



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2023 – 04:13 pm BST

PDB ID : 8BJJ
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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

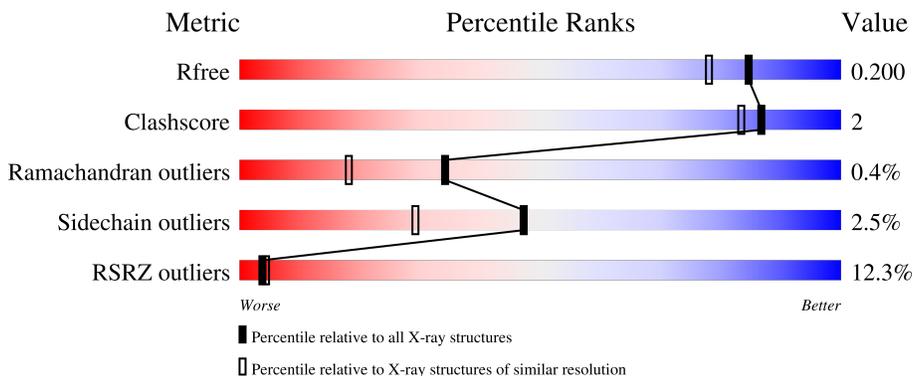
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

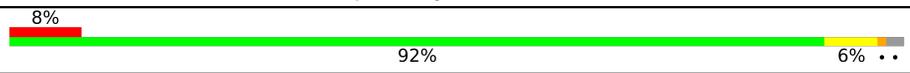
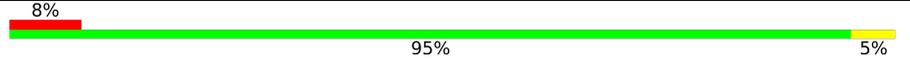
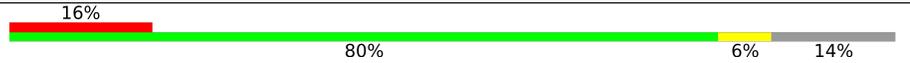
The reported resolution of this entry is 1.70 Å.

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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (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	
2	C	139	
3	B	413	

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
			Total	C	N	O	S			
1	A	367	2979	1898	495	563	23	0	18	0

- Molecule 2 is a protein called Profilin-1.

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

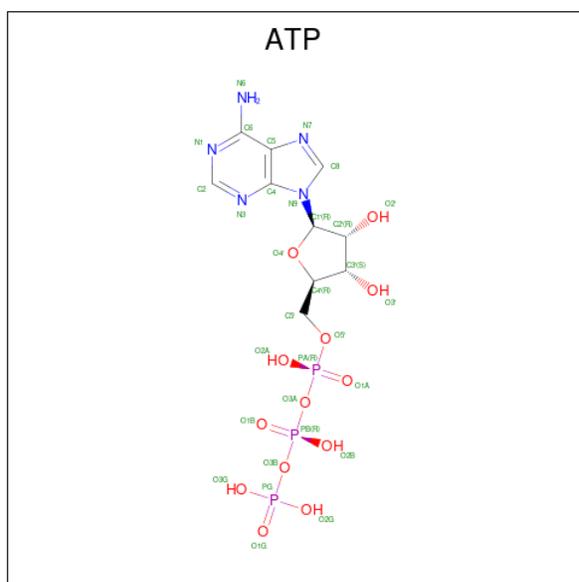
- Molecule 3 is a protein called Putative Adenylate cyclase.

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

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 (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

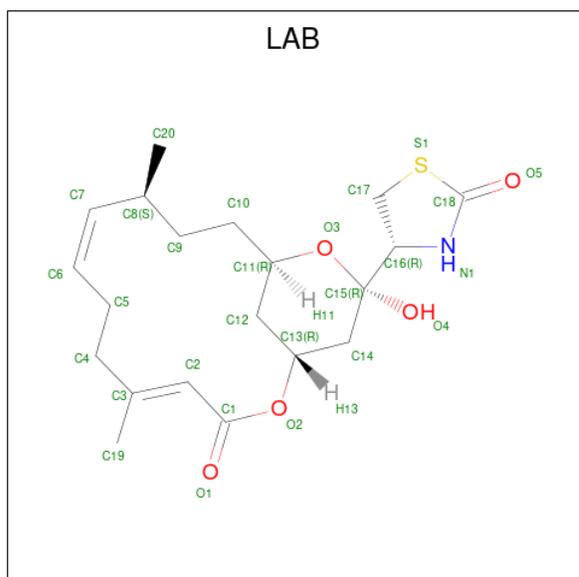


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	31	10	5	13	3	0	0

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

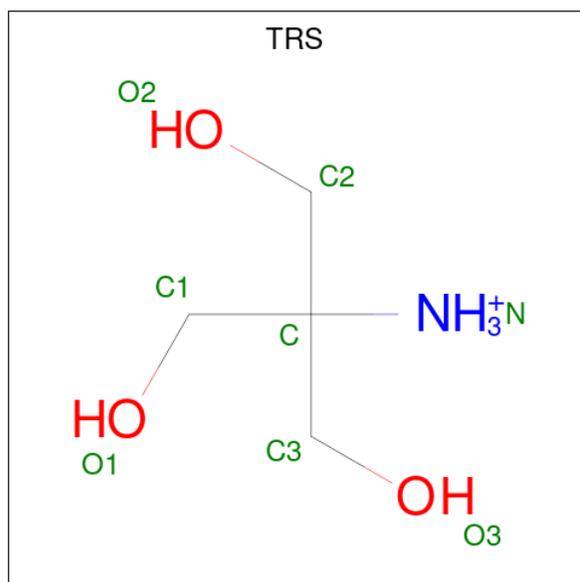
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	1	1	1	0	0

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



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

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



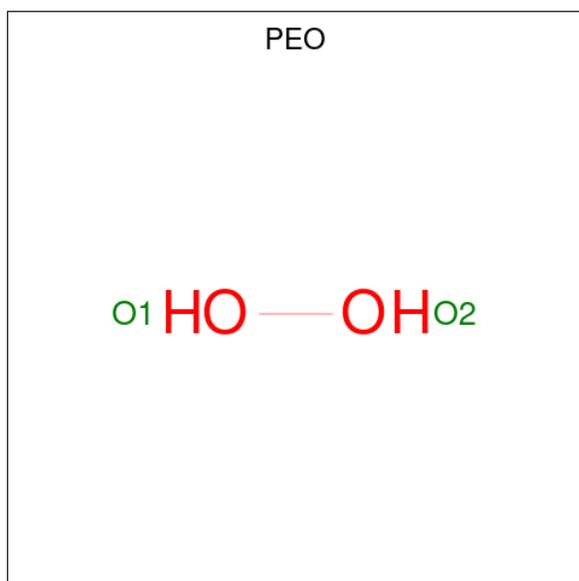
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	8	4	1	3	0	0
7	B	1	8	4	1	3	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO₄) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



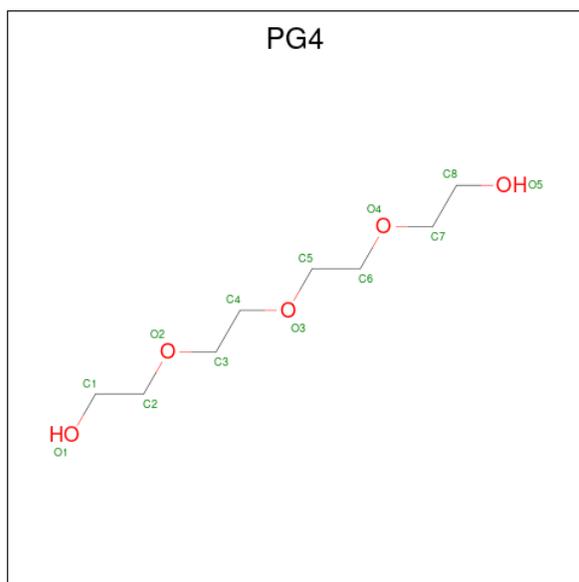
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H₂O₂).



