



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2025 – 10:37 AM JST

PDB ID : 9JZC / pdb_00009jzc
Title : PfDXR - Mn²⁺ - NADPH - MAMK251 quaternary complex
Authors : Takada, S.; Sakamoto, Y.; Tanaka, N.
Deposited on : 2024-10-14
Resolution : 1.77 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

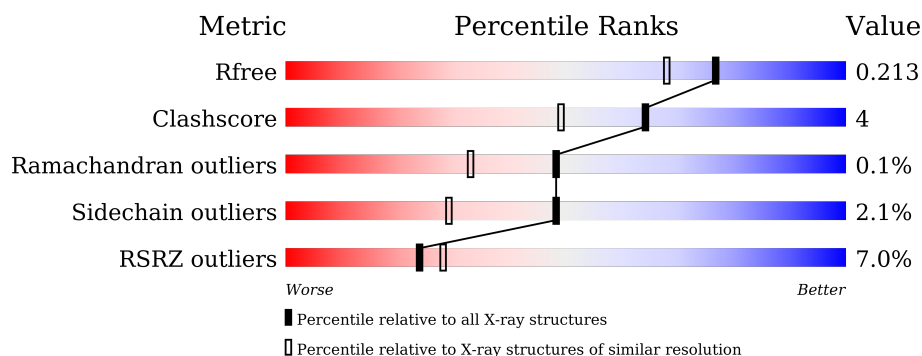
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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}	164625	1191 (1.78-1.78)
Clashscore	180529	1282 (1.78-1.78)
Ramachandran outliers	177936	1270 (1.78-1.78)
Sidechain outliers	177891	1270 (1.78-1.78)
RSRZ outliers	164620	1191 (1.78-1.78)

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	<div> <div>11%</div> <div> <div></div> <div>75%</div> <div>8%</div> <div>16%</div> </div> </div>
1	B	488	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>6%</div> <div>16%</div> </div> </div>

2 Entry composition [i](#)

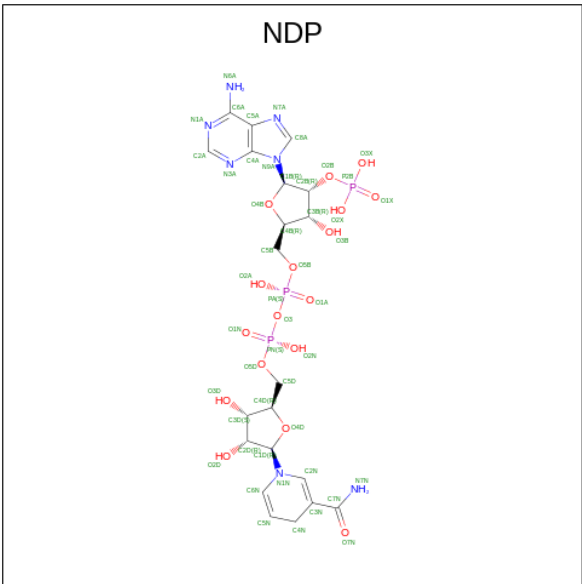
There are 7 unique types of molecules in this entry. The entry contains 7108 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	408	Total	C	N	O	S	0	0	0
			3259	2092	533	614	20			
1	B	408	Total	C	N	O	S	0	0	0
			3259	2092	533	614	20			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).

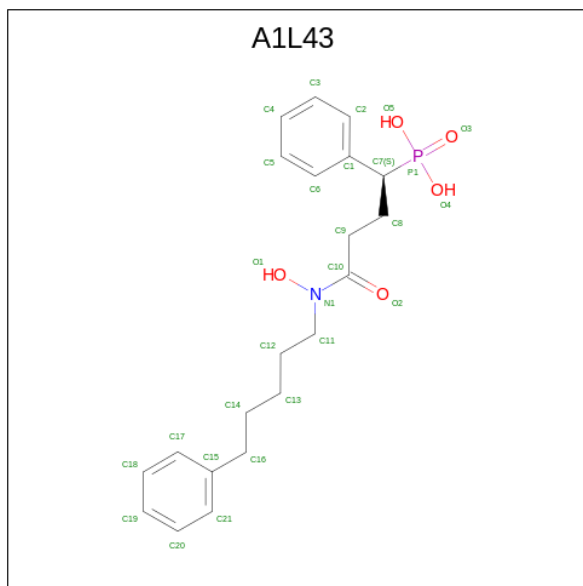


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- 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-oxidanylidene-4-[oxidanyl(5-phenylpentyl)amino]-1-phenyl-butyl]p
hosphonic acid (CCD ID: A1L43) (formula: C₂₁H₂₈NO₅P) (labeled as "Ligand of Interest"
by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			28	21	1	5	1		
4	B	1	Total	C	N	O	P	0	0
			28	21	1	5	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

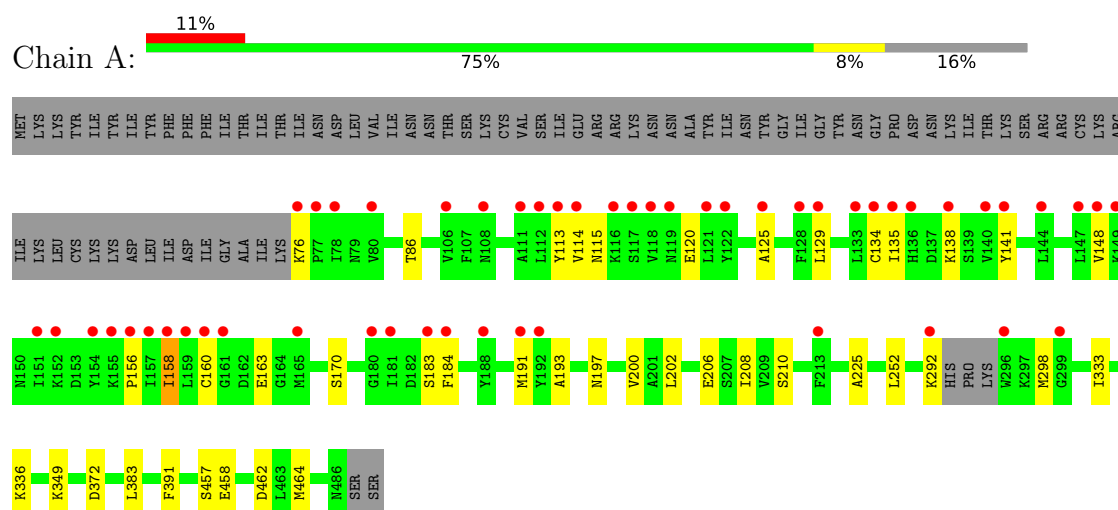
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	177	Total	O	0	0
			177	177		
7	B	244	Total	O	0	0
			244	244		

