



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 11:05 PM BST

PDB ID : 5YU3  
Title : Structural basis for recognition of L-lysine, L-ornithine, and L-2,4-diamino butyric acid by lysine cyclodeaminase  
Authors : Min, K.J.; Yoon, H.J.; Matsuura, A.; Kim, Y.H.; Lee, H.H.  
Deposited on : 2017-11-20  
Resolution : 1.79 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 2.14.4.dev1  
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) : 2.14.4.dev1

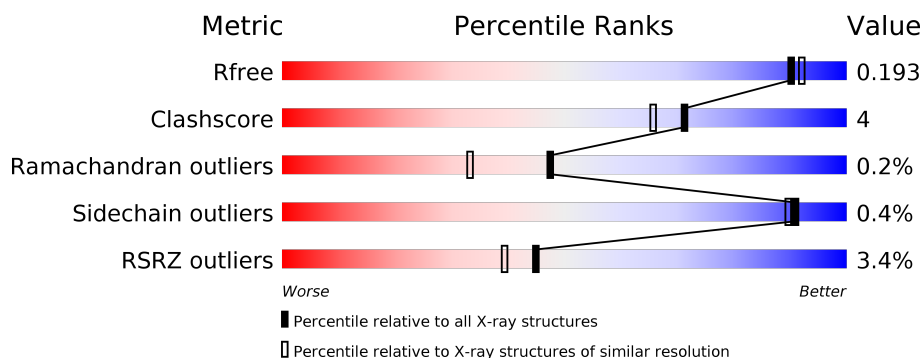
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.79 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>88%</span> <span>11%</span> </div> </div>
1	B	344	<div> <div style="width: 6%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>6%</span> <span>87%</span> <span>13%</span> </div> </div>
1	C	344	<div> <div style="width: 3%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>84%</span> <span>14%</span> </div> </div>
1	D	344	<div> <div style="width: 4%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>90%</span> <span>10%</span> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11889 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 Lysine cyclodeaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2573	1608	470	488	7			
1	B	344	Total	C	N	O	S	0	0	0
			2573	1608	470	488	7			
1	C	344	Total	C	N	O	S	0	0	0
			2573	1608	470	488	7			
1	D	344	Total	C	N	O	S	0	0	0
			2573	1608	470	488	7			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

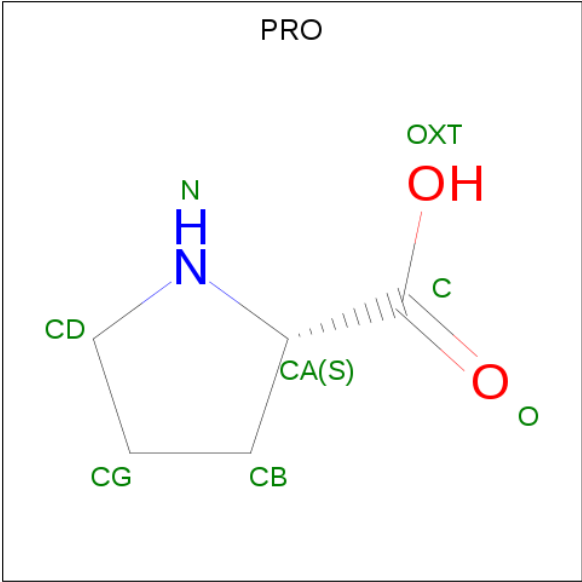
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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

- Molecule 4 is PROLINE (three-letter code: PRO) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 8 5 1 2	0	0
4	B	1	Total C N O 8 5 1 2	0	0
4	C	1	Total C N O 8 5 1 2	0	0
4	D	1	Total C N O 8 5 1 2	0	0

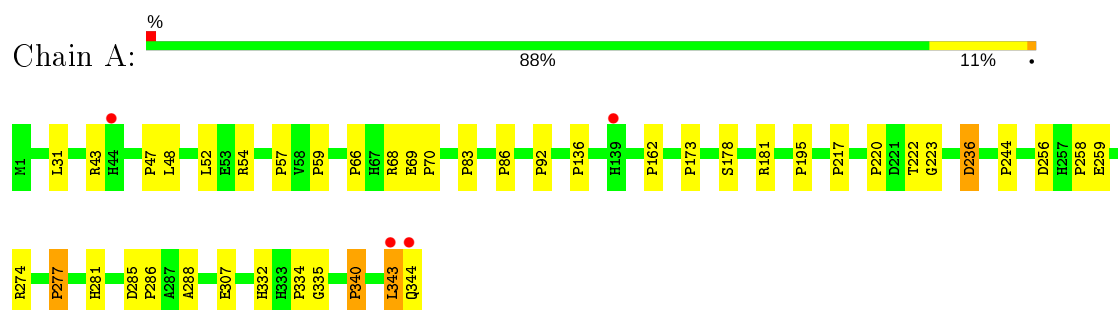
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	345	Total O 345 345	0	0
5	B	316	Total O 316 316	0	0
5	C	400	Total O 400 400	0	0
5	D	324	Total O 324 324	0	0

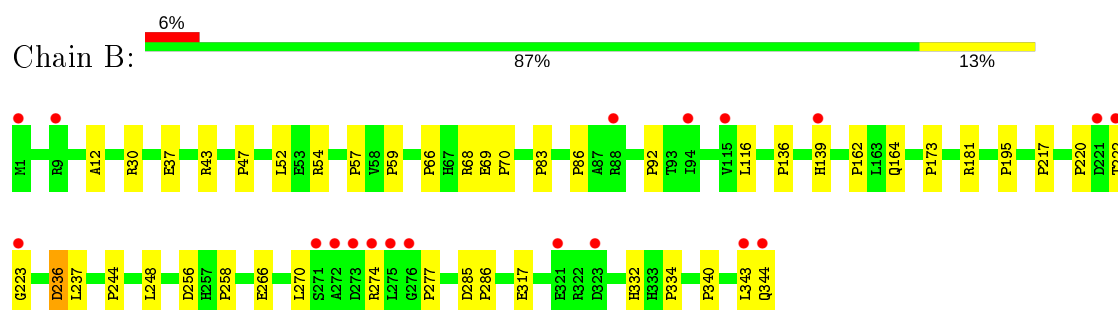
### 3 Residue-property plots [i](#)

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.

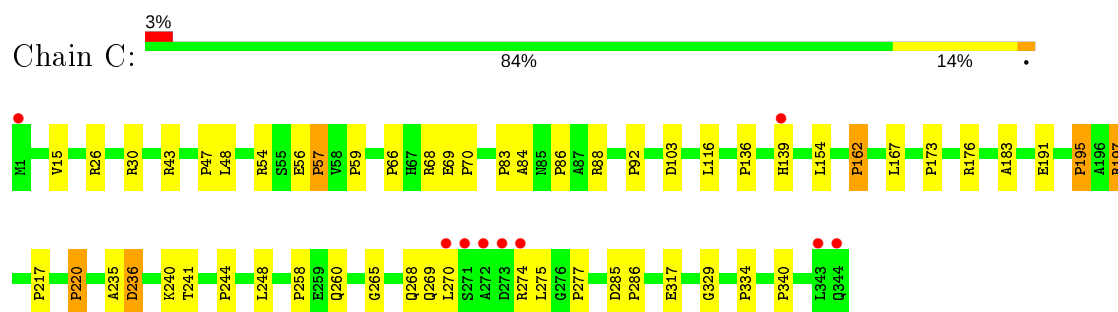
#### • Molecule 1: Lysine cyclodeaminase



