



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 03:31 AM UTC

PDB ID : 6KSD / pdb_00006ksd
Title : Structural basis for domain rotation during adenylation of active site K123 and fragment library screening against NAD⁺ -dependent DNA ligase from Mycobacterium tuberculosis
Authors : Ramachandran, R.; Shukla, A.; Afsar, M.
Deposited on : 2019-08-23
Resolution : 2.50 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	:	FAILED
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

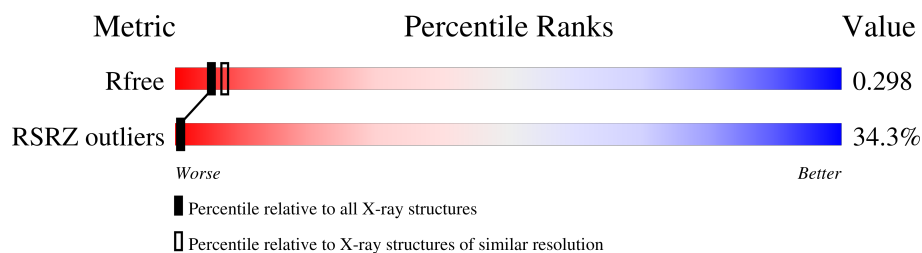
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4735 atoms, of which 2229 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.

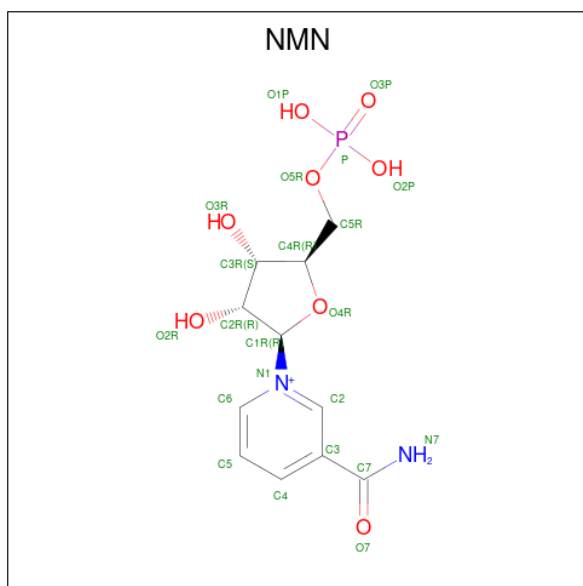
- Molecule 1 is a protein called DNA ligase A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	321	4576	1483	2201	434	454	4	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	ALA	LYS	engineered mutation	UNP P9WNV1

- Molecule 2 is BETA-NICOTINAMIDE RIBOSE MONOPHOSPHATE (CCD ID: NMN) (formula: $C_{11}H_{16}N_2O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
2	A	1	72	22	28	4	16	2	0	1

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total	O	0	0
			72	72		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	95.75Å 95.75Å 199.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.56 – 2.50 46.56 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.56-2.50) 99.0 (46.56-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.266 , 0.295 0.298 , 0.298	Depositor DCC
R_{free} test set	966 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	52.3	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4735	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	SO4	A	404	-	4,4,4	0.25	0	6,6,6	0.38	0
3	SO4	A	403	-	4,4,4	0.29	0	6,6,6	0.59	0
2	NMN	A	401[B]	-	21,23,23	3.93	6 (28%)	27,34,34	1.95	6 (22%)
2	NMN	A	401[A]	-	21,23,23	3.97	6 (28%)	27,34,34	1.97	7 (25%)
3	SO4	A	402	-	4,4,4	0.24	0	6,6,6	0.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NMN	A	401[B]	-	-	3/14/30/30	0/2/2/2
2	NMN	A	401[A]	-	-	1/14/30/30	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401[A]	NMN	C5R-C4R	13.03	1.90	1.51
2	A	401[B]	NMN	C5R-C4R	12.79	1.90	1.51
2	A	401[A]	NMN	P-O5R	9.96	1.91	1.60
2	A	401[B]	NMN	P-O5R	9.91	1.91	1.60
2	A	401[B]	NMN	O5R-C5R	-4.18	1.28	1.44
2	A	401[A]	NMN	O5R-C5R	-4.13	1.29	1.44
2	A	401[B]	NMN	C2-N1	3.80	1.39	1.35
2	A	401[A]	NMN	C2-N1	3.72	1.39	1.35
2	A	401[A]	NMN	C7-N7	3.64	1.39	1.33
2	A	401[B]	NMN	C7-N7	3.64	1.39	1.33
2	A	401[A]	NMN	C2R-C3R	2.50	1.60	1.53
2	A	401[B]	NMN	C2R-C3R	2.33	1.59	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401[B]	NMN	C3-C7-N7	5.66	124.71	117.74
2	A	401[A]	NMN	C3-C7-N7	5.55	124.57	117.74
2	A	401[B]	NMN	O7-C7-N7	-4.46	116.18	122.62
2	A	401[A]	NMN	O7-C7-N7	-4.39	116.27	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401[A]	NMN	O2P-P-O5R	-3.58	97.34	106.67
2	A	401[B]	NMN	O2P-P-O5R	-3.56	97.39	106.67
2	A	401[B]	NMN	O5R-P-O3P	-3.02	98.28	106.44
2	A	401[A]	NMN	O5R-P-O3P	-2.91	98.58	106.44
2	A	401[A]	NMN	C6-N1-C2	-2.89	119.42	121.88
2	A	401[B]	NMN	C6-N1-C2	-2.87	119.44	121.88
2	A	401[A]	NMN	C4R-O4R-C1R	-2.47	107.66	109.92
2	A	401[B]	NMN	O1P-P-O3P	2.22	119.49	110.83
2	A	401[A]	NMN	O1P-P-O3P	2.22	119.48	110.83

There are no chirality outliers.

