



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:05 PM UTC

PDB ID : 9IE2 / pdb\_00009ie2  
Title : Human Deoxyhypusine Synthase Fragment Screening Campaign - ligand VT00224  
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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](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

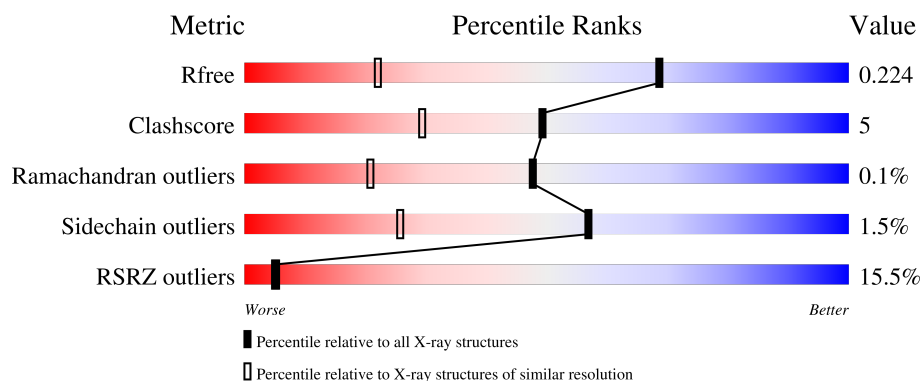
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.39 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  $\geq 3$ , 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>15%</div> <div>85%</div> <div>8% .. 5%</div> </div>
1	B	369	<div> <div>14%</div> <div>86%</div> <div>8% • 5%</div> </div>

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	X4P	A	403[A]	-	X	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6176 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.

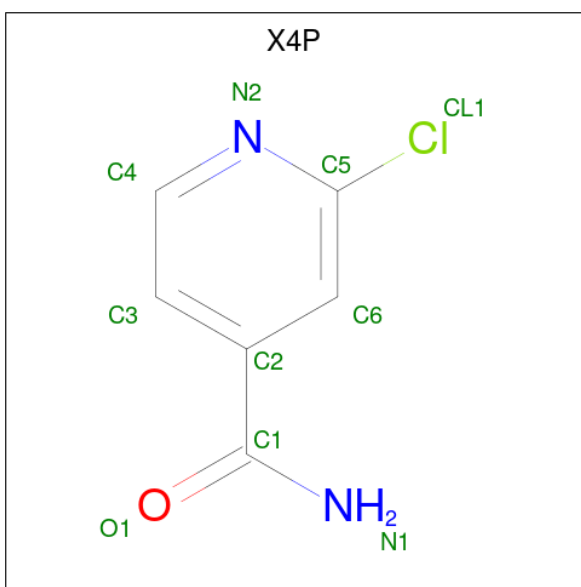
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	8	0
			2776	1768	471	521	16			
1	B	351	Total	C	N	O	S	0	9	0
			2794	1779	472	526	17			

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



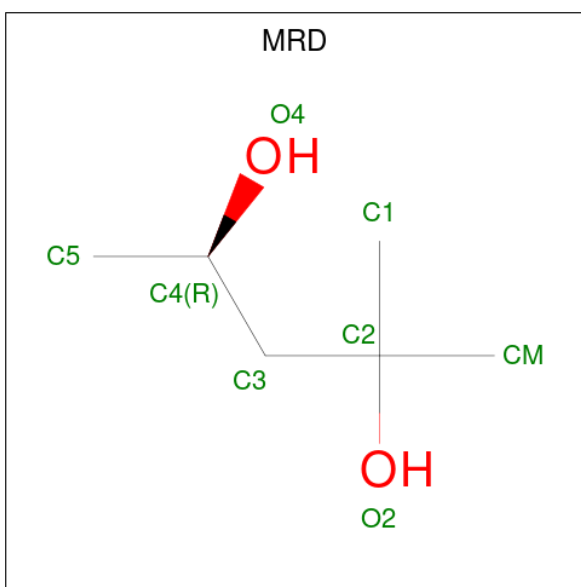
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 2-chloropyridine-4-carboxamide (CCD ID: X4P) (formula:  $C_6H_5ClN_2O$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			10	6	1	2	1		
3	A	1	Total	C	Cl	N	O	0	1
			20	12	2	4	2		
3	B	1	Total	C	Cl	N	O	0	0
			10	6	1	2	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		

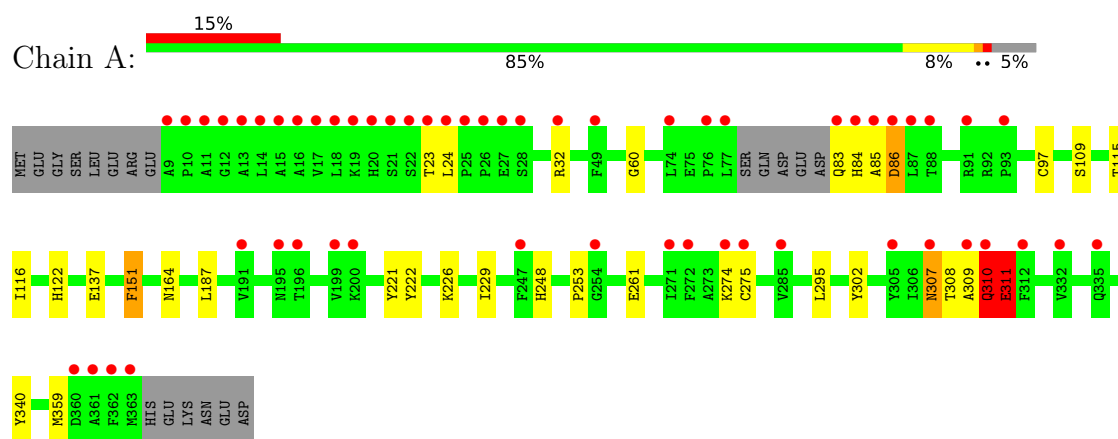
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	237	Total 237	O 237	0	0
5	B	233	Total 233	O 233	0	0

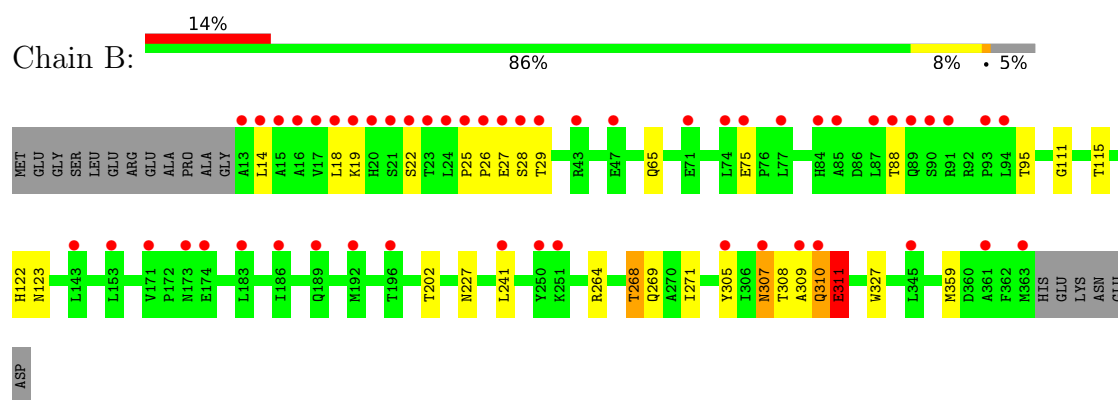
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	105.04Å 105.04Å 160.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.10 – 1.39 46.10 – 1.39	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.10-1.39) 99.8 (46.10-1.39)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.02 (at 1.39Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, $R_{free}$	0.205 , 0.217 0.214 , 0.224	Depositor DCC
$R_{free}$ test set	10101 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 35.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6176	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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: MRD, CSS, X4P, 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	1.20	9/2843 (0.3%)	1.38	17/3854 (0.4%)
1	B	1.25	12/2867 (0.4%)	1.39	19/3887 (0.5%)
All	All	1.22	21/5710 (0.4%)	1.38	36/7741 (0.5%)

