



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:35 AM UTC

PDB ID : 6KJM / pdb_00006kjm
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 : 2019-07-22
Resolution : 2.20 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

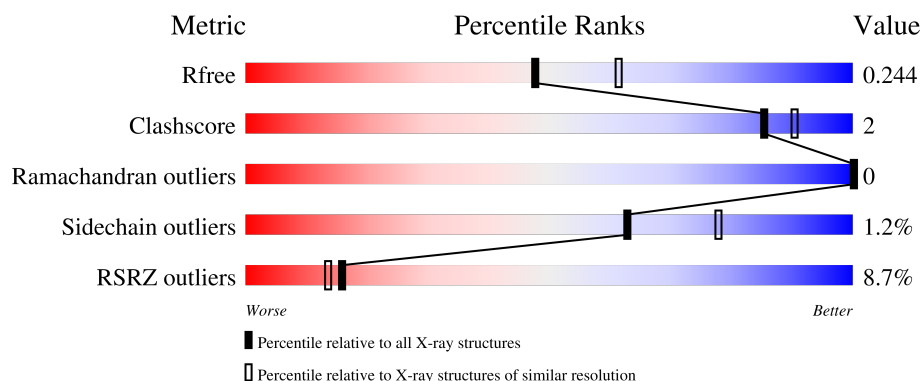
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	334	8% 30% 64% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5016 atoms, of which 2368 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.

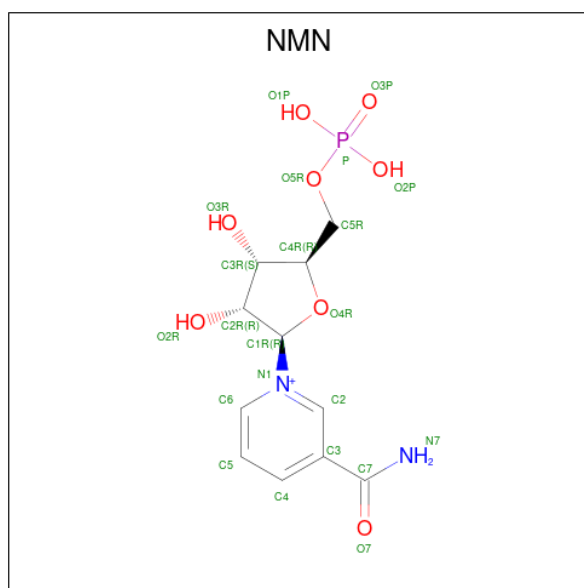
- Molecule 1 is a protein called DNA ligase A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	321	4820	1555	2342	448	471	4	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

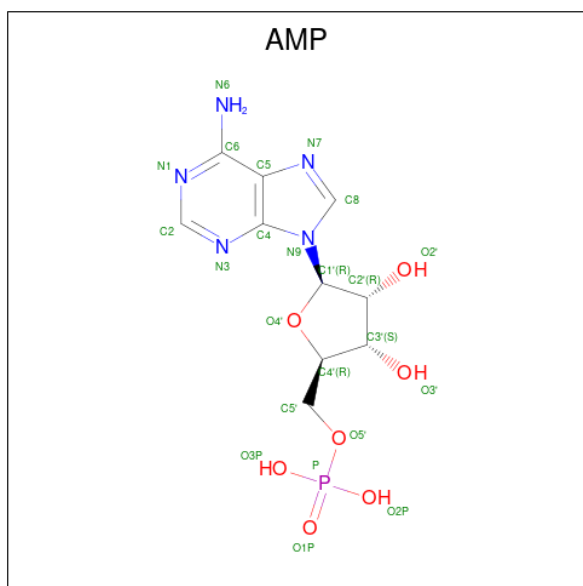
Chain	Residue	Modelled	Actual	Comment	Reference
A	329	HIS	-	expression tag	UNP P9WNV1
A	330	HIS	-	expression tag	UNP P9WNV1
A	331	HIS	-	expression tag	UNP P9WNV1
A	332	HIS	-	expression tag	UNP P9WNV1
A	333	HIS	-	expression tag	UNP P9WNV1
A	334	HIS	-	expression tag	UNP P9WNV1

- 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).



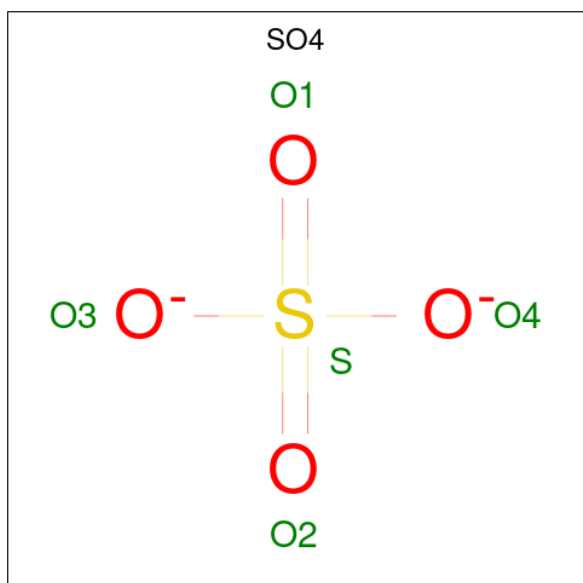
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total	C	H	N	O	P	0	0
			36	11	14	2	8	1		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			35	10	12	5	7	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).



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

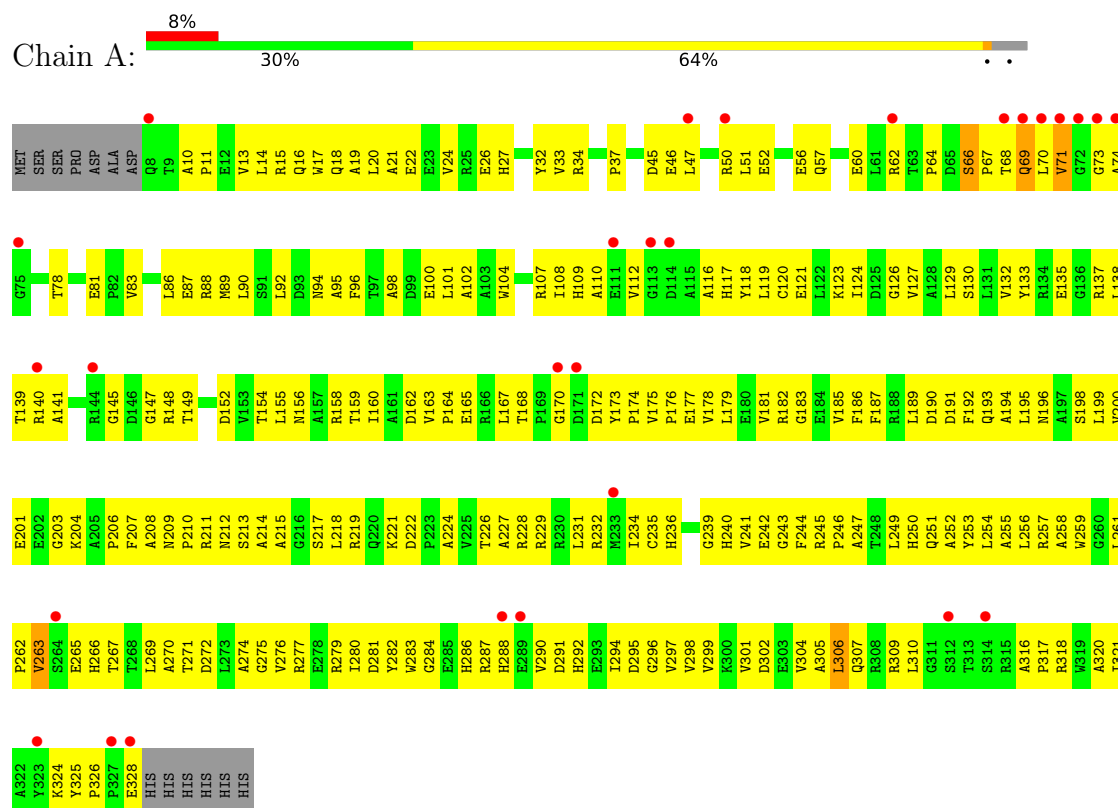
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	105	Total	O	0	0
			105	105		

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: DNA ligase A



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	95.73Å 95.73Å 201.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.23 – 2.20 43.23 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.23-2.20) 99.9 (43.23-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.216 , 0.246 0.234 , 0.244	Depositor DCC
R_{free} test set	1418 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5016	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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: SO4, NMN, AMP

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	2.65	216/2535 (8.5%)	1.26	18/3458 (0.5%)

