Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 04:07 PM EST

PDB ID	:	6BB1
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'-bipyridi n]-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*
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:

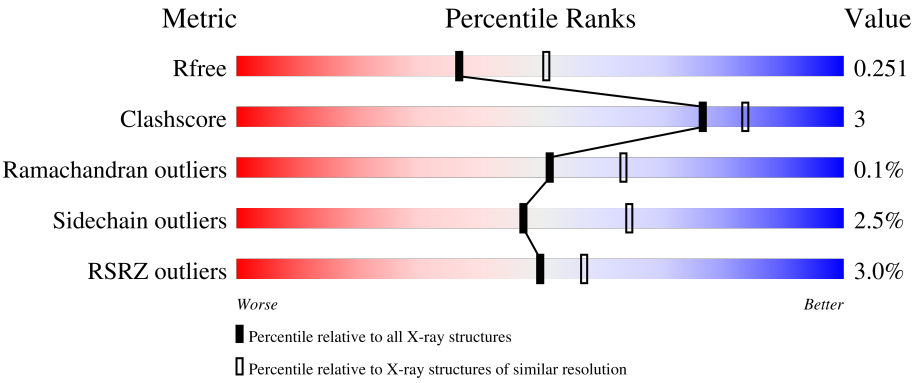
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 >=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 <=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	2% 88% 9% •
1	B	331	5% 89% 8% •
1	C	331	% 89% 10% ••
1	D	331	2% 91% 8% •

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Mol	Chain	Length	Quality of chain
1	E	331	3% 82% 11% 6%
1	F	331	3% 87% 8% 5%
1	G	331	4% 87% 10%
1	H	331	2% 87% 11%

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
5	LAC	C	803	-	X	-	-

2 Entry composition (i)

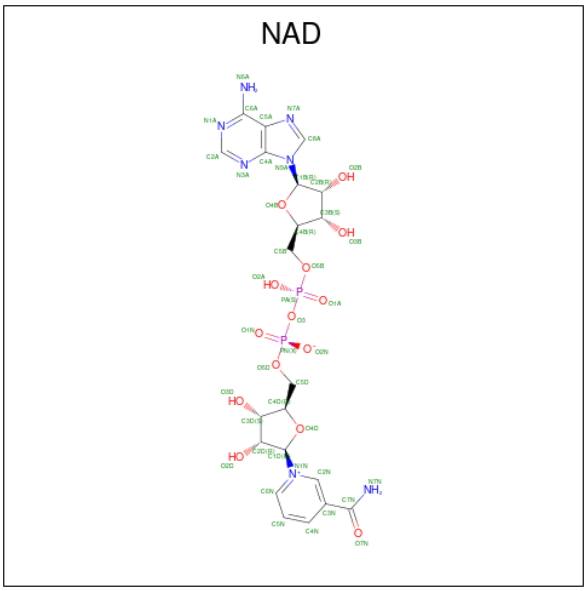
There are 6 unique types of molecules in this entry. The entry contains 21329 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

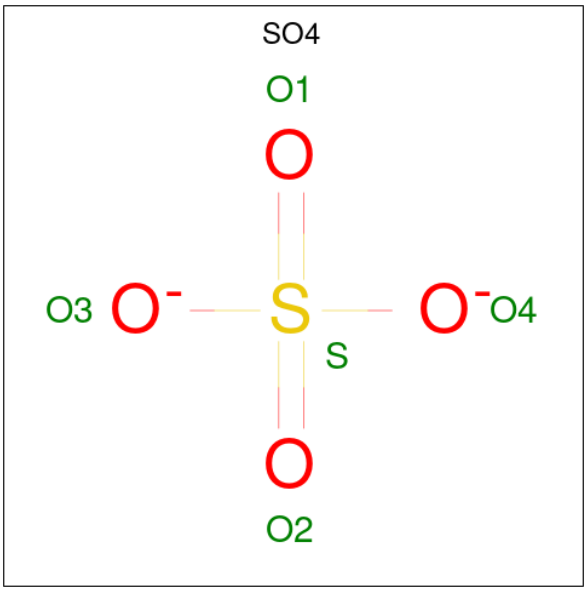
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2503	1602	426	462	13			
1	B	322	Total	C	N	O	S	0	0	0
			2492	1596	422	461	13			
1	C	328	Total	C	N	O	S	0	0	0
			2545	1626	436	470	13			
1	D	329	Total	C	N	O	S	0	0	0
			2550	1629	436	472	13			
1	E	310	Total	C	N	O	S	0	0	0
	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

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



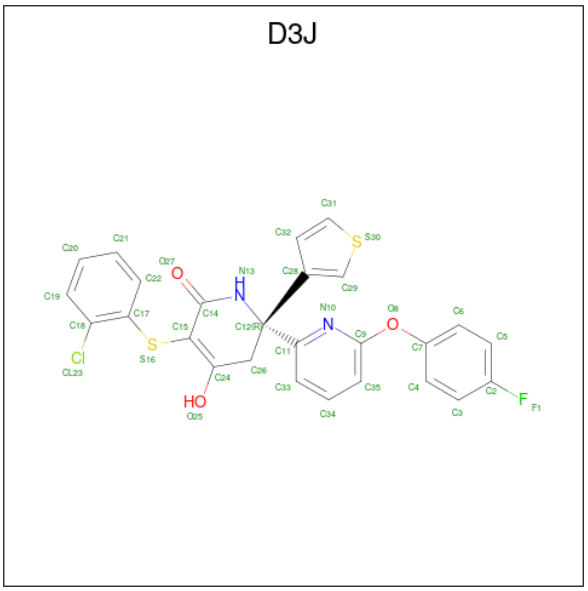
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



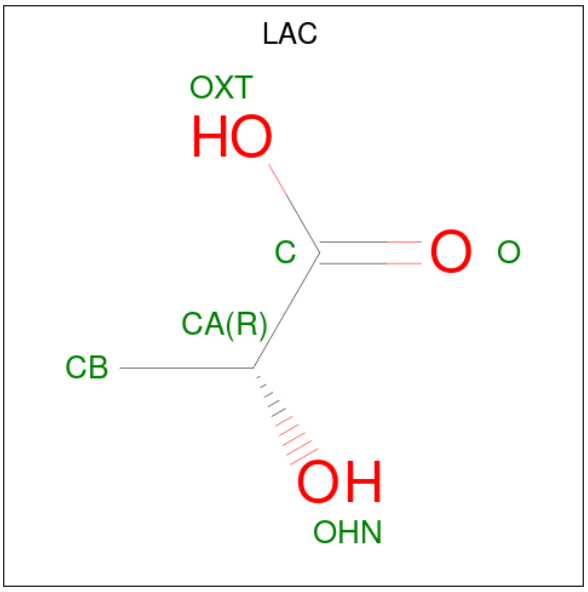
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0

- 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 (three-letter code: D3J) (formula: $C_{26}H_{18}ClFN_2O_3S_2$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	A	1	Total	C	Cl	F	N	O	S	0	0
			35	26	1	1	2	3	2		
4	B	1	Total	C	Cl	F	N	O	S	0	0
			35	26	1	1	2	3	2		
4	D	1	Total	C	Cl	F	N	O	S	0	0
			35	26	1	1	2	3	2		
4	E	1	Total	C	Cl	F	N	O	S	0	0
			35	26	1	1	2	3	2		
4	F	1	Total	C	Cl	F	N	O	S	0	0
			35	26	1	1	2	3	2		
4	G	1	Total	C	Cl	F	N	O	S	0	0
			35	26	1	1	2	3	2		

- Molecule 5 is LACTIC ACID (three-letter code: LAC) (formula: $C_3H_6O_3$).



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

- Molecule 6 is water.

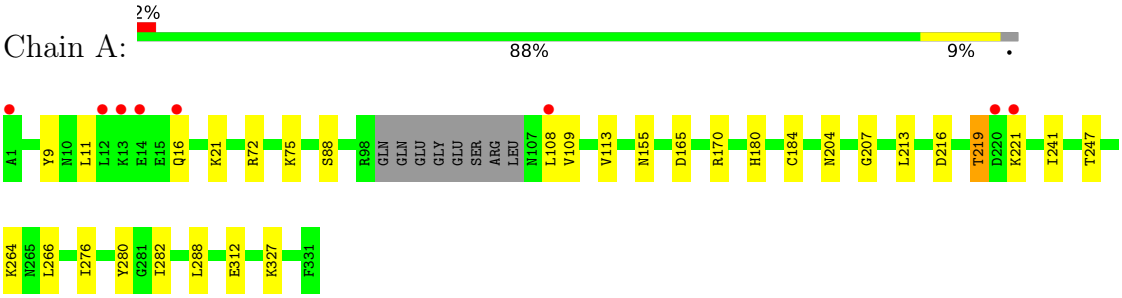
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	111	Total O 111 111	0	0
6	B	104	Total O 104 104	0	0
6	C	115	Total O 115 115	0	0
6	D	99	Total O 99 99	0	0
6	E	67	Total O 67 67	0	0
6	F	83	Total O 83 83	0	0
6	G	74	Total O 74 74	0	0
6	H	118	Total O 118 118	0	0

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.

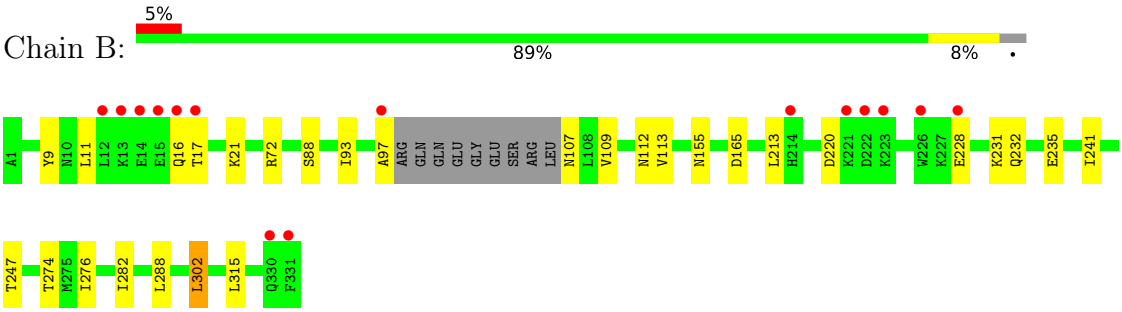
• Molecule 1: L-lactate dehydrogenase A chain

Chain A:



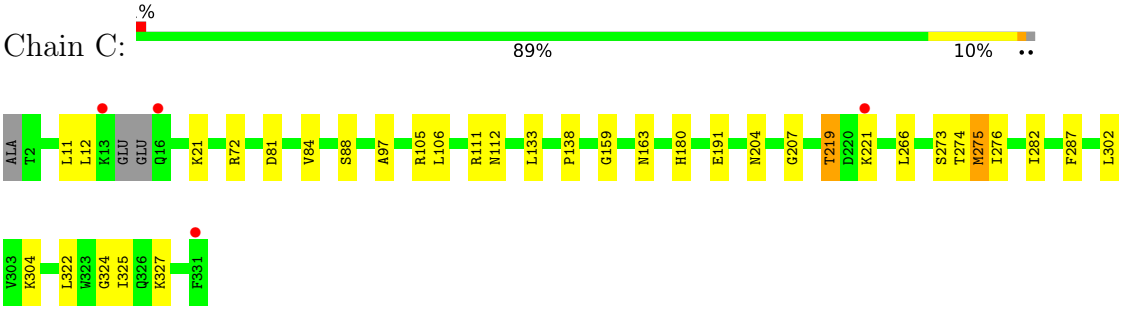
• Molecule 1: L-lactate dehydrogenase A chain

Chain B:



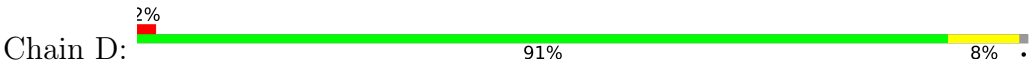
• Molecule 1: L-lactate dehydrogenase A chain

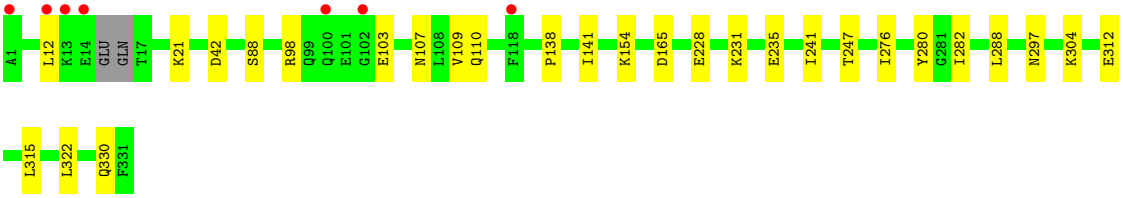
Chain C:



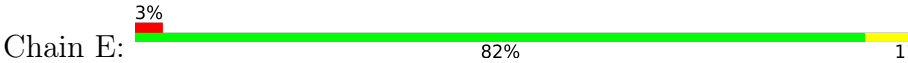
• Molecule 1: L-lactate dehydrogenase A chain

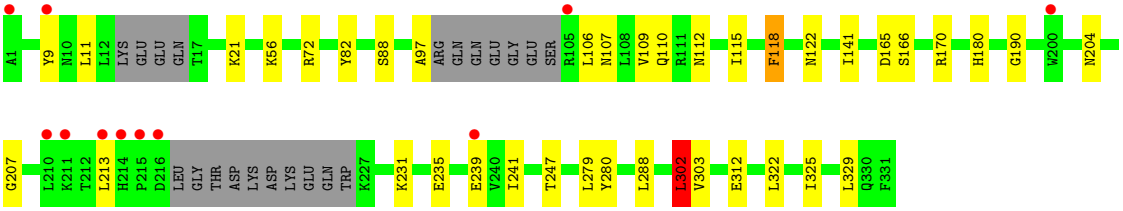
Chain D:



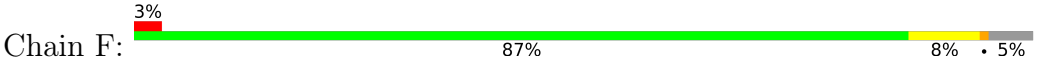


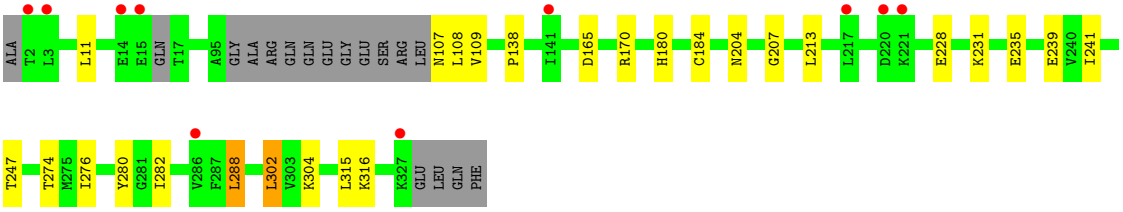
• Molecule 1: L-lactate dehydrogenase A chain