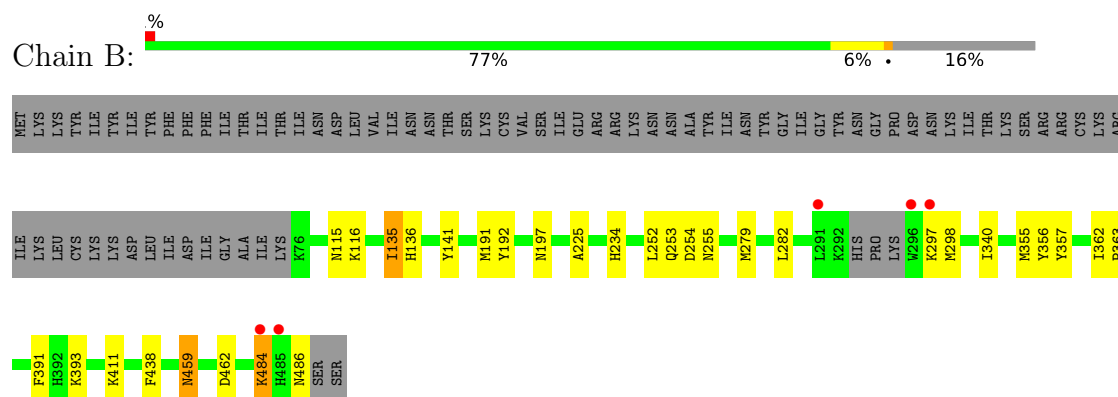
3 Residue-property plots [i](#)

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: 1-deoxy-D-xylulose 5-phosphate reductoisomerase, apicoplasmic



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.46Å 77.52Å 111.47Å 90.00° 92.19° 90.00°	Depositor
Resolution (Å)	40.43 – 1.77 40.43 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.43-1.77) 99.6 (40.43-1.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.169 , 0.203 0.180 , 0.213	Depositor DCC
R_{free} test set	4452 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7108	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NDP, A1L43, GOL, MN

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	0.59	0/3319	1.05	0/4480
1	B	0.63	0/3319	1.09	4/4480 (0.1%)
All	All	0.61	0/6638	1.07	4/8960 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	298	MET	CG-SD-CE	-7.02	85.45	100.90
1	B	282	LEU	N-CA-CB	-5.60	101.60	110.22
1	B	253	GLN	CB-CA-C	5.41	119.08	109.72
1	B	234	HIS	CA-CB-CG	-5.24	108.56	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3259	0	3306	30	0
1	B	3259	0	3306	18	0
2	A	48	0	26	4	0
2	B	48	0	26	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	28	0	0	0	0
4	B	28	0	0	0	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	B	3	0	0	0	0
7	A	177	0	0	13	0
7	B	244	0	0	3	0
All	All	7108	0	6680	51	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 (51) 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:135:ILE:HD11	1:B:141:TYR:HA	1.35	1.03
1:A:372:ASP:HB2	7:A:747:HOH:O	1.82	0.79
1:A:206:GLU:CD	7:A:602:HOH:O	2.26	0.78
1:B:135:ILE:CD1	1:B:141:TYR:HA	2.15	0.76
1:A:183:SER:HA	1:A:206:GLU:OE1	1.87	0.75
1:A:120:GLU:N	1:A:120:GLU:OE1	2.20	0.74
1:B:191:MET:HE3	1:B:192:TYR:CE2	2.25	0.72
1:A:206:GLU:CG	7:A:602:HOH:O	2.38	0.71
2:A:501:NDP:H8A	7:A:647:HOH:O	1.88	0.71
1:A:191:MET:HE1	1:A:464:MET:HE2	1.74	0.68
1:B:135:ILE:HD11	1:B:141:TYR:CA	2.18	0.66
1:A:113:TYR:CZ	2:A:501:NDP:H2A	2.33	0.63
1:A:372:ASP:CB	7:A:747:HOH:O	2.43	0.63
1:B:484:LYS:HA	1:B:484:LYS:HE2	1.85	0.58
1:B:279:MET:HE1	1:B:438:PHE:CZ	2.40	0.56
1:A:134:CYS:SG	7:A:704:HOH:O	2.41	0.55
1:A:206:GLU:HG3	7:A:602:HOH:O	2.05	0.55
1:B:355:MET:HE2	7:B:611:HOH:O	2.07	0.54
1:A:336:LYS:HE3	7:A:671:HOH:O	2.09	0.52
1:B:393:LYS:HG2	7:B:690:HOH:O	2.09	0.52
1:B:254:ASP:O	1:B:255:ASN:HB2	2.12	0.49
1:B:459:ASN:OD1	1:B:462:ASP:OD2	2.31	0.48
1:A:202:LEU:HD23	1:A:208:ILE:HD11	1.96	0.48
1:A:156:PRO:HG2	1:A:158:ILE:HD11	1.96	0.48
1:A:138:LYS:HD3	1:A:160:CYS:SG	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501:NDP:C5N	7:A:631:HOH:O	2.62	0.47
2:A:501:NDP:H42N	7:A:631:HOH:O	2.15	0.47
1:A:292:LYS:HA	1:A:292:LYS:HE2	1.97	0.46
1:A:333:ILE:HD11	1:A:391:PHE:HB3	1.98	0.46
1:A:141:TYR:CD1	1:A:160:CYS:HB2	2.52	0.45
1:A:197:ASN:HA	1:A:225:ALA:HB2	1.98	0.44
1:A:138:LYS:CD	1:A:160:CYS:SG	3.06	0.44
1:A:193:ALA:HB1	1:A:200:VAL:HG22	2.01	0.43
1:A:115:ASN:C	1:A:115:ASN:HD22	2.27	0.43
1:A:298:MET:HB3	7:A:604:HOH:O	2.19	0.43
1:B:197:ASN:HA	1:B:225:ALA:HB2	2.01	0.43
1:A:183:SER:CB	7:A:664:HOH:O	2.67	0.42
1:B:135:ILE:CD1	1:B:141:TYR:CA	2.90	0.42
1:A:372:ASP:CG	7:A:747:HOH:O	2.62	0.42
1:B:340:ILE:HD12	1:B:391:PHE:HZ	1.83	0.42
1:A:457:SER:OG	1:A:462:ASP:HB2	2.20	0.41
1:A:135:ILE:O	1:A:160:CYS:HA	2.20	0.41
1:A:148:VAL:HG11	1:A:156:PRO:HG3	2.02	0.41
1:B:362:ILE:HB	1:B:363:PRO:HD3	2.01	0.41
1:A:86:THR:HG23	1:A:114:VAL:HG11	2.02	0.41
1:A:349:LYS:HA	1:A:349:LYS:HD3	1.89	0.41
1:B:355:MET:CE	7:B:611:HOH:O	2.65	0.41
1:A:125:ALA:O	1:A:129:LEU:HD13	2.21	0.41
1:B:115:ASN:HD22	1:B:136:HIS:HB3	1.87	0.40
1:B:191:MET:HE3	1:B:192:TYR:CD2	2.56	0.40
1:B:356:TYR:CG	1:B:357:TYR:N	2.90	0.40

