



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 01:55 PM BST

PDB ID : 6BAG
Title : Lactate Dehydrogenase in complex with inhibitor (R)-5-((2-chlorophenyl)thio)-6'-((4-fluorophenyl)amino)-4-hydroxy-2-(thiophen-3-yl)-2,3-dihydro-[2,2'-bi-pyridin]-6(1H)-one
Authors : Ultsch, M.; Eigenbrot, C.
Deposited on : 2017-10-12
Resolution : 2.40 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 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 : 2.13.1
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) : 2.13.1

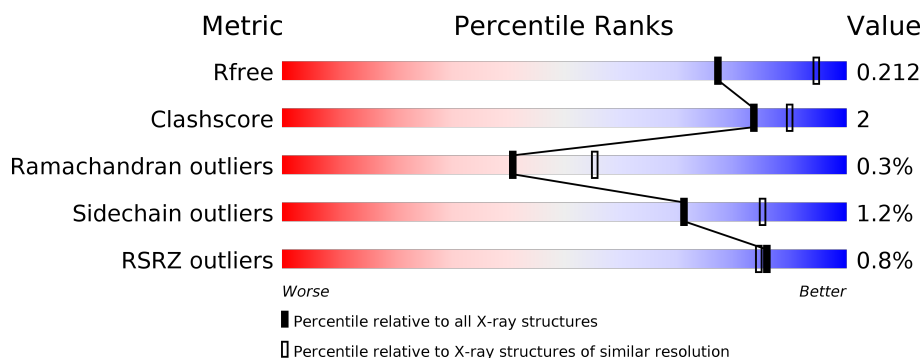
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	331	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>5% ..</div> </div> </div>
1	B	331	<div> <div></div> <div>92%</div> <div>8%</div> </div>
1	C	331	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>8% •</div> </div> </div>
1	D	331	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>

2 Entry composition [i](#)

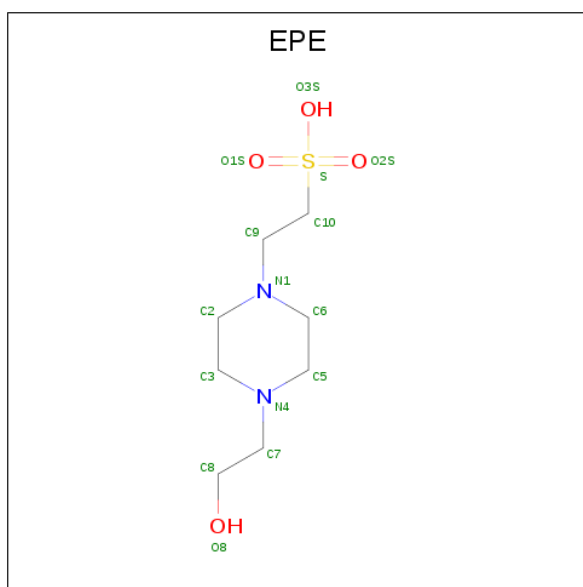
There are 6 unique types of molecules in this entry. The entry contains 11026 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	327	Total	C	N	O	S	0	1	0
			2536	1622	430	471	13			
1	B	331	Total	C	N	O	S	0	3	0
			2589	1657	442	477	13			
1	C	325	Total	C	N	O	S	0	1	0
			2522	1614	428	467	13			
1	D	331	Total	C	N	O	S	0	2	0
			2581	1652	439	477	13			

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

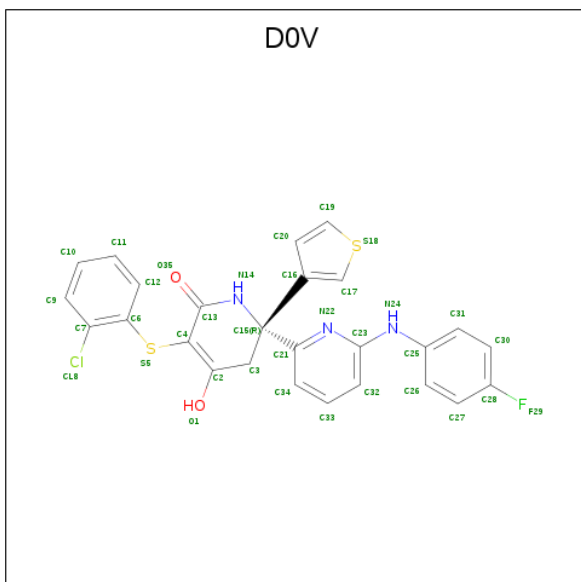
- # NAD
-
- The image displays the chemical structure of Nicotinamide Adenine Dinucleotide (NAD), a crucial coenzyme. The molecule is composed of two nucleotides linked by a pyrophosphate bridge. The top nucleotide consists of an adenine base (a purine ring system with an amino group at the 6-position) attached to a ribose sugar. The bottom nucleotide consists of a nicotinamide base (a pyrimidine ring system with a carbonyl group at the 3-position and an amino group at the 4-position) attached to another ribose sugar. The two ribose sugars are connected via their 5' and 3' phosphate groups, forming a pyrophosphate linkage. The structure is color-coded: adenine is blue, ribose is green, pyrophosphate is red, and nicotinamide is blue. Stereochemistry is indicated with wedges and dashes on the sugar rings.

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is (2R)-5-[(2-chlorophenyl)sulfanyl]-6'-[(4-fluorophenyl)amino]-4-hydroxy-2-(thiophen-3-yl)-2,3-dihydro[2,2'-bipyridin]-6(1H)-one (three-letter code: D0V) (formula: C₂₆H₁₉ClFN₃O₂S₂).



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

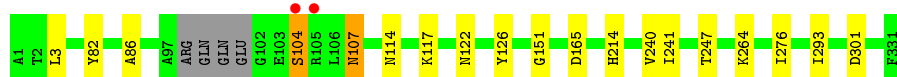
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	97	Total	O	0	0
			97	97		
6	B	113	Total	O	0	0
			113	113		
6	C	87	Total	O	0	0
			87	87		
6	D	120	Total	O	0	0
			120	120		

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.

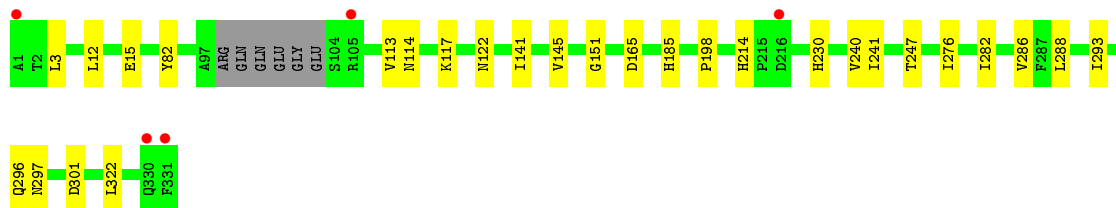
- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain



- Molecule 1: L-lactate dehydrogenase A chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.80 Å 81.01 Å 102.76 Å 90.00° 98.53° 90.00°	Depositor
Resolution (Å)	47.07 – 2.40 47.07 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.07-2.40) 99.7 (47.07-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.39 Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.175 , 0.213 0.175 , 0.212	Depositor DCC
R_{free} test set	1046 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11026	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: D0V, EPE, SO4, NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.46	0/2582	0.61	0/3491
1	B	0.46	0/2643	0.62	0/3573
1	C	0.46	0/2568	0.60	0/3473
1	D	0.48	0/2632	0.62	0/3559
All	All	0.47	0/10425	0.61	0/14096

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2536	0	2626	11	0
1	B	2589	0	2689	17	0
1	C	2522	0	2615	17	0
1	D	2581	0	2676	12	0
2	A	15	0	17	1	0
2	B	15	0	17	1	0
2	C	15	0	17	1	0
3	A	44	0	25	0	0
3	B	44	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	44	0	25	0	0
3	D	44	0	25	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	1	0
4	D	5	0	0	1	0
5	A	35	0	0	0	0
5	B	35	0	0	0	0
5	C	35	0	0	0	0
5	D	35	0	0	0	0
6	A	97	0	0	1	0
6	B	113	0	0	0	0
6	C	87	0	0	0	0
6	D	120	0	0	0	0
All	All	11026	0	10757	51	0