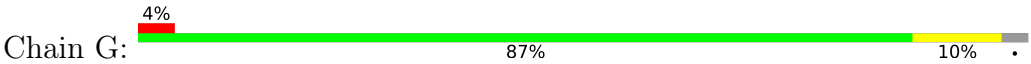


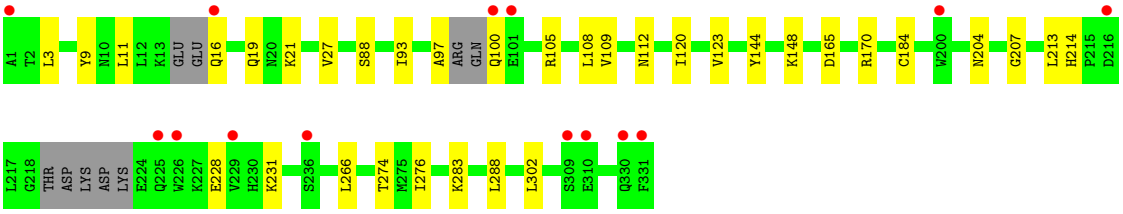
• Molecule 1: L-lactate dehydrogenase A chain



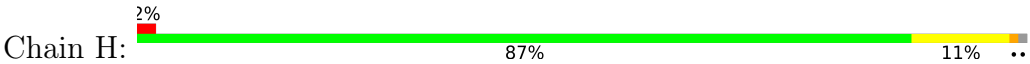


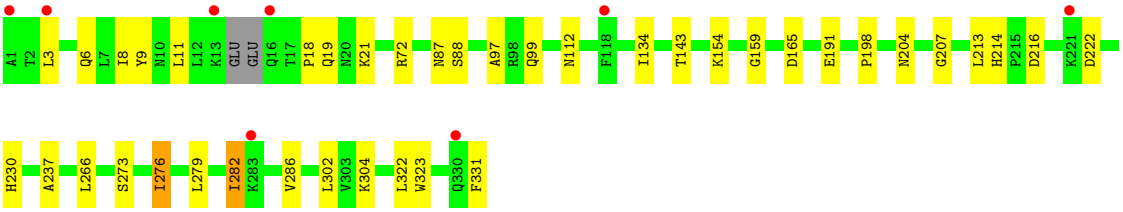
• Molecule 1: L-lactate dehydrogenase A chain





• Molecule 1: L-lactate dehydrogenase A chain





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.04 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.204 , 0.238 0.214 , 0.251	Depositor DCC
R_{free} test set	1094 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å^2)	33.8	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 41.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21329	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.49	0/2546	0.65	0/3443
1	B	0.50	0/2535	0.66	1/3429 (0.0%)
1	C	0.49	0/2588	0.67	0/3498
1	D	0.49	0/2593	0.65	0/3505
1	E	0.48	0/2429	0.66	1/3284 (0.0%)
1	F	0.46	0/2472	0.63	0/3344
1	G	0.47	0/2530	0.64	0/3419
1	H	0.51	0/2593	0.68	0/3505
All	All	0.49	0/20286	0.65	2/27427 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	16	GLN	C-N-CA	5.61	135.72	121.70
1	E	302	LEU	CA-CB-CG	5.43	127.80	115.30

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	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2492	0	2582	13	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	22	0
1	H	2550	0	2643	22	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
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	126	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 (126) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:C:219:THR:HG23	1:C:221:LYS:H	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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)

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	319/331 (96%)	308 (97%)	11 (3%)	0	100	100
1	B	318/331 (96%)	307 (96%)	10 (3%)	1 (0%)	41	50
1	C	324/331 (98%)	314 (97%)	10 (3%)	0	100	100
1	D	325/331 (98%)	314 (97%)	11 (3%)	0	100	100
1	E	302/331 (91%)	296 (98%)	6 (2%)	0	100	100
1	F	308/331 (93%)	299 (97%)	9 (3%)	0	100	100
1	G	314/331 (95%)	303 (96%)	10 (3%)	1 (0%)	41	50
1	H	325/331 (98%)	315 (97%)	10 (3%)	0	100	100
All	All	2535/2648 (96%)	2456 (97%)	77 (3%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	17	THR
1	G	27	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	280/287 (98%)	273 (98%)	7 (2%)	47	65
1	B	279/287 (97%)	272 (98%)	7 (2%)	47	65
1	C	285/287 (99%)	280 (98%)	5 (2%)	59	75
1	D	285/287 (99%)	282 (99%)	3 (1%)	73	86
1	E	268/287 (93%)	257 (96%)	11 (4%)	30	43
1	F	274/287 (96%)	267 (97%)	7 (3%)	46	63
1	G	278/287 (97%)	272 (98%)	6 (2%)	52	69
1	H	285/287 (99%)	276 (97%)	9 (3%)	39	54
All	All	2234/2296 (97%)	2179 (98%)	55 (2%)	47	65

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ARG
1	A	75	LYS
1	A	108	LEU
1	A	165	ASP
1	A	213	LEU
1	A	219	THR
1	A	327	LYS
1	B	72	ARG
1	B	93	ILE
1	B	107	ASN
1	B	165	ASP
1	B	213	LEU
1	B	220	ASP
1	B	302	LEU
1	C	72	ARG
1	C	111	ARG
1	C	133	LEU
1	C	219	THR
1	C	275	MET
1	D	98	ARG
1	D	165	ASP
1	D	315	LEU
1	E	56	LYS
1	E	72	ARG

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Mol	Chain	Res	Type
1	E	106	LEU
1	E	107	ASN
1	E	110	GLN
1	E	118	PHE
1	E	165	ASP
1	E	213	LEU
1	E	231	LYS
1	E	302	LEU
1	E	329	LEU
1	F	107	ASN
1	F	108	LEU
1	F	165	ASP
1	F	213	LEU
1	F	288	LEU
1	F	302	LEU
1	F	315	LEU
1	G	16	GLN
1	G	19	GLN
1	G	93	ILE
1	G	165	ASP
1	G	213	LEU
1	G	283	LYS
1	H	19	GLN
1	H	72	ARG
1	H	99	GLN
1	H	165	ASP
1	H	213	LEU
1	H	276	ILE
1	H	279	LEU
1	H	282	ILE
1	H	331	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	112	ASN
1	A	122	ASN
1	A	204	ASN
1	A	230	HIS
1	B	112	ASN
1	B	122	ASN

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Mol	Chain	Res	Type
1	B	204	ASN
1	B	230	HIS
1	B	297	ASN
1	C	16	GLN
1	C	112	ASN
1	C	204	ASN
1	C	230	HIS
1	D	20	ASN
1	D	100	GLN
1	D	107	ASN
1	D	110	GLN
1	D	204	ASN
1	D	230	HIS
1	D	297	ASN
1	D	330	GLN
1	E	112	ASN
1	E	204	ASN
1	E	230	HIS
1	F	112	ASN
1	F	122	ASN
1	F	204	ASN
1	F	230	HIS
1	G	112	ASN
1	G	204	ASN
1	G	230	HIS
1	H	6	GLN
1	H	16	GLN
1	H	107	ASN
1	H	112	ASN
1	H	204	ASN
1	H	230	HIS
1	H	326	GLN

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 monosaccharides 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	$\#\|Z\| > 2$
3	SO4	B	802	-	4,4,4	0.20	0	6,6,6	0.12	0
2	NAD	H	801	-	42,48,48	1.84	9 (21%)	50,73,73	1.55	9 (18%)
3	SO4	D	802	-	4,4,4	0.22	0	6,6,6	0.31	0
2	NAD	E	801	-	42,48,48	1.86	8 (19%)	50,73,73	1.39	6 (12%)
5	LAC	C	803	-	5,5,5	1.07	1 (20%)	4,6,6	1.62	1 (25%)
3	SO4	C	802	-	4,4,4	0.11	0	6,6,6	0.15	0
3	SO4	F	802	-	4,4,4	0.18	0	6,6,6	0.22	0
4	D3J	D	804	-	35,39,39	1.30	2 (5%)	40,56,56	2.06	8 (20%)
4	D3J	G	803	-	35,39,39	1.33	2 (5%)	40,56,56	2.13	8 (20%)
4	D3J	A	803	-	35,39,39	1.40	3 (8%)	40,56,56	2.22	8 (20%)
3	SO4	H	802	-	4,4,4	0.15	0	6,6,6	0.15	0
2	NAD	B	801	-	42,48,48	1.86	11 (26%)	50,73,73	1.29	7 (14%)
3	SO4	A	802	-	4,4,4	0.36	0	6,6,6	0.30	0
4	D3J	B	803	-	35,39,39	1.27	2 (5%)	40,56,56	1.94	6 (15%)
2	NAD	A	801	-	42,48,48	1.89	10 (23%)	50,73,73	1.30	7 (14%)
2	NAD	G	801	-	42,48,48	1.70	8 (19%)	50,73,73	1.31	6 (12%)
4	D3J	E	802	-	35,39,39	1.27	2 (5%)	40,56,56	2.12	7 (17%)
4	D3J	F	803	-	35,39,39	1.30	2 (5%)	40,56,56	2.20	7 (17%)
3	SO4	G	802	-	4,4,4	0.17	0	6,6,6	0.13	0
2	NAD	F	801	-	42,48,48	1.88	9 (21%)	50,73,73	1.20	4 (8%)
3	SO4	D	803	-	4,4,4	0.16	0	6,6,6	0.21	0
2	NAD	C	801	-	42,48,48	1.83	10 (23%)	50,73,73	1.42	5 (10%)
2	NAD	D	801	-	42,48,48	1.88	11 (26%)	50,73,73	1.26	4 (8%)

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	D3J	G	803	-	-	1/12/38/38	0/5/5/5
2	NAD	H	801	-	-	5/26/62/62	0/5/5/5
2	NAD	B	801	-	-	5/26/62/62	0/5/5/5
2	NAD	E	801	-	-	5/26/62/62	0/5/5/5
4	D3J	F	803	-	-	4/12/38/38	0/5/5/5
5	LAC	C	803	-	-	4/4/4/4	-
4	D3J	B	803	-	-	2/12/38/38	0/5/5/5
2	NAD	A	801	-	-	5/26/62/62	0/5/5/5
2	NAD	G	801	-	-	4/26/62/62	0/5/5/5
2	NAD	F	801	-	-	5/26/62/62	0/5/5/5
4	D3J	D	804	-	-	1/12/38/38	0/5/5/5
4	D3J	E	802	-	-	2/12/38/38	0/5/5/5
4	D3J	A	803	-	-	3/12/38/38	0/5/5/5
2	NAD	C	801	-	-	5/26/62/62	0/5/5/5
2	NAD	D	801	-	-	5/26/62/62	0/5/5/5

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	NAD	C7N-N7N	5.75	1.43	1.33
2	E	801	NAD	C7N-N7N	5.60	1.43	1.33
2	D	801	NAD	C7N-N7N	5.57	1.43	1.33
2	C	801	NAD	C7N-N7N	5.33	1.43	1.33
4	G	803	D3J	C29-C28	-5.31	1.33	1.37
2	H	801	NAD	C7N-N7N	4.98	1.42	1.33
2	F	801	NAD	C7N-N7N	4.94	1.42	1.33
2	G	801	NAD	C7N-N7N	4.74	1.42	1.33
4	A	803	D3J	C29-C28	-4.59	1.34	1.37
2	H	801	NAD	C2B-C3B	-4.53	1.40	1.53
2	B	801	NAD	C7N-N7N	4.48	1.41	1.33
2	A	801	NAD	C2B-C3B	-4.43	1.41	1.53
4	A	803	D3J	C29-S30	4.41	1.76	1.70
2	F	801	NAD	C2B-C3B	-4.40	1.41	1.53
4	E	802	D3J	C29-S30	4.38	1.76	1.70
4	D	804	D3J	C29-S30	4.33	1.76	1.70
2	E	801	NAD	C2B-C3B	-4.31	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	NAD	C2B-C3B	-4.26	1.41	1.53
4	F	803	D3J	C29-C28	-4.25	1.34	1.37
2	B	801	NAD	C2B-C3B	-4.23	1.41	1.53
4	F	803	D3J	C29-S30	4.22	1.76	1.70
4	D	804	D3J	C29-C28	-4.14	1.34	1.37
4	B	803	D3J	C29-C28	-4.06	1.34	1.37
2	C	801	NAD	C2B-C3B	-4.05	1.42	1.53
2	G	801	NAD	C2B-C3B	-4.03	1.42	1.53
4	B	803	D3J	C29-S30	3.80	1.75	1.70
4	E	802	D3J	C29-C28	-3.78	1.34	1.37
2	B	801	NAD	O2D-C2D	-3.71	1.34	1.43
2	F	801	NAD	C6A-N6A	3.57	1.47	1.34
2	B	801	NAD	C6A-N6A	3.56	1.47	1.34
2	C	801	NAD	O2D-C2D	-3.50	1.34	1.43
2	E	801	NAD	C2B-C1B	-3.47	1.48	1.53
2	F	801	NAD	O2D-C2D	-3.38	1.35	1.43
2	C	801	NAD	C6A-N6A	3.36	1.46	1.34
2	D	801	NAD	O2D-C2D	-3.35	1.35	1.43
2	E	801	NAD	C6A-N6A	3.30	1.46	1.34
2	A	801	NAD	C6A-N6A	3.30	1.46	1.34
2	H	801	NAD	C6A-N6A	3.23	1.45	1.34
2	G	801	NAD	C6A-N6A	3.22	1.45	1.34
2	E	801	NAD	O2D-C2D	-3.19	1.35	1.43
4	G	803	D3J	C29-S30	3.18	1.75	1.70
2	D	801	NAD	C6A-N6A	3.16	1.45	1.34
2	A	801	NAD	O2D-C2D	-3.12	1.35	1.43
2	G	801	NAD	O2D-C2D	-3.09	1.35	1.43
2	D	801	NAD	C2B-C1B	-3.06	1.49	1.53
2	H	801	NAD	O2D-C2D	-3.04	1.35	1.43
2	A	801	NAD	C2B-C1B	-3.03	1.49	1.53
2	B	801	NAD	C2B-C1B	-3.00	1.49	1.53
2	H	801	NAD	C2B-C1B	-2.94	1.49	1.53
2	F	801	NAD	C2B-C1B	-2.87	1.49	1.53
2	C	801	NAD	C2B-C1B	-2.81	1.49	1.53
2	E	801	NAD	C5D-C4D	-2.61	1.43	1.51
2	G	801	NAD	C2B-C1B	-2.60	1.49	1.53
2	D	801	NAD	C5B-C4B	-2.50	1.43	1.51
2	C	801	NAD	C2N-N1N	2.48	1.38	1.35
2	C	801	NAD	C5D-C4D	-2.47	1.43	1.51
2	C	801	NAD	C2D-C1D	-2.45	1.50	1.53
2	D	801	NAD	C5D-C4D	-2.43	1.44	1.51
2	C	801	NAD	C5B-C4B	-2.43	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	801	NAD	C5B-C4B	-2.39	1.44	1.51
2	F	801	NAD	C5D-C4D	-2.38	1.44	1.51
2	D	801	NAD	C2D-C1D	-2.35	1.50	1.53
2	F	801	NAD	C5B-C4B	-2.34	1.44	1.51
2	A	801	NAD	C5B-C4B	-2.30	1.44	1.51
2	G	801	NAD	C5D-C4D	-2.30	1.44	1.51
2	B	801	NAD	C5B-C4B	-2.30	1.44	1.51
2	A	801	NAD	O4B-C4B	-2.29	1.39	1.45
2	B	801	NAD	C5D-C4D	-2.28	1.44	1.51
2	H	801	NAD	C5B-C4B	-2.27	1.44	1.51
2	E	801	NAD	O4B-C4B	-2.27	1.39	1.45
2	D	801	NAD	O4B-C1B	-2.27	1.37	1.41
2	A	801	NAD	C5D-C4D	-2.26	1.44	1.51
2	G	801	NAD	C5B-C4B	-2.25	1.44	1.51
2	B	801	NAD	C2D-C1D	-2.23	1.50	1.53
2	B	801	NAD	O4B-C1B	-2.21	1.38	1.41
2	F	801	NAD	O4B-C4B	-2.21	1.40	1.45
2	H	801	NAD	O4B-C4B	-2.18	1.40	1.45
2	H	801	NAD	C5D-C4D	-2.18	1.44	1.51
2	B	801	NAD	O4B-C4B	-2.17	1.40	1.45
2	G	801	NAD	C2D-C1D	-2.14	1.50	1.53
2	A	801	NAD	C2D-C1D	-2.13	1.50	1.53
2	F	801	NAD	C2A-N3A	2.13	1.35	1.32
4	A	803	D3J	C3-C2	2.11	1.41	1.37
2	C	801	NAD	C2A-N3A	2.10	1.35	1.32
2	H	801	NAD	O4B-C1B	-2.09	1.38	1.41
2	B	801	NAD	C2D-C3D	-2.08	1.47	1.53
2	D	801	NAD	O4B-C4B	-2.08	1.40	1.45
2	D	801	NAD	O5B-C5B	-2.03	1.37	1.44
5	C	803	LAC	OXT-C	-2.02	1.23	1.30
2	A	801	NAD	O5B-C5B	-2.02	1.37	1.44