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	4
1	B	0	1
All	All	0	5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	29	THR	C-N	-16.00	1.12	1.33
1	B	65	GLN	CD-OE1	7.33	1.37	1.23
1	B	307[A]	ASN	C-O	7.08	1.32	1.23
1	B	307[B]	ASN	C-O	7.08	1.32	1.23
1	A	310[A]	GLN	C-O	6.98	1.32	1.23
1	A	310[B]	GLN	C-O	6.98	1.32	1.23
1	A	307[A]	ASN	C-O	6.45	1.31	1.23
1	A	307[B]	ASN	C-O	6.45	1.31	1.23
1	A	311[A]	GLU	C-O	5.99	1.31	1.24
1	A	311[B]	GLU	C-O	5.99	1.31	1.24
1	B	271	ILE	C-O	-5.82	1.17	1.24
1	A	60	GLY	C-O	5.54	1.30	1.23
1	A	122	HIS	CE1-NE2	5.23	1.37	1.32
1	B	311[A]	GLU	C-O	5.12	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	311[B]	GLU	C-O	5.12	1.30	1.24
1	B	111	GLY	C-O	5.09	1.29	1.24
1	A	248	HIS	C-O	5.08	1.30	1.24
1	B	268[A]	THR	C-O	5.03	1.29	1.24
1	B	268[B]	THR	C-O	5.03	1.29	1.24
1	B	310[A]	GLN	C-O	5.00	1.29	1.23
1	B	310[B]	GLN	C-O	5.00	1.29	1.23

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	311[A]	GLU	N-CA-C	12.71	126.32	111.71
1	B	311[B]	GLU	N-CA-C	12.71	126.32	111.71
1	B	241[A]	LEU	CA-C-O	10.48	131.66	120.55
1	B	241[B]	LEU	CA-C-O	10.48	131.66	120.55
1	B	65	GLN	CG-CD-NE2	-10.05	101.33	116.40
1	B	311[A]	GLU	CA-C-O	8.80	130.04	120.10
1	B	311[B]	GLU	CA-C-O	8.80	130.04	120.10
1	B	268[A]	THR	CA-C-O	7.91	129.04	120.10
1	B	268[B]	THR	CA-C-O	7.91	129.04	120.10
1	B	268[A]	THR	N-CA-C	7.85	120.74	111.71
1	B	268[B]	THR	N-CA-C	7.85	120.74	111.71
1	A	229	ILE	O-C-N	7.46	126.07	121.37
1	B	241[A]	LEU	N-CA-C	7.35	119.29	111.28
1	B	241[B]	LEU	N-CA-C	7.35	119.29	111.28
1	B	65	GLN	OE1-CD-NE2	7.27	129.87	122.60
1	A	24	LEU	CA-C-N	6.42	124.34	119.66
1	A	24	LEU	C-N-CA	6.42	124.34	119.66
1	A	310[A]	GLN	CA-C-O	5.99	127.88	121.05
1	A	310[B]	GLN	CA-C-O	5.99	127.88	121.05
1	B	307[A]	ASN	CA-C-O	5.78	127.77	121.06
1	B	307[B]	ASN	CA-C-O	5.78	127.77	121.06
1	B	305	TYR	CA-CB-CG	5.54	123.87	113.90
1	A	311[A]	GLU	CA-C-O	5.40	126.49	120.82
1	A	311[B]	GLU	CA-C-O	5.40	126.49	120.82
1	B	202	THR	O-C-N	-5.36	118.28	121.71
1	A	221	TYR	CA-C-O	-5.22	113.62	119.79
1	B	29	THR	O-C-N	-5.22	116.16	122.48
1	A	310[A]	GLN	N-CA-C	5.21	118.43	110.20
1	A	310[B]	GLN	N-CA-C	5.21	118.43	110.20
1	A	116	ILE	O-C-N	5.16	127.15	121.83
1	A	151	PHE	CA-C-O	-5.09	115.15	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	PRO	N-CA-CB	5.09	108.06	103.33
1	A	116	ILE	CA-C-O	-5.05	115.50	120.85
1	A	187	LEU	CA-C-O	-5.04	114.40	120.10
1	A	307[A]	ASN	CA-C-O	5.01	126.88	121.06
1	A	307[B]	ASN	CA-C-O	5.01	126.88	121.06

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	310[A]	GLN	Mainchain
1	A	85	ALA	Mainchain
1	A	86[A]	ASP	Mainchain
1	B	311[B]	GLU	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	2776	0	2762	26	2
1	B	2794	0	2785	36	0
2	A	44	0	26	2	0
2	B	44	0	26	5	0
3	A	30	0	0	3	0
3	B	10	0	0	3	0
4	B	8	0	14	0	0
5	A	237	0	0	5	2
5	B	233	0	0	7	0
All	All	6176	0	5613	61	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 5.

All (61) 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:311[A]:GLU:HG2	3:B:403:X4P:CL1	1.94	1.03
1:B:27:GLU:O	5:B:501:HOH:O	1.92	0.85
1:B:307[B]:ASN:ND2	1:B:309:ALA:H	1.75	0.85
1:A:261:GLU:HG2	5:A:514:HOH:O	1.76	0.83
1:B:307[B]:ASN:ND2	5:B:503:HOH:O	2.13	0.81
1:A:309:ALA:C	1:A:310[A]:GLN:CA	2.56	0.78
1:B:307[B]:ASN:OD1	1:B:309:ALA:HB3	1.87	0.73
1:A:137[B]:GLU:OE1	5:A:502:HOH:O	2.11	0.68
1:A:310[A]:GLN:NE2	5:A:507:HOH:O	2.29	0.65
1:B:75:GLU:OE1	5:B:504:HOH:O	2.14	0.65
1:B:14:LEU:C	1:B:14:LEU:HD13	2.22	0.65
1:B:307[B]:ASN:CG	1:B:309:ALA:H	2.05	0.65
1:B:14:LEU:HD11	1:B:18:LEU:HD11	1.77	0.64
1:B:309:ALA:HB2	2:B:402:NAD:O2B	1.98	0.63
1:A:226:LYS:NZ	5:A:508:HOH:O	2.32	0.61
1:B:25:PRO:O	1:B:28:SER:HB2	2.01	0.61
1:A:83:GLN:HG3	1:A:84:HIS:N	2.18	0.59
1:A:309:ALA:HB2	2:A:401:NAD:O2B	2.03	0.58
1:B:264:ARG:O	1:B:268[A]:THR:HG23	2.04	0.57
1:A:359:MET:O	1:A:359:MET:HE3	2.06	0.55
1:B:307[B]:ASN:CG	5:B:503:HOH:O	2.45	0.54
1:A:295:LEU:HD12	1:A:295:LEU:O	2.06	0.54
1:A:359:MET:HE3	1:A:359:MET:HA	1.90	0.53
1:B:311[A]:GLU:CG	3:B:403:X4P:CL1	2.82	0.52
1:A:340:TYR:C	3:A:403[A]:X4P:CL1	2.90	0.51
1:B:307[B]:ASN:HD21	1:B:309:ALA:HB2	1.76	0.50
1:B:307[B]:ASN:ND2	1:B:308:THR:N	2.61	0.49
1:B:307[B]:ASN:HD22	2:B:402:NAD:H1B	1.77	0.49
1:B:307[B]:ASN:HD21	1:B:309:ALA:H	1.55	0.48
1:B:311[B]:GLU:OE2	5:B:505:HOH:O	2.16	0.48
1:A:307[B]:ASN:OD1	2:A:401:NAD:H1B	2.13	0.48
1:B:307[B]:ASN:HD21	1:B:309:ALA:CB	2.27	0.48
1:A:222:TYR:OH	1:A:226:LYS:NZ	2.45	0.48
1:A:97:CYS:SG	1:A:275:CYS:SG	3.12	0.48
1:B:309:ALA:HB2	2:B:402:NAD:HO2A	1.77	0.48
1:B:307[B]:ASN:ND2	1:B:309:ALA:N	2.53	0.48
1:B:19:LYS:O	1:B:22:SER:OG	2.31	0.47
1:A:275:CYS:SG	1:A:302:TYR:HE2	2.38	0.47
1:A:164:ASN:HB3	1:B:327:TRP:CE2	2.51	0.45
1:B:88:THR:O	5:B:507:HOH:O	2.21	0.44
1:A:309:ALA:O	1:A:310[A]:GLN:CA	2.66	0.44
1:B:307[B]:ASN:HD21	1:B:309:ALA:N	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:LEU:HD11	1:B:18:LEU:CD1	2.43	0.44
3:A:403[B]:X4P:N1	1:B:310[B]:GLN:HG3	2.33	0.44
1:A:310[B]:GLN:CD	5:A:507:HOH:O	2.62	0.43
1:B:269:GLN:NE2	5:B:506:HOH:O	2.50	0.43
1:A:310[A]:GLN:NE2	3:A:403[A]:X4P:N1	2.64	0.43
1:B:122:HIS:CE1	1:B:359[B]:MET:HE1	2.53	0.43
1:B:14:LEU:CD1	1:B:18:LEU:CD1	2.96	0.43
1:B:27:GLU:H	1:B:27:GLU:CD	2.26	0.42
1:A:151:PHE:HB2	3:B:403:X4P:C4	2.50	0.42
1:B:123:ASN:OD1	1:B:227:ASN:HB3	2.20	0.42
1:A:307[B]:ASN:OD1	1:A:308:THR:N	2.53	0.41
1:B:307[B]:ASN:ND2	2:B:402:NAD:H1B	2.36	0.41
1:A:359:MET:HE3	1:A:359:MET:CA	2.51	0.41
1:B:307[B]:ASN:ND2	2:B:402:NAD:O2B	2.53	0.41
1:B:14:LEU:C	1:B:14:LEU:CD1	2.93	0.40
1:A:32:ARG:HB2	1:A:32:ARG:CZ	2.51	0.40
1:A:83:GLN:CG	1:A:84:HIS:N	2.85	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)
1:A:310[B]:GLN:CB	5:A:507:HOH:O[4_555]	2.04	0.16
1:A:310[B]:GLN:CG	5:A:507:HOH:O[4_555]	2.15	0.05

