



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:15 AM UTC

PDB ID : 8BXX / pdb_00008bxx
Title : Crystal structure of formate dehydrogenase FDH2 enzyme from *Granulicella mallensis* MP5ACTX8 in complex with NAD and azide.
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Deposited on : 2022-12-10
Resolution : 1.97 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

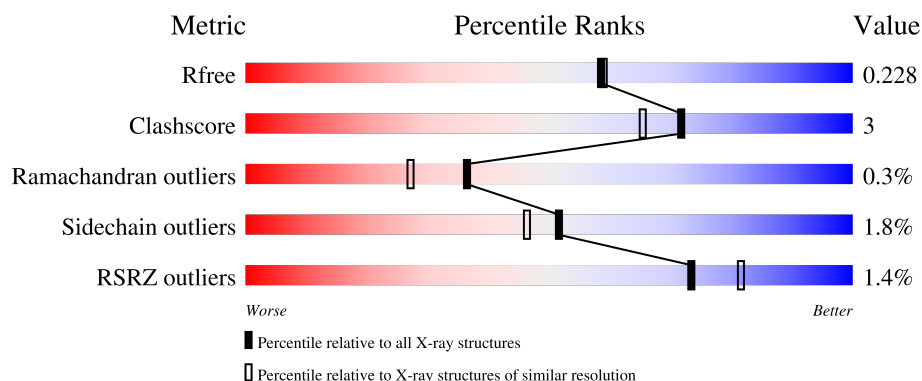
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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

Mol	Chain	Length	Quality of chain
1	AA	386	
1	BB	386	
1	CC	386	
1	DD	386	

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
3	AZI	AA	402	-	X	-	-
3	AZI	BB	402	-	X	-	-
3	AZI	CC	402	-	X	-	-
3	AZI	DD	402	-	X	-	-

2 Entry composition [i](#)

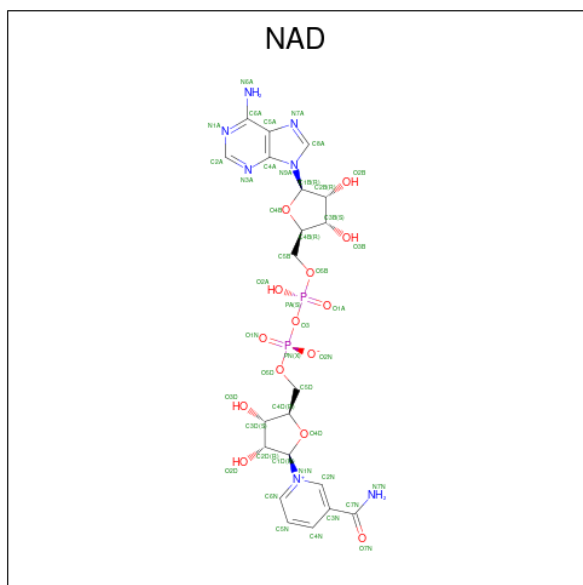
There are 5 unique types of molecules in this entry. The entry contains 12689 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Formate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	370	Total	C	N	O	S	0	0	0
			2885	1841	493	539	12			
1	BB	370	Total	C	N	O	S	0	0	0
			2885	1841	493	539	12			
1	CC	370	Total	C	N	O	S	0	0	0
			2885	1841	493	539	12			
1	DD	370	Total	C	N	O	S	0	2	0
			2908	1856	498	542	12			

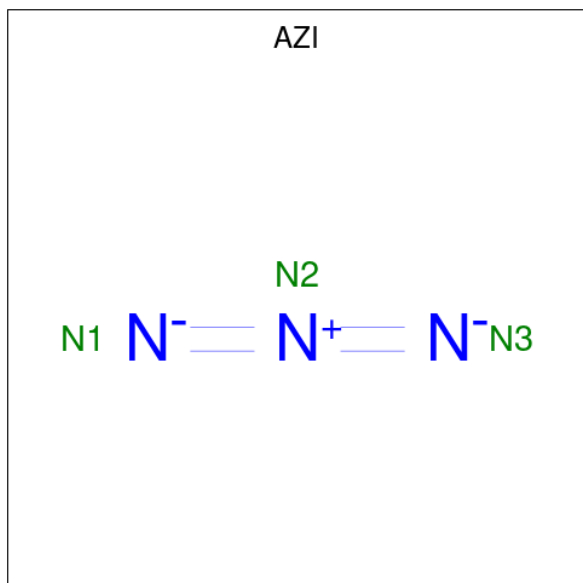
- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	CC	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	DD	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is AZIDE ION (CCD ID: AZI) (formula: N_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AA	1	Total	N	0	0
			3	3		
3	BB	1	Total	N	0	0
			3	3		
3	CC	1	Total	N	0	0
			3	3		
3	DD	1	Total	N	0	0
			3	3		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AA	1	Total	C	O	0	0
			4	2	2		
4	BB	1	Total	C	O	0	0
			4	2	2		
4	CC	1	Total	C	O	0	0
			4	2	2		
4	DD	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

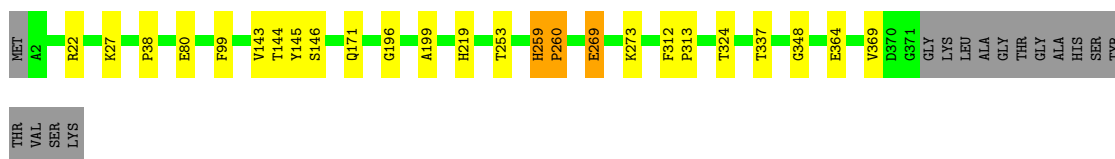
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AA	239	Total	O	0	0
			239	239		
5	BB	236	Total	O	0	0
			236	236		
5	CC	243	Total	O	0	0
			243	243		
5	DD	204	Total	O	0	0
			204	204		

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.

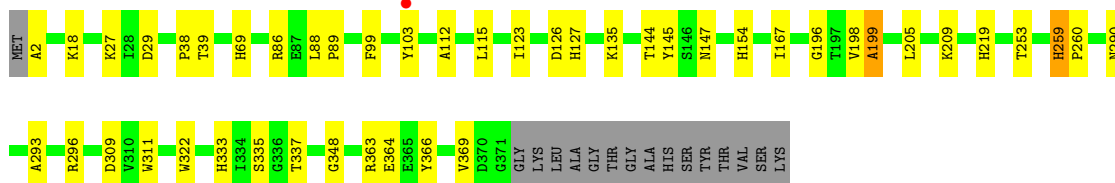
- Molecule 1: Formate dehydrogenase

Chain AA: 



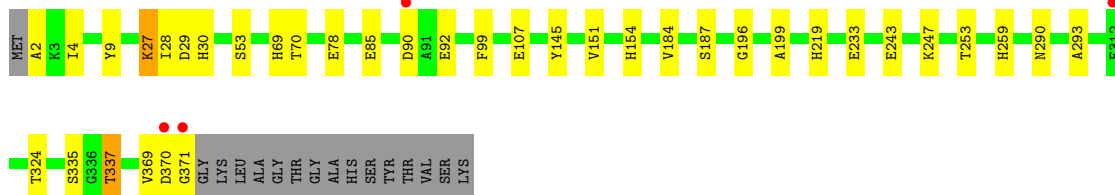
- Molecule 1: Formate dehydrogenase

Chain BB: 



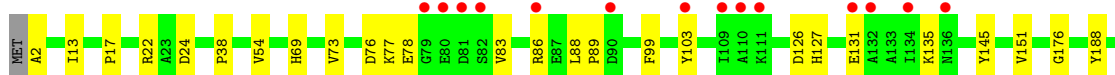
- Molecule 1: Formate dehydrogenase

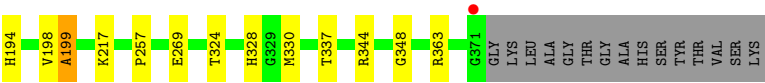
Chain CC: 



