



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:54 PM UTC

PDB ID : 6KRH / pdb_00006krh
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 : 2019-08-21
Resolution : 2.60 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

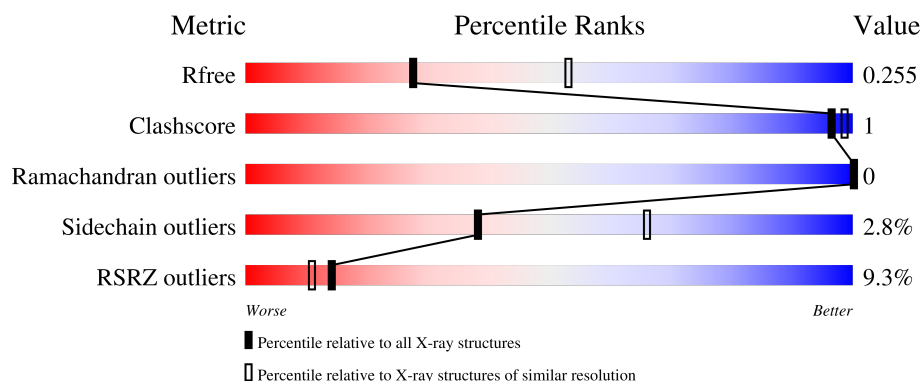
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

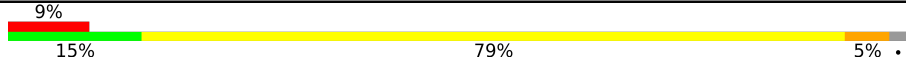
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	327	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5039 atoms, of which 2425 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.

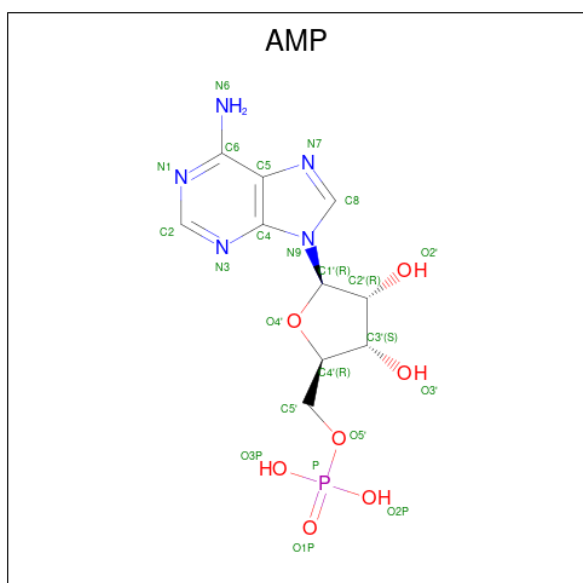
- Molecule 1 is a protein called DNA ligase A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	321	4905	1571	2399	453	478	4	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

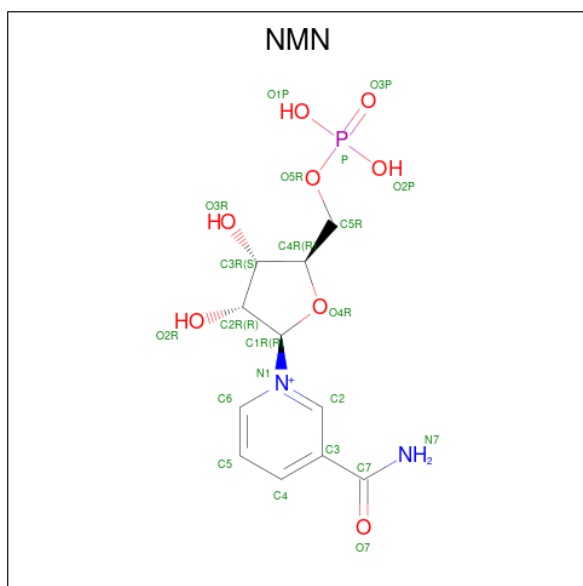
Chain	Residue	Modelled	Actual	Comment	Reference
A	236	TYR	HIS	engineered mutation	UNP P9WNV1
A	329	HIS	-	expression tag	UNP P9WNV1
A	330	HIS	-	expression tag	UNP P9WNV1
A	331	HIS	-	expression tag	UNP P9WNV1
A	332	HIS	-	expression tag	UNP P9WNV1
A	333	HIS	-	expression tag	UNP P9WNV1
A	334	HIS	-	expression tag	UNP P9WNV1

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



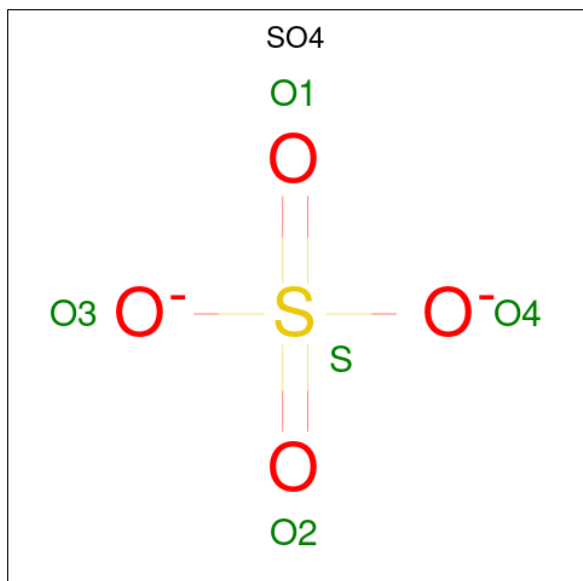
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total	C	H	N	O	P	0	0
			35	10	12	5	7	1		

- Molecule 3 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	
3	A	1	Total	C	H	N	O	P	0	0
			36	11	14	2	8	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		

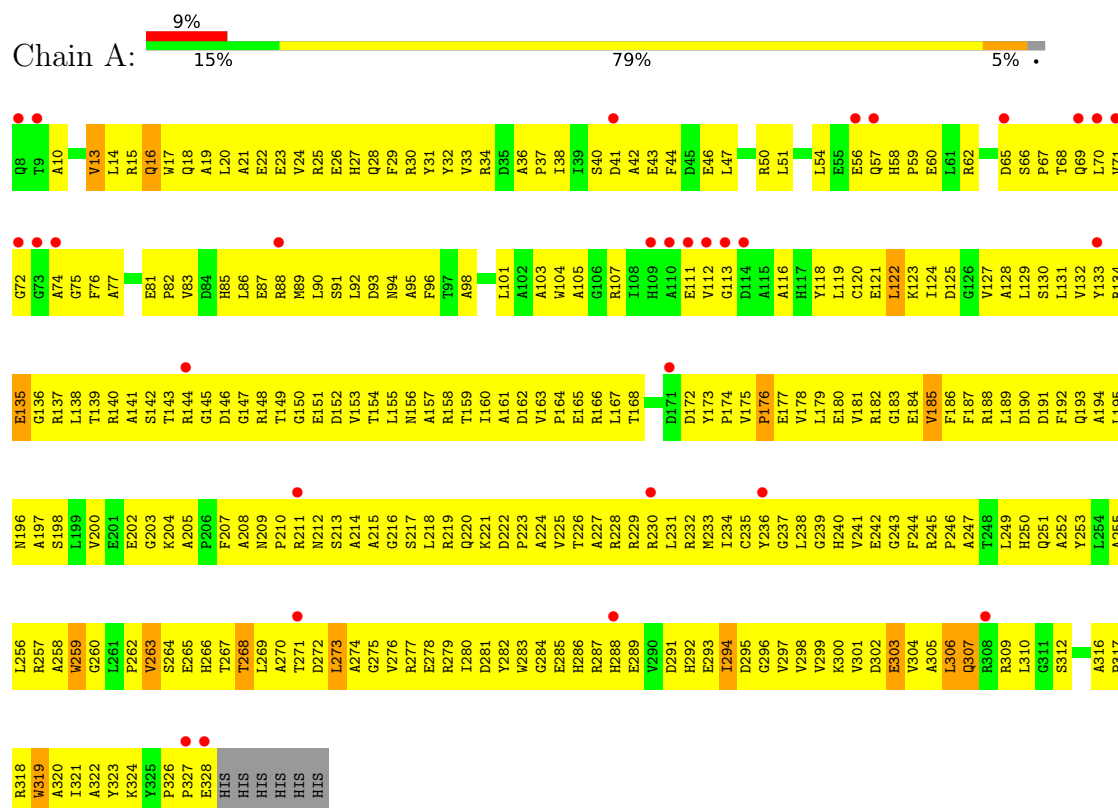
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	43	Total	O	0	0
			43	43		

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	95.55Å 95.55Å 200.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.13 – 2.60 43.13 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.13-2.60) 99.9 (43.13-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.224 , 0.264 0.242 , 0.255	Depositor DCC
R_{free} test set	880 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5039	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: NMN, SO4, 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	3.40	338/2564 (13.2%)	1.46	34/3493 (1.0%)

