



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:36 AM UTC

PDB ID : 8BJJ / pdb_00008bjj
Title : ExoY Nucleotidyl Cyclase domain from *Vibrio nigripulchritudo* MARTX toxin,
bound to ATP-Mg-actin, human profilin 1 and a sulfate ion
Authors : Teixeira-Nunes, M.; Renault, L.; Retailleau, P.
Deposited on : 2022-11-04
Resolution : 1.70 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

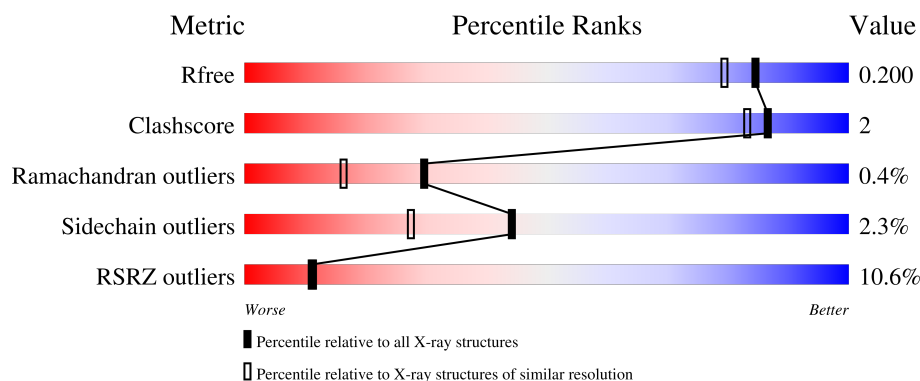
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	375	6% 92% 5% ..
2	C	139	8% 94% 6%
3	B	413	14% 79% 6% 14%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 7763 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 Actin, alpha skeletal muscle, intermediate form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	18	0
			2979	1898	495	563	23			

- Molecule 2 is a protein called Profilin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	139	Total	C	N	O	S	0	2	0
			1057	666	181	203	7			

- Molecule 3 is a protein called Putative Adenylate cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	355	Total	C	N	O	S	0	15	0
			2886	1828	481	569	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	451	GLY	-	expression tag	UNP A0A6N3LUE9
B	452	PRO	-	expression tag	UNP A0A6N3LUE9
B	453	GLY	-	expression tag	UNP A0A6N3LUE9
B	454	SER	-	expression tag	UNP A0A6N3LUE9

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

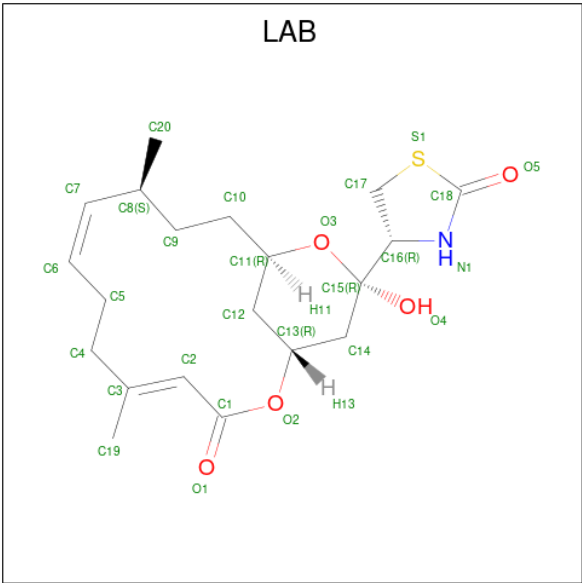


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

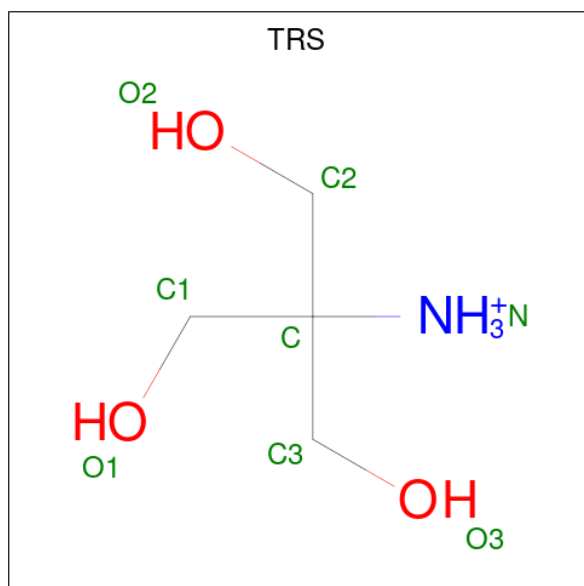
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is LATRUNCULIN B (CCD ID: LAB) (formula: C₂₀H₂₉NO₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			27	20	1	5	1		

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



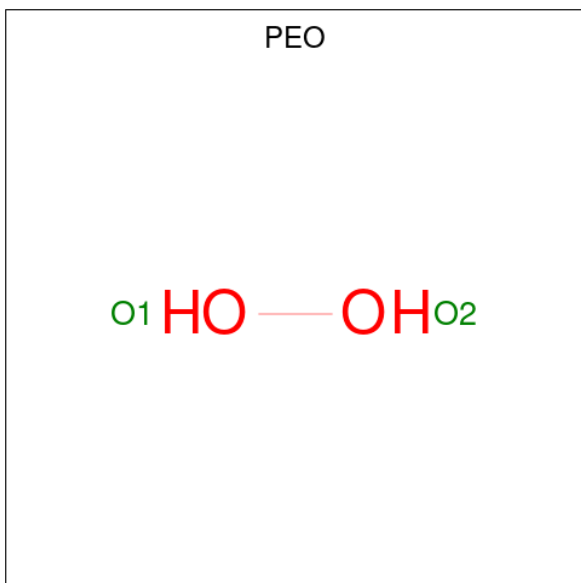
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			8	4	1	3		
7	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).



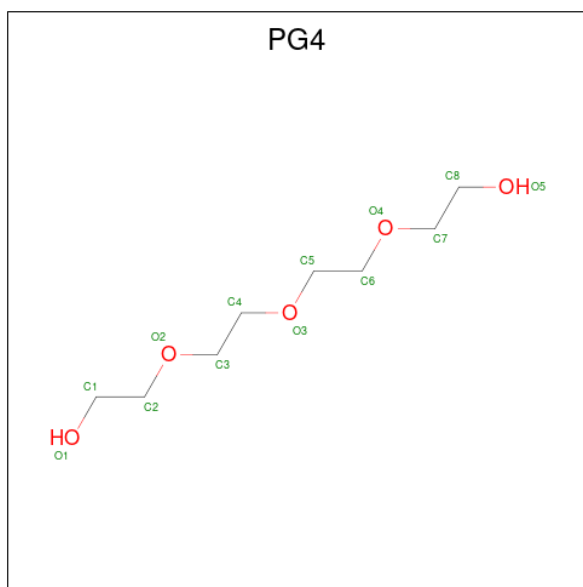
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is HYDROGEN PEROXIDE (CCD ID: PEO) (formula: H_2O_2).