There are no symmetry-related clashes.

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	404/488 (83%)	394 (98%)	9 (2%)	1 (0%)	44	29
1	B	404/488 (83%)	393 (97%)	11 (3%)	0	100	100
All	All	808/976 (83%)	787 (97%)	20 (2%)	1 (0%)	48	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	PHE

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	375/449 (84%)	367 (98%)	8 (2%)	48	29
1	B	375/449 (84%)	367 (98%)	8 (2%)	48	29
All	All	750/898 (84%)	734 (98%)	16 (2%)	48	29

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	LYS
1	A	158	ILE
1	A	163	GLU
1	A	170	SER
1	A	210	SER
1	A	252	LEU
1	A	383	LEU
1	A	458	GLU
1	B	116	LYS
1	B	135	ILE
1	B	252	LEU
1	B	297	LYS
1	B	411	LYS
1	B	459	ASN
1	B	484	LYS

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Mol	Chain	Res	Type
1	B	486	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	115	ASN
1	A	150	ASN
1	A	224	ASN
1	A	253	GLN
1	A	255	ASN
1	A	260	ASN
1	A	284	ASN
1	A	407	GLN
1	A	428	ASN
1	B	92	ASN
1	B	105	ASN
1	B	115	ASN
1	B	119	ASN
1	B	172	ASN
1	B	255	ASN
1	B	261	ASN
1	B	432	ASN
1	B	446	GLN
1	B	486	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 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
5	GOL	B	507	-	5,5,5	0.20	0	5,5,5	0.92	0
2	NDP	A	501	-	45,52,52	0.76	1 (2%)	53,80,80	0.96	2 (3%)
4	A1L43	B	503	3	28,29,29	1.68	7 (25%)	29,38,38	1.04	1 (3%)
5	GOL	A	504	-	5,5,5	0.25	0	5,5,5	0.66	0
4	A1L43	A	503	3	28,29,29	1.27	4 (14%)	29,38,38	1.32	3 (10%)
2	NDP	B	501	-	45,52,52	0.94	2 (4%)	53,80,80	1.08	4 (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
5	GOL	B	507	-	-	0/4/4/4	-
2	NDP	A	501	-	-	7/30/77/77	0/5/5/5
4	A1L43	B	503	3	-	4/27/27/27	0/2/2/2
5	GOL	A	504	-	-	2/4/4/4	-
4	A1L43	A	503	3	-	2/27/27/27	0/2/2/2
2	NDP	B	501	-	-	5/30/77/77	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	A1L43	P1-O5	-4.54	1.47	1.54
4	A	503	A1L43	O1-N1	-4.05	1.37	1.40
4	B	503	A1L43	P1-C7	3.52	1.86	1.82
4	B	503	A1L43	P1-O3	3.30	1.55	1.49
4	A	503	A1L43	P1-O3	3.20	1.55	1.49
4	B	503	A1L43	O2-C10	2.94	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NDP	P2B-O2B	2.89	1.64	1.59
4	B	503	A1L43	C11-N1	2.54	1.51	1.46
2	B	501	NDP	C4N-C3N	-2.38	1.45	1.49
2	A	501	NDP	P2B-O2B	2.25	1.63	1.59
4	A	503	A1L43	P1-C7	2.23	1.85	1.82
4	B	503	A1L43	C5-C6	2.19	1.43	1.38
4	A	503	A1L43	C6-C1	2.18	1.42	1.39
4	B	503	A1L43	C1-C7	2.09	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NDP	O2N-PN-O1N	3.65	130.30	112.24
4	A	503	A1L43	O5-P1-O3	-2.94	106.06	113.45
4	B	503	A1L43	O3-P1-C7	-2.94	105.12	113.35
4	A	503	A1L43	C21-C15-C17	2.83	122.62	118.17
2	A	501	NDP	O2N-PN-O1N	2.82	126.18	112.24
2	B	501	NDP	O3X-P2B-O2X	2.68	117.88	107.64
4	A	503	A1L43	C8-C7-C1	-2.58	109.17	113.42
2	B	501	NDP	C5A-C6A-N6A	2.57	124.25	120.35
2	B	501	NDP	C3B-C2B-C1B	-2.44	98.30	102.89
2	A	501	NDP	C5A-C6A-N6A	2.12	123.57	120.35