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	803	D3J	C9-N10-C11	8.27	123.61	117.24
4	A	803	D3J	C9-N10-C11	7.98	123.39	117.24
4	G	803	D3J	C9-N10-C11	7.23	122.81	117.24
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	D	804	D3J	C9-N10-C11	6.72	122.42	117.24
4	E	802	D3J	C9-N10-C11	6.68	122.39	117.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	803	D3J	C9-N10-C11	6.23	122.04	117.24
4	B	803	D3J	C12-N13-C14	5.92	121.74	117.33
4	F	803	D3J	C12-N13-C14	5.75	121.61	117.33
2	H	801	NAD	N3A-C2A-N1A	-5.52	120.05	128.68
4	G	803	D3J	C28-C29-S30	-5.49	108.75	112.29
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
4	F	803	D3J	C28-C29-S30	-5.33	108.86	112.29
2	C	801	NAD	N3A-C2A-N1A	-5.25	120.47	128.68
2	A	801	NAD	N3A-C2A-N1A	-4.94	120.95	128.68
4	A	803	D3J	C17-S16-C15	4.73	108.82	102.81
2	E	801	NAD	N3A-C2A-N1A	-4.67	121.37	128.68
2	B	801	NAD	N3A-C2A-N1A	-4.67	121.37	128.68
4	A	803	D3J	C28-C29-S30	-4.61	109.32	112.29
2	D	801	NAD	N3A-C2A-N1A	-4.55	121.57	128.68
2	G	801	NAD	N3A-C2A-N1A	-4.26	122.02	128.68
4	E	802	D3J	C17-S16-C15	3.78	107.61	102.81
4	D	804	D3J	C28-C29-S30	-3.69	109.92	112.29
4	F	803	D3J	C17-S16-C15	3.69	107.49	102.81
2	E	801	NAD	C3N-C7N-N7N	3.66	122.15	117.75
2	F	801	NAD	N3A-C2A-N1A	-3.61	123.03	128.68
2	G	801	NAD	C4A-C5A-N7A	-3.60	105.65	109.40
4	E	802	D3J	C12-C11-N10	3.52	121.51	116.12
4	B	803	D3J	C15-C14-N13	3.45	120.04	114.39
4	D	804	D3J	C17-S16-C15	3.37	107.09	102.81
2	C	801	NAD	PN-O3-PA	-3.32	121.44	132.83
4	B	803	D3J	C26-C12-N13	3.31	112.10	108.09
4	B	803	D3J	C28-C29-S30	-3.23	110.21	112.29
2	H	801	NAD	C3N-C2N-N1N	3.20	123.55	120.43
2	H	801	NAD	PN-O3-PA	-3.07	122.31	132.83
5	C	803	LAC	CB-CA-C	3.05	117.55	110.63
4	G	803	D3J	C12-C11-N10	2.95	120.63	116.12
2	F	801	NAD	C4A-C5A-N7A	-2.94	106.34	109.40
4	F	803	D3J	O8-C9-C35	2.92	121.22	115.35
4	G	803	D3J	C15-C14-N13	2.88	119.11	114.39
4	E	802	D3J	C15-C14-N13	2.88	119.10	114.39
4	A	803	D3J	C15-C14-N13	2.88	119.10	114.39
2	F	801	NAD	PN-O3-PA	-2.87	122.98	132.83
2	D	801	NAD	PN-O3-PA	-2.87	122.98	132.83
2	E	801	NAD	O7N-C7N-N7N	-2.82	118.57	122.58
4	F	803	D3J	C15-C14-N13	2.81	118.98	114.39
4	A	803	D3J	O8-C9-C35	2.76	120.89	115.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	802	D3J	C33-C11-N10	-2.72	118.61	122.20
2	H	801	NAD	C6N-N1N-C2N	-2.69	119.53	121.97
2	A	801	NAD	PN-O3-PA	-2.69	123.61	132.83
2	G	801	NAD	O5D-C5D-C4D	2.68	118.22	108.99
2	E	801	NAD	PN-O3-PA	-2.68	123.64	132.83
4	A	803	D3J	C33-C11-N10	-2.66	118.70	122.20
2	D	801	NAD	C3N-C7N-N7N	2.64	120.92	117.75
2	A	801	NAD	C3N-C7N-N7N	2.64	120.92	117.75
4	D	804	D3J	C12-C11-N10	2.62	120.13	116.12
2	B	801	NAD	PN-O3-PA	-2.62	123.84	132.83
2	G	801	NAD	PN-O3-PA	-2.58	123.98	132.83
2	C	801	NAD	O4B-C1B-C2B	-2.56	103.18	106.93
4	F	803	D3J	C33-C11-N10	-2.56	118.83	122.20
4	E	802	D3J	C28-C29-S30	-2.55	110.65	112.29
2	E	801	NAD	O4B-C1B-C2B	-2.50	103.27	106.93
2	H	801	NAD	O5D-C5D-C4D	2.49	117.57	108.99
2	E	801	NAD	O5D-C5D-C4D	2.49	117.55	108.99
2	G	801	NAD	O7N-C7N-N7N	-2.49	119.05	122.58
2	B	801	NAD	O5D-C5D-C4D	2.49	117.55	108.99
2	B	801	NAD	O7N-C7N-N7N	-2.49	119.05	122.58
2	D	801	NAD	O5D-C5D-C4D	2.47	117.49	108.99
2	H	801	NAD	C5N-C4N-C3N	-2.42	117.47	120.34
2	G	801	NAD	O7N-C7N-C3N	2.41	122.52	119.63
4	G	803	D3J	C33-C11-N10	-2.41	119.03	122.20
4	G	803	D3J	C17-S16-C15	2.41	105.87	102.81
2	B	801	NAD	O4B-C1B-C2B	-2.41	103.41	106.93
4	A	803	D3J	C3-C2-C5	-2.39	119.65	122.83
4	D	804	D3J	C15-C14-N13	2.36	118.26	114.39
2	C	801	NAD	C3N-C7N-N7N	2.35	120.57	117.75
2	F	801	NAD	O5D-C5D-C4D	2.34	117.04	108.99
2	A	801	NAD	O5D-C5D-C4D	2.33	117.02	108.99
2	C	801	NAD	O5D-C5D-C4D	2.30	116.92	108.99
2	B	801	NAD	O7N-C7N-C3N	2.30	122.39	119.63
2	H	801	NAD	C1B-N9A-C4A	-2.25	122.69	126.64
2	H	801	NAD	C6N-C5N-C4N	2.23	122.68	119.44
4	D	804	D3J	C22-C17-C18	2.21	120.46	117.52
4	D	804	D3J	C33-C11-N10	-2.20	119.31	122.20
4	G	803	D3J	C7-O8-C9	2.19	124.08	118.83
2	A	801	NAD	O4B-C1B-C2B	-2.14	103.80	106.93
2	B	801	NAD	C4A-C5A-N7A	-2.13	107.18	109.40
2	H	801	NAD	C3N-C7N-N7N	2.12	120.30	117.75
4	B	803	D3J	C7-O8-C9	2.10	123.87	118.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	NAD	C4A-C5A-N7A	-2.05	107.26	109.40
2	A	801	NAD	C1B-N9A-C4A	-2.03	123.08	126.64

There are no chirality outliers.

All (56) 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
4	F	803	D3J	C24-C15-S16-C17
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	N10-C9-O8-C7
4	F	803	D3J	N10-C9-O8-C7
4	A	803	D3J	C35-C9-O8-C7
4	F	803	D3J	C35-C9-O8-C7
4	A	803	D3J	C33-C11-C12-C26
4	D	804	D3J	C33-C11-C12-C26

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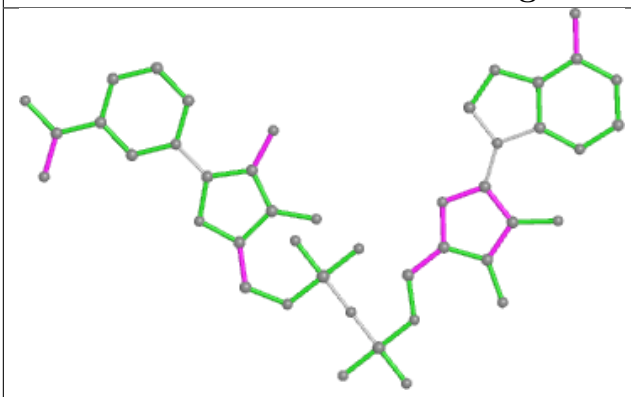
Mol	Chain	Res	Type	Atoms
4	G	803	D3J	C33-C11-C12-C26
4	B	803	D3J	C24-C15-S16-C17
4	E	802	D3J	C35-C9-O8-C7
2	E	801	NAD	O4B-C4B-C5B-O5B
2	B	801	NAD	O4B-C4B-C5B-O5B
2	G	801	NAD	O4B-C4B-C5B-O5B
2	A	801	NAD	C2D-C1D-N1N-C6N
2	B	801	NAD	C2D-C1D-N1N-C6N
2	C	801	NAD	C2D-C1D-N1N-C6N
2	D	801	NAD	C2D-C1D-N1N-C6N
2	E	801	NAD	C2D-C1D-N1N-C6N
2	F	801	NAD	C2D-C1D-N1N-C6N
2	H	801	NAD	C2D-C1D-N1N-C6N
2	A	801	NAD	O4B-C4B-C5B-O5B
2	C	801	NAD	O4B-C4B-C5B-O5B
2	D	801	NAD	O4B-C4B-C5B-O5B
2	F	801	NAD	O4B-C4B-C5B-O5B
2	H	801	NAD	O4B-C4B-C5B-O5B
4	B	803	D3J	C33-C11-C12-C26
4	E	802	D3J	C33-C11-C12-C26
4	F	803	D3J	C33-C11-C12-C26

There are no ring outliers.

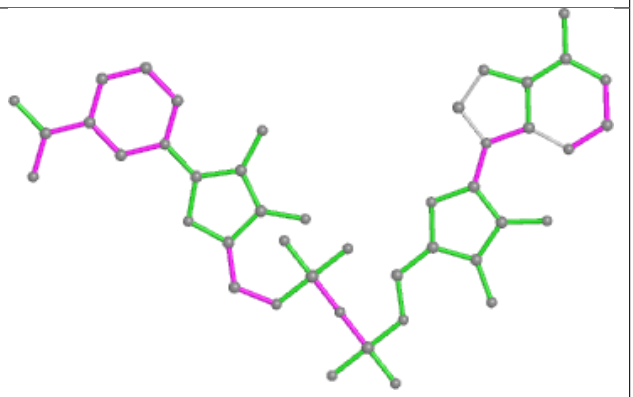
No monomer is involved in short contacts.

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 then 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.