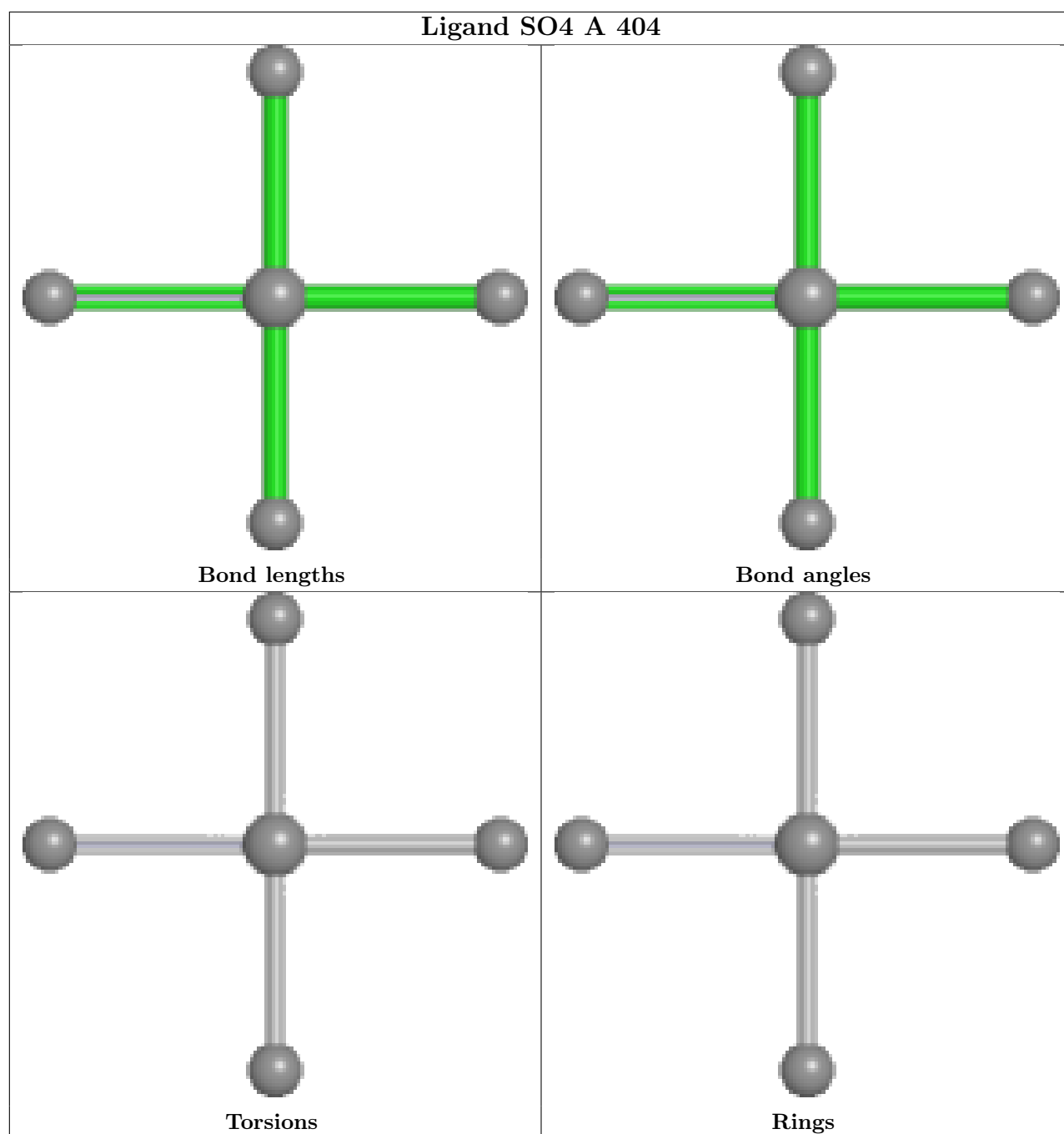
All (4) torsion outliers are listed below:

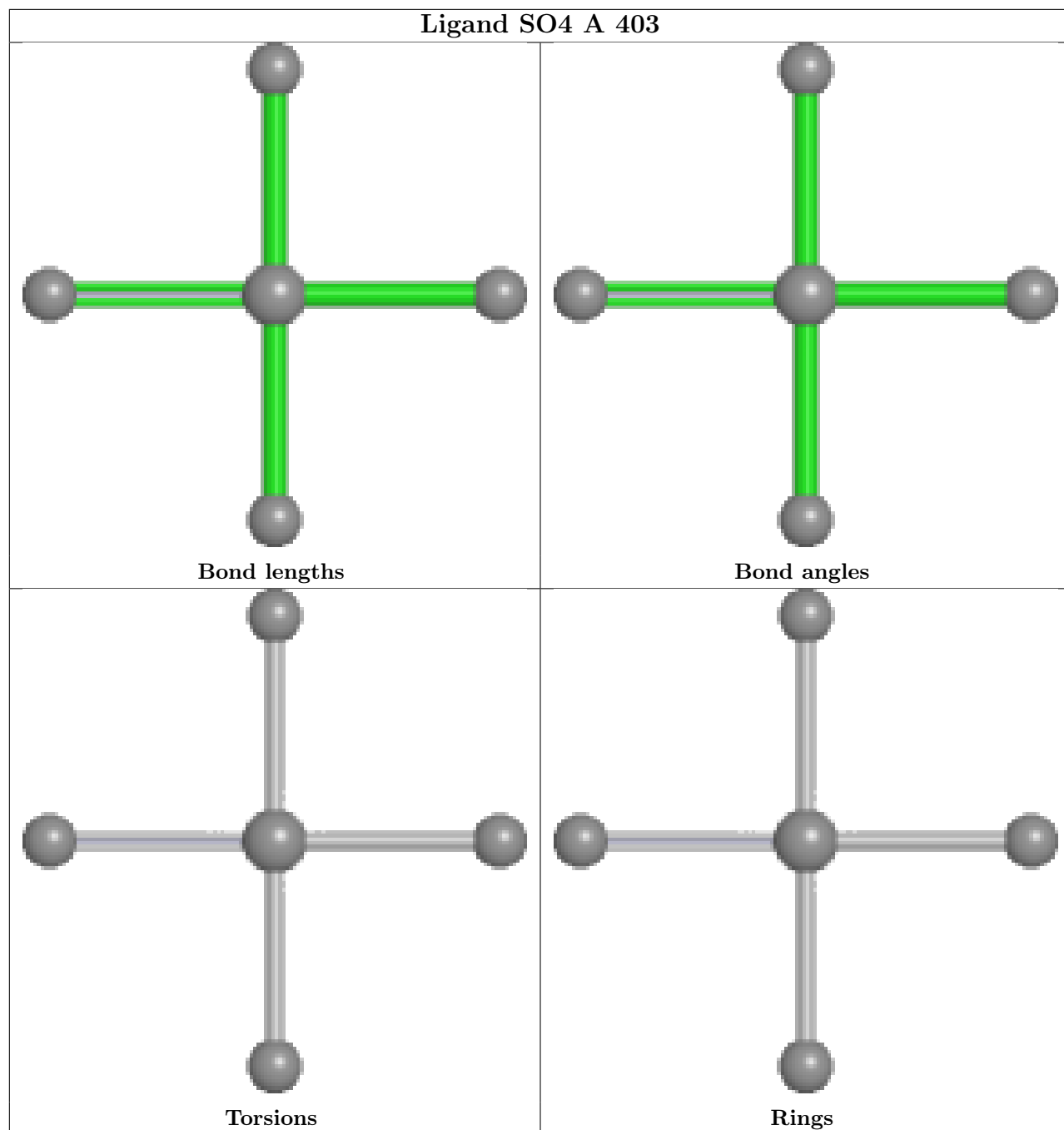
Mol	Chain	Res	Type	Atoms
2	A	401[B]	NMN	O4R-C4R-C5R-O5R
2	A	401[B]	NMN	C3R-C4R-C5R-O5R
2	A	401[B]	NMN	C4R-C5R-O5R-P
2	A	401[A]	NMN	C4R-C5R-O5R-P

There are no ring outliers.

