



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:27 AM UTC

PDB ID : 8A39 / pdb_00008a39
Title : Crystal Structure of PaaX from Escherichia coli W
Authors : Molina, R.; Alba-Perez, A.; Hermoso, J.A.
Deposited on : 2022-06-07
Resolution : 2.30 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)
Xtrriage (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

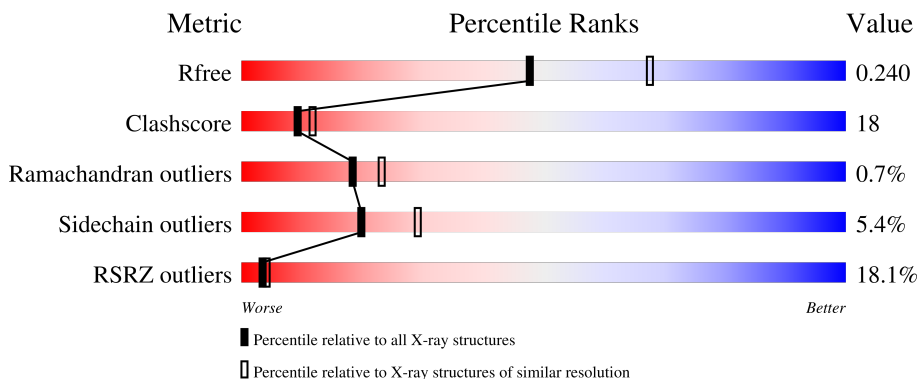
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	AP1	316	 22% 66% 26%
1	BP1	316	 12% 73% 21%
1	CP1	316	 19% 72% 21%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	AP1	403	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7465 atoms, of which 16 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-binding transcriptional repressor of phenylacetic acid degradation, aryl-CoA responsive.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AP1	305	Total	C	N	O	S	1	0	0
			2397	1544	422	429	2			
1	BP1	305	Total	C	N	O	S	1	0	0
			2397	1544	422	429	2			
1	CP1	305	Total	C	N	O	S	1	0	0
			2397	1544	422	429	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AP1	168	ALA	CYS	conflict	UNP A0A024L404
AP1	189	ALA	CYS	conflict	UNP A0A024L404
AP1	264	ALA	CYS	conflict	UNP A0A024L404
AP1	312	ALA	CYS	conflict	UNP A0A024L404
BP1	168	ALA	CYS	conflict	UNP A0A024L404
BP1	189	ALA	CYS	conflict	UNP A0A024L404
BP1	264	ALA	CYS	conflict	UNP A0A024L404
BP1	312	ALA	CYS	conflict	UNP A0A024L404
CP1	168	ALA	CYS	conflict	UNP A0A024L404
CP1	189	ALA	CYS	conflict	UNP A0A024L404
CP1	264	ALA	CYS	conflict	UNP A0A024L404
CP1	312	ALA	CYS	conflict	UNP A0A024L404

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AP1	1	Total C O 6 3 3	0	0
2	AP1	1	Total C H O 14 3 8 3	0	0
2	AP1	1	Total C H O 14 3 8 3	0	0
2	BP1	1	Total C O 6 3 3	0	0
2	BP1	1	Total C O 6 3 3	0	0
2	CP1	1	Total C O 6 3 3	0	0
2	CP1	1	Total C O 6 3 3	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AP1	1	Total	O	S	0	0
			5	4	1		
3	AP1	1	Total	O	S	0	0
			5	4	1		
3	AP1	1	Total	O	S	0	0
			5	4	1		
3	BP1	1	Total	O	S	0	0
			5	4	1		
3	BP1	1	Total	O	S	0	0
			5	4	1		
3	CP1	1	Total	O	S	0	0
			5	4	1		
3	CP1	1	Total	O	S	0	0
			5	4	1		

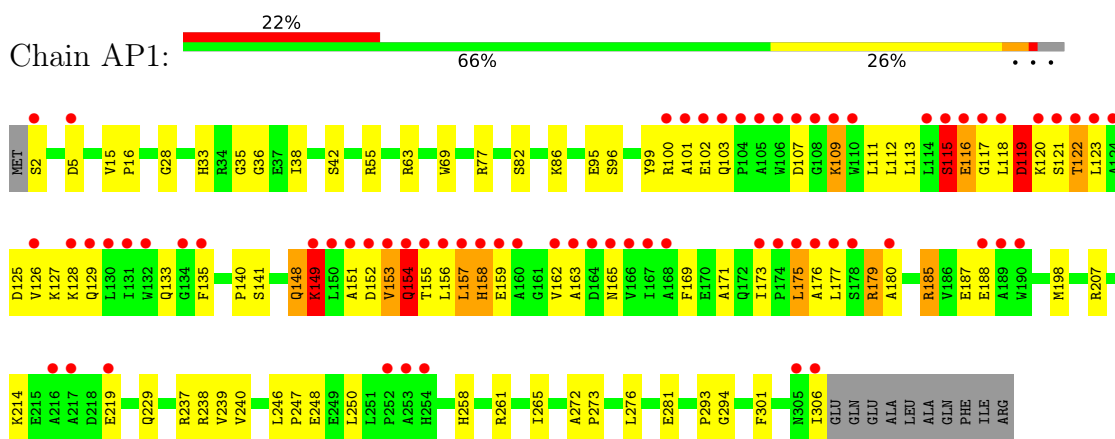
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AP1	68	Total	O	0	0
			68	68		
4	BP1	47	Total	O	0	0
			47	47		
4	CP1	66	Total	O	0	0
			66	66		

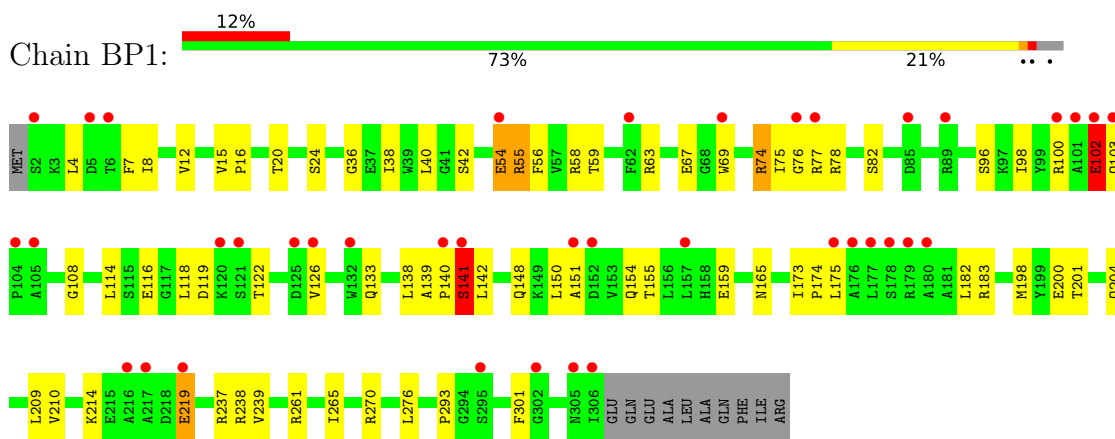
3 Residue-property plots

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.

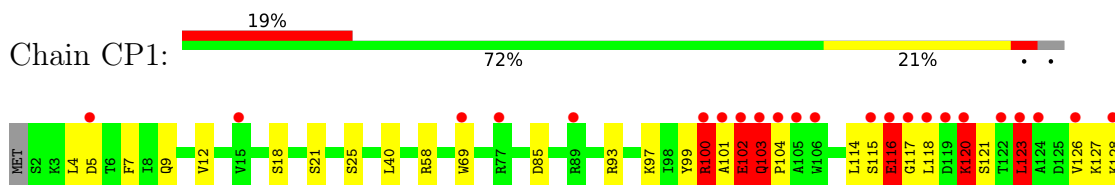
- Molecule 1: DNA-binding transcriptional repressor of phenylacetic acid degradation, aryl-CoA responsive

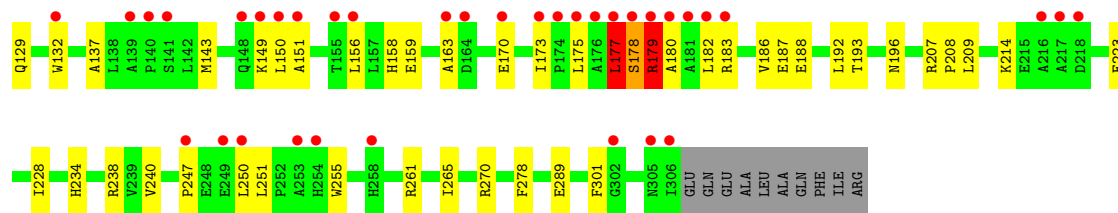


- Molecule 1: DNA-binding transcriptional repressor of phenylacetic acid degradation, aryl-CoA responsive



- Molecule 1: DNA-binding transcriptional repressor of phenylacetic acid degradation, aryl-CoA responsive





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.88Å 106.23Å 85.87Å 90.00° 108.33° 90.00°	Depositor
Resolution (Å)	44.20 – 2.30 44.20 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.20-2.30) 99.4 (44.20-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.197 , 0.241 0.196 , 0.240	Depositor DCC
R_{free} test set	956 reflections (1.50%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtrriage
Anisotropy	0.164	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7465	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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: SO4, GOL

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	AP1	0.36	0/2453	0.74	12/3328 (0.4%)
1	BP1	0.32	1/2453 (0.0%)	0.57	4/3328 (0.1%)
1	CP1	0.40	1/2453 (0.0%)	0.80	15/3328 (0.5%)
All	All	0.36	2/7359 (0.0%)	0.71	31/9984 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AP1	0	4
1	CP1	0	7
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BP1	210	VAL	CA-CB	7.59	1.58	1.54
1	CP1	179	ARG	CG-CD	5.39	1.68	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CP1	179	ARG	CB-CG-CD	12.00	138.89	111.30
1	CP1	120	LYS	CD-CE-NZ	-9.30	82.14	111.90
1	AP1	149	LYS	CA-CB-CG	8.65	131.40	114.10
1	AP1	127	LYS	CG-CD-CE	-8.58	91.56	111.30
1	CP1	103	GLN	N-CA-CB	8.45	124.10	109.57
1	BP1	102	GLU	CA-C-N	7.90	136.06	121.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BP1	102	GLU	C-N-CA	7.90	136.06	121.69
1	CP1	93	ARG	CB-CG-CD	-7.37	94.34	111.30
1	BP1	74	ARG	CA-CB-CG	-7.08	99.94	114.10
1	AP1	148	GLN	CA-CB-CG	6.92	127.93	114.10
1	AP1	119	ASP	CB-CA-C	-6.41	97.67	110.42
1	AP1	157	LEU	CA-C-N	-6.40	110.58	120.31
1	AP1	157	LEU	C-N-CA	-6.40	110.58	120.31
1	AP1	115	SER	CA-C-N	-6.28	110.41	122.09
1	AP1	115	SER	C-N-CA	-6.28	110.41	122.09
1	CP1	179	ARG	N-CA-C	6.20	124.01	110.80
1	CP1	102	GLU	CA-CB-CG	-6.17	101.76	114.10
1	CP1	177	LEU	CB-CG-CD1	5.93	128.50	110.70
1	CP1	116	GLU	CB-CG-CD	5.89	122.61	112.60
1	CP1	177	LEU	CB-CG-CD2	-5.76	93.41	110.70
1	CP1	116	GLU	CA-CB-CG	5.74	125.58	114.10
1	AP1	154	GLN	CA-C-N	-5.62	112.68	120.38
1	AP1	154	GLN	C-N-CA	-5.62	112.68	120.38
1	BP1	74	ARG	CB-CG-CD	5.60	124.17	111.30
1	CP1	100	ARG	N-CA-CB	-5.47	101.24	110.49
1	CP1	116	GLU	CB-CA-C	5.45	120.14	110.16
1	AP1	149	LYS	CB-CG-CD	5.42	123.78	111.30
1	CP1	179	ARG	CG-CD-NE	5.42	123.94	112.00
1	CP1	123	LEU	CD1-CG-CD2	5.34	122.56	110.80
1	CP1	100	ARG	CA-CB-CG	5.20	124.50	114.10
1	AP1	154	GLN	CB-CA-C	5.18	119.01	110.88

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AP1	115	SER	Peptide
1	AP1	119	ASP	Peptide
1	AP1	149	LYS	Peptide
1	AP1	154	GLN	Sidechain
1	CP1	101	ALA	Peptide
1	CP1	103	GLN	Peptide
1	CP1	116	GLU	Sidechain
1	CP1	159	GLU	Peptide
1	CP1	178	SER	Peptide
1	CP1	179	ARG	Sidechain
1	CP1	99	TYR	Peptide

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	AP1	2397	0	2428	108	0
1	BP1	2397	0	2428	56	0
1	CP1	2397	0	2428	97	0
2	AP1	18	16	23	6	0
2	BP1	12	0	16	5	0
2	CP1	12	0	16	3	0
3	AP1	15	0	0	0	0
3	BP1	10	0	0	0	0
3	CP1	10	0	0	0	0
4	AP1	68	0	0	6	0
4	BP1	47	0	0	4	0
4	CP1	66	0	0	5	0
All	All	7449	16	7339	264	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 18.

