WORLDWIDE PDB

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Full wwPDB X-ray Structure Validation Report (i)

Sep 6, 2022 – 02:27 pm BST

PDB ID	:	7QVS
Title	:	Pseudomonas aeruginosa nicotinamide adenine dinucleotide kinase (NADK) structure in complex with NADP
Authors	:	Rahimova, R.; Gelin, M.; Labesse, G.; Lionne, C.
Deposited on	:	2022-01-23
Resolution	:	2.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.
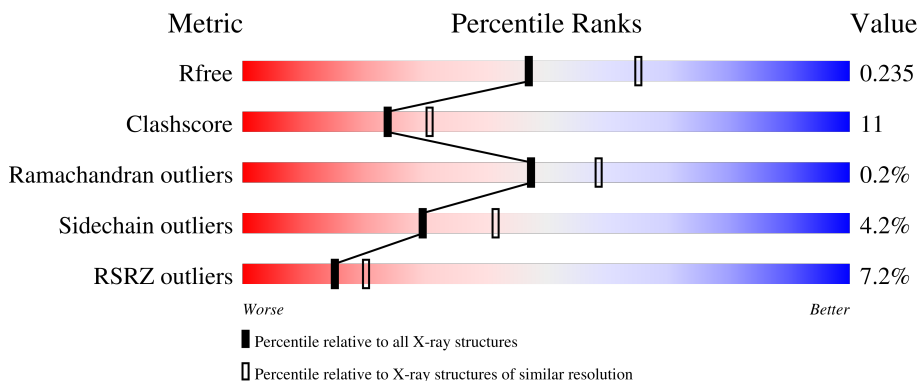
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	303	
1	B	303	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4659 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 NAD kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	5	0
			2181	1380	384	402	15			
1	B	283	Total	C	N	O	S	0	2	0
			2103	1334	368	387	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	296	LEU	-	expression tag	UNP A0A071KS55
A	297	GLU	-	expression tag	UNP A0A071KS55
A	298	HIS	-	expression tag	UNP A0A071KS55
A	299	HIS	-	expression tag	UNP A0A071KS55
A	300	HIS	-	expression tag	UNP A0A071KS55
A	301	HIS	-	expression tag	UNP A0A071KS55
A	302	HIS	-	expression tag	UNP A0A071KS55
A	303	HIS	-	expression tag	UNP A0A071KS55
B	296	LEU	-	expression tag	UNP A0A071KS55
B	297	GLU	-	expression tag	UNP A0A071KS55
B	298	HIS	-	expression tag	UNP A0A071KS55
B	299	HIS	-	expression tag	UNP A0A071KS55
B	300	HIS	-	expression tag	UNP A0A071KS55
B	301	HIS	-	expression tag	UNP A0A071KS55
B	302	HIS	-	expression tag	UNP A0A071KS55
B	303	HIS	-	expression tag	UNP A0A071KS55

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 96	C 42	N 14	O 34	P 6	0	1

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total 108	O 108	0	0
4	B	113	Total 113	O 113	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: NAD kinase
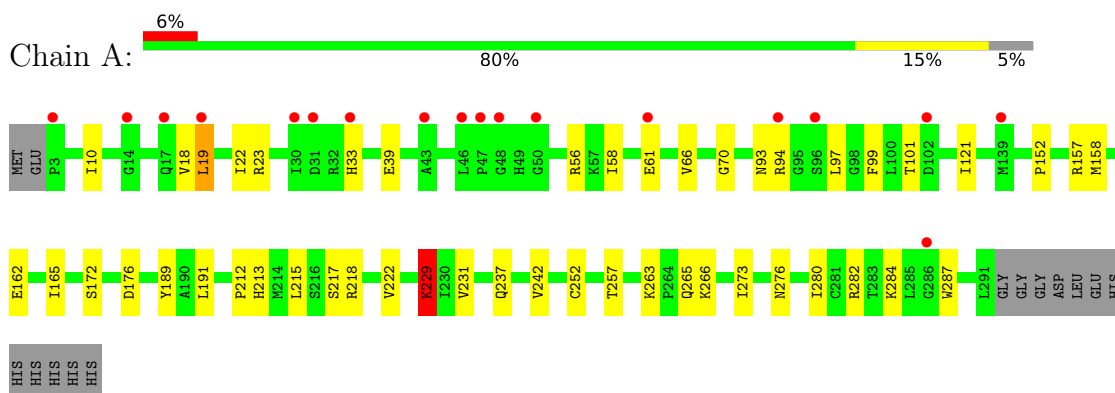
- Molecule 1: NAD kinase
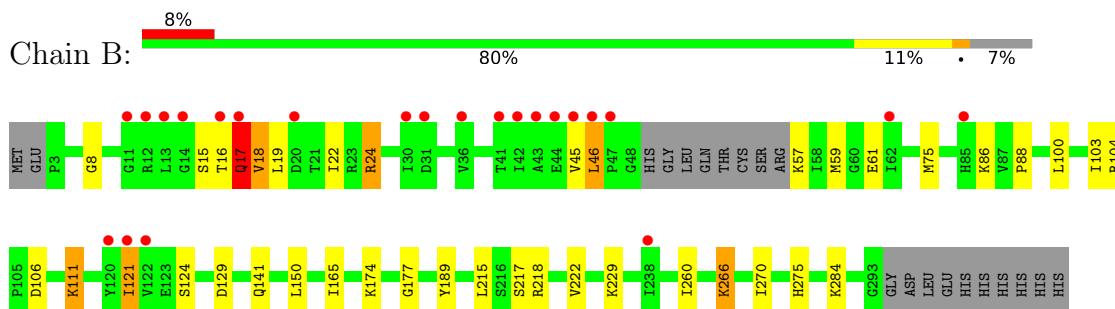
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	88.77Å 88.77Å 174.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.59 – 2.30 29.59 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.59-2.30) 99.8 (29.59-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.96 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122, PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.197 , 0.236 0.196 , 0.235	Depositor DCC
R_{free} test set	1570 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	31.5	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4659	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4, NAP

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	0.50	0/2241	0.77	8/3040 (0.3%)
1	B	0.65	4/2146 (0.2%)	0.85	8/2912 (0.3%)
All	All	0.58	4/4387 (0.1%)	0.81	16/5952 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	6	0
1	B	0	2
All	All	6	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	17[A]	GLN	N-CA	-12.46	1.21	1.46
1	B	17[B]	GLN	N-CA	-12.46	1.21	1.46
1	B	17[A]	GLN	CA-C	9.76	1.78	1.52
1	B	17[B]	GLN	CA-C	9.76	1.78	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17[A]	GLN	N-CA-C	14.96	151.39	111.00
1	B	17[B]	GLN	N-CA-C	14.96	151.39	111.00
1	B	17[A]	GLN	CA-C-N	-9.50	96.31	117.20
1	B	17[B]	GLN	CA-C-N	-9.50	96.31	117.20
1	B	17[A]	GLN	CA-C-O	-8.28	102.71	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17[B]	GLN	CA-C-O	-8.28	102.71	120.10
1	A	229[A]	LYS	N-CA-CB	8.12	125.22	110.60
1	A	229[B]	LYS	N-CA-CB	8.12	125.22	110.60
1	B	17[A]	GLN	CB-CA-C	-7.89	94.61	110.40
1	B	17[B]	GLN	CB-CA-C	-7.89	94.61	110.40
1	A	229[A]	LYS	CB-CA-C	7.86	126.13	110.40
1	A	229[B]	LYS	CB-CA-C	7.86	126.13	110.40
1	A	33[A]	HIS	CB-CA-C	7.29	124.97	110.40
1	A	33[B]	HIS	CB-CA-C	7.29	124.97	110.40
1	A	33[A]	HIS	N-CA-CB	6.42	122.15	110.60
1	A	33[B]	HIS	N-CA-CB	6.42	122.15	110.60

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	33[A]	HIS	CA
1	A	33[B]	HIS	CA
1	A	102[A]	ASP	CA
1	A	102[B]	ASP	CA
1	A	229[A]	LYS	CA
1	A	229[B]	LYS	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	17[A]	GLN	Mainchain
1	B	17[B]	GLN	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	2181	0	2166	44	0
1	B	2103	0	2097	48	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	48	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	96	0	48	6	0
4	A	108	0	0	5	0
4	B	113	0	0	2	0
All	All	4659	0	4335	97	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 11.

