



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2023 – 04:11 PM EDT

PDB ID : 8FTM
Title : Setx-ssRNA-ADP-SO4 complex
Authors : Williams, R.S.; Appel, C.D.
Deposited on : 2023-01-12
Resolution : 3.01 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

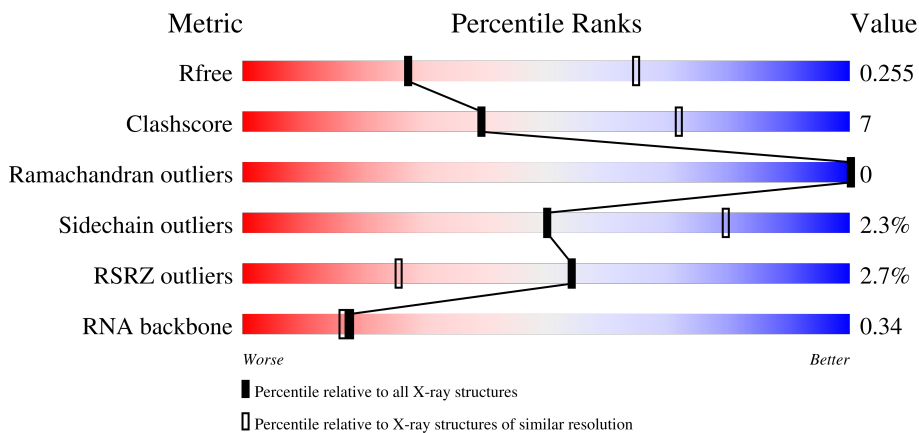
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)
RNA backbone	3102	1066 (3.30-2.74)

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	793	 4% 71% 18% 10%
1	B	793	 % 74% 18% 8%
2	C	15	 40% 27% 13% 20%
2	D	15	 13% 40% 13% 33%

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
4	SO4	B	2006	-	-	X	-

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 11842 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 5'-3' RNA helicase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	714	5628	3562	985	1050	31	0	0	1
1	B	731	5766	3638	1013	1084	31	0	0	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1086	SER	-	expression tag	UNP G0S163
B	1086	SER	-	expression tag	UNP G0S163

- Molecule 2 is a RNA chain called RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3').

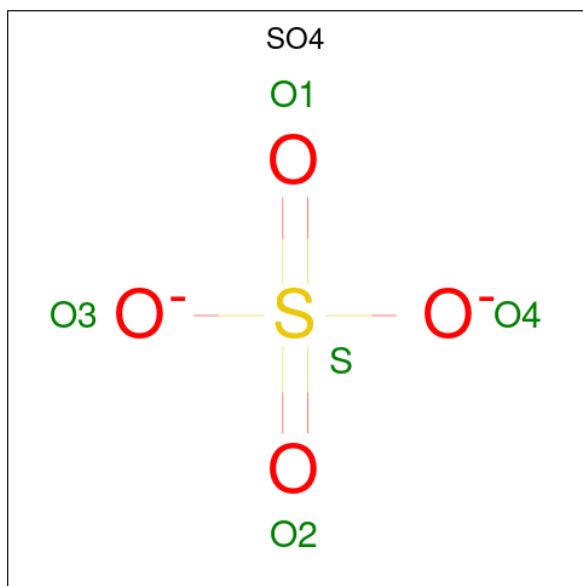
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	12	205	90	20	84	11	0	0	1
2	D	10	165	72	16	68	9	0	0	1

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
3	A	1	27	10	5	10	2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

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

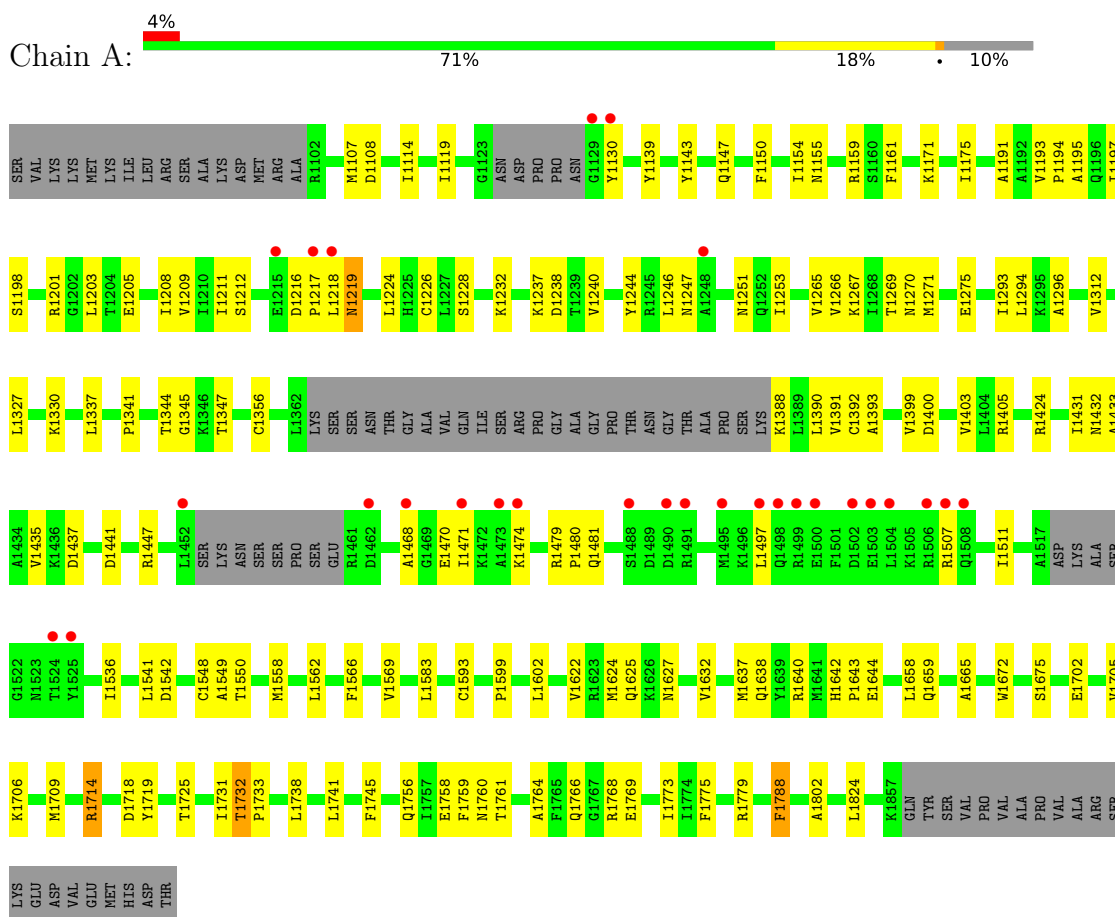
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total O 3 3	0	0
5	B	3	Total O 3 3	0	0

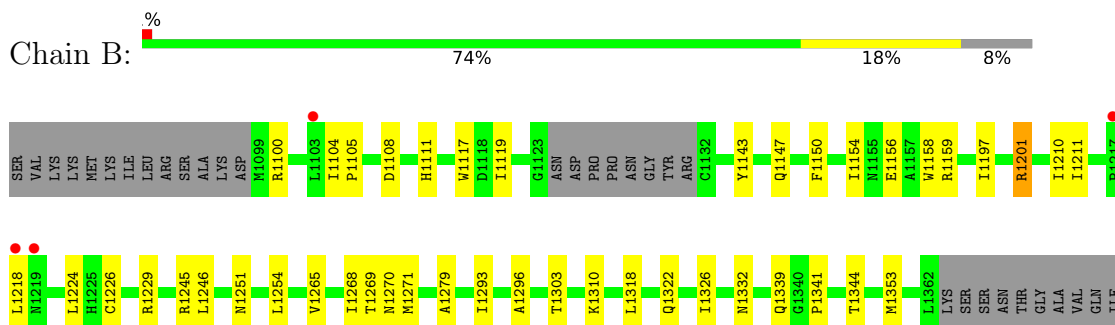
3 Residue-property plots [i](#)

