



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 08:53 AM UTC

PDB ID : 9IE9 / pdb_00009ie9
Title : Human Deoxyhypusine Synthase Fragment Screening Campaign - ligand VT00254
Authors : Wilk, P.; Water-Wilk, E.; Krojer, T.; Grudnik, P.
Deposited on : 2025-02-15
Resolution : 1.39 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

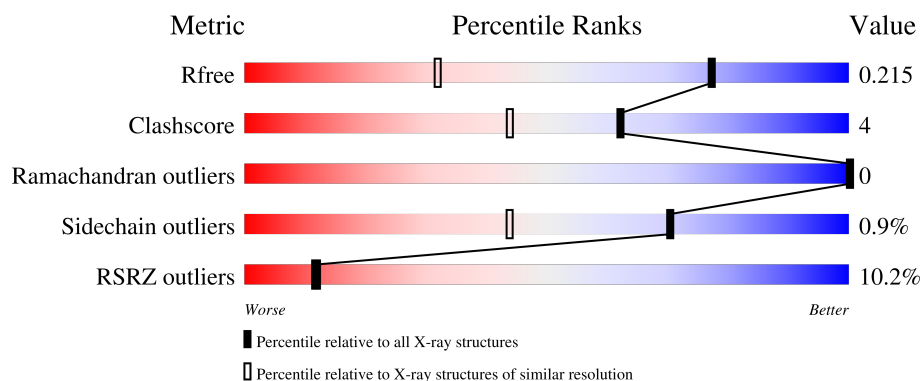
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.39 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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 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	A	369	 12% 85% 8% • 5%
1	B	369	 7% 84% 6% • 9%

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	A1I3L	A	402	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6168 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 Deoxyhypusine synthase.

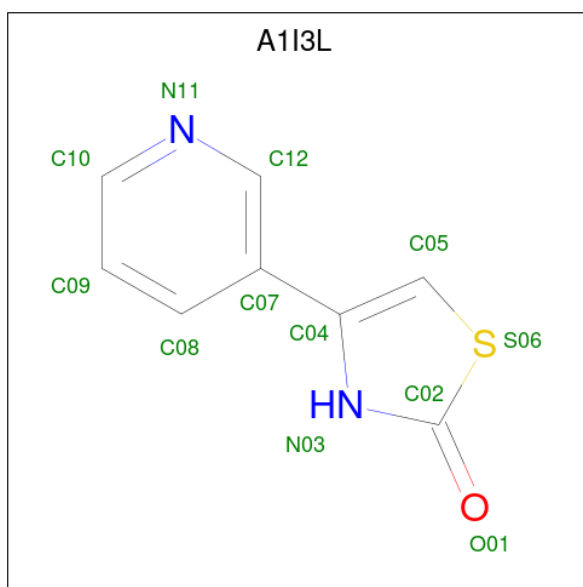
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	9	0
			2771	1767	469	518	17			
1	B	336	Total	C	N	O	S	0	10	0
			2697	1720	456	504	17			

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



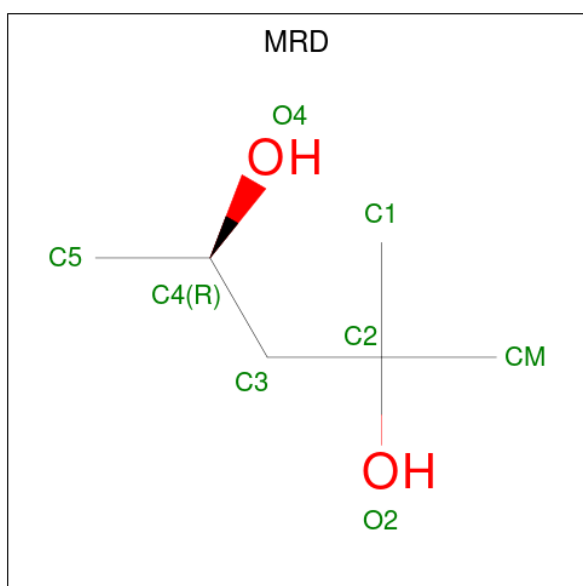
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
2	B	1	Total	C	N	O	P	0	1
			88	42	14	28	4		

- Molecule 3 is 4-pyridin-3-yl-3 {H}-1,3-thiazol-2-one (CCD ID: A1I3L) (formula: $C_8H_6N_2OS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	8	2	1	1		
3	B	1	Total	C	N	O	S	0	0
			12	8	2	1	1		

- Molecule 4 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			8	6	2		

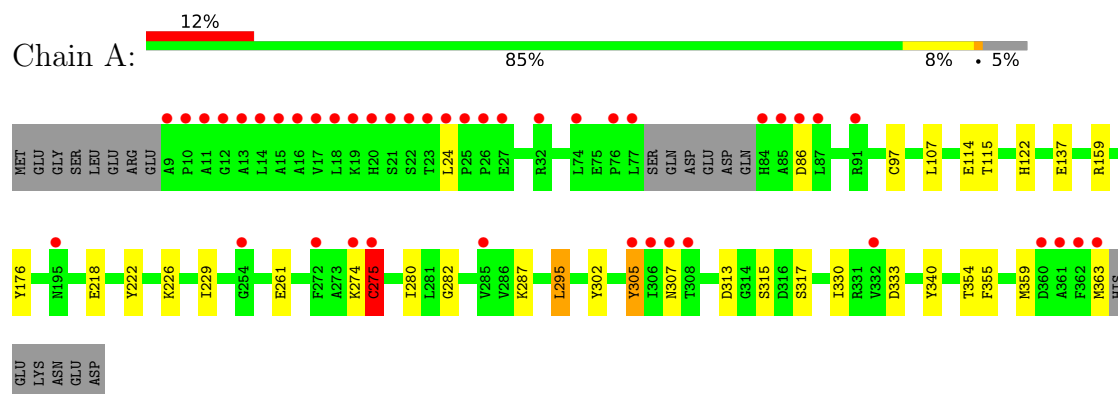
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	246	Total 246	O 246	0	0
5	B	246	Total 246	O 246	0	0

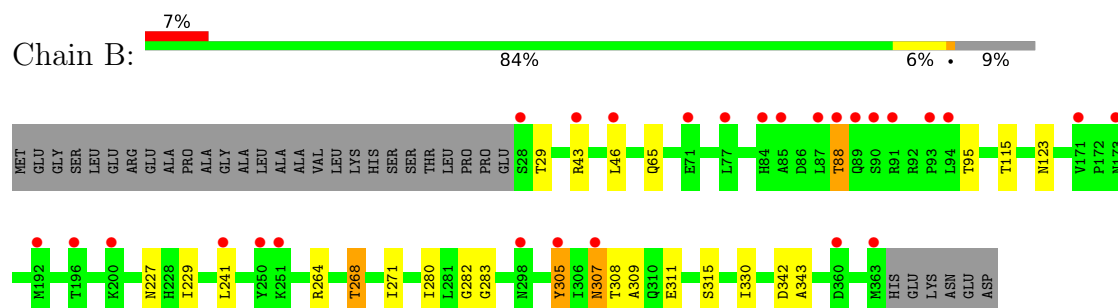
3 Residue-property plots

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: Deoxyhypusine synthase



• Molecule 1: Deoxyhypusine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.86Å 104.86Å 160.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.08 – 1.39 46.08 – 1.39	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.08-1.39) 99.8 (46.08-1.39)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 1.39Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.190 , 0.206 0.200 , 0.215	Depositor DCC
R_{free} test set	10088 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6168	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1I3L, CSS, MRD, 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	1.28	16/2842 (0.6%)	1.46	25/3852 (0.6%)
1	B	1.21	9/2771 (0.3%)	1.41	25/3754 (0.7%)
All	All	1.25	25/5613 (0.4%)	1.44	50/7606 (0.7%)