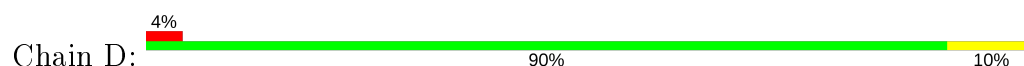
#### • Molecule 1: Lysine cyclodeaminase

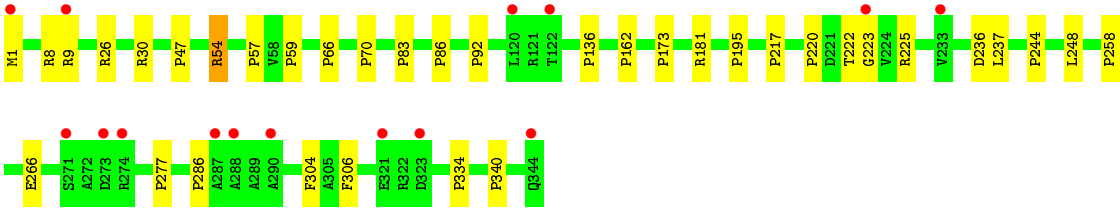


#### • Molecule 1: Lysine cyclodeaminase



#### • Molecule 1: Lysine cyclodeaminase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	271.53Å 64.78Å 106.86Å 90.00° 104.20° 90.00°	Depositor
Resolution (Å)	37.25 – 1.79 37.25 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.6 (37.25-1.79) 99.4 (37.25-1.79)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.85 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, $R_{free}$	0.166 , 0.193 0.166 , 0.193	Depositor DCC
$R_{free}$ test set	8337 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.2	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 52.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11889	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 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	0.79	24/2623 (0.9%)	0.65	3/3576 (0.1%)
1	B	0.79	24/2623 (0.9%)	0.65	3/3576 (0.1%)
1	C	0.79	24/2623 (0.9%)	0.70	4/3576 (0.1%)
1	D	0.78	24/2623 (0.9%)	0.73	3/3576 (0.1%)
All	All	0.79	96/10492 (0.9%)	0.68	13/14304 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	57	PRO	CA-CB	-12.68	1.28	1.53
1	A	217	PRO	CA-CB	-12.63	1.28	1.53
1	A	57	PRO	CA-CB	-12.63	1.28	1.53
1	B	217	PRO	CA-CB	-12.50	1.28	1.53
1	C	57	PRO	CA-CB	-12.37	1.28	1.53
1	D	217	PRO	CA-CB	-12.14	1.29	1.53
1	C	217	PRO	CA-CB	-11.77	1.30	1.53
1	D	57	PRO	CA-CB	-11.59	1.30	1.53
1	B	57	PRO	N-CA	6.40	1.58	1.47
1	C	57	PRO	N-CA	6.27	1.57	1.47
1	B	57	PRO	CG-CD	-6.13	1.30	1.50
1	D	136	PRO	CG-CD	-6.11	1.30	1.50
1	A	57	PRO	N-CA	6.09	1.57	1.47
1	D	286	PRO	CG-CD	-6.09	1.30	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	286	PRO	CG-CD	-6.09	1.30	1.50
1	C	47	PRO	CG-CD	-6.09	1.30	1.50
1	A	173	PRO	CG-CD	-6.07	1.30	1.50
1	A	59	PRO	CG-CD	-6.06	1.30	1.50
1	B	59	PRO	CG-CD	-6.06	1.30	1.50
1	D	70	PRO	CG-CD	-6.06	1.30	1.50
1	A	277	PRO	CG-CD	-6.06	1.30	1.50
1	B	277	PRO	CG-CD	-6.06	1.30	1.50
1	A	57	PRO	CG-CD	-6.05	1.30	1.50
1	A	286	PRO	CG-CD	-6.04	1.30	1.50
1	C	217	PRO	N-CA	6.04	1.57	1.47
1	A	70	PRO	CG-CD	-6.01	1.30	1.50
1	A	92	PRO	CG-CD	-6.01	1.30	1.50
1	B	217	PRO	CG-CD	-6.01	1.30	1.50
1	B	136	PRO	CG-CD	-6.01	1.30	1.50
1	B	217	PRO	N-CA	6.00	1.57	1.47
1	D	47	PRO	CG-CD	-5.99	1.30	1.50
1	A	217	PRO	CG-CD	-5.99	1.30	1.50
1	B	334	PRO	CG-CD	-5.98	1.30	1.50
1	C	340	PRO	CG-CD	-5.97	1.30	1.50
1	D	277	PRO	CG-CD	-5.97	1.30	1.50
1	C	173	PRO	CG-CD	-5.97	1.30	1.50
1	B	340	PRO	CG-CD	-5.95	1.31	1.50
1	C	136	PRO	CG-CD	-5.95	1.31	1.50
1	D	340	PRO	CG-CD	-5.95	1.31	1.50
1	B	244	PRO	CG-CD	-5.94	1.31	1.50
1	B	220	PRO	CG-CD	-5.94	1.31	1.50
1	C	334	PRO	CG-CD	-5.94	1.31	1.50
1	C	286	PRO	CG-CD	-5.94	1.31	1.50
1	C	59	PRO	CG-CD	-5.93	1.31	1.50
1	B	258	PRO	CG-CD	-5.92	1.31	1.50
1	D	334	PRO	CG-CD	-5.92	1.31	1.50
1	B	47	PRO	CG-CD	-5.92	1.31	1.50
1	B	70	PRO	CG-CD	-5.91	1.31	1.50
1	D	57	PRO	CG-CD	-5.91	1.31	1.50
1	B	92	PRO	CG-CD	-5.91	1.31	1.50
1	C	277	PRO	CG-CD	-5.91	1.31	1.50
1	C	57	PRO	CG-CD	-5.90	1.31	1.50
1	B	83	PRO	CG-CD	-5.90	1.31	1.50
1	A	334	PRO	CG-CD	-5.89	1.31	1.50
1	D	92	PRO	CG-CD	-5.89	1.31	1.50
1	A	136	PRO	CG-CD	-5.88	1.31	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	220	PRO	CG-CD	-5.88	1.31	1.50
1	A	47	PRO	CG-CD	-5.86	1.31	1.50
1	C	217	PRO	CG-CD	-5.86	1.31	1.50
1	D	173	PRO	CG-CD	-5.86	1.31	1.50
1	C	258	PRO	CG-CD	-5.86	1.31	1.50
1	D	244	PRO	CG-CD	-5.84	1.31	1.50
1	D	57	PRO	N-CA	5.84	1.57	1.47
1	D	217	PRO	CG-CD	-5.84	1.31	1.50
1	A	195	PRO	CG-CD	-5.84	1.31	1.50
1	D	220	PRO	CG-CD	-5.83	1.31	1.50
1	A	66	PRO	CG-CD	-5.83	1.31	1.50
1	A	86	PRO	CG-CD	-5.82	1.31	1.50
1	D	258	PRO	CG-CD	-5.81	1.31	1.50
1	C	220	PRO	CG-CD	-5.79	1.31	1.50
1	D	195	PRO	CG-CD	-5.78	1.31	1.50
1	B	86	PRO	CG-CD	-5.76	1.31	1.50
1	B	173	PRO	CG-CD	-5.76	1.31	1.50
1	A	162	PRO	CG-CD	-5.75	1.31	1.50
1	B	66	PRO	CG-CD	-5.75	1.31	1.50
1	C	162	PRO	CG-CD	-5.75	1.31	1.50
1	A	340	PRO	CG-CD	-5.72	1.31	1.50
1	C	86	PRO	CG-CD	-5.72	1.31	1.50
1	D	83	PRO	CG-CD	-5.71	1.31	1.50
1	A	244	PRO	CG-CD	-5.70	1.31	1.50
1	B	195	PRO	CG-CD	-5.70	1.31	1.50
1	C	92	PRO	CG-CD	-5.66	1.31	1.50
1	D	66	PRO	CG-CD	-5.66	1.31	1.50
1	A	258	PRO	CG-CD	-5.66	1.31	1.50
1	C	66	PRO	CG-CD	-5.65	1.31	1.50
1	D	162	PRO	CG-CD	-5.64	1.32	1.50
1	C	195	PRO	CG-CD	-5.63	1.32	1.50
1	B	162	PRO	CG-CD	-5.59	1.32	1.50
1	C	70	PRO	CG-CD	-5.58	1.32	1.50
1	A	83	PRO	CG-CD	-5.57	1.32	1.50
1	D	59	PRO	CG-CD	-5.56	1.32	1.50
1	D	86	PRO	CG-CD	-5.54	1.32	1.50
1	C	83	PRO	CG-CD	-5.44	1.32	1.50
1	D	217	PRO	N-CA	5.30	1.56	1.47
1	C	244	PRO	CG-CD	-5.26	1.33	1.50
1	A	217	PRO	N-CA	5.25	1.56	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	54	ARG	NE-CZ-NH2	-13.93	113.34	120.30
1	D	54	ARG	NE-CZ-NH1	13.36	126.98	120.30
1	B	54	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	B	54	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	256	ASP	CB-CG-OD1	5.71	123.44	118.30
1	C	54	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	54	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	D	54	ARG	CD-NE-CZ	5.47	131.25	123.60
1	C	220	PRO	N-CD-CG	5.19	110.99	103.20
1	C	176	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	B	256	ASP	CB-CG-OD1	5.05	122.84	118.30
1	A	54	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	C	54	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	343	LEU	Peptide

