



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 10:36 PM UTC

PDB ID : 6BB1 / pdb\_00006bb1  
Title : Lactate Dehydrogenase in complex with inhibitor (R)-5-((2-chlorophenyl)thio)-6'--(4-fluorophenoxy)-4-hydroxy-2-(thiophen-3-yl)-2,3-dihydro-[2,2'-bipyridin]-6(1H)-one  
Authors : Ultsch, M.; Eigenbrot, C.  
Deposited on : 2017-10-16  
Resolution : 2.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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The following versions of software and data (see [references ⓘ](#)) 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

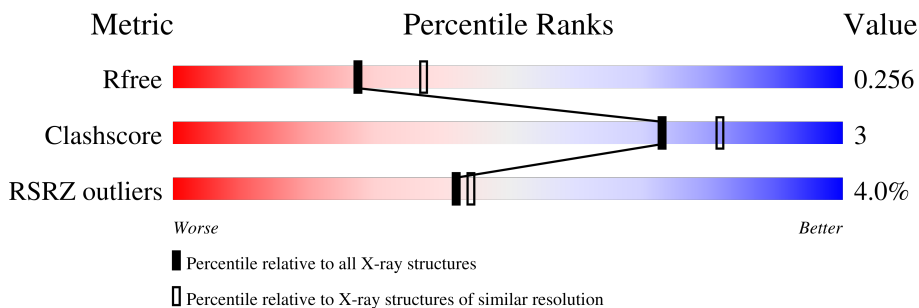
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	331	4% (poor fit), 89% (0-1 outliers), 8% (2-3 outliers), 0% (4+ outliers), 0% (not modelled)
1	B	331	5% (poor fit), 88% (0-1 outliers), 9% (2-3 outliers), 0% (4+ outliers), 0% (not modelled)
1	C	331	0% (poor fit), 87% (0-1 outliers), 12% (2-3 outliers), 0% (4+ outliers), 0% (not modelled)
1	D	331	0% (poor fit), 91% (0-1 outliers), 8% (2-3 outliers), 0% (4+ outliers), 0% (not modelled)
1	E	331	5% (poor fit), 83% (0-1 outliers), 10% (2-3 outliers), 6% (4+ outliers), 0% (not modelled)
1	F	331	7% (poor fit), 87% (0-1 outliers), 8% (2-3 outliers), 5% (4+ outliers), 0% (not modelled)
1	G	331	6% (poor fit), 86% (0-1 outliers), 11% (2-3 outliers), 0% (4+ outliers), 0% (not modelled)

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Mol	Chain	Length	Quality of chain
1	H	331	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a small red segment on the left labeled '2%', a large green segment in the middle labeled '88%', and a small yellow segment on the right labeled '11%'. A small grey dot is visible at the far right end of the bar.</p>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21329 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 L-lactate dehydrogenase A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	323	2503	1602	426	462	13	0	0	0
1	B	322	2492	1596	422	461	13	0	0	0
1	C	328	2545	1626	436	470	13	0	0	0
1	D	329	2550	1629	436	472	13	0	0	0
1	E	310	2390	1534	407	436	13	0	0	0
1	F	314	2431	1558	412	448	13	0	0	0
1	G	322	2489	1594	424	458	13	0	0	0
1	H	329	2550	1629	437	471	13	0	0	0

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

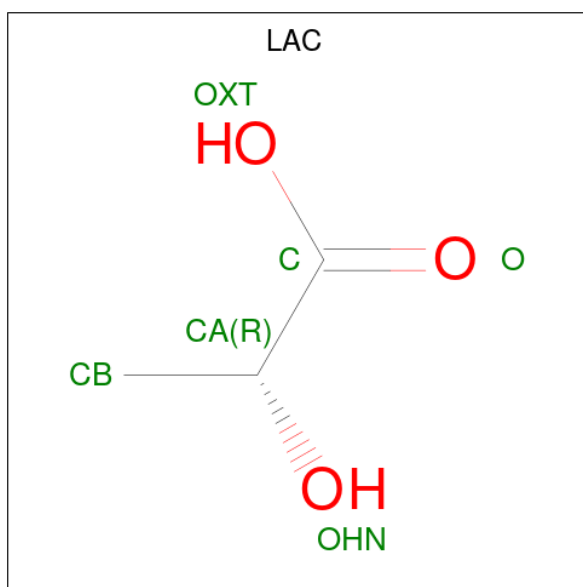




Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0
3	B	1	5	4	1	0	0
3	C	1	5	4	1	0	0
3	D	1	5	4	1	0	0
3	D	1	5	4	1	0	0
3	F	1	5	4	1	0	0
3	G	1	5	4	1	0	0
3	H	1	5	4	1	0	0

- Molecule 4 is (2R)-5-[(2-chlorophenyl)sulfanyl]-6'--(4-fluorophenoxy)-4-hydroxy-2-(thiophen-3-yl)-2,3-dihydro[2,2'-bipyridin]-6(1H)-one (CCD ID: D3J) (formula: C<sub>26</sub>H<sub>18</sub>ClFN<sub>2</sub>O<sub>3</sub>S<sub>2</sub>).





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

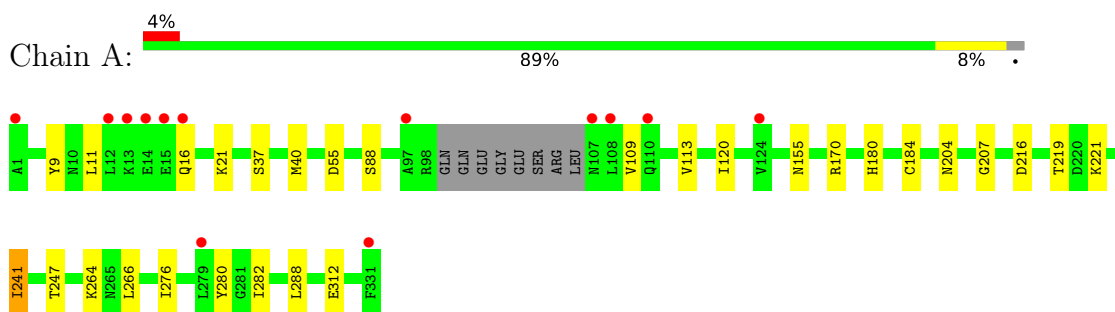
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	111	Total O 111 111	0	0
6	B	104	Total O 104 104	0	0
6	C	115	Total O 115 115	0	0
6	D	99	Total O 99 99	0	0
6	E	67	Total O 67 67	0	0
6	F	83	Total O 83 83	0	0
6	G	74	Total O 74 74	0	0
6	H	118	Total O 118 118	0	0

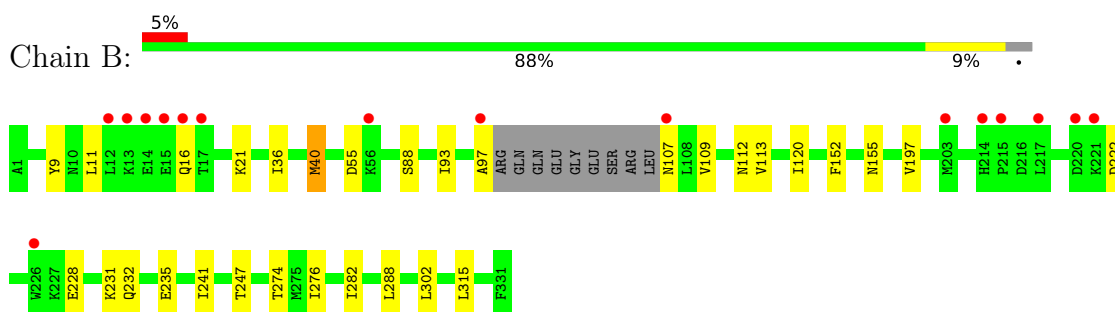
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

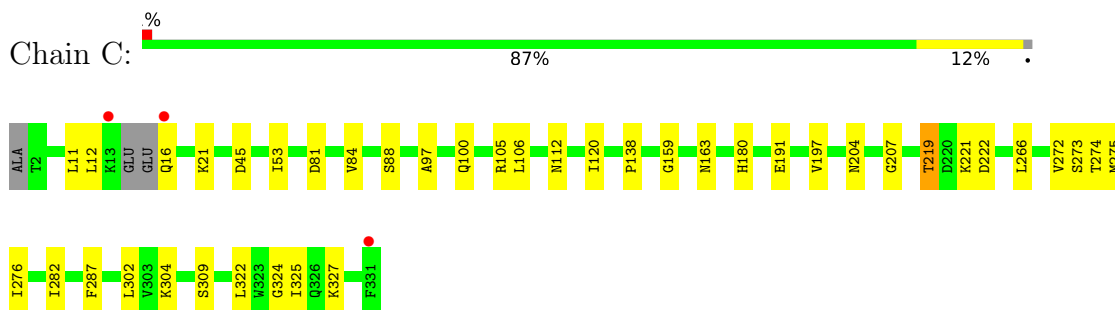
- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain

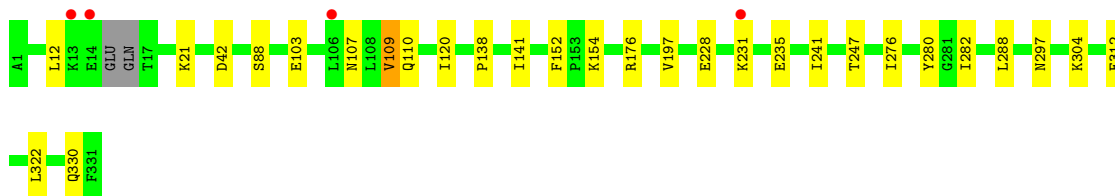


- Molecule 1: L-lactate dehydrogenase A chain

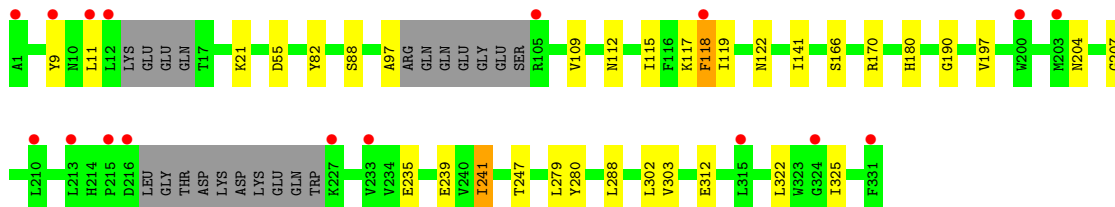
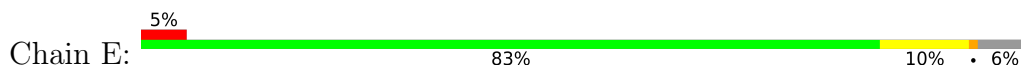


- Molecule 1: L-lactate dehydrogenase A chain

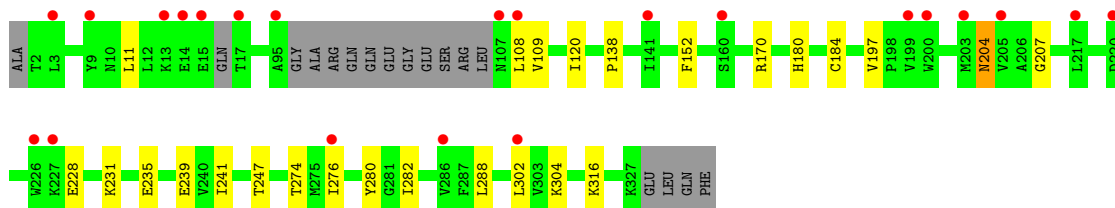
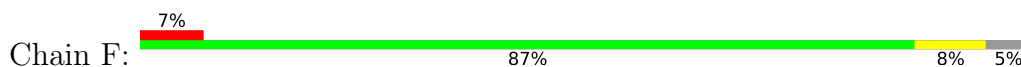




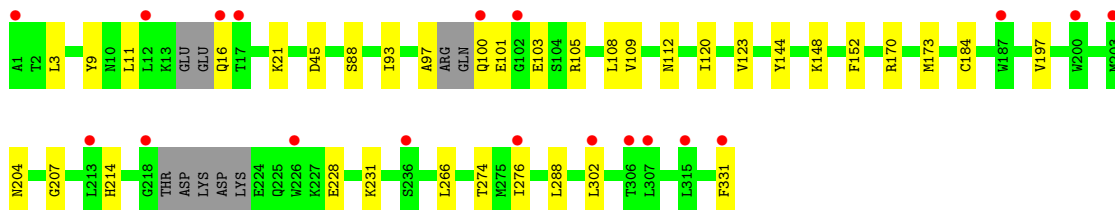
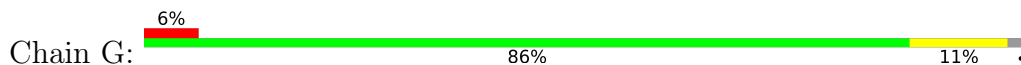
- Molecule 1: L-lactate dehydrogenase A chain



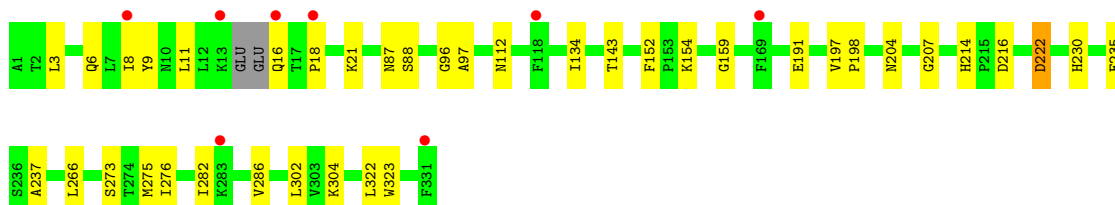
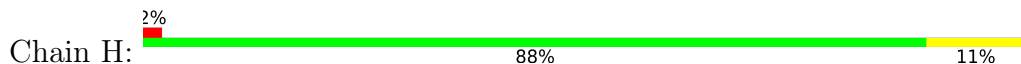
- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.60Å 155.30Å 265.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.74 – 2.30 48.74 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.6 (48.74-2.30) 95.7 (48.74-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 2.29Å)	Xtrriage
Refinement program	BUSTER 2.11.6	Depositor
R, $R_{free}$	0.204 , 0.238 (Not available) , 0.256	Depositor DCC
$R_{free}$ test set	1094 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.8	Xtrriage
Anisotropy	0.495	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 38.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21329	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, LAC, NAD, D3J

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	0.83	2/2546 (0.1%)	1.29	1/3443 (0.0%)
1	B	0.85	2/2535 (0.1%)	1.32	9/3429 (0.3%)
1	C	0.84	2/2588 (0.1%)	1.31	11/3498 (0.3%)
1	D	0.83	1/2593 (0.0%)	1.28	4/3505 (0.1%)
1	E	0.82	1/2429 (0.0%)	1.34	8/3284 (0.2%)
1	F	0.80	1/2472 (0.0%)	1.29	5/3344 (0.1%)
1	G	0.80	0/2530	1.30	9/3419 (0.3%)
1	H	0.87	0/2593	1.34	8/3505 (0.2%)
All	All	0.83	9/20286 (0.0%)	1.31	55/27427 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	120	ILE	CA-CB	8.04	1.58	1.54
1	C	272	VAL	CA-C	5.83	1.59	1.52
1	A	120	ILE	CA-CB	5.75	1.57	1.54
1	F	120	ILE	CA-CB	5.57	1.56	1.54
1	C	120	ILE	CA-CB	5.47	1.56	1.54
1	A	241	ILE	CG1-CD1	-5.38	1.30	1.51
1	B	40	MET	SD-CE	-5.20	1.66	1.79
1	D	120	ILE	CA-CB	5.17	1.56	1.54
1	E	241	ILE	CG1-CD1	-5.12	1.31	1.51

