



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:07 PM UTC

PDB ID : 1QSG / pdb_00001qsg
Title : CRYSTAL STRUCTURE OF ENOYL REDUCTASE INHIBITION BY TRI-CLOSAN
Authors : Stewart, M.J.; Parikh, S.; Xiao, G.; Tonge, P.J.; Kisker, C.
Deposited on : 1999-06-21
Resolution : 1.75 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

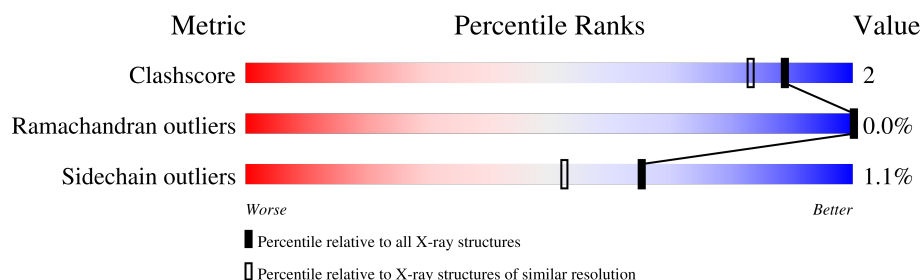
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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))
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	265	88% 10% .
1	B	265	89% 8% ..
1	C	265	91% 6% .
1	D	265	89% 9% .
1	E	265	86% 9% ..
1	F	265	88% 9% ..
1	G	265	88% 8% ..
1	H	265	90% 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
2	GLC	A	1303	X	-	-	-
2	GLC	B	1306	X	-	-	-
2	GLC	C	1309	X	-	-	-
2	GLC	D	1312	X	-	-	-
2	GLC	E	1315	X	-	-	-
2	GLC	F	1318	X	-	-	-
2	GLC	G	1321	X	-	-	-
2	GLC	H	1324	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17287 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 ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1918	1209	331	365	13			
1	B	258	Total	C	N	O	S	0	0	0
			1918	1209	331	365	13			
1	C	258	Total	C	N	O	S	0	0	0
			1918	1209	331	365	13			
1	D	258	Total	C	N	O	S	0	0	0
			1918	1209	331	365	13			
1	E	258	Total	C	N	O	S	0	0	0
			1918	1209	331	365	13			
1	F	258	Total	C	N	O	S	0	0	0
			1918	1209	331	365	13			
1	G	259	Total	C	N	O	S	0	0	0
			1927	1214	332	368	13			
1	H	258	Total	C	N	O	S	0	0	0
			1918	1209	331	365	13			

There are 24 discrepancies between the modelled and reference sequences:

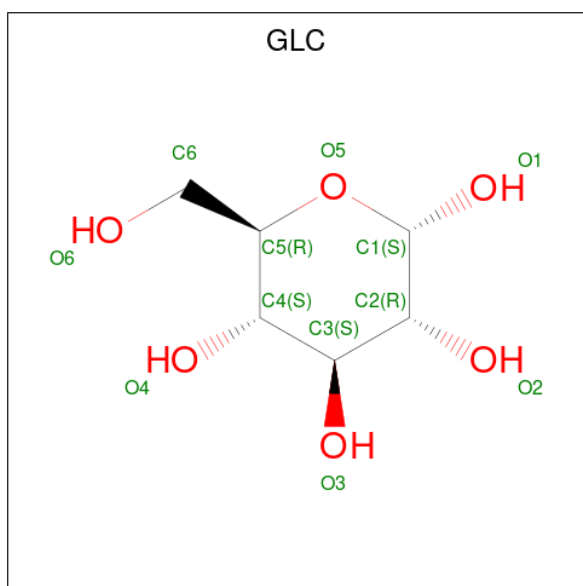
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P29132
A	-1	SER	-	expression tag	UNP P29132
A	0	HIS	-	expression tag	UNP P29132
B	-2	GLY	-	expression tag	UNP P29132
B	-1	SER	-	expression tag	UNP P29132
B	0	HIS	-	expression tag	UNP P29132
C	-2	GLY	-	expression tag	UNP P29132
C	-1	SER	-	expression tag	UNP P29132
C	0	HIS	-	expression tag	UNP P29132
D	-2	GLY	-	expression tag	UNP P29132
D	-1	SER	-	expression tag	UNP P29132
D	0	HIS	-	expression tag	UNP P29132
E	-2	GLY	-	expression tag	UNP P29132

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	expression tag	UNP P29132
E	0	HIS	-	expression tag	UNP P29132
F	-2	GLY	-	expression tag	UNP P29132
F	-1	SER	-	expression tag	UNP P29132
F	0	HIS	-	expression tag	UNP P29132
G	-2	GLY	-	expression tag	UNP P29132
G	-1	SER	-	expression tag	UNP P29132
G	0	HIS	-	expression tag	UNP P29132
H	-2	GLY	-	expression tag	UNP P29132
H	-1	SER	-	expression tag	UNP P29132
H	0	HIS	-	expression tag	UNP P29132

- Molecule 2 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



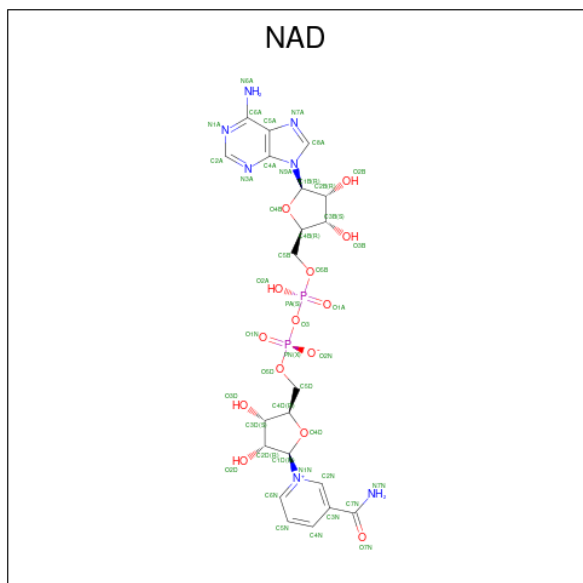
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			12	6	6		
2	E	1	Total	C	O	0	0
			12	6	6		
2	F	1	Total	C	O	0	0
			12	6	6		

Continued on next page...

Continued from previous page...

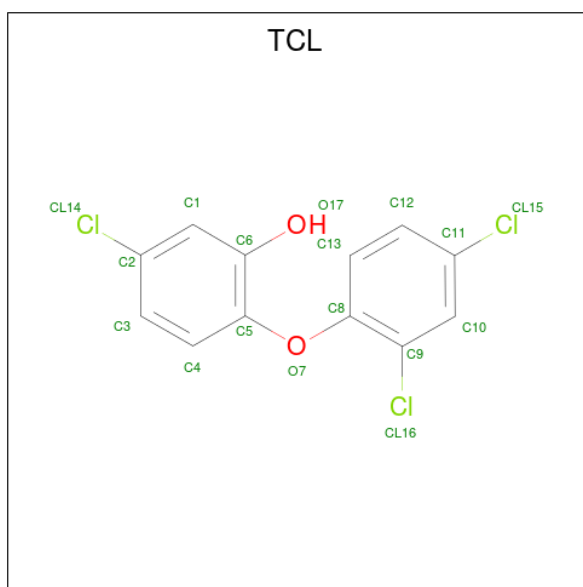
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total C O 12 6 6	0	0
2	H	1	Total C O 12 6 6	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$).



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

- Molecule 4 is TRICLOSAN (CCD ID: TCL) (formula: $\text{C}_{12}\text{H}_7\text{Cl}_3\text{O}_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	O	0	0
			17	12	3	2		
4	B	1	Total	C	Cl	O	0	0
			17	12	3	2		
4	C	1	Total	C	Cl	O	0	0
			17	12	3	2		
4	D	1	Total	C	Cl	O	0	0
			17	12	3	2		
4	E	1	Total	C	Cl	O	0	0
			17	12	3	2		
4	F	1	Total	C	Cl	O	0	0
			17	12	3	2		
4	G	1	Total	C	Cl	O	0	0
			17	12	3	2		
4	H	1	Total	C	Cl	O	0	0
			17	12	3	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	214	Total	O	0	0
			214	214		
5	B	165	Total	O	0	0
			165	165		
5	C	177	Total	O	0	0
			177	177		
5	D	180	Total	O	0	0
			180	180		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	144	Total 144	O 144	0	0
5	F	132	Total 132	O 132	0	0
5	G	188	Total 188	O 188	0	0
5	H	150	Total 150	O 150	0	0

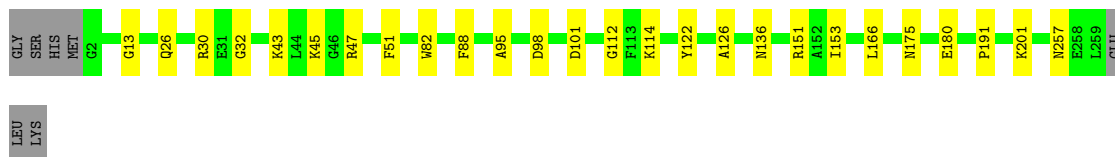
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

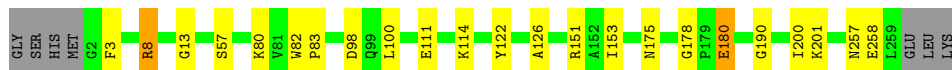
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE

Chain A: 



• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE

Chain B: 



• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE

Chain C: 



• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE

Chain D: 



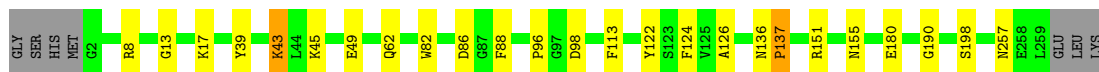
• Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE

Chain E: 



● Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE

Chain F:  88% 9% ..



● Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE

Chain G:  88% 8% ..



● Molecule 1: ENOYL-[ACYL-CARRIER-PROTEIN] REDUCTASE

Chain H:  90% 7% .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.73Å 82.08Å 84.18Å 89.54° 87.43° 77.77°	Depositor
Resolution (Å)	20.00 – 1.75	Depositor
% Data completeness (in resolution range)	94.2 (20.00-1.75)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.172 , 0.215	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17287	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, TCL, NAD

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	0.89	0/1950	1.57	16/2634 (0.6%)
1	B	0.81	0/1950	1.54	19/2634 (0.7%)
1	C	0.84	0/1950	1.51	16/2634 (0.6%)
1	D	0.80	0/1950	1.51	10/2634 (0.4%)
1	E	0.68	0/1950	1.42	11/2634 (0.4%)
1	F	0.70	0/1950	1.48	10/2634 (0.4%)
1	G	0.77	0/1959	1.53	16/2646 (0.6%)
1	H	0.76	0/1950	1.51	13/2634 (0.5%)
All	All	0.78	0/15609	1.51	111/21084 (0.5%)

There are no bond length outliers.