All (338) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	283	TRP	C-O	-10.59	1.10	1.24
1	A	211	ARG	C-O	-9.91	1.12	1.24
1	A	209	ASN	C-O	-9.71	1.14	1.24
1	A	303	GLU	CA-CB	-9.66	1.38	1.53
1	A	161	ALA	C-O	-9.47	1.12	1.24
1	A	235	CYS	C-O	-9.47	1.12	1.23
1	A	226	THR	C-O	-9.47	1.13	1.24
1	A	66	SER	C-O	-9.41	1.11	1.23
1	A	181	VAL	C-O	-9.39	1.14	1.24
1	A	237	GLY	C-O	-9.20	1.14	1.23
1	A	132	VAL	C-O	-9.19	1.14	1.24
1	A	189	LEU	C-O	-9.18	1.13	1.24
1	A	123	LYS	N-CA	-9.17	1.34	1.46
1	A	149	THR	C-O	-9.11	1.13	1.24
1	A	143	THR	C-O	-9.08	1.11	1.23
1	A	130	SER	C-O	-9.06	1.13	1.24
1	A	269	LEU	C-O	-9.03	1.13	1.23
1	A	179	LEU	C-O	-9.00	1.13	1.23
1	A	121	GLU	C-O	-8.95	1.12	1.23
1	A	41	ASP	C-O	-8.90	1.12	1.24
1	A	173	TYR	C-O	-8.89	1.16	1.24
1	A	297	VAL	C-O	-8.87	1.14	1.24
1	A	207	PHE	C-O	-8.77	1.13	1.23
1	A	183	GLY	C-O	-8.74	1.15	1.23
1	A	265	GLU	C-O	-8.71	1.12	1.24
1	A	142	SER	C-O	-8.70	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	187	PHE	C-O	-8.64	1.13	1.23
1	A	305	ALA	C-O	-8.63	1.13	1.24
1	A	120	CYS	C-O	-8.61	1.14	1.24
1	A	241	VAL	C-O	-8.60	1.15	1.23
1	A	76	PHE	C-O	-8.60	1.14	1.23
1	A	105	ALA	CA-CB	-8.59	1.39	1.53
1	A	182	ARG	C-O	-8.59	1.13	1.23
1	A	123	LYS	CA-CB	-8.57	1.41	1.53
1	A	234	ILE	C-O	-8.57	1.15	1.24
1	A	233	MET	C-O	-8.53	1.13	1.23
1	A	131	LEU	C-O	-8.50	1.13	1.23
1	A	263	VAL	C-O	-8.47	1.14	1.23
1	A	256	LEU	C-O	-8.44	1.14	1.24
1	A	180	GLU	C-O	-8.40	1.13	1.24
1	A	18	GLN	C-O	-8.39	1.13	1.24
1	A	89	MET	C-O	-8.34	1.14	1.23
1	A	216	GLY	C-O	-8.33	1.14	1.23
1	A	151	GLU	C-O	-8.32	1.13	1.23
1	A	232	ARG	C-O	-8.31	1.13	1.23
1	A	27	HIS	C-O	-8.29	1.13	1.24
1	A	279	ARG	C-O	-8.26	1.14	1.24
1	A	127	VAL	C-O	-8.24	1.14	1.24
1	A	221	LYS	C-O	-8.24	1.14	1.24
1	A	299	VAL	C-O	-8.19	1.15	1.24
1	A	219	ARG	C-O	-8.12	1.14	1.23
1	A	156	ASN	C-O	-8.09	1.14	1.24
1	A	178	VAL	C-O	-8.09	1.16	1.24
1	A	82	PRO	C-O	-8.07	1.14	1.23
1	A	175	VAL	C-O	-8.04	1.15	1.25
1	A	86	LEU	C-O	-8.02	1.14	1.24
1	A	298	VAL	C-O	-8.02	1.14	1.24
1	A	122	LEU	C-O	-7.99	1.14	1.24
1	A	28	GLN	C-O	-7.98	1.14	1.24
1	A	144	ARG	CZ-NH2	-7.96	1.23	1.33
1	A	159	THR	C-O	-7.95	1.13	1.24
1	A	246	PRO	C-O	-7.93	1.15	1.23
1	A	193	GLN	C-O	-7.93	1.14	1.24
1	A	140	ARG	C-O	-7.91	1.14	1.23
1	A	253	TYR	C-O	-7.91	1.14	1.24
1	A	301	VAL	C-O	-7.90	1.15	1.24
1	A	321	ILE	C-O	-7.88	1.15	1.23
1	A	116	ALA	C-O	-7.82	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	296	GLY	C-O	-7.81	1.14	1.23
1	A	32	TYR	C-O	-7.80	1.15	1.24
1	A	129	LEU	C-O	-7.79	1.14	1.23
1	A	255	ALA	C-O	-7.77	1.14	1.24
1	A	136	GLY	C-O	-7.77	1.14	1.24
1	A	70	LEU	CA-C	-7.75	1.41	1.52
1	A	210	PRO	C-O	-7.73	1.14	1.24
1	A	160	ILE	C-O	-7.73	1.15	1.24
1	A	208	ALA	C-O	-7.73	1.14	1.24
1	A	191	ASP	C-O	-7.71	1.14	1.24
1	A	24	VAL	C-O	-7.69	1.15	1.24
1	A	104	TRP	C-O	-7.67	1.15	1.24
1	A	295	ASP	C-O	-7.66	1.13	1.24
1	A	194	ALA	C-O	-7.63	1.15	1.24
1	A	141	ALA	C-O	-7.61	1.14	1.23
1	A	163	VAL	CA-C	-7.60	1.47	1.53
1	A	137	ARG	C-O	-7.58	1.14	1.23
1	A	44	PHE	C-O	-7.54	1.15	1.24
1	A	242	GLU	C-O	-7.54	1.15	1.24
1	A	267	THR	C-O	-7.52	1.14	1.23
1	A	58	HIS	C-O	-7.51	1.15	1.24
1	A	20	LEU	C-O	-7.46	1.15	1.24
1	A	17	TRP	C-O	-7.46	1.14	1.24
1	A	275	GLY	C-O	-7.45	1.14	1.23
1	A	247	ALA	CA-C	-7.43	1.42	1.52
1	A	68	THR	C-O	-7.42	1.17	1.23
1	A	139	THR	C-O	-7.42	1.13	1.23
1	A	75	GLY	C-O	-7.42	1.14	1.24
1	A	195	LEU	C-O	-7.41	1.15	1.24
1	A	134	ARG	C-O	-7.40	1.15	1.24
1	A	176	PRO	C-O	-7.33	1.14	1.23
1	A	289	GLU	C-O	-7.31	1.14	1.24
1	A	266	HIS	C-O	-7.30	1.13	1.23
1	A	138	LEU	C-O	-7.29	1.15	1.24
1	A	300	LYS	C-O	-7.28	1.15	1.23
1	A	324	LYS	C-O	-7.27	1.15	1.24
1	A	218	LEU	C-O	-7.27	1.15	1.24
1	A	21	ALA	C-O	-7.24	1.15	1.24
1	A	217	SER	C-O	-7.24	1.15	1.24
1	A	188	ARG	C-O	-7.23	1.14	1.23
1	A	258	ALA	C-O	-7.21	1.15	1.24
1	A	236	TYR	CE1-CZ	-7.20	1.21	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	197	ALA	C-O	-7.19	1.15	1.24
1	A	107	ARG	C-O	-7.16	1.15	1.24
1	A	276	VAL	C-O	-7.15	1.15	1.24
1	A	177	GLU	C-O	-7.15	1.15	1.24
1	A	153	VAL	C-O	-7.14	1.15	1.24
1	A	83	VAL	C-O	-7.12	1.16	1.23
1	A	147	GLY	C-O	-7.08	1.14	1.23
1	A	284	GLY	C-O	-7.07	1.15	1.23
1	A	320	ALA	C-O	-7.05	1.15	1.23
1	A	243	GLY	C-O	-7.02	1.15	1.24
1	A	29	PHE	C-O	-7.02	1.15	1.24
1	A	23	GLU	C-O	-7.00	1.15	1.24
1	A	96	PHE	C-O	-6.98	1.14	1.24
1	A	119	LEU	C-O	-6.98	1.15	1.23
1	A	164	PRO	C-O	-6.98	1.16	1.23
1	A	163	VAL	N-CA	-6.96	1.41	1.46
1	A	165	GLU	C-O	-6.95	1.15	1.24
1	A	223	PRO	C-O	-6.95	1.15	1.24
1	A	144	ARG	C-O	-6.91	1.16	1.24
1	A	294	ILE	C-O	-6.91	1.16	1.24
1	A	95	ALA	C-O	-6.89	1.16	1.24
1	A	123	LYS	C-O	-6.89	1.15	1.24
1	A	174	PRO	C-O	-6.89	1.16	1.23
1	A	166	ARG	C-O	-6.88	1.15	1.23
1	A	274	ALA	CA-C	-6.85	1.43	1.52
1	A	37	PRO	C-O	-6.85	1.15	1.23
1	A	135	GLU	C-O	-6.84	1.14	1.23
1	A	121	GLU	CA-C	-6.83	1.44	1.52
1	A	252	ALA	C-O	-6.82	1.16	1.24
1	A	18	GLN	CA-C	-6.80	1.43	1.52
1	A	200	VAL	C-O	-6.80	1.15	1.24
1	A	260	GLY	C-O	-6.79	1.14	1.24
1	A	306	LEU	C-O	-6.79	1.16	1.24
1	A	168	THR	C-O	-6.76	1.15	1.24
1	A	185	VAL	C-O	-6.75	1.15	1.24
1	A	239	GLY	C-O	-6.74	1.14	1.23
1	A	318	ARG	C-O	-6.74	1.14	1.23
1	A	46	GLU	C-O	-6.74	1.16	1.24
1	A	152	ASP	C-O	-6.73	1.15	1.24
1	A	322	ALA	C-O	-6.70	1.15	1.24
1	A	36	ALA	C-O	-6.67	1.16	1.24
1	A	184	GLU	C-O	-6.67	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	LEU	C-O	-6.64	1.15	1.24
1	A	272	ASP	C-O	-6.63	1.16	1.23
1	A	68	THR	CA-C	-6.63	1.47	1.53
1	A	26	GLU	C-O	-6.63	1.15	1.24
1	A	158	ARG	C-O	-6.59	1.15	1.24
1	A	319	TRP	C-O	-6.59	1.15	1.24
1	A	244	PHE	C-O	-6.58	1.15	1.24
1	A	51	LEU	C-O	-6.57	1.15	1.24
1	A	184	GLU	CD-OE1	-6.57	1.12	1.25
1	A	266	HIS	CA-C	-6.55	1.44	1.53
1	A	92	LEU	C-O	-6.55	1.15	1.23
1	A	316	ALA	C-O	-6.55	1.15	1.24
1	A	81	GLU	C-O	-6.54	1.15	1.23
1	A	133	TYR	C-O	-6.51	1.16	1.24
1	A	62	ARG	C-O	-6.49	1.16	1.24
1	A	22	GLU	C-O	-6.47	1.16	1.24
1	A	287	ARG	C-O	-6.47	1.16	1.24
1	A	105	ALA	C-O	-6.46	1.16	1.24
1	A	118	TYR	C-O	-6.45	1.16	1.24
1	A	151	GLU	CA-C	-6.42	1.45	1.52
1	A	231	LEU	C-O	-6.42	1.15	1.23
1	A	229	ARG	C-O	-6.40	1.16	1.23
1	A	182	ARG	CZ-NH2	-6.39	1.25	1.33
1	A	262	PRO	C-O	-6.38	1.15	1.24
1	A	182	ARG	N-CA	-6.37	1.38	1.45
1	A	213	SER	C-O	-6.35	1.16	1.24
1	A	214	ALA	C-O	-6.34	1.15	1.24
1	A	47	LEU	C-O	-6.33	1.16	1.24
1	A	146	ASP	C-O	-6.32	1.15	1.24
1	A	186	PHE	C-O	-6.31	1.16	1.23
1	A	25	ARG	C-O	-6.30	1.16	1.24
1	A	38	ILE	C-O	-6.29	1.14	1.23
1	A	293	GLU	C-O	-6.27	1.16	1.23
1	A	163	VAL	C-O	-6.25	1.16	1.24
1	A	215	ALA	C-O	-6.22	1.16	1.24
1	A	238	LEU	N-CA	-6.22	1.38	1.46
1	A	87	GLU	C-O	-6.22	1.16	1.23
1	A	125	ASP	N-CA	-6.21	1.38	1.46
