



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:18 AM UTC

PDB ID : 9JZA / pdb_00009jza
Title : PfDXR - Mn²⁺ - NADPH - MAMK218 quaternary complex
Authors : Takada, S.; Sakamoto, Y.; Tanaka, N.
Deposited on : 2024-10-14
Resolution : 1.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

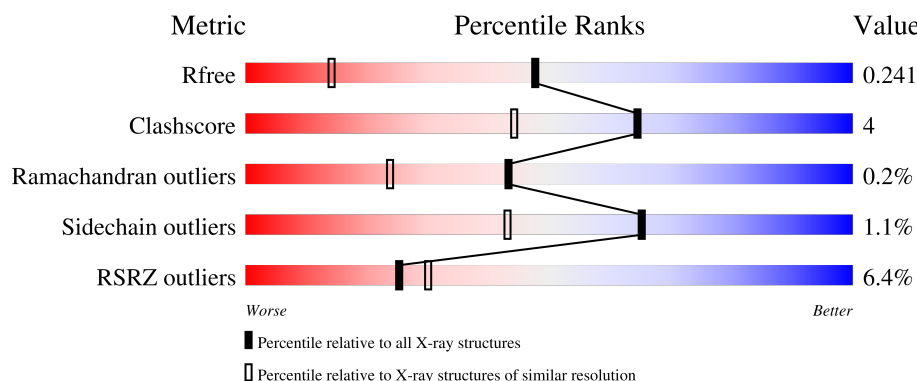
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	488	6% 75% 7% 17%
1	B	488	5% 72% 11% 17%

2 Entry composition [i](#)

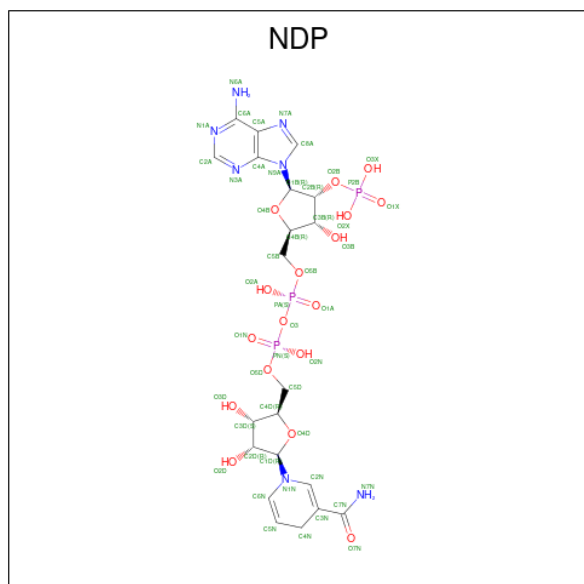
There are 6 unique types of molecules in this entry. The entry contains 7078 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	406	Total	C	N	O	S	0	1	0
			3244	2079	530	615	20			
1	B	406	Total	C	N	O	S	0	1	0
			3244	2079	530	615	20			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).

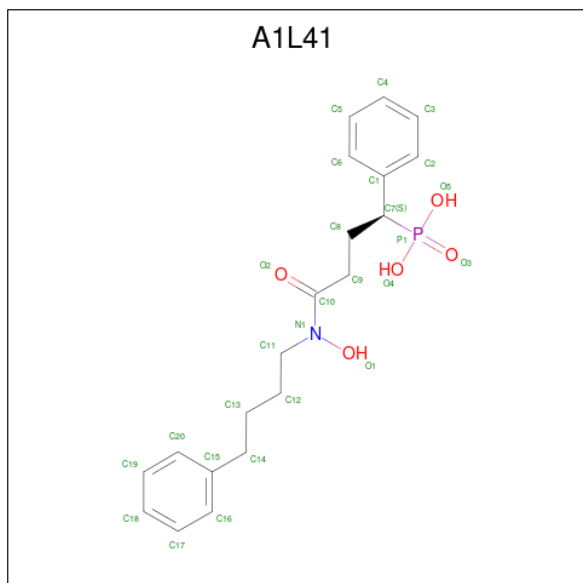


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- 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 1 1	0	0
3	B	1	Total Mn 1 1	0	0

- Molecule 4 is [(1 {S})-4-oxidanylidene-4-[oxidanyl(4-phenylbutyl)amino]-1-phenyl-butyl]p
hosphonic acid (CCD ID: A1L41) (formula: C₂₀H₂₆NO₅P) (labeled as "Ligand of Interest"
by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 37 30 1 5 1	0	1
4	B	1	Total C N O P 37 30 1 5 1	0	1

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	181	Total O 181 181	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	234	Total 234	O 234	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.54Å 77.51Å 111.27Å 90.00° 92.38° 90.00°	Depositor
Resolution (Å)	42.89 – 1.55 42.89 – 1.55	Depositor EDS
% Data completeness (in resolution range)	97.3 (42.89-1.55) 97.3 (42.89-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.189 , 0.211 (Not available) , 0.241	Depositor DCC
R_{free} test set	6391 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7078	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, MN, CA, A1L41

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	0.70	0/3302	1.17	9/4457 (0.2%)
1	B	0.74	0/3302	1.21	9/4457 (0.2%)
All	All	0.72	0/6604	1.19	18/8914 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	279	MET	CG-SD-CE	-9.08	80.92	100.90
1	A	399	PHE	CA-CB-CG	-8.21	105.59	113.80
1	B	305	ASP	CA-CB-CG	7.64	120.24	112.60
1	B	234	HIS	CA-CB-CG	-6.32	107.48	113.80
1	A	116	LYS	CB-CA-C	-6.25	99.38	109.13
1	B	348	ASP	CA-CB-CG	6.23	118.83	112.60
1	B	231	ASP	CB-CA-C	5.86	119.14	109.70
1	A	231	ASP	CB-CA-C	5.86	118.63	109.84
1	B	265	ILE	CA-C-O	-5.81	114.29	120.39
1	B	137	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	273	PRO	N-CA-CB	-5.61	98.25	103.46
1	A	420	ASN	CA-CB-CG	-5.56	107.04	112.60
1	B	392	HIS	CA-CB-CG	5.48	119.28	113.80
1	A	286	THR	CA-CB-OG1	-5.25	101.72	109.60
1	A	264	LYS	CA-CB-CG	5.22	124.55	114.10
1	A	195	MET	CG-SD-CE	5.17	112.27	100.90
1	A	371	PRO	N-CA-CB	-5.08	97.01	102.60
1	B	399	PHE	CA-CB-CG	-5.08	108.72	113.80

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	3244	0	3286	18	0
1	B	3244	0	3286	34	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	37	0	0	1	0
4	B	37	0	0	4	0
5	B	3	0	0	0	0
6	A	181	0	0	1	0
6	B	234	0	0	11	0
All	All	7078	0	6624	52	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 4.