All (216) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	GLN	CA-C	-9.75	1.40	1.52
1	A	256	LEU	C-O	-9.70	1.12	1.24
1	A	214	ALA	C-O	-9.00	1.13	1.24
1	A	70	LEU	CA-C	-8.88	1.42	1.52
1	A	213	SER	C-O	-8.85	1.13	1.24
1	A	317	PRO	C-O	-8.69	1.14	1.23
1	A	277	ARG	C-O	-8.64	1.14	1.24
1	A	175	VAL	C-O	-8.64	1.14	1.25
1	A	252	ALA	C-O	-8.64	1.14	1.24
1	A	263	VAL	C-O	-8.30	1.14	1.23
1	A	198	SER	C-O	-8.20	1.14	1.24
1	A	226	THR	C-O	-8.17	1.14	1.24
1	A	287	ARG	C-O	-8.17	1.13	1.24
1	A	127	VAL	C-O	-8.01	1.15	1.24
1	A	241	VAL	C-O	-7.98	1.16	1.24
1	A	183	GLY	C-O	-7.94	1.15	1.23
1	A	33	VAL	C-O	-7.92	1.15	1.24
1	A	266	HIS	C-O	-7.90	1.14	1.24
1	A	249	LEU	C-O	-7.89	1.14	1.24
1	A	152	ASP	C-O	-7.88	1.15	1.24
1	A	189	LEU	C-O	-7.88	1.14	1.24
1	A	235	CYS	C-O	-7.88	1.14	1.24
1	A	272	ASP	C-O	-7.71	1.15	1.23
1	A	283	TRP	C-O	-7.71	1.14	1.24
1	A	187	PHE	C-O	-7.70	1.14	1.23
1	A	200	VAL	C-O	-7.58	1.14	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	PHE	C-O	-7.56	1.14	1.23
1	A	100	GLU	C-O	-7.55	1.15	1.24
1	A	244	PHE	C-O	-7.51	1.14	1.24
1	A	165	GLU	C-O	-7.50	1.15	1.24
1	A	17	TRP	C-O	-7.50	1.15	1.24
1	A	162	ASP	C-O	-7.47	1.14	1.24
1	A	190	ASP	C-O	-7.43	1.15	1.24
1	A	181	VAL	C-O	-7.42	1.16	1.24
1	A	26	GLU	C-O	-7.35	1.15	1.24
1	A	210	PRO	C-O	-7.32	1.15	1.24
1	A	163	VAL	C-O	-7.30	1.16	1.24
1	A	279	ARG	C-O	-7.30	1.15	1.24
1	A	121	GLU	C-O	-7.25	1.15	1.23
1	A	284	GLY	C-O	-7.25	1.15	1.23
1	A	259	TRP	C-O	-7.25	1.14	1.24
1	A	245	ARG	C-O	-7.18	1.16	1.24
1	A	195	LEU	C-O	-7.17	1.15	1.24
1	A	123	LYS	C-O	-7.14	1.15	1.24
1	A	52	GLU	C-O	-7.12	1.15	1.24
1	A	174	PRO	C-O	-7.11	1.16	1.23
1	A	281	ASP	C-O	-7.11	1.15	1.24
1	A	160	ILE	C-O	-7.09	1.17	1.24
1	A	255	ALA	C-O	-7.09	1.15	1.24
1	A	211	ARG	C-O	-7.09	1.15	1.24
1	A	224	ALA	C-O	-7.07	1.15	1.24
1	A	164	PRO	C-O	-7.06	1.16	1.23
1	A	18	GLN	C-O	-7.03	1.16	1.24
1	A	20	LEU	C-O	-7.03	1.15	1.24
1	A	177	GLU	C-O	-7.00	1.16	1.24
1	A	217	SER	C-O	-6.98	1.15	1.24
1	A	298	VAL	C-O	-6.94	1.16	1.24
1	A	10	ALA	C-O	-6.93	1.15	1.24
1	A	129	LEU	C-O	-6.92	1.16	1.23
1	A	261	LEU	C-O	-6.91	1.14	1.24
1	A	116	ALA	C-O	-6.89	1.15	1.24
1	A	262	PRO	C-O	-6.87	1.16	1.23
1	A	253	TYR	C-O	-6.84	1.15	1.24
1	A	307	GLN	C-O	-6.84	1.16	1.24
1	A	258	ALA	C-O	-6.82	1.16	1.24
1	A	83	VAL	C-O	-6.79	1.17	1.24
1	A	159	THR	C-O	-6.79	1.15	1.24
1	A	296	GLY	C-O	-6.78	1.14	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	227	ALA	C-O	-6.76	1.15	1.24
1	A	209	ASN	C-O	-6.75	1.17	1.24
1	A	242	GLU	C-O	-6.75	1.16	1.24
1	A	155	LEU	C-O	-6.74	1.16	1.24
1	A	221	LYS	C-O	-6.74	1.15	1.24
1	A	90	LEU	C-O	-6.74	1.15	1.23
1	A	301	VAL	C-O	-6.66	1.17	1.24
1	A	27	HIS	C-O	-6.65	1.15	1.24
1	A	130	SER	C-O	-6.63	1.16	1.24
1	A	305	ALA	C-O	-6.63	1.16	1.24
1	A	196	ASN	C-O	-6.61	1.16	1.24
1	A	104	TRP	C-O	-6.60	1.16	1.24
1	A	110	ALA	C-O	-6.59	1.15	1.24
1	A	16	GLN	C-O	-6.59	1.16	1.24
1	A	86	LEU	C-O	-6.58	1.16	1.24
1	A	186	PHE	C-O	-6.57	1.16	1.23
1	A	246	PRO	C-O	-6.52	1.16	1.23
1	A	149	THR	C-O	-6.49	1.16	1.24
1	A	11	PRO	C-O	-6.49	1.15	1.24
1	A	51	LEU	C-O	-6.48	1.16	1.24
1	A	109	HIS	C-O	-6.46	1.16	1.24
1	A	231	LEU	C-O	-6.43	1.15	1.23
1	A	295	ASP	C-O	-6.43	1.15	1.24
1	A	14	LEU	C-O	-6.41	1.16	1.24
1	A	215	ALA	C-O	-6.40	1.16	1.24
1	A	126	GLY	C-O	-6.39	1.15	1.23
1	A	257	ARG	C-O	-6.38	1.16	1.24
1	A	193	GLN	C-O	-6.37	1.16	1.24
1	A	201	GLU	C-O	-6.36	1.16	1.24
1	A	88	ARG	C-O	-6.34	1.16	1.23
1	A	251	GLN	C-O	-6.34	1.16	1.24
1	A	275	GLY	C-O	-6.28	1.16	1.23
1	A	137	ARG	C-O	-6.27	1.16	1.24
1	A	288	HIS	C-O	-6.24	1.16	1.24
1	A	276	VAL	C-O	-6.23	1.17	1.24
1	A	265	GLU	C-O	-6.22	1.15	1.24
1	A	299	VAL	C-O	-6.21	1.17	1.24
1	A	95	ALA	C-O	-6.19	1.17	1.24
1	A	173	TYR	C-O	-6.18	1.18	1.24
1	A	64	PRO	C-O	-6.17	1.16	1.24
1	A	78	THR	C-O	-6.10	1.16	1.24
1	A	148	ARG	C-O	-6.09	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	THR	C-O	-6.08	1.17	1.24
1	A	135	GLU	C-O	-6.05	1.15	1.23
1	A	102	ALA	C-O	-6.03	1.17	1.24
1	A	240	HIS	C-O	-6.03	1.16	1.23
1	A	247	ALA	C-O	-6.02	1.16	1.24
1	A	145	GLY	C-O	-6.02	1.16	1.24
1	A	178	VAL	C-O	-6.01	1.18	1.24
1	A	98	ALA	C-O	-6.00	1.17	1.24
1	A	232	ARG	C-O	-6.00	1.16	1.23
1	A	271	THR	C-O	-5.99	1.16	1.24
1	A	168	THR	C-O	-5.98	1.16	1.24
1	A	32	TYR	C-O	-5.98	1.17	1.24
1	A	81	GLU	C-O	-5.97	1.16	1.24
1	A	120	CYS	C-O	-5.97	1.17	1.24
1	A	229	ARG	C-O	-5.97	1.16	1.24
1	A	206	PRO	C-O	-5.94	1.15	1.23
1	A	291	ASP	C-O	-5.93	1.15	1.24
1	A	101	LEU	C-O	-5.88	1.17	1.24
1	A	47	LEU	C-O	-5.87	1.17	1.24
1	A	112	VAL	C-O	-5.86	1.17	1.24
1	A	280	ILE	C-O	-5.84	1.17	1.24
1	A	70	LEU	N-CA	-5.81	1.38	1.46
1	A	282	TYR	C-O	-5.80	1.17	1.24
1	A	326	PRO	C-O	-5.80	1.20	1.25
1	A	234	ILE	C-O	-5.80	1.17	1.24
1	A	212	ASN	C-O	-5.79	1.17	1.24
1	A	310	LEU	C-O	-5.78	1.17	1.24
1	A	192	PHE	C-O	-5.77	1.17	1.24
1	A	24	VAL	C-O	-5.77	1.17	1.24
1	A	158	ARG	C-O	-5.76	1.16	1.24
1	A	218	LEU	C-O	-5.75	1.17	1.24
1	A	236	HIS	C-O	-5.73	1.15	1.23
1	A	309	ARG	C-O	-5.72	1.17	1.24
1	A	92	LEU	C-O	-5.71	1.17	1.23
1	A	45	ASP	C-O	-5.70	1.17	1.24
1	A	306	LEU	C-O	-5.67	1.17	1.24
1	A	191	ASP	C-O	-5.65	1.17	1.24
1	A	292	HIS	C-O	-5.65	1.16	1.23
1	A	117	HIS	C-O	-5.65	1.16	1.23
1	A	34	ARG	C-O	-5.62	1.16	1.24
1	A	203	GLY	C-O	-5.60	1.16	1.23
1	A	94	ASN	C-O	-5.57	1.16	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	LEU	C-O	-5.56	1.17	1.24
1	A	124	ILE	C-O	-5.56	1.17	1.24
1	A	108	ILE	N-CA	-5.55	1.39	1.46
1	A	179	LEU	C-O	-5.55	1.17	1.23
1	A	133	TYR	C-O	-5.54	1.17	1.24
1	A	140	ARG	C-O	-5.54	1.17	1.23
1	A	139	THR	C-O	-5.54	1.16	1.23
1	A	60	GLU	C-O	-5.54	1.16	1.24
1	A	132	VAL	C-O	-5.54	1.18	1.24
1	A	219	ARG	C-O	-5.54	1.16	1.23
1	A	185	VAL	C-O	-5.54	1.17	1.24
1	A	138	LEU	C-O	-5.52	1.17	1.24
1	A	172	ASP	C-O	-5.48	1.17	1.24
1	A	141	ALA	C-O	-5.47	1.17	1.23
1	A	239	GLY	C-O	-5.47	1.16	1.23
1	A	297	VAL	C-O	-5.47	1.18	1.24
1	A	302	ASP	CG-OD2	-5.47	1.15	1.25
1	A	274	ALA	C-O	-5.46	1.17	1.24
1	A	66	SER	C-O	-5.44	1.17	1.24
1	A	326	PRO	CA-CB	-5.44	1.48	1.53
1	A	270	ALA	C-O	-5.43	1.17	1.23
1	A	156	ASN	C-O	-5.42	1.17	1.24
1	A	254	LEU	C-O	-5.42	1.17	1.24
1	A	213	SER	N-CA	-5.42	1.39	1.46
1	A	324	LYS	C-O	-5.41	1.17	1.23
1	A	107	ARG	C-O	-5.39	1.17	1.24
1	A	228	ARG	C-O	-5.38	1.17	1.24
1	A	320	ALA	C-O	-5.37	1.17	1.23
1	A	118	TYR	C-O	-5.37	1.18	1.24
1	A	167	LEU	N-CA	-5.31	1.39	1.46
1	A	13	VAL	C-O	-5.30	1.18	1.24
1	A	50	ARG	C-O	-5.30	1.18	1.24
1	A	204	LYS	C-O	-5.28	1.17	1.23
1	A	176	PRO	C-O	-5.27	1.17	1.23
1	A	182	ARG	CZ-NH1	-5.26	1.25	1.32
1	A	304	VAL	C-O	-5.26	1.18	1.24
1	A	182	ARG	C-O	-5.25	1.17	1.23
1	A	15	ARG	C-O	-5.25	1.18	1.24
1	A	194	ALA	C-O	-5.23	1.18	1.24
1	A	250	HIS	C-O	-5.20	1.18	1.24
1	A	318	ARG	C-O	-5.19	1.17	1.24
1	A	22	GLU	C-O	-5.19	1.18	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	LEU	C-O	-5.18	1.17	1.24
1	A	147	GLY	C-O	-5.18	1.17	1.23
1	A	46	GLU	C-O	-5.17	1.18	1.24
1	A	316	ALA	C-O	-5.17	1.17	1.24
1	A	19	ALA	C-O	-5.16	1.18	1.24
1	A	208	ALA	C-O	-5.15	1.17	1.24
1	A	87	GLU	C-O	-5.15	1.17	1.23
1	A	222	ASP	C-O	-5.15	1.18	1.24
1	A	321	ILE	C-O	-5.13	1.17	1.23
1	A	243	GLY	C-O	-5.13	1.16	1.24
1	A	294	ILE	C-O	-5.09	1.18	1.24
1	A	182	ARG	N-CA	-5.09	1.40	1.45
1	A	71	VAL	C-O	-5.08	1.16	1.23
1	A	56	GLU	C-O	-5.08	1.18	1.24
1	A	21	ALA	C-O	-5.08	1.18	1.24
1	A	37	PRO	C-O	-5.08	1.17	1.23
1	A	96	PHE	C-O	-5.06	1.17	1.24
1	A	267	THR	C-O	-5.04	1.17	1.23
1	A	269	LEU	C-O	-5.04	1.18	1.24
1	A	290	VAL	C-O	-5.02	1.17	1.24
1	A	280	ILE	N-CA	-5.02	1.40	1.46
1	A	57	GLN	C-O	-5.01	1.17	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	THR	N-CA-C	8.80	122.14	111.40
1	A	71	VAL	CB-CA-C	8.37	122.83	112.45
1	A	316	ALA	N-CA-C	8.05	115.46	108.22
1	A	325	TYR	CA-C-N	7.01	124.78	119.66
1	A	325	TYR	C-N-CA	7.01	124.78	119.66
1	A	71	VAL	N-CA-CB	-6.95	104.66	111.89
1	A	286	HIS	N-CA-C	6.49	121.26	112.88
1	A	68	THR	CB-CA-C	-6.43	99.98	110.79
1	A	209	ASN	N-CA-C	6.38	115.65	108.25
1	A	73	GLY	O-C-N	6.38	128.31	122.19
1	A	74	ALA	CA-C-N	5.78	132.73	121.41
1	A	74	ALA	C-N-CA	5.78	132.73	121.41
1	A	291	ASP	N-CA-C	5.76	120.00	113.15
1	A	172	ASP	N-CA-C	5.68	117.56	111.36
1	A	32	TYR	N-CA-C	5.58	117.17	111.14
1	A	118	TYR	N-CA-C	5.50	117.38	108.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	GLY	O-C-N	-5.24	118.69	123.57
1	A	257	ARG	CB-CA-C	-5.16	102.78	110.88