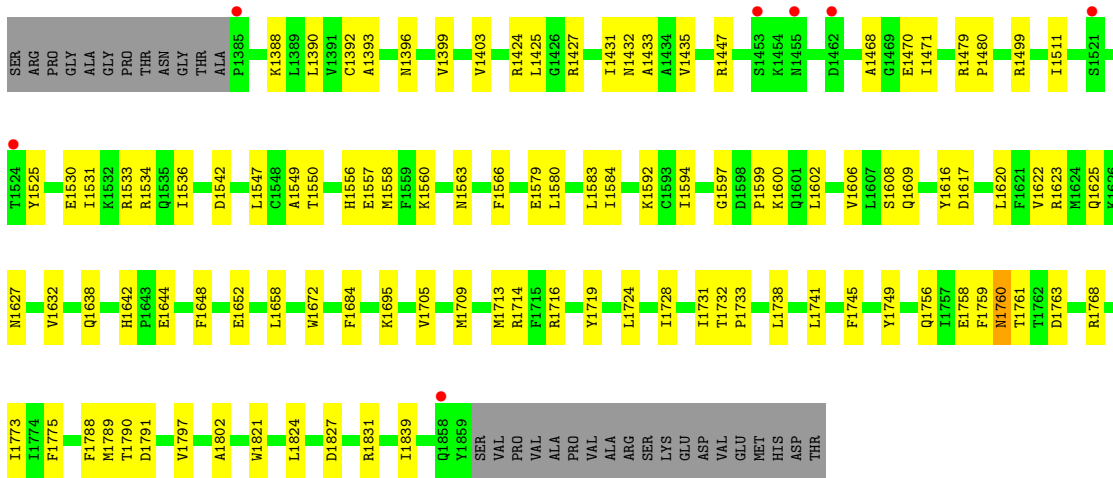
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 5'-3' RNA helicase-like protein



- Molecule 1: 5'-3' RNA helicase-like protein

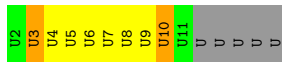
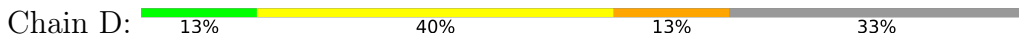




• Molecule 2: RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



• Molecule 2: RNA (5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.70Å 107.32Å 162.03Å 90.00° 99.64° 90.00°	Depositor
Resolution (Å)	44.54 – 3.01 44.54 – 3.01	Depositor EDS
% Data completeness (in resolution range)	98.3 (44.54-3.01) 98.3 (44.54-3.01)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.212 , 0.251 0.215 , 0.255	Depositor DCC
R_{free} test set	1999 reflections (5.33%)	wwPDB-VP
Wilson B-factor (Å ²)	70.7	Xtrriage
Anisotropy	0.461	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11842	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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: ADP, SO4

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	0.24	0/5725	0.48	0/7727
1	B	0.25	0/5866	0.48	0/7915
2	C	0.14	0/224	0.74	0/346
2	D	0.18	0/180	0.78	0/278
All	All	0.24	0/11995	0.50	0/16266

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	5628	0	5681	87	0
1	B	5766	0	5841	85	0
2	C	205	0	100	5	0
2	D	165	0	80	7	0
3	A	27	0	12	1	0
4	A	15	0	0	0	0
4	B	30	0	0	2	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
All	All	11842	0	11714	173	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 7.