## 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	2573	0	2564	19	0
1	B	2573	0	2564	22	0
1	C	2573	0	2564	27	0
1	D	2573	0	2564	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	44	0	26	0	0
3	B	44	0	26	0	0
3	C	44	0	26	0	0
3	D	44	0	26	0	0
4	A	8	0	7	0	0
4	B	8	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	8	0	7	1	0
4	D	8	0	7	0	0
5	A	345	0	0	7	0
5	B	316	0	0	2	0
5	C	400	0	0	7	0
5	D	324	0	0	6	0
All	All	11889	0	10388	74	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 4.

All (74) 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:329:GLY:O	5:D:501:HOH:O	1.81	0.95
1:A:274:ARG:NH2	5:A:501:HOH:O	2.02	0.93
1:B:139:HIS:NE2	1:B:164:GLN:OE1	2.02	0.92
1:B:222:THR:HG22	1:B:223:GLY:H	1.43	0.83
1:B:139:HIS:CD2	1:B:164:GLN:CD	2.52	0.82
1:B:69:GLU:OE2	5:B:501:HOH:O	2.00	0.79
1:B:139:HIS:NE2	1:B:164:GLN:CD	2.36	0.78
1:C:274:ARG:HD3	1:C:274:ARG:O	1.84	0.77
1:C:139:HIS:NE2	5:C:503:HOH:O	2.19	0.74
1:C:265:GLY:O	1:C:268:GLN:HG3	1.88	0.73
1:A:285:ASP:O	5:A:502:HOH:O	2.09	0.71
1:C:268:GLN:NE2	5:C:502:HOH:O	2.20	0.68
1:B:139:HIS:CD2	1:B:164:GLN:NE2	2.63	0.67
1:D:8:ARG:N	5:D:501:HOH:O	2.19	0.66
1:D:8:ARG:HG2	5:D:501:HOH:O	1.96	0.65
1:C:240:LYS:O	5:C:502:HOH:O	2.15	0.64
1:B:236:ASP:OD1	1:B:237:LEU:N	2.27	0.59
1:A:335:GLY:H	1:A:344:GLN:HB2	1.70	0.56
1:B:139:HIS:HD2	1:B:164:GLN:NE2	2.02	0.56
1:B:222:THR:HG22	1:B:223:GLY:N	2.18	0.54
1:B:30:ARG:NH2	1:B:317:GLU:OE2	2.36	0.54
1:C:48:LEU:HD23	1:C:260:GLN:HG3	1.90	0.53
1:C:241:THR:HG21	1:C:269:GLN:CG	2.39	0.53
1:A:332:HIS:NE2	1:A:343:LEU:HA	2.24	0.52
1:B:248:LEU:HD11	1:B:266:GLU:HB3	1.93	0.51
1:B:139:HIS:CE1	1:B:164:GLN:HB2	2.46	0.51
1:B:270:LEU:HD22	1:B:274:ARG:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:LEU:HG	1:C:270:LEU:HD11	1.92	0.50
1:A:281:HIS:O	5:A:502:HOH:O	2.19	0.50
1:C:235:ALA:O	4:C:403:PRO:HD2	2.10	0.50
1:A:68:ARG:HB2	1:B:52:LEU:HD13	1.92	0.50
1:D:225:ARG:NH2	5:D:508:HOH:O	2.35	0.50
1:A:335:GLY:H	1:A:344:GLN:CB	2.25	0.49
1:C:84:ALA:HB1	1:C:88:ARG:HG3	1.94	0.49
1:A:222:THR:OG1	1:A:223:GLY:N	2.45	0.49
1:A:43:ARG:NH1	1:A:69:GLU:OE1	2.45	0.49
1:D:222:THR:OG1	1:D:223:GLY:N	2.44	0.49
1:B:37:GLU:OE1	1:B:43:ARG:HD2	2.13	0.48
1:C:162:PRO:O	5:C:504:HOH:O	2.20	0.48
1:C:15:VAL:HG21	1:C:116:LEU:HD21	1.96	0.48
1:A:236:ASP:O	5:A:503:HOH:O	2.20	0.48
1:A:277:PRO:HG2	1:A:288:ALA:HB1	1.95	0.47
1:D:304:PHE:CE2	1:D:306:PHE:HB3	2.49	0.47
1:B:222:THR:CG2	1:B:223:GLY:H	2.21	0.47
1:C:241:THR:HG21	1:C:269:GLN:HG3	1.96	0.47
1:C:195:PRO:HB2	1:C:220:PRO:HD3	1.96	0.47
1:A:181:ARG:NH1	5:A:511:HOH:O	2.42	0.46
1:C:154:LEU:HD23	1:C:183:ALA:HB1	1.98	0.46
1:D:1:MET:N	5:D:502:HOH:O	2.25	0.46
1:C:103:ASP:O	1:D:54:ARG:HD2	2.17	0.45
1:B:332:HIS:CE1	1:B:343:LEU:HA	2.52	0.45
1:C:285:ASP:OD1	5:C:505:HOH:O	2.21	0.45
1:C:167:LEU:CD2	1:C:191:GLU:HG3	2.46	0.45
1:C:43:ARG:NH1	1:C:69:GLU:OE1	2.50	0.45
1:A:343:LEU:HD22	1:B:12:ALA:HA	2.00	0.44
1:A:52:LEU:HD13	1:B:68:ARG:HB2	2.00	0.44
1:A:48:LEU:HD21	1:A:259:GLU:HG2	1.99	0.43
1:D:26:ARG:O	1:D:30:ARG:HG2	2.19	0.43
1:A:178:SER:HA	5:A:758:HOH:O	2.17	0.43
1:D:248:LEU:HD21	1:D:266:GLU:HB3	2.01	0.43
1:D:181:ARG:HD3	5:D:778:HOH:O	2.19	0.43
1:A:31:LEU:HD11	1:A:307:GLU:HG2	2.01	0.42
1:C:197:ARG:NH1	5:C:510:HOH:O	2.41	0.42
1:C:275:LEU:HD22	5:C:623:HOH:O	2.18	0.42
1:C:68:ARG:CZ	1:D:54:ARG:HG2	2.50	0.42
1:D:236:ASP:OD1	1:D:237:LEU:N	2.39	0.42
1:C:30:ARG:NH2	1:C:317:GLU:OE2	2.44	0.42
1:A:332:HIS:HE1	1:A:340:PRO:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:ARG:O	1:C:30:ARG:HG2	2.20	0.41
1:A:343:LEU:HD21	1:B:116:LEU:HD22	2.03	0.41
1:C:56:GLU:HA	1:C:57:PRO:C	2.42	0.41
1:B:285:ASP:HB3	5:B:684:HOH:O	2.20	0.40
5:A:794:HOH:O	1:B:181:ARG:HD3	2.20	0.40
1:C:167:LEU:HD23	1:C:191:GLU:HG3	2.03	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	342/344 (99%)	332 (97%)	9 (3%)	1 (0%)	41	27
1	B	342/344 (99%)	332 (97%)	9 (3%)	1 (0%)	41	27
1	C	342/344 (99%)	332 (97%)	9 (3%)	1 (0%)	41	27
1	D	342/344 (99%)	334 (98%)	8 (2%)	0	100	100
All	All	1368/1376 (99%)	1330 (97%)	35 (3%)	3 (0%)	47	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	ASP
1	B	236	ASP
1	C	236	ASP