## 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	353/369 (96%)	349 (99%)	4 (1%)	0	100	100
1	B	357/369 (97%)	351 (98%)	5 (1%)	1 (0%)	36	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	710/738 (96%)	700 (99%)	9 (1%)	1 (0%)	48 21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	26	PRO

### 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%)	291 (97%)	8 (3%)	39 10
1	B	304/309 (98%)	300 (99%)	4 (1%)	61 30
All	All	603/618 (98%)	591 (98%)	12 (2%)	57 17

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	THR
1	A	86[A]	ASP
1	A	86[B]	ASP
1	A	109	SER
1	A	115	THR
1	A	274	LYS
1	A	311[A]	GLU
1	A	311[B]	GLU
1	B	95	THR
1	B	115	THR
1	B	311[A]	GLU
1	B	311[B]	GLU

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

Mol	Chain	Res	Type
1	B	20	HIS
1	B	37	ASN
1	B	228	HIS

### 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	0.78	0	2,6,8	0.95	0
1	CSS	A	177	1	4,6,7	0.92	0	2,6,8	0.34	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	$\# Z  > 2$
2	NAD	A	401	-	46,48,48	0.52	0	64,73,73	0.67	1 (1%)
2	NAD	B	402	-	46,48,48	0.54	0	64,73,73	0.66	1 (1%)
3	X4P	A	403[B]	-	10,10,10	2.80	4 (40%)	12,13,13	1.86	3 (25%)
3	X4P	A	402	-	10,10,10	2.95	7 (70%)	12,13,13	2.40	4 (33%)
3	X4P	A	403[A]	-	10,10,10	3.52	7 (70%)	12,13,13	2.50	6 (50%)
4	MRD	B	401	-	7,7,7	0.25	0	9,10,10	0.87	0
3	X4P	B	403	-	10,10,10	2.71	6 (60%)	12,13,13	2.23	5 (41%)

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	A	401	-	-	5/30/62/62	0/5/5/5
2	NAD	B	402	-	-	5/30/62/62	0/5/5/5
3	X4P	A	403[B]	-	-	0/4/4/4	0/1/1/1
3	X4P	A	402	-	-	0/4/4/4	0/1/1/1
3	X4P	A	403[A]	-	-	0/4/4/4	0/1/1/1
4	MRD	B	401	-	-	0/5/5/5	-
3	X4P	B	403	-	-	0/4/4/4	0/1/1/1

All (24) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403[B]	X4P	C1-N1	6.21	1.44	1.33
3	A	403[A]	X4P	C1-N1	6.09	1.44	1.33
3	A	402	X4P	C1-N1	5.92	1.43	1.33
3	B	403	X4P	C1-N1	5.62	1.43	1.33
3	A	403[A]	X4P	O1-C1	-5.03	1.14	1.24
3	A	403[A]	X4P	C4-N2	-4.16	1.25	1.34
3	A	403[B]	X4P	O1-C1	-4.03	1.16	1.24
3	A	402	X4P	C6-C2	-3.65	1.34	1.39
3	B	403	X4P	O1-C1	-3.48	1.17	1.24
3	A	403[A]	X4P	C3-C2	-3.45	1.34	1.39
3	A	402	X4P	C3-C2	-3.35	1.34	1.39
3	A	403[A]	X4P	C6-C2	-3.34	1.34	1.39
3	A	403[A]	X4P	C5-N2	-3.17	1.25	1.32
3	B	403	X4P	C6-C2	-2.95	1.35	1.39
3	A	402	X4P	O1-C1	-2.94	1.18	1.24
3	A	403[B]	X4P	C4-N2	-2.75	1.28	1.34
3	A	403[B]	X4P	C6-C2	-2.69	1.35	1.39
3	A	403[A]	X4P	C2-C1	-2.51	1.46	1.50
3	A	402	X4P	C4-N2	-2.48	1.29	1.34
3	B	403	X4P	C4-N2	-2.43	1.29	1.34
3	B	403	X4P	C2-C1	2.43	1.54	1.50
3	A	402	X4P	C3-C4	-2.21	1.34	1.38
3	A	402	X4P	C5-N2	-2.07	1.28	1.32
3	B	403	X4P	C3-C2	-2.07	1.36	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	X4P	C6-C5-N2	-4.92	121.31	125.59
3	A	403[A]	X4P	C4-N2-C5	4.35	121.83	115.58
3	B	403	X4P	C6-C5-N2	-4.33	121.82	125.59
3	A	403[A]	X4P	O1-C1-C2	-4.21	114.45	119.60
3	A	402	X4P	C4-N2-C5	4.15	121.56	115.58
3	A	403[B]	X4P	C4-N2-C5	4.04	121.39	115.58
3	A	403[A]	X4P	C6-C5-N2	-3.56	122.50	125.59
3	B	403	X4P	C4-N2-C5	3.46	120.56	115.58
3	A	403[A]	X4P	C2-C1-N1	3.44	121.97	117.74
3	A	402	X4P	C3-C4-N2	-3.41	119.79	123.97
3	A	403[B]	X4P	C3-C4-N2	-3.24	120.01	123.97
3	A	403[B]	X4P	C6-C5-N2	-3.10	122.90	125.59
3	B	403	X4P	C3-C4-N2	-2.97	120.33	123.97
3	A	403[A]	X4P	C3-C4-N2	-2.63	120.75	123.97
2	A	401	NAD	C6N-N1N-C2N	-2.54	119.72	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	NAD	C6N-N1N-C2N	-2.45	119.80	121.88
3	A	403[A]	X4P	C6-C5-CL1	2.36	121.95	118.92
3	A	402	X4P	C6-C5-CL1	2.31	121.89	118.92
3	B	403	X4P	CL1-C5-N2	2.30	120.29	115.98
3	B	403	X4P	O1-C1-C2	2.10	122.17	119.60

There are no chirality outliers.