All (173) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1725:THR:HB	1:B:1499:ARG:HH22	1.48	0.78
1:B:1159:ARG:HG3	1:B:1608:SER:HA	1.66	0.76
1:A:1400:ASP:OD1	1:A:1424:ARG:NH1	2.18	0.76
1:A:1218:LEU:HD11	1:A:1266:VAL:HG21	1.71	0.71
1:B:1332:ASN:O	1:B:1592:LYS:NZ	2.22	0.71
1:B:1424:ARG:NH1	1:B:1425:LEU:O	2.23	0.71
1:B:1602:LEU:HG	1:B:1797:VAL:HG21	1.74	0.70
1:B:1716:ARG:HE	1:B:1724:LEU:HD12	1.58	0.68
1:B:1556:HIS:HE2	2:D:10:U:H2'	1.59	0.67
1:A:1198:SER:HA	1:A:1203:LEU:HD13	1.81	0.62
1:B:1763:ASP:OD2	2:D:5:U:O2'	2.18	0.62
1:B:1197:ILE:HG23	1:B:1201:ARG:HH21	1.64	0.62
1:A:1638:GLN:HB3	1:A:1658:LEU:HD11	1.83	0.61
1:B:1251:ASN:HB3	1:B:1254:LEU:HG	1.83	0.61
1:A:1175:ILE:HG22	1:A:1193:VAL:HG22	1.83	0.60
1:B:1579:GLU:HG3	1:B:1620:LEU:HB2	1.82	0.60
1:A:1468:ALA:HB2	1:A:1511:ILE:HG21	1.84	0.60
1:A:1209:VAL:HG12	1:A:1267:LYS:HA	1.84	0.59
1:A:1171:LYS:HB2	1:A:1201:ARG:HH21	1.67	0.59
1:B:1104:ILE:HD11	1:B:1560:LYS:HD3	1.83	0.59
1:A:1388:LYS:NZ	1:A:1541:LEU:O	2.34	0.59
1:B:1218:LEU:HD21	1:B:1268:ILE:HD11	1.83	0.58
1:B:1684:PHE:HB3	1:B:1839:ILE:HD13	1.85	0.58
1:A:1733:PRO:HD3	1:A:1775:PHE:HE1	1.68	0.58
1:A:1247:ASN:O	1:A:1251:ASN:ND2	2.37	0.57
1:B:1100:ARG:NH2	1:B:1563:ASN:OD1	2.32	0.57
1:A:1330:LYS:HD2	1:A:1356:CYS:SG	2.45	0.57
1:A:1599:PRO:HB3	1:A:1622:VAL:HG22	1.87	0.56
1:B:1600:LYS:NZ	4:B:2006:SO4:S	2.78	0.56
1:B:1105:PRO:HG2	1:B:1279:ALA:HA	1.87	0.56
1:B:1425:LEU:HD11	1:B:1547:LEU:HD23	1.87	0.56
1:B:1296:ALA:HB3	1:B:1627:ASN:HD22	1.70	0.56
1:B:1713:MET:SD	1:B:1749:TYR:OH	2.58	0.55
1:A:1471:ILE:HD13	1:A:1507:ARG:HB3	1.89	0.55
1:B:1758:GLU:OE1	1:B:1768:ARG:NH2	2.33	0.55
1:A:1672:TRP:HA	1:A:1719:TYR:CZ	2.42	0.54
1:A:1470:GLU:HG2	1:A:1474:LYS:HE2	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1789:MET:HG3	1:B:1821:TRP:HE1	1.72	0.54
1:A:1731:ILE:HA	1:A:1760:ASN:O	2.07	0.54
1:A:1345:GLY:HA2	3:A:2001:ADP:H5'1	1.90	0.53
2:D:6:U:H2'	2:D:7:U:C6	2.43	0.53
1:B:1119:ILE:HD13	1:B:1210:ILE:HD12	1.90	0.53
1:B:1625:GLN:HG3	1:B:1632:VAL:HG21	1.91	0.53
1:A:1764:ALA:HB2	2:C:6:U:H5''	1.91	0.53
1:A:1643:PRO:HG2	1:A:1665:ALA:HB2	1.90	0.52
1:A:1441:ASP:OD2	2:C:10:U:N3	2.42	0.52
1:B:1579:GLU:OE2	1:B:1623:ARG:NH2	2.38	0.52
1:A:1107:MET:HE2	1:A:1275:GLU:HG2	1.92	0.52
1:A:1205:GLU:HG2	1:A:1232:LYS:HA	1.92	0.52
1:A:1431:ILE:HG23	1:A:1435:VAL:HG23	1.92	0.51
1:A:1388:LYS:HZ1	1:A:1542:ASP:HA	1.76	0.51
1:B:1638:GLN:HB3	1:B:1658:LEU:HD11	1.93	0.51
1:B:1731:ILE:HA	1:B:1760:ASN:O	2.10	0.51
1:B:1602:LEU:HD11	1:B:1763:ASP:HA	1.92	0.50
1:B:1211:ILE:HD13	1:B:1265:VAL:HG22	1.93	0.50
1:A:1625:GLN:HG3	1:A:1632:VAL:HG21	1.93	0.50
1:A:1270:ASN:OD1	1:A:1271:MET:N	2.45	0.50
1:B:1724:LEU:HD13	1:B:1728:ILE:HD11	1.93	0.50
1:A:1779:ARG:NH2	2:C:2:U:O4	2.45	0.50
1:B:1773:ILE:HB	1:B:1802:ALA:HB2	1.94	0.50
1:A:1296:ALA:HB3	1:A:1627:ASN:HD22	1.76	0.49
1:B:1530:GLU:O	1:B:1533:ARG:HB3	2.12	0.49
1:A:1208:ILE:HD11	1:A:1271:MET:SD	2.52	0.49
1:A:1219:ASN:OD1	1:A:1219:ASN:N	2.44	0.49
1:B:1556:HIS:ND1	1:B:1558:MET:HG3	2.27	0.49
1:B:1392:CYS:HA	1:B:1549:ALA:O	2.11	0.49
1:B:1672:TRP:HA	1:B:1719:TYR:CZ	2.48	0.49
1:A:1191:ALA:HB3	1:A:1244:TYR:HE1	1.79	0.48
1:A:1758:GLU:OE1	1:A:1768:ARG:NH2	2.46	0.48
1:A:1195:ALA:HA	1:A:1240:VAL:HG23	1.94	0.48
1:B:1827:ASP:OD2	1:B:1831:ARG:NH2	2.44	0.48
1:B:1269:THR:OG1	1:B:1270:ASN:N	2.45	0.47
1:B:1531:ILE:HG13	1:B:1534:ARG:HH21	1.80	0.47
1:A:1269:THR:OG1	1:A:1270:ASN:N	2.46	0.47
1:A:1738:LEU:HD11	1:A:1759:PHE:HB3	1.96	0.47
1:B:1390:LEU:HD22	1:B:1566:PHE:CD2	2.50	0.47
1:A:1481:GLN:HB3	1:A:1497:LEU:HD13	1.96	0.47
1:A:1642:HIS:CE1	1:A:1644:GLU:HG3	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1270:ASN:OD1	1:B:1271:MET:N	2.47	0.47
1:B:1468:ALA:HB2	1:B:1511:ILE:HG21	1.95	0.47
1:B:1447:ARG:HD3	1:B:1536:ILE:HG23	1.96	0.47
1:B:1468:ALA:O	1:B:1471:ILE:HG13	2.15	0.47
1:B:1341:PRO:HD2	1:B:1344:THR:HG21	1.96	0.47
1:A:1569:VAL:O	1:A:1593:CYS:HA	2.16	0.46
1:A:1732:THR:O	1:A:1761:THR:HA	2.14	0.46
1:B:1716:ARG:NH2	1:B:1756:GLN:OE1	2.43	0.46
1:B:1580:LEU:O	1:B:1584:ILE:HG13	2.15	0.46
1:B:1648:PHE:CE1	1:B:1652:GLU:HG3	2.51	0.46
1:B:1403:VAL:HG21	1:B:1424:ARG:HD3	1.97	0.46
1:A:1432:ASN:OD1	1:A:1433:ALA:N	2.49	0.46