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

All (51) 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:A:104:SER:HB3	1:A:107:ASN:HB2	1.77	0.66
1:D:154:LYS:HE2	1:D:275:MET:HG2	1.82	0.61
1:A:264:LYS:HE3	6:A:533:HOH:O	2.01	0.60
1:D:106:LEU:HB3	1:D:110:GLN:HB2	1.84	0.59
1:B:276:ILE:HG12	1:B:288:LEU:HB2	1.86	0.56
1:C:3:LEU:HD13	1:D:214:HIS:HB2	1.88	0.56
1:C:151:GLY:O	2:C:401:EPE:H72	2.05	0.55
1:C:276:ILE:HG12	1:C:288:LEU:HB2	1.88	0.54
1:B:276:ILE:HD11	1:B:286:VAL:CG2	2.38	0.54
1:B:16:GLN:HB3	1:C:296:GLN:NE2	2.22	0.54
1:D:293[A]:ILE:HD12	1:D:301:ASP:HB2	1.89	0.53
1:A:3:LEU:HD13	1:B:214:HIS:HB2	1.91	0.53
1:B:276:ILE:HD11	1:B:286:VAL:HG23	1.92	0.52
1:A:214:HIS:HB2	1:B:3:LEU:HD13	1.92	0.50
1:C:114:ASN:HA	1:C:117:LYS:HD3	1.94	0.50
1:D:269:VAL:HG22	1:D:293[B]:ILE:HG13	1.93	0.48
1:A:151:GLY:O	2:A:401:EPE:H71	2.12	0.48
1:B:276:ILE:HD13	1:B:282:ILE:HD13	1.94	0.48
1:B:153:PRO:HA	2:B:401:EPE:H91	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:HIS:HD2	4:D:802:SO4:O2	1.99	0.45
1:B:293:ILE:HD12	1:B:301:ASP:HB2	1.99	0.45
1:C:276:ILE:HD11	1:C:286:VAL:HG23	1.98	0.44
1:B:168:ARG:HH12	1:B:247:THR:HG21	1.81	0.44
1:B:240:VAL:HG11	1:B:247:THR:HG22	2.00	0.44
1:C:113:VAL:HG22	1:C:145:VAL:HG21	2.00	0.44
1:C:185:HIS:HD2	4:C:403:SO4:O4	2.00	0.44
1:C:241:ILE:CD1	1:C:247:THR:HG23	2.48	0.44
1:B:103:GLU:OE2	1:B:111:ARG:HD3	2.17	0.43
1:B:82:TYR:CG	1:B:122:ASN:HB3	2.53	0.43
1:D:241:ILE:CD1	1:D:247:THR:HG23	2.48	0.43
1:C:276:ILE:HD11	1:C:286:VAL:CG2	2.49	0.43
1:C:276:ILE:HD13	1:C:282:ILE:HD13	2.00	0.43
1:D:86:ALA:HA	1:D:126:TYR:HB3	2.01	0.43
1:A:240:VAL:HG11	1:A:247:THR:HG22	2.01	0.43
1:A:241:ILE:CD1	1:A:247:THR:HG23	2.48	0.42
1:A:82:TYR:CG	1:A:122:ASN:HB3	2.53	0.42
1:C:214:HIS:HB2	1:D:3:LEU:HD13	2.01	0.42
1:A:293:ILE:HD12	1:A:301:ASP:HB2	2.01	0.42
1:C:293:ILE:HD12	1:C:301:ASP:HB2	2.00	0.42
1:C:82:TYR:CG	1:C:122:ASN:HB3	2.53	0.42
1:B:241:ILE:CD1	1:B:247:THR:HG23	2.50	0.42
1:C:240:VAL:HG11	1:C:247:THR:HG22	2.02	0.42
1:A:114:ASN:HA	1:A:117:LYS:HD3	2.00	0.41
1:B:86:ALA:HA	1:B:126:TYR:HB3	2.03	0.41
1:D:82:TYR:CG	1:D:122:ASN:HB3	2.55	0.41
1:C:198:PRO:HG3	1:C:230:HIS:CG	2.56	0.41
1:B:72[B]:ARG:HE	1:B:72[B]:ARG:HB2	1.71	0.41
1:A:86:ALA:HA	1:A:126:TYR:HB3	2.02	0.41
1:D:141:ILE:HG13	1:D:322:LEU:HD22	2.02	0.41
1:C:141:ILE:HG13	1:C:322:LEU:HD22	2.03	0.41
1:B:180:HIS:HB2	1:D:266:LEU:O	2.21	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	324/331 (98%)	316 (98%)	7 (2%)	1 (0%)	41	55
1	B	332/331 (100%)	323 (97%)	7 (2%)	2 (1%)	25	36
1	C	322/331 (97%)	315 (98%)	7 (2%)	0	100	100
1	D	331/331 (100%)	323 (98%)	7 (2%)	1 (0%)	41	55
All	All	1309/1324 (99%)	1277 (98%)	28 (2%)	4 (0%)	41	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	SER
1	B	101	GLU
1	D	100	GLN
1	B	14	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	284/287 (99%)	281 (99%)	3 (1%)	73	87
1	B	290/287 (101%)	288 (99%)	2 (1%)	84	92
1	C	283/287 (99%)	279 (99%)	4 (1%)	67	82
1	D	289/287 (101%)	284 (98%)	5 (2%)	60	78
All	All	1146/1148 (100%)	1132 (99%)	14 (1%)	71	85

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	165	ASP

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Mol	Chain	Res	Type
1	A	276	ILE
1	B	19	GLN
1	B	165	ASP
1	C	12	LEU
1	C	15	GLU
1	C	165	ASP
1	C	297	ASN
1	D	15	GLU
1	D	103	GLU
1	D	107	ASN
1	D	110	GLN
1	D	165	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	185	HIS
1	C	185	HIS
1	C	296	GLN
1	D	16	GLN
1	D	185	HIS

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](#)

15 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	SO4	B	403	-	4,4,4	0.25	0	6,6,6	0.15	0
3	NAD	A	402	-	42,48,48	1.82	8 (19%)	50,73,73	1.30	5 (10%)
4	SO4	A	403	-	4,4,4	0.08	0	6,6,6	0.38	0
3	NAD	B	402	-	42,48,48	1.86	9 (21%)	50,73,73	1.26	7 (14%)
4	SO4	C	403	-	4,4,4	0.42	0	6,6,6	0.19	0
2	EPE	B	401	-	15,15,15	1.26	1 (6%)	18,20,20	0.30	0
2	EPE	A	401	-	15,15,15	1.46	1 (6%)	18,20,20	0.53	0
3	NAD	D	801	-	42,48,48	1.81	8 (19%)	50,73,73	1.30	6 (12%)
5	D0V	C	404	-	35,39,39	1.33	2 (5%)	40,56,56	1.89	6 (15%)
5	D0V	B	404	-	35,39,39	1.27	2 (5%)	40,56,56	1.76	5 (12%)
5	D0V	A	404	-	35,39,39	1.15	2 (5%)	40,56,56	1.73	8 (20%)
5	D0V	D	803	-	35,39,39	1.48	2 (5%)	40,56,56	1.89	6 (15%)
2	EPE	C	401	-	15,15,15	1.05	1 (6%)	18,20,20	0.42	0
4	SO4	D	802	-	4,4,4	0.29	0	6,6,6	0.38	0
3	NAD	C	402	-	42,48,48	1.84	8 (19%)	50,73,73	1.26	7 (14%)

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
3	NAD	A	402	-	-	4/26/62/62	0/5/5/5
3	NAD	B	402	-	-	4/26/62/62	0/5/5/5
2	EPE	B	401	-	-	5/9/19/19	0/1/1/1
2	EPE	A	401	-	-	2/9/19/19	0/1/1/1
3	NAD	D	801	-	-	4/26/62/62	0/5/5/5
5	D0V	C	404	-	-	1/12/38/38	0/5/5/5
5	D0V	B	404	-	-	1/12/38/38	0/5/5/5
5	D0V	A	404	-	-	1/12/38/38	0/5/5/5
5	D0V	D	803	-	-	1/12/38/38	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EPE	C	401	-	-	4/9/19/19	0/1/1/1
3	NAD	C	402	-	-	4/26/62/62	0/5/5/5

