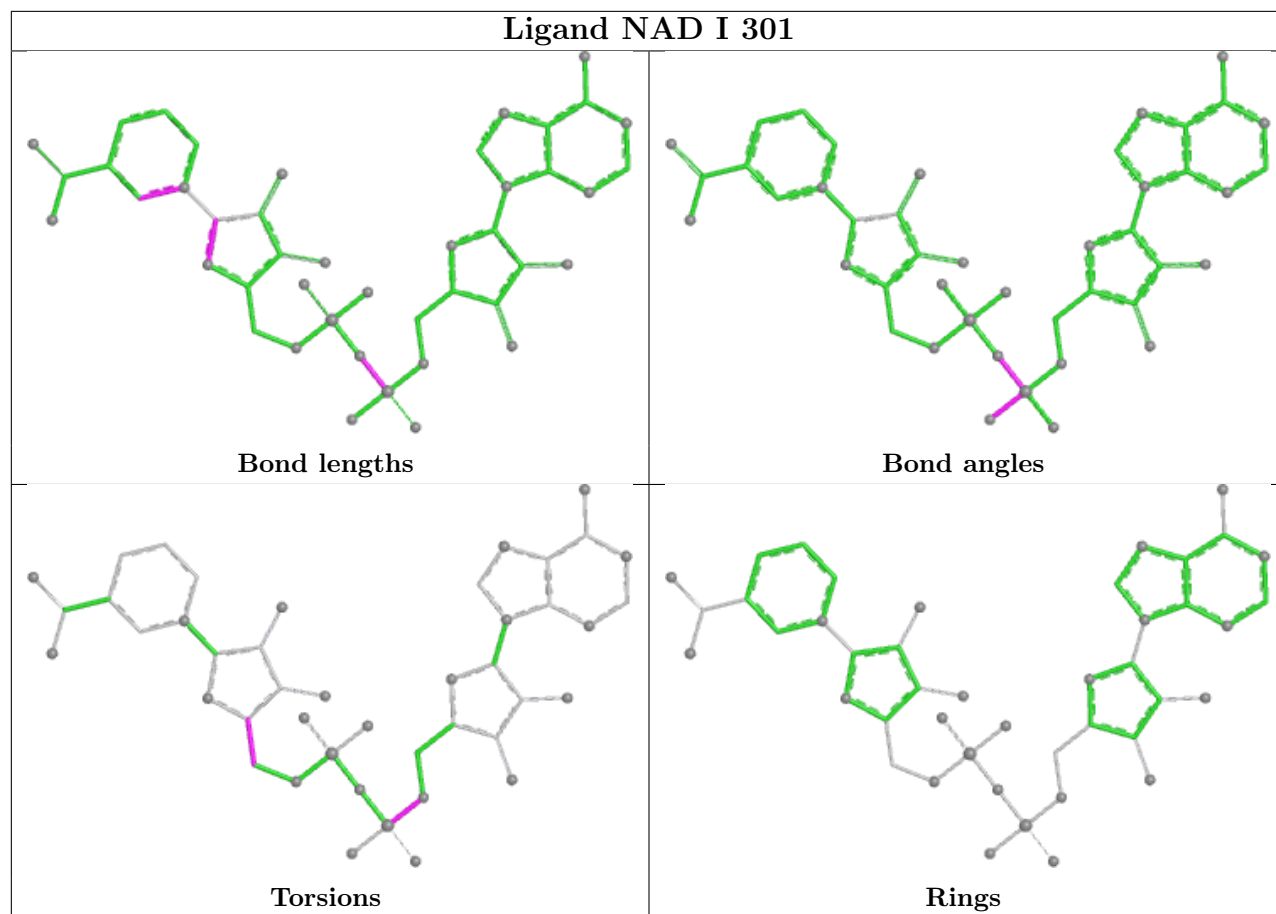
Ligand 68O I 302

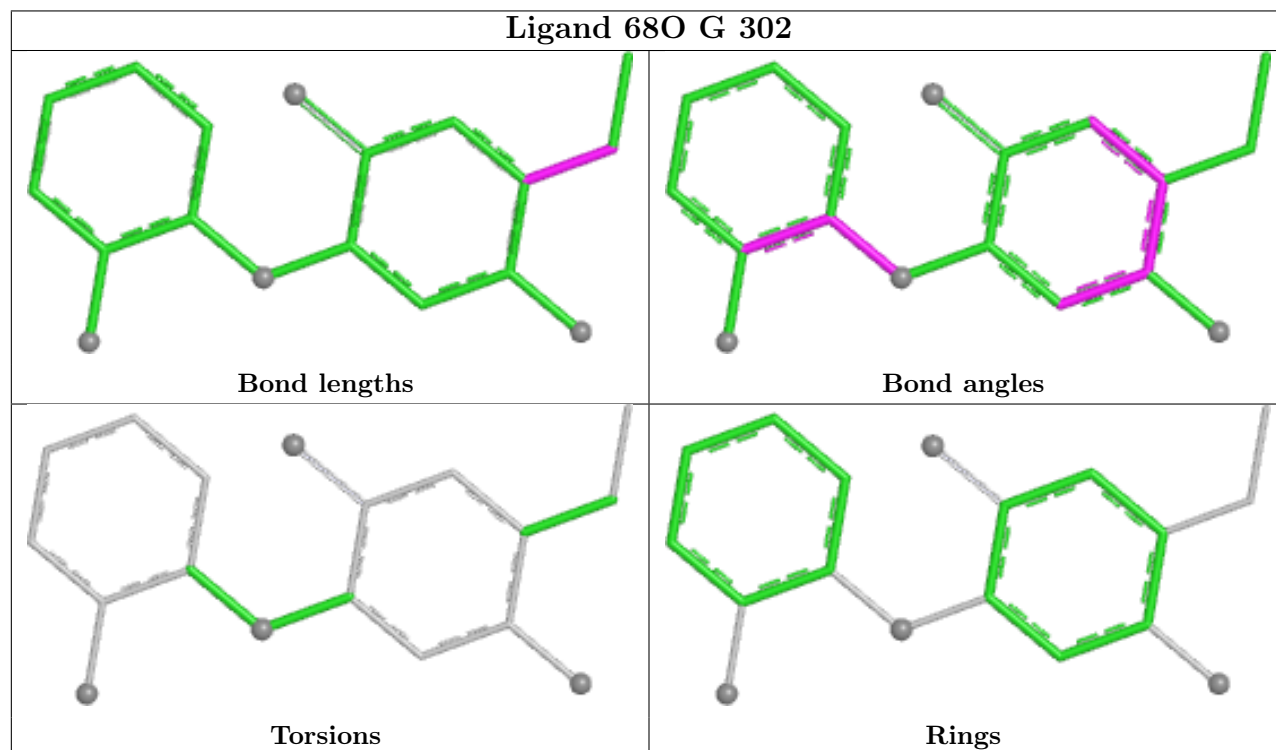
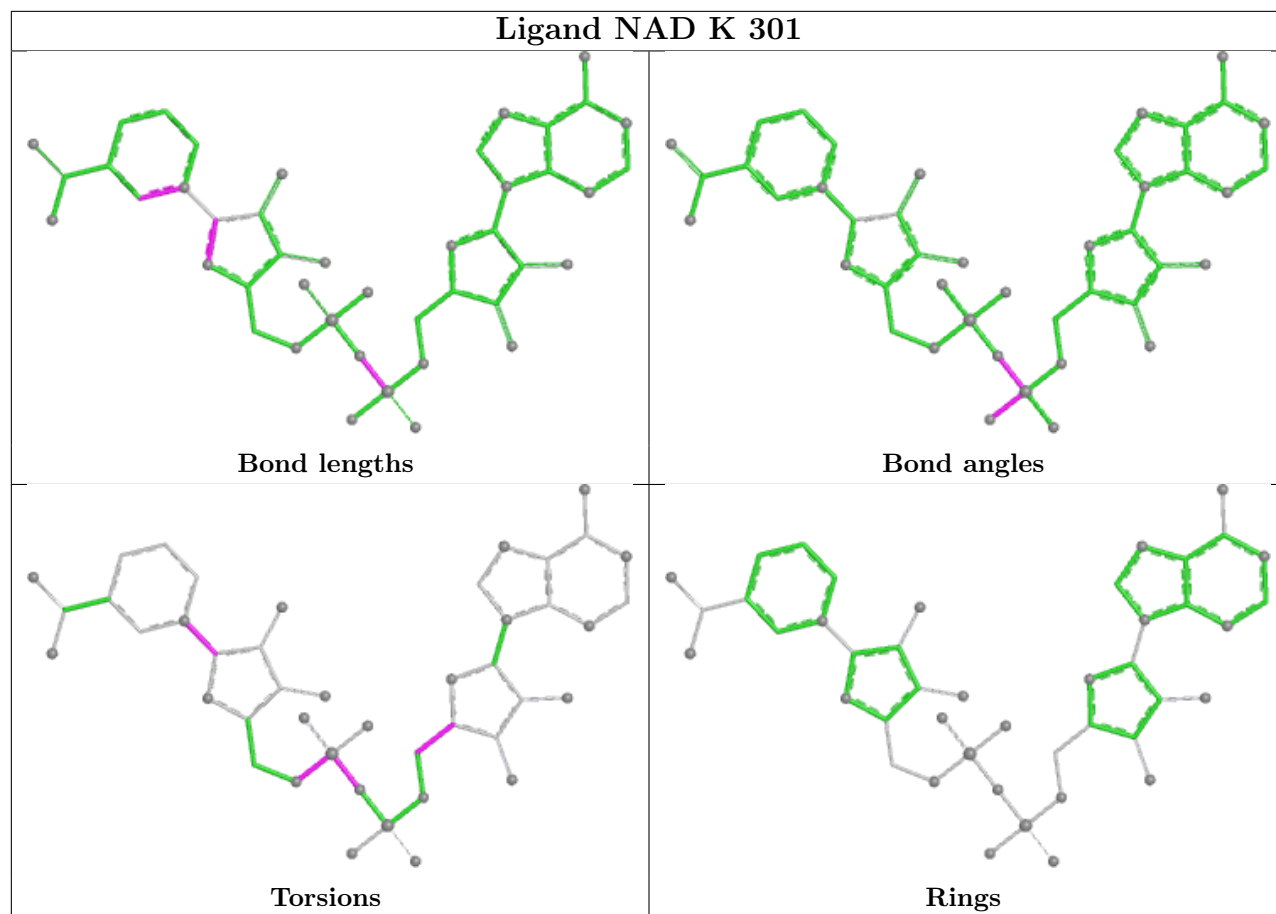