- Molecule 1: Formate dehydrogenase

Chain DD: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.07Å 128.81Å 85.66Å 90.00° 100.40° 90.00°	Depositor
Resolution (Å)	62.10 – 1.97 62.10 – 1.97	Depositor EDS
% Data completeness (in resolution range)	97.8 (62.10-1.97) 94.0 (62.10-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.188 , 0.234 (Not available) , 0.228	Depositor DCC
R_{free} test set	5278 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	15.5	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12689	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.14% 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: EDO, NAD, AZI

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	AA	0.65	1/2957 (0.0%)	1.07	2/4025 (0.0%)
1	BB	0.64	0/2957	1.05	3/4025 (0.1%)
1	CC	0.66	1/2957 (0.0%)	1.06	4/4025 (0.1%)
1	DD	0.63	0/2981	1.07	5/4057 (0.1%)
All	All	0.64	2/11852 (0.0%)	1.06	14/16132 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CC	233	GLU	C-O	-5.52	1.17	1.24
1	AA	80	GLU	CD-OE2	-5.17	1.15	1.25

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DD	324	THR	CA-CB-OG1	-6.33	100.11	109.60
1	AA	144	THR	CA-CB-OG1	-5.88	100.78	109.60
1	DD	76	ASP	CA-CB-CG	5.80	118.40	112.60
1	BB	144	THR	CA-CB-OG1	-5.69	101.06	109.60
1	CC	337	THR	CB-CA-C	5.58	120.09	111.28
1	CC	324	THR	CA-CB-OG1	-5.55	101.28	109.60
1	CC	27	LYS	CA-C-N	-5.52	115.76	123.10
1	CC	27	LYS	C-N-CA	-5.52	115.76	123.10
1	DD	363	ARG	CB-CA-C	-5.40	101.08	109.61
1	DD	176	GLY	CA-C-N	-5.27	117.74	122.43
1	DD	176	GLY	C-N-CA	-5.27	117.74	122.43
1	BB	39	THR	CA-CB-OG1	-5.11	101.93	109.60
1	AA	324	THR	CA-CB-OG1	-5.09	101.96	109.60
1	BB	167	ILE	N-CA-CB	5.02	114.37	110.45

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	AA	2885	0	2868	15	0
1	BB	2885	0	2868	24	0
1	CC	2885	0	2868	19	0
1	DD	2908	0	2888	23	0
2	AA	44	0	26	0	0
2	BB	44	0	26	0	0
2	CC	44	0	26	2	0
2	DD	44	0	26	2	0
3	AA	3	0	0	0	0
3	BB	3	0	0	0	0
3	CC	3	0	0	0	0
3	DD	3	0	0	0	0
4	AA	4	0	6	0	0
4	BB	4	0	6	3	0
4	CC	4	0	6	0	0
4	DD	4	0	6	0	0
5	AA	239	0	0	4	0
5	BB	236	0	0	1	0
5	CC	243	0	0	7	0
5	DD	204	0	0	1	0
All	All	12689	0	11620	77	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 (77) 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:AA:171:GLN:HG2	5:AA:709:HOH:O	1.40	1.18
1:BB:127:HIS:NE2	4:BB:403:EDO:H21	1.79	0.96
1:BB:364:GLU:HG3	5:BB:723:HOH:O	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CC:634:HOH:O	1:DD:13:ILE:HD11	1.85	0.74
1:AA:259:HIS:HB2	1:AA:260:PRO:HD2	1.74	0.69
1:AA:364:GLU:HG3	5:AA:728:HOH:O	1.95	0.66
1:DD:2:ALA:N	1:DD:69:HIS:HD1	1.98	0.62
1:BB:259:HIS:HB2	1:BB:260:PRO:CD	2.30	0.61
1:AA:273:LYS:HE2	5:AA:661:HOH:O	1.99	0.61
1:CC:2:ALA:N	1:CC:69:HIS:HD1	2.00	0.59
1:BB:27:LYS:HE2	1:BB:29:ASP:HB3	1.85	0.58
1:CC:370:ASP:OD1	1:CC:371:GLY:N	2.37	0.58
1:AA:259:HIS:HB2	1:AA:260:PRO:CD	2.35	0.57
1:BB:127:HIS:CD2	4:BB:403:EDO:H12	2.39	0.57
1:CC:99:PHE:CE2	1:CC:337:THR:HB	2.42	0.54
1:AA:22:ARG:HD3	1:DD:188:TYR:CE1	2.42	0.53
1:CC:92:GLU:HB2	5:CC:503:HOH:O	2.07	0.53
1:DD:194:HIS:CE1	1:DD:217:LYS:HD2	2.44	0.53
1:DD:131:GLU:O	1:DD:135:LYS:HG2	2.09	0.52
5:AA:583:HOH:O	1:BB:86:ARG:HD2	2.09	0.52
1:CC:29:ASP:OD2	1:CC:30:HIS:HD2	1.91	0.52
1:BB:127:HIS:NE2	4:BB:403:EDO:C2	2.63	0.51
1:CC:290:ASN:HB3	1:CC:293:ALA:HB3	1.93	0.50
1:CC:259:HIS:HE1	2:CC:401:NAD:N7A	2.09	0.49
1:BB:99:PHE:CE2	1:BB:337:THR:HB	2.48	0.49
1:CC:196:GLY:HA2	1:CC:219:HIS:O	2.13	0.49
1:CC:243:GLU:HG3	1:CC:247:LYS:HE3	1.95	0.49
1:DD:103[A]:TYR:CE2	1:DD:127:HIS:HA	2.48	0.48
1:AA:269:GLU:OE1	1:BB:296:ARG:HD3	2.13	0.48
1:BB:311:TRP:CZ3	1:BB:322:TRP:HB2	2.48	0.48
1:CC:27:LYS:HD3	5:CC:675:HOH:O	2.13	0.48
1:BB:259:HIS:HB2	1:BB:260:PRO:HD3	1.96	0.47
1:DD:99:PHE:CE2	1:DD:337:THR:HB	2.50	0.47
1:DD:54:VAL:HG13	1:DD:73:VAL:HG12	1.96	0.47
1:BB:154:HIS:CG	1:BB:335:SER:HB3	2.49	0.46
1:BB:2:ALA:N	1:BB:69:HIS:HD1	2.14	0.46
1:BB:309:ASP:O	1:BB:333:HIS:HA	2.15	0.46
1:DD:88:LEU:N	1:DD:89:PRO:CD	2.78	0.45
1:AA:143:VAL:HG12	1:AA:146:SER:HB3	1.99	0.45
1:CC:90:ASP:OD1	5:CC:501:HOH:O	2.21	0.45
1:BB:196:GLY:HA2	1:BB:219:HIS:O	2.16	0.45
1:BB:290:ASN:HB3	1:BB:293:ALA:HB3	1.99	0.45
1:BB:198:VAL:O	1:BB:199:ALA:HB3	2.17	0.44
1:DD:77:LYS:NZ	1:DD:78:GLU:OE2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BB:112:ALA:HB1	1:BB:115:LEU:HB2	2.00	0.43
1:DD:328:HIS:ND1	1:DD:330:MET:HG2	2.34	0.43
1:CC:107:GLU:HB3	5:CC:660:HOH:O	2.18	0.43
1:CC:154:HIS:CG	1:CC:335:SER:HB3	2.53	0.43
1:BB:88:LEU:N	1:BB:89:PRO:CD	2.82	0.43
1:DD:38:PRO:HG2	1:DD:344:ARG:O	2.19	0.43
1:DD:198:VAL:O	1:DD:199:ALA:HB3	2.19	0.43
1:CC:107:GLU:HG2	5:CC:589:HOH:O	2.19	0.42
1:CC:184:VAL:HA	1:CC:187:SER:HB2	2.02	0.42
1:DD:17:PRO:HA	5:DD:579:HOH:O	2.19	0.42
1:DD:86[A]:ARG:O	1:DD:89:PRO:HD2	2.19	0.42
1:DD:151:VAL:HG21	2:DD:401:NAD:C4N	2.50	0.42
1:AA:273:LYS:HD3	1:AA:273:LYS:HA	1.77	0.42
1:DD:194:HIS:NE2	1:DD:217:LYS:HD2	2.35	0.42
1:AA:22:ARG:HD3	1:DD:188:TYR:CD1	2.55	0.42
1:DD:38:PRO:HB3	1:DD:348:GLY:HA2	2.01	0.42
1:DD:83:VAL:HG22	1:DD:86[A]:ARG:NH2	2.34	0.42
1:AA:38:PRO:HB3	1:AA:348:GLY:HA2	2.01	0.41
1:BB:38:PRO:HB3	1:BB:348:GLY:HA2	2.01	0.41
1:AA:22:ARG:HG2	1:DD:188:TYR:CZ	2.55	0.41
1:AA:196:GLY:HA2	1:AA:219:HIS:O	2.20	0.41
1:CC:9:TYR:O	1:CC:53:SER:HA	2.20	0.41
1:AA:312:PHE:HA	1:AA:313:PRO:HA	1.89	0.41
1:BB:363:ARG:HB2	1:BB:366:TYR:CD2	2.55	0.41
1:CC:4:ILE:N	1:CC:4:ILE:HD12	2.36	0.41
1:CC:28:ILE:HB	5:CC:713:HOH:O	2.20	0.41
1:DD:257:PRO:HD3	2:DD:401:NAD:H52A	2.03	0.41
1:BB:103:TYR:CD1	1:BB:127:HIS:HB2	2.56	0.40
1:BB:123:ILE:HD12	1:BB:147:ASN:OD1	2.21	0.40
1:AA:99:PHE:CE2	1:AA:337:THR:HB	2.55	0.40
1:BB:205:LEU:HG	1:BB:209:LYS:HE3	2.03	0.40
1:DD:22:ARG:NH1	1:DD:24:ASP:O	2.54	0.40
1:CC:151:VAL:HG21	2:CC:401:NAD:C4N	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	368/386 (95%)	349 (95%)	18 (5%)	1 (0%)	36	27
1	BB	368/386 (95%)	357 (97%)	10 (3%)	1 (0%)	36	27
1	CC	368/386 (95%)	355 (96%)	12 (3%)	1 (0%)	36	27
1	DD	370/386 (96%)	357 (96%)	12 (3%)	1 (0%)	36	27
All	All	1474/1544 (96%)	1418 (96%)	52 (4%)	4 (0%)	36	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	199	ALA
1	CC	199	ALA
1	DD	199	ALA
1	BB	199	ALA