All (264) 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:CP1:118:LEU:HD11	1:CP1:123:LEU:HD12	1.32	1.12
1:BP1:261:ARG:NH1	4:BP1:501:HOH:O	1.89	1.06
1:BP1:173:ILE:HD12	1:BP1:182:LEU:HD22	1.39	1.05
1:AP1:119:ASP:OD1	1:AP1:122:THR:N	1.92	1.03
1:AP1:149:LYS:HB2	1:AP1:152:ASP:H	1.24	1.02
1:AP1:294:GLY:HA3	2:AP1:403:GOL:H11	1.43	0.98
1:CP1:100:ARG:O	1:CP1:261:ARG:NH2	1.96	0.98
1:CP1:100:ARG:NE	1:CP1:102:GLU:OE2	1.98	0.95
1:CP1:238:ARG:NH2	4:CP1:501:HOH:O	1.99	0.95
1:CP1:103:GLN:HE22	1:CP1:247:PRO:HA	1.31	0.95
1:AP1:149:LYS:CB	1:AP1:152:ASP:H	1.84	0.91
1:AP1:121:SER:O	1:AP1:125:ASP:HB2	1.72	0.90
1:CP1:97:LYS:O	1:CP1:100:ARG:HD3	1.73	0.88
1:AP1:15:VAL:HG13	1:AP1:16:PRO:HD2	1.55	0.87
1:AP1:175:LEU:HD21	1:AP1:177:LEU:HB2	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CP1:127:LYS:HG3	1:CP1:143:MET:HE3	1.57	0.86
1:AP1:173:ILE:HD12	1:AP1:173:ILE:O	1.75	0.86
1:CP1:173:ILE:HB	1:CP1:179:ARG:HH22	1.40	0.86
1:CP1:118:LEU:CD1	1:CP1:123:LEU:HD12	2.07	0.85
1:AP1:103:GLN:NE2	1:AP1:246:LEU:O	2.09	0.85
1:AP1:179:ARG:HD3	1:AP1:180:ALA:H	1.42	0.84
1:CP1:149:LYS:NZ	1:CP1:170:GLU:OE2	2.10	0.84
1:AP1:86:LYS:NZ	4:AP1:501:HOH:O	2.12	0.83
1:AP1:294:GLY:HA3	2:AP1:403:GOL:C1	2.08	0.83
1:AP1:176:ALA:O	1:AP1:179:ARG:HD2	1.79	0.83
1:AP1:247:PRO:HD2	1:AP1:250:LEU:HD12	1.60	0.83
1:BP1:140:PRO:O	1:BP1:141:SER:HB3	1.79	0.82
1:AP1:198:MET:HE2	1:AP1:239:VAL:HG22	1.63	0.81
1:AP1:135:PHE:CE1	1:AP1:148:GLN:HG3	2.16	0.80
1:AP1:185:ARG:NH2	1:AP1:188:GLU:OE1	2.14	0.80
1:CP1:116:GLU:OE1	1:CP1:117:GLY:N	2.14	0.80
1:AP1:149:LYS:HG3	1:AP1:151:ALA:HB3	1.63	0.80
1:CP1:182:LEU:HD13	1:CP1:182:LEU:O	1.81	0.79
1:BP1:15:VAL:HG22	1:BP1:16:PRO:HD2	1.65	0.79
1:BP1:108:GLY:O	4:BP1:502:HOH:O	2.00	0.79
1:CP1:120:LYS:HA	1:CP1:123:LEU:HB2	1.65	0.79
1:AP1:119:ASP:CG	1:AP1:122:THR:H	1.92	0.77
1:AP1:149:LYS:HB2	1:AP1:152:ASP:N	2.00	0.77
1:BP1:103:GLN:CD	1:BP1:103:GLN:H	1.92	0.76
1:CP1:149:LYS:HD3	1:CP1:150:LEU:H	1.50	0.76
1:AP1:158:HIS:ND1	1:AP1:163:ALA:HB2	2.00	0.76
1:BP1:173:ILE:CD1	1:BP1:182:LEU:HD22	2.16	0.75
1:AP1:149:LYS:HB2	1:AP1:152:ASP:HB2	1.68	0.75
1:BP1:201:THR:OG1	2:BP1:401:GOL:H32	1.87	0.75
1:AP1:149:LYS:HG2	1:AP1:152:ASP:OD2	1.86	0.74
1:BP1:63:ARG:O	1:BP1:67:GLU:HG3	1.86	0.74
1:CP1:127:LYS:HG3	1:CP1:143:MET:CE	2.18	0.74
1:CP1:182:LEU:HD13	1:CP1:182:LEU:C	2.13	0.74
1:AP1:119:ASP:O	1:AP1:123:LEU:HD12	1.88	0.73
1:AP1:153:VAL:HG23	1:AP1:157:LEU:HG	1.68	0.73
1:AP1:135:PHE:HE1	1:AP1:148:GLN:HG3	1.50	0.73
1:CP1:173:ILE:HB	1:CP1:179:ARG:NH2	2.03	0.73
1:CP1:187:GLU:OE1	1:CP1:188:GLU:HG3	1.89	0.73
1:AP1:158:HIS:CE1	1:AP1:163:ALA:HB1	2.24	0.72
1:CP1:103:GLN:HE22	1:CP1:247:PRO:CA	2.02	0.71
1:AP1:111:LEU:HD11	1:AP1:113:LEU:HD21	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BP1:8:ILE:O	1:BP1:12:VAL:HG12	1.90	0.71
1:CP1:179:ARG:CD	1:CP1:182:LEU:HB3	2.21	0.71
1:AP1:133:GLN:O	1:AP1:148:GLN:NE2	2.23	0.71
1:BP1:270:ARG:NH2	1:CP1:289:GLU:OE2	2.24	0.71
1:BP1:174:PRO:O	1:BP1:175:LEU:HD23	1.91	0.70
1:BP1:133:GLN:HB3	1:BP1:148:GLN:NE2	2.07	0.70
1:AP1:149:LYS:HB2	1:AP1:152:ASP:CB	2.22	0.69
1:AP1:158:HIS:CE1	1:AP1:163:ALA:CB	2.75	0.69
1:AP1:179:ARG:HD3	1:AP1:180:ALA:N	2.08	0.69
1:AP1:175:LEU:HD11	1:AP1:177:LEU:HD23	1.75	0.69
1:CP1:158:HIS:HA	1:CP1:163:ALA:HB2	1.74	0.69
1:AP1:101:ALA:O	1:AP1:102:GLU:HB2	1.91	0.69
1:AP1:237:ARG:HA	1:AP1:240:VAL:HG12	1.75	0.68
1:BP1:74:ARG:HD2	1:BP1:77:ARG:HA	1.74	0.68
1:CP1:173:ILE:CB	1:CP1:179:ARG:HH22	2.06	0.68
1:AP1:115:SER:O	1:AP1:116:GLU:HB2	1.93	0.68
1:AP1:149:LYS:HB3	1:AP1:151:ALA:N	2.09	0.68
1:BP1:100:ARG:HB3	4:BP1:501:HOH:O	1.94	0.68
2:BP1:402:GOL:H2	2:CP1:401:GOL:H11	1.75	0.67
1:CP1:261:ARG:NH1	4:CP1:502:HOH:O	2.16	0.67
1:AP1:119:ASP:OD2	1:AP1:122:THR:OG1	2.12	0.67
1:BP1:133:GLN:HB3	1:BP1:148:GLN:HE21	1.61	0.65
1:AP1:100:ARG:O	1:AP1:261:ARG:NH1	2.26	0.65
1:CP1:103:GLN:NE2	1:CP1:247:PRO:HA	2.10	0.64
1:CP1:156:LEU:HD12	1:CP1:156:LEU:O	1.98	0.64
1:BP1:102:GLU:HA	1:BP1:103:GLN:OE1	1.98	0.64
1:AP1:294:GLY:CA	2:AP1:403:GOL:H11	2.23	0.63
1:BP1:4:LEU:HD12	1:BP1:219:GLU:OE1	1.99	0.63
1:AP1:111:LEU:HD11	1:AP1:113:LEU:CD2	2.29	0.62
1:BP1:15:VAL:CG2	1:BP1:16:PRO:HD2	2.29	0.62
1:AP1:158:HIS:ND1	1:AP1:163:ALA:CB	2.61	0.62
1:CP1:100:ARG:HG3	1:CP1:102:GLU:OE1	1.98	0.62
1:AP1:112:LEU:O	1:AP1:113:LEU:HD23	2.00	0.62
1:AP1:175:LEU:HG	1:AP1:177:LEU:H	1.65	0.62
1:BP1:24:SER:HB2	1:BP1:237:ARG:HH12	1.65	0.62
1:CP1:247:PRO:HD2	1:CP1:250:LEU:HD12	1.82	0.61
1:BP1:98:ILE:HD11	1:BP1:237:ARG:HG3	1.82	0.61
1:BP1:151:ALA:HA	1:BP1:154:GLN:HG3	1.81	0.61
1:CP1:179:ARG:HD3	1:CP1:182:LEU:HB3	1.83	0.61
1:AP1:149:LYS:O	1:AP1:153:VAL:HG12	2.01	0.61
1:CP1:182:LEU:HD13	1:CP1:186:VAL:HG13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AP1:273:PRO:HG3	1:AP1:306:ILE:HG12	1.83	0.61
1:CP1:173:ILE:HG21	1:CP1:179:ARG:NH2	2.16	0.61
1:CP1:102:GLU:CG	1:CP1:103:GLN:N	2.60	0.61
1:CP1:115:SER:O	1:CP1:123:LEU:HD11	2.00	0.61
1:BP1:114:LEU:HD13	1:BP1:142:LEU:HD13	1.83	0.60
1:CP1:173:ILE:CG2	1:CP1:179:ARG:NH2	2.65	0.60
1:AP1:276:LEU:HD11	1:AP1:293:PRO:HG3	1.83	0.59
1:AP1:140:PRO:O	1:AP1:141:SER:HB3	2.02	0.59
1:AP1:122:THR:O	1:AP1:126:VAL:HG23	2.01	0.59
1:CP1:100:ARG:HB3	1:CP1:261:ARG:NH1	2.18	0.59
1:CP1:100:ARG:HB3	1:CP1:261:ARG:HH12	1.68	0.59
1:AP1:153:VAL:CG2	1:AP1:157:LEU:HG	2.33	0.59
1:CP1:175:LEU:HD21	1:CP1:178:SER:H	1.67	0.58
1:AP1:28:GLY:HA3	2:AP1:401:GOL:H11	1.84	0.58
1:AP1:129:GLN:OE1	1:AP1:156:LEU:HD11	2.04	0.58
1:AP1:175:LEU:CD1	1:AP1:177:LEU:HD23	2.33	0.58
1:AP1:116:GLU:CD	1:AP1:117:GLY:H	2.11	0.58
1:CP1:128:LYS:HE2	1:CP1:132:TRP:HE1	1.69	0.58
1:BP1:54:GLU:HG2	1:BP1:55:ARG:N	2.17	0.57
1:BP1:103:GLN:OE1	1:BP1:103:GLN:N	2.23	0.57
1:BP1:139:ALA:HB1	1:BP1:140:PRO:HD2	1.86	0.57
1:CP1:182:LEU:C	1:CP1:182:LEU:CD1	2.77	0.57
1:CP1:173:ILE:HD12	1:CP1:179:ARG:HH12	1.69	0.57
1:AP1:117:GLY:C	1:AP1:118:LEU:HD23	2.29	0.57
1:BP1:74:ARG:HG3	1:BP1:75:ILE:N	2.19	0.57
1:AP1:111:LEU:HD13	1:AP1:111:LEU:C	2.30	0.57
1:CP1:103:GLN:HB3	1:CP1:104:PRO:O	2.05	0.56
1:CP1:179:ARG:HD3	1:CP1:182:LEU:CB	2.35	0.56
2:BP1:402:GOL:H2	2:CP1:401:GOL:C1	2.35	0.56
1:CP1:214:LYS:HE3	1:CP1:270:ARG:NH2	2.20	0.56
1:BP1:59:THR:O	1:BP1:63:ARG:HG3	2.05	0.56
1:CP1:149:LYS:CD	1:CP1:150:LEU:H	2.17	0.56
1:CP1:177:LEU:O	1:CP1:178:SER:OG	2.17	0.56
1:AP1:149:LYS:O	1:AP1:153:VAL:CG1	2.53	0.56
1:AP1:112:LEU:HD21	1:AP1:171:ALA:CB	2.36	0.56
1:BP1:276:LEU:HD21	1:BP1:293:PRO:HG3	1.86	0.56
1:BP1:40:LEU:HD23	1:BP1:40:LEU:C	2.30	0.56
1:CP1:100:ARG:HG3	1:CP1:102:GLU:CD	2.31	0.56
1:AP1:229:GLN:OE1	1:AP1:272:ALA:HA	2.05	0.55
1:AP1:118:LEU:HB3	1:AP1:122:THR:HB	1.89	0.55
1:BP1:54:GLU:HG2	1:BP1:55:ARG:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BP1:54:GLU:CD	1:BP1:54:GLU:H	2.15	0.54
1:AP1:135:PHE:CE1	1:AP1:148:GLN:CG	2.90	0.54
1:AP1:35:GLY:C	2:BP1:401:GOL:H11	2.31	0.54
1:CP1:173:ILE:CB	1:CP1:179:ARG:NH2	2.67	0.54
1:AP1:15:VAL:HG13	1:AP1:16:PRO:CD	2.32	0.54
1:CP1:100:ARG:HG2	1:CP1:261:ARG:NH1	2.24	0.53
1:CP1:100:ARG:HE	1:CP1:102:GLU:CD	2.09	0.53
1:BP1:122:THR:O	1:BP1:126:VAL:HG12	2.08	0.53
1:AP1:122:THR:HG22	1:AP1:162:VAL:HG11	1.90	0.52
1:BP1:20:THR:O	1:BP1:24:SER:OG	2.25	0.52
1:CP1:182:LEU:CD1	1:CP1:186:VAL:HG13	2.39	0.52
1:CP1:179:ARG:CD	1:CP1:182:LEU:CB	2.87	0.52
1:CP1:137:ALA:HB2	1:CP1:143:MET:HE1	1.92	0.52
1:AP1:38:ILE:HG12	1:AP1:42:SER:HB2	1.92	0.52
1:AP1:112:LEU:HD21	1:AP1:171:ALA:HB3	1.92	0.52
1:CP1:100:ARG:HH12	1:CP1:240:VAL:HG13	1.75	0.52
1:CP1:102:GLU:HG2	1:CP1:103:GLN:H	1.75	0.52
1:BP1:214:LYS:NZ	4:BP1:504:HOH:O	2.42	0.51
1:AP1:112:LEU:HB2	1:AP1:169:PHE:HB2	1.91	0.51
1:AP1:179:ARG:CD	1:AP1:179:ARG:H	2.23	0.51
1:AP1:111:LEU:HD12	1:AP1:135:PHE:HE2	1.76	0.51
1:CP1:100:ARG:CG	1:CP1:102:GLU:OE1	2.58	0.51
1:BP1:40:LEU:HD11	1:BP1:58:ARG:HG2	1.92	0.51
1:CP1:100:ARG:HH12	1:CP1:240:VAL:CG1	2.24	0.50
1:AP1:118:LEU:HD21	1:AP1:165:ASN:ND2	2.27	0.50
1:AP1:129:GLN:O	1:AP1:133:GLN:HB2	2.11	0.50
1:CP1:25:SER:OG	1:CP1:234:HIS:HD2	1.95	0.50
1:AP1:107:ASP:OD2	1:AP1:109:LYS:HG2	2.11	0.50
1:AP1:149:LYS:CG	1:AP1:152:ASP:OD2	2.56	0.50
1:BP1:118:LEU:HD11	1:BP1:165:ASN:HB2	1.93	0.50
1:AP1:175:LEU:CD2	1:AP1:177:LEU:HB2	2.34	0.50
1:BP1:38:ILE:HG12	1:BP1:42:SER:HB2	1.93	0.50
1:BP1:36:GLY:O	1:BP1:82:SER:HA	2.12	0.50
1:AP1:265:ILE:HG12	1:AP1:301:PHE:CG	2.48	0.49
1:AP1:281:GLU:OE1	4:AP1:502:HOH:O	2.19	0.49
1:CP1:179:ARG:O	1:CP1:180:ALA:C	2.51	0.49
1:CP1:129:GLN:OE1	1:CP1:156:LEU:HD11	2.13	0.49
1:AP1:149:LYS:HG2	1:AP1:152:ASP:CG	2.38	0.49
1:CP1:265:ILE:HG12	1:CP1:301:PHE:CG	2.48	0.49
1:CP1:179:ARG:HG3	1:CP1:183:ARG:HG3	1.94	0.49
1:AP1:117:GLY:O	1:AP1:118:LEU:HD23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BP1:119:ASP:OD2	1:BP1:122:THR:OG1	2.20	0.49
1:CP1:102:GLU:HG2	1:CP1:103:GLN:N	2.27	0.48
1:AP1:33:HIS:HA	2:AP1:403:GOL:H2	1.95	0.48
1:AP1:198:MET:CE	1:AP1:239:VAL:HG22	2.38	0.48
1:CP1:251:LEU:HD13	1:CP1:255:TRP:CD1	2.49	0.48
1:CP1:9:GLN:O	1:CP1:12:VAL:HG12	2.14	0.48
1:CP1:40:LEU:C	1:CP1:40:LEU:HD23	2.39	0.48
1:CP1:179:ARG:HD2	1:CP1:182:LEU:HD12	1.96	0.48
1:AP1:149:LYS:HB3	1:AP1:152:ASP:H	1.74	0.48
1:CP1:102:GLU:CG	1:CP1:103:GLN:H	2.27	0.48
1:CP1:156:LEU:HD12	1:CP1:156:LEU:C	2.39	0.48
2:CP1:401:GOL:H32	4:CP1:517:HOH:O	2.13	0.48
1:BP1:118:LEU:HD11	1:BP1:165:ASN:CB	2.44	0.47
1:AP1:207:ARG:NH1	4:AP1:504:HOH:O	2.38	0.47
1:CP1:179:ARG:NH1	1:CP1:182:LEU:HG	2.30	0.47
1:AP1:55:ARG:HH21	2:AP1:402:GOL:H32	1.79	0.47
1:AP1:185:ARG:CZ	1:AP1:185:ARG:HA	2.45	0.47
1:BP1:118:LEU:CD1	1:BP1:165:ASN:CB	2.93	0.47
1:CP1:18:SER:HB3	1:CP1:21:SER:HB3	1.95	0.47
1:CP1:182:LEU:HD11	1:CP1:186:VAL:CG1	2.45	0.47
1:CP1:149:LYS:CD	1:CP1:150:LEU:N	2.78	0.46
1:CP1:179:ARG:HH11	1:CP1:182:LEU:HG	1.80	0.46
1:CP1:183:ARG:O	1:CP1:186:VAL:HG22	2.15	0.46
1:CP1:175:LEU:CD2	1:CP1:178:SER:H	2.29	0.46
1:AP1:122:THR:CG2	1:AP1:162:VAL:HG11	2.45	0.46
1:AP1:248:GLU:OE1	1:AP1:258:HIS:CE1	2.68	0.46
1:AP1:179:ARG:HD2	1:AP1:179:ARG:H	1.80	0.46
1:BP1:150:LEU:O	1:BP1:154:GLN:HG2	2.16	0.46
1:CP1:4:LEU:HD23	1:CP1:4:LEU:HA	1.79	0.46
1:CP1:58:ARG:NH1	4:CP1:503:HOH:O	2.17	0.46
1:AP1:154:GLN:HE21	1:AP1:158:HIS:CE1	2.34	0.45
1:BP1:7:PHE:CE2	1:BP1:209:LEU:HD22	2.51	0.45
1:BP1:133:GLN:O	1:BP1:148:GLN:NE2	2.49	0.45
1:BP1:198:MET:HB3	1:BP1:239:VAL:HG13	1.99	0.45
1:CP1:118:LEU:CD1	1:CP1:123:LEU:CD1	2.88	0.45
1:CP1:209:LEU:HD21	1:CP1:228:ILE:HG23	1.98	0.45
1:CP1:179:ARG:HD2	1:CP1:182:LEU:CG	2.46	0.45
1:AP1:115:SER:O	1:AP1:116:GLU:CB	2.58	0.45
1:AP1:116:GLU:CG	1:AP1:117:GLY:H	2.30	0.45
1:CP1:196:ASN:OD1	1:CP1:255:TRP:HA	2.17	0.45
1:AP1:2:SER:OG	1:AP1:219:GLU:OE1	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AP1:112:LEU:CD2	1:AP1:171:ALA:HB2	2.46	0.44
1:AP1:118:LEU:HD21	1:AP1:165:ASN:HD22	1.83	0.44
1:AP1:149:LYS:CB	1:AP1:152:ASP:N	2.67	0.44
1:AP1:100:ARG:HG2	1:AP1:102:GLU:H	1.82	0.44
1:AP1:154:GLN:O	1:AP1:155:THR:C	2.52	0.44
1:BP1:200:GLU:O	1:BP1:204:GLN:HG3	2.17	0.44
1:CP1:182:LEU:CD1	1:CP1:186:VAL:CG1	2.95	0.44
1:BP1:155:THR:HG22	1:BP1:159:GLU:OE1	2.18	0.44
1:BP1:54:GLU:CD	1:BP1:54:GLU:N	2.76	0.44
1:CP1:102:GLU:O	1:CP1:103:GLN:C	2.59	0.43
1:AP1:111:LEU:HD12	1:AP1:135:PHE:CE2	2.53	0.43
1:CP1:97:LYS:HE3	1:CP1:97:LYS:HB3	1.63	0.43
1:AP1:95:GLU:HG3	1:AP1:99:TYR:HD2	1.83	0.43
1:AP1:149:LYS:HB3	1:AP1:151:ALA:H	1.81	0.43
1:BP1:138:LEU:HD12	1:BP1:138:LEU:HA	1.87	0.43
1:AP1:214:LYS:NZ	4:AP1:510:HOH:O	2.52	0.43
1:BP1:74:ARG:HG3	1:BP1:78:ARG:O	2.19	0.43
1:AP1:179:ARG:CD	1:AP1:179:ARG:N	2.80	0.43
1:AP1:126:VAL:HG21	1:AP1:162:VAL:HG21	2.00	0.42
1:BP1:74:ARG:HH11	1:BP1:77:ARG:C	2.27	0.42
1:CP1:100:ARG:CD	1:CP1:102:GLU:OE2	2.67	0.42
1:BP1:74:ARG:HD2	1:BP1:76:GLY:O	2.20	0.42
1:CP1:173:ILE:CD1	1:CP1:179:ARG:HH22	2.32	0.42
1:CP1:223:GLU:HB2	1:CP1:278:PHE:CE1	2.55	0.42
1:CP1:149:LYS:HG3	1:CP1:151:ALA:H	1.85	0.42
1:CP1:7:PHE:CE1	1:CP1:209:LEU:HD22	2.55	0.42
1:AP1:112:LEU:C	1:AP1:113:LEU:HD23	2.45	0.42
1:AP1:276:LEU:HD12	4:AP1:546:HOH:O	2.19	0.42
1:CP1:118:LEU:O	1:CP1:118:LEU:HD12	2.19	0.42
1:AP1:155:THR:HG23	1:AP1:156:LEU:N	2.34	0.41
1:CP1:100:ARG:CG	1:CP1:102:GLU:CD	2.93	0.41
1:BP1:55:ARG:HD3	1:BP1:56:PHE:N	2.36	0.41
1:CP1:214:LYS:NZ	4:CP1:510:HOH:O	2.54	0.41
4:AP1:509:HOH:O	2:BP1:401:GOL:H12	2.20	0.41
1:BP1:265:ILE:HG12	1:BP1:301:PHE:CG	2.56	0.41
1:CP1:187:GLU:OE2	1:CP1:193:THR:OG1	2.28	0.41
1:AP1:36:GLY:O	1:AP1:82:SER:HA	2.21	0.41
1:CP1:100:ARG:NE	1:CP1:102:GLU:CD	2.74	0.40
1:CP1:177:LEU:C	1:CP1:178:SER:HG	2.22	0.40
1:CP1:187:GLU:HG2	1:CP1:192:LEU:HB2	2.03	0.40
1:CP1:207:ARG:HB3	1:CP1:208:PRO:HD3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AP1:96:SER:O	1:AP1:100:ARG:HB2	2.22	0.40
1:AP1:112:LEU:CD2	1:AP1:171:ALA:CB	3.00	0.40
1:BP1:116:GLU:O	1:BP1:165:ASN:HB3	2.21	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	AP1	303/316 (96%)	294 (97%)	9 (3%)	0	100	100
1	BP1	303/316 (96%)	298 (98%)	3 (1%)	2 (1%)	18	23
1	CP1	303/316 (96%)	290 (96%)	9 (3%)	4 (1%)	9	10
All	All	909/948 (96%)	882 (97%)	21 (2%)	6 (1%)	18	23