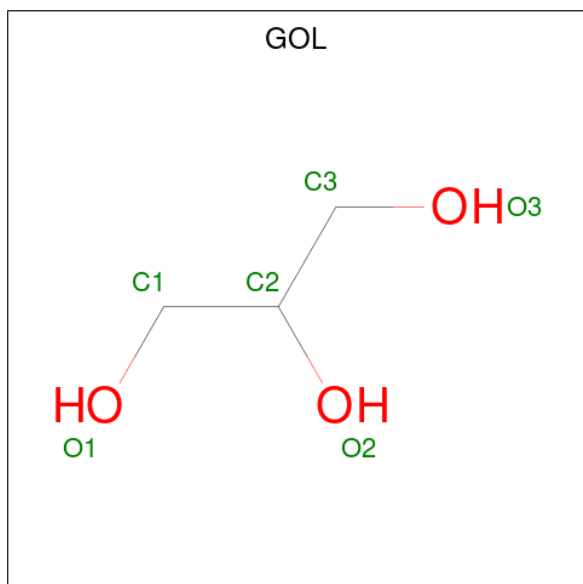
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total	O	0	0
			2	2		
9	C	1	Total	O	0	0
			2	2		

- Molecule 10 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 11 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

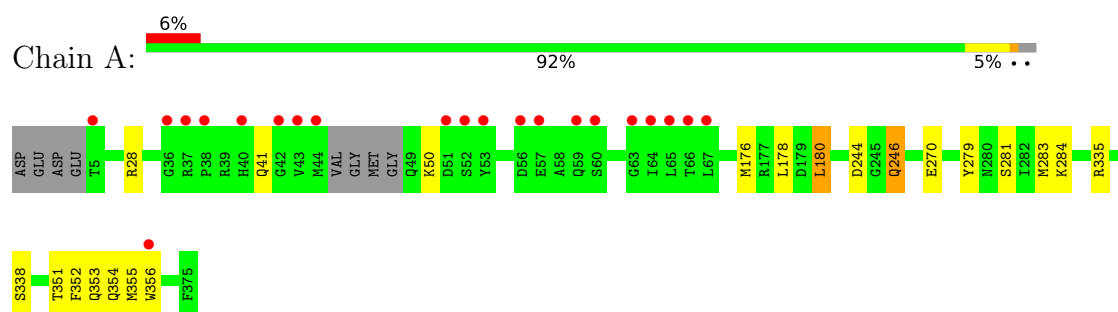
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	335	Total	O	0	1
			336	336		
12	C	113	Total	O	0	0
			113	113		
12	B	274	Total	O	0	3
			274	274		

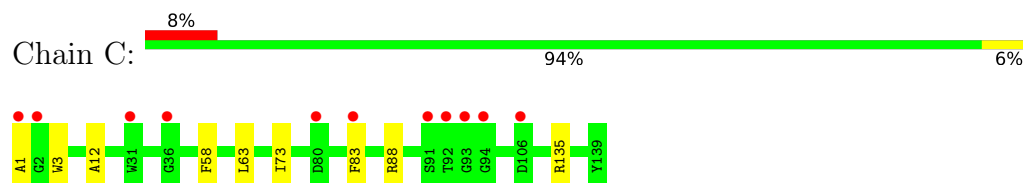
3 Residue-property plots

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.

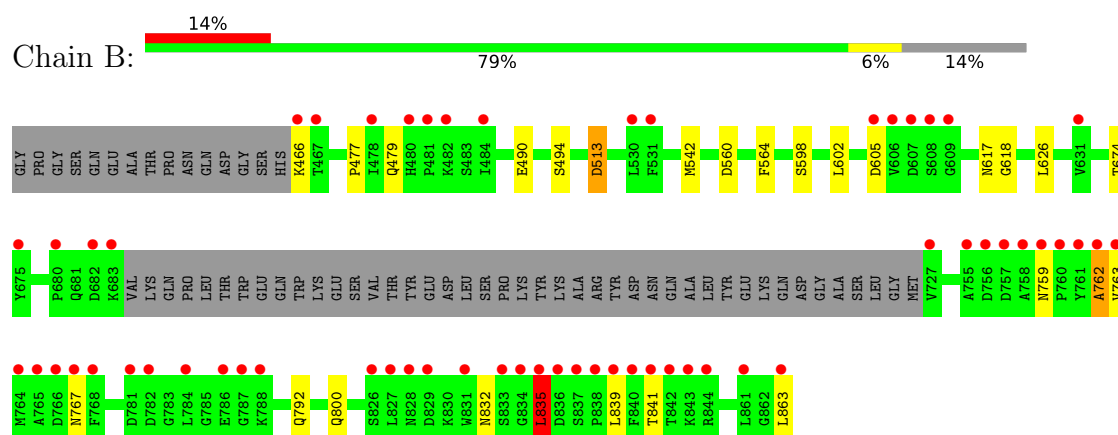
- Molecule 1: Actin, alpha skeletal muscle, intermediate form



- Molecule 2: Profilin-1



- Molecule 3: Putative Adenylate cyclase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.19Å 63.20Å 93.45Å 90.00° 91.04° 90.00°	Depositor
Resolution (Å)	44.20 – 1.70 44.20 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.20-1.70) 99.8 (44.20-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 1.70Å)	Xtriage
Refinement program	BUSTER 2.10.3 (20-MAY-2020)	Depositor
R, R_{free}	0.175 , 0.195 0.178 , 0.200	Depositor DCC
R_{free} test set	5186 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7763	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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: PG4, LAB, GOL, MG, TRS, PEO, SO4, ATP

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	0.72	0/3096	0.94	0/4190
2	C	0.67	0/1081	0.94	1/1460 (0.1%)
3	B	0.65	1/2986 (0.0%)	0.91	3/4037 (0.1%)
All	All	0.68	1/7163 (0.0%)	0.93	4/9687 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	762	ALA	CA-C	5.62	1.60	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	564	PHE	CA-CB-CG	-5.99	107.81	113.80
3	B	513	ASP	CA-CB-CG	5.67	118.27	112.60
2	C	12	ALA	N-CA-C	5.61	117.40	111.28
3	B	605	ASP	CA-CB-CG	5.00	117.60	112.60

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	2979	0	2980	13	0
2	C	1057	0	1067	7	0
3	B	2886	0	2853	10	0
4	A	31	0	12	0	0
5	A	1	0	0	0	0
6	A	27	0	29	0	0
7	A	8	0	12	0	0
7	B	8	0	12	0	0
8	A	5	0	0	0	0
8	B	15	0	0	1	0
9	C	4	0	0	1	0
10	B	13	0	18	1	0
11	B	6	0	8	2	0
12	A	336	0	0	2	0
12	B	274	0	0	1	0
12	C	113	0	0	0	0
All	All	7763	0	6991	30	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 (30) 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)
9:C:201:PEO:O1	9:C:201:PEO:O2	1.54	1.20
3:B:762:ALA:HB1	3:B:835:LEU:HD11	1.70	0.74
3:B:792:GLN:HB2	10:B:905:PG4:H72	1.68	0.74
3:B:598:SER:HB3	12:B:1310:HOH:O	2.00	0.60
2:C:1:ALA:CB	2:C:3:TRP:HD1	2.16	0.58
3:B:618:GLY:H	11:B:906:GOL:H2	1.68	0.58
1:A:353:GLN:HA	1:A:356[B]:TRP:CD1	2.39	0.57
1:A:353:GLN:HA	1:A:356[B]:TRP:HD1	1.68	0.57
2:C:1:ALA:HB3	2:C:3:TRP:HD1	1.72	0.54
1:A:335:ARG:HA	1:A:338[B]:SER:OG	2.08	0.54
3:B:490[A]:GLU:HG2	8:B:903:SO4:O3	2.08	0.53
3:B:602:LEU:HD21	3:B:626:LEU:HD12	1.91	0.53
3:B:494:SER:OG	3:B:800[B]:GLN:OE1	2.28	0.51
1:A:351:THR:HB	3:B:863:LEU:HD11	1.92	0.50
1:A:244:ASP:OD1	1:A:246[A]:GLN:HB2	2.13	0.49
1:A:176:MET:HG2	1:A:281[B]:SER:OG	2.14	0.48
3:B:617:ASN:HB2	11:B:906:GOL:H32	1.95	0.48
1:A:178:LEU:HD21	1:A:180:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352[B]:PHE:HD1	1:A:355:MET:SD	2.40	0.45
2:C:83:PHE:HD2	2:C:135:ARG:NH2	2.14	0.45
1:A:28:ARG:HG2	12:A:582:HOH:O	2.19	0.43
1:A:279:TYR:CZ	1:A:283:MET:HG3	2.53	0.43
2:C:1:ALA:HB1	2:C:3:TRP:CD1	2.54	0.43
1:A:352[B]:PHE:CD1	1:A:355:MET:SD	3.12	0.42
1:A:284:LYS:NZ	12:A:502:HOH:O	2.52	0.41
2:C:73[B]:ILE:HD11	2:C:88:ARG:HB2	2.01	0.41
1:A:176:MET:CG	1:A:281[B]:SER:OG	2.69	0.41
2:C:1:ALA:CB	2:C:3:TRP:CD1	3.02	0.40
2:C:63:LEU:HD12	2:C:63:LEU:C	2.47	0.40
3:B:466:LYS:HG2	3:B:477:PRO:HG2	2.04	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	381/375 (102%)	375 (98%)	6 (2%)	0	100	100
2	C	139/139 (100%)	131 (94%)	8 (6%)	0	100	100
3	B	366/413 (89%)	351 (96%)	12 (3%)	3 (1%)	16	5
All	All	886/927 (96%)	857 (97%)	26 (3%)	3 (0%)	30	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	763	VAL
3	B	835	LEU
3	B	759	ASN