### 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	261/261 (100%)	261 (100%)	0	100	100
1	B	261/261 (100%)	260 (100%)	1 (0%)	91	89
1	C	261/261 (100%)	259 (99%)	2 (1%)	81	78
1	D	261/261 (100%)	260 (100%)	1 (0%)	91	89
All	All	1044/1044 (100%)	1040 (100%)	4 (0%)	91	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	344	GLN
1	C	197	ARG
1	C	236	ASP
1	D	9	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	GLN
1	A	281	HIS
1	D	139	HIS

### 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 monosaccharides in this entry.



## 5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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	PRO	A	403	-	5,8,8	10.00	3 (60%)	6,10,10	1.30	1 (16%)
3	NAD	B	402	-	42,48,48	0.86	1 (2%)	50,73,73	1.24	7 (14%)
3	NAD	A	402	-	42,48,48	0.88	1 (2%)	50,73,73	1.27	7 (14%)
3	NAD	D	402	-	42,48,48	0.90	2 (4%)	50,73,73	1.17	7 (14%)
3	NAD	C	402	-	42,48,48	0.85	1 (2%)	50,73,73	1.22	6 (12%)
4	PRO	C	403	-	5,8,8	10.11	4 (80%)	6,10,10	1.99	1 (16%)
4	PRO	D	403	-	5,8,8	9.92	3 (60%)	6,10,10	1.89	1 (16%)
4	PRO	B	403	-	5,8,8	10.11	3 (60%)	6,10,10	1.01	0

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	PRO	A	403	-	-	0/0/11/11	0/1/1/1
3	NAD	B	402	-	-	5/26/62/62	0/5/5/5
3	NAD	A	402	-	-	5/26/62/62	0/5/5/5
3	NAD	D	402	-	-	5/26/62/62	0/5/5/5
3	NAD	C	402	-	-	5/26/62/62	0/5/5/5
4	PRO	C	403	-	-	0/0/11/11	0/1/1/1
4	PRO	D	403	-	-	0/0/11/11	0/1/1/1
4	PRO	B	403	-	-	0/0/11/11	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	PRO	CB-CA	-21.97	1.28	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	403	PRO	CB-CA	-21.82	1.28	1.54
4	A	403	PRO	CB-CA	-21.77	1.28	1.54
4	D	403	PRO	CB-CA	-21.60	1.28	1.54
4	C	403	PRO	CG-CD	-4.58	1.28	1.51
4	B	403	PRO	CG-CD	-4.46	1.29	1.51
4	A	403	PRO	CG-CD	-4.33	1.30	1.51
4	D	403	PRO	CG-CD	-4.17	1.30	1.51
4	C	403	PRO	CD-N	-2.74	1.39	1.49
3	C	402	NAD	C2A-N3A	2.58	1.36	1.32
3	A	402	NAD	C5A-C4A	2.49	1.47	1.40
4	A	403	PRO	CG-CB	2.45	1.62	1.51
4	D	403	PRO	CG-CB	2.42	1.61	1.51
3	D	402	NAD	C5A-C4A	2.31	1.47	1.40
4	C	403	PRO	CG-CB	2.29	1.61	1.51
4	B	403	PRO	CG-CB	2.23	1.61	1.51
3	B	402	NAD	O4D-C1D	2.14	1.44	1.41
3	D	402	NAD	C2A-N3A	2.05	1.35	1.32

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	403	PRO	CD-N-CA	-4.54	94.89	107.06
4	C	403	PRO	CD-N-CA	-4.34	95.42	107.06
3	A	402	NAD	N3A-C2A-N1A	-4.13	122.23	128.68
3	B	402	NAD	N3A-C2A-N1A	-3.87	122.63	128.68
3	C	402	NAD	N3A-C2A-N1A	-3.74	122.83	128.68
3	D	402	NAD	N3A-C2A-N1A	-3.38	123.39	128.68
3	C	402	NAD	C1B-N9A-C4A	-3.07	121.24	126.64
4	A	403	PRO	CD-N-CA	-3.00	99.00	107.06
3	A	402	NAD	O4B-C1B-C2B	-2.79	102.85	106.93
3	A	402	NAD	C1B-N9A-C4A	-2.76	121.80	126.64
3	A	402	NAD	C2A-N1A-C6A	2.75	123.45	118.75
3	A	402	NAD	O4D-C1D-C2D	-2.72	102.96	106.93
3	B	402	NAD	O4D-C1D-C2D	-2.48	103.30	106.93
3	B	402	NAD	C5N-C4N-C3N	-2.42	117.48	120.34
3	D	402	NAD	O4B-C1B-C2B	-2.39	103.43	106.93
3	D	402	NAD	O4D-C1D-C2D	-2.36	103.47	106.93
3	B	402	NAD	O4B-C1B-C2B	-2.36	103.48	106.93
3	B	402	NAD	C1B-N9A-C4A	-2.33	122.56	126.64
3	B	402	NAD	C2A-N1A-C6A	2.31	122.70	118.75
3	A	402	NAD	C4A-C5A-N7A	-2.21	107.10	109.40
3	D	402	NAD	C2A-N1A-C6A	2.20	122.52	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	NAD	C5N-C4N-C3N	-2.19	117.75	120.34
3	C	402	NAD	N6A-C6A-N1A	2.19	123.11	118.57
3	D	402	NAD	C1B-N9A-C4A	-2.12	122.92	126.64
3	C	402	NAD	C2A-N1A-C6A	2.10	122.35	118.75
3	C	402	NAD	C4A-C5A-N7A	-2.08	107.23	109.40
3	D	402	NAD	C4A-C5A-N7A	-2.07	107.24	109.40
3	B	402	NAD	C4A-C5A-N7A	-2.03	107.28	109.40
3	C	402	NAD	O4B-C1B-C2B	-2.02	103.97	106.93
3	D	402	NAD	C5N-C4N-C3N	-2.00	117.97	120.34

There are no chirality outliers.