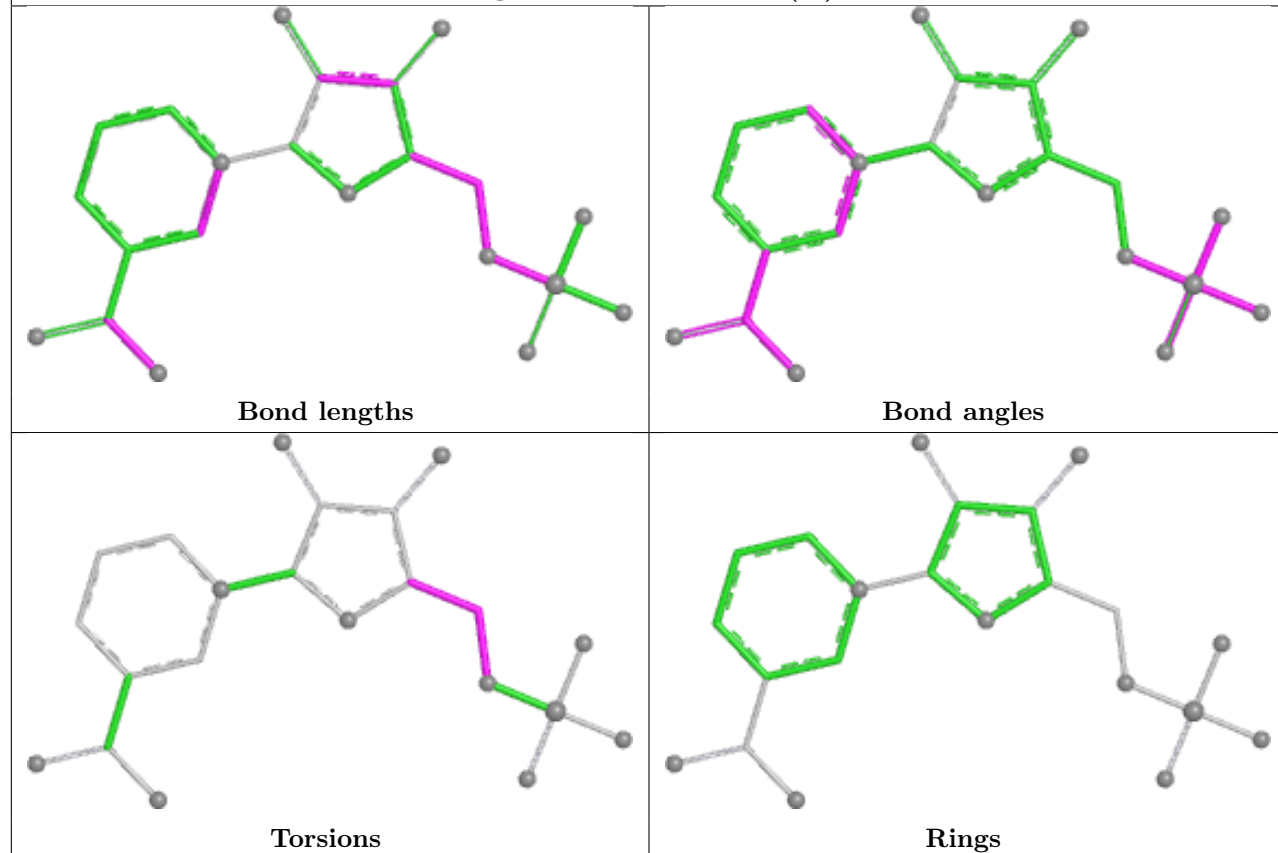
No monomer is involved in short contacts.

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.