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	3
1	B	0	1
All	All	0	4

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	355	PHE	CA-C	-10.46	1.39	1.52
1	A	275[A]	CYS	N-CA	10.24	1.58	1.46
1	A	275[B]	CYS	N-CA	10.24	1.58	1.46
1	A	354	THR	CA-CB	9.34	1.69	1.53
1	B	65	GLN	CD-OE1	7.93	1.38	1.23
1	B	307[A]	ASN	C-O	7.50	1.32	1.23
1	B	307[B]	ASN	C-O	7.50	1.32	1.23
1	A	305[A]	TYR	C-O	7.34	1.32	1.24
1	A	305[B]	TYR	C-O	7.34	1.32	1.24
1	B	305[A]	TYR	C-O	6.84	1.32	1.24
1	B	305[B]	TYR	C-O	6.84	1.32	1.24
1	A	287[A]	LYS	C-O	6.80	1.32	1.24
1	A	287[B]	LYS	C-O	6.80	1.32	1.24
1	A	355	PHE	CA-CB	6.72	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	271	ILE	C-O	-6.18	1.17	1.24
1	B	229	ILE	N-CA	5.71	1.50	1.46
1	A	317[A]	SER	C-O	5.56	1.30	1.24
1	A	317[B]	SER	C-O	5.56	1.30	1.24
1	A	122	HIS	CE1-NE2	5.51	1.38	1.32
1	A	114	GLU	N-CA	5.39	1.52	1.46
1	A	354	THR	C-N	-5.34	1.26	1.33
1	B	43[A]	ARG	C-O	5.11	1.30	1.24
1	B	43[B]	ARG	C-O	5.11	1.30	1.24
1	A	307[A]	ASN	C-O	5.08	1.30	1.23
1	A	307[B]	ASN	C-O	5.08	1.30	1.23

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46[A]	LEU	CA-C-O	10.57	131.76	120.55
1	B	46[B]	LEU	CA-C-O	10.57	131.76	120.55
1	B	241[A]	LEU	CA-C-O	10.51	131.69	120.55
1	B	241[B]	LEU	CA-C-O	10.51	131.69	120.55
1	B	65	GLN	CG-CD-NE2	-10.28	100.99	116.40
1	A	218[A]	GLU	CA-C-O	10.21	132.33	119.05
1	A	218[B]	GLU	CA-C-O	10.21	132.33	119.05
1	B	43[A]	ARG	CA-C-O	9.86	131.00	120.55
1	B	43[B]	ARG	CA-C-O	9.86	131.00	120.55
1	B	43[A]	ARG	N-CA-C	9.70	121.86	111.28
1	B	43[B]	ARG	N-CA-C	9.70	121.86	111.28
1	B	46[A]	LEU	N-CA-C	9.40	121.53	111.28
1	B	46[B]	LEU	N-CA-C	9.40	121.53	111.28
1	B	268[A]	THR	CA-C-O	9.17	130.47	120.10
1	B	268[B]	THR	CA-C-O	9.17	130.47	120.10
1	A	307[A]	ASN	CA-C-O	8.52	130.94	121.06
1	A	307[B]	ASN	CA-C-O	8.52	130.94	121.06
1	A	317[A]	SER	CA-C-O	8.06	129.10	120.55
1	A	317[B]	SER	CA-C-O	8.06	129.10	120.55
1	A	24	LEU	CA-C-N	7.96	125.47	119.66
1	A	24	LEU	C-N-CA	7.96	125.47	119.66
1	B	65	GLN	OE1-CD-NE2	7.69	130.29	122.60
1	A	274	LYS	CA-C-N	7.59	135.29	121.94
1	A	274	LYS	C-N-CA	7.59	135.29	121.94
1	B	305[A]	TYR	CA-C-O	7.54	128.61	120.32
1	B	305[B]	TYR	CA-C-O	7.54	128.61	120.32
1	B	241[A]	LEU	N-CA-C	7.48	119.43	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	241[B]	LEU	N-CA-C	7.48	119.43	111.28
1	A	229	ILE	O-C-N	7.32	125.98	121.37
1	A	218[A]	GLU	N-CA-C	6.77	120.80	112.54
1	A	218[B]	GLU	N-CA-C	6.77	120.80	112.54
1	A	317[A]	SER	N-CA-C	6.75	118.64	111.28
1	A	317[B]	SER	N-CA-C	6.75	118.64	111.28
1	A	287[A]	LYS	CA-C-O	6.39	127.19	120.42
1	A	287[B]	LYS	CA-C-O	6.39	127.19	120.42
1	B	307[A]	ASN	CA-C-O	6.26	128.11	120.60
1	B	307[B]	ASN	CA-C-O	6.26	128.11	120.60
1	A	287[A]	LYS	N-CA-C	6.23	118.15	111.36
1	A	287[B]	LYS	N-CA-C	6.23	118.15	111.36
1	B	29	THR	CA-CB-OG1	-5.51	101.34	109.60
1	A	275[A]	CYS	CA-C-O	-5.39	113.91	120.54
1	A	275[B]	CYS	CA-C-O	-5.39	113.91	120.54
1	B	305[A]	TYR	CA-C-N	-5.39	115.55	123.10
1	B	305[A]	TYR	C-N-CA	-5.39	115.55	123.10
1	B	305[B]	TYR	CA-C-N	-5.39	115.55	123.10
1	B	305[B]	TYR	C-N-CA	-5.39	115.55	123.10
1	A	355	PHE	CA-CB-CG	5.30	119.10	113.80
1	A	275[A]	CYS	CB-CA-C	-5.14	98.94	109.38
1	A	275[B]	CYS	CB-CA-C	-5.14	98.94	109.38
1	A	333	ASP	CA-CB-CG	5.08	117.68	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	275[A]	CYS	Mainchain
1	A	275[B]	CYS	Mainchain
1	A	86[A]	ASP	Mainchain
1	B	283	GLY	Mainchain

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	2771	0	2761	23	0
1	B	2697	0	2691	18	1
2	A	88	0	52	6	0
2	B	88	0	52	8	0
3	A	12	0	0	0	0
3	B	12	0	0	1	1
4	B	8	0	14	0	0
5	A	246	0	0	10	1
5	B	246	0	0	7	1
All	All	6168	0	5570	46	2