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	118	PHE	CA-CB-CG	9.35	123.15	113.80
1	A	55	ASP	CA-CB-CG	9.16	121.76	112.60
1	B	55	ASP	CA-CB-CG	8.75	121.35	112.60
1	E	55	ASP	CA-CB-CG	7.79	120.39	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	GLN	N-CA-C	-7.58	99.60	110.59
1	G	331	PHE	CA-CB-CG	6.78	120.58	113.80
1	H	16	GLN	CA-C-N	6.69	130.83	120.60
1	H	16	GLN	C-N-CA	6.69	130.83	120.60
1	F	108	LEU	CA-C-N	6.60	128.95	120.70
1	F	108	LEU	C-N-CA	6.60	128.95	120.70
1	G	16	GLN	CA-C-N	6.31	129.17	120.39
1	G	16	GLN	C-N-CA	6.31	129.17	120.39
1	C	309	SER	CA-C-N	6.23	128.63	120.28
1	C	309	SER	C-N-CA	6.23	128.63	120.28
1	E	118	PHE	CA-C-N	6.01	128.22	120.88
1	E	118	PHE	C-N-CA	6.01	128.22	120.88
1	H	197	VAL	N-CA-C	6.00	114.02	107.60
1	C	197	VAL	N-CA-C	5.87	113.88	107.60
1	H	222	ASP	CA-CB-CG	5.87	118.47	112.60
1	C	53	ILE	CA-C-N	5.84	128.91	120.79
1	C	53	ILE	C-N-CA	5.84	128.91	120.79
1	C	16	GLN	CA-C-N	5.82	129.50	120.60
1	C	16	GLN	C-N-CA	5.82	129.50	120.60
1	C	45	ASP	CA-CB-CG	5.80	118.40	112.60
1	D	176	ARG	CB-CG-CD	5.77	124.56	111.30
1	C	219	THR	CB-CA-C	5.71	119.98	109.71
1	B	16	GLN	CA-C-N	5.70	135.72	121.80
1	B	16	GLN	C-N-CA	5.70	135.72	121.80
1	G	93	ILE	CB-CG1-CD1	5.68	125.72	113.80
1	D	152	PHE	CA-CB-CG	5.63	119.43	113.80
1	G	197	VAL	N-CA-C	5.62	113.61	107.60
1	G	152	PHE	CA-CB-CG	5.58	119.38	113.80
1	B	107	ASN	CA-C-N	5.57	129.51	120.60
1	B	107	ASN	C-N-CA	5.57	129.51	120.60
1	B	197	VAL	N-CA-C	5.55	113.54	107.60
1	D	109	VAL	N-CA-CB	5.54	116.44	110.62
1	B	93	ILE	CB-CG1-CD1	5.54	125.43	113.80
1	E	117	LYS	CA-C-N	5.50	129.90	120.71
1	E	117	LYS	C-N-CA	5.50	129.90	120.71
1	F	152	PHE	CA-CB-CG	5.46	119.26	113.80
1	B	152	PHE	CA-CB-CG	5.41	119.21	113.80
1	E	197	VAL	N-CA-C	5.38	113.36	107.60
1	B	222	ASP	CA-CB-CG	5.32	117.92	112.60
1	C	222	ASP	CA-CB-CG	5.30	117.90	112.60
1	H	96	GLY	CA-C-N	5.28	128.21	120.71
1	H	96	GLY	C-N-CA	5.28	128.21	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	45	ASP	CA-CB-CG	5.26	117.86	112.60
1	F	197	VAL	N-CA-C	5.24	113.21	107.60
1	H	152	PHE	CA-CB-CG	5.21	119.02	113.80
1	F	204	ASN	N-CA-C	5.12	116.63	108.79
1	E	119	ILE	N-CA-C	5.07	115.35	110.74
1	G	173	MET	CA-C-N	5.02	125.51	119.94
1	G	173	MET	C-N-CA	5.02	125.51	119.94
1	D	197	VAL	N-CA-C	5.02	112.97	107.60
1	H	235	GLU	N-CA-C	5.01	118.54	112.23

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	2503	0	2595	21	0
1	B	2492	0	2582	16	0
1	C	2545	0	2635	21	0
1	D	2550	0	2641	17	0
1	E	2390	0	2492	21	0
1	F	2431	0	2523	15	0
1	G	2489	0	2579	23	0
1	H	2550	0	2643	23	0
2	A	44	0	25	0	0
2	B	44	0	25	0	0
2	C	44	0	25	0	0
2	D	44	0	25	0	0
2	E	44	0	25	0	0
2	F	44	0	25	0	0
2	G	44	0	25	0	0
2	H	44	0	25	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0
4	A	35	0	0	0	0
4	B	35	0	0	0	0
4	D	35	0	0	0	0
4	E	35	0	0	0	0
4	F	35	0	0	0	0
4	G	35	0	0	0	0
5	C	6	0	0	0	0
6	A	111	0	0	0	0
6	B	104	0	0	1	0
6	C	115	0	0	1	0
6	D	99	0	0	0	0
6	E	67	0	0	1	0
6	F	83	0	0	0	0
6	G	74	0	0	0	0
6	H	118	0	0	1	0
All	All	21329	0	20890	131	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 (131) 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:C:97:ALA:H	1:C:112:ASN:HD21	1.20	0.90
1:E:97:ALA:H	1:E:112:ASN:HD21	1.17	0.88
1:D:110:GLN:HE22	1:D:330:GLN:H	1.23	0.83
1:G:97:ALA:H	1:G:112:ASN:HD21	1.25	0.82
1:F:170:ARG:HD3	1:F:184:CYS:O	1.81	0.81
1:A:264:LYS:HE2	1:D:42:ASP:HB3	1.67	0.74
1:B:302:LEU:HD13	1:C:11:LEU:HD21	1.72	0.72
1:G:170:ARG:CD	1:G:184:CYS:O	2.41	0.69
1:A:170:ARG:HD3	1:A:184:CYS:O	1.93	0.69
1:A:170:ARG:CD	1:A:184:CYS:O	2.42	0.68
1:G:170:ARG:HD3	1:G:184:CYS:O	1.94	0.67
1:H:97:ALA:H	1:H:112:ASN:HD21	1.43	0.66
1:C:163:ASN:HB3	6:C:957:HOH:O	1.97	0.64
1:C:159:GLY:HA3	1:C:273:SER:HB2	1.80	0.64
1:G:97:ALA:H	1:G:112:ASN:ND2	1.96	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:ILE:HG12	1:D:288:LEU:HB2	1.83	0.60
1:C:275:MET:HG2	1:C:287:PHE:CE1	2.37	0.59
1:H:276:ILE:HD12	1:H:282:ILE:HG12	1.85	0.59
1:D:109:VAL:HG22	1:D:138:PRO:HG2	1.85	0.59
1:B:288:LEU:HD11	1:B:315:LEU:HD21	1.85	0.58
1:D:231:LYS:O	1:D:235:GLU:HG2	2.04	0.58
1:D:276:ILE:HD13	1:D:282:ILE:HD13	1.84	0.57
1:E:11:LEU:HD12	1:H:154:LYS:HE3	1.84	0.57
1:E:11:LEU:HD21	1:H:302:LEU:HD13	1.86	0.57
1:C:106:LEU:HD22	1:C:325:ILE:HD13	1.86	0.57
1:G:170:ARG:HD2	1:G:184:CYS:O	2.04	0.57
1:B:276:ILE:HD13	1:B:282:ILE:HD13	1.86	0.57
1:F:280:TYR:O	1:F:316:LYS:HE3	2.06	0.56
1:A:9:TYR:HB2	1:D:304:LYS:HD2	1.86	0.56
1:C:191:GLU:HG3	1:C:322:LEU:HD21	1.86	0.56
1:H:159:GLY:HA3	1:H:273:SER:HB2	1.87	0.56
1:E:97:ALA:H	1:E:112:ASN:ND2	1.94	0.55
1:E:115:ILE:O	1:E:118:PHE:HB3	2.06	0.55
1:C:105:ARG:O	1:C:138:PRO:HG3	2.06	0.55
1:E:302:LEU:HD22	1:H:9:TYR:HB3	1.88	0.55
1:A:170:ARG:HD2	1:A:184:CYS:O	2.07	0.55
1:B:11:LEU:HD11	1:C:302:LEU:HD13	1.88	0.54
1:A:155:ASN:ND2	1:D:12:LEU:HD11	2.22	0.54
1:A:276:ILE:HD13	1:A:282:ILE:HD13	1.88	0.54
1:B:274:THR:HG21	1:B:302:LEU:HD11	1.90	0.53
1:G:274:THR:HG21	1:G:302:LEU:HD11	1.91	0.53
1:E:190:GLY:HA2	1:E:288:LEU:HD13	1.90	0.52
1:F:274:THR:HG21	1:F:302:LEU:HD11	1.89	0.52
1:F:276:ILE:HG12	1:F:288:LEU:HB2	1.91	0.52
1:H:18:PRO:HG2	1:H:87:ASN:HB2	1.91	0.52
1:F:276:ILE:HD13	1:F:282:ILE:HD13	1.92	0.52
1:G:100:GLN:HG3	1:G:108:LEU:HD22	1.91	0.52
1:G:144:TYR:OH	1:G:148:LYS:HE2	2.10	0.52
1:A:276:ILE:HG12	1:A:288:LEU:HB2	1.92	0.51
1:F:302:LEU:HD13	1:G:11:LEU:HD21	1.91	0.51
1:C:204:ASN:HD22	1:C:207:GLY:H	1.59	0.51
1:E:280:TYR:HB3	1:E:312:GLU:HG3	1.93	0.51
1:G:276:ILE:HG12	1:G:288:LEU:HB2	1.94	0.50
1:E:109:VAL:HG11	1:E:325:ILE:HG21	1.95	0.49
1:E:279:LEU:HD21	1:E:302:LEU:HD21	1.94	0.49
1:H:3:LEU:HA	1:H:6:GLN:HE21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:ILE:HG13	1:E:322:LEU:HD22	1.95	0.48
1:A:219:THR:HG23	1:A:221:LYS:H	1.77	0.48
1:H:191:GLU:HG3	1:H:322:LEU:HD21	1.95	0.48
1:B:36:ILE:HG13	1:B:40:MET:HE2	1.95	0.48
1:F:11:LEU:HD11	1:G:302:LEU:HD13	1.94	0.48
1:G:105:ARG:O	1:G:109:VAL:HG23	2.13	0.48
1:E:235:GLU:O	1:E:239:GLU:HG2	2.14	0.48
1:C:276:ILE:HD13	1:C:282:ILE:HD13	1.95	0.48
1:F:204:ASN:HD22	1:F:207:GLY:H	1.62	0.48
6:E:906:HOH:O	1:H:11:LEU:HD21	2.13	0.47
1:D:280:TYR:HB3	1:D:312:GLU:HG3	1.97	0.47
1:H:204:ASN:HD22	1:H:207:GLY:H	1.63	0.47
1:F:109:VAL:HG22	1:F:138:PRO:HG2	1.97	0.47
1:H:237:ALA:CB	6:H:969:HOH:O	2.63	0.46
1:H:286:VAL:HG22	1:H:323:TRP:HB2	1.96	0.46
1:F:304:LYS:HD2	1:G:9:TYR:HB2	1.97	0.46
1:H:134:ILE:HD13	1:H:143:THR:HG23	1.97	0.46
1:B:241:ILE:CD1	1:B:247:THR:HG23	2.46	0.46
1:D:241:ILE:CD1	1:D:247:THR:HG23	2.46	0.46
1:F:235:GLU:O	1:F:239:GLU:HG2	2.15	0.46
1:A:40:MET:SD	1:B:40:MET:HE3	2.57	0.45
1:A:216:ASP:O	1:A:219:THR:HG22	2.16	0.45
6:B:959:HOH:O	1:C:11:LEU:HG	2.16	0.45
1:A:37:SER:HA	1:B:40:MET:HE1	1.98	0.45
1:C:219:THR:HG23	1:C:221:LYS:H	1.82	0.45
1:H:154:LYS:HD3	1:H:275:MET:HE3	1.99	0.45
1:A:266:LEU:O	1:C:180:HIS:HB2	2.17	0.44
1:E:166:SER:O	1:E:170:ARG:HG3	2.18	0.44
1:G:204:ASN:HD22	1:G:207:GLY:H	1.64	0.44
1:E:21:LYS:HB3	1:E:88:SER:HA	1.98	0.44
1:A:280:TYR:HB3	1:A:312:GLU:HG3	1.99	0.44
1:B:97:ALA:H	1:B:112:ASN:HD21	1.63	0.44
1:D:110:GLN:NE2	1:D:330:GLN:H	2.02	0.44
1:D:21:LYS:HB3	1:D:88:SER:HA	1.99	0.44
1:H:216:ASP:HB3	1:H:222:ASP:HB3	1.99	0.44
1:B:232:GLN:HA	1:B:235:GLU:HB2	1.99	0.44
1:B:155:ASN:ND2	1:C:12:LEU:HD11	2.33	0.43
1:F:180:HIS:HB2	1:H:266:LEU:O	2.18	0.43
1:F:228:GLU:HA	1:F:231:LYS:HB2	2.00	0.43
1:G:214:HIS:HB2	1:H:3:LEU:HD13	1.99	0.43
1:B:109:VAL:O	1:B:113:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLN:HG3	1:D:297:ASN:HD21	1.83	0.43
1:B:228:GLU:HA	1:B:231:LYS:HB2	2.00	0.43
1:E:241:ILE:CD1	1:E:247:THR:HG23	2.48	0.43
1:D:103:GLU:HG3	1:D:107:ASN:HD22	1.82	0.43
1:A:204:ASN:HD22	1:A:207:GLY:H	1.66	0.42
1:A:241:ILE:CD1	1:A:247:THR:HG23	2.48	0.42
1:B:21:LYS:HB3	1:B:88:SER:HA	2.01	0.42
1:C:274:THR:O	1:C:287:PHE:HA	2.19	0.42
1:A:11:LEU:HD12	1:D:154:LYS:HE3	2.01	0.42
1:B:9:TYR:HB2	1:C:304:LYS:HD2	2.01	0.42
1:A:21:LYS:HB3	1:A:88:SER:HA	2.01	0.42
1:E:180:HIS:HB2	1:G:266:LEU:O	2.18	0.42
1:G:97:ALA:N	1:G:112:ASN:HD21	2.05	0.42
1:G:3:LEU:HD13	1:H:214:HIS:HB2	2.01	0.42
1:G:228:GLU:HA	1:G:231:LYS:HB2	2.00	0.42
1:H:198:PRO:HG3	1:H:230:HIS:CG	2.55	0.42
1:C:81:ASP:O	1:C:84:VAL:HG22	2.20	0.41
1:C:324:GLY:HA2	1:C:327:LYS:HE3	2.02	0.41
1:G:101:GLU:C	1:G:103:GLU:H	2.28	0.41
1:A:109:VAL:O	1:A:113:VAL:HG23	2.20	0.41
1:C:21:LYS:HB3	1:C:88:SER:HA	2.02	0.41
1:E:204:ASN:HD22	1:E:207:GLY:H	1.69	0.41
1:G:21:LYS:HB3	1:G:88:SER:HA	2.02	0.41
1:E:112:ASN:HD22	1:E:115:ILE:HD12	1.86	0.41
1:D:228:GLU:HA	1:D:231:LYS:HB2	2.01	0.41
1:F:241:ILE:CD1	1:F:247:THR:HG23	2.51	0.41
1:A:180:HIS:HB2	1:C:266:LEU:O	2.22	0.40
1:E:9:TYR:HB2	1:H:304:LYS:HE2	2.03	0.40
1:E:82:TYR:CG	1:E:122:ASN:HB3	2.55	0.40
1:H:21:LYS:HB3	1:H:88:SER:HA	2.03	0.40
1:D:141:ILE:HG13	1:D:322:LEU:HD22	2.03	0.40
1:E:303:VAL:HG22	1:H:8:ILE:HD13	2.04	0.40
1:G:120:ILE:HA	1:G:123:VAL:HG22	2.03	0.40
1:F:11:LEU:CD1	1:G:302:LEU:HD13	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

There are no protein backbone outliers to report in this entry.

