



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:14 AM UTC

PDB ID : 9IDF / pdb\_00009idf  
Title : Human Deoxyhypusine Synthase Fragment Screening Campaign - ligand VT00127  
Authors : Wilk, P.; Water-Wilk, E.; Krojer, T.; Grudnik, P.  
Deposited on : 2025-02-15  
Resolution : 1.43 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.

The types of validation reports are described at

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

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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

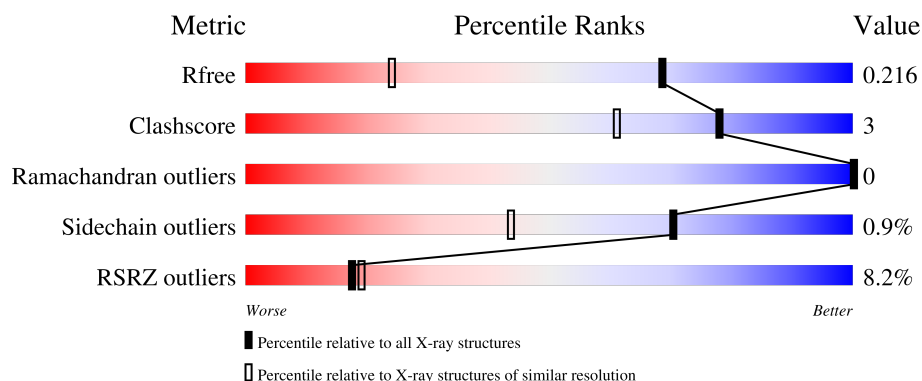
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.43 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	3234 (1.46-1.42)
Clashscore	190562	3289 (1.46-1.42)
Ramachandran outliers	187476	3248 (1.46-1.42)
Sidechain outliers	187428	3248 (1.46-1.42)
RSRZ outliers	180081	3234 (1.46-1.42)

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  $\geq 3$ , 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	369	<div> <div>10%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>• 5%</div> </div> </div>
1	B	369	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>•</div> <div>9%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6073 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.

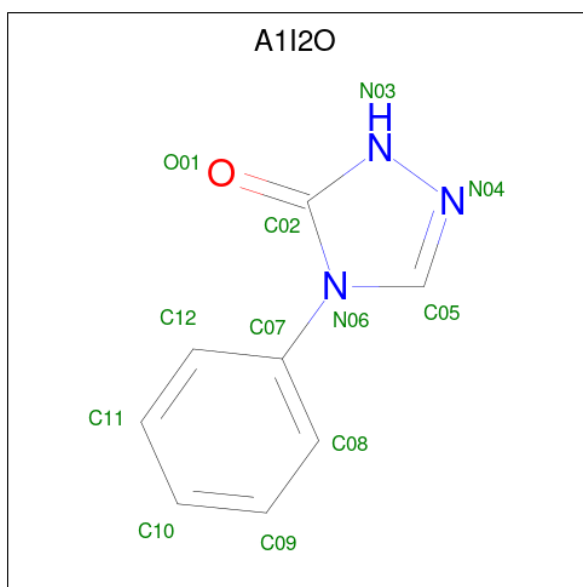
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	0	11	0
			2797	1787	471	522	17			
1	B	336	Total	C	N	O	S	0	5	0
			2664	1692	452	503	17			

- 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	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 4-phenyl-1 {H}-1,2,4-triazol-5-one (CCD ID: A1I2O) (formula:  $C_8H_7N_3O$ ) (labeled as "Ligand of Interest" by depositor).



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

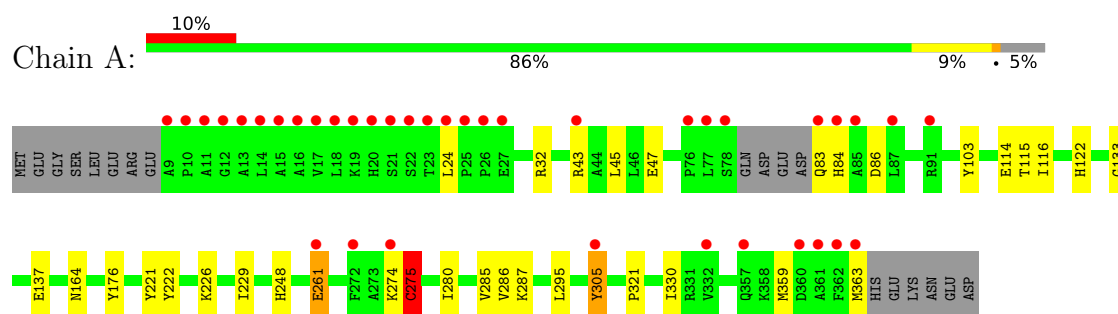
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	249	Total	O	0	1
			250	250		
4	B	250	Total	O	0	0
			250	250		

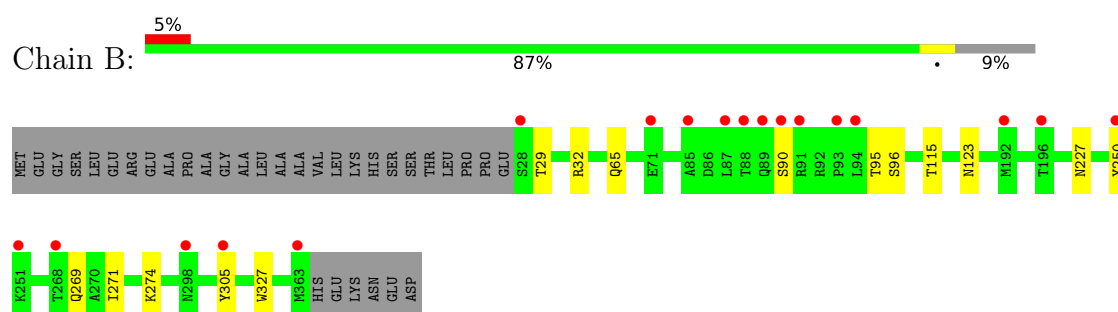
### 3 Residue-property plots [i](#)