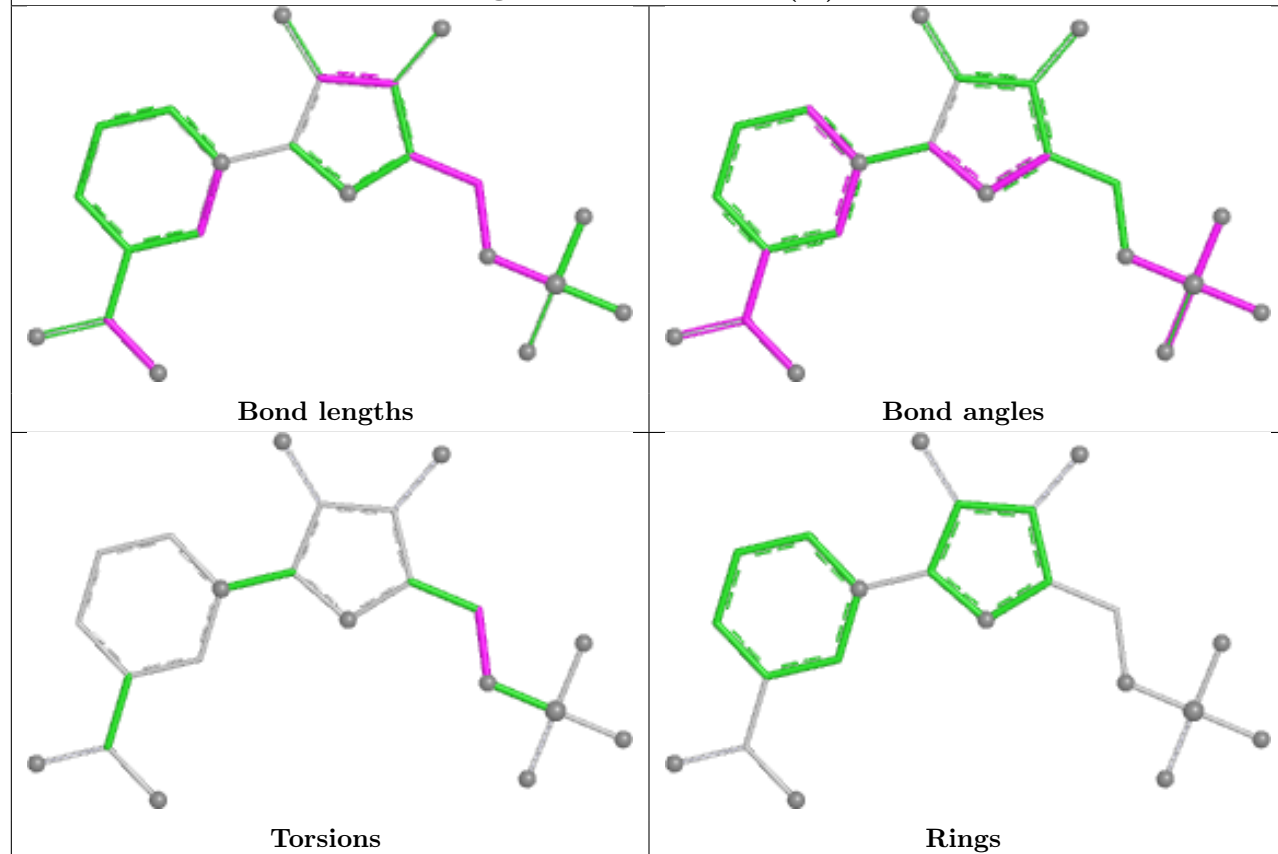


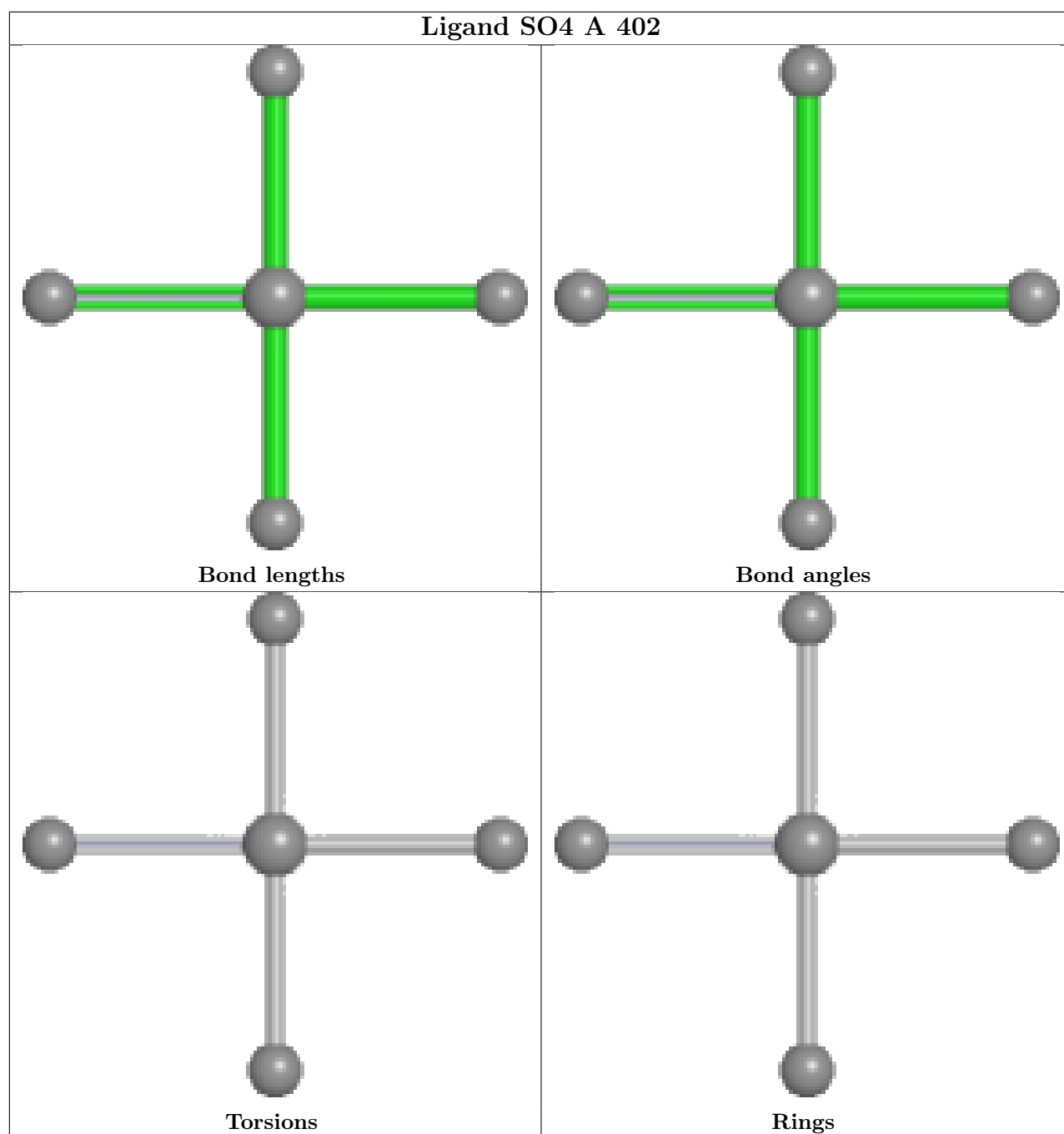


Ligand NMN A 401 (B)



Ligand NMN A 401 (A)