All (97) 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:124:SER:HB3	1:B:266:LYS:CD	1.60	1.30
3:B:402[B]:NAP:O4D	3:B:402[B]:NAP:C4D	1.64	1.26
3:B:402[A]:NAP:C4D	3:B:402[A]:NAP:O4D	1.65	1.25
1:B:124:SER:CB	1:B:266:LYS:HD3	1.72	1.19
1:A:229[B]:LYS:HD3	1:A:257:THR:HB	1.21	1.17
1:A:58:ILE:CD1	1:A:61:GLU:HG3	1.80	1.10
1:A:58:ILE:HD12	1:A:61:GLU:HG3	1.08	1.08
1:B:24:ARG:HG2	1:B:24:ARG:HH11	1.28	0.99
1:A:229[A]:LYS:HE3	4:A:542:HOH:O	1.64	0.97
1:A:229[A]:LYS:CE	4:A:542:HOH:O	2.12	0.96
1:A:58:ILE:HD12	1:A:61:GLU:CG	1.98	0.93
1:B:17[A]:GLN:CA	1:B:18:VAL:N	2.33	0.91
1:B:17[B]:GLN:CA	1:B:18:VAL:N	2.36	0.87
1:B:15:SER:O	1:B:19:LEU:HD12	1.74	0.87
1:B:124:SER:HB3	1:B:266:LYS:HD3	0.86	0.83
1:B:121:ILE:HD11	1:B:275:HIS:HB3	1.65	0.79
1:B:266:LYS:NZ	1:B:266:LYS:HB3	1.98	0.77
1:B:15:SER:HB3	1:B:18:VAL:HB	1.69	0.74
1:A:229[B]:LYS:HD3	1:A:257:THR:CB	2.09	0.74
1:B:18:VAL:CG1	1:B:19:LEU:N	2.52	0.72
1:B:18:VAL:HG12	1:B:19:LEU:N	2.04	0.72
1:A:229[A]:LYS:HE2	4:A:542:HOH:O	1.81	0.70
1:A:58:ILE:CD1	1:A:61:GLU:CG	2.66	0.67
1:A:93:ASN:OD1	1:A:101:THR:OG1	2.14	0.65
1:B:24:ARG:HG2	1:B:24:ARG:NH1	2.05	0.65
1:B:124:SER:HB3	1:B:266:LYS:CG	2.25	0.65
1:A:266:LYS:HE2	4:A:562:HOH:O	1.98	0.64
1:B:18:VAL:HG12	1:B:19:LEU:H	1.64	0.62
1:A:229[B]:LYS:NZ	1:A:257:THR:HG21	2.15	0.62
1:A:229[B]:LYS:CD	1:A:257:THR:HB	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LEU:O	1:A:218:ARG:NH1	2.34	0.61
1:B:229:LYS:NZ	4:B:501:HOH:O	2.33	0.61
1:B:124:SER:CB	1:B:266:LYS:CD	2.52	0.59
1:A:158[A]:MET:CE	1:A:213:HIS:HB2	2.34	0.57
1:B:24:ARG:HH11	1:B:24:ARG:CG	2.09	0.57
1:B:15:SER:OG	1:B:17[A]:GLN:NE2	2.38	0.56
1:B:129:ASP:OD1	1:B:141:GLN:NE2	2.40	0.55
1:A:276:ASN:O	1:A:280:ILE:HG12	2.07	0.54
1:A:58:ILE:HG13	1:A:58:ILE:O	2.09	0.52
1:A:165:ILE:HD13	1:A:222:VAL:HG11	1.92	0.52
1:B:45:VAL:C	1:B:46:LEU:HD23	2.30	0.52
1:A:19:LEU:HD12	1:A:23:ARG:HH12	1.75	0.51
1:A:162:GLU:HG2	1:A:172:SER:HB3	1.93	0.51
1:A:19:LEU:HD12	1:A:23:ARG:NH1	2.25	0.51
1:B:266:LYS:HB3	1:B:266:LYS:HZ2	1.72	0.51
1:B:75:MET:HG2	1:B:100:LEU:HB3	1.93	0.50
1:A:229[B]:LYS:HZ3	1:A:257:THR:HG21	1.77	0.49
1:B:150:LEU:O	1:B:177:GLY:HA3	2.13	0.49
1:A:10:ILE:HD12	1:A:66:VAL:HG11	1.95	0.49
1:B:165:ILE:HD13	1:B:222:VAL:HG11	1.95	0.49
1:A:152:PRO:HD3	1:A:176:ASP:O	2.13	0.48
1:A:157:ARG:NH2	1:A:237:GLN:HB2	2.28	0.48
1:A:158[A]:MET:HE1	1:A:213:HIS:HB2	1.97	0.47
1:A:121:ILE:HG13	1:A:273:ILE:HA	1.96	0.46
1:B:88:PRO:HB2	1:B:270:ILE:HD11	1.97	0.46
3:B:402[B]:NAP:O4D	3:B:402[B]:NAP:C5D	2.53	0.46
1:B:215:LEU:O	1:B:218:ARG:NH1	2.49	0.45
1:A:212:PRO:HG3	1:A:217:SER:HB3	1.98	0.45
1:B:24:ARG:NH1	1:B:24:ARG:CG	2.72	0.45
1:A:58:ILE:HD11	1:A:61:GLU:HG3	1.89	0.44
1:A:70:GLY:HA2	1:A:94:ARG:HG3	1.98	0.44
3:B:402[A]:NAP:O4D	3:B:402[A]:NAP:C5D	2.55	0.44
1:A:157:ARG:HH22	1:A:237:GLN:HB2	1.83	0.44
1:A:231:VAL:HG22	1:A:257:THR:HG22	1.99	0.44
1:A:282:ARG:HG3	1:A:287:TRP:HB2	1.99	0.44
1:B:88:PRO:CB	1:B:270:ILE:HD11	2.48	0.44
1:A:58:ILE:CD1	1:A:61:GLU:HB2	2.48	0.43
1:B:22:ILE:HD13	1:B:22:ILE:HA	1.85	0.43
1:B:266:LYS:HB3	1:B:266:LYS:HZ1	1.81	0.43
1:B:129:ASP:O	1:B:260:ILE:HA	2.18	0.42
1:A:158[A]:MET:HE3	1:A:213:HIS:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17[A]:GLN:CA	1:B:18:VAL:H	2.27	0.42
1:A:18:VAL:O	1:A:22:ILE:HD12	2.20	0.42
1:A:229[B]:LYS:HZ2	1:A:257:THR:HG21	1.85	0.41
3:B:402[A]:NAP:H51A	3:B:402[A]:NAP:O1N	2.20	0.41
1:A:39:GLU:O	1:A:39:GLU:HG3	2.20	0.41
1:B:104:ARG:NH1	1:B:106:ASP:OD1	2.53	0.41
4:A:520:HOH:O	3:B:402[B]:NAP:H6N	2.21	0.41
1:B:103:ILE:HG12	1:B:111:LYS:HG2	2.03	0.41
1:A:99:PHE:CE2	1:A:284:LYS:HD3	2.55	0.41
1:A:242:VAL:HG23	1:A:252:CYS:SG	2.61	0.41
1:A:265:GLN:N	1:A:265:GLN:CD	2.74	0.41
1:B:8:GLY:HA3	1:B:59:MET:HE3	2.03	0.41
1:B:19:LEU:HD23	1:B:46:LEU:CD2	2.51	0.41
1:B:57:LYS:N	4:B:509:HOH:O	2.52	0.41
1:A:265:GLN:CD	1:A:265:GLN:H	2.24	0.41
1:A:191:LEU:HD21	1:B:215:LEU:HD11	2.03	0.40
1:A:97:LEU:HD13	1:A:280:ILE:HD12	2.02	0.40
1:B:266:LYS:NZ	1:B:266:LYS:CB	2.72	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	292/303 (96%)	284 (97%)	8 (3%)	0	100	100
1	B	281/303 (93%)	271 (96%)	8 (3%)	2 (1%)	22	26
All	All	573/606 (95%)	555 (97%)	16 (3%)	2 (0%)	47	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	17[A]	GLN
1	B	17[B]	GLN