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 (46) 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:B:307[B]:ASN:ND2	5:B:502:HOH:O	1.70	1.25
2:B:402[A]:NAD:O1A	5:B:504:HOH:O	1.81	0.96
2:A:401[A]:NAD:O1A	5:A:503:HOH:O	1.85	0.94
1:A:261:GLU:HG2	5:A:522:HOH:O	1.76	0.84
1:B:280:ILE:HD12	1:B:305[B]:TYR:CE2	2.22	0.74
1:B:307[B]:ASN:CG	5:B:502:HOH:O	2.19	0.73
1:A:137[A]:GLU:CD	5:A:504:HOH:O	2.33	0.71
2:B:402[A]:NAD:O7N	5:B:506:HOH:O	2.09	0.70
1:A:137[A]:GLU:OE2	5:A:504:HOH:O	2.10	0.69
1:A:305[A]:TYR:OH	1:A:330:ILE:HD11	1.92	0.69
1:A:137[B]:GLU:OE1	5:A:505:HOH:O	2.12	0.66
1:B:307[B]:ASN:OD1	1:B:308:THR:N	2.35	0.60
2:A:401[B]:NAD:N7N	5:A:504:HOH:O	2.28	0.58
1:B:280:ILE:HD12	1:B:305[B]:TYR:HE2	1.67	0.57
1:A:159:ARG:NH2	5:A:508:HOH:O	2.34	0.56
1:A:226:LYS:NZ	5:A:513:HOH:O	2.34	0.55
1:A:275[A]:CYS:SG	1:A:302:TYR:HE2	2.30	0.55
1:A:359:MET:O	1:A:359:MET:HE3	2.08	0.53
2:A:401[A]:NAD:H3B	1:B:315:SER:CB	2.38	0.53
1:A:295:LEU:HD12	1:A:295:LEU:O	2.07	0.53
1:A:107:LEU:HD21	2:A:401[A]:NAD:N6A	2.23	0.53
1:A:159:ARG:NE	5:A:508:HOH:O	2.23	0.53
1:B:88:THR:O	5:B:508:HOH:O	2.18	0.53
2:A:401[A]:NAD:H3B	1:B:315:SER:HB3	1.91	0.52
1:B:305[B]:TYR:OH	1:B:330:ILE:HD11	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ASP:OD2	2:B:402[A]:NAD:H2B	2.09	0.52
1:A:359:MET:HE3	1:A:359:MET:HA	1.94	0.49
1:A:315:SER:CB	2:B:402[A]:NAD:H3B	2.42	0.49
1:A:159:ARG:CZ	5:A:508:HOH:O	2.61	0.48
1:A:222:TYR:OH	1:A:226:LYS:NZ	2.47	0.47
1:B:307[B]:ASN:HD21	1:B:309:ALA:HB3	1.80	0.46
1:B:264:ARG:O	1:B:268[A]:THR:HG23	2.16	0.45
1:B:342:ASP:HA	2:B:402[A]:NAD:N1A	2.31	0.44
1:A:137[B]:GLU:OE2	1:A:176:TYR:OH	2.29	0.44
1:B:309:ALA:HB2	2:B:402[B]:NAD:O2B	2.18	0.44
1:B:343:ALA:N	2:B:402[A]:NAD:N1A	2.50	0.43
1:B:305[A]:TYR:OH	5:B:507:HOH:O	2.16	0.43
1:A:97:CYS:HA	1:A:275[A]:CYS:HB3	2.00	0.43
1:A:282:GLY:HA2	2:A:401[A]:NAD:H1B	1.99	0.43
3:B:403:A1I3L:C12	5:B:503:HOH:O	0.73	0.43
1:B:282:GLY:HA2	2:B:402[A]:NAD:H1B	2.00	0.42
1:A:280:ILE:HD12	1:A:305[A]:TYR:CE2	2.54	0.42
1:B:307[B]:ASN:ND2	1:B:309:ALA:HB3	2.34	0.42
1:A:359:MET:HE2	1:A:363:MET:SD	2.60	0.41
1:B:123:ASN:OD1	1:B:227:ASN:HB3	2.20	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:713:HOH:O	5:B:722:HOH:O[4_555]	1.83	0.37
1:B:311:GLU:OE2	3:B:403:A1I3L:C05[4_555]	1.89	0.31

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	A	353/369 (96%)	349 (99%)	4 (1%)	0	100	100
1	B	343/369 (93%)	338 (98%)	5 (2%)	0	100	100
All	All	696/738 (94%)	687 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	299/309 (97%)	297 (99%)	2 (1%)	76	52
1	B	293/309 (95%)	290 (99%)	3 (1%)	68	40
All	All	592/618 (96%)	587 (99%)	5 (1%)	70	48

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	THR
1	A	295	LEU
1	B	88	THR
1	B	95	THR
1	B	115	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	37	ASN
1	B	310	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSS	B	177	1	4,6,7	0.78	0	2,6,8	1.09	0
1	CSS	A	177	1	4,6,7	0.66	0	2,6,8	0.31	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
1	CSS	B	177	1	-	0/1/5/7	-
1	CSS	A	177	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	A1I3L	B	403	-	13,13,13	6.99	6 (46%)	15,17,17	2.77	8 (53%)
2	NAD	B	402[A]	-	46,48,48	0.59	0	64,73,73	0.74	2 (3%)
4	MRD	B	401	-	7,7,7	0.22	0	9,10,10	0.84	0
2	NAD	A	401[A]	-	46,48,48	0.61	1 (2%)	64,73,73	0.72	2 (3%)
2	NAD	B	402[B]	-	46,48,48	0.54	1 (2%)	64,73,73	0.63	1 (1%)
3	A1I3L	A	402	-	13,13,13	6.91	7 (53%)	15,17,17	3.13	9 (60%)
2	NAD	A	401[B]	-	46,48,48	0.52	1 (2%)	64,73,73	0.61	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
3	A1I3L	B	403	-	-	0/4/4/4	0/2/2/2
2	NAD	B	402[A]	-	-	9/30/62/62	0/5/5/5
4	MRD	B	401	-	-	0/5/5/5	-
2	NAD	A	401[A]	-	-	8/30/62/62	0/5/5/5
2	NAD	B	402[B]	-	-	5/30/62/62	0/5/5/5
3	A1I3L	A	402	-	-	0/4/4/4	0/2/2/2
2	NAD	A	401[B]	-	-	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)
3	B	403	A1I3L	C04-N03	13.82	1.64	1.37
3	A	402	A1I3L	C04-N03	13.71	1.64	1.37
3	B	403	A1I3L	C05-C04	13.66	1.56	1.35
3	A	402	A1I3L	C05-C04	13.38	1.56	1.35
3	B	403	A1I3L	C02-N03	10.56	1.50	1.36
3	A	402	A1I3L	C02-N03	10.39	1.50	1.36
3	A	402	A1I3L	C02-S06	-9.62	1.66	1.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	A1I3L	C02-S06	-9.45	1.66	1.78
3	B	403	A1I3L	C05-S06	-5.13	1.59	1.71
3	A	402	A1I3L	C05-S06	-4.92	1.59	1.71
3	B	403	A1I3L	O01-C02	-4.44	1.15	1.22
3	A	402	A1I3L	O01-C02	-4.12	1.16	1.22
2	B	402[B]	NAD	C2N-N1N	2.29	1.37	1.35
2	A	401[A]	NAD	C2N-N1N	2.18	1.37	1.35
2	A	401[B]	NAD	C2N-N1N	2.02	1.37	1.35
3	A	402	A1I3L	C10-N11	-2.02	1.28	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	A1I3L	O01-C02-N03	-6.46	119.18	125.76
3	B	403	A1I3L	O01-C02-N03	-6.42	119.23	125.76
3	A	402	A1I3L	O01-C02-S06	5.95	132.25	124.59
3	B	403	A1I3L	O01-C02-S06	5.43	131.59	124.59
3	A	402	A1I3L	C10-N11-C12	3.98	123.83	116.85
3	A	402	A1I3L	C07-C04-N03	-3.38	118.49	122.76
3	B	403	A1I3L	C04-C05-S06	-3.37	106.81	111.48
3	A	402	A1I3L	C08-C07-C04	-3.22	115.92	120.81
3	A	402	A1I3L	C12-C07-C04	2.98	127.18	121.76
3	A	402	A1I3L	C04-C05-S06	-2.71	107.72	111.48
3	B	403	A1I3L	C04-N03-C02	-2.61	107.17	112.37
2	B	402[B]	NAD	C6N-N1N-C2N	-2.60	119.66	121.88
2	A	401[B]	NAD	C6N-N1N-C2N	-2.50	119.75	121.88
2	A	401[A]	NAD	C2B-C1B-N9A	-2.45	107.22	113.30
3	B	403	A1I3L	C12-C07-C04	-2.39	117.41	121.76
3	A	402	A1I3L	C05-C04-N03	-2.36	108.57	111.67
2	B	402[A]	NAD	C6N-N1N-C2N	-2.33	119.90	121.88
2	A	401[A]	NAD	C5N-C4N-C3N	-2.32	118.08	120.36
3	B	403	A1I3L	C08-C07-C12	2.31	120.19	117.61
2	B	402[A]	NAD	O2B-C2B-C1B	2.31	118.05	110.10
3	A	402	A1I3L	C07-C12-N11	-2.14	120.32	123.50
3	B	403	A1I3L	C09-C08-C07	-2.10	118.30	120.36
3	B	403	A1I3L	C10-N11-C12	2.02	120.39	116.85