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	NAD	C7N-N7N	5.75	1.43	1.33
3	D	801	NAD	C7N-N7N	5.73	1.43	1.33
3	A	402	NAD	C7N-N7N	5.62	1.43	1.33
2	A	401	EPE	C10-S	-5.49	1.69	1.77
3	B	402	NAD	C7N-N7N	5.43	1.43	1.33
5	D	803	D0V	C17-C16	-5.34	1.33	1.37
5	C	404	D0V	C17-C16	-4.81	1.34	1.37
2	B	401	EPE	C10-S	-4.80	1.70	1.77
3	B	402	NAD	C2B-C3B	-4.43	1.41	1.53
3	A	402	NAD	C2B-C3B	-4.42	1.41	1.53
5	D	803	D0V	C17-S18	4.26	1.76	1.70
3	D	801	NAD	C2B-C3B	-4.20	1.41	1.53
5	C	404	D0V	C17-S18	4.11	1.76	1.70
5	B	404	D0V	C17-C16	-4.11	1.34	1.37
3	C	402	NAD	C2B-C3B	-4.08	1.42	1.53
5	B	404	D0V	C17-S18	3.85	1.75	1.70
2	C	401	EPE	C10-S	-3.85	1.72	1.77
5	A	404	D0V	C17-S18	3.66	1.75	1.70
5	A	404	D0V	C17-C16	-3.48	1.34	1.37
3	D	801	NAD	C6A-N6A	3.35	1.46	1.34
3	C	402	NAD	C6A-N6A	3.34	1.46	1.34
3	B	402	NAD	C6A-N6A	3.26	1.46	1.34
3	A	402	NAD	C6A-N6A	3.17	1.45	1.34
3	B	402	NAD	O2D-C2D	-3.02	1.35	1.43
3	C	402	NAD	O2D-C2D	-2.98	1.36	1.43
3	D	801	NAD	O2D-C2D	-2.87	1.36	1.43
3	A	402	NAD	O2D-C2D	-2.87	1.36	1.43
3	D	801	NAD	C2B-C1B	-2.71	1.49	1.53
3	B	402	NAD	C2B-C1B	-2.70	1.49	1.53
3	B	402	NAD	C5D-C4D	-2.56	1.43	1.51
3	D	801	NAD	C5D-C4D	-2.43	1.44	1.51
3	A	402	NAD	C2B-C1B	-2.42	1.50	1.53
3	C	402	NAD	C5D-C4D	-2.38	1.44	1.51
3	C	402	NAD	C2B-C1B	-2.34	1.50	1.53
3	A	402	NAD	C5D-C4D	-2.31	1.44	1.51
3	B	402	NAD	O4B-C4B	-2.30	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	NAD	C2D-C1D	-2.29	1.50	1.53
3	C	402	NAD	C2N-N1N	2.15	1.37	1.35
3	D	801	NAD	O4B-C4B	-2.14	1.40	1.45
3	A	402	NAD	C5B-C4B	-2.13	1.45	1.51
3	C	402	NAD	C5B-C4B	-2.07	1.45	1.51
3	B	402	NAD	C5B-C4B	-2.06	1.45	1.51
3	D	801	NAD	C5B-C4B	-2.03	1.45	1.51
3	B	402	NAD	C2D-C1D	-2.03	1.50	1.53

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	404	D0V	C15-N14-C13	6.92	122.48	117.33
5	A	404	D0V	C15-N14-C13	6.61	122.25	117.33
5	B	404	D0V	C15-N14-C13	5.99	121.79	117.33
5	D	803	D0V	C15-N14-C13	5.68	121.56	117.33
5	D	803	D0V	C16-C17-S18	-5.61	108.68	112.29
3	D	801	NAD	N3A-C2A-N1A	-4.90	121.02	128.68
3	C	402	NAD	N3A-C2A-N1A	-4.86	121.08	128.68
3	B	402	NAD	N3A-C2A-N1A	-4.84	121.12	128.68
3	A	402	NAD	N3A-C2A-N1A	-4.84	121.12	128.68
5	C	404	D0V	C16-C17-S18	-4.75	109.23	112.29
5	B	404	D0V	C16-C17-S18	-4.51	109.39	112.29
5	D	803	D0V	C23-N22-C21	3.92	123.73	118.17
5	D	803	D0V	C6-S5-C4	3.51	107.27	102.81
5	A	404	D0V	C23-N22-C21	3.48	123.10	118.17
5	B	404	D0V	C23-N22-C21	3.21	122.72	118.17
5	D	803	D0V	C4-C13-N14	3.19	119.61	114.39
5	C	404	D0V	C4-C13-N14	3.12	119.50	114.39
3	D	801	NAD	C3N-C7N-N7N	3.04	121.40	117.75
5	C	404	D0V	C23-N22-C21	3.02	122.45	118.17
5	A	404	D0V	C16-C17-S18	-2.91	110.42	112.29
5	B	404	D0V	C4-C13-N14	2.87	119.09	114.39
3	A	402	NAD	C3N-C7N-N7N	2.84	121.15	117.75
5	A	404	D0V	C6-S5-C4	2.79	106.35	102.81
3	B	402	NAD	O4B-C1B-C2B	-2.59	103.15	106.93
5	C	404	D0V	C3-C15-N14	2.54	111.16	108.09
3	A	402	NAD	O7N-C7N-N7N	-2.53	118.99	122.58
5	A	404	D0V	C3-C15-N14	2.52	111.14	108.09
5	A	404	D0V	C34-C21-N22	-2.38	119.07	122.20
5	A	404	D0V	C4-C13-N14	2.38	118.28	114.39
3	D	801	NAD	C4A-C5A-N7A	-2.36	106.94	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	801	NAD	O5D-C5D-C4D	2.35	117.07	108.99
3	D	801	NAD	O7N-C7N-N7N	-2.34	119.26	122.58
5	D	803	D0V	C32-C23-N22	-2.33	119.23	123.16
5	C	404	D0V	C32-C23-N22	-2.29	119.29	123.16
5	B	404	D0V	C32-C23-N22	-2.28	119.32	123.16
3	C	402	NAD	C4A-C5A-N7A	-2.27	107.04	109.40
3	D	801	NAD	O4B-C1B-C2B	-2.24	103.65	106.93
3	B	402	NAD	O5D-C5D-C4D	2.22	116.62	108.99
3	A	402	NAD	O5D-C5D-C4D	2.21	116.61	108.99
3	B	402	NAD	PN-O3-PA	-2.21	125.25	132.83
3	C	402	NAD	O5D-C5D-C4D	2.18	116.48	108.99
3	B	402	NAD	O7N-C7N-N7N	-2.16	119.50	122.58
3	C	402	NAD	C3N-C7N-N7N	2.16	120.34	117.75
3	B	402	NAD	C3N-C7N-N7N	2.14	120.32	117.75
3	B	402	NAD	C4A-C5A-N7A	-2.12	107.19	109.40
5	A	404	D0V	C15-C21-N22	2.11	119.35	116.12
3	A	402	NAD	C4A-C5A-N7A	-2.07	107.25	109.40
3	C	402	NAD	PN-O3-PA	-2.05	125.78	132.83
3	C	402	NAD	O4B-C1B-C2B	-2.04	103.95	106.93
3	C	402	NAD	O7N-C7N-N7N	-2.02	119.70	122.58

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	NAD	O4D-C1D-N1N-C2N
3	A	402	NAD	O4D-C1D-N1N-C6N
3	A	402	NAD	C2D-C1D-N1N-C2N
3	B	402	NAD	O4D-C1D-N1N-C2N
3	B	402	NAD	O4D-C1D-N1N-C6N
3	B	402	NAD	C2D-C1D-N1N-C2N
3	D	801	NAD	O4D-C1D-N1N-C2N
3	D	801	NAD	O4D-C1D-N1N-C6N
3	D	801	NAD	C2D-C1D-N1N-C2N
2	C	401	EPE	S-C10-C9-N1
2	C	401	EPE	C9-C10-S-O1S
3	C	402	NAD	O4D-C1D-N1N-C2N
3	C	402	NAD	O4D-C1D-N1N-C6N
3	C	402	NAD	C2D-C1D-N1N-C2N
2	C	401	EPE	C9-C10-S-O3S
2	B	401	EPE	C10-C9-N1-C2
2	C	401	EPE	C9-C10-S-O2S

