



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2026 – 12:15 PM JST

PDB ID : 9V5Z / pdb\_00009v5z  
Title : PfDXR - Mn<sup>2+</sup> - SHOK314 - NADPH quaternary complex  
Authors : Takada, S.; Sakamoto, Y.; Tanaka, N.  
Deposited on : 2025-05-26  
Resolution : 1.58 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 : 1.8.5 (274361), CSD as541be (2020)  
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

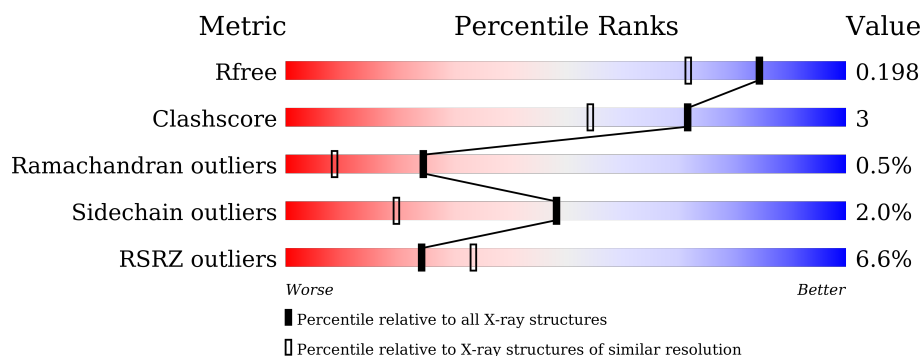
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.58 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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	488	<div> <div>8%</div> <div>77%</div> <div>6%</div> <div>16%</div> </div>
1	B	488	<div> <div>3%</div> <div>75%</div> <div>9%</div> <div>16%</div> </div>

## 2 Entry composition [i](#)

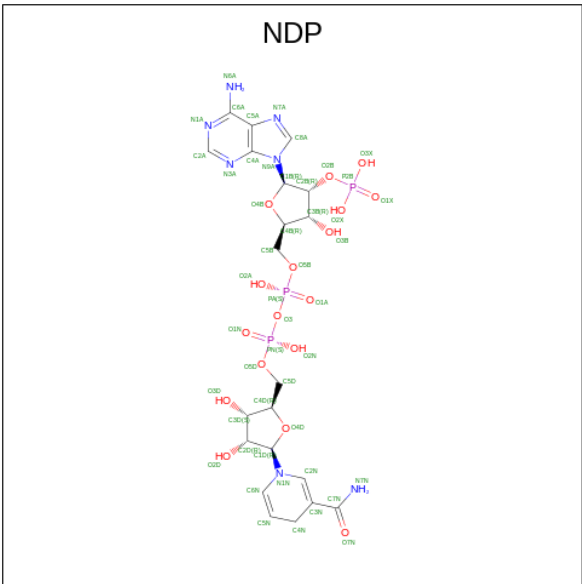
There are 6 unique types of molecules in this entry. The entry contains 7210 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1-deoxy-D-xylulose 5-phosphate reductoisomerase, apicoplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3285	2109	539	617	20			
1	B	411	Total	C	N	O	S	0	0	0
			3285	2109	539	617	20			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).

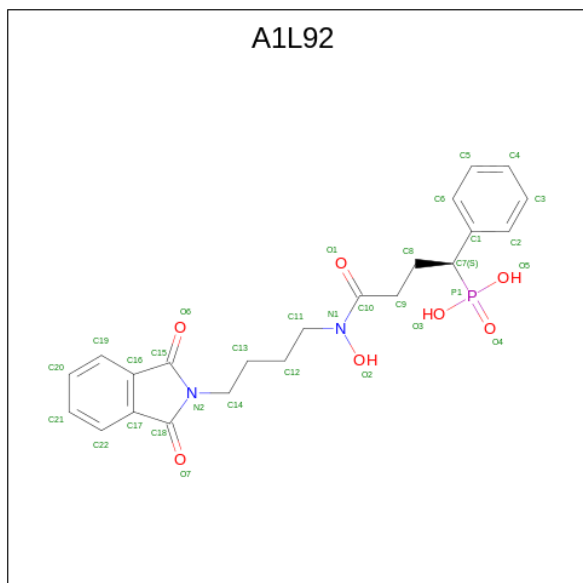


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		

- Molecule 4 is [(1 {S})-4-[4-[1,3-bis(oxidanylidene)isoindol-2-yl]butyl-oxidanyl-amino]-4-oxidanylidene-1-phenyl-butyl]phosphonic acid (CCD ID: A1L92) (formula: C<sub>22</sub>H<sub>25</sub>N<sub>2</sub>O<sub>7</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	22	2	7	1		
4	B	1	Total	C	N	O	P	0	0
			32	22	2	7	1		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total	Ca	0	0
			3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	217	Total	O	0	0
			217	217		

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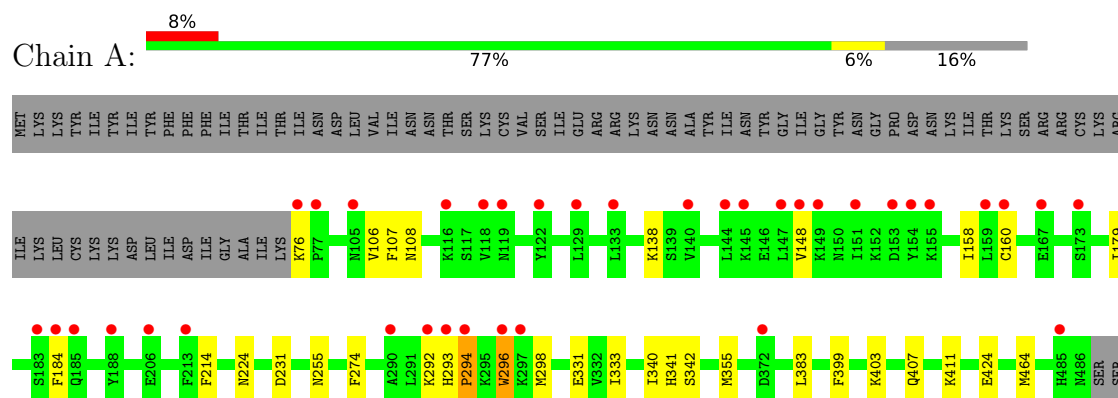
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	258	Total 258	O 258	0	0