1	A	144	ARG	CZ-NH1	-6.20	1.24	1.32
1	A	317	PRO	C-O	-6.17	1.16	1.23
1	A	94	ASN	C-O	-6.14	1.16	1.23
1	A	72	GLY	C-O	-6.14	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	ASP	C-O	-6.14	1.16	1.23
1	A	203	GLY	C-O	-6.12	1.16	1.24
1	A	319	TRP	N-CA	-6.11	1.38	1.46
1	A	198	SER	C-O	-6.10	1.17	1.24
1	A	204	LYS	C-O	-6.10	1.16	1.23
1	A	153	VAL	N-CA	-6.10	1.38	1.46
1	A	247	ALA	C-O	-6.10	1.16	1.24
1	A	309	ARG	C-O	-6.09	1.16	1.24
1	A	145	GLY	C-O	-6.09	1.16	1.24
1	A	245	ARG	C-O	-6.08	1.17	1.24
1	A	240	HIS	C-O	-6.05	1.16	1.24
1	A	16	GLN	C-O	-6.03	1.17	1.24
1	A	155	LEU	C-O	-6.03	1.16	1.24
1	A	270	ALA	C-O	-6.02	1.16	1.23
1	A	266	HIS	N-CA	-6.02	1.39	1.46
1	A	326	PRO	C-O	-6.01	1.17	1.24
1	A	162	ASP	C-O	-6.01	1.16	1.24
1	A	192	PHE	C-O	-5.99	1.17	1.24
1	A	251	GLN	C-O	-5.99	1.16	1.24
1	A	291	ASP	C-O	-5.98	1.16	1.24
1	A	257	ARG	C-O	-5.98	1.17	1.24
1	A	236	TYR	C-O	-5.98	1.16	1.24
1	A	310	LEU	C-O	-5.97	1.16	1.24
1	A	324	LYS	CA-CB	-5.97	1.44	1.53
1	A	41	ASP	CA-C	-5.97	1.44	1.52
1	A	288	HIS	C-O	-5.96	1.16	1.24
1	A	13	VAL	C-O	-5.95	1.17	1.24
1	A	197	ALA	N-CA	-5.94	1.39	1.46
1	A	60	GLU	C-O	-5.94	1.16	1.24
1	A	154	THR	C-O	-5.93	1.17	1.24
1	A	19	ALA	C-O	-5.92	1.17	1.24
1	A	213	SER	N-CA	-5.92	1.39	1.46
1	A	167	LEU	C-O	-5.91	1.16	1.23
1	A	307	GLN	C-O	-5.90	1.17	1.24
1	A	93	ASP	C-O	-5.90	1.16	1.23
1	A	43	GLU	C-O	-5.89	1.17	1.24
1	A	196	ASN	C-O	-5.87	1.17	1.24
1	A	244	PHE	N-CA	-5.87	1.39	1.46
1	A	16	GLN	CA-C	-5.87	1.45	1.52
1	A	42	ALA	C-O	-5.86	1.17	1.24
1	A	125	ASP	CG-OD1	-5.86	1.14	1.25
1	A	229	ARG	CZ-NH2	-5.85	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	ARG	CD-NE	5.84	1.54	1.46
1	A	282	TYR	C-O	-5.84	1.17	1.24
1	A	277	ARG	C-O	-5.82	1.16	1.24
1	A	312	SER	C-O	-5.81	1.16	1.23
1	A	249	LEU	C-O	-5.81	1.16	1.24
1	A	40	SER	C-O	-5.78	1.15	1.23
1	A	278	GLU	C-O	-5.77	1.17	1.24
1	A	259	TRP	C-O	-5.77	1.16	1.24
1	A	224	ALA	C-O	-5.77	1.16	1.24
1	A	220	GLN	C-O	-5.75	1.16	1.24
1	A	285	GLU	C-O	-5.74	1.16	1.24
1	A	268	THR	C-O	-5.74	1.16	1.23
1	A	190	ASP	C-O	-5.74	1.17	1.24
1	A	89	MET	N-CA	-5.74	1.38	1.46
1	A	134	ARG	CZ-NH1	-5.73	1.24	1.32
1	A	157	ALA	C-O	-5.72	1.16	1.24
1	A	88	ARG	C-O	-5.71	1.17	1.23
1	A	50	ARG	CA-C	-5.70	1.45	1.52
1	A	17	TRP	CA-C	-5.70	1.45	1.52
1	A	185	VAL	N-CA	-5.70	1.39	1.46
1	A	274	ALA	C-O	-5.70	1.17	1.24
1	A	198	SER	N-CA	-5.69	1.39	1.46
1	A	281	ASP	C-O	-5.69	1.17	1.24
1	A	15	ARG	C-O	-5.68	1.17	1.24
1	A	34	ARG	CZ-NH1	-5.65	1.24	1.32
1	A	54	LEU	C-O	-5.62	1.17	1.24
1	A	90	LEU	C-O	-5.61	1.16	1.23
1	A	323	TYR	C-O	-5.60	1.17	1.24
1	A	40	SER	CA-C	-5.57	1.45	1.53
1	A	280	ILE	N-CA	-5.56	1.39	1.46
1	A	194	ALA	N-CA	-5.55	1.39	1.46
1	A	305	ALA	CA-C	-5.54	1.45	1.52
1	A	151	GLU	CA-CB	-5.54	1.44	1.53
1	A	189	LEU	CA-C	-5.53	1.45	1.52
1	A	103	ALA	C-O	-5.53	1.17	1.24
1	A	228	ARG	N-CA	-5.51	1.38	1.46
1	A	226	THR	CB-CG2	-5.51	1.34	1.52
1	A	227	ALA	C-O	-5.51	1.17	1.24
1	A	134	ARG	CZ-NH2	-5.50	1.26	1.33
1	A	220	GLN	N-CA	-5.50	1.39	1.46
1	A	140	ARG	CZ-NH1	-5.49	1.25	1.32
1	A	33	VAL	C-O	-5.49	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	ARG	CZ-NH2	-5.47	1.26	1.33
1	A	250	HIS	C-O	-5.47	1.17	1.24
1	A	180	GLU	CD-OE2	-5.45	1.15	1.25
1	A	74	ALA	C-O	-5.45	1.16	1.24
1	A	202	GLU	C-O	-5.44	1.16	1.24
1	A	124	ILE	C-O	-5.44	1.17	1.24
1	A	286	HIS	C-O	-5.42	1.16	1.24
1	A	30	ARG	C-O	-5.41	1.17	1.24
1	A	77	ALA	C-O	-5.41	1.17	1.23
1	A	101	LEU	C-O	-5.40	1.17	1.24
1	A	140	ARG	CZ-NH2	-5.39	1.26	1.33
1	A	304	VAL	C-O	-5.37	1.16	1.24
1	A	123	LYS	CA-C	-5.36	1.46	1.52
1	A	247	ALA	N-CA	-5.36	1.39	1.46
1	A	222	ASP	C-O	-5.35	1.17	1.24
1	A	150	GLY	C-O	-5.34	1.16	1.23
1	A	302	ASP	CG-OD1	-5.34	1.15	1.25
1	A	50	ARG	C-O	-5.33	1.17	1.24
1	A	67	PRO	C-O	-5.33	1.17	1.24
1	A	111	GLU	C-O	-5.33	1.17	1.24
1	A	212	ASN	C-O	-5.33	1.17	1.24
1	A	231	LEU	N-CA	-5.33	1.38	1.45
1	A	65	ASP	C-O	-5.31	1.16	1.23
1	A	46	GLU	CA-C	-5.30	1.46	1.52
1	A	318	ARG	N-CA	-5.28	1.39	1.46
1	A	271	THR	C-O	-5.28	1.17	1.24
1	A	86	LEU	CA-C	-5.28	1.46	1.52
1	A	71	VAL	C-O	-5.27	1.18	1.24
1	A	292	HIS	C-O	-5.27	1.17	1.23
1	A	31	TYR	C-O	-5.26	1.17	1.24
1	A	166	ARG	N-CA	-5.25	1.39	1.45
1	A	155	LEU	N-CA	-5.25	1.39	1.46
1	A	148	ARG	C-O	-5.25	1.17	1.24
1	A	273	LEU	C-O	-5.24	1.17	1.24
1	A	152	ASP	CG-OD2	-5.24	1.15	1.25
1	A	205	ALA	C-O	-5.23	1.17	1.23
1	A	85	HIS	C-O	-5.23	1.17	1.23
1	A	225	VAL	C-O	-5.22	1.18	1.24
1	A	91	SER	C-O	-5.18	1.16	1.24
1	A	57	GLN	C-O	-5.17	1.18	1.24
1	A	217	SER	CB-OG	-5.17	1.31	1.42
1	A	28	GLN	N-CA	-5.16	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	303	GLU	C-O	-5.16	1.17	1.24
1	A	95	ALA	CA-C	-5.12	1.46	1.52
1	A	214	ALA	CA-C	-5.12	1.45	1.52
1	A	257	ARG	N-CA	-5.12	1.40	1.46
1	A	10	ALA	C-O	-5.10	1.17	1.24
1	A	76	PHE	CA-C	-5.09	1.46	1.53
1	A	44	PHE	CA-C	-5.09	1.46	1.52
1	A	98	ALA	C-O	-5.08	1.17	1.24
1	A	166	ARG	CZ-NH2	-5.08	1.26	1.33
1	A	302	ASP	C-O	-5.07	1.17	1.24
1	A	128	ALA	C-O	-5.06	1.17	1.24
1	A	25	ARG	N-CA	-5.04	1.40	1.46
1	A	287	ARG	CZ-NH2	-5.04	1.26	1.33
1	A	172	ASP	C-O	-5.04	1.18	1.24
1	A	105	ALA	CA-C	-5.03	1.46	1.52
1	A	180	GLU	CD-OE1	-5.01	1.15	1.25
1	A	186	PHE	N-CA	-5.01	1.40	1.46
1	A	193	GLN	CA-C	-5.01	1.46	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	VAL	CB-CA-C	13.69	128.78	110.99
1	A	113	GLY	N-CA-C	11.75	141.03	113.18
1	A	74	ALA	N-CA-C	7.70	122.89	109.80
1	A	56	GLU	N-CA-C	-6.77	103.36	111.69
1	A	327	PRO	O-C-N	6.75	130.33	122.23
1	A	71	VAL	N-CA-C	-6.74	96.56	107.28
1	A	118	TYR	N-CA-C	6.67	119.28	108.41
1	A	112	VAL	N-CA-C	6.61	120.15	113.47
1	A	144	ARG	CA-CB-CG	6.55	127.20	114.10
1	A	230	ARG	N-CA-C	6.52	118.90	109.71
1	A	123	LYS	CD-CE-NZ	-6.48	91.17	111.90
1	A	327	PRO	CA-C-N	6.46	133.32	121.70
1	A	327	PRO	C-N-CA	6.46	133.32	121.70
1	A	186	PHE	N-CA-C	6.41	117.96	108.60
1	A	316	ALA	N-CA-C	6.30	113.89	108.22
1	A	59	PRO	CB-CA-C	-6.21	103.03	111.85
1	A	59	PRO	N-CA-C	5.63	121.16	113.84
1	A	287	ARG	N-CA-C	5.62	118.17	111.71
1	A	328	GLU	N-CA-CB	5.60	120.02	110.50
1	A	163	VAL	N-CA-C	5.51	112.57	107.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	SER	N-CA-C	5.44	118.54	110.48
1	A	46	GLU	N-CA-C	-5.42	105.29	111.14
1	A	237	GLY	O-C-N	-5.40	117.30	123.51
1	A	293	GLU	N-CA-C	5.40	118.06	109.96
1	A	142	SER	N-CA-C	5.36	117.21	109.07
1	A	302	ASP	N-CA-C	5.26	118.86	112.23
1	A	123	LYS	CG-CD-CE	-5.13	99.50	111.30
1	A	70	LEU	CA-C-N	-5.12	116.27	123.13
1	A	70	LEU	C-N-CA	-5.12	116.27	123.13
1	A	291	ASP	N-CA-C	5.11	119.38	113.20
1	A	123	LYS	CB-CG-CD	-5.08	99.61	111.30
1	A	105	ALA	N-CA-C	5.07	117.70	111.82
1	A	154	THR	N-CA-CB	5.05	117.54	110.12
1	A	69	GLN	N-CA-C	-5.02	102.43	109.96