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	AA	311/322 (97%)	304 (98%)	7 (2%)	44	37
1	BB	311/322 (97%)	304 (98%)	7 (2%)	44	37
1	CC	311/322 (97%)	305 (98%)	6 (2%)	50	44
1	DD	313/322 (97%)	310 (99%)	3 (1%)	68	65
All	All	1246/1288 (97%)	1223 (98%)	23 (2%)	51	46

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	27	LYS
1	AA	145	TYR
1	AA	253	THR
1	AA	259	HIS
1	AA	260	PRO
1	AA	269	GLU
1	AA	369	VAL
1	BB	18	LYS
1	BB	126	ASP
1	BB	135	LYS
1	BB	145	TYR
1	BB	253	THR
1	BB	259	HIS
1	BB	369	VAL
1	CC	70	THR
1	CC	78	GLU
1	CC	85	GLU
1	CC	145	TYR
1	CC	253	THR
1	CC	369	VAL
1	DD	126	ASP
1	DD	145	TYR
1	DD	269	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	30	HIS
1	AA	35	GLN
1	AA	42	GLN
1	AA	136	ASN
1	AA	255	ASN
1	BB	35	GLN
1	BB	136	ASN
1	BB	154	HIS
1	BB	171	GLN
1	BB	314	GLN
1	CC	30	HIS
1	CC	35	GLN
1	CC	136	ASN
1	CC	154	HIS

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Mol	Chain	Res	Type
1	CC	232	ASN
1	CC	255	ASN
1	CC	259	HIS
1	DD	136	ASN
1	DD	223	GLN
1	DD	255	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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	AZI	BB	402	-	2,2,2	3.90	2 (100%)	0,1,1	-	-
4	EDO	BB	403	-	3,3,3	0.29	0	2,2,2	0.28	0
2	NAD	DD	401	-	46,48,48	0.83	3 (6%)	64,73,73	0.90	1 (1%)
4	EDO	DD	403	-	3,3,3	0.15	0	2,2,2	0.22	0
3	AZI	CC	402	-	2,2,2	3.49	2 (100%)	0,1,1	-	-
3	AZI	AA	402	-	2,2,2	3.44	2 (100%)	0,1,1	-	-
4	EDO	CC	403	-	3,3,3	0.22	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	AA	403	-	3,3,3	0.20	0	2,2,2	0.38	0
2	NAD	BB	401	-	46,48,48	0.86	2 (4%)	64,73,73	0.77	0
2	NAD	CC	401	-	46,48,48	1.03	3 (6%)	64,73,73	0.71	1 (1%)
3	AZI	DD	402	-	2,2,2	3.80	2 (100%)	0,1,1	-	-
2	NAD	AA	401	-	46,48,48	0.63	0	64,73,73	0.88	1 (1%)

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	EDO	BB	403	-	-	1/1/1/1	-
2	NAD	DD	401	-	-	4/30/62/62	0/5/5/5
4	EDO	DD	403	-	-	0/1/1/1	-
4	EDO	CC	403	-	-	0/1/1/1	-
4	EDO	AA	403	-	-	0/1/1/1	-
2	NAD	BB	401	-	-	3/30/62/62	0/5/5/5
2	NAD	CC	401	-	-	3/30/62/62	0/5/5/5
2	NAD	AA	401	-	-	2/30/62/62	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CC	401	NAD	C2N-N1N	4.74	1.40	1.35
3	BB	402	AZI	N1-N2	-4.11	1.14	1.23
3	DD	402	AZI	N1-N2	-3.96	1.15	1.23
3	AA	402	AZI	N3-N2	-3.79	1.15	1.23
2	BB	401	NAD	C2N-N1N	3.78	1.39	1.35
3	CC	402	AZI	N3-N2	-3.78	1.15	1.23
3	BB	402	AZI	N3-N2	-3.68	1.15	1.23
3	DD	402	AZI	N3-N2	-3.64	1.15	1.23
2	CC	401	NAD	O4D-C1D	3.58	1.45	1.40
3	CC	402	AZI	N1-N2	-3.17	1.16	1.23
3	AA	402	AZI	N1-N2	-3.04	1.16	1.23
2	DD	401	NAD	C2N-N1N	2.69	1.37	1.35
2	DD	401	NAD	O4D-C1D	2.47	1.44	1.40
2	CC	401	NAD	PN-O3	2.34	1.62	1.59
2	DD	401	NAD	PN-O3	2.13	1.61	1.59
2	BB	401	NAD	PN-O3	2.10	1.61	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DD	401	NAD	C6N-N1N-C2N	-3.40	118.99	121.88
2	AA	401	NAD	C6N-N1N-C2N	-3.06	119.27	121.88
2	CC	401	NAD	O2A-PA-O1A	2.18	122.57	112.44

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AA	401	NAD	O4D-C1D-N1N-C6N
2	BB	401	NAD	O4D-C1D-N1N-C6N
2	CC	401	NAD	O4D-C1D-N1N-C6N
2	DD	401	NAD	O4D-C1D-N1N-C6N
4	BB	403	EDO	O1-C1-C2-O2
2	DD	401	NAD	O4B-C4B-C5B-O5B
2	CC	401	NAD	O4B-C4B-C5B-O5B
2	BB	401	NAD	O4B-C4B-C5B-O5B
2	AA	401	NAD	O4D-C1D-N1N-C2N
2	BB	401	NAD	O4D-C1D-N1N-C2N
2	CC	401	NAD	O4D-C1D-N1N-C2N
2	DD	401	NAD	O4D-C1D-N1N-C2N
2	DD	401	NAD	C3B-C4B-C5B-O5B