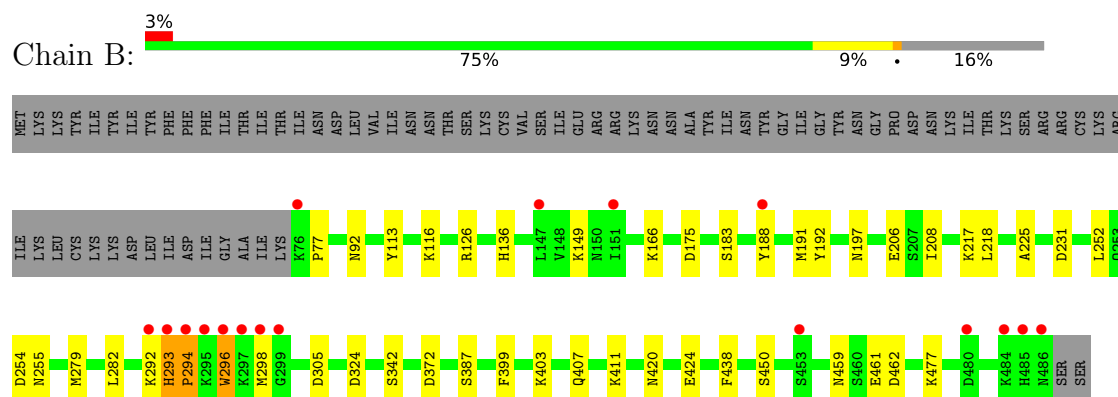
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase, apicoplactic



- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase, apicoplactic



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.58Å 76.88Å 111.15Å 90.00° 92.54° 90.00°	Depositor
Resolution (Å)	45.01 – 1.58 45.01 – 1.58	Depositor EDS
% Data completeness (in resolution range)	95.9 (45.01-1.58) 96.2 (45.01-1.58)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.163 , 0.186 0.177 , 0.198	Depositor DCC
$R_{free}$ test set	5807 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.3	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 39.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7210	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.92% 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: MN, NDP, CA, A1L92

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.68	0/3348	1.11	7/4521 (0.2%)
1	B	0.73	0/3348	1.14	8/4521 (0.2%)
All	All	0.71	0/6696	1.12	15/9042 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	PHE	CA-CB-CG	7.17	120.97	113.80
1	A	231	ASP	CB-CA-C	6.72	119.93	109.84
1	B	77	PRO	N-CA-CB	6.29	108.82	103.35
1	B	305	ASP	CA-CB-CG	6.19	118.79	112.60
1	B	324	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	424	GLU	N-CA-CB	5.60	118.28	109.94
1	B	231	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	399	PHE	CA-CB-CG	-5.54	108.26	113.80
1	B	399	PHE	CA-CB-CG	-5.41	108.39	113.80
1	A	298	MET	CG-SD-CE	-5.36	89.12	100.90
1	B	293	HIS	CA-CB-CG	5.25	119.05	113.80
1	B	282	LEU	N-CA-CB	-5.17	102.25	110.22
1	A	255	ASN	CA-CB-CG	-5.14	107.46	112.60
1	A	224	ASN	CA-CB-CG	-5.13	107.47	112.60
1	B	175	ASP	CA-CB-CG	5.08	117.68	112.60

There are no chirality outliers.

There are no planarity outliers.



## 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	3285	0	3334	19	0
1	B	3285	0	3334	26	0
2	A	48	0	26	0	0
2	B	48	0	26	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	32	0	0	0	0
4	B	32	0	0	0	0
5	B	3	0	0	0	0
6	A	217	0	0	5	0
6	B	258	0	0	11	0
All	All	7210	0	6720	45	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (45) 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:372:ASP:HB3	6:B:772:HOH:O	1.58	1.03
1:B:188:TYR:HB2	6:B:831:HOH:O	1.78	0.82
1:A:292:LYS:O	1:A:294:PRO:HD3	1.78	0.82
1:A:214:PHE:CE2	1:A:464:MET:HE3	2.16	0.80
1:B:459:ASN:ND2	1:B:462:ASP:OD2	2.21	0.73
1:B:459:ASN:HD21	1:B:462:ASP:CG	2.00	0.69
1:A:138:LYS:HD3	1:A:160:CYS:SG	2.32	0.69
1:B:217:LYS:HE3	6:B:644:HOH:O	1.94	0.67
1:A:214:PHE:CD2	1:A:464:MET:CE	2.81	0.64
1:B:191:MET:HE3	1:B:192:TYR:CE2	2.32	0.64
1:B:279:MET:HE1	1:B:438:PHE:CZ	2.33	0.64
1:A:106:VAL:HG23	1:A:107:PHE:CD2	2.37	0.59
1:B:166:LYS:HE2	1:B:192:TYR:CZ	2.40	0.57
1:A:214:PHE:CE2	1:A:464:MET:CE	2.88	0.55
1:B:372:ASP:CB	6:B:772:HOH:O	2.34	0.55
1:A:138:LYS:HA	1:A:160:CYS:SG	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASN:ND2	6:A:604:HOH:O	2.42	0.52
1:A:411:LYS:HE3	6:A:630:HOH:O	2.08	0.52
1:B:459:ASN:ND2	1:B:462:ASP:CG	2.67	0.51
1:B:113:TYR:OH	1:B:136:HIS:HD2	1.94	0.51
1:B:206:GLU:HG2	6:B:668:HOH:O	2.12	0.50
1:A:296:TRP:HA	1:A:296:TRP:CE3	2.48	0.48
1:B:403:LYS:HE3	1:B:407:GLN:NE2	2.29	0.48
1:A:331:GLU:OE2	1:A:333:ILE:HD11	2.14	0.47
1:B:296:TRP:CD1	6:B:608:HOH:O	2.67	0.47
1:A:331:GLU:CD	1:A:333:ILE:HD11	2.39	0.47
1:B:191:MET:HG3	1:B:218:LEU:HD11	1.97	0.46
1:B:217:LYS:CE	6:B:644:HOH:O	2.59	0.46
1:B:296:TRP:NE1	6:B:608:HOH:O	2.47	0.45
1:A:333:ILE:HD13	6:A:676:HOH:O	2.17	0.44
1:B:292:LYS:O	1:B:294:PRO:HD3	2.17	0.44
1:B:183:SER:O	6:B:602:HOH:O	2.21	0.43
1:A:340:ILE:HG12	1:A:355:MET:HG2	2.00	0.43
1:A:184:PHE:HA	6:A:768:HOH:O	2.19	0.42
1:B:197:ASN:HA	1:B:225:ALA:HB2	2.02	0.42
1:A:403:LYS:HE2	1:A:407:GLN:NE2	2.35	0.42
1:A:214:PHE:CZ	1:A:464:MET:HE3	2.55	0.42
1:A:148:VAL:HG11	1:A:158:ILE:HD11	2.02	0.41
1:B:149:LYS:HG3	6:B:613:HOH:O	2.20	0.41
1:B:403:LYS:NZ	6:B:610:HOH:O	2.48	0.40
1:B:450:SER:OG	1:B:477:LYS:HE2	2.21	0.40
1:B:420:ASN:O	1:B:424:GLU:HG3	2.21	0.40
1:A:341:HIS:HD2	6:A:786:HOH:O	2.03	0.40
1:B:126:ARG:HH11	1:B:126:ARG:HG3	1.86	0.40
1:B:254:ASP:O	1:B:255:ASN:HB2	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	409/488 (84%)	397 (97%)	10 (2%)	2 (0%)	24	9
1	B	409/488 (84%)	399 (98%)	8 (2%)	2 (0%)	24	9
All	All	818/976 (84%)	796 (97%)	18 (2%)	4 (0%)	24	9