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	2506	2399	2394	4	0
2	A	23	12	11	1	0
3	A	22	14	14	0	0
4	A	20	0	0	0	0
5	A	43	0	0	0	0
All	All	2614	2425	2419	5	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 1.

All (5) 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:307:GLN:HG2	1:A:319:TRP:CD2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:GLU:HB2	1:A:306:LEU:HD13	1.85	0.58
2:A:401:AMP:H2'	2:A:401:AMP:N3	2.20	0.57
1:A:176:PRO:HD3	1:A:259:TRP:CZ2	2.47	0.49
1:A:122:LEU:HB3	1:A:294:ILE:HD12	1.97	0.46

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	319/327 (98%)	313 (98%)	6 (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	252/267 (94%)	245 (97%)	7 (3%)	38	66

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	16	GLN

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Mol	Chain	Res	Type
1	A	135	GLU
1	A	185	VAL
1	A	263	VAL
1	A	268	THR
1	A	273	LEU

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	85	HIS
1	A	109	HIS
1	A	220	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	0.21	0	6,6,6	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	403	-	4,4,4	0.43	0	6,6,6	0.08	0
4	SO4	A	404	-	4,4,4	0.22	0	6,6,6	0.33	0
3	NMN	A	402	-	21,23,23	2.30	8 (38%)	27,34,34	2.35	8 (29%)
2	AMP	A	401	-	25,25,25	2.84	15 (60%)	37,38,38	2.30	14 (37%)
4	SO4	A	405	-	4,4,4	0.26	0	6,6,6	0.17	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	AMP	A	401	-	-	7/10/26/26	0/3/3/3
3	NMN	A	402	-	-	6/14/30/30	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	AMP	C8-N9	-6.09	1.27	1.37
2	A	401	AMP	C5-N7	-5.58	1.28	1.39
2	A	401	AMP	C4-N9	-4.98	1.27	1.37
3	A	402	NMN	O7-C7	-4.92	1.15	1.24
2	A	401	AMP	C2-N3	-4.06	1.26	1.33
3	A	402	NMN	C2-N1	-3.72	1.30	1.35
3	A	402	NMN	C5-C4	-3.45	1.33	1.38
2	A	401	AMP	P-O2P	-3.27	1.42	1.54
2	A	401	AMP	C4-N3	-3.22	1.28	1.34
3	A	402	NMN	C7-N7	-3.15	1.27	1.33
3	A	402	NMN	C4-C3	-3.10	1.34	1.39
2	A	401	AMP	P-O3P	-2.95	1.43	1.54
2	A	401	AMP	C3'-C4'	-2.78	1.45	1.53
3	A	402	NMN	C6-N1	-2.74	1.29	1.35
3	A	402	NMN	O4R-C4R	-2.64	1.39	1.45
2	A	401	AMP	O3'-C3'	-2.59	1.36	1.43
2	A	401	AMP	C2-N1	-2.48	1.29	1.33
2	A	401	AMP	C2'-C3'	-2.37	1.46	1.53
2	A	401	AMP	O2'-C2'	-2.28	1.37	1.43
2	A	401	AMP	C6-N1	-2.18	1.29	1.35
2	A	401	AMP	O4'-C4'	-2.17	1.40	1.45
2	A	401	AMP	O5'-C5'	-2.05	1.36	1.44
3	A	402	NMN	C3-C7	-2.01	1.47	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	AMP	C5-C4-N3	-5.80	118.73	126.72
3	A	402	NMN	O2P-P-O5R	-5.66	91.90	106.67
3	A	402	NMN	O7-C7-N7	-5.45	114.73	122.62
3	A	402	NMN	C3-C7-N7	5.42	124.41	117.74
2	A	401	AMP	N3-C4-N9	5.23	136.06	127.17
2	A	401	AMP	C2-N3-C4	4.08	121.80	111.83
2	A	401	AMP	C1'-N9-C8	-3.75	118.76	127.09
2	A	401	AMP	C4-N9-C8	3.75	109.68	105.74
2	A	401	AMP	O4'-C4'-C3'	-3.47	98.26	105.15
2	A	401	AMP	N3-C2-N1	-3.43	123.40	128.58
2	A	401	AMP	C4-C5-N7	-3.36	106.73	110.58
3	A	402	NMN	O1P-P-O5R	3.19	115.00	106.67
2	A	401	AMP	O2P-P-O1P	3.06	122.75	110.83
3	A	402	NMN	C4R-O4R-C1R	2.79	112.48	109.92
3	A	402	NMN	C4-C3-C7	-2.60	113.99	121.06
2	A	401	AMP	C2-N1-C6	2.54	122.90	118.73
2	A	401	AMP	O4'-C4'-C5'	2.53	117.44	109.33
3	A	402	NMN	O2P-P-O1P	2.45	117.00	107.80
3	A	402	NMN	C2-C3-C7	2.39	126.35	119.46
2	A	401	AMP	C5-N7-C8	2.34	107.12	103.45
2	A	401	AMP	C4-N9-C1'	2.11	131.56	126.63
2	A	401	AMP	C4'-O4'-C1'	-2.02	105.01	109.47

There are no chirality outliers.