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	151	ARG	CD-NE-CZ	10.14	138.60	124.40
1	D	98	ASP	CA-CB-CG	10.03	122.62	112.60
1	G	8	ARG	CD-NE-CZ	9.39	137.55	124.40
1	C	8	ARG	CD-NE-CZ	9.30	137.42	124.40
1	B	153	ILE	CA-C-O	9.15	125.18	119.51
1	E	3	PHE	CA-CB-CG	8.53	122.33	113.80
1	B	151	ARG	CD-NE-CZ	7.83	135.37	124.40
1	A	166	LEU	O-C-N	-7.65	114.19	122.07
1	A	153	ILE	CA-C-O	7.45	124.13	119.51
1	A	98	ASP	CA-CB-CG	7.37	119.97	112.60
1	C	78	LEU	CA-C-N	7.25	129.20	120.14
1	C	78	LEU	C-N-CA	7.25	129.20	120.14
1	G	111	GLU	CB-CG-CD	7.25	124.92	112.60
1	E	153	ILE	CA-C-O	7.21	123.98	119.51
1	F	98	ASP	CA-CB-CG	7.16	119.76	112.60
1	B	100	LEU	N-CA-C	7.06	120.55	112.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	95	ALA	O-C-N	6.97	126.83	121.88
1	B	98	ASP	CA-CB-CG	6.86	119.46	112.60
1	A	151	ARG	CD-NE-CZ	6.72	133.81	124.40
1	G	13	GLY	N-CA-C	6.72	125.26	114.90
1	E	106	ASN	OD1-CG-ND2	-6.71	115.89	122.60
1	G	151	ARG	CD-NE-CZ	6.69	133.77	124.40
1	A	88	PHE	CA-CB-CG	6.66	120.46	113.80
1	C	45	LYS	N-CA-C	6.56	118.98	111.11
1	B	258	GLU	CA-C-N	6.54	133.48	121.70
1	B	258	GLU	C-N-CA	6.54	133.48	121.70
1	H	40	GLN	N-CA-C	6.51	118.46	111.36
1	F	88	PHE	CA-CB-CG	6.46	120.26	113.80
1	E	100	LEU	N-CA-C	6.44	121.73	111.81
1	E	101	ASP	CA-CB-CG	6.42	119.02	112.60
1	G	153	ILE	CA-C-O	6.40	123.48	119.51
1	C	157	ASN	OD1-CG-ND2	-6.34	116.26	122.60
1	C	3	PHE	CA-CB-CG	6.30	120.10	113.80
1	A	51	PHE	CA-CB-CG	6.30	120.10	113.80
1	A	136	ASN	CA-CB-CG	6.23	118.83	112.60
1	B	258	GLU	CA-C-O	6.20	128.15	121.02
1	G	88	PHE	CA-CB-CG	6.16	119.96	113.80
1	B	200	ILE	N-CA-CB	6.14	118.00	111.00
1	D	13	GLY	N-CA-C	6.14	123.83	115.30
1	H	88	PHE	CA-CB-CG	6.13	119.93	113.80
1	F	151	ARG	CD-NE-CZ	6.06	132.88	124.40
1	G	62	GLN	OE1-CD-NE2	6.06	128.66	122.60
1	B	13	GLY	N-CA-C	6.05	124.22	114.90
1	F	113	PHE	CA-CB-CG	6.05	119.85	113.80
1	A	32	GLY	N-CA-C	6.02	123.67	115.30
1	D	100	LEU	N-CA-C	6.01	119.36	112.57
1	B	111	GLU	CA-C-N	6.00	126.60	119.94
1	B	111	GLU	C-N-CA	6.00	126.60	119.94
1	E	106	ASN	CA-CB-CG	6.00	118.60	112.60
1	D	86	ASP	N-CA-C	5.98	119.89	112.59
1	D	51	PHE	CA-CB-CG	5.97	119.77	113.80
1	A	112	GLY	CA-C-N	5.95	128.17	120.44
1	A	112	GLY	C-N-CA	5.95	128.17	120.44
1	F	13	GLY	N-CA-C	5.93	124.21	115.08
1	H	13	GLY	N-CA-C	5.91	123.81	115.30
1	A	13	GLY	N-CA-C	5.87	123.46	115.30
1	D	137	PRO	CA-C-O	-5.85	114.67	121.34
1	A	82	TRP	CA-C-N	5.82	125.51	119.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	TRP	C-N-CA	5.82	125.51	119.05
1	B	190	GLY	N-CA-C	-5.78	105.00	112.10
1	F	190	GLY	N-CA-C	-5.71	105.08	112.10
1	E	107	ALA	N-CA-C	5.67	119.38	112.23
1	C	224	ASP	CA-CB-CG	5.67	118.27	112.60
1	B	3	PHE	CA-CB-CG	5.66	119.46	113.80
1	G	96	PRO	N-CA-CB	5.65	108.23	103.25
1	D	157	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	F	124	PHE	CA-CB-CG	5.63	119.43	113.80
1	G	37	PHE	N-CA-C	5.61	118.37	109.50
1	F	137	PRO	N-CA-CB	5.59	108.29	103.31
1	F	96	PRO	N-CA-CB	5.56	108.15	103.25
1	B	180	GLU	O-C-N	-5.55	115.23	122.39
1	H	214	THR	CA-C-N	5.54	125.00	119.24
1	H	214	THR	C-N-CA	5.54	125.00	119.24
1	C	100	LEU	N-CA-C	5.47	118.75	112.57
1	C	212	ALA	N-CA-C	5.46	118.16	111.82
1	H	100	LEU	N-CA-C	5.46	118.74	112.57
1	H	137	PRO	N-CA-CB	5.43	108.03	103.25
1	G	223	GLU	CB-CG-CD	5.39	121.76	112.60
1	D	154	PRO	N-CA-CB	5.38	108.03	103.19
1	C	40	GLN	OE1-CD-NE2	-5.35	117.25	122.60
1	D	224	ASP	CA-CB-CG	5.33	117.93	112.60
1	G	191	PRO	N-CA-CB	5.30	108.04	103.27
1	B	57	SER	N-CA-C	5.30	118.37	109.95
1	G	3	PHE	CA-CB-CG	5.29	119.09	113.80
1	G	78	LEU	CA-C-N	5.29	126.75	120.14
1	G	78	LEU	C-N-CA	5.29	126.75	120.14
1	C	146	TYR	CA-C-N	5.28	127.88	120.28
1	C	146	TYR	C-N-CA	5.28	127.88	120.28
1	B	8	ARG	CD-NE-CZ	5.27	131.77	124.40
1	H	90	HIS	CA-CB-CG	5.26	119.06	113.80
1	B	83	PRO	N-CA-CB	5.26	109.09	103.52
1	H	32	GLY	N-CA-C	5.26	122.84	115.43
1	C	154	PRO	N-CA-CB	5.24	107.86	103.25
1	A	191	PRO	N-CA-CB	5.23	107.97	103.36
1	H	212	ALA	N-CA-C	5.23	118.12	111.69
1	C	137	PRO	N-CA-CB	5.21	107.94	103.31
1	E	86	ASP	N-CA-C	5.20	118.94	112.59
1	G	218	ARG	CA-C-O	-5.18	115.69	121.23
1	A	45	LYS	N-CA-C	5.15	116.58	111.07
1	F	86	ASP	N-CA-C	5.15	118.88	112.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	107	ALA	N-CA-C	5.14	118.70	112.23
1	G	8	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	C	82	TRP	O-C-N	-5.10	116.78	121.37
1	H	124	PHE	CA-CB-CG	5.09	118.89	113.80
1	E	257	ASN	CA-C-N	5.09	131.25	121.54
1	E	257	ASN	C-N-CA	5.09	131.25	121.54
1	B	178	GLY	CA-C-N	5.08	125.36	119.47
1	B	178	GLY	C-N-CA	5.08	125.36	119.47
1	H	200	ILE	N-CA-CB	5.05	117.12	111.21
1	E	213	VAL	N-CA-C	5.00	117.70	112.90
1	A	95	ALA	O-C-N	-5.00	118.35	121.85

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	1918	0	1909	9	0
1	B	1918	0	1909	8	0
1	C	1918	0	1909	4	0
1	D	1918	0	1909	8	0
1	E	1918	0	1909	15	0
1	F	1918	0	1909	10	0
1	G	1927	0	1915	10	0
1	H	1918	0	1909	4	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
2	C	12	0	12	0	0
2	D	12	0	12	1	0
2	E	12	0	12	0	0
2	F	12	0	12	0	0
2	G	12	0	11	0	0
2	H	12	0	12	0	0
3	A	44	0	26	0	0
3	B	44	0	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	44	0	25	0	0
3	D	44	0	26	0	0
3	E	44	0	24	2	0
3	F	44	0	25	0	0
3	G	44	0	25	0	0
3	H	44	0	25	0	0
4	A	17	0	7	0	0
4	B	17	0	7	0	0
4	C	17	0	7	0	0
4	D	17	0	7	0	0
4	E	17	0	7	1	0
4	F	17	0	7	0	0
4	G	17	0	7	0	0
4	H	17	0	7	0	0
5	A	214	0	0	1	0
5	B	165	0	0	2	0
5	C	177	0	0	2	0
5	D	180	0	0	2	0
5	E	144	0	0	1	0
5	F	132	0	0	2	0
5	G	188	0	0	3	0
5	H	150	0	0	1	0
All	All	17287	0	15630	59	0

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

All (59) 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:E:259:LEU:HD22	1:H:205:LYS:HD3	1.60	0.83
1:E:257:ASN:HD21	1:G:175:ASN:HD21	1.31	0.78
1:B:175:ASN:HD21	1:D:257:ASN:HD21	1.34	0.76
1:E:175:ASN:HD21	1:G:257:ASN:HD21	1.33	0.76
1:G:213:VAL:HG11	1:G:258:GLU:HG3	1.71	0.71
1:A:175:ASN:HD21	1:C:257:ASN:HD21	1.37	0.70
1:E:49:GLU:HG2	1:E:60:VAL:HG11	1.74	0.70
1:A:114:LYS:HD2	1:B:114:LYS:HD2	1.77	0.67
1:A:257:ASN:HD21	1:C:175:ASN:HD21	1.43	0.66
1:F:257:ASN:HD21	1:H:175:ASN:HD21	1.48	0.62
1:B:8:ARG:HH11	1:B:82:TRP:CD1	2.20	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:17:LYS:HD3	5:G:1357:HOH:O	2.02	0.59
1:B:80:LYS:HE3	5:B:1443:HOH:O	2.04	0.58
3:E:1313:NAD:H51N	4:E:1314:TCL:CL16	2.41	0.57
1:E:195:LEU:HD23	5:E:1424:HOH:O	2.08	0.53
1:F:8:ARG:HH11	1:F:82:TRP:CD1	2.28	0.52
1:D:94:PHE:CD2	2:D:1312:GLC:H2	2.45	0.51
3:E:1313:NAD:H2N	3:E:1313:NAD:H52N	1.93	0.51
1:A:26:GLN:NE2	5:A:1444:HOH:O	2.43	0.51
1:E:101:ASP:OD1	1:E:201:LYS:HD2	2.11	0.50
1:A:101:ASP:OD1	1:A:201:LYS:HD2	2.11	0.50
1:F:198:SER:HB3	5:F:1417:HOH:O	2.12	0.50
1:C:26:GLN:NE2	5:C:1449:HOH:O	2.45	0.49
1:B:114:LYS:HE2	5:B:1432:HOH:O	2.12	0.49
1:E:45:LYS:O	1:E:49:GLU:HG3	2.13	0.48
1:G:101:ASP:OD1	1:G:201:LYS:HD2	2.14	0.48
1:E:99:GLN:OE1	1:E:108:VAL:HA	2.14	0.48
1:B:257:ASN:HD21	1:D:175:ASN:HD21	1.60	0.48
1:A:47:ARG:NH2	1:H:72:ASP:OD1	2.47	0.47
1:D:101:ASP:OD1	1:D:201:LYS:HD2	2.15	0.47
1:F:122:TYR:CE2	1:F:126:ALA:HB2	2.50	0.47
1:F:43:LYS:NZ	5:F:1427:HOH:O	2.45	0.46
1:B:122:TYR:CE2	1:B:126:ALA:HB2	2.51	0.46
1:D:8:ARG:NH1	5:D:1404:HOH:O	2.35	0.46
1:D:122:TYR:CE2	1:D:126:ALA:HB2	2.50	0.46
1:B:8:ARG:HD3	1:B:82:TRP:NE1	2.30	0.46
1:H:38:THR:HA	1:H:61:LEU:O	2.16	0.45
1:F:155:ASN:ND2	1:G:260:GLU:OE2	2.47	0.44
1:G:114:LYS:HD3	1:G:114:LYS:C	2.42	0.44
1:D:204:ARG:HG2	5:D:1444:HOH:O	2.17	0.44
1:E:204:ARG:HD2	1:E:204:ARG:O	2.18	0.43
1:E:44:LEU:O	1:E:45:LYS:C	2.62	0.43
1:E:38:THR:HA	1:E:61:LEU:O	2.19	0.42
1:G:213:VAL:CG1	1:G:258:GLU:HG3	2.44	0.42
1:D:38:THR:HA	1:D:61:LEU:O	2.19	0.42
1:E:122:TYR:CE2	1:E:126:ALA:HB2	2.55	0.42
1:F:8:ARG:HD3	1:F:82:TRP:NE1	2.34	0.42
1:E:114:LYS:HD3	1:E:114:LYS:C	2.45	0.42
1:G:220:VAL:HG22	5:G:1397:HOH:O	2.20	0.42
1:C:8:ARG:NH1	5:C:1371:HOH:O	2.49	0.41
1:F:39:TYR:OH	1:F:45:LYS:HD2	2.20	0.41
1:F:136:ASN:HB3	1:F:137:PRO:HD2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:TYR:CE2	1:A:126:ALA:HB2	2.54	0.41
1:E:258:GLU:H	1:E:258:GLU:HG3	1.29	0.41
1:A:30:ARG:HH11	1:A:30:ARG:HD3	1.73	0.41
1:F:45:LYS:HE3	1:F:49:GLU:OE2	2.21	0.41
1:A:43:LYS:HE3	5:H:1373:HOH:O	2.20	0.40
1:E:194:THR:H	1:E:197:ALA:HB3	1.86	0.40
1:G:47:ARG:HG2	5:G:1484:HOH:O	2.22	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	256/265 (97%)	250 (98%)	6 (2%)	0	100	100
1	B	256/265 (97%)	249 (97%)	7 (3%)	0	100	100
1	C	256/265 (97%)	250 (98%)	6 (2%)	0	100	100
1	D	256/265 (97%)	250 (98%)	6 (2%)	0	100	100
1	E	256/265 (97%)	249 (97%)	6 (2%)	1 (0%)	30	15
1	F	256/265 (97%)	247 (96%)	9 (4%)	0	100	100
1	G	257/265 (97%)	251 (98%)	6 (2%)	0	100	100
1	H	256/265 (97%)	245 (96%)	11 (4%)	0	100	100
All	All	2049/2120 (97%)	1991 (97%)	57 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	258	GLU

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	197/203 (97%)	196 (100%)	1 (0%)	81	75
1	B	197/203 (97%)	195 (99%)	2 (1%)	68	56
1	C	197/203 (97%)	196 (100%)	1 (0%)	81	75
1	D	197/203 (97%)	195 (99%)	2 (1%)	68	56
1	E	197/203 (97%)	195 (99%)	2 (1%)	68	56
1	F	197/203 (97%)	193 (98%)	4 (2%)	48	29
1	G	198/203 (98%)	195 (98%)	3 (2%)	57	41
1	H	197/203 (97%)	195 (99%)	2 (1%)	68	56
All	All	1577/1624 (97%)	1560 (99%)	17 (1%)	65	52