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	2478	2342	2359	8	0
2	A	22	14	14	3	0
3	A	23	12	9	0	0
4	A	20	0	0	0	0
5	A	105	0	0	0	0
All	All	2648	2368	2382	11	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 2.

All (11) 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:A:62:ARG:HD3	1:A:69:GLN:HE21	1.04	1.18
1:A:62:ARG:HD3	1:A:69:GLN:NE2	1.88	0.88
1:A:62:ARG:CD	1:A:69:GLN:HE21	1.91	0.77
1:A:328:GLU:N	1:A:328:GLU:OE1	2.28	0.67
2:A:401:NMN:O3P	2:A:401:NMN:HC6	1.98	0.63
1:A:67:PRO:HA	1:A:71:VAL:HG23	1.95	0.48
2:A:401:NMN:HC6	2:A:401:NMN:H5R2	1.95	0.47
1:A:67:PRO:HA	1:A:71:VAL:CG2	2.46	0.45
2:A:401:NMN:H5R2	2:A:401:NMN:C6	2.47	0.43
1:A:66:SER:O	1:A:71:VAL:HG22	2.18	0.43
1:A:69:GLN:O	1:A:69:GLN:HG3	2.20	0.42

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	319/334 (96%)	311 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	247/273 (90%)	244 (99%)	3 (1%)	63	78

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	MET
1	A	263	VAL
1	A	306	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN

5.3.3 RNA [i](#)

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 ⓘ

6 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	$\# Z > 2$
4	SO4	A	406	-	4,4,4	0.43	0	6,6,6	0.07	0
3	AMP	A	402	-	25,25,25	3.56	17 (68%)	37,38,38	2.07	13 (35%)
4	SO4	A	404	-	4,4,4	0.42	0	6,6,6	0.07	0
4	SO4	A	403	-	4,4,4	0.42	0	6,6,6	0.07	0
2	NMN	A	401	-	21,23,23	4.24	13 (61%)	27,34,34	4.29	15 (55%)
4	SO4	A	405	-	4,4,4	0.43	0	6,6,6	0.08	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
3	AMP	A	402	-	-	3/10/26/26	0/3/3/3
2	NMN	A	401	-	-	6/14/30/30	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	AMP	C2'-C3'	-9.89	1.26	1.53
2	A	401	NMN	O4R-C1R	-9.64	1.28	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NMN	O4R-C4R	8.21	1.63	1.45
3	A	402	AMP	O4'-C4'	-7.02	1.29	1.45
2	A	401	NMN	C3R-C4R	-6.64	1.36	1.53
2	A	401	NMN	O7-C7	-6.39	1.12	1.24
3	A	402	AMP	C8-N9	-5.77	1.27	1.37
2	A	401	NMN	C7-N7	5.65	1.43	1.33
2	A	401	NMN	C2-N1	-5.25	1.29	1.35
3	A	402	AMP	C5-N7	-4.27	1.31	1.39
3	A	402	AMP	C4-N9	-3.70	1.30	1.37
3	A	402	AMP	C2-N3	-3.57	1.27	1.33
2	A	401	NMN	C5R-C4R	3.43	1.61	1.51
3	A	402	AMP	C6-N6	3.40	1.42	1.34
2	A	401	NMN	C6-N1	-3.21	1.28	1.35
2	A	401	NMN	C4-C3	-3.13	1.34	1.39
3	A	402	AMP	P-O2P	-3.08	1.43	1.54
2	A	401	NMN	P-O3P	-3.03	1.41	1.50
3	A	402	AMP	C5-C4	-2.98	1.33	1.39
3	A	402	AMP	O2'-C2'	-2.94	1.35	1.43
3	A	402	AMP	C2-N1	-2.90	1.28	1.33
2	A	401	NMN	C3-C7	-2.83	1.46	1.50
3	A	402	AMP	C8-N7	-2.70	1.26	1.31
3	A	402	AMP	C3'-C4'	2.62	1.59	1.53
3	A	402	AMP	O4'-C1'	2.61	1.48	1.42
3	A	402	AMP	O3'-C3'	-2.31	1.37	1.43
2	A	401	NMN	P-O2P	-2.11	1.47	1.54
2	A	401	NMN	O2R-C2R	-2.09	1.37	1.43
3	A	402	AMP	C6-N1	-2.01	1.30	1.35
3	A	402	AMP	C4-N3	-2.01	1.30	1.34