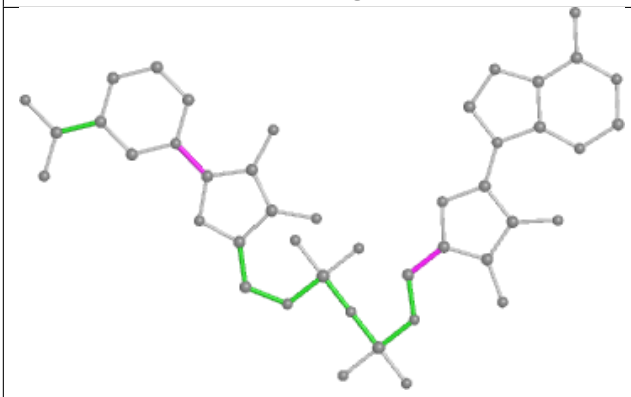
Ligand NAD H 801



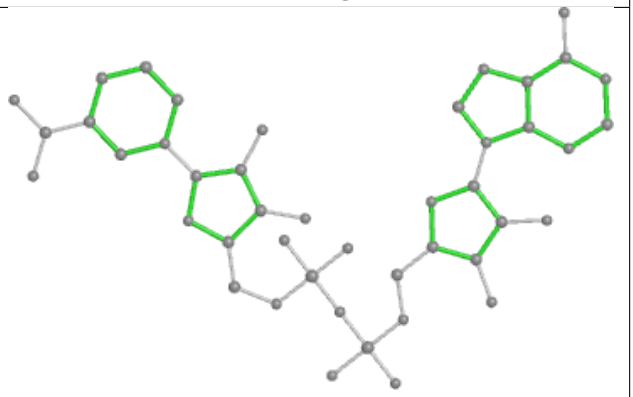
Bond lengths



Bond angles

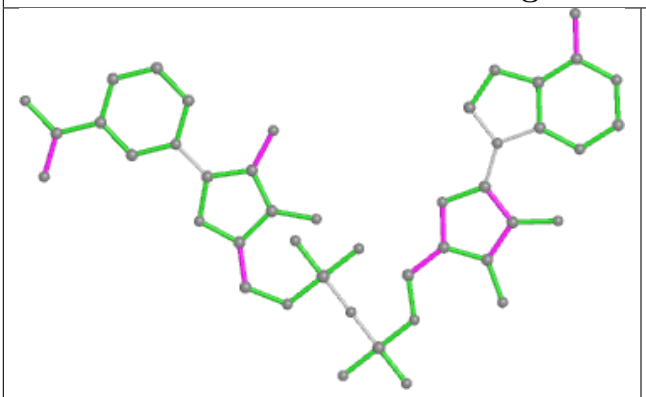


Torsions

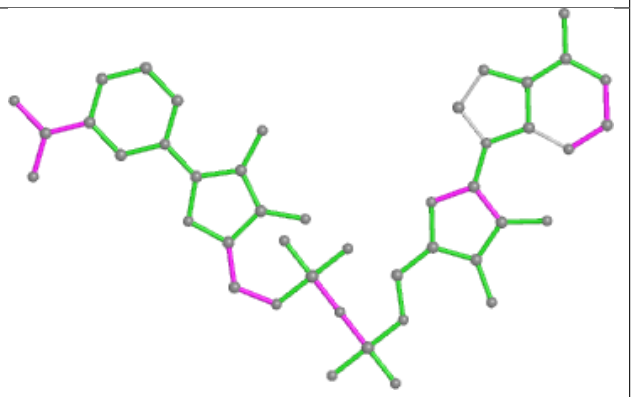


Rings

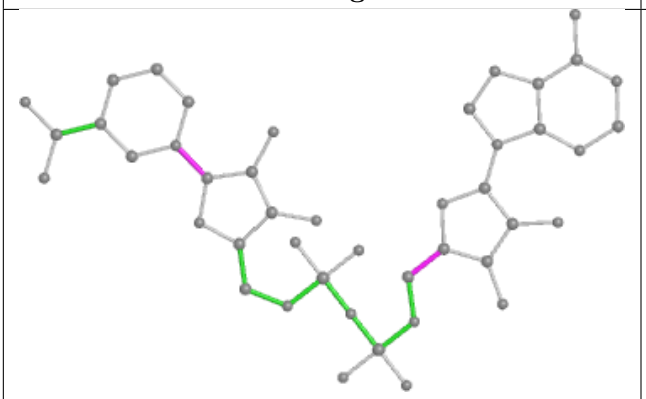
Ligand NAD E 801



Bond lengths



Bond angles



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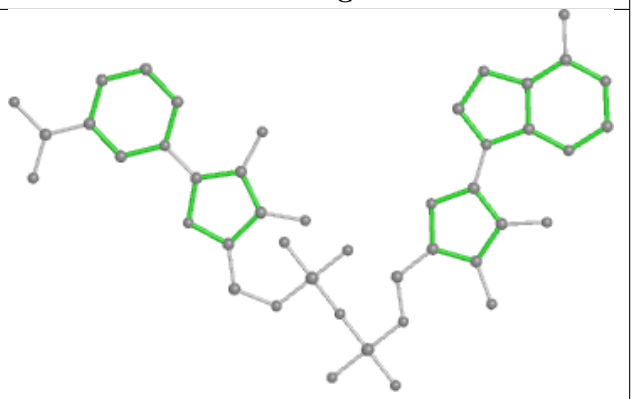
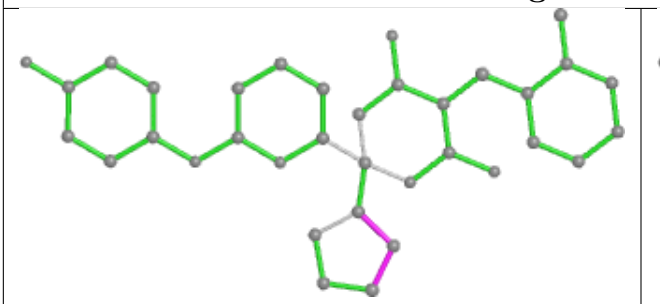
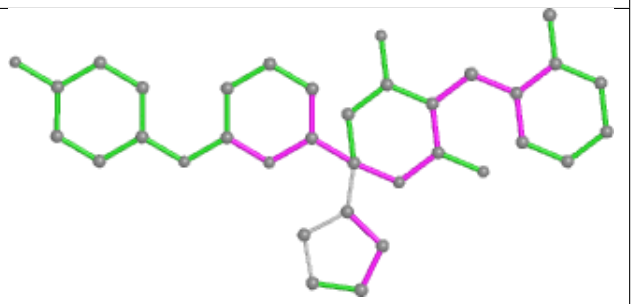


Rings

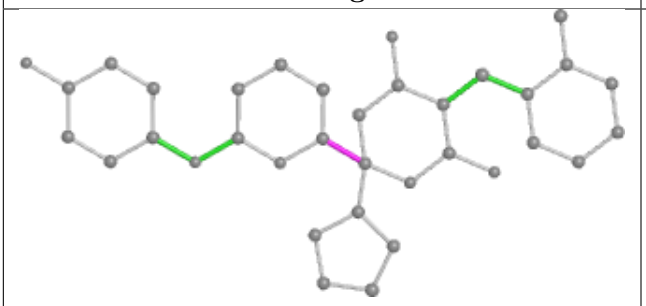
Ligand D3J D 804



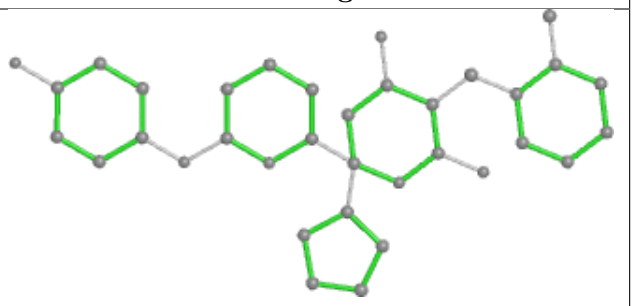
Bond lengths



Bond angles

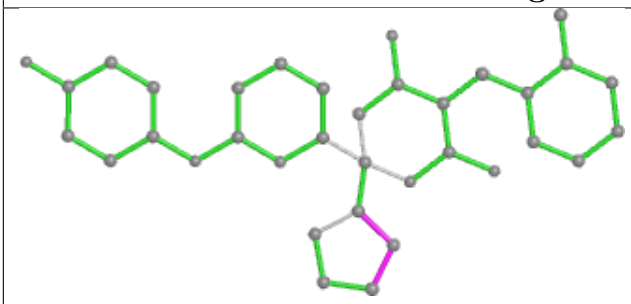


Torsions

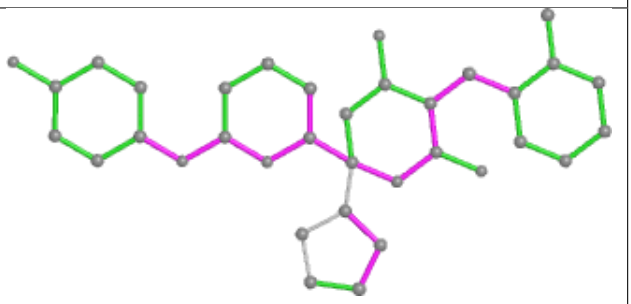


Rings

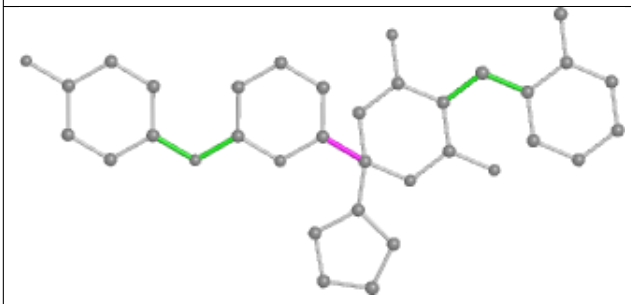
Ligand D3J G 803



Bond lengths



Bond angles



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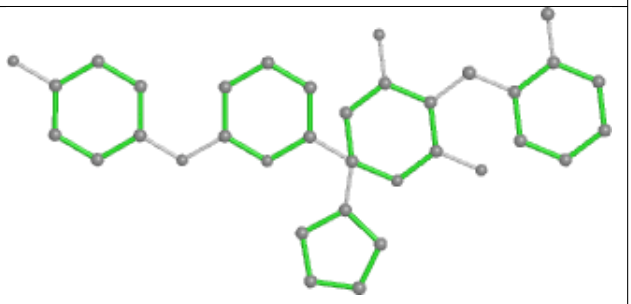
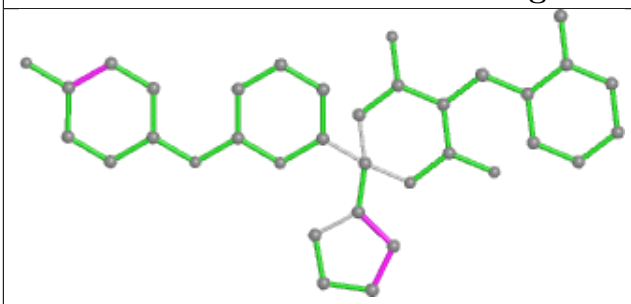


Rings

Ligand D3J A 803



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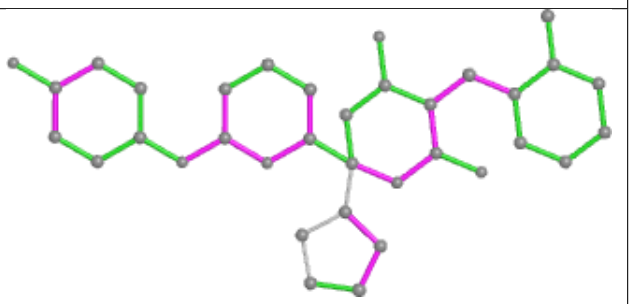
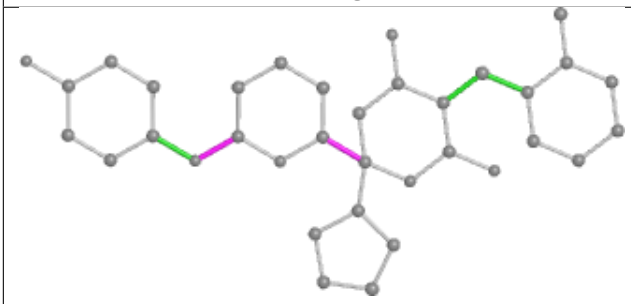


Bond angles



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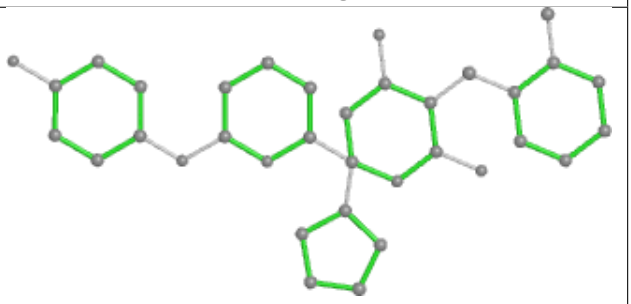
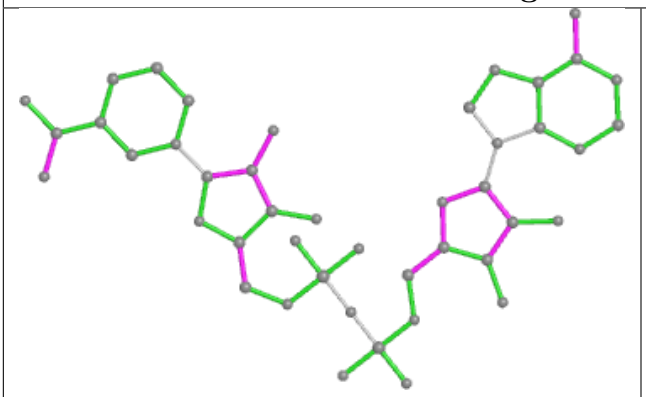
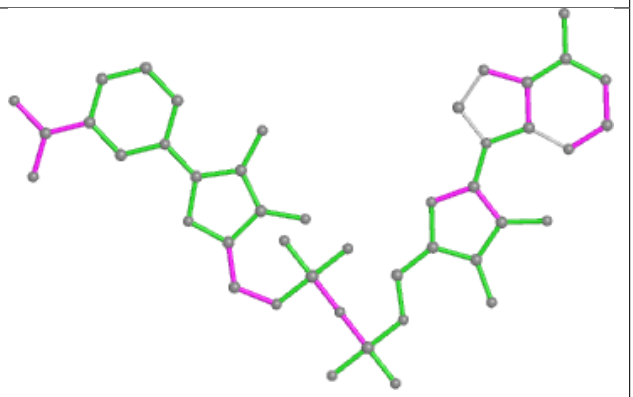