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	GLU
1	B	180	GLU
1	B	201	LYS
1	C	206	MET
1	D	114	LYS
1	D	180	GLU
1	E	17	LYS
1	E	195	LEU
1	F	17	LYS
1	F	43	LYS
1	F	62	GLN
1	F	180	GLU
1	G	17	LYS
1	G	111	GLU
1	G	258	GLU
1	H	180	GLU
1	H	258	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	209	HIS
1	A	257	ASN
1	B	41	ASN
1	B	257	ASN
1	C	26	GLN
1	C	157	ASN
1	C	257	ASN
1	D	26	GLN
1	D	62	GLN
1	D	257	ASN
1	E	26	GLN
1	E	62	GLN
1	E	257	ASN
1	F	29	HIS
1	F	257	ASN
1	G	157	ASN
1	G	257	ASN
1	H	26	GLN
1	H	40	GLN
1	H	54	GLN
1	H	209	HIS
1	H	257	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$
4	TCL	B	1305	-	18,18,18	1.04	2 (11%)	25,25,25	1.05	1 (4%)
2	GLC	F	1318	-	12,12,12	1.00	0	17,17,17	2.25	5 (29%)
3	NAD	D	1310	-	46,48,48	2.07	13 (28%)	64,73,73	2.22	18 (28%)
4	TCL	A	1302	-	18,18,18	1.13	1 (5%)	25,25,25	1.17	2 (8%)
3	NAD	H	1322	-	46,48,48	2.08	16 (34%)	64,73,73	2.31	18 (28%)
3	NAD	F	1316	-	46,48,48	2.06	13 (28%)	64,73,73	2.25	21 (32%)
3	NAD	C	1307	-	46,48,48	2.34	16 (34%)	64,73,73	2.21	18 (28%)
3	NAD	G	1319	-	46,48,48	2.32	16 (34%)	64,73,73	2.42	15 (23%)
2	GLC	B	1306	-	12,12,12	1.12	1 (8%)	17,17,17	1.63	2 (11%)
4	TCL	C	1308	-	18,18,18	1.05	0	25,25,25	1.11	2 (8%)
3	NAD	E	1313	-	46,48,48	2.27	15 (32%)	64,73,73	2.53	24 (37%)
2	GLC	E	1315	-	12,12,12	1.07	0	17,17,17	1.91	3 (17%)
3	NAD	B	1304	-	46,48,48	2.14	16 (34%)	64,73,73	2.49	20 (31%)
2	GLC	H	1324	-	12,12,12	0.86	0	17,17,17	2.71	7 (41%)
3	NAD	A	1301	-	46,48,48	2.26	16 (34%)	64,73,73	2.48	18 (28%)
4	TCL	E	1314	-	18,18,18	0.93	1 (5%)	25,25,25	0.98	2 (8%)
4	TCL	F	1317	-	18,18,18	0.85	0	25,25,25	1.05	1 (4%)
2	GLC	C	1309	-	12,12,12	1.21	0	17,17,17	1.76	3 (17%)
2	GLC	G	1321	-	12,12,12	0.92	0	17,17,17	2.60	7 (41%)
4	TCL	H	1323	-	18,18,18	1.03	0	25,25,25	1.06	2 (8%)
2	GLC	A	1303	-	12,12,12	1.08	1 (8%)	17,17,17	2.88	9 (52%)
4	TCL	G	1320	-	18,18,18	1.16	0	25,25,25	1.04	1 (4%)
4	TCL	D	1311	-	18,18,18	0.89	0	25,25,25	1.32	2 (8%)
2	GLC	D	1312	-	12,12,12	0.87	1 (8%)	17,17,17	2.21	4 (23%)

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
4	TCL	B	1305	-	-	0/4/4/4	0/2/2/2
2	GLC	F	1318	-	1/1/5/5	0/2/22/22	0/1/1/1
3	NAD	D	1310	-	-	5/30/62/62	0/5/5/5
4	TCL	A	1302	-	-	0/4/4/4	0/2/2/2
3	NAD	H	1322	-	-	8/30/62/62	0/5/5/5
3	NAD	F	1316	-	-	6/30/62/62	0/5/5/5
3	NAD	C	1307	-	-	6/30/62/62	0/5/5/5
3	NAD	G	1319	-	-	6/30/62/62	0/5/5/5
2	GLC	B	1306	-	1/1/5/5	2/2/22/22	0/1/1/1
4	TCL	C	1308	-	-	0/4/4/4	0/2/2/2
3	NAD	E	1313	-	-	7/30/62/62	0/5/5/5
2	GLC	E	1315	-	1/1/5/5	1/2/22/22	0/1/1/1
3	NAD	B	1304	-	-	7/30/62/62	0/5/5/5
2	GLC	H	1324	-	1/1/5/5	2/2/22/22	0/1/1/1
3	NAD	A	1301	-	-	6/30/62/62	0/5/5/5
4	TCL	E	1314	-	-	0/4/4/4	0/2/2/2
4	TCL	F	1317	-	-	0/4/4/4	0/2/2/2
2	GLC	C	1309	-	1/1/5/5	2/2/22/22	0/1/1/1
2	GLC	G	1321	-	1/1/5/5	0/2/22/22	0/1/1/1
4	TCL	H	1323	-	-	0/4/4/4	0/2/2/2
2	GLC	A	1303	-	1/1/5/5	0/2/22/22	0/1/1/1
4	TCL	G	1320	-	-	0/4/4/4	0/2/2/2
4	TCL	D	1311	-	-	0/4/4/4	0/2/2/2
2	GLC	D	1312	-	1/1/5/5	1/2/22/22	0/1/1/1

All (128) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1307	NAD	PN-O3	8.16	1.68	1.59
3	E	1313	NAD	PN-O3	7.52	1.67	1.59
3	G	1319	NAD	PN-O3	6.64	1.66	1.59
3	A	1301	NAD	PN-O3	6.45	1.66	1.59
3	B	1304	NAD	PN-O3	6.15	1.66	1.59
3	D	1310	NAD	PN-O3	5.89	1.65	1.59
3	F	1316	NAD	PN-O3	5.66	1.65	1.59
3	C	1307	NAD	C3N-C7N	5.57	1.58	1.50
3	D	1310	NAD	C2N-N1N	5.53	1.41	1.35
3	H	1322	NAD	C2N-N1N	5.51	1.41	1.35
3	H	1322	NAD	C3N-C7N	5.51	1.58	1.50
3	B	1304	NAD	C2N-N1N	5.33	1.40	1.35
3	A	1301	NAD	C2N-N1N	5.22	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1313	NAD	O4D-C4D	5.18	1.56	1.45
3	B	1304	NAD	C3N-C7N	5.11	1.58	1.50
3	H	1322	NAD	PN-O3	4.90	1.64	1.59
3	F	1316	NAD	C2N-N1N	4.86	1.40	1.35
3	C	1307	NAD	C2N-N1N	4.85	1.40	1.35
3	D	1310	NAD	C3N-C7N	4.74	1.57	1.50
3	G	1319	NAD	C2N-N1N	4.71	1.40	1.35
3	G	1319	NAD	C3N-C7N	4.65	1.57	1.50
3	G	1319	NAD	O4D-C1D	4.53	1.46	1.40
3	F	1316	NAD	C3N-C7N	4.46	1.57	1.50
3	E	1313	NAD	C3N-C7N	4.44	1.57	1.50
3	G	1319	NAD	O4D-C4D	4.40	1.54	1.45
3	A	1301	NAD	O4D-C4D	4.20	1.54	1.45
3	E	1313	NAD	C2N-N1N	4.16	1.39	1.35
3	A	1301	NAD	O4D-C1D	3.97	1.46	1.40
3	E	1313	NAD	C2A-N3A	3.93	1.40	1.33
3	F	1316	NAD	O4D-C4D	3.91	1.53	1.45
3	A	1301	NAD	C3N-C7N	3.91	1.56	1.50
3	A	1301	NAD	C2A-N3A	3.75	1.40	1.33
3	C	1307	NAD	O4D-C4D	3.74	1.53	1.45
3	F	1316	NAD	O4D-C1D	3.70	1.45	1.40
3	H	1322	NAD	C2A-N3A	3.68	1.40	1.33
3	G	1319	NAD	C5N-C4N	3.59	1.45	1.38
3	G	1319	NAD	C2A-N3A	3.57	1.40	1.33
3	D	1310	NAD	O4D-C4D	3.50	1.52	1.45
3	A	1301	NAD	O3B-C3B	3.37	1.51	1.43
3	H	1322	NAD	O4D-C4D	3.32	1.52	1.45
3	B	1304	NAD	O2B-C2B	-3.30	1.34	1.43
3	D	1310	NAD	C4A-N3A	3.30	1.40	1.34
3	E	1313	NAD	O3D-C3D	-3.28	1.34	1.43
3	B	1304	NAD	O4D-C4D	3.28	1.52	1.45
3	C	1307	NAD	C2A-N3A	3.27	1.39	1.33
3	G	1319	NAD	C4A-N3A	3.14	1.40	1.34
3	G	1319	NAD	O3B-C3B	3.14	1.50	1.43
3	A	1301	NAD	C4A-N3A	3.14	1.40	1.34
3	F	1316	NAD	C2A-N3A	3.12	1.39	1.33
3	F	1316	NAD	O2B-C2B	-3.09	1.35	1.43
3	G	1319	NAD	C5A-N7A	-3.01	1.33	1.39
3	C	1307	NAD	O4D-C1D	3.00	1.44	1.40
3	B	1304	NAD	O4B-C4B	2.99	1.51	1.45
3	D	1310	NAD	O4D-C1D	2.97	1.44	1.40
3	E	1313	NAD	C3D-C4D	2.95	1.60	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1322	NAD	O2B-C2B	-2.94	1.35	1.43
3	C	1307	NAD	O2B-C2B	-2.88	1.35	1.43
3	A	1301	NAD	C5N-C4N	2.85	1.43	1.38
3	G	1319	NAD	O4B-C4B	2.80	1.51	1.45
3	B	1304	NAD	C4A-N3A	2.78	1.39	1.34
3	C	1307	NAD	C4A-N3A	2.76	1.39	1.34
3	A	1301	NAD	O4B-C4B	2.76	1.51	1.45
3	B	1304	NAD	O3B-C3B	2.75	1.49	1.43
3	B	1304	NAD	C5A-N7A	-2.73	1.34	1.39
3	D	1310	NAD	C2A-N3A	2.73	1.38	1.33
3	C	1307	NAD	O3B-C3B	2.72	1.49	1.43
3	E	1313	NAD	O2B-C2B	-2.67	1.36	1.43
3	A	1301	NAD	C5A-N7A	-2.65	1.34	1.39
3	E	1313	NAD	C4A-N9A	2.64	1.43	1.37
3	C	1307	NAD	O4B-C4B	2.62	1.50	1.45
3	F	1316	NAD	O3B-C3B	2.60	1.49	1.43
3	D	1310	NAD	C3B-C4B	2.60	1.59	1.53
3	D	1310	NAD	O3B-C3B	2.59	1.49	1.43
3	G	1319	NAD	C4N-C3N	2.59	1.43	1.39
3	B	1304	NAD	C5N-C4N	2.59	1.43	1.38
3	C	1307	NAD	C5A-C6A	2.57	1.48	1.41
3	C	1307	NAD	C5A-N7A	-2.56	1.34	1.39
3	G	1319	NAD	O2B-C2B	-2.56	1.36	1.43
3	H	1322	NAD	C4A-N9A	2.53	1.42	1.37
3	E	1313	NAD	C5A-C6A	2.53	1.48	1.41
3	D	1310	NAD	O4B-C4B	2.51	1.50	1.45
3	F	1316	NAD	C4A-N3A	2.51	1.39	1.34
3	A	1301	NAD	C5A-C6A	2.49	1.47	1.41
3	F	1316	NAD	C5A-N7A	-2.48	1.34	1.39
3	B	1304	NAD	C3B-C4B	2.47	1.59	1.53
3	F	1316	NAD	C3B-C4B	2.44	1.59	1.53
3	H	1322	NAD	O3B-C3B	2.41	1.48	1.43
3	B	1304	NAD	O4D-C1D	2.41	1.44	1.40
3	F	1316	NAD	C5A-C6A	2.41	1.47	1.41
3	H	1322	NAD	C4A-N3A	2.39	1.38	1.34
3	E	1313	NAD	C3B-C4B	2.39	1.59	1.53
3	E	1313	NAD	C5A-N7A	-2.36	1.34	1.39
2	A	1303	GLC	C4-C3	2.35	1.58	1.52
2	D	1312	GLC	C4-C3	2.35	1.58	1.52
3	G	1319	NAD	C5A-C6A	2.34	1.47	1.41
3	G	1319	NAD	O2D-C2D	-2.34	1.37	1.43
3	H	1322	NAD	O4B-C4B	2.33	1.50	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1301	NAD	O2D-C2D	-2.32	1.37	1.43
3	E	1313	NAD	C4A-N3A	2.32	1.38	1.34
3	D	1310	NAD	C5A-N7A	-2.32	1.34	1.39
3	D	1310	NAD	C3D-C4D	2.28	1.58	1.53
3	D	1310	NAD	O2D-C2D	-2.26	1.37	1.43
3	H	1322	NAD	C5A-N7A	-2.25	1.35	1.39
3	C	1307	NAD	C4A-N9A	2.25	1.42	1.37
3	H	1322	NAD	O2D-C2D	-2.25	1.37	1.43
3	B	1304	NAD	C4A-N9A	2.25	1.42	1.37
3	B	1304	NAD	C2A-N3A	2.22	1.37	1.33
3	E	1313	NAD	O4B-C4B	2.20	1.49	1.45
3	A	1301	NAD	C3B-C4B	2.19	1.58	1.53
3	A	1301	NAD	C4A-N9A	2.16	1.42	1.37
3	C	1307	NAD	C3B-C4B	2.16	1.58	1.53
3	B	1304	NAD	C5A-C6A	2.16	1.47	1.41
3	H	1322	NAD	C5N-C4N	2.16	1.42	1.38
3	H	1322	NAD	C5A-C6A	2.15	1.47	1.41
2	B	1306	GLC	C4-C3	2.14	1.57	1.52
4	B	1305	TCL	O17-C6	2.13	1.40	1.36
3	C	1307	NAD	C5N-C4N	2.11	1.42	1.38
4	A	1302	TCL	O17-C6	2.09	1.40	1.36
3	F	1316	NAD	O2D-C2D	-2.08	1.37	1.43
3	B	1304	NAD	C5A-C4A	2.08	1.42	1.39
3	H	1322	NAD	C3B-C4B	2.08	1.58	1.53
3	G	1319	NAD	C5A-C4A	2.06	1.42	1.39
4	E	1314	TCL	O17-C6	2.05	1.40	1.36
3	C	1307	NAD	O3D-C3D	-2.05	1.37	1.43
3	H	1322	NAD	C3D-C4D	2.04	1.58	1.53
3	E	1313	NAD	O3B-C3B	2.04	1.48	1.43
3	A	1301	NAD	C4N-C3N	2.03	1.42	1.39
4	B	1305	TCL	O7-C8	2.01	1.43	1.39