All (13) torsion outliers are listed below:

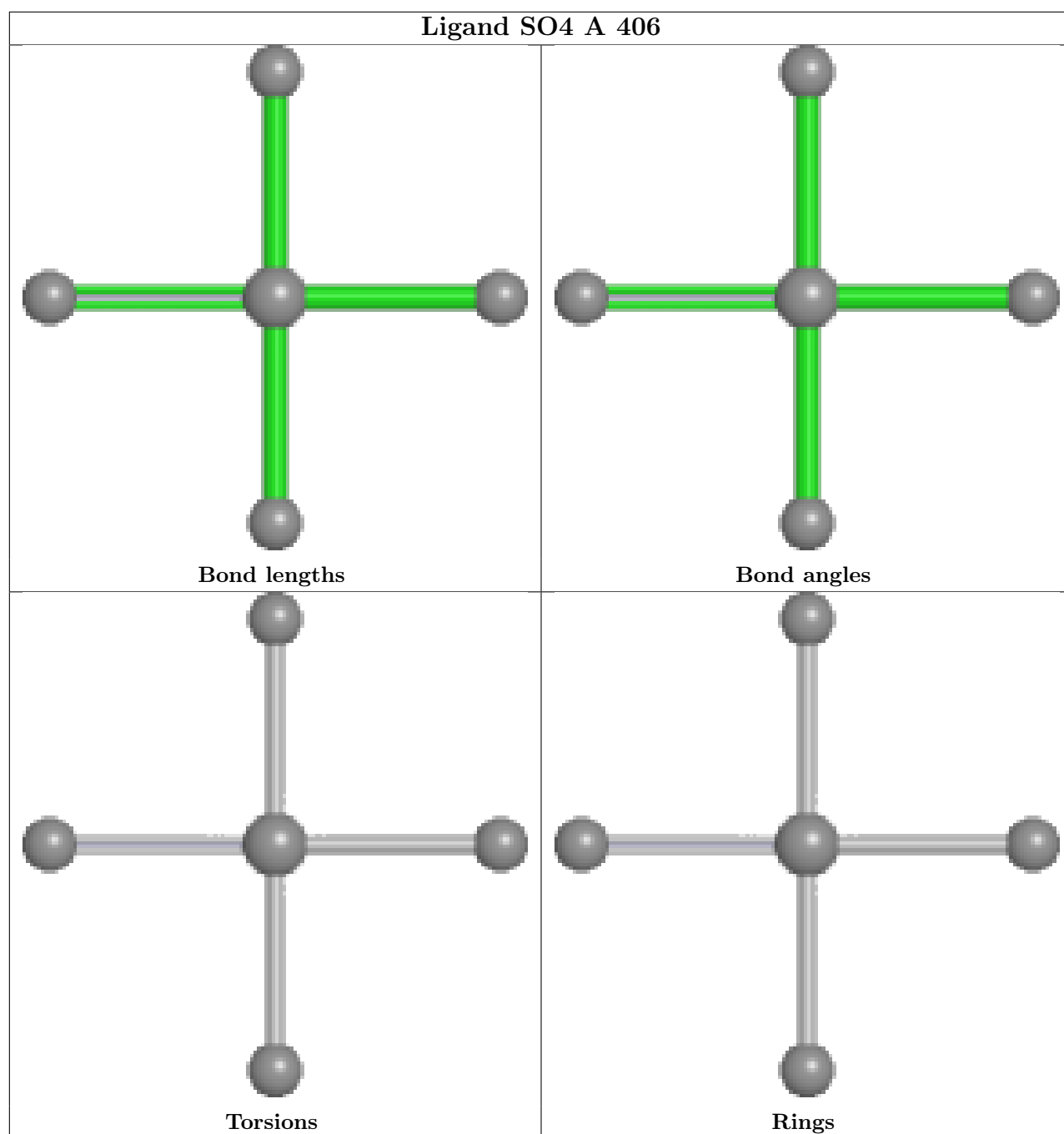
Mol	Chain	Res	Type	Atoms
2	A	401	AMP	C5'-O5'-P-O1P
2	A	401	AMP	C5'-O5'-P-O2P
2	A	401	AMP	C5'-O5'-P-O3P
2	A	401	AMP	O4'-C4'-C5'-O5'
3	A	402	NMN	C5R-O5R-P-O3P
3	A	402	NMN	C5R-O5R-P-O1P
3	A	402	NMN	C5R-O5R-P-O2P
3	A	402	NMN	O4R-C4R-C5R-O5R
2	A	401	AMP	C3'-C4'-C5'-O5'
3	A	402	NMN	C3R-C4R-C5R-O5R
2	A	401	AMP	C2'-C1'-N9-C8
2	A	401	AMP	C2'-C1'-N9-C4
3	A	402	NMN	C4R-C5R-O5R-P

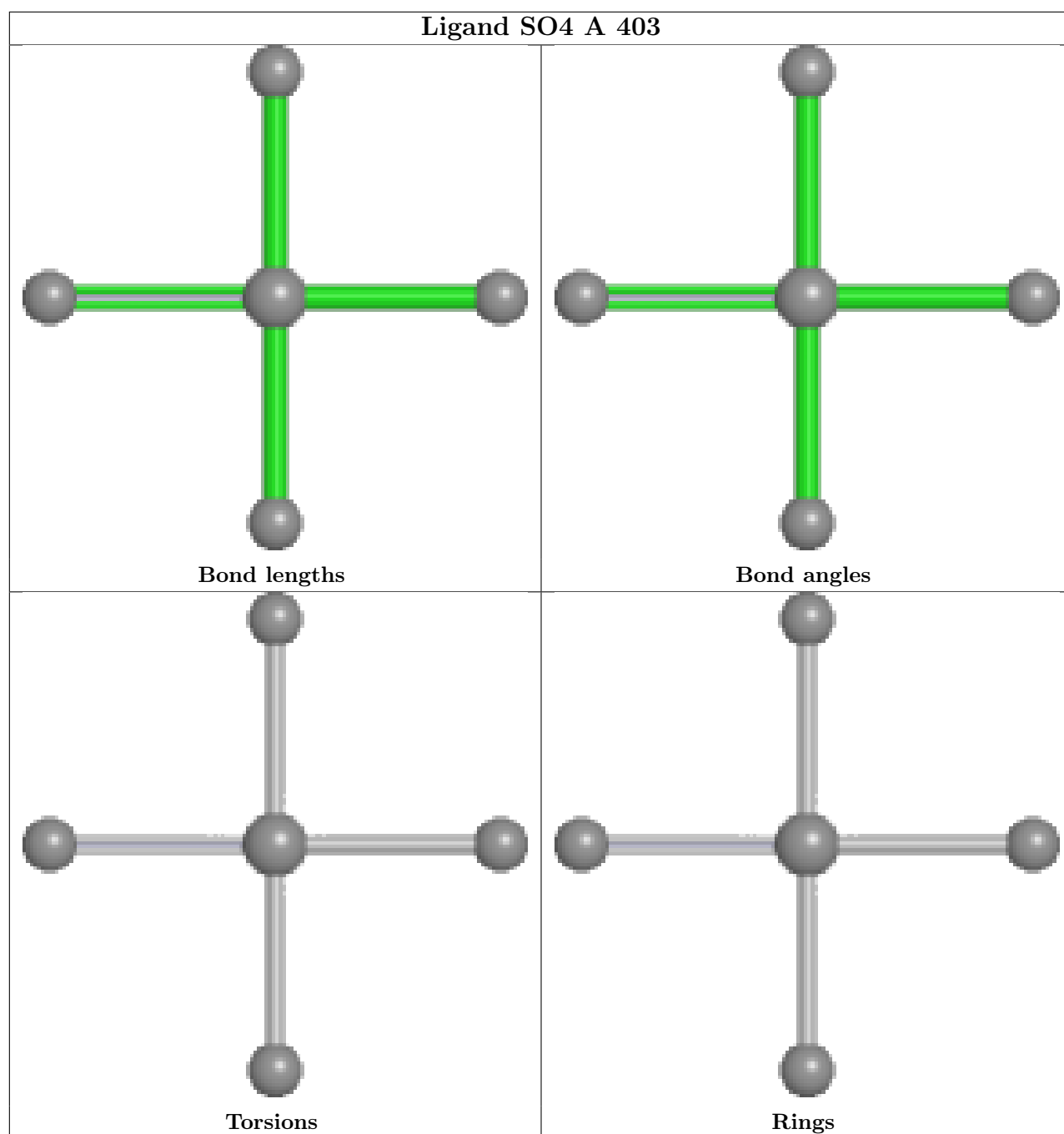
There are no ring outliers.

