



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:35 PM UTC

PDB ID : 9IEA / pdb\_00009iea  
Title : Human Deoxyhypusine Synthase Fragment Screening Campaign - ligand VT00257  
Authors : Wilk, P.; Water-Wilk, E.; Krojer, T.; Grudnik, P.  
Deposited on : 2025-02-15  
Resolution : 1.30 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

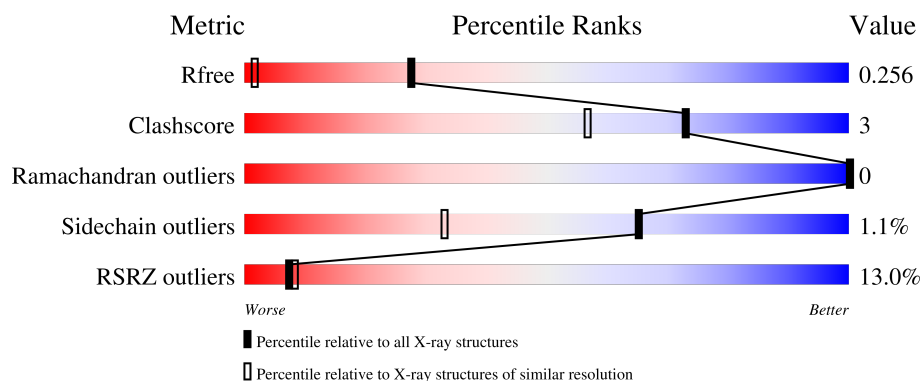
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.30 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	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (1.30-1.30)

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	 10% 82% 7% • 11%
1	B	369	 13% 85% 5% • 9%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5897 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.

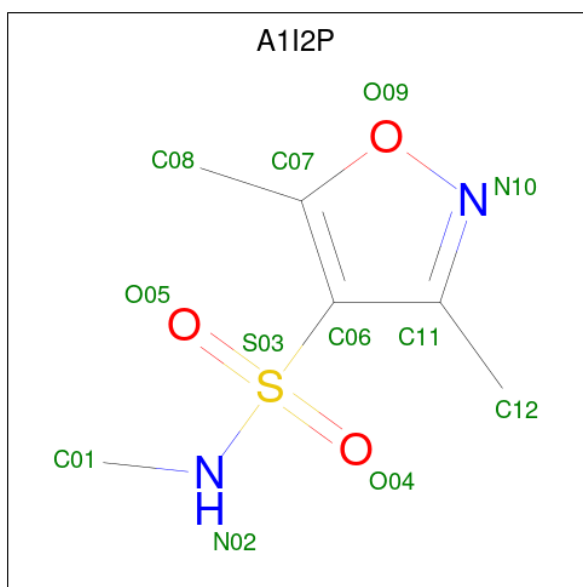
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	6	0
			2619	1667	445	490	17			
1	B	335	Total	C	N	O	S	0	9	0
			2681	1708	453	503	17			

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



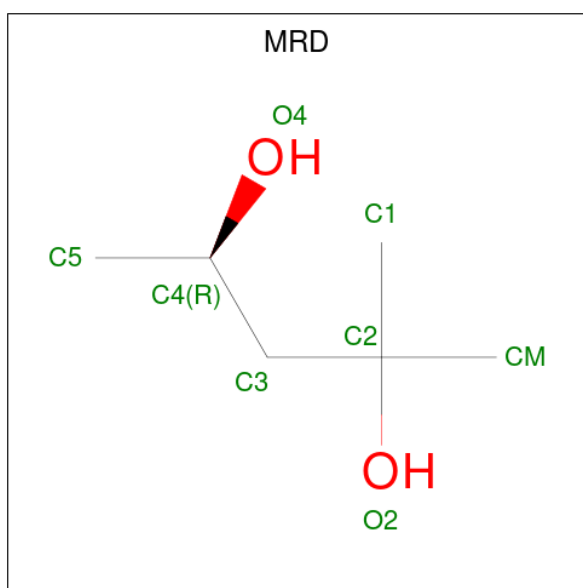
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is {N},3,5-trimethyl-1,2-oxazole-4-sulfonamide (CCD ID: A1I2P) (formula:  $C_6H_{10}N_2O_3S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	2	3	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	2	3	1		

- Molecule 4 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



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

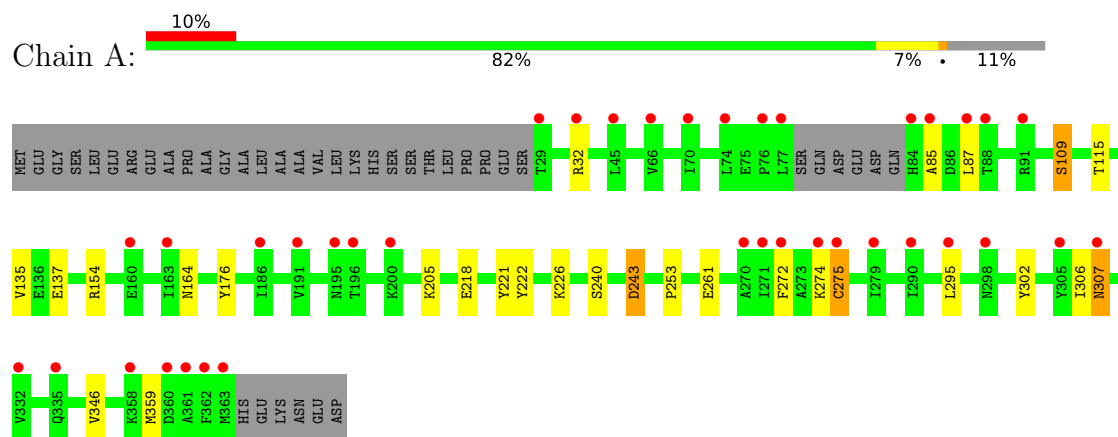
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	242	Total 242	O 242	0	0
5	B	235	Total 235	O 235	0	0