All (205) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1301	NAD	C2N-C3N-C4N	9.52	129.33	118.26
3	H	1322	NAD	C2N-C3N-C4N	9.02	128.74	118.26
3	B	1304	NAD	C2N-C3N-C4N	8.84	128.54	118.26
3	G	1319	NAD	C2N-C3N-C4N	8.71	128.39	118.26
3	D	1310	NAD	C2N-C3N-C4N	8.51	128.15	118.26
3	C	1307	NAD	C2N-C3N-C4N	8.49	128.13	118.26
3	F	1316	NAD	C2N-C3N-C4N	8.26	127.86	118.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1313	NAD	C2N-C3N-C4N	8.02	127.58	118.26
3	G	1319	NAD	C5N-C4N-C3N	-7.90	112.60	120.36
3	H	1322	NAD	C5N-C4N-C3N	-7.59	112.90	120.36
3	E	1313	NAD	C5N-C4N-C3N	-7.46	113.03	120.36
3	A	1301	NAD	C5N-C4N-C3N	-7.45	113.04	120.36
3	C	1307	NAD	C5N-C4N-C3N	-7.30	113.18	120.36
3	B	1304	NAD	O7N-C7N-C3N	-7.02	111.01	119.60
3	B	1304	NAD	C5N-C4N-C3N	-6.99	113.49	120.36
3	F	1316	NAD	C5N-C4N-C3N	-6.33	114.14	120.36
3	G	1319	NAD	C3N-C7N-N7N	5.97	125.09	117.74
3	D	1310	NAD	C5N-C4N-C3N	-5.93	114.53	120.36
2	D	1312	GLC	O5-C5-C6	5.90	121.07	106.44
3	A	1301	NAD	C2A-N1A-C6A	5.77	128.21	118.73
3	G	1319	NAD	C2A-N1A-C6A	5.76	128.19	118.73
2	F	1318	GLC	C1-O5-C5	5.72	124.72	113.65
2	H	1324	GLC	O5-C5-C4	5.71	119.98	109.70
2	H	1324	GLC	O5-C1-C2	5.62	120.18	110.30
3	E	1313	NAD	C2A-N1A-C6A	5.48	127.73	118.73
2	A	1303	GLC	O5-C1-C2	5.37	119.74	110.30
2	G	1321	GLC	O5-C1-C2	5.21	119.47	110.30
3	E	1313	NAD	C5D-C4D-C3D	-5.14	96.72	115.21
3	A	1301	NAD	C3N-C7N-N7N	5.13	124.06	117.74
3	D	1310	NAD	C2A-N1A-C6A	5.13	127.16	118.73
3	A	1301	NAD	O7N-C7N-C3N	-5.10	113.36	119.60
2	A	1303	GLC	O3-C3-C2	5.05	122.27	110.38
3	F	1316	NAD	C2A-N1A-C6A	4.87	126.74	118.73
2	E	1315	GLC	C1-O5-C5	4.73	122.80	113.65
3	B	1304	NAD	C2A-N1A-C6A	4.71	126.47	118.73
3	E	1313	NAD	N3A-C2A-N1A	-4.69	121.48	128.58
3	F	1316	NAD	C4A-N9A-C8A	-4.50	101.02	105.74
3	H	1322	NAD	O7N-C7N-C3N	-4.49	114.11	119.60
3	A	1301	NAD	N3A-C2A-N1A	-4.48	121.80	128.58
2	E	1315	GLC	O5-C5-C4	4.37	117.57	109.70
3	H	1322	NAD	C2A-N1A-C6A	4.27	125.75	118.73
3	E	1313	NAD	O4D-C4D-C5D	-4.26	95.69	109.33
2	C	1309	GLC	C1-O5-C5	4.23	121.83	113.65
2	G	1321	GLC	O1-C1-C2	4.16	121.05	108.98
2	G	1321	GLC	O3-C3-C2	4.15	120.16	110.38
2	A	1303	GLC	O2-C2-C1	4.14	118.81	109.25
2	H	1324	GLC	O4-C4-C3	4.12	120.10	110.38
3	B	1304	NAD	C5A-C4A-N3A	-4.10	121.07	126.72
2	B	1306	GLC	O5-C5-C4	4.07	117.04	109.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1307	NAD	C2A-N1A-C6A	4.05	125.38	118.73
3	F	1316	NAD	N3A-C2A-N1A	-4.05	122.45	128.58
3	D	1310	NAD	N3A-C2A-N1A	-4.04	122.47	128.58
3	B	1304	NAD	N3A-C2A-N1A	-4.00	122.53	128.58
2	F	1318	GLC	O5-C5-C4	3.90	116.72	109.70
3	A	1301	NAD	C4A-N9A-C8A	-3.90	101.65	105.74
2	C	1309	GLC	O5-C5-C4	3.89	116.70	109.70
3	G	1319	NAD	N3A-C2A-N1A	-3.81	122.81	128.58
3	E	1313	NAD	C4D-O4D-C1D	-3.80	106.44	109.92
3	G	1319	NAD	O7N-C7N-C3N	-3.80	114.96	119.60
2	G	1321	GLC	O5-C5-C6	3.78	115.80	106.44
3	E	1313	NAD	C4A-N9A-C8A	-3.74	101.81	105.74
3	C	1307	NAD	C4A-N9A-C8A	-3.71	101.84	105.74
3	H	1322	NAD	C4A-N9A-C8A	-3.71	101.84	105.74
3	E	1313	NAD	O3D-C3D-C2D	3.70	123.68	111.82
3	F	1316	NAD	C6N-N1N-C2N	3.65	124.98	121.88
3	F	1316	NAD	C5A-C4A-N3A	-3.60	121.75	126.72
3	G	1319	NAD	C4A-N9A-C8A	-3.60	101.96	105.74
2	D	1312	GLC	O5-C1-C2	3.60	116.63	110.30
3	B	1304	NAD	C6N-N1N-C2N	3.56	124.91	121.88
3	D	1310	NAD	C6N-N1N-C2N	3.52	124.87	121.88
2	B	1306	GLC	C1-O5-C5	3.49	120.41	113.65
2	G	1321	GLC	C3-C4-C5	-3.46	103.96	110.23
3	B	1304	NAD	C3N-C7N-N7N	3.46	122.00	117.74
3	H	1322	NAD	N3A-C2A-N1A	-3.44	123.38	128.58
3	D	1310	NAD	C2B-C3B-C4B	3.42	109.21	102.61
2	H	1324	GLC	O1-C1-O5	3.41	120.55	110.41
3	C	1307	NAD	C5A-C4A-N3A	-3.41	122.02	126.72
3	G	1319	NAD	C6N-N1N-C2N	3.40	124.77	121.88
2	A	1303	GLC	O4-C4-C5	-3.39	100.98	109.32
2	A	1303	GLC	O5-C5-C6	3.38	114.82	106.44
3	C	1307	NAD	C3N-C7N-N7N	3.37	121.89	117.74
3	E	1313	NAD	C6N-N1N-C2N	3.31	124.70	121.88
3	G	1319	NAD	C4B-O4B-C1B	-3.25	102.29	109.47
3	C	1307	NAD	N3A-C2A-N1A	-3.23	123.69	128.58
3	D	1310	NAD	C5A-C4A-N3A	-3.22	122.28	126.72
2	F	1318	GLC	O5-C1-C2	3.19	115.91	110.30
3	A	1301	NAD	C6N-N1N-C2N	3.19	124.59	121.88
3	E	1313	NAD	C3N-C7N-N7N	3.18	121.66	117.74
3	B	1304	NAD	C4A-N9A-C8A	-3.17	102.41	105.74
3	H	1322	NAD	C5A-C4A-N3A	-3.13	122.41	126.72
2	A	1303	GLC	O2-C2-C3	3.10	117.69	110.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1310	NAD	C3B-C2B-C1B	-3.10	95.60	101.46
2	G	1321	GLC	O4-C4-C5	-3.09	101.71	109.32
3	C	1307	NAD	O7N-C7N-C3N	-3.09	115.82	119.60
2	H	1324	GLC	C1-O5-C5	3.09	119.63	113.65
3	H	1322	NAD	C4B-O4B-C1B	-3.04	102.75	109.47
2	H	1324	GLC	O1-C1-C2	3.03	117.78	108.98
4	C	1308	TCL	C1-C6-C5	3.02	122.73	119.81
3	B	1304	NAD	O7N-C7N-N7N	3.00	126.95	122.62
3	A	1301	NAD	C2B-C3B-C4B	2.99	108.39	102.61
3	B	1304	NAD	C4B-O4B-C1B	-2.97	102.91	109.47
2	A	1303	GLC	C3-C4-C5	-2.95	104.89	110.23
2	G	1321	GLC	O2-C2-C1	2.88	115.90	109.25
3	H	1322	NAD	C3N-C7N-N7N	2.88	121.29	117.74
3	E	1313	NAD	C2B-C3B-C4B	2.87	108.16	102.61
3	A	1301	NAD	C1B-N9A-C8A	2.81	133.34	127.09
3	D	1310	NAD	C3N-C7N-N7N	2.80	121.19	117.74
2	A	1303	GLC	C1-C2-C3	2.77	116.01	110.36
3	H	1322	NAD	C6A-C5A-C4A	2.77	120.96	117.18
3	B	1304	NAD	N3A-C4A-N9A	2.76	131.86	127.17
3	B	1304	NAD	C1B-N9A-C8A	2.75	133.21	127.09
3	C	1307	NAD	C2B-C3B-C4B	2.75	107.92	102.61
3	E	1313	NAD	C1B-N9A-C8A	2.73	133.15	127.09
3	D	1310	NAD	C4A-N9A-C8A	-2.73	102.88	105.74
4	C	1308	TCL	C6-C1-C2	-2.71	115.91	118.96
3	F	1316	NAD	C6A-C5A-C4A	2.68	120.84	117.18
2	D	1312	GLC	C3-C4-C5	-2.68	105.37	110.23
3	H	1322	NAD	C2D-C3D-C4D	2.68	107.79	102.61
3	C	1307	NAD	O2A-PA-O3	2.67	114.49	107.27
4	A	1302	TCL	C13-C12-C11	-2.66	116.56	119.24
3	D	1310	NAD	C1B-N9A-C8A	2.66	133.00	127.09
3	C	1307	NAD	C6A-C5A-C4A	2.63	120.77	117.18
3	E	1313	NAD	C5A-C4A-N3A	-2.62	123.10	126.72
3	D	1310	NAD	C6A-C5A-C4A	2.62	120.76	117.18
2	A	1303	GLC	O1-C1-C2	2.59	116.49	108.98
2	E	1315	GLC	O5-C1-C2	2.59	114.85	110.30
2	F	1318	GLC	O3-C3-C4	2.59	116.47	110.38
3	H	1322	NAD	C2B-C3B-C4B	2.58	107.60	102.61
3	C	1307	NAD	C6N-N1N-C2N	2.58	124.07	121.88
3	B	1304	NAD	C6A-C5A-C4A	2.57	120.69	117.18
3	B	1304	NAD	C2D-C3D-C4D	2.49	107.42	102.61
3	A	1301	NAD	C4D-O4D-C1D	-2.49	107.65	109.92
3	A	1301	NAD	C5A-C4A-N3A	-2.48	123.31	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1322	NAD	C3B-C2B-C1B	-2.48	96.78	101.46
4	A	1302	TCL	C4-C3-C2	-2.47	116.75	119.24
3	H	1322	NAD	C6N-N1N-C2N	2.46	123.97	121.88
3	G	1319	NAD	C5A-C4A-N3A	-2.45	123.35	126.72
3	E	1313	NAD	O2N-PN-O3	2.45	113.89	107.27
3	C	1307	NAD	O2N-PN-O1N	2.45	123.82	112.44
4	H	1323	TCL	O7-C5-C4	2.44	127.13	120.74
4	E	1314	TCL	C8-O7-C5	2.41	123.84	118.09
3	F	1316	NAD	C2B-C3B-C4B	2.41	107.26	102.61
3	H	1322	NAD	O2A-PA-O1A	2.39	123.55	112.44
4	D	1311	TCL	O7-C5-C6	2.39	120.62	116.59
3	G	1319	NAD	C5A-C6A-N1A	-2.38	111.46	117.51
3	C	1307	NAD	C2D-C3D-C4D	2.37	107.19	102.61
2	D	1312	GLC	C4-C3-C2	-2.36	106.69	110.83
3	D	1310	NAD	C4A-C5A-N7A	-2.35	107.89	110.58
2	C	1309	GLC	O5-C1-C2	2.35	114.43	110.30
3	A	1301	NAD	C4B-O4B-C1B	-2.35	104.28	109.47
3	C	1307	NAD	C1B-N9A-C8A	2.35	132.30	127.09
3	E	1313	NAD	C6A-C5A-C4A	2.34	120.38	117.18
3	E	1313	NAD	C2D-C3D-C4D	-2.32	98.12	102.61
3	A	1301	NAD	C2B-C1B-N9A	-2.32	107.54	113.30
3	D	1310	NAD	C2D-C3D-C4D	2.30	107.06	102.61
3	E	1313	NAD	C4B-O4B-C1B	-2.29	104.40	109.47
3	D	1310	NAD	C5A-N7A-C8A	2.29	107.04	103.45
3	D	1310	NAD	C4B-O4B-C1B	-2.27	104.45	109.47
3	A	1301	NAD	C5A-N7A-C8A	2.27	107.02	103.45
3	B	1304	NAD	O3-PA-O1A	-2.27	103.88	110.70
3	F	1316	NAD	O3B-C3B-C4B	-2.26	104.60	111.08
4	D	1311	TCL	C4-C5-C6	-2.25	117.21	119.87
3	A	1301	NAD	C5A-C4A-N9A	2.25	108.26	105.81
3	E	1313	NAD	C5A-C6A-N1A	-2.24	111.83	117.51
3	E	1313	NAD	O2N-PN-O1N	2.23	122.81	112.44
3	F	1316	NAD	O7N-C7N-C3N	-2.20	116.90	119.60
4	G	1320	TCL	C1-C6-C5	2.20	121.94	119.81
3	E	1313	NAD	C3B-C2B-C1B	-2.20	97.30	101.46
3	F	1316	NAD	O4D-C4D-C5D	-2.19	102.31	109.33
3	E	1313	NAD	C2B-C1B-N9A	-2.19	107.87	113.30
3	H	1322	NAD	O4D-C4D-C3D	-2.19	100.81	105.15
3	F	1316	NAD	O2N-PN-O1N	2.18	122.60	112.44
3	B	1304	NAD	O2B-C2B-C3B	2.18	118.81	111.82
4	H	1323	TCL	C1-C6-C5	2.18	121.92	119.81
3	G	1319	NAD	C6A-C5A-C4A	2.18	120.16	117.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1319	NAD	N6A-C6A-N1A	2.18	123.23	118.38
3	F	1316	NAD	C2D-C3D-C4D	2.17	106.81	102.61
2	H	1324	GLC	C6-C5-C4	-2.17	107.68	113.02
3	H	1322	NAD	C1B-N9A-C8A	2.17	131.92	127.09
3	A	1301	NAD	C5A-C6A-N1A	-2.17	112.00	117.51
4	F	1317	TCL	C1-C6-C5	2.15	121.89	119.81
3	D	1310	NAD	C5A-C6A-N1A	-2.14	112.07	117.51
2	F	1318	GLC	O4-C4-C3	2.14	115.42	110.38
3	C	1307	NAD	C4B-O4B-C1B	-2.14	104.74	109.47
3	E	1313	NAD	O3-PA-O1A	-2.13	104.28	110.70
3	A	1301	NAD	C6A-C5A-C4A	2.13	120.08	117.18
4	B	1305	TCL	C13-C12-C11	-2.12	117.11	119.24
3	F	1316	NAD	C5A-C6A-N1A	-2.11	112.15	117.51
3	H	1322	NAD	O4D-C4D-C5D	-2.11	102.58	109.33
3	F	1316	NAD	O2A-PA-O1A	2.10	122.23	112.44
3	D	1310	NAD	O4B-C4B-C3B	-2.10	100.99	105.15
4	E	1314	TCL	C6-C1-C2	-2.09	116.61	118.96
3	G	1319	NAD	C5A-N7A-C8A	2.09	106.73	103.45
3	F	1316	NAD	C4B-O4B-C1B	-2.08	104.88	109.47
3	G	1319	NAD	O7N-C7N-N7N	-2.07	119.62	122.62
3	B	1304	NAD	C5D-C4D-C3D	2.06	122.63	115.21
3	C	1307	NAD	O3D-C3D-C4D	-2.06	105.17	111.08
3	F	1316	NAD	C1B-N9A-C8A	2.05	131.65	127.09
3	F	1316	NAD	C3N-C7N-N7N	2.05	120.26	117.74
3	F	1316	NAD	O3-PN-O1N	-2.04	104.58	110.70
3	F	1316	NAD	C5A-C4A-N9A	2.03	108.02	105.81
3	B	1304	NAD	C5A-N7A-C8A	2.02	106.63	103.45
3	E	1313	NAD	C6N-C5N-C4N	2.01	122.35	119.45
3	C	1307	NAD	O3-PA-O1A	-2.01	104.65	110.70
3	B	1304	NAD	C2B-C3B-C4B	2.01	106.50	102.61