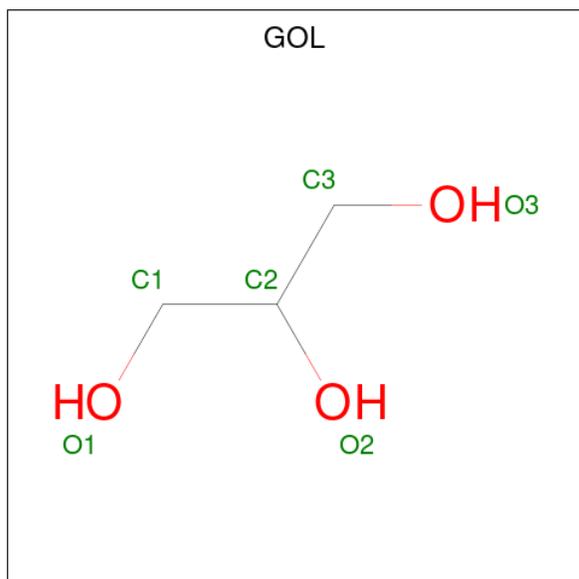
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total O 2 2	0	0
9	C	1	Total O 2 2	0	0

- Molecule 10 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 11 is GLYCEROL (three-letter code: 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		

4 Data and refinement statistics i

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)	Xtrriage
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 (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtrriage
Anisotropy	0.020	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7763	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, PG4, PEO, MG, TRS, LAB, 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	0.44	0/3096	0.59	0/4190
2	C	0.41	0/1081	0.60	0/1460
3	B	0.39	0/2986	0.56	0/4037
All	All	0.41	0/7163	0.58	0/9687

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	14	0
2	C	1057	0	1067	6	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352[B]:PHE:HE1	1:A:355:MET:HE2	1.86	0.41
2:C:1:ALA:CB	2:C:3:TRP:CD1	3.02	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 [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	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%)	19	6
All	All	886/927 (96%)	857 (97%)	26 (3%)	3 (0%)	34	24

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 [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	330/318 (104%)	318 (96%)	12 (4%)	35	16
2	C	115/113 (102%)	114 (99%)	1 (1%)	78	70
3	B	324/358 (90%)	314 (97%)	10 (3%)	40	21
All	All	769/789 (98%)	746 (97%)	23 (3%)	47	22

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	44	MET
1	A	95[A]	ARG
1	A	95[B]	ARG
1	A	116	ARG
1	A	246[A]	GLN
1	A	246[B]	GLN
1	A	270[A]	GLU
1	A	270[B]	GLU
1	A	354	GLN
1	A	356[A]	TRP
1	A	356[B]	TRP
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

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 monosaccharides 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	0.38	0	6,6,6	0.18	0
6	LAB	A	403	-	28,29,29	0.28	0	30,41,41	0.73	0
9	PEO	C	201	-	1,1,1	1.15	0	-		
4	ATP	A	401	5	26,33,33	0.84	0	31,52,52	0.75	1 (3%)
11	GOL	B	906	-	5,5,5	0.04	0	5,5,5	0.19	0
7	TRS	B	904	-	7,7,7	0.18	0	9,9,9	0.20	0
8	SO4	B	902	-	4,4,4	0.14	0	6,6,6	0.13	0
8	SO4	B	901	-	4,4,4	0.18	0	6,6,6	0.14	0
8	SO4	B	903	-	4,4,4	0.41	0	6,6,6	0.43	0
9	PEO	C	202	-	1,1,1	0.78	0	-		
10	PG4	B	905	-	12,12,12	0.17	0	11,11,11	0.13	0
7	TRS	A	404	-	7,7,7	0.18	0	9,9,9	0.35	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
6	LAB	A	403	-	-	2/21/49/49	0/2/3/3
4	ATP	A	401	5	-	2/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	GOL	B	906	-	-	0/4/4/4	-
7	TRS	B	904	-	-	0/9/9/9	-
10	PG4	B	905	-	-	2/10/10/10	-
7	TRS	A	404	-	-	0/9/9/9	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	ATP	C5-C6-N6	2.12	123.58	120.35

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	401	ATP	PG-O3B-PB-O1B
10	B	905	PG4	O2-C3-C4-O3
6	A	403	LAB	O2-C1-C2-C3
6	A	403	LAB	O1-C1-C2-C3
4	A	401	ATP	PG-O3B-PB-O2B
10	B	905	PG4	O3-C5-C6-O4

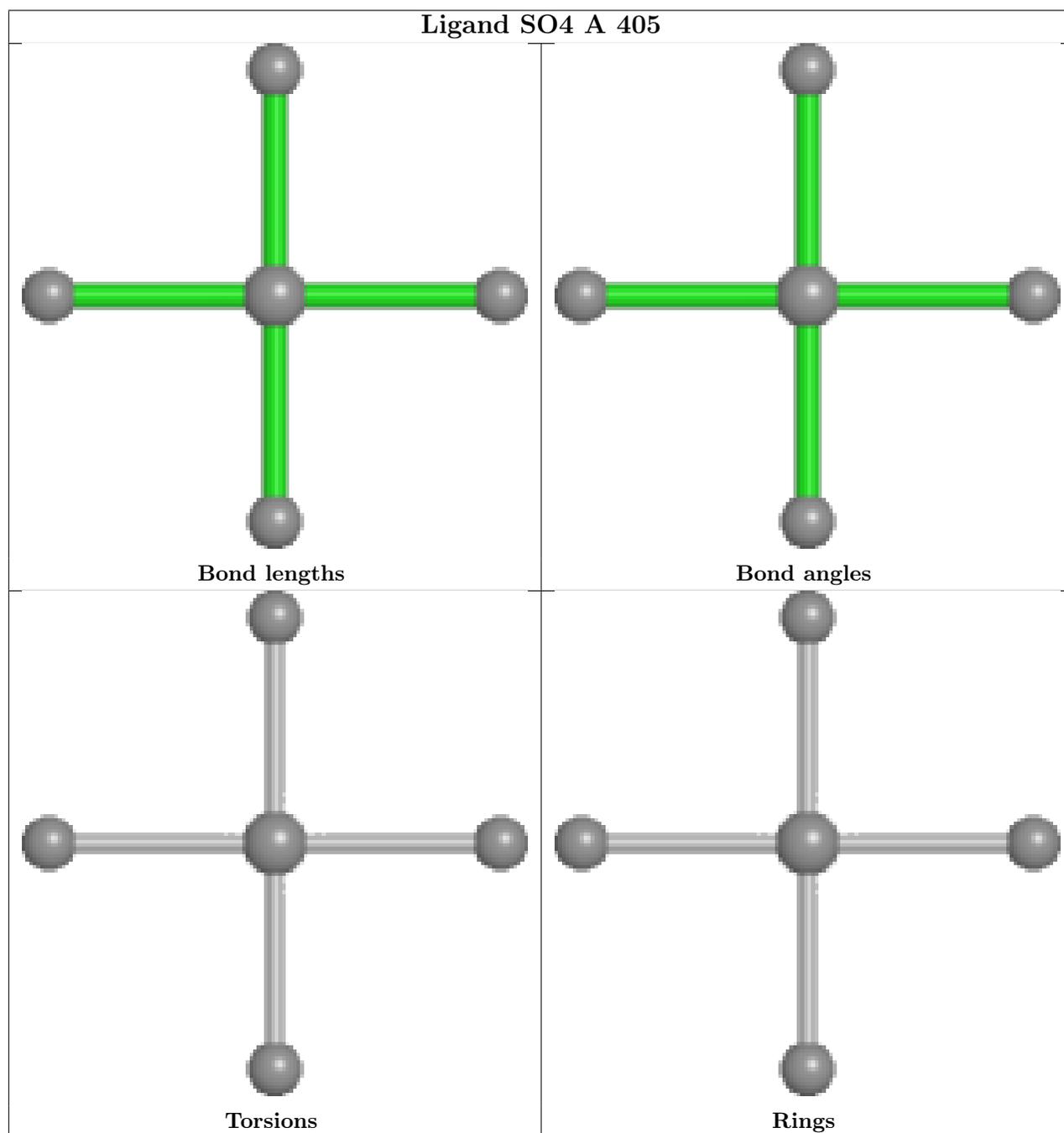
There are no ring outliers.