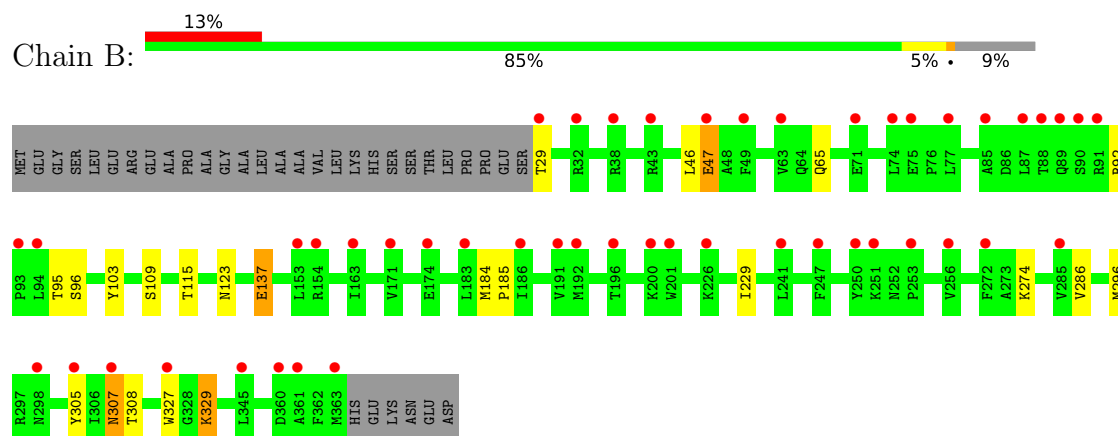
### 3 Residue-property plots [i](#)

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: 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, $\alpha$ , $\beta$ , $\gamma$	104.81Å 104.81Å 160.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.07 – 1.30 46.07 – 1.30	Depositor EDS
% Data completeness (in resolution range)	84.5 (46.07-1.30) 84.5 (46.07-1.30)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.96 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, $R_{free}$	0.237 , 0.253 0.243 , 0.256	Depositor DCC
$R_{free}$ test set	10500 reflections (4.21%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5897	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: CSS, NAD, A1I2P, MRD

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	1.16	5/2676 (0.2%)	1.30	11/3624 (0.3%)
1	B	1.14	5/2751 (0.2%)	1.30	13/3726 (0.3%)
All	All	1.15	10/5427 (0.2%)	1.30	24/7350 (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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	307[A]	ASN	C-O	6.49	1.31	1.23
1	B	307[B]	ASN	C-O	6.49	1.31	1.23
1	A	307[A]	ASN	C-O	6.25	1.31	1.23
1	A	307[B]	ASN	C-O	6.25	1.31	1.23
1	A	253	PRO	C-O	-5.85	1.17	1.23
1	B	229	ILE	N-CA	5.25	1.50	1.46
1	A	275[A]	CYS	N-CA	5.13	1.52	1.45
1	A	275[B]	CYS	N-CA	5.13	1.52	1.45
1	B	137[A]	GLU	C-O	5.11	1.30	1.24
1	B	137[B]	GLU	C-O	5.11	1.30	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46[A]	LEU	CA-C-O	10.95	132.15	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46[B]	LEU	CA-C-O	10.95	132.15	120.55
1	A	218[A]	GLU	CA-C-O	10.12	132.21	119.05
1	A	218[B]	GLU	CA-C-O	10.12	132.21	119.05
1	B	46[A]	LEU	N-CA-C	9.48	121.61	111.28
1	B	46[B]	LEU	N-CA-C	9.48	121.61	111.28
1	A	218[A]	GLU	N-CA-C	7.11	121.55	113.01
1	A	218[B]	GLU	N-CA-C	7.11	121.55	113.01
1	B	65	GLN	CG-CD-NE2	-6.51	106.64	116.40
1	B	307[A]	ASN	CA-C-O	5.81	127.80	121.06
1	B	307[B]	ASN	CA-C-O	5.81	127.80	121.06
1	A	307[A]	ASN	CA-C-O	5.78	127.64	120.54
1	A	307[B]	ASN	CA-C-O	5.78	127.64	120.54
1	B	329[A]	LYS	CA-C-O	5.71	126.39	119.31
1	B	329[B]	LYS	CA-C-O	5.71	126.39	119.31
1	A	243	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	305	TYR	CA-CB-CG	5.42	123.66	113.90
1	A	275[A]	CYS	N-CA-CB	-5.17	102.82	111.20
1	A	275[B]	CYS	N-CA-CB	-5.17	102.82	111.20
1	B	29	THR	CA-CB-OG1	-5.16	101.85	109.60
1	B	137[A]	GLU	CA-C-O	5.01	125.74	119.97
1	B	137[B]	GLU	CA-C-O	5.01	125.74	119.97
1	A	154	ARG	CA-C-N	5.01	125.54	119.98
1	A	154	ARG	C-N-CA	5.01	125.54	119.98

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	85	ALA	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	2619	0	2595	20	0
1	B	2681	0	2672	12	0
2	A	44	0	26	1	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	4	0
3	B	12	0	0	2	0
4	B	8	0	14	0	0
5	A	242	0	0	7	2
5	B	235	0	0	4	2
All	All	5897	0	5333	34	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 3.