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NDP	C5B-O5B-PA-O1A
2	A	501	NDP	O4D-C1D-N1N-C6N
2	A	501	NDP	O4B-C4B-C5B-O5B
2	A	501	NDP	C3B-C4B-C5B-O5B
4	A	503	A1L43	C13-C14-C16-C15
2	B	501	NDP	PN-O3-PA-O1A
2	B	501	NDP	O4D-C1D-N1N-C6N
4	B	503	A1L43	C13-C14-C16-C15
2	A	501	NDP	C5B-O5B-PA-O3
5	A	504	GOL	O2-C2-C3-O3
4	B	503	A1L43	C17-C15-C16-C14
4	B	503	A1L43	C21-C15-C16-C14
2	B	501	NDP	PN-O3-PA-O2A
2	B	501	NDP	O4B-C4B-C5B-O5B
2	A	501	NDP	C1B-C2B-O2B-P2B

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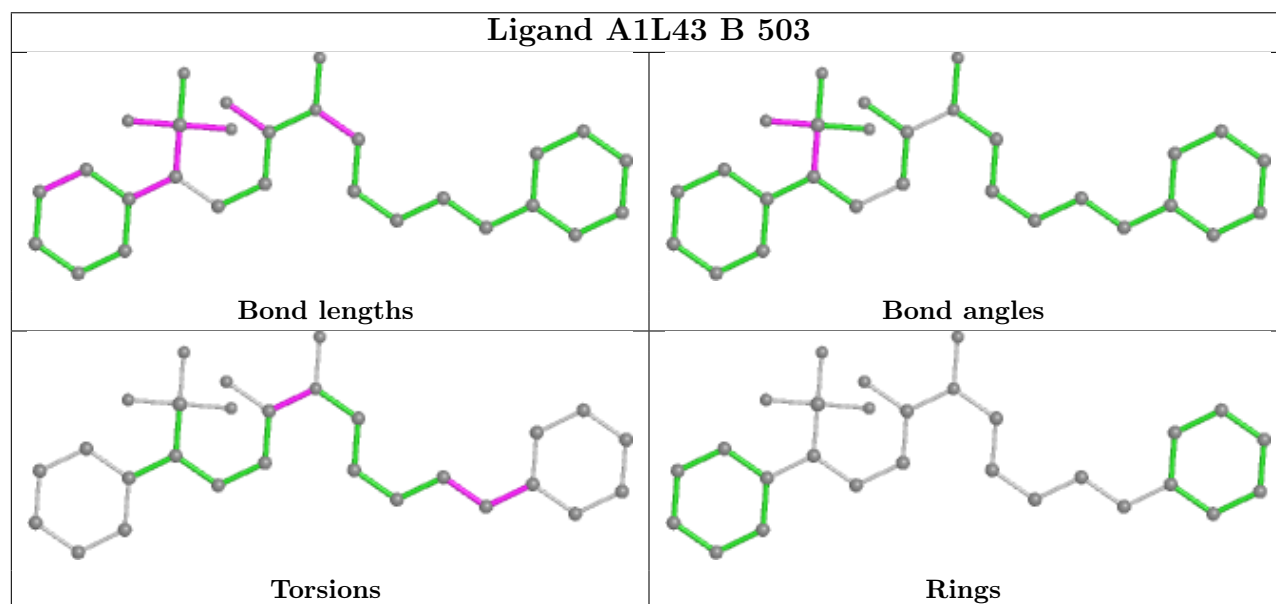
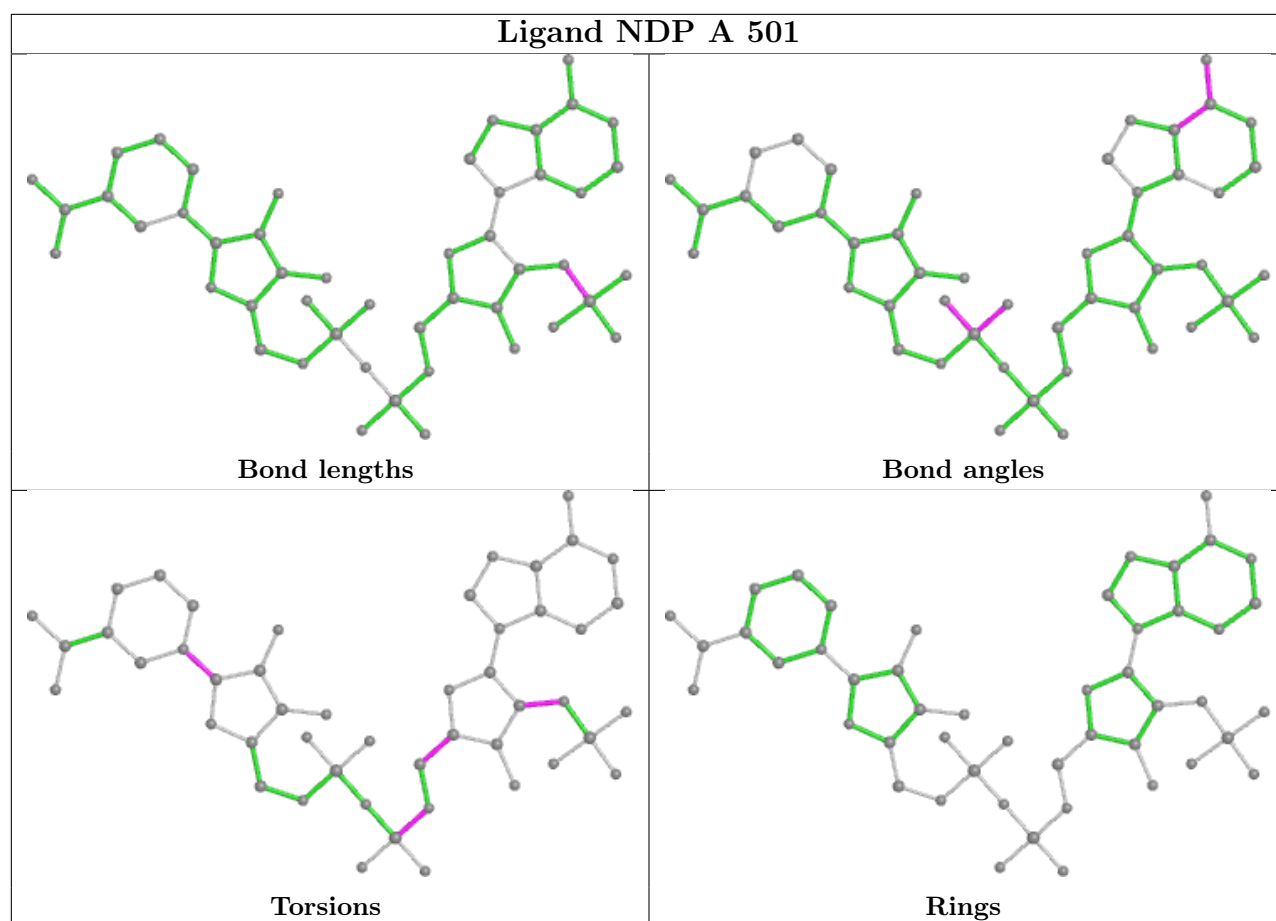
Mol	Chain	Res	Type	Atoms
2	B	501	NDP	C1B-C2B-O2B-P2B
4	A	503	A1L43	O2-C10-N1-O1
4	B	503	A1L43	O2-C10-N1-O1
5	A	504	GOL	C1-C2-C3-O3
2	A	501	NDP	C3B-C2B-O2B-P2B