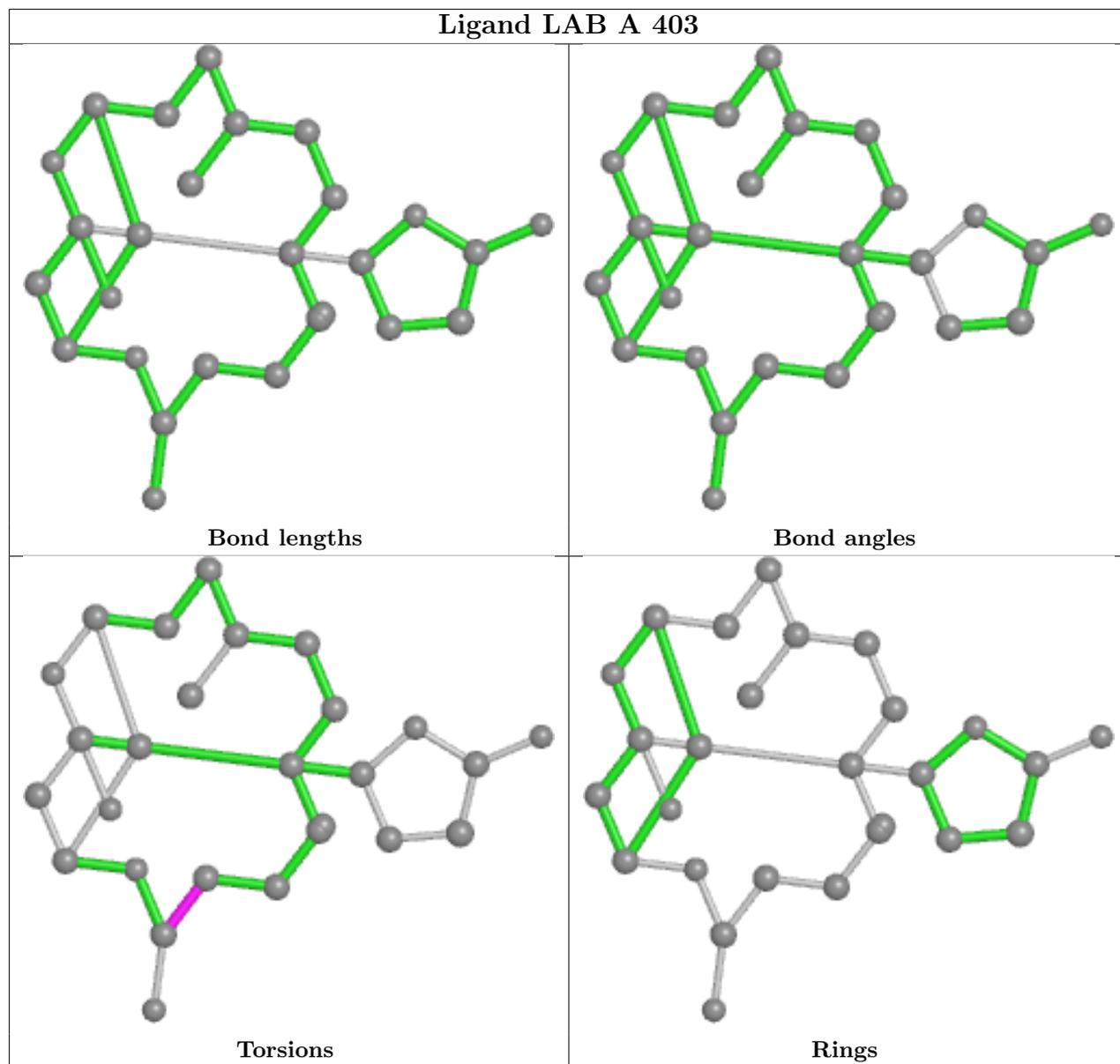
4 monomers are involved in 5 short contacts:

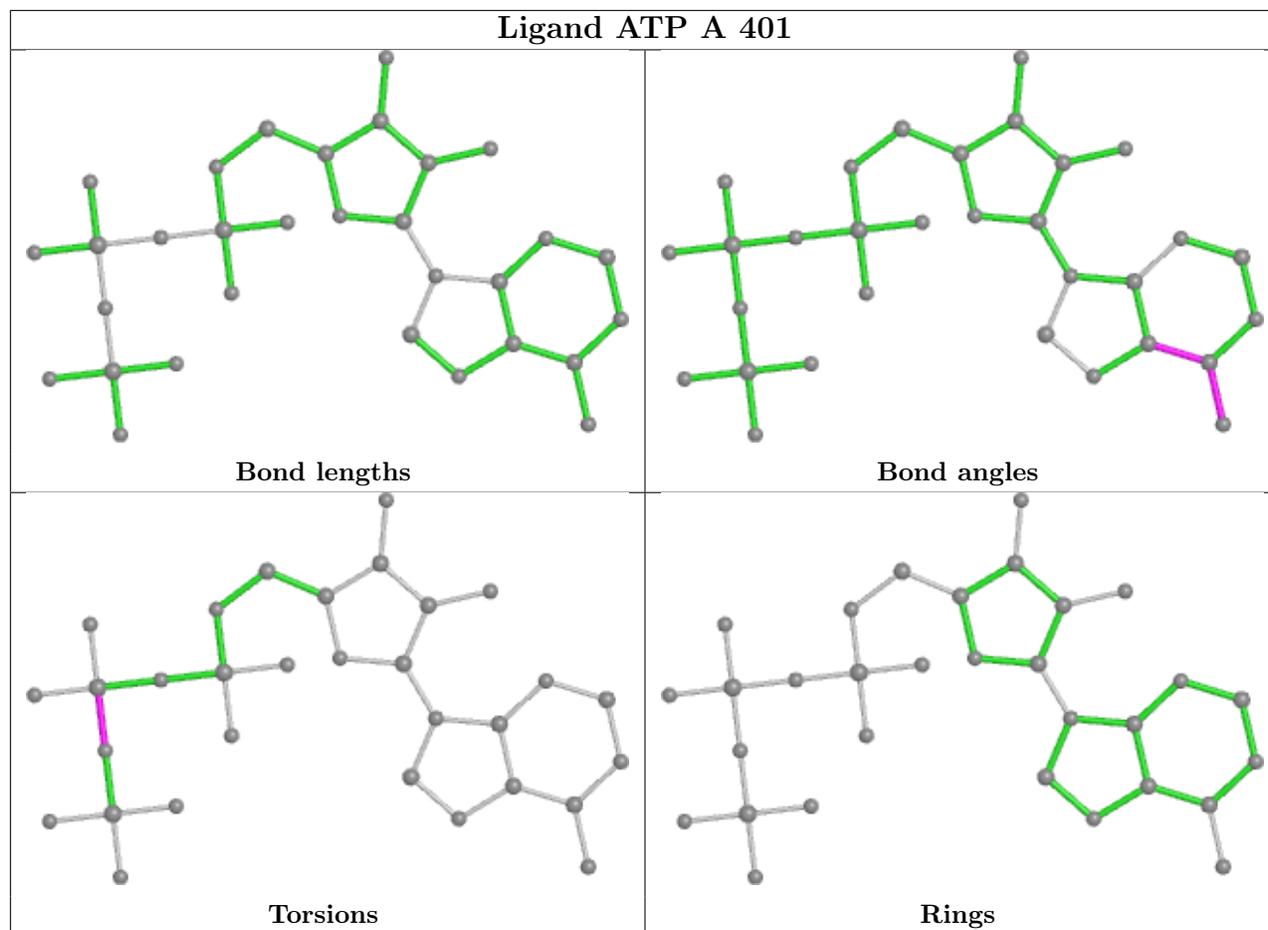
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	201	PEO	1	0
11	B	906	GOL	2	0
8	B	903	SO4	1	0
10	B	905	PG4	1	0