All (52) 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:355:MET:HE2	6:B:769:HOH:O	1.76	0.84
1:A:106:VAL:HG23	1:A:107:PHE:CD2	2.27	0.70
1:B:108:ASN:HB3	6:B:801:HOH:O	1.96	0.65
1:B:359[B]:ASP:H	4:B:503[B]:A1L41:C19	2.12	0.62
1:B:279:MET:HE1	1:B:397:GLU:HG2	1.82	0.60
4:A:503[B]:A1L41:C12	4:A:503[B]:A1L41:C20	2.76	0.60
1:B:355:MET:CE	6:B:769:HOH:O	2.39	0.59
1:B:449:GLU:HG2	6:B:746:HOH:O	2.02	0.59
1:A:227:ILE:HD12	1:A:252:LEU:HD13	1.85	0.59
1:B:359[B]:ASP:H	4:B:503[B]:A1L41:C20	2.16	0.59
1:B:310:MET:HE1	1:B:419:LEU:HD11	1.85	0.58
1:A:191:MET:CE	1:A:464:MET:HE3	2.36	0.56
1:B:459:ASN:HD21	1:B:462:ASP:CG	2.14	0.55
1:A:191:MET:HE2	1:A:464:MET:HE3	1.87	0.55
1:B:258:LYS:HE2	6:B:815:HOH:O	2.07	0.55
1:B:359[B]:ASP:N	4:B:503[B]:A1L41:C20	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:LYS:N	1:B:77:PRO:CD	2.73	0.51
1:A:292:LYS:HA	1:A:292:LYS:HE2	1.94	0.50
1:B:254:ASP:O	6:B:601:HOH:O	2.20	0.49
1:A:146:GLU:HG3	1:A:147:LEU:N	2.28	0.48
1:A:217:LYS:HA	1:A:217:LYS:HE2	1.95	0.48
1:B:254:ASP:O	1:B:255:ASN:HB2	2.13	0.47
1:B:403:LYS:HE3	1:B:407:GLN:NE2	2.31	0.46
1:B:480:ASP:HB2	6:B:768:HOH:O	2.15	0.46
1:A:143:GLU:HA	1:A:146:GLU:HG2	1.98	0.46
1:A:358:PRO:O	1:A:359[B]:ASP:HB2	2.16	0.46
1:B:261:ASN:ND2	6:B:602:HOH:O	2.36	0.46
1:A:298:MET:HE3	1:A:302:ILE:HG23	1.98	0.45
1:B:411:LYS:HE3	1:B:415:TYR:CE2	2.52	0.45
1:A:138:LYS:HD3	1:A:160:CYS:SG	2.58	0.44
1:A:144:LEU:O	1:A:148:VAL:HG23	2.18	0.44
1:A:214:PHE:CE2	1:A:464:MET:CE	3.01	0.44
1:B:114:VAL:HG22	1:B:121:LEU:HD22	1.99	0.44
1:A:333:ILE:HD11	1:B:384:ALA:HB2	1.99	0.44
1:B:358:PRO:HA	4:B:503[B]:A1L41:C16	2.47	0.44
1:B:76:LYS:N	1:B:77:PRO:HD2	2.33	0.43
1:B:191:MET:HG3	1:B:218:LEU:HD11	2.00	0.43
1:B:393:LYS:HG2	6:B:636:HOH:O	2.18	0.43
1:B:449:GLU:CG	6:B:746:HOH:O	2.63	0.42
1:A:338:CYS:O	1:A:341:HIS:HE1	2.03	0.42
1:B:230:VAL:O	1:B:231:ASP:C	2.61	0.42
1:A:359[B]:ASP:OD1	6:A:601:HOH:O	2.22	0.42
1:A:430:PHE:CG	1:A:440:ILE:HD11	2.55	0.42
1:B:119:ASN:ND2	1:B:147:LEU:HD11	2.35	0.41
1:A:269:SER:HB2	1:A:312:LYS:HE3	2.02	0.41
1:B:129:LEU:N	1:B:130:PRO:CD	2.84	0.41
1:B:79:ASN:OD1	1:B:108:ASN:HB2	2.21	0.41
1:B:274:PHE:CZ	1:B:290:ALA:HB2	2.57	0.41
1:B:369:THR:O	1:B:370:TRP:C	2.64	0.41
1:B:363:PRO:HD3	6:B:707:HOH:O	2.21	0.40
1:B:252:LEU:HD11	1:B:322:LEU:HD23	2.04	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	403/488 (83%)	394 (98%)	9 (2%)	0	100	100
1	B	403/488 (83%)	387 (96%)	14 (4%)	2 (0%)	24	8
All	All	806/976 (83%)	781 (97%)	23 (3%)	2 (0%)	43	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	183	SER
1	B	299	GLY

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	374/449 (83%)	370 (99%)	4 (1%)	65	43
1	B	374/449 (83%)	370 (99%)	4 (1%)	65	43
All	All	748/898 (83%)	740 (99%)	8 (1%)	65	43

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	217	LYS
1	A	252	LEU
1	A	355	MET
1	A	484	LYS

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Mol	Chain	Res	Type
1	B	116	LYS
1	B	292	LYS
1	B	387	SER
1	B	461	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	92	ASN
1	A	108	ASN
1	A	136	HIS
1	A	197	ASN
1	A	253	GLN
1	A	260	ASN
1	A	284	ASN
1	A	341	HIS
1	B	119	ASN
1	B	172	ASN
1	B	197	ASN
1	B	260	ASN
1	B	407	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	A1L41	A	503[A]	-	27,28,28	2.75	6 (22%)	28,37,37	2.49	6 (21%)
2	NDP	B	501	-	51,52,52	1.10	4 (7%)	71,80,80	1.20	7 (9%)
4	A1L41	B	503[A]	-	27,28,28	4.09	7 (25%)	28,37,37	1.99	5 (17%)
4	A1L41	A	503[B]	-	27,28,28	3.12	6 (22%)	28,37,37	2.53	6 (21%)
4	A1L41	B	503[B]	-	27,28,28	4.23	7 (25%)	28,37,37	2.83	7 (25%)
2	NDP	A	501	-	51,52,52	0.77	1 (1%)	71,80,80	0.88	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1L41	A	503[A]	-	-	7/26/26/26	0/2/2/2
2	NDP	B	501	-	-	3/34/77/77	0/5/5/5
4	A1L41	B	503[A]	-	-	5/26/26/26	0/2/2/2
4	A1L41	A	503[B]	-	-	7/26/26/26	0/2/2/2
4	A1L41	B	503[B]	-	-	5/26/26/26	0/2/2/2
2	NDP	A	501	-	-	7/34/77/77	0/5/5/5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503[A]	A1L41	O1-N1	17.20	1.52	1.40
4	B	503[B]	A1L41	O1-N1	17.20	1.52	1.40
4	A	503[B]	A1L41	C11-N1	-11.17	1.28	1.46
4	B	503[B]	A1L41	C11-N1	-10.57	1.29	1.46
4	B	503[A]	A1L41	C11-N1	-9.34	1.31	1.46
4	A	503[A]	A1L41	O1-N1	8.96	1.46	1.40
4	A	503[B]	A1L41	O1-N1	8.96	1.46	1.40
4	A	503[A]	A1L41	C11-N1	-8.49	1.32	1.46
4	B	503[B]	A1L41	C12-C11	-5.41	1.30	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503[A]	A1L41	C12-C11	-4.92	1.32	1.51
4	A	503[B]	A1L41	C12-C11	-4.90	1.32	1.51
2	B	501	NDP	P2B-O2B	4.14	1.66	1.59
4	A	503[A]	A1L41	C12-C11	-4.10	1.35	1.51
2	A	501	NDP	P2B-O2B	3.83	1.66	1.59
4	A	503[A]	A1L41	C1-C7	-3.50	1.46	1.52
4	A	503[B]	A1L41	C1-C7	-3.50	1.46	1.52
4	B	503[A]	A1L41	C10-N1	-3.33	1.30	1.35
4	B	503[B]	A1L41	C10-N1	-3.33	1.30	1.35
2	B	501	NDP	P2B-O2X	-3.17	1.43	1.54
4	B	503[A]	A1L41	C3-C2	3.09	1.44	1.38
4	B	503[B]	A1L41	C3-C2	3.09	1.44	1.38
4	B	503[A]	A1L41	P1-C7	2.68	1.85	1.81
4	B	503[B]	A1L41	P1-C7	2.68	1.85	1.81
2	B	501	NDP	PN-O3	2.60	1.62	1.59
2	B	501	NDP	P2B-O3X	-2.53	1.45	1.54
4	B	503[A]	A1L41	P1-O3	2.40	1.53	1.49
4	B	503[B]	A1L41	P1-O3	2.40	1.53	1.49
4	A	503[A]	A1L41	C9-C10	2.08	1.55	1.51
4	A	503[B]	A1L41	C9-C10	2.08	1.55	1.51
4	A	503[A]	A1L41	C2-C1	2.04	1.42	1.39
4	A	503[B]	A1L41	C2-C1	2.04	1.42	1.39