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	294	PRO
1	B	342	SER
1	A	342	SER
1	A	294	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	378/449 (84%)	373 (99%)	5 (1%)	61	37
1	B	378/449 (84%)	368 (97%)	10 (3%)	40	11
All	All	756/898 (84%)	741 (98%)	15 (2%)	48	20

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	LYS
1	A	179	ILE
1	A	293	HIS
1	A	296	TRP
1	A	383	LEU
1	B	92	ASN
1	B	116	LYS
1	B	208	ILE
1	B	252	LEU
1	B	293	HIS
1	B	296	TRP
1	B	298	MET

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Mol	Chain	Res	Type
1	B	387	SER
1	B	411	LYS
1	B	461	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	108	ASN
1	A	136	HIS
1	A	260	ASN
1	A	284	ASN
1	A	293	HIS
1	A	341	HIS
1	A	407	GLN
1	A	428	ASN
1	B	105	ASN
1	B	119	ASN
1	B	136	HIS
1	B	172	ASN
1	B	276	ASN
1	B	284	ASN
1	B	328	ASN
1	B	407	GLN
1	B	452	ASN
1	B	459	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	A1L92	B	503	3	33,34,34	2.55	10 (30%)	39,48,48	2.08	14 (35%)
4	A1L92	A	503	3	33,34,34	2.37	9 (27%)	39,48,48	2.56	14 (35%)
2	NDP	A	501	-	49,52,52	0.67	1 (2%)	66,80,80	0.81	3 (4%)
2	NDP	B	501	-	49,52,52	1.07	4 (8%)	66,80,80	1.13	5 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1L92	B	503	3	-	1/26/42/42	0/3/3/3
4	A1L92	A	503	3	-	2/26/42/42	0/3/3/3
2	NDP	A	501	-	-	4/34/77/77	0/5/5/5
2	NDP	B	501	-	-	3/34/77/77	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	A1L92	O2-N1	5.67	1.44	1.40
4	B	503	A1L92	C18-N2	-5.63	1.32	1.39
4	B	503	A1L92	O2-N1	5.60	1.44	1.40
4	A	503	A1L92	O7-C18	5.42	1.33	1.22
4	B	503	A1L92	P1-O5	-5.34	1.46	1.54
4	A	503	A1L92	O6-C15	4.99	1.32	1.22
4	B	503	A1L92	P1-C7	4.97	1.88	1.82
4	B	503	A1L92	C15-N2	-4.58	1.34	1.39
4	B	503	A1L92	O6-C15	4.51	1.31	1.22
4	A	503	A1L92	C15-N2	-4.35	1.34	1.39
4	A	503	A1L92	P1-O4	4.34	1.56	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NDP	P2B-O2B	4.31	1.67	1.59
4	B	503	A1L92	O7-C18	4.25	1.30	1.22
4	A	503	A1L92	P1-O3	-4.24	1.48	1.54
4	A	503	A1L92	P1-C7	3.90	1.87	1.82
4	A	503	A1L92	C18-N2	-3.16	1.35	1.39
4	A	503	A1L92	C9-C10	2.95	1.57	1.51
4	B	503	A1L92	C10-N1	2.94	1.38	1.34
2	A	501	NDP	P2B-O2B	2.78	1.64	1.59
4	B	503	A1L92	O1-C10	2.60	1.28	1.23
2	B	501	NDP	P2B-O3X	-2.39	1.45	1.54
2	B	501	NDP	PN-O2N	-2.31	1.44	1.55
2	B	501	NDP	P2B-O2X	-2.21	1.46	1.54
4	B	503	A1L92	C1-C7	2.10	1.55	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	A1L92	C16-C15-N2	6.41	110.43	105.88
4	A	503	A1L92	C17-C18-N2	5.77	109.98	105.88
4	A	503	A1L92	O6-C15-N2	5.39	130.07	124.81
4	B	503	A1L92	C17-C18-N2	5.33	109.66	105.88
4	A	503	A1L92	C18-N2-C15	-4.85	108.08	112.03
4	A	503	A1L92	O6-C15-C16	-4.72	119.50	128.68
4	B	503	A1L92	C14-N2-C18	4.68	128.59	123.88
4	B	503	A1L92	C16-C15-N2	3.97	108.70	105.88
4	A	503	A1L92	C14-N2-C15	3.86	127.77	123.88
2	B	501	NDP	O3X-P2B-O2X	3.49	120.98	107.64
4	B	503	A1L92	C16-C17-C18	-3.47	105.25	108.26
4	A	503	A1L92	O7-C18-C17	-3.37	122.12	128.68
4	A	503	A1L92	C16-C17-C18	-3.22	105.47	108.26
4	A	503	A1L92	O7-C18-N2	3.16	127.89	124.81
4	B	503	A1L92	O6-C15-N2	2.87	127.61	124.81
4	B	503	A1L92	O6-C15-C16	-2.82	123.19	128.68
2	B	501	NDP	C3B-C2B-C1B	-2.77	97.68	102.89
2	B	501	NDP	O2N-PN-O1N	2.74	125.79	112.24
2	B	501	NDP	C3N-C7N-N7N	2.66	122.40	117.67
2	B	501	NDP	PN-O3-PA	-2.62	123.84	132.83
4	A	503	A1L92	C17-C16-C15	-2.62	105.99	108.26
4	B	503	A1L92	C14-N2-C15	-2.61	121.25	123.88
4	A	503	A1L92	O4-P1-C7	-2.57	106.16	113.35
4	B	503	A1L92	C17-C16-C15	-2.55	106.05	108.26
4	A	503	A1L92	C22-C17-C18	2.55	133.78	129.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NDP	O2N-PN-O1N	2.53	124.74	112.24
4	B	503	A1L92	C19-C16-C15	2.53	133.75	129.63
4	A	503	A1L92	C3-C4-C5	2.49	124.56	119.93
4	B	503	A1L92	C18-N2-C15	-2.31	110.14	112.03
4	B	503	A1L92	C2-C1-C7	-2.31	117.10	120.82
4	B	503	A1L92	C2-C1-C6	2.31	121.17	118.29
4	A	503	A1L92	C2-C1-C6	2.30	121.16	118.29
2	A	501	NDP	O3X-P2B-O2X	2.26	116.29	107.64
2	A	501	NDP	C3B-C2B-C1B	-2.08	98.97	102.89
4	B	503	A1L92	O3-P1-O5	2.04	113.13	107.64
4	B	503	A1L92	O2-N1-C11	2.03	118.67	113.59

There are no chirality outliers.