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401[A]	NAD	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
2	A	401[A]	NAD	C2N-C3N-C7N-O7N
2	A	401[A]	NAD	C2N-C3N-C7N-N7N
2	B	402[A]	NAD	PA-O3-PN-O5D
2	B	402[A]	NAD	C5D-O5D-PN-O3
2	B	402[A]	NAD	C5D-O5D-PN-O1N
2	B	402[B]	NAD	C5D-O5D-PN-O1N
2	A	401[A]	NAD	C4N-C3N-C7N-O7N
2	A	401[A]	NAD	C4N-C3N-C7N-N7N
2	B	402[A]	NAD	C2N-C3N-C7N-N7N
2	A	401[A]	NAD	PA-O3-PN-O5D
2	A	401[B]	NAD	PA-O3-PN-O5D
2	B	402[B]	NAD	PA-O3-PN-O5D
2	B	402[A]	NAD	C2N-C3N-C7N-O7N
2	A	401[A]	NAD	C5D-O5D-PN-O3
2	B	402[A]	NAD	C5D-O5D-PN-O2N
2	B	402[B]	NAD	C5D-O5D-PN-O3
2	B	402[B]	NAD	C5D-O5D-PN-O2N
2	B	402[A]	NAD	C4N-C3N-C7N-N7N
2	B	402[A]	NAD	C4N-C3N-C7N-O7N
2	B	402[A]	NAD	PA-O3-PN-O1N
2	A	401[A]	NAD	PA-O3-PN-O1N
2	A	401[B]	NAD	PA-O3-PN-O1N
2	B	402[B]	NAD	PA-O3-PN-O2N

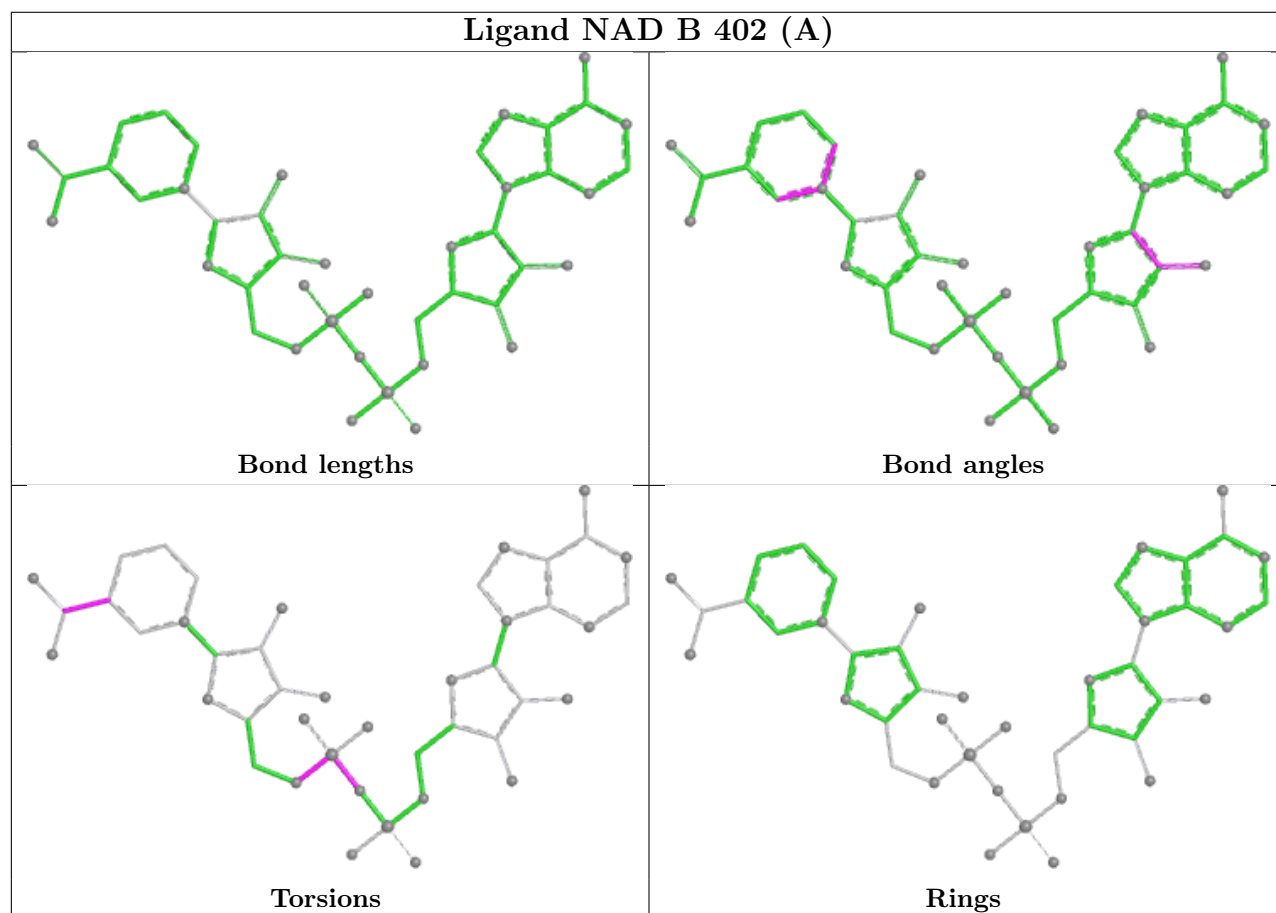
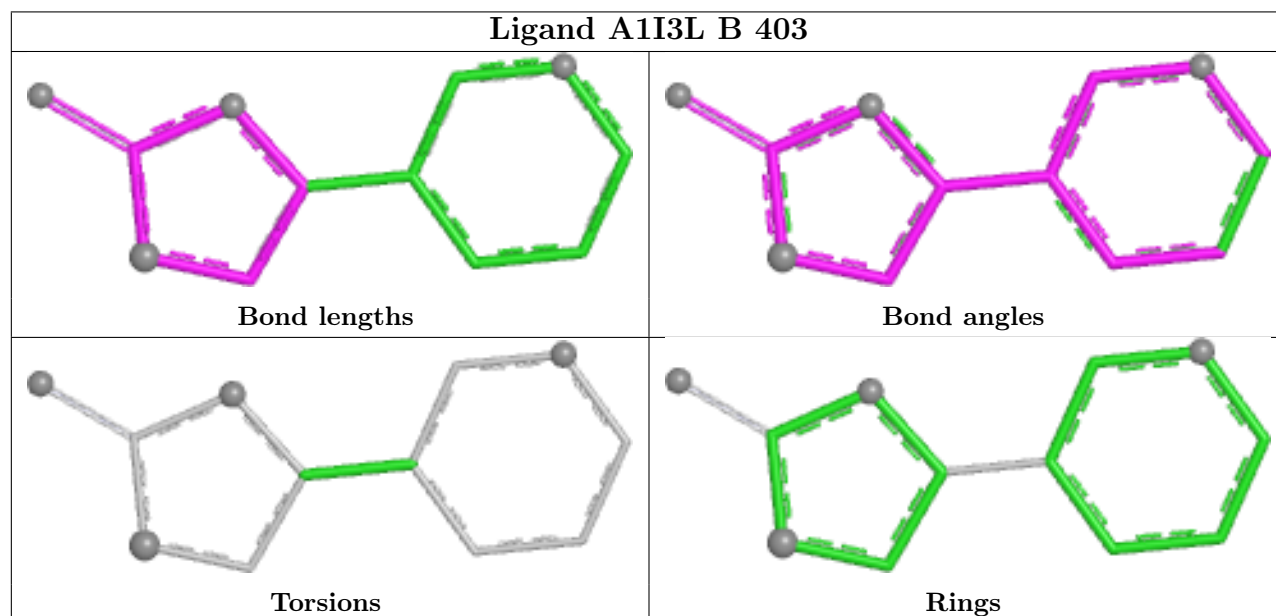
There are no ring outliers.