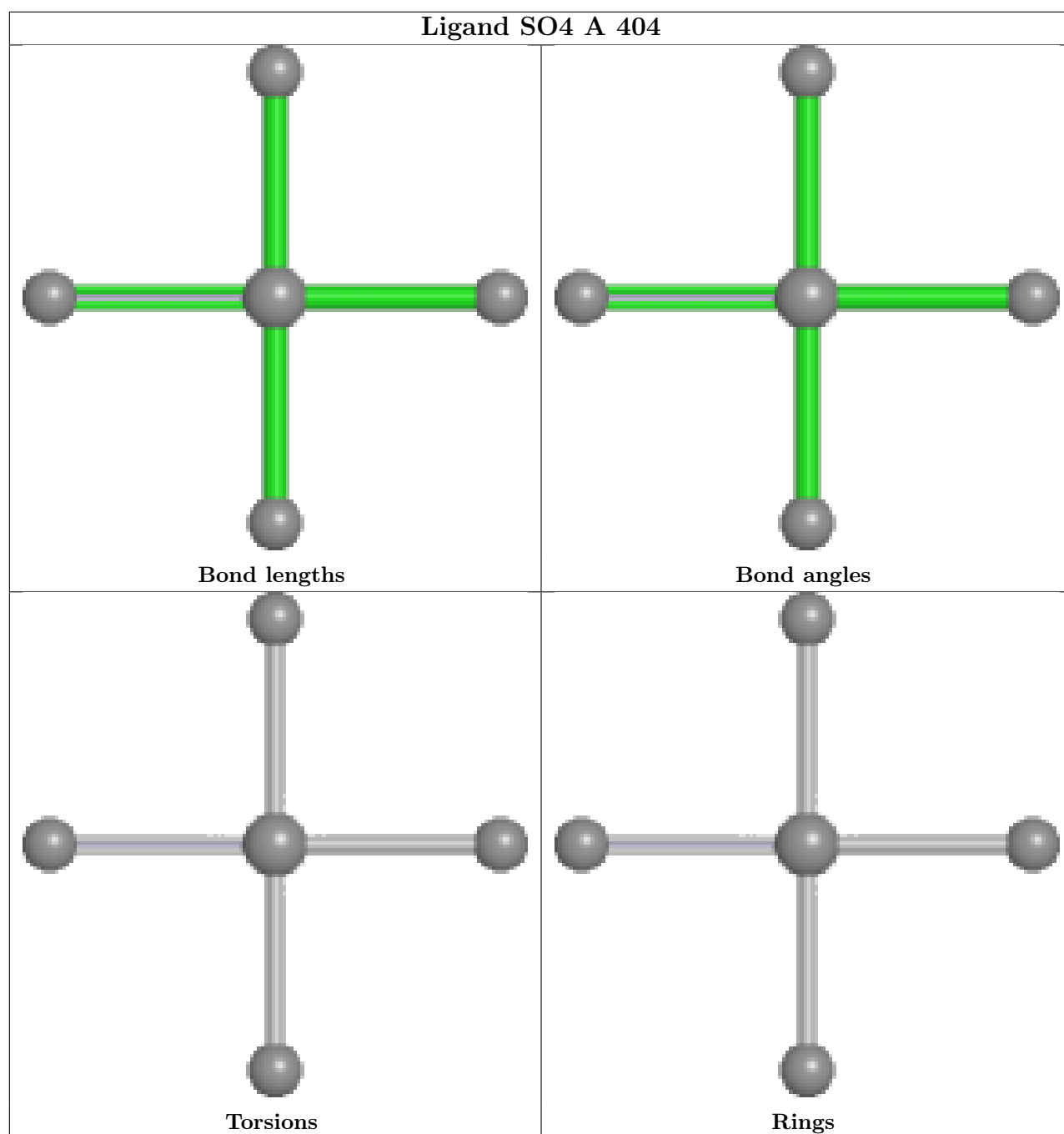
1 monomer is involved in 1 short contact:

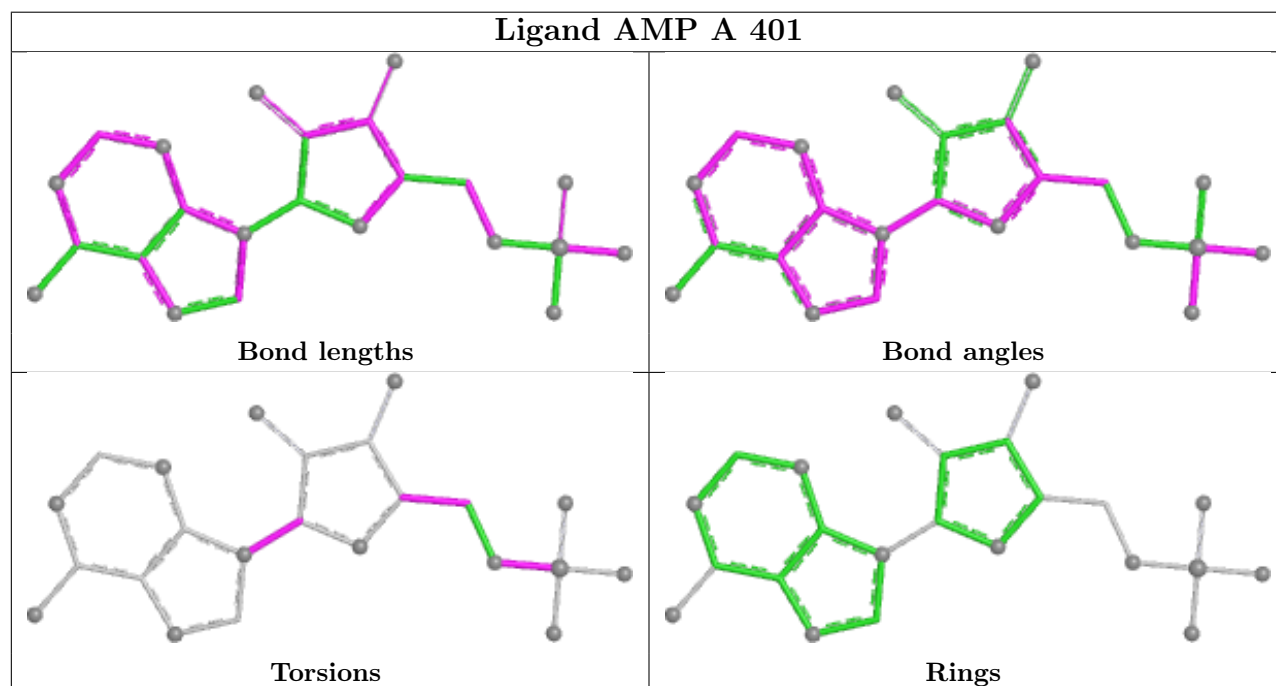
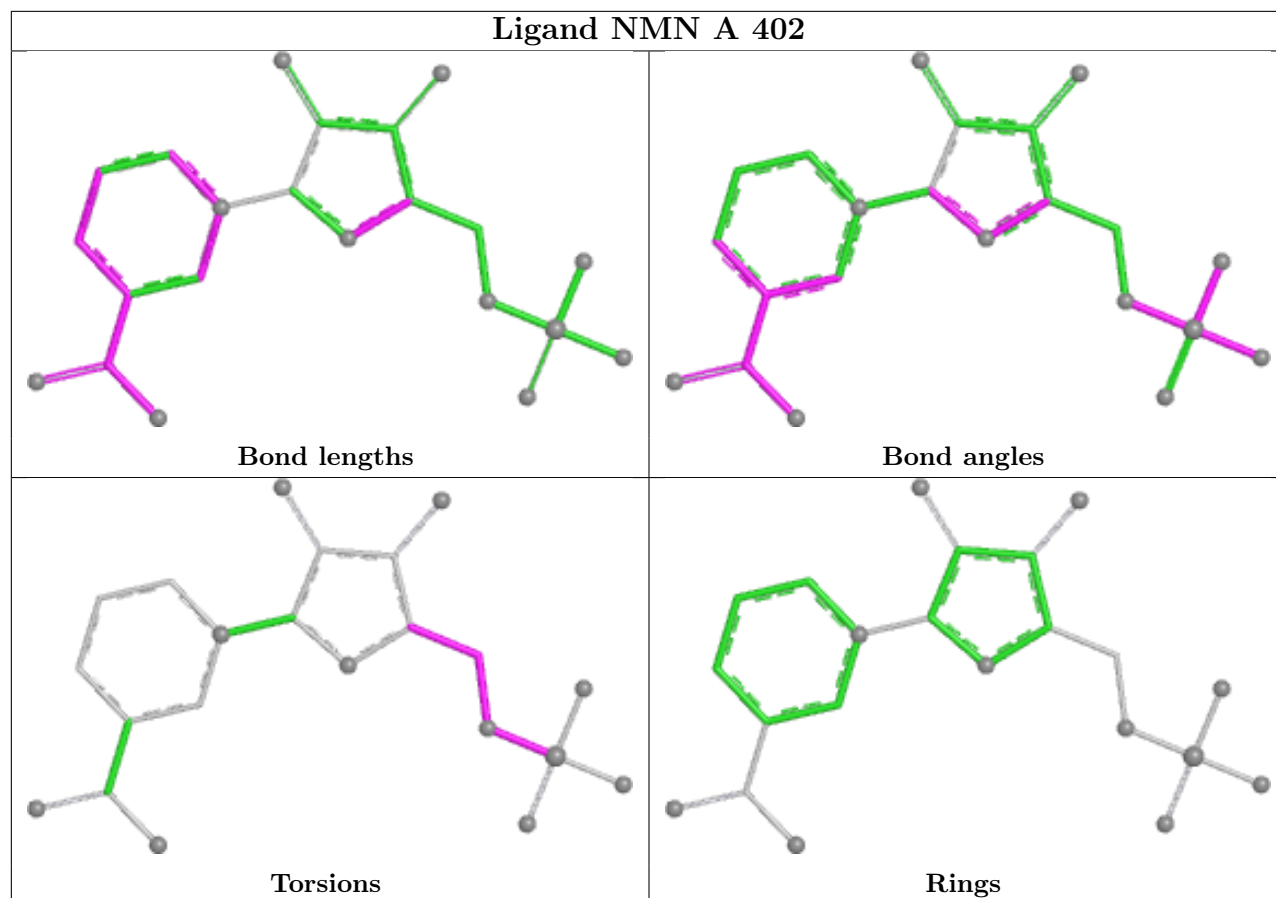
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	AMP	1	0