All (10) torsion outliers are listed below:

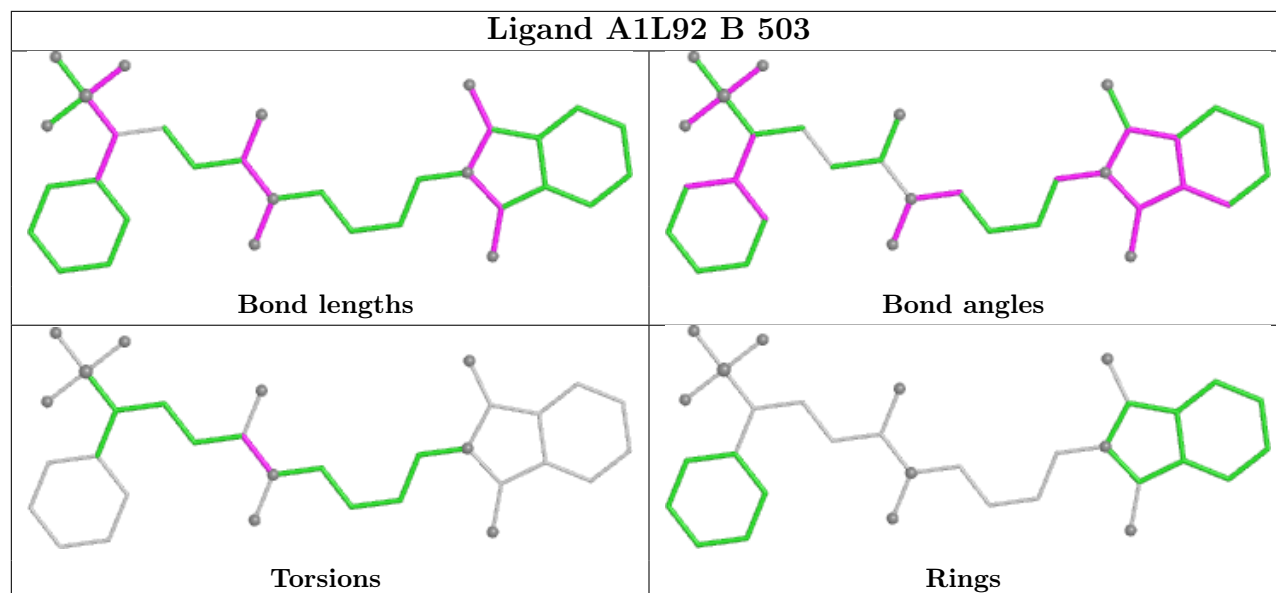
Mol	Chain	Res	Type	Atoms
2	A	501	NDP	O4D-C1D-N1N-C6N
2	B	501	NDP	O4D-C1D-N1N-C6N
2	B	501	NDP	O4B-C4B-C5B-O5B
2	A	501	NDP	PN-O3-PA-O1A
2	B	501	NDP	PN-O3-PA-O1A
2	A	501	NDP	C1B-C2B-O2B-P2B
4	A	503	A1L92	C12-C11-N1-O2
4	A	503	A1L92	O1-C10-N1-O2
4	B	503	A1L92	O1-C10-N1-O2
2	A	501	NDP	O4B-C4B-C5B-O5B

There are no ring outliers.

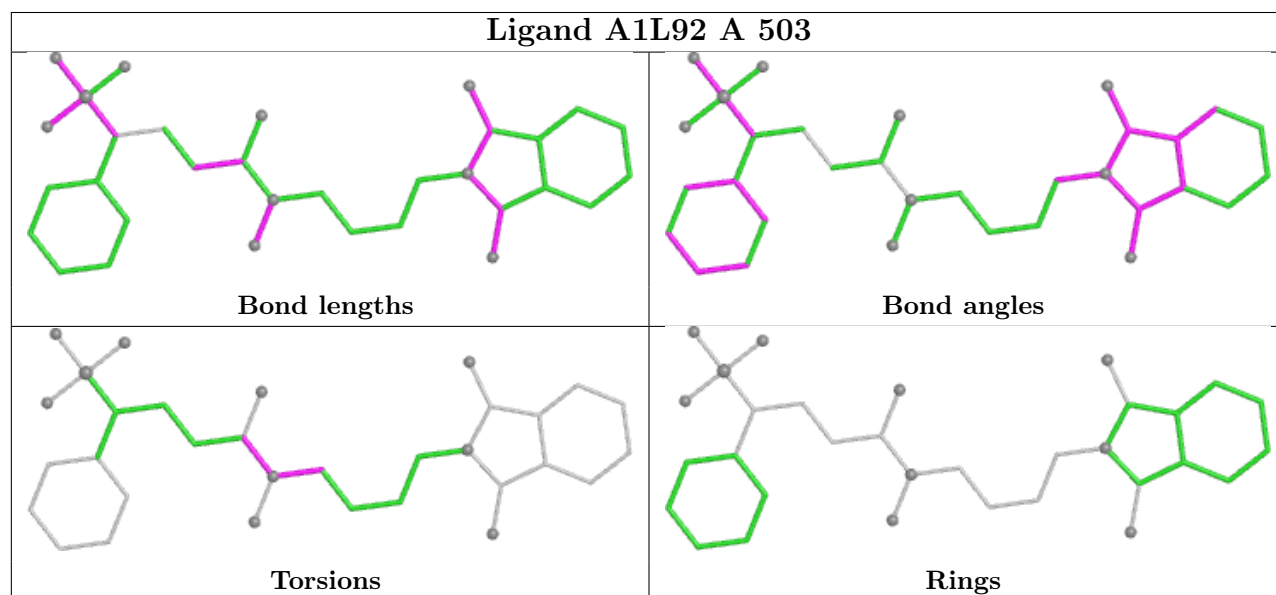
No monomer is involved in short contacts.

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.