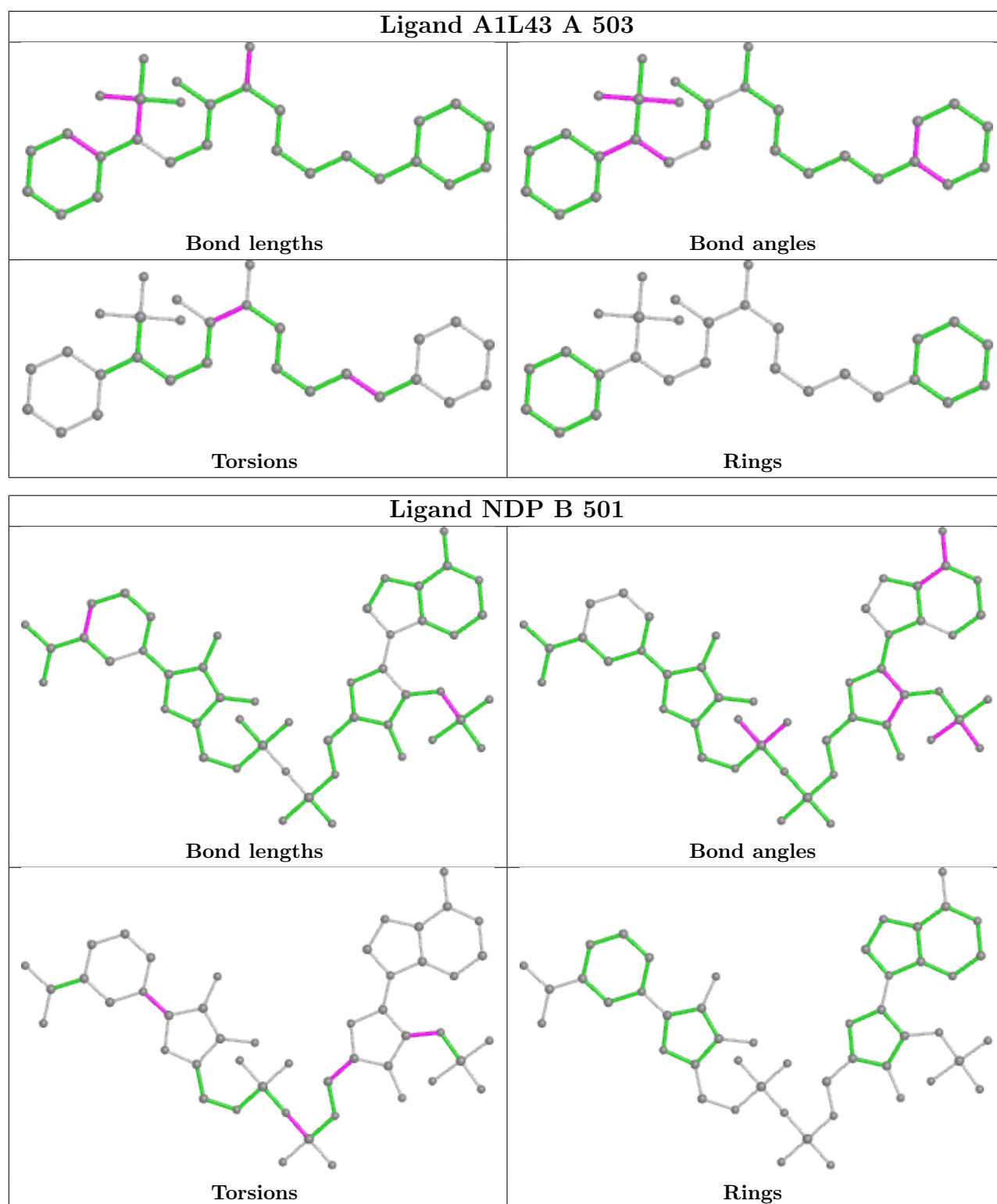
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NDP	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.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	408/488 (83%)	0.41	52 (12%) 9 10	17, 32, 82, 106	0
1	B	408/488 (83%)	-0.12	5 (1%) 76 81	17, 26, 52, 86	0
All	All	816/976 (83%)	0.15	57 (6%) 24 28	17, 28, 68, 106	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	296	TRP	5.7
1	A	188	TYR	5.3
1	A	144	LEU	5.3
1	A	148	VAL	5.1
1	A	114	VAL	4.9
1	A	147	LEU	4.5
1	B	297	LYS	4.3
1	A	296	TRP	4.1
1	A	140	VAL	4.1
1	A	128	PHE	4.1
1	A	118	VAL	4.1
1	A	133	LEU	3.9
1	A	122	TYR	3.8
1	A	154	TYR	3.8
1	A	158	ILE	3.3
1	B	485	HIS	3.3
1	A	151	ILE	3.3
1	A	77	PRO	3.3
1	A	161	GLY	3.2
1	A	125	ALA	3.1
1	A	141	TYR	3.1
1	A	119	ASN	3.1
1	A	135	ILE	3.1
1	A	113	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	121	LEU	3.0
1	A	180	GLY	2.8
1	A	292	LYS	2.8
1	A	116	LYS	2.8
1	A	134	CYS	2.7
1	A	129	LEU	2.6
1	A	159	LEU	2.6
1	B	291	LEU	2.5
1	A	157	ILE	2.5
1	A	160	CYS	2.4
1	A	111	ALA	2.4
1	A	117	SER	2.4
1	A	183	SER	2.4
1	A	112	LEU	2.4
1	A	156	PRO	2.3
1	A	155	LYS	2.3
1	A	192	TYR	2.3
1	A	78	ILE	2.2
1	A	213	PHE	2.2
1	A	184	PHE	2.2
1	A	76	LYS	2.2
1	B	484	LYS	2.2
1	A	138	LYS	2.2
1	A	299	GLY	2.2
1	A	165	MET	2.1
1	A	181	ILE	2.1
1	A	106	VAL	2.1
1	A	191	MET	2.1
1	A	149	LYS	2.1
1	A	80	VAL	2.1
1	A	152	LYS	2.1
1	A	136	HIS	2.0
1	A	108	ASN	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](#)