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NMN	O1P-P-O5R	10.92	135.14	106.67
2	A	401	NMN	O2P-P-O5R	-8.75	83.86	106.67
2	A	401	NMN	C3-C7-N7	8.30	127.97	117.74
2	A	401	NMN	O7-C7-N7	-6.74	112.88	122.62
2	A	401	NMN	O5R-C5R-C4R	6.43	130.88	108.99
2	A	401	NMN	O1P-P-O3P	-6.40	85.91	110.83
2	A	401	NMN	O2P-P-O1P	4.94	126.33	107.80
3	A	402	AMP	C5-C4-N3	-4.82	120.08	126.72
2	A	401	NMN	O4R-C4R-C3R	-4.34	96.55	105.15
3	A	402	AMP	N3-C2-N1	-4.30	122.07	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	AMP	N3-C4-N9	3.92	133.84	127.17
3	A	402	AMP	C2-N3-C4	3.81	121.14	111.83
2	A	401	NMN	C5R-C4R-C3R	-3.45	102.81	115.21
3	A	402	AMP	C4-C5-N7	-2.94	107.22	110.58
3	A	402	AMP	C4-N9-C8	2.83	108.71	105.74
3	A	402	AMP	C4'-O4'-C1'	-2.77	103.34	109.47
3	A	402	AMP	O5'-C5'-C4'	-2.71	99.75	108.99
3	A	402	AMP	C5-N7-C8	2.69	107.67	103.45
3	A	402	AMP	N9-C8-N7	-2.56	110.31	113.94
2	A	401	NMN	O5R-P-O3P	2.55	113.32	106.44
3	A	402	AMP	O4'-C4'-C3'	-2.45	100.29	105.15
2	A	401	NMN	O4R-C4R-C5R	2.41	117.04	109.33
2	A	401	NMN	O3R-C3R-C2R	-2.33	104.36	111.82
3	A	402	AMP	O2'-C2'-C3'	2.27	119.10	111.82
2	A	401	NMN	O2R-C2R-C3R	2.20	118.85	111.82
2	A	401	NMN	C6-N1-C1R	2.19	124.02	119.73
2	A	401	NMN	C5-C6-N1	2.14	123.31	120.38
3	A	402	AMP	O3'-C3'-C2'	2.02	118.30	111.82

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NMN	C5R-O5R-P-O1P
2	A	401	NMN	C5R-O5R-P-O2P
2	A	401	NMN	C3R-C4R-C5R-O5R
2	A	401	NMN	O4R-C4R-C5R-O5R
2	A	401	NMN	C4R-C5R-O5R-P
3	A	402	AMP	C2'-C1'-N9-C4
3	A	402	AMP	C2'-C1'-N9-C8
2	A	401	NMN	C5R-O5R-P-O3P
3	A	402	AMP	O4'-C1'-N9-C8

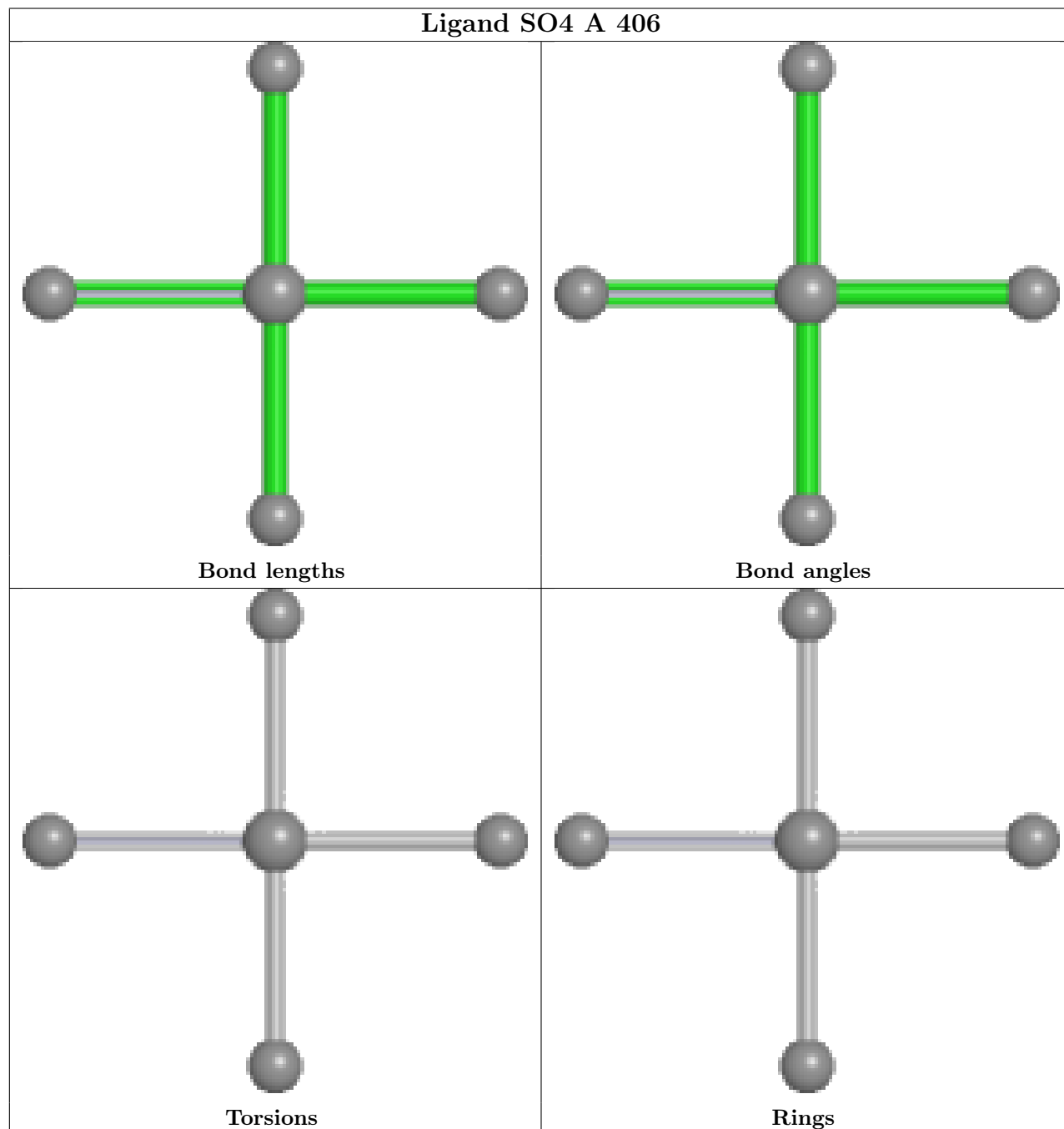
There are no ring outliers.

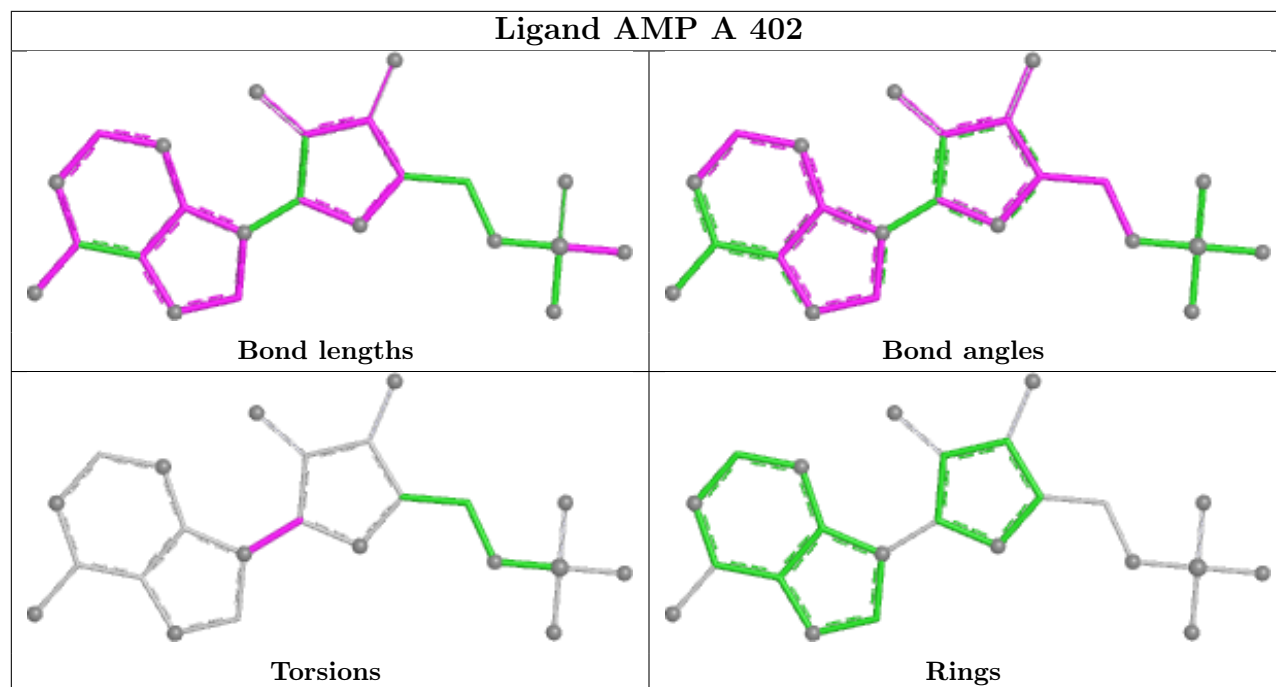
1 monomer is involved in 3 short contacts:

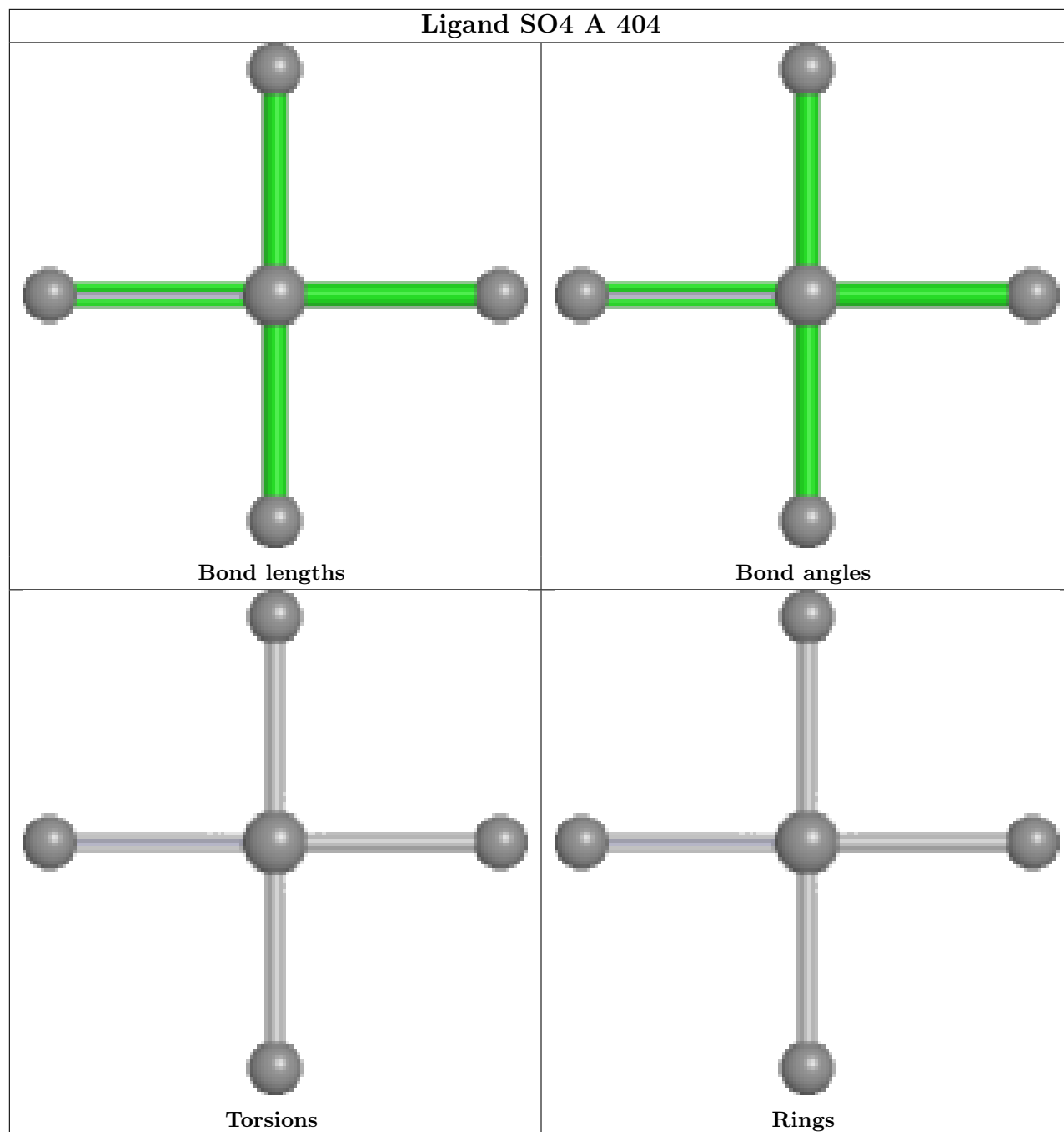
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NMN	3	0

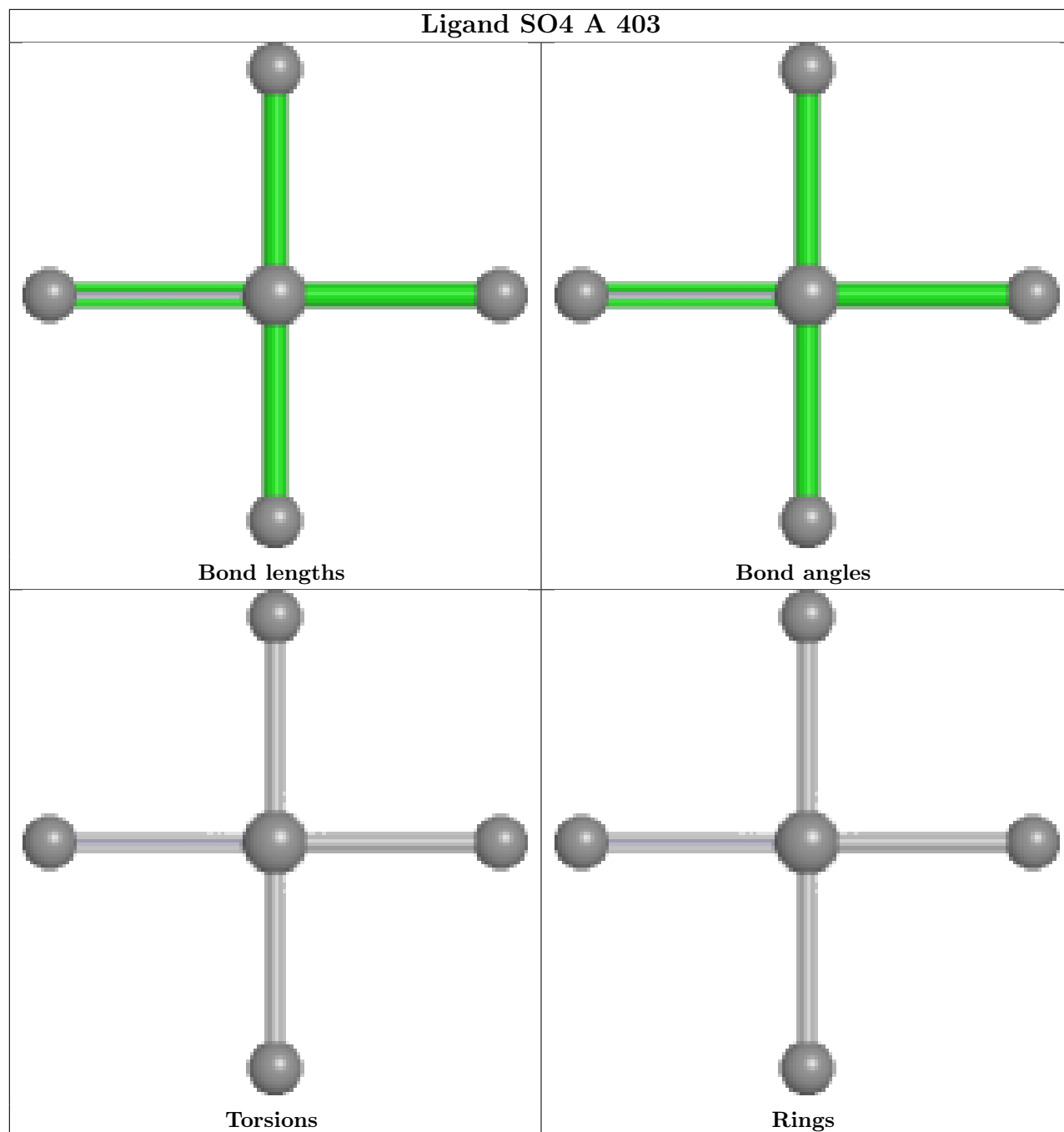
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