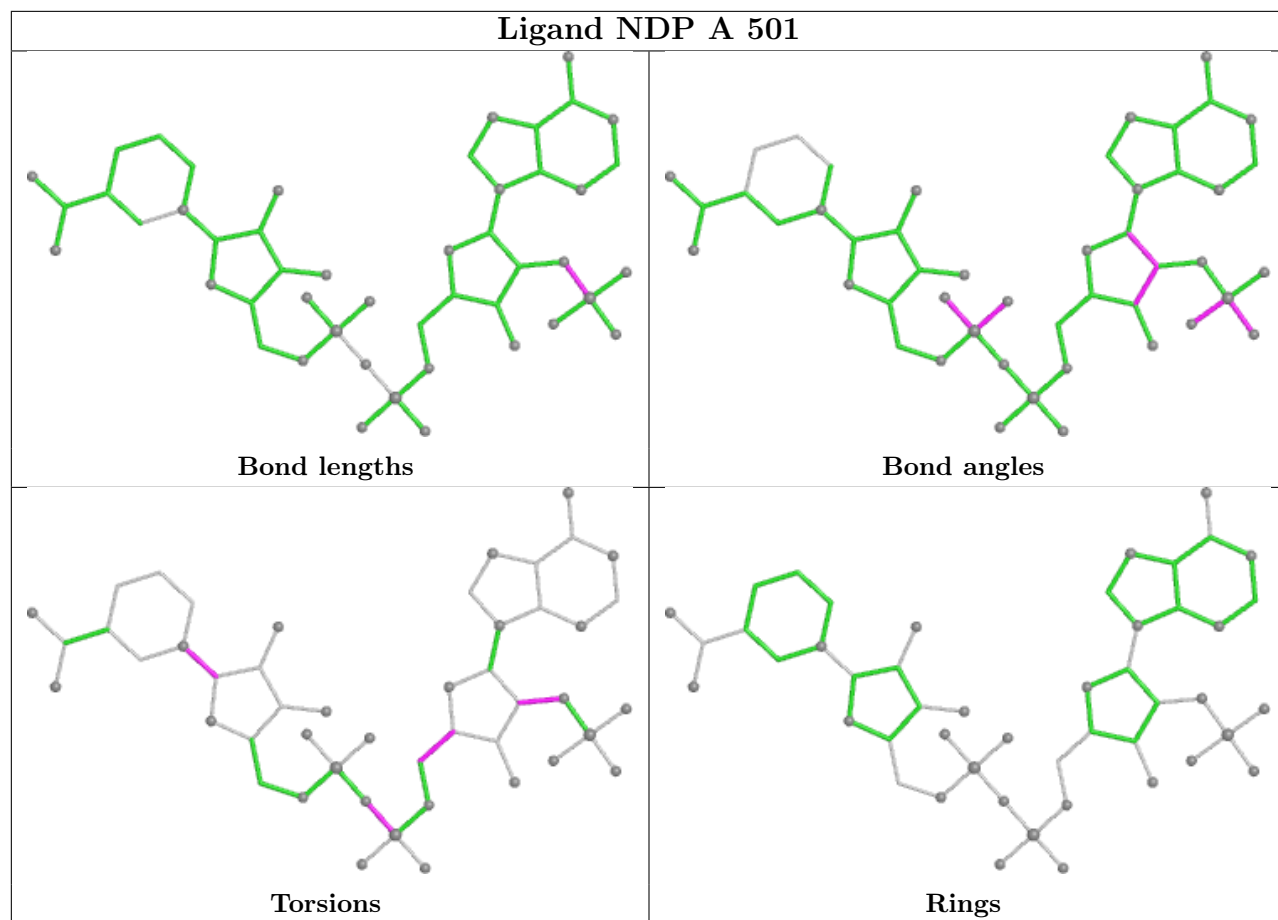
## Ligand A1L92 B 503

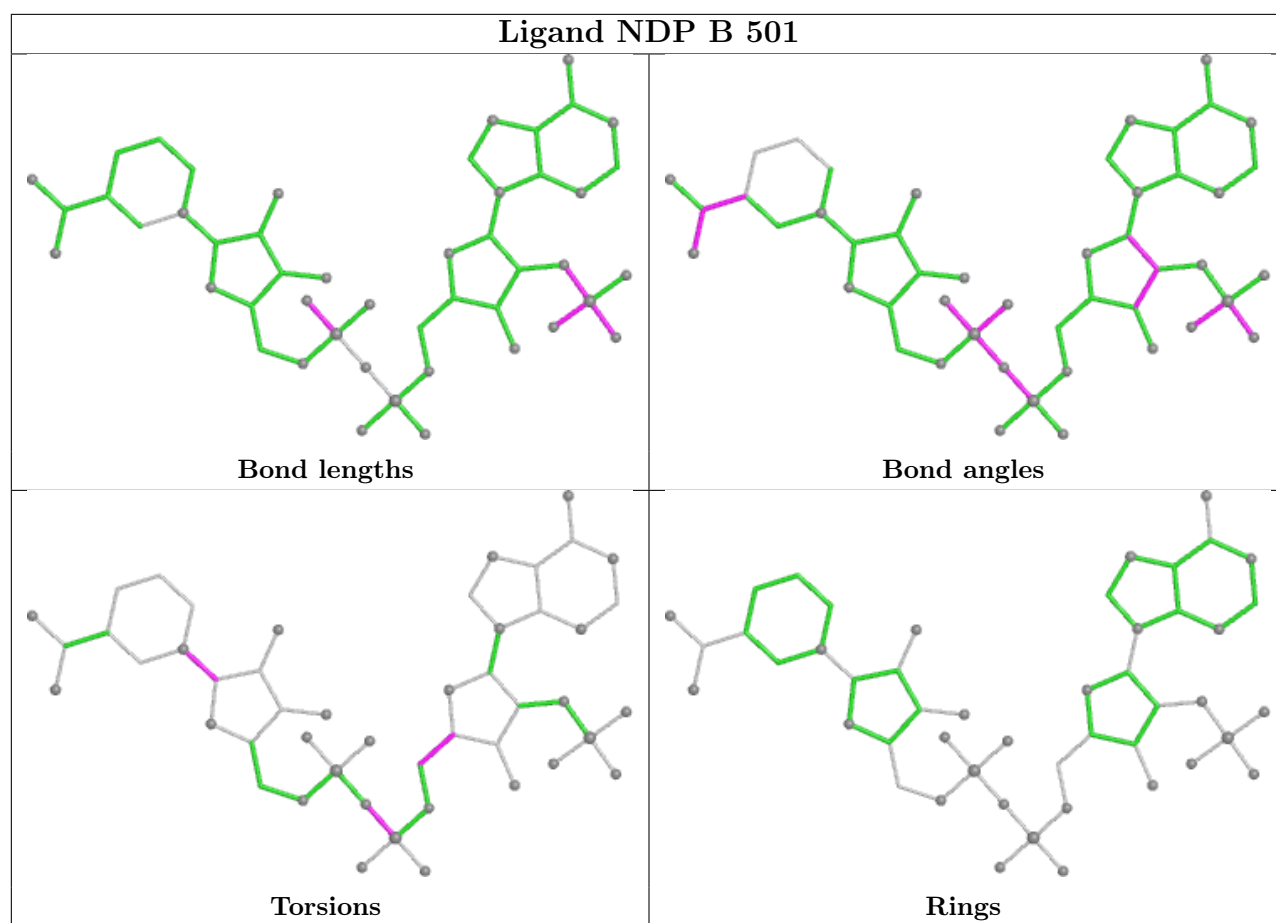


## Ligand A1L92 A 503









## 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	411/488 (84%)	0.44	37 (9%) 15 23	13, 24, 55, 90	0
1	B	411/488 (84%)	0.23	17 (4%) 41 53	12, 21, 43, 120	0
All	All	822/976 (84%)	0.33	54 (6%) 24 33	12, 22, 52, 120	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	294	PRO	7.8
1	B	296	TRP	6.8
1	A	296	TRP	5.3
1	B	292	LYS	4.8
1	A	184	PHE	4.6
1	B	293	HIS	4.6
1	B	299	GLY	4.5
1	A	294	PRO	4.5
1	B	297	LYS	4.3
1	B	295	LYS	3.9
1	A	293	HIS	3.9
1	A	183	SER	3.9
1	A	290	ALA	3.7
1	A	140	VAL	3.6
1	A	147	LEU	3.5
1	A	77	PRO	3.4
1	B	298	MET	3.4
1	A	292	LYS	3.2
1	A	188	TYR	3.2
1	B	486	ASN	3.1