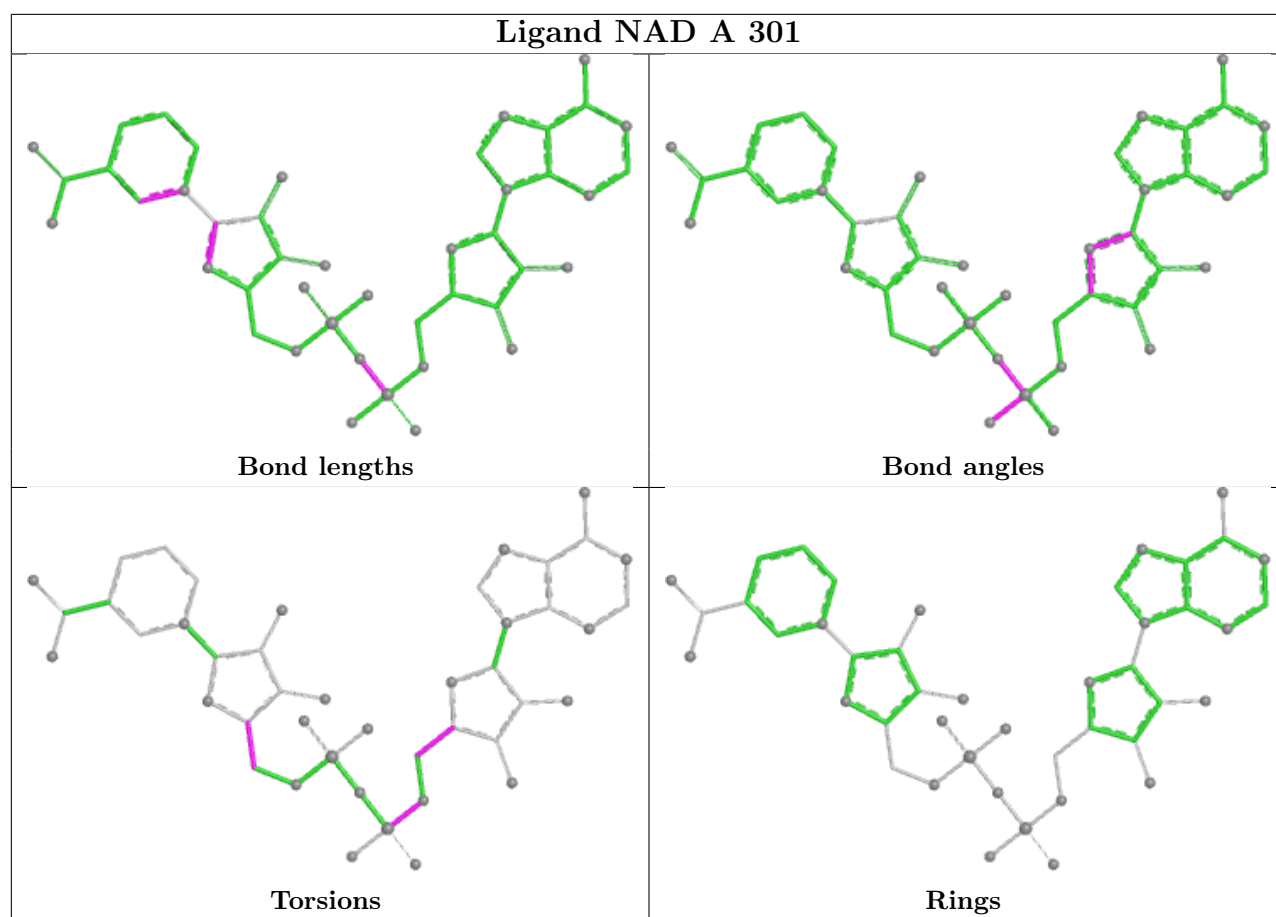
Ligand NAD C 301











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	257/276 (93%)	1.72	76 (29%) 1 1	38, 55, 80, 168	0
1	B	257/276 (93%)	1.78	89 (34%) 1 1	42, 58, 84, 114	0
1	C	257/276 (93%)	2.06	124 (48%) 0 0	40, 60, 84, 142	0
1	D	257/276 (93%)	1.80	99 (38%) 1 0	35, 50, 70, 116	0
1	E	257/276 (93%)	2.24	137 (53%) 0 0	36, 60, 89, 129	1 (0%)
1	F	257/276 (93%)	1.70	80 (31%) 1 1	27, 51, 75, 115	1 (0%)
1	G	257/276 (93%)	1.68	73 (28%) 1 1	32, 53, 80, 109	1 (0%)
1	H	257/276 (93%)	1.88	111 (43%) 0 0	44, 62, 87, 97	0
1	I	257/276 (93%)	1.58	60 (23%) 2 2	45, 57, 79, 105	0
1	J	257/276 (93%)	1.58	72 (28%) 1 1	35, 56, 76, 114	1 (0%)
1	K	257/276 (93%)	1.63	82 (31%) 1 1	32, 55, 79, 122	1 (0%)
1	L	257/276 (93%)	1.81	95 (36%) 1 0	46, 61, 86, 124	0
All	All	3084/3312 (93%)	1.79	1098 (35%) 1 1	27, 56, 82, 168	5 (0%)

All (1098) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	189	ALA	6.5
1	E	18	ARG	6.3
1	B	137	ASP	6.2
1	E	60	VAL	6.2
1	G	202	SER	6.1
1	F	193	LYS	6.0
1	H	198	SER	5.6
1	E	220	VAL	5.6
1	D	256	GLY	5.3
1	E	139	ALA	5.3
1	L	26	LYS	5.2