All (20) torsion outliers are listed below:

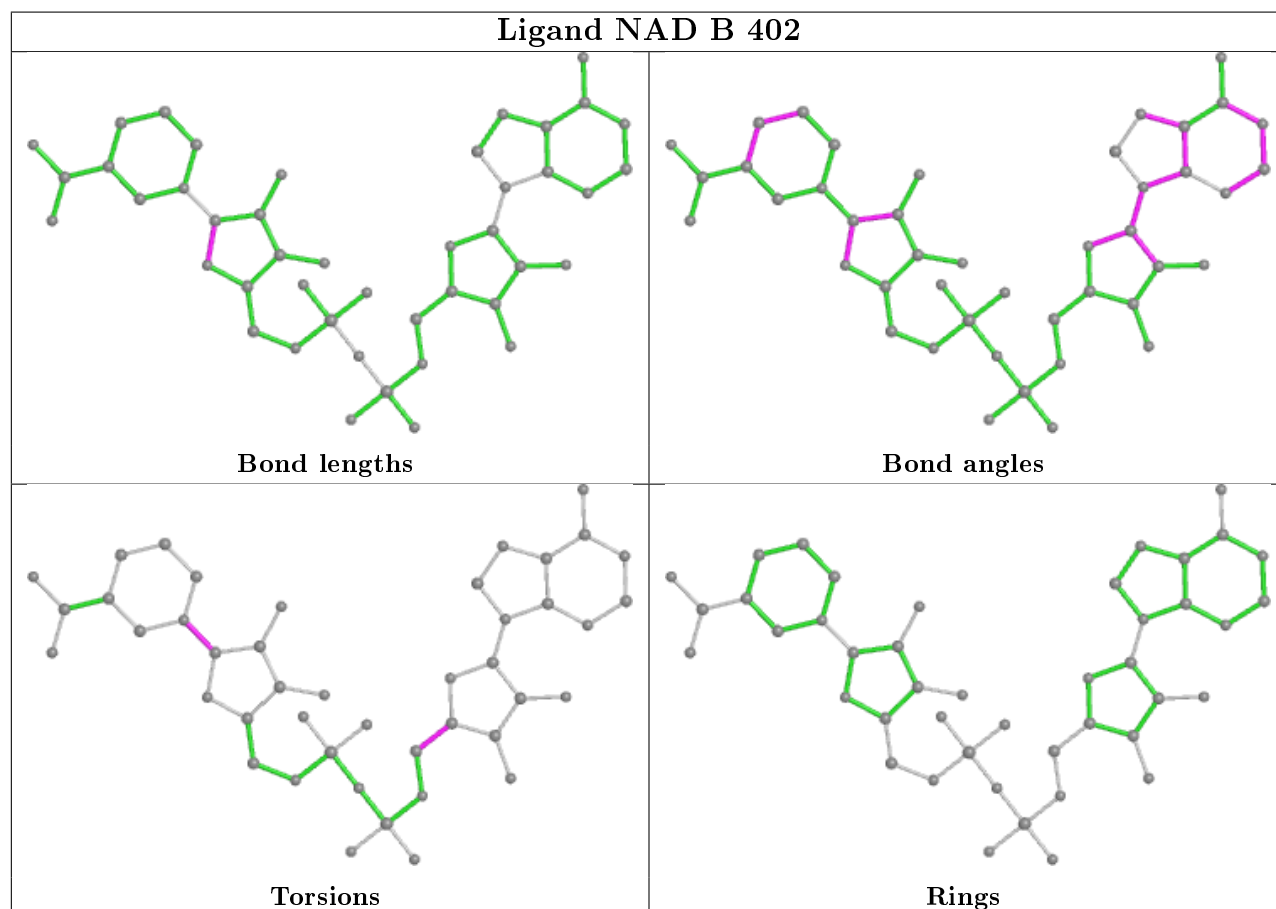
Mol	Chain	Res	Type	Atoms
3	B	402	NAD	O4D-C1D-N1N-C2N
3	B	402	NAD	O4D-C1D-N1N-C6N
3	B	402	NAD	C2D-C1D-N1N-C2N
3	B	402	NAD	C2D-C1D-N1N-C6N
3	A	402	NAD	O4D-C1D-N1N-C2N
3	A	402	NAD	O4D-C1D-N1N-C6N
3	A	402	NAD	C2D-C1D-N1N-C2N
3	A	402	NAD	C2D-C1D-N1N-C6N
3	D	402	NAD	O4D-C1D-N1N-C2N
3	D	402	NAD	O4D-C1D-N1N-C6N
3	D	402	NAD	C2D-C1D-N1N-C2N
3	D	402	NAD	C2D-C1D-N1N-C6N
3	C	402	NAD	O4D-C1D-N1N-C2N
3	C	402	NAD	O4D-C1D-N1N-C6N
3	C	402	NAD	C2D-C1D-N1N-C2N
3	C	402	NAD	C2D-C1D-N1N-C6N
3	C	402	NAD	O4B-C4B-C5B-O5B
3	B	402	NAD	O4B-C4B-C5B-O5B
3	A	402	NAD	O4B-C4B-C5B-O5B
3	D	402	NAD	O4B-C4B-C5B-O5B

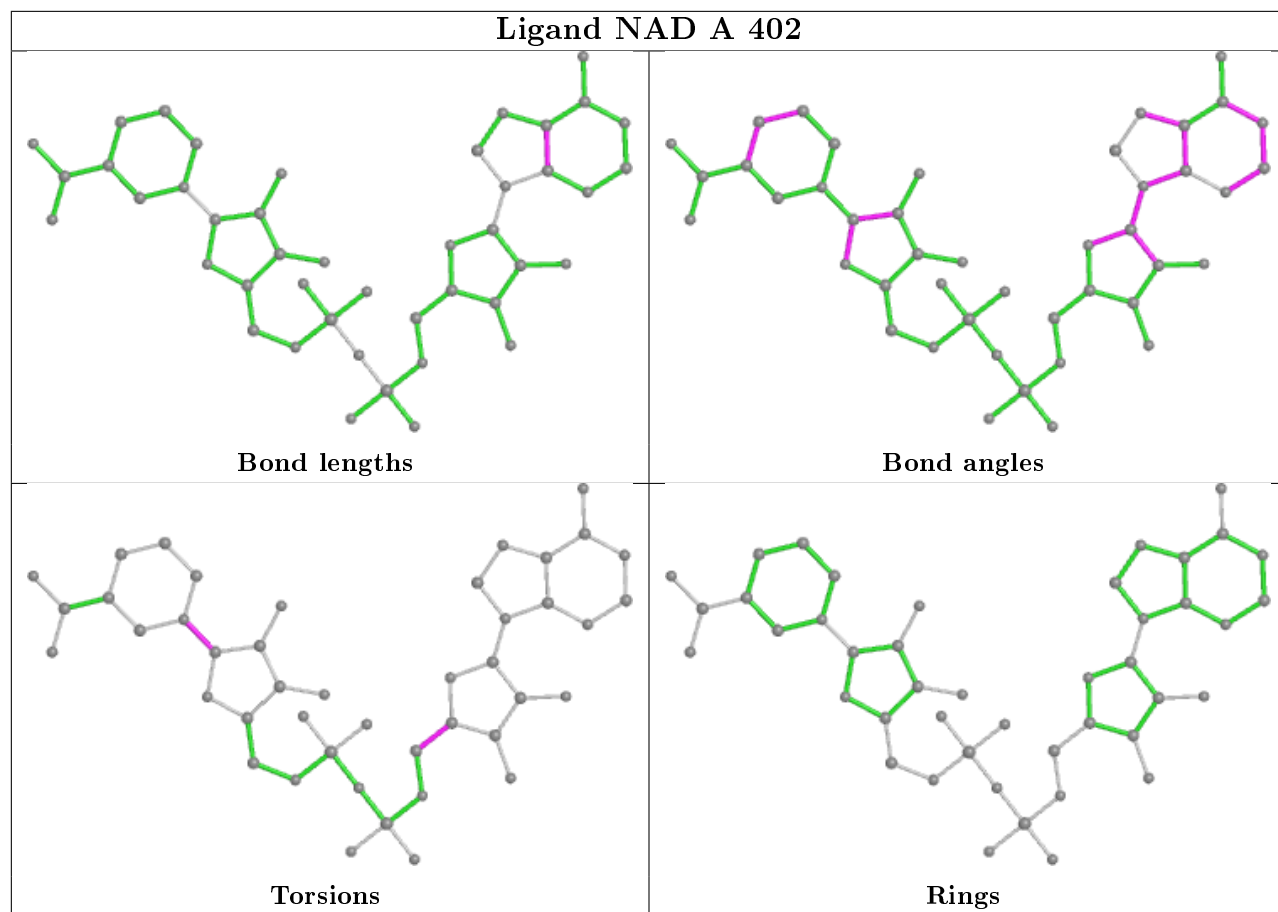
There are no ring outliers.