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BP1	141	SER
1	CP1	100	ARG
1	CP1	179	ARG
1	BP1	102	GLU
1	CP1	102	GLU
1	CP1	120	LYS

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	AP1	248/257 (96%)	228 (92%)	20 (8%)	11	14
1	BP1	248/257 (96%)	240 (97%)	8 (3%)	34	51
1	CP1	248/257 (96%)	236 (95%)	12 (5%)	23	35
All	All	744/771 (96%)	704 (95%)	40 (5%)	20	29

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AP1	5	ASP
1	AP1	63	ARG
1	AP1	69	TRP
1	AP1	77	ARG
1	AP1	109	LYS
1	AP1	115	SER
1	AP1	116	GLU
1	AP1	119	ASP
1	AP1	120	LYS
1	AP1	122	THR
1	AP1	128	LYS
1	AP1	149	LYS
1	AP1	153	VAL
1	AP1	158	HIS
1	AP1	159	GLU
1	AP1	175	LEU
1	AP1	179	ARG
1	AP1	185	ARG
1	AP1	187	GLU
1	AP1	238	ARG
1	BP1	54	GLU
1	BP1	55	ARG
1	BP1	69	TRP
1	BP1	96	SER
1	BP1	141	SER
1	BP1	183	ARG
1	BP1	219	GLU
1	BP1	238	ARG
1	CP1	5	ASP
1	CP1	69	TRP
1	CP1	85	ASP
1	CP1	100	ARG

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Mol	Chain	Res	Type
1	CP1	102	GLU
1	CP1	114	LEU
1	CP1	116	GLU
1	CP1	120	LYS
1	CP1	121	SER
1	CP1	123	LEU
1	CP1	126	VAL
1	CP1	177	LEU

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

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](#)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	AP1	405	-	4,4,4	0.22	0	6,6,6	0.17	0
3	SO4	AP1	406	-	4,4,4	0.26	0	6,6,6	0.06	0
2	GOL	BP1	402	-	5,5,5	1.00	0	5,5,5	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	AP1	404	-	4,4,4	0.28	0	6,6,6	0.17	0
2	GOL	AP1	403	-	5,5,5	1.38	1 (20%)	5,5,5	1.50	1 (20%)
3	SO4	BP1	404	-	4,4,4	0.25	0	6,6,6	0.14	0
2	GOL	AP1	402	-	5,5,5	1.18	0	5,5,5	1.18	1 (20%)
3	SO4	CP1	403	-	4,4,4	0.25	0	6,6,6	0.08	0
3	SO4	CP1	404	-	4,4,4	0.25	0	6,6,6	0.29	0
2	GOL	AP1	401	-	5,5,5	0.95	0	5,5,5	0.97	0
2	GOL	CP1	401	-	5,5,5	0.84	0	5,5,5	1.23	1 (20%)
2	GOL	BP1	401	-	5,5,5	0.99	0	5,5,5	1.28	1 (20%)
3	SO4	BP1	403	-	4,4,4	0.25	0	6,6,6	0.10	0
2	GOL	CP1	402	-	5,5,5	0.99	0	5,5,5	1.14	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	GOL	BP1	402	-	-	2/4/4/4	-
2	GOL	AP1	403	-	-	1/4/4/4	-
2	GOL	AP1	402	-	-	0/4/4/4	-
2	GOL	AP1	401	-	-	2/4/4/4	-
2	GOL	CP1	401	-	-	2/4/4/4	-
2	GOL	BP1	401	-	-	4/4/4/4	-
2	GOL	CP1	402	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AP1	403	GOL	C3-C2	2.09	1.59	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AP1	403	GOL	C3-C2-C1	-2.91	101.11	111.80
2	BP1	401	GOL	C3-C2-C1	-2.32	103.28	111.80
2	CP1	401	GOL	C3-C2-C1	-2.12	104.01	111.80
2	AP1	402	GOL	C3-C2-C1	-2.07	104.19	111.80

There are no chirality outliers.

All (13) torsion outliers are listed below:

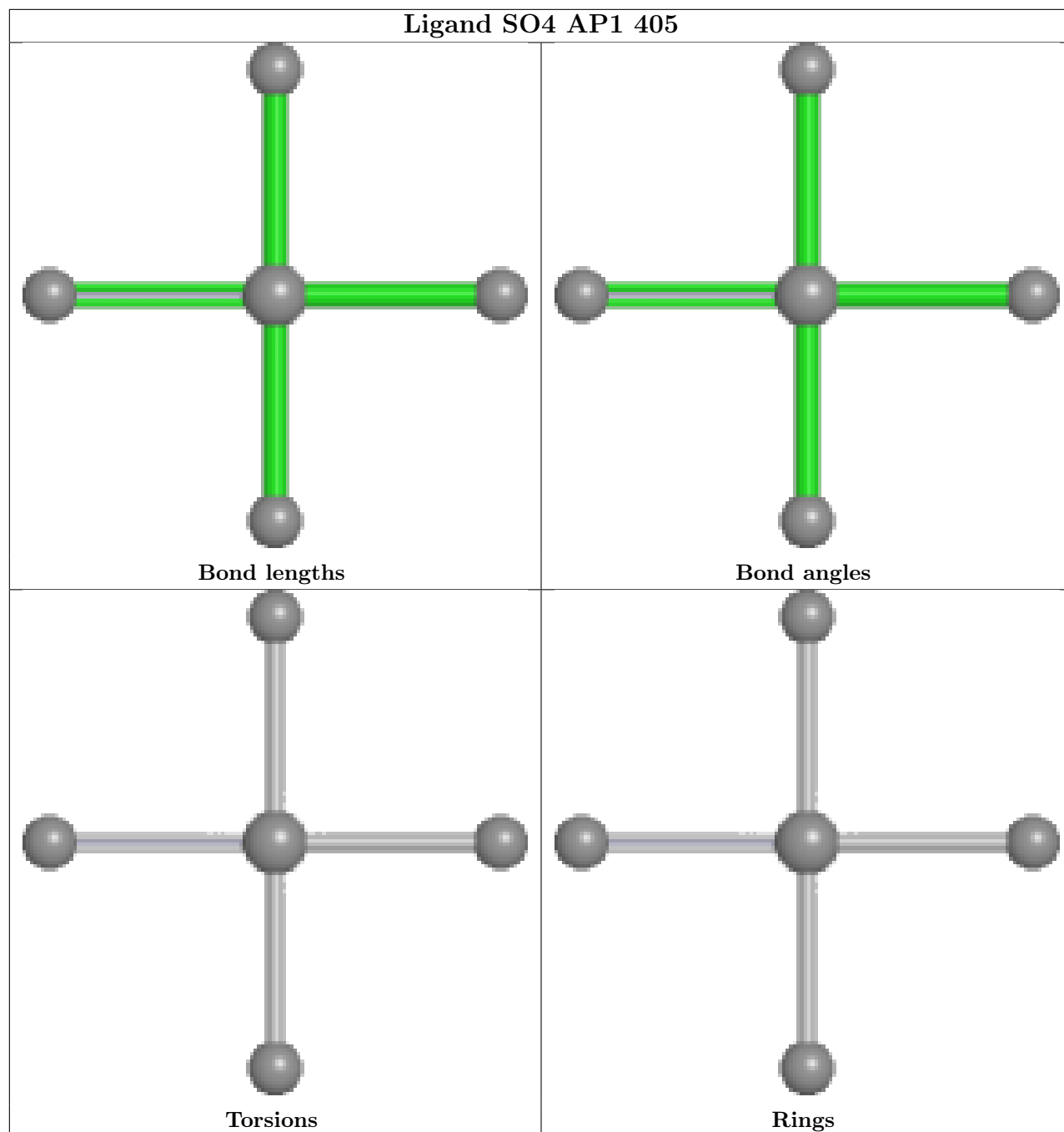
Mol	Chain	Res	Type	Atoms
2	BP1	401	GOL	O1-C1-C2-C3
2	BP1	401	GOL	C1-C2-C3-O3
2	BP1	402	GOL	O1-C1-C2-O2
2	BP1	402	GOL	O1-C1-C2-C3
2	CP1	401	GOL	C1-C2-C3-O3
2	CP1	402	GOL	C1-C2-C3-O3
2	BP1	401	GOL	O1-C1-C2-O2
2	CP1	402	GOL	O2-C2-C3-O3
2	AP1	401	GOL	O1-C1-C2-C3
2	BP1	401	GOL	O2-C2-C3-O3
2	CP1	401	GOL	O2-C2-C3-O3
2	AP1	401	GOL	O1-C1-C2-O2
2	AP1	403	GOL	O1-C1-C2-O2

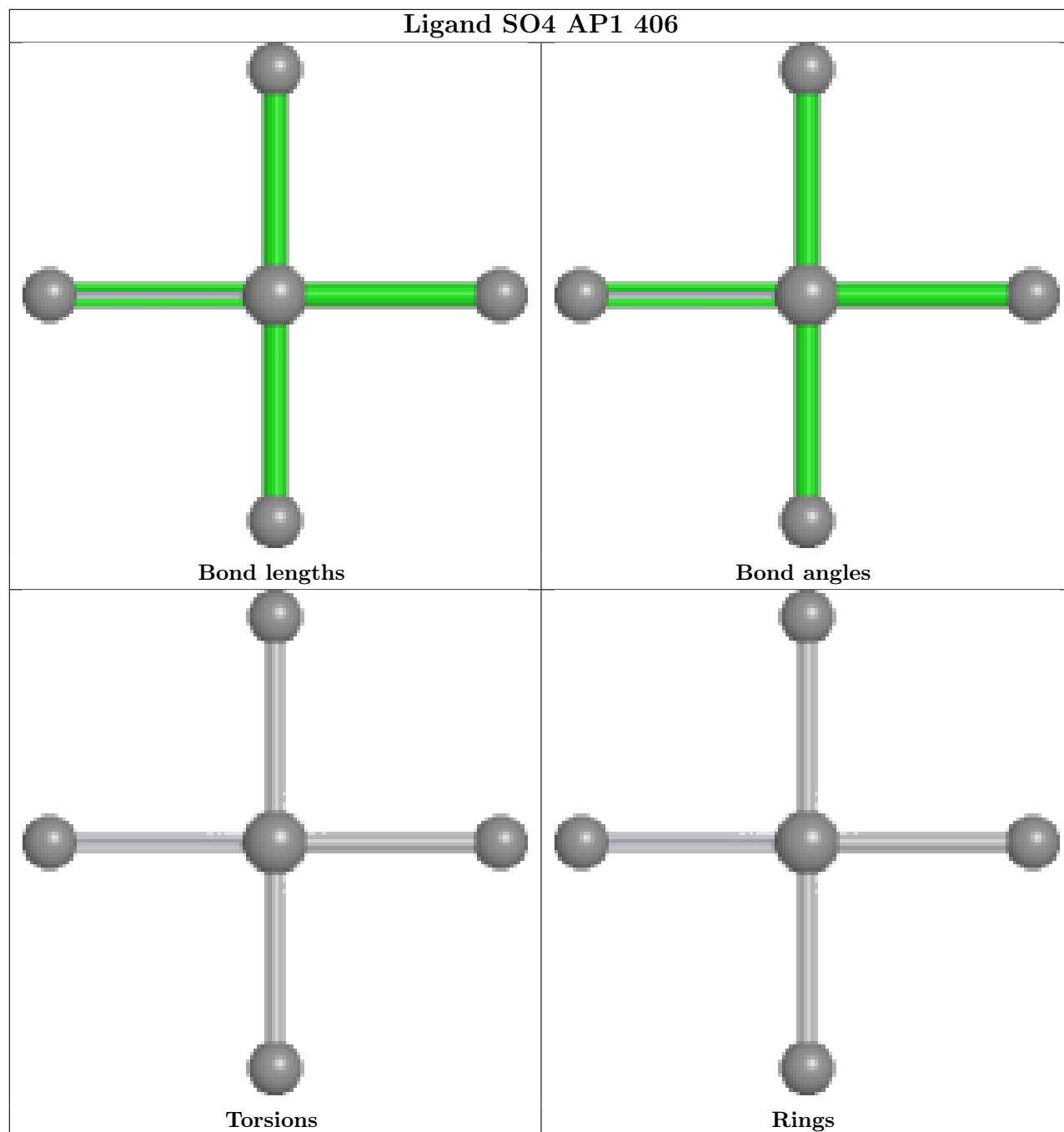
There are no ring outliers.

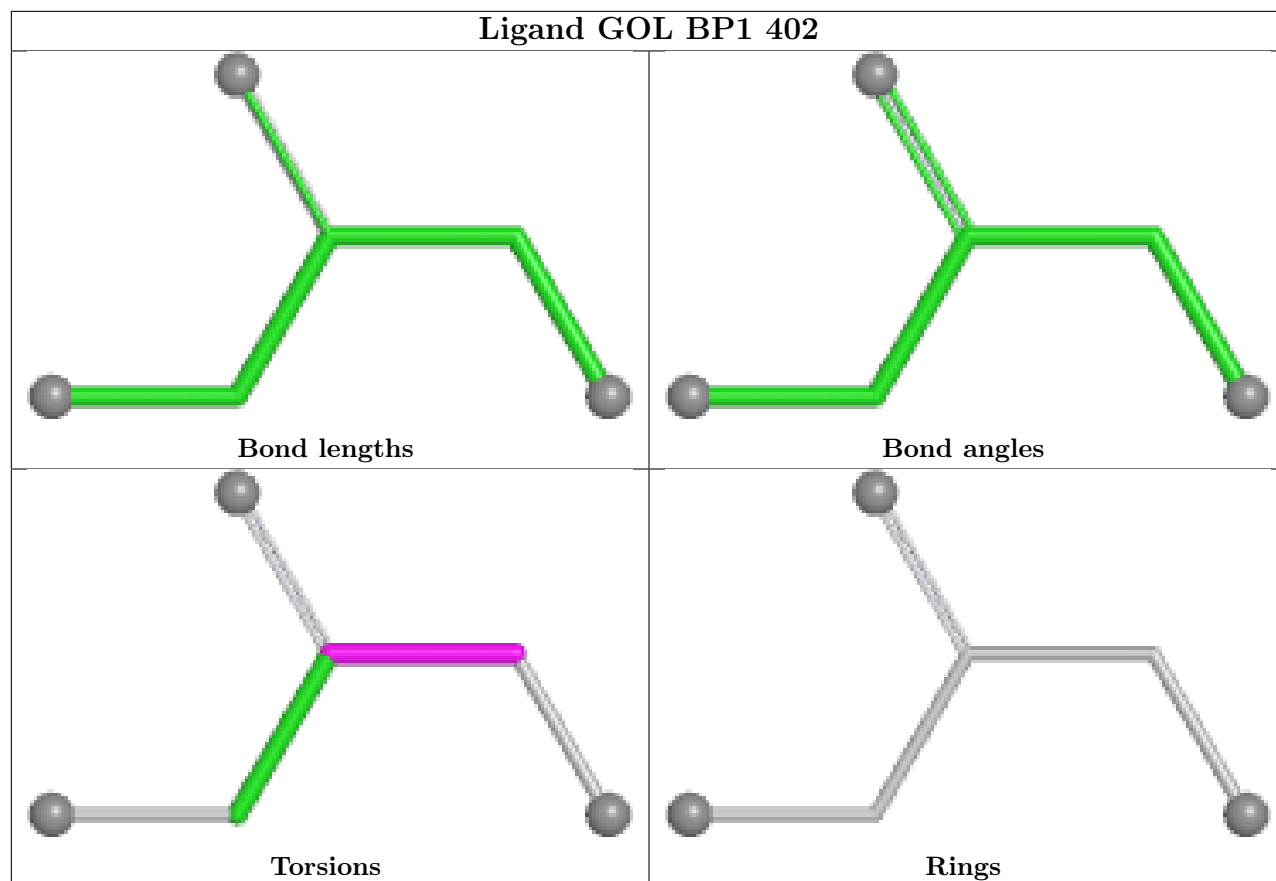
6 monomers are involved in 12 short contacts:

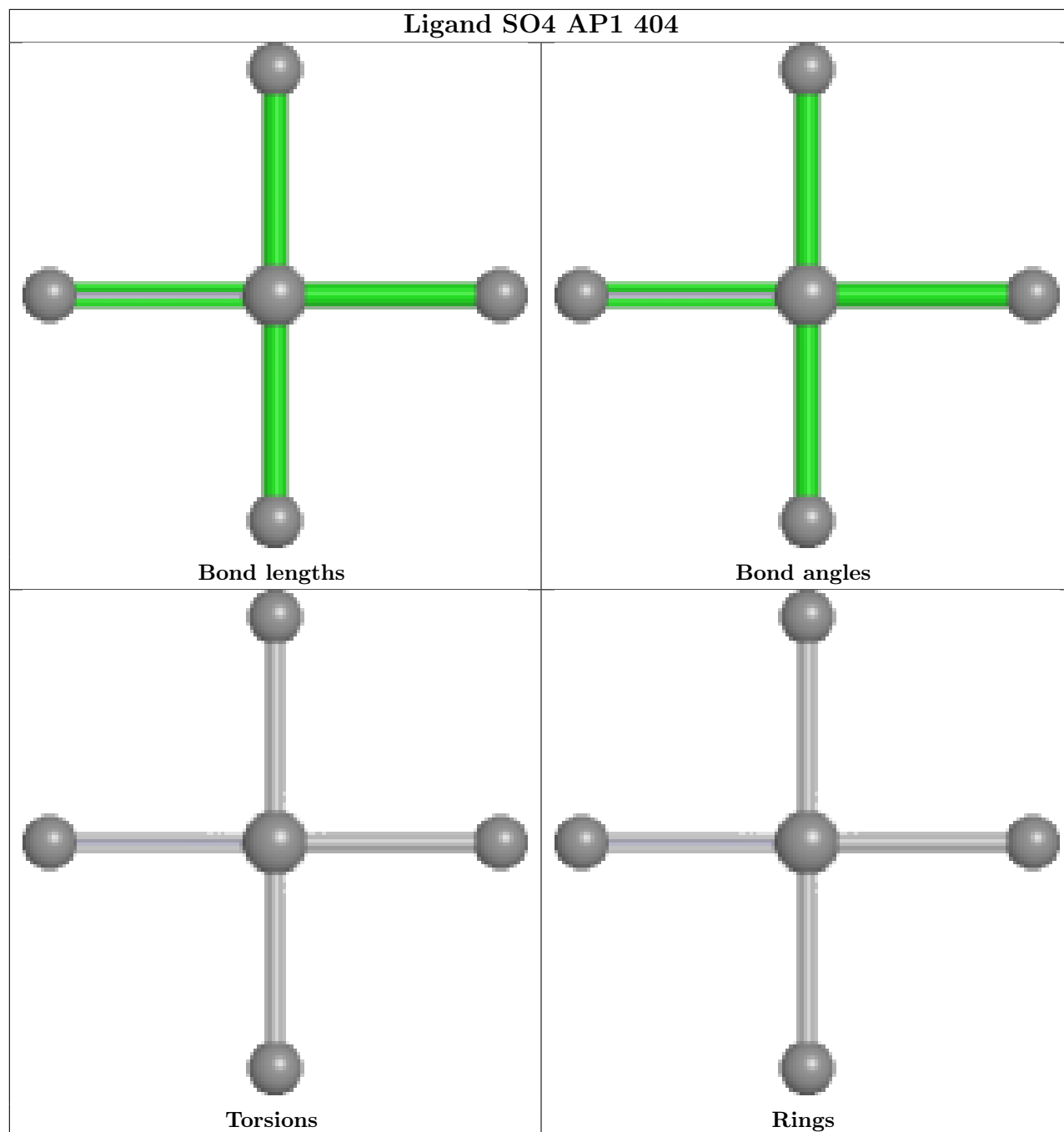
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BP1	402	GOL	2	0
2	AP1	403	GOL	4	0
2	AP1	402	GOL	1	0
2	AP1	401	GOL	1	0
2	CP1	401	GOL	3	0
2	BP1	401	GOL	3	0

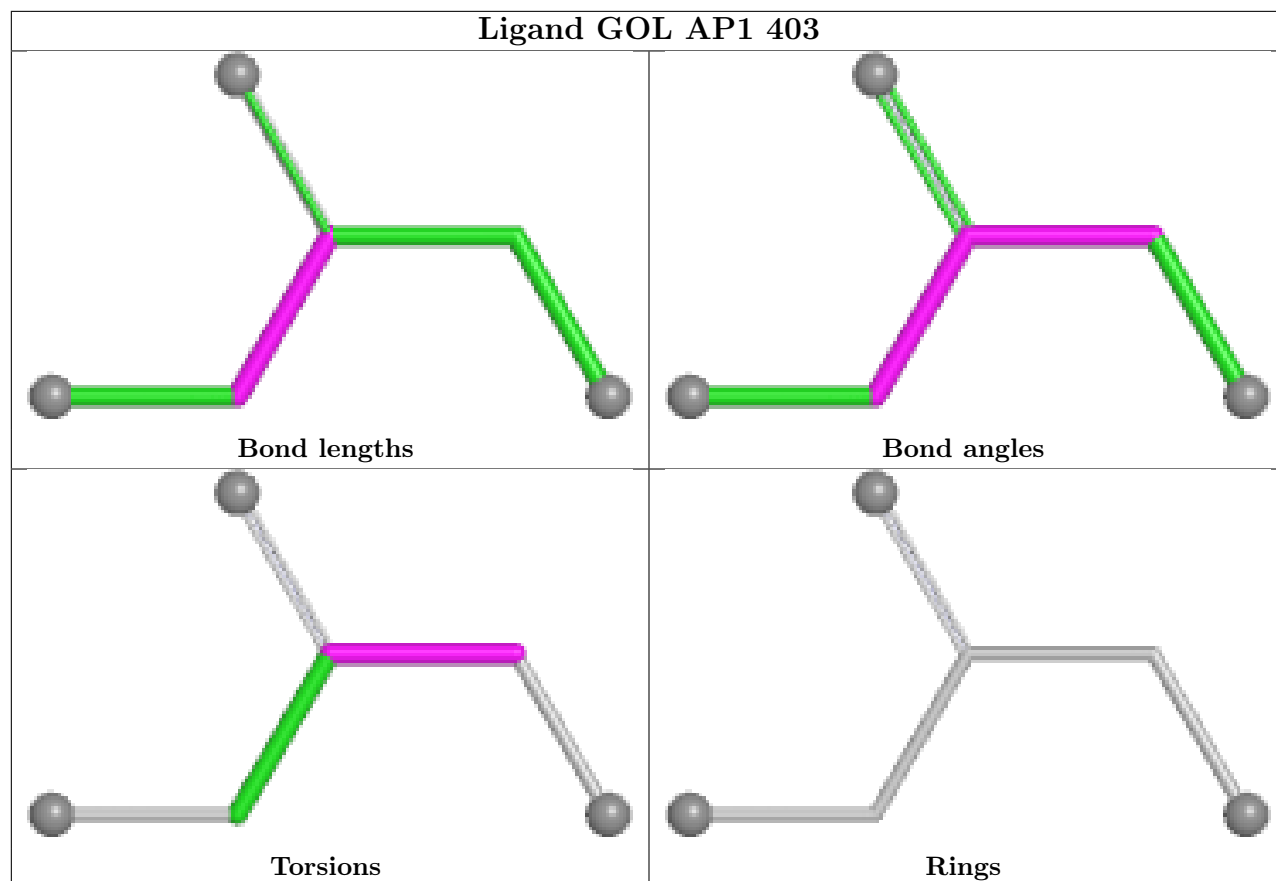
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