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

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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](#)

23 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	D3J	A	803	-	37,39,39	1.01	2 (5%)	42,56,56	2.00	7 (16%)
2	NAD	B	801	-	46,48,48	1.87	9 (19%)	64,73,73	1.68	16 (25%)
3	SO4	C	802	-	4,4,4	0.23	0	6,6,6	0.16	0
2	NAD	G	801	-	46,48,48	1.72	7 (15%)	64,73,73	1.90	16 (25%)
3	SO4	D	802	-	4,4,4	0.30	0	6,6,6	0.31	0
2	NAD	H	801	-	46,48,48	1.96	10 (21%)	64,73,73	1.86	17 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAD	F	801	-	46,48,48	1.94	9 (19%)	64,73,73	1.65	13 (20%)
3	SO4	F	802	-	4,4,4	0.20	0	6,6,6	0.14	0
4	D3J	F	803	-	37,39,39	0.92	1 (2%)	42,56,56	1.94	6 (14%)
3	SO4	G	802	-	4,4,4	0.24	0	6,6,6	0.15	0
2	NAD	E	801	-	46,48,48	1.94	9 (19%)	64,73,73	1.78	15 (23%)
2	NAD	D	801	-	46,48,48	1.91	11 (23%)	64,73,73	1.71	15 (23%)
3	SO4	B	802	-	4,4,4	0.31	0	6,6,6	0.13	0
3	SO4	H	802	-	4,4,4	0.25	0	6,6,6	0.16	0
2	NAD	C	801	-	46,48,48	1.96	9 (19%)	64,73,73	1.78	13 (20%)
4	D3J	D	804	-	37,39,39	0.97	1 (2%)	42,56,56	1.91	7 (16%)
4	D3J	B	803	-	37,39,39	0.97	0	42,56,56	1.81	5 (11%)
3	SO4	D	803	-	4,4,4	0.27	0	6,6,6	0.18	0
3	SO4	A	802	-	4,4,4	0.43	0	6,6,6	0.32	0
5	LAC	C	803	-	4,5,5	1.25	1 (25%)	2,6,6	0.77	0
4	D3J	G	803	-	37,39,39	0.86	0	42,56,56	1.88	6 (14%)
2	NAD	A	801	-	46,48,48	1.96	10 (21%)	64,73,73	1.67	14 (21%)
4	D3J	E	802	-	37,39,39	0.93	1 (2%)	42,56,56	1.96	7 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	D	801	-	-	4/30/62/62	0/5/5/5
4	D3J	A	803	-	-	2/13/38/38	0/5/5/5
5	LAC	C	803	-	-	4/4/4/4	-
4	D3J	G	803	-	-	0/13/38/38	0/5/5/5
4	D3J	F	803	-	-	3/13/38/38	0/5/5/5
2	NAD	B	801	-	-	5/30/62/62	0/5/5/5
2	NAD	A	801	-	-	5/30/62/62	0/5/5/5
4	D3J	D	804	-	-	0/13/38/38	0/5/5/5
2	NAD	G	801	-	-	4/30/62/62	0/5/5/5
4	D3J	E	802	-	-	2/13/38/38	0/5/5/5
2	NAD	H	801	-	-	4/30/62/62	0/5/5/5
2	NAD	C	801	-	-	4/30/62/62	0/5/5/5
2	NAD	F	801	-	-	4/30/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	E	801	-	-	5/30/62/62	0/5/5/5
4	D3J	B	803	-	-	0/13/38/38	0/5/5/5

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	NAD	C7N-N7N	5.96	1.43	1.33
2	E	801	NAD	C7N-N7N	5.80	1.43	1.33
2	D	801	NAD	C7N-N7N	5.78	1.43	1.33
2	C	801	NAD	C7N-N7N	5.53	1.43	1.33
2	H	801	NAD	C7N-N7N	5.16	1.42	1.33
2	F	801	NAD	C7N-N7N	5.13	1.42	1.33
2	F	801	NAD	C6A-N6A	5.04	1.47	1.34
2	B	801	NAD	C6A-N6A	5.02	1.47	1.34
2	G	801	NAD	C7N-N7N	4.92	1.42	1.33
2	C	801	NAD	PA-O3	4.76	1.64	1.59
2	C	801	NAD	C6A-N6A	4.74	1.46	1.34
2	H	801	NAD	PA-O3	4.70	1.64	1.59
2	B	801	NAD	C7N-N7N	4.65	1.41	1.33
2	E	801	NAD	C6A-N6A	4.65	1.46	1.34
2	A	801	NAD	C6A-N6A	4.64	1.46	1.34
2	H	801	NAD	C2B-C3B	-4.59	1.40	1.53
2	H	801	NAD	C6A-N6A	4.55	1.45	1.34
2	G	801	NAD	C6A-N6A	4.53	1.45	1.34
2	A	801	NAD	C2B-C3B	-4.48	1.41	1.53
2	F	801	NAD	C2B-C3B	-4.45	1.41	1.53
2	D	801	NAD	C6A-N6A	4.45	1.45	1.34
2	E	801	NAD	C2B-C3B	-4.36	1.41	1.53
2	D	801	NAD	C2B-C3B	-4.31	1.41	1.53
2	B	801	NAD	C2B-C3B	-4.28	1.41	1.53
2	C	801	NAD	C2B-C3B	-4.10	1.42	1.53
2	G	801	NAD	C2B-C3B	-4.08	1.42	1.53
2	B	801	NAD	O2D-C2D	-3.52	1.34	1.43
2	C	801	NAD	O2D-C2D	-3.32	1.34	1.43
2	F	801	NAD	O2D-C2D	-3.21	1.35	1.43
2	E	801	NAD	PN-O3	3.20	1.63	1.59
2	D	801	NAD	O2D-C2D	-3.17	1.35	1.43
2	E	801	NAD	O2D-C2D	-3.03	1.35	1.43
2	A	801	NAD	O2D-C2D	-2.96	1.35	1.43
2	G	801	NAD	O2D-C2D	-2.93	1.35	1.43
2	H	801	NAD	O2D-C2D	-2.88	1.35	1.43
2	C	801	NAD	C2N-N1N	2.72	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	NAD	PA-O3	2.69	1.62	1.59
2	E	801	NAD	C5D-C4D	-2.69	1.43	1.51
2	A	801	NAD	PN-O3	2.60	1.62	1.59
2	D	801	NAD	C5B-C4B	-2.59	1.43	1.51
2	C	801	NAD	C5D-C4D	-2.55	1.43	1.51
2	D	801	NAD	C5A-N7A	-2.52	1.34	1.39
2	D	801	NAD	C5D-C4D	-2.51	1.44	1.51
2	B	801	NAD	C5A-N7A	-2.51	1.34	1.39
2	C	801	NAD	C5B-C4B	-2.50	1.44	1.51
2	F	801	NAD	PN-O3	2.49	1.62	1.59
2	E	801	NAD	C5B-C4B	-2.47	1.44	1.51
2	F	801	NAD	C5D-C4D	-2.46	1.44	1.51
2	F	801	NAD	C5B-C4B	-2.41	1.44	1.51
2	A	801	NAD	C5B-C4B	-2.38	1.44	1.51
2	G	801	NAD	C5D-C4D	-2.37	1.44	1.51
2	B	801	NAD	C5B-C4B	-2.37	1.44	1.51
2	B	801	NAD	C5D-C4D	-2.35	1.44	1.51
2	H	801	NAD	C5B-C4B	-2.34	1.44	1.51
2	A	801	NAD	C5D-C4D	-2.33	1.44	1.51
2	G	801	NAD	C8A-N7A	2.33	1.36	1.31
2	G	801	NAD	C5B-C4B	-2.32	1.44	1.51
2	A	801	NAD	O4B-C4B	-2.30	1.39	1.45
2	E	801	NAD	O4B-C4B	-2.28	1.39	1.45
2	C	801	NAD	C8A-N7A	2.27	1.36	1.31
2	E	801	NAD	C5A-N7A	-2.27	1.34	1.39
2	H	801	NAD	C5D-C4D	-2.25	1.44	1.51
2	H	801	NAD	C5A-N7A	-2.24	1.35	1.39
2	F	801	NAD	O4B-C4B	-2.22	1.40	1.45
2	F	801	NAD	C8A-N7A	2.20	1.35	1.31
4	A	803	D3J	C29-S30	2.20	1.76	1.70
2	H	801	NAD	O4B-C4B	-2.19	1.40	1.45
2	D	801	NAD	PN-O3	2.19	1.61	1.59
4	E	802	D3J	C29-S30	2.18	1.76	1.70
2	B	801	NAD	O4B-C4B	-2.18	1.40	1.45
4	D	804	D3J	C29-S30	2.16	1.76	1.70
4	F	803	D3J	C29-S30	2.11	1.76	1.70
2	B	801	NAD	C2D-C3D	-2.11	1.47	1.53
5	C	803	LAC	OXT-C	-2.11	1.23	1.30
2	D	801	NAD	C8A-N7A	2.09	1.35	1.31
2	D	801	NAD	O4B-C4B	-2.09	1.40	1.45
4	A	803	D3J	C3-C2	2.08	1.41	1.37
2	H	801	NAD	C2N-N1N	2.07	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	NAD	O5B-C5B	-2.02	1.37	1.44
2	A	801	NAD	O5B-C5B	-2.00	1.37	1.44

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	803	D3J	C9-N10-C11	7.77	123.61	117.20
4	A	803	D3J	C9-N10-C11	7.50	123.39	117.20
4	E	802	D3J	C12-N13-C14	7.15	122.65	117.33
4	D	804	D3J	C12-N13-C14	6.97	122.52	117.33
4	G	803	D3J	C9-N10-C11	6.79	122.81	117.20
4	D	804	D3J	C9-N10-C11	6.32	122.42	117.20
4	E	802	D3J	C9-N10-C11	6.28	122.39	117.20
4	B	803	D3J	C12-N13-C14	5.92	121.74	117.33
4	B	803	D3J	C9-N10-C11	5.86	122.04	117.20
4	F	803	D3J	C12-N13-C14	5.75	121.61	117.33
2	H	801	NAD	N3A-C2A-N1A	-5.64	120.05	128.58
2	G	801	NAD	C5A-C4A-N3A	-5.56	119.06	126.72
4	A	803	D3J	C12-N13-C14	5.45	121.39	117.33
4	G	803	D3J	C12-N13-C14	5.43	121.37	117.33
2	C	801	NAD	N3A-C2A-N1A	-5.36	120.47	128.58
2	A	801	NAD	N3A-C2A-N1A	-5.04	120.95	128.58
2	E	801	NAD	C5A-C4A-N3A	-4.79	120.12	126.72
2	E	801	NAD	N3A-C2A-N1A	-4.76	121.37	128.58
2	B	801	NAD	N3A-C2A-N1A	-4.76	121.37	128.58
4	A	803	D3J	C17-S16-C15	4.73	108.82	102.81
2	D	801	NAD	N3A-C2A-N1A	-4.63	121.57	128.58
2	D	801	NAD	C5A-C4A-N3A	-4.51	120.51	126.72
2	F	801	NAD	C5A-C4A-N3A	-4.50	120.53	126.72
2	B	801	NAD	C5A-C4A-N3A	-4.46	120.58	126.72
2	C	801	NAD	C5A-C4A-N3A	-4.46	120.58	126.72
2	G	801	NAD	N3A-C2A-N1A	-4.33	122.02	128.58
2	G	801	NAD	C4A-C5A-N7A	-4.31	105.65	110.58
2	G	801	NAD	N9A-C8A-N7A	-4.27	107.89	113.94
2	A	801	NAD	C5A-C4A-N3A	-4.07	121.11	126.72
2	G	801	NAD	C5A-N7A-C8A	3.99	109.72	103.45
2	H	801	NAD	N9A-C8A-N7A	-3.99	108.28	113.94
2	D	801	NAD	N9A-C8A-N7A	-3.86	108.46	113.94
2	G	801	NAD	C2A-N3A-C4A	3.86	121.26	111.83
4	E	802	D3J	C17-S16-C15	3.78	107.61	102.81
2	H	801	NAD	C4A-N9A-C8A	3.72	109.65	105.74
2	F	801	NAD	C4A-C5A-N7A	-3.71	106.34	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	803	D3J	C17-S16-C15	3.69	107.49	102.81
2	B	801	NAD	N9A-C8A-N7A	-3.67	108.72	113.94
2	F	801	NAD	N3A-C2A-N1A	-3.66	123.03	128.58
2	E	801	NAD	C2A-N3A-C4A	3.66	120.76	111.83
2	H	801	NAD	C5A-C4A-N3A	-3.63	121.71	126.72
2	C	801	NAD	C2A-N3A-C4A	3.60	120.62	111.83
2	E	801	NAD	C3N-C7N-N7N	3.58	122.15	117.74
2	F	801	NAD	N9A-C8A-N7A	-3.57	108.87	113.94
2	A	801	NAD	N9A-C8A-N7A	-3.56	108.89	113.94
2	C	801	NAD	N9A-C8A-N7A	-3.55	108.91	113.94
2	B	801	NAD	C2A-N3A-C4A	3.52	120.42	111.83
2	G	801	NAD	N3A-C4A-N9A	3.47	133.07	127.17
2	C	801	NAD	C4A-N9A-C8A	3.47	109.38	105.74
2	E	801	NAD	N3A-C4A-N9A	3.46	133.06	127.17
2	C	801	NAD	N3A-C4A-N9A	3.42	132.99	127.17
2	H	801	NAD	C2A-N3A-C4A	3.42	120.18	111.83
2	D	801	NAD	C2A-N3A-C4A	3.42	120.17	111.83
2	E	801	NAD	N9A-C8A-N7A	-3.41	109.10	113.94
2	A	801	NAD	C2A-N3A-C4A	3.40	120.13	111.83
2	G	801	NAD	O4B-C1B-N9A	3.37	114.57	108.09
2	F	801	NAD	C5A-N7A-C8A	3.37	108.75	103.45
4	D	804	D3J	C17-S16-C15	3.37	107.09	102.81
2	D	801	NAD	N3A-C4A-N9A	3.36	132.88	127.17
4	B	803	D3J	C26-C12-N13	3.31	112.10	108.09
2	H	801	NAD	O2A-PA-O3	3.28	116.15	107.27
2	B	801	NAD	C5A-N7A-C8A	3.28	108.61	103.45
2	D	801	NAD	C5A-N7A-C8A	3.27	108.60	103.45
2	H	801	NAD	N3A-C4A-N9A	3.27	132.72	127.17
4	G	803	D3J	C12-C28-C29	-3.25	121.90	126.64
2	C	801	NAD	C4B-O4B-C1B	-3.18	102.44	109.47
2	H	801	NAD	C5A-N7A-C8A	3.15	108.41	103.45
2	D	801	NAD	C4A-N9A-C8A	3.12	109.02	105.74
4	B	803	D3J	C15-C14-N13	3.12	120.04	113.96
2	B	801	NAD	N3A-C4A-N9A	3.11	132.46	127.17
2	A	801	NAD	C4A-N9A-C8A	3.06	108.95	105.74
2	G	801	NAD	C4A-N9A-C8A	3.04	108.93	105.74
2	B	801	NAD	C4A-C5A-N7A	-2.98	107.18	110.58
2	F	801	NAD	N3A-C4A-N9A	2.98	132.23	127.17
2	E	801	NAD	C4D-O4D-C1D	-2.97	107.20	109.92
2	A	801	NAD	C5A-N7A-C8A	2.95	108.09	103.45
2	H	801	NAD	C5N-C4N-C3N	-2.94	117.47	120.36
2	F	801	NAD	C4A-N9A-C8A	2.92	108.81	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	NAD	N3A-C4A-N9A	2.92	132.14	127.17
2	F	801	NAD	C2A-N3A-C4A	2.92	118.95	111.83
2	E	801	NAD	O4B-C1B-N9A	2.91	113.68	108.09
2	A	801	NAD	C4A-C5A-N7A	-2.90	107.26	110.58
2	G	801	NAD	C4B-O4B-C1B	-2.89	103.08	109.47
2	D	801	NAD	C4A-C5A-N7A	-2.85	107.32	110.58
2	E	801	NAD	C5A-N7A-C8A	2.83	107.89	103.45
2	E	801	NAD	C4A-N9A-C8A	2.81	108.69	105.74
2	H	801	NAD	C4D-O4D-C1D	-2.81	107.35	109.92
2	E	801	NAD	O7N-C7N-N7N	-2.80	118.57	122.62
2	H	801	NAD	C4B-O4B-C1B	-2.79	103.31	109.47
2	F	801	NAD	C4D-O4D-C1D	-2.77	107.38	109.92
2	H	801	NAD	C6N-N1N-C2N	-2.76	119.53	121.88
2	C	801	NAD	O4B-C1B-N9A	2.76	113.40	108.09
4	E	802	D3J	C33-C11-N10	-2.72	118.61	122.29
2	F	801	NAD	O4B-C1B-N9A	2.71	113.30	108.09
2	G	801	NAD	O5D-C5D-C4D	2.71	118.22	108.99
2	F	801	NAD	C4B-O4B-C1B	-2.69	103.53	109.47
2	D	801	NAD	C4B-O4B-C1B	-2.69	103.53	109.47
2	B	801	NAD	C4A-N9A-C8A	2.68	108.55	105.74
2	E	801	NAD	C4A-C5A-N7A	-2.66	107.54	110.58
4	A	803	D3J	C33-C11-N10	-2.65	118.70	122.29
2	A	801	NAD	C4D-O4D-C1D	-2.65	107.50	109.92
4	G	803	D3J	C15-C14-N13	2.64	119.11	113.96
4	E	802	D3J	C15-C14-N13	2.64	119.10	113.96
4	A	803	D3J	C15-C14-N13	2.63	119.10	113.96
2	A	801	NAD	C4B-O4B-C1B	-2.63	103.66	109.47
2	D	801	NAD	C3N-C7N-N7N	2.58	120.92	117.74
2	A	801	NAD	C3N-C7N-N7N	2.58	120.92	117.74
4	D	804	D3J	C12-C28-C29	-2.58	122.88	126.64
4	F	803	D3J	C15-C14-N13	2.58	118.98	113.96
4	F	803	D3J	C33-C11-N10	-2.56	118.83	122.29
2	D	801	NAD	C4D-O4D-C1D	-2.56	107.58	109.92
4	B	803	D3J	C12-C28-C29	-2.52	122.96	126.64
2	H	801	NAD	O5D-C5D-C4D	2.52	117.57	108.99
2	E	801	NAD	O5D-C5D-C4D	2.51	117.55	108.99
2	B	801	NAD	O5D-C5D-C4D	2.51	117.55	108.99
2	C	801	NAD	C4D-O4D-C1D	-2.51	107.63	109.92
2	D	801	NAD	O5D-C5D-C4D	2.50	117.49	108.99
2	E	801	NAD	C4B-O4B-C1B	-2.49	103.96	109.47
2	G	801	NAD	O7N-C7N-N7N	-2.47	119.05	122.62
2	B	801	NAD	O7N-C7N-N7N	-2.47	119.05	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	NAD	C4B-O4B-C1B	-2.46	104.03	109.47
2	A	801	NAD	O4B-C1B-N9A	2.45	112.80	108.09
2	H	801	NAD	O4B-C1B-N9A	2.44	112.78	108.09
2	C	801	NAD	C5A-N7A-C8A	2.43	107.27	103.45
4	G	803	D3J	C33-C11-N10	-2.41	119.03	122.29
4	G	803	D3J	C17-S16-C15	2.41	105.87	102.81
4	A	803	D3J	C3-C2-C5	-2.40	119.65	122.80
2	G	801	NAD	O7N-C7N-C3N	2.39	122.52	119.60
2	B	801	NAD	O4B-C1B-N9A	2.38	112.66	108.09
2	F	801	NAD	O5D-C5D-C4D	2.36	117.04	108.99
2	A	801	NAD	O5D-C5D-C4D	2.36	117.02	108.99
4	F	803	D3J	C12-C28-C29	-2.33	123.24	126.64
2	C	801	NAD	O5D-C5D-C4D	2.33	116.92	108.99
2	D	801	NAD	O4B-C1B-N9A	2.33	112.56	108.09
2	G	801	NAD	C6A-C5A-N7A	2.32	136.56	132.09
2	C	801	NAD	C3N-C7N-N7N	2.30	120.57	117.74
2	B	801	NAD	O7N-C7N-C3N	2.28	122.39	119.60
2	B	801	NAD	C4D-O4D-C1D	-2.26	107.86	109.92
4	E	802	D3J	C12-C28-C29	-2.25	123.36	126.64
4	A	803	D3J	C12-C28-C29	-2.24	123.36	126.64
2	H	801	NAD	C6N-C5N-C4N	2.24	122.68	119.45
2	D	801	NAD	O3-PA-O1A	-2.24	103.97	110.70
4	D	804	D3J	C22-C17-C18	2.23	120.46	117.55
4	D	804	D3J	C33-C11-N10	-2.21	119.31	122.29
2	C	801	NAD	C4A-C5A-N7A	-2.20	108.06	110.58
4	D	804	D3J	C15-C14-N13	2.20	118.26	113.96
2	G	801	NAD	C4D-O4D-C1D	-2.20	107.91	109.92
2	G	801	NAD	O3-PA-O1A	-2.20	104.10	110.70
2	H	801	NAD	C4A-C5A-N7A	-2.15	108.13	110.58
2	D	801	NAD	C6N-N1N-C1D	2.13	123.91	119.73
2	E	801	NAD	C6N-N1N-C1D	2.10	123.86	119.73
2	H	801	NAD	C3N-C7N-N7N	2.08	120.30	117.74
2	B	801	NAD	O2N-PN-O3	2.07	112.88	107.27
4	E	802	D3J	O25-C24-C26	2.05	118.98	114.24
2	F	801	NAD	C6N-N1N-C1D	2.03	123.71	119.73
2	B	801	NAD	C6N-N1N-C1D	2.02	123.69	119.73
2	A	801	NAD	C6A-C5A-N7A	2.02	135.98	132.09