All (10) 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-O1N
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	A	401	NAD	C5D-O5D-PN-O2N
2	B	402	NAD	C5D-O5D-PN-O3
2	B	402	NAD	C5D-O5D-PN-O2N
2	B	402	NAD	PA-O3-PN-O2N
2	A	401	NAD	PA-O3-PN-O2N

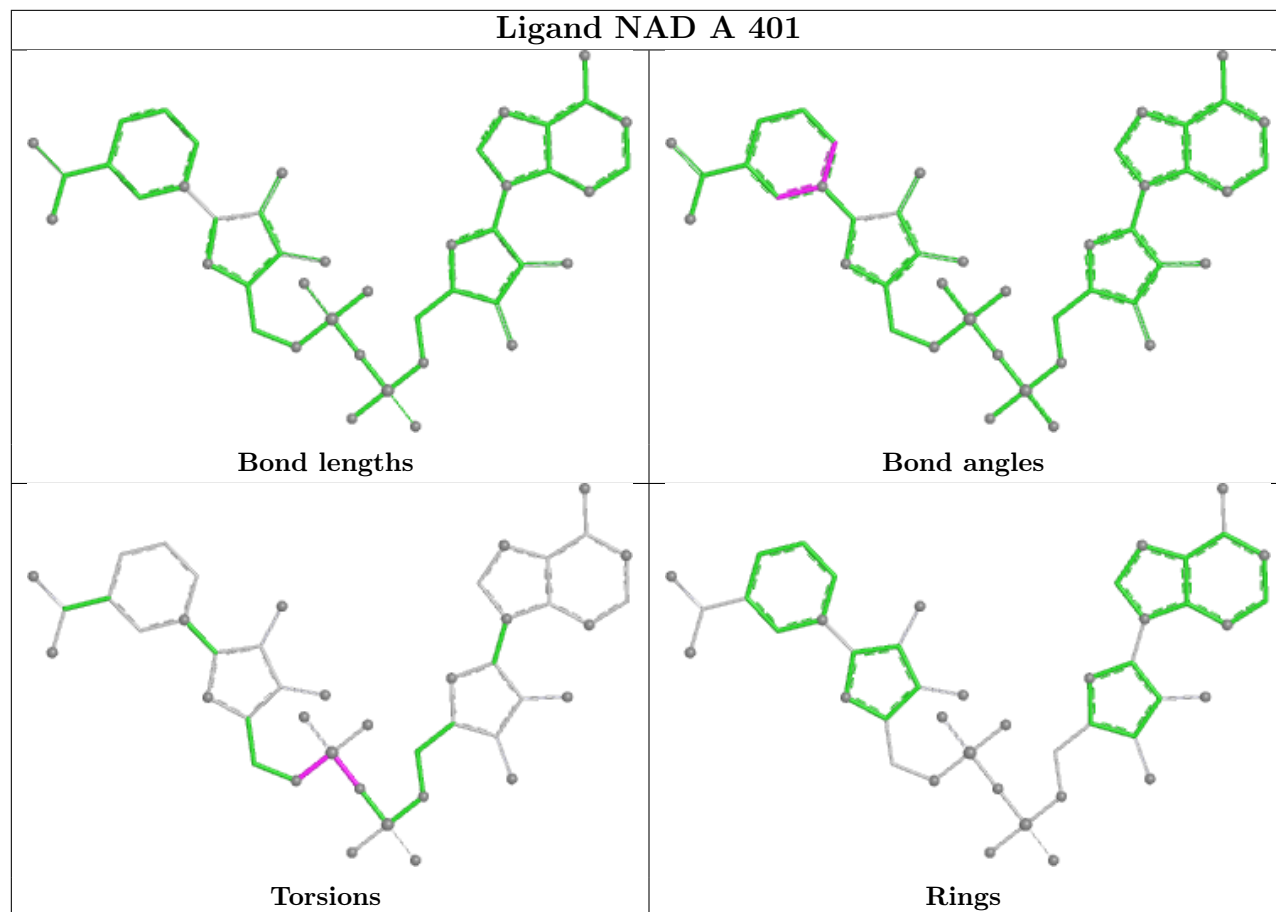
There are no ring outliers.

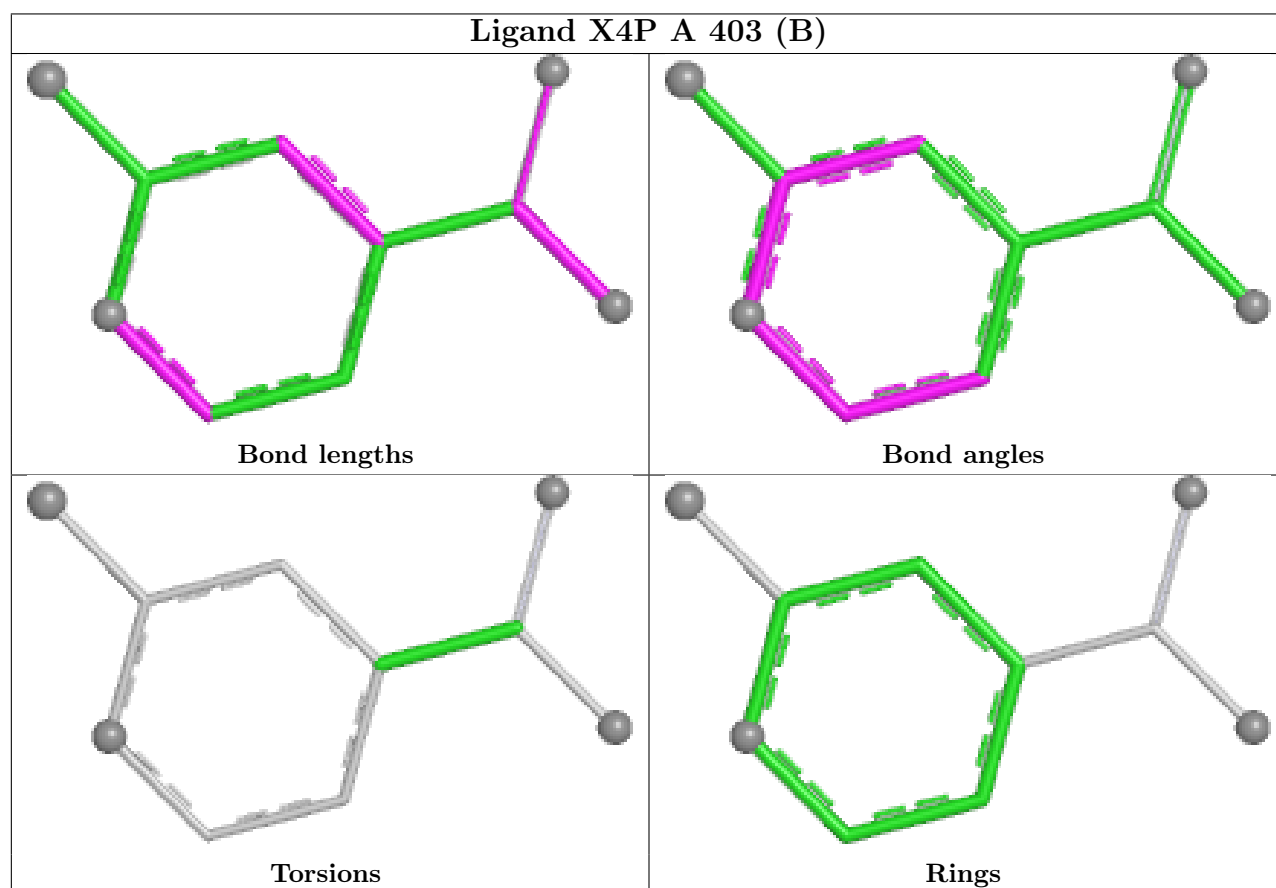
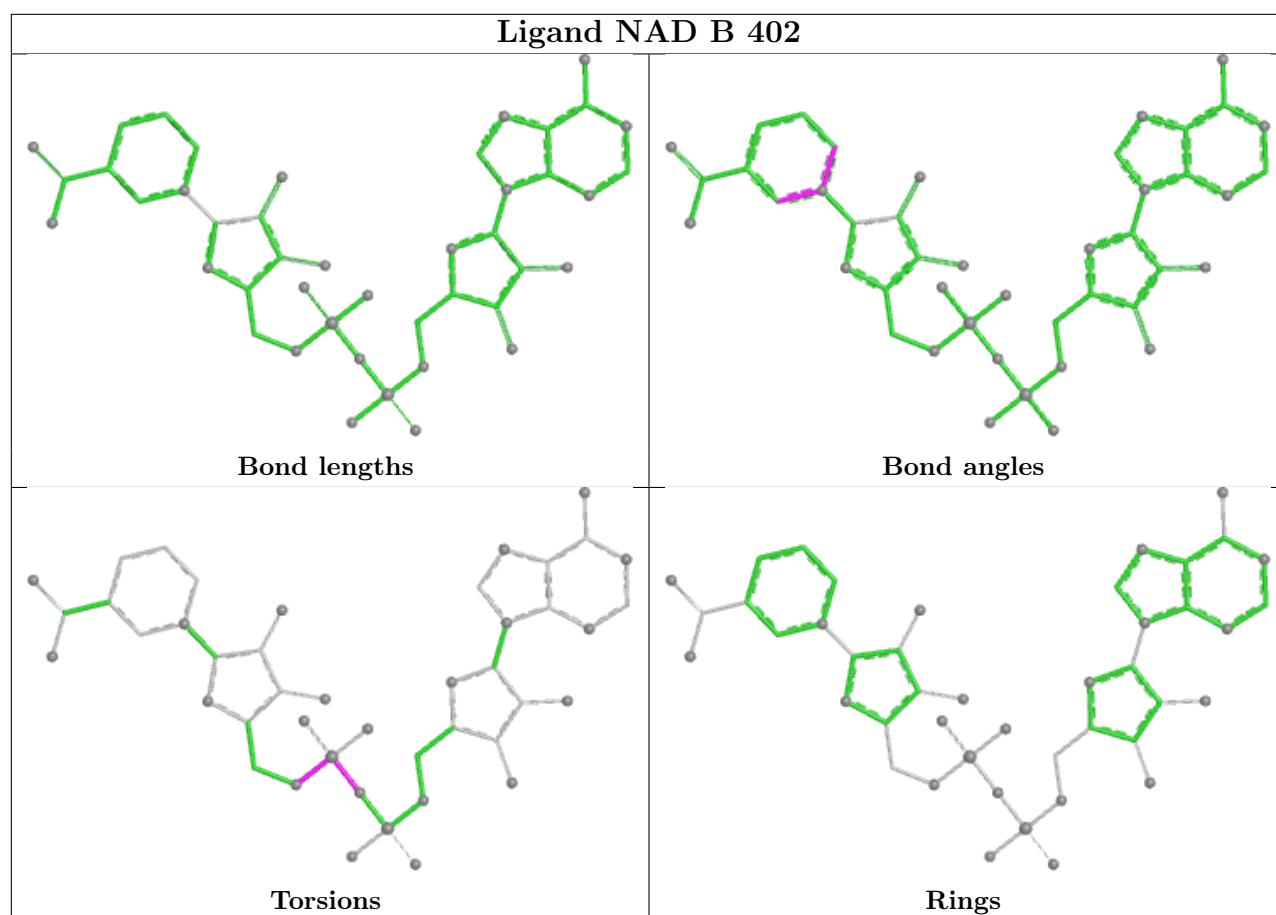
5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAD	2	0
2	B	402	NAD	5	0
3	A	403[B]	X4P	1	0
3	A	403[A]	X4P	2	0
3	B	403	X4P	3	0