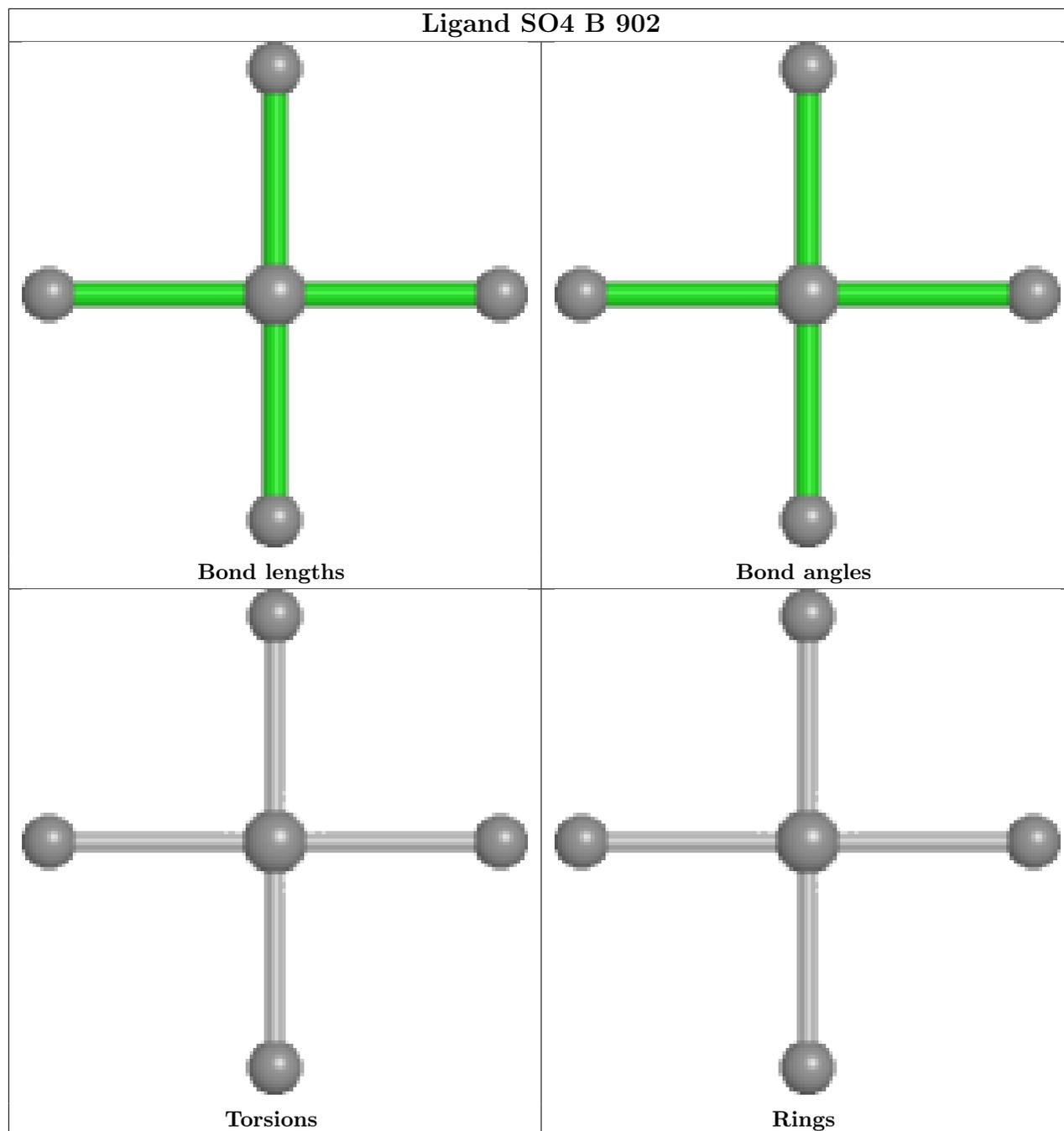
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

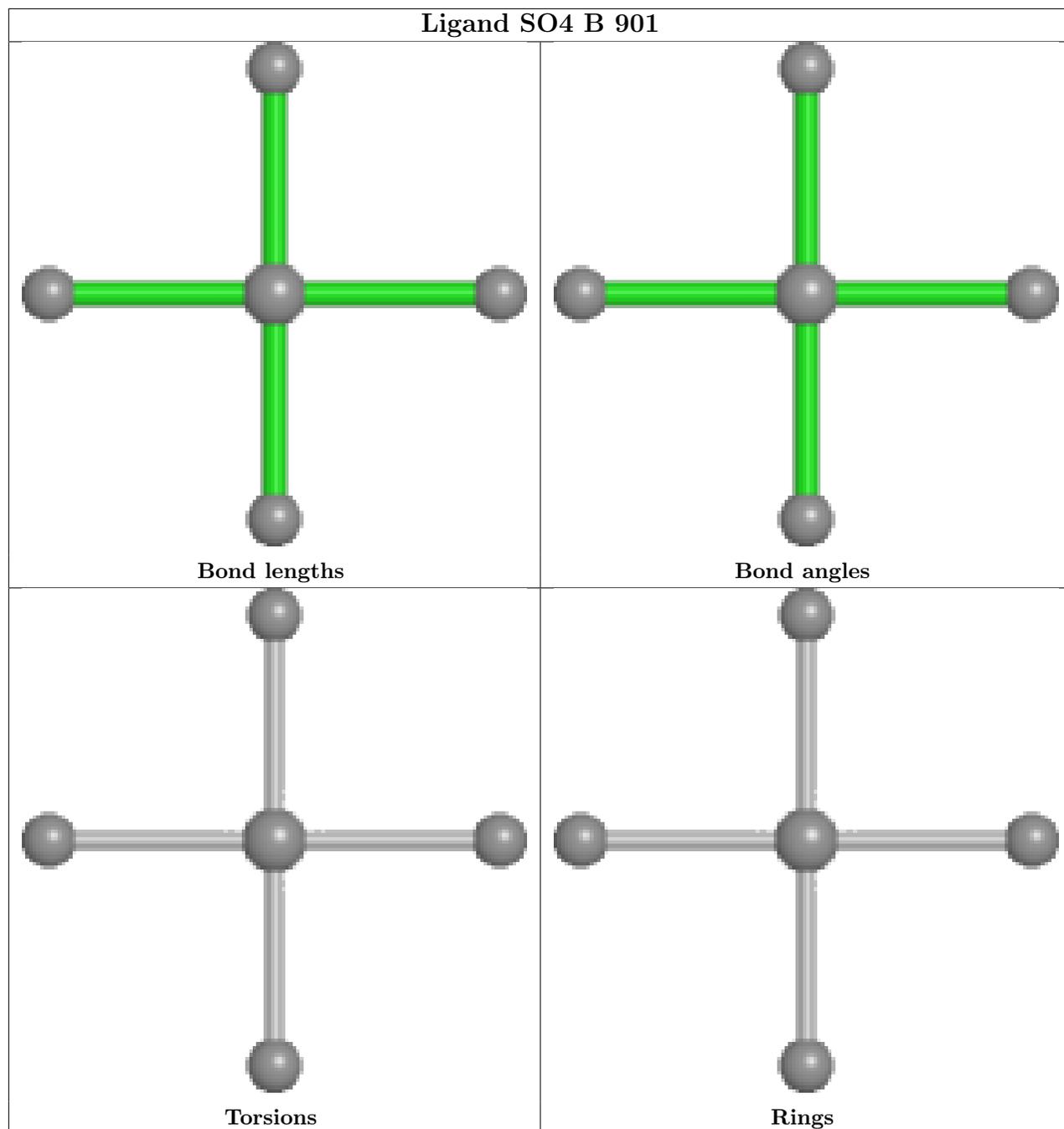
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