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	NAD	O4D-C1D-N1N-C2N
2	A	801	NAD	O4D-C1D-N1N-C6N
2	A	801	NAD	C2D-C1D-N1N-C2N
2	B	801	NAD	O4D-C1D-N1N-C2N
2	B	801	NAD	O4D-C1D-N1N-C6N
2	B	801	NAD	C2D-C1D-N1N-C2N
2	C	801	NAD	O4D-C1D-N1N-C2N
2	C	801	NAD	O4D-C1D-N1N-C6N
2	C	801	NAD	C2D-C1D-N1N-C2N
2	D	801	NAD	O4D-C1D-N1N-C2N
2	D	801	NAD	O4D-C1D-N1N-C6N
2	D	801	NAD	C2D-C1D-N1N-C2N
2	E	801	NAD	O4D-C1D-N1N-C2N
2	E	801	NAD	O4D-C1D-N1N-C6N
2	E	801	NAD	C2D-C1D-N1N-C2N
2	F	801	NAD	O4D-C1D-N1N-C2N
2	F	801	NAD	O4D-C1D-N1N-C6N
2	F	801	NAD	C2D-C1D-N1N-C2N
2	G	801	NAD	O4D-C1D-N1N-C2N
2	G	801	NAD	O4D-C1D-N1N-C6N
2	G	801	NAD	C2D-C1D-N1N-C2N
2	H	801	NAD	O4D-C1D-N1N-C2N
2	H	801	NAD	O4D-C1D-N1N-C6N
2	H	801	NAD	C2D-C1D-N1N-C2N
5	C	803	LAC	O-C-CA-CB
5	C	803	LAC	O-C-CA-OHN
5	C	803	LAC	OXT-C-CA-CB
5	C	803	LAC	OXT-C-CA-OHN
4	A	803	D3J	C35-C9-O8-C7
4	F	803	D3J	C35-C9-O8-C7
4	A	803	D3J	N10-C9-O8-C7
4	F	803	D3J	N10-C9-O8-C7
2	A	801	NAD	C2D-C1D-N1N-C6N
2	B	801	NAD	C2D-C1D-N1N-C6N
2	C	801	NAD	C2D-C1D-N1N-C6N
2	D	801	NAD	C2D-C1D-N1N-C6N
2	E	801	NAD	C2D-C1D-N1N-C6N
2	F	801	NAD	C2D-C1D-N1N-C6N
2	H	801	NAD	C2D-C1D-N1N-C6N
4	E	802	D3J	C35-C9-O8-C7
4	F	803	D3J	C24-C15-S16-C17
2	E	801	NAD	O4B-C4B-C5B-O5B
2	B	801	NAD	O4B-C4B-C5B-O5B

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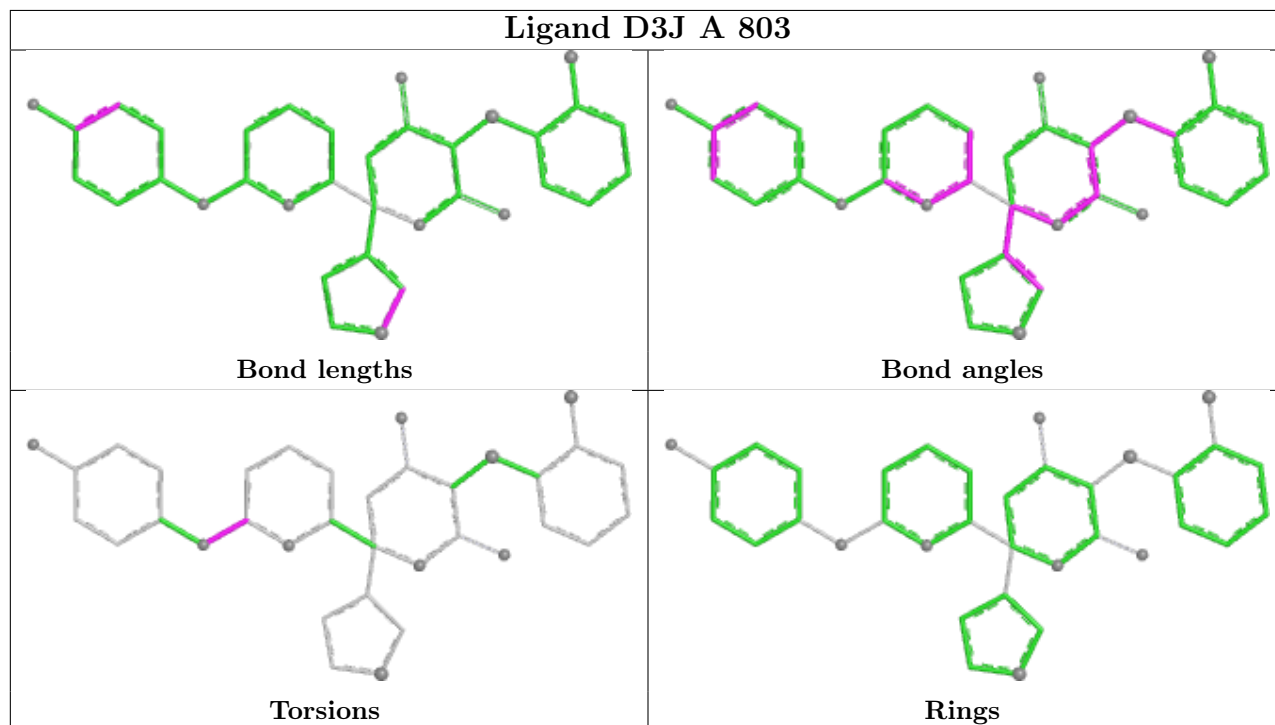
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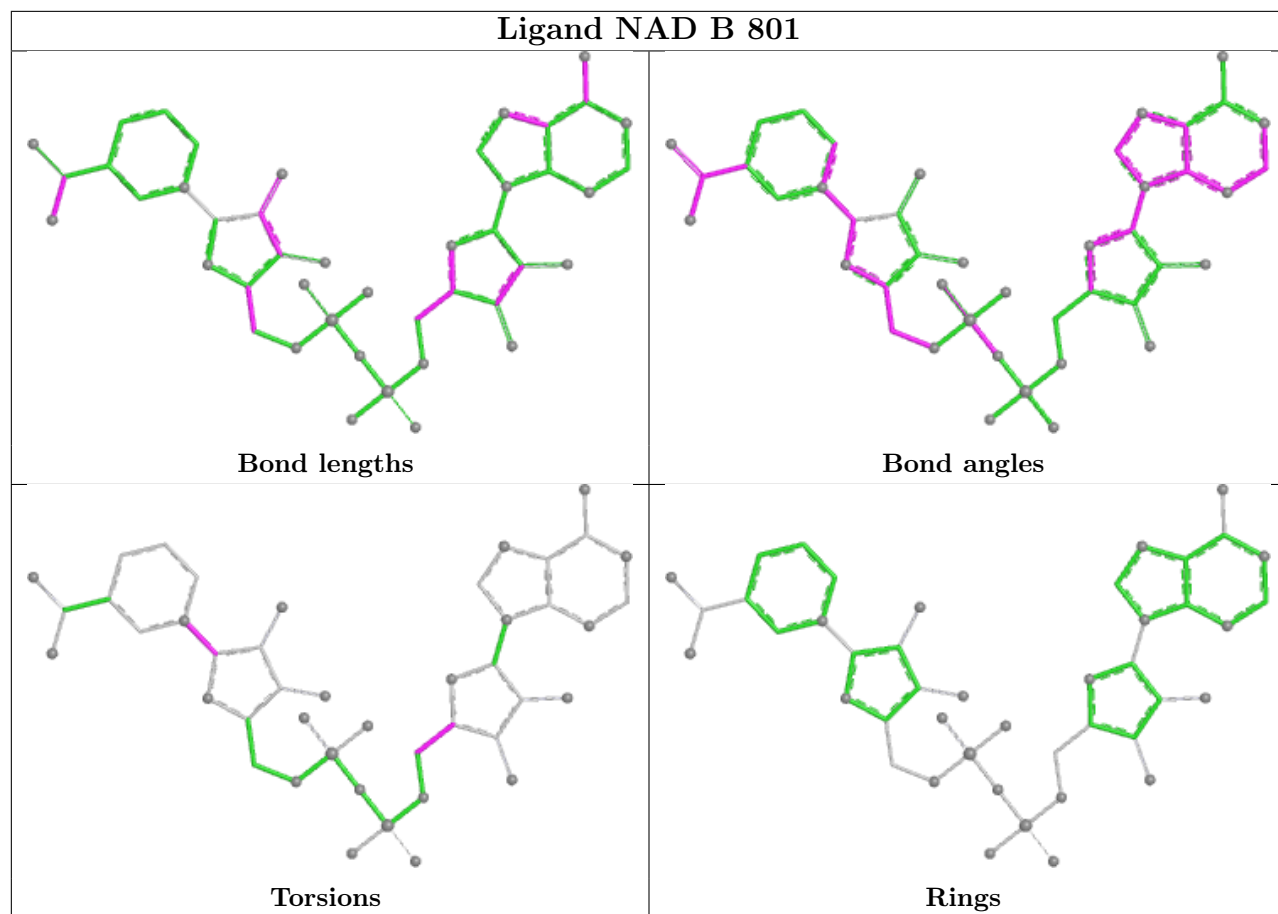
Mol	Chain	Res	Type	Atoms
4	E	802	D3J	N10-C9-O8-C7
2	A	801	NAD	C2B-C1B-N9A-C8A
2	G	801	NAD	O4B-C4B-C5B-O5B

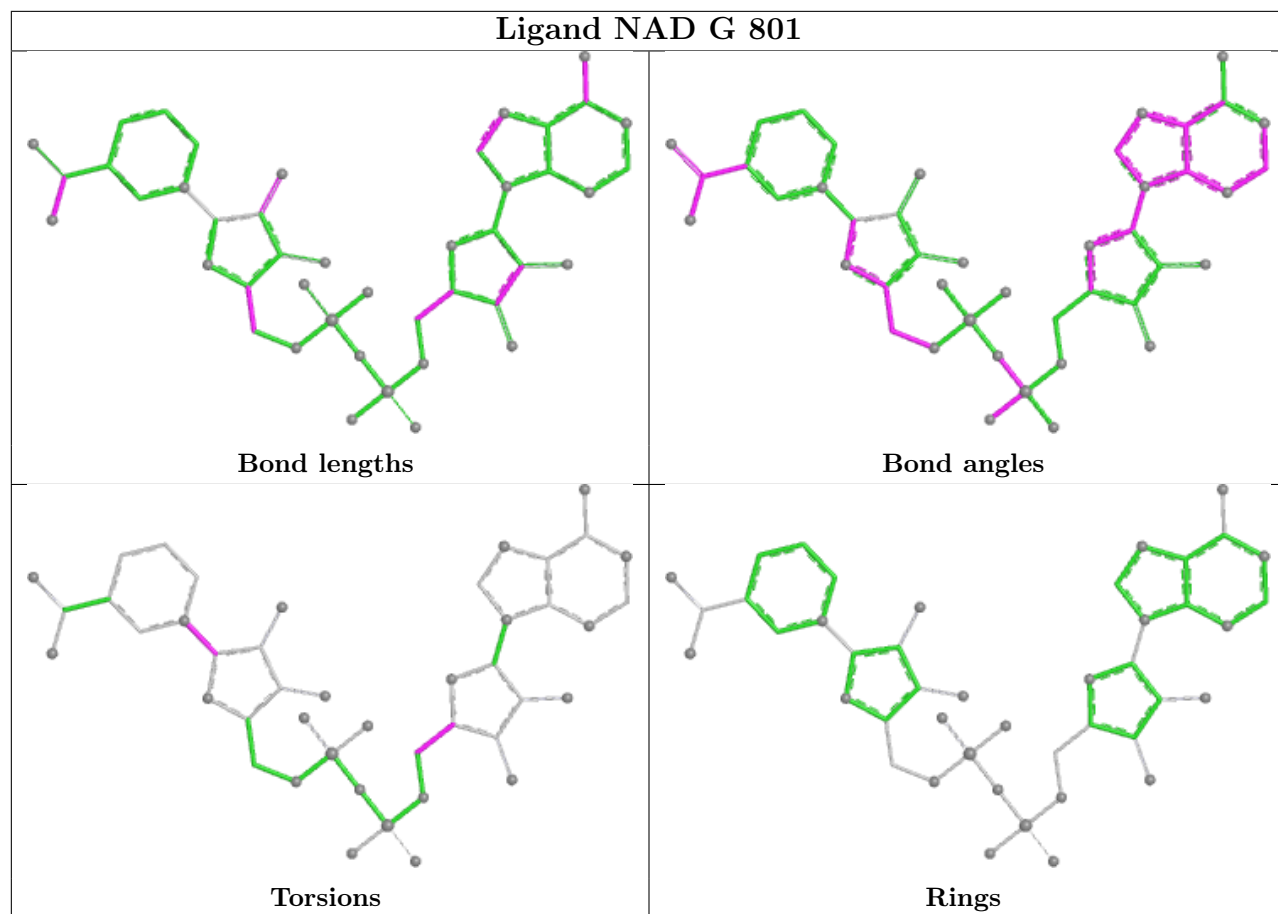
There are no ring outliers.