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	234/256 (91%)	228 (97%)	6 (3%)	46	63
1	B	222/256 (87%)	207 (93%)	15 (7%)	16	21
All	All	456/512 (89%)	435 (95%)	21 (5%)	30	38

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	56	ARG
1	A	189	TYR
1	A	229[A]	LYS
1	A	229[B]	LYS
1	A	263	LYS
1	B	16	THR
1	B	17[A]	GLN
1	B	17[B]	GLN
1	B	18	VAL
1	B	24	ARG
1	B	46	LEU
1	B	61	GLU
1	B	86	LYS
1	B	111	LYS
1	B	121	ILE
1	B	174	LYS
1	B	189	TYR
1	B	217	SER
1	B	266	LYS
1	B	284	LYS

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

Mol	Chain	Res	Type
1	A	241	GLN
1	B	85	HIS
1	B	173	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	PO4	A	401	-	4,4,4	0.94	0	6,6,6	0.35	0
3	NAP	B	402[B]	-	45,52,52	3.31	17 (37%)	56,80,80	1.32	6 (10%)
2	PO4	B	401	-	4,4,4	0.84	0	6,6,6	0.69	0
3	NAP	B	402[A]	-	45,52,52	3.36	18 (40%)	56,80,80	1.21	7 (12%)
3	NAP	A	402	-	45,52,52	3.20	17 (37%)	56,80,80	1.34	6 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	B	402[A]	-	-	9/31/67/67	0/5/5/5
3	NAP	A	402	-	-	5/31/67/67	0/5/5/5
3	NAP	B	402[B]	-	-	9/31/67/67	0/5/5/5

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402[A]	NAP	O4D-C4D	9.30	1.65	1.45
3	B	402[B]	NAP	O4D-C4D	8.90	1.64	1.45
3	A	402	NAP	C3B-C4B	-8.07	1.32	1.53
3	B	402[B]	NAP	C3B-C4B	-8.05	1.32	1.53
3	B	402[A]	NAP	C3B-C4B	-8.00	1.32	1.53
3	B	402[A]	NAP	C3D-C4D	-7.92	1.32	1.53
3	A	402	NAP	C3D-C4D	-7.62	1.33	1.53
3	B	402[B]	NAP	C3D-C4D	-7.45	1.34	1.53
3	A	402	NAP	O4D-C4D	7.44	1.61	1.45
3	B	402[A]	NAP	O4B-C4B	6.97	1.60	1.45
3	B	402[B]	NAP	O4D-C1D	-6.86	1.31	1.41
3	A	402	NAP	O4D-C1D	-6.84	1.31	1.41
3	B	402[B]	NAP	O4B-C4B	6.74	1.60	1.45
3	B	402[A]	NAP	O4D-C1D	-6.45	1.32	1.41
3	A	402	NAP	O4B-C4B	6.25	1.59	1.45
3	B	402[A]	NAP	O4B-C1B	-6.17	1.32	1.41
3	A	402	NAP	O4B-C1B	-6.13	1.32	1.41
3	B	402[B]	NAP	O4B-C1B	-6.01	1.32	1.41
3	A	402	NAP	P2B-O2B	5.37	1.69	1.59
3	B	402[A]	NAP	C7N-N7N	5.14	1.42	1.33
3	A	402	NAP	C7N-N7N	4.99	1.42	1.33
3	B	402[B]	NAP	P2B-O2B	4.96	1.68	1.59
3	B	402[B]	NAP	C7N-N7N	4.89	1.42	1.33
3	B	402[A]	NAP	O2D-C2D	-4.78	1.31	1.43
3	B	402[B]	NAP	O2D-C2D	-4.58	1.32	1.43
3	B	402[A]	NAP	P2B-O2B	4.53	1.67	1.59
3	A	402	NAP	O2D-C2D	-3.98	1.33	1.43
3	B	402[A]	NAP	O3B-C3B	3.78	1.51	1.43
3	B	402[B]	NAP	O3B-C3B	3.59	1.51	1.43
3	A	402	NAP	O3B-C3B	3.39	1.51	1.43
3	B	402[B]	NAP	P2B-O1X	3.19	1.60	1.50
3	B	402[A]	NAP	P2B-O1X	3.06	1.60	1.50
3	B	402[A]	NAP	C6A-N6A	3.00	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	NAP	C2D-C1D	2.95	1.58	1.53
3	B	402[B]	NAP	C6A-N6A	2.93	1.44	1.34
3	A	402	NAP	C6A-N6A	2.85	1.44	1.34
3	A	402	NAP	P2B-O1X	2.67	1.59	1.50
3	A	402	NAP	C2A-N1A	-2.66	1.29	1.33
3	B	402[A]	NAP	C2A-N1A	-2.47	1.29	1.33
3	B	402[A]	NAP	PA-O5B	2.47	1.69	1.59
3	B	402[B]	NAP	C2D-C3D	2.41	1.59	1.53
3	B	402[A]	NAP	C2D-C1D	2.38	1.57	1.53
3	B	402[B]	NAP	C2N-N1N	-2.34	1.32	1.35
3	A	402	NAP	C2N-N1N	-2.32	1.32	1.35
3	B	402[B]	NAP	PA-O5B	2.28	1.68	1.59
3	B	402[B]	NAP	C2A-N1A	-2.22	1.29	1.33
3	B	402[B]	NAP	O3D-C3D	2.21	1.48	1.43
3	B	402[A]	NAP	O3D-C3D	2.11	1.47	1.43
3	A	402	NAP	O3D-C3D	2.09	1.47	1.43
3	B	402[A]	NAP	C2D-C3D	2.03	1.58	1.53
3	B	402[A]	NAP	C8A-N7A	-2.02	1.31	1.34
3	A	402	NAP	C8A-N7A	-2.00	1.31	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402[B]	NAP	N3A-C2A-N1A	-4.33	121.91	128.68
3	B	402[A]	NAP	N3A-C2A-N1A	-4.31	121.94	128.68
3	A	402	NAP	C3N-C2N-N1N	-4.00	116.52	120.43
3	A	402	NAP	N3A-C2A-N1A	-3.91	122.57	128.68
3	B	402[B]	NAP	C6N-N1N-C2N	3.45	125.12	121.97
3	A	402	NAP	C2N-C3N-C4N	3.21	121.90	118.26
3	B	402[B]	NAP	C3N-C2N-N1N	-3.07	117.43	120.43
3	A	402	NAP	C6N-N1N-C2N	2.91	124.63	121.97
3	B	402[B]	NAP	C4A-C5A-N7A	-2.80	106.48	109.40
3	B	402[A]	NAP	C3D-C2D-C1D	2.76	105.13	100.98
3	B	402[A]	NAP	C4A-C5A-N7A	-2.73	106.56	109.40
3	B	402[B]	NAP	C2N-C3N-C4N	2.65	121.26	118.26
3	A	402	NAP	C1B-N9A-C4A	-2.59	122.09	126.64
3	B	402[A]	NAP	C6N-N1N-C2N	2.50	124.25	121.97
3	B	402[A]	NAP	C3N-C2N-N1N	-2.41	118.07	120.43
3	A	402	NAP	C4A-C5A-N7A	-2.40	106.90	109.40
3	B	402[A]	NAP	C2B-C3B-C4B	2.30	107.00	101.99
3	B	402[B]	NAP	C5N-C4N-C3N	-2.19	117.75	120.34
3	B	402[A]	NAP	C2N-C3N-C4N	2.01	120.54	118.26