1	A	213	PHE	3.1
1	B	485	HIS	3.0
1	B	76	LYS	3.0
1	A	149	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	154	TYR	2.9
1	A	151	ILE	2.9
1	A	76	LYS	2.7
1	A	372	ASP	2.7
1	B	484	LYS	2.6
1	A	153	ASP	2.6
1	A	185	GLN	2.6
1	B	188	TYR	2.6
1	A	144	LEU	2.5
1	B	151	ILE	2.4
1	A	118	VAL	2.4
1	A	122	TYR	2.4
1	A	119	ASN	2.4
1	A	297	LYS	2.3
1	A	167	GLU	2.3
1	A	133	LEU	2.3
1	A	485	HIS	2.2
1	A	155	LYS	2.2
1	B	453	SER	2.2
1	A	159	LEU	2.2
1	B	147	LEU	2.2
1	A	148	VAL	2.2
1	A	160	CYS	2.1
1	A	173	SER	2.1
1	A	129	LEU	2.1
1	A	105	ASN	2.1
1	B	480	ASP	2.1
1	A	145	LYS	2.1
1	A	206	GLU	2.1
1	A	116	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

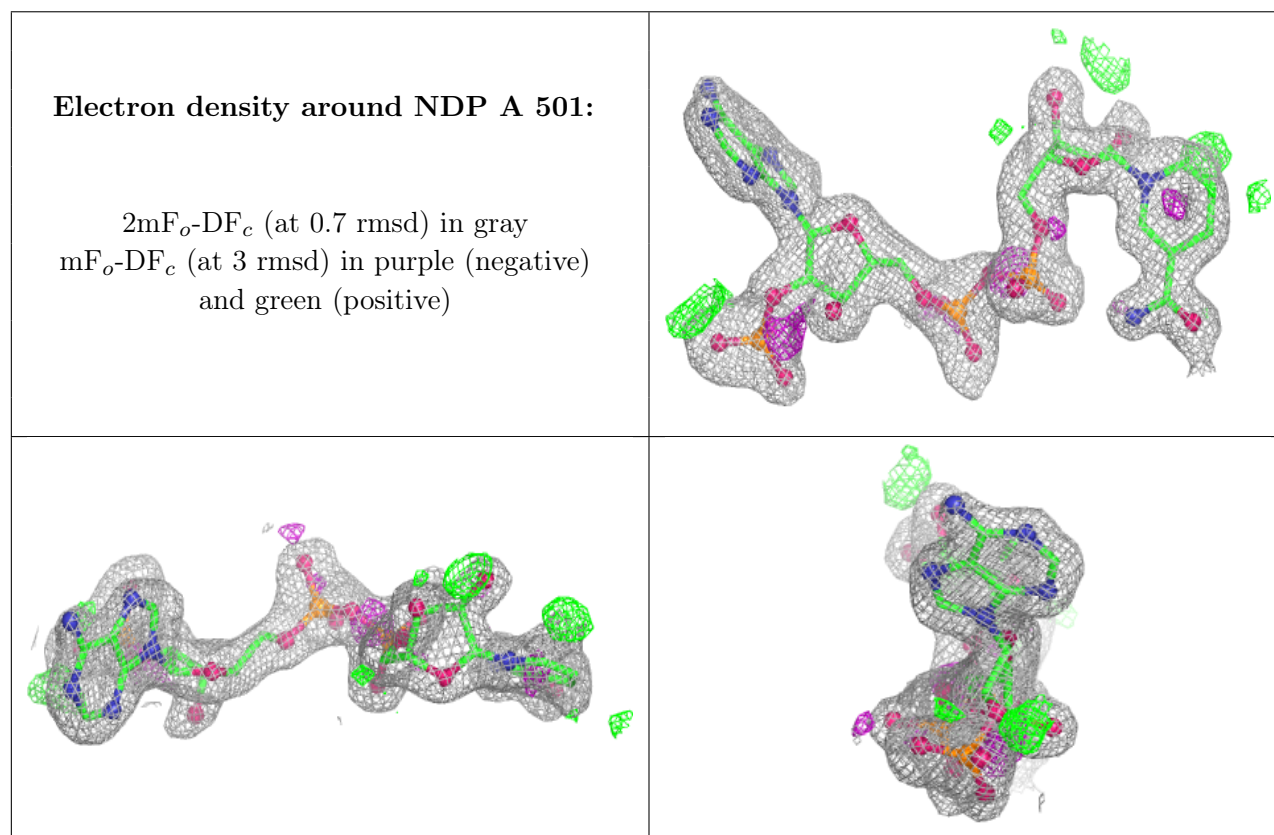
There are no oligosaccharides in this entry.