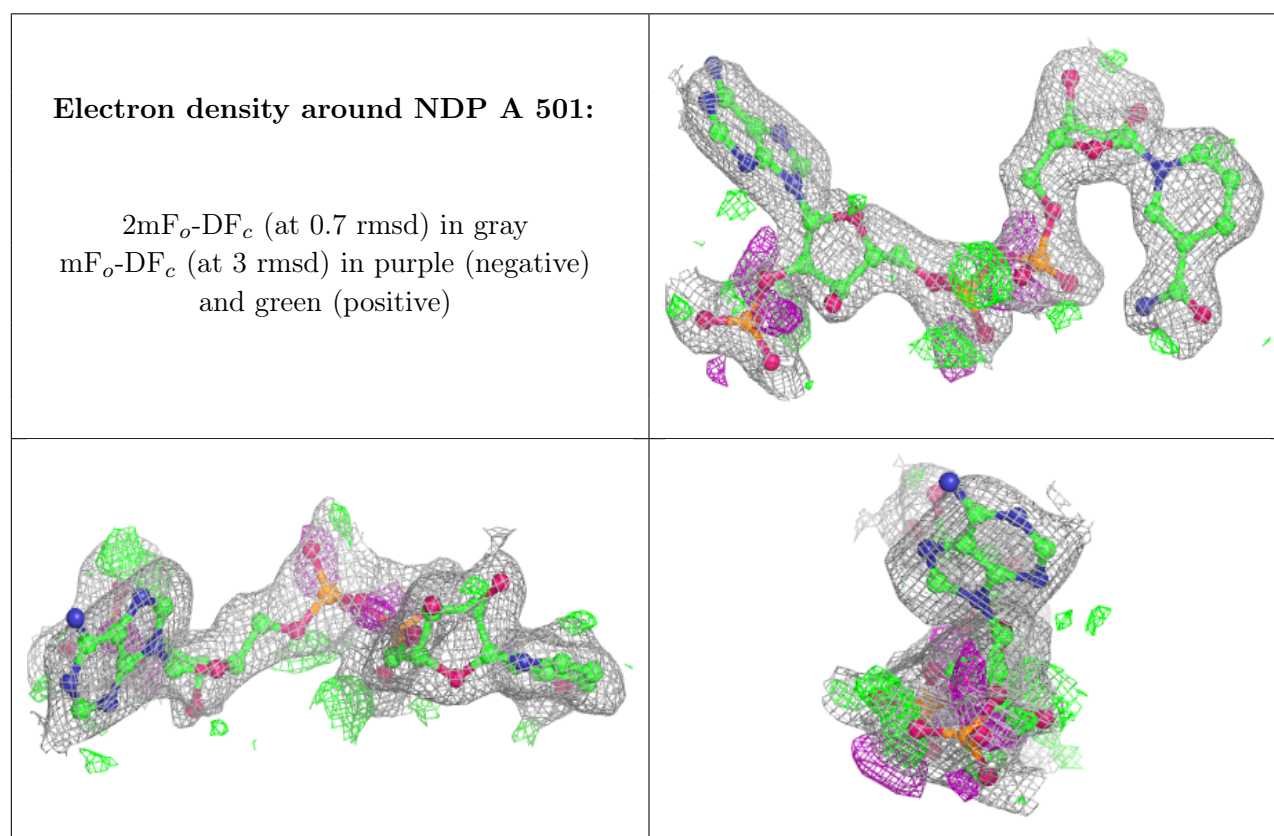
There are no oligosaccharides in this entry.

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.

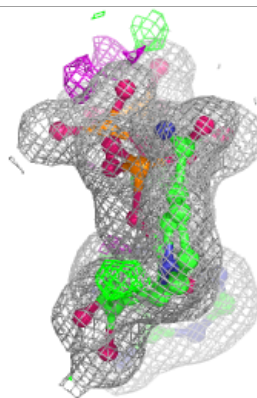
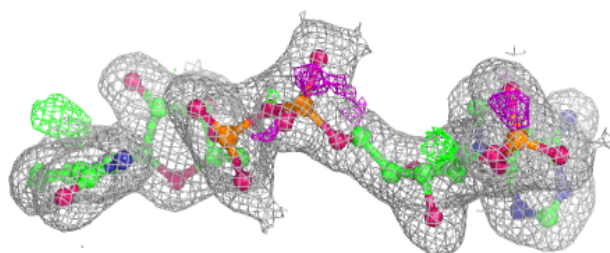
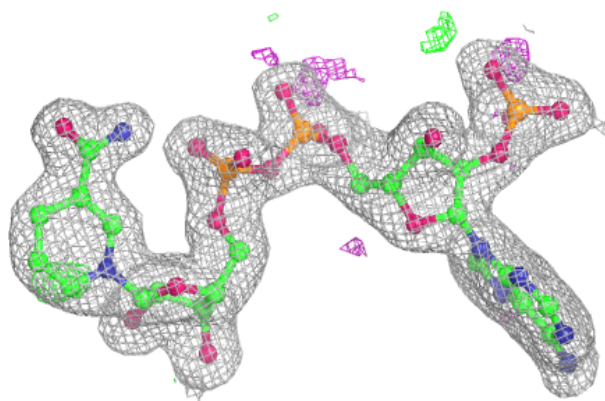
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NDP	A	501	48/48	0.84	0.12	31,53,70,72	0
5	GOL	B	507	6/6	0.92	0.12	22,27,31,32	0
5	GOL	A	504	6/6	0.93	0.10	27,29,34,35	0
2	NDP	B	501	48/48	0.97	0.06	19,25,29,31	0
4	A1L43	A	503	28/28	0.97	0.09	20,28,71,76	0
6	CA	B	505	1/1	0.97	0.07	33,33,33,33	0
4	A1L43	B	503	28/28	0.98	0.08	15,24,57,60	0
3	MN	B	502	1/1	0.99	0.02	18,18,18,18	0
6	CA	B	504	1/1	0.99	0.06	21,21,21,21	0
3	MN	A	502	1/1	0.99	0.02	21,21,21,21	0
6	CA	B	506	1/1	0.99	0.05	32,32,32,32	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.