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402[A]	NAP	O4D-C4D-C5D-O5D
3	B	402[A]	NAP	C3D-C4D-C5D-O5D
3	B	402[B]	NAP	C5B-O5B-PA-O1A
3	B	402[B]	NAP	C5B-O5B-PA-O2A
3	B	402[B]	NAP	PA-O3-PN-O5D
3	B	402[B]	NAP	C3B-C2B-O2B-P2B
3	A	402	NAP	C3B-C2B-O2B-P2B
3	B	402[A]	NAP	C3B-C2B-O2B-P2B
3	A	402	NAP	C1B-C2B-O2B-P2B
3	B	402[A]	NAP	C1B-C2B-O2B-P2B
3	B	402[A]	NAP	O4B-C4B-C5B-O5B
3	A	402	NAP	PN-O3-PA-O5B
3	B	402[A]	NAP	PA-O3-PN-O5D
3	B	402[B]	NAP	PN-O3-PA-O5B
3	B	402[A]	NAP	C2B-O2B-P2B-O2X
3	B	402[A]	NAP	C2B-O2B-P2B-O3X
3	B	402[B]	NAP	C5B-O5B-PA-O3
3	B	402[B]	NAP	C2B-O2B-P2B-O2X
3	B	402[B]	NAP	C1B-C2B-O2B-P2B
3	B	402[B]	NAP	PN-O3-PA-O1A
3	B	402[A]	NAP	C3B-C4B-C5B-O5B
3	A	402	NAP	C2B-O2B-P2B-O3X
3	A	402	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402[B]	NAP	3	0
3	B	402[A]	NAP	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 then 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
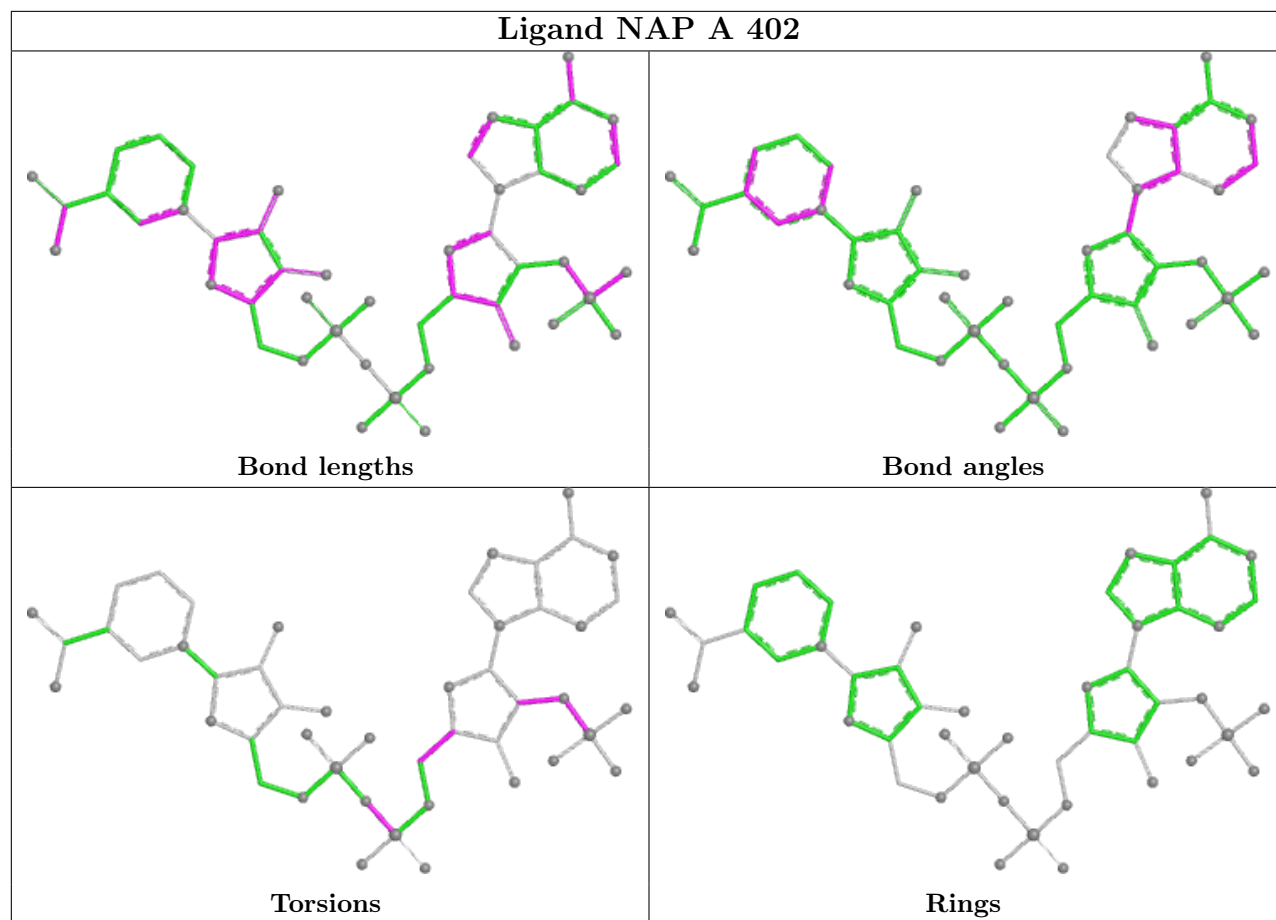
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PO4 A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP B 402 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand PO4 B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP B 402 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP A 402