5 monomers are involved in 16 short contacts:

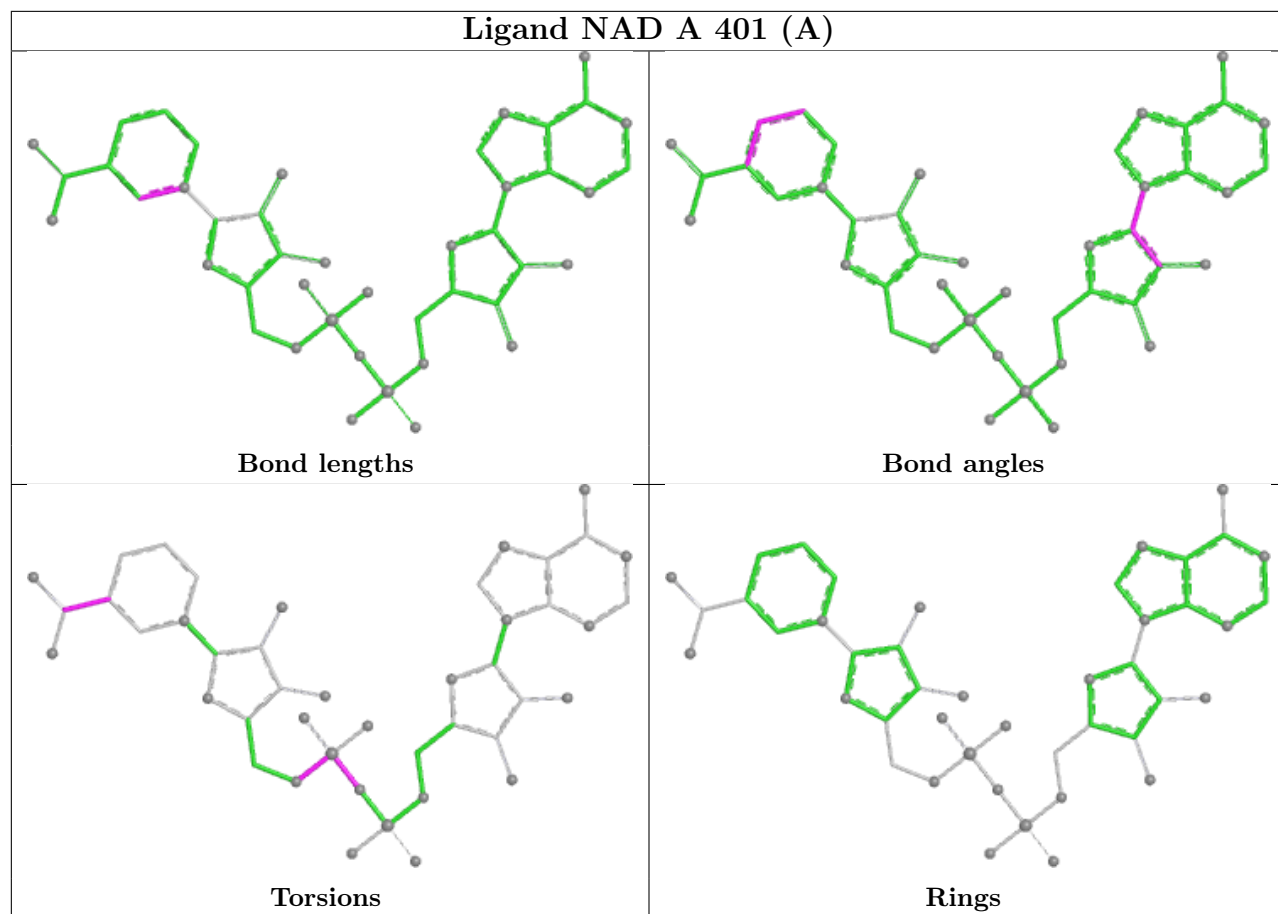
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	403	A1I3L	1	1
2	B	402[A]	NAD	7	0
2	A	401[A]	NAD	5	0
2	B	402[B]	NAD	1	0
2	A	401[B]	NAD	1	0

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

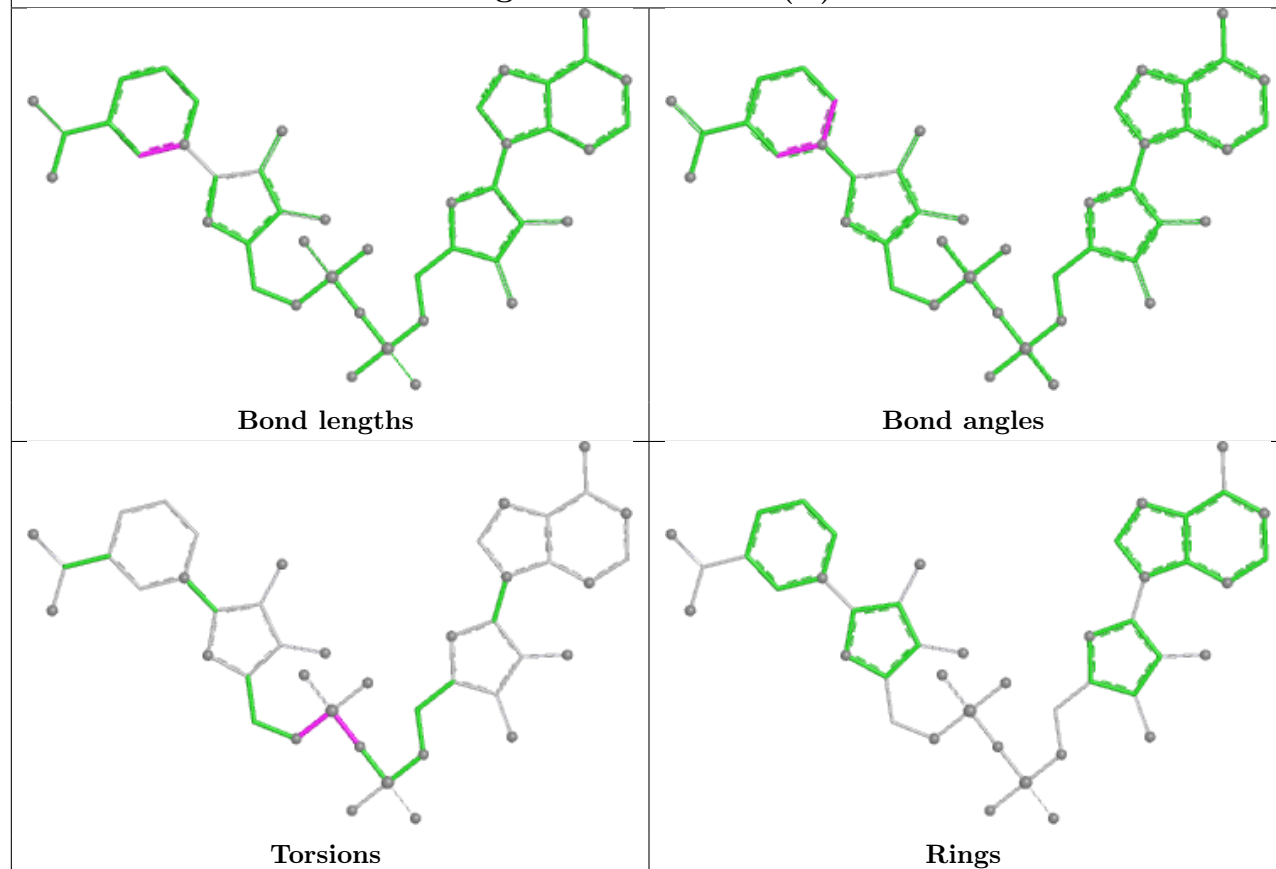
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