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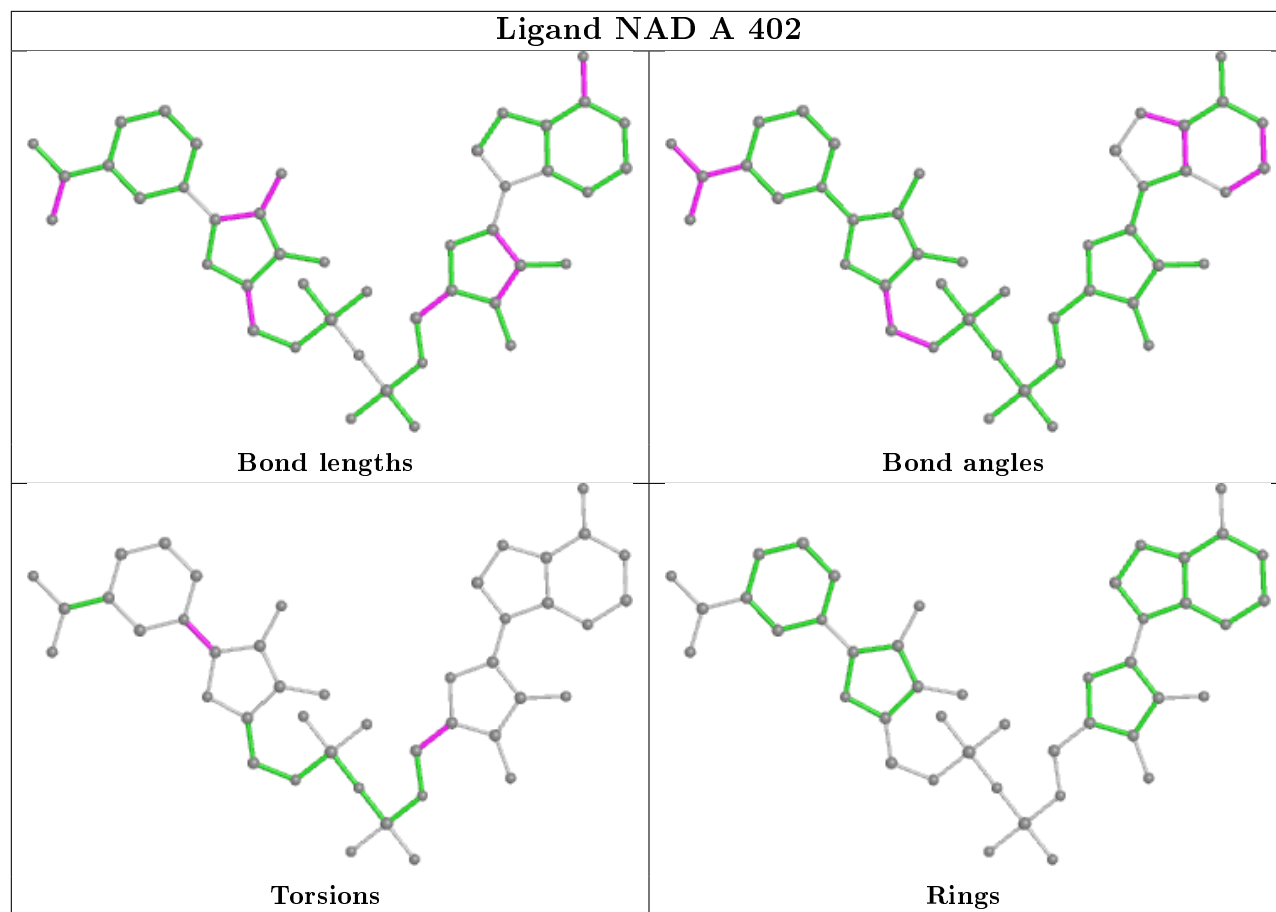
Mol	Chain	Res	Type	Atoms
5	C	404	D0V	C3-C15-C21-C34
5	A	404	D0V	C3-C15-C21-C34
2	B	401	EPE	C8-C7-N4-C5
2	A	401	EPE	C8-C7-N4-C3
2	B	401	EPE	C10-C9-N1-C6
2	B	401	EPE	C8-C7-N4-C3
2	A	401	EPE	C8-C7-N4-C5
3	A	402	NAD	O4B-C4B-C5B-O5B
3	B	402	NAD	O4B-C4B-C5B-O5B
3	D	801	NAD	O4B-C4B-C5B-O5B
3	C	402	NAD	O4B-C4B-C5B-O5B
2	B	401	EPE	S-C10-C9-N1
5	B	404	D0V	C3-C15-C21-C34
5	D	803	D0V	C3-C15-C21-C34

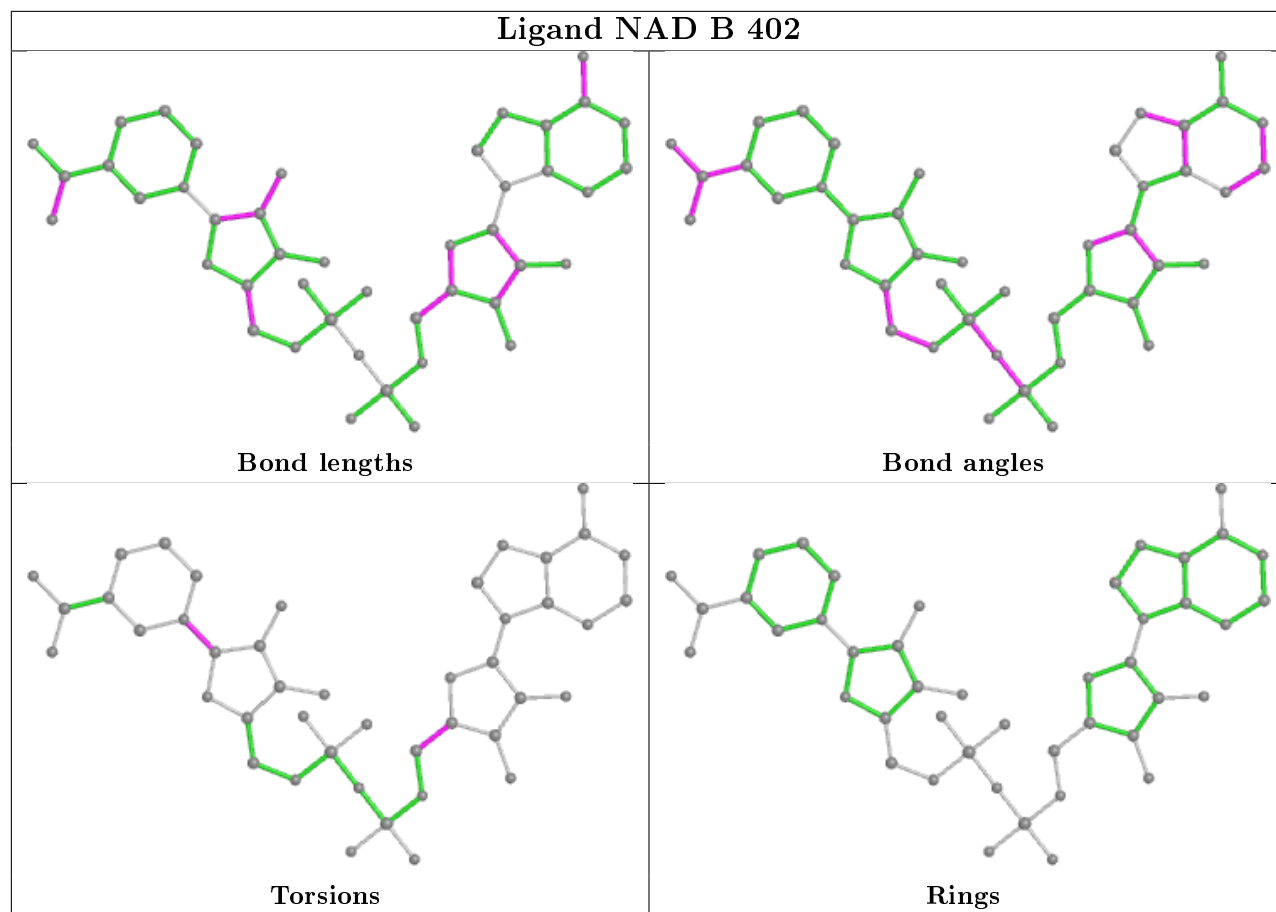
There are no ring outliers.