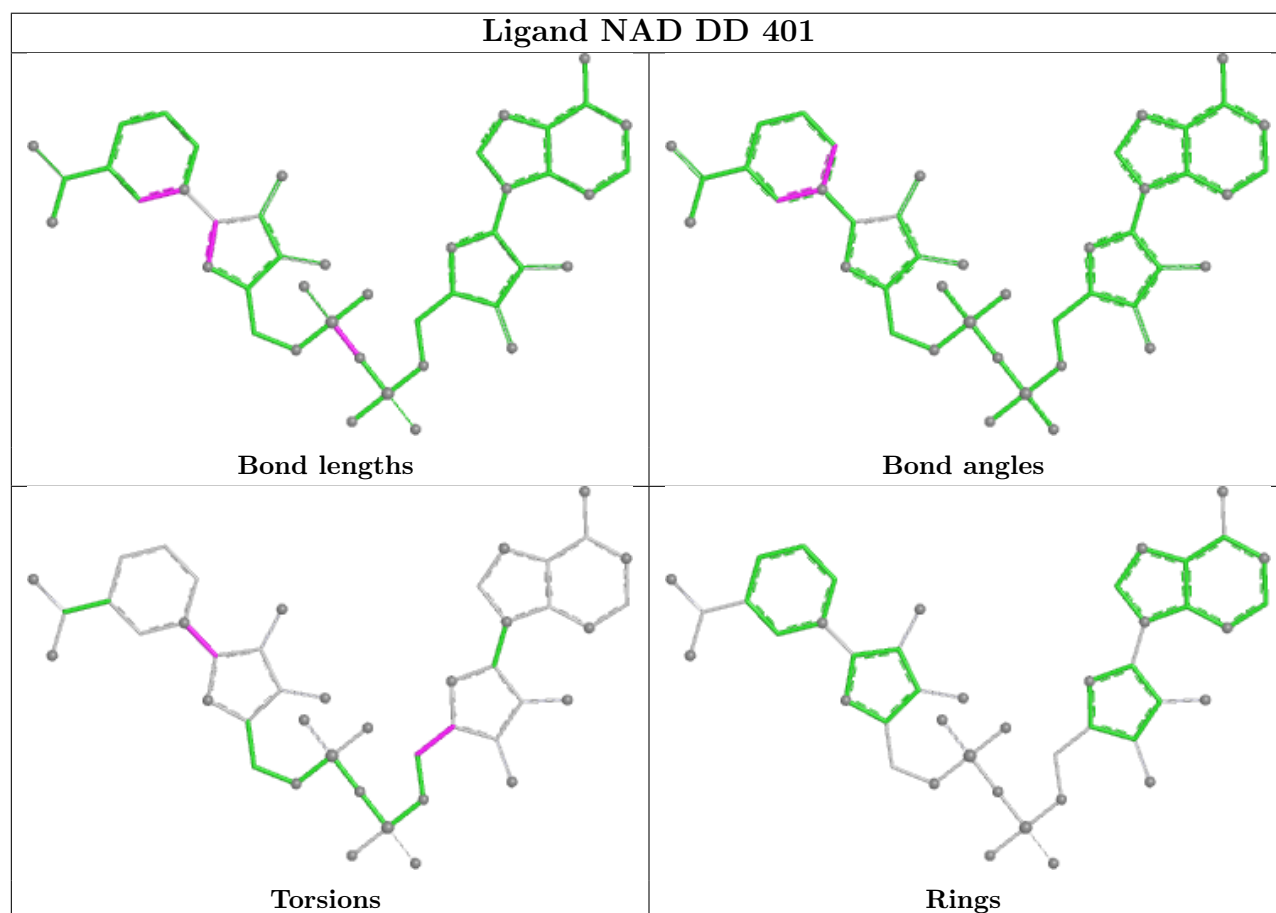
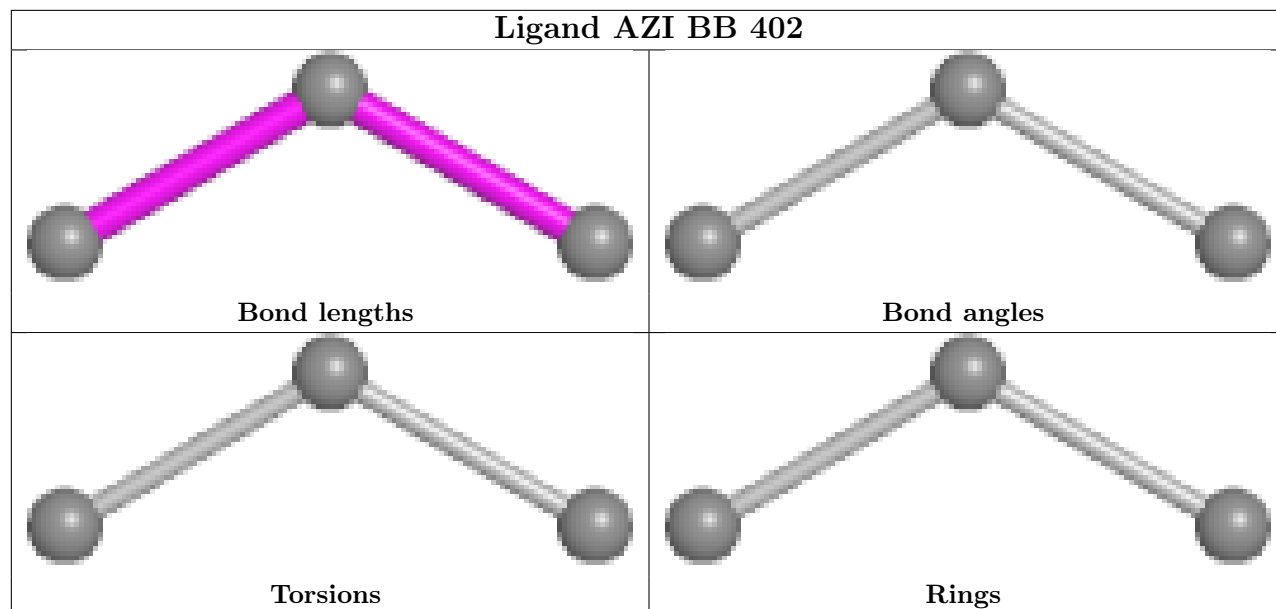
There are no ring outliers.