1:B:1388:LYS:NZ	1:B:1542:ASP:HA	2.30	0.46
1:A:1347:THR:HG21	1:A:1405:ARG:HG3	1.97	0.46
1:A:1171:LYS:HB2	1:A:1201:ARG:NH2	2.30	0.46
1:B:1432:ASN:OD1	1:B:1433:ALA:N	2.48	0.46
1:A:1675:SER:OG	1:A:1719:TYR:OH	2.26	0.46
1:B:1732:THR:O	1:B:1761:THR:HA	2.15	0.46
1:A:1237:LYS:HG3	1:A:1238:ASP:H	1.81	0.46
1:B:1733:PRO:HD3	1:B:1775:PHE:HE1	1.81	0.46
1:A:1143:TYR:O	1:A:1147:GLN:HG2	2.16	0.45
1:B:1427:ARG:HD3	2:D:10:U:H5''	1.97	0.45
1:B:1606:VAL:HG21	1:B:1617:ASP:HA	1.97	0.45
1:A:1159:ARG:HA	1:A:1159:ARG:HD2	1.74	0.45
1:A:1388:LYS:NZ	1:A:1542:ASP:HA	2.31	0.45
1:B:1709:MET:HG2	1:B:1745:PHE:CE1	2.51	0.45
1:B:1642:HIS:CE1	1:B:1644:GLU:HG3	2.51	0.45
1:A:1212:SER:HB3	1:A:1217:PRO:HB3	1.98	0.45
1:A:1393:ALA:O	1:A:1550:THR:HA	2.17	0.45
1:A:1437:ASP:N	1:A:1437:ASP:OD1	2.49	0.45
1:A:1150:PHE:O	1:A:1154:ILE:HG12	2.17	0.45
1:A:1447:ARG:HD2	1:A:1536:ILE:HG23	1.99	0.45
1:B:1393:ALA:O	1:B:1550:THR:HA	2.17	0.45
1:A:1341:PRO:HD2	1:A:1344:THR:HG21	1.98	0.45
1:A:1130:TYR:CE1	1:A:1154:ILE:HG21	2.52	0.45
1:A:1392:CYS:HA	1:A:1549:ALA:O	2.16	0.44
1:A:1602:LEU:HB2	1:A:1766:GLN:OE1	2.17	0.44
1:A:1725:THR:HA	1:A:1756:GLN:HG3	2.00	0.44
1:B:1229:ARG:HE	1:B:1271:MET:HE2	1.82	0.44
1:B:1600:LYS:NZ	4:B:2006:SO4:O4	2.45	0.44
1:A:1558:MET:HG2	1:A:1562:LEU:HD12	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1293:ILE:HD13	1:A:1583:LEU:HD22	2.00	0.44
1:A:1705:VAL:HG13	1:A:1741:LEU:HD23	2.00	0.44
1:B:1353:MET:SD	1:B:1594:ILE:HD13	2.58	0.44
1:B:1599:PRO:HB3	1:B:1622:VAL:HG22	1.98	0.44
1:A:1390:LEU:HD22	1:A:1566:PHE:CD2	2.52	0.44
1:B:1318:LEU:HB3	1:B:1322:GLN:HB2	1.99	0.44
1:A:1479:ARG:HB3	1:A:1480:PRO:HD3	1.99	0.43
1:B:1293:ILE:HD13	1:B:1583:LEU:HD22	2.00	0.43
1:B:1648:PHE:CZ	1:B:1652:GLU:HG3	2.53	0.43
1:A:1399:VAL:O	1:A:1403:VAL:HG23	2.19	0.43
1:B:1339:GLN:HA	1:B:1597:GLY:O	2.18	0.43
1:B:1738:LEU:HD11	1:B:1759:PHE:HB3	2.01	0.43
1:B:1789:MET:HG3	1:B:1821:TRP:NE1	2.33	0.43
1:B:1156:GLU:HB2	1:B:1616:TYR:CE2	2.53	0.43
1:B:1609:GLN:HG2	2:D:3:U:C5	2.53	0.43
1:A:1337:LEU:HD11	1:A:1624:MET:HB2	2.00	0.43
1:B:1150:PHE:O	1:B:1154:ILE:HG12	2.19	0.43
1:A:1709:MET:HG2	1:A:1745:PHE:CE1	2.53	0.43
1:A:1773:ILE:HB	1:A:1802:ALA:HB2	2.00	0.43
1:A:1312:VAL:HG21	1:A:1327:LEU:HD21	2.00	0.43
1:A:1432:ASN:HB3	1:A:1435:VAL:HG22	2.01	0.43
1:A:1470:GLU:O	1:A:1474:LYS:HG3	2.19	0.43
1:A:1391:VAL:O	1:A:1548:CYS:HA	2.19	0.42
1:A:1216:ASP:HB3	1:A:1219:ASN:OD1	2.19	0.42
1:B:1117:TRP:CH2	1:B:1158:TRP:HB2	2.55	0.42
1:B:1399:VAL:O	1:B:1403:VAL:HG23	2.19	0.42
1:A:1119:ILE:HG23	1:A:1161:PHE:CZ	2.55	0.42
1:A:1191:ALA:HB3	1:A:1244:TYR:CE1	2.54	0.42
1:A:1211:ILE:HG23	1:A:1265:VAL:HG22	2.02	0.42
1:B:1296:ALA:HB3	1:B:1627:ASN:ND2	2.35	0.41
1:B:1705:VAL:HG13	1:B:1741:LEU:HD23	2.02	0.41
1:A:1228:SER:OG	1:A:1244:TYR:HB3	2.20	0.41
1:B:1210:ILE:O	1:B:1265:VAL:HA	2.20	0.41
1:B:1427:ARG:HD3	2:D:10:U:C5'	2.51	0.41
1:A:1139:TYR:HB2	1:A:1294:LEU:HD22	2.02	0.41
1:A:1194:PRO:HG2	1:A:1197:ILE:HD12	2.03	0.41
1:B:1431:ILE:HG23	1:B:1435:VAL:HG23	2.03	0.41
1:B:1557:GLU:HA	1:B:1560:LYS:HE3	2.03	0.41
1:A:1271:MET:HE2	1:A:1275:GLU:HG3	2.02	0.41
1:A:1637:MET:HG2	1:A:1659:GLN:HG3	2.03	0.41
1:A:1702:GLU:HG3	1:A:1706:LYS:HE3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1788:PHE:HB3	2:C:3:U:O2'	2.21	0.41
1:B:1393:ALA:HB3	1:B:1399:VAL:HG23	2.03	0.41
2:C:7:U:H2'	2:C:8:U:O4'	2.20	0.41
1:A:1640:ARG:NE	1:A:1769:GLU:OE1	2.52	0.41
1:B:1224:LEU:HD23	1:B:1224:LEU:HA	1.90	0.41
1:B:1396:ASN:ND2	2:D:8:U:OP1	2.41	0.41
1:B:1479:ARG:HB3	1:B:1480:PRO:HD3	2.03	0.40
1:A:1212:SER:HA	1:A:1224:LEU:O	2.21	0.40
1:A:1224:LEU:HB3	1:A:1253:ILE:HG22	2.02	0.40
1:B:1716:ARG:NE	1:B:1724:LEU:HD12	2.29	0.40
1:B:1143:TYR:O	1:B:1147:GLN:HG2	2.21	0.40
1:B:1547:LEU:HD22	1:B:1566:PHE:CZ	2.56	0.40
1:A:1714:ARG:HE	1:A:1718:ASP:CG	2.25	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	704/793 (89%)	677 (96%)	27 (4%)	0	100	100
1	B	725/793 (91%)	694 (96%)	31 (4%)	0	100	100
All	All	1429/1586 (90%)	1371 (96%)	58 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	607/681 (89%)	597 (98%)	10 (2%)	62	86
1	B	628/681 (92%)	610 (97%)	18 (3%)	42	75
All	All	1235/1362 (91%)	1207 (98%)	28 (2%)	50	79