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	330/318 (104%)	322 (98%)	8 (2%)	43	26
2	C	115/113 (102%)	114 (99%)	1 (1%)	70	62
3	B	324/358 (90%)	313 (97%)	11 (3%)	32	16
All	All	769/789 (98%)	749 (97%)	20 (3%)	44	23

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	50	LYS
1	A	180	LEU
1	A	246[A]	GLN
1	A	246[B]	GLN
1	A	270[A]	GLU
1	A	270[B]	GLU
1	A	354	GLN
2	C	58	PHE
3	B	479	GLN
3	B	513	ASP
3	B	542	MET
3	B	560	ASP
3	B	674	THR
3	B	767[A]	ASN
3	B	767[B]	ASN
3	B	832	ASN
3	B	835	LEU
3	B	839	LEU
3	B	841	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS

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Mol	Chain	Res	Type
1	A	297	ASN
2	C	133	HIS
3	B	576	ASN

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](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	SO4	A	405	-	4,4,4	0.45	0	6,6,6	0.17	0
7	TRS	B	904	-	7,7,7	0.20	0	9,9,9	0.24	0
6	LAB	A	403	-	28,29,29	0.50	1 (3%)	29,41,41	0.73	1 (3%)
7	TRS	A	404	-	7,7,7	0.21	0	9,9,9	0.41	0
8	SO4	B	901	-	4,4,4	0.21	0	6,6,6	0.17	0
9	PEO	C	201	-	1,1,1	0.83	0	-		
8	SO4	B	903	-	4,4,4	0.46	0	6,6,6	0.43	0
10	PG4	B	905	-	12,12,12	0.17	0	11,11,11	0.13	0
9	PEO	C	202	-	1,1,1	0.56	0	-		
11	GOL	B	906	-	5,5,5	0.05	0	5,5,5	0.17	0
4	ATP	A	401	5	32,33,33	0.59	0	48,52,52	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SO4	B	902	-	4,4,4	0.24	0	6,6,6	0.11	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
7	TRS	B	904	-	-	0/9/9/9	-
6	LAB	A	403	-	-	2/21/49/49	0/2/3/3
7	TRS	A	404	-	-	0/9/9/9	-
10	PG4	B	905	-	-	1/10/10/10	-
11	GOL	B	906	-	-	0/4/4/4	-
4	ATP	A	401	5	-	2/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	403	LAB	C15-C16	2.32	1.58	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	403	LAB	C3-C2-C1	2.00	132.14	127.36

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	401	ATP	PG-O3B-PB-O1B
6	A	403	LAB	O2-C1-C2-C3
10	B	905	PG4	O2-C3-C4-O3
6	A	403	LAB	O1-C1-C2-C3
4	A	401	ATP	PG-O3B-PB-O2B

There are no ring outliers.

4 monomers are involved in 5 short contacts:

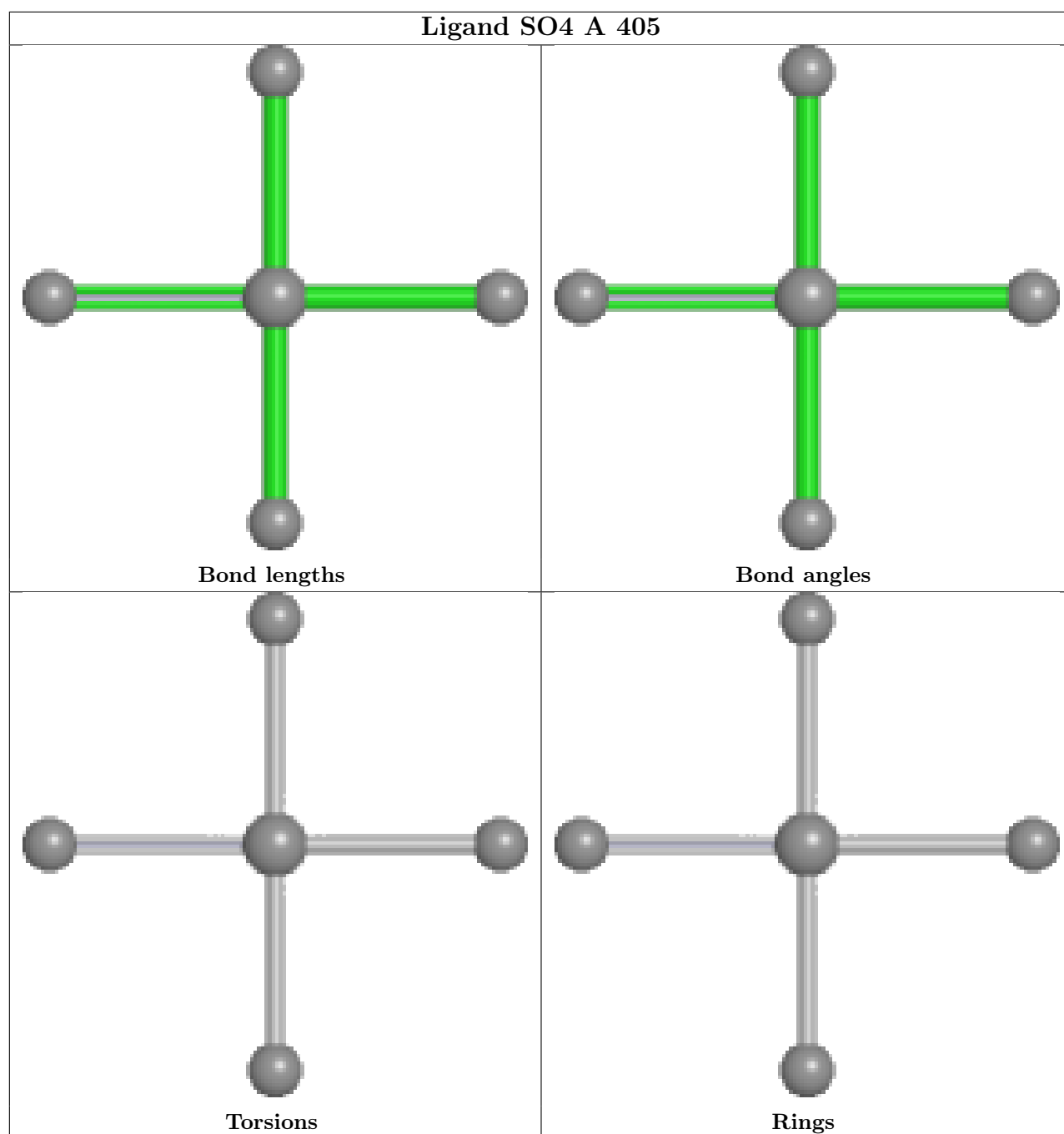
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	201	PEO	1	0