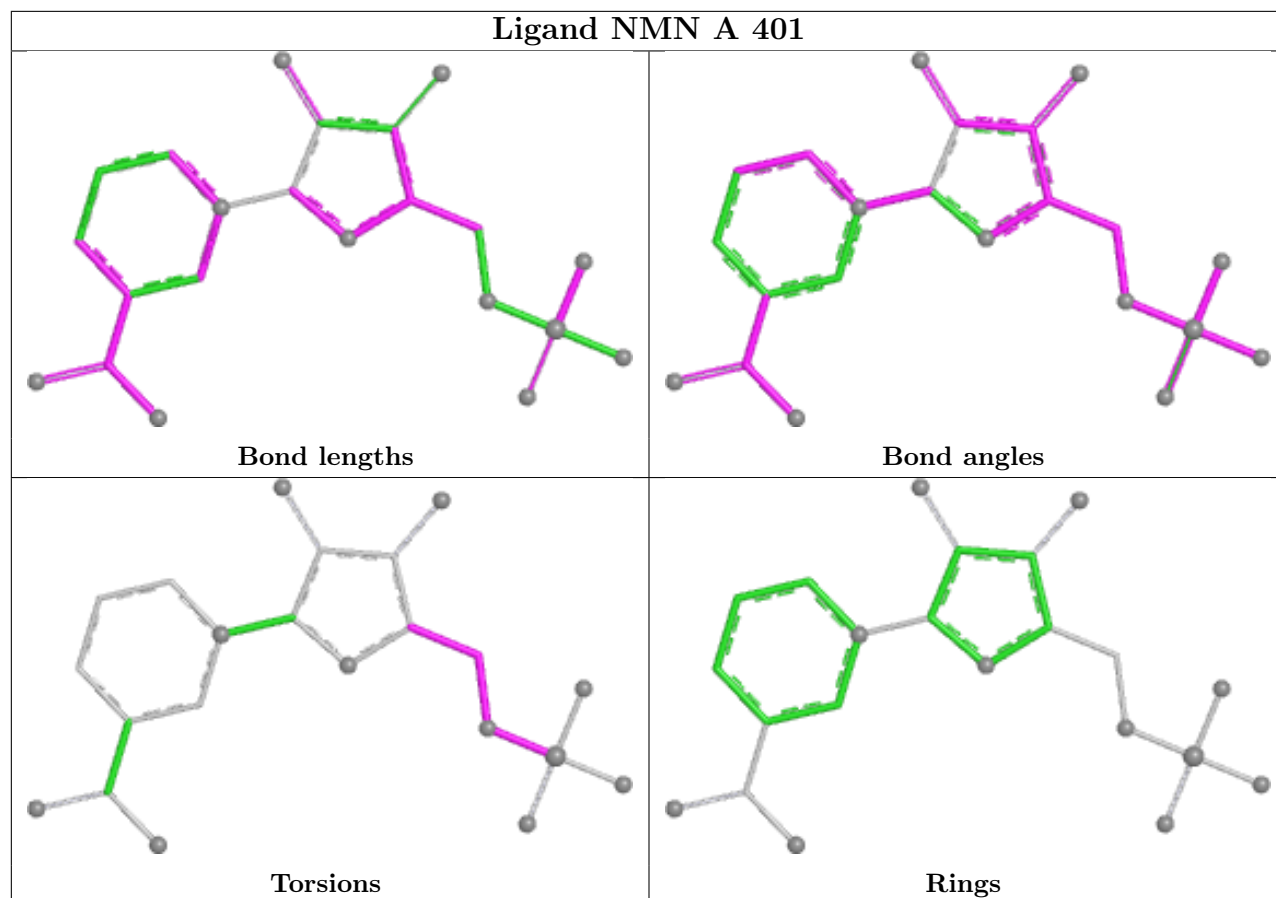
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

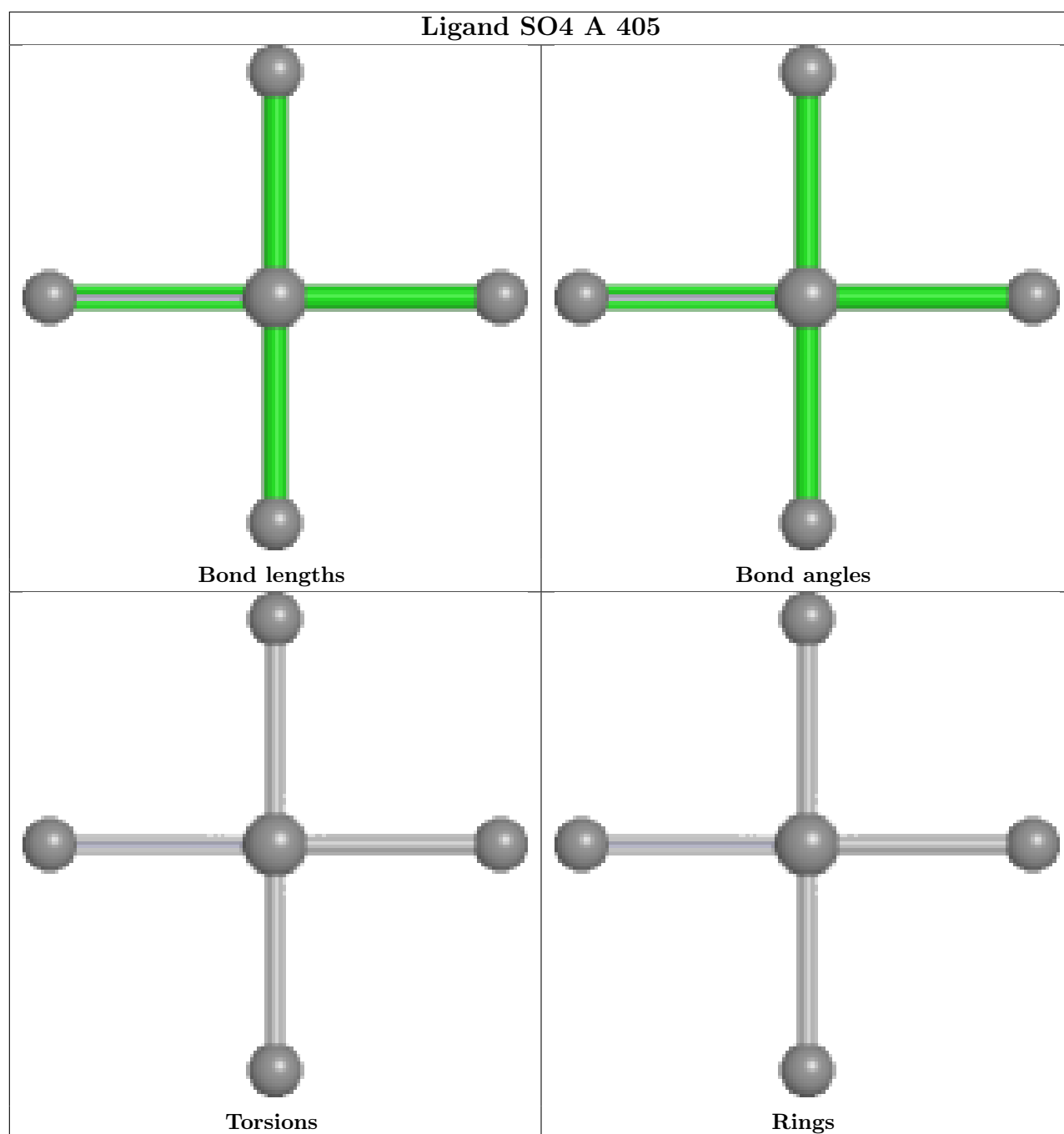












5.7 Other polymers [i](#)

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	321/334 (96%)	0.44	28 (8%) 16 13	24, 37, 59, 79	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	GLN	11.9
1	A	70	LEU	8.5
1	A	71	VAL	7.1
1	A	73	GLY	6.2
1	A	328	GLU	5.9
1	A	113	GLY	5.6
1	A	114	ASP	5.0
1	A	170	GLY	4.9
1	A	68	THR	4.1
1	A	74	ALA	3.8
1	A	314	SER	3.7
1	A	264	SER	3.4
1	A	171	ASP	3.4
1	A	323	TYR	3.3
1	A	72	GLY	3.1
1	A	8	GLN	2.9
1	A	327	PRO	2.6
1	A	75	GLY	2.5
1	A	62	ARG	2.5
1	A	289	GLU	2.3
1	A	144	ARG	2.2
1	A	288	HIS	2.2
1	A	312	SER	2.2
1	A	233	MET	2.2
1	A	47	LEU	2.1
1	A	111	GLU	2.0
1	A	50	ARG	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	140	ARG	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](#)