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1108	ASP
1	A	1114	ILE
1	A	1155	ASN
1	A	1219	ASN
1	A	1226	CYS
1	A	1246	LEU
1	A	1714	ARG
1	A	1732	THR
1	A	1788	PHE
1	A	1824	LEU
1	B	1108	ASP
1	B	1111	HIS
1	B	1201	ARG
1	B	1226	CYS
1	B	1245	ARG
1	B	1246	LEU
1	B	1303	THR
1	B	1310	LYS
1	B	1326	ILE
1	B	1470	GLU
1	B	1525	TYR
1	B	1695	LYS
1	B	1714	ARG
1	B	1760	ASN
1	B	1788	PHE
1	B	1790	THR
1	B	1791	ASP
1	B	1824	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1247	ASN
1	A	1633	HIS
1	A	1710	GLN
1	B	1222	GLN
1	B	1830	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	9/15 (60%)	2 (22%)	0
2	D	8/15 (53%)	4 (50%)	0
All	All	17/30 (56%)	6 (35%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	2	U
2	C	3	U
2	D	3	U
2	D	4	U
2	D	9	U
2	D	10	U

There are no RNA pucker outliers to report.

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](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	B	2003	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	B	2006	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	2002	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	B	2005	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	B	2004	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	2003	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	B	2002	-	4,4,4	0.14	0	6,6,6	0.06	0
3	ADP	A	2001	-	24,29,29	0.96	1 (4%)	29,45,45	1.45	4 (13%)
4	SO4	A	2004	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	B	2001	-	4,4,4	0.14	0	6,6,6	0.06	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	2001	-	-	4/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	ADP	C5-C4	2.51	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	ADP	PA-O3A-PB	-3.42	121.09	132.83
3	A	2001	ADP	C3'-C2'-C1'	3.36	106.04	100.98
3	A	2001	ADP	N3-C2-N1	-3.20	123.68	128.68
3	A	2001	ADP	C4-C5-N7	-2.53	106.76	109.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

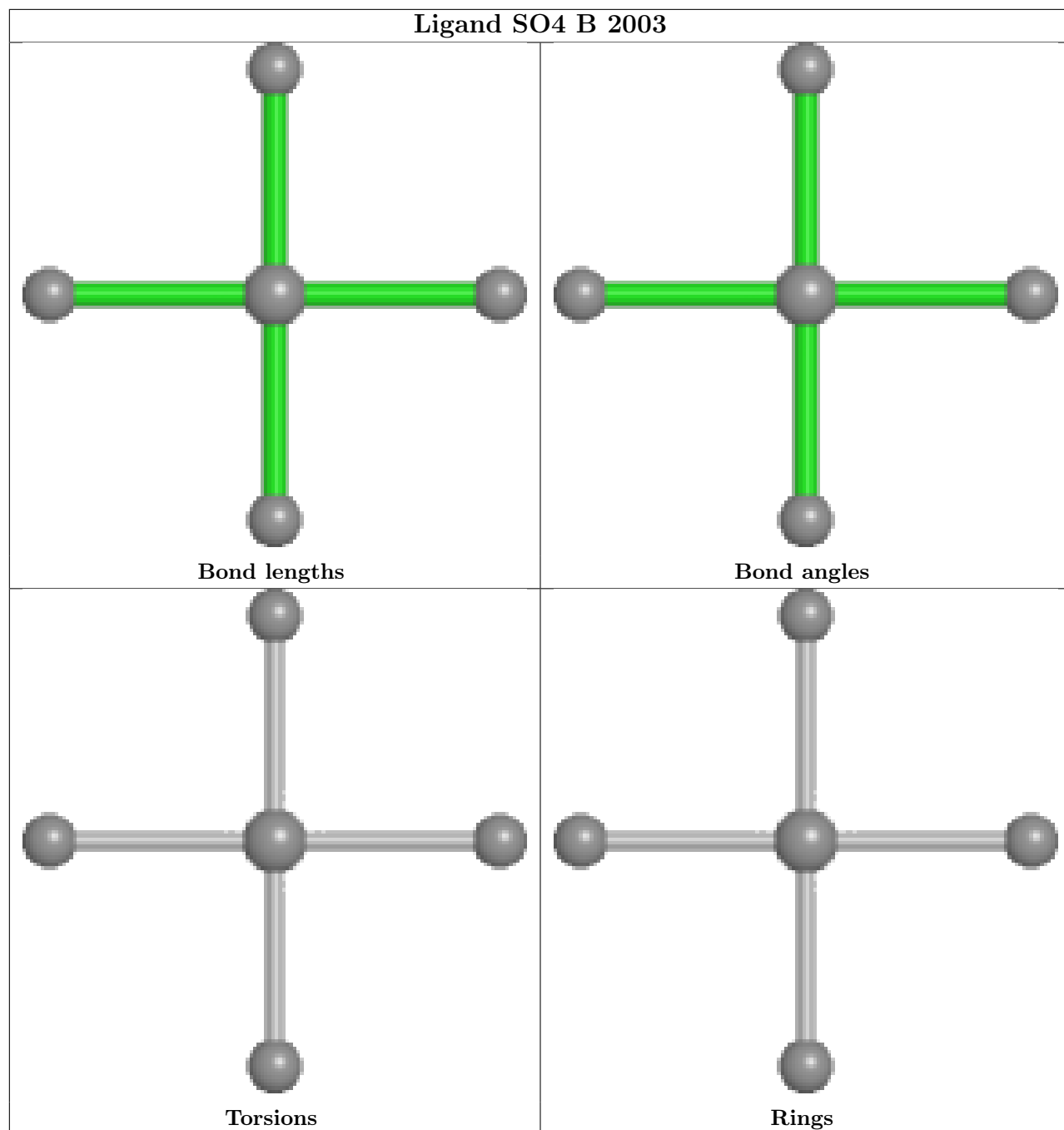
Mol	Chain	Res	Type	Atoms
3	A	2001	ADP	PA-O3A-PB-O2B
3	A	2001	ADP	PA-O3A-PB-O3B
3	A	2001	ADP	C5'-O5'-PA-O1A
3	A	2001	ADP	O4'-C4'-C5'-O5'