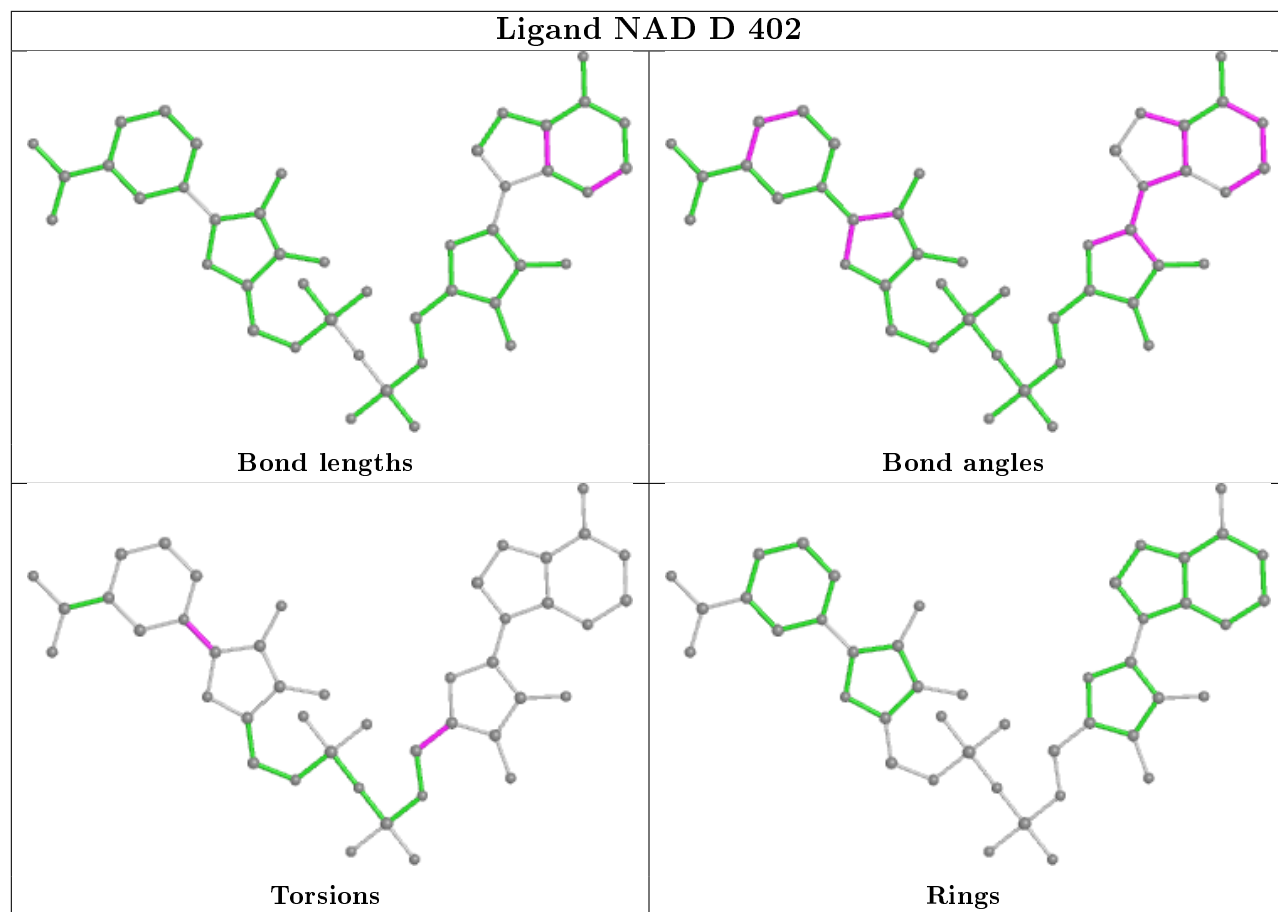
1 monomer is involved in 1 short contact:

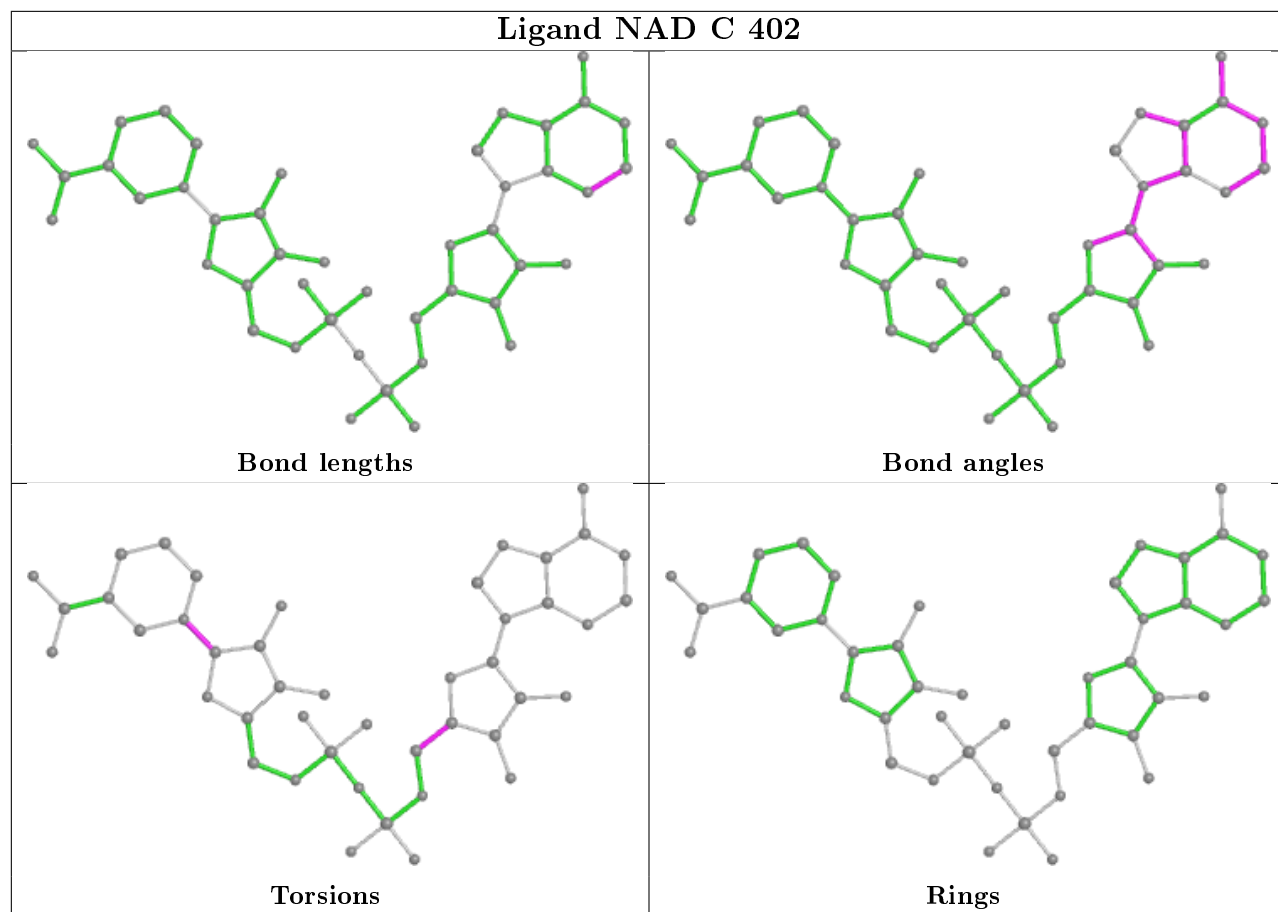
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	403	PRO	1	0