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: 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, $\alpha$ , $\beta$ , $\gamma$	105.11Å 105.11Å 160.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.09 – 1.43 46.09 – 1.43	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.09-1.43) 100.0 (46.09-1.43)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, $R_{free}$	0.191 , 0.206 (Not available) , 0.216	Depositor DCC
$R_{free}$ test set	11074 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.6	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 36.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6073	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1I2O, NAD, CSS

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	1.23	9/2871 (0.3%)	1.38	17/3895 (0.4%)
1	B	1.15	2/2721 (0.1%)	1.24	6/3687 (0.2%)
All	All	1.19	11/5592 (0.2%)	1.32	23/7582 (0.3%)

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	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275[A]	CYS	N-CA	10.39	1.58	1.46
1	A	275[B]	CYS	N-CA	10.39	1.58	1.46
1	A	305[A]	TYR	C-O	8.87	1.34	1.24
1	A	305[B]	TYR	C-O	8.87	1.34	1.24
1	B	65	GLN	CD-OE1	7.18	1.37	1.23
1	A	122	HIS	CE1-NE2	6.87	1.39	1.32
1	A	261[A]	GLU	C-O	5.42	1.30	1.24
1	A	261[B]	GLU	C-O	5.42	1.30	1.24
1	A	114	GLU	N-CA	5.19	1.52	1.46
1	B	271	ILE	C-O	-5.18	1.18	1.24
1	A	248	HIS	C-O	5.10	1.30	1.24

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	GLN	CG-CD-NE2	-9.69	101.86	116.40
1	A	275[A]	CYS	CA-C-O	-7.91	110.82	120.54
1	A	275[B]	CYS	CA-C-O	-7.91	110.82	120.54
1	A	261[A]	GLU	CA-C-O	7.69	129.05	119.05
1	A	261[B]	GLU	CA-C-O	7.69	129.05	119.05
1	A	229	ILE	O-C-N	7.54	126.12	121.37
1	B	65	GLN	OE1-CD-NE2	6.75	129.35	122.60
1	A	305[A]	TYR	CA-C-O	6.38	127.10	120.40
1	A	305[B]	TYR	CA-C-O	6.38	127.10	120.40
1	A	24	LEU	CA-C-N	6.38	126.95	120.38
1	A	24	LEU	C-N-CA	6.38	126.95	120.38
1	A	274	LYS	CA-C-N	6.11	132.70	121.94
1	A	274	LYS	C-N-CA	6.11	132.70	121.94
1	B	32	ARG	NE-CZ-NH2	-5.87	113.91	119.20
1	A	221	TYR	CA-C-O	-5.69	113.08	119.79
1	A	305[A]	TYR	CB-CA-C	-5.60	100.86	110.16
1	A	305[B]	TYR	CB-CA-C	-5.60	100.86	110.16
1	B	29	THR	CA-CB-OG1	-5.43	101.45	109.60
1	A	229	ILE	CA-C-O	-5.12	115.36	119.25
1	B	250	TYR	CB-CA-C	5.11	118.97	110.90
1	A	116	ILE	CA-C-O	-5.09	115.46	120.85
1	A	133	GLY	O-C-N	5.06	127.05	122.19
1	B	305	TYR	CA-CB-CG	5.04	122.98	113.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	275[A]	CYS	Mainchain
1	A	275[B]	CYS	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	2797	0	2790	27	0
1	B	2664	0	2643	4	0
2	A	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	44	0	26	1	0
3	A	12	0	0	0	0
3	B	12	0	0	0	0
4	A	250	0	0	7	1
4	B	250	0	0	1	1
All	All	6073	0	5485	30	1

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 (30) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275[B]:CYS:SG	4:A:716:HOH:O	2.01	1.16
1:A:261[A]:GLU:HG2	4:A:533[A]:HOH:O	1.74	0.85
1:A:305[B]:TYR:CD2	1:A:321:PRO:HG3	2.18	0.79
1:A:47:GLU:OE1	4:A:502:HOH:O	2.03	0.74
1:A:305[B]:TYR:CE2	1:A:321:PRO:HG3	2.23	0.73
1:A:305[A]:TYR:OH	1:A:330:ILE:HD11	2.00	0.62
1:A:280:ILE:HD12	1:A:305[A]:TYR:CE2	2.34	0.62
1:A:359:MET:O	1:A:359:MET:HE3	2.02	0.59
1:A:285[B]:VAL:HG12	2:B:401:NAD:O3D	2.03	0.58
1:A:226:LYS:NZ	4:A:506:HOH:O	2.31	0.57
1:A:83:GLN:HG3	1:A:84:HIS:N	2.20	0.56
1:A:137[B]:GLU:OE1	4:A:503:HOH:O	2.17	0.56
1:A:295:LEU:HD12	1:A:295:LEU:O	2.06	0.54
1:A:103:TYR:N	1:A:286[A]:VAL:HG11	2.22	0.54
1:A:287:LYS:HE2	1:A:305[B]:TYR:CE1	2.47	0.50
1:B:269:GLN:NE2	4:B:507:HOH:O	2.44	0.49
1:A:261[B]:GLU:HG3	4:A:533[B]:HOH:O	2.11	0.49
1:A:222:TYR:OH	1:A:226:LYS:NZ	2.47	0.47
1:B:123:ASN:OD1	1:B:227:ASN:HB3	2.16	0.45
1:A:359:MET:HE3	1:A:359:MET:HA	1.99	0.43
1:A:359:MET:HE2	1:A:363:MET:SD	2.59	0.43
1:A:305[B]:TYR:HD2	1:A:321:PRO:HG3	1.78	0.42
1:A:164:ASN:HB3	1:B:327:TRP:CE2	2.54	0.42
1:A:137[B]:GLU:OE2	1:A:176:TYR:OH	2.28	0.42
1:B:96:SER:HA	1:B:274:LYS:HD3	2.02	0.42
1:A:43:ARG:NE	4:A:502:HOH:O	2.52	0.41
1:A:83:GLN:CG	1:A:84:HIS:N	2.84	0.40
1:A:32:ARG:HB2	1:A:32:ARG:CZ	2.51	0.40