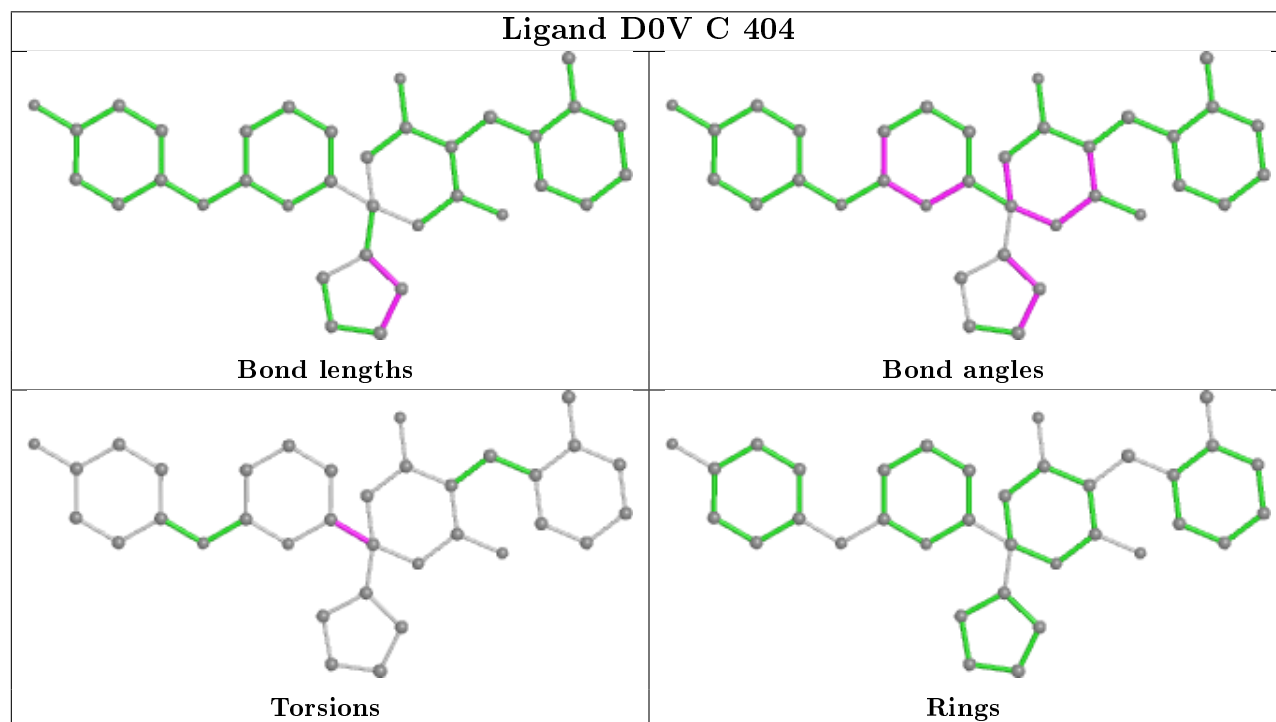
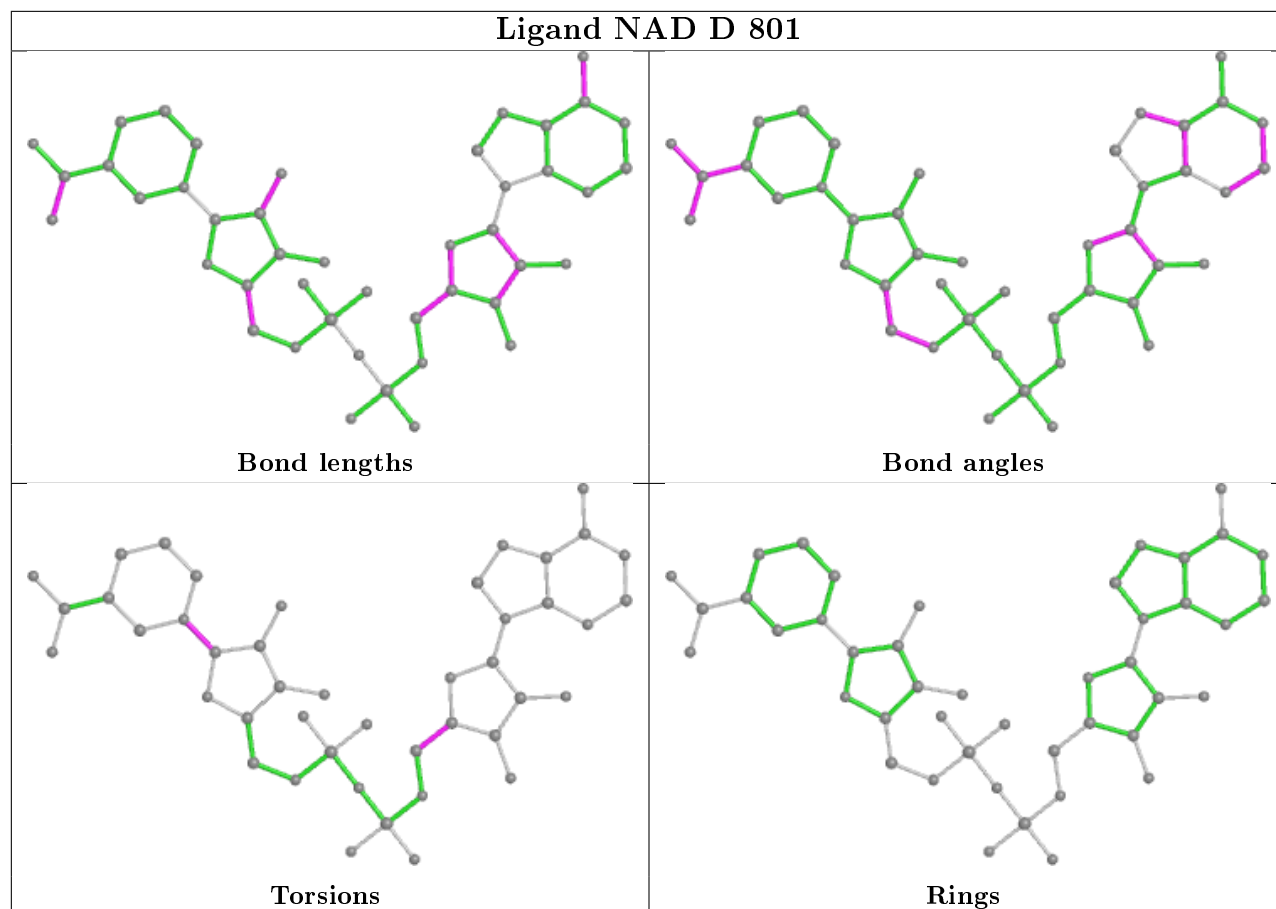
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	403	SO4	1	0
2	B	401	EPE	1	0
2	A	401	EPE	1	0
2	C	401	EPE	1	0
4	D	802	SO4	1	0

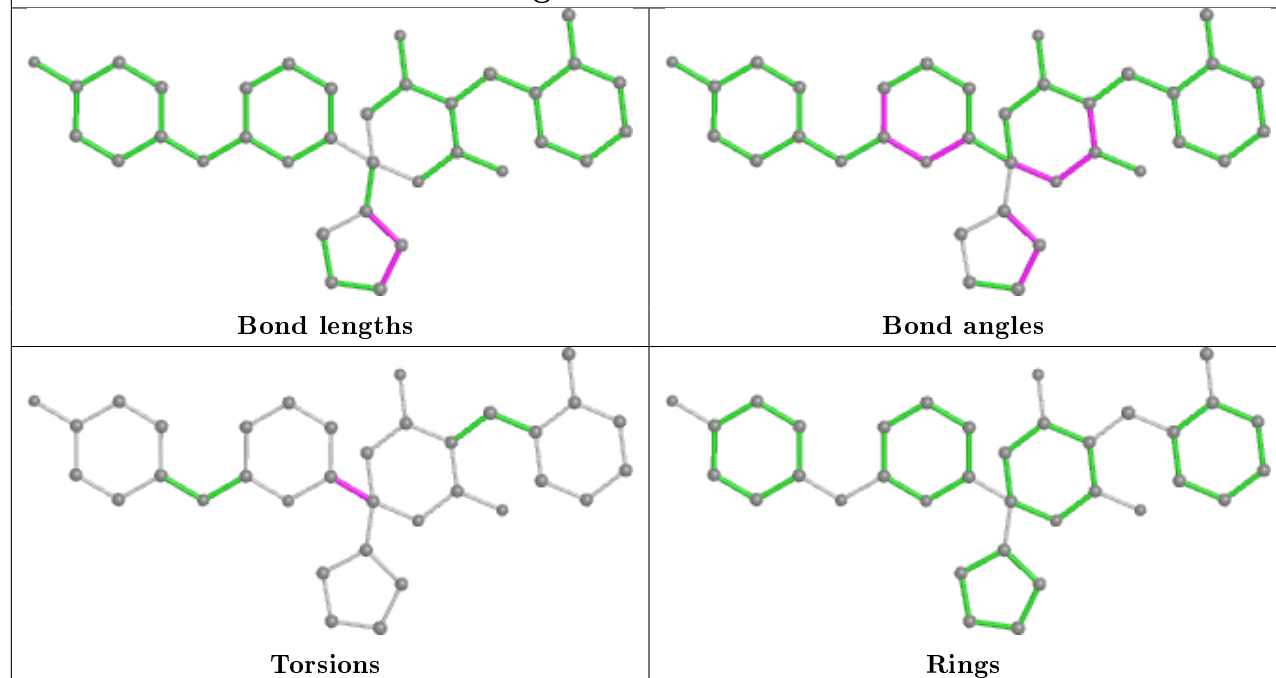
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