All (34) 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:240:SER:OG	3:A:402:A1I2P:C01	1.73	1.36
3:B:403:A1I2P:C12	5:B:526:HOH:O	1.78	1.26
1:B:137[B]:GLU:OE1	5:B:504:HOH:O	1.86	0.93
3:B:403:A1I2P:N10	5:B:505:HOH:O	2.05	0.89
1:B:307[B]:ASN:OD1	1:B:308:THR:N	2.10	0.83
1:A:240:SER:CB	3:A:402:A1I2P:C01	2.59	0.80
3:A:402:A1I2P:N10	5:A:505:HOH:O	2.25	0.69
1:A:261:GLU:HG2	5:A:508:HOH:O	1.96	0.65
1:A:32:ARG:HD2	5:A:612:HOH:O	2.05	0.56
1:A:359:MET:O	1:A:359:MET:HE3	2.07	0.55
1:B:92:ARG:NH1	1:B:123:ASN:OD1	2.33	0.54
1:A:275[A]:CYS:SG	1:A:302:TYR:HE1	2.31	0.53
1:A:222:TYR:OH	1:A:226:LYS:NZ	2.43	0.52
1:B:109:SER:OG	1:B:137[A]:GLU:OE1	2.25	0.51
1:A:205:LYS:NZ	5:A:508:HOH:O	2.40	0.49
1:A:137[B]:GLU:OE2	5:A:502:HOH:O	2.18	0.49
1:A:359:MET:HE3	1:A:359:MET:HA	1.94	0.48
1:A:226:LYS:NZ	5:A:514:HOH:O	2.47	0.48
1:A:306:ILE:HD13	1:A:346:VAL:HG12	1.97	0.46
1:A:243:ASP:OD2	3:A:402:A1I2P:N02	2.47	0.46
1:A:295:LEU:HD12	1:A:295:LEU:O	2.16	0.45
1:B:307[A]:ASN:HA	2:B:402:NAD:H2A	1.99	0.44
1:A:87:LEU:HD13	1:A:272:PHE:CE1	2.52	0.44
1:A:307[B]:ASN:OD1	2:A:401:NAD:H1B	2.17	0.43
5:A:529:HOH:O	1:B:296:MET:HE2	2.19	0.43
1:B:103:TYR:N	1:B:286[A]:VAL:HG11	2.34	0.43
1:A:137[B]:GLU:OE2	1:A:176:TYR:OH	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:GLU:O	1:B:47:GLU:HG3	2.19	0.42
1:B:96:SER:HA	1:B:274:LYS:HD3	2.02	0.42
1:A:109:SER:OG	1:A:137[A]:GLU:OE1	2.34	0.41
1:A:164:ASN:HB3	1:B:327:TRP:CE2	2.55	0.41
1:B:329[B]:LYS:HE3	5:B:512:HOH:O	2.21	0.41
1:B:184:MET:HB2	1:B:185:PRO:HD3	2.03	0.41
1:A:135:VAL:HA	1:A:221:TYR:CE2	2.56	0.40

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:704:HOH:O	5:B:708:HOH:O[4_555]	1.87	0.33
5:A:525:HOH:O	5:B:542:HOH:O[2_444]	2.18	0.02

## 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	330/369 (89%)	326 (99%)	4 (1%)	0	100	100
1	B	341/369 (92%)	335 (98%)	6 (2%)	0	100	100
All	All	671/738 (91%)	661 (98%)	10 (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	282/309 (91%)	279 (99%)	3 (1%)	65	33
1	B	291/309 (94%)	288 (99%)	3 (1%)	68	37
All	All	573/618 (93%)	567 (99%)	6 (1%)	65	37

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

Mol	Chain	Res	Type
1	A	109	SER
1	A	115	THR
1	A	274	LYS
1	B	47	GLU
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	84	HIS
1	A	228	HIS
1	B	65	GLN
1	B	189	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	A	177	1	4,6,7	0.55	0	2,6,8	0.15	0
1	CSS	B	177	1	4,6,7	0.65	0	2,6,8	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
1	CSS	A	177	1	-	0/1/5/7	-
1	CSS	B	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](#)

5 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	A1I2P	B	403	-	10,12,12	2.66	3 (30%)	10,18,18	5.66	6 (60%)
4	MRD	B	401	-	7,7,7	0.36	0	9,10,10	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	A1I2P	A	402	-	10,12,12	2.73	4 (40%)	10,18,18	4.26	6 (60%)
2	NAD	A	401	-	46,48,48	0.81	1 (2%)	64,73,73	1.00	4 (6%)
2	NAD	B	402	-	46,48,48	0.91	2 (4%)	64,73,73	0.91	3 (4%)

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	A1I2P	B	403	-	-	5/7/9/9	0/1/1/1
4	MRD	B	401	-	-	0/5/5/5	-
3	A1I2P	A	402	-	-	3/7/9/9	0/1/1/1
2	NAD	A	401	-	-	5/30/62/62	0/5/5/5
2	NAD	B	402	-	-	5/30/62/62	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	A1I2P	S03-N02	5.86	1.70	1.61
3	B	403	A1I2P	S03-N02	5.19	1.69	1.61
3	B	403	A1I2P	O09-N10	-4.52	1.34	1.42
2	B	402	NAD	C2N-N1N	4.11	1.39	1.35
3	A	402	A1I2P	O09-N10	-3.95	1.35	1.42
3	B	403	A1I2P	O09-C07	-2.93	1.29	1.34
3	A	402	A1I2P	O09-C07	-2.40	1.30	1.34
2	B	402	NAD	PA-O2A	-2.22	1.45	1.55
3	A	402	A1I2P	C01-N02	-2.18	1.43	1.46
2	A	401	NAD	PA-O2A	-2.14	1.45	1.55

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	A1I2P	O05-S03-O04	-11.84	98.11	119.82
3	B	403	A1I2P	C11-C06-S03	10.98	135.40	127.23
3	A	402	A1I2P	O05-S03-O04	-10.22	101.08	119.82
3	A	402	A1I2P	O09-C07-C08	5.26	124.72	116.59
3	B	403	A1I2P	O09-C07-C08	4.89	124.15	116.59
3	B	403	A1I2P	O04-S03-N02	3.66	113.81	107.06
3	A	402	A1I2P	O05-S03-N02	3.66	113.80	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	NAD	O2A-PA-O1A	3.48	128.65	112.44
3	B	403	A1I2P	C07-O09-N10	3.27	112.14	108.51
3	A	402	A1I2P	C12-C11-N10	3.26	125.53	119.86
3	A	402	A1I2P	C07-O09-N10	3.25	112.12	108.51
2	A	401	NAD	O2A-PA-O1A	3.12	126.94	112.44
2	A	401	NAD	C6N-N1N-C2N	-2.64	119.63	121.88
3	A	402	A1I2P	O04-S03-N02	2.57	111.80	107.06
3	B	403	A1I2P	C12-C11-C06	2.20	132.69	129.58
2	B	402	NAD	C6N-N1N-C2N	-2.20	120.01	121.88
2	A	401	NAD	O7N-C7N-C3N	-2.18	116.93	119.60
2	A	401	NAD	O3-PA-O1A	-2.12	104.31	110.70
2	B	402	NAD	O3-PN-O1N	-2.03	104.59	110.70