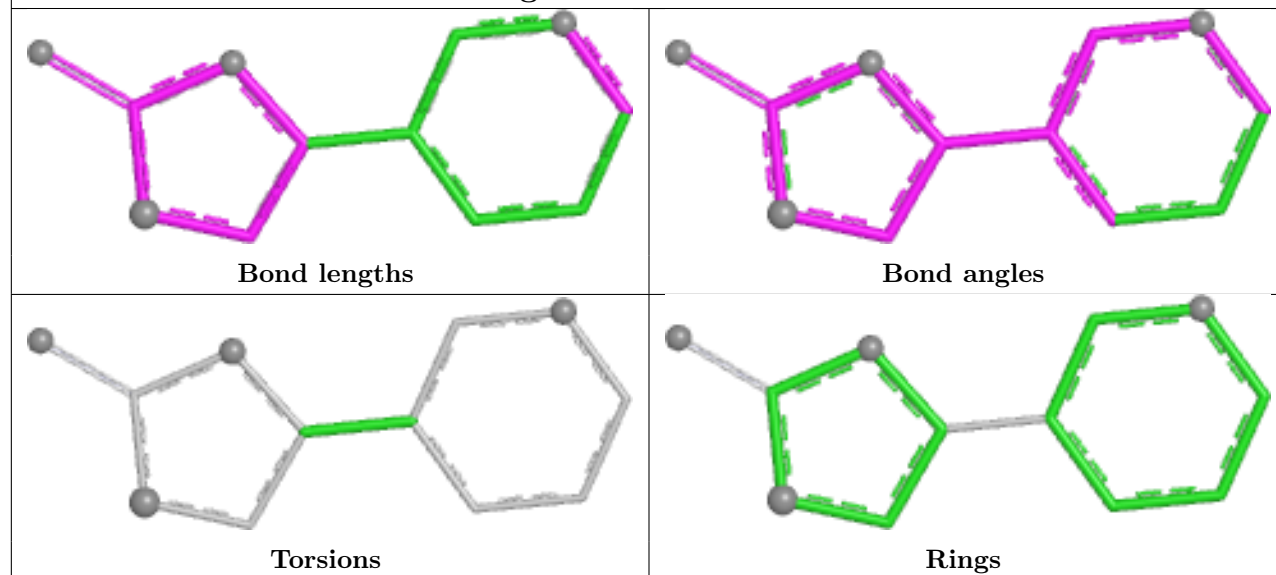
Ligand NAD A 401 (A)

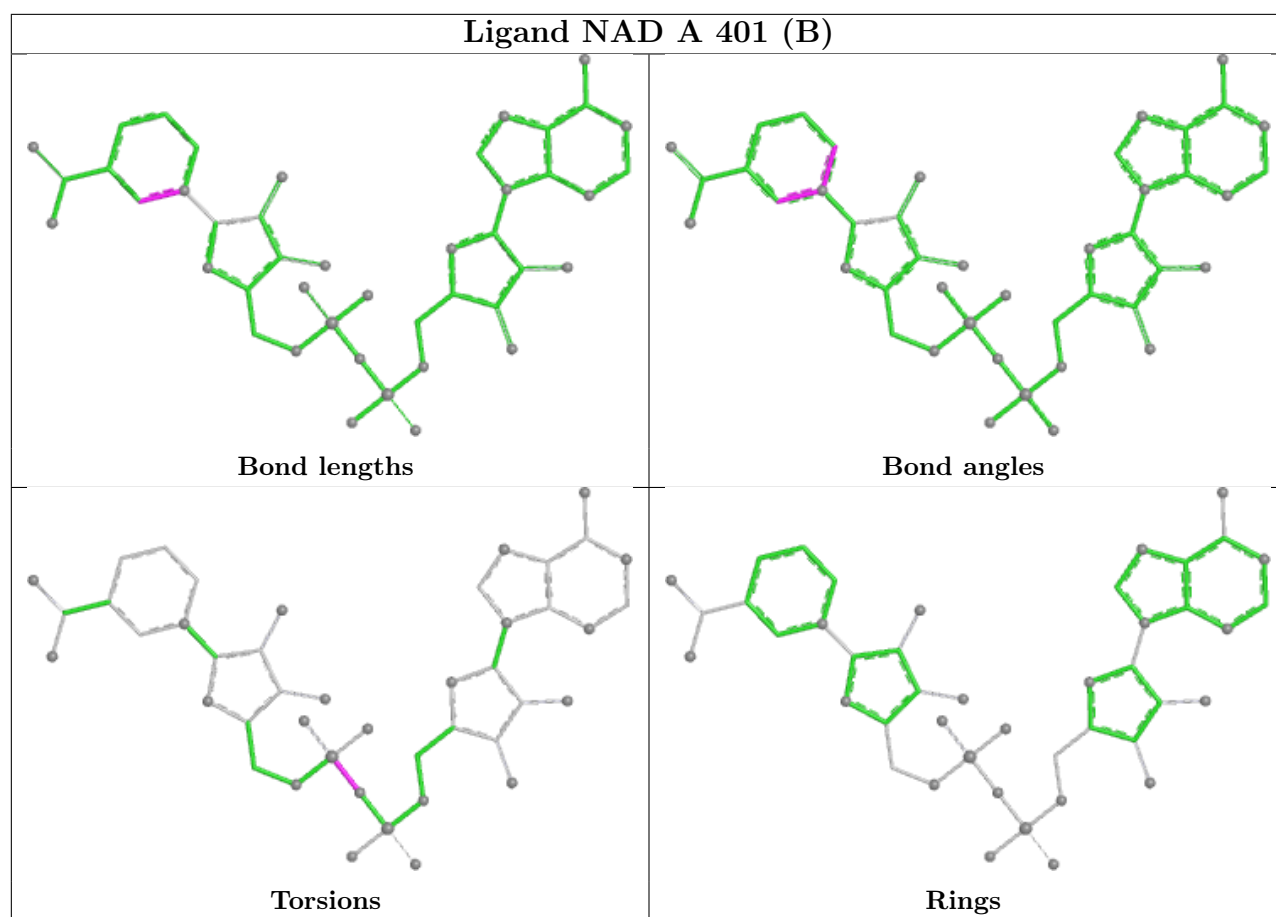


Ligand NAD B 402 (B)