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503[B]	A1L41	C12-C11-N1	10.98	133.72	111.11
4	A	503[B]	A1L41	C12-C11-N1	9.64	130.95	111.11
4	A	503[A]	A1L41	C12-C11-N1	9.03	129.69	111.11
4	B	503[A]	A1L41	C12-C11-N1	7.17	125.87	111.11
4	A	503[A]	A1L41	O1-N1-C11	6.87	129.85	113.76
4	B	503[B]	A1L41	O1-N1-C11	6.81	129.72	113.76
4	A	503[B]	A1L41	O1-N1-C11	6.43	128.81	113.76
4	B	503[A]	A1L41	O1-N1-C11	4.12	123.40	113.76
4	B	503[A]	A1L41	O2-C10-C9	-3.83	110.90	121.26
4	B	503[B]	A1L41	O2-C10-C9	-3.83	110.90	121.26
4	A	503[A]	A1L41	O2-C10-C9	-3.44	111.95	121.26
4	A	503[B]	A1L41	O2-C10-C9	-3.44	111.95	121.26
2	B	501	NDP	O3X-P2B-O2X	3.40	120.54	107.80
2	B	501	NDP	O3X-P2B-O2B	-3.28	93.06	105.85
4	B	503[B]	A1L41	C17-C16-C15	-3.11	116.24	120.61
2	B	501	NDP	C3B-C2B-C1B	-2.90	97.25	102.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NDP	O2N-PN-O1N	2.90	125.94	112.44
4	B	503[A]	A1L41	C13-C12-C11	2.59	124.94	113.17
4	A	503[A]	A1L41	C13-C12-C11	2.52	124.64	113.17
2	B	501	NDP	O7N-C7N-C3N	-2.48	116.22	120.90
2	B	501	NDP	O3-PN-O1N	-2.48	103.24	110.70
4	A	503[B]	A1L41	C13-C14-C15	-2.44	104.55	113.67
4	B	503[B]	A1L41	C18-C17-C16	2.43	123.24	120.24
2	A	501	NDP	O3-PA-O1A	-2.42	103.42	110.70
4	B	503[B]	A1L41	C18-C19-C20	-2.39	117.29	120.24
4	A	503[A]	A1L41	O5-P1-O3	-2.32	107.63	113.45
4	A	503[B]	A1L41	O5-P1-O3	-2.32	107.63	113.45
4	B	503[B]	A1L41	C16-C15-C20	2.31	121.66	118.23
4	A	503[A]	A1L41	O4-P1-O3	-2.23	107.86	113.45
4	A	503[B]	A1L41	O4-P1-O3	-2.23	107.86	113.45
2	B	501	NDP	P2B-O2B-C2B	-2.17	117.63	123.43
4	B	503[A]	A1L41	C18-C17-C16	-2.10	117.64	120.24

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503[A]	A1L41	C12-C11-N1-O1
4	A	503[B]	A1L41	C12-C11-N1-C10
4	A	503[B]	A1L41	C12-C11-N1-O1
4	B	503[A]	A1L41	C12-C11-N1-C10
4	B	503[A]	A1L41	C12-C11-N1-O1
4	B	503[A]	A1L41	N1-C10-C9-C8
4	B	503[B]	A1L41	C12-C11-N1-C10
4	B	503[B]	A1L41	C12-C11-N1-O1
4	B	503[B]	A1L41	N1-C10-C9-C8
4	A	503[A]	A1L41	C11-C12-C13-C14
4	B	503[A]	A1L41	C12-C13-C14-C15
4	B	503[B]	A1L41	C12-C13-C14-C15
4	A	503[B]	A1L41	C11-C12-C13-C14
2	B	501	NDP	PN-O3-PA-O1A
2	A	501	NDP	O4D-C1D-N1N-C6N
2	B	501	NDP	O4D-C1D-N1N-C6N
2	A	501	NDP	C2B-O2B-P2B-O1X
2	A	501	NDP	C1B-C2B-O2B-P2B
2	A	501	NDP	PN-O3-PA-O1A
4	A	503[A]	A1L41	C13-C14-C15-C16
4	A	503[B]	A1L41	C13-C14-C15-C20

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Mol	Chain	Res	Type	Atoms
4	A	503[A]	A1L41	C13-C14-C15-C20
4	A	503[B]	A1L41	C13-C14-C15-C16
2	A	501	NDP	PN-O3-PA-O2A
4	A	503[A]	A1L41	C12-C11-N1-C10
4	A	503[A]	A1L41	N1-C10-C9-C8
4	A	503[B]	A1L41	N1-C10-C9-C8
2	A	501	NDP	C3B-C2B-O2B-P2B
2	B	501	NDP	PN-O3-PA-O2A
2	A	501	NDP	C2B-O2B-P2B-O2X
4	A	503[A]	A1L41	O2-C10-N1-O1
4	A	503[B]	A1L41	O2-C10-N1-O1
4	B	503[A]	A1L41	O2-C10-N1-O1
4	B	503[B]	A1L41	O2-C10-N1-O1

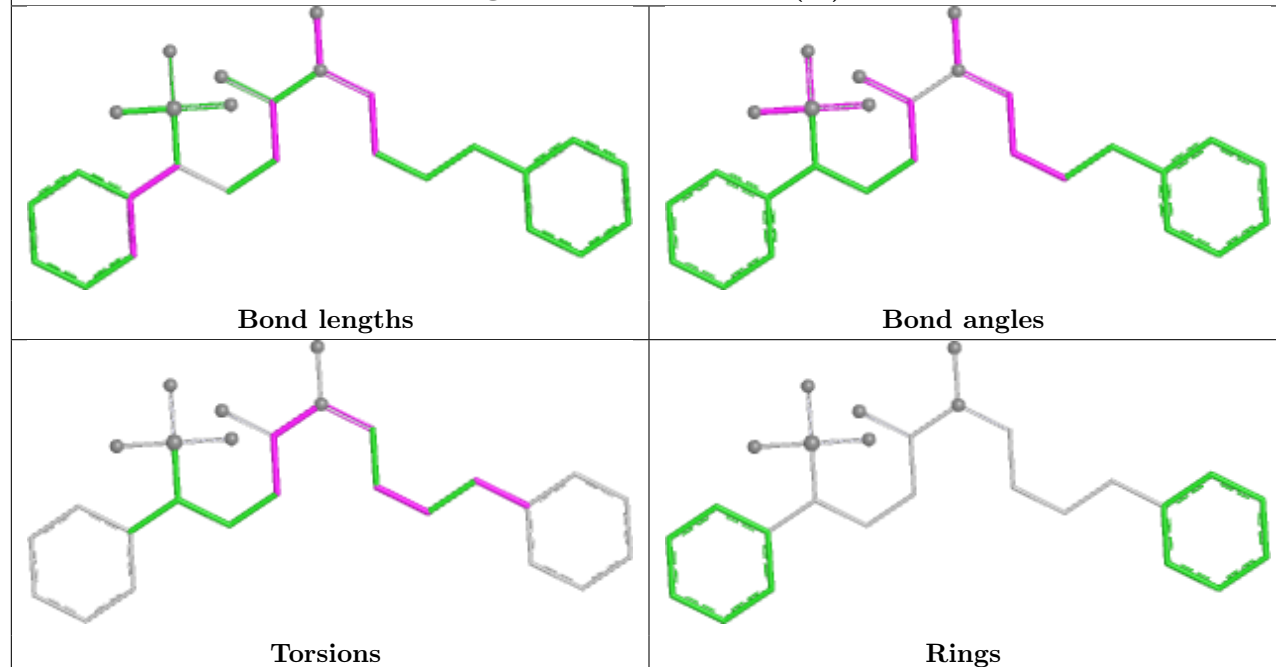
There are no ring outliers.