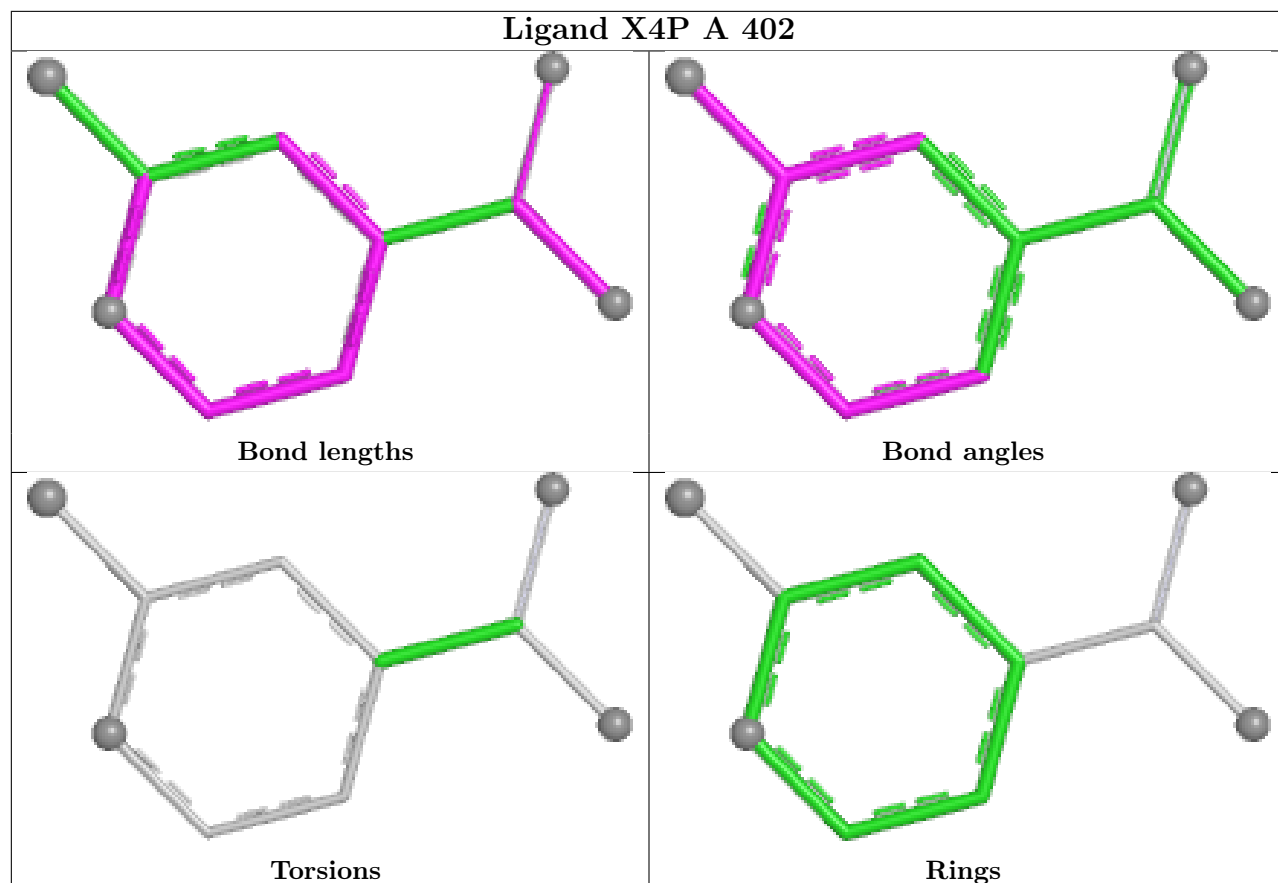
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