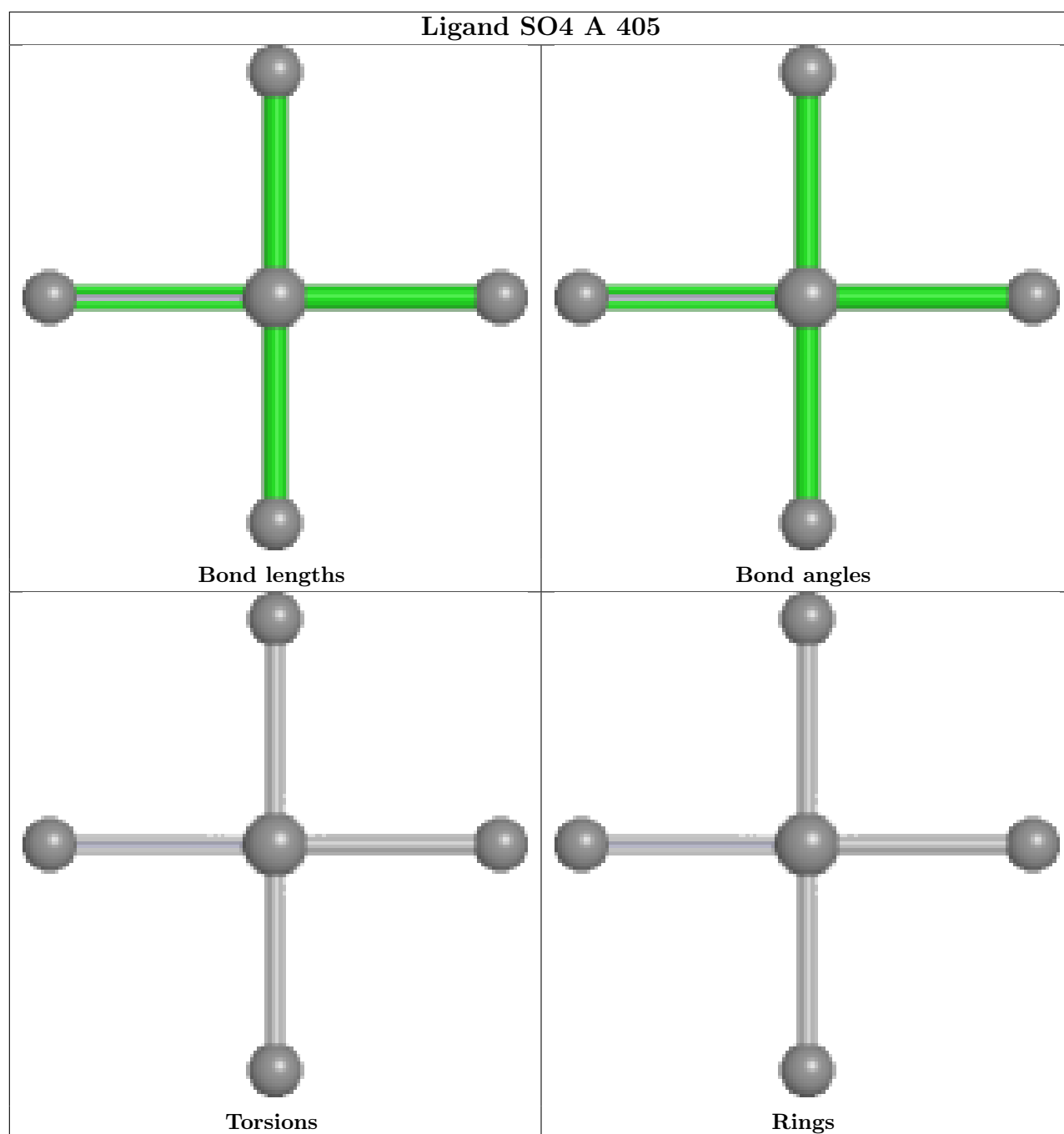
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	321/327 (98%)	0.53	30 (9%) 14 11	28, 46, 77, 188	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	112	VAL	13.8
1	A	113	GLY	10.1
1	A	70	LEU	9.8
1	A	69	GLN	7.9
1	A	72	GLY	6.5
1	A	73	GLY	6.4
1	A	328	GLU	5.6
1	A	110	ALA	5.5
1	A	171	ASP	4.7
1	A	327	PRO	4.7
1	A	71	VAL	4.6
1	A	74	ALA	4.6
1	A	8	GLN	4.4
1	A	56	GLU	4.0
1	A	88	ARG	3.9
1	A	41	ASP	3.4
1	A	211	ARG	2.9
1	A	111	GLU	2.9
1	A	144	ARG	2.9
1	A	288	HIS	2.9
1	A	114	ASP	2.7
1	A	109	HIS	2.6
1	A	230	ARG	2.6
1	A	236	TYR	2.6
1	A	57	GLN	2.4
1	A	133	TYR	2.2
1	A	9	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	65	ASP	2.2
1	A	308	ARG	2.0
1	A	271	THR	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](#)

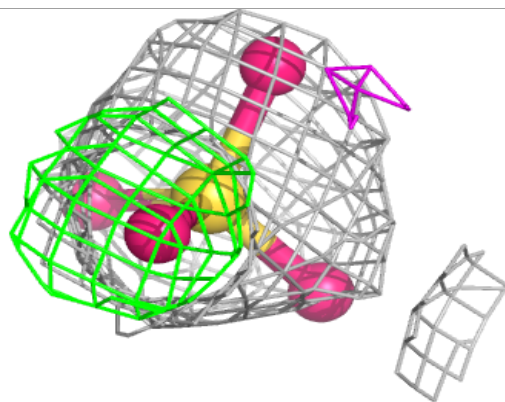
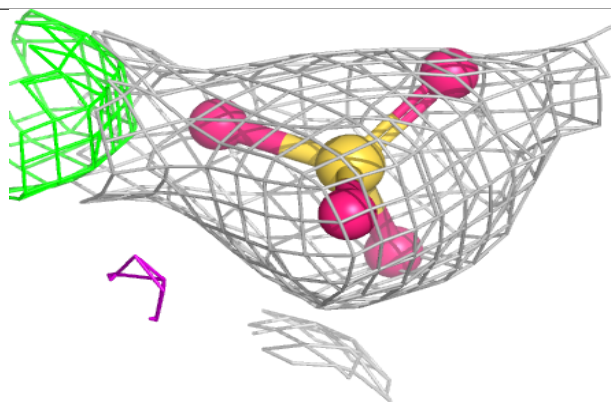
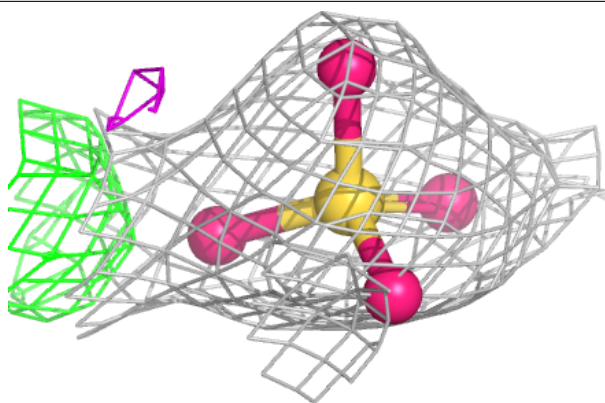
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	A	406	5/5	0.81	0.27	82,89,89,91	0
4	SO4	A	405	5/5	0.85	0.17	89,90,98,98	0
3	NMN	A	402	22/22	0.85	0.18	50,76,105,107	0
2	AMP	A	401	23/23	0.90	0.11	35,60,84,96	0
4	SO4	A	403	5/5	0.98	0.06	43,48,48,52	0
4	SO4	A	404	5/5	0.98	0.08	38,39,41,56	0

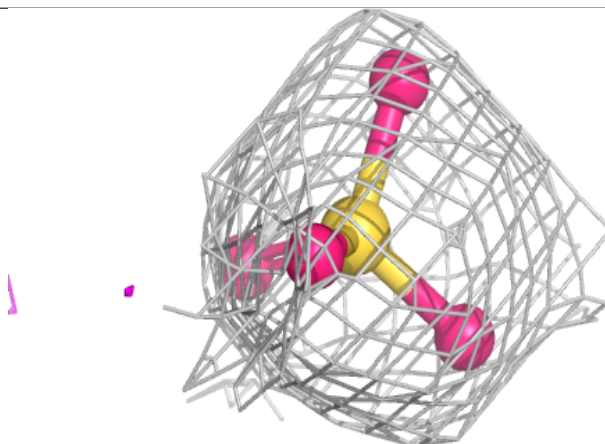
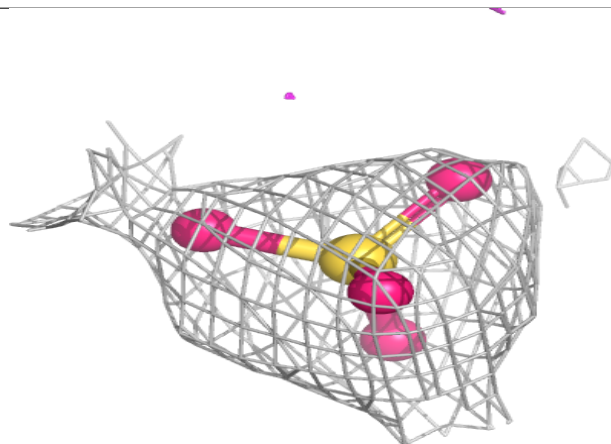
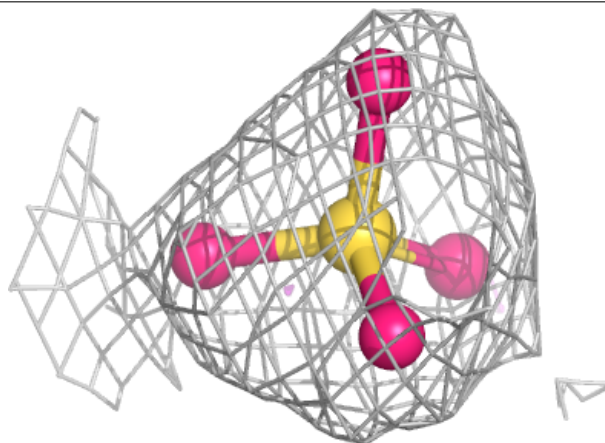
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