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1303	GLC	C2
2	B	1306	GLC	C1
2	C	1309	GLC	C1
2	D	1312	GLC	C2
2	E	1315	GLC	C1
2	F	1318	GLC	C1
2	G	1321	GLC	C2
2	H	1324	GLC	C1

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1301	NAD	C5D-O5D-PN-O3
3	A	1301	NAD	C5D-O5D-PN-O1N
3	A	1301	NAD	C5D-O5D-PN-O2N
3	A	1301	NAD	O4D-C1D-N1N-C2N
3	B	1304	NAD	C5D-O5D-PN-O3
3	B	1304	NAD	C5D-O5D-PN-O2N
3	B	1304	NAD	O4D-C1D-N1N-C2N
3	B	1304	NAD	O4D-C1D-N1N-C6N
3	C	1307	NAD	C5D-O5D-PN-O3
3	C	1307	NAD	C5D-O5D-PN-O1N
3	C	1307	NAD	C5D-O5D-PN-O2N
3	C	1307	NAD	O4D-C1D-N1N-C2N
3	C	1307	NAD	O4D-C1D-N1N-C6N
3	D	1310	NAD	C5D-O5D-PN-O3
3	D	1310	NAD	C5D-O5D-PN-O1N
3	D	1310	NAD	C5D-O5D-PN-O2N
3	D	1310	NAD	O4D-C1D-N1N-C2N
3	D	1310	NAD	O4D-C1D-N1N-C6N
3	E	1313	NAD	C5D-O5D-PN-O3
3	E	1313	NAD	C5D-O5D-PN-O1N
3	E	1313	NAD	O4D-C4D-C5D-O5D
3	E	1313	NAD	O4D-C1D-N1N-C2N
3	E	1313	NAD	O4D-C1D-N1N-C6N
3	F	1316	NAD	C5D-O5D-PN-O3
3	F	1316	NAD	C5D-O5D-PN-O1N
3	F	1316	NAD	C5D-O5D-PN-O2N
3	F	1316	NAD	O4D-C1D-N1N-C2N
3	G	1319	NAD	C5D-O5D-PN-O3
3	G	1319	NAD	C5D-O5D-PN-O1N
3	G	1319	NAD	C5D-O5D-PN-O2N
3	G	1319	NAD	O4D-C1D-N1N-C2N
3	H	1322	NAD	C5D-O5D-PN-O3
3	H	1322	NAD	C5D-O5D-PN-O1N
3	H	1322	NAD	C5D-O5D-PN-O2N
3	H	1322	NAD	O4D-C1D-N1N-C2N
3	H	1322	NAD	O4D-C1D-N1N-C6N
2	H	1324	GLC	O5-C5-C6-O6
3	E	1313	NAD	C3D-C4D-C5D-O5D
2	D	1312	GLC	C4-C5-C6-O6
2	C	1309	GLC	C4-C5-C6-O6
2	B	1306	GLC	C4-C5-C6-O6
2	E	1315	GLC	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

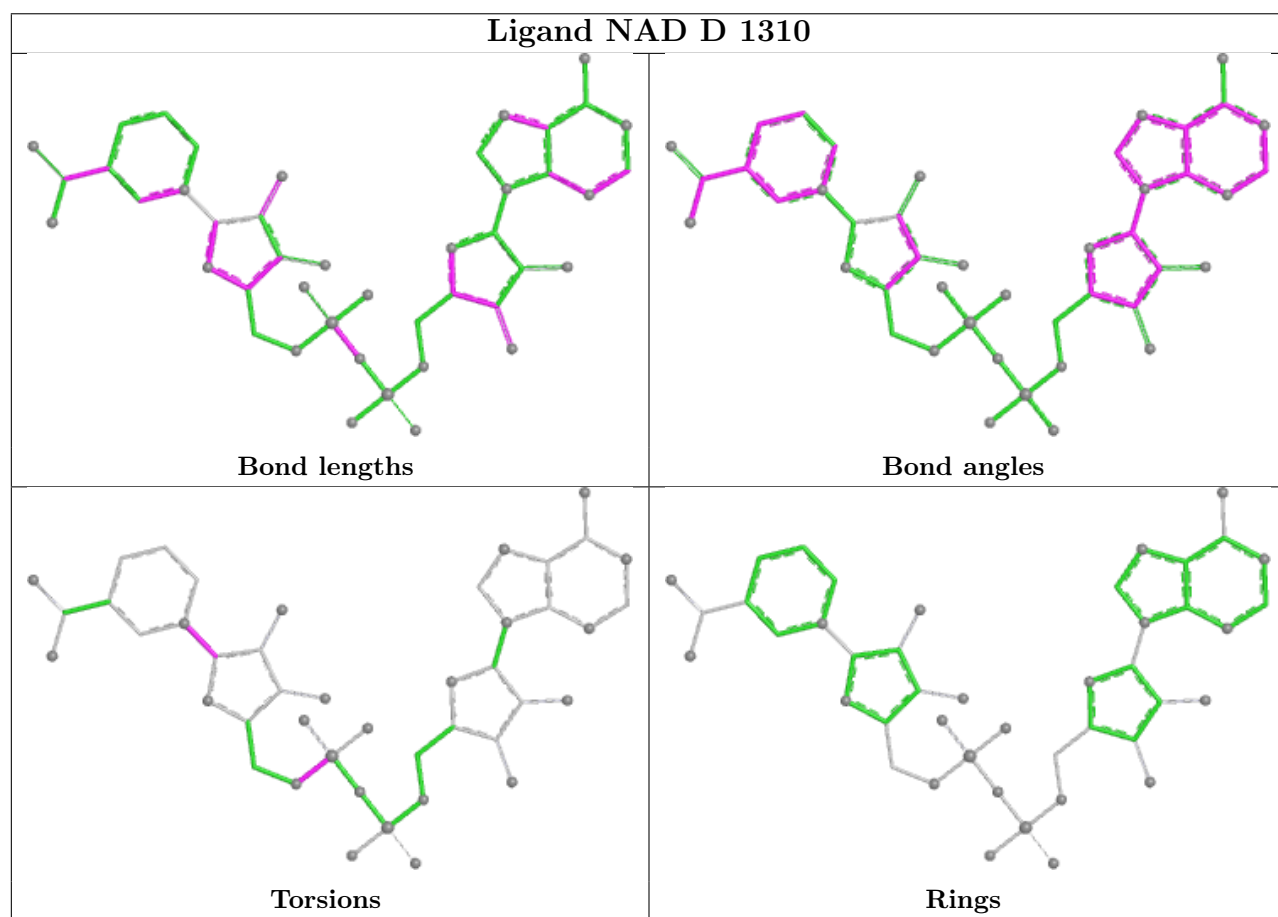
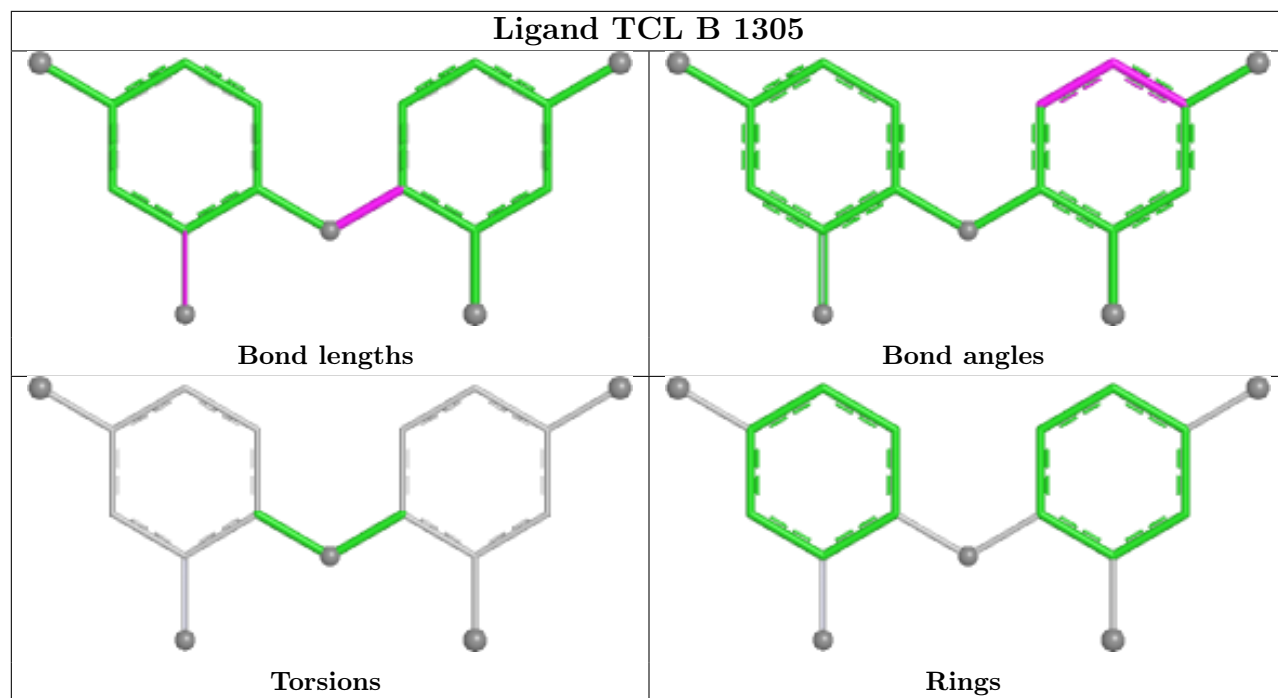
Mol	Chain	Res	Type	Atoms
3	H	1322	NAD	PA-O3-PN-O1N
2	H	1324	GLC	C4-C5-C6-O6
3	B	1304	NAD	C5D-O5D-PN-O1N
3	E	1313	NAD	C5D-O5D-PN-O2N
3	A	1301	NAD	O4D-C1D-N1N-C6N
3	F	1316	NAD	O4D-C1D-N1N-C6N
3	G	1319	NAD	O4D-C1D-N1N-C6N
3	F	1316	NAD	PA-O3-PN-O2N
3	H	1322	NAD	PA-O3-PN-O2N
3	A	1301	NAD	PN-O3-PA-O5B
3	H	1322	NAD	O4B-C4B-C5B-O5B
2	C	1309	GLC	O5-C5-C6-O6
2	B	1306	GLC	O5-C5-C6-O6
3	B	1304	NAD	PA-O3-PN-O1N
3	B	1304	NAD	PA-O3-PN-O2N
3	C	1307	NAD	PA-O3-PN-O2N
3	G	1319	NAD	PA-O3-PN-O2N