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 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	321/321 (100%)	1.87	110 (34%) 1 1	30, 62, 103, 141	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	LEU	11.6
1	A	68	THR	8.6
1	A	9	THR	8.5
1	A	73	GLY	7.3
1	A	69	GLN	6.3
1	A	115	ALA	6.0
1	A	8	GLN	5.9
1	A	126	GLY	5.8
1	A	113	GLY	5.6
1	A	49	ARG	5.4
1	A	72	GLY	5.1
1	A	114	ASP	5.1
1	A	178	VAL	4.9
1	A	116	ALA	4.9
1	A	57	GLN	4.8
1	A	74	ALA	4.8
1	A	306	LEU	4.6
1	A	171	ASP	4.6
1	A	58	HIS	4.2
1	A	170	GLY	4.2
1	A	32	TYR	4.1
1	A	44	PHE	4.1
1	A	10	ALA	4.0
1	A	18	GLN	4.0
1	A	327	PRO	4.0
1	A	60	GLU	4.0
1	A	112	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	305	ALA	3.9
1	A	328	GLU	3.8
1	A	137	ARG	3.7
1	A	111	GLU	3.7
1	A	51	LEU	3.7
1	A	110	ALA	3.6
1	A	13	VAL	3.6
1	A	14	LEU	3.5
1	A	109	HIS	3.5
1	A	105	ALA	3.5
1	A	75	GLY	3.4
1	A	39	ILE	3.3
1	A	103	ALA	3.3
1	A	172	ASP	3.3
1	A	71	VAL	3.2
1	A	106	GLY	3.2
1	A	311	GLY	3.2
1	A	252	ALA	3.2
1	A	133	TYR	3.1
1	A	309	ARG	3.1
1	A	118	TYR	3.1
1	A	102	ALA	3.0
1	A	181	VAL	3.0
1	A	91	SER	2.9
1	A	20	LEU	2.8
1	A	310	LEU	2.8
1	A	56	GLU	2.8
1	A	231	LEU	2.8
1	A	67	PRO	2.8
1	A	246	PRO	2.8
1	A	304	VAL	2.8
1	A	65	ASP	2.8
1	A	54	LEU	2.7
1	A	313	THR	2.7
1	A	40	SER	2.7
1	A	274	ALA	2.7
1	A	299	VAL	2.7
1	A	42	ALA	2.7
1	A	46	GLU	2.7
1	A	117	HIS	2.7
1	A	15	ARG	2.7
1	A	319	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	41	ASP	2.6
1	A	233	MET	2.6
1	A	124	ILE	2.6
1	A	48	LEU	2.6
1	A	90	LEU	2.6
1	A	228	ARG	2.5
1	A	47	LEU	2.5
1	A	101	LEU	2.5
1	A	182	ARG	2.5
1	A	61	LEU	2.5
1	A	38	ILE	2.4
1	A	269	LEU	2.4
1	A	17	TRP	2.4
1	A	244	PHE	2.4
1	A	24	VAL	2.4
1	A	94	ASN	2.4
1	A	96	PHE	2.4
1	A	37	PRO	2.3
1	A	63	THR	2.3
1	A	108	ILE	2.3
1	A	270	ALA	2.3
1	A	179	LEU	2.3
1	A	301	VAL	2.3
1	A	98	ALA	2.3
1	A	247	ALA	2.3
1	A	277	ARG	2.3
1	A	307	GLN	2.2
1	A	33	VAL	2.2
1	A	230	ARG	2.2
1	A	12	GLU	2.2
1	A	88	ARG	2.2
1	A	31	TYR	2.2
1	A	288	HIS	2.2
1	A	16	GLN	2.2
1	A	127	VAL	2.1
1	A	260	GLY	2.1
1	A	55	GLU	2.1
1	A	59	PRO	2.1
1	A	163	VAL	2.0
1	A	312	SER	2.0
1	A	238	LEU	2.0

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

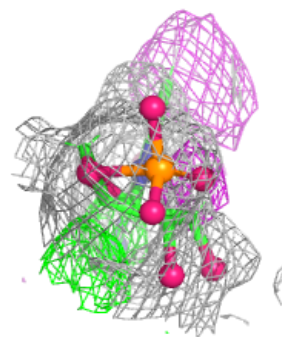
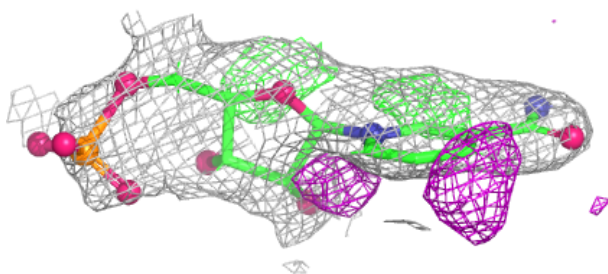
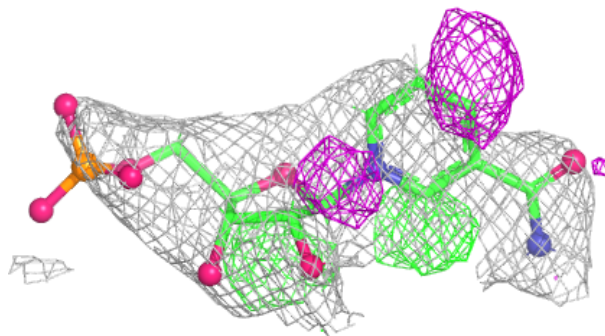
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NMN	A	401[A]	22/22	0.56	0.31	74,99,126,129	36
2	NMN	A	401[B]	22/22	0.56	0.31	74,99,126,128	36
3	SO4	A	404	5/5	0.85	0.21	81,83,89,92	0
3	SO4	A	403	5/5	0.93	0.17	54,56,71,73	0
3	SO4	A	402	5/5	0.96	0.10	53,58,67,72	0