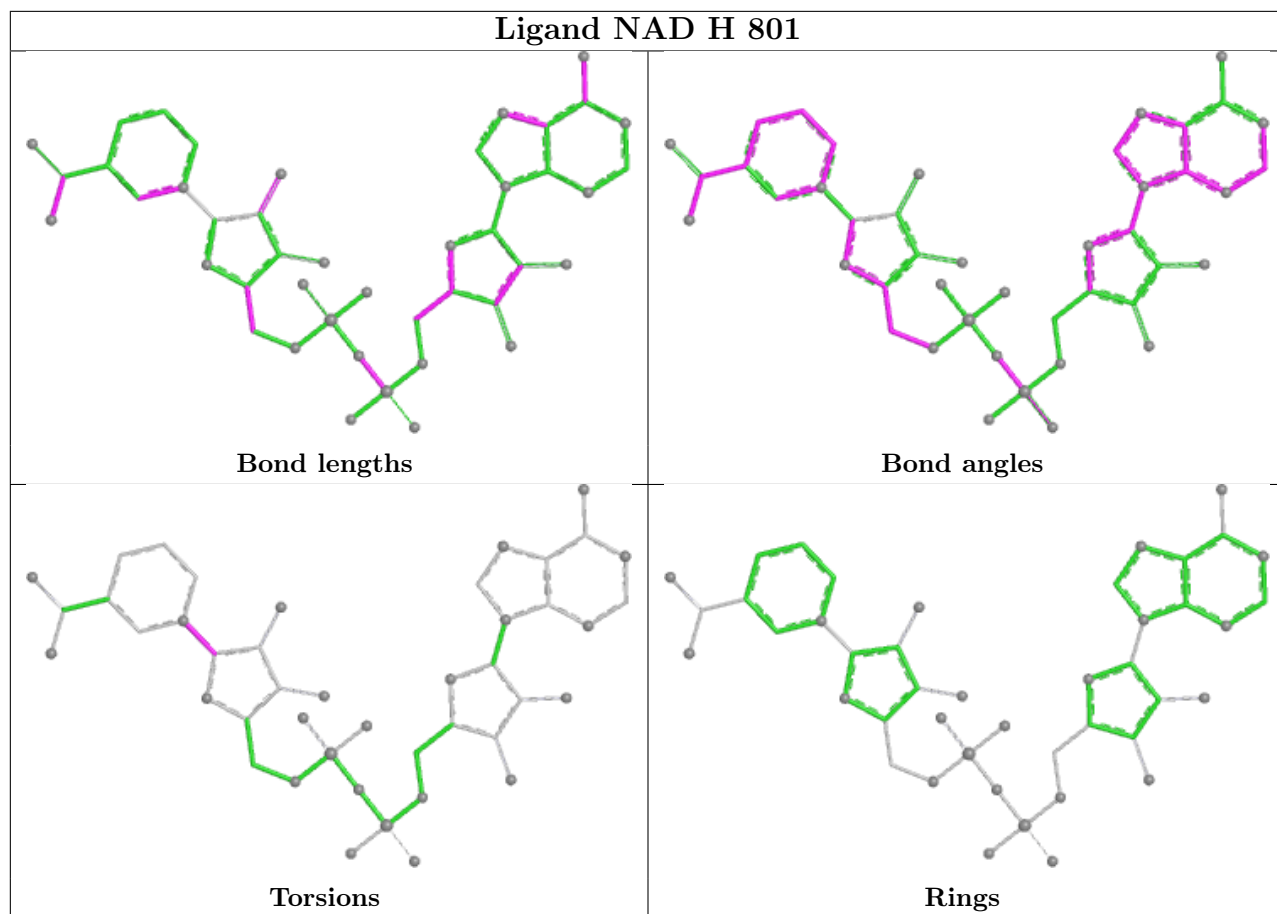
No monomer is involved in short contacts.

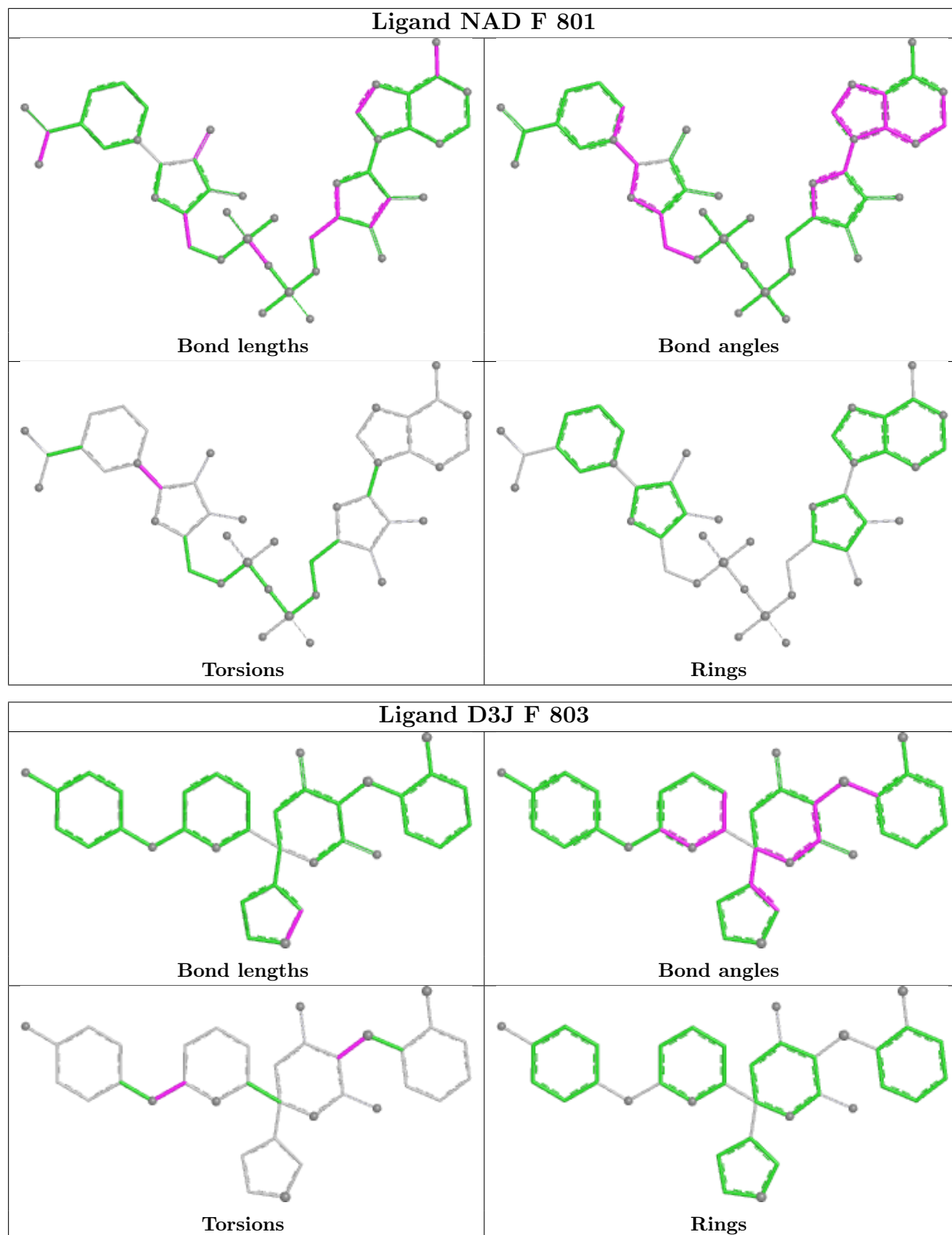
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