2 monomers are involved in 5 short contacts:

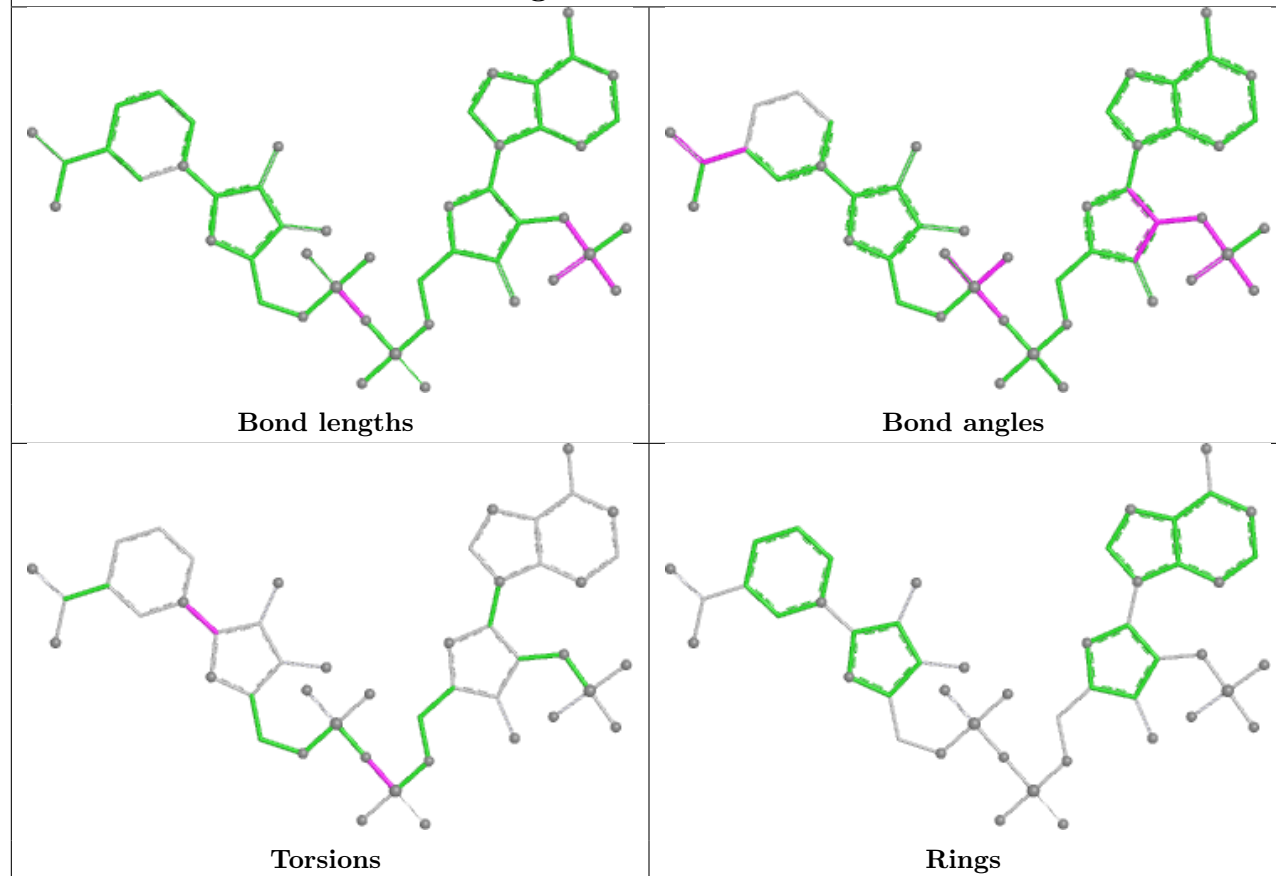
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503[B]	A1L41	1	0
4	B	503[B]	A1L41	4	0

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.

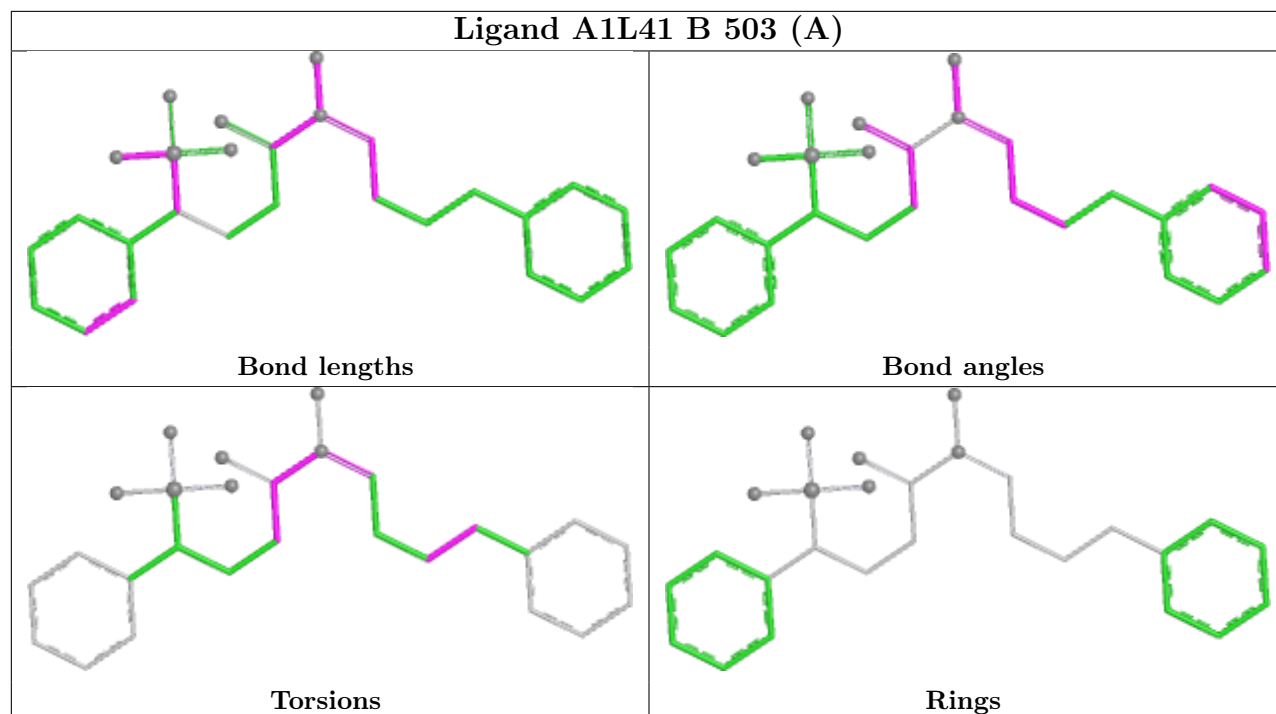
Ligand A1L41 A 503 (A)