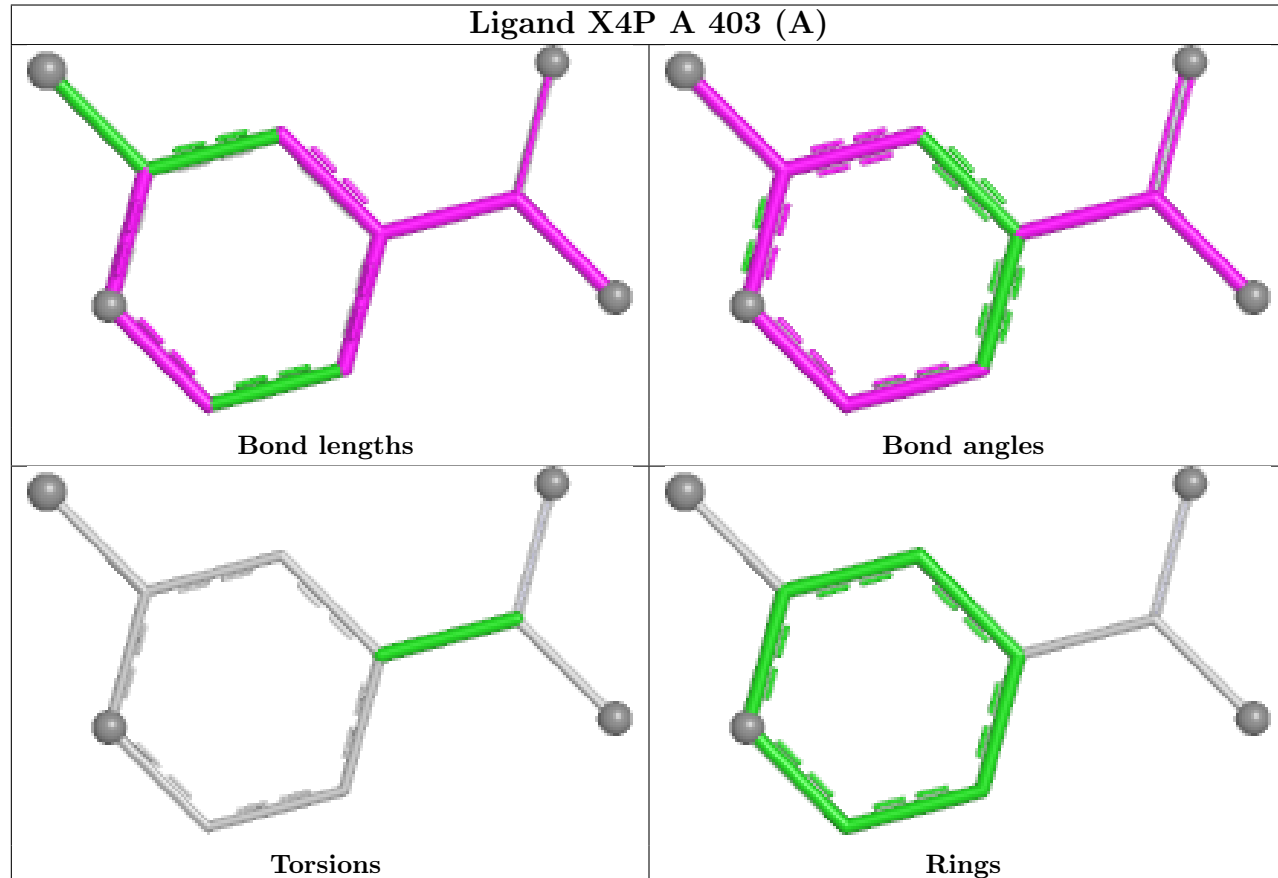


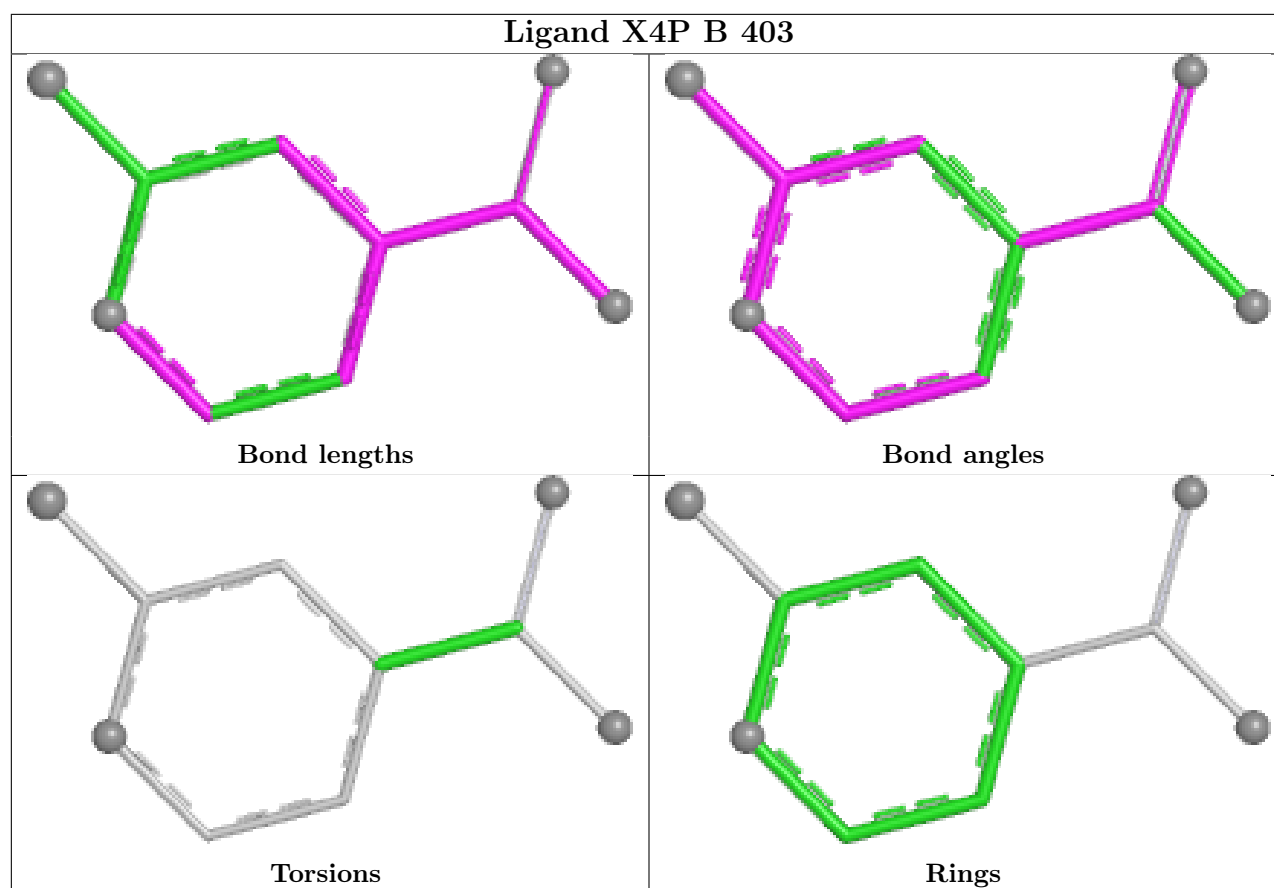


## Ligand X4P A 402



## Ligand X4P A 403 (A)





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	29:THR	C	30:GLN	N	1.12

## 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	349/369 (94%)	1.15	56 (16%) <b>5</b> <b>5</b>	11, 27, 64, 115	11 (3%)
1	B	350/369 (94%)	1.22	52 (14%) <b>5</b> <b>6</b>	13, 27, 46, 80	10 (2%)
All	All	699/738 (94%)	1.19	108 (15%) <b>5</b> <b>5</b>	11, 27, 54, 115	21 (3%)

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	24	LEU	13.1
1	B	15	ALA	11.9
1	B	17	VAL	11.5
1	B	18	LEU	11.1
1	B	13	ALA	11.0
1	B	23	THR	10.7
1	A	14	LEU	10.7
1	B	25	PRO	10.4
1	B	19	LYS	9.9
1	B	16	ALA	9.9
1	B	14	LEU	9.6
1	B	22	SER	9.4
1	A	18	LEU	9.3
1	B	20	HIS	9.2
1	A	11	ALA	8.1
1	B	21	SER	8.1
1	B	28	SER	8.0
1	B	27	GLU	7.9
1	A	17	VAL	7.8
1	A	87	LEU	7.5
1	A	10	PRO	7.4
1	A	9	ALA	7.3
1	B	26	PRO	7.1
1	A	77	LEU	6.8