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.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	344/344 (100%)	-0.19	4 (1%) 79 76	14, 20, 31, 54	0
1	B	344/344 (100%)	0.05	19 (5%) 25 20	14, 21, 36, 63	0
1	C	344/344 (100%)	-0.16	9 (2%) 56 51	11, 17, 27, 58	0
1	D	344/344 (100%)	0.05	15 (4%) 34 28	12, 21, 37, 54	0
All	All	1376/1376 (100%)	-0.06	47 (3%) 45 39	11, 20, 34, 63	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	274	ARG	7.3
1	C	272	ALA	6.8
1	C	273	ASP	5.7
1	A	344	GLN	5.6
1	C	271	SER	5.5
1	C	344	GLN	5.5
1	C	270	LEU	5.0
1	B	275	LEU	4.9
1	A	343	LEU	4.7
1	B	273	ASP	4.2
1	C	343	LEU	4.2
1	D	1	MET	3.7
1	B	1	MET	3.6
1	D	287	ALA	3.2
1	B	344	GLN	3.2
1	D	290	ALA	3.2
1	C	274	ARG	3.1
1	B	276	GLY	3.1
1	B	223	GLY	3.0
1	B	321	GLU	2.9
1	D	274	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	88	ARG	2.9
1	B	271	SER	2.8
1	C	1	MET	2.8
1	B	139	HIS	2.8
1	D	344	GLN	2.7
1	B	272	ALA	2.5
1	B	115	VAL	2.5
1	B	343	LEU	2.5
1	D	223	GLY	2.5
1	A	139	HIS	2.5
1	D	271	SER	2.5
1	D	288	ALA	2.4
1	D	273	ASP	2.4
1	D	233	VAL	2.4
1	D	9	ARG	2.4
1	B	222	THR	2.4
1	D	120	LEU	2.3
1	B	221	ASP	2.3
1	B	94	ILE	2.2
1	B	323	ASP	2.2
1	B	9	ARG	2.2
1	C	139	HIS	2.2
1	D	321	GLU	2.1
1	D	323	ASP	2.1
1	A	44	HIS	2.1
1	D	122	THR	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](#)

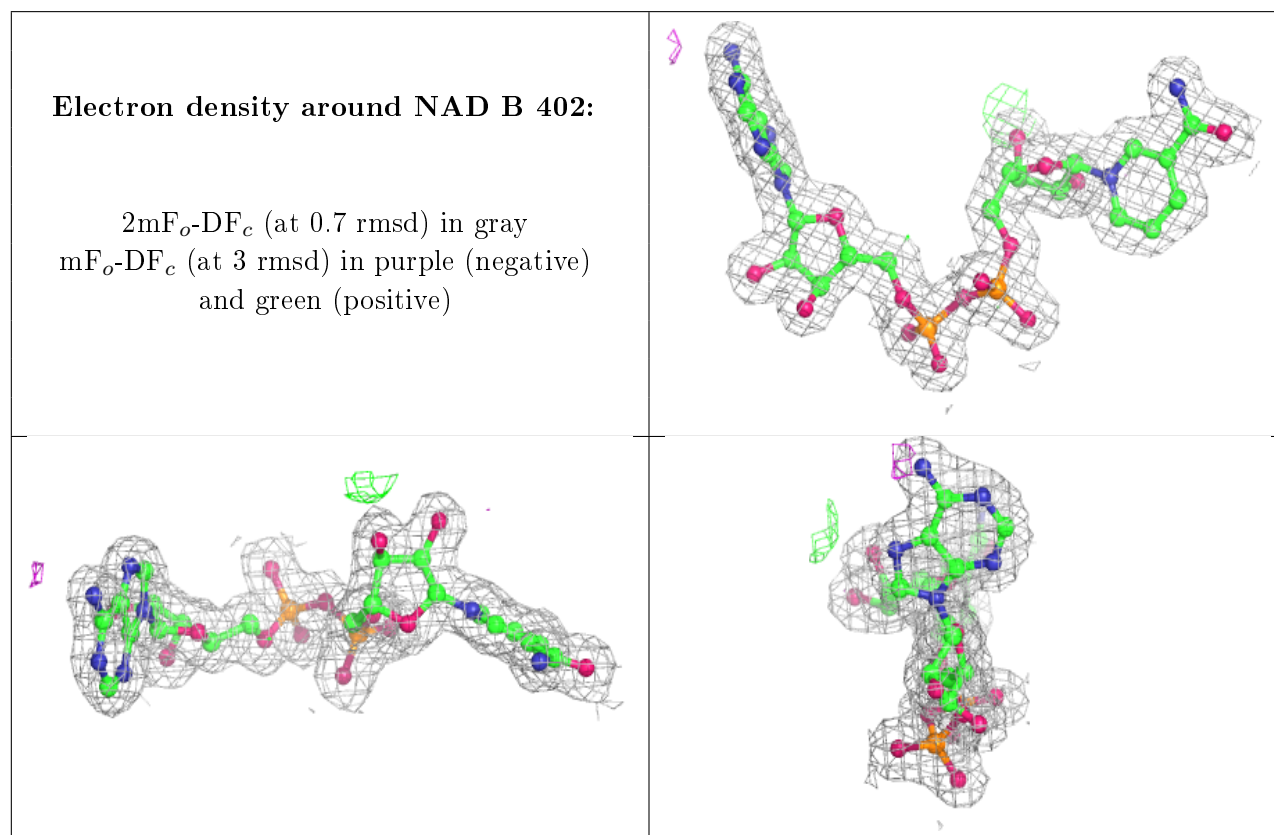
There are no monosaccharides in this entry.