## 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.

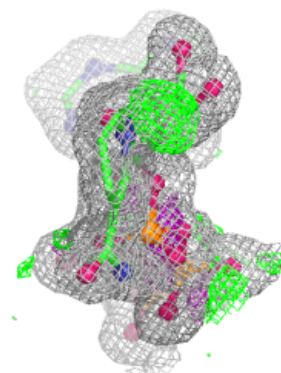
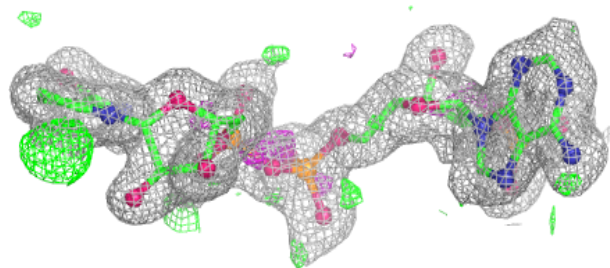
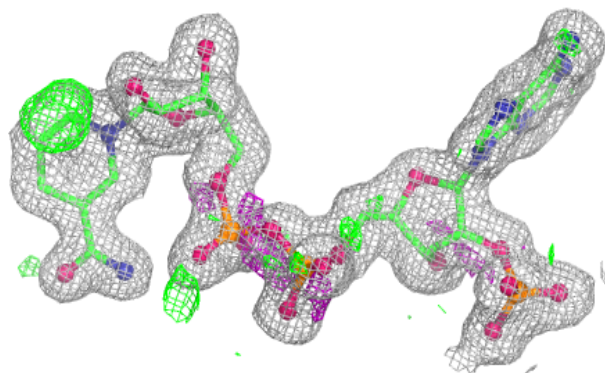
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NDP	A	501	48/48	0.93	0.09	27,31,37,42	0
2	NDP	B	501	48/48	0.96	0.06	16,19,22,23	0
4	A1L92	A	503	32/32	0.97	0.06	17,23,31,34	0
5	CA	B	505	1/1	0.97	0.07	23,23,23,23	0
4	A1L92	B	503	32/32	0.98	0.05	13,18,25,26	0
5	CA	B	506	1/1	0.98	0.10	23,23,23,23	0
5	CA	B	504	1/1	0.99	0.06	15,15,15,15	0
3	MN	A	502	1/1	0.99	0.02	15,15,15,15	0
3	MN	B	502	1/1	0.99	0.04	12,12,12,12	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.

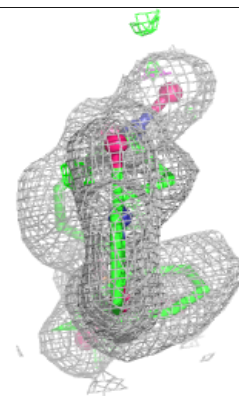
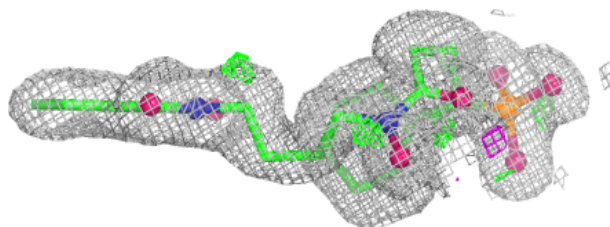
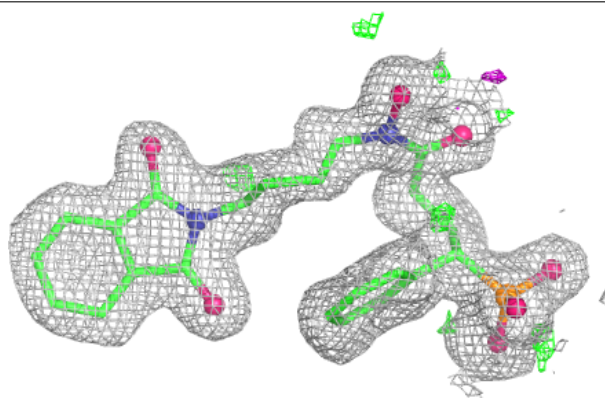


**Electron density around NDP B 501:**

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

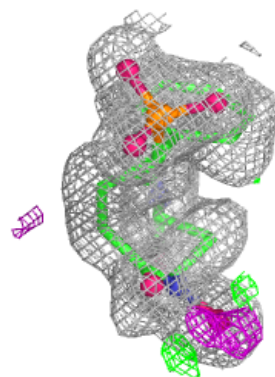
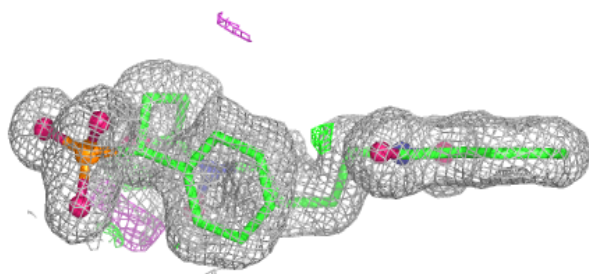
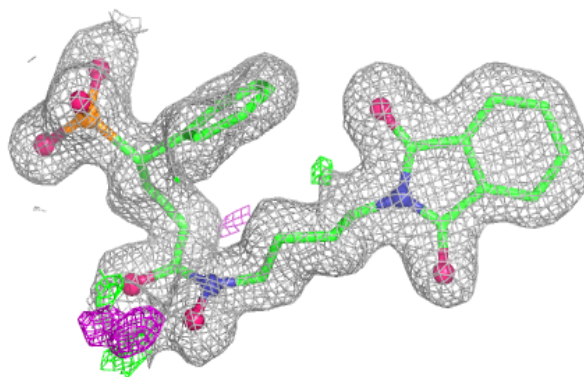
**Electron density around A1L92 A 503:**