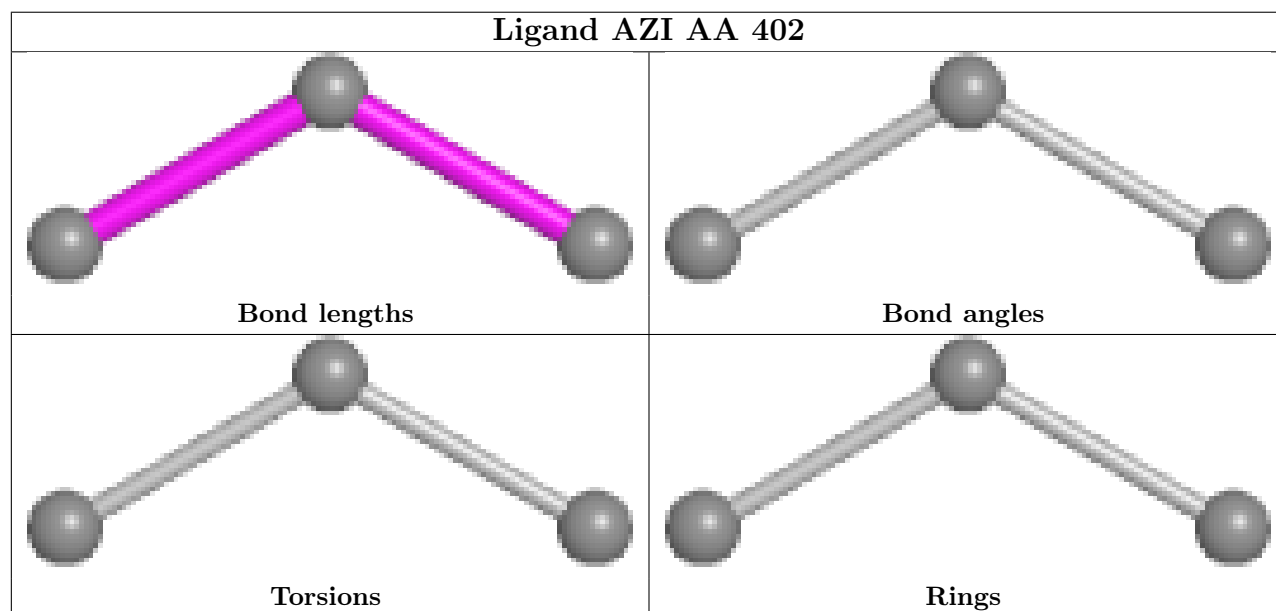
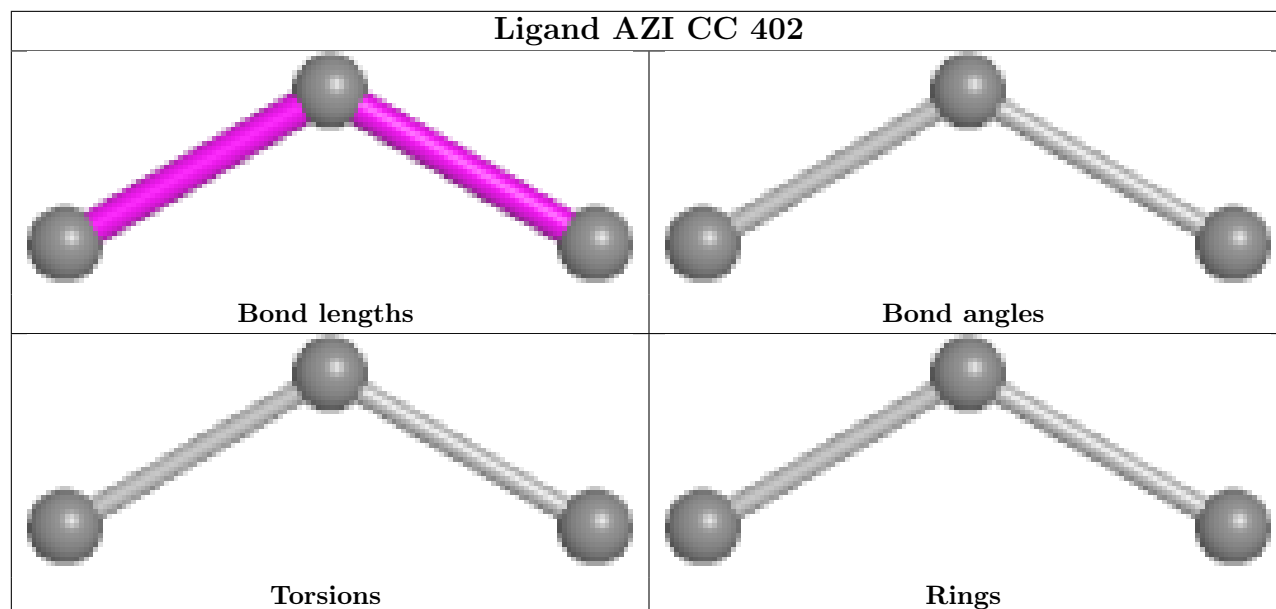
3 monomers are involved in 7 short contacts:

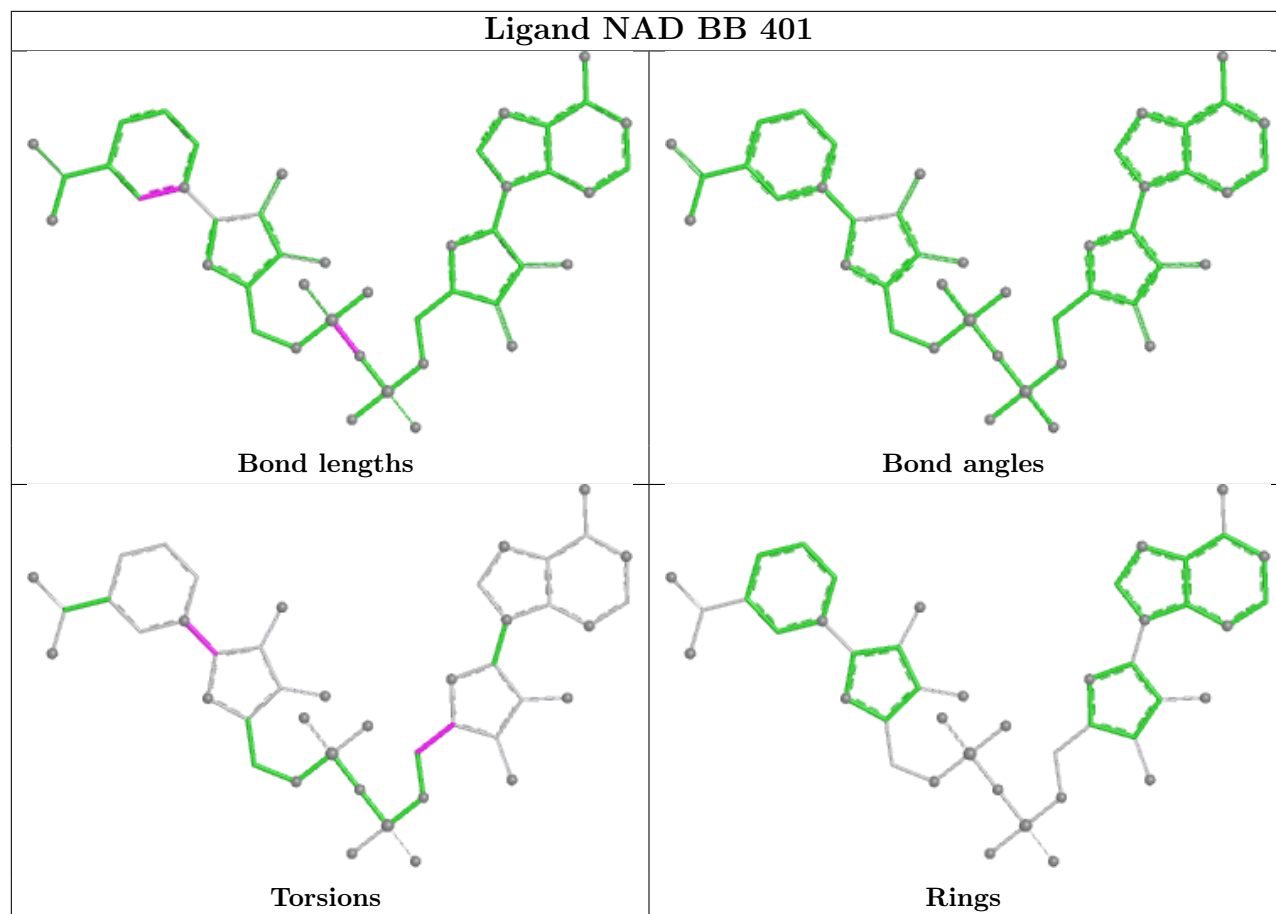
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	BB	403	EDO	3	0
2	DD	401	NAD	2	0
2	CC	401	NAD	2	0