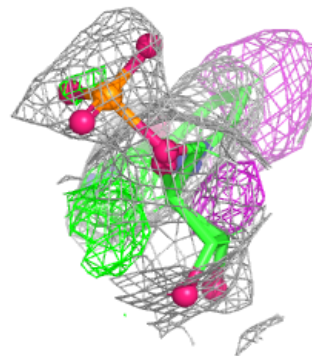
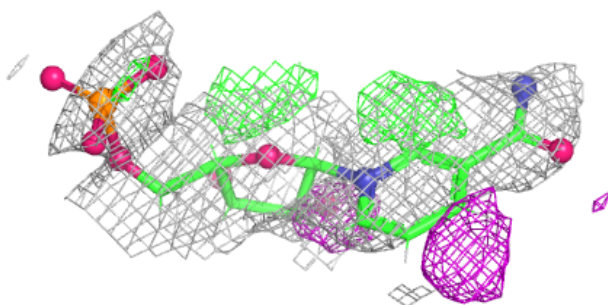
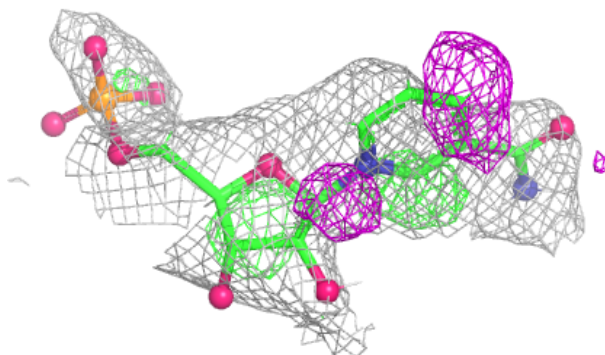
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NMN A 401 (A):

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

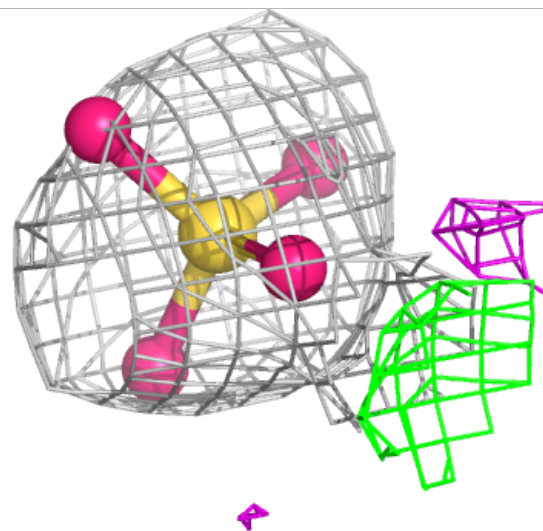
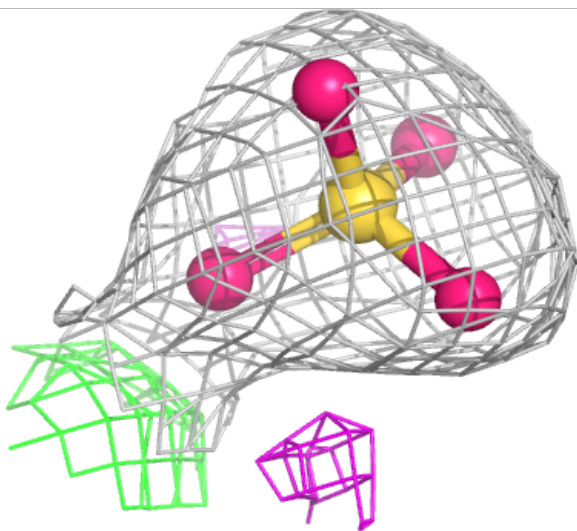
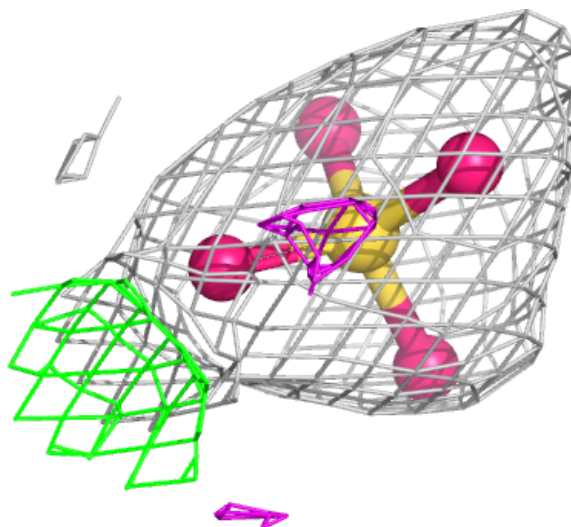
**Electron density around NMN A 401 (B):**