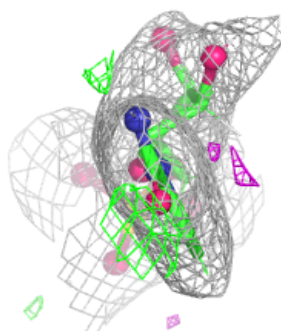
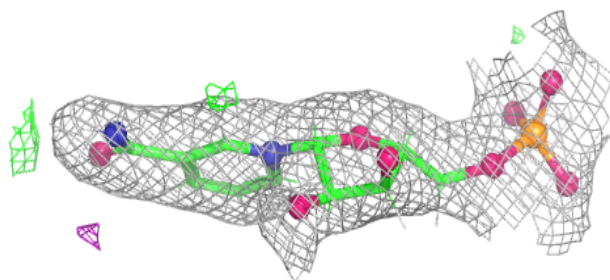
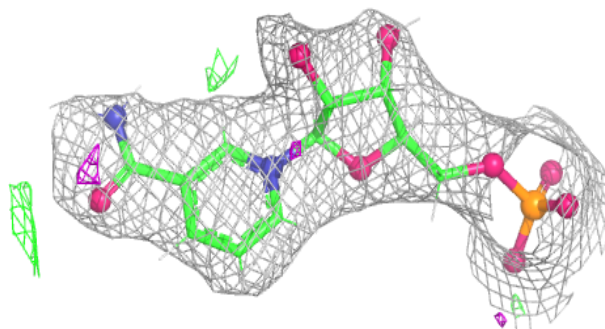
**Electron density around SO4 A 405:**

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

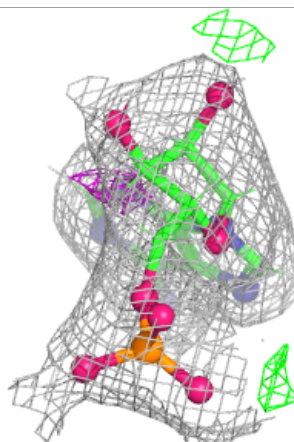
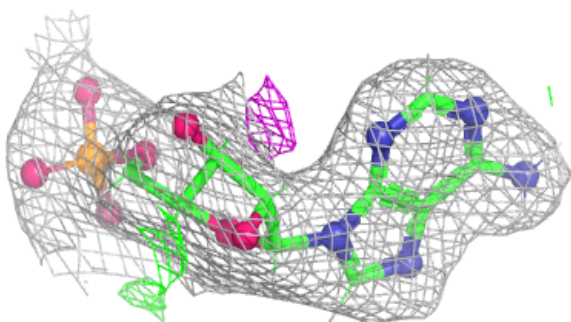
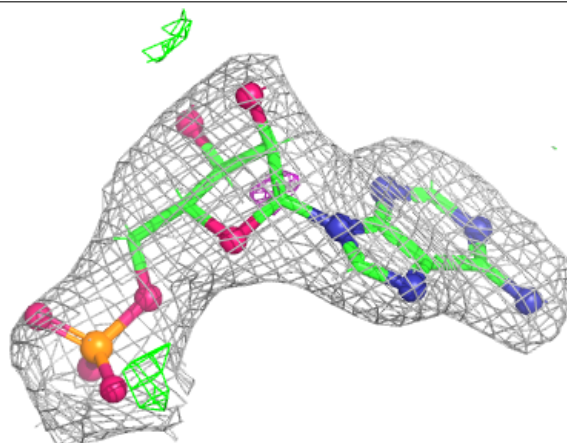


Electron density around NMN A 402:

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

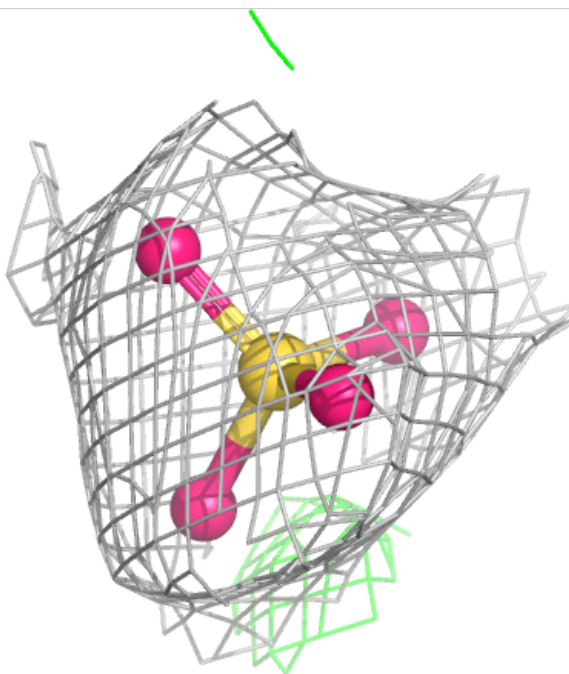
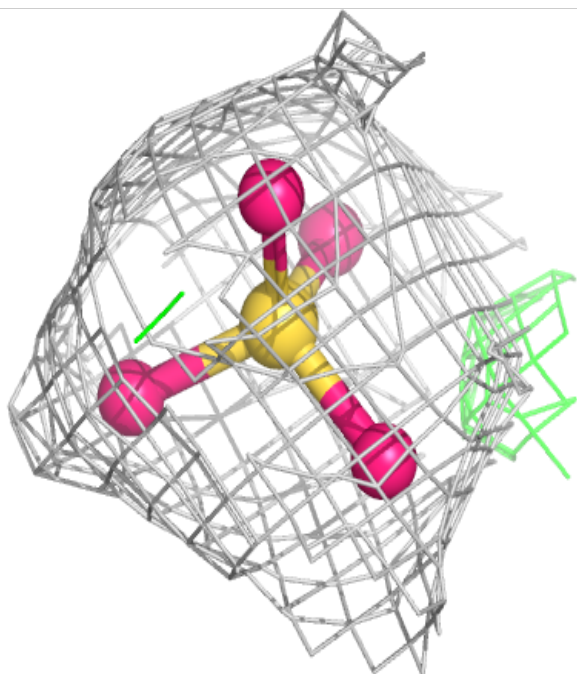
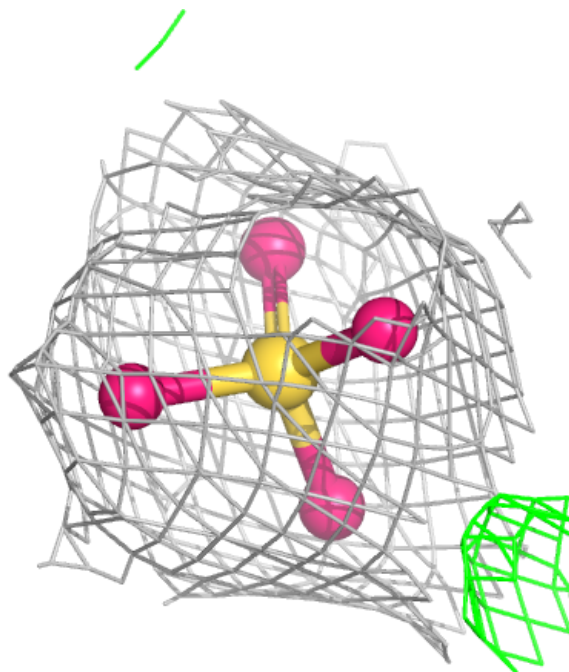
**Electron density around AMP A 401:**

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



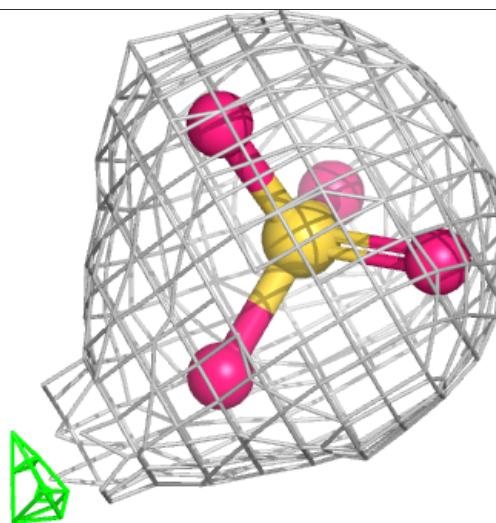
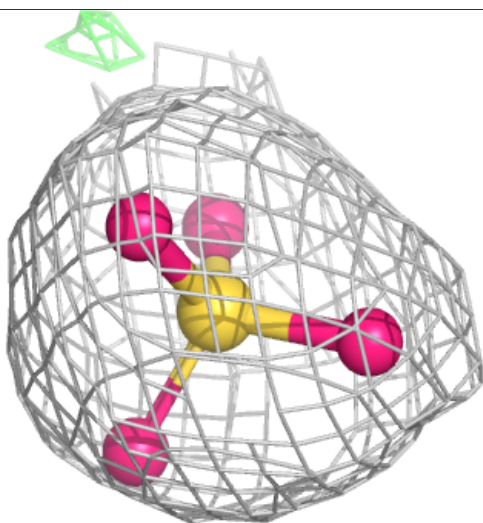
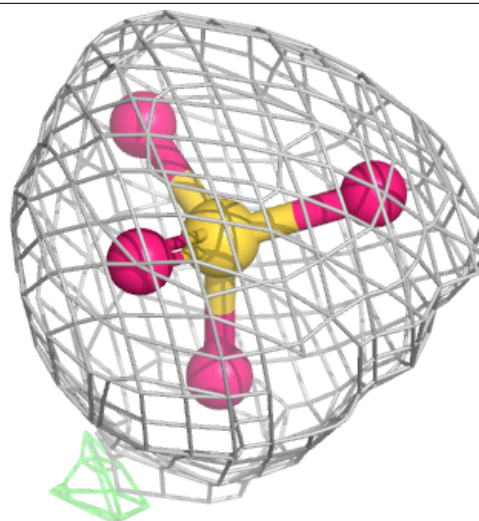
Electron density around SO4 A 403:

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



Electron density around SO4 A 404:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.