Bond lengths

Bond angles

Torsions

Rings
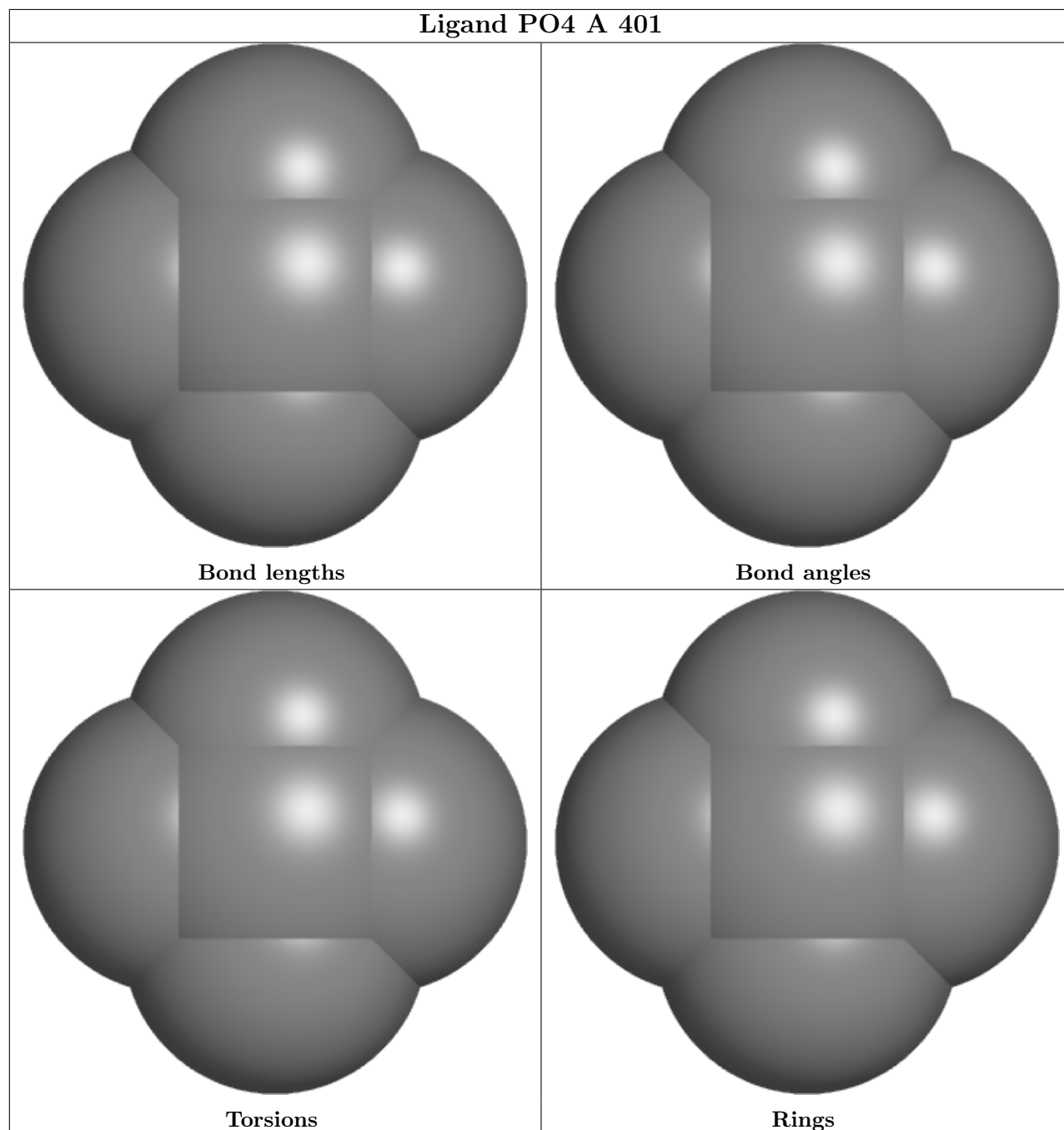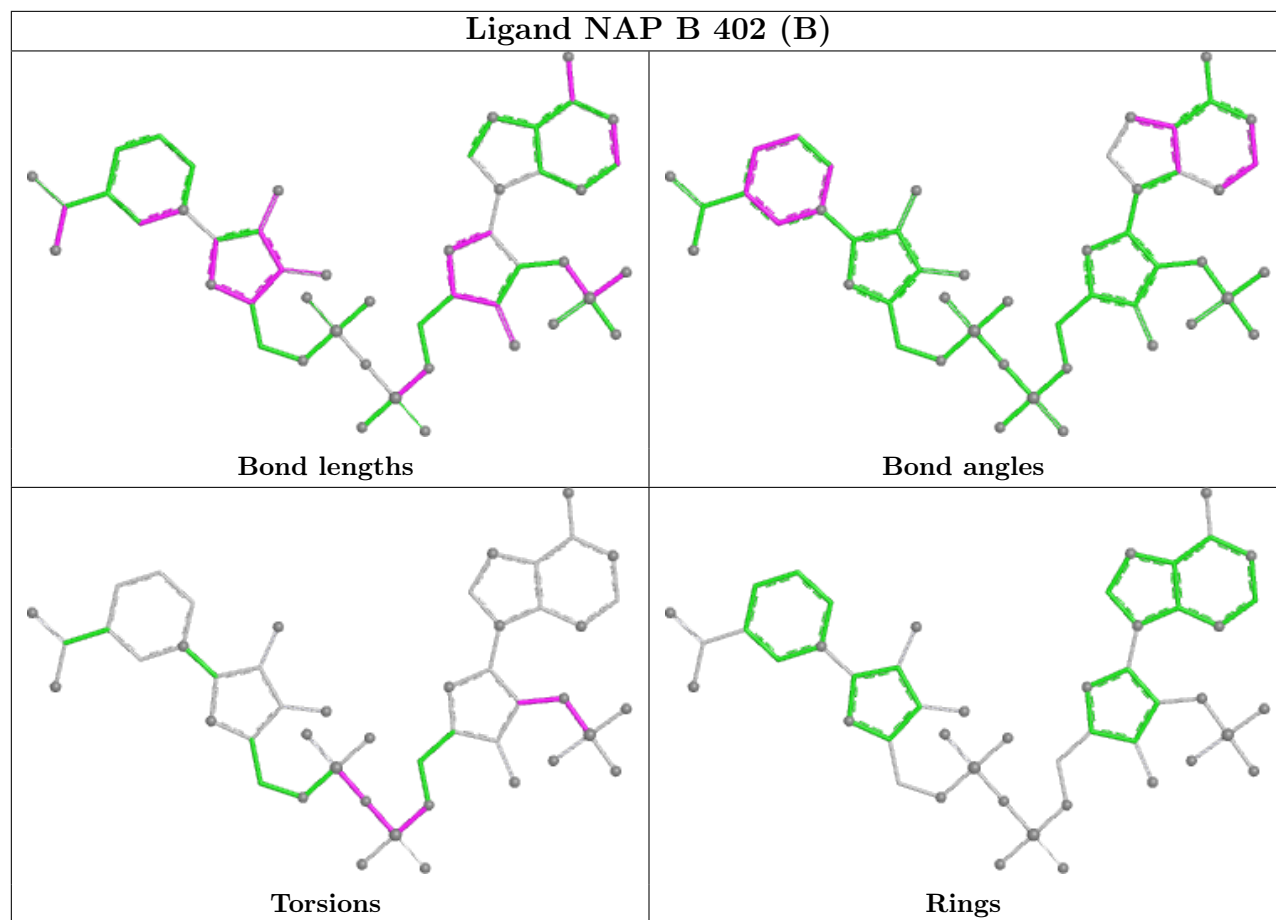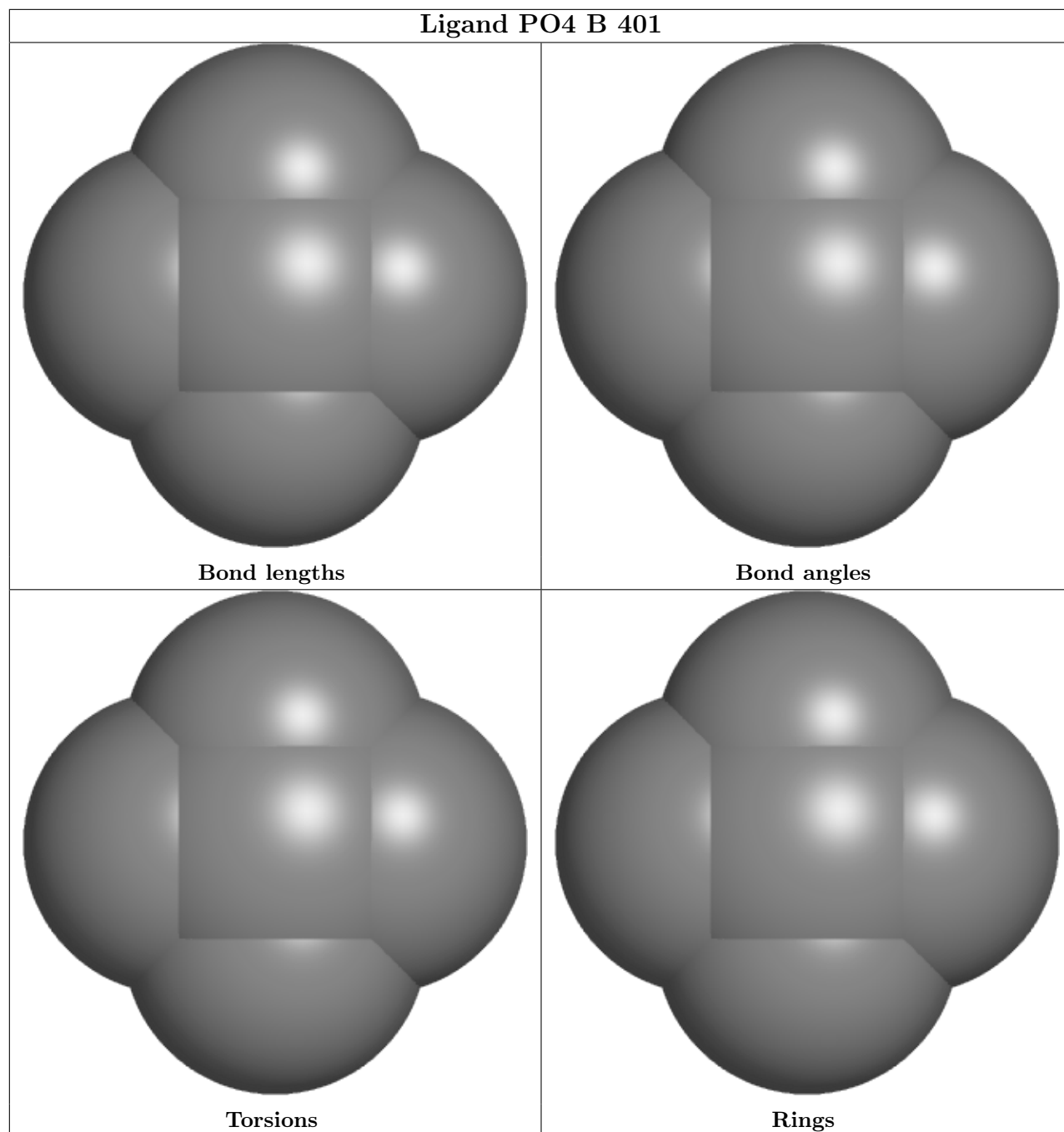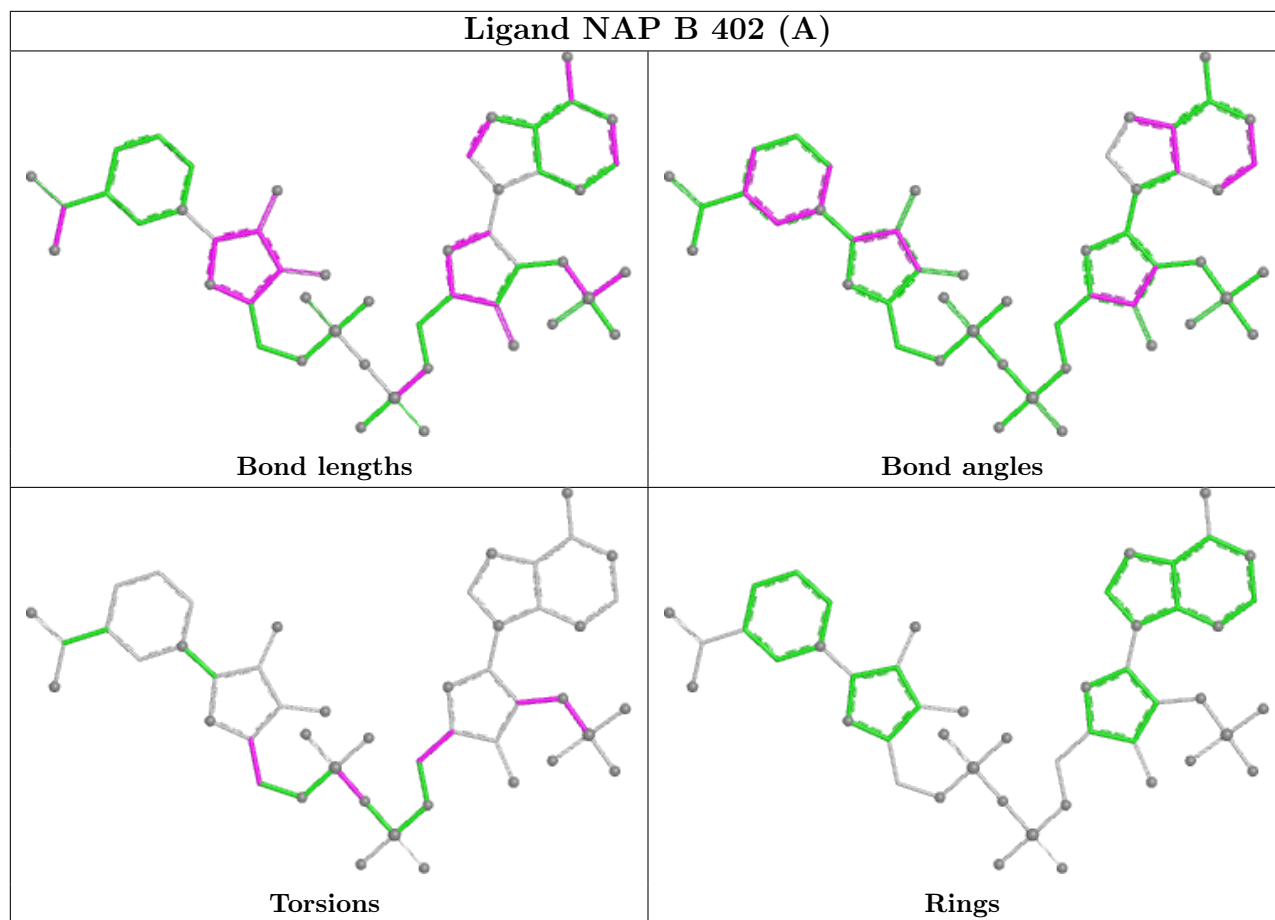
5.7 Other polymers ⓘ