Rings

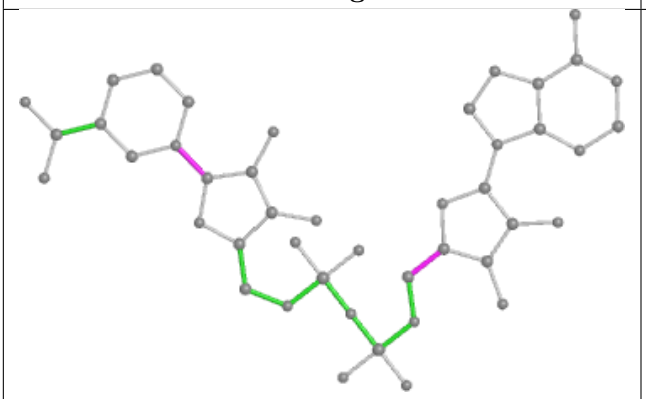
Ligand NAD B 801



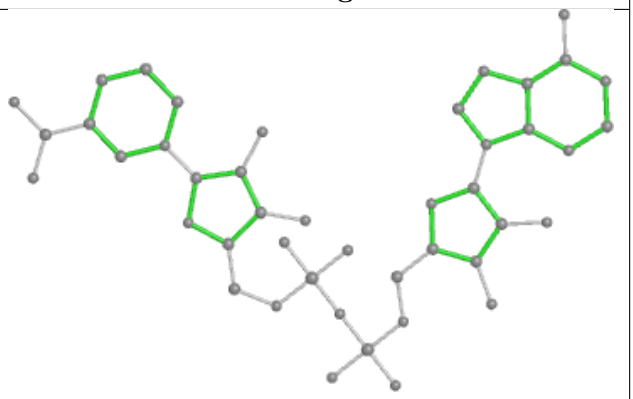
Bond lengths



Bond angles

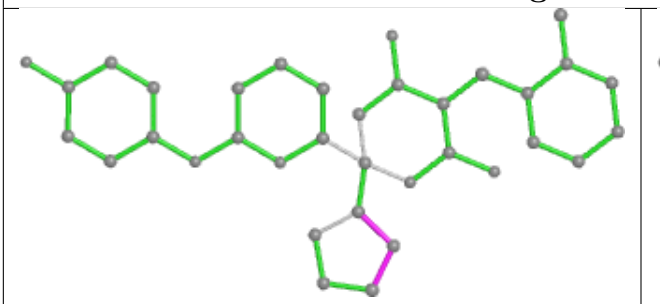


Torsions

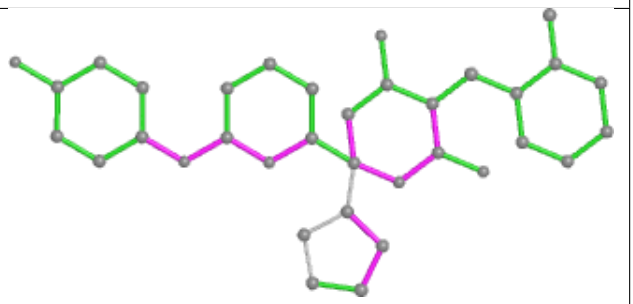


Rings

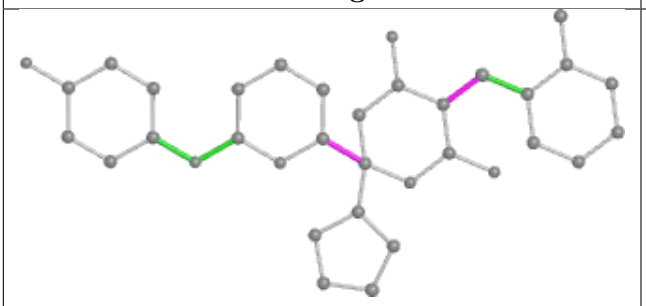
Ligand D3J B 803



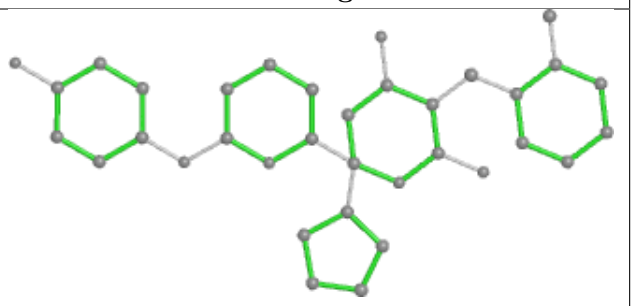
Bond lengths



Bond angles

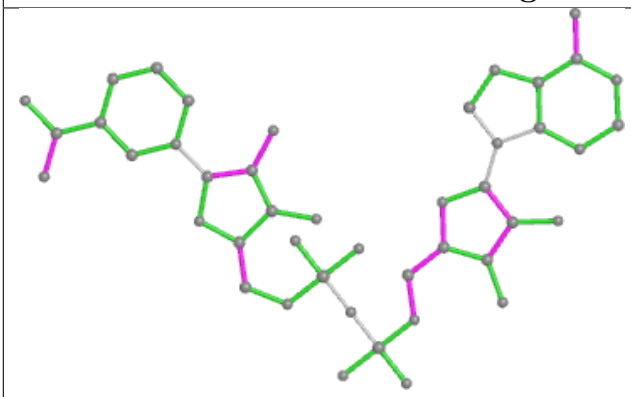


Torsions

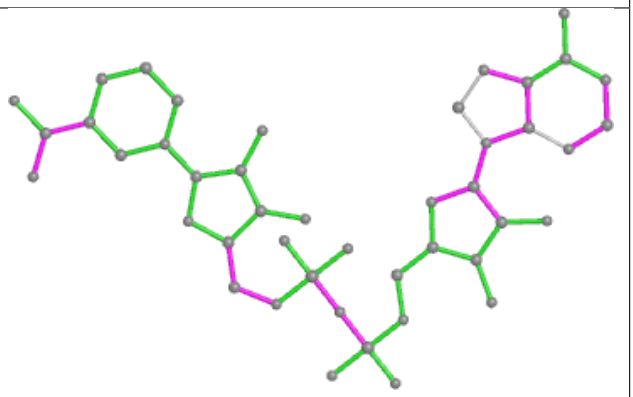


Rings

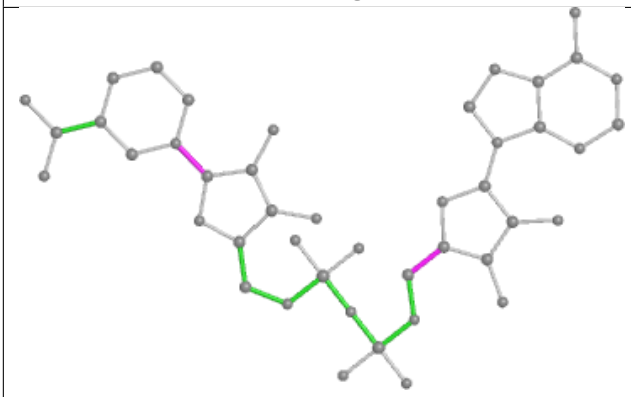
Ligand NAD A 801



Bond lengths



Bond angles



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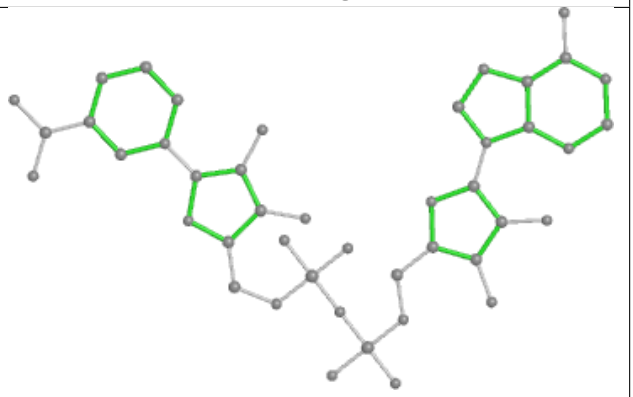
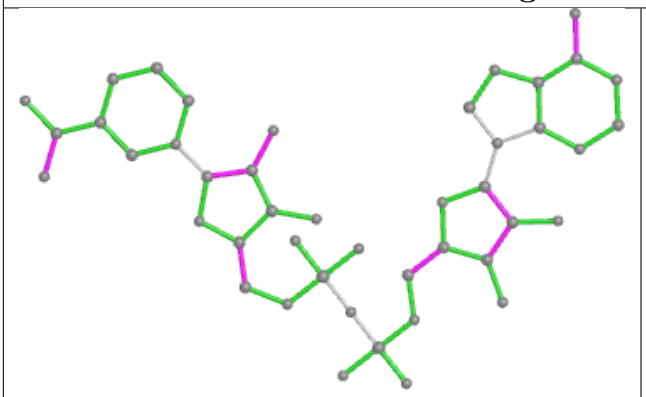
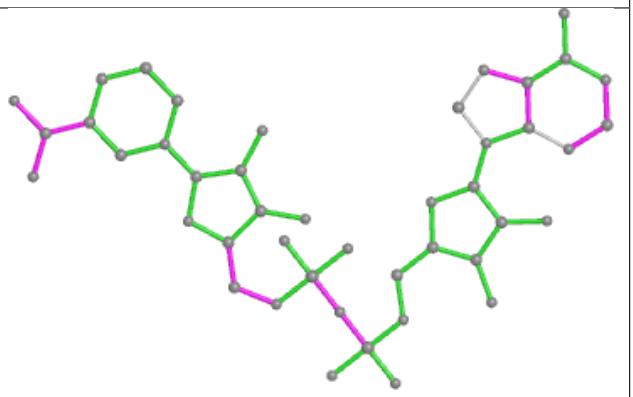


Rings

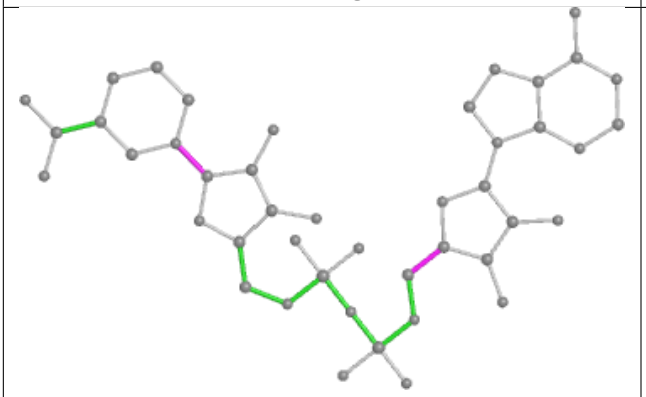
Ligand NAD G 801



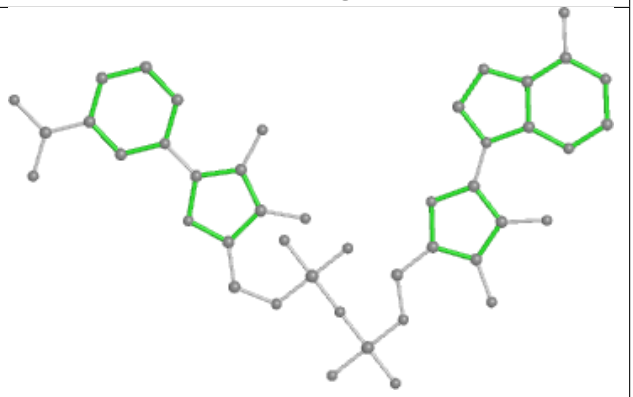
Bond lengths



Bond angles

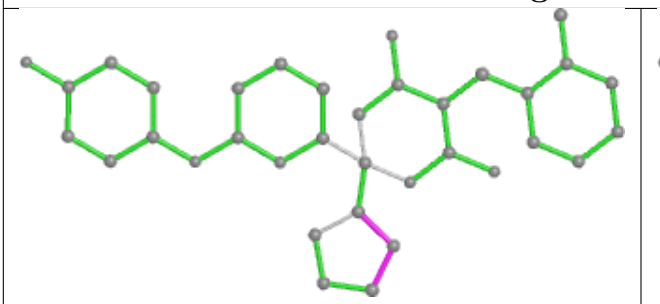


Torsions

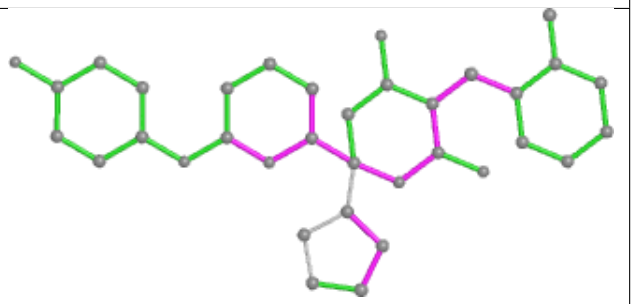


Rings

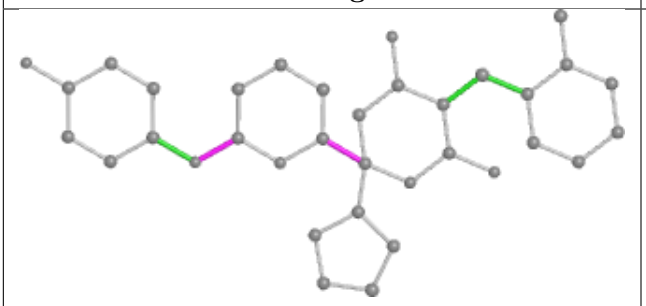
Ligand D3J E 802



Bond lengths



Bond angles



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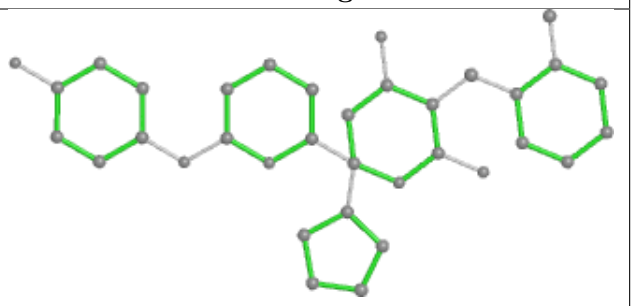
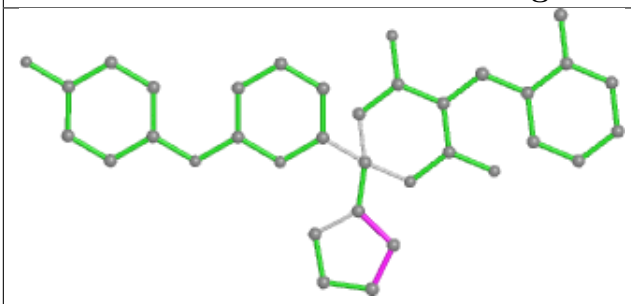
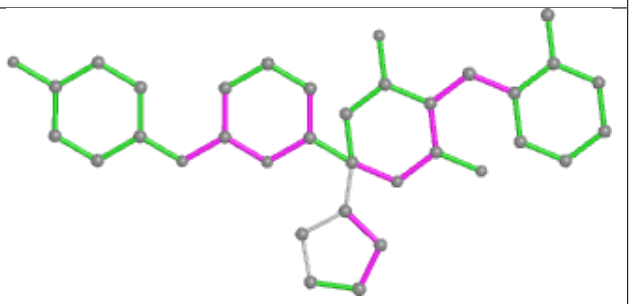