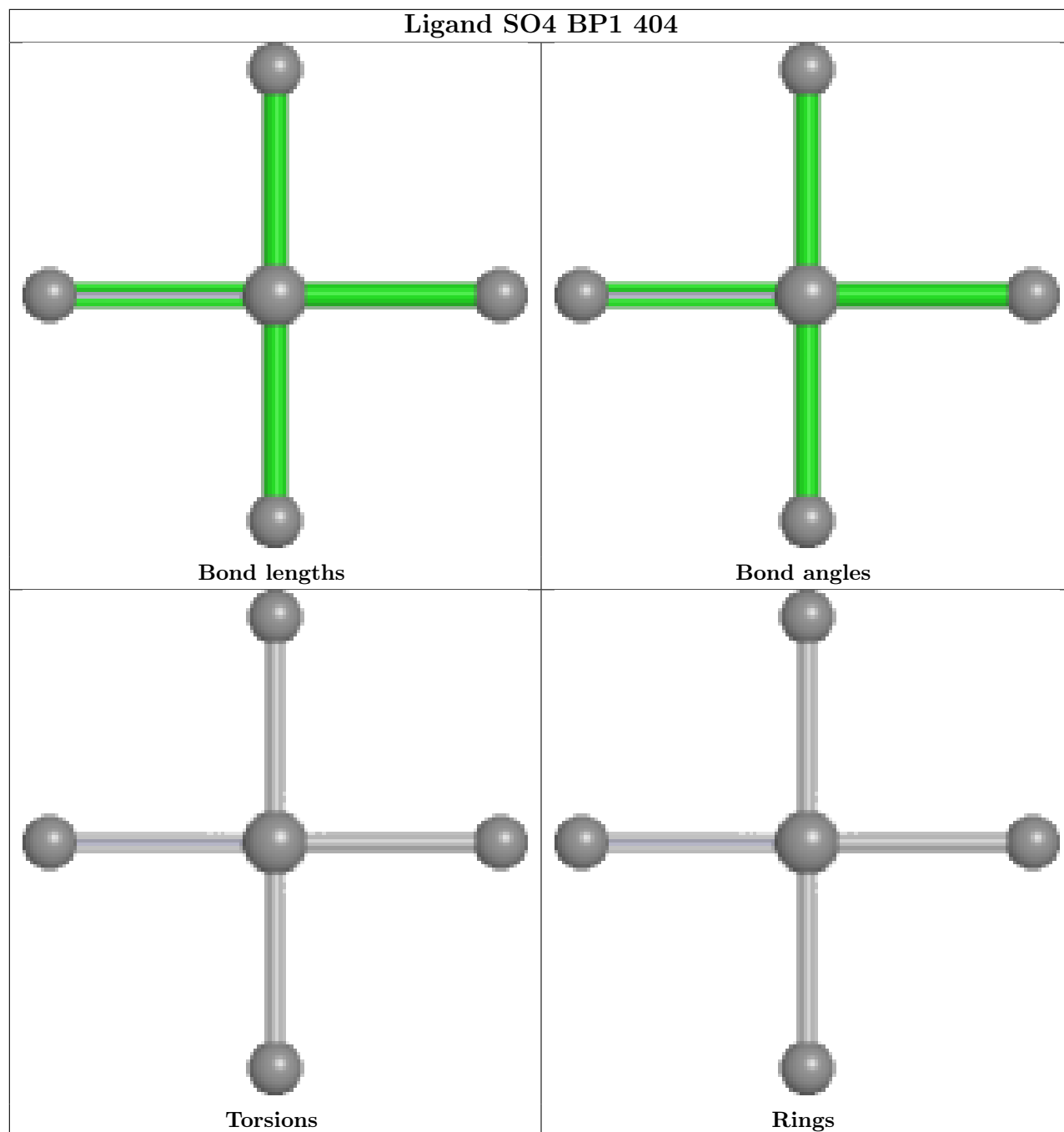


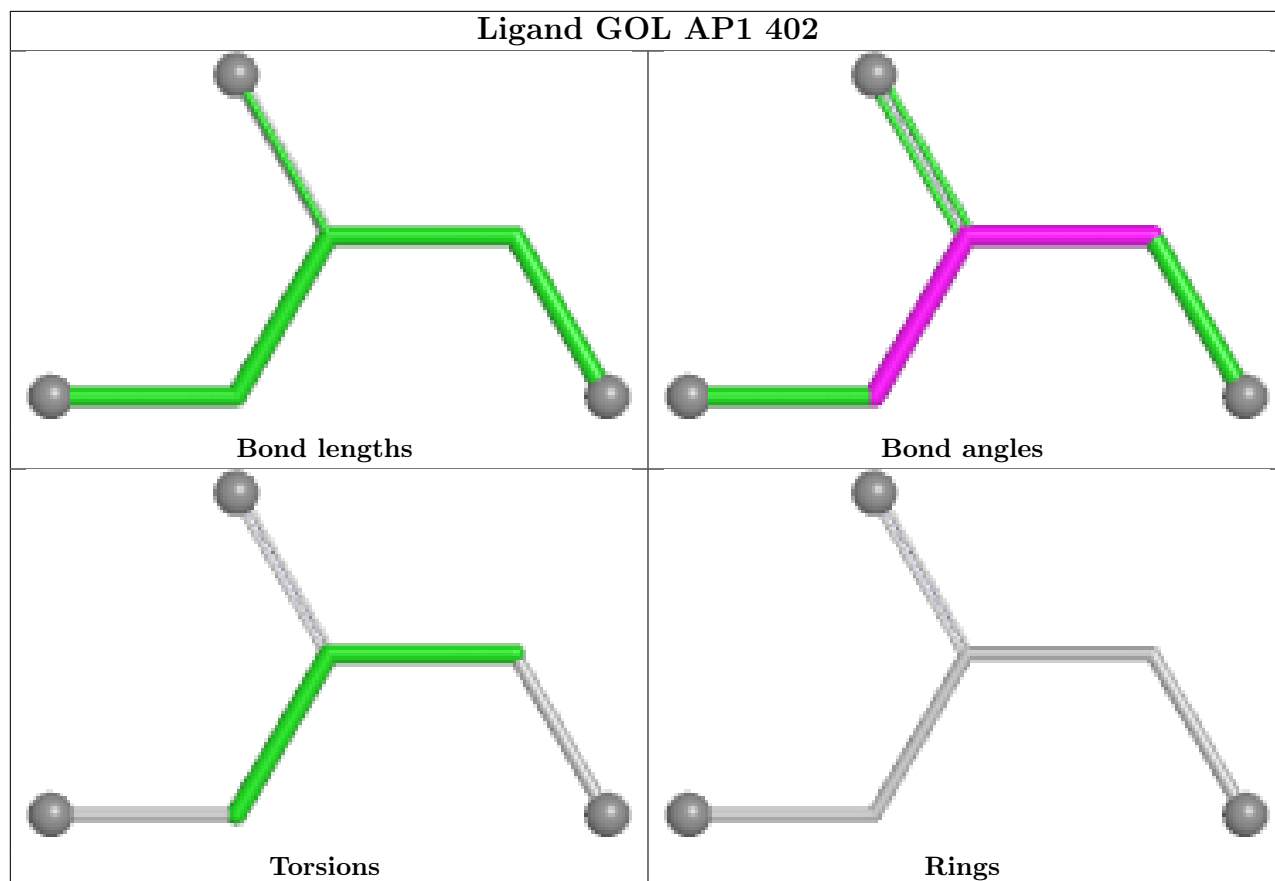


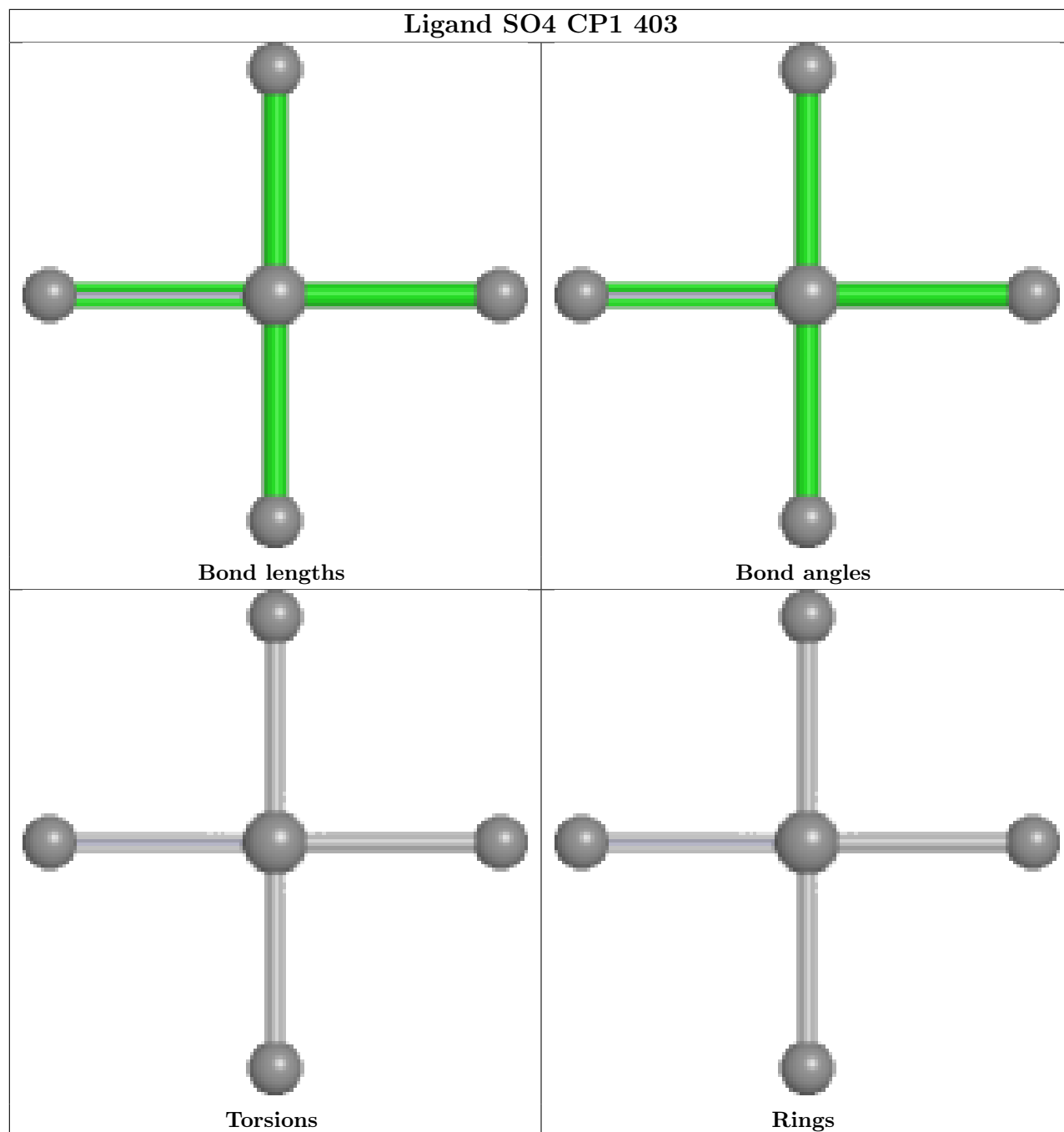


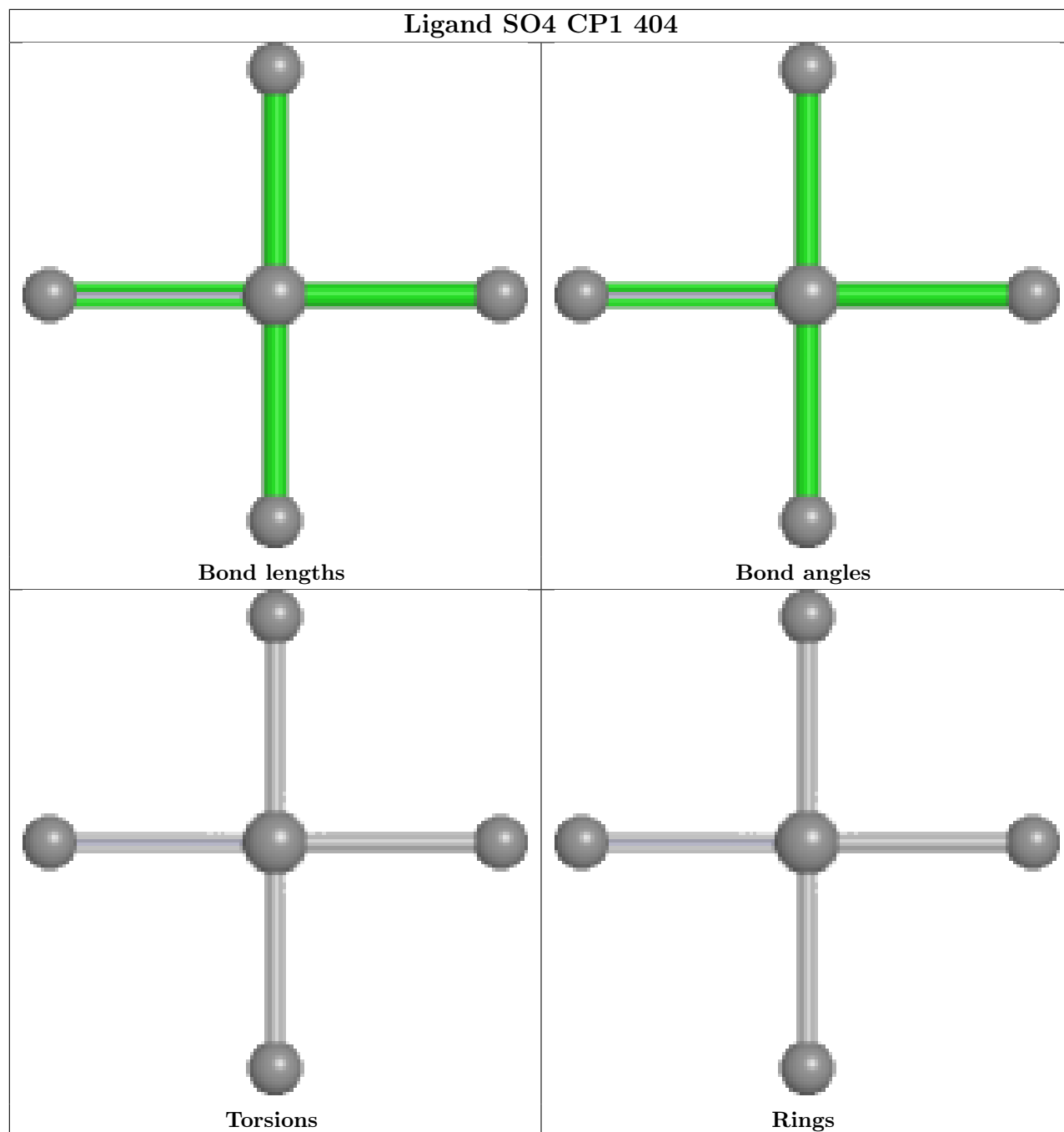


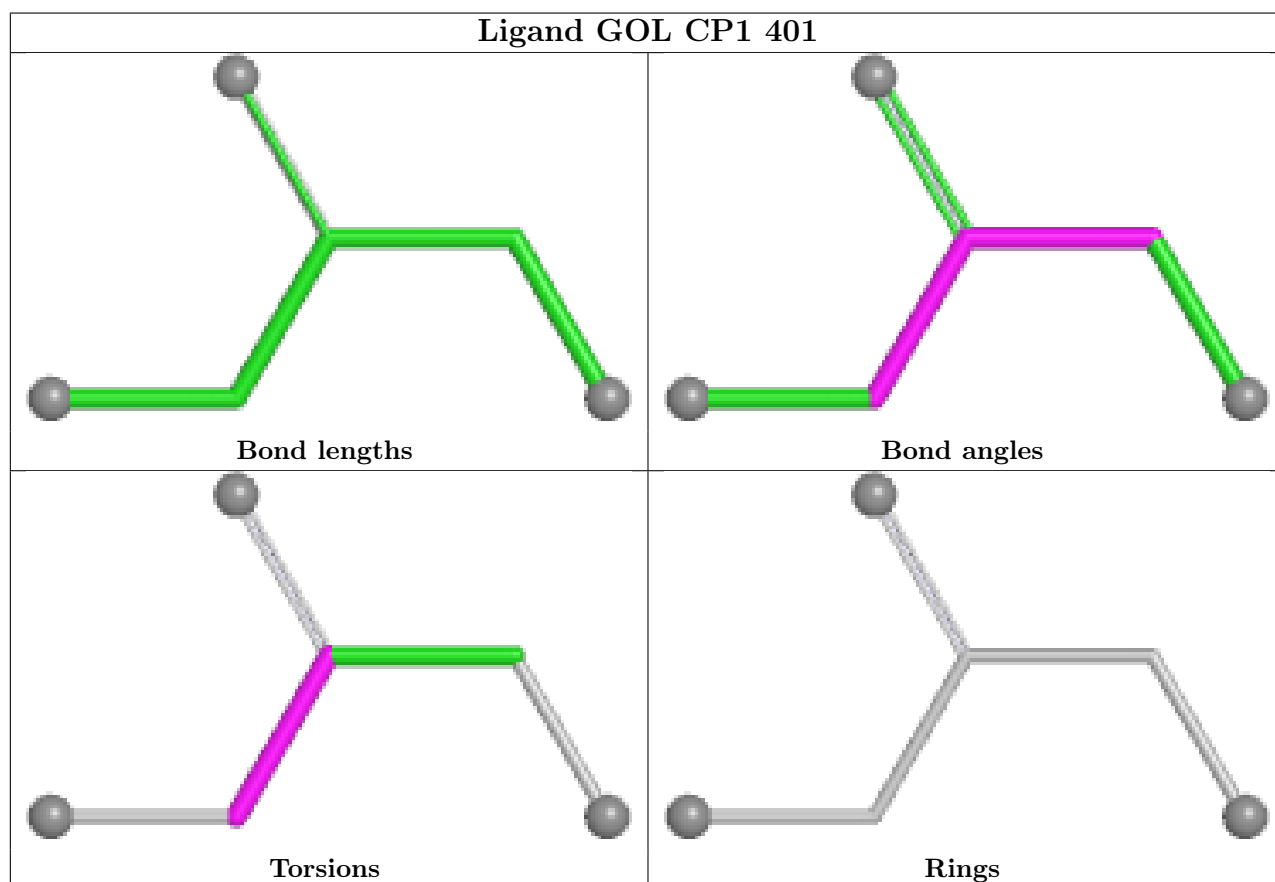
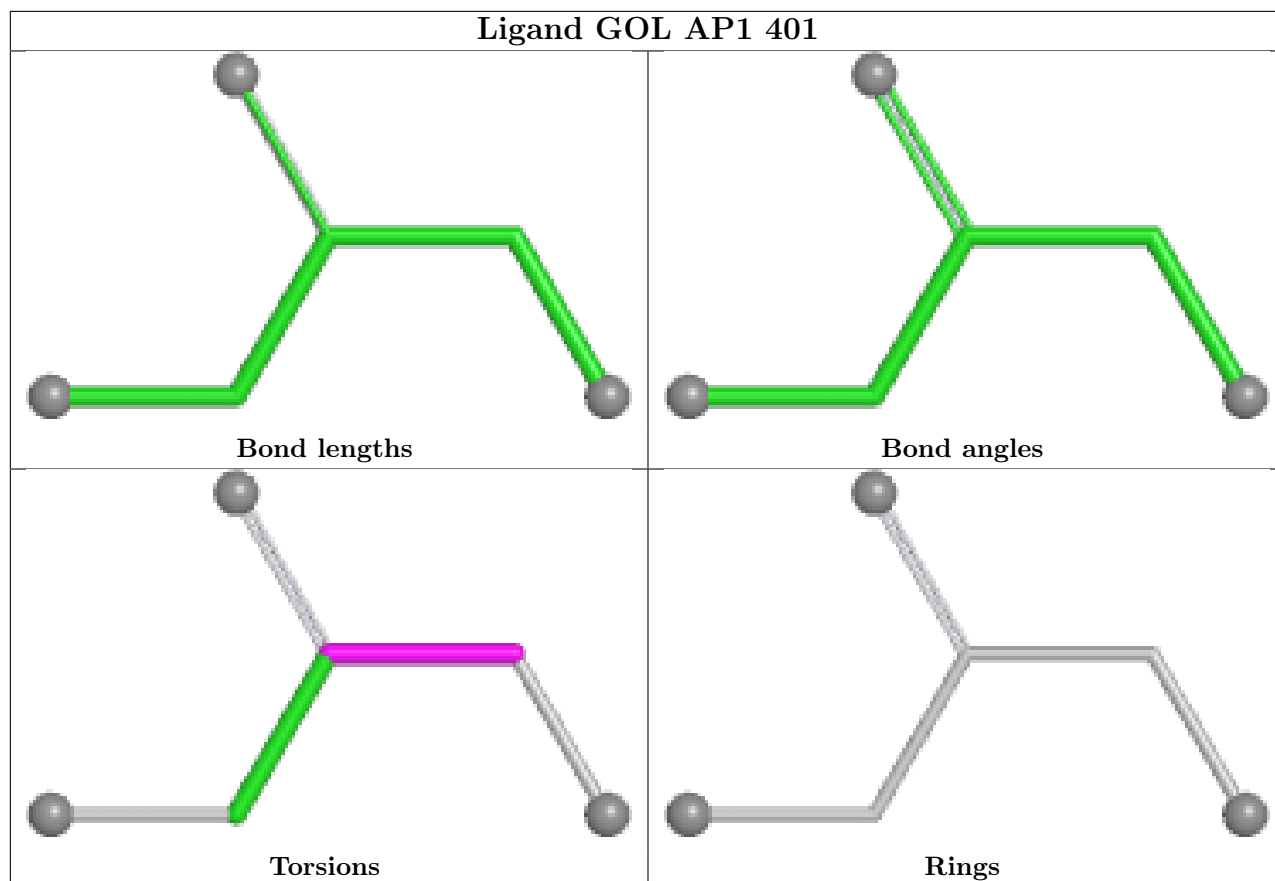