All (1) 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)
4:A:715:HOH:O	4:B:715:HOH:O[4_555]	2.11	0.09

## 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	357/369 (97%)	351 (98%)	6 (2%)	0	100	100
1	B	338/369 (92%)	332 (98%)	6 (2%)	0	100	100
All	All	695/738 (94%)	683 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	302/309 (98%)	299 (99%)	3 (1%)	68	39
1	B	288/309 (93%)	285 (99%)	3 (1%)	68	39
All	All	590/618 (96%)	584 (99%)	6 (1%)	70	39

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86[A]	ASP
1	A	86[B]	ASP
1	A	115	THR
1	B	90	SER
1	B	95	THR
1	B	115	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	B	37	ASN
1	B	228	HIS
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 ⓘ

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	0.67	0	2,6,8	1.20	0
1	CSS	A	177	1	4,6,7	0.74	0	2,6,8	0.15	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](#)

4 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
2	NAD	B	401	-	46,48,48	0.70	1 (2%)	64,73,73	0.68	2 (3%)
2	NAD	A	401	-	46,48,48	0.98	3 (6%)	64,73,73	1.07	3 (4%)
3	A1I2O	A	402	-	13,13,13	4.59	4 (30%)	16,17,17	2.68	4 (25%)
3	A1I2O	B	402	-	13,13,13	5.33	5 (38%)	16,17,17	2.19	4 (25%)

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
2	NAD	B	401	-	-	5/30/62/62	0/5/5/5
2	NAD	A	401	-	-	6/30/62/62	0/5/5/5
3	A1I2O	A	402	-	-	2/4/4/4	0/2/2/2
3	A1I2O	B	402	-	-	0/4/4/4	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	A1I2O	C05-N04	15.45	1.44	1.29
3	A	402	A1I2O	C05-N04	13.82	1.43	1.29
3	B	402	A1I2O	C02-N03	9.81	1.44	1.35
3	A	402	A1I2O	C02-N03	7.88	1.42	1.35
3	B	402	A1I2O	C05-N06	3.84	1.43	1.37
3	A	402	A1I2O	O01-C02	-3.23	1.17	1.23
3	B	402	A1I2O	N03-N04	3.10	1.42	1.36
3	B	402	A1I2O	O01-C02	-2.95	1.17	1.23
2	A	401	NAD	C2N-N1N	2.76	1.38	1.35
2	A	401	NAD	PA-O2A	-2.62	1.43	1.55
2	A	401	NAD	C6N-C5N	-2.54	1.33	1.38
2	B	401	NAD	PA-O2A	-2.07	1.45	1.55
3	A	402	A1I2O	C05-N06	2.01	1.40	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	A1I2O	N03-C02-N06	8.49	108.99	103.44
3	B	402	A1I2O	N03-C02-N06	6.77	107.87	103.44
2	A	401	NAD	C6N-N1N-C2N	-4.25	118.26	121.88
3	B	402	A1I2O	C05-N04-N03	3.88	108.35	104.14
3	A	402	A1I2O	C05-N04-N03	3.65	108.10	104.14
3	A	402	A1I2O	O01-C02-N03	-3.48	124.53	129.30
2	A	401	NAD	O2A-PA-O1A	3.16	127.14	112.44
3	B	402	A1I2O	O01-C02-N03	-2.64	125.67	129.30
3	A	402	A1I2O	C08-C07-N06	2.53	122.92	119.62
2	B	401	NAD	C6N-N1N-C2N	-2.22	119.99	121.88
2	B	401	NAD	O2A-PA-O1A	2.18	122.57	112.44
2	A	401	NAD	O3-PA-O1A	-2.17	104.18	110.70
3	B	402	A1I2O	N06-C05-N04	-2.10	107.56	111.45

There are no chirality outliers.

All (13) torsion outliers are listed below:

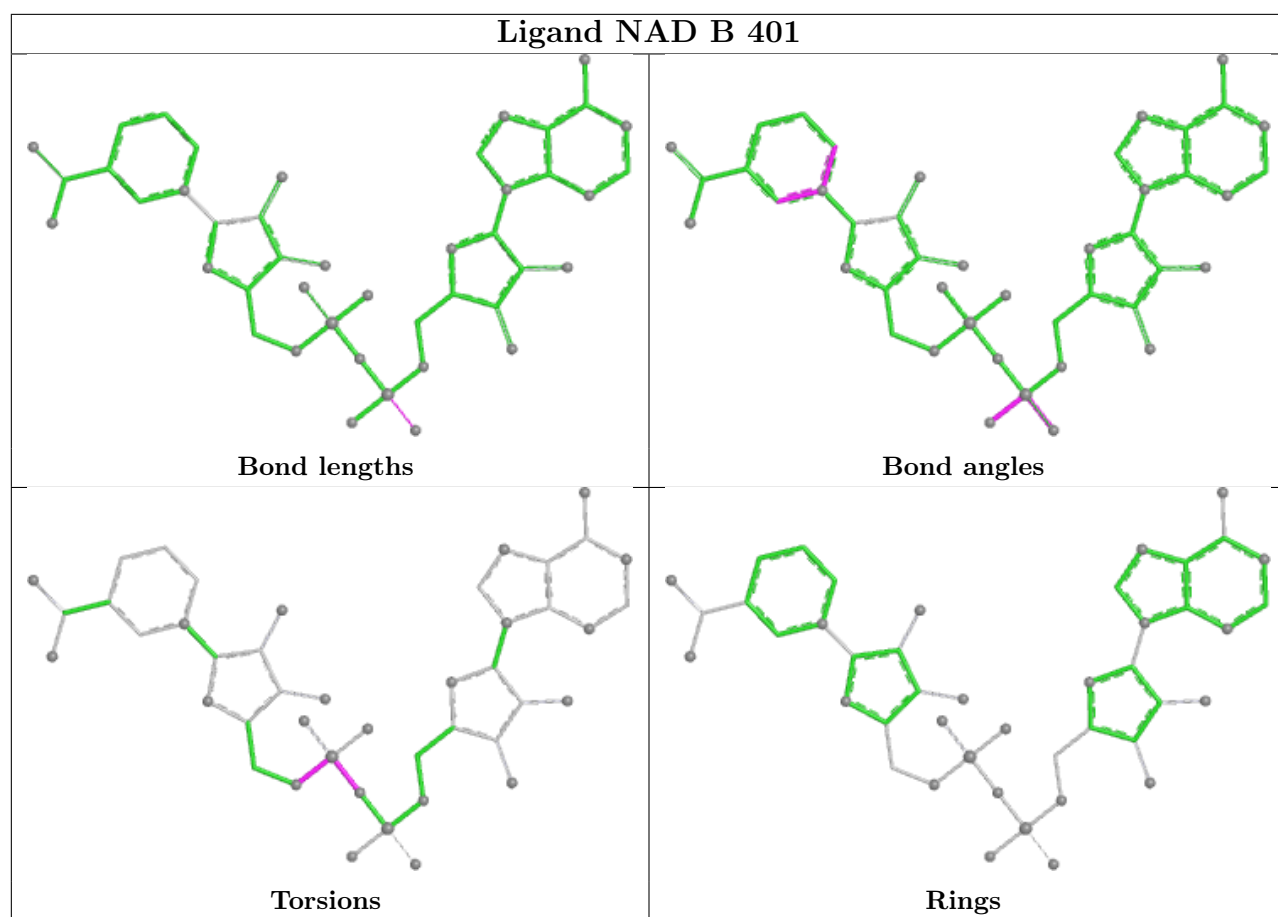
Mol	Chain	Res	Type	Atoms
2	A	401	NAD	C5D-O5D-PN-O1N
2	B	401	NAD	C5D-O5D-PN-O3
2	B	401	NAD	C5D-O5D-PN-O1N
3	A	402	A1I2O	C12-C07-N06-C02
2	A	401	NAD	PA-O3-PN-O5D
2	B	401	NAD	PA-O3-PN-O5D
2	A	401	NAD	C5D-O5D-PN-O3
2	A	401	NAD	C5D-O5D-PN-O2N
2	B	401	NAD	C5D-O5D-PN-O2N
3	A	402	A1I2O	C08-C07-N06-C02
2	B	401	NAD	PA-O3-PN-O2N
2	A	401	NAD	PA-O3-PN-O1N
2	A	401	NAD	PA-O3-PN-O2N