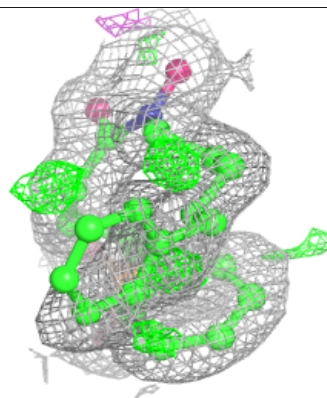
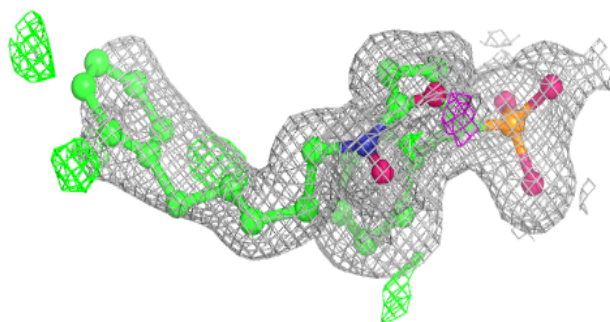
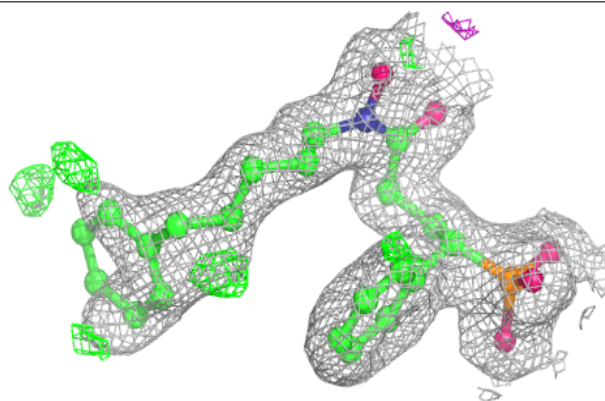


Electron density around NDP B 501:

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

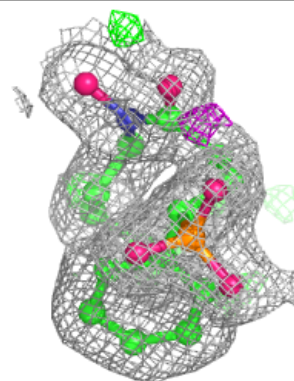
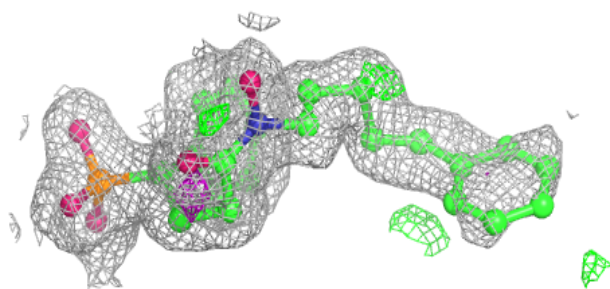
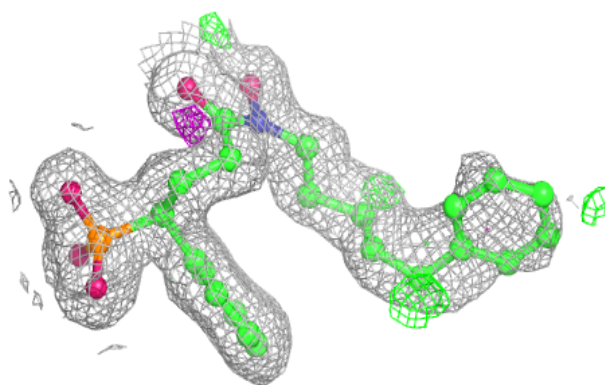
**Electron density around A1L43 A 503:**