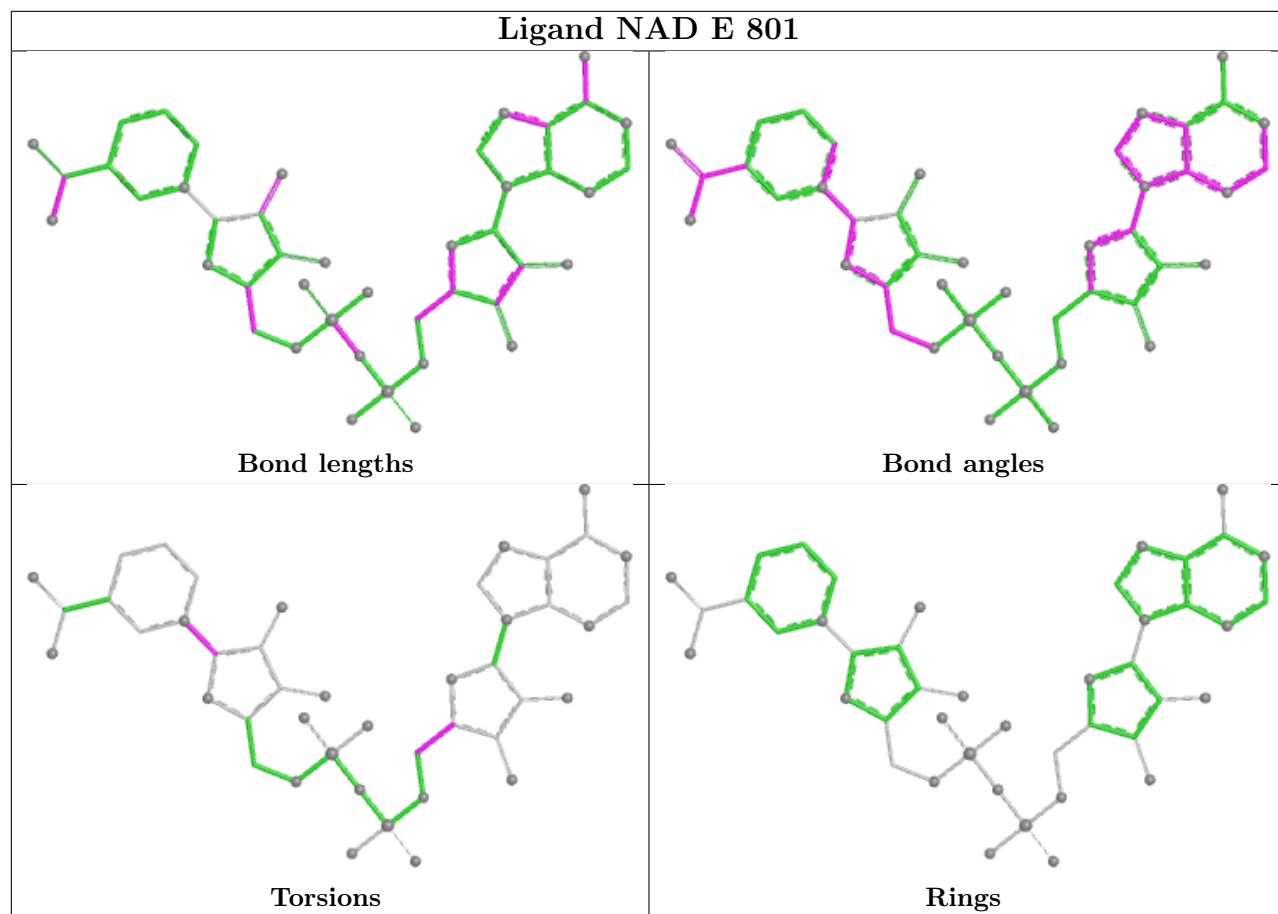


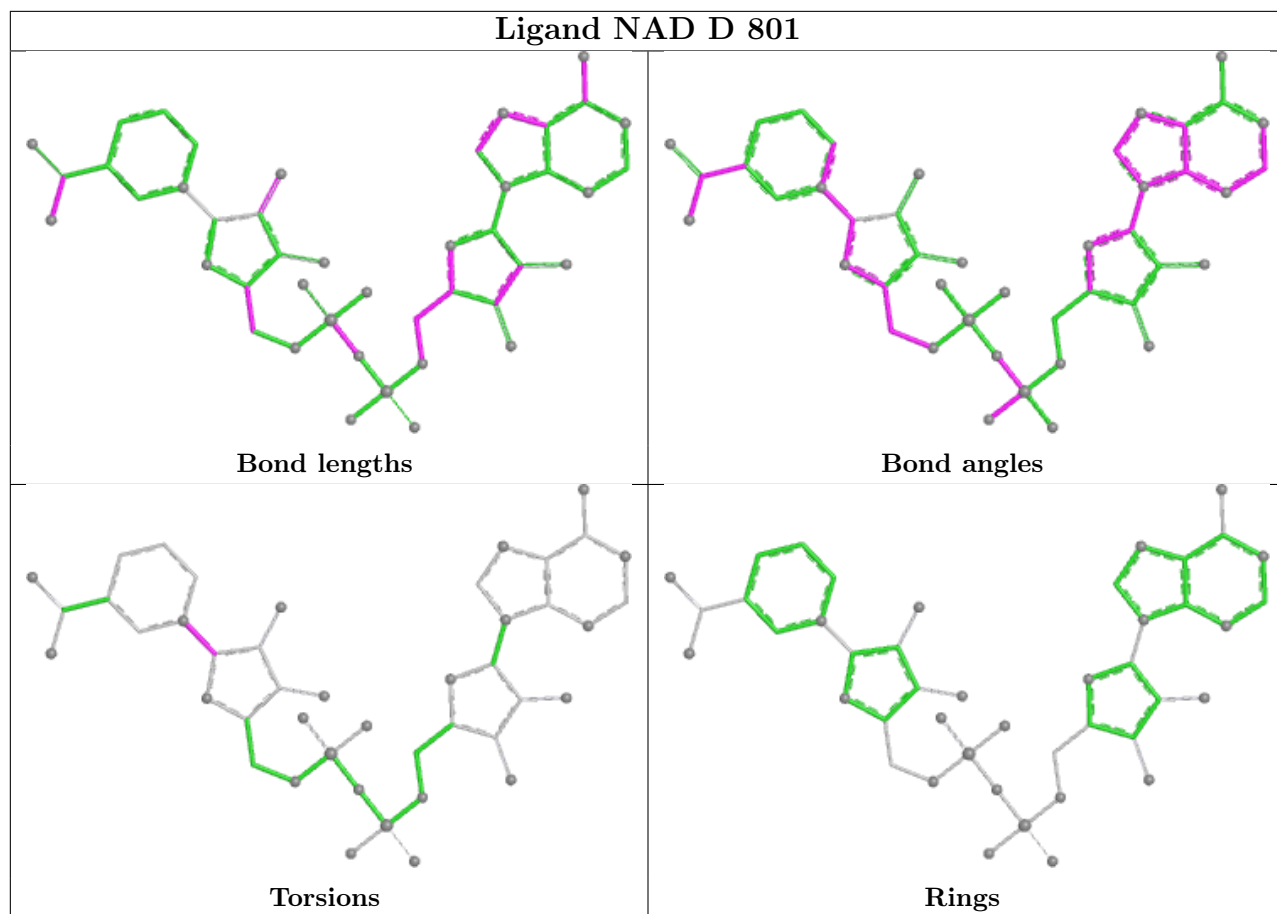


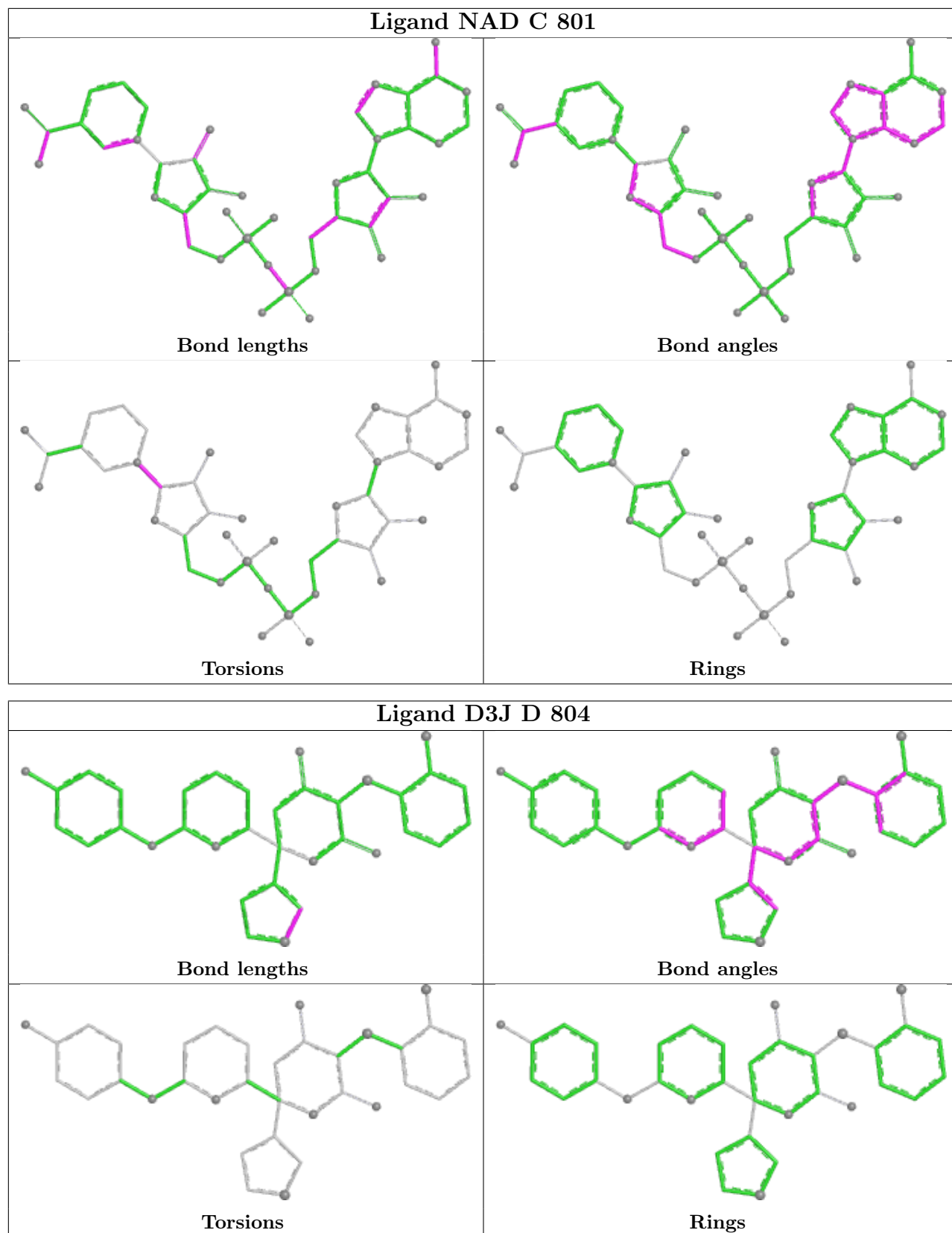


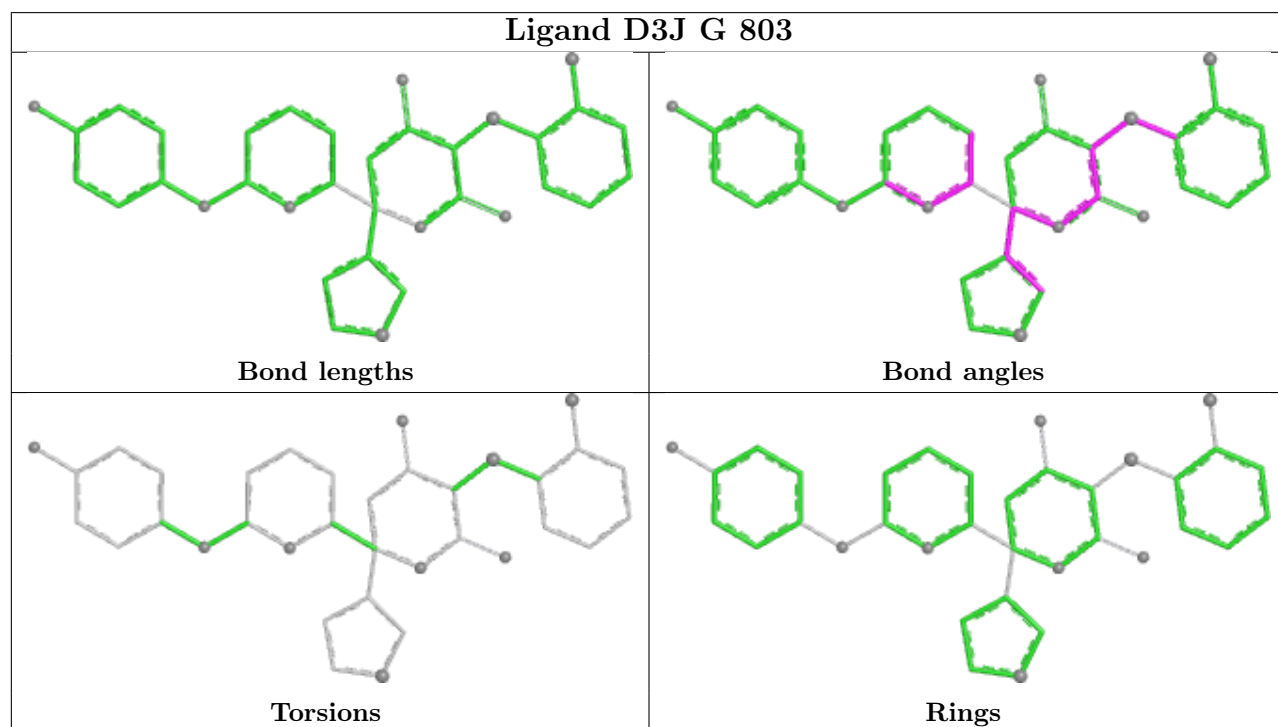
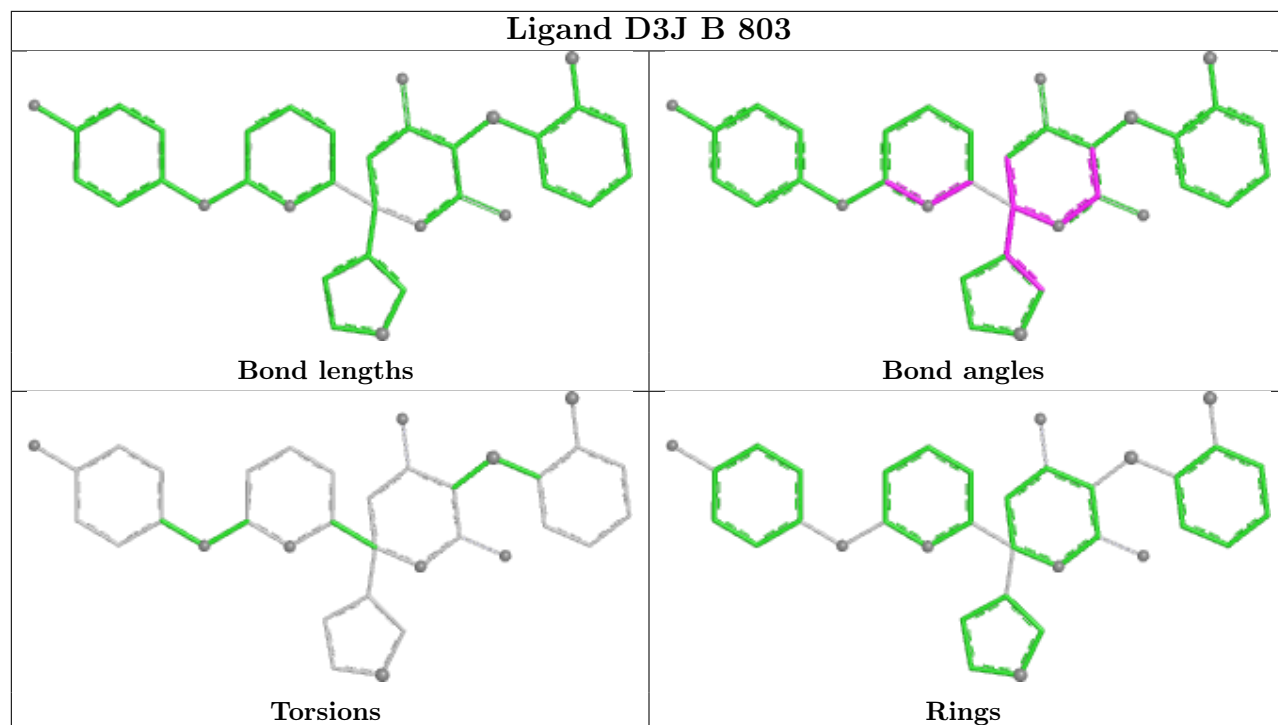


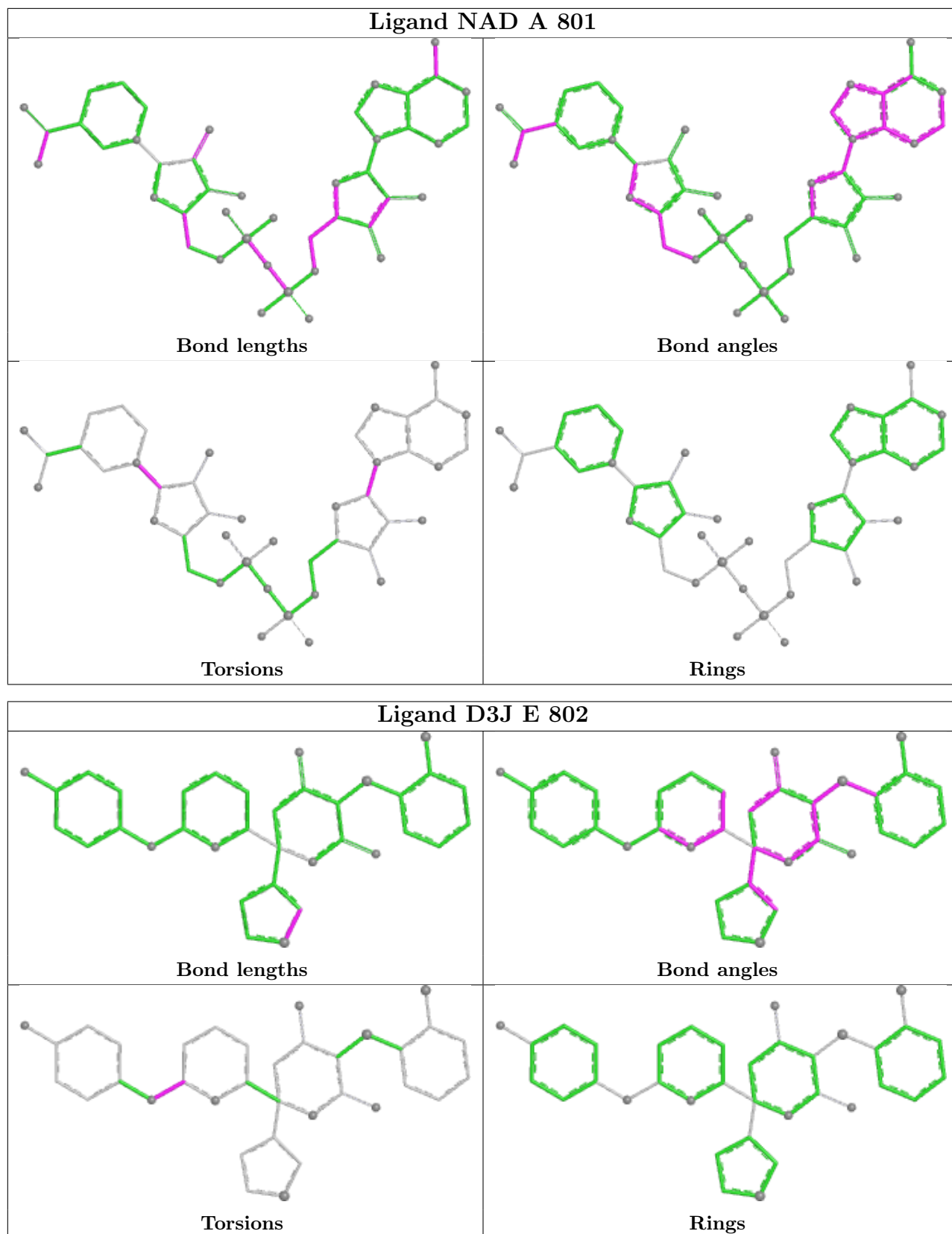












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	323/331 (97%)	0.24	13 (4%) 42 44	17, 32, 62, 84	5 (1%)
1	B	322/331 (97%)	0.29	16 (4%) 34 35	19, 34, 68, 97	6 (1%)
1	C	328/331 (99%)	0.23	3 (0%) 81 82	21, 36, 64, 106	1 (0%)
1	D	329/331 (99%)	0.12	4 (1%) 76 77	19, 34, 62, 82	3 (0%)
1	E	310/331 (93%)	0.50	17 (5%) 30 32	25, 41, 69, 142	0
1	F	314/331 (94%)	0.65	22 (7%) 22 24	25, 40, 72, 102	3 (0%)
1	G	322/331 (97%)	0.49	19 (5%) 28 30	21, 40, 84, 109	2 (0%)
1	H	329/331 (99%)	0.24	8 (2%) 59 62	24, 35, 65, 87	2 (0%)
All	All	2577/2648 (97%)	0.34	102 (3%) 42 44	17, 36, 69, 142	22 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	16	GLN	12.2
1	A	13	LYS	11.6
1	D	13	LYS	10.3
1	A	14	GLU	9.9
1	B	12	LEU	9.0
1	B	17	THR	8.4
1	A	16	GLN	8.1
1	D	14	GLU	7.0
1	F	15	GLU	6.9
1	H	13	LYS	6.4
1	A	12	LEU	6.4
1	H	16	GLN	6.2
1	D	231	LYS	6.1
1	B	15	GLU	6.1
1	A	15	GLU	5.7
1	B	16	GLN	5.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	16	GLN	5.3
1	B	14	GLU	5.1
1	G	12	LEU	5.0
1	B	13	LYS	4.6
1	F	13	LYS	4.4
1	B	226	TRP	4.0
1	B	97	ALA	3.9
1	E	1	ALA	3.5
1	E	210	LEU	3.3
1	F	14	GLU	3.3
1	E	216	ASP	3.3
1	F	217	LEU	3.1
1	A	97	ALA	3.0
1	H	331	PHE	3.0
1	G	236	SER	3.0
1	G	218	GLY	3.0
1	G	1	ALA	2.9
1	F	17	THR	2.9
1	E	203	MET	2.9
1	G	213	LEU	2.9
1	G	331	PHE	2.9
1	F	141	ILE	2.8
1	E	200	TRP	2.8
1	A	279	LEU	2.7
1	E	213	LEU	2.7
1	B	217	LEU	2.7
1	F	108	LEU	2.7
1	F	107	ASN	2.7
1	F	3	LEU	2.7
1	C	13	LYS	2.6
1	B	107	ASN	2.6
1	F	95	ALA	2.6
1	E	233	VAL	2.6
1	E	12	LEU	2.6
1	A	1	ALA	2.6
1	G	17	THR	2.6
1	G	276	ILE	2.6
1	E	227	LYS	2.5
1	F	220	ASP	2.5
1	G	102	GLY	2.5
1	A	124	VAL	2.4
1	F	227	LYS	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	200	TRP	2.4
1	B	215	PRO	2.4
1	H	283	LYS	2.4
1	G	226	TRP	2.4
1	A	107	ASN	2.3
1	E	9	TYR	2.3
1	B	221	LYS	2.3
1	F	203	MET	2.3
1	B	214	HIS	2.3
1	C	331	PHE	2.3
1	G	100	GLN	2.3
1	A	108	LEU	2.3
1	F	302	LEU	2.3
1	B	56	LYS	2.3
1	B	203	MET	2.3
1	E	11	LEU	2.3
1	F	9	TYR	2.3
1	H	8	ILE	2.3
1	A	110	GLN	2.2
1	H	118	PHE	2.2
1	F	226	TRP	2.2
1	E	331	PHE	2.2
1	H	169	PHE	2.2
1	B	220	ASP	2.2
1	E	105	ARG	2.2
1	E	315	LEU	2.2
1	G	315	LEU	2.2
1	F	205	VAL	2.2
1	G	187	TRP	2.1
1	G	203	MET	2.1
1	H	18	PRO	2.1
1	E	324	GLY	2.1
1	F	276	ILE	2.1
1	F	200	TRP	2.1
1	F	160	SER	2.1
1	G	306	THR	2.1
1	G	307	LEU	2.1
1	A	331	PHE	2.1
1	D	106	LEU	2.0
1	F	199	VAL	2.0
1	F	286	VAL	2.0
1	E	118	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	302	LEU	2.0
1	E	215	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