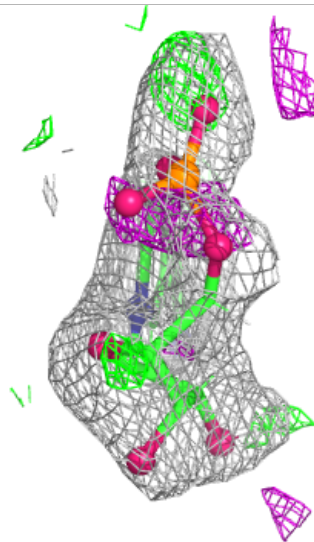
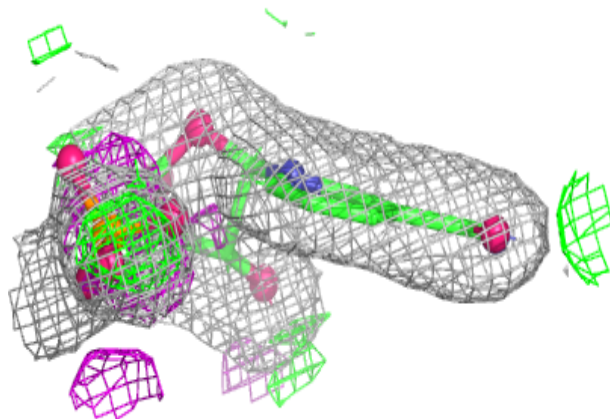
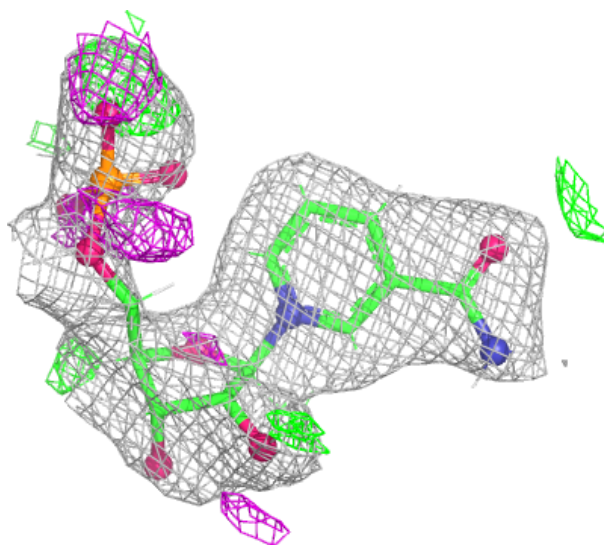
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NMN	A	401	22/22	0.77	0.20	35,54,84,96	0
4	SO4	A	405	5/5	0.79	0.15	77,79,80,92	0
4	SO4	A	406	5/5	0.89	0.28	79,81,89,93	0
3	AMP	A	402	23/23	0.91	0.11	24,37,58,70	0
4	SO4	A	404	5/5	0.94	0.14	32,41,48,55	0
4	SO4	A	403	5/5	0.97	0.10	29,36,44,45	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.

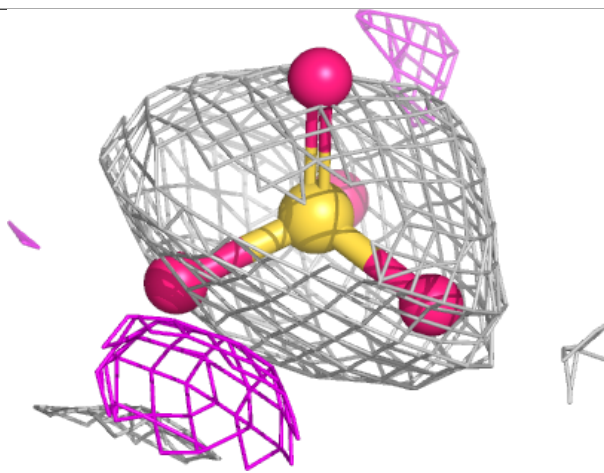
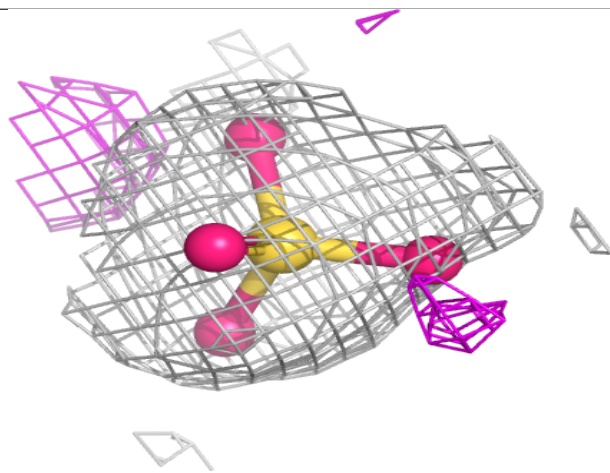
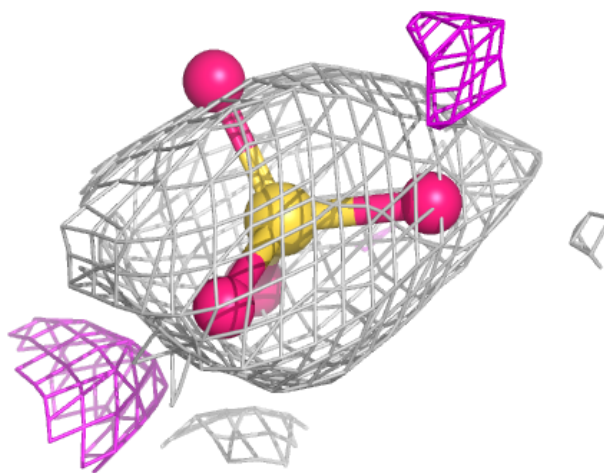
Electron density around NMN A 401:

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



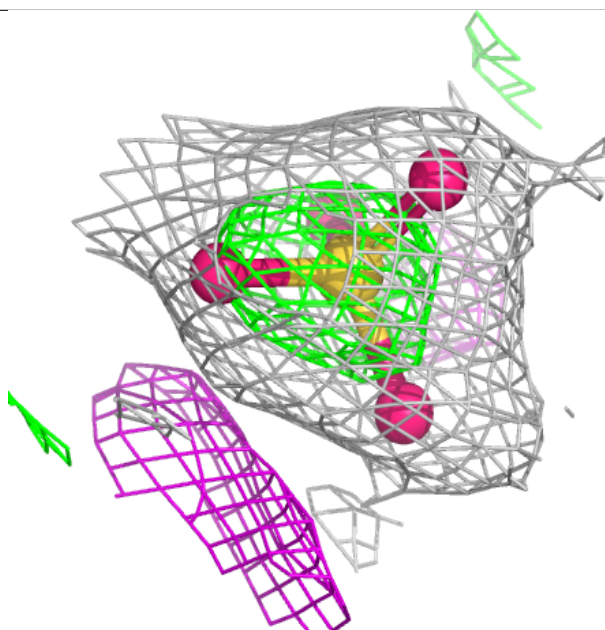
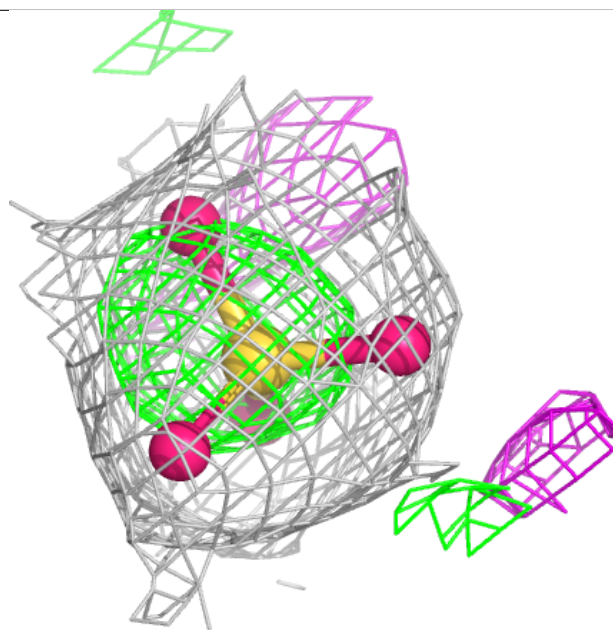
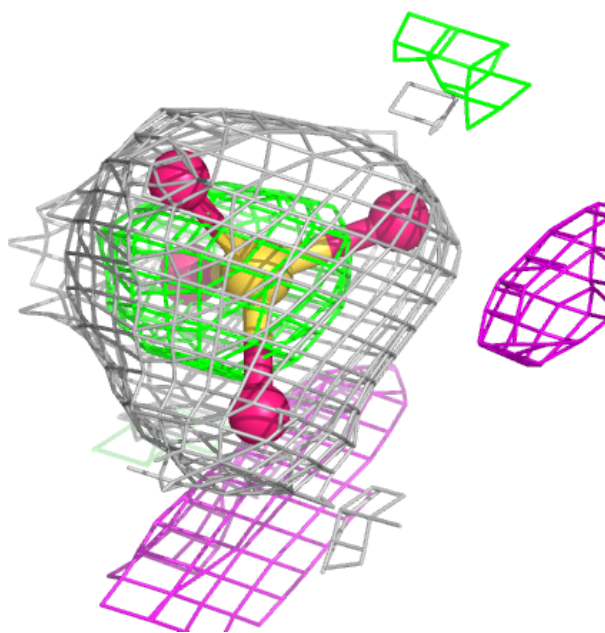
Electron density around SO4 A 405:

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



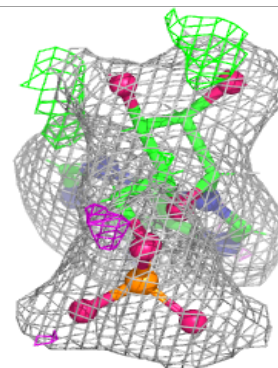
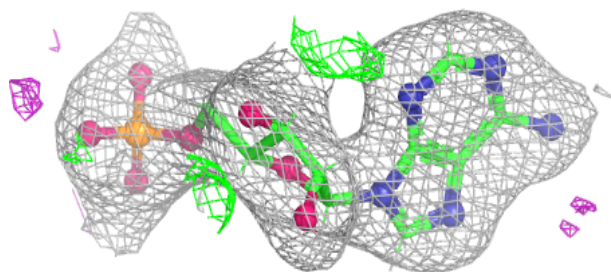
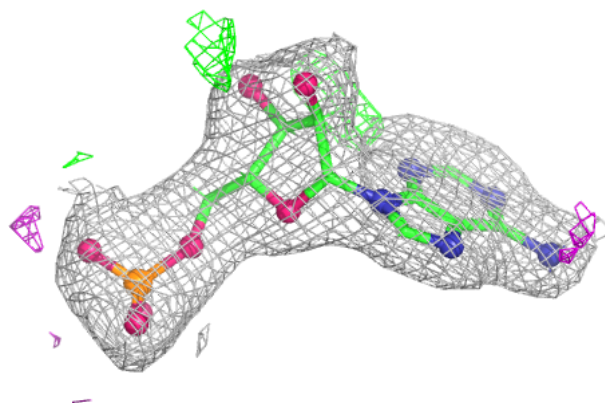
Electron density around SO4 A 406:

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



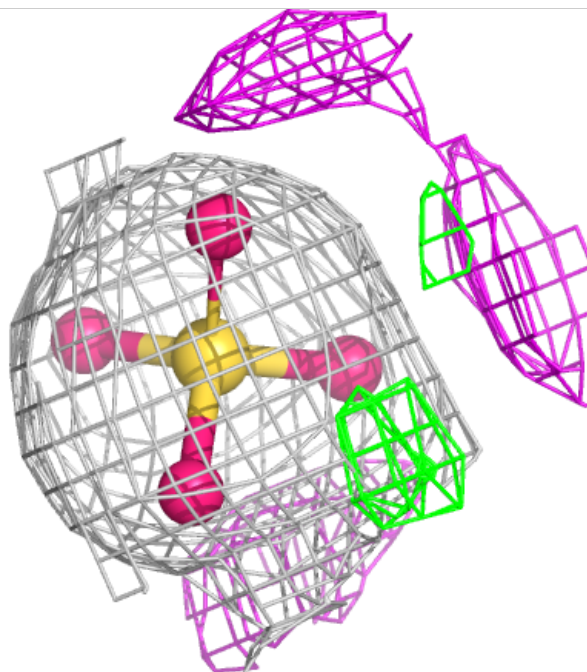
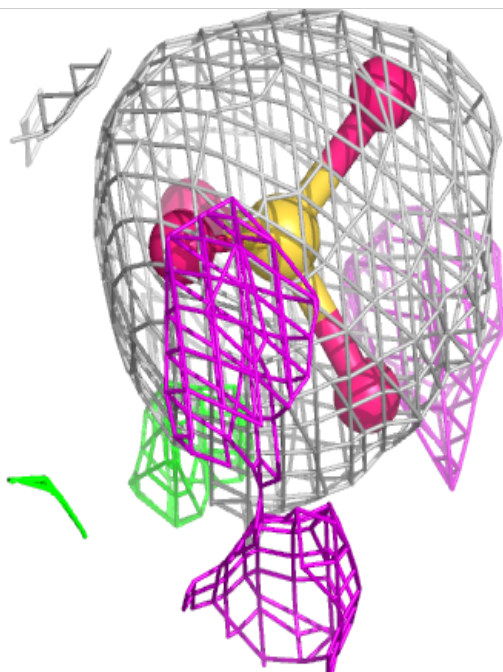
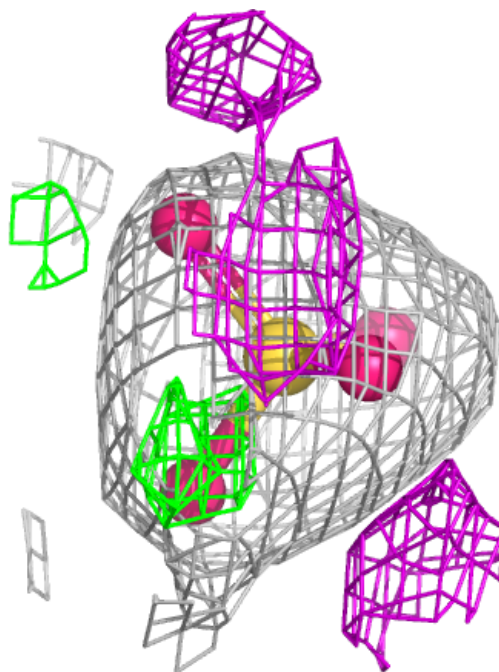
Electron density around AMP A 402:

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



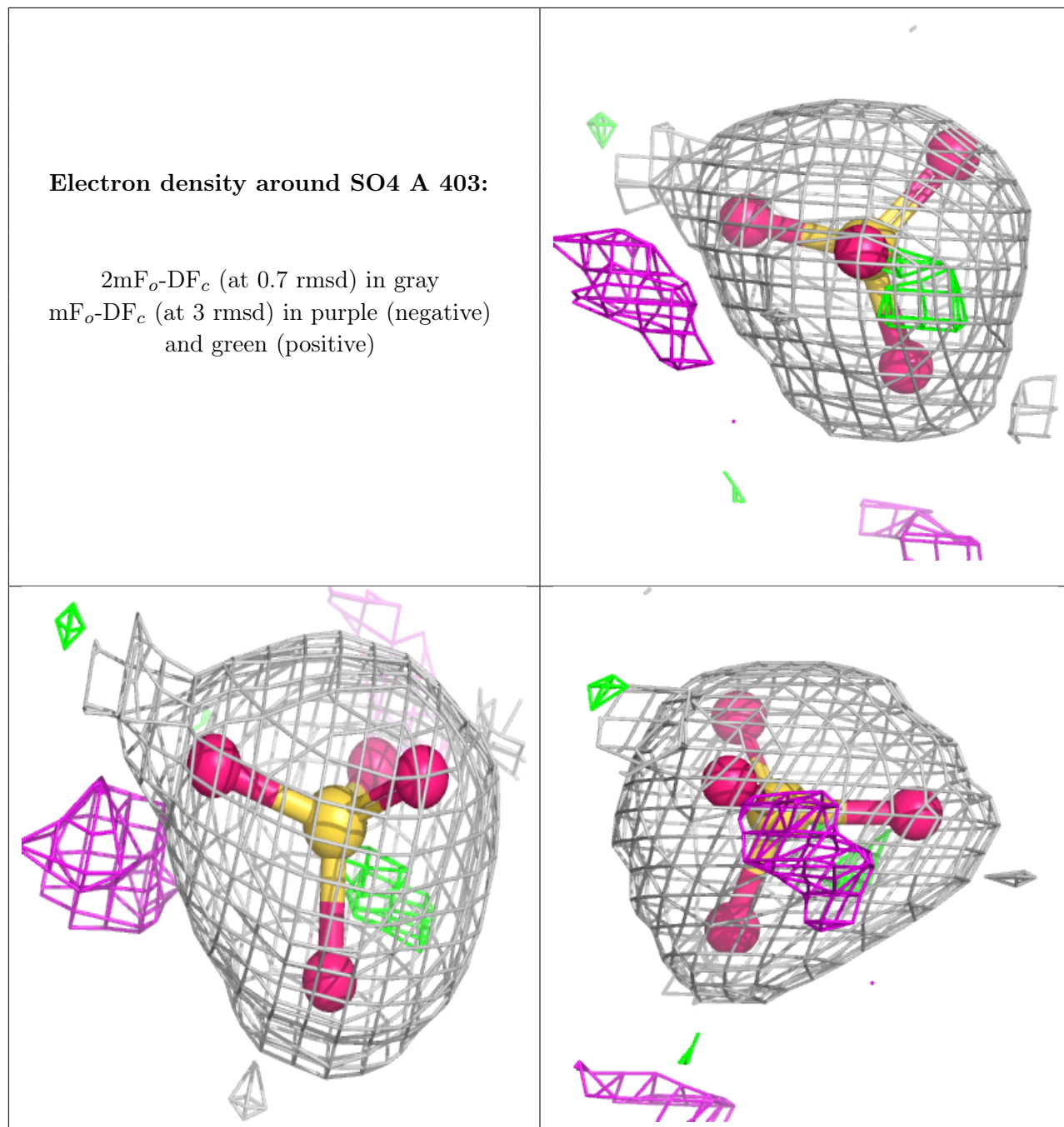
Electron density around SO4 A 404:

$2mF_o-DF_c$ (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)



6.5 Other polymers ⓘ

There are no such residues in this entry.