Ligand A1I3L A 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	A	348/369 (94%)	1.05	43 (12%) 8 8	11, 27, 66, 117	12 (3%)
1	B	335/369 (90%)	0.72	27 (8%) 18 18	13, 27, 47, 80	11 (3%)
All	All	683/738 (92%)	0.89	70 (10%) 12 12	11, 27, 54, 117	23 (3%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	18	LEU	10.9
1	A	14	LEU	10.9
1	A	10	PRO	7.5
1	A	26	PRO	7.4
1	A	87	LEU	7.3
1	A	9	ALA	7.2
1	A	77	LEU	7.1
1	A	11	ALA	7.0
1	A	24	LEU	6.9
1	A	16	ALA	6.8
1	A	15	ALA	6.4
1	A	17	VAL	6.0
1	B	89	GLN	5.9
1	A	19	LYS	5.6
1	B	305[A]	TYR	5.4
1	A	25	PRO	5.4
1	A	91	ARG	5.3
1	A	84	HIS	5.3
1	B	250	TYR	4.9
1	A	361	ALA	4.7
1	A	363	MET	4.6
1	A	20	HIS	4.6
1	B	94	LEU	4.5
1	A	362	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	13	ALA	4.3
1	A	85	ALA	4.3
1	A	21	SER	4.2
1	B	85	ALA	4.2
1	A	23	THR	4.0
1	B	28	SER	4.0
1	A	12	GLY	3.9
1	B	43[A]	ARG	3.9
1	A	274	LYS	3.8
1	A	22	SER	3.7
1	B	251	LYS	3.6
1	B	90	SER	3.5
1	A	275[A]	CYS	3.4
1	B	192	MET	3.3
1	B	307[A]	ASN	3.2
1	A	305[A]	TYR	3.2
1	B	93	PRO	3.2
1	A	306	ILE	3.2
1	B	241[A]	LEU	3.2
1	A	76	PRO	3.1
1	B	363	MET	3.0
1	B	88	THR	3.0
1	A	308	THR	2.9
1	A	74	LEU	2.9
1	A	272	PHE	2.8
1	B	196	THR	2.5
1	A	307[A]	ASN	2.5
1	A	86[A]	ASP	2.5
1	B	87	LEU	2.5
1	B	298	ASN	2.4
1	A	27	GLU	2.4
1	A	195	ASN	2.4
1	B	91	ARG	2.4
1	A	360	ASP	2.4
1	B	77	LEU	2.3
1	B	173	ASN	2.3
1	A	32	ARG	2.2
1	B	84	HIS	2.2
1	A	332	VAL	2.2
1	B	171	VAL	2.2
1	B	360	ASP	2.1
1	A	285	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	200	LYS	2.1
1	B	46[A]	LEU	2.1
1	A	254	GLY	2.0
1	B	71	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	CSS	B	177	7/8	0.91	0.14	32,36,49,86	0
1	CSS	A	177	7/8	0.93	0.10	26,28,39,51	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

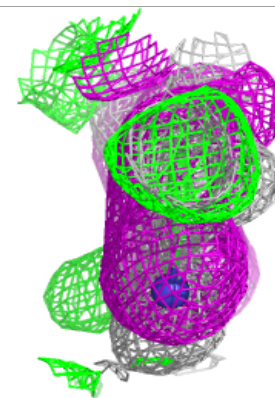
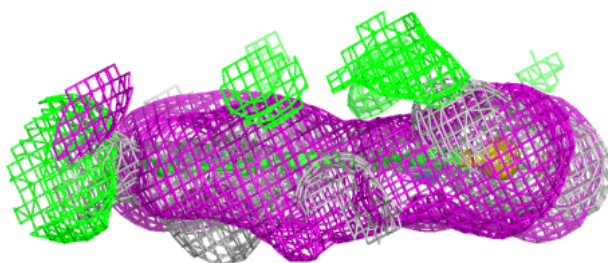
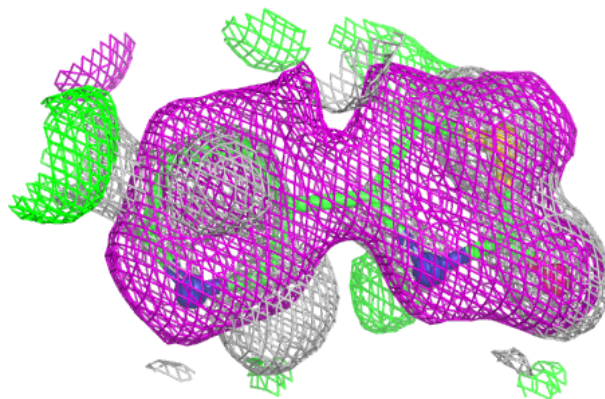
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	A1I3L	B	403	12/12	0.75	0.19	20,20,20,20	12
3	A1I3L	A	402	12/12	0.77	0.18	20,20,20,20	12
2	NAD	A	401[A]	44/44	0.90	0.14	18,22,31,38	44
2	NAD	A	401[B]	44/44	0.90	0.14	18,22,31,38	44
4	MRD	B	401	8/8	0.92	0.15	38,41,47,50	8
2	NAD	B	402[B]	44/44	0.93	0.14	18,22,33,38	44
2	NAD	B	402[A]	44/44	0.93	0.14	18,22,33,38	44

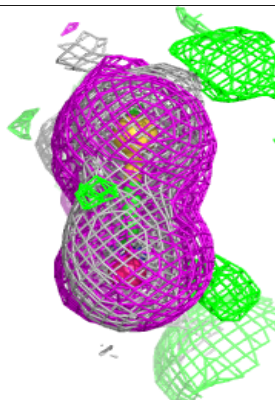
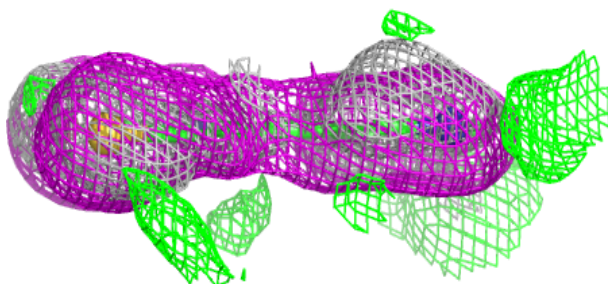
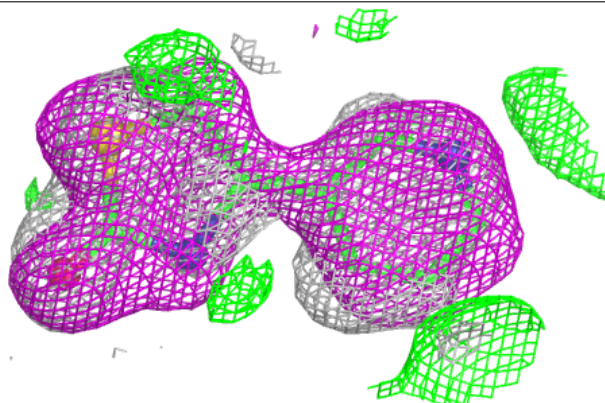
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1I3L B 403:

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

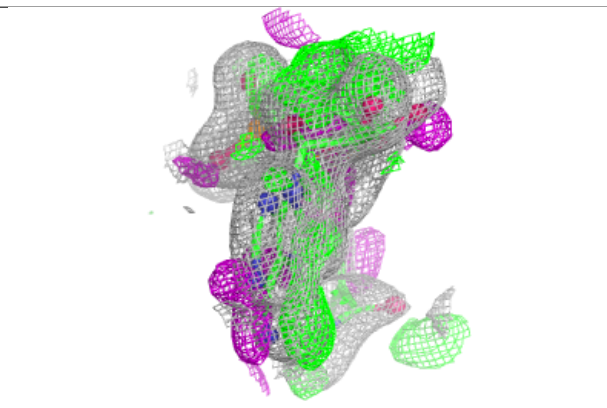
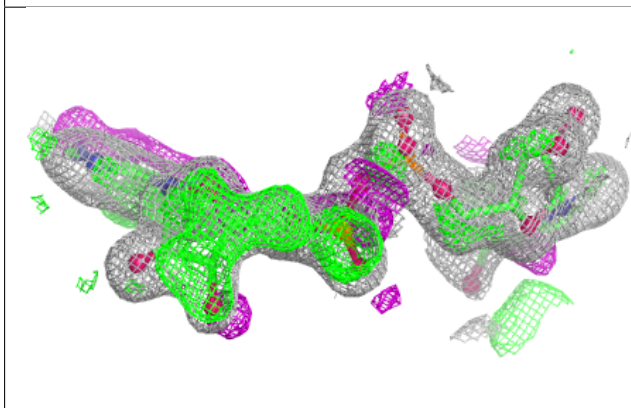
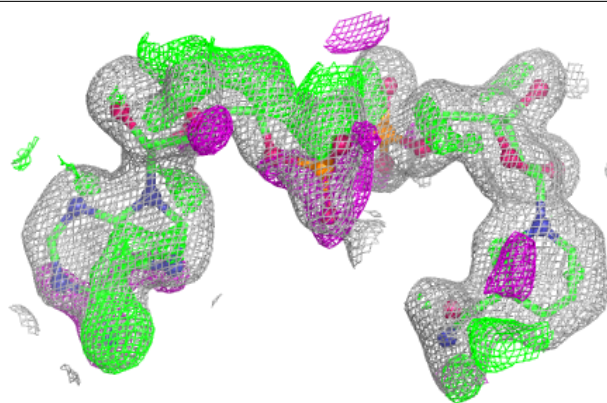
**Electron density around A1I3L A 402:**