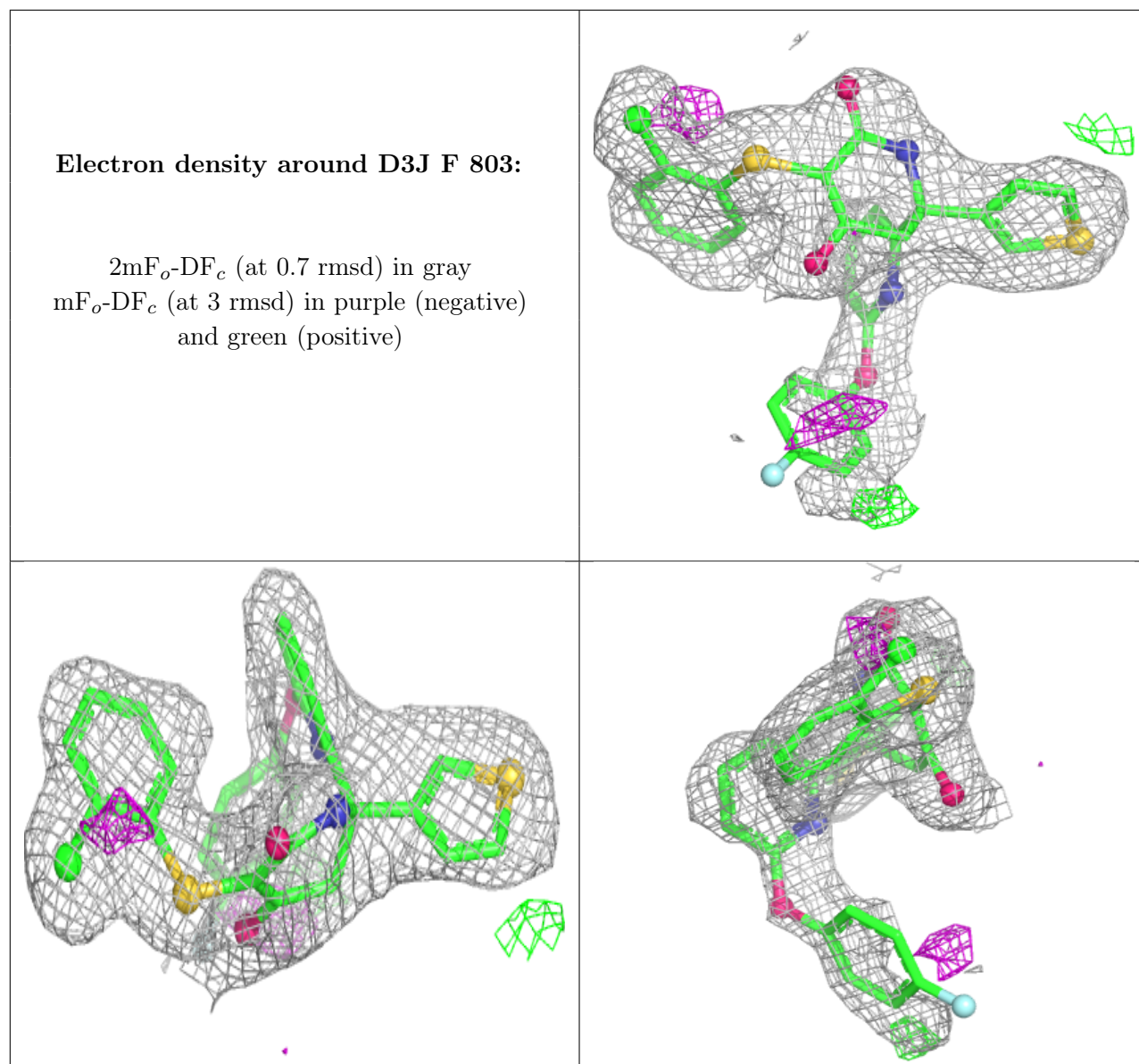
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	G	802	5/5	0.69	0.21	50,51,52,52	5
3	SO4	D	803	5/5	0.76	0.14	90,90,91,92	0
3	SO4	C	802	5/5	0.81	0.11	100,100,100,100	0
4	D3J	F	803	35/35	0.87	0.13	37,53,83,86	0
3	SO4	A	802	5/5	0.88	0.13	55,55,58,59	0
2	NAD	F	801	44/44	0.89	0.10	41,46,51,54	0
3	SO4	D	802	5/5	0.90	0.14	32,36,37,39	5
3	SO4	B	802	5/5	0.91	0.17	71,71,72,73	0
4	D3J	E	802	35/35	0.91	0.10	40,52,71,72	0
3	SO4	F	802	5/5	0.91	0.13	33,33,35,38	5
2	NAD	E	801	44/44	0.93	0.09	31,41,46,48	0
4	D3J	A	803	35/35	0.93	0.10	29,36,58,61	0
4	D3J	G	803	35/35	0.93	0.09	40,49,63,63	0
5	LAC	C	803	6/6	0.93	0.08	36,39,39,40	0
2	NAD	B	801	44/44	0.94	0.08	32,37,42,49	0
4	D3J	B	803	35/35	0.94	0.08	31,41,54,55	0
4	D3J	D	804	35/35	0.95	0.08	33,39,55,63	0
2	NAD	A	801	44/44	0.95	0.07	27,32,37,41	0
3	SO4	H	802	5/5	0.95	0.11	46,47,48,50	0
2	NAD	C	801	44/44	0.95	0.07	20,28,32,34	0
2	NAD	H	801	44/44	0.95	0.07	27,32,36,38	0

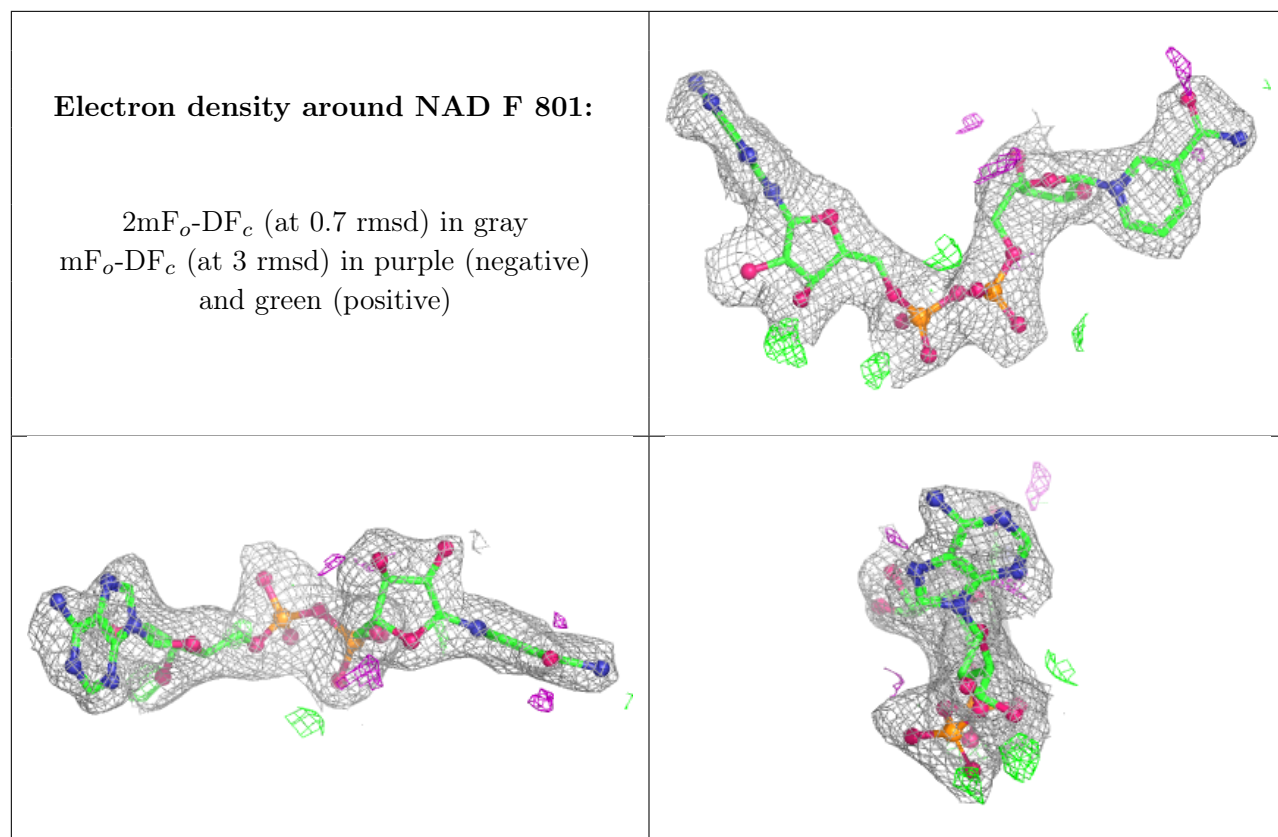
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAD	D	801	44/44	0.96	0.06	27,34,39,40	0
2	NAD	G	801	44/44	0.96	0.07	26,30,44,45	0

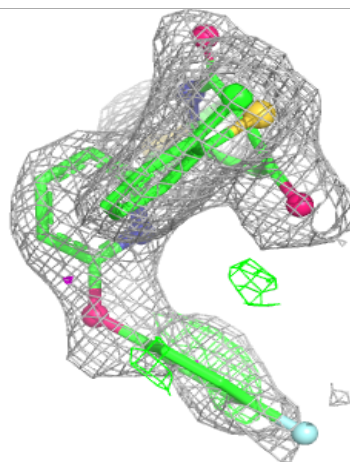
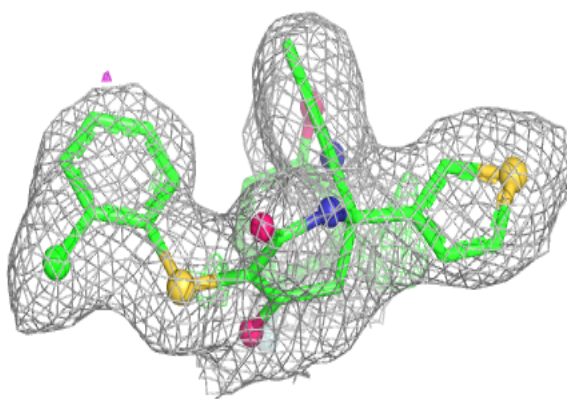
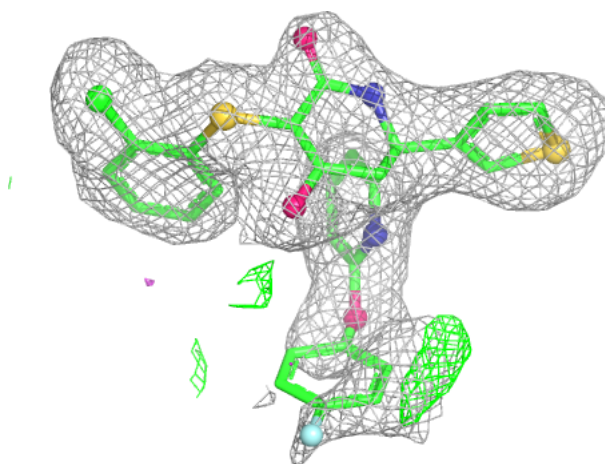
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





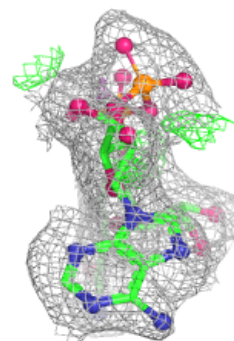
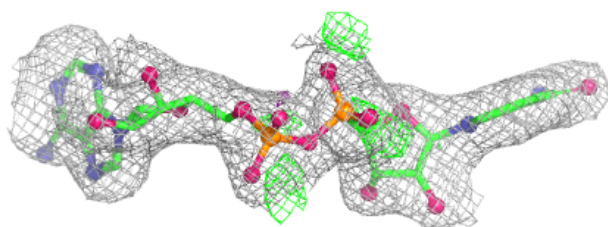
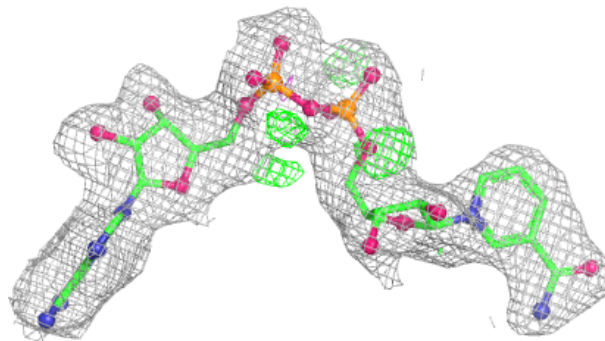
**Electron density around D3J E 802:**

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



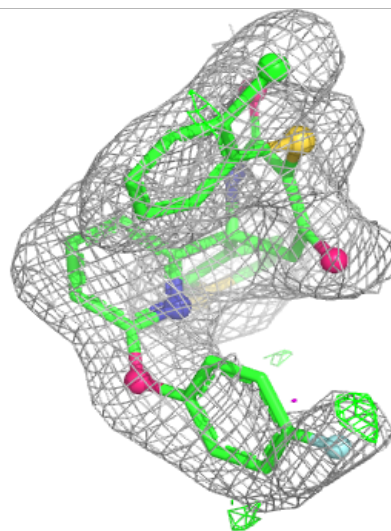
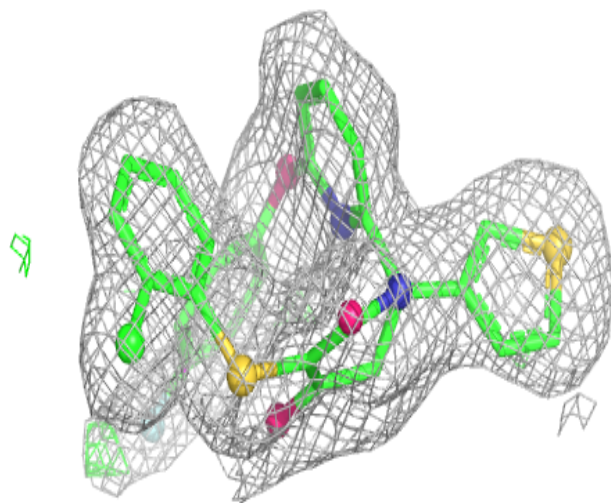
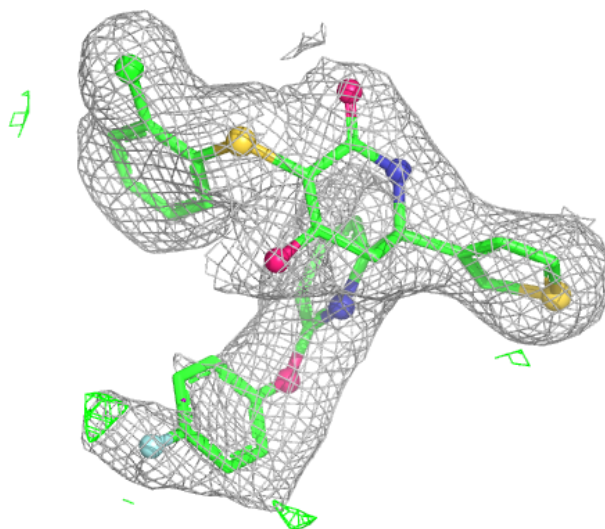
**Electron density around NAD E 801:**

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



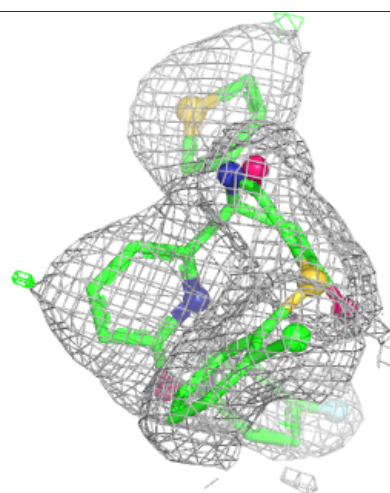
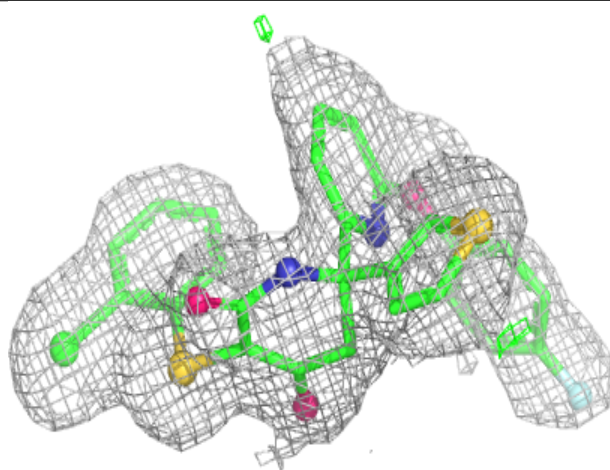
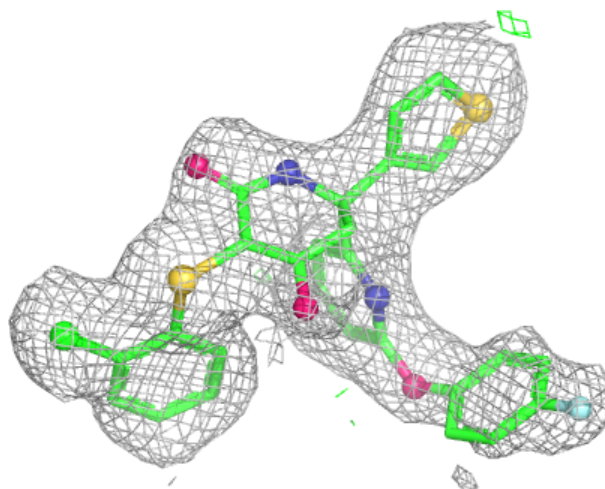
**Electron density around D3J A 803:**