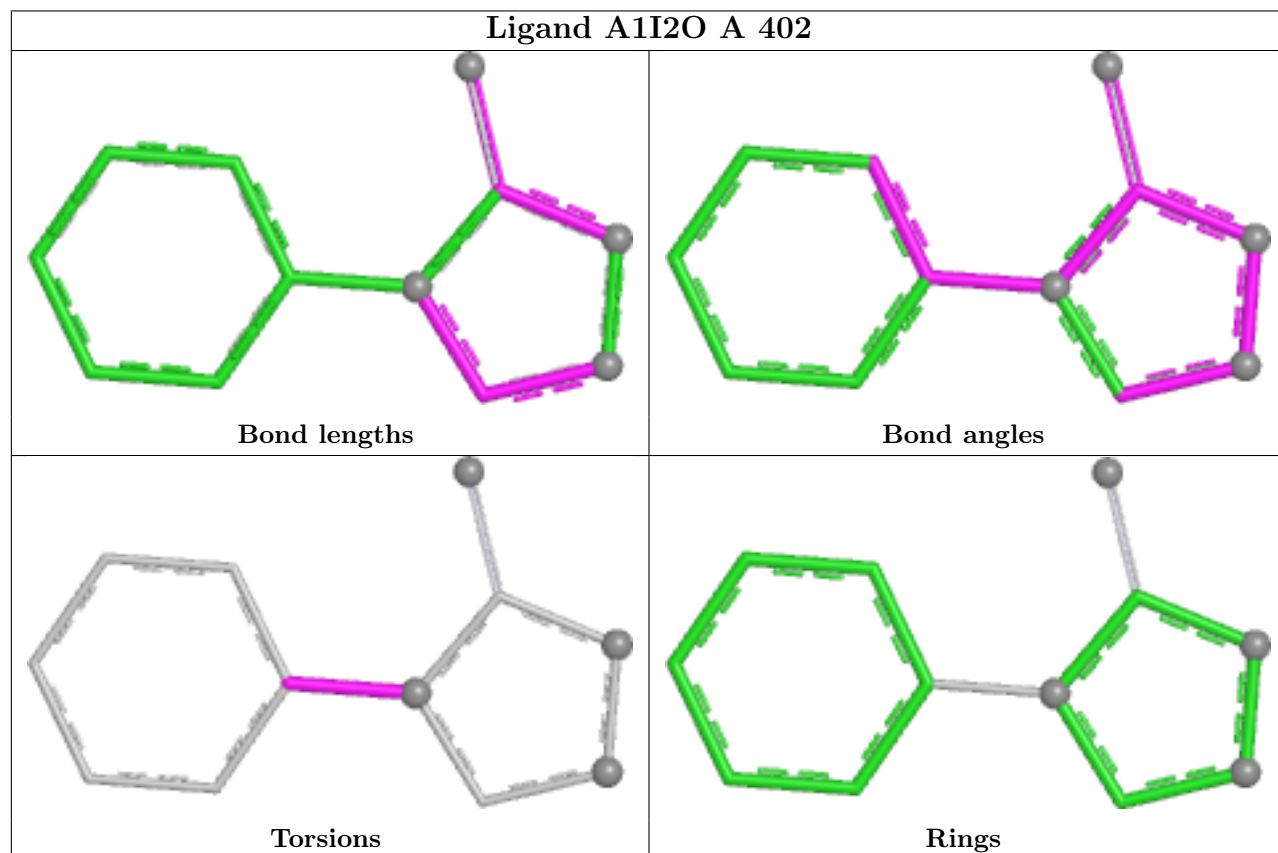
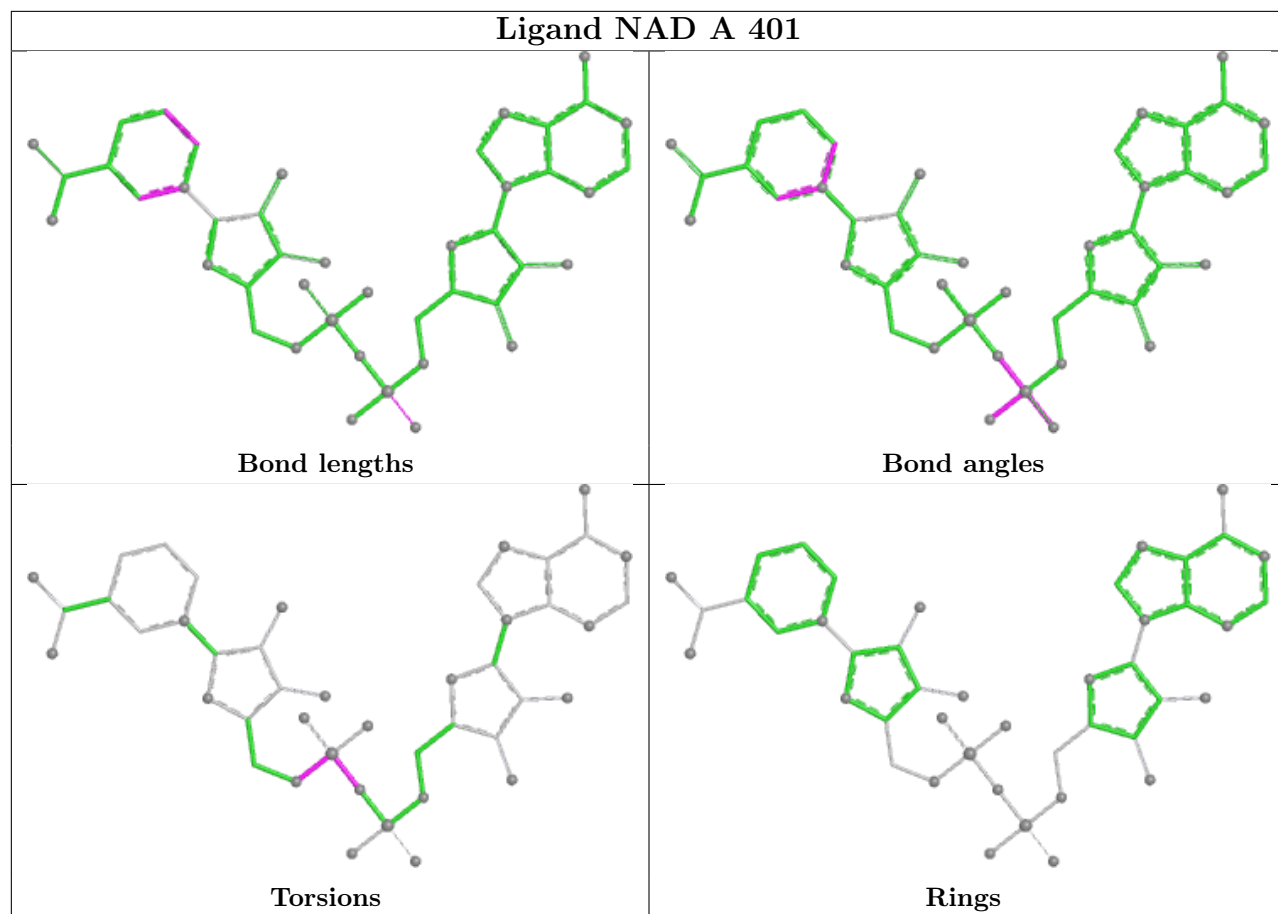
There are no ring outliers.