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

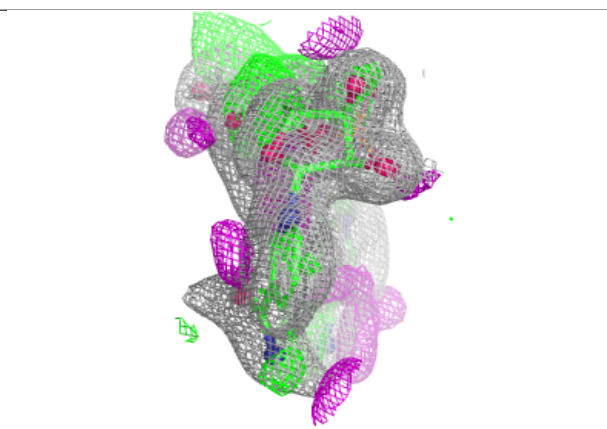
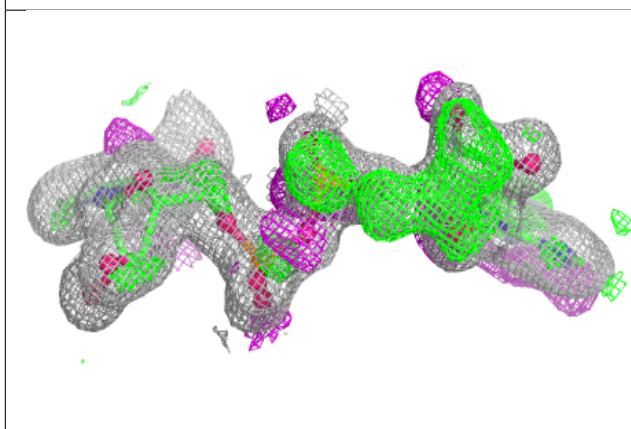
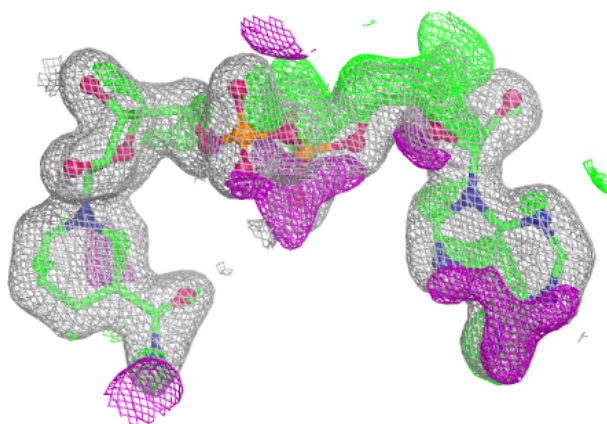


Electron density around NAD A 401 (A):

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

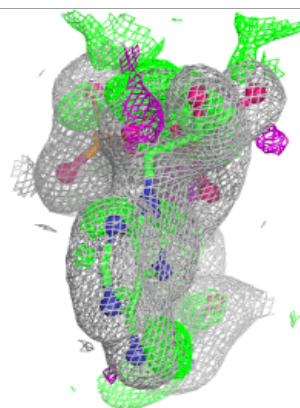
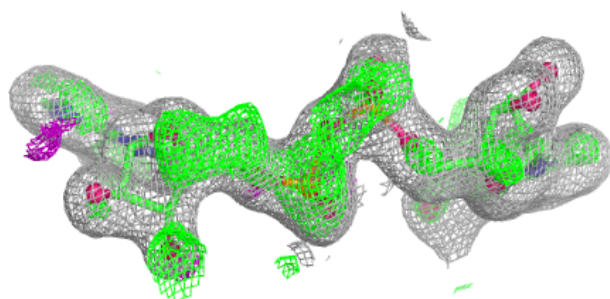
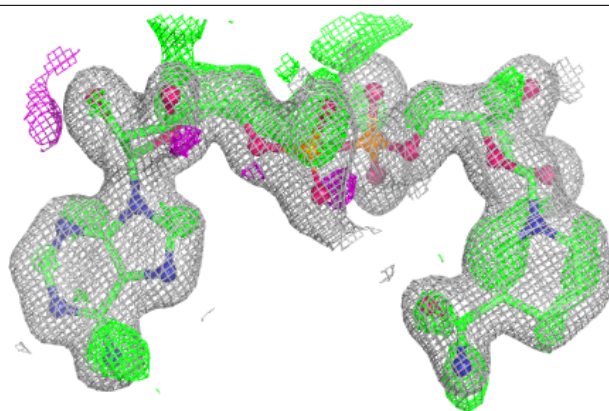
**Electron density around NAD A 401 (B):**

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

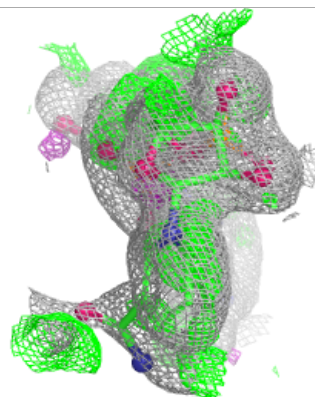
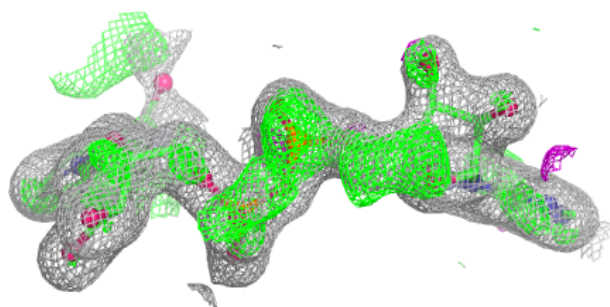
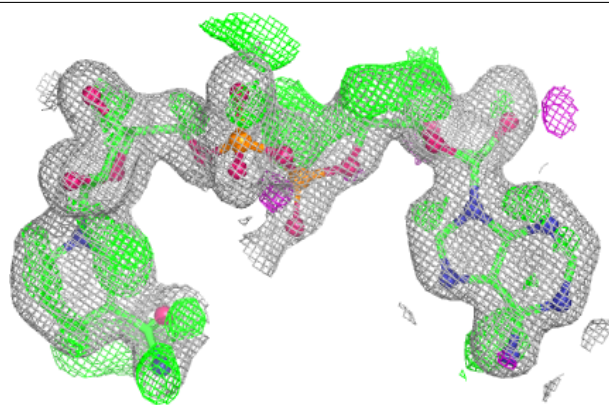


Electron density around NAD B 402 (B):

$2mF_o-DF_c$ (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 (A):**

$2mF_o-DF_c$ (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.