Rings

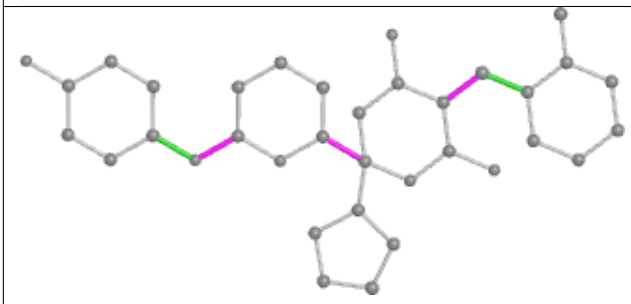
Ligand D3J F 803



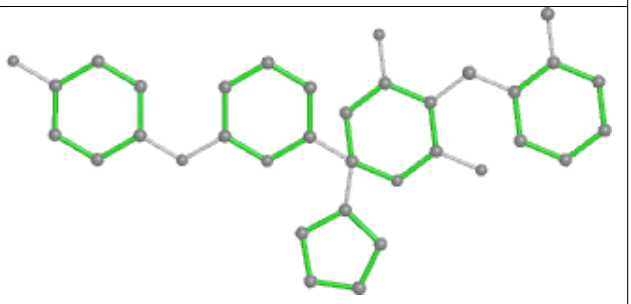
Bond lengths



Bond angles

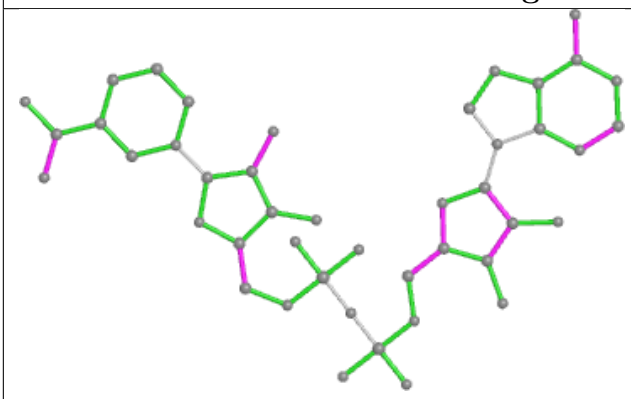


Torsions

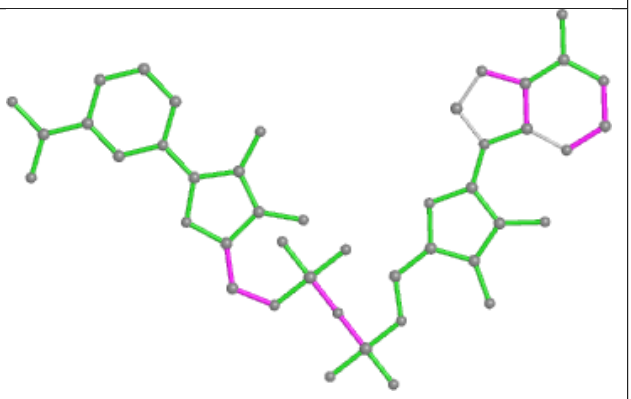


Rings

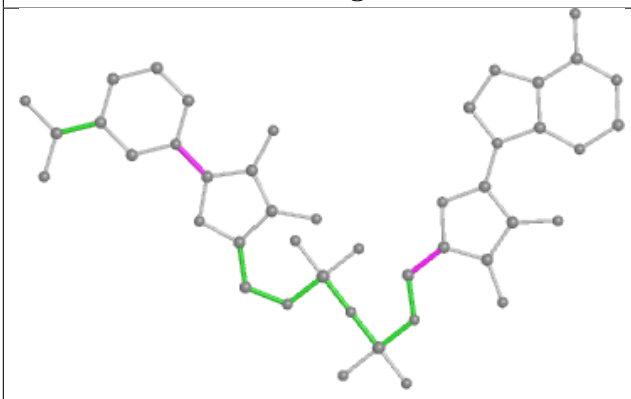
Ligand NAD F 801



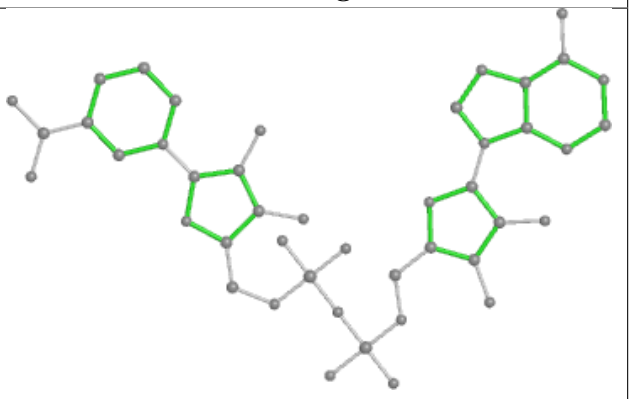
Bond lengths



Bond angles

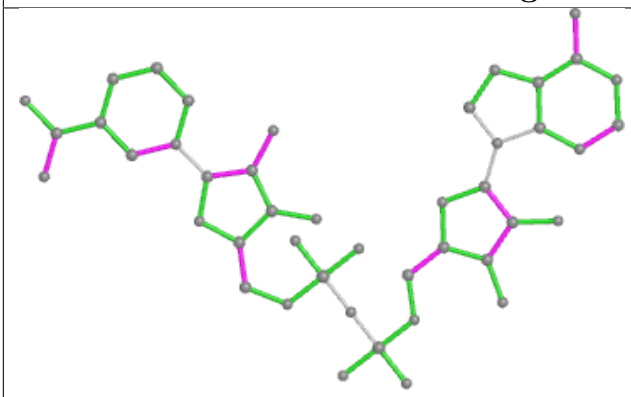


Torsions

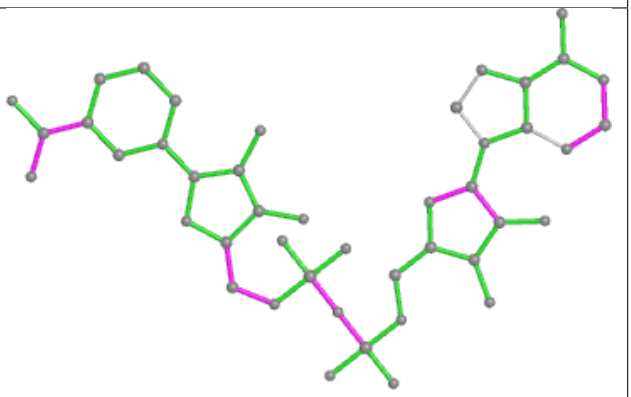


Rings

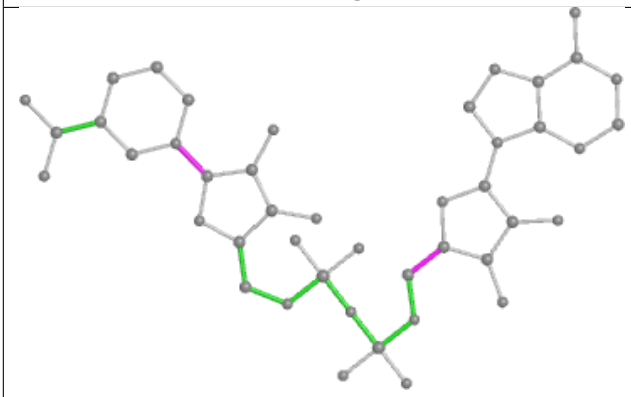
Ligand NAD C 801



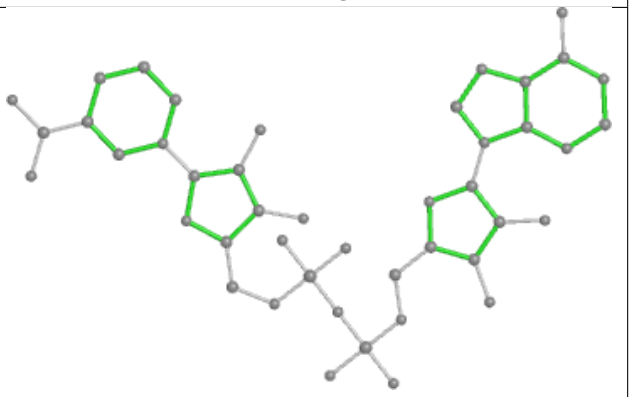
Bond lengths



Bond angles

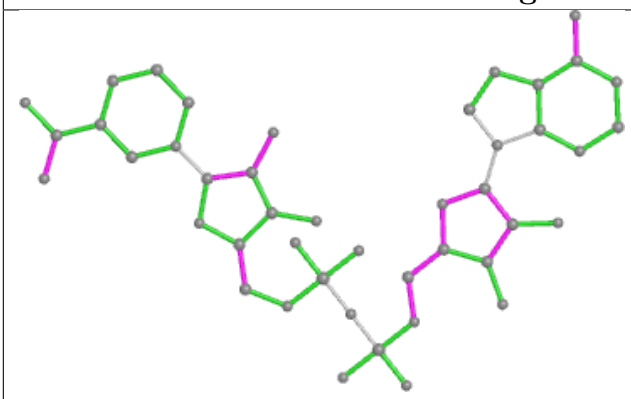


Torsions

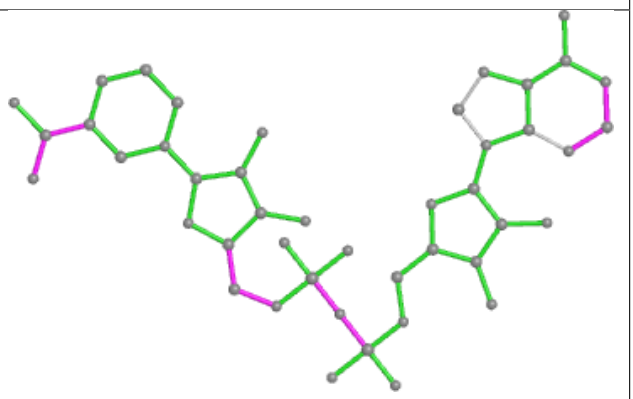


Rings

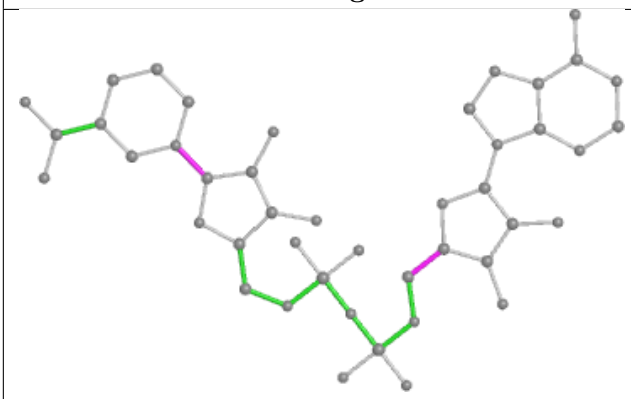
Ligand NAD D 801



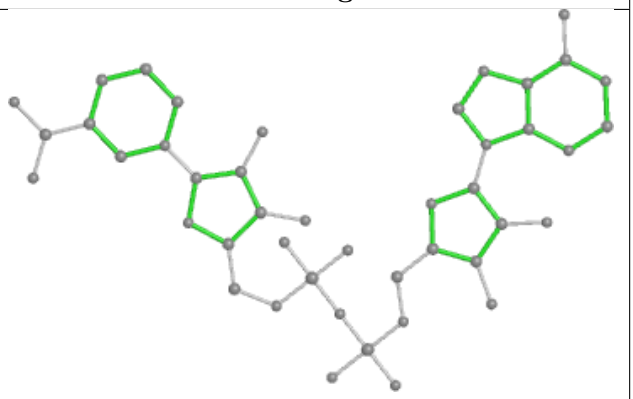
Bond lengths



Bond angles



Torsions



Rings

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	323/331 (97%)	-0.21	8 (2%)	57	64	20, 33, 62, 84	5 (1%)
1	B	322/331 (97%)	-0.10	15 (4%)	31	38	19, 34, 68, 97	6 (1%)
1	C	328/331 (99%)	-0.18	4 (1%)	79	83	21, 36, 64, 106	1 (0%)
1	D	329/331 (99%)	-0.31	7 (2%)	63	70	21, 34, 62, 82	3 (0%)
1	E	310/331 (93%)	0.05	11 (3%)	44	51	25, 41, 69, 142	0
1	F	314/331 (94%)	0.09	10 (3%)	47	54	25, 41, 72, 102	3 (0%)
1	G	322/331 (97%)	0.01	14 (4%)	35	42	24, 40, 84, 109	2 (0%)
1	H	329/331 (99%)	-0.26	8 (2%)	59	66	24, 35, 66, 90	2 (0%)
All	All	2577/2648 (97%)	-0.12	77 (2%)	50	57	19, 37, 70, 142	22 (0%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	16	GLN	7.1
1	G	16	GLN	6.9
1	F	15	GLU	5.8
1	E	213	LEU	5.7
1	B	12	LEU	5.6
1	B	17	THR	5.6
1	B	14	GLU	5.2
1	C	13	LYS	5.2
1	G	331	PHE	5.1
1	E	214	HIS	5.0
1	H	13	LYS	4.8
1	H	16	GLN	4.5
1	H	221	LYS	4.4
1	A	13	LYS	4.4
1	D	14	GLU	4.2
1	B	15	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	G	1	ALA	4.2
1	D	1	ALA	4.1
1	E	1	ALA	4.1
1	E	216	ASP	3.9
1	G	225	GLN	3.8
1	H	1	ALA	3.7
1	G	226	TRP	3.7
1	E	105	ARG	3.6
1	A	12	LEU	3.6
1	A	14	GLU	3.6
1	D	13	LYS	3.5
1	H	330	GLN	3.5
1	F	14	GLU	3.5
1	B	331	PHE	3.4
1	A	1	ALA	3.4
1	F	3	LEU	3.3
1	C	16	GLN	3.1
1	F	221	LYS	3.1
1	F	220	ASP	3.1
1	C	221	LYS	3.0
1	B	226	TRP	2.9
1	E	210	LEU	2.8
1	G	100	GLN	2.8
1	E	211	LYS	2.7
1	F	141	ILE	2.7
1	F	217	LEU	2.7
1	G	101	GLU	2.7
1	A	108	LEU	2.7
1	F	286	VAL	2.7
1	B	221	LYS	2.6
1	H	118	PHE	2.6
1	E	9	TYR	2.6
1	B	214	HIS	2.5
1	F	2	THR	2.5
1	G	200	TRP	2.5
1	A	16	GLN	2.5
1	A	220	ASP	2.5
1	G	216	ASP	2.5
1	B	13	LYS	2.5
1	G	330	GLN	2.5
1	A	221	LYS	2.3
1	G	309	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	229	VAL	2.3
1	H	3	LEU	2.3
1	B	223	LYS	2.3
1	B	330	GLN	2.2
1	D	102	GLY	2.2
1	G	236	SER	2.2
1	D	100	GLN	2.2
1	H	283	LYS	2.2
1	E	200	TRP	2.2
1	F	327	LYS	2.2
1	B	222	ASP	2.2
1	E	215	PRO	2.2
1	C	331	PHE	2.1
1	E	239	GLU	2.1
1	D	118	PHE	2.1
1	B	228	GLU	2.1
1	D	12	LEU	2.1
1	G	310	GLU	2.0
1	B	97	ALA	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 monosaccharides 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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	D3J	F	803	35/35	0.90	0.18	37,53,83,86	0
3	SO4	G	802	5/5	0.91	0.18	50,51,52,52	5
3	SO4	D	803	5/5	0.91	0.15	90,90,91,92	0
4	D3J	E	802	35/35	0.92	0.14	40,52,71,72	0

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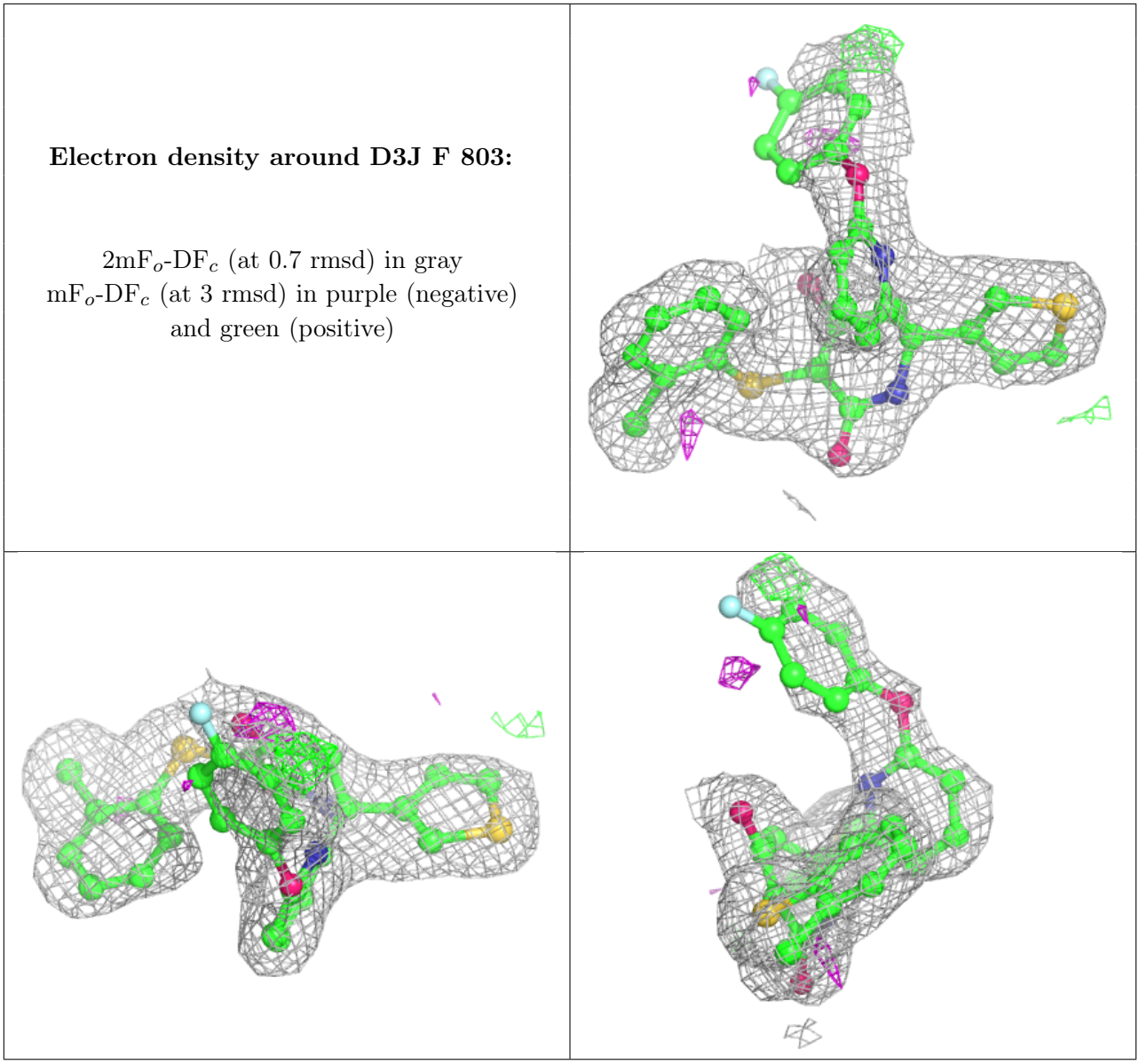
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	C	802	5/5	0.92	0.15	100,100,100,100	0
3	SO4	A	802	5/5	0.93	0.14	55,55,58,59	0
2	NAD	F	801	44/44	0.93	0.14	41,46,51,54	0
4	D3J	B	803	35/35	0.94	0.14	31,41,54,55	0
3	SO4	D	802	5/5	0.94	0.24	32,36,37,39	5
4	D3J	A	803	35/35	0.94	0.11	29,36,58,61	0
2	NAD	E	801	44/44	0.95	0.12	31,41,46,48	0
4	D3J	G	803	35/35	0.95	0.10	40,49,63,63	0
2	NAD	A	801	44/44	0.96	0.09	27,32,37,41	0
2	NAD	B	801	44/44	0.96	0.10	32,37,42,49	0
4	D3J	D	804	35/35	0.96	0.09	33,39,55,63	0
2	NAD	H	801	44/44	0.96	0.09	27,32,36,38	0
3	SO4	F	802	5/5	0.96	0.13	33,33,35,38	5
2	NAD	C	801	44/44	0.96	0.10	20,28,32,34	0
5	LAC	C	803	6/6	0.96	0.13	36,39,39,40	0
2	NAD	G	801	44/44	0.97	0.09	26,30,44,45	0
3	SO4	B	802	5/5	0.97	0.11	71,71,72,73	0
2	NAD	D	801	44/44	0.98	0.07	27,34,39,40	0
3	SO4	H	802	5/5	0.99	0.13	46,47,48,50	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.