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAD	C5D-O5D-PN-O1N
2	B	402	NAD	C5D-O5D-PN-O3
2	B	402	NAD	C5D-O5D-PN-O1N
3	A	402	A1I2P	C07-C06-S03-O04
3	A	402	A1I2P	C11-C06-S03-O04
3	B	403	A1I2P	C01-N02-S03-O04
3	B	403	A1I2P	C01-N02-S03-O05
3	B	403	A1I2P	C01-N02-S03-C06
3	B	403	A1I2P	C07-C06-S03-O05
3	B	403	A1I2P	C11-C06-S03-O05
2	A	401	NAD	PA-O3-PN-O5D
2	B	402	NAD	PA-O3-PN-O5D
2	A	401	NAD	C5D-O5D-PN-O3
2	B	402	NAD	C5D-O5D-PN-O2N
3	A	402	A1I2P	C07-C06-S03-O05
2	A	401	NAD	PA-O3-PN-O1N
2	A	401	NAD	PA-O3-PN-O2N
2	B	402	NAD	PA-O3-PN-O2N

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	403	A1I2P	2	0

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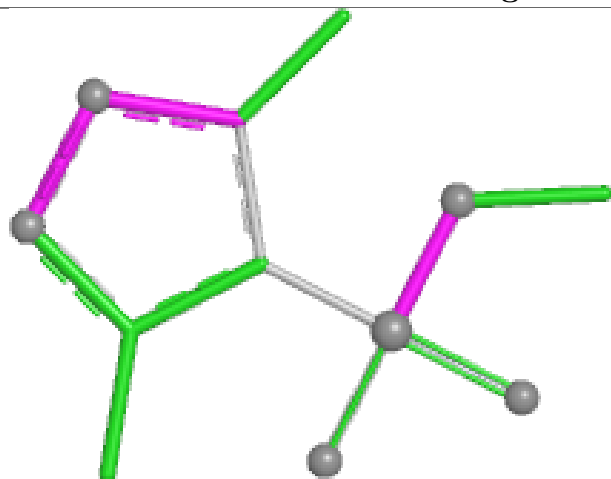
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	A1I2P	4	0
2	A	401	NAD	1	0
2	B	402	NAD	1	0

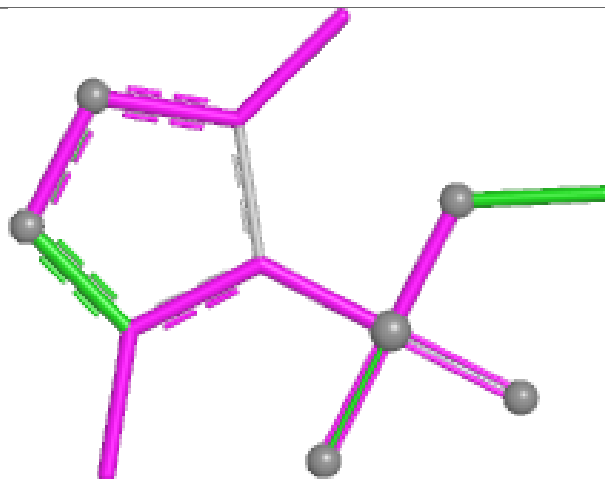
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