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



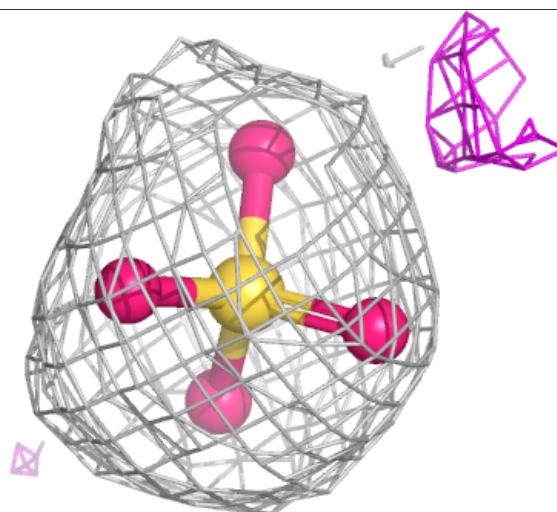
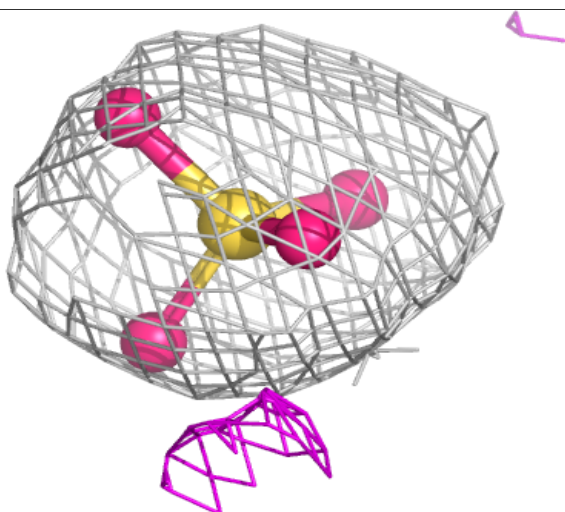
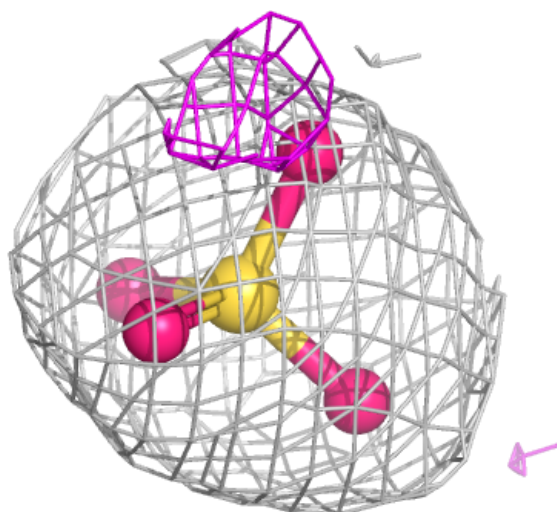
Electron density around SO4 A 404:

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



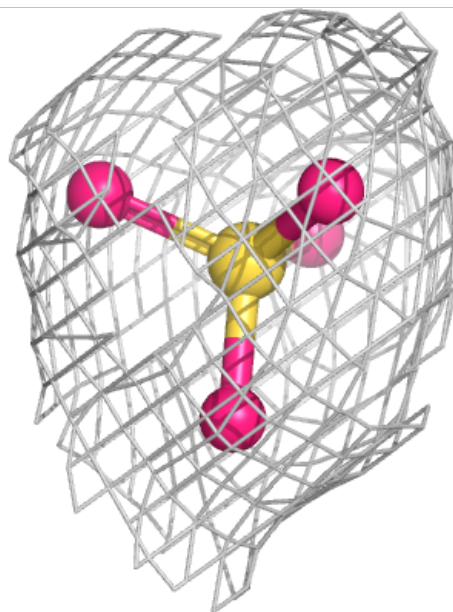
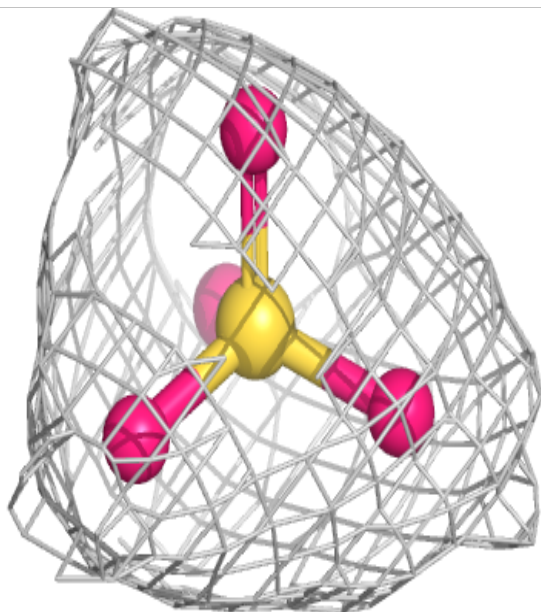
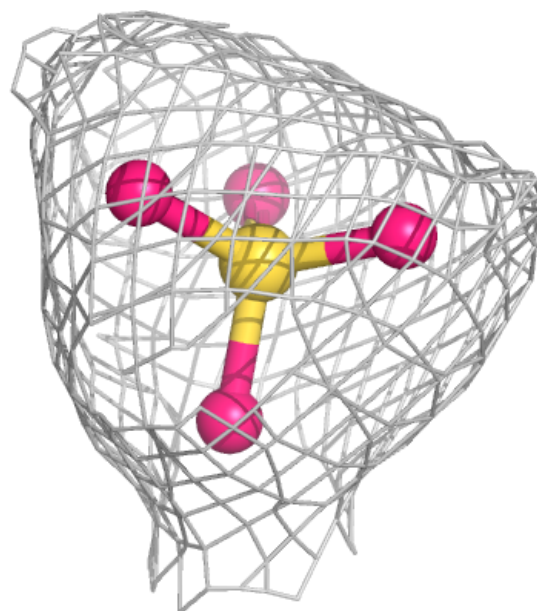
Electron density around SO4 A 403:

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



Electron density around SO4 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)



5.5 Other polymers ⓘ

There are no such residues in this entry.