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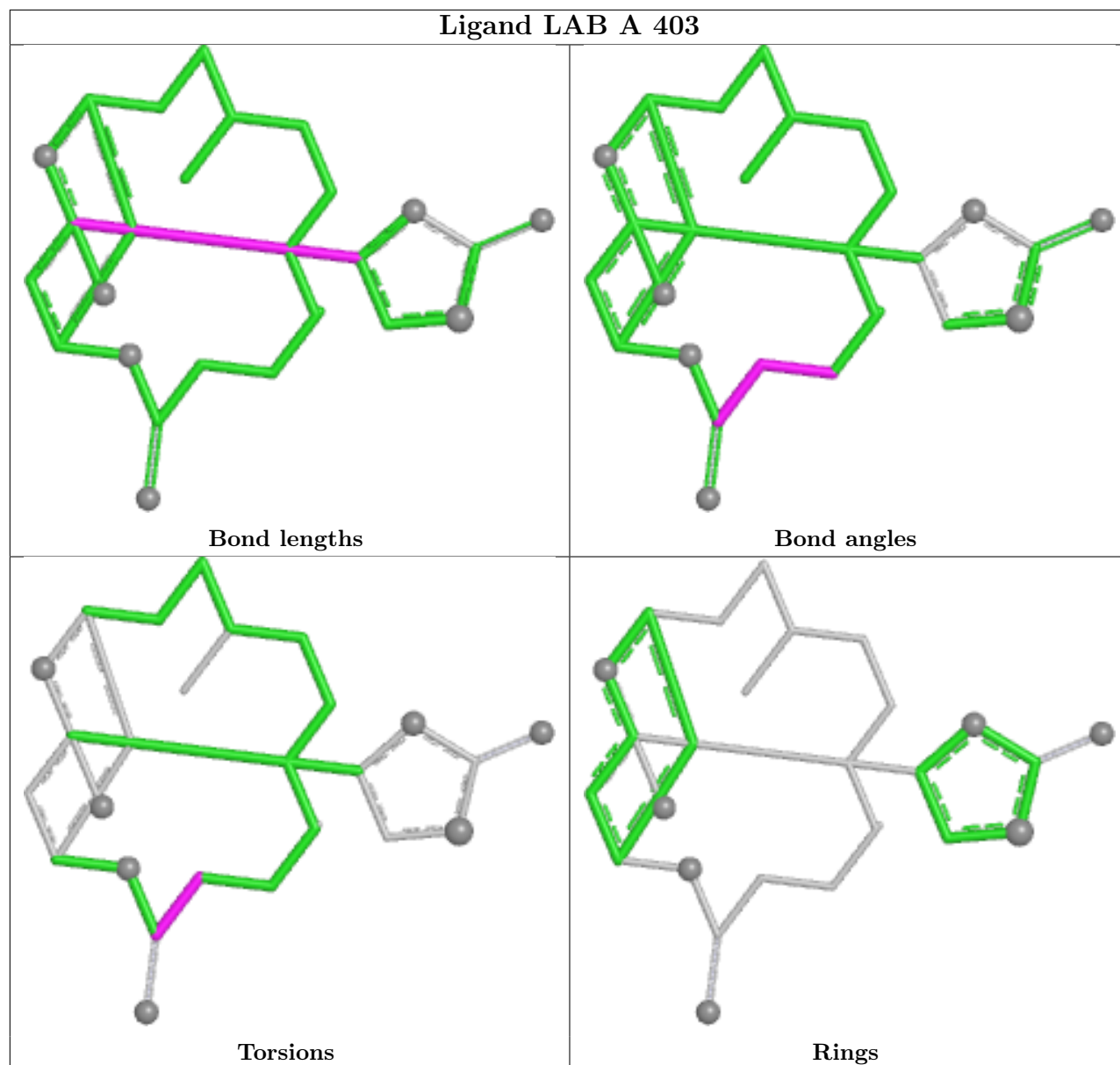
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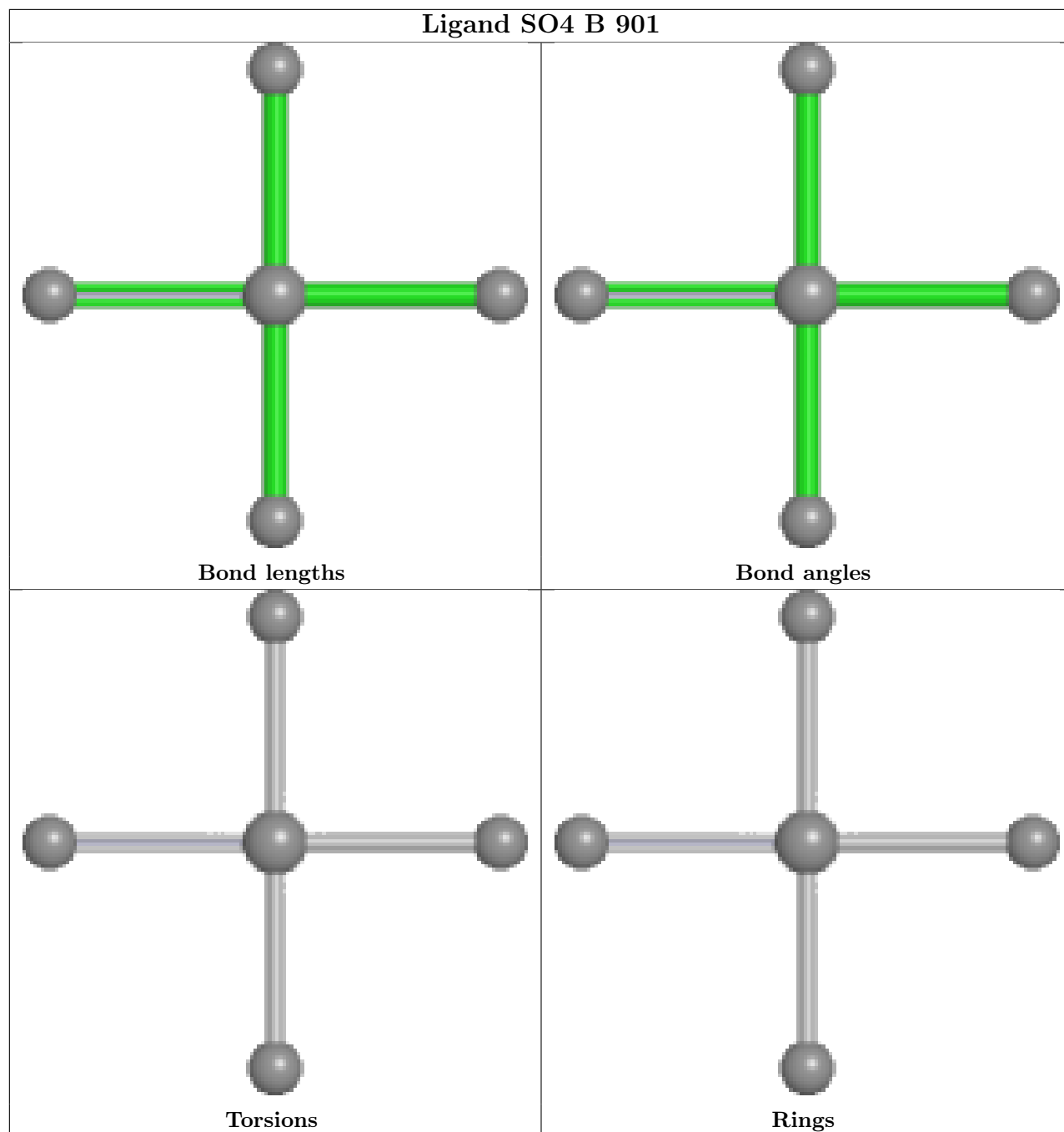
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	903	SO4	1	0
10	B	905	PG4	1	0
11	B	906	GOL	2	0