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

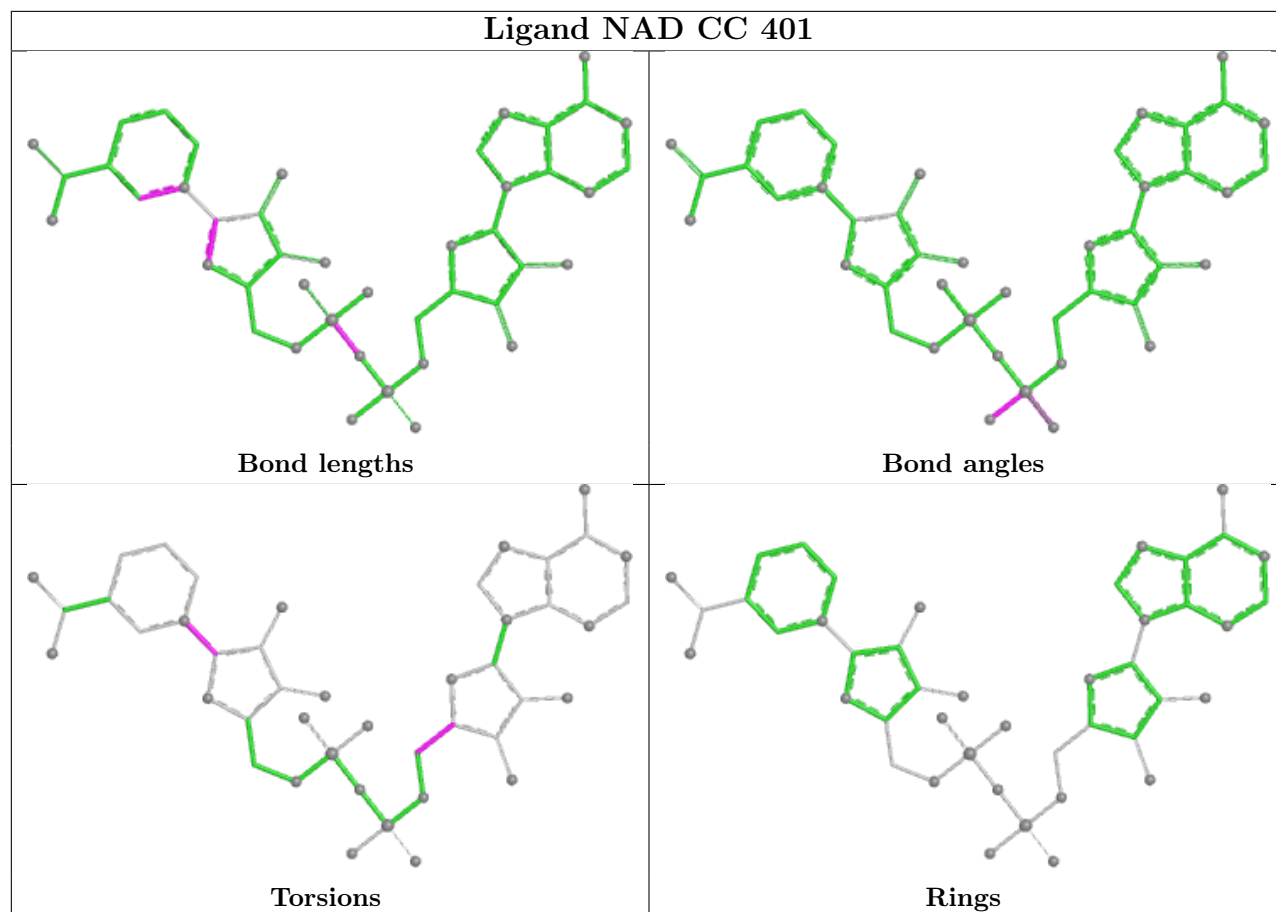
equivalents in the CSD to analyse the geometry.