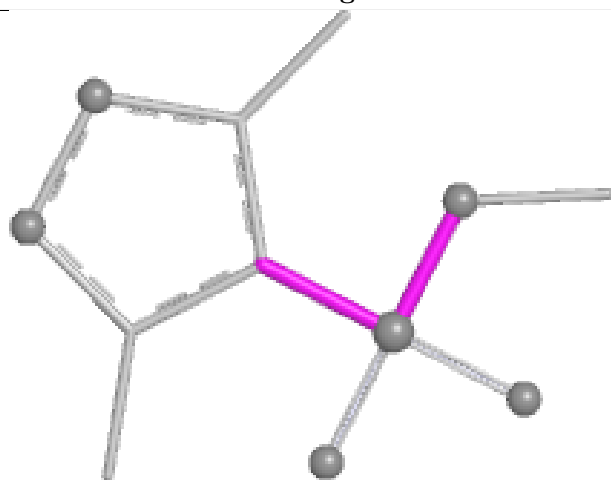
## Ligand A1I2P B 403



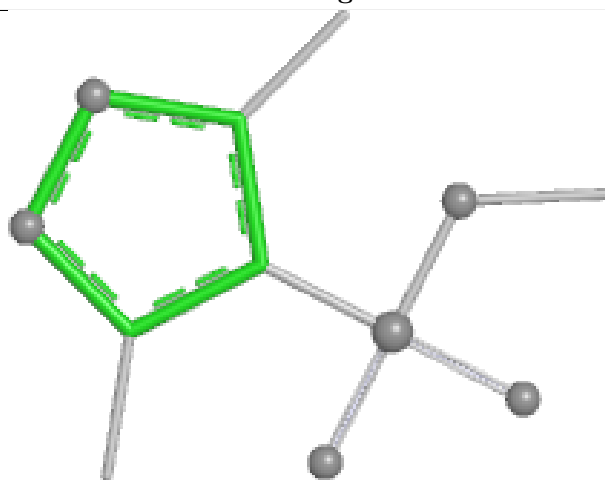
Bond lengths



Bond angles

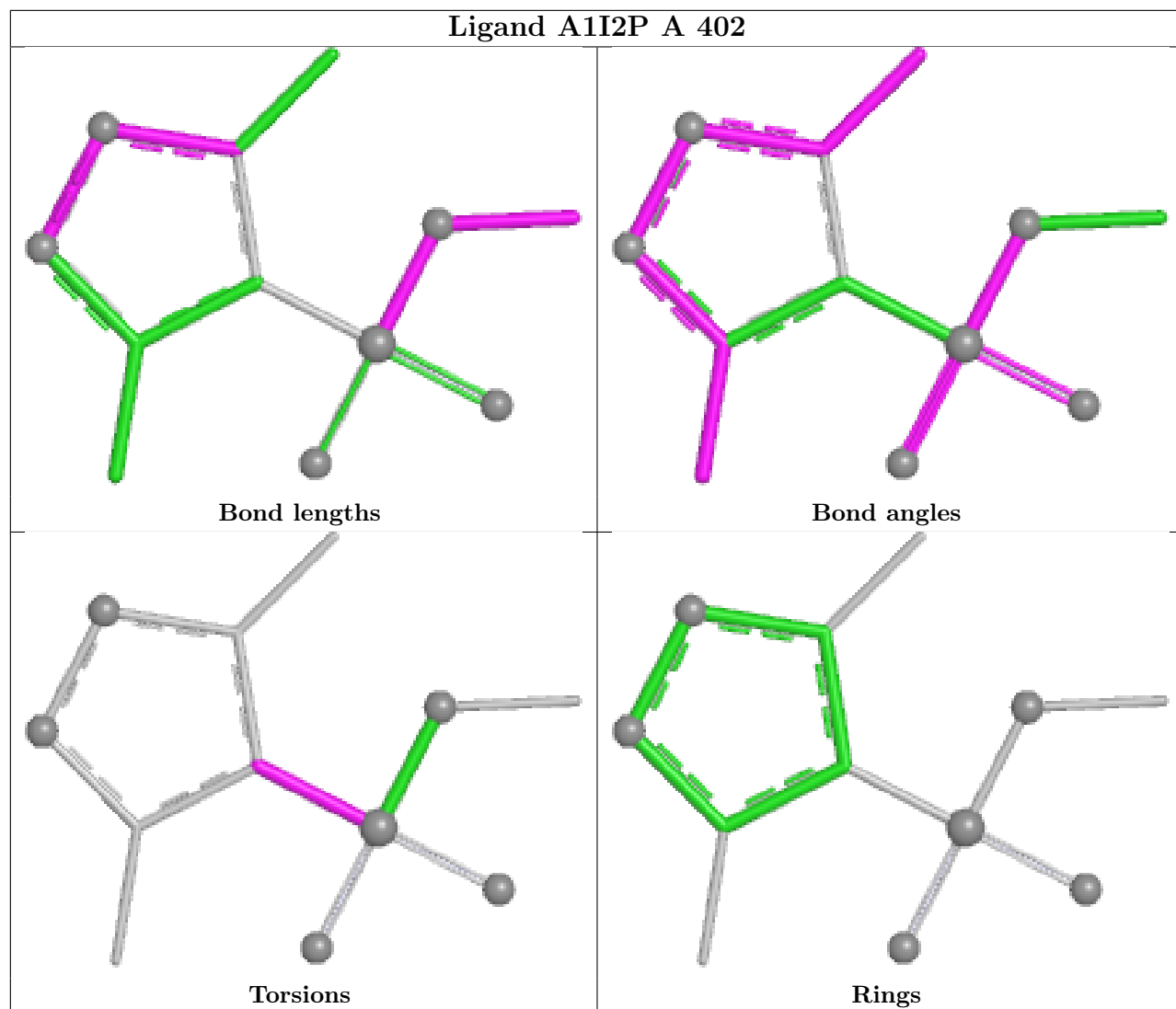


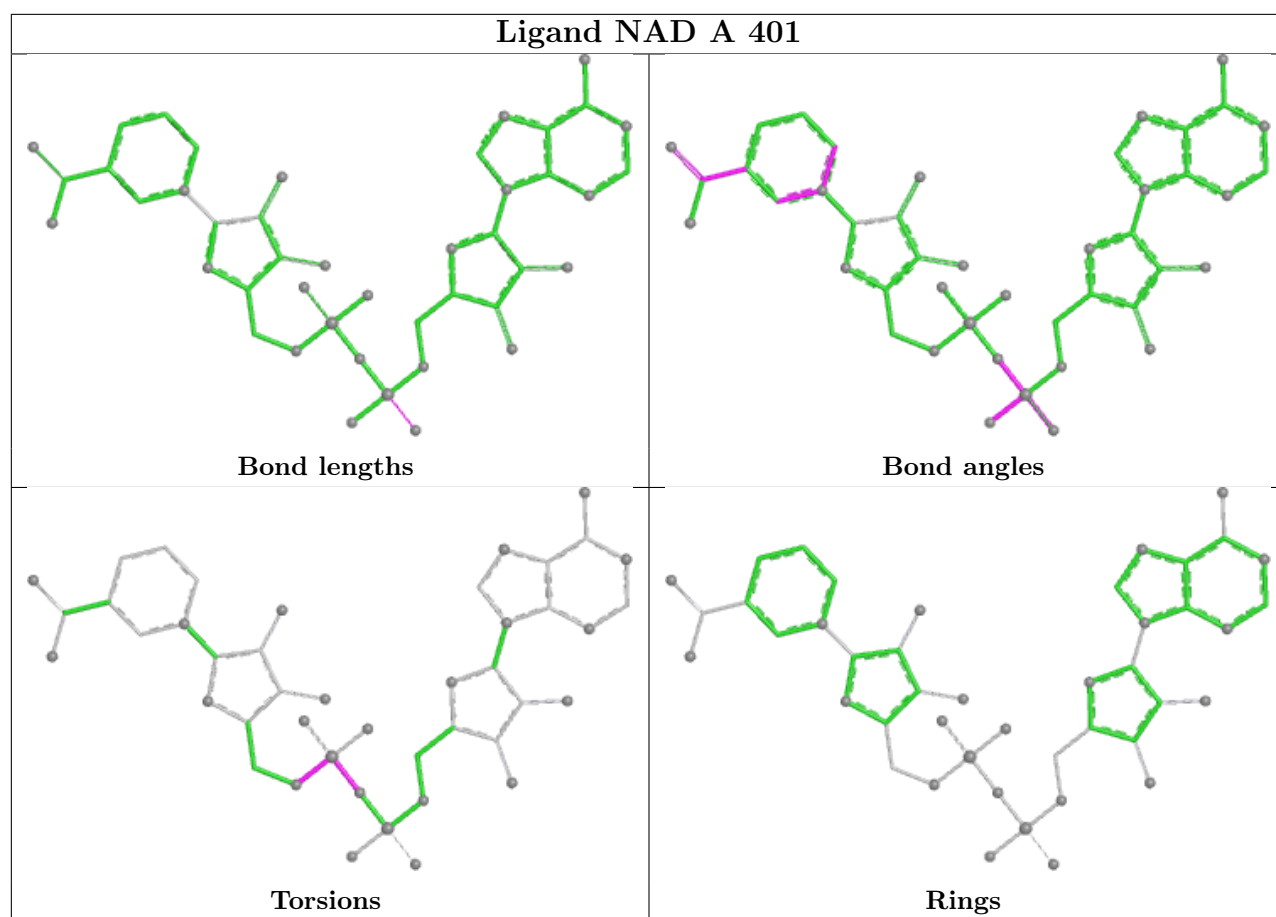
Torsions

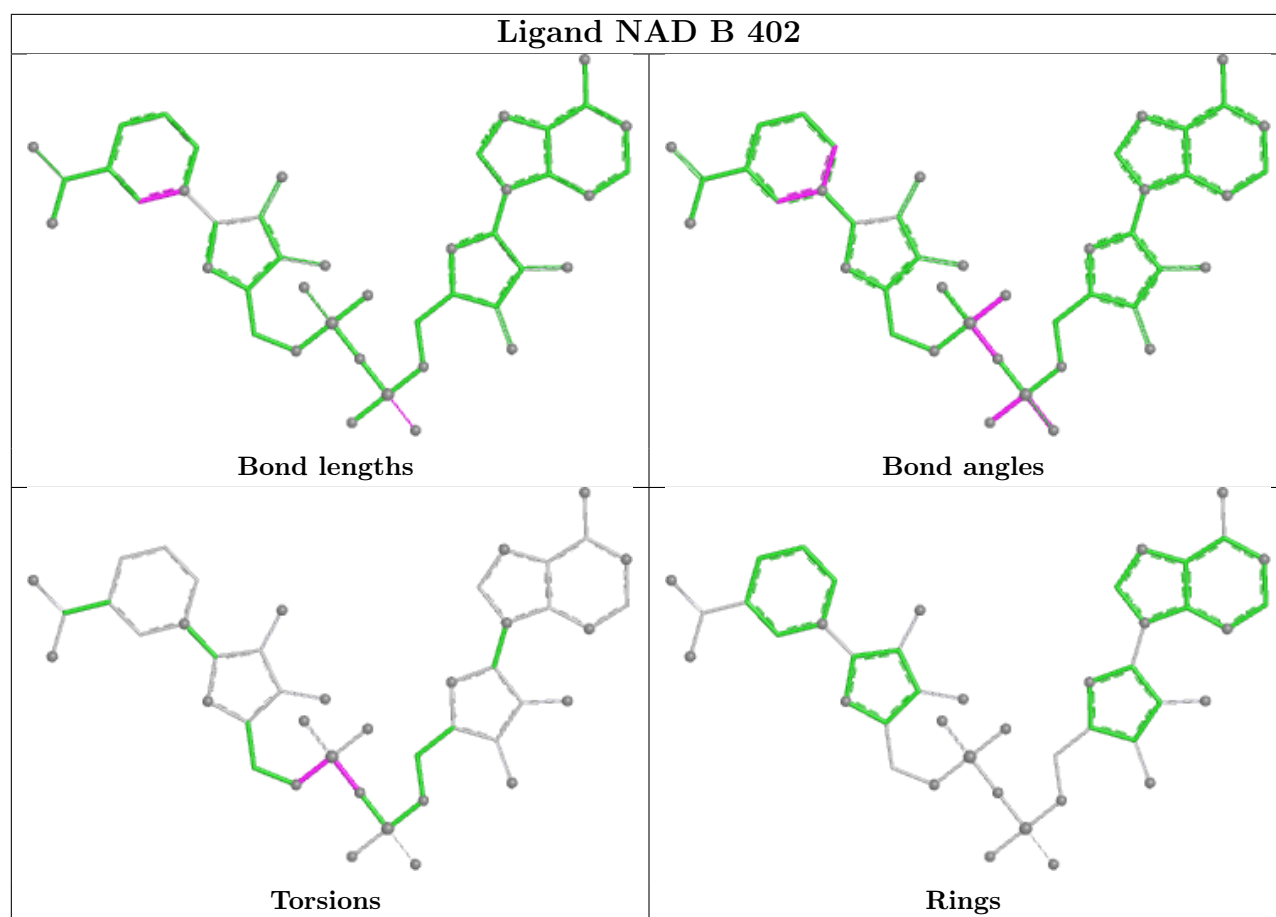


Rings

## Ligand A1I2P 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, 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	328/369 (88%)	1.06	38 (11%) <b>9</b> <b>10</b>	13, 29, 47, 88	6 (1%)
1	B	334/369 (90%)	1.00	48 (14%) <b>6</b> <b>6</b>	15, 29, 49, 80	10 (2%)
All	All	662/738 (89%)	1.03	86 (12%) <b>7</b> <b>8</b>	13, 29, 48, 88	16 (2%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	87	LEU	7.5
1	A	77	LEU	6.6
1	B	89	GLN	6.4
1	A	91	ARG	5.4
1	B	94	LEU	5.0
1	A	84	HIS	4.9
1	A	305	TYR	4.8
1	B	29	THR	4.6
1	B	251	LYS	4.6
1	A	85	ALA	4.3
1	A	363	MET	4.3
1	B	305	TYR	4.1
1	B	85	ALA	4.0
1	A	362	PHE	4.0
1	B	307[A]	ASN	3.8