## 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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

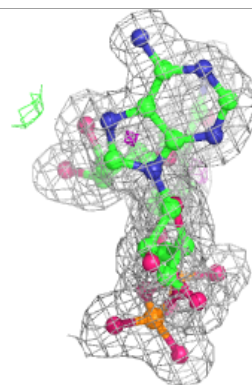
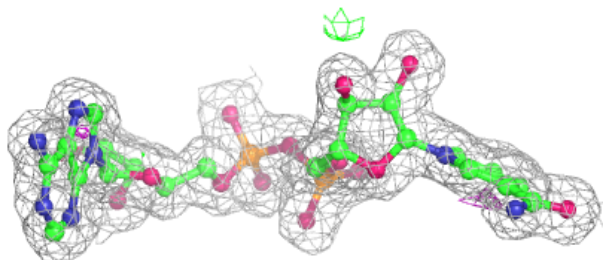
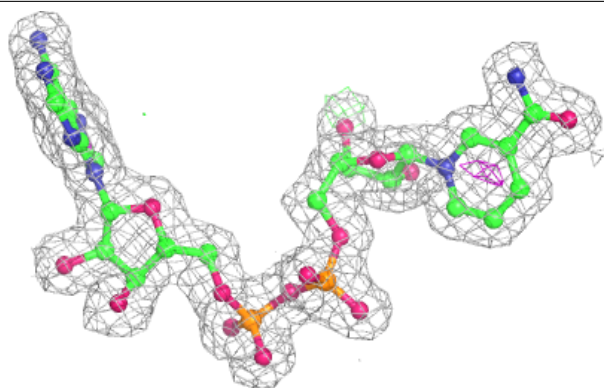
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PRO	C	403	8/8	0.82	0.14	18,24,27,34	0
4	PRO	D	403	8/8	0.86	0.14	20,24,27,31	0
4	PRO	A	403	8/8	0.88	0.14	20,26,30,32	0
4	PRO	B	403	8/8	0.91	0.13	20,27,31,33	0
3	NAD	B	402	44/44	0.97	0.09	14,16,19,21	0
3	NAD	A	402	44/44	0.97	0.07	13,16,19,20	0
3	NAD	D	402	44/44	0.97	0.10	13,15,17,18	0
3	NAD	C	402	44/44	0.98	0.08	9,12,14,15	0
2	NA	A	401	1/1	0.99	0.15	17,17,17,17	0
2	NA	D	401	1/1	0.99	0.16	18,18,18,18	0
2	NA	B	401	1/1	1.00	0.13	18,18,18,18	0
2	NA	C	401	1/1	1.00	0.20	10,10,10,10	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.

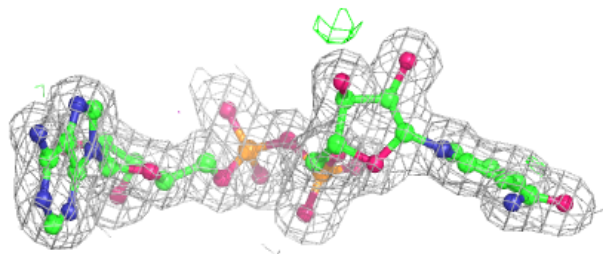
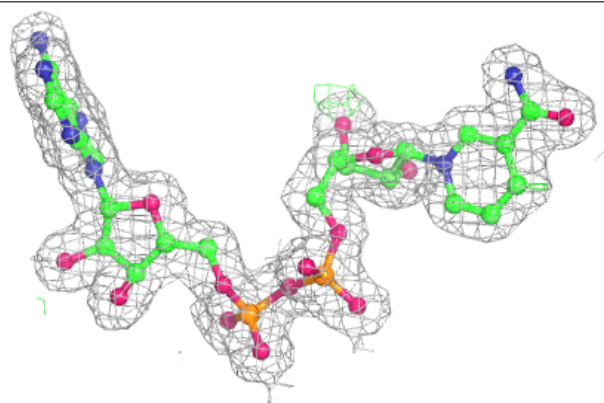


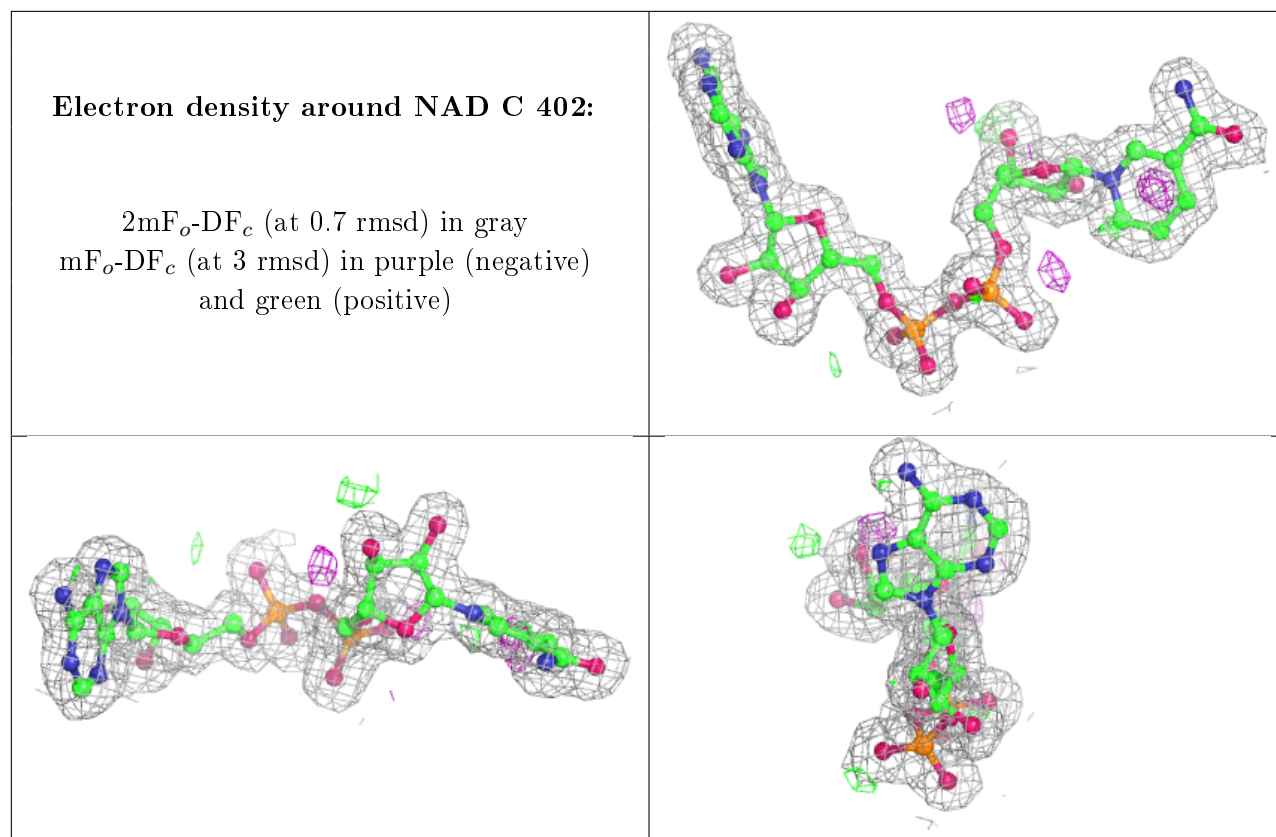
**Electron density around NAD A 402:**

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

**Electron density around NAD D 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 ⓘ

There are no such residues in this entry.