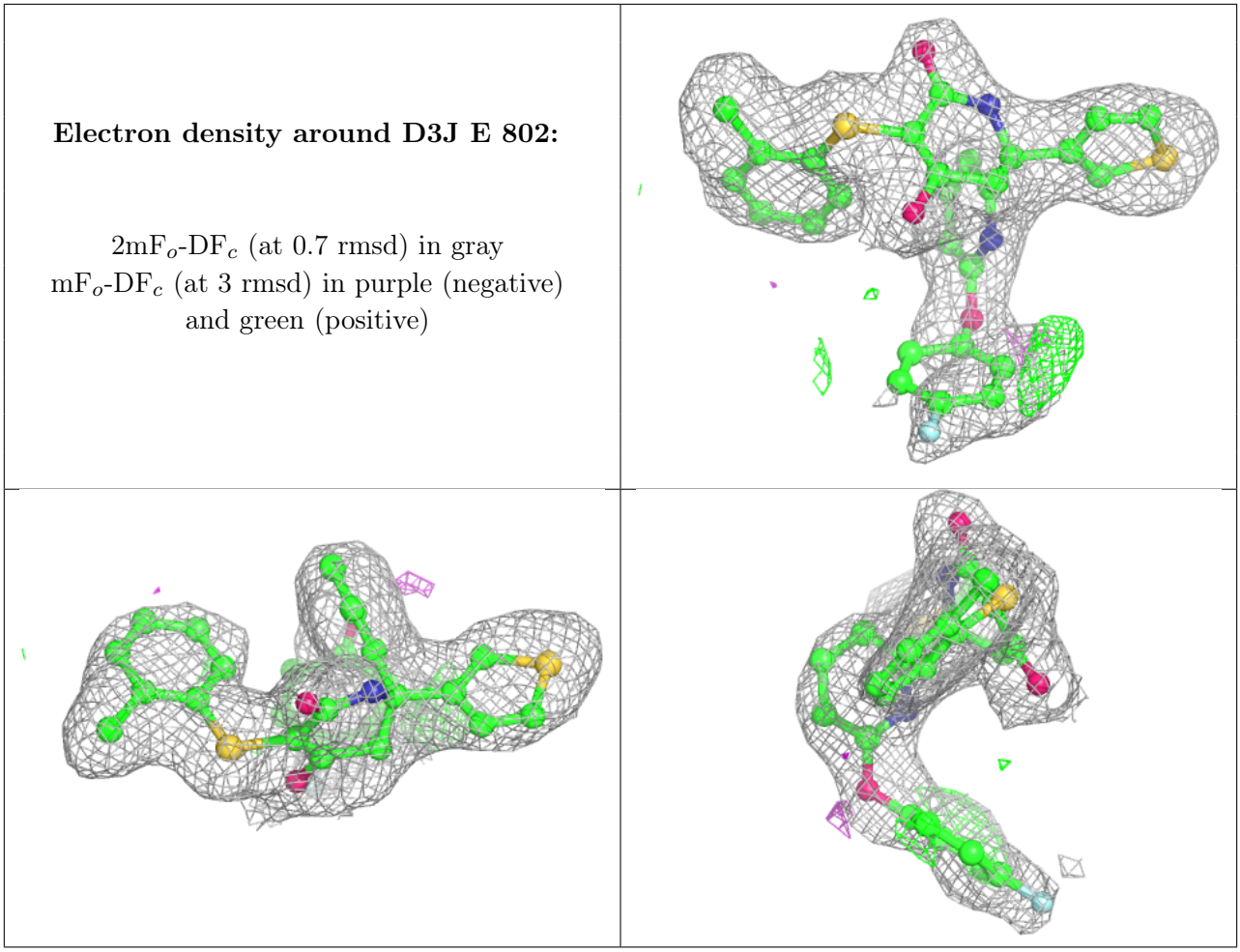
Electron density around D3J F 803:

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



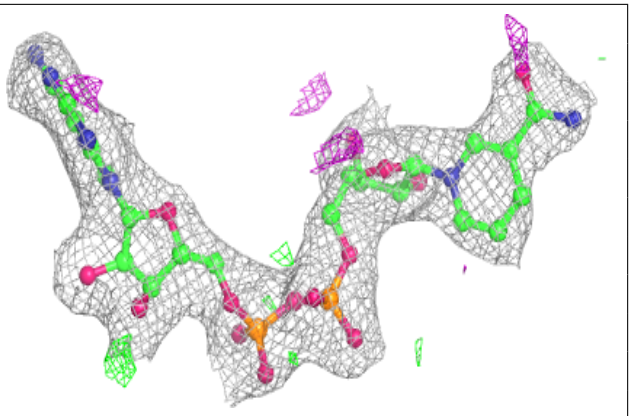
Electron density around D3J E 802:

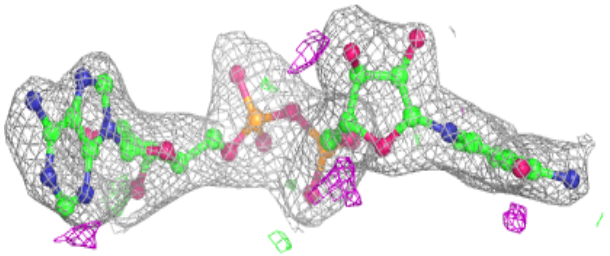
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

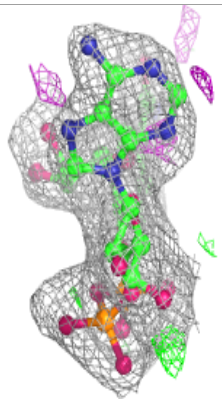


Electron density around NAD F 801:

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

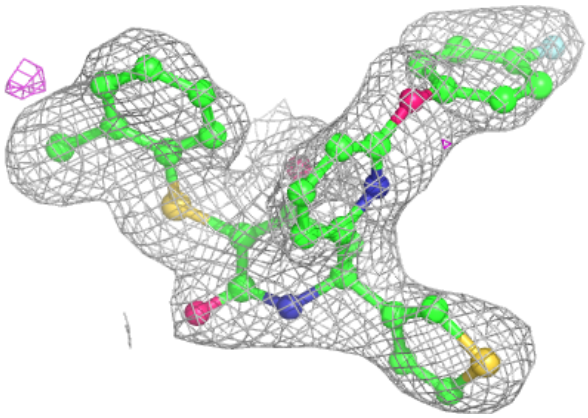


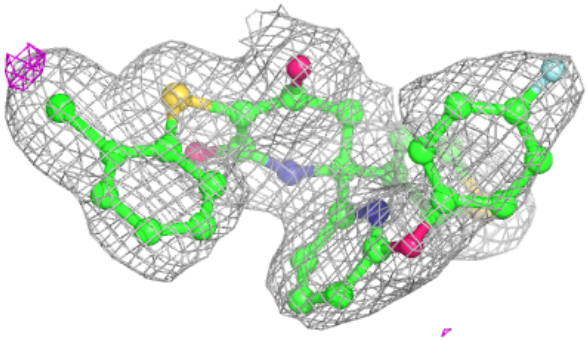


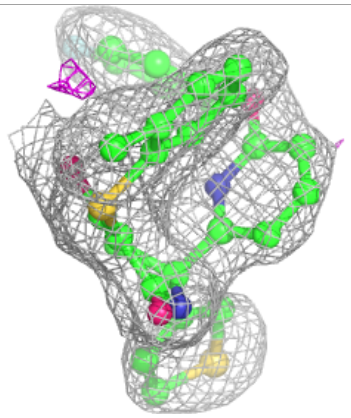


Electron density around D3J B 803:

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

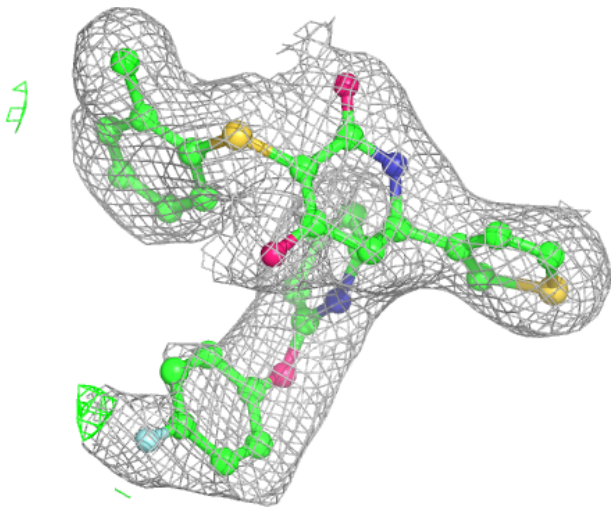


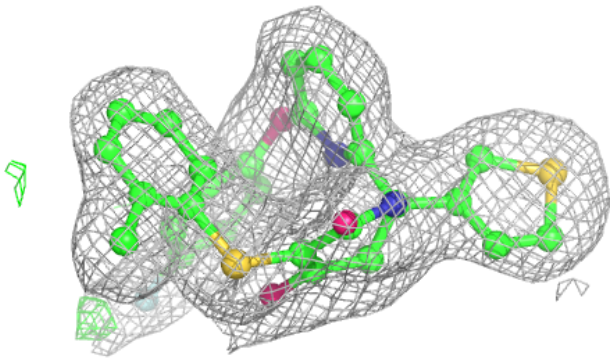


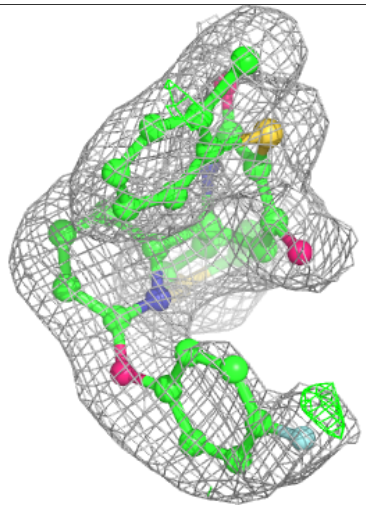


Electron density around D3J A 803:

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

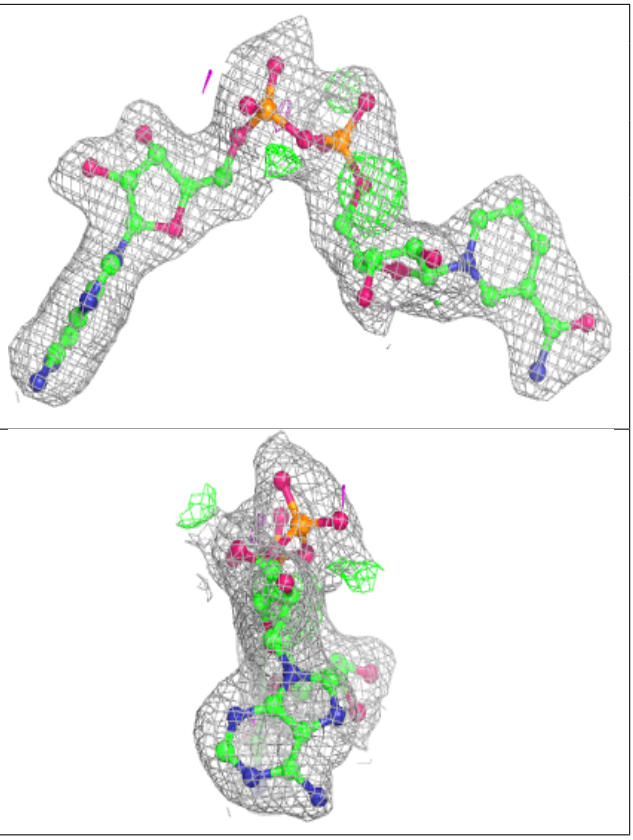






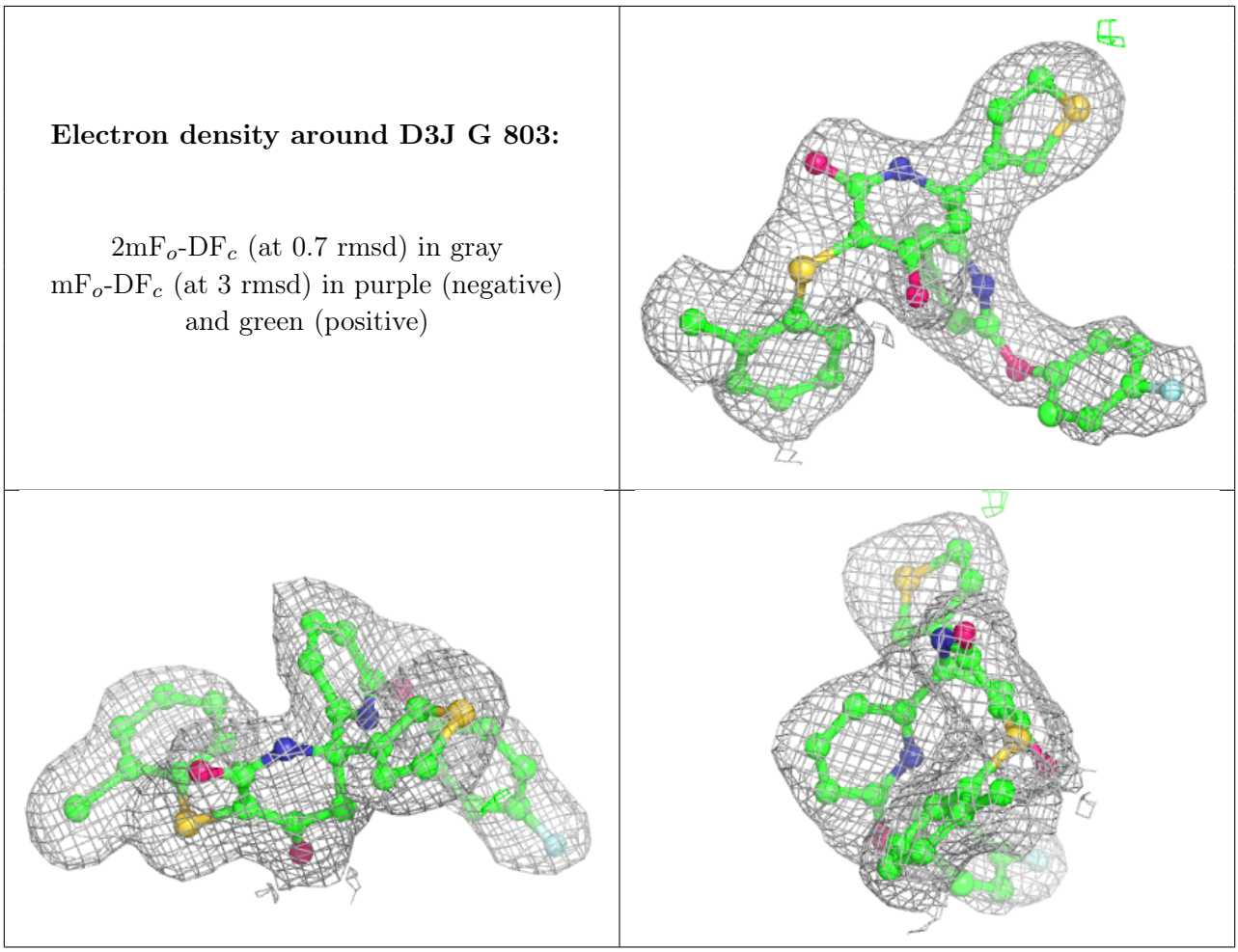
Electron density around NAD E 801:

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



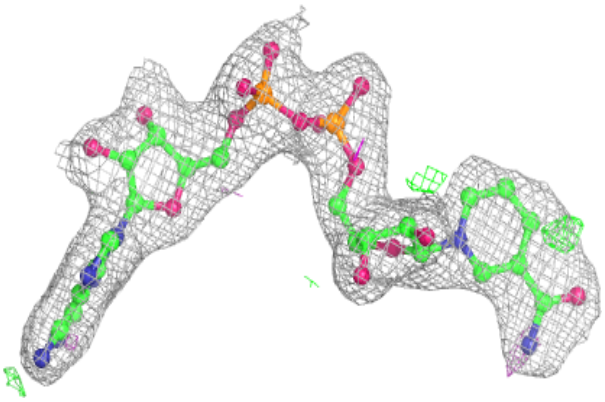
Electron density around D3J G 803:

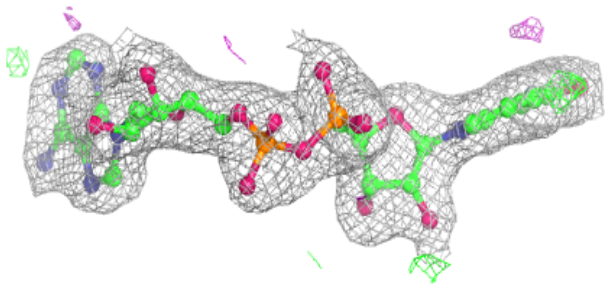
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

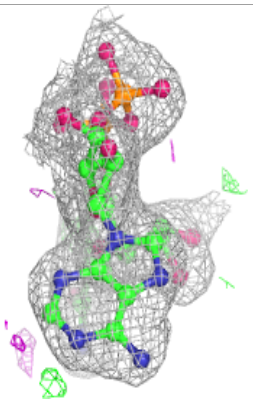


Electron density around NAD A 801:

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

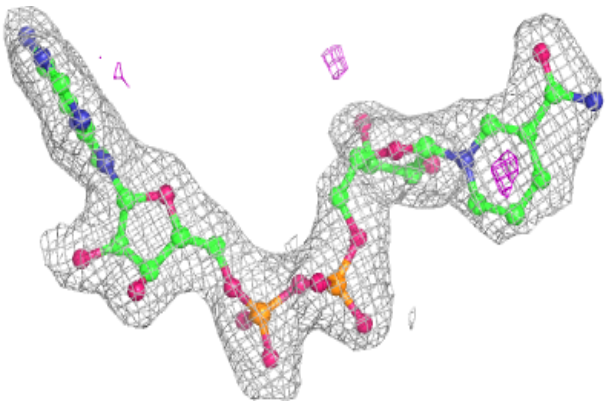


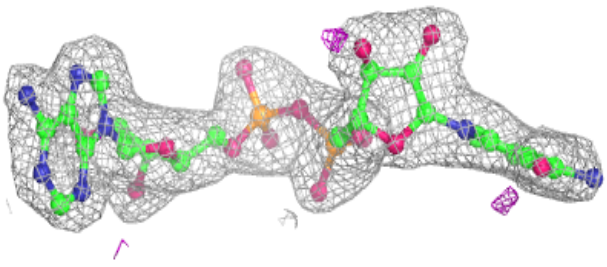


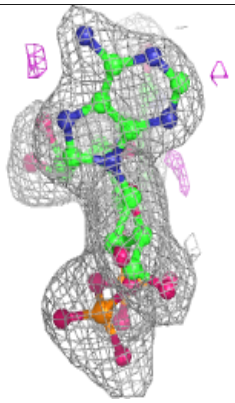


Electron density around NAD B 801:

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

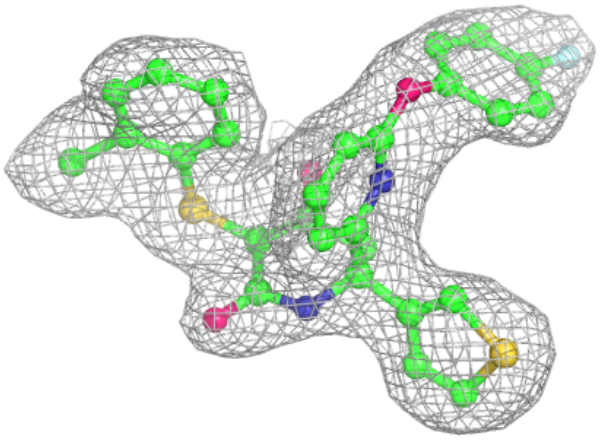


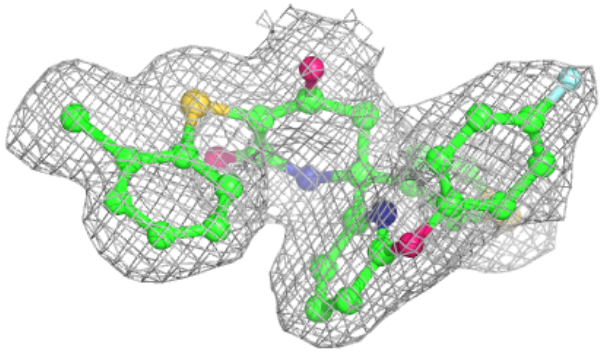


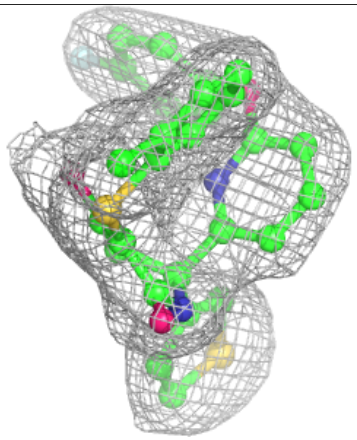


Electron density around D3J D 804:

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

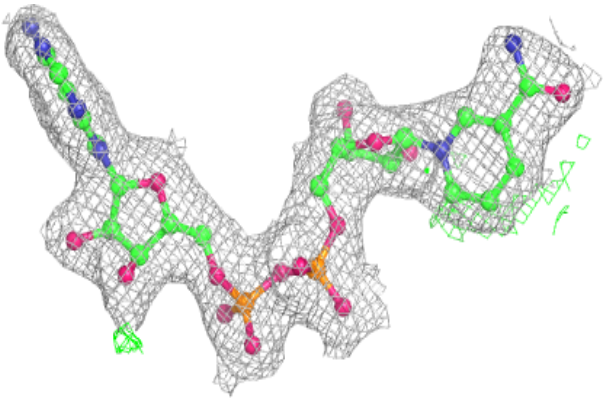


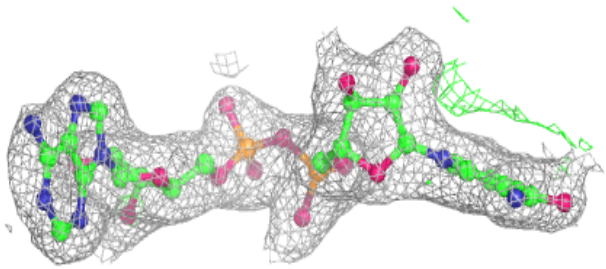


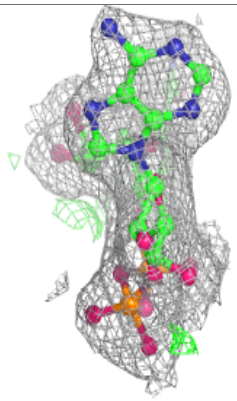


Electron density around NAD H 801:

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

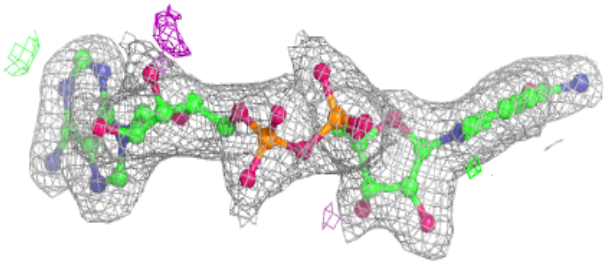


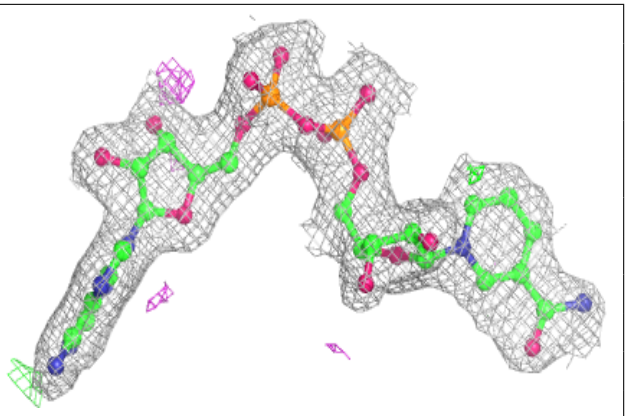


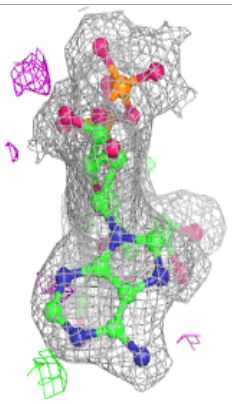


Electron density around NAD C 801:

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

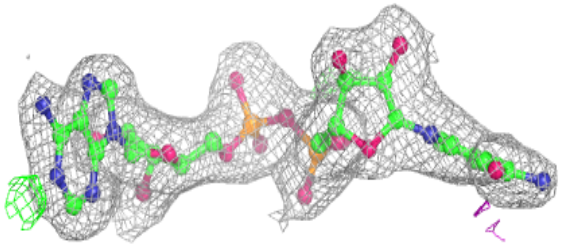


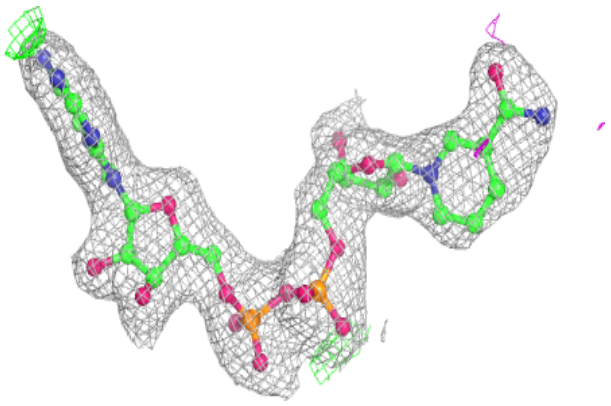


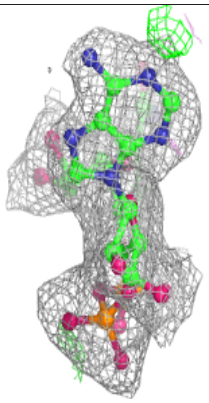


Electron density around NAD G 801:

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

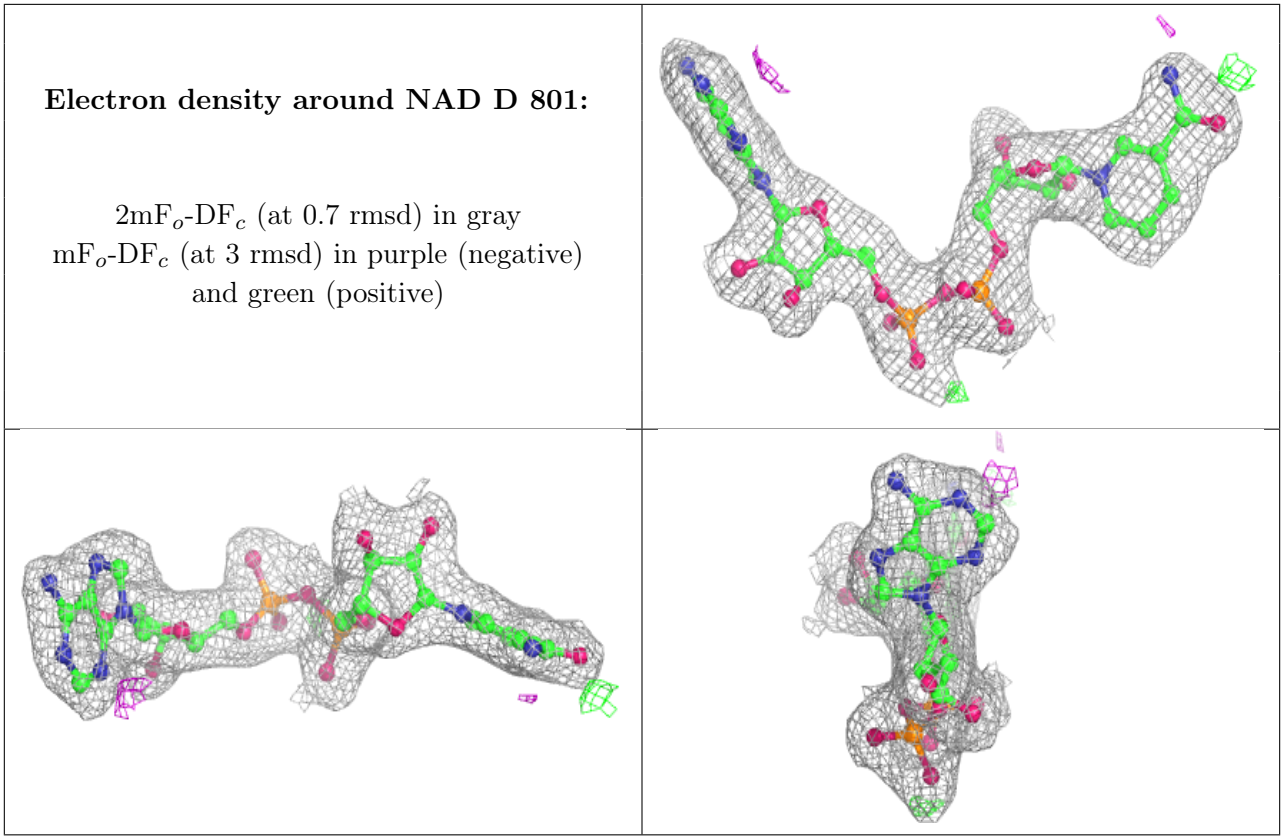






Electron density around NAD D 801:

$2mF_o$-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.