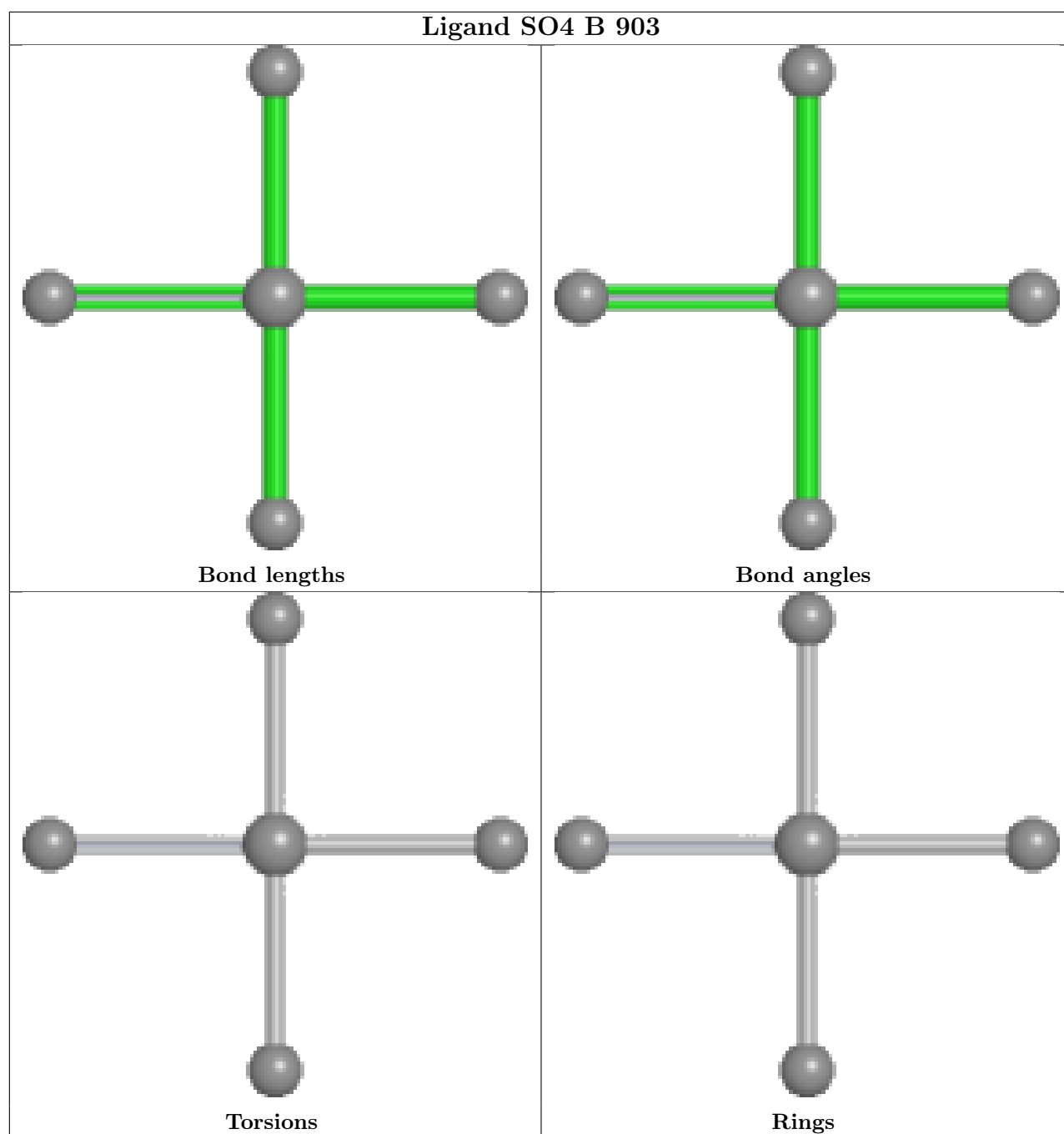
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