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Mol	Chain	Res	Type	RSRZ
1	B	29	THR	6.7
1	A	26	PRO	6.4
1	B	89	GLN	6.2
1	A	91	ARG	5.9
1	A	24	LEU	5.8
1	A	19	LYS	5.5
1	A	363	MET	5.5
1	A	16	ALA	5.4
1	A	15	ALA	5.4
1	A	275	CYS	5.3
1	A	20	HIS	5.3
1	A	361	ALA	5.2
1	A	12	GLY	5.1
1	A	13	ALA	4.8
1	B	250	TYR	4.8
1	A	310[A]	GLN	4.8
1	A	85	ALA	4.6
1	B	85	ALA	4.5
1	A	362	PHE	4.4
1	A	23	THR	4.3
1	B	309	ALA	4.3
1	A	84	HIS	4.2
1	A	274	LYS	4.1
1	B	310[A]	GLN	4.0
1	A	83	GLN	3.9
1	A	25	PRO	3.7
1	B	90	SER	3.7
1	B	192	MET	3.7
1	A	21	SER	3.7
1	A	312	PHE	3.7
1	B	94	LEU	3.5
1	B	241[A]	LEU	3.4
1	A	22	SER	3.4
1	B	93	PRO	3.4
1	A	307[A]	ASN	3.3
1	B	251	LYS	3.2
1	A	305	TYR	3.2
1	B	196	THR	3.2
1	B	363	MET	3.2
1	A	309	ALA	3.1
1	B	307[A]	ASN	3.1
1	A	74	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	87	LEU	2.8
1	B	91	ARG	2.7
1	A	195	ASN	2.7
1	B	361	ALA	2.7
1	A	76	PRO	2.7
1	B	88	THR	2.6
1	A	332	VAL	2.6
1	A	272	PHE	2.6
1	A	360	ASP	2.6
1	A	27	GLU	2.6
1	A	32	ARG	2.5
1	B	173	ASN	2.5
1	B	305	TYR	2.4
1	A	199	VAL	2.4
1	A	93	PRO	2.4
1	B	77	LEU	2.3
1	A	86[A]	ASP	2.3
1	B	84	HIS	2.3
1	A	28	SER	2.3
1	A	196	THR	2.3
1	B	174	GLU	2.3
1	A	254	GLY	2.3
1	B	43	ARG	2.2
1	A	200	LYS	2.2
1	B	345	LEU	2.2
1	B	71	GLU	2.2
1	A	271	ILE	2.1
1	B	171	VAL	2.1
1	B	74	LEU	2.1
1	B	153	LEU	2.1
1	A	191	VAL	2.1
1	A	285	VAL	2.1
1	A	88	THR	2.1
1	A	335	GLN	2.1
1	B	75	GLU	2.1
1	B	189	GLN	2.1
1	A	49[A]	PHE	2.1
1	B	186	ILE	2.1
1	B	143	LEU	2.0
1	B	183	LEU	2.0
1	A	247	PHE	2.0
1	B	47	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	0.91	0.14	34,35,49,88	0
1	CSS	A	177	7/8	0.94	0.09	25,28,40,51	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

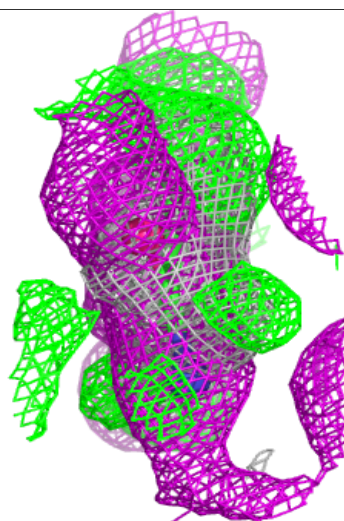
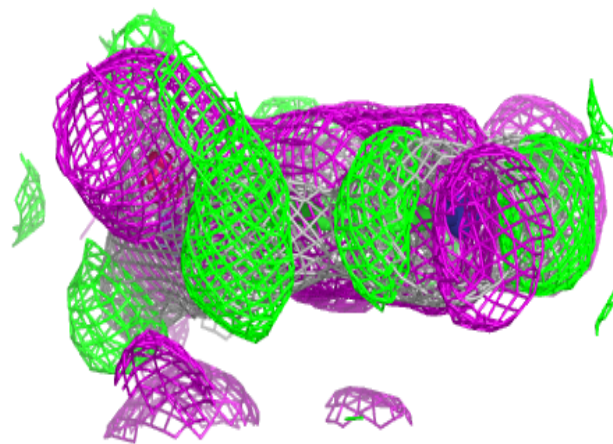
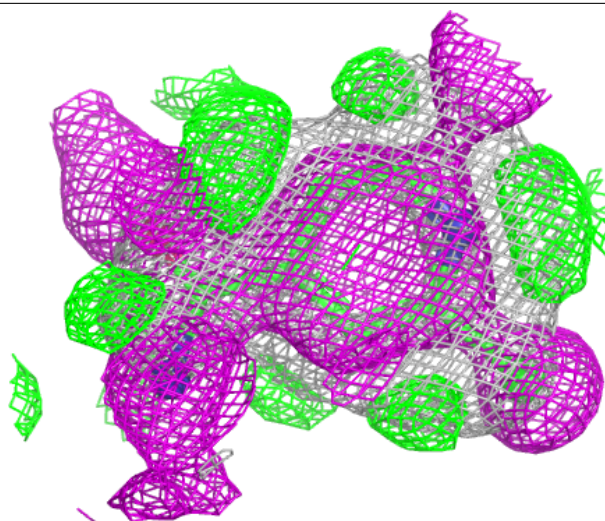
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	X4P	A	403[A]	10/10	0.55	0.21	20,20,20,20	10
3	X4P	A	403[B]	10/10	0.55	0.21	20,20,20,20	10
3	X4P	B	403	10/10	0.69	0.21	20,20,20,20	10
3	X4P	A	402	10/10	0.74	0.22	20,20,20,20	10
4	MRD	B	401	8/8	0.89	0.19	38,42,46,52	8
2	NAD	B	402	44/44	0.97	0.08	18,22,31,34	44
2	NAD	A	401	44/44	0.97	0.07	18,21,29,36	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.

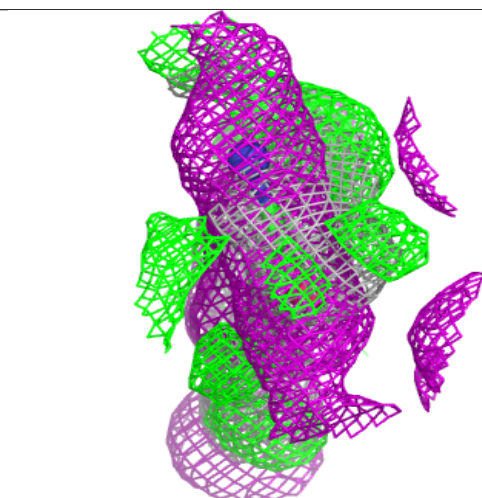
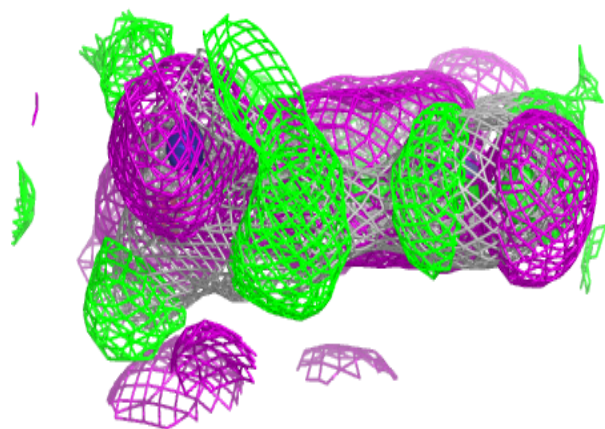
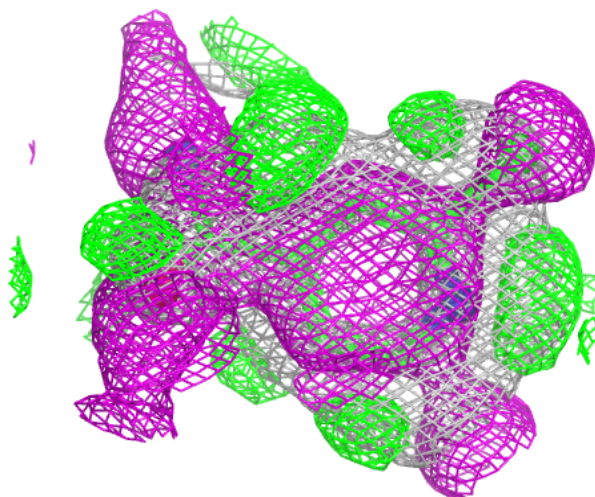
**Electron density around X4P A 403 (A):**