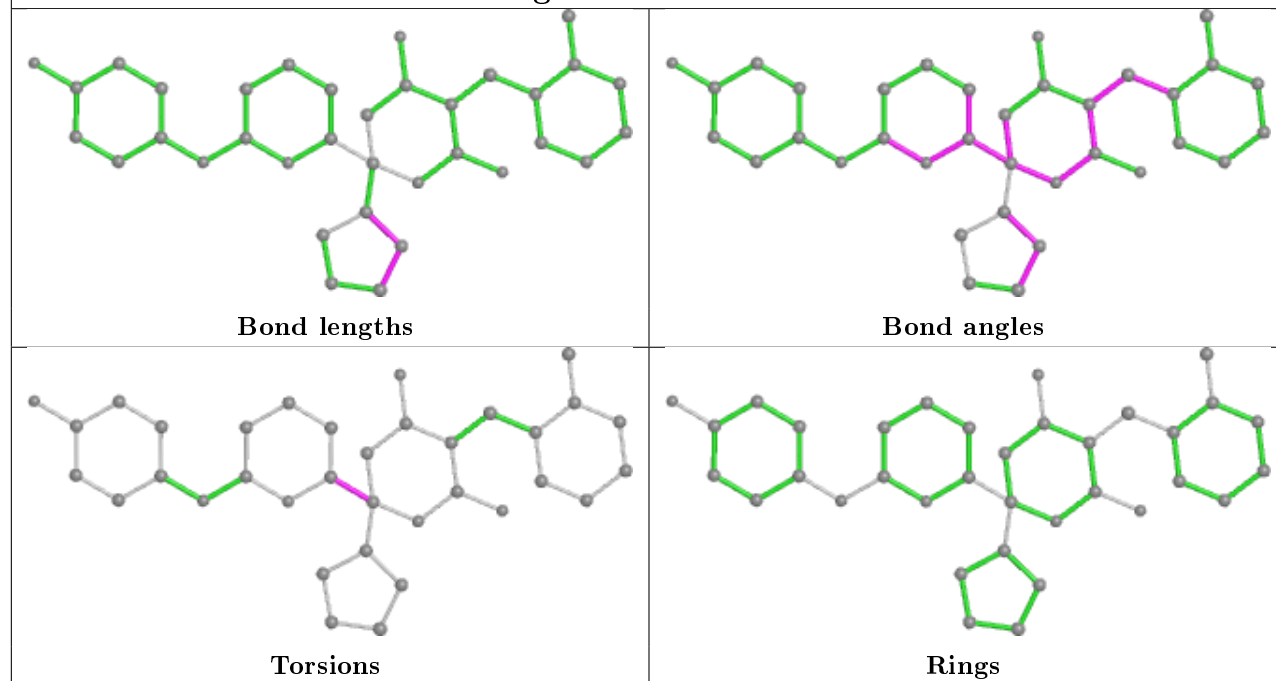


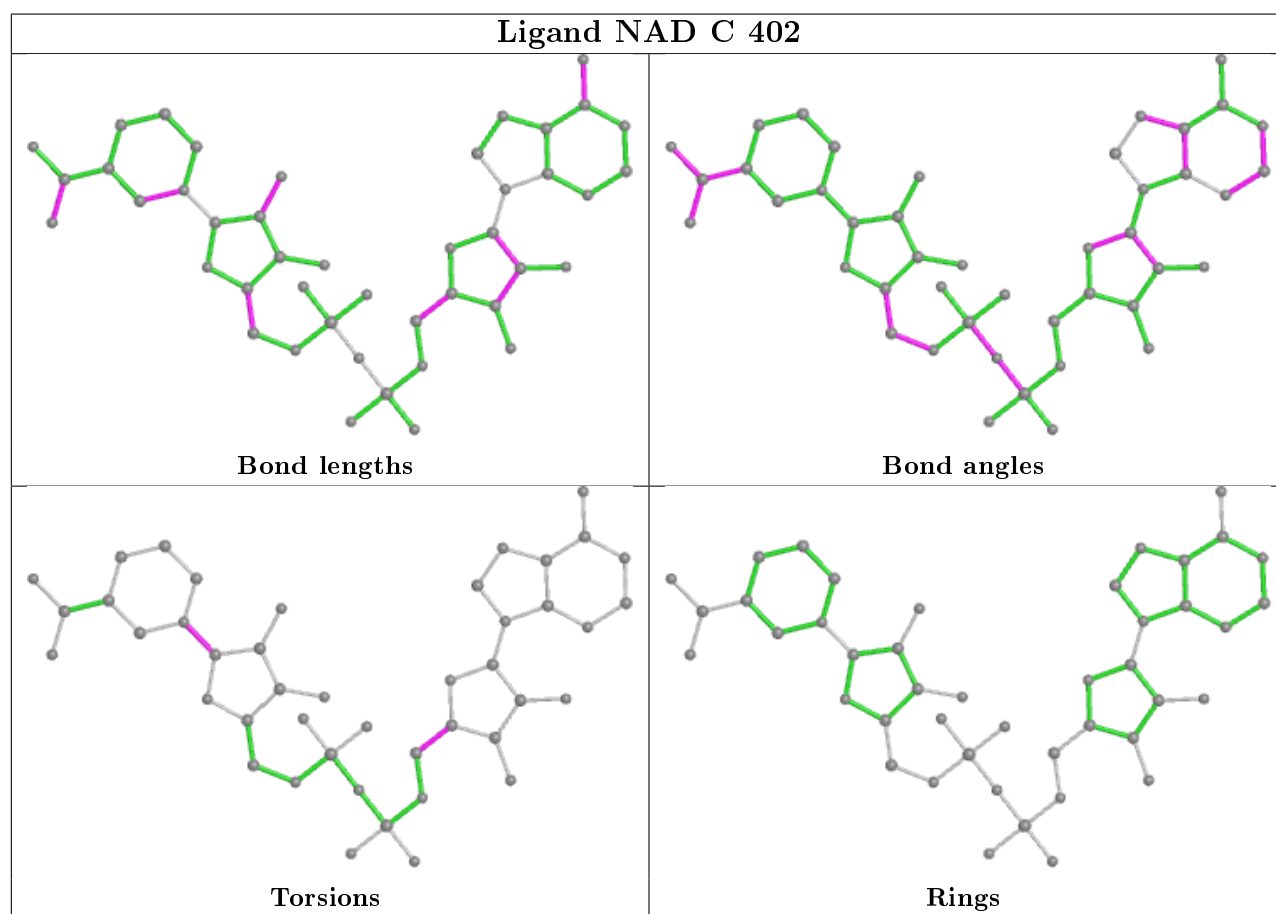
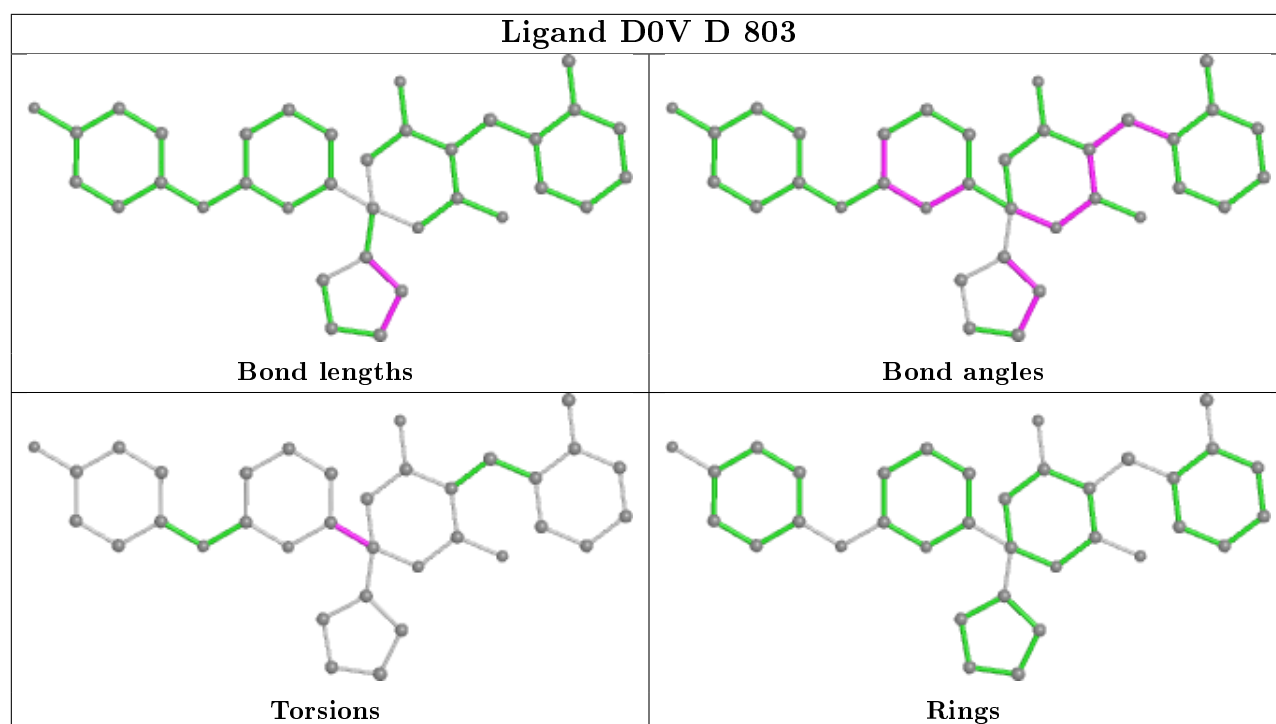