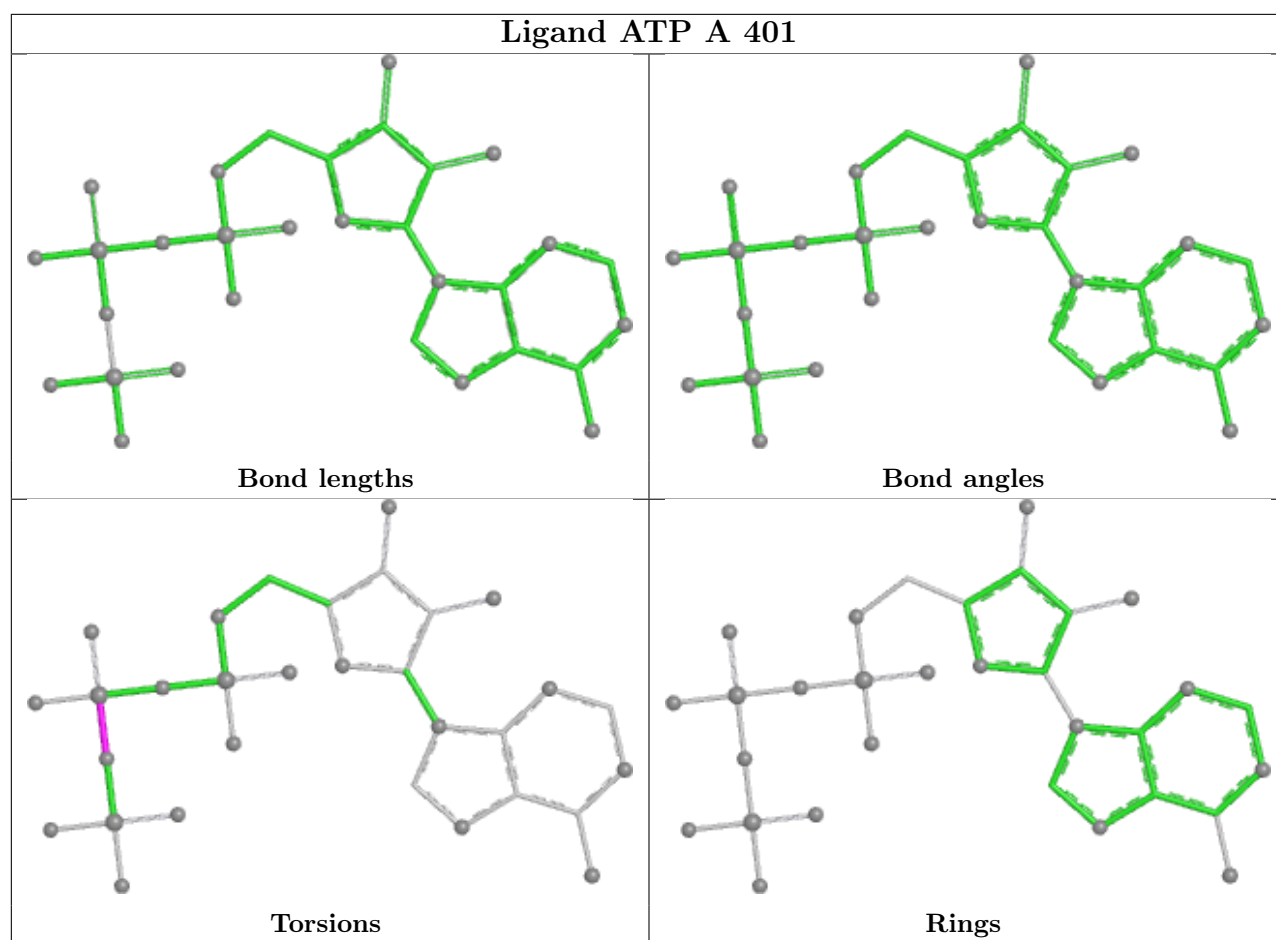


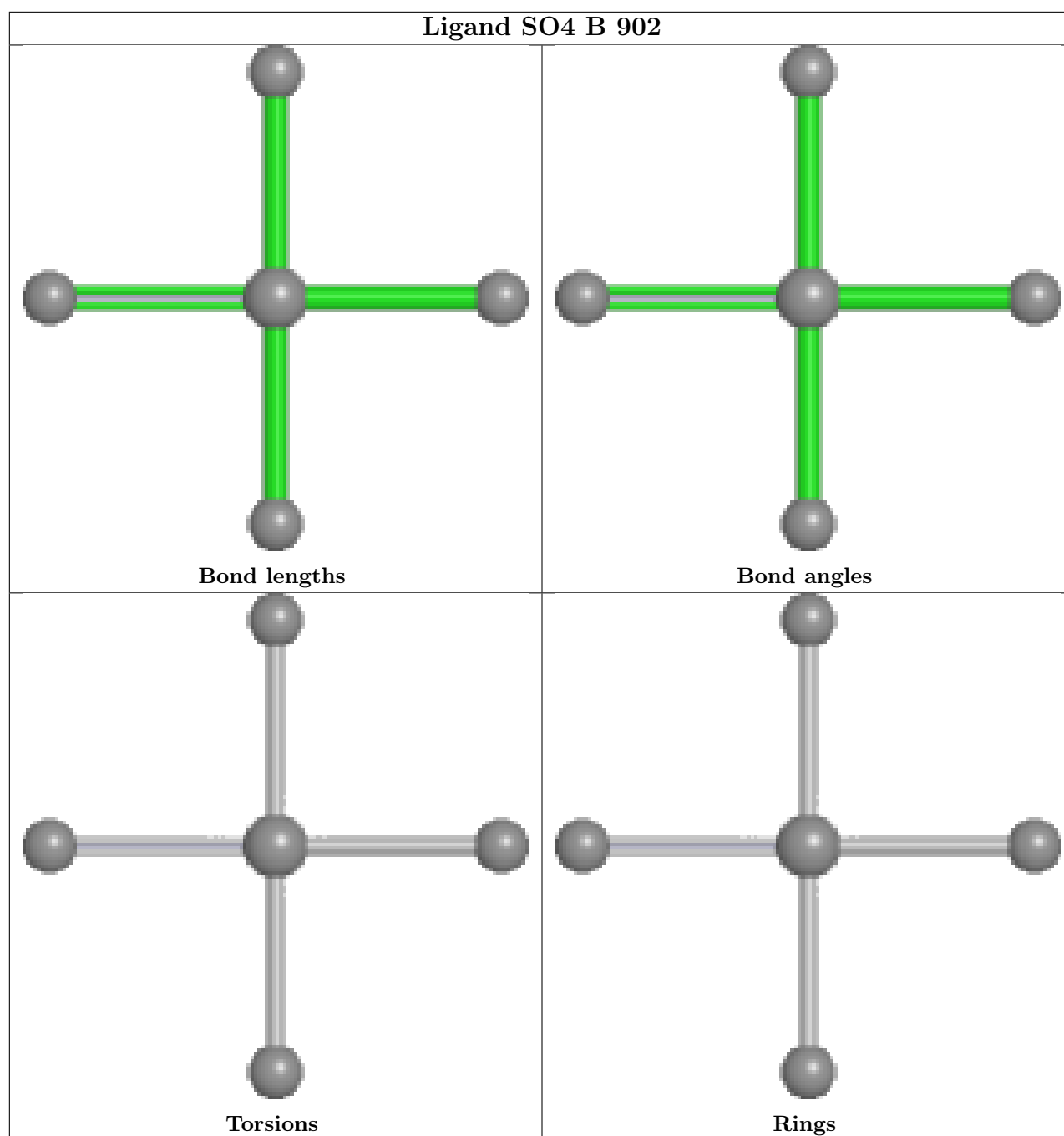
Ligand LAB A 403











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	367/375 (97%)	0.15	21 (5%)	29	32	11, 23, 49, 104	18 (4%)
2	C	139/139 (100%)	0.43	11 (7%)	18	20	11, 31, 51, 61	2 (1%)
3	B	355/413 (85%)	0.87	59 (16%)	4	4	12, 31, 77, 95	15 (4%)
All	All	861/927 (92%)	0.49	91 (10%)	11	11	11, 27, 62, 104	35 (4%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	835	LEU	9.0
3	B	763	VAL	7.3
3	B	839	LEU	7.2
3	B	836	ASP	7.0
3	B	762	ALA	6.5
3	B	761	TYR	6.4
3	B	760	PRO	6.4
3	B	759	ASN	6.2
3	B	727	VAL	5.9
3	B	827	LEU	5.6
1	A	43	VAL	5.5
3	B	765	ALA	5.5
2	C	1	ALA	5.4
3	B	840	PHE	5.2
3	B	838	PRO	5.2
3	B	755	ALA	4.7
3	B	758	ALA	4.7
2	C	93	GLY	4.6
3	B	480[A]	HIS	4.5
3	B	831	TRP	4.4
3	B	766	ASP	4.4
1	A	40	HIS	4.3
3	B	828	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
3	B	606	VAL	4.1
3	B	842	THR	4.1
3	B	764	MET	4.1
3	B	841	THR	4.1
3	B	757	ASP	4.1
1	A	64	ILE	3.9
3	B	837	SER	3.8
2	C	92	THR	3.8
2	C	94	GLY	3.8
1	A	5	THR	3.6
3	B	826	SER	3.6
1	A	53	TYR	3.6
3	B	787	GLY	3.5
1	A	65	LEU	3.5
1	A	38	PRO	3.5
3	B	863	LEU	3.5
1	A	60	SER	3.4
3	B	609	GLY	3.3
1	A	44	MET	3.3
2	C	80	ASP	3.2
3	B	784	LEU	3.1
3	B	786	GLU	3.1
3	B	843	LYS	3.0
3	B	756	ASP	3.0
1	A	66	THR	3.0
1	A	51	ASP	2.9
3	B	829	ASP	2.9
2	C	91	SER	2.8
1	A	42	GLY	2.8
1	A	36	GLY	2.8
3	B	531	PHE	2.7
1	A	63	GLY	2.7
3	B	833	SER	2.7
3	B	844	ARG	2.7
3	B	478	ILE	2.7
3	B	631	VAL	2.6
1	A	37	ARG	2.6
3	B	767[A]	ASN	2.6
3	B	834	GLY	2.5
2	C	83	PHE	2.5
2	C	2	GLY	2.5
3	B	607	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
3	B	484	ILE	2.4
3	B	675	TYR	2.4
3	B	530	LEU	2.4
3	B	605	ASP	2.4
3	B	861	LEU	2.3
3	B	466	LYS	2.3
1	A	56	ASP	2.3
3	B	482	LYS	2.3
3	B	608	SER	2.3
3	B	683	LYS	2.3
3	B	481	PRO	2.2
2	C	106	ASP	2.2
1	A	356[A]	TRP	2.2
1	A	67	LEU	2.2
1	A	59[A]	GLN	2.2
3	B	781	ASP	2.2
2	C	31	TRP	2.2
3	B	680	PRO	2.2
1	A	52	SER	2.2
2	C	36	GLY	2.1
3	B	467	THR	2.1
3	B	782	ASP	2.1
1	A	57	GLU	2.1
3	B	682	ASP	2.1
3	B	768	PHE	2.1
3	B	788	LYS	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](#)

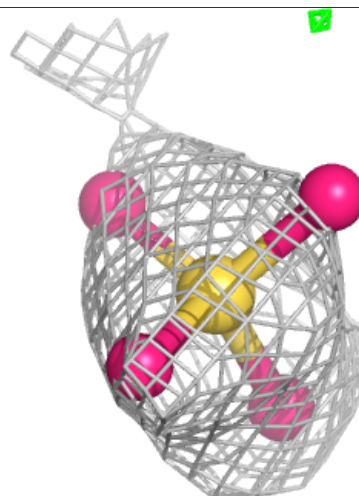
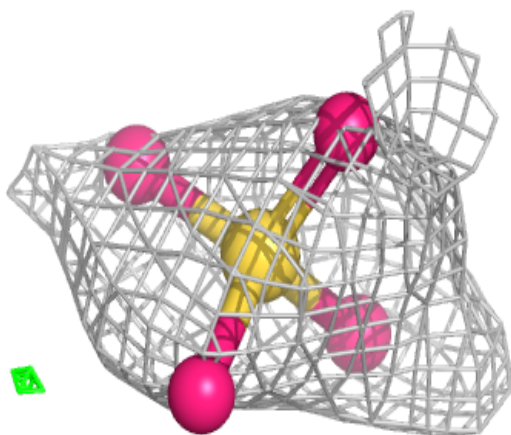
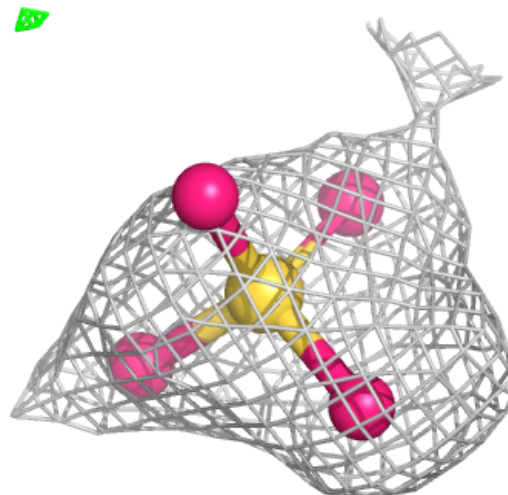
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	PG4	B	905	13/13	0.81	0.17	60,60,62,62	0
11	GOL	B	906	6/6	0.82	0.17	52,53,53,53	0
7	TRS	B	904	8/8	0.83	0.12	38,38,39,39	0
9	PEO	C	201	2/2	0.83	0.34	45,45,45,45	0
8	SO4	B	902	5/5	0.84	0.17	51,51,51,51	5
8	SO4	B	901	5/5	0.86	0.11	60,60,60,61	0
7	TRS	A	404	8/8	0.88	0.10	30,31,31,32	0
9	PEO	C	202	2/2	0.90	0.10	57,57,57,57	0
8	SO4	A	405	5/5	0.94	0.09	44,44,44,44	0
6	LAB	A	403	27/27	0.95	0.08	22,24,27,28	0
8	SO4	B	903	5/5	0.96	0.07	34,34,35,35	0
4	ATP	A	401	31/31	0.99	0.04	16,18,21,24	0
5	MG	A	402	1/1	1.00	0.06	16,16,16,16	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.