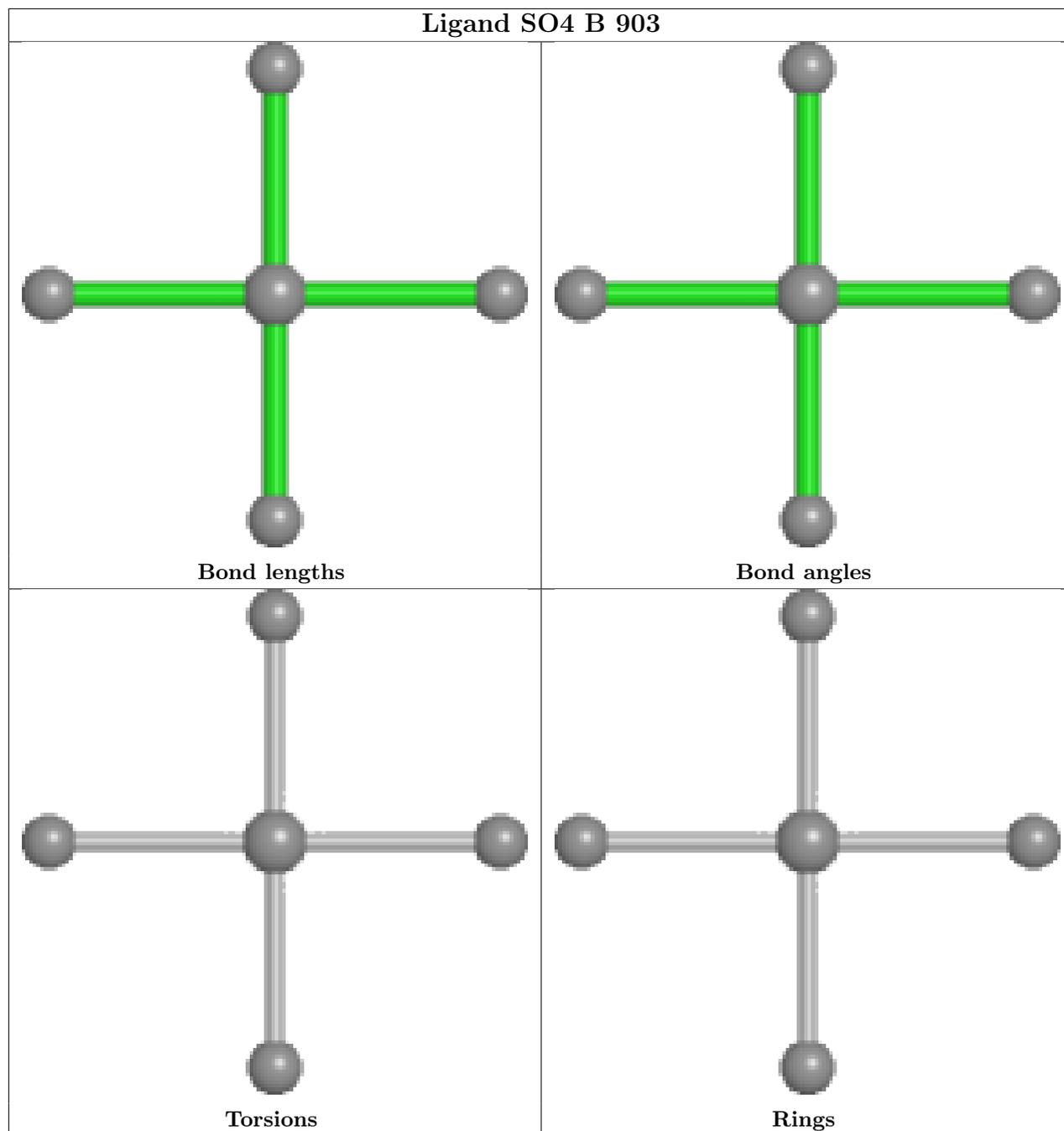












5.7 Other polymers [i](#)

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	367/375 (97%)	0.43	29 (7%)	12 14	14, 24, 49, 104	0
2	C	139/139 (100%)	0.28	11 (7%)	12 14	18, 31, 51, 61	0
3	B	355/413 (85%)	0.96	66 (18%)	1 1	18, 32, 77, 95	0
All	All	861/927 (92%)	0.63	106 (12%)	4 4	14, 28, 62, 104	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	759	ASN	18.8
3	B	760	PRO	13.4
3	B	839	LEU	12.8
3	B	761	TYR	12.2
3	B	835	LEU	11.9
1	A	42	GLY	10.4
3	B	727	VAL	9.7
3	B	836	ASP	9.6
2	C	1	ALA	9.5
1	A	43	VAL	9.5
3	B	837	SER	9.3
1	A	64	ILE	8.7
3	B	757	ASP	8.6
3	B	840	PHE	7.8
3	B	758	ALA	7.7
3	B	606	VAL	7.6
3	B	863	LEU	7.4
1	A	40	HIS	7.3
3	B	762	ALA	7.2
3	B	786	GLU	6.8
3	B	841	THR	6.7
1	A	65	LEU	6.5
1	A	49	GLN	6.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	B	478	ILE	6.4
1	A	5	THR	6.4
3	B	683	LYS	6.1
1	A	39	ARG	6.1
1	A	41	GLN	5.8
3	B	763	VAL	5.6
3	B	480[A]	HIS	5.5
3	B	844	ARG	5.4
3	B	828	ASN	5.1
1	A	60	SER	5.0
1	A	38	PRO	5.0
3	B	827	LEU	4.9
3	B	787	GLY	4.9
3	B	765	ALA	4.8
3	B	833	SER	4.8
3	B	607	ASP	4.7
1	A	53	TYR	4.7
2	C	93	GLY	4.6
3	B	479	GLN	4.6
3	B	842	THR	4.5
3	B	631	VAL	4.4
1	A	51	ASP	4.4
3	B	633	ASP	4.4
3	B	781	ASP	4.3
3	B	788	LYS	4.2
1	A	44	MET	4.1
3	B	755	ALA	4.1
3	B	766	ASP	4.0
3	B	843	LYS	4.0
1	A	66	THR	4.0
2	C	94	GLY	3.9
3	B	784	LEU	3.9
3	B	531	PHE	3.7
3	B	756	ASP	3.7
2	C	139	TYR	3.6
3	B	632	ASP	3.6
1	A	50	LYS	3.5
2	C	92	THR	3.4
3	B	832	ASN	3.3
3	B	476	GLU	3.3
3	B	831	TRP	3.2
3	B	838	PRO	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	37	ARG	3.0
3	B	477	PRO	3.0
3	B	608	SER	3.0
1	A	61	LYS	3.0
3	B	482	LYS	2.9
1	A	36	GLY	2.9
3	B	466	LYS	2.9
1	A	58	ALA	2.8
3	B	573	LEU	2.8
1	A	62	ARG	2.8
3	B	764	MET	2.8
2	C	106	ASP	2.7
3	B	782	ASP	2.7
3	B	682	ASP	2.7
1	A	163	VAL	2.6
3	B	862	GLY	2.6
3	B	754	GLY	2.5
2	C	2	GLY	2.4
2	C	26	ASP	2.4
2	C	6	TYR	2.4
3	B	681	GLN	2.4
3	B	829	ASP	2.4
3	B	634	LYS	2.3
1	A	59[A]	GLN	2.3
3	B	729	ASP	2.3
2	C	3	TRP	2.3
3	B	746	ASP	2.3
3	B	605	ASP	2.2
1	A	270[A]	GLU	2.2
3	B	467	THR	2.2
1	A	354	GLN	2.2
3	B	474	VAL	2.1
1	A	52	SER	2.1
1	A	353	GLN	2.1
3	B	481	PRO	2.1
3	B	785	GLY	2.1
2	C	83	PHE	2.1
3	B	530	LEU	2.1
1	A	234	SER	2.0
3	B	468	TYR	2.0
1	A	56	ASP	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 monosaccharides in this entry.