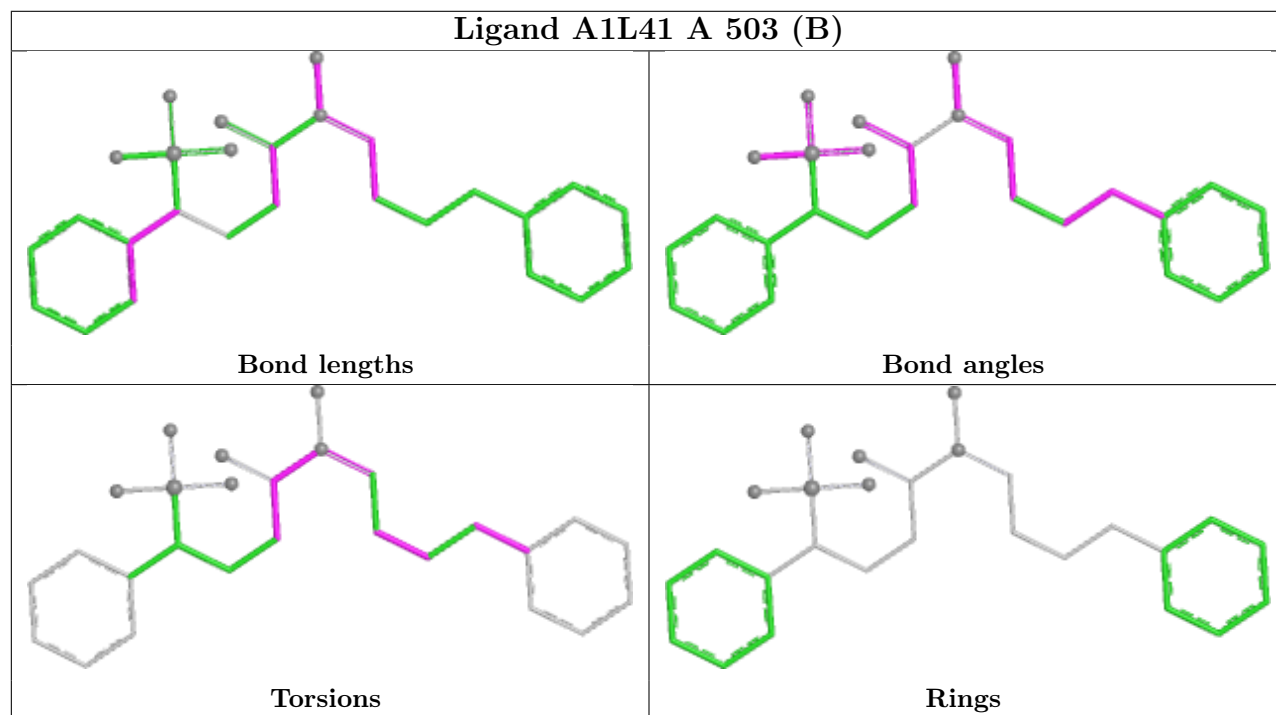
Ligand NDP B 501



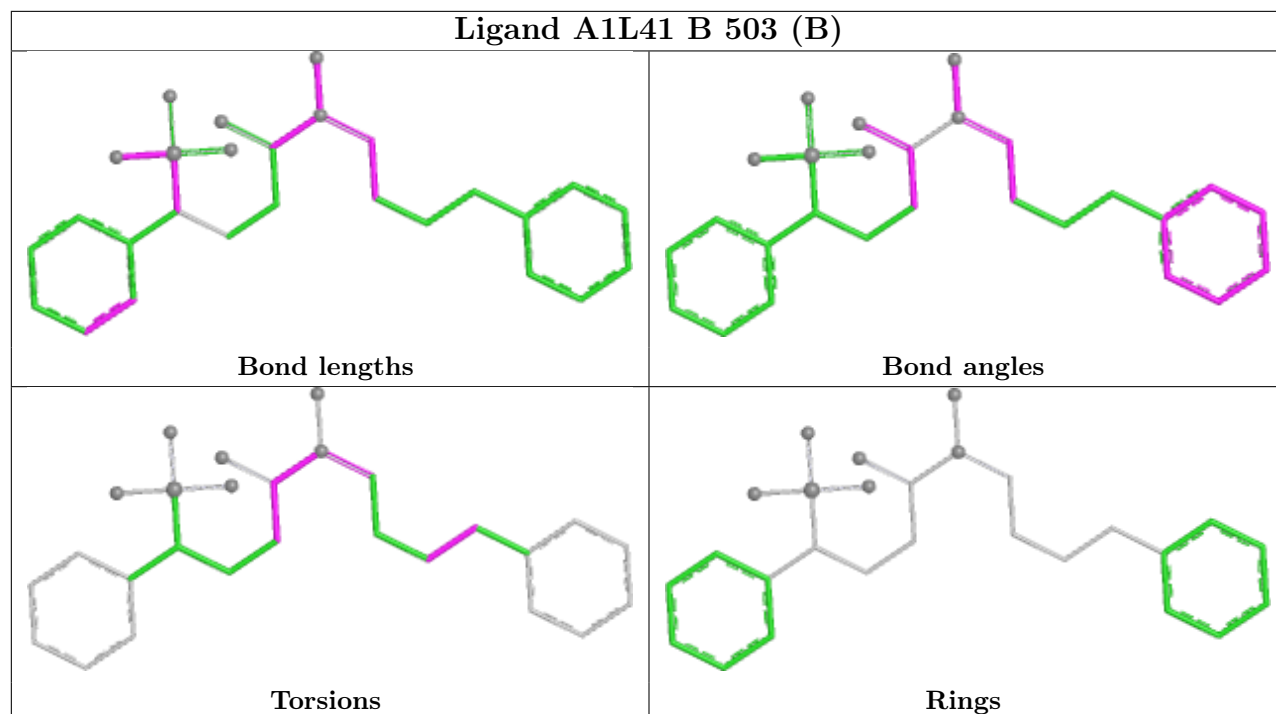
Ligand A1L41 B 503 (A)



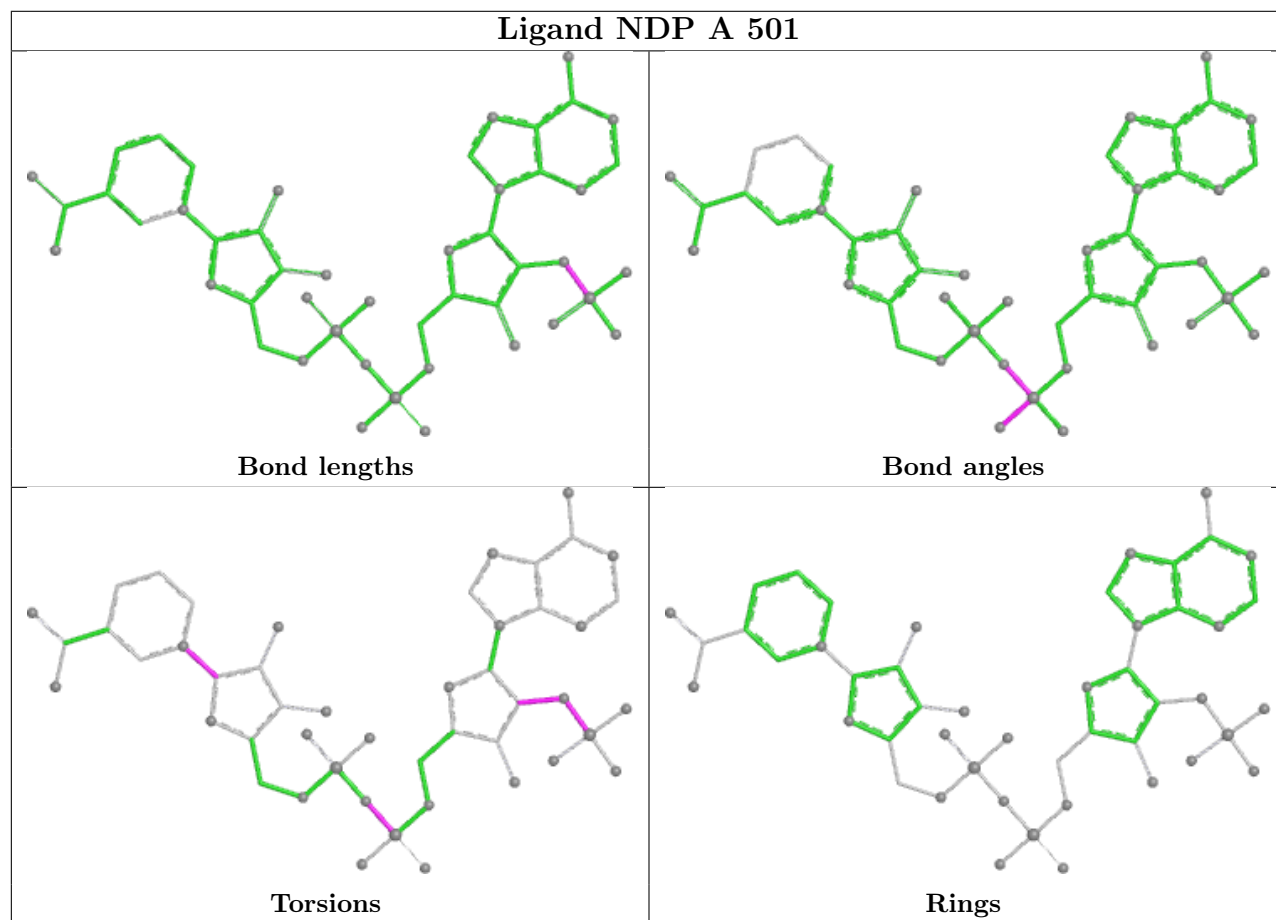
Ligand A1L41 A 503 (B)