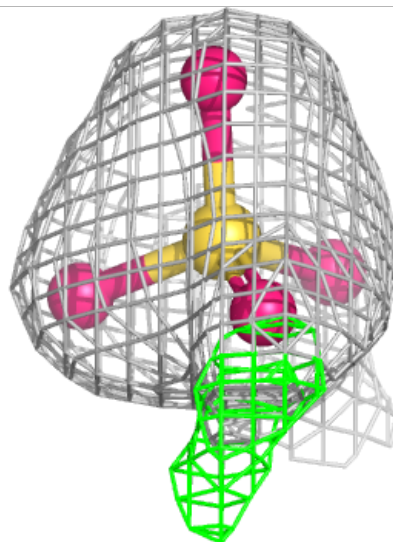
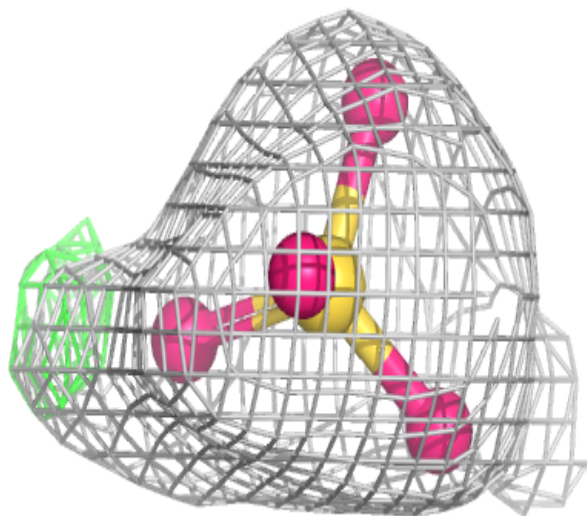
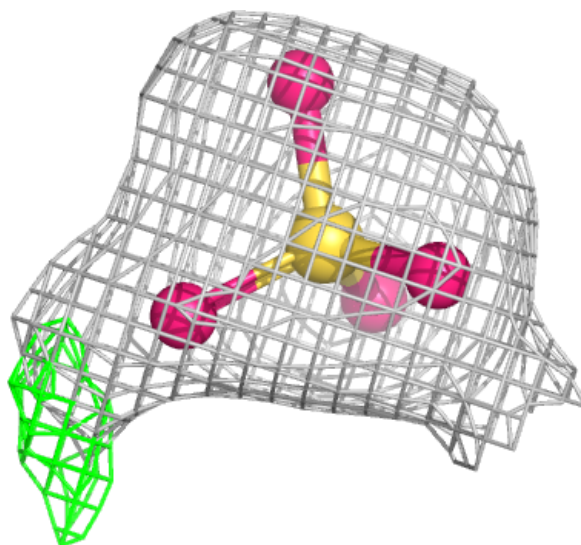
Electron density around SO4 B 902:

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



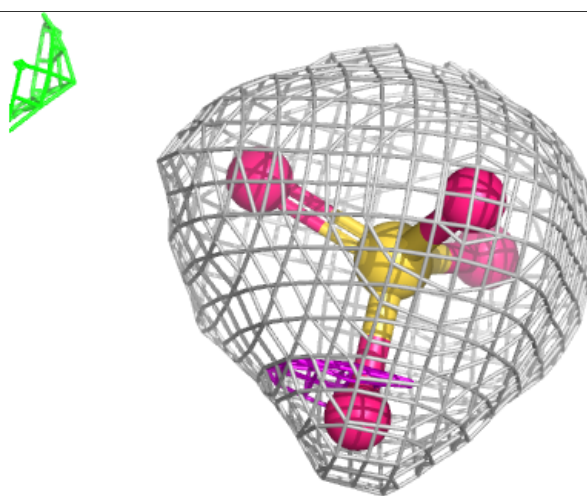
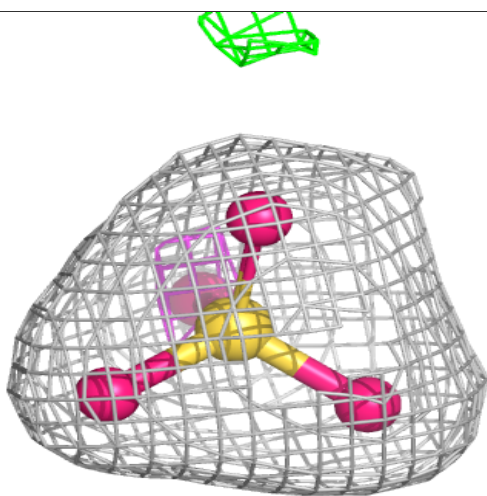
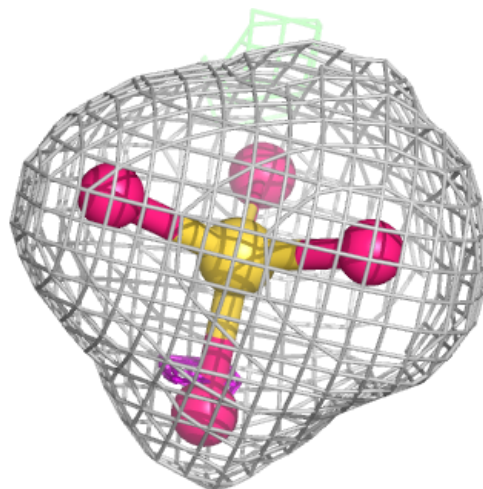
Electron density around SO4 B 901:

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



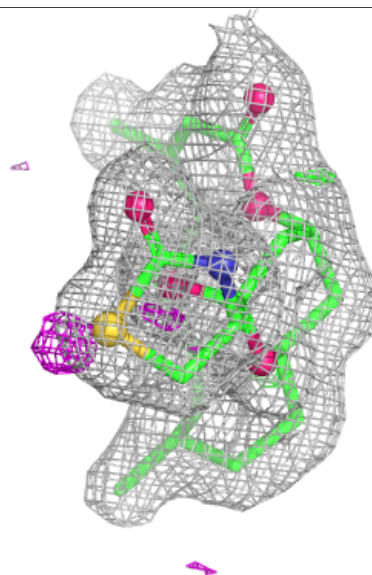
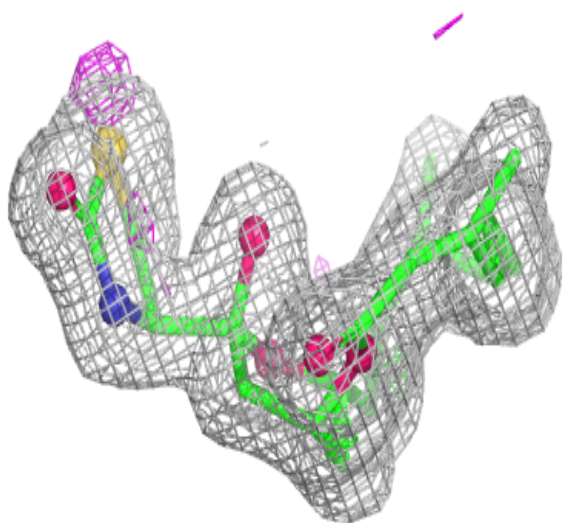
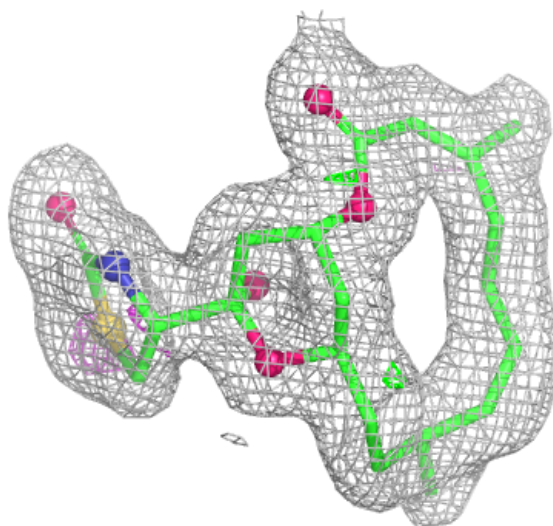
Electron density around SO4 A 405:

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



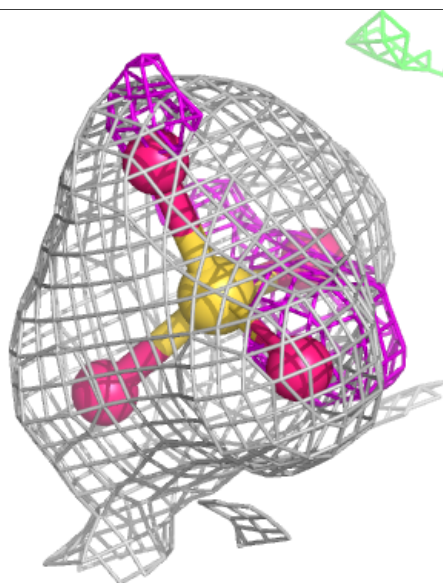
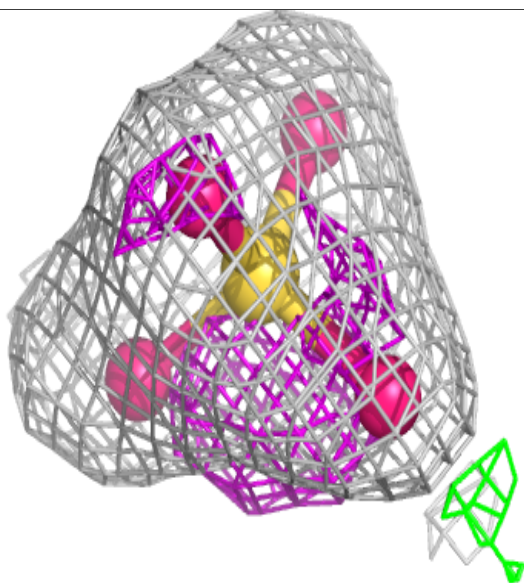
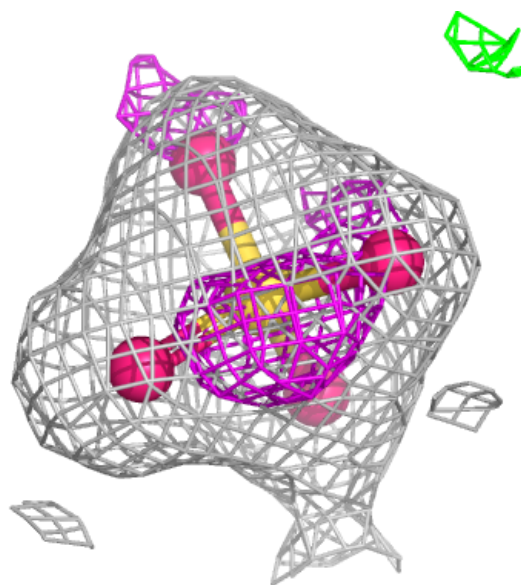
Electron density around LAB A 403:

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



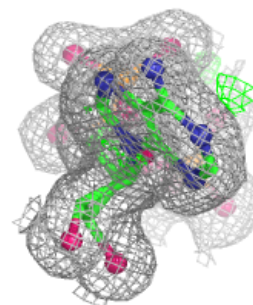
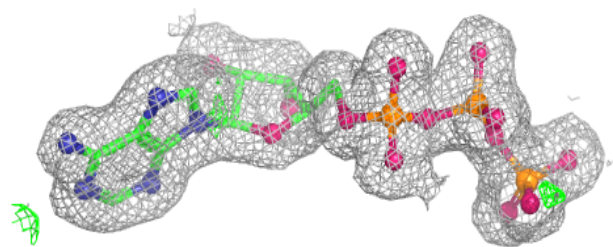
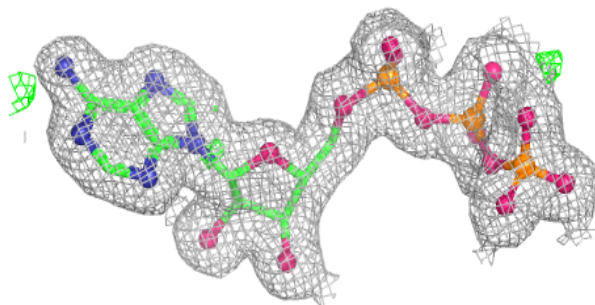
Electron density around SO4 B 903:

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



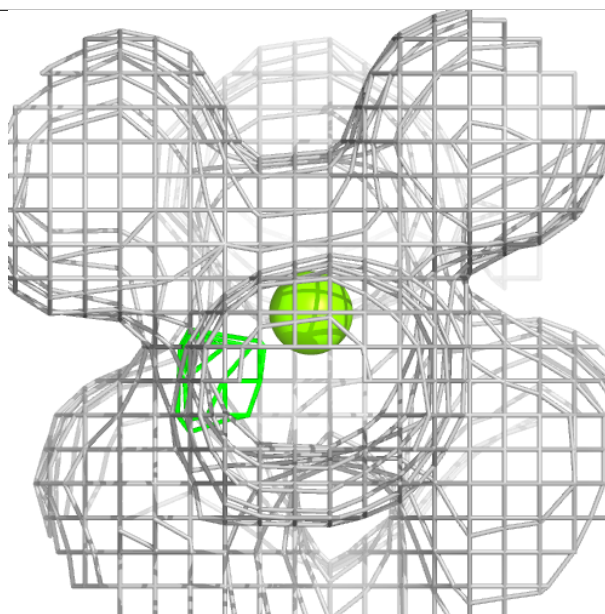
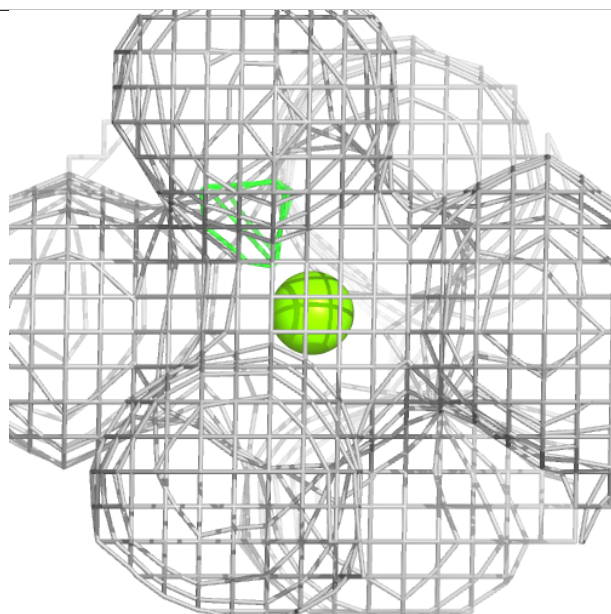
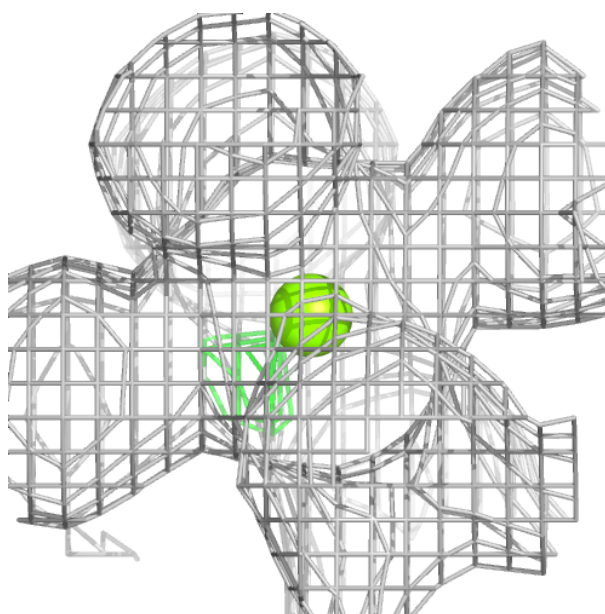
Electron density around ATP A 401:

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



Electron density around MG 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.