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



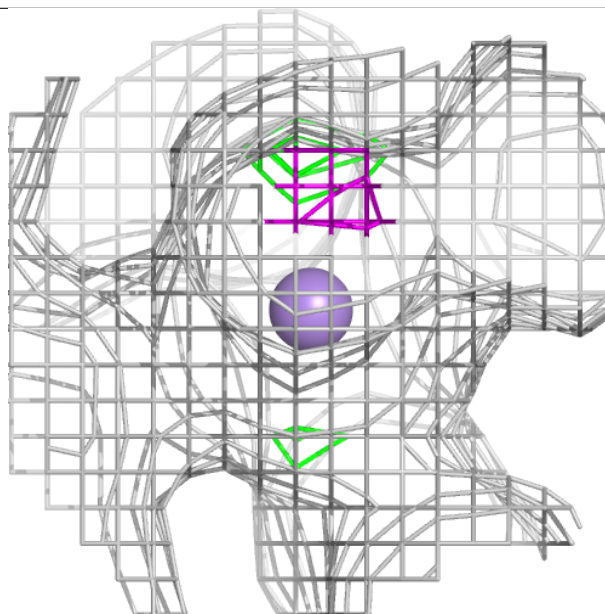
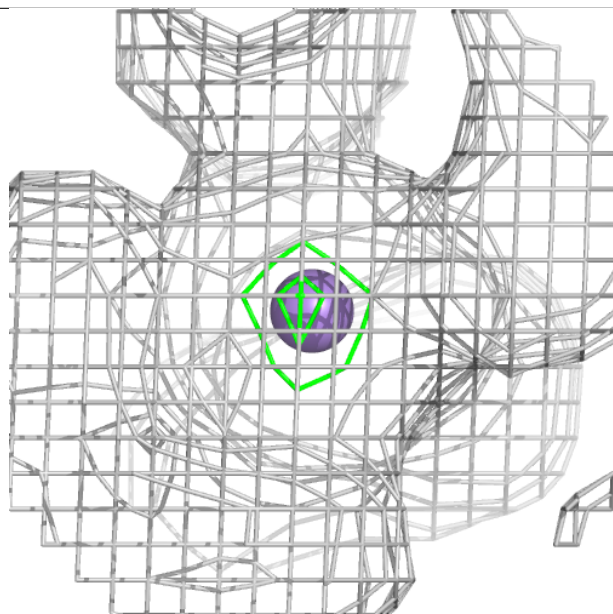
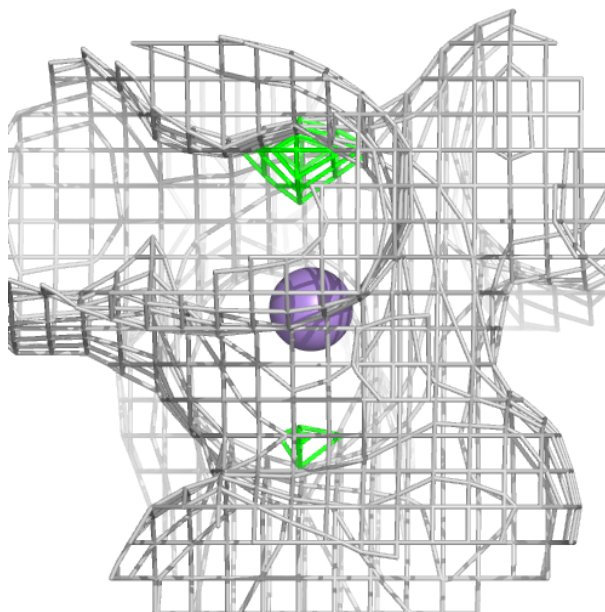
Electron density around A1L43 B 503:

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



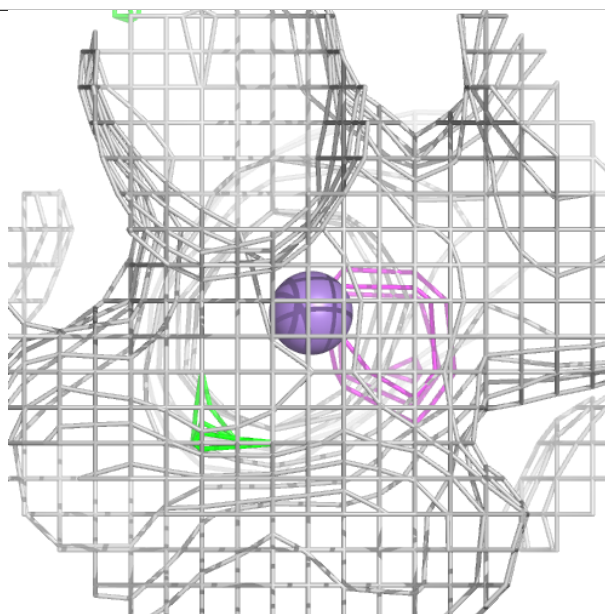
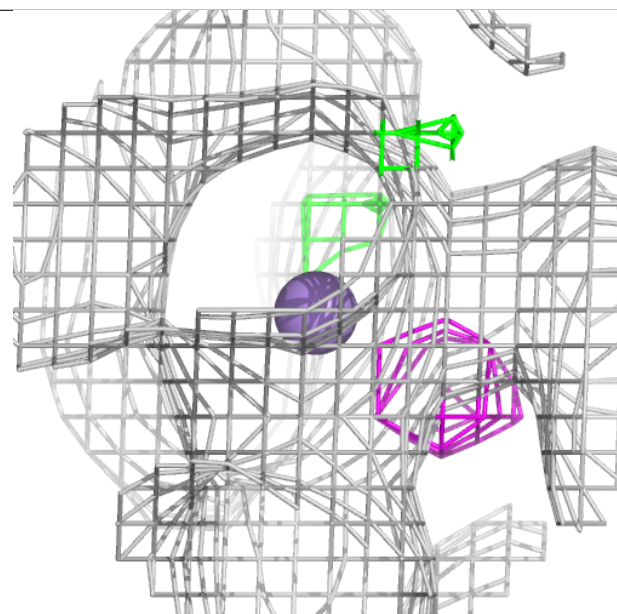
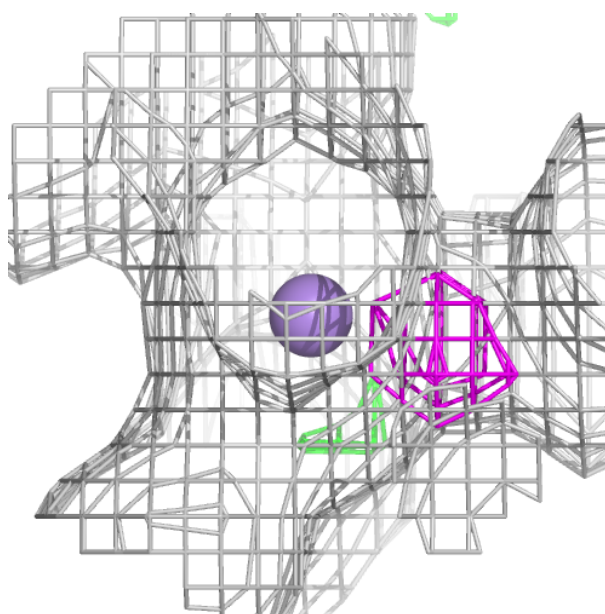
Electron density around MN B 502:

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



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)



6.5 Other polymers ⓘ

There are no such residues in this entry.