1	A	361	ALA	3.7
1	B	171	VAL	3.5
1	B	192	MET	3.4
1	B	71	GLU	3.4
1	B	87	LEU	3.3
1	B	241	LEU	3.2
1	A	29	THR	3.2
1	B	363	MET	3.2
1	A	307[A]	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	76	PRO	3.1
1	A	272	PHE	3.1
1	B	88	THR	3.1
1	B	196	THR	3.0
1	A	360	ASP	3.0
1	A	274	LYS	3.0
1	B	250	TYR	3.0
1	A	186	ILE	3.0
1	A	279	ILE	3.0
1	B	247	PHE	2.9
1	A	74	LEU	2.9
1	A	290	ILE	2.9
1	B	153	LEU	2.8
1	A	332	VAL	2.8
1	A	70	ILE	2.8
1	B	43	ARG	2.8
1	B	77	LEU	2.8
1	A	195	ASN	2.6
1	B	174	GLU	2.6
1	B	75	GLU	2.6
1	A	271	ILE	2.6
1	B	38	ARG	2.5
1	A	275[A]	CYS	2.5
1	B	74	LEU	2.5
1	B	163	ILE	2.5
1	B	93	PRO	2.5
1	B	298	ASN	2.4
1	B	200	LYS	2.4
1	A	295	LEU	2.4
1	A	66	VAL	2.4
1	B	360	ASP	2.4
1	B	90	SER	2.4
1	A	45	LEU	2.3
1	A	200	LYS	2.3
1	A	163	ILE	2.3
1	A	298	ASN	2.3
1	A	335	GLN	2.3
1	B	186	ILE	2.3
1	B	256	VAL	2.3
1	B	327	TRP	2.2
1	B	91	ARG	2.2
1	A	160	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	47	GLU	2.2
1	A	191	VAL	2.2