Ligand A1L41 B 503 (B)



Ligand NDP A 501



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	406/488 (83%)	0.60	30 (7%)	20 24	14, 26, 56, 88	1 (0%)
1	B	406/488 (83%)	0.40	22 (5%)	31 38	13, 23, 47, 82	1 (0%)
All	All	812/976 (83%)	0.50	52 (6%)	25 30	13, 24, 53, 88	2 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	LYS	4.9
1	B	141	TYR	4.8
1	B	188	TYR	4.3
1	A	147	LEU	4.0
1	A	151	ILE	3.7
1	A	140	VAL	3.5
1	A	291	LEU	3.4
1	B	292	LYS	3.4
1	A	141	TYR	3.4
1	B	299	GLY	3.3
1	B	485	HIS	3.2
1	A	148	VAL	3.2
1	A	183	SER	3.0
1	B	486	ASN	2.9
1	A	298	MET	2.9
1	A	184	PHE	2.8
1	A	106	VAL	2.7
1	A	77	PRO	2.7
1	A	152	LYS	2.7
1	A	154	TYR	2.6
1	A	149	LYS	2.6
1	B	484	LYS	2.6
1	A	192	TYR	2.6
1	A	76	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	188	TYR	2.5
1	A	118	VAL	2.5
1	A	135	ILE	2.5
1	B	76	LYS	2.5
1	A	144	LEU	2.4
1	A	485	HIS	2.4
1	B	150	ASN	2.4
1	B	147	LEU	2.4
1	A	122	TYR	2.4
1	B	160	CYS	2.3
1	B	148	VAL	2.3
1	A	155	LYS	2.3
1	A	142	GLU	2.3
1	A	299	GLY	2.2
1	A	252	LEU	2.2
1	B	151	ILE	2.2
1	B	459	ASN	2.2
1	A	484	LYS	2.2
1	B	140	VAL	2.2
1	B	144	LEU	2.2
1	B	458	GLU	2.2
1	B	158	ILE	2.1
1	B	213	PHE	2.1
1	B	457	SER	2.1
1	B	291	LEU	2.1
1	A	121	LEU	2.0
1	A	302	ILE	2.0
1	B	462	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

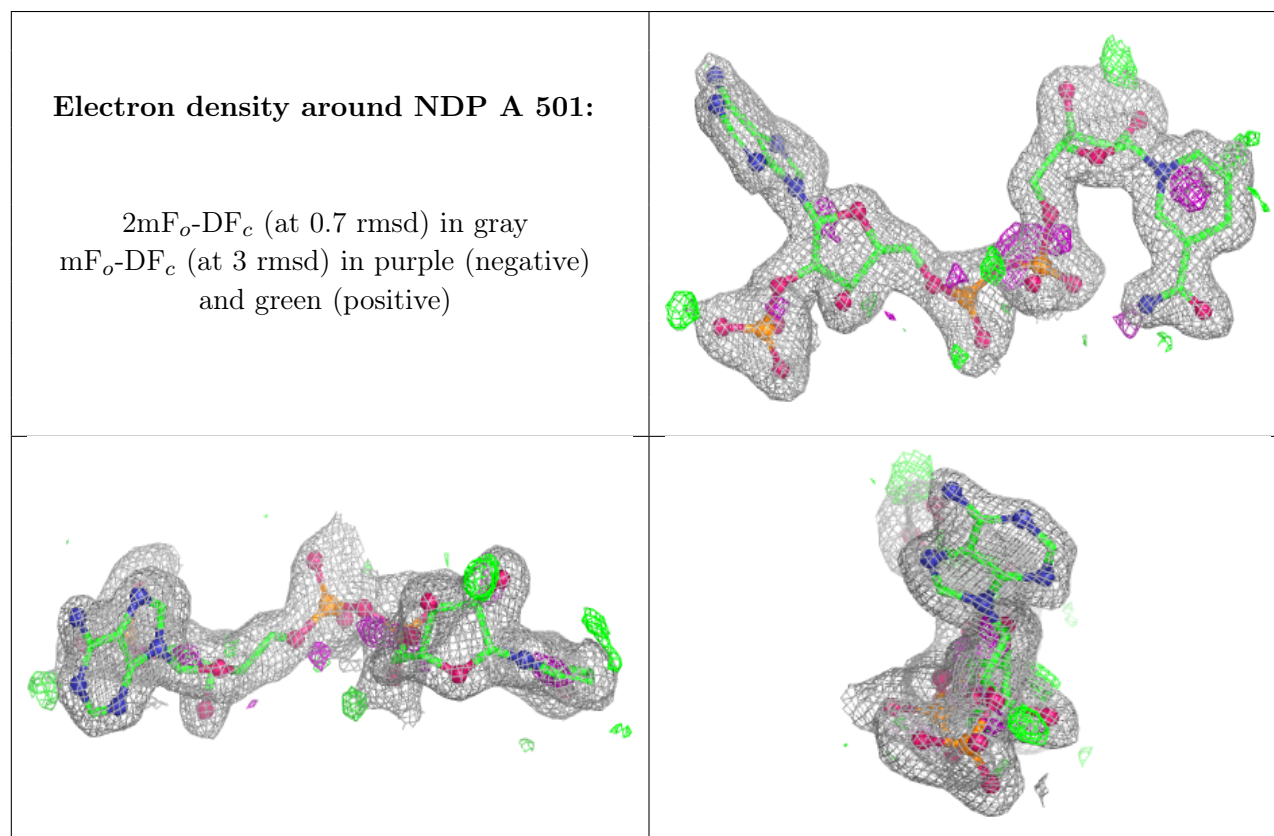
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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

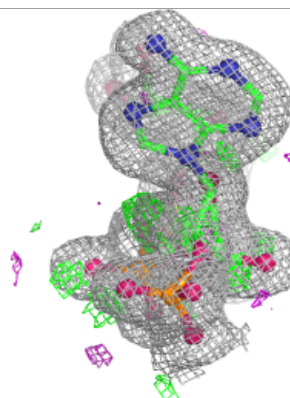
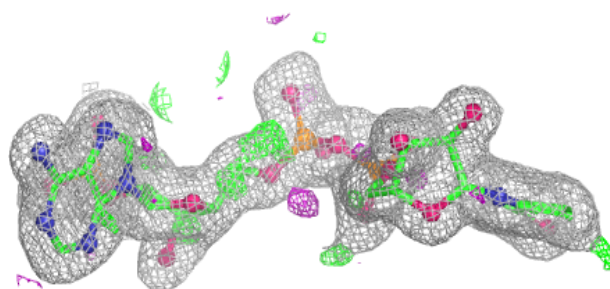
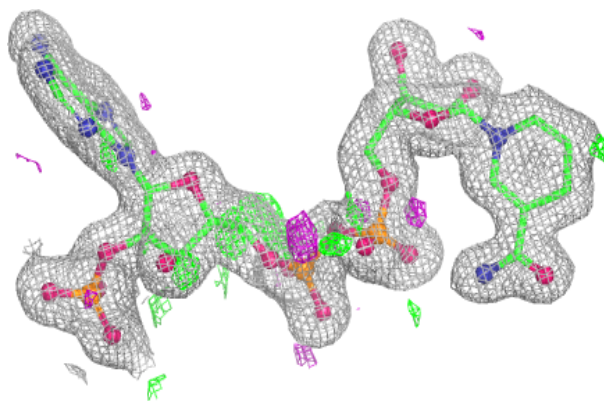
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NDP	A	501	48/48	0.92	0.10	25,32,36,38	0
2	NDP	B	501	48/48	0.96	0.07	16,23,27,29	0
4	A1L41	A	503[A]	27/27	0.96	0.10	18,21,27,28	10
4	A1L41	A	503[B]	27/27	0.96	0.10	18,21,31,32	10
5	CA	B	505	1/1	0.96	0.07	27,27,27,27	0
4	A1L41	B	503[B]	27/27	0.97	0.10	13,18,24,26	10
4	A1L41	B	503[A]	27/27	0.97	0.10	13,20,33,34	10
5	CA	B	506	1/1	0.97	0.08	30,30,30,30	0
5	CA	B	504	1/1	1.00	0.04	17,17,17,17	0
3	MN	A	502	1/1	1.00	0.02	16,16,16,16	0
3	MN	B	502	1/1	1.00	0.01	14,14,14,14	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.