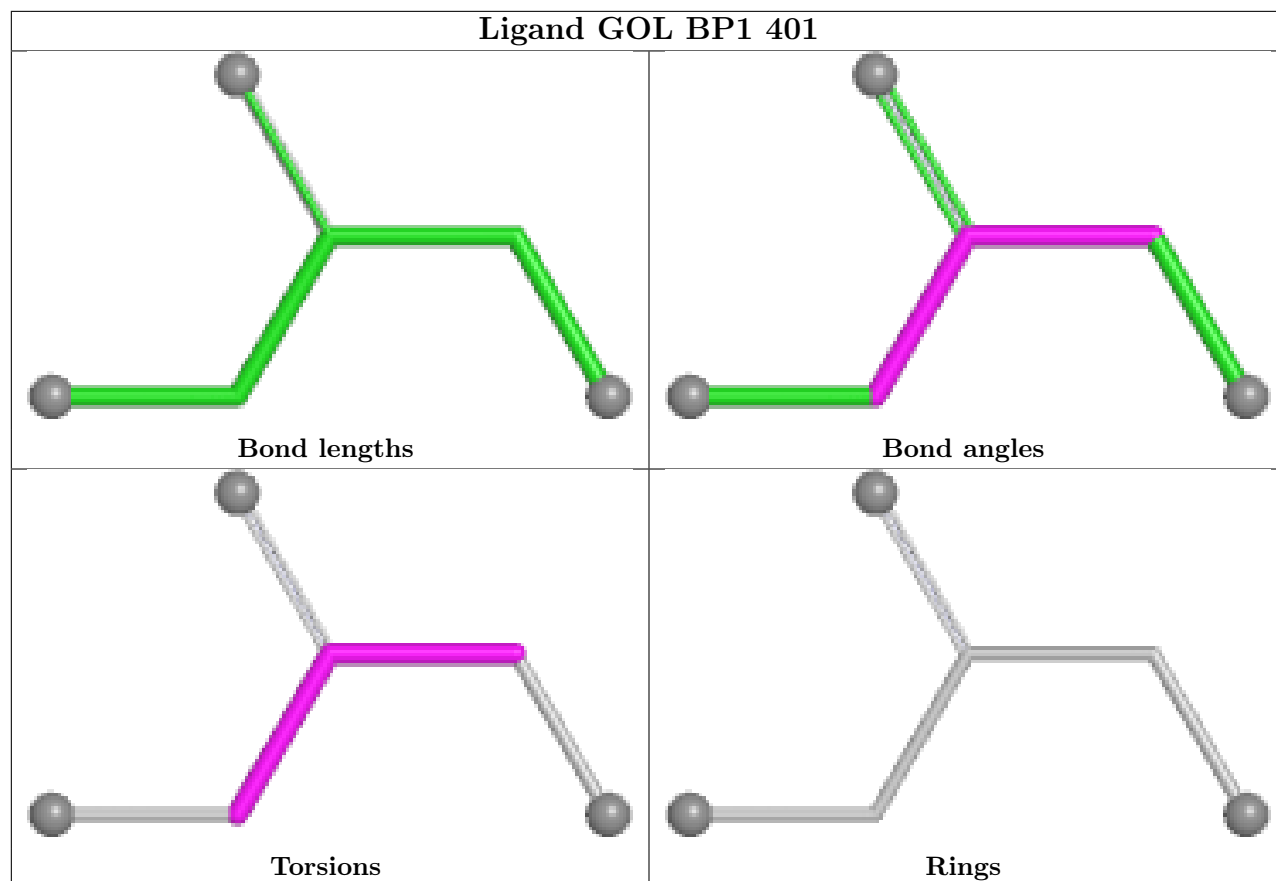


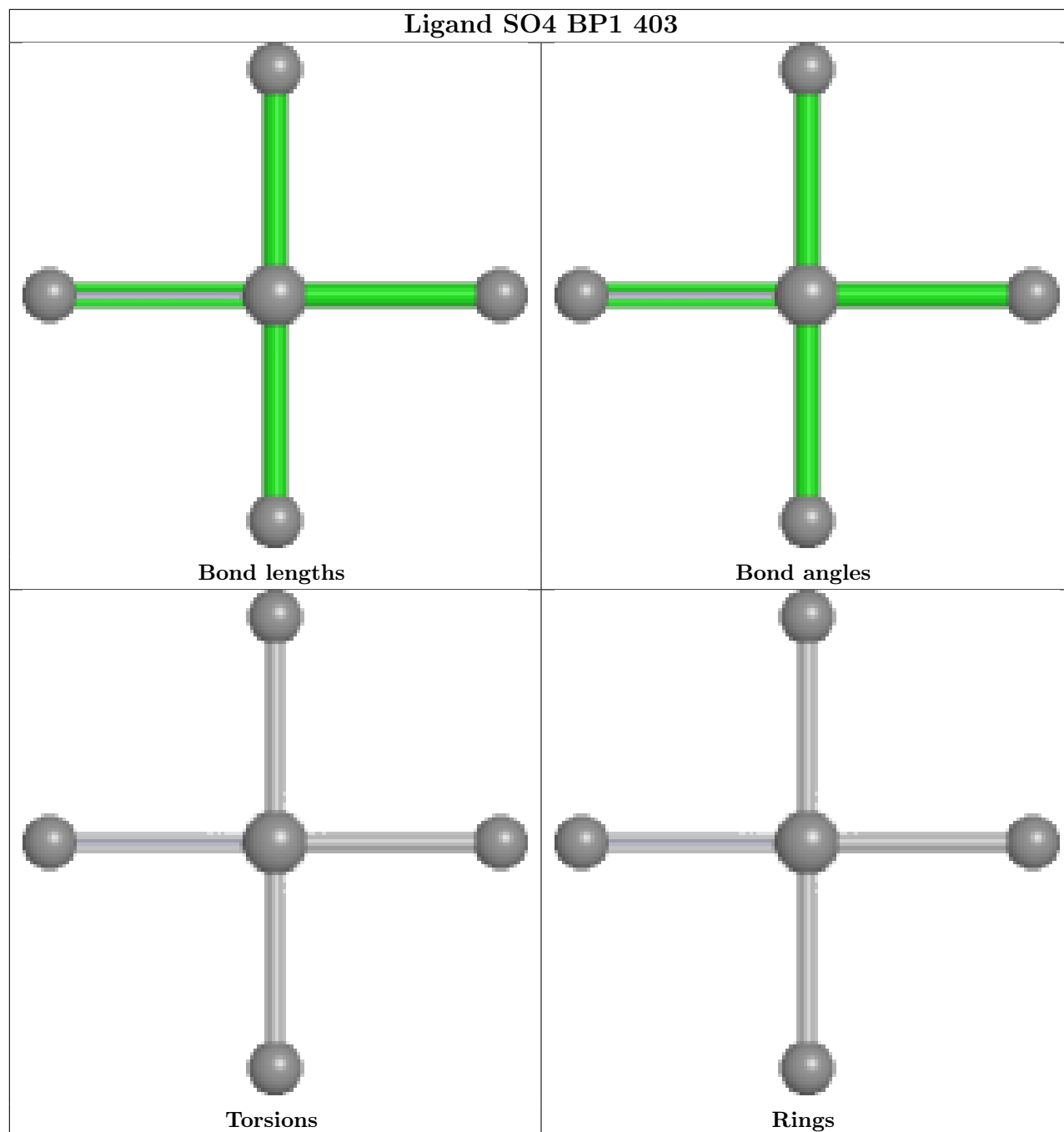


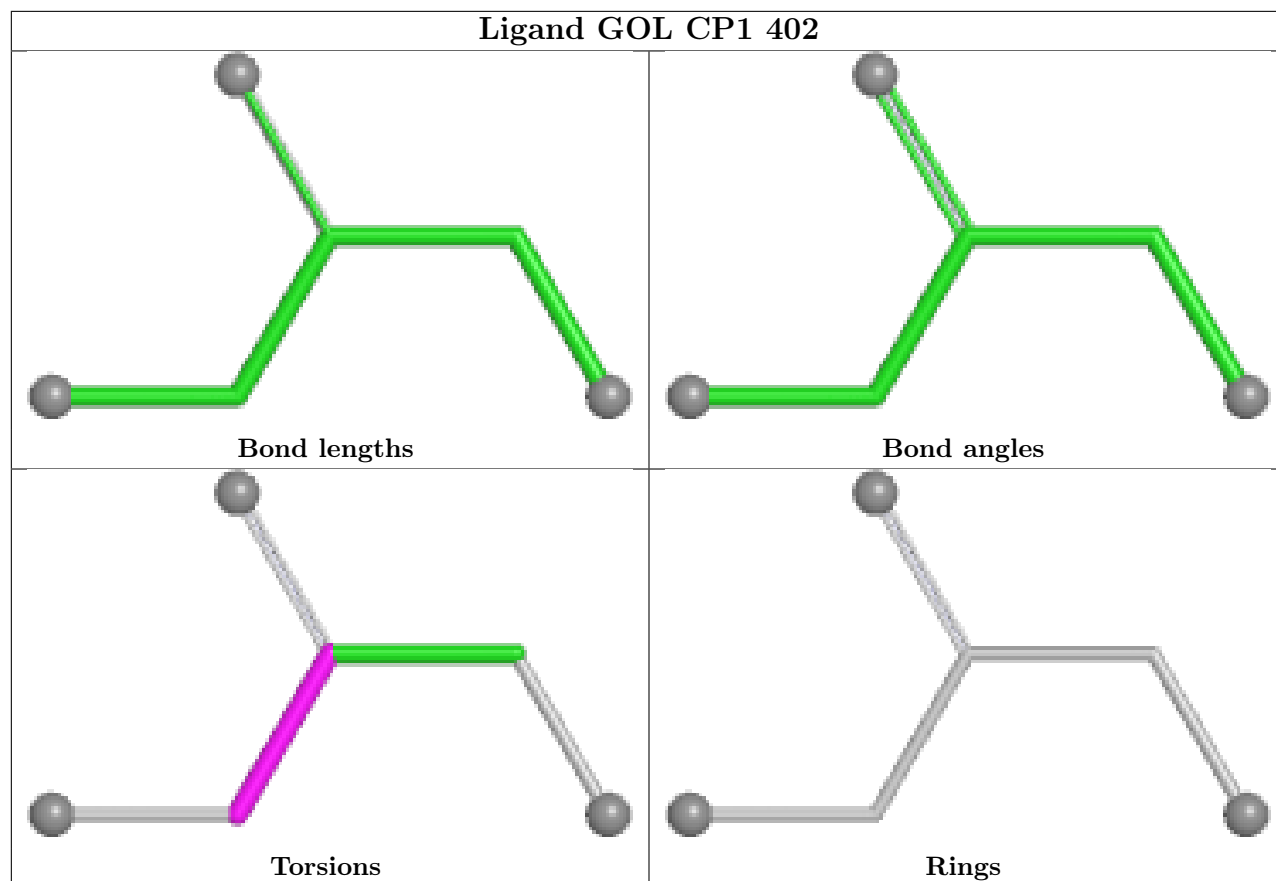












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AP1	305/316 (96%)	0.90	68 (22%) 2 2	27, 50, 129, 154	1 (0%)
1	BP1	305/316 (96%)	0.54	39 (12%) 7 8	25, 49, 97, 122	1 (0%)
1	CP1	305/316 (96%)	0.85	59 (19%) 3 3	27, 57, 120, 153	1 (0%)
All	All	915/948 (96%)	0.77	166 (18%) 3 4	25, 52, 122, 154	3 (0%)

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BP1	306	ILE	8.3
1	CP1	177	LEU	8.0
1	CP1	175	LEU	7.7
1	AP1	104	PRO	7.4
1	AP1	306	ILE	7.4
1	CP1	100	ARG	6.7
1	AP1	177	LEU	6.4
1	CP1	306	ILE	6.2
1	CP1	179	ARG	6.1
1	BP1	101	ALA	6.1
1	BP1	178	SER	5.8
1	AP1	105	ALA	5.8
1	AP1	132	TRP	5.7
1	AP1	252	PRO	5.6
1	AP1	156	LEU	5.5
1	BP1	103	GLN	5.5
1	CP1	101	ALA	5.3
1	AP1	103	GLN	5.2
1	AP1	253	ALA	5.2
1	CP1	176	ALA	5.2
1	AP1	151	ALA	5.2
1	AP1	217	ALA	5.0
1	AP1	155	THR	4.9

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Mol	Chain	Res	Type	RSRZ
1	CP1	140	PRO	4.8
1	AP1	175	LEU	4.7
1	CP1	102	GLU	4.7
1	AP1	115	SER	4.5
1	CP1	174	PRO	4.5
1	CP1	178	SER	4.5
1	AP1	101	ALA	4.5
1	AP1	150	LEU	4.4
1	CP1	155	THR	4.4
1	AP1	254	HIS	4.4
1	AP1	157	LEU	4.3
1	BP1	176	ALA	4.2
1	AP1	176	ALA	4.2
1	AP1	163	ALA	4.1
1	CP1	132	TRP	4.0
1	AP1	129	GLN	4.0
1	CP1	126	VAL	3.9
1	AP1	135	PHE	3.9
1	AP1	178	SER	3.9
1	CP1	302	GLY	3.9
1	CP1	120	LYS	3.9
1	CP1	164	ASP	3.8
1	CP1	151	ALA	3.7
1	BP1	177	LEU	3.7
1	AP1	162	VAL	3.7
1	BP1	132	TRP	3.7
1	BP1	175	LEU	3.7
1	AP1	5	ASP	3.7
1	AP1	153	VAL	3.7
1	AP1	152	ASP	3.6
1	CP1	218	ASP	3.6
1	AP1	107	ASP	3.6
1	CP1	250	LEU	3.5
1	AP1	124	ALA	3.5
1	CP1	105	ALA	3.5
1	AP1	173	ILE	3.4
1	AP1	134	GLY	3.4
1	CP1	104	PRO	3.4
1	BP1	2	SER	3.4
1	AP1	219	GLU	3.3
1	BP1	102	GLU	3.3
1	AP1	158	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	AP1	114	LEU	3.3
1	AP1	130	LEU	3.3
1	AP1	174	PRO	3.2
1	CP1	181	ALA	3.2
1	AP1	216	ALA	3.2
1	CP1	122	THR	3.2
1	BP1	89	ARG	3.1
1	AP1	128	LYS	3.1
1	BP1	125	ASP	3.1
1	AP1	190	TRP	3.1
1	CP1	149	LYS	3.1
1	CP1	103	GLN	3.1
1	CP1	217	ALA	3.1
1	AP1	126	VAL	3.0
1	AP1	102	GLU	3.0
1	AP1	166	VAL	3.0
1	CP1	182	LEU	3.0
1	AP1	106	TRP	3.0
1	CP1	173	ILE	2.9
1	AP1	120	LYS	2.9
1	AP1	131	ILE	2.9
1	BP1	219	GLU	2.9
1	AP1	100	ARG	2.9
1	CP1	180	ALA	2.9
1	CP1	253	ALA	2.9
1	BP1	302	GLY	2.9
1	AP1	2	SER	2.8
1	CP1	117	GLY	2.8
1	CP1	216	ALA	2.8
1	AP1	305	ASN	2.8
1	CP1	118	LEU	2.8
1	BP1	105	ALA	2.8
1	CP1	128	LYS	2.8
1	CP1	69	TRP	2.8
1	AP1	108	GLY	2.7
1	AP1	109	LYS	2.7
1	BP1	5	ASP	2.7
1	CP1	119	ASP	2.7
1	BP1	54	GLU	2.7
1	CP1	183	ARG	2.7
1	BP1	151	ALA	2.7
1	AP1	149	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	CP1	150	LEU	2.7
1	CP1	124	ALA	2.6
1	CP1	249	GLU	2.6
1	BP1	104	PRO	2.6
1	BP1	141	SER	2.6
1	BP1	179	ARG	2.6
1	BP1	121	SER	2.6
1	AP1	160	ALA	2.5
1	BP1	305	ASN	2.5
1	AP1	122	THR	2.5
1	AP1	123	LEU	2.5
1	BP1	69	TRP	2.4
1	CP1	163	ALA	2.4
1	BP1	62	PHE	2.4
1	CP1	305	ASN	2.4
1	CP1	156	LEU	2.4
1	CP1	116	GLU	2.4
1	BP1	100	ARG	2.3
1	CP1	254	HIS	2.3
1	BP1	216	ALA	2.3
1	CP1	89	ARG	2.3
1	AP1	110	TRP	2.3
1	CP1	15	VAL	2.3
1	BP1	140	PRO	2.3
1	CP1	77	ARG	2.3
1	CP1	106	TRP	2.3
1	AP1	121	SER	2.3
1	AP1	188	GLU	2.3
1	AP1	118	LEU	2.2
1	AP1	189	ALA	2.2
1	CP1	148	GLN	2.2
1	AP1	164	ASP	2.2
1	AP1	117	GLY	2.2
1	AP1	180	ALA	2.2
1	BP1	76	GLY	2.2
1	CP1	258	HIS	2.2
1	BP1	180	ALA	2.2
1	BP1	295	SER	2.2
1	AP1	159	GLU	2.2
1	CP1	139	ALA	2.2
1	AP1	154	GLN	2.1
1	CP1	115	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	CP1	123	LEU	2.1
1	BP1	152	ASP	2.1
1	AP1	168	ALA	2.1
1	BP1	120	LYS	2.1
1	CP1	247	PRO	2.1
1	BP1	6	THR	2.1
1	BP1	217	ALA	2.1
1	AP1	116	GLU	2.1
1	CP1	170	GLU	2.1
1	BP1	77	ARG	2.1
1	CP1	141	SER	2.0
1	AP1	165	ASN	2.0
1	BP1	85	ASP	2.0
1	BP1	157	LEU	2.0
1	CP1	5	ASP	2.0
1	AP1	167	ILE	2.0
1	BP1	126	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

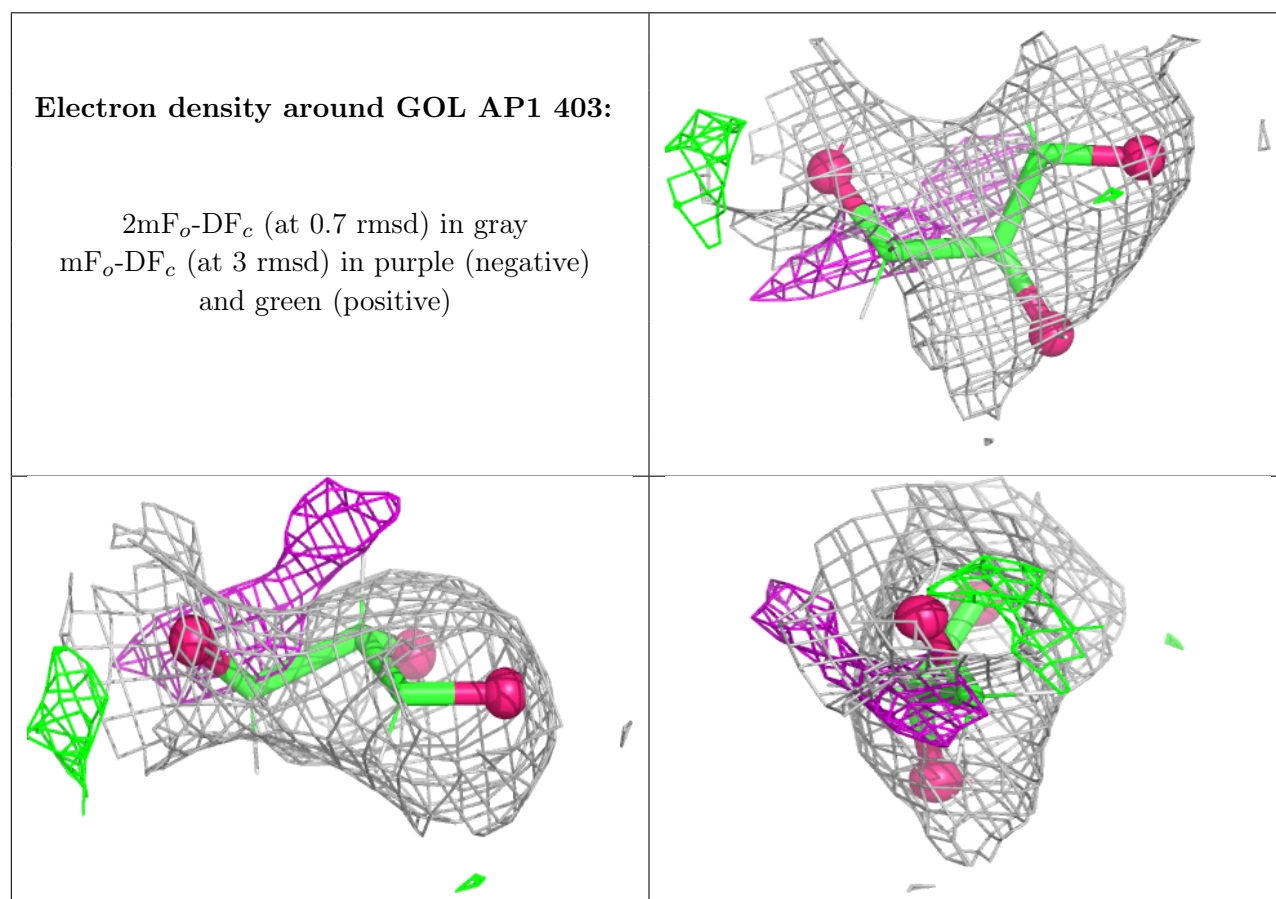
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	AP1	403	6/6	0.84	0.18	54,71,99,99	0
3	SO4	BP1	403	5/5	0.85	0.15	70,82,112,125	0
2	GOL	AP1	401	6/6	0.89	0.13	43,48,52,53	0
2	GOL	AP1	402	6/6	0.90	0.13	44,57,83,83	0
3	SO4	BP1	404	5/5	0.90	0.10	71,80,110,121	0
2	GOL	BP1	401	6/6	0.91	0.14	35,46,52,66	0