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Mol	Chain	Res	Type	RSRZ
1	E	61	PHE	5.2
1	E	258	MET	5.1
1	E	44	PHE	5.1
1	I	257	GLY	5.0
1	E	104	PHE	4.9
1	I	44	PHE	4.8
1	C	174	ALA	4.8
1	D	137	ASP	4.7
1	E	17	ASN	4.7
1	A	257	GLY	4.6
1	L	15	LEU	4.6
1	H	201	LYS	4.5
1	E	201	LYS	4.5
1	E	51	PHE	4.5
1	E	193	LYS	4.4
1	G	87	GLY	4.4
1	B	102	GLY	4.4
1	L	202	SER	4.4
1	H	195	LEU	4.4
1	I	138	ASP	4.4
1	D	48	ILE	4.4
1	D	97	ARG	4.3
1	L	82	TRP	4.3
1	G	198	SER	4.3
1	H	97	ARG	4.3
1	E	48	ILE	4.3
1	B	257	GLY	4.3
1	F	61	PHE	4.3
1	L	43	ARG	4.2
1	D	202	SER	4.2
1	A	137	ASP	4.2
1	C	138	ASP	4.2
1	A	44	PHE	4.2
1	J	50	GLU	4.2
1	G	201	LYS	4.2
1	J	258	MET	4.1
1	L	136	SER	4.1
1	B	193	LYS	4.1
1	A	258	MET	4.1
1	D	136	SER	4.1
1	L	212	SER	4.1
1	E	83	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	K	138	ASP	4.1
1	K	193	LYS	4.1
1	C	238	SER	4.1
1	D	99	ALA	4.0
1	C	2	GLY	4.0
1	E	251	PHE	4.0
1	J	255	VAL	4.0
1	E	140	SER	4.0
1	E	26	LYS	4.0
1	K	217	LYS	4.0
1	E	203	PHE	4.0
1	H	17	ASN	4.0
1	B	258	MET	4.0
1	G	97	ARG	4.0
1	B	221	THR	3.9
1	C	161	LEU	3.9
1	J	193	LYS	3.9
1	B	201	LYS	3.9
1	G	11	LEU	3.9
1	A	213	ASN	3.9
1	F	50	GLU	3.9
1	F	138	ASP	3.9
1	J	18	ARG	3.9
1	H	120	SER	3.9
1	A	100	ILE	3.9
1	H	196	ALA	3.9
1	A	99	ALA	3.9
1	E	125	PRO	3.8
1	K	180	LYS	3.8
1	C	159	MET	3.8
1	F	2	GLY	3.8
1	B	252	ASN	3.8
1	C	155	ASN	3.8
1	E	95	ALA	3.8
1	L	89	VAL	3.8
1	A	97	ARG	3.8
1	H	83	ASP	3.8
1	E	210	VAL	3.8
1	E	137[A]	ASP	3.8
1	E	57	SER	3.8
1	F	202	SER	3.8
1	F	47	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	200	ILE	3.7
1	E	189	ALA	3.7
1	B	97	ARG	3.7
1	J	203	PHE	3.7
1	E	142	LEU	3.7
1	E	39	TYR	3.7
1	H	202	SER	3.7
1	J	84	SER	3.7
1	J	107	GLY	3.7
1	F	59	LEU	3.7
1	G	15	LEU	3.7
1	B	192	ILE	3.7
1	C	24	ILE	3.7
1	L	199	GLY	3.7
1	G	19	SER	3.7
1	C	9	ILE	3.6
1	C	208	ASP	3.6
1	B	107	GLY	3.6
1	I	202	SER	3.6
1	K	60	VAL	3.6
1	D	49	THR	3.6
1	E	6	GLY	3.6
1	A	152	ALA	3.6
1	H	133	PRO	3.6
1	B	233	LEU	3.6
1	H	87	GLY	3.6
1	G	76	ALA	3.6
1	F	44	PHE	3.6
1	J	65	VAL	3.6
1	E	188	SER	3.6
1	C	43	ARG	3.5
1	I	2	GLY	3.5
1	C	201	LYS	3.5
1	F	113	PHE	3.5
1	H	161	LEU	3.5
1	F	15	LEU	3.5
1	E	97	ARG	3.5
1	D	138	ASP	3.5
1	K	5	ASP	3.5
1	A	66	ALA	3.5
1	J	139	ALA	3.5
1	B	26	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	22	TYR	3.5
1	E	99	ALA	3.5
1	H	41	GLY	3.5
1	A	93	GLY	3.5
1	L	13	GLY	3.5
1	H	258	MET	3.5
1	F	180	LYS	3.5
1	C	139	ALA	3.5
1	H	215	PRO	3.5
1	C	78	LEU	3.5
1	H	26	LYS	3.4
1	H	95	ALA	3.4
1	C	239	GLY	3.4
1	E	186	ALA	3.4
1	C	41	GLY	3.4
1	C	202	SER	3.4
1	G	23	GLY	3.4
1	E	195	LEU	3.4
1	D	47	ARG	3.4
1	A	26	LYS	3.4
1	G	199	GLY	3.4
1	L	157	ASN	3.4
1	L	9	ILE	3.3
1	B	79	LYS	3.3
1	D	201	LYS	3.3
1	E	50	GLU	3.3
1	J	237	ALA	3.3
1	E	34	GLU	3.3
1	E	223	GLU	3.3
1	I	233	LEU	3.3
1	L	11	LEU	3.3
1	J	59	LEU	3.3
1	H	242	ALA	3.3
1	F	189	ALA	3.3
1	A	60	VAL	3.3
1	J	82	TRP	3.3
1	E	12	THR	3.3
1	F	18	ARG	3.3
1	J	47	ARG	3.3
1	H	144	LEU	3.3
1	I	127	LEU	3.3
1	C	199	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	87	GLY	3.3
1	K	2	GLY	3.3
1	H	130	ALA	3.3
1	H	205	LYS	3.3
1	J	83	ASP	3.3
1	K	173	LEU	3.3
1	C	229	GLY	3.3
1	E	165	ALA	3.3
1	B	219	ASN	3.3
1	H	252	ASN	3.3
1	F	100	ILE	3.3
1	G	157	ASN	3.3
1	K	83	ASP	3.3
1	B	127	LEU	3.2
1	D	161	LEU	3.2
1	C	140	SER	3.2
1	A	256	GLY	3.2
1	H	75	PHE	3.2
1	B	96	PRO	3.2
1	G	194	THR	3.2
1	D	194	THR	3.2
1	J	32	GLY	3.2
1	I	39	TYR	3.2
1	E	92	ILE	3.2
1	L	222	ILE	3.2
1	B	83	ASP	3.2
1	A	201	LYS	3.2
1	G	41	GLY	3.2
1	H	230	ALA	3.2
1	E	192	ILE	3.2
1	E	200	ILE	3.2
1	H	20	ILE	3.2
1	C	200	ILE	3.2
1	A	83	ASP	3.2
1	L	235	ASP	3.2
1	F	43	ARG	3.2
1	C	207	LEU	3.2
1	C	128	ALA	3.2
1	K	206	ILE	3.2
1	F	60	VAL	3.2
1	D	75	PHE	3.2
1	L	44	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	108	LEU	3.1
1	E	15	LEU	3.1
1	E	233	LEU	3.1
1	L	233	LEU	3.1
1	J	14	LEU	3.1
1	C	168	ALA	3.1
1	G	164	ALA	3.1
1	D	139	ALA	3.1
1	D	228	ALA	3.1
1	E	24	ILE	3.1
1	C	209	PHE	3.1
1	D	94	PHE	3.1
1	E	155	ASN	3.1
1	F	137	ASP	3.1
1	B	236	LEU	3.1
1	C	11	LEU	3.1
1	B	223	GLU	3.1
1	E	257	GLY	3.1
1	A	2	GLY	3.1
1	J	257	GLY	3.1
1	C	192	ILE	3.1
1	A	69	ALA	3.1
1	F	174	ALA	3.1
1	C	120	SER	3.1
1	F	16	SER	3.1
1	D	188	SER	3.1
1	A	43	ARG	3.1
1	I	26	LYS	3.1
1	K	258	MET	3.1
1	F	17	ASN	3.1
1	F	14	LEU	3.1
1	D	50	GLU	3.1
1	F	49	THR	3.1
1	D	257	GLY	3.1
1	E	119	ILE	3.1
1	E	206	ILE	3.1
1	F	92	ILE	3.1
1	B	198	SER	3.1
1	C	114	ARG	3.1
1	J	44	PHE	3.1
1	C	258	MET	3.1
1	A	146	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	158	THR	3.1
1	E	38	THR	3.1
1	E	102	GLY	3.1
1	E	194	THR	3.1
1	D	109	THR	3.1
1	K	201	LYS	3.1
1	B	47	ARG	3.1
1	F	170	VAL	3.1
1	H	249	SER	3.1
1	A	238	SER	3.1
1	K	85	LEU	3.0
1	B	17	ASN	3.0
1	A	246	HIS	3.0
1	K	208	ASP	3.0
1	C	196	ALA	3.0
1	A	76	ALA	3.0
1	L	36	ALA	3.0
1	B	251	PHE	3.0
1	C	198	SER	3.0
1	A	19	SER	3.0
1	D	234	SER	3.0
1	C	127	LEU	3.0
1	C	195	LEU	3.0
1	C	233	LEU	3.0
1	D	232	LEU	3.0
1	E	56	GLY	3.0
1	E	100	ILE	3.0
1	G	6	GLY	3.0
1	G	93	GLY	3.0
1	L	258	MET	3.0
1	G	228	ALA	3.0
1	C	61	PHE	3.0
1	H	154	PRO	3.0
1	C	17	ASN	3.0
1	E	93	GLY	3.0
1	E	222	ILE	3.0
1	D	92	ILE	3.0
1	K	9	ILE	3.0
1	E	52	ALA	3.0
1	L	174	ALA	3.0
1	C	60	VAL	3.0
1	C	170	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	198	SER	3.0
1	F	201	LYS	3.0
1	D	17	ASN	3.0
1	E	86	ASP	3.0
1	K	235	ASP	3.0
1	C	222	ILE	3.0
1	A	92	ILE	3.0
1	E	190	GLY	3.0
1	C	13	GLY	3.0
1	G	143	THR	3.0
1	G	99	ALA	3.0
1	C	145	SER	2.9
1	D	22	TYR	2.9
1	B	200	ILE	2.9
1	E	20	ILE	2.9
1	H	241	THR	2.9
1	B	237	ALA	2.9
1	L	99	ALA	2.9
1	H	254	VAL	2.9
1	C	255	VAL	2.9
1	H	11	LEU	2.9
1	H	191	PRO	2.9
1	C	214	SER	2.9
1	I	18	ARG	2.9
1	D	122	TYR	2.9
1	A	115	ILE	2.9
1	L	200	ILE	2.9
1	B	199	GLY	2.9
1	F	87	GLY	2.9
1	E	164	ALA	2.9
1	C	197	ALA	2.9
1	J	126	ALA	2.9
1	E	113	PHE	2.9
1	E	225	VAL	2.9
1	A	255	VAL	2.9
1	D	220	VAL	2.9
1	K	65	VAL	2.9
1	E	141	LEU	2.9
1	A	34	GLU	2.9
1	B	238	SER	2.9
1	E	249	SER	2.9
1	K	16	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	206	ILE	2.9
1	E	226	GLY	2.9
1	C	99	ALA	2.9
1	G	197	ALA	2.9
1	D	131	ALA	2.9
1	H	184	VAL	2.9
1	C	51	PHE	2.9
1	D	255	VAL	2.9
1	K	233	LEU	2.9
1	D	214	SER	2.9
1	C	86	ASP	2.9
1	J	72	ASP	2.9
1	B	230	ALA	2.9
1	H	228	ALA	2.9
1	A	14	LEU	2.9
1	F	76	ALA	2.9
1	C	113	PHE	2.9
1	B	19	SER	2.8
1	C	234	SER	2.8
1	J	112	ASN	2.8
1	G	217	LYS	2.8
1	F	177	LEU	2.8
1	G	27	ALA	2.8
1	I	255	VAL	2.8
1	A	211	GLU	2.8
1	I	258	MET	2.8
1	B	205	LYS	2.8
1	C	83	ASP	2.8
1	F	190	GLY	2.8
1	F	257	GLY	2.8
1	D	199	GLY	2.8
1	I	190	GLY	2.8
1	K	107	GLY	2.8
1	E	59	LEU	2.8
1	B	149	ALA	2.8
1	D	21	ALA	2.8
1	L	152	ALA	2.8
1	L	228	ALA	2.8
1	B	113	PHE	2.8
1	H	231	PHE	2.8
1	H	255	VAL	2.8
1	F	89	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	244	VAL	2.8
1	E	43	ARG	2.8
1	F	140	SER	2.8
1	I	140	SER	2.8
1	G	185	ASN	2.8
1	E	14	LEU	2.8
1	E	135	LEU	2.8
1	A	15	LEU	2.8
1	A	195	LEU	2.8
1	D	141	LEU	2.8
1	H	25	ALA	2.8
1	C	76	ALA	2.8
1	C	131	ALA	2.8
1	G	159	MET	2.8
1	K	98	GLU	2.8
1	I	43	ARG	2.8
1	L	191	PRO	2.8
1	H	48	ILE	2.8
1	C	100	ILE	2.8
1	D	24	ILE	2.8
1	J	48	ILE	2.8
1	E	145	SER	2.8
1	D	249	SER	2.8
1	K	136	SER	2.8
1	H	219	ASN	2.8
1	A	185	ASN	2.8
1	G	17	ASN	2.8
1	C	87	GLY	2.8
1	C	232	LEU	2.8
1	G	207	LEU	2.8
1	G	257	GLY	2.8
1	G	80	THR	2.8
1	D	258	MET	2.8
1	G	37	PHE	2.8
1	I	60	VAL	2.8
1	L	27	ALA	2.8
1	A	104	PHE	2.8
1	E	8	ARG	2.8
1	L	28	CYS	2.7
1	H	217	LYS	2.7
1	G	100	ILE	2.7
1	K	192	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	136	SER	2.7
1	F	19	SER	2.7
1	K	17	ASN	2.7
1	L	41	GLY	2.7
1	E	64	ASP	2.7
1	E	184	VAL	2.7
1	C	149	ALA	2.7
1	A	150	GLU	2.7
1	F	130	ALA	2.7
1	C	47	ARG	2.7
1	F	184	VAL	2.7
1	J	43	ARG	2.7
1	B	153	ILE	2.7
1	C	92	ILE	2.7
1	B	207	LEU	2.7
1	C	134	MET	2.7
1	C	148	GLY	2.7
1	A	148	GLY	2.7
1	L	16	SER	2.7
1	J	198	SER	2.7
1	B	151	ARG	2.7
1	E	228	ALA	2.7
1	C	221	THR	2.7
1	D	158	THR	2.7
1	I	168	ALA	2.7
1	K	62	PRO	2.7
1	K	154	PRO	2.7
1	C	156	TYR	2.7
1	C	180	LYS	2.7
1	B	100	ILE	2.7
1	I	200	ILE	2.7
1	K	100	ILE	2.7
1	J	9	ILE	2.7
1	E	10	LEU	2.7
1	E	232	LEU	2.7
1	A	105	LEU	2.7
1	H	199	GLY	2.7
1	B	112	ASN	2.7
1	E	47	ARG	2.7
1	E	120	SER	2.7
1	H	40	VAL	2.7
1	F	203	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	184	VAL	2.7
1	L	241	THR	2.7
1	J	220	VAL	2.7
1	E	79	LYS	2.7
1	J	39	TYR	2.7
1	F	10	LEU	2.7
1	J	15	LEU	2.7
1	D	2	GLY	2.7
1	K	6	GLY	2.7
1	E	54	GLU	2.7
1	C	185	ASN	2.7
1	F	227	ASN	2.7
1	J	227	ASN	2.7
1	H	76	ALA	2.7
1	D	170	VAL	2.7
1	I	230	ALA	2.7
1	K	237	ALA	2.7
1	L	33	ALA	2.7
1	F	42	ASP	2.7
1	H	4	LEU	2.6
1	H	142	LEU	2.6
1	F	85	LEU	2.6
1	K	15	LEU	2.6
1	F	13	GLY	2.6
1	I	6	GLY	2.6
1	K	243	GLU	2.6
1	E	16	SER	2.6
1	C	157	ASN	2.6
1	A	193	LYS	2.6
1	G	45	LYS	2.6
1	G	155	ASN	2.6
1	B	203	PHE	2.6
1	H	66	ALA	2.6
1	A	149	ALA	2.6
1	A	175	VAL	2.6
1	D	212	SER	2.6
1	K	255	VAL	2.6
1	J	57	SER	2.6
1	J	238	SER	2.6
1	G	44	PHE	2.6
1	L	158	THR	2.6
1	A	106	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	159	MET	2.6
1	A	153	ILE	2.6
1	L	92	ILE	2.6
1	L	206	ILE	2.6
1	F	233	LEU	2.6
1	G	108	LEU	2.6
1	J	233	LEU	2.6
1	H	256	GLY	2.6
1	C	150	GLU	2.6
1	L	180	LYS	2.6
1	B	3	PHE	2.6
1	B	16	SER	2.6
1	B	61	PHE	2.6
1	E	65	VAL	2.6
1	E	234	SER	2.6
1	H	131	ALA	2.6
1	H	209	PHE	2.6
1	G	40	VAL	2.6
1	F	96	PRO	2.6
1	G	230	ALA	2.6
1	D	55	PHE	2.6
1	D	61	PHE	2.6
1	L	255	VAL	2.6
1	C	191	PRO	2.6
1	A	154	PRO	2.6
1	J	99	ALA	2.6
1	A	248	ASP	2.6
1	L	138	ASP	2.6
1	C	48	ILE	2.6
1	J	100	ILE	2.6
1	F	195	LEU	2.6
1	L	232	LEU	2.6
1	I	50	GLU	2.6
1	F	178	GLY	2.6
1	C	219	ASN	2.6
1	G	182	VAL	2.6
1	I	247	VAL	2.6
1	L	230	ALA	2.6
1	J	60	VAL	2.6
1	C	82	TRP	2.6
1	A	143	THR	2.6
1	F	238	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	82	TRP	2.6
1	K	19	SER	2.6
1	J	212	SER	2.6
1	C	137	ASP	2.6
1	D	100	ILE	2.6
1	I	92	ILE	2.6
1	B	4	LEU	2.6
1	C	141	LEU	2.6
1	F	88	LEU	2.6
1	F	236	LEU	2.6
1	L	207	LEU	2.6
1	H	22	TYR	2.6
1	H	156	TYR	2.6
1	F	217	LYS	2.6
1	G	98	GLU	2.6
1	C	178	GLY	2.6
1	J	190	GLY	2.6
1	H	101	ALA	2.6
1	A	182	VAL	2.6
1	C	44	PHE	2.6
1	D	197	ALA	2.6
1	K	36	ALA	2.6
1	L	162	ALA	2.6
1	E	19	SER	2.5
1	A	206	ILE	2.5
1	C	142	LEU	2.5
1	D	207	LEU	2.5
1	K	216	LEU	2.5
1	L	193	LYS	2.5
1	J	7	LYS	2.5
1	D	211	GLU	2.5
1	B	148	GLY	2.5
1	E	41	GLY	2.5
1	C	6	GLY	2.5
1	G	60	VAL	2.5
1	E	168	ALA	2.5
1	H	70	GLN	2.5
1	H	139	ALA	2.5
1	C	33	ALA	2.5
1	D	44	PHE	2.5
1	K	242	ALA	2.5
1	K	253	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	253	ALA	2.5
1	E	158	THR	2.5
1	C	80	THR	2.5
1	L	49	THR	2.5
1	H	188	SER	2.5
1	H	82	TRP	2.5
1	E	68	ASP	2.5
1	E	35	LEU	2.5
1	H	216	LEU	2.5
1	A	4	LEU	2.5
1	A	144	LEU	2.5
1	I	151	ARG	2.5
1	C	50	GLU	2.5
1	I	58	GLU	2.5
1	L	50	GLU	2.5
1	C	107	GLY	2.5
1	G	256	GLY	2.5
1	D	93	GLY	2.5
1	L	87	GLY	2.5
1	I	189	ALA	2.5
1	H	63	CYS	2.5
1	B	42	ASP	2.5
1	D	71	ILE	2.5
1	E	161	LEU	2.5
1	D	35	LEU	2.5
1	B	211	GLU	2.5
1	G	156	TYR	2.5
1	E	2	GLY	2.5
1	C	257	GLY	2.5
1	F	107	GLY	2.5
1	H	65	VAL	2.5
1	D	60	VAL	2.5
1	E	94	PHE	2.5
1	E	101	ALA	2.5
1	E	197	ALA	2.5
1	F	99	ALA	2.5
1	K	228	ALA	2.5
1	J	52	ALA	2.5
1	J	130	ALA	2.5
1	J	228	ALA	2.5
1	K	219	ASN	2.5
1	B	71	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	16	SER	2.5
1	K	47	ARG	2.5
1	K	120	SER	2.5
1	B	72	ASP	2.5
1	F	82	TRP	2.5
1	E	81	HIS	2.5
1	H	98	GLU	2.5
1	I	87	GLY	2.5
1	I	199	GLY	2.5
1	K	39	TYR	2.5
1	L	239	GLY	2.5
1	E	133	PRO	2.5
1	G	62	PRO	2.5
1	B	220	VAL	2.5
1	L	40	VAL	2.5
1	L	182	VAL	2.5
1	L	210	VAL	2.5
1	H	165	ALA	2.5
1	L	168	ALA	2.5
1	J	61	PHE	2.5
1	K	45	LYS	2.4
1	B	14	LEU	2.4
1	L	20	ILE	2.4
1	B	63	CYS	2.4
1	B	234	SER	2.4
1	C	212	SER	2.4
1	I	176	SER	2.4
1	E	235	ASP	2.4
1	H	257	GLY	2.4
1	K	190	GLY	2.4
1	L	190	GLY	2.4
1	E	180	LYS	2.4
1	E	182	VAL	2.4
1	H	60	VAL	2.4
1	D	45	LYS	2.4
1	L	225	VAL	2.4
1	B	76	ALA	2.4
1	B	242	ALA	2.4
1	E	196	ALA	2.4
1	D	66	ALA	2.4
1	J	162	ALA	2.4
1	H	80	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	12	THR	2.4
1	E	115	ILE	2.4
1	H	200	ILE	2.4
1	G	192	ILE	2.4
1	D	127	LEU	2.4
1	D	222	ILE	2.4
1	L	105	LEU	2.4
1	J	200	ILE	2.4
1	L	145	SER	2.4
1	K	223	GLU	2.4
1	E	229	GLY	2.4
1	B	60	VAL	2.4
1	C	89	VAL	2.4
1	E	121	ALA	2.4
1	E	242	ALA	2.4
1	C	104	PHE	2.4
1	C	230	ALA	2.4
1	I	61	PHE	2.4
1	I	66	ALA	2.4
1	K	131	ALA	2.4
1	C	15	LEU	2.4
1	G	10	LEU	2.4
1	D	223	GLU	2.4
1	H	45	LYS	2.4
1	E	87	GLY	2.4
1	D	210	VAL	2.4
1	B	139	ALA	2.4
1	E	55	PHE	2.4
1	E	75	PHE	2.4
1	E	152	ALA	2.4
1	H	197	ALA	2.4
1	F	209	PHE	2.4
1	I	94	PHE	2.4
1	E	108	LEU	2.4
1	I	195	LEU	2.4
1	K	35	LEU	2.4
1	H	143	THR	2.4
1	B	31	GLU	2.4
1	F	120	SER	2.4
1	F	136	SER	2.4
1	F	243	GLU	2.4
1	I	19	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	249	SER	2.4
1	J	188	SER	2.4
1	D	67	ASP	2.4
1	J	208	ASP	2.4
1	G	96	PRO	2.4
1	K	257	GLY	2.4
1	L	229	GLY	2.4
1	J	13	GLY	2.4
1	B	21	ALA	2.4
1	E	25	ALA	2.4
1	E	126	ALA	2.4
1	L	51	PHE	2.4
1	E	105	LEU	2.3
1	H	15	LEU	2.3
1	A	39	TYR	2.3
1	K	195	LEU	2.3
1	B	143	THR	2.3
1	H	109	THR	2.3
1	J	81	HIS	2.3
1	I	157	ASN	2.3
1	E	150	GLU	2.3
1	H	223	GLU	2.3
1	L	150	GLU	2.3
1	H	138	ASP	2.3
1	C	235	ASP	2.3
1	I	123	SER	2.3
1	K	137	ASP	2.3
1	J	201	LYS	2.3
1	H	190	GLY	2.3
1	L	2	GLY	2.3
1	E	124	PHE	2.3
1	B	15	LEU	2.3
1	E	207	LEU	2.3
1	C	108	LEU	2.3
1	A	88	LEU	2.3
1	A	197	ALA	2.3
1	K	21	ALA	2.3
1	L	179	ALA	2.3
1	C	81	HIS	2.3
1	G	34	GLU	2.3
1	H	46	ASP	2.3
1	C	136	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	212	SER	2.3
1	D	91	SER	2.3
1	J	64	ASP	2.3
1	H	107	GLY	2.3
1	G	47	ARG	2.3
1	E	63	CYS	2.3
1	G	184	VAL	2.3
1	I	89	VAL	2.3
1	L	247	VAL	2.3
1	B	11	LEU	2.3
1	G	61	PHE	2.3
1	F	196	ALA	2.3
1	D	85	LEU	2.3
1	D	195	LEU	2.3
1	J	113	PHE	2.3
1	J	251	PHE	2.3
1	H	237	ALA	2.3
1	C	119	ILE	2.3
1	G	24	ILE	2.3
1	F	241	THR	2.3
1	L	172	TYR	2.3
1	D	134	MET	2.3
1	G	227	ASN	2.3
1	G	252	ASN	2.3
1	E	154	PRO	2.3
1	I	83	ASP	2.3
1	J	42	ASP	2.3
1	H	240	VAL	2.3
1	L	170	VAL	2.3
1	E	4	LEU	2.3
1	E	166	LEU	2.3
1	H	147	LEU	2.3
1	C	144	LEU	2.3
1	C	173	LEU	2.3
1	D	88	LEU	2.3
1	I	75	PHE	2.3
1	I	141	LEU	2.3
1	L	14	LEU	2.3
1	E	66	ALA	2.3
1	H	36	ALA	2.3
1	H	189	ALA	2.3
1	H	192	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	152	ALA	2.3
1	G	186	ALA	2.3
1	D	9	ILE	2.3
1	D	33	ALA	2.3
1	L	52	ALA	2.3
1	D	81	HIS	2.3
1	E	49	THR	2.3
1	K	245	MET	2.3
1	L	80	THR	2.3
1	L	201	LYS	2.3
1	B	122	TYR	2.3
1	C	122	TYR	2.3
1	E	211	GLU	2.3
1	K	58	GLU	2.3
1	J	155	ASN	2.3
1	F	68	ASP	2.3
1	F	97	ARG	2.3
1	D	57	SER	2.3
1	J	202	SER	2.3
1	H	239	GLY	2.3
1	F	6	GLY	2.3
1	K	199	GLY	2.3
1	B	10	LEU	2.3
1	C	244	VAL	2.3
1	G	254	VAL	2.3
1	D	4	LEU	2.3
1	D	182	VAL	2.3
1	I	182	VAL	2.3
1	K	184	VAL	2.3
1	J	144	LEU	2.3
1	B	209	PHE	2.3
1	H	251	PHE	2.3
1	D	231	PHE	2.3
1	K	94	PHE	2.3
1	D	253	ALA	2.2
1	L	53	ALA	2.2
1	A	17	ASN	2.2
1	J	213	ASN	2.2
1	A	47	ARG	2.2
1	I	96	PRO	2.2
1	B	248	ASP	2.2
1	F	118	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	64	ASP	2.2
1	B	181	GLY	2.2
1	C	226	GLY	2.2
1	C	147	LEU	2.2
1	A	40	VAL	2.2
1	K	220	VAL	2.2
1	L	175	VAL	2.2
1	J	195	LEU	2.2
1	B	20	ILE	2.2
1	K	44	PHE	2.2
1	K	203	PHE	2.2
1	C	95	ALA	2.2
1	A	230	ALA	2.2
1	C	34	GLU	2.2
1	C	38	THR	2.2
1	B	2	GLY	2.2
1	C	77	SER	2.2
1	C	250	GLY	2.2
1	K	14	LEU	2.2
1	B	45	LYS	2.2
1	H	79	LYS	2.2
1	H	182	VAL	2.2
1	A	225	VAL	2.2
1	A	254	VAL	2.2
1	F	65	VAL	2.2
1	B	222	ILE	2.2
1	H	37	PHE	2.2
1	F	51	PHE	2.2
1	F	71	ILE	2.2
1	D	113	PHE	2.2
1	F	52	ALA	2.2
1	D	164	ALA	2.2
1	H	146	TYR	2.2
1	H	155	ASN	2.2
1	L	39	TYR	2.2
1	K	96	PRO	2.2
1	H	78	LEU	2.2
1	H	137	ASP	2.2
1	C	59	LEU	2.2
1	A	108	LEU	2.2
1	G	86	ASP	2.2
1	D	56	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	161	LEU	2.2
1	L	93	GLY	2.2
1	L	256	GLY	2.2
1	A	136	SER	2.2
1	B	225	VAL	2.2
1	I	175	VAL	2.2
1	K	244	VAL	2.2
1	J	184	VAL	2.2
1	F	9	ILE	2.2
1	G	20	ILE	2.2
1	L	187	ILE	2.2
1	J	124	PHE	2.2
1	B	27	ALA	2.2
1	H	73	ALA	2.2
1	H	164	ALA	2.2
1	I	237	ALA	2.2
1	K	66	ALA	2.2
1	J	189	ALA	2.2
1	H	50	GLU	2.2
1	J	49	THR	2.2
1	D	114	ARG	2.2
1	I	97	ARG	2.2
1	D	39	TYR	2.2
1	D	156	TYR	2.2
1	D	213	ASN	2.2
1	C	26	LYS	2.2
1	E	178	GLY	2.2
1	H	2	GLY	2.2
1	G	85	LEU	2.2
1	L	6	GLY	2.2
1	H	68	ASP	2.2
1	H	208	ASP	2.2
1	F	258	MET	2.2
1	G	42	ASP	2.2
1	F	176	SER	2.2
1	I	238	SER	2.2
1	C	20	ILE	2.2
1	I	90	HIS	2.2
1	I	254	VAL	2.2
1	H	104	PHE	2.2
1	D	104	PHE	2.2
1	B	101	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	126	ALA	2.1
1	B	128	ALA	2.1
1	B	186	ALA	2.1
1	C	179	ALA	2.1
1	F	139	ALA	2.1
1	D	53	ALA	2.1
1	K	82	TRP	2.1
1	D	58	GLU	2.1
1	J	243	GLU	2.1
1	L	18	ARG	2.1
1	H	185	ASN	2.1
1	G	4	LEU	2.1
1	K	59	LEU	2.1
1	L	78	LEU	2.1
1	K	204	GLY	2.1
1	B	68	ASP	2.1
1	E	46	ASP	2.1
1	G	92	ILE	2.1
1	D	86	ASP	2.1
1	I	20	ILE	2.1
1	I	42	ASP	2.1
1	K	140	SER	2.1
1	K	153	ILE	2.1
1	L	248	ASP	2.1
1	J	182	VAL	2.1
1	A	113	PHE	2.1
1	D	124	PHE	2.1
1	D	203	PHE	2.1
1	J	51	PHE	2.1
1	B	95	ALA	2.1
1	B	152	ALA	2.1
1	A	139	ALA	2.1
1	G	33	ALA	2.1
1	G	73	ALA	2.1
1	G	196	ALA	2.1
1	D	36	ALA	2.1
1	B	43	ARG	2.1
1	D	43	ARG	2.1
1	L	47	ARG	2.1
1	A	49	THR	2.1
1	F	80	THR	2.1
1	A	85	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	185	ASN	2.1
1	K	144	LEU	2.1
1	E	204	GLY	2.1
1	H	6	GLY	2.1
1	H	102	GLY	2.1
1	D	6	GLY	2.1
1	I	41	GLY	2.1
1	I	178	GLY	2.1
1	E	71	ILE	2.1
1	A	187	ILE	2.1
1	F	192	ILE	2.1
1	K	42	ASP	2.1
1	L	64	ASP	2.1
1	B	94	PHE	2.1
1	H	123	SER	2.1
1	K	189	ALA	2.1
1	L	131	ALA	2.1
1	J	33	ALA	2.1
1	L	30	ARG	2.1
1	B	217	LYS	2.1
1	D	217	LYS	2.1
1	L	133	PRO	2.1
1	G	233	LEU	2.1
1	D	59	LEU	2.1
1	K	78	LEU	2.1
1	D	157	ASN	2.1
1	I	155	ASN	2.1
1	E	13	GLY	2.1
1	E	172	TYR	2.1
1	H	81	HIS	2.1
1	B	92	ILE	2.1
1	H	9	ILE	2.1
1	K	200	ILE	2.1
1	L	240	VAL	2.1
1	C	118	ASP	2.1
1	A	37	PHE	2.1
1	I	37	PHE	2.1
1	L	3	PHE	2.1
1	L	75	PHE	2.1
1	L	86	ASP	2.1
1	E	76	ALA	2.1
1	H	169	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	253	ALA	2.1
1	C	66	ALA	2.1
1	A	101	ALA	2.1
1	A	126	ALA	2.1
1	K	238	SER	2.1
1	F	110	ARG	2.1
1	D	243	GLU	2.1
1	A	217	LYS	2.1
1	H	105	LEU	2.1
1	C	85	LEU	2.1
1	K	10	LEU	2.1
1	B	239	GLY	2.1
1	D	87	GLY	2.1
1	J	93	GLY	2.1
1	H	187	ILE	2.1
1	C	115	ILE	2.1
1	I	187	ILE	2.1
1	K	92	ILE	2.1
1	J	172	TYR	2.1
1	C	254	VAL	2.1
1	I	240	VAL	2.1
1	E	110	ARG	2.0
1	C	5	ASP	2.0
1	C	46	ASP	2.0
1	A	138	ASP	2.0
1	G	94	PHE	2.1
1	G	203	PHE	2.1
1	L	55	PHE	2.1
1	L	94	PHE	2.1
1	E	53	ALA	2.0
1	C	228	ALA	2.0
1	F	98	GLU	2.0
1	A	16	SER	2.0
1	G	168	ALA	2.0
1	I	131	ALA	2.0
1	I	201	LYS	2.0
1	A	158	THR	2.0
1	E	132	LEU	2.0
1	H	85	LEU	2.0
1	C	74	LEU	2.0
1	L	144	LEU	2.0
1	F	117	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	190	GLY	2.0
1	B	39	TYR	2.0
1	B	65	VAL	2.0
1	B	172	TYR	2.0
1	E	255	VAL	2.0
1	C	220	VAL	2.0
1	A	172	TYR	2.0
1	F	240	VAL	2.0
1	J	170	VAL	2.0
1	C	124	PHE	2.0
1	D	98	GLU	2.0
1	K	50	GLU	2.0
1	F	230	ALA	2.0
1	D	26	LYS	2.0
1	D	189	ALA	2.0
1	L	42	ASP	2.0
1	C	217	LYS	2.0
1	L	121	ALA	2.0
1	I	159	MET	2.0
1	K	134	MET	2.0
1	A	215	PRO	2.0
1	J	143	THR	2.0
1	C	135	LEU	2.0
1	L	224	GLN	2.0
1	E	9	ILE	2.0
1	E	112	ASN	2.0
1	H	92	ILE	2.0
1	H	227	ASN	2.0
1	A	155	ASN	2.0
1	G	13	GLY	2.0
1	G	213	ASN	2.0
1	K	222	ILE	2.0
1	L	17	ASN	2.0
1	E	247	VAL	2.0
1	C	40	VAL	2.0
1	D	8	ARG	2.0
1	K	97	ARG	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 ⓘ