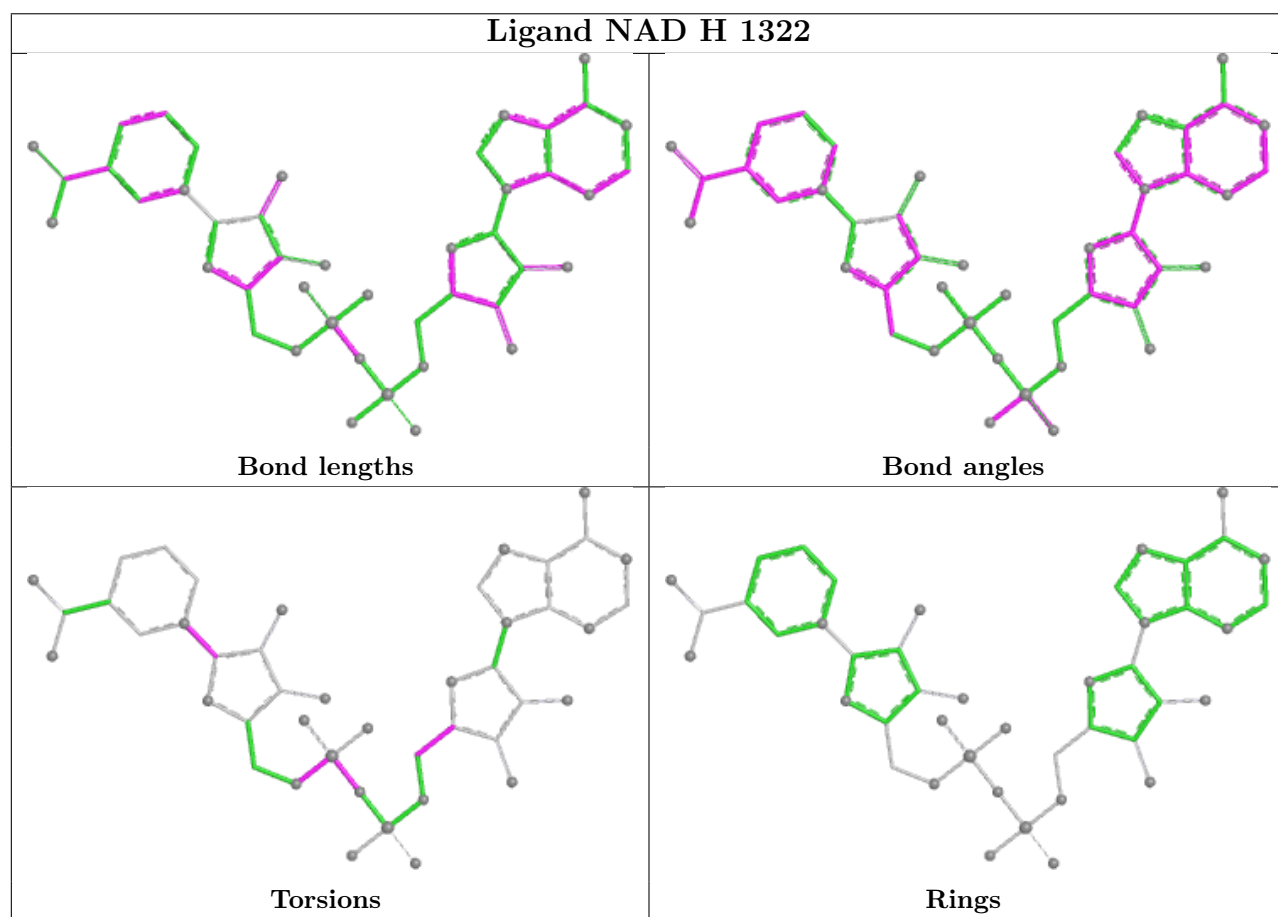
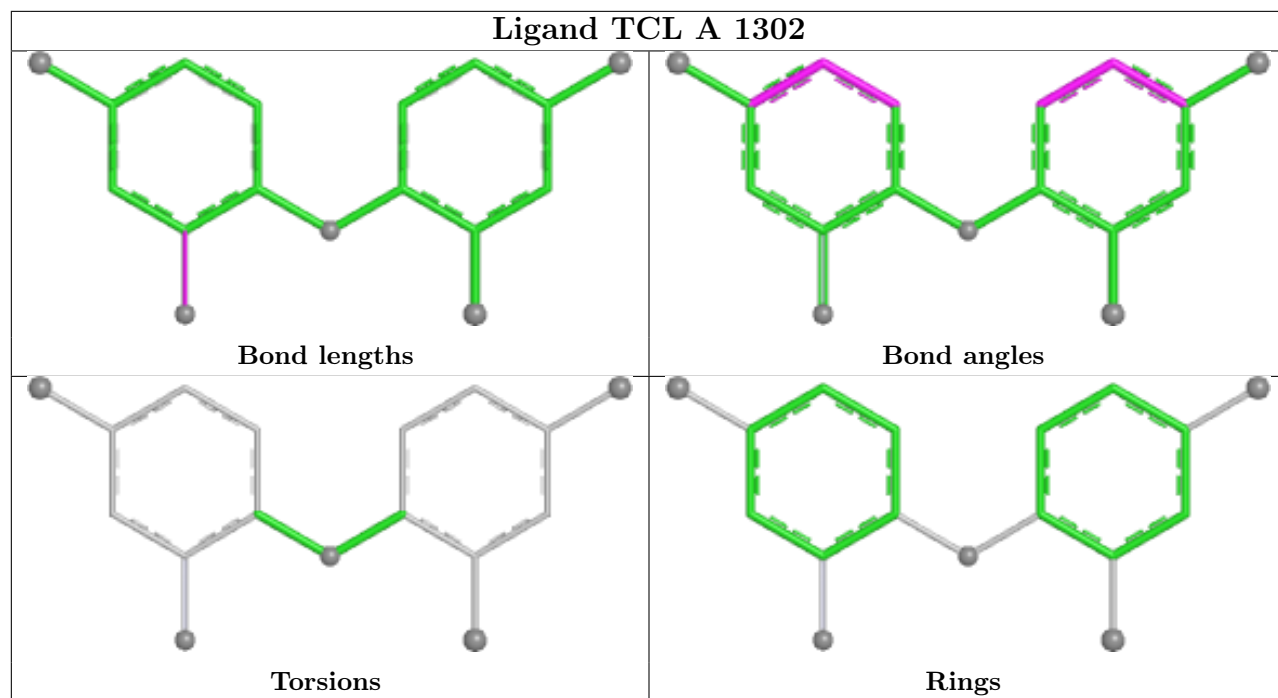
There are no ring outliers.

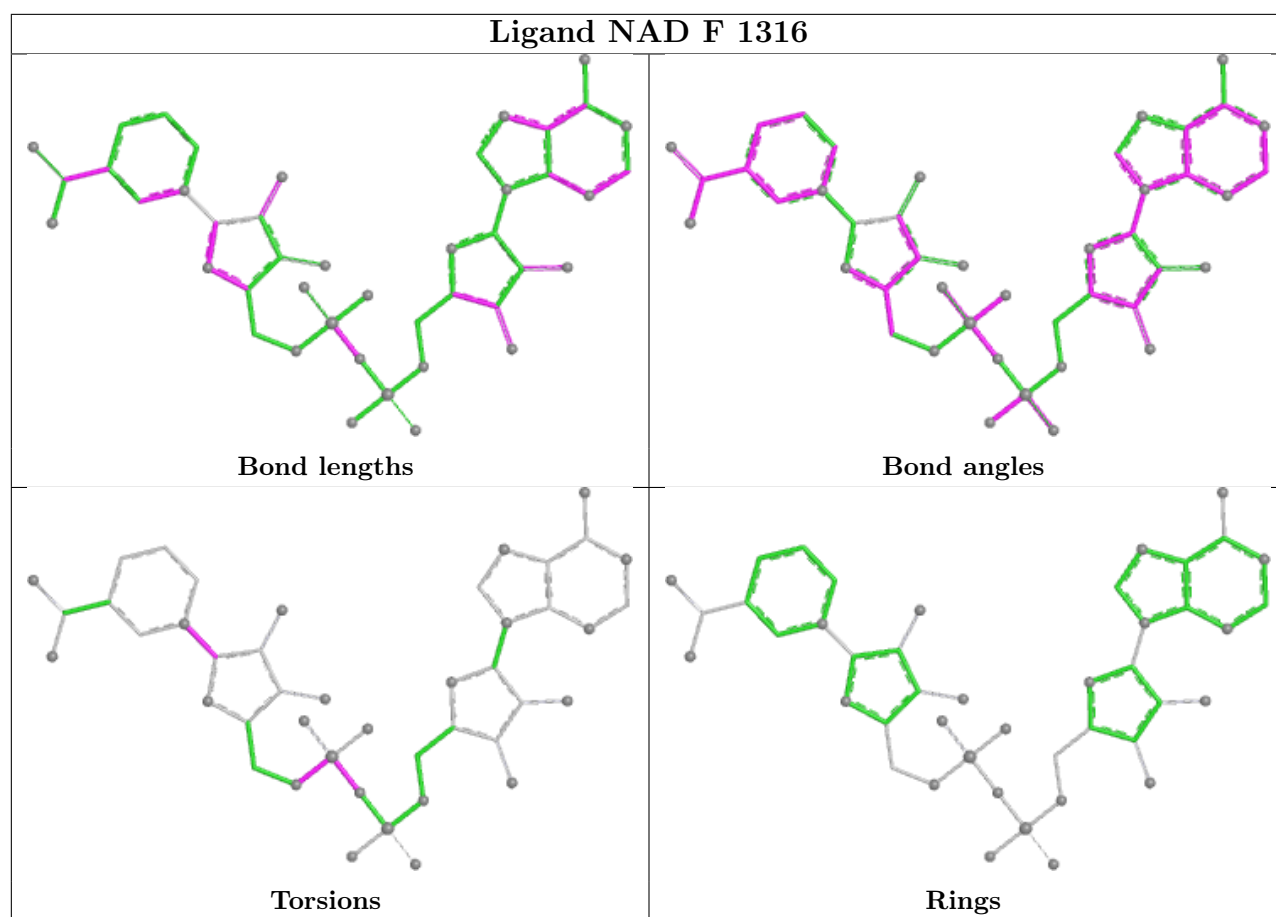
3 monomers are involved in 3 short contacts:

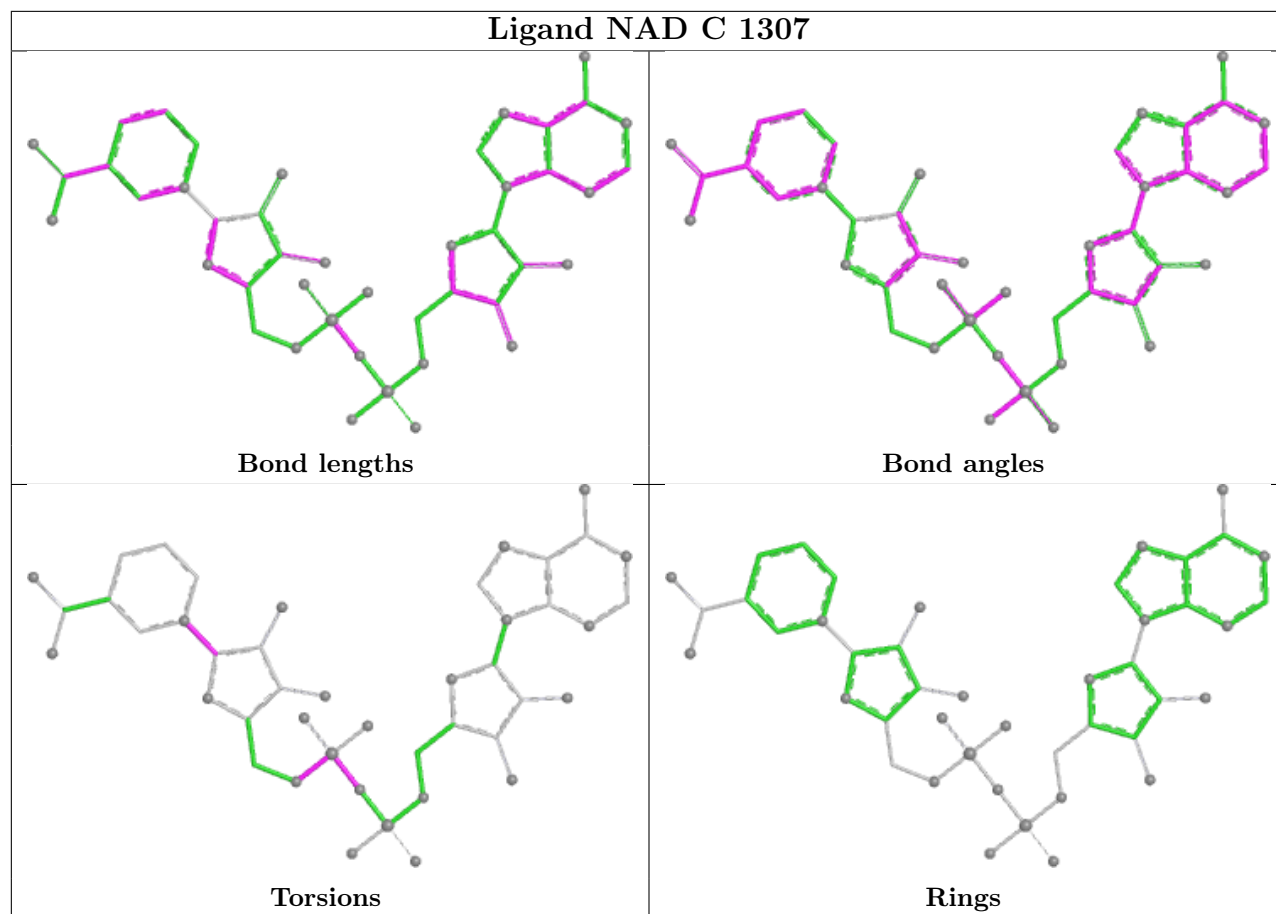
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1313	NAD	2	0
4	E	1314	TCL	1	0
2	D	1312	GLC	1	0