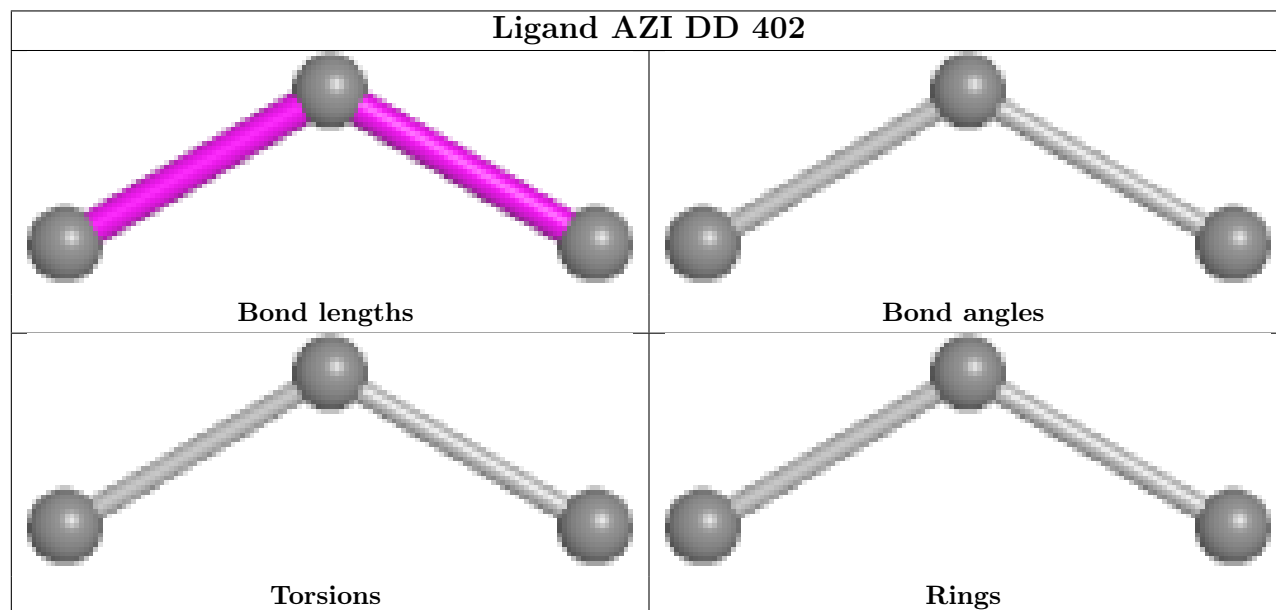


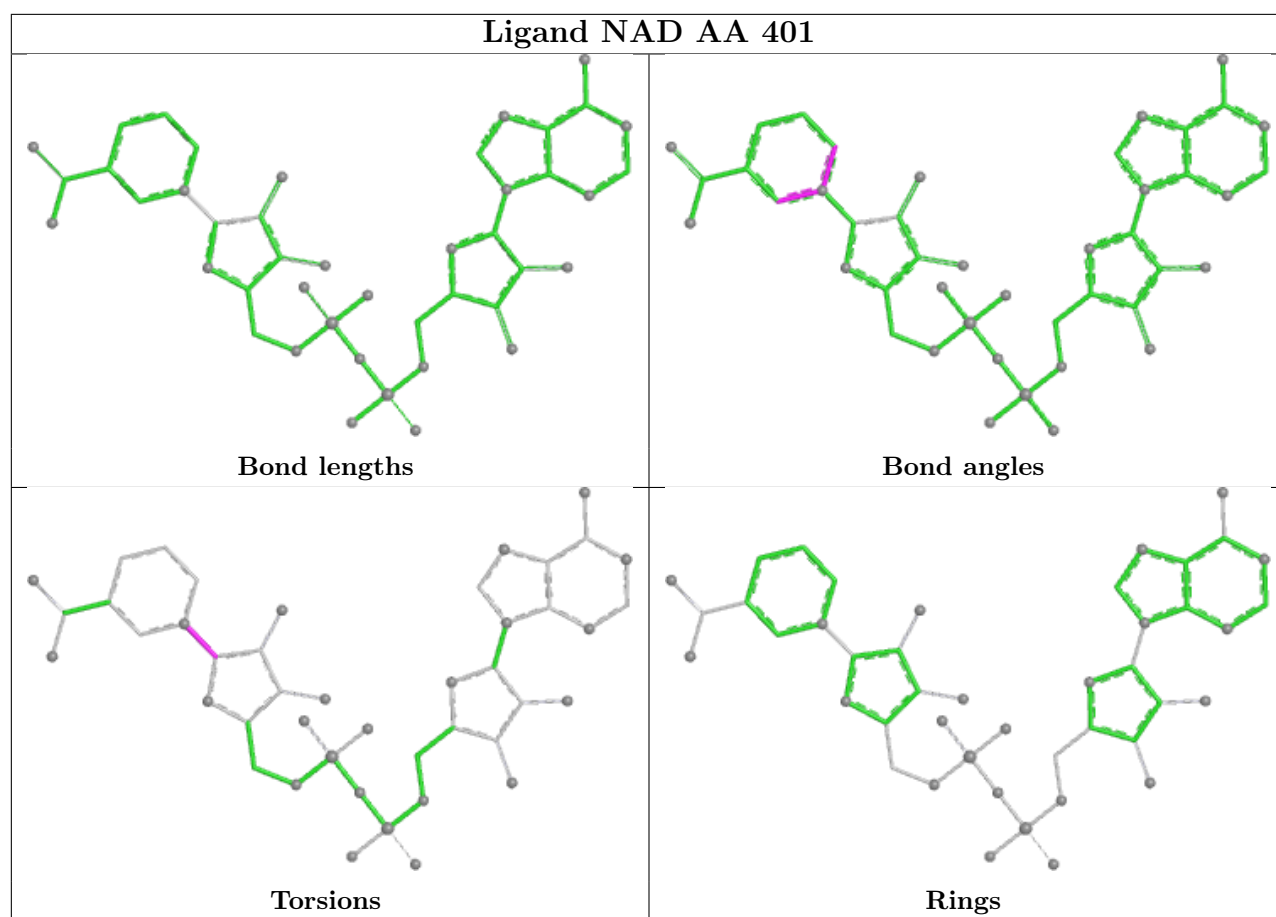


Ligand NAD CC 401



Ligand AZI DD 402





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	370/386 (95%)	-0.31	0 100 100	5, 13, 26, 37	0
1	BB	370/386 (95%)	-0.23	1 (0%) 90 93	6, 13, 27, 44	0
1	CC	370/386 (95%)	-0.39	4 (1%) 78 84	4, 10, 24, 57	0
1	DD	370/386 (95%)	-0.06	15 (4%) 41 51	6, 13, 38, 55	2 (0%)
All	All	1480/1544 (95%)	-0.24	20 (1%) 73 81	4, 12, 30, 57	2 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DD	86[A]	ARG	3.8
1	BB	103	TYR	3.6
1	CC	371	GLY	3.5
1	DD	103[A]	TYR	3.1
1	DD	81	ASP	3.0
1	DD	80	GLU	3.0
1	DD	134	ILE	2.8
1	DD	111	LYS	2.8
1	CC	90	ASP	2.7
1	DD	110	ALA	2.7
1	DD	90	ASP	2.5
1	DD	109	ILE	2.5
1	DD	136	ASN	2.4
1	DD	82	SER	2.4
1	DD	79	GLY	2.3
1	CC	370	ASP	2.2
1	DD	132	ALA	2.2
1	DD	131	GLU	2.1
1	CC	312	PHE	2.1
1	DD	371	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

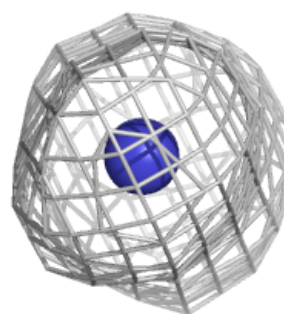
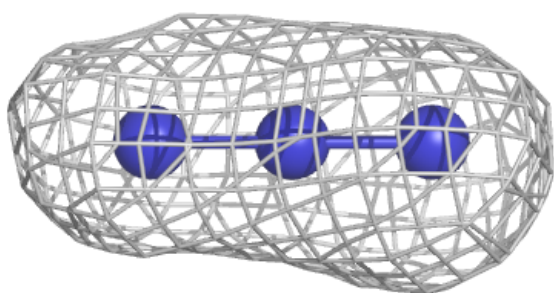
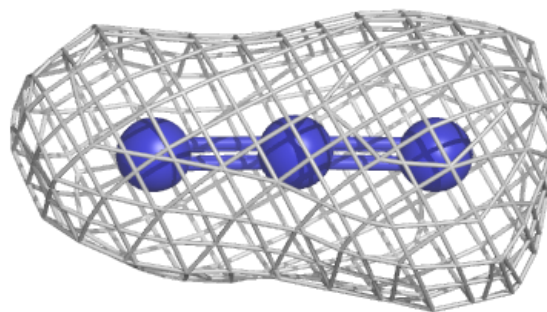
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	BB	403	4/4	0.87	0.19	24,31,34,34	0
4	EDO	AA	403	4/4	0.93	0.11	21,27,27,29	0
3	AZI	AA	402	3/3	0.94	0.07	12,12,13,14	0
4	EDO	DD	403	4/4	0.94	0.12	25,30,31,31	0
3	AZI	DD	402	3/3	0.96	0.06	12,12,12,14	0
2	NAD	DD	401	44/44	0.97	0.05	9,12,18,18	0
4	EDO	CC	403	4/4	0.97	0.12	14,15,16,17	0
2	NAD	BB	401	44/44	0.97	0.05	10,13,17,18	0
2	NAD	CC	401	44/44	0.98	0.05	6,8,12,13	0
3	AZI	BB	402	3/3	0.98	0.04	11,11,12,12	0
3	AZI	CC	402	3/3	0.98	0.04	6,6,6,6	0
2	NAD	AA	401	44/44	0.98	0.05	8,11,14,15	0

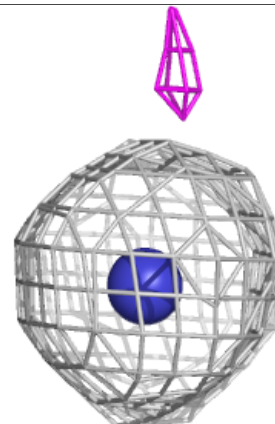
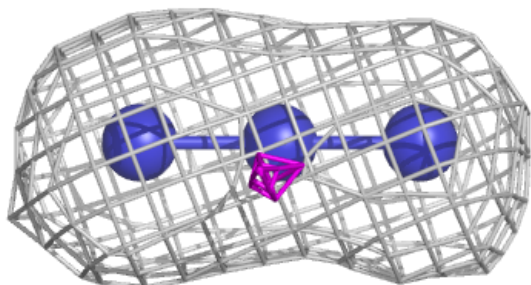
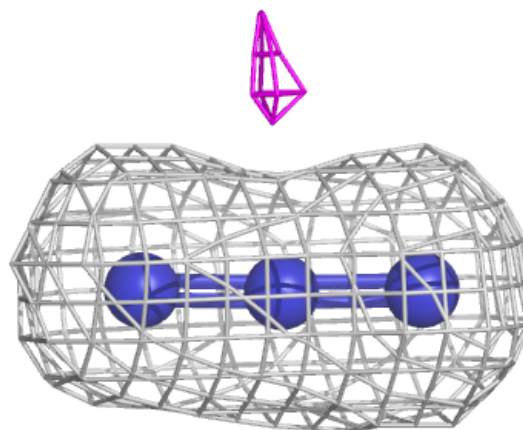
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AZI AA 402:

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

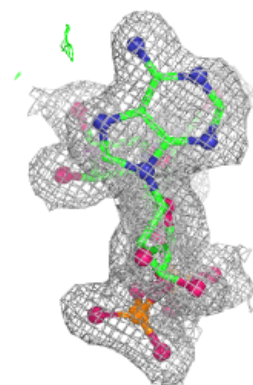
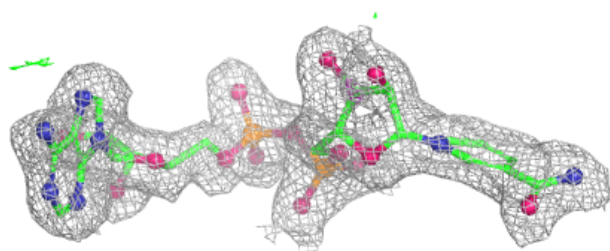
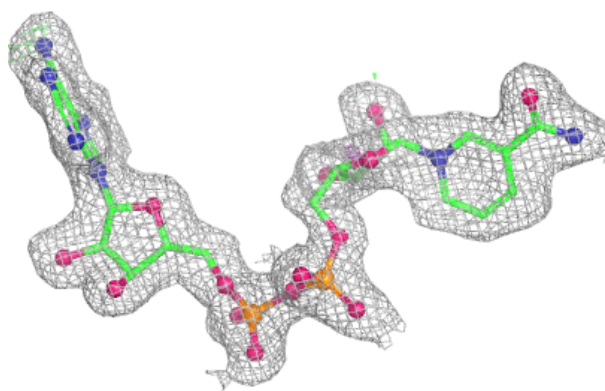
**Electron density around AZI DD 402:**