Ligand D0V B 404



Ligand D0V A 404





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	327/331 (98%)	-0.56	2 (0%) 89 88	23, 32, 57, 96	0
1	B	331/331 (100%)	-0.61	1 (0%) 94 93	21, 32, 57, 87	0
1	C	325/331 (98%)	-0.23	5 (1%) 73 72	22, 35, 64, 93	0
1	D	331/331 (100%)	-0.48	2 (0%) 89 88	21, 30, 63, 93	0
All	All	1314/1324 (99%)	-0.47	10 (0%) 86 84	21, 32, 59, 96	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	ALA	4.7
1	C	331	PHE	4.6
1	C	105	ARG	3.8
1	C	1	ALA	3.5
1	A	104	SER	3.4
1	C	330	GLN	2.6
1	A	105	ARG	2.5
1	B	1	ALA	2.3
1	C	216	ASP	2.2
1	D	98	ARG	2.1

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 ⓘ

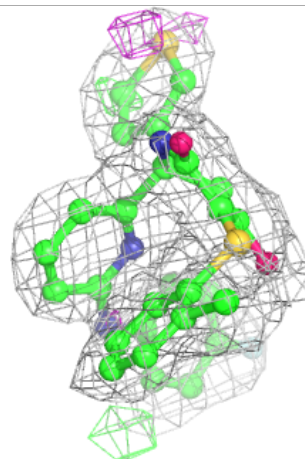
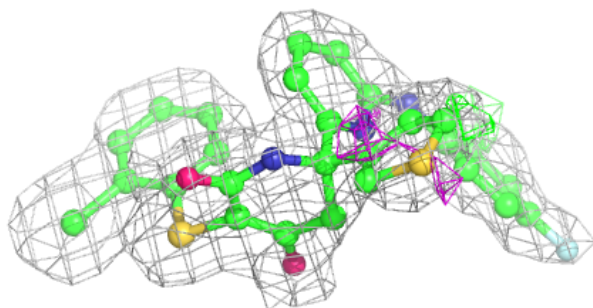
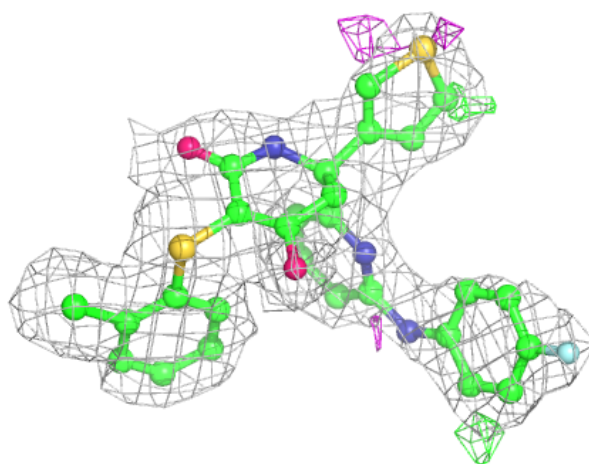
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EPE	A	401	15/15	0.87	0.32	33,39,44,45	15
2	EPE	C	401	15/15	0.90	0.19	49,53,55,55	15
2	EPE	B	401	15/15	0.92	0.20	51,56,65,66	15
5	D0V	B	404	35/35	0.94	0.13	31,39,54,59	0
5	D0V	C	404	35/35	0.95	0.12	31,37,49,53	0
3	NAD	C	402	44/44	0.95	0.12	30,36,43,48	0
5	D0V	D	803	35/35	0.96	0.12	31,36,53,58	0
4	SO4	C	403	5/5	0.96	0.12	43,47,51,52	0
5	D0V	A	404	35/35	0.96	0.14	30,35,42,43	0
3	NAD	B	402	44/44	0.97	0.09	27,34,39,43	0
3	NAD	D	801	44/44	0.97	0.11	25,33,39,41	0
3	NAD	A	402	44/44	0.97	0.10	31,35,37,39	0
4	SO4	A	403	5/5	0.97	0.11	62,62,64,64	0
4	SO4	D	802	5/5	0.98	0.07	38,40,42,43	0
4	SO4	B	403	5/5	0.98	0.09	42,45,47,48	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.

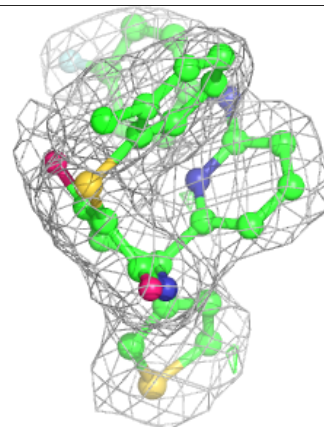
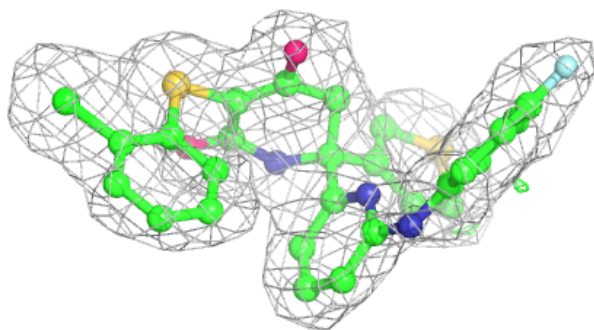
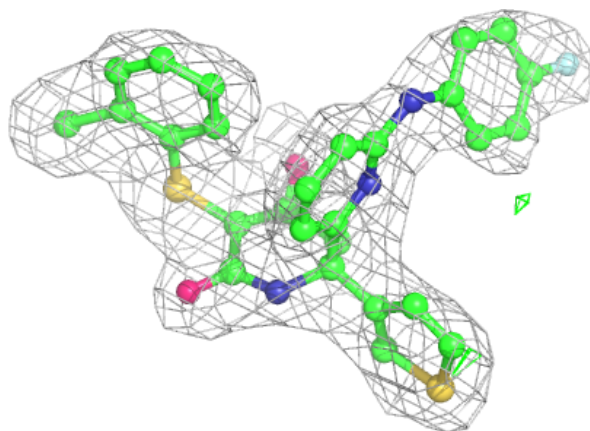
Electron density around D0V B 404:

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

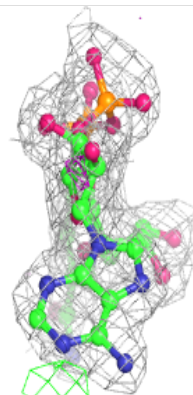
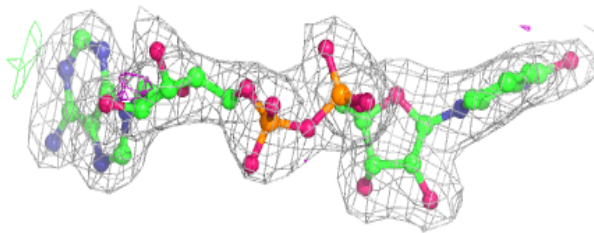
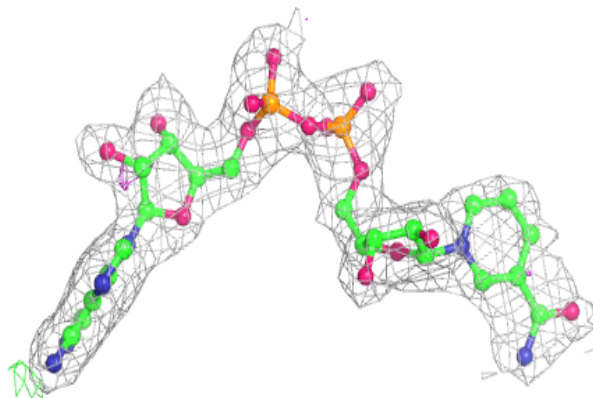


Electron density around D0V C 404:

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

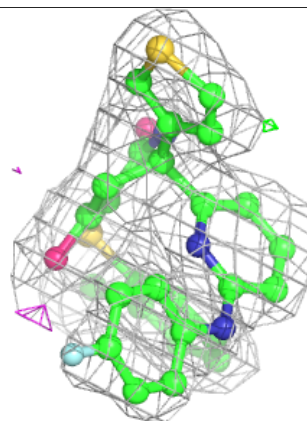
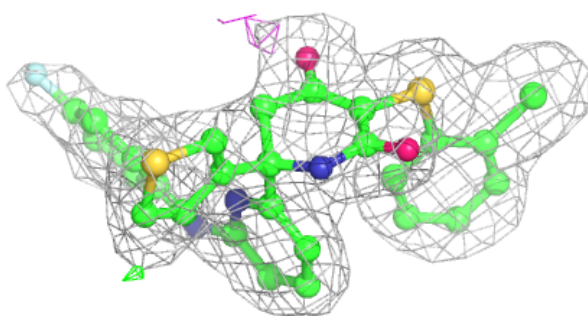
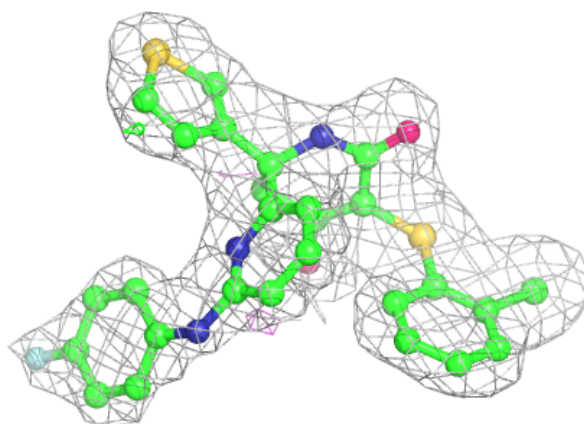
**Electron density around NAD C 402:**

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



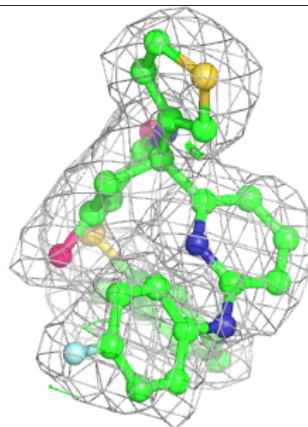
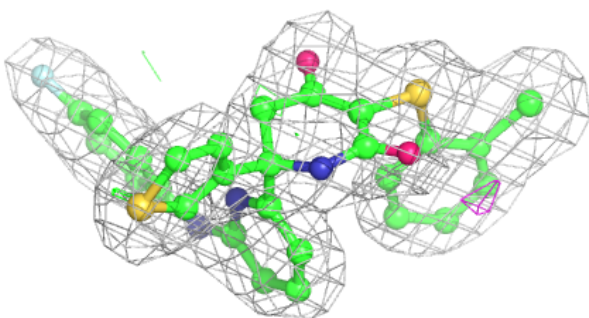
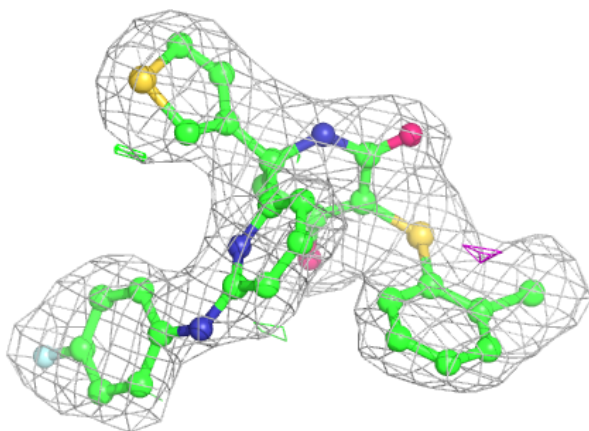
Electron density around D0V D 803:

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

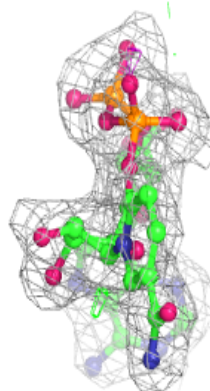
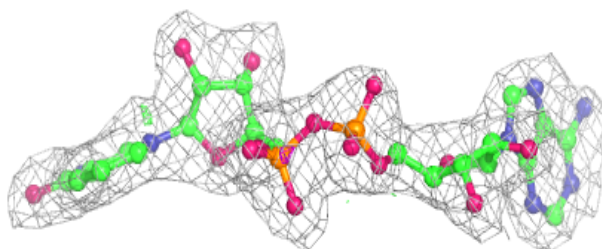
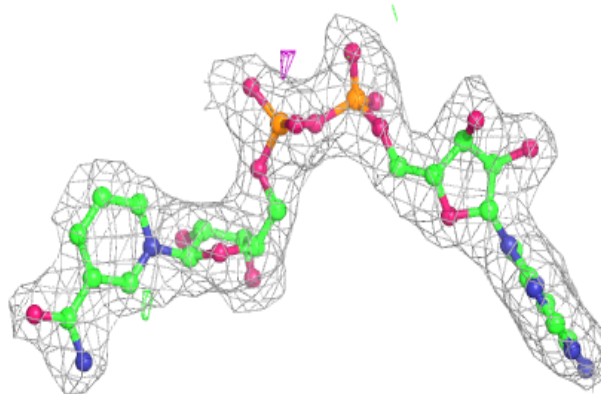


Electron density around D0V A 404:

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

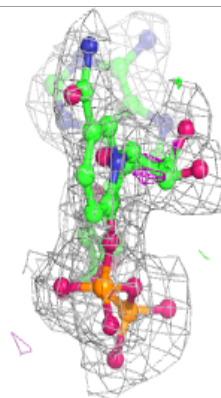
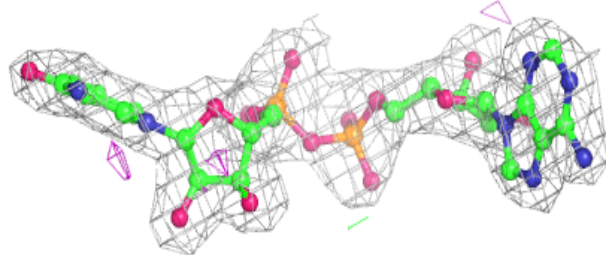
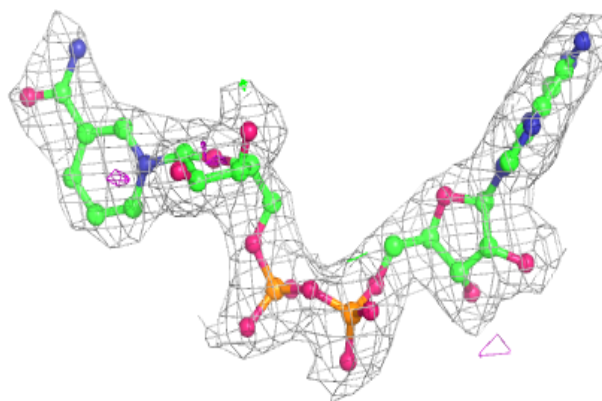
**Electron density around NAD B 402:**

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

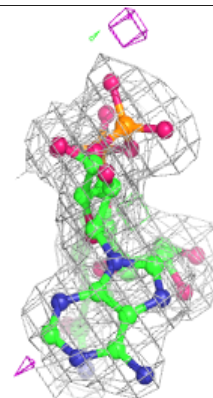
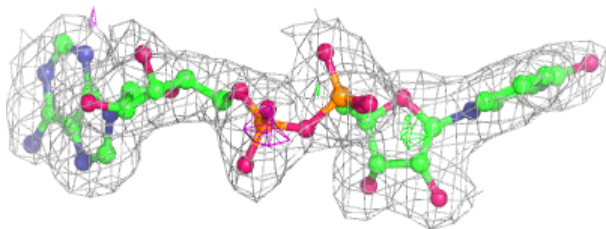
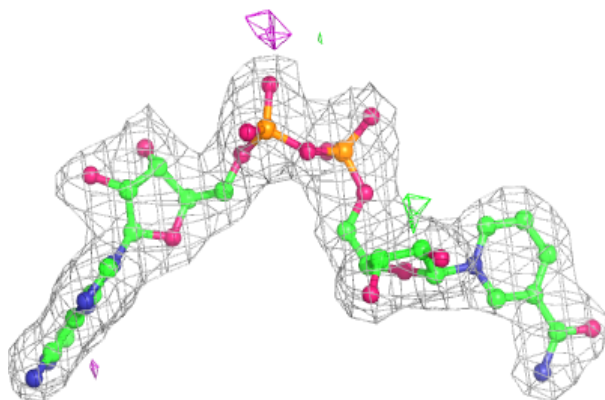


Electron density around NAD D 801:

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

**Electron density around NAD A 402:**

$2mF_o-DF_c$ (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.