1 monomer is involved in 1 short contact:

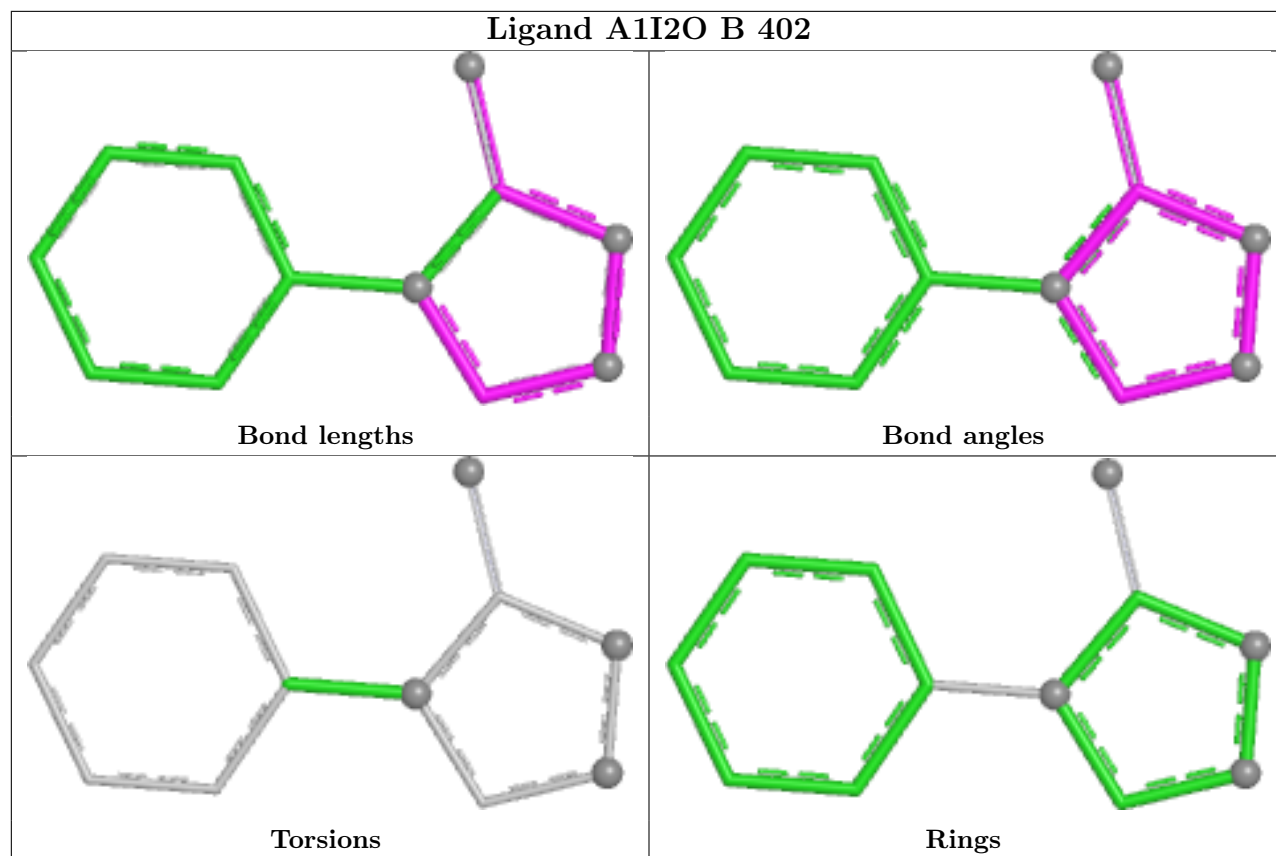
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	NAD	1	0

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.









## 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	350/369 (94%)	0.75	38 (10%)	10 12	11, 27, 78, 134	14 (4%)
1	B	335/369 (90%)	0.40	18 (5%)	31 32	17, 27, 46, 82	6 (1%)
All	All	685/738 (92%)	0.58	56 (8%)	17 19	11, 27, 58, 134	20 (2%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	LEU	10.8
1	A	18	LEU	10.6
1	A	78	SER	8.5
1	A	10	PRO	8.1
1	A	17	VAL	7.1
1	A	11	ALA	6.8
1	A	9	ALA	6.7
1	A	16	ALA	6.3
1	A	87	LEU	6.3
1	A	305[A]	TYR	6.1
1	B	89	GLN	6.0
1	A	26	PRO	6.0
1	A	15	ALA	5.4
1	A	19	LYS	5.3
1	A	13	ALA	5.1
1	A	84	HIS	4.9
1	A	20	HIS	4.9
1	A	24	LEU	4.7
1	A	91	ARG	4.7
1	A	25	PRO	4.6
1	A	12	GLY	4.2
1	A	83	GLN	4.1
1	A	77	LEU	4.0
1	A	363	MET	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	85	ALA	3.9
1	A	22	SER	3.9
1	A	21	SER	3.8
1	A	274	LYS	3.7
1	A	23	THR	3.7
1	B	28	SER	3.7
1	B	94	LEU	3.5
1	A	261[A]	GLU	3.5
1	A	361	ALA	3.5
1	B	250	TYR	3.5
1	B	251	LYS	3.5
1	B	85	ALA	3.3
1	A	362	PHE	3.2
1	B	88	THR	3.1
1	B	192	MET	2.7
1	B	87	LEU	2.7
1	B	90	SER	2.7
1	A	43	ARG	2.7
1	A	272	PHE	2.5
1	B	363	MET	2.4
1	B	268	THR	2.4
1	A	360	ASP	2.3
1	B	93	PRO	2.3
1	A	357	GLN	2.3
1	B	91	ARG	2.3
1	A	76	PRO	2.2
1	A	332	VAL	2.2
1	B	298	ASN	2.1
1	B	71	GLU	2.1
1	B	196	THR	2.0
1	B	305	TYR	2.0
1	A	27	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, 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(Å <sup>2</sup> )	Q<0.9
1	CSS	B	177	7/8	0.90	0.13	34,36,50,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CSS	A	177	7/8	0.93	0.11	26,28,41,52	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