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	289/303 (95%)	0.21	18 (6%)	20	26	14, 34, 77, 96	0
1	B	283/303 (93%)	0.38	23 (8%)	12	16	17, 37, 86, 118	1 (0%)
All	All	572/606 (94%)	0.29	41 (7%)	15	20	14, 36, 82, 118	1 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	62	ILE	5.4
1	A	33[A]	HIS	5.2
1	B	43	ALA	5.0
1	B	42	ILE	4.5
1	B	16	THR	4.5
1	A	47	PRO	4.1
1	B	13	LEU	3.9
1	A	14	GLY	3.9
1	B	46	LEU	3.5
1	A	30	ILE	3.4
1	B	14	GLY	3.3
1	B	41	THR	3.2
1	B	44	GLU	3.1
1	B	20	ASP	3.0
1	B	47	PRO	2.9
1	A	46	LEU	2.9
1	B	121	ILE	2.8
1	A	102[A]	ASP	2.7
1	A	48	GLY	2.7
1	B	120	TYR	2.6
1	A	17	GLN	2.6
1	A	31	ASP	2.6
1	B	11	GLY	2.5
1	B	12	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	17[A]	GLN	2.5
1	A	96	SER	2.4
1	B	45	VAL	2.4
1	B	31	ASP	2.3
1	A	61	GLU	2.3
1	A	43	ALA	2.3
1	B	85	HIS	2.2
1	B	36	VAL	2.2
1	B	122	VAL	2.2
1	A	3	PRO	2.2
1	B	30	ILE	2.2
1	A	94	ARG	2.2
1	A	286	GLY	2.2
1	A	50	GLY	2.1
1	A	139	MET	2.1
1	A	19	LEU	2.1
1	B	238	ILE	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 monosaccharides in this entry.