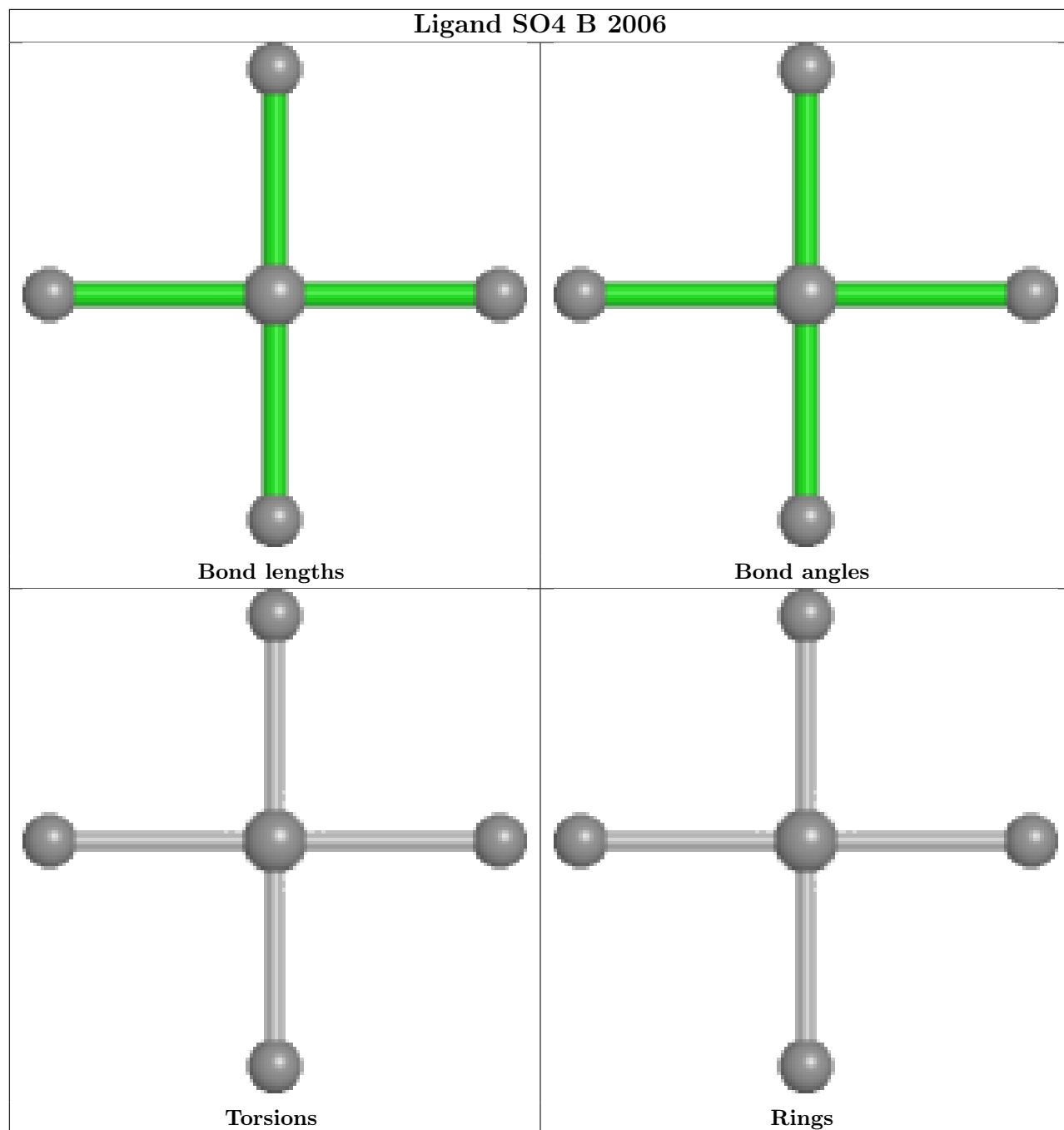
There are no ring outliers.

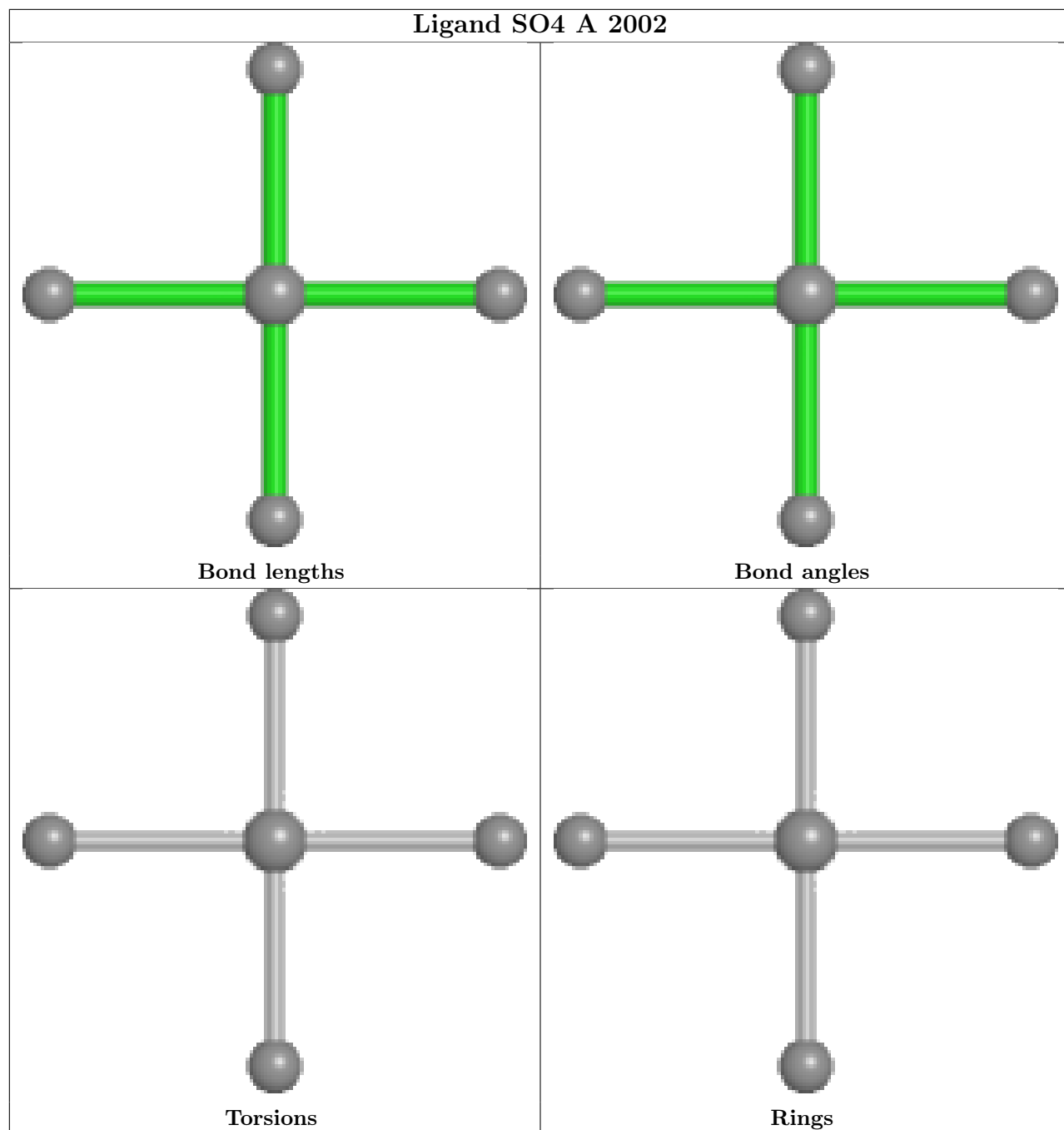
2 monomers are involved in 3 short contacts:

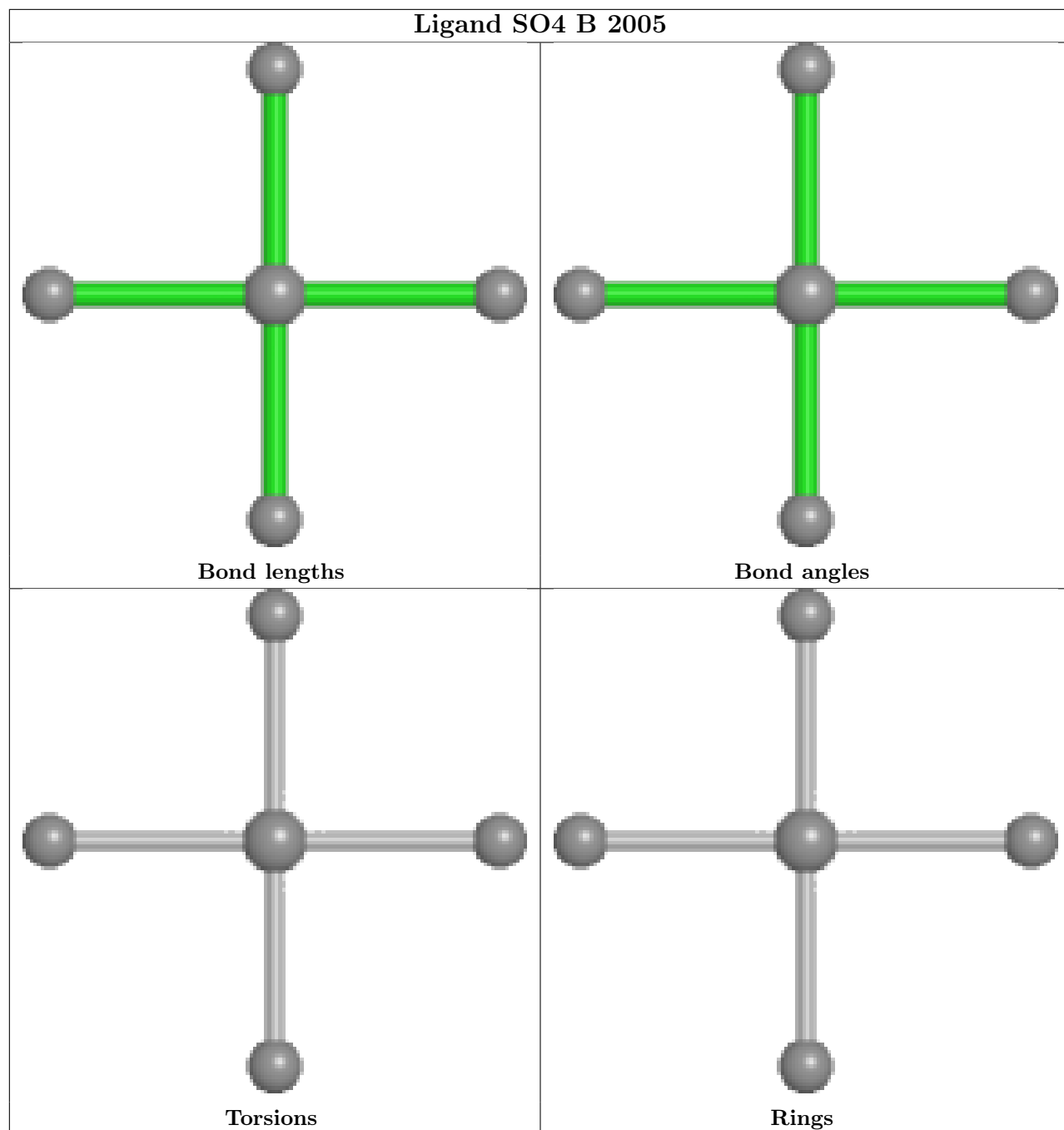
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2006	SO4	2	0
3	A	2001	ADP	1	0

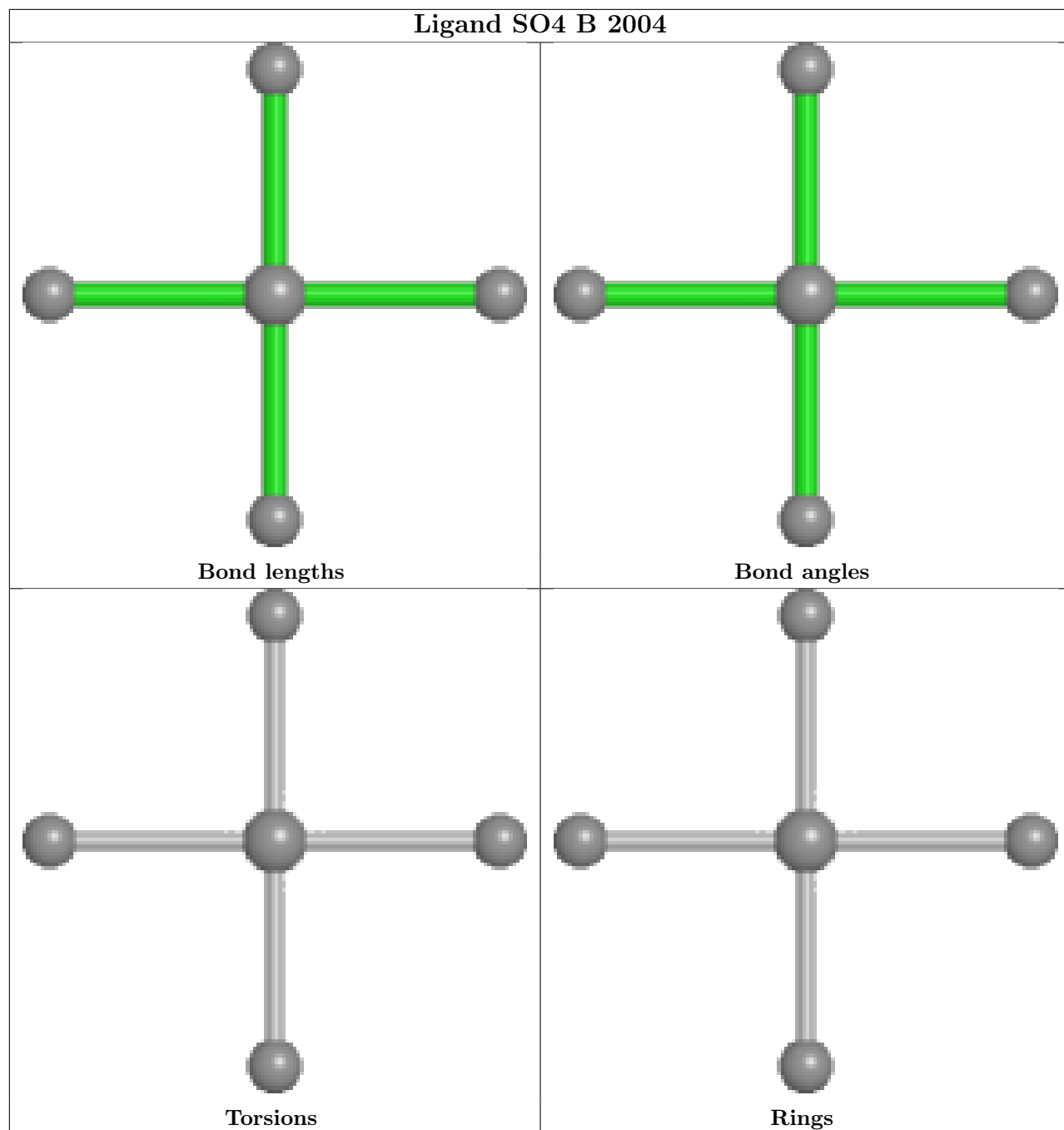
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