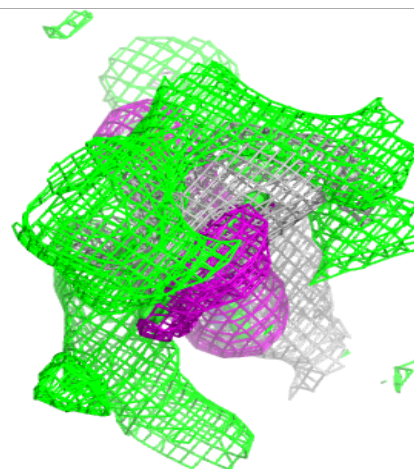
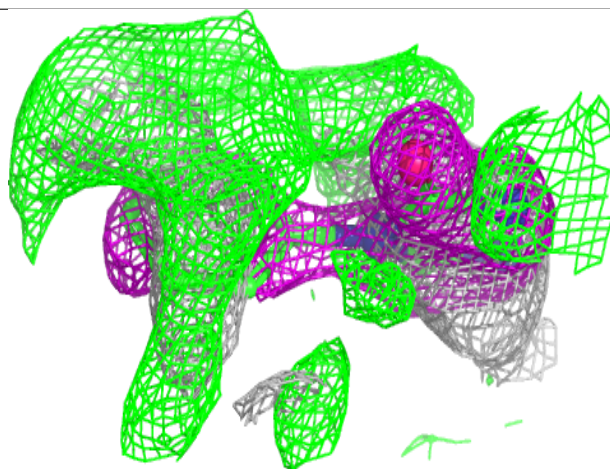
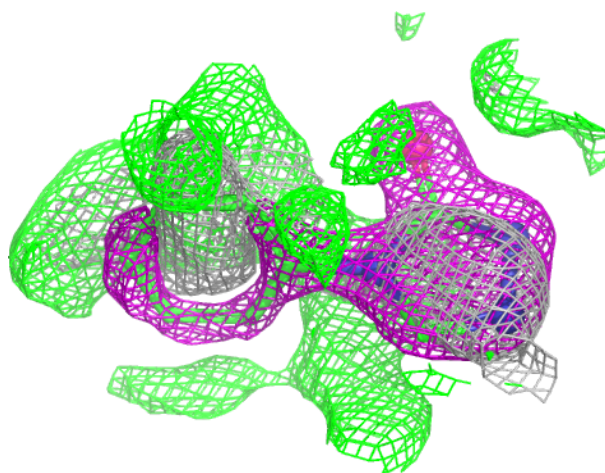
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	A1I2O	A	402	12/12	0.31	0.28	20,20,20,20	12
3	A1I2O	B	402	12/12	0.51	0.22	20,20,20,20	12
2	NAD	B	401	44/44	0.97	0.07	19,23,32,35	44
2	NAD	A	401	44/44	0.98	0.06	19,21,31,38	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.

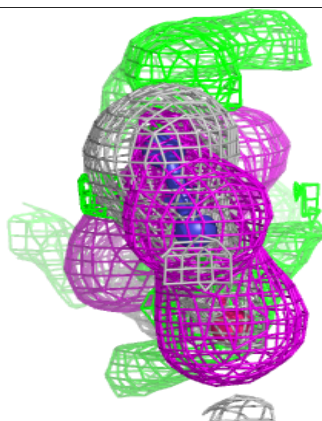
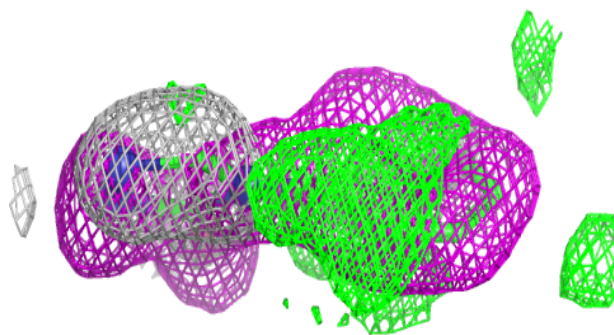
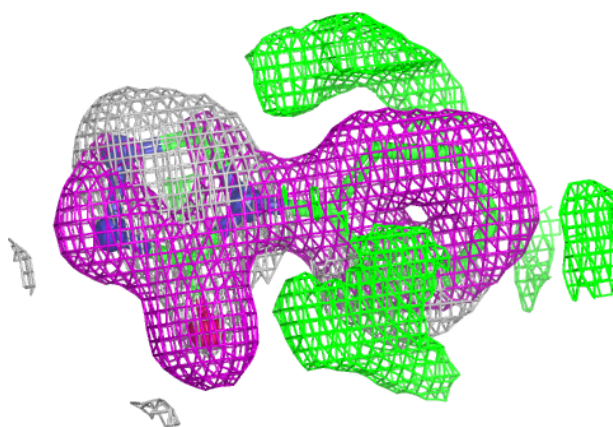
**Electron density around A1I2O A 402:**