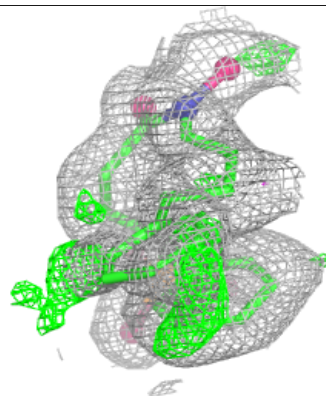
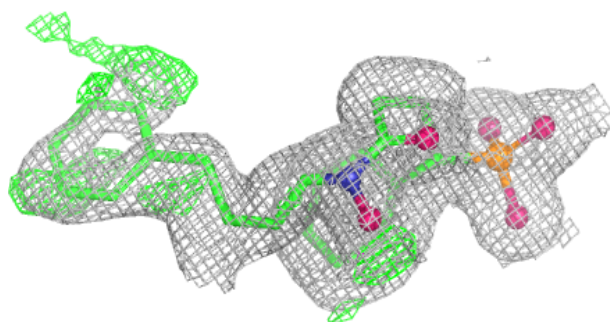
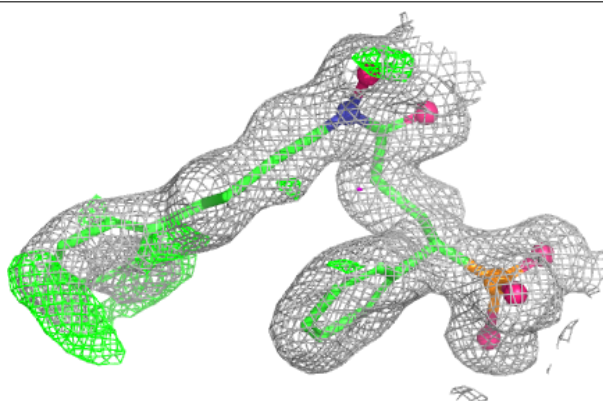


Electron density around NDP B 501:

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

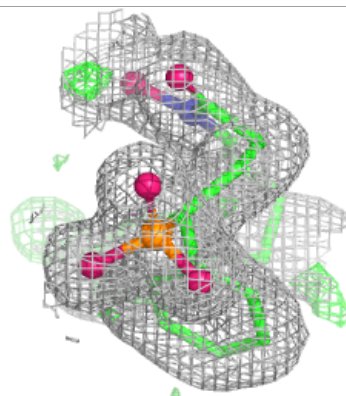
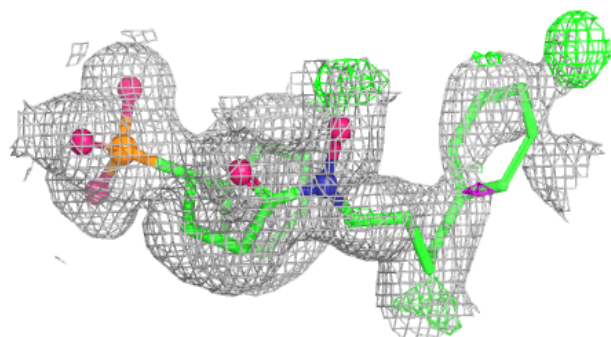
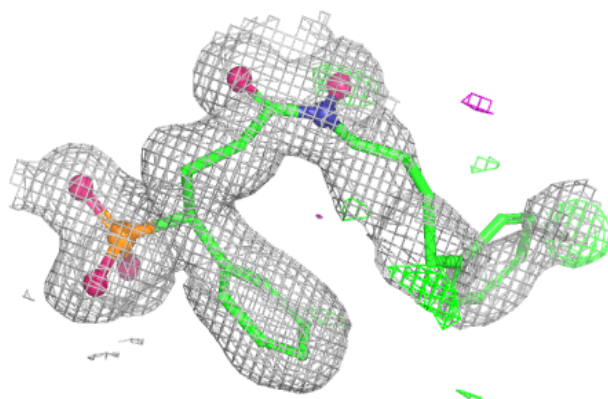
**Electron density around A1L41 A 503 (A):**

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

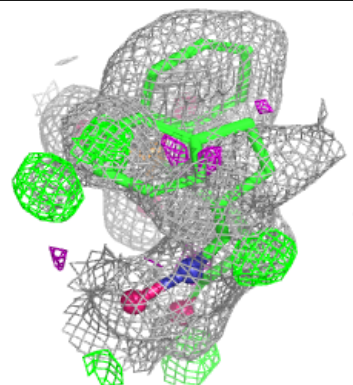
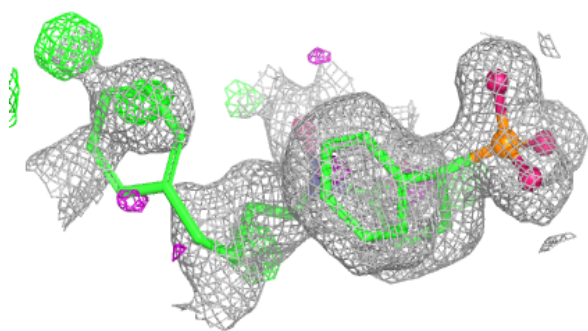
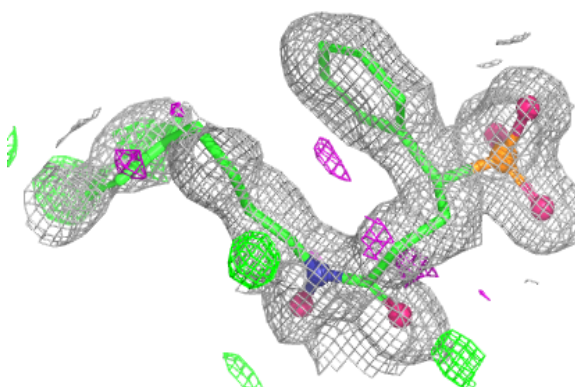


Electron density around A1L41 A 503 (B):

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

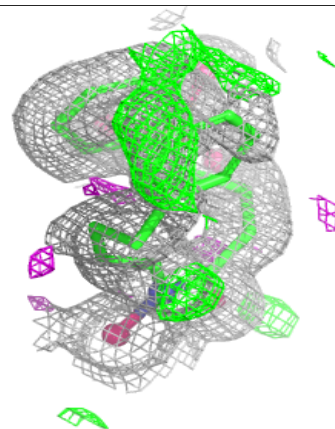
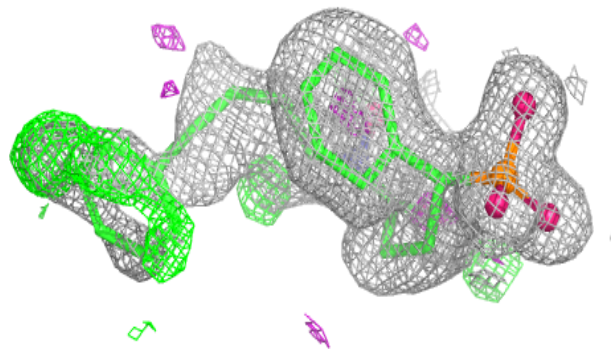
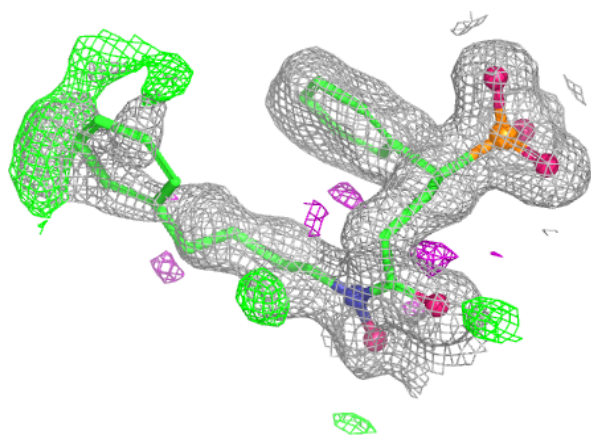
**Electron density around A1L41 B 503 (B):**