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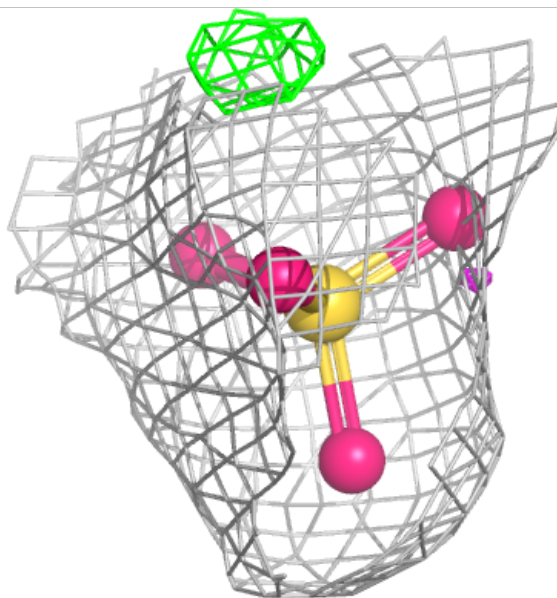
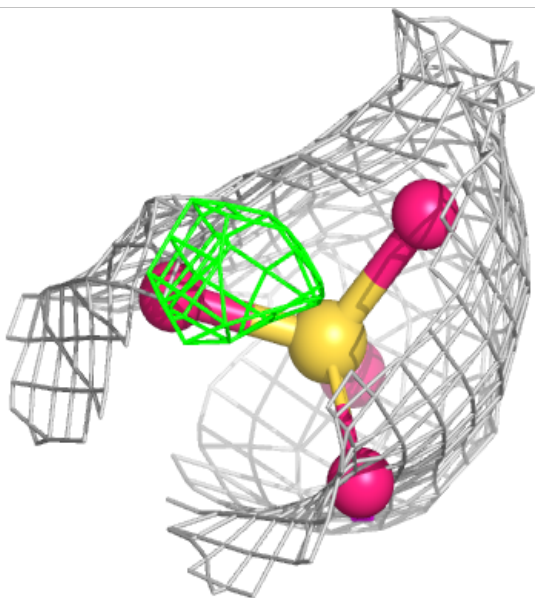
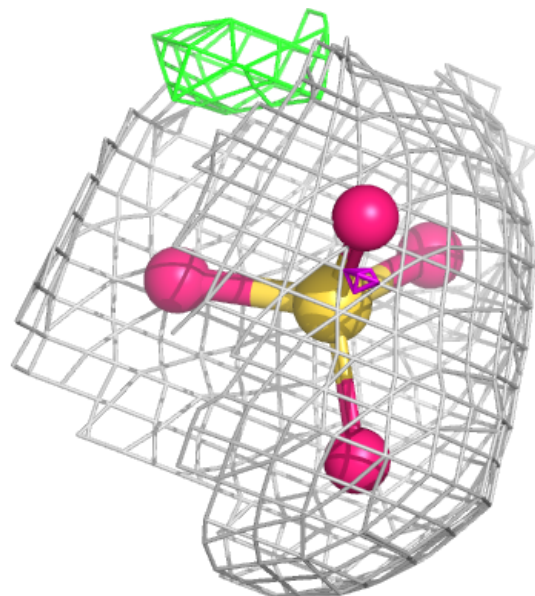
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	AP1	406	5/5	0.91	0.10	61,81,94,127	0
3	SO4	CP1	403	5/5	0.91	0.11	66,78,106,109	0
3	SO4	AP1	405	5/5	0.92	0.10	47,48,93,95	0
2	GOL	CP1	401	6/6	0.94	0.10	41,46,51,56	0
2	GOL	BP1	402	6/6	0.94	0.10	46,51,56,62	0
2	GOL	CP1	402	6/6	0.95	0.10	35,41,47,51	0
3	SO4	AP1	404	5/5	0.97	0.08	54,57,66,70	0
3	SO4	CP1	404	5/5	0.97	0.08	35,42,70,72	0

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



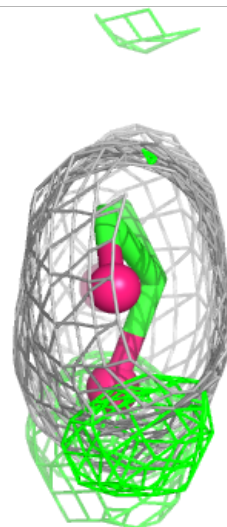
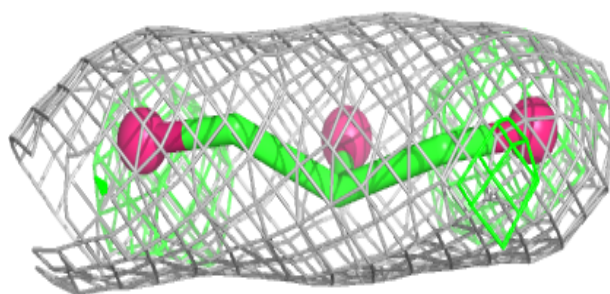
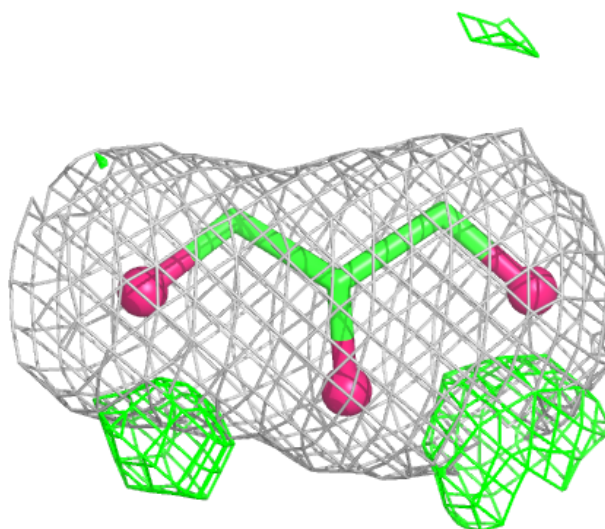
Electron density around SO4 BP1 403:

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



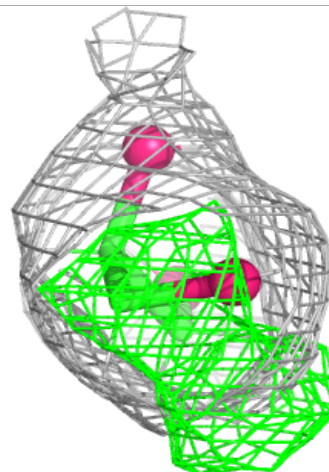
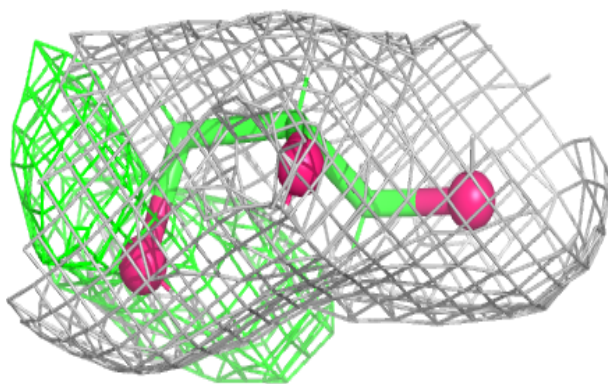
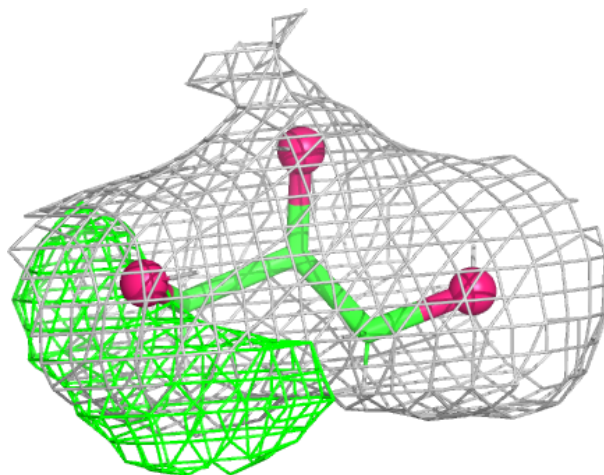
Electron density around GOL AP1 401:

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



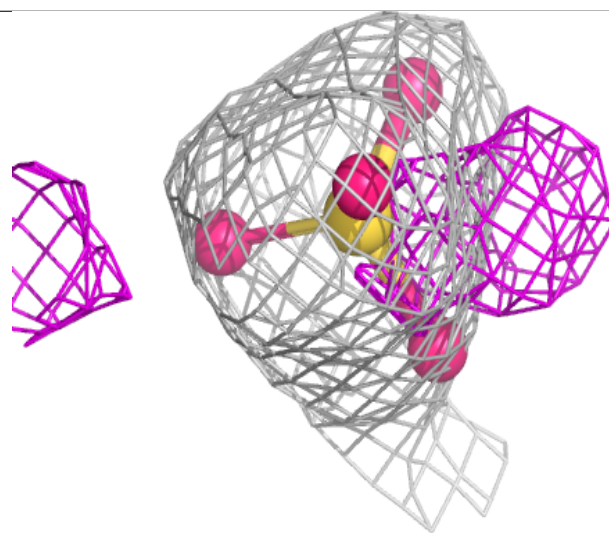
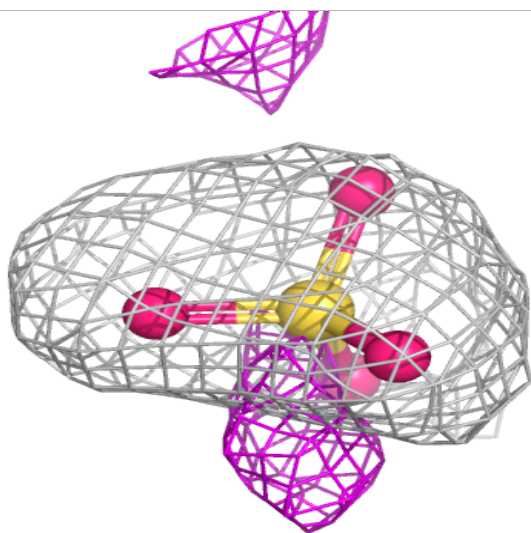
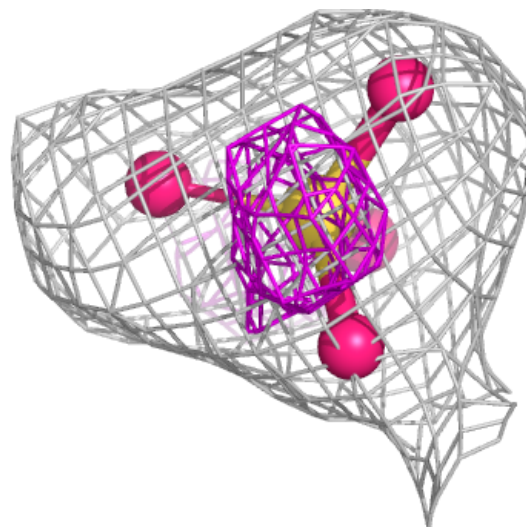
Electron density around GOL AP1 402:

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



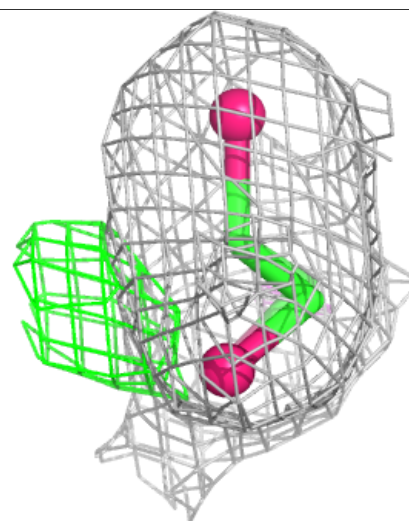
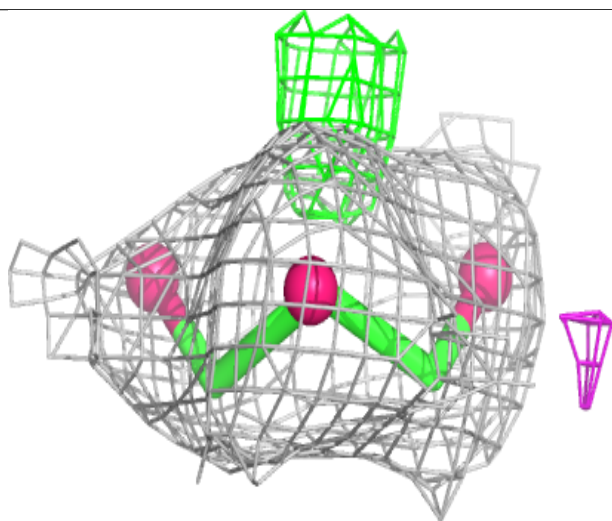
Electron density around SO4 BP1 404:

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



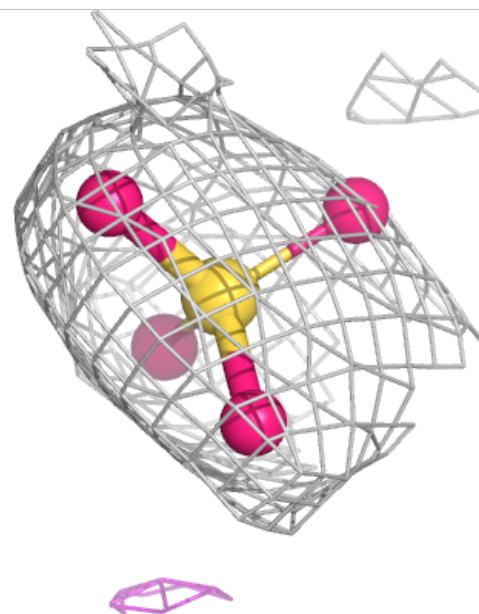
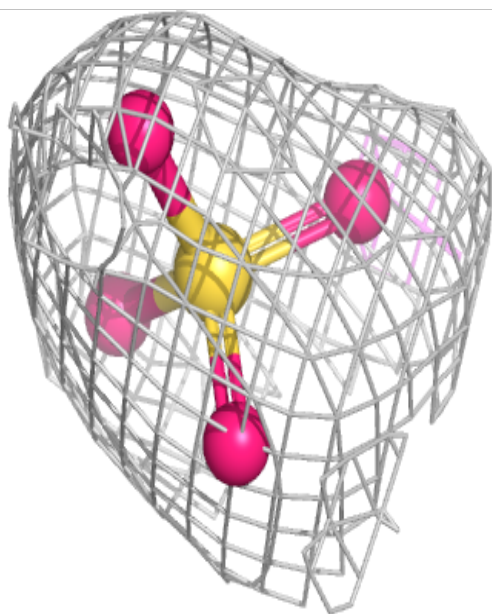
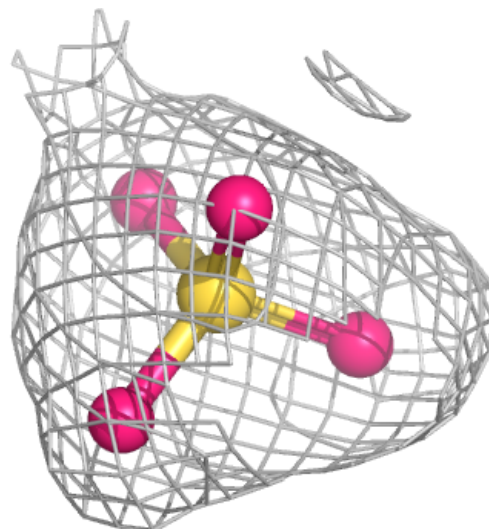
Electron density around GOL BP1 401:

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



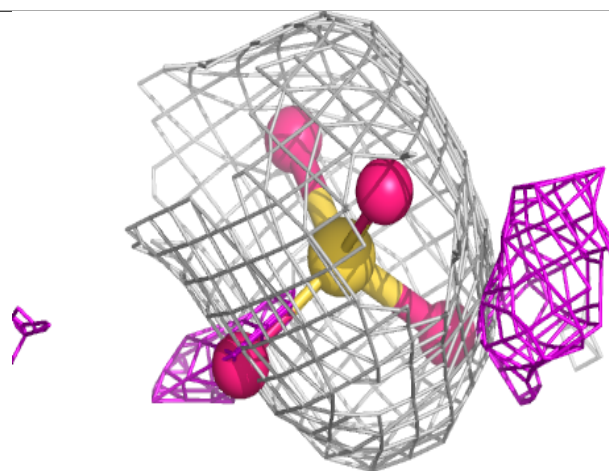
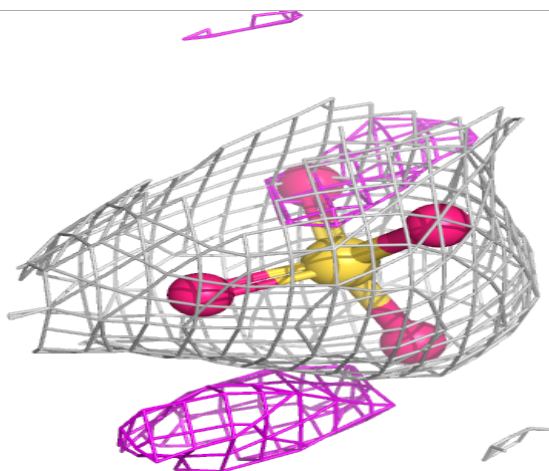
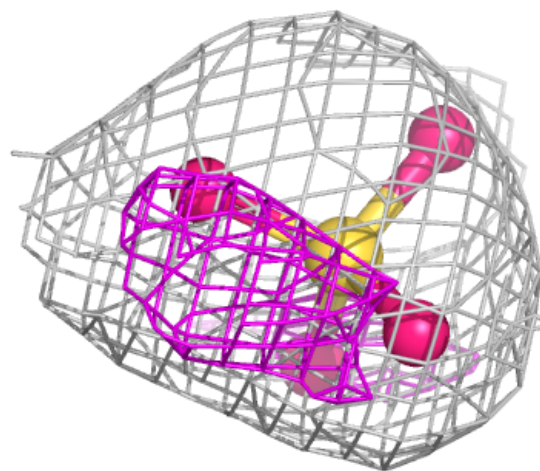
Electron density around SO4 AP1 406:

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



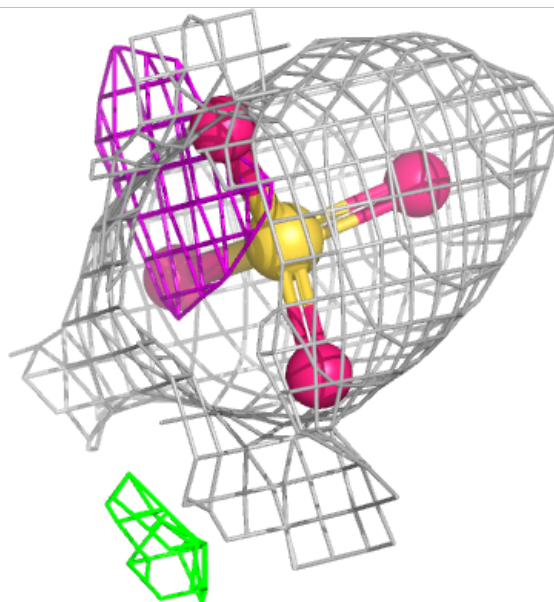
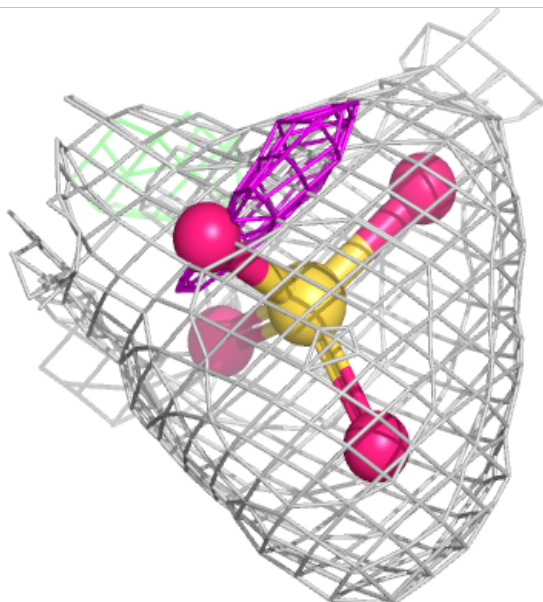
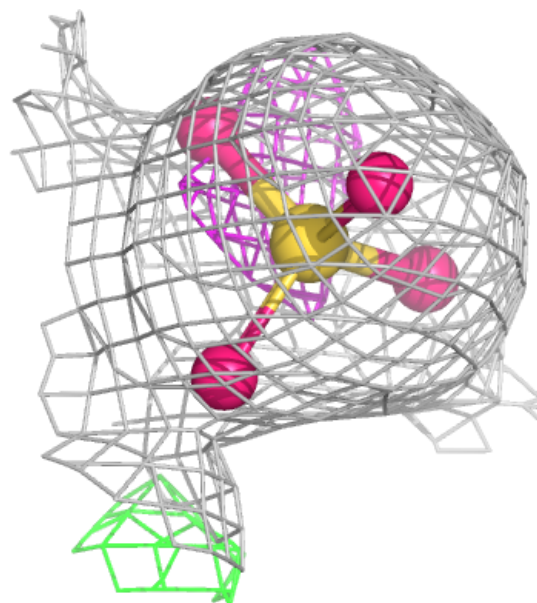
Electron density around SO4 CP1 403:

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



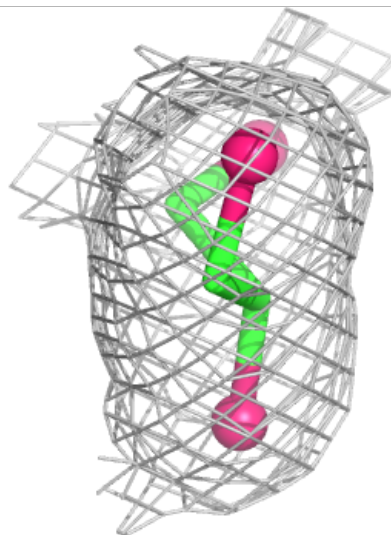
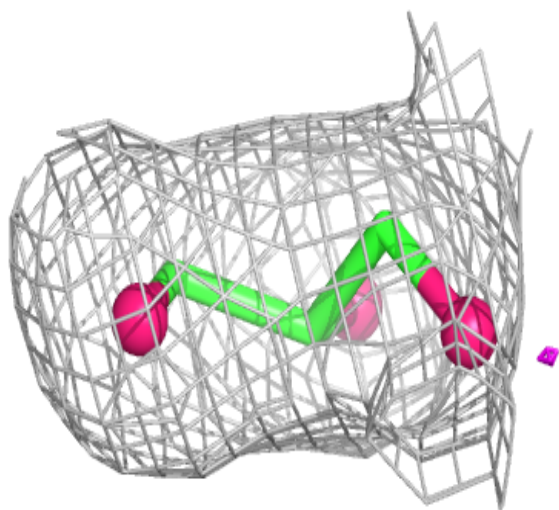
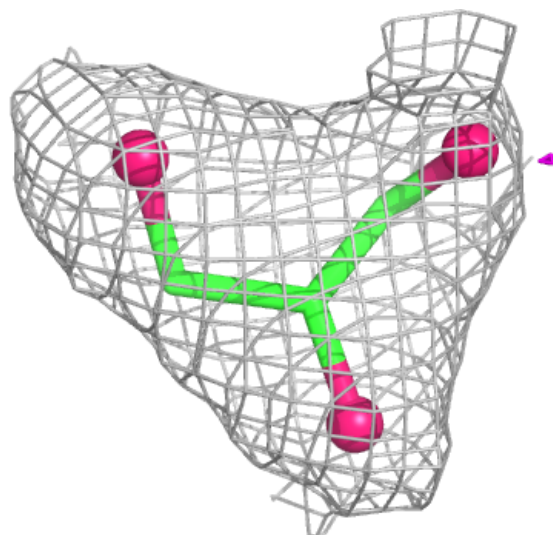
Electron density around SO4 AP1 405:

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



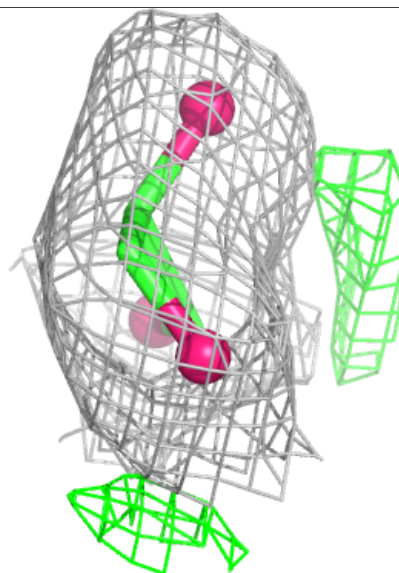
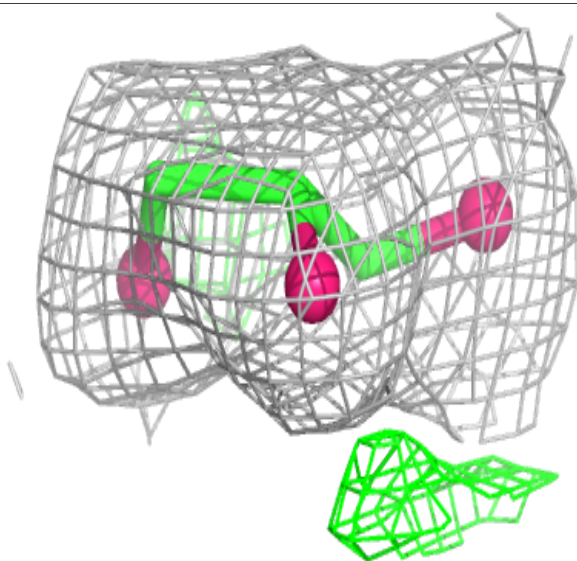
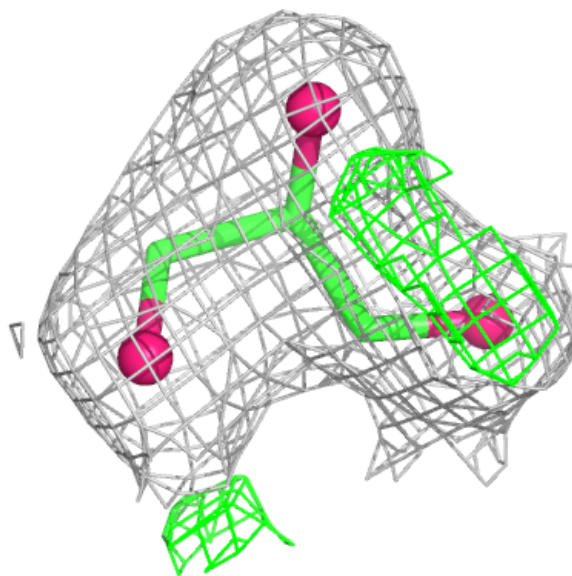
Electron density around GOL CP1 401:

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



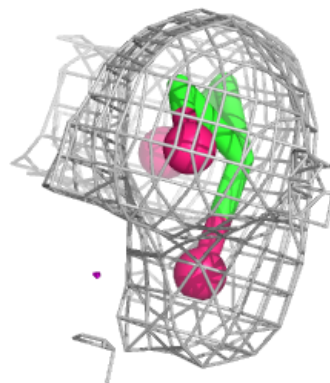
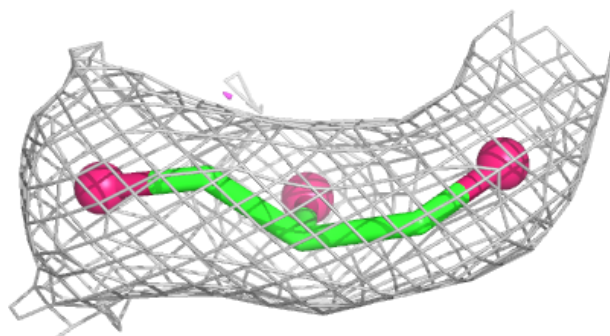
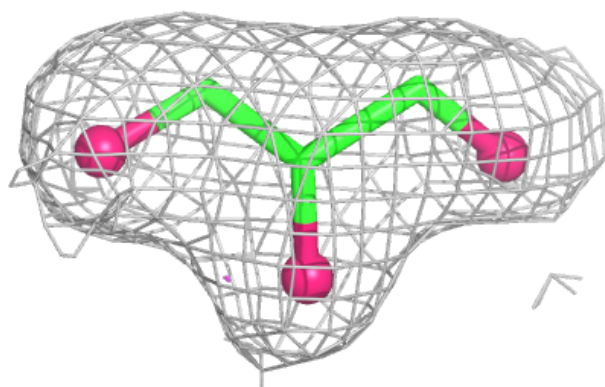
Electron density around GOL BP1 402:

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



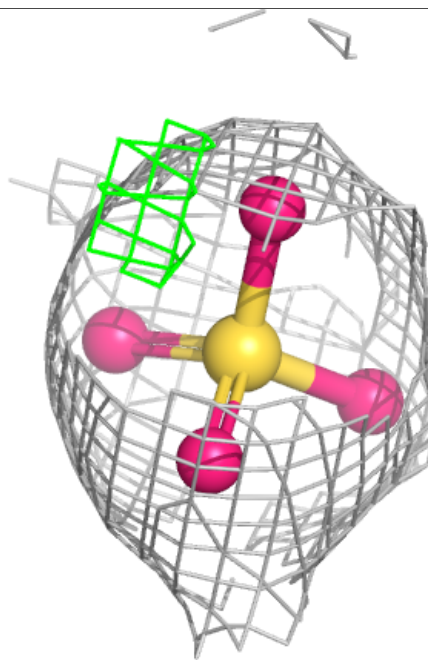
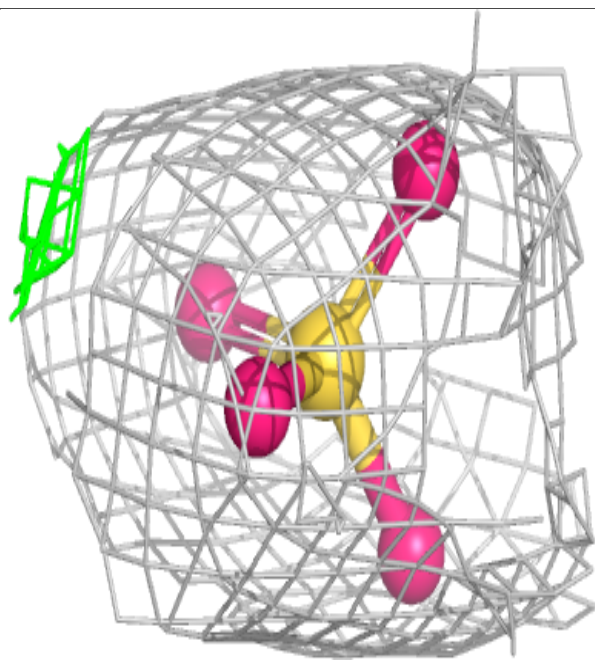
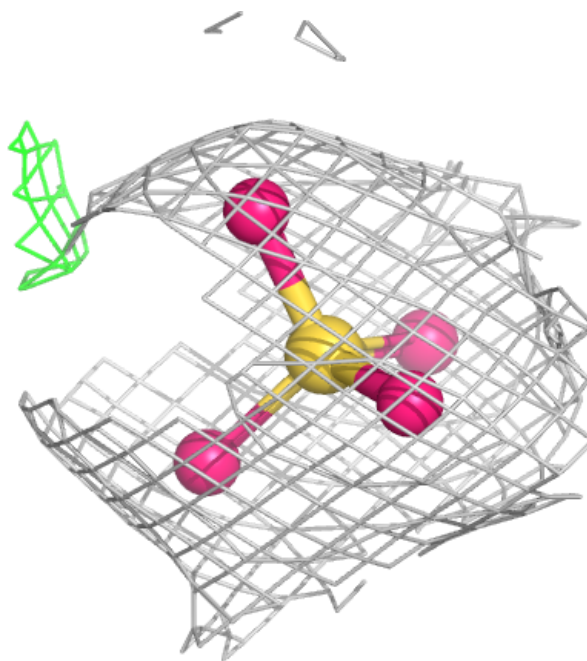
Electron density around GOL CP1 402:

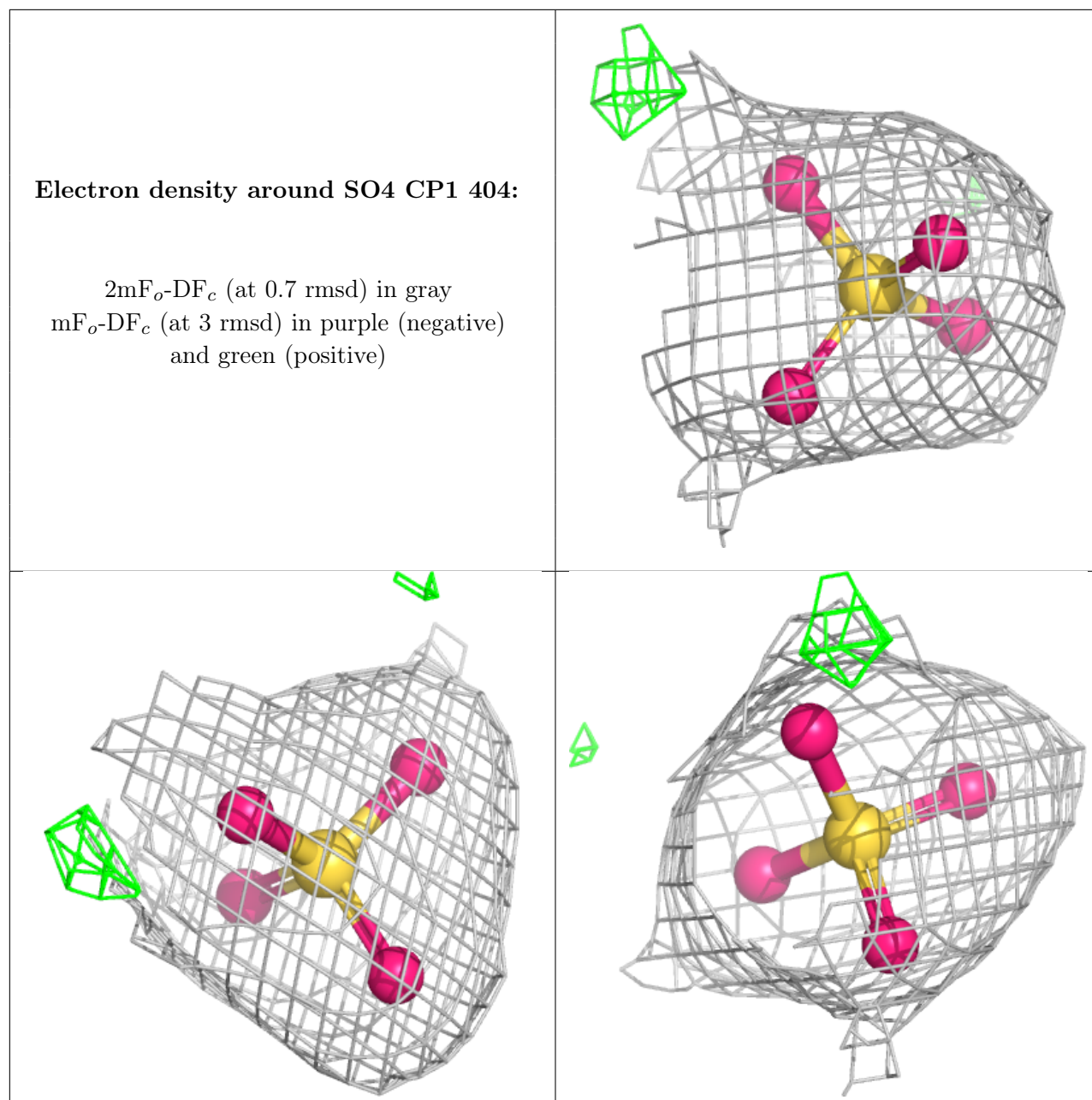
$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)



Electron density around SO4 AP1 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.