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



**Electron density around A1L92 B 503:**

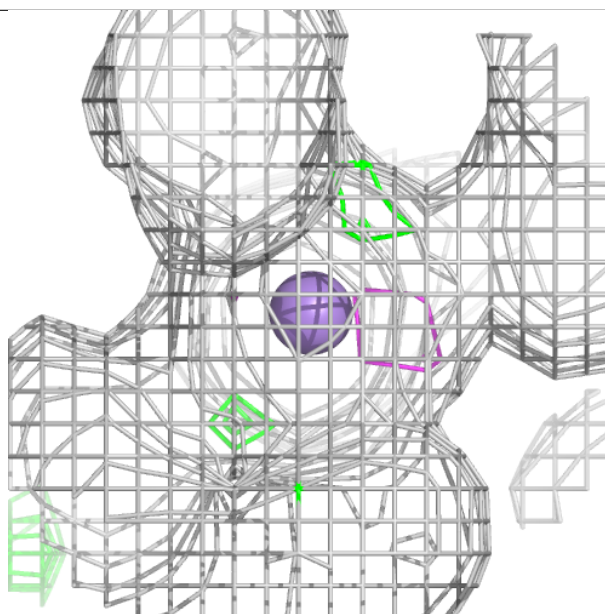
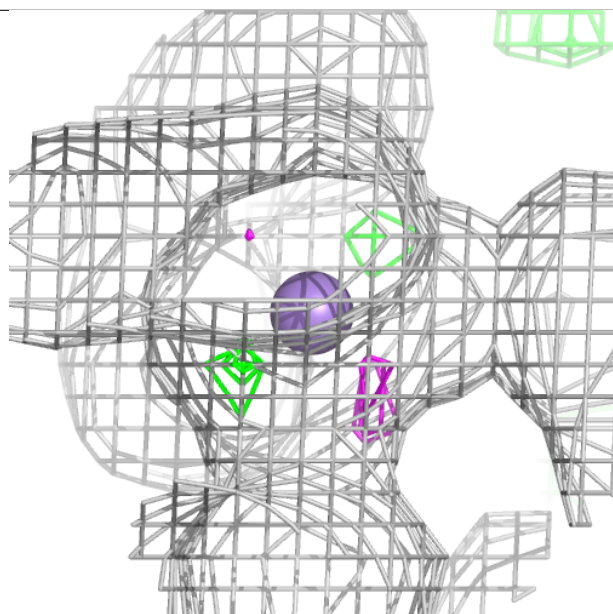
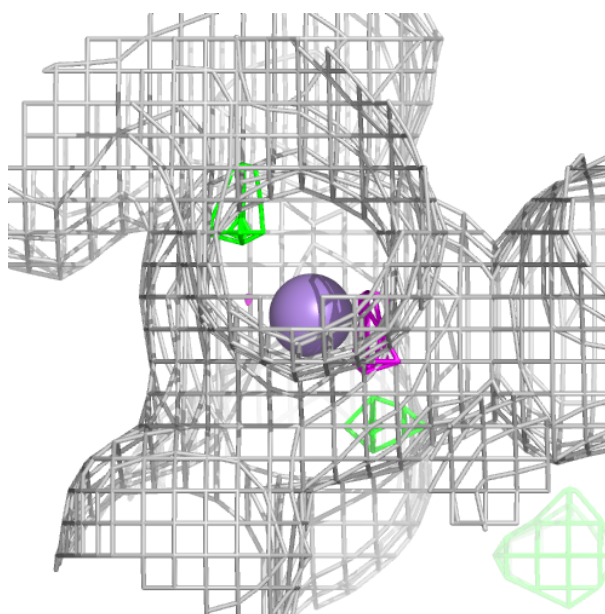
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MN A 502:**

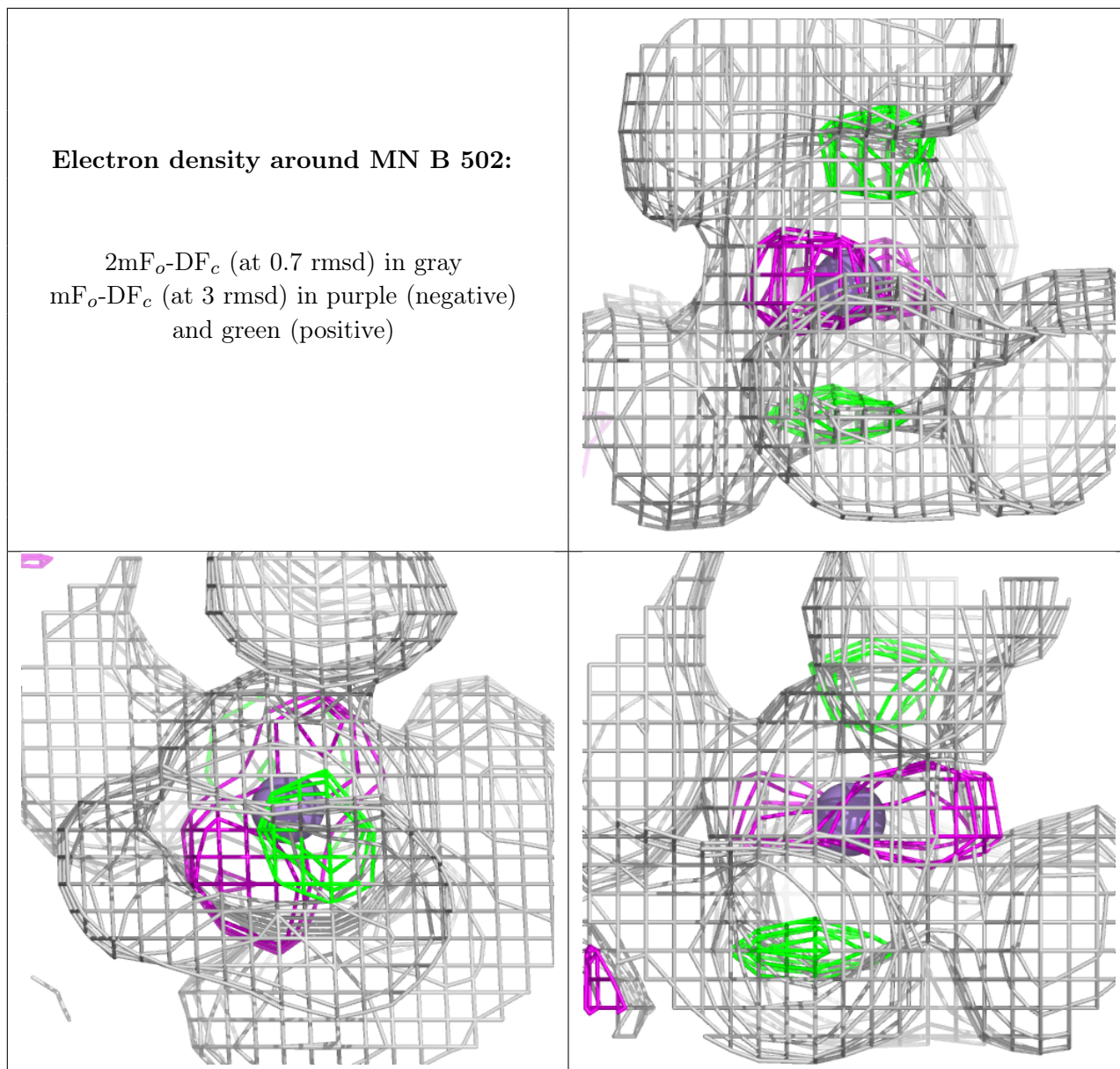
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MN B 502:**

$2mF_o-DF_c$  (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.