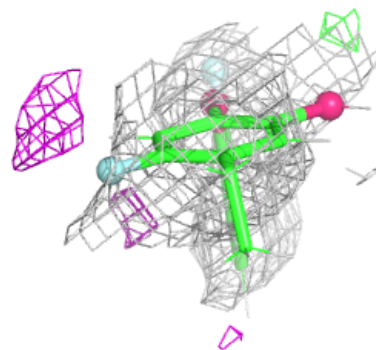
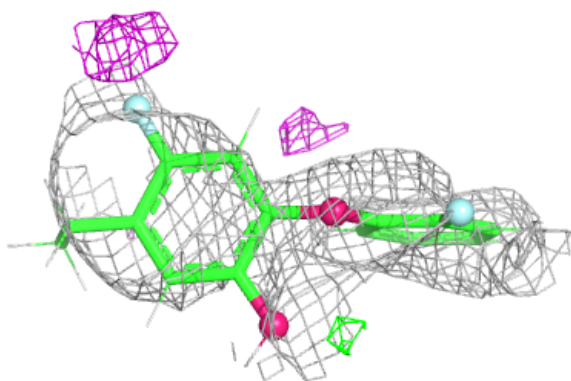
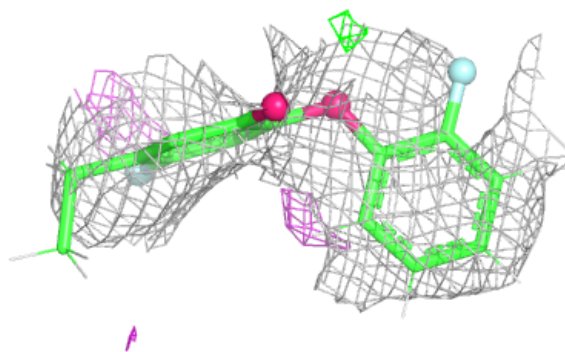
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	68O	C	302	18/18	0.71	0.19	49,51,61,61	0
3	68O	K	302	18/18	0.72	0.18	46,47,56,57	0
2	NAD	E	301	44/44	0.74	0.16	48,54,67,81	0
3	68O	I	302	18/18	0.75	0.17	48,51,61,61	0
3	68O	E	302	18/18	0.75	0.20	56,57,69,69	0
2	NAD	C	301	44/44	0.76	0.15	44,54,66,67	0
3	68O	F	302	18/18	0.78	0.17	47,47,57,57	0
3	68O	H	302	18/18	0.78	0.17	42,44,52,53	0
2	NAD	H	301	44/44	0.78	0.16	45,58,71,72	0
2	NAD	F	301	44/44	0.79	0.16	40,48,58,61	0
2	NAD	J	301	44/44	0.81	0.16	50,55,66,69	0
3	68O	D	302	18/18	0.81	0.15	40,43,52,53	0
3	68O	J	302	18/18	0.81	0.15	46,48,58,58	0
3	68O	L	302	18/18	0.82	0.17	53,54,64,65	0
2	NAD	G	301	44/44	0.82	0.16	39,51,71,73	0
2	NAD	B	301	44/44	0.83	0.17	44,50,60,62	0
2	NAD	A	301	44/44	0.83	0.17	46,51,61,63	0
3	68O	G	302	18/18	0.83	0.16	39,43,52,53	0
2	NAD	K	301	44/44	0.83	0.16	42,51,63,65	0
2	NAD	L	301	44/44	0.84	0.14	52,55,67,68	0
3	68O	B	302	18/18	0.84	0.16	48,49,59,60	0
2	NAD	D	301	44/44	0.86	0.13	36,48,58,58	0
2	NAD	I	301	44/44	0.86	0.14	44,53,65,65	0
3	68O	A	302	18/18	0.89	0.14	43,48,58,58	0