6.4 Ligands [i](#)

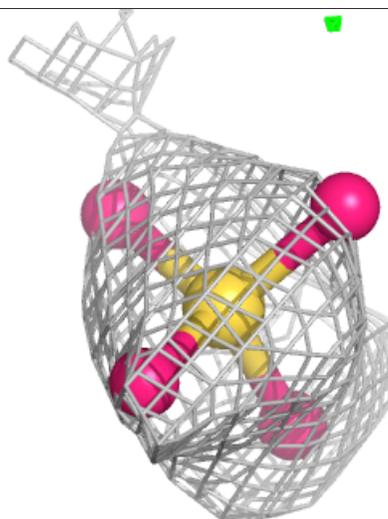
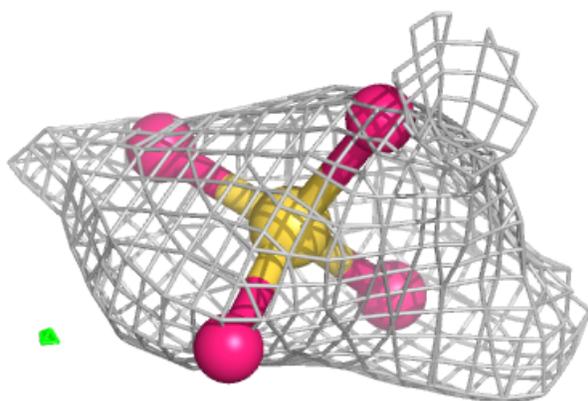
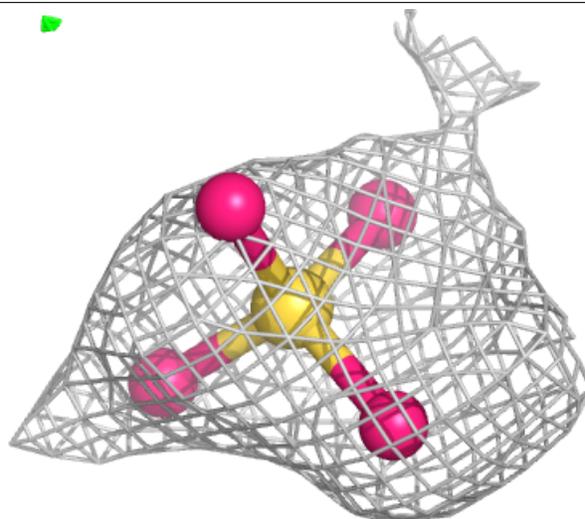
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	PEO	C	202	2/2	0.72	0.15	57,57,57,57	0
10	PG4	B	905	13/13	0.75	0.13	60,60,62,62	0
9	PEO	C	201	2/2	0.81	0.44	45,45,45,45	0
7	TRS	B	904	8/8	0.83	0.17	38,38,39,39	0
11	GOL	B	906	6/6	0.83	0.19	52,53,53,53	0
8	SO4	B	902	5/5	0.88	0.18	51,51,51,51	5
7	TRS	A	404	8/8	0.90	0.15	30,31,31,32	0
8	SO4	B	901	5/5	0.95	0.10	60,60,60,61	0
6	LAB	A	403	27/27	0.95	0.09	22,24,27,28	0
8	SO4	A	405	5/5	0.97	0.10	44,44,44,44	0
8	SO4	B	903	5/5	0.98	0.09	34,34,35,35	0
4	ATP	A	401	31/31	0.99	0.13	16,18,21,24	0
5	MG	A	402	1/1	1.00	0.15	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.

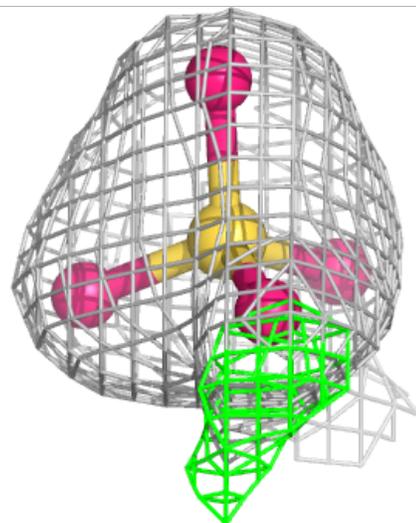
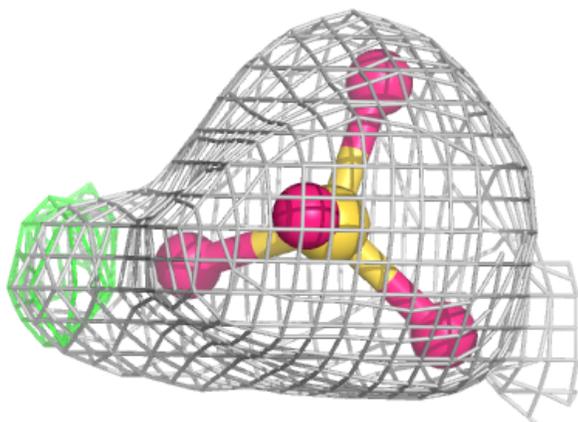
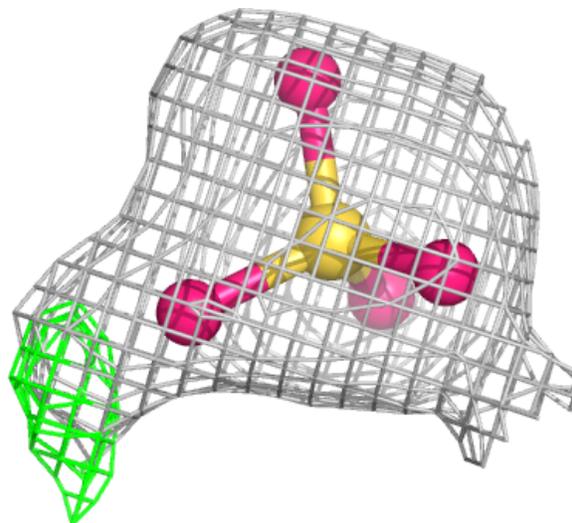
Electron density around SO4 B 902:

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



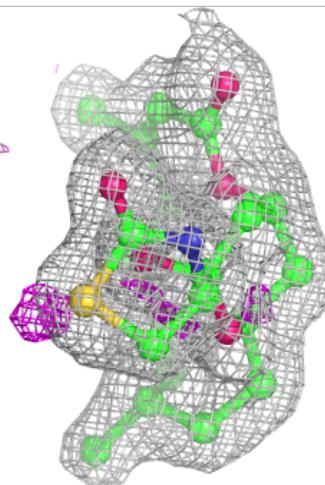
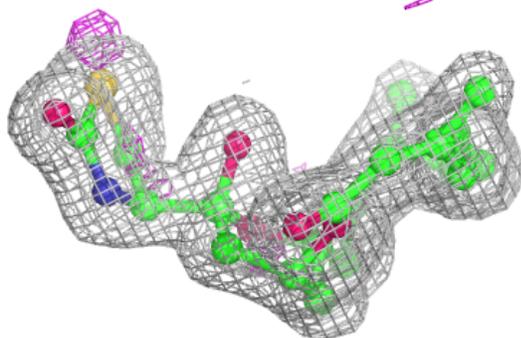
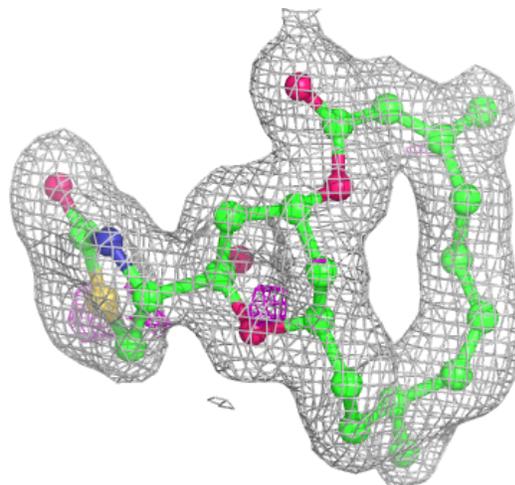
Electron density around SO4 B 901:

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



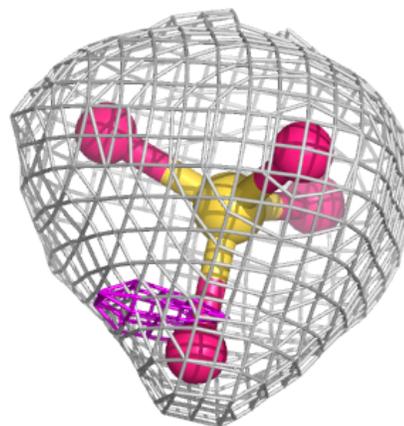
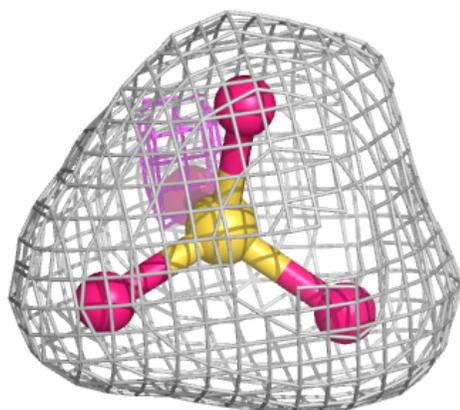
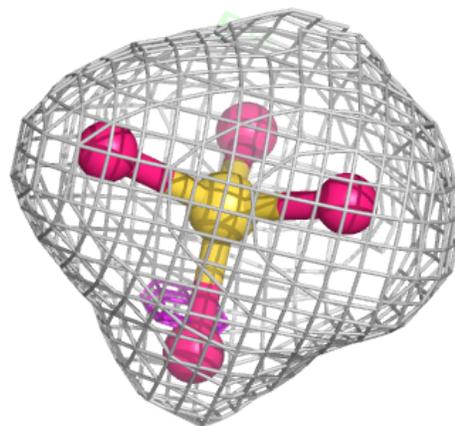
Electron density around LAB A 403:

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



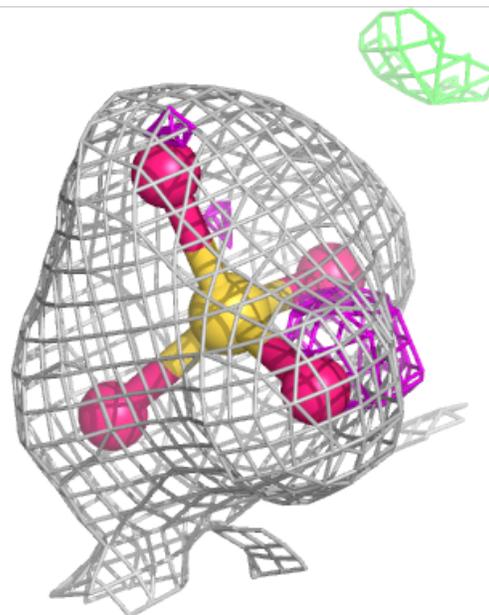
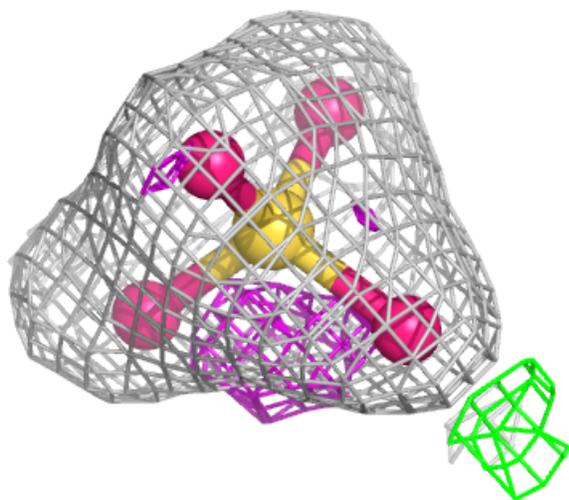
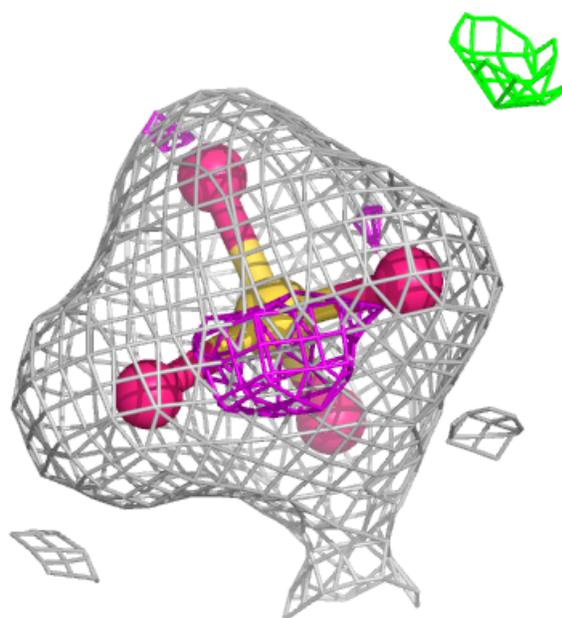
Electron density around SO4 A 405:

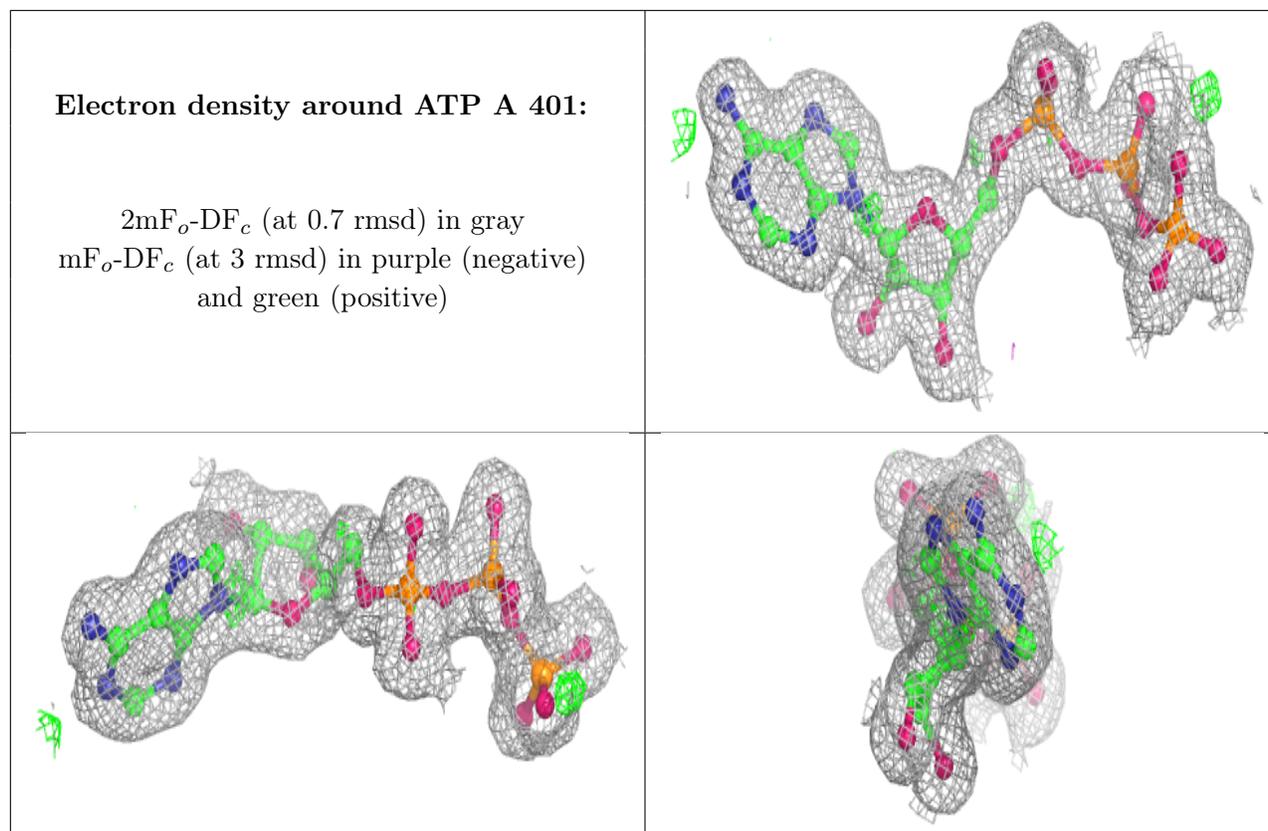
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

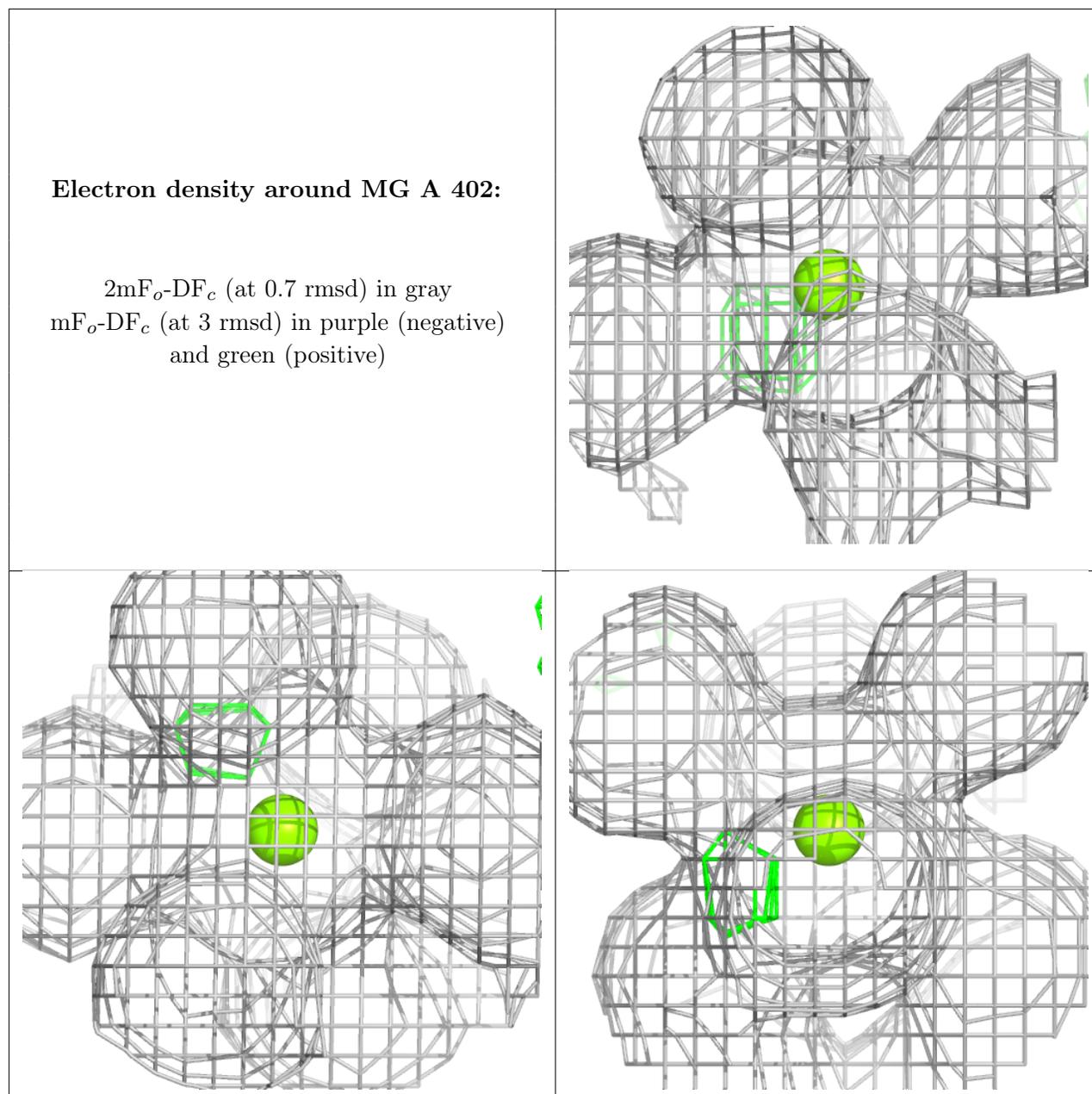


Electron density around SO4 B 903:

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







6.5 Other polymers [i](#)

There are no such residues in this entry.