6.4 Ligands ⓘ

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
3	NAP	B	402[A]	48/48	0.83	0.21	22,27,41,44	48
3	NAP	B	402[B]	48/48	0.83	0.21	21,27,44,48	48
2	PO4	A	401	5/5	0.92	0.20	40,45,53,58	0
3	NAP	A	402	48/48	0.92	0.13	17,23,37,42	0
2	PO4	B	401	5/5	0.96	0.18	54,56,56,61	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.
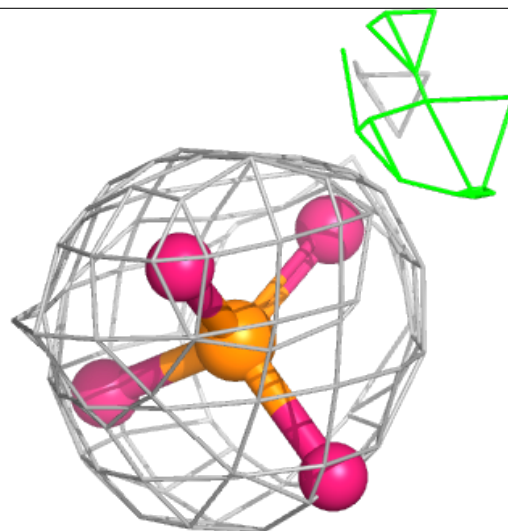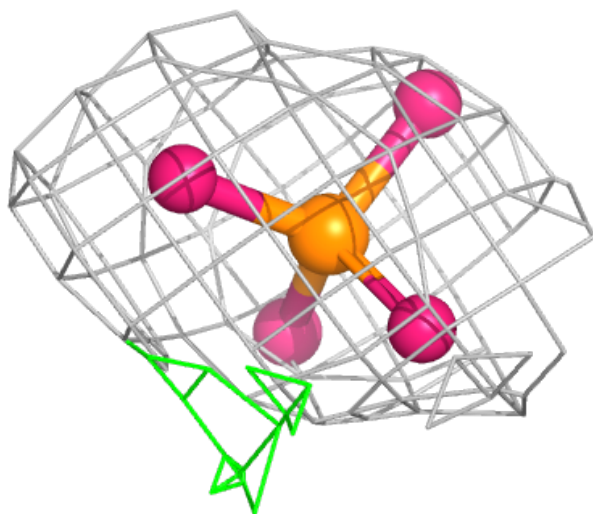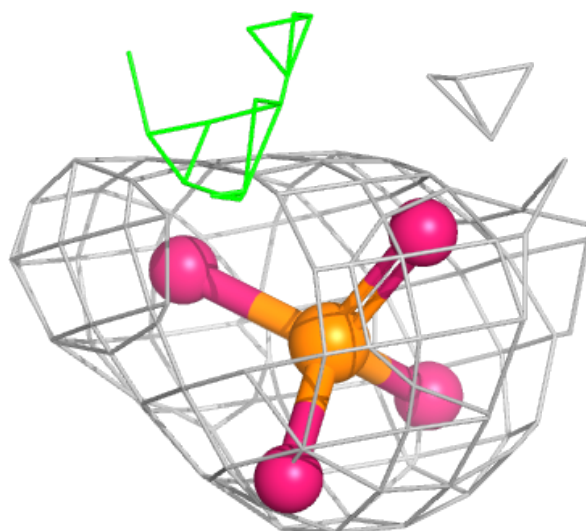
Electron density around NAP B 402 (A):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
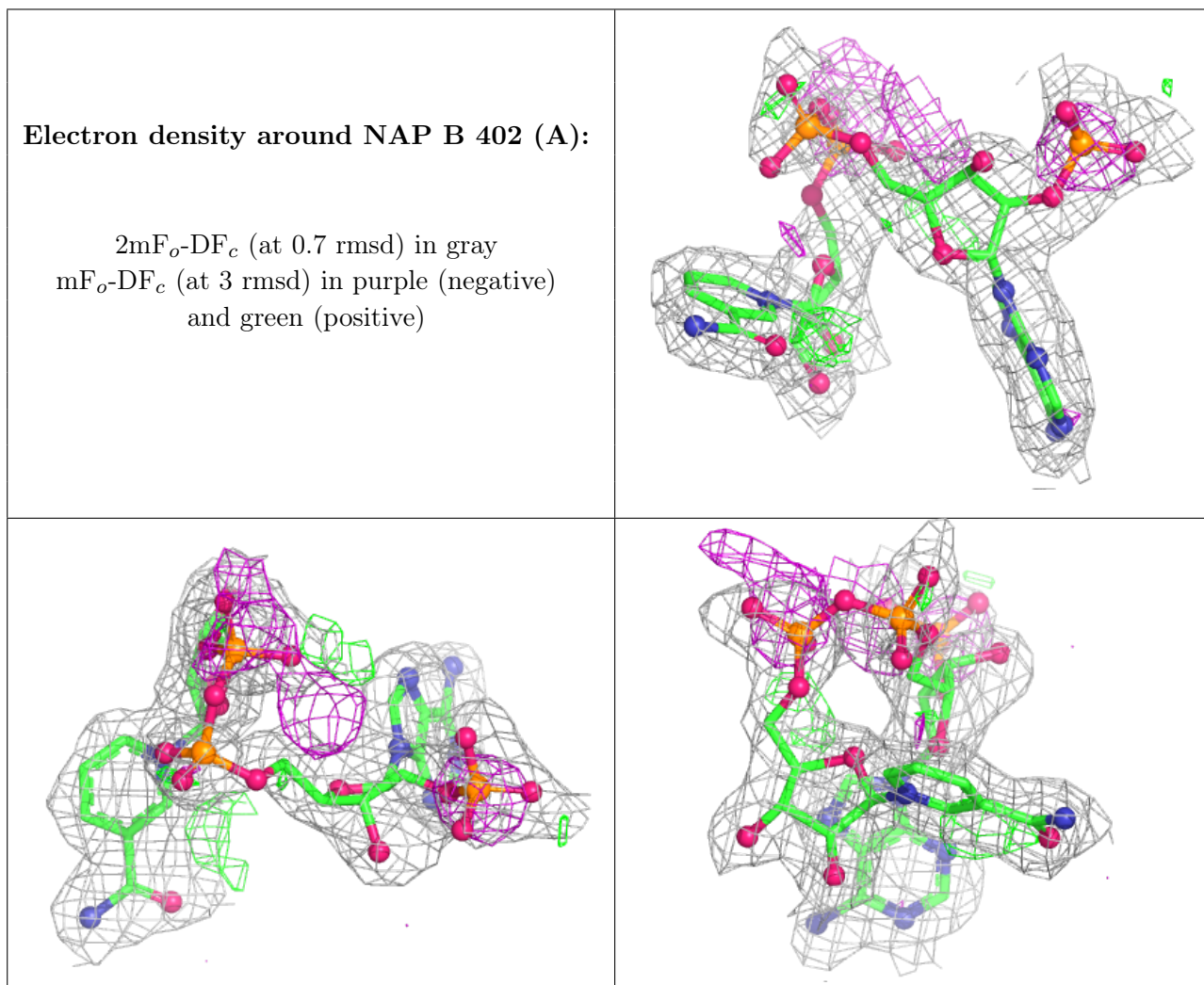