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

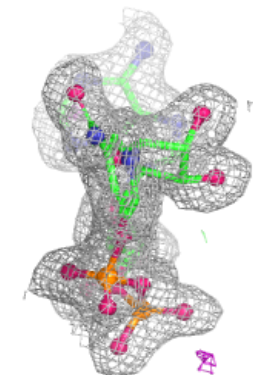
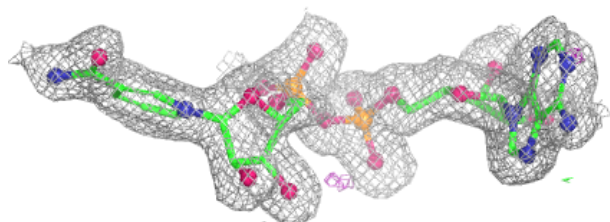
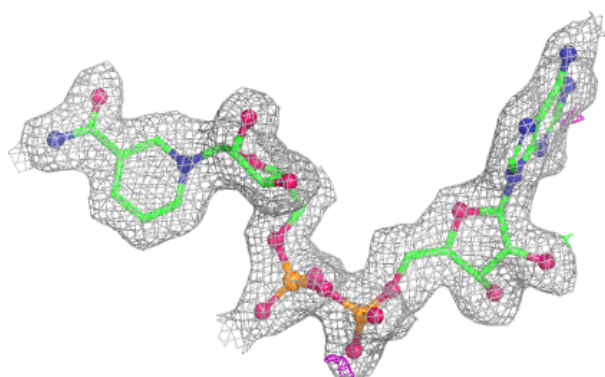


Electron density around NAD DD 401:

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

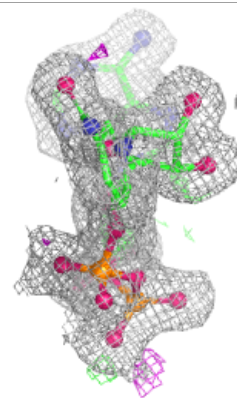
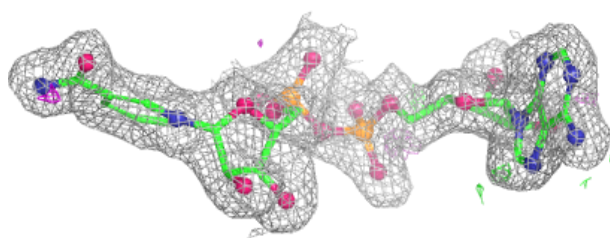
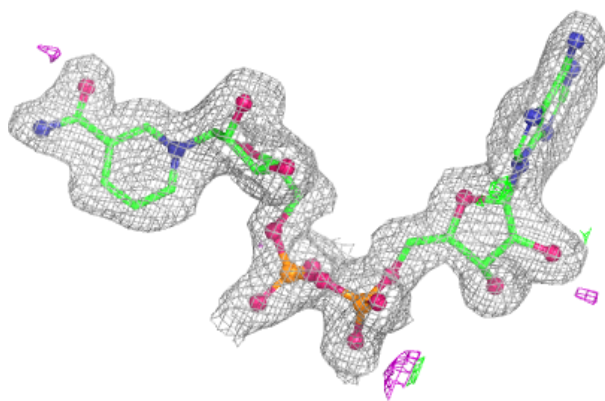
**Electron density around NAD BB 401:**

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

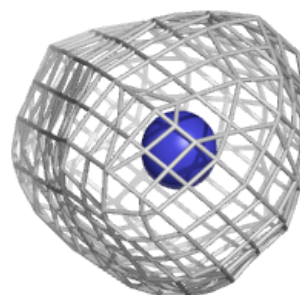
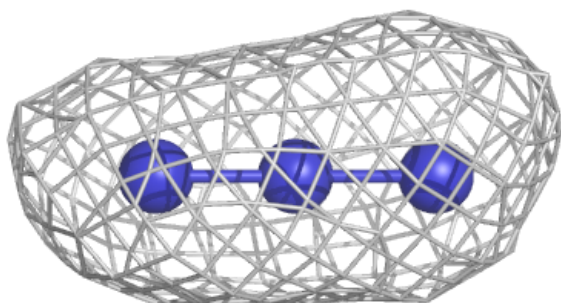
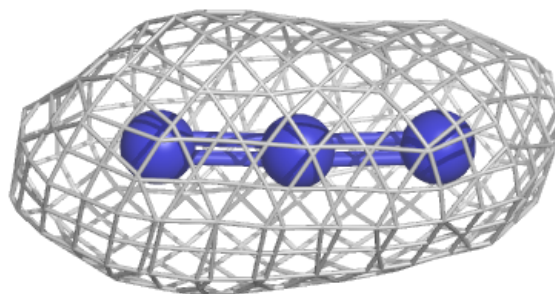


Electron density around NAD CC 401:

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and green (positive)

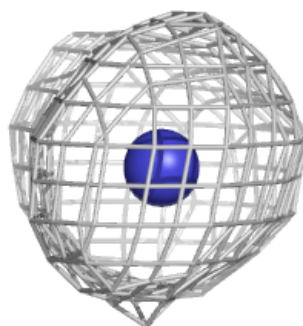
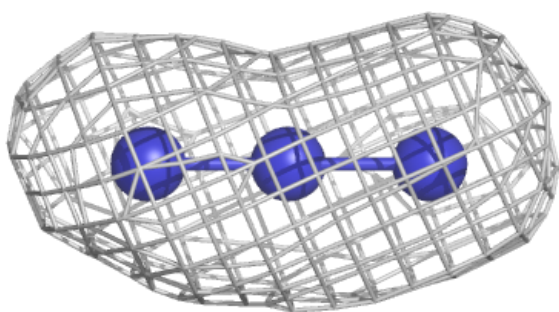
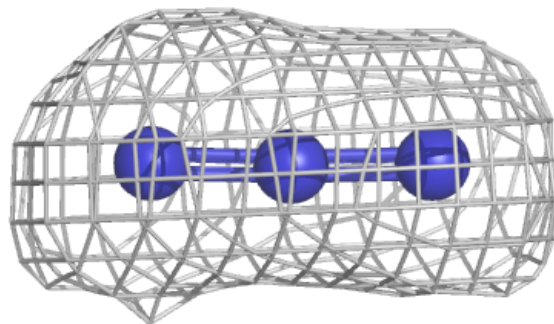
**Electron density around AZI BB 402:**

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

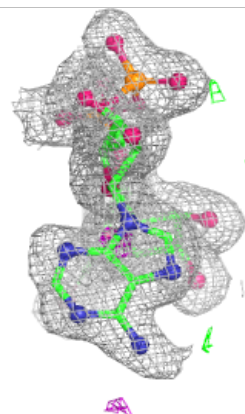
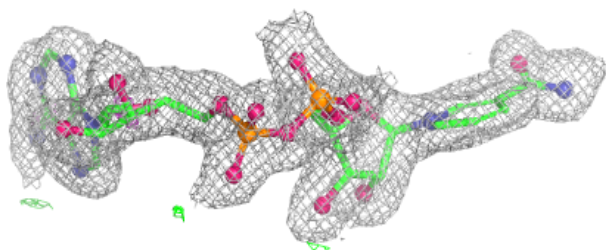
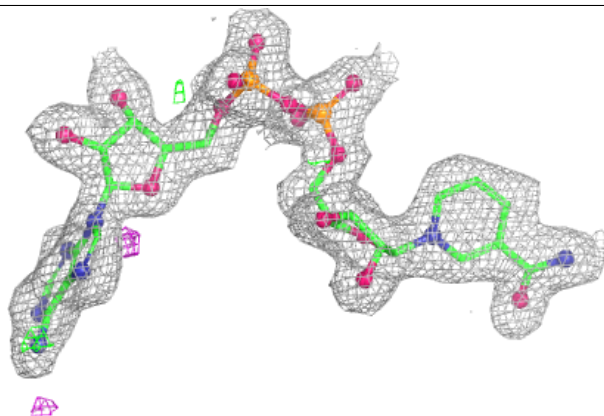


Electron density around AZI CC 402:

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

**Electron density around NAD AA 401:**

$2mF_o-DF_c$ (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.