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



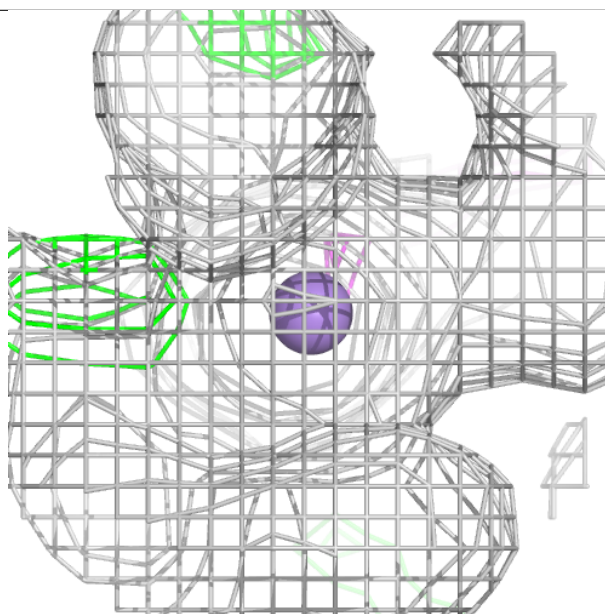
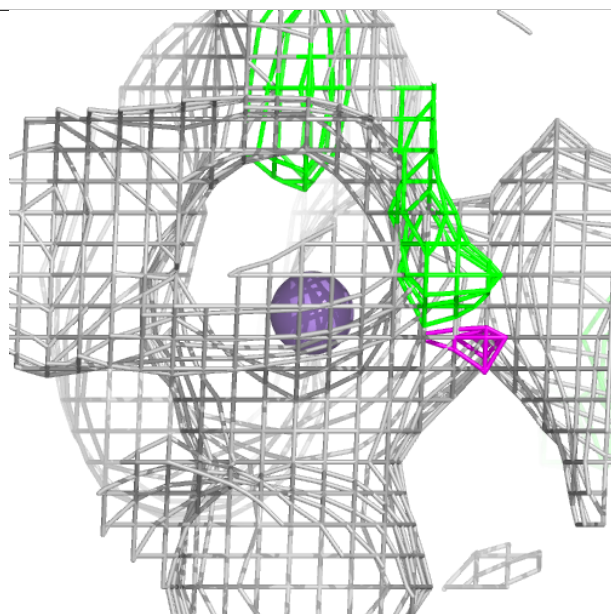
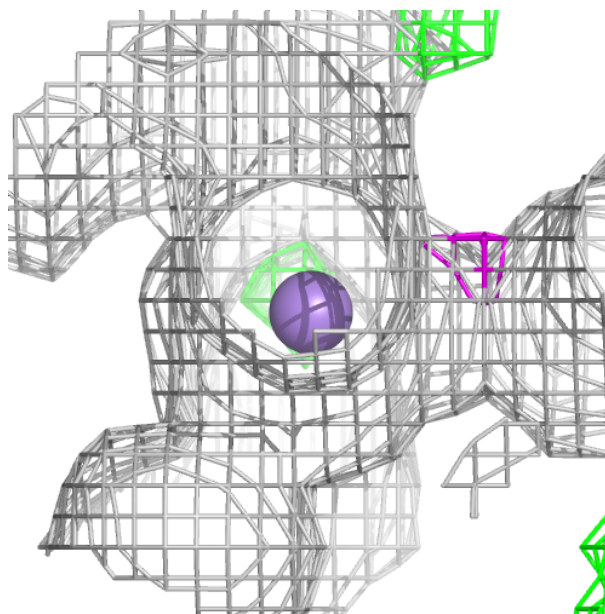
Electron density around A1L41 B 503 (A):

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



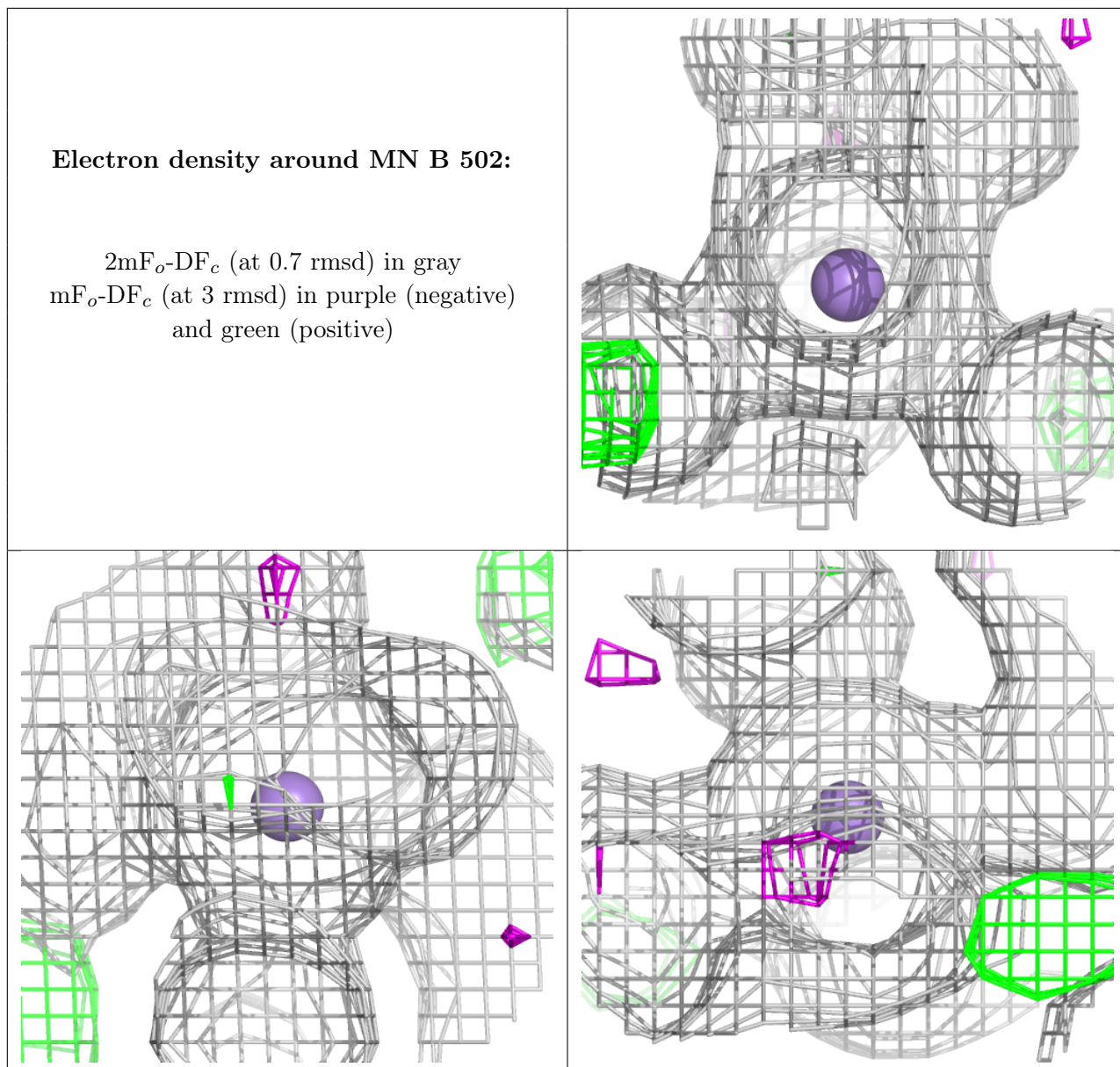
Electron density around MN A 502:

$2mF_o-DF_c$ (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.