Electron density around NAP B 402 (B):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
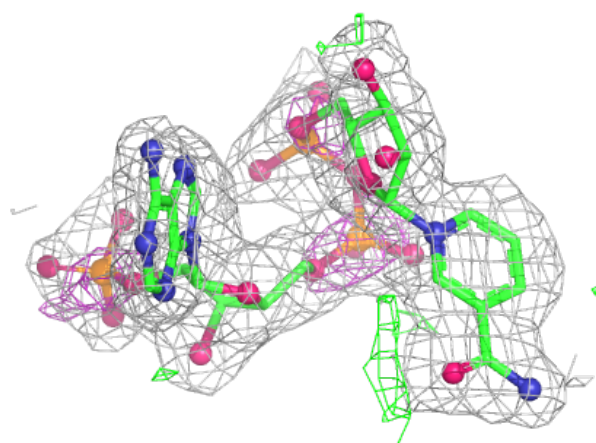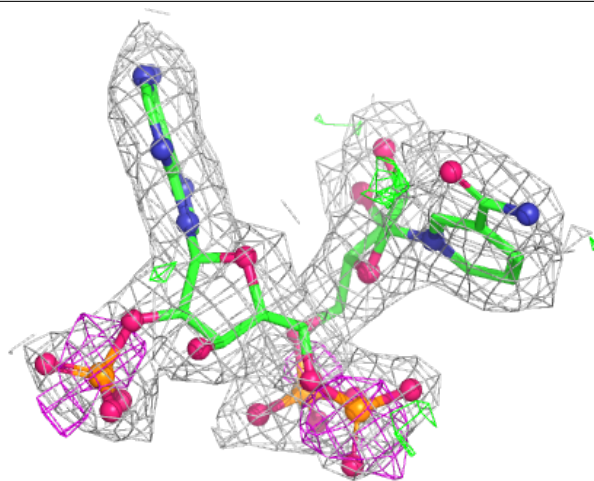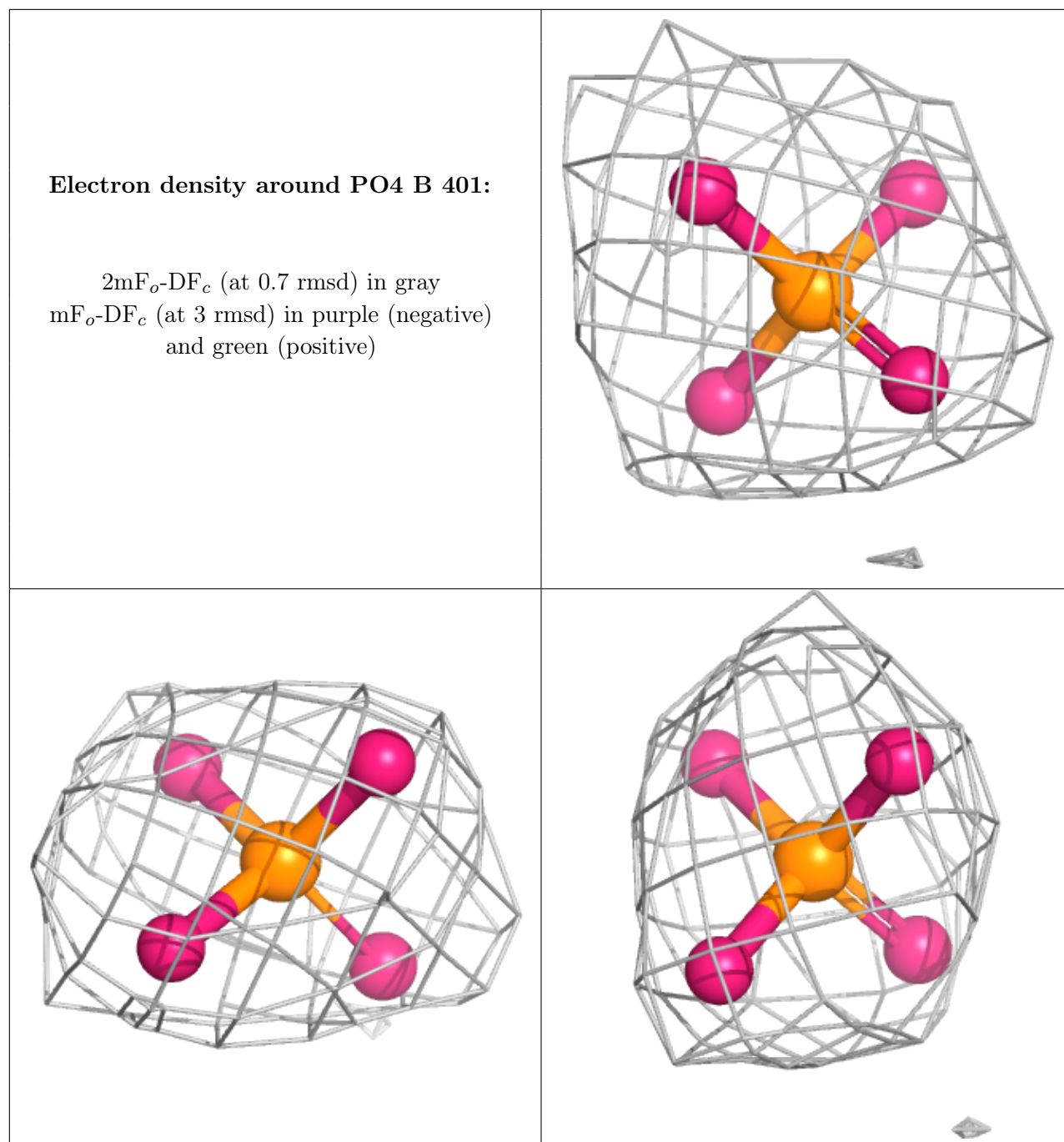and green (positive)
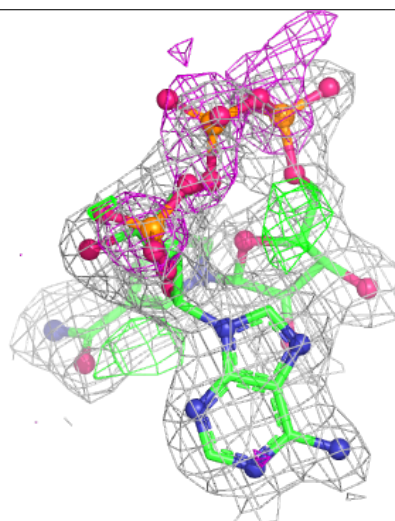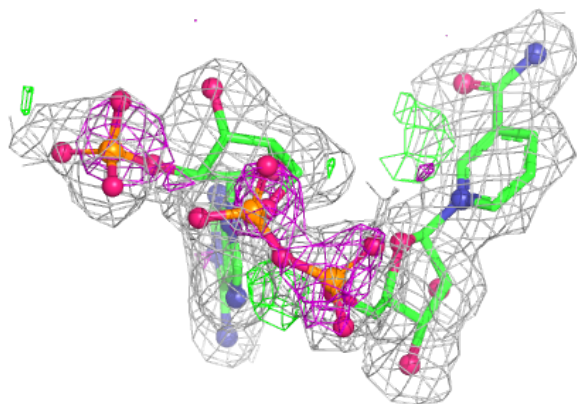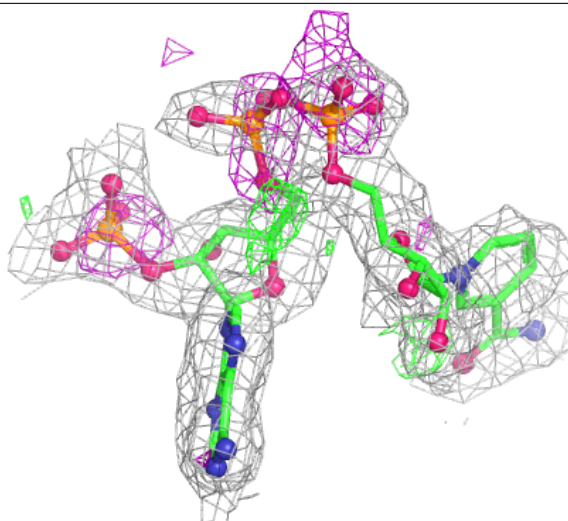
Electron density around PO4 A 401:

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

Electron density around NAP 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 PO4 B 401:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.