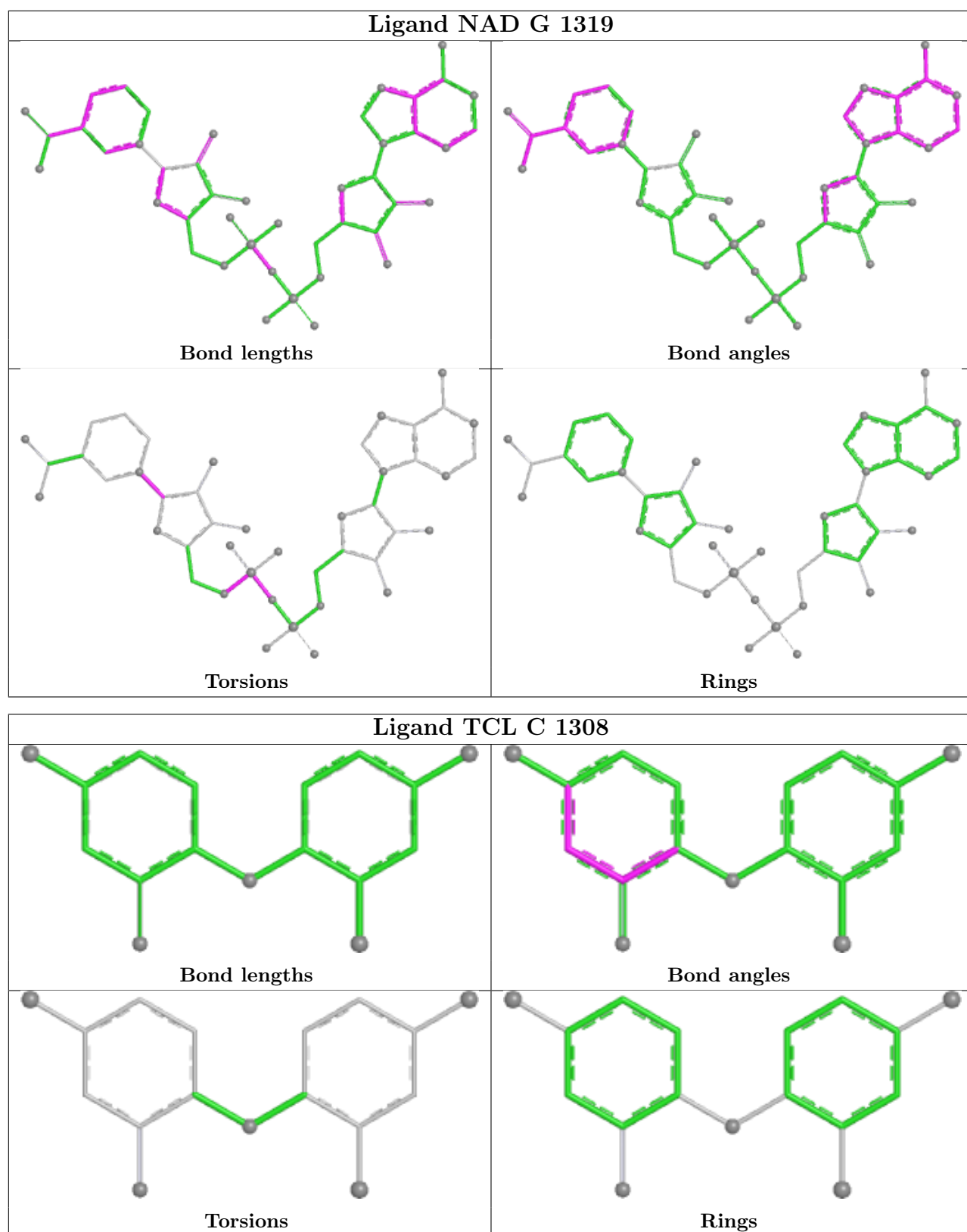
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