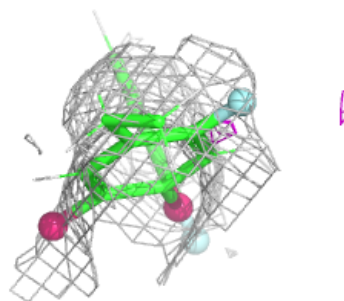
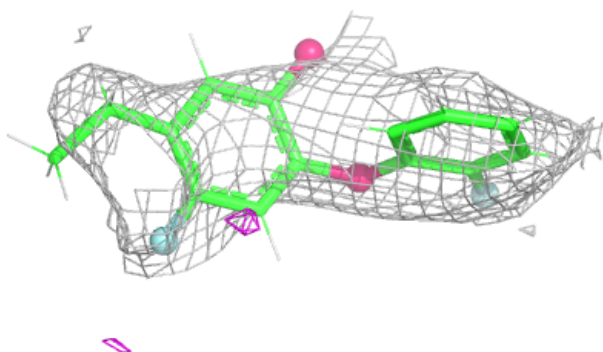
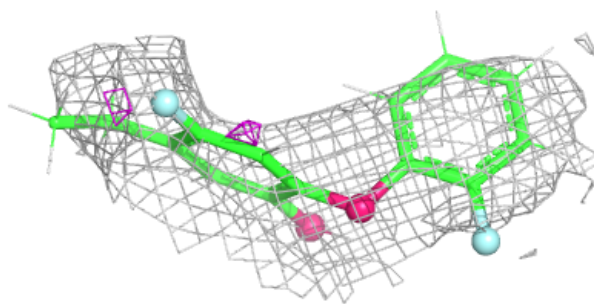
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 68O C 302:

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

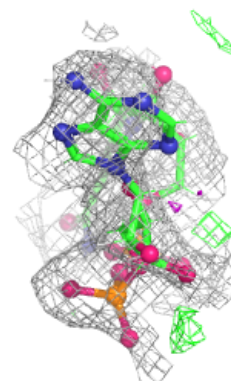
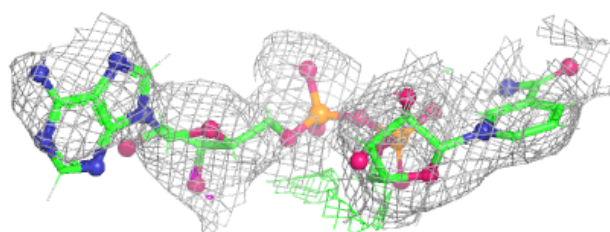
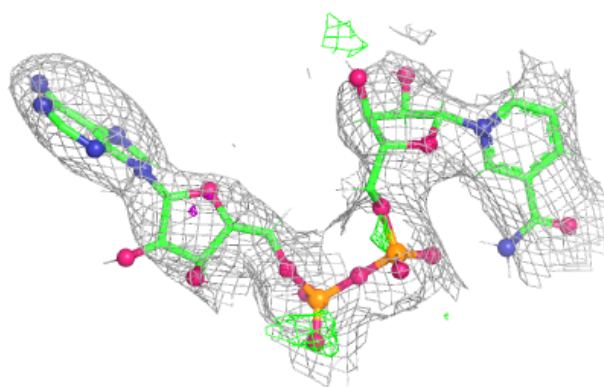
**Electron density around 68O K 302:**

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

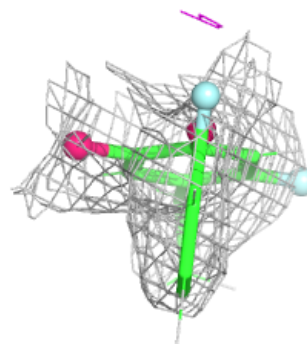
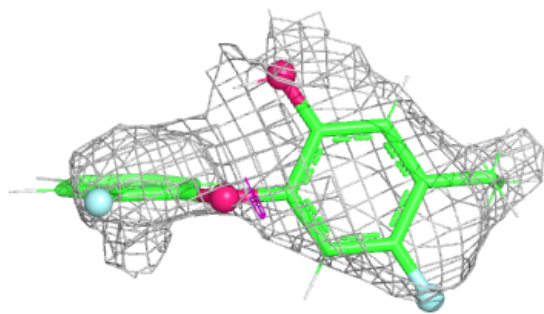
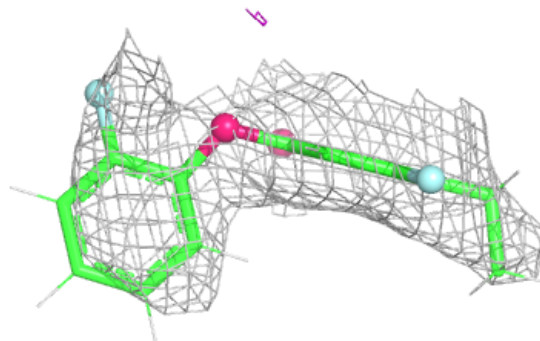


Electron density around NAD E 301:

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

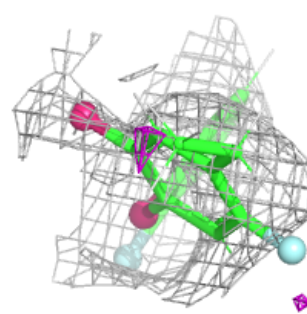
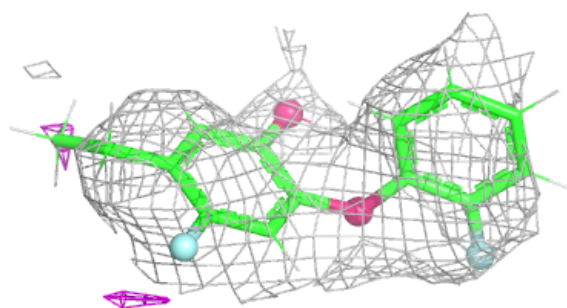
**Electron density around 68O I 302:**

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

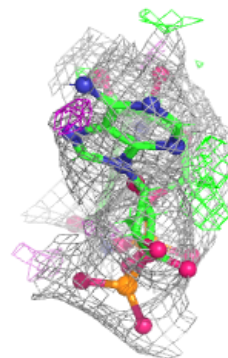
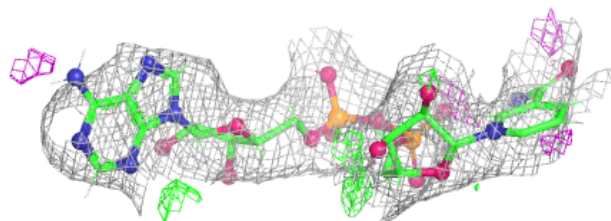
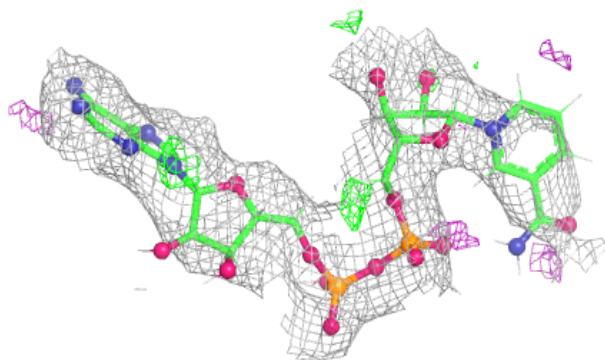


Electron density around 68O E 302:

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

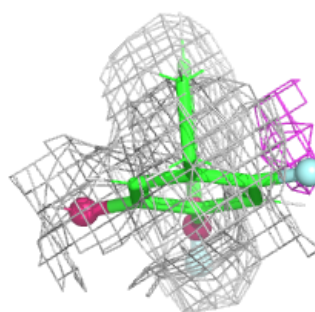
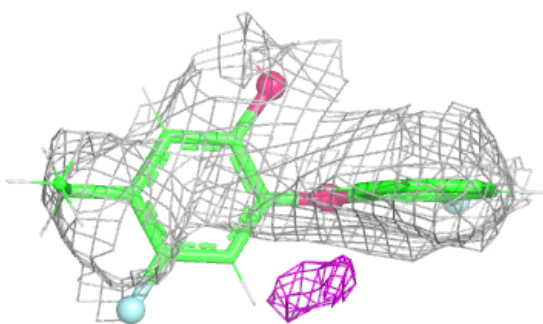
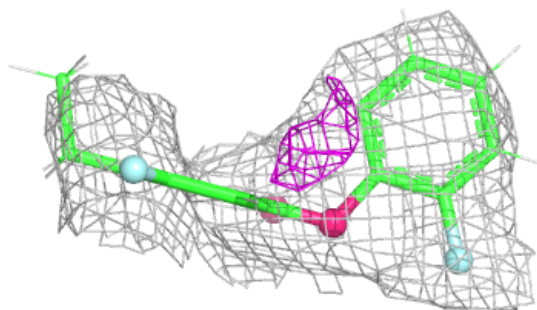
**Electron density around NAD C 301:**

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

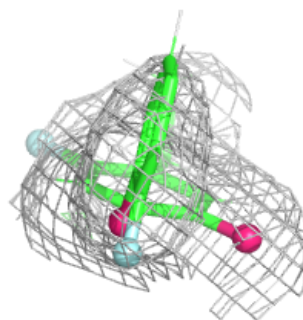
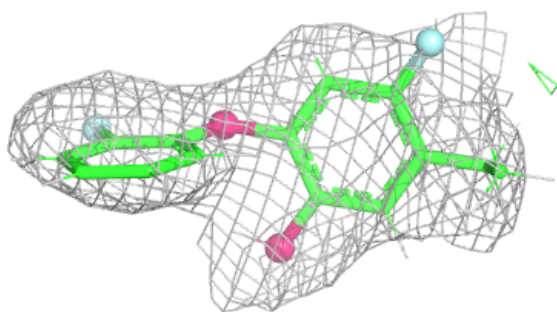
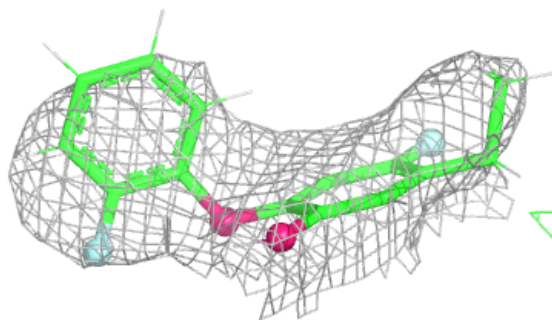


Electron density around 68O F 302:

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

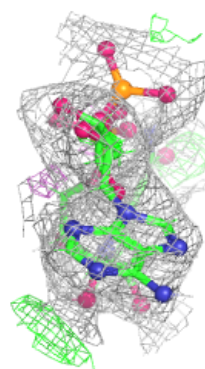
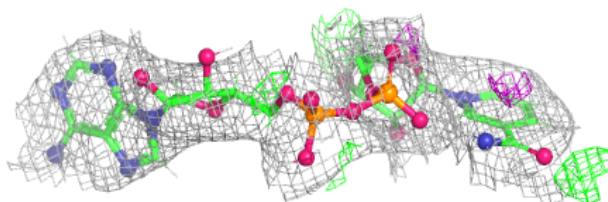
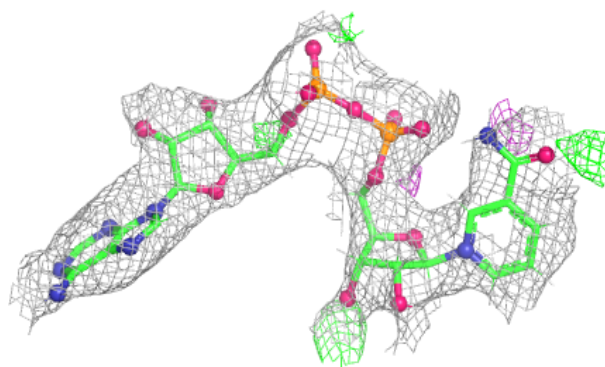
**Electron density around 68O H 302:**