1	B	285	VAL	2.2
1	B	32	ARG	2.2
1	B	272	PHE	2.2
1	A	196	THR	2.2
1	A	358	LYS	2.2
1	B	183	LEU	2.1
1	B	345	LEU	2.1
1	A	32	ARG	2.1
1	B	154	ARG	2.1
1	B	201	TRP	2.1
1	A	270	ALA	2.1
1	A	88	THR	2.1
1	B	49[A]	PHE	2.1
1	B	191	VAL	2.1
1	B	361	ALA	2.0
1	B	226	LYS	2.0
1	B	253	PRO	2.0
1	B	63	VAL	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	0.87	0.16	36,37,54,98	0
1	CSS	A	177	7/8	0.94	0.08	28,29,42,51	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,

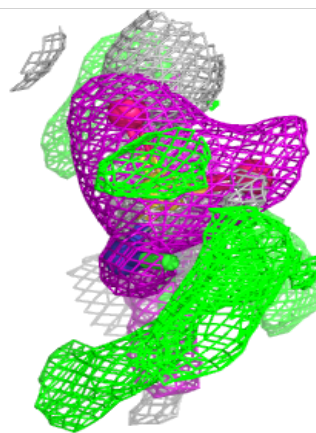
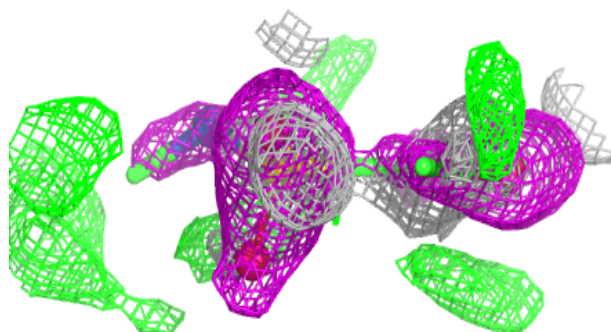
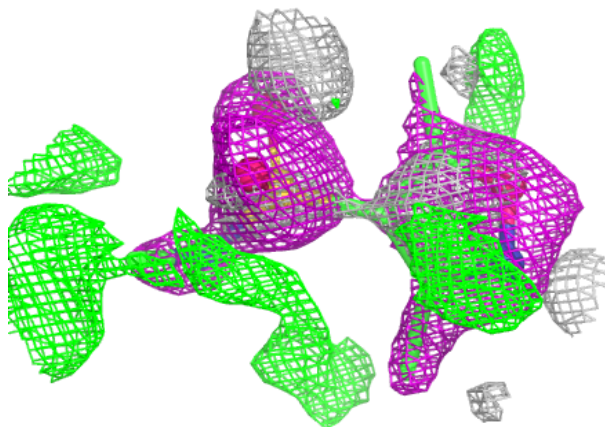
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	A1I2P	B	403	12/12	0.54	0.28	20,20,20,20	12
3	A1I2P	A	402	12/12	0.70	0.24	20,20,20,20	12
4	MRD	B	401	8/8	0.90	0.19	38,40,44,48	8
2	NAD	B	402	44/44	0.97	0.07	20,24,34,43	44
2	NAD	A	401	44/44	0.97	0.07	19,24,33,43	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 A1I2P B 403:**