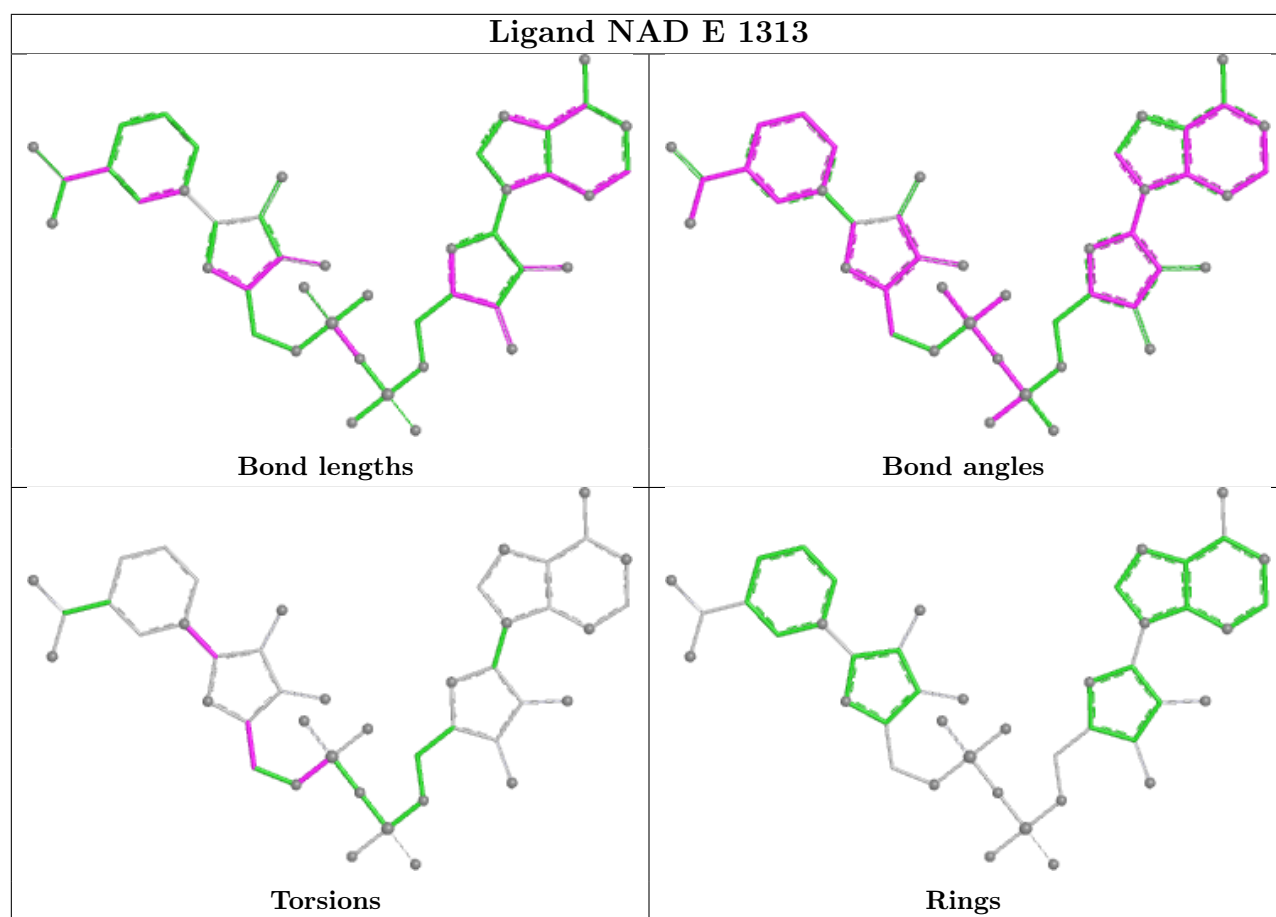


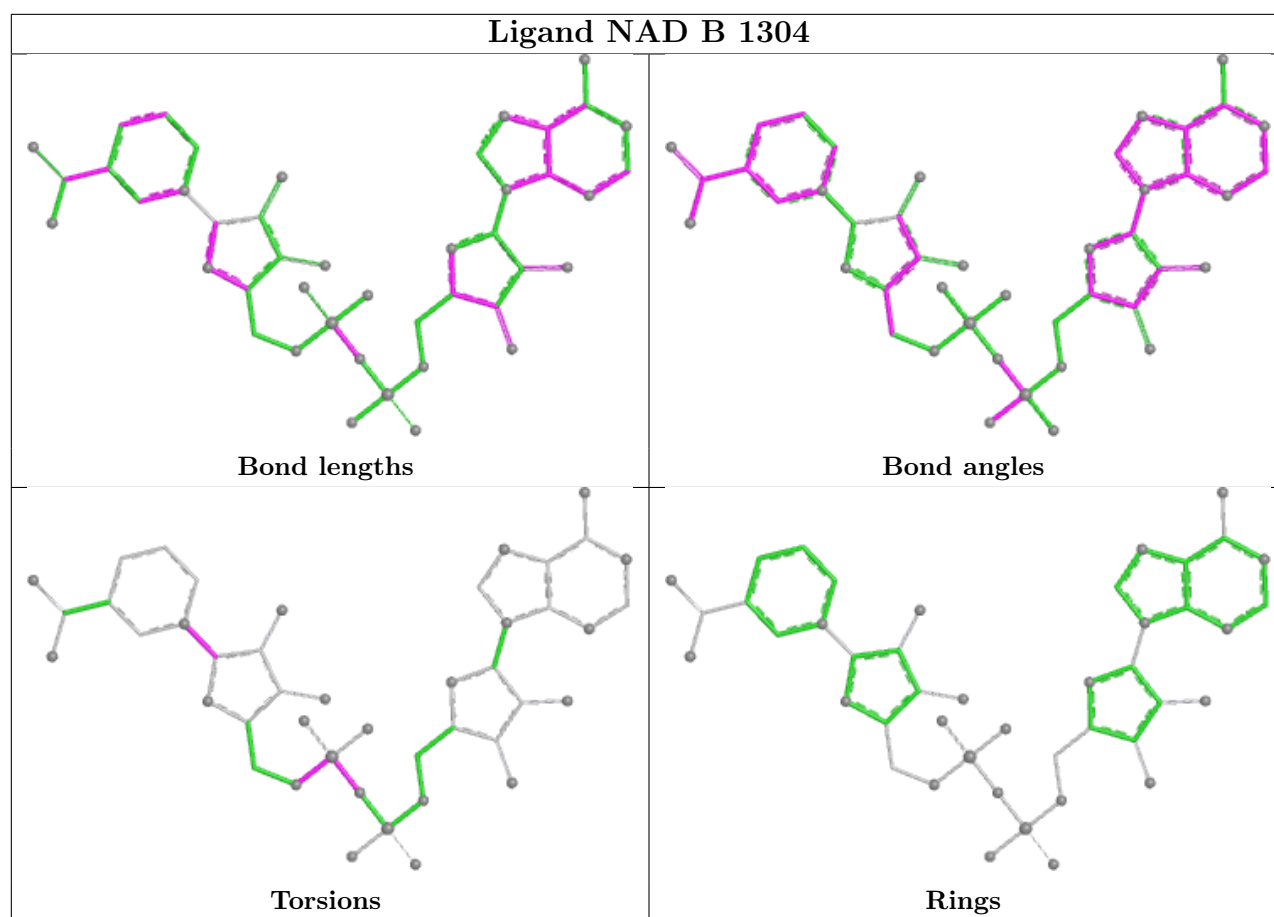




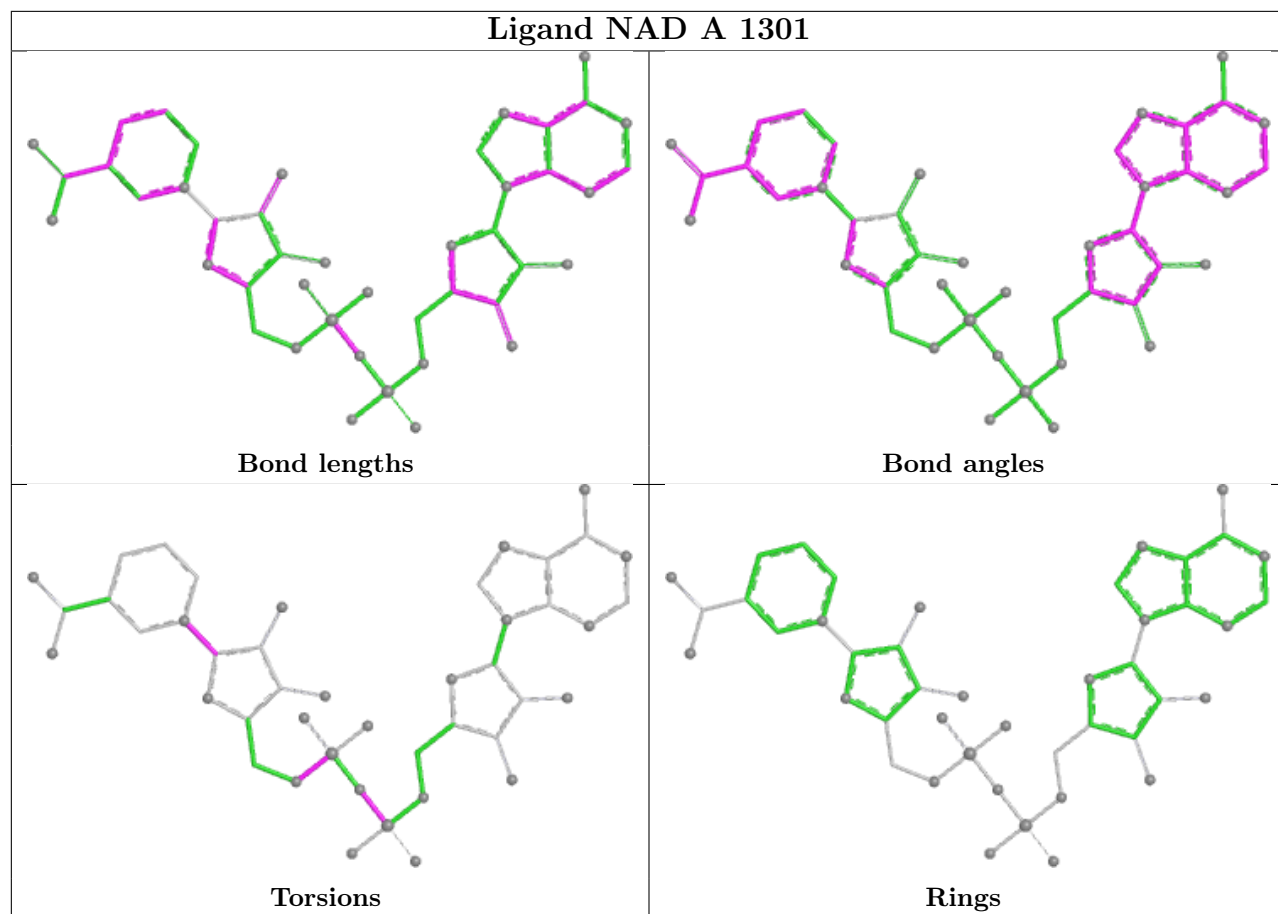




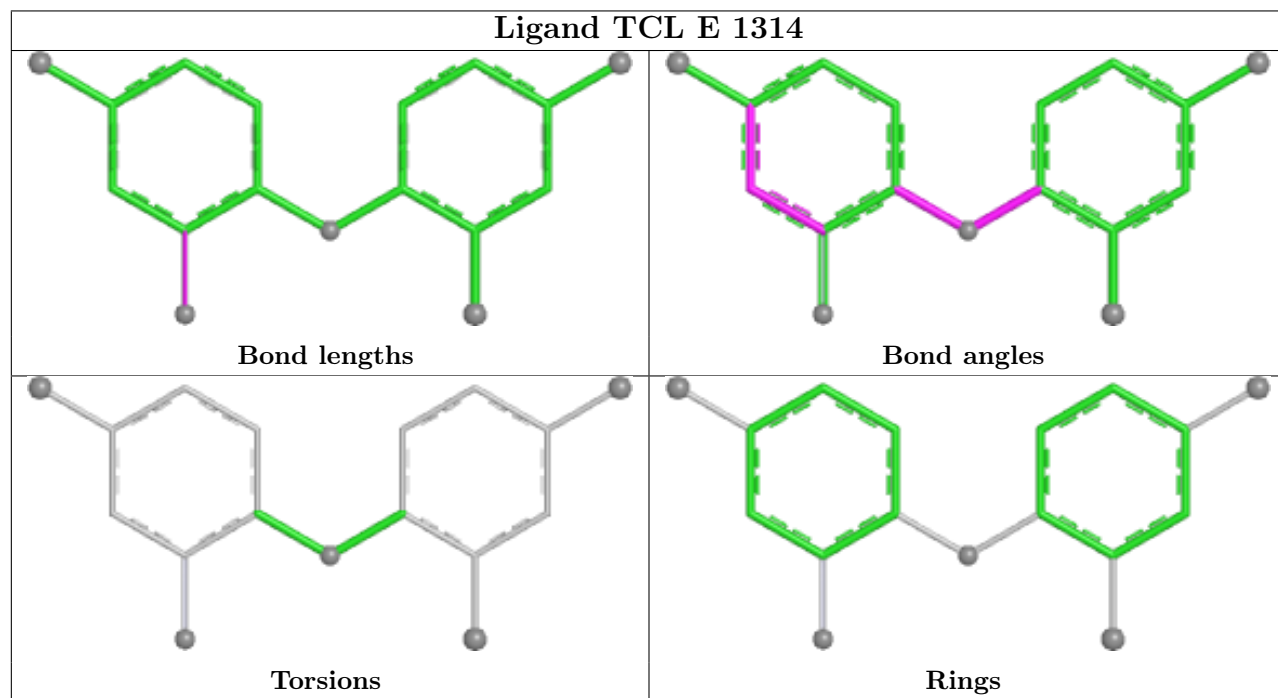


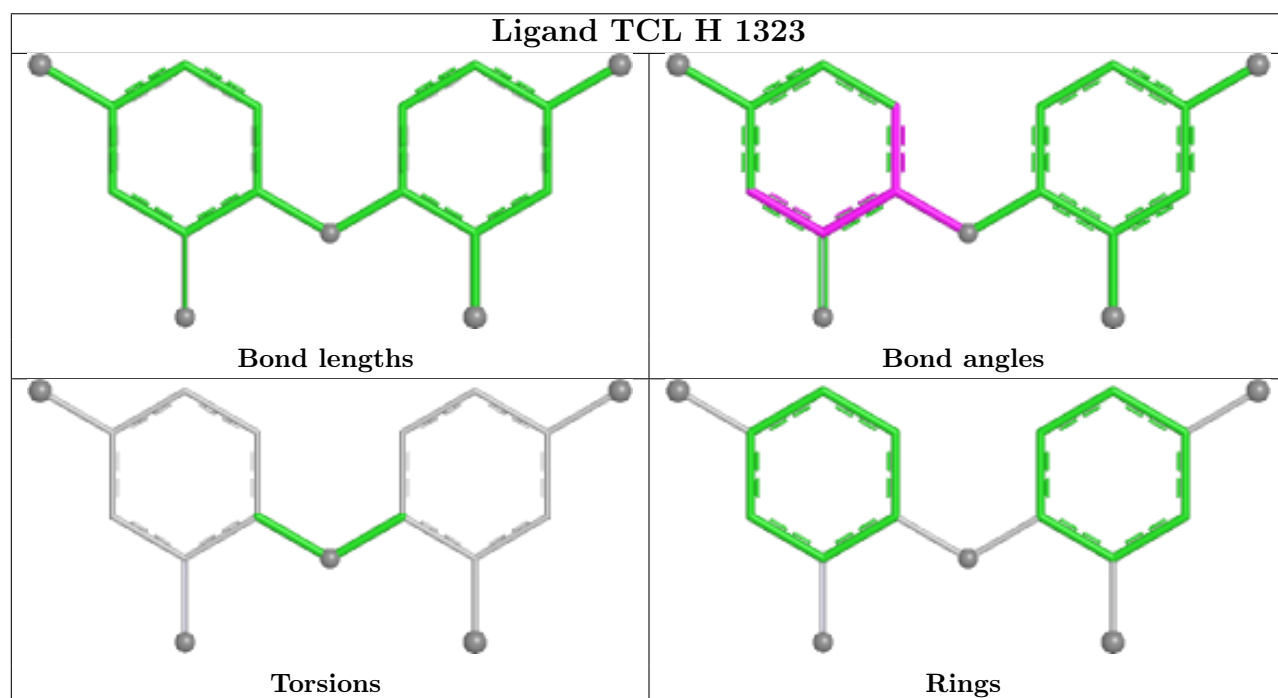
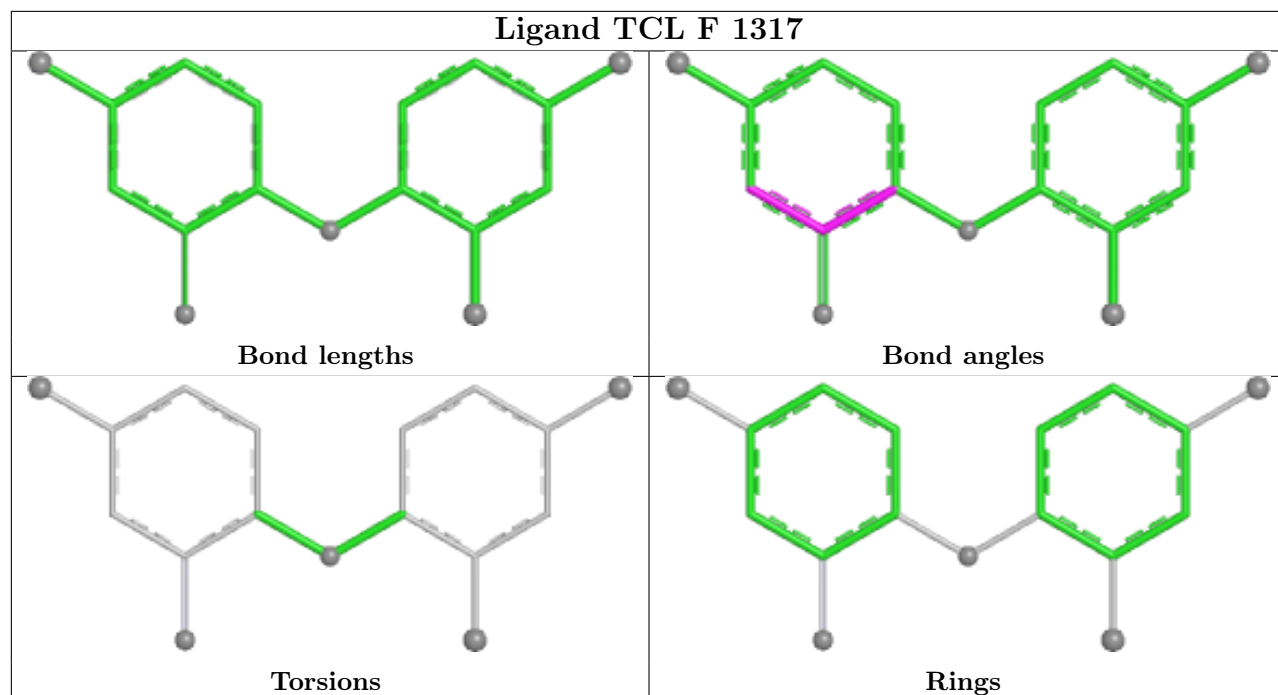


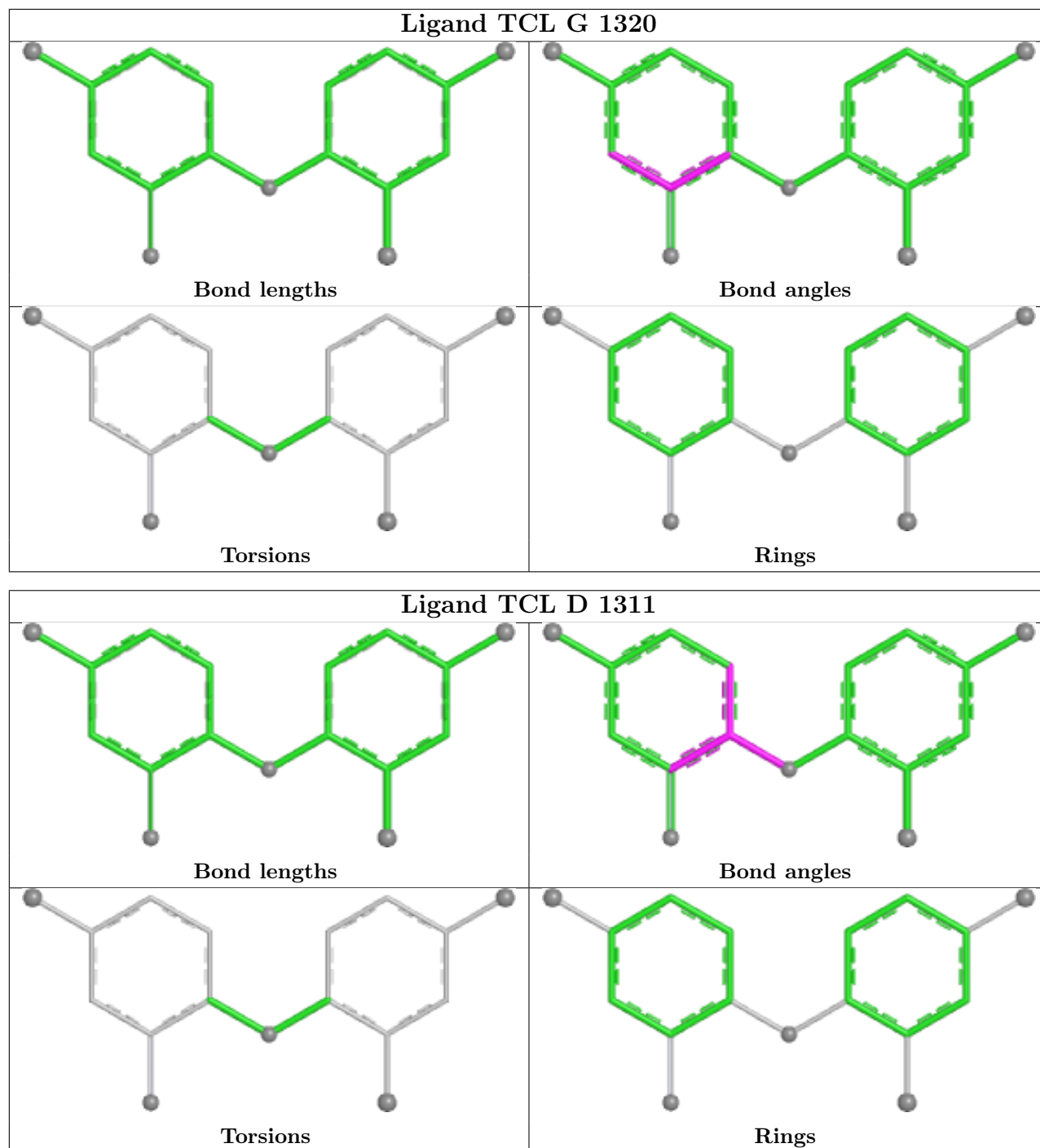
Ligand NAD A 1301



Ligand TCL E 1314







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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.