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



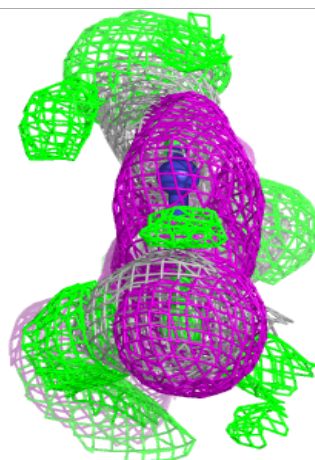
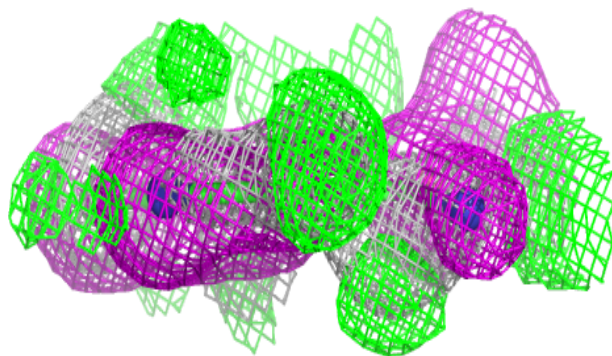
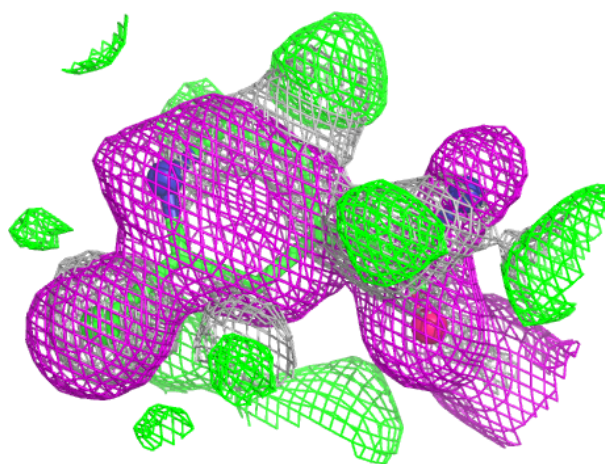
**Electron density around X4P A 403 (B):**

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



**Electron density around X4P B 403:**

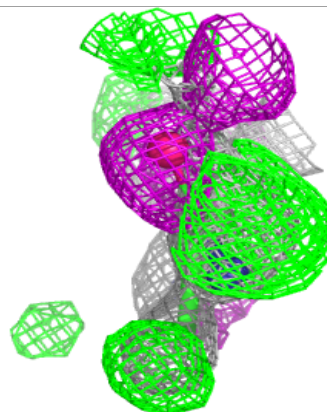
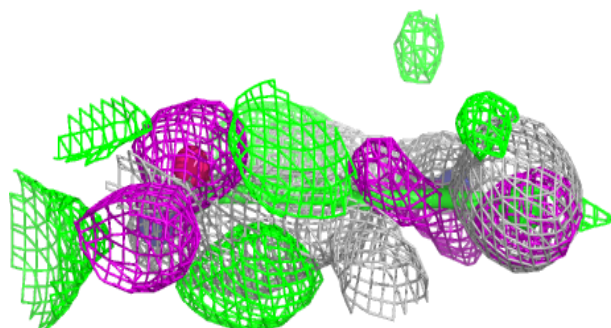
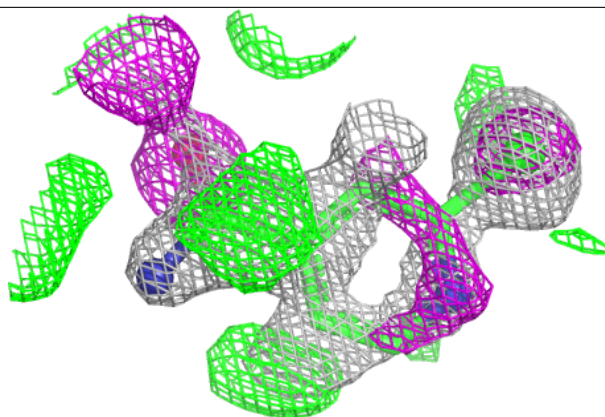
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



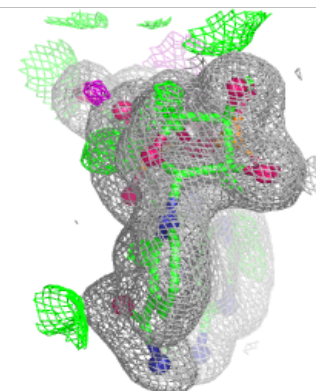
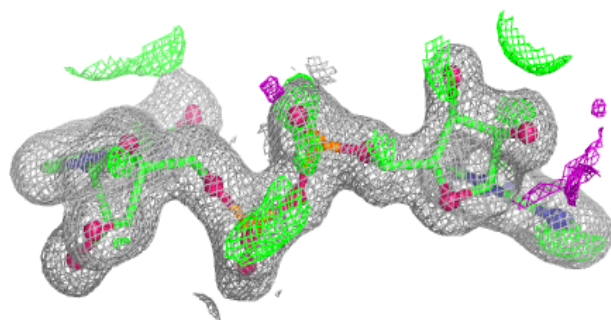
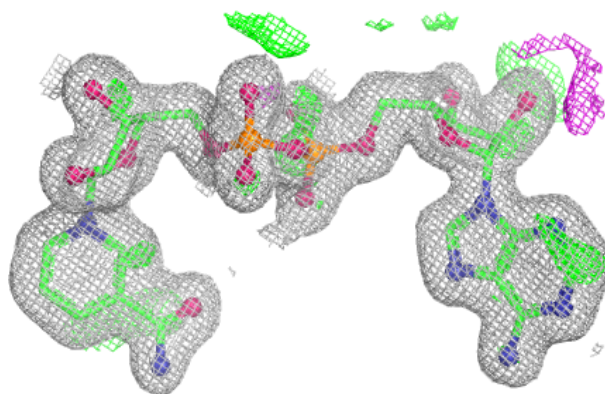


**Electron density around X4P A 402:**

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

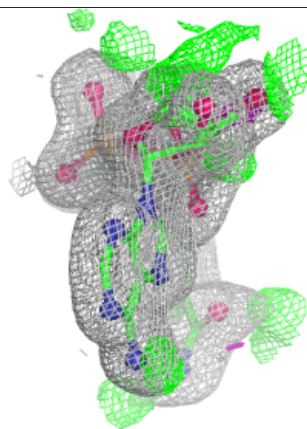
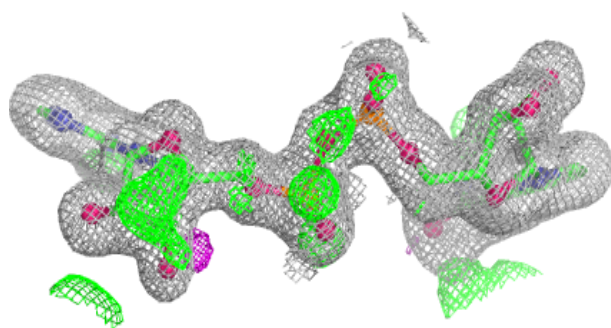
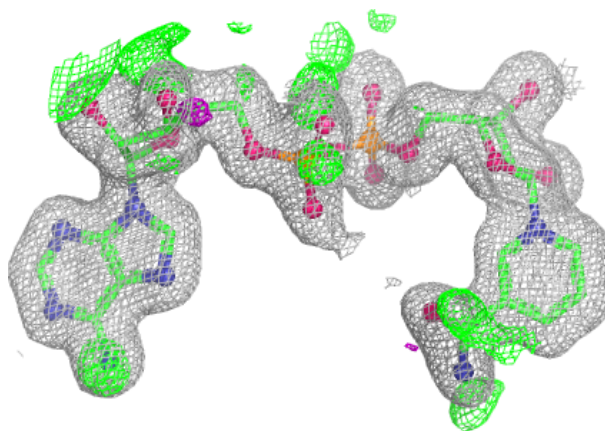
**Electron density around NAD B 402:**

$2mF_o-DF_c$  (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 ⓘ

There are no such residues in this entry.