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

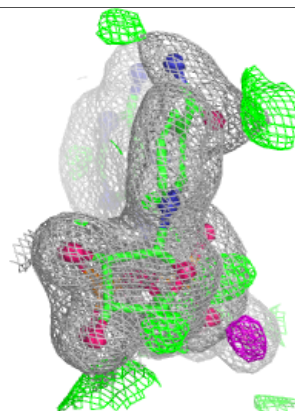
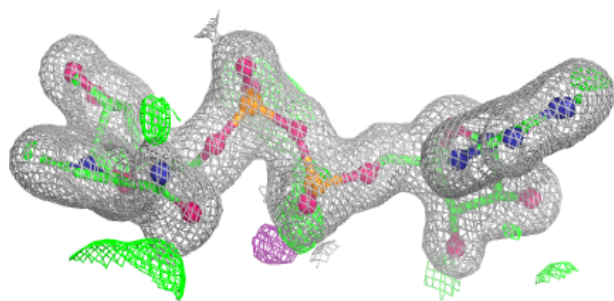
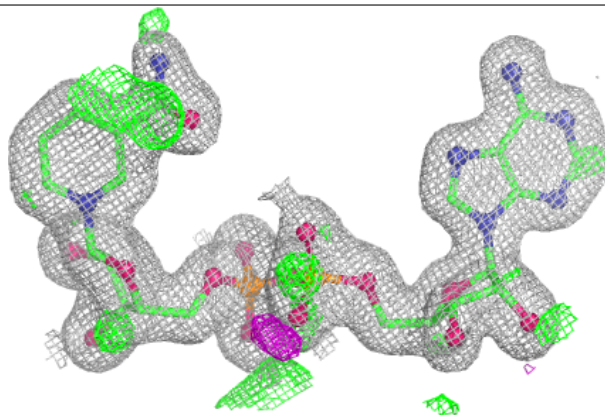


**Electron density around A1I2O B 402:**

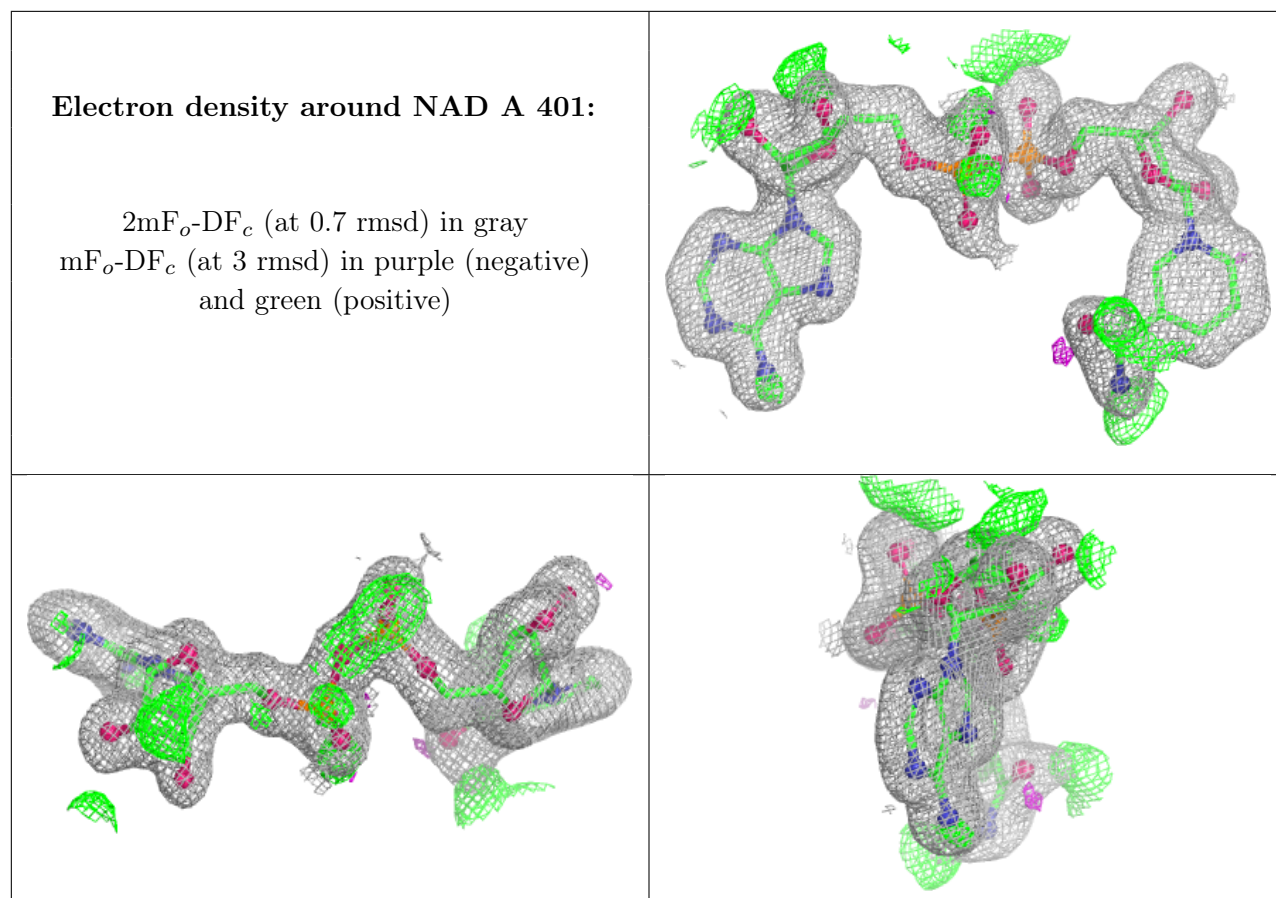
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around NAD B 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 ⓘ

There are no such residues in this entry.