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

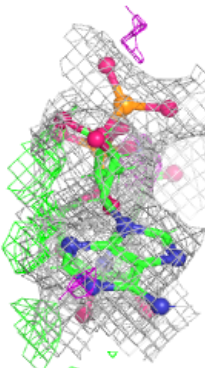
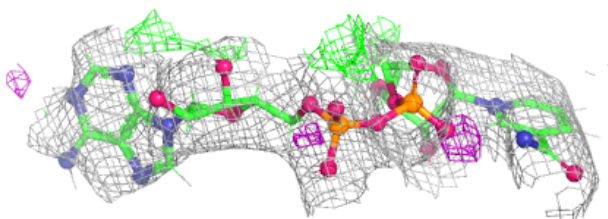
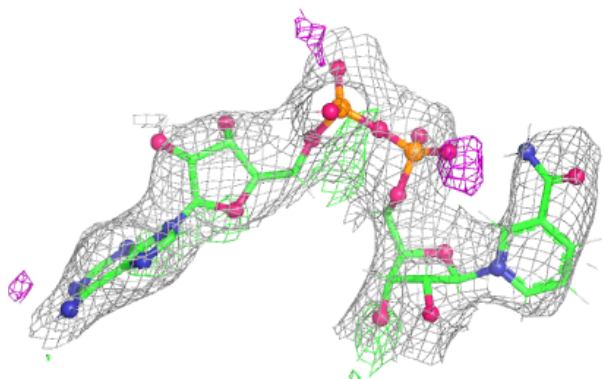


Electron density around NAD H 301:

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

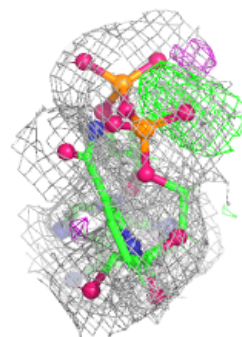
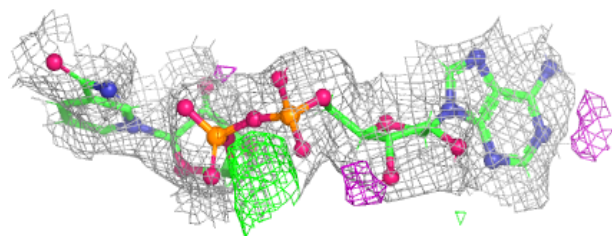
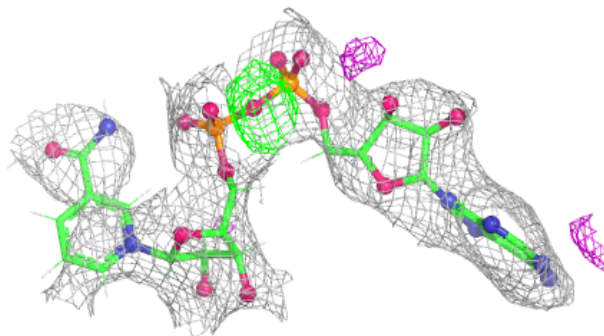
**Electron density around NAD F 301:**

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

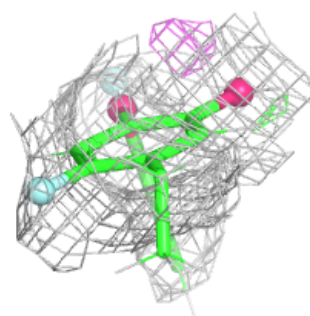
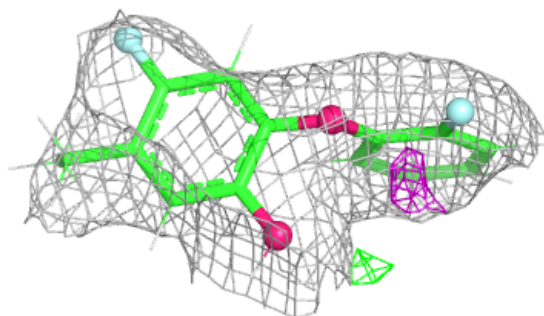
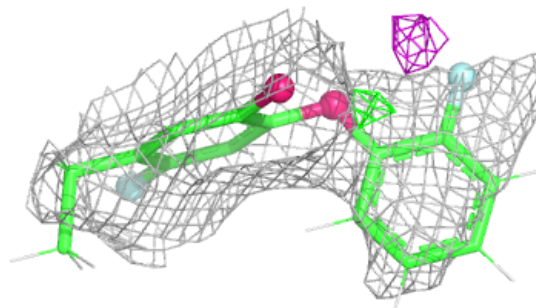


Electron density around NAD J 301:

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

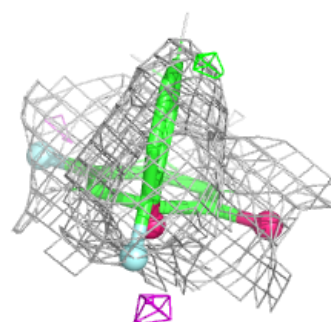
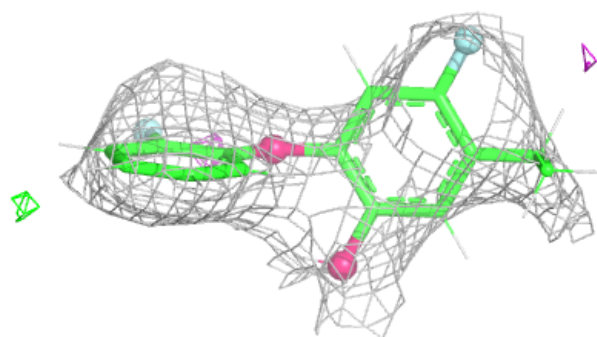
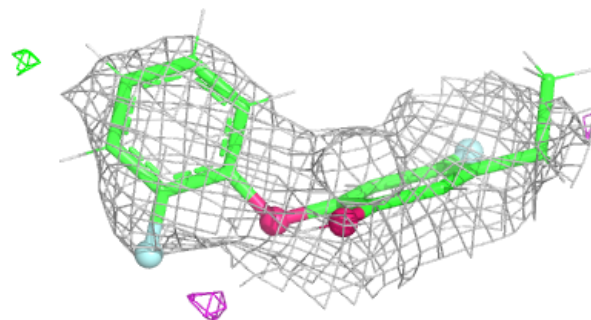
**Electron density around 68O D 302:**

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

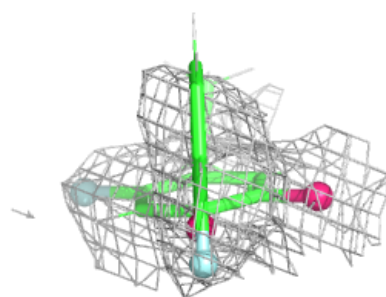
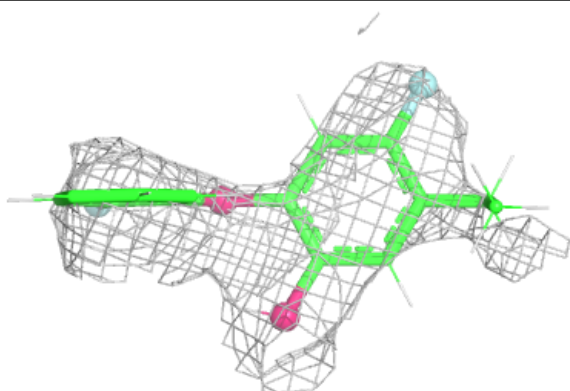
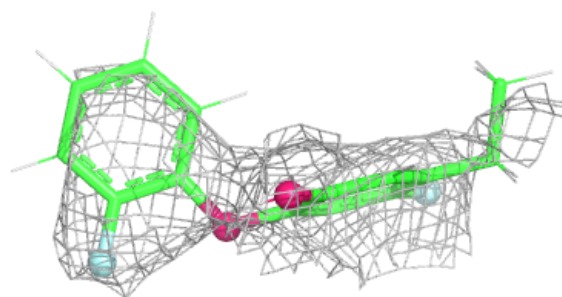


Electron density around 68O J 302:

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

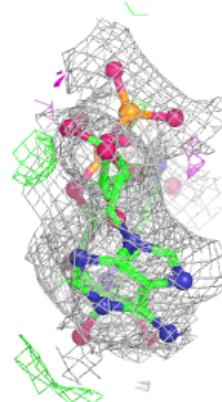
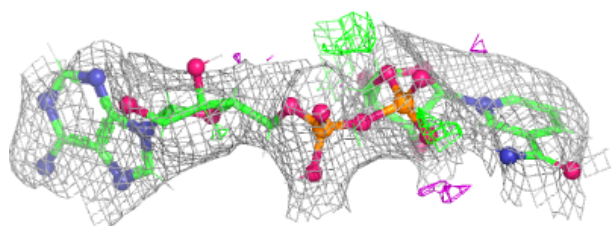
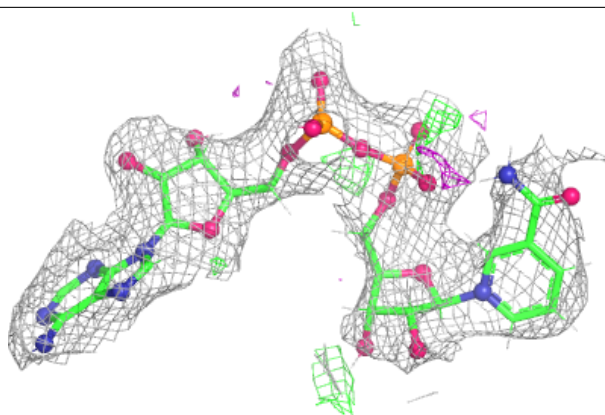
**Electron density around 68O L 302:**

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

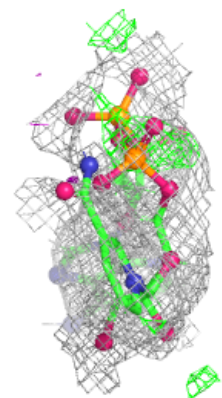
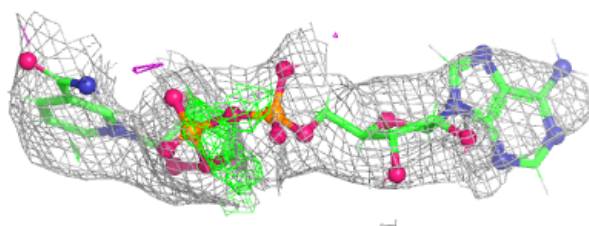
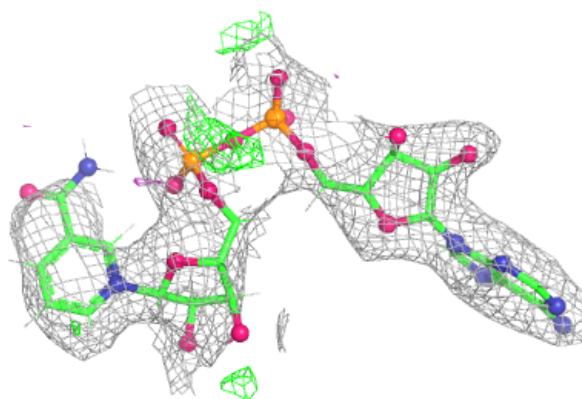


Electron density around NAD G 301:

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

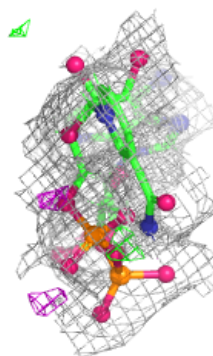
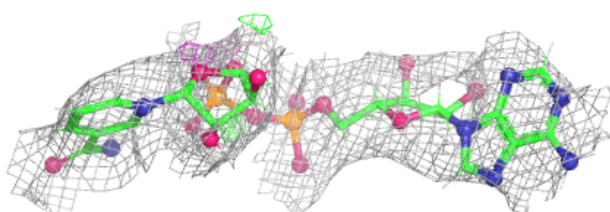
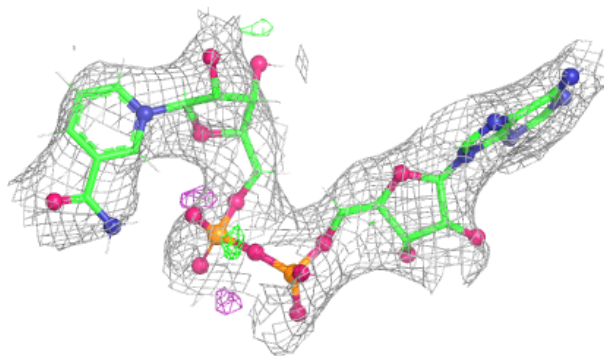
**Electron density around NAD B 301:**

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

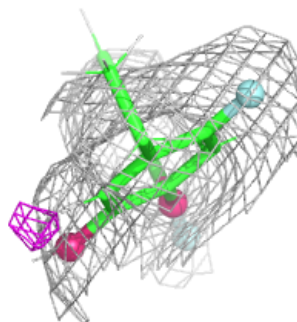
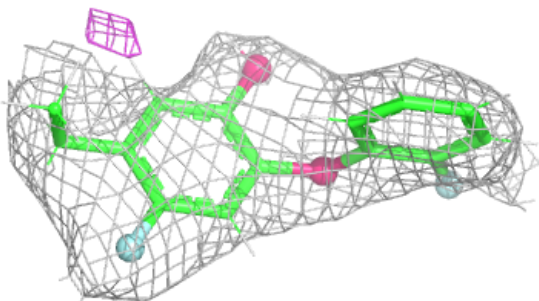
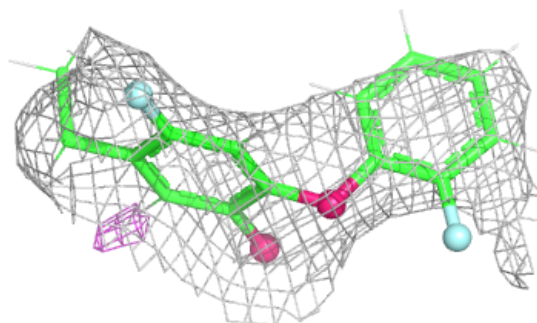


Electron density around NAD A 301:

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

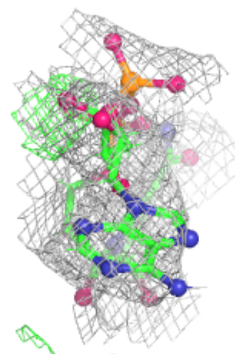
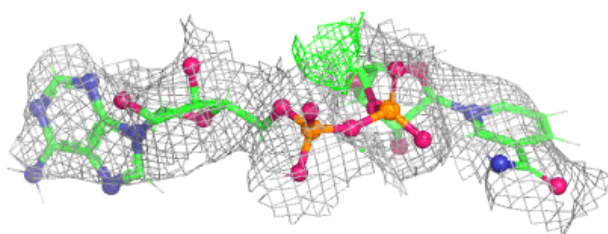
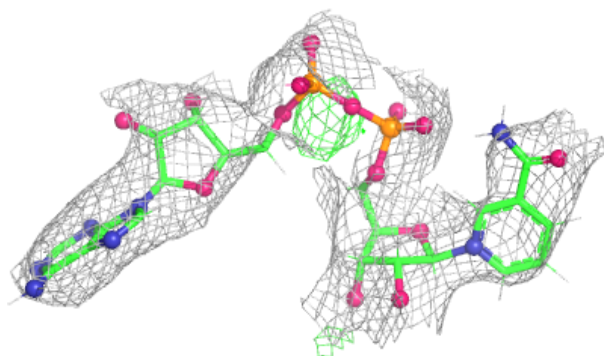
**Electron density around 68O G 302:**

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

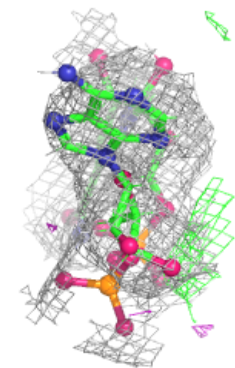
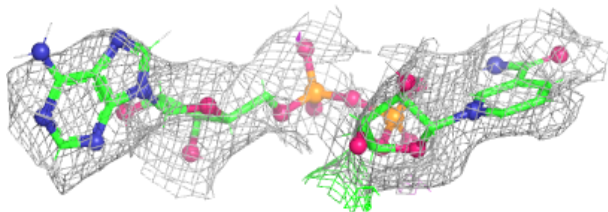
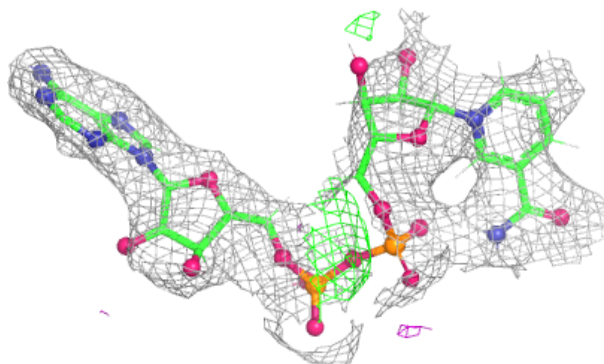


Electron density around NAD K 301:

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

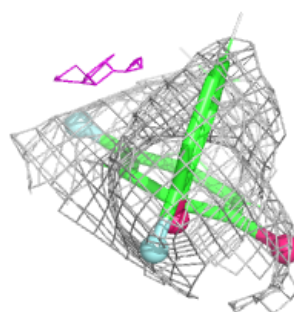
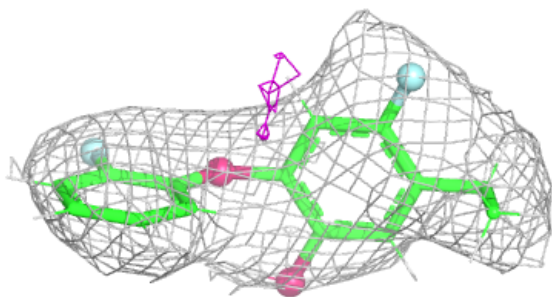
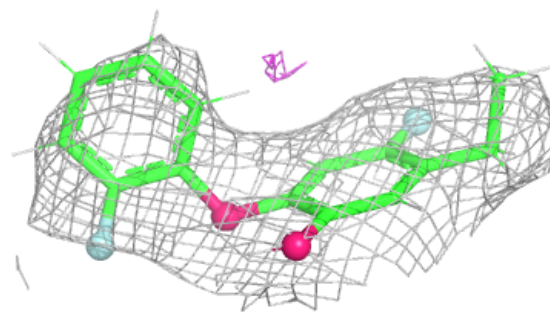
**Electron density around NAD L 301:**

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

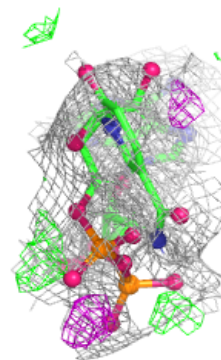
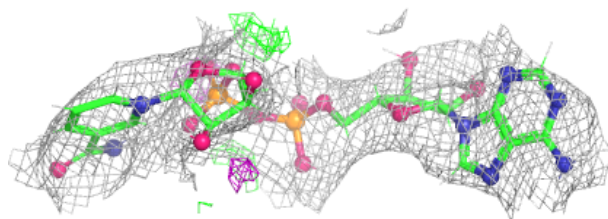
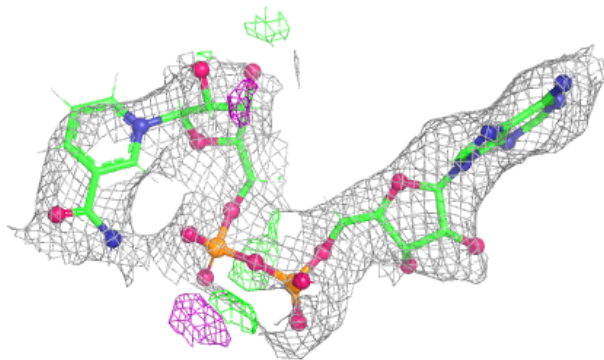


Electron density around 68O B 302:

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

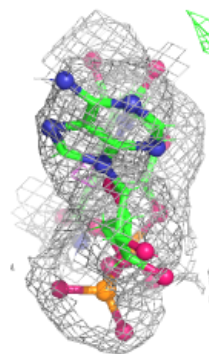
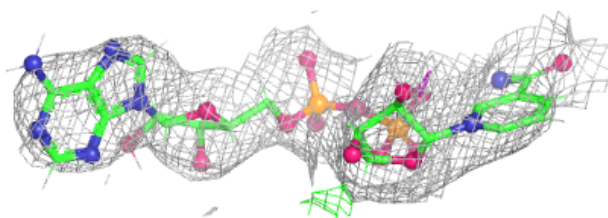
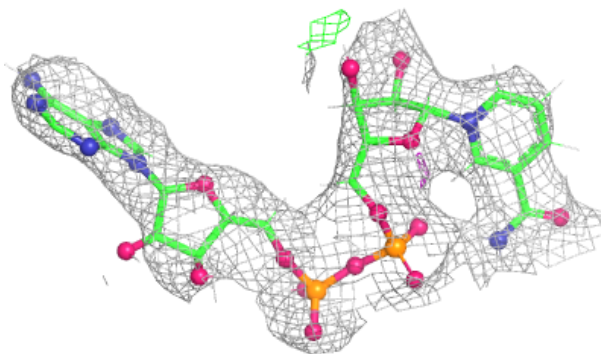
**Electron density around NAD D 301:**

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

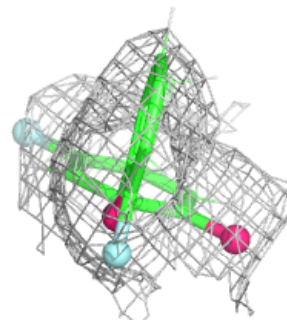
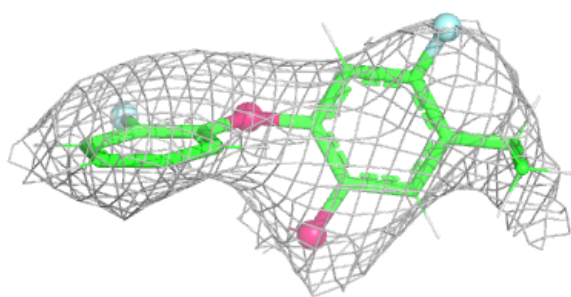
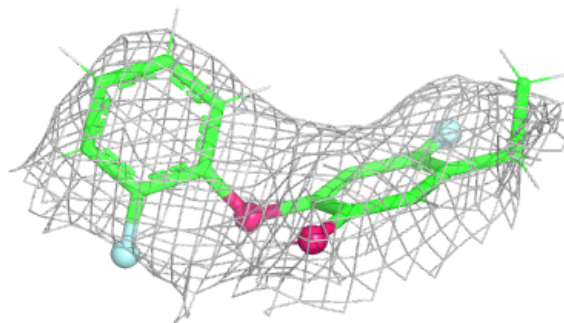


Electron density around NAD I 301:

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

**Electron density around 68O A 302:**

$2mF_o-DF_c$ (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.