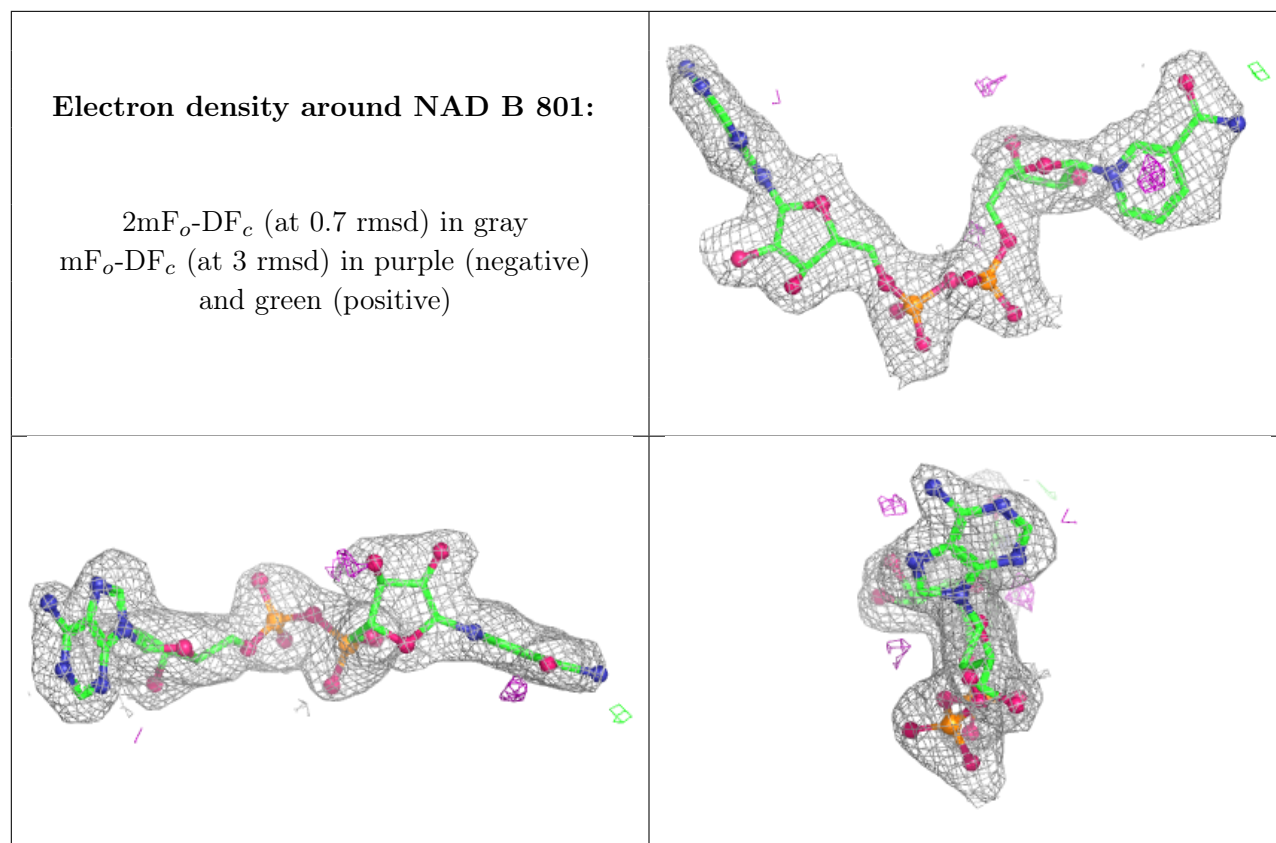
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around D3J G 803:**

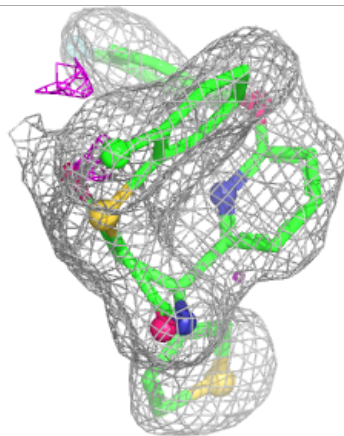
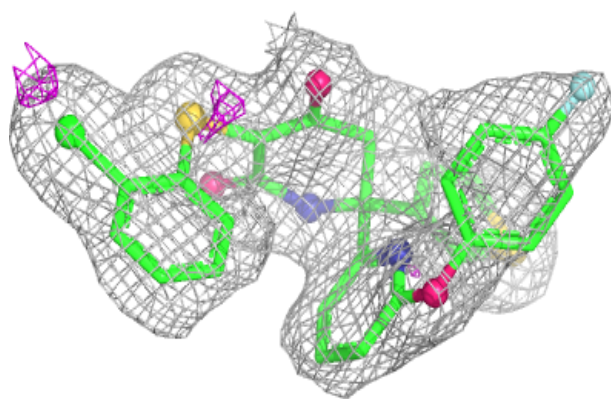
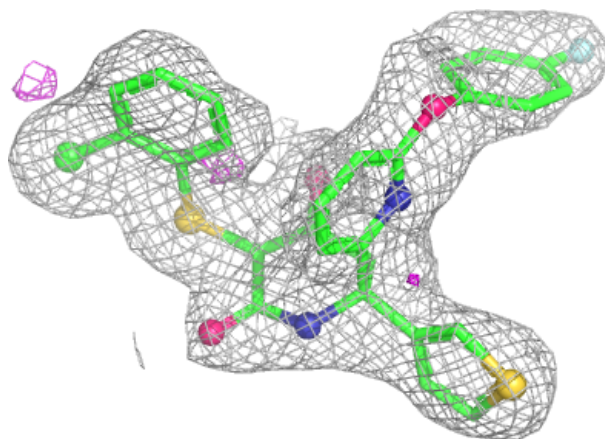
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





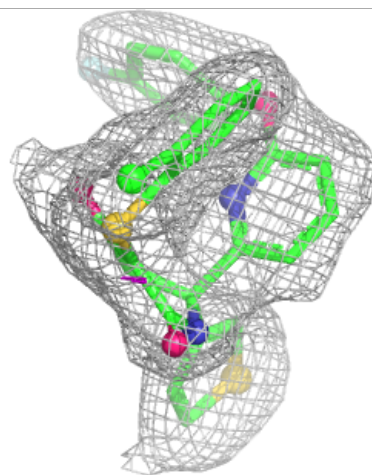
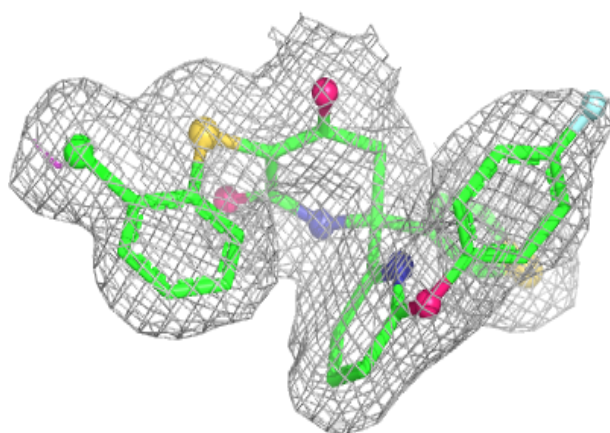
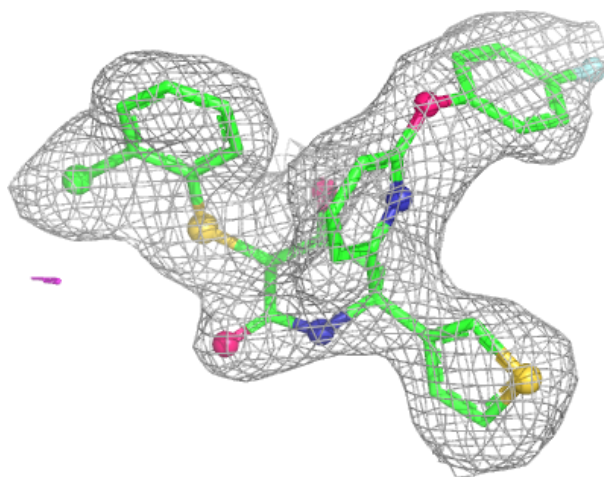
**Electron density around D3J B 803:**

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



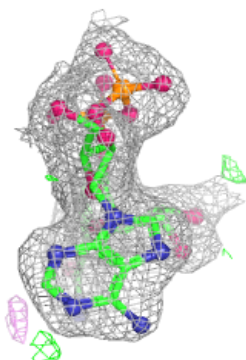
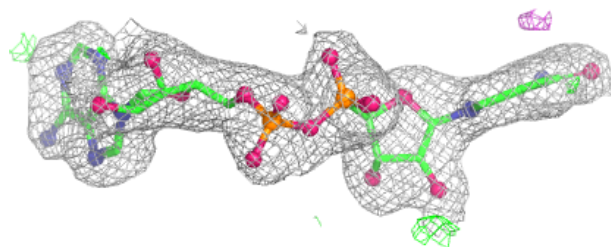
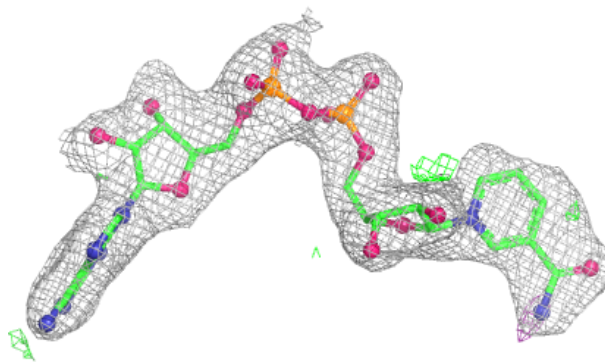
**Electron density around D3J D 804:**

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and green (positive)

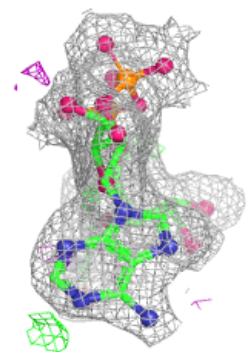
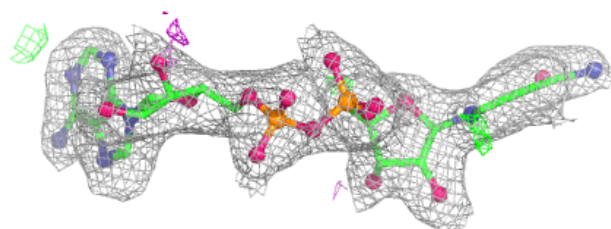
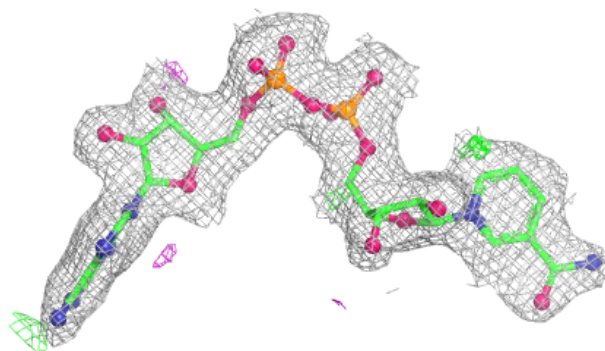


**Electron density around NAD A 801:**

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

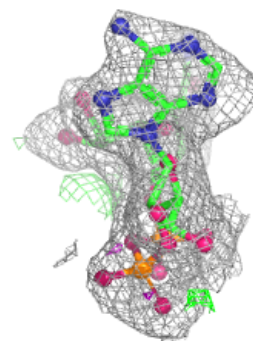
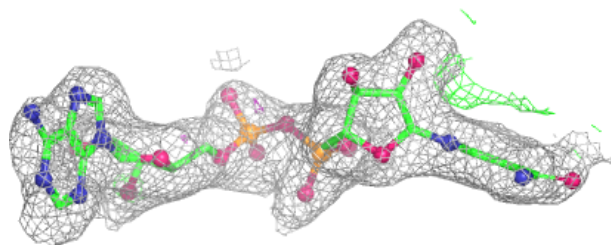
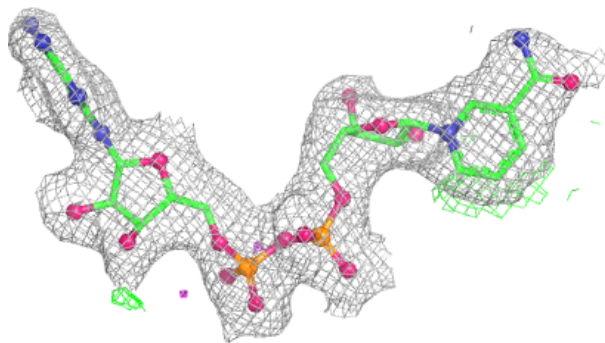
**Electron density around NAD C 801:**

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

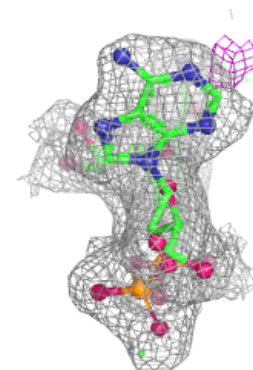
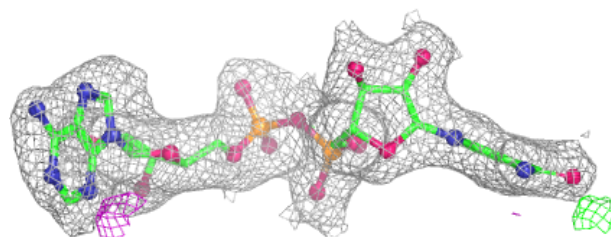
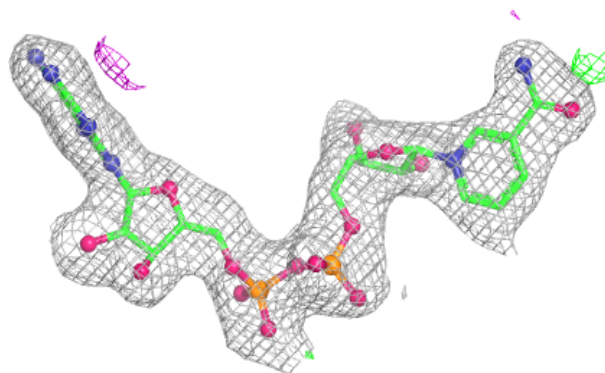


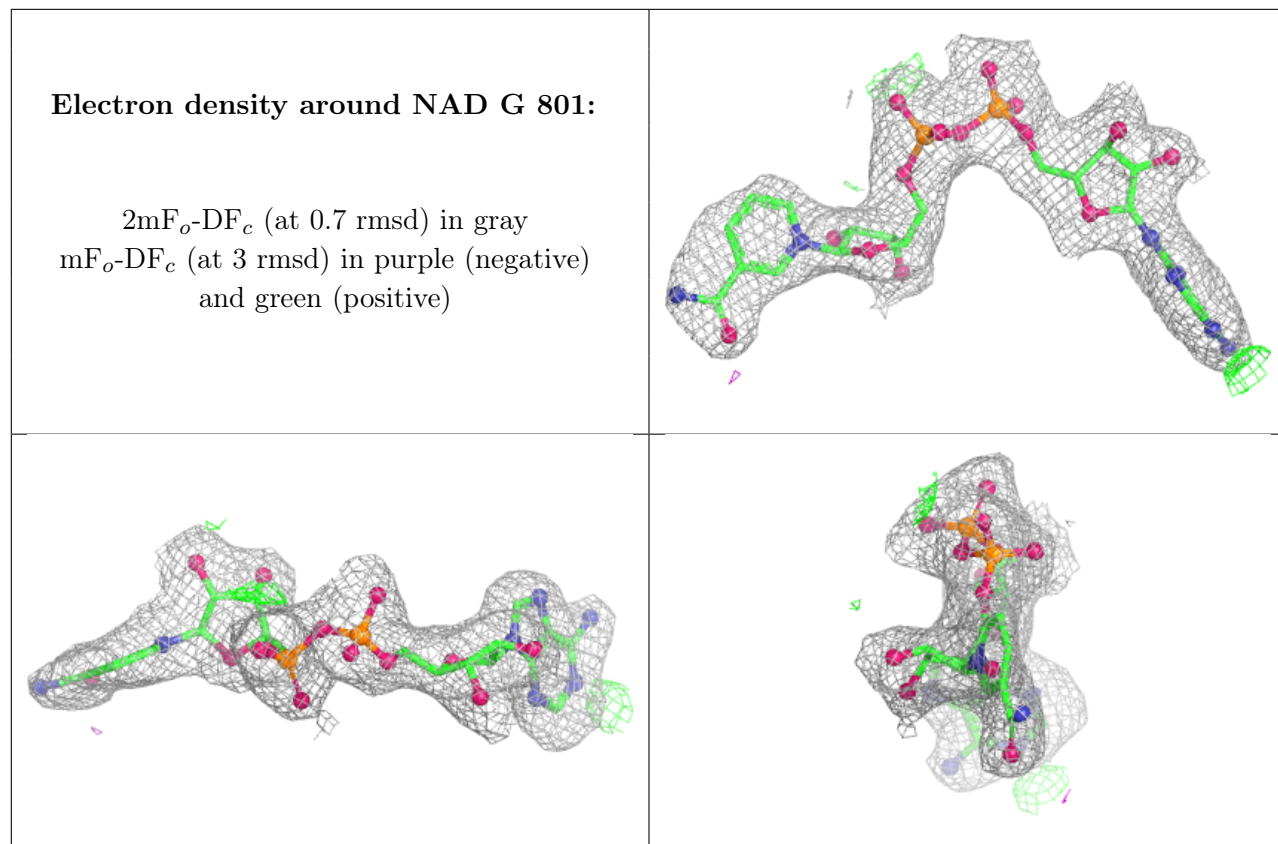
**Electron density around NAD H 801:**

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

**Electron density around NAD D 801:**

$2mF_o-DF_c$  (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.