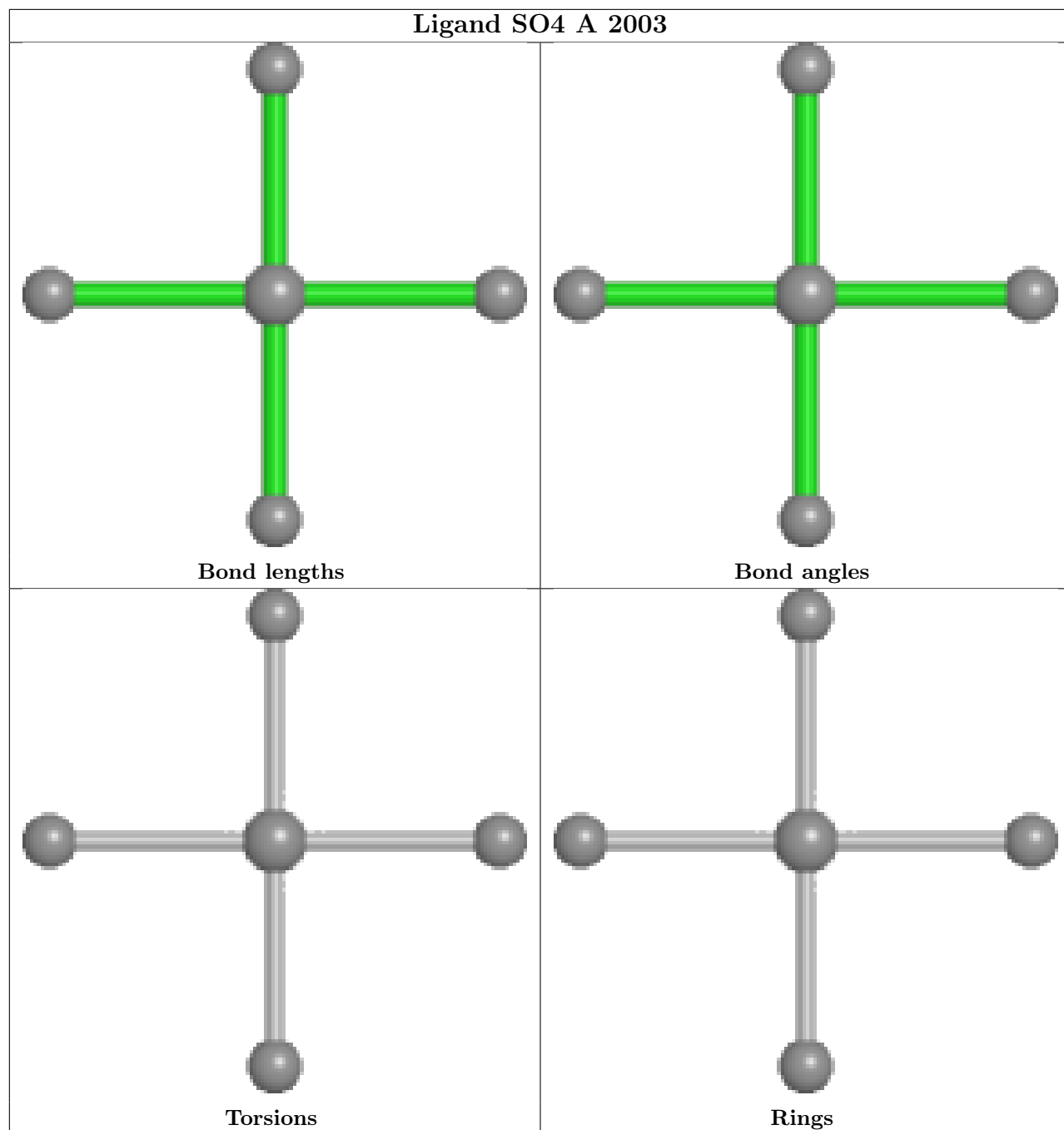


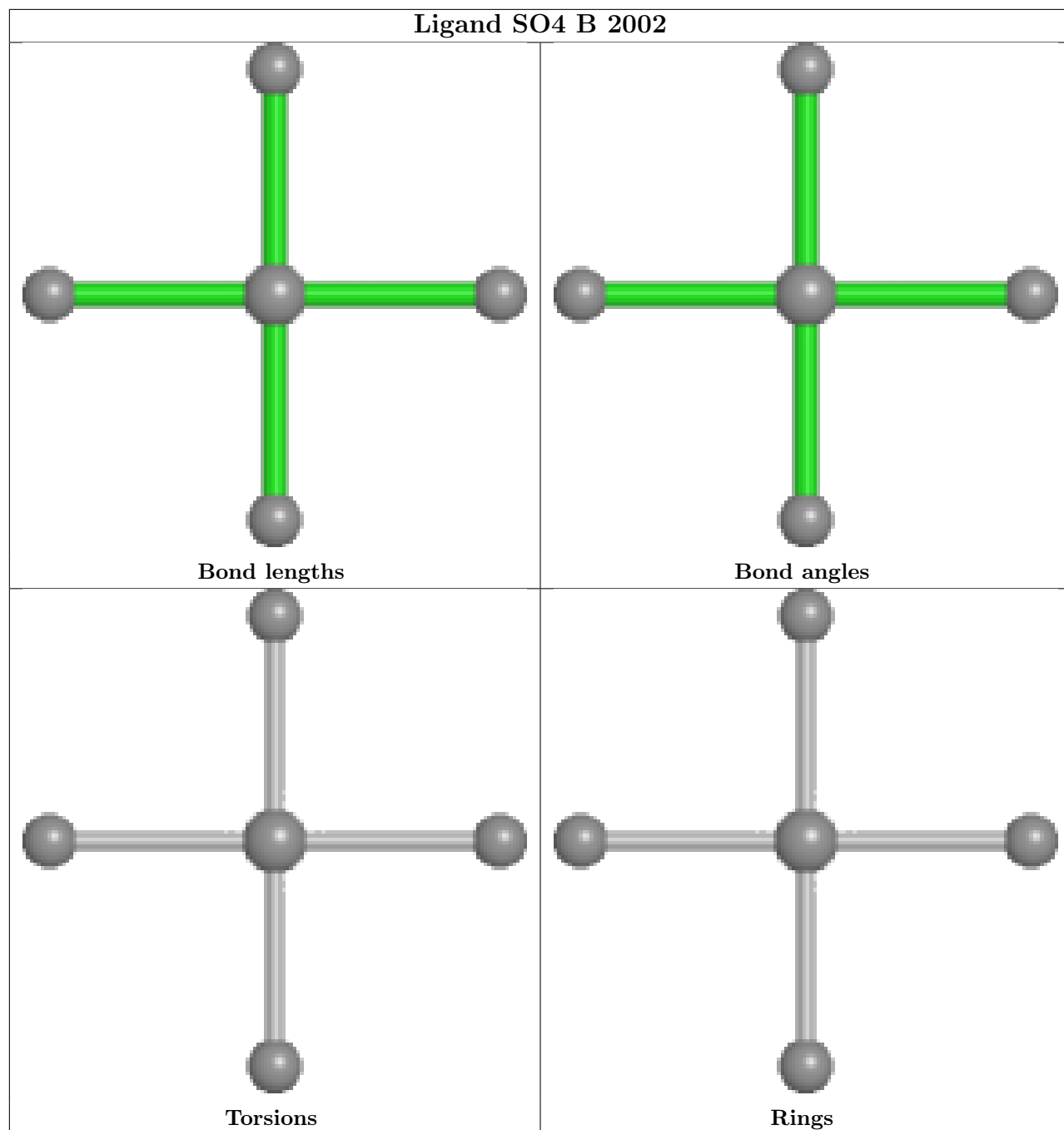


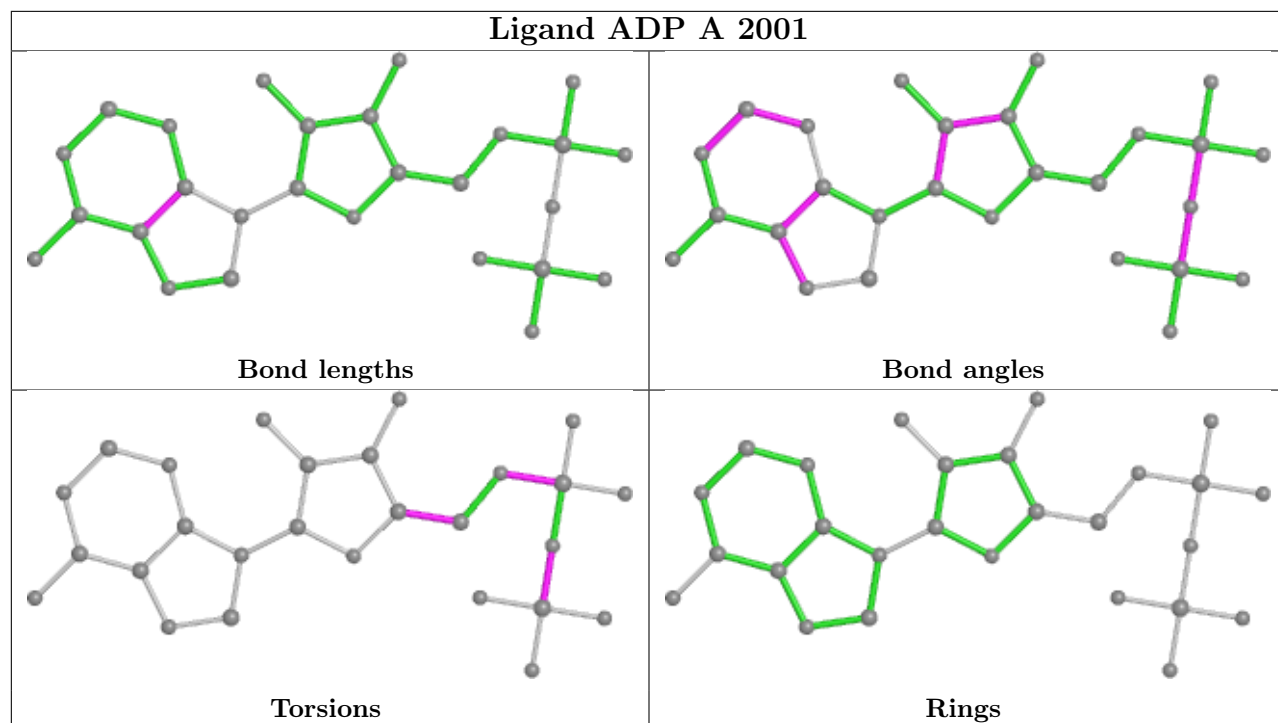


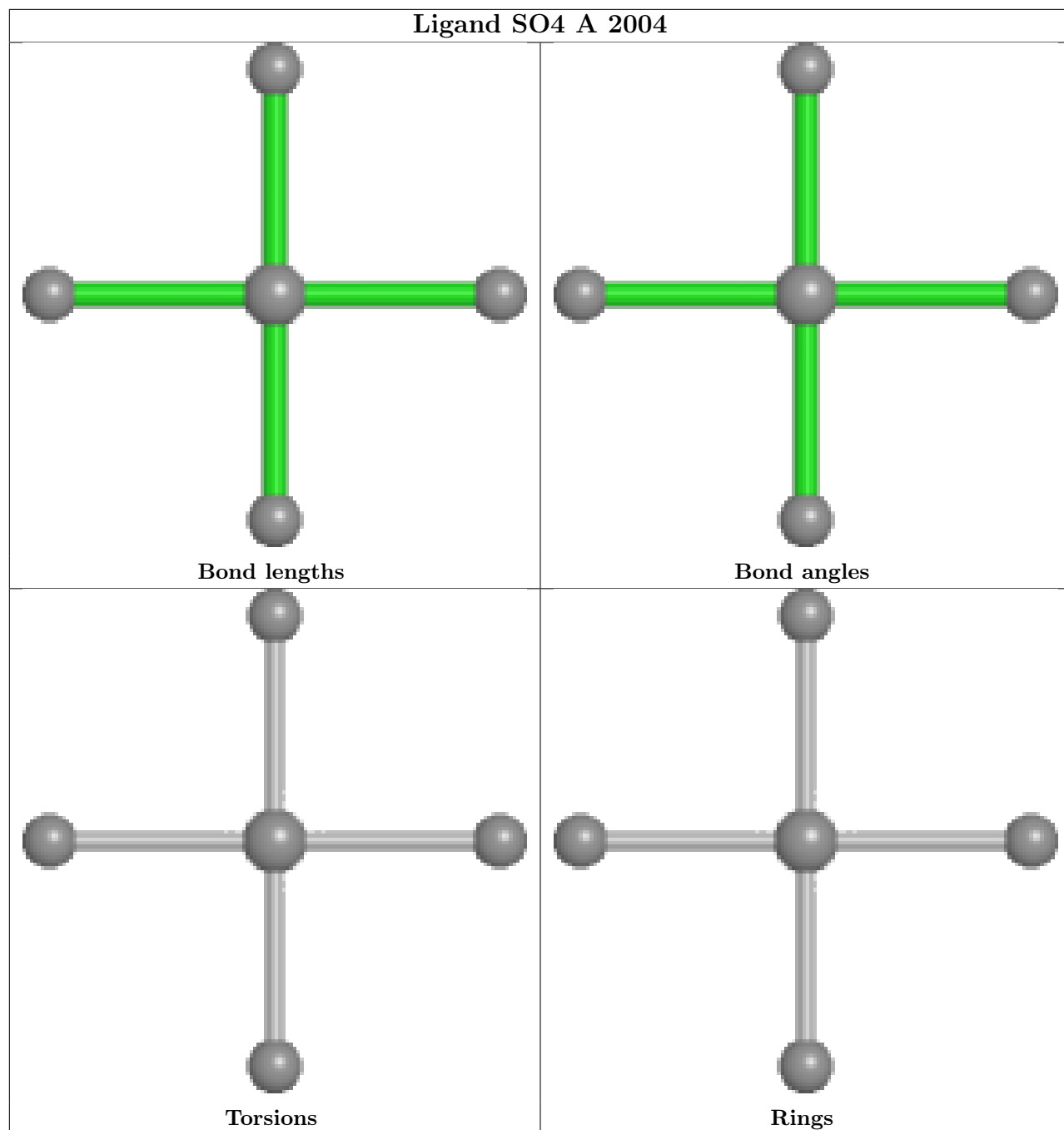