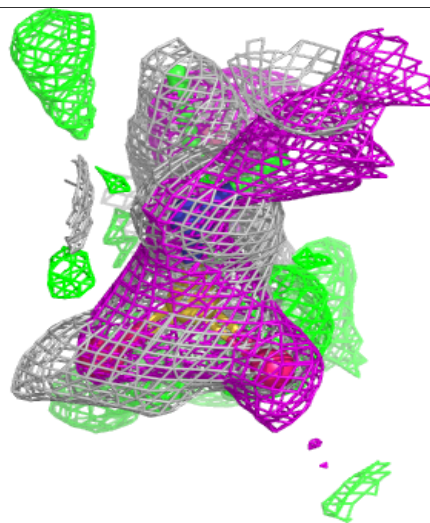
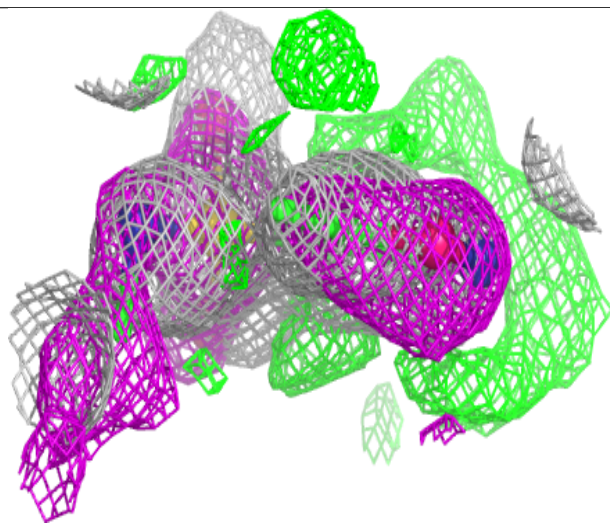
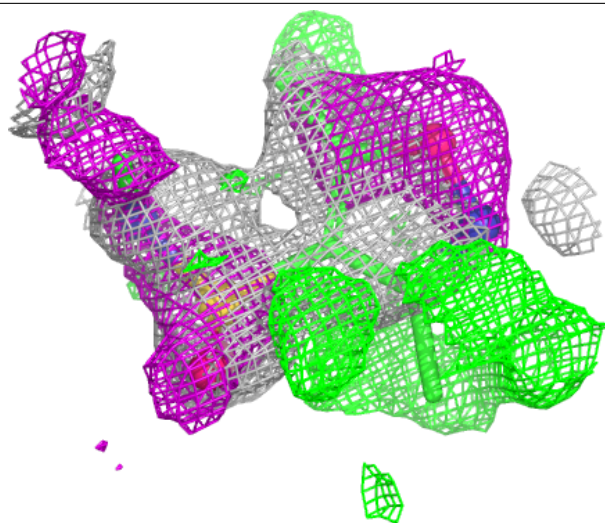
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





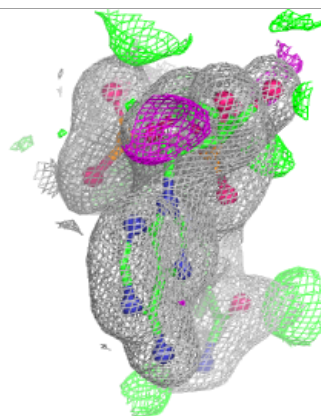
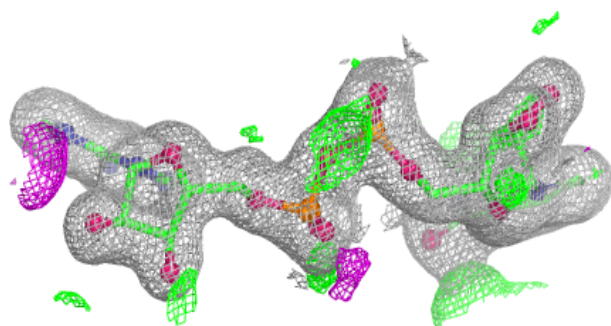
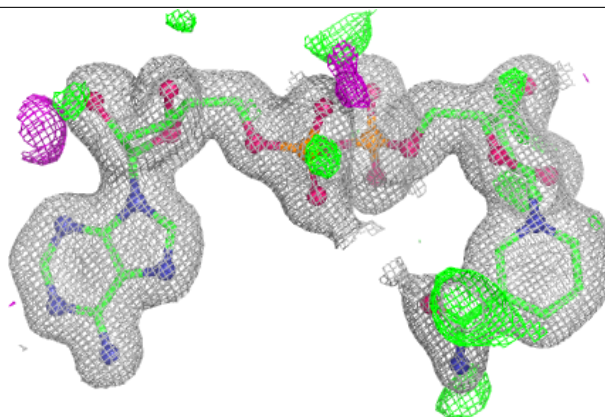
**Electron density around A1I2P A 402:**

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

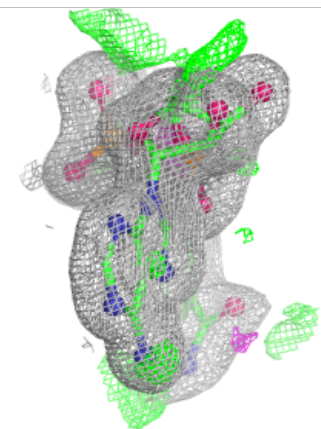
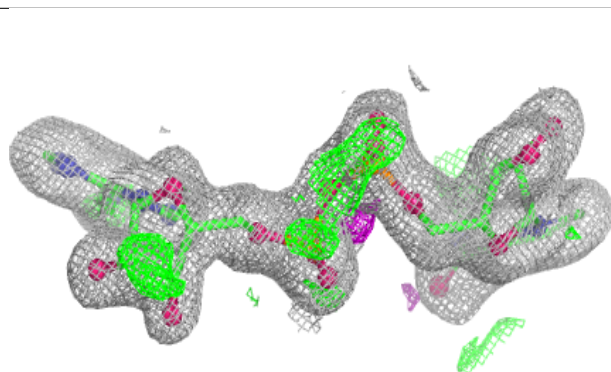
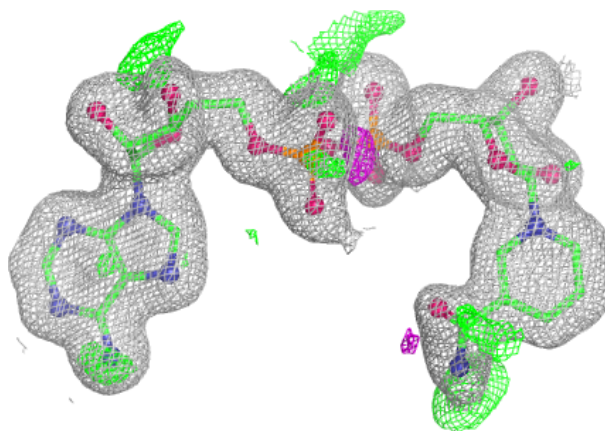


**Electron density around NAD B 402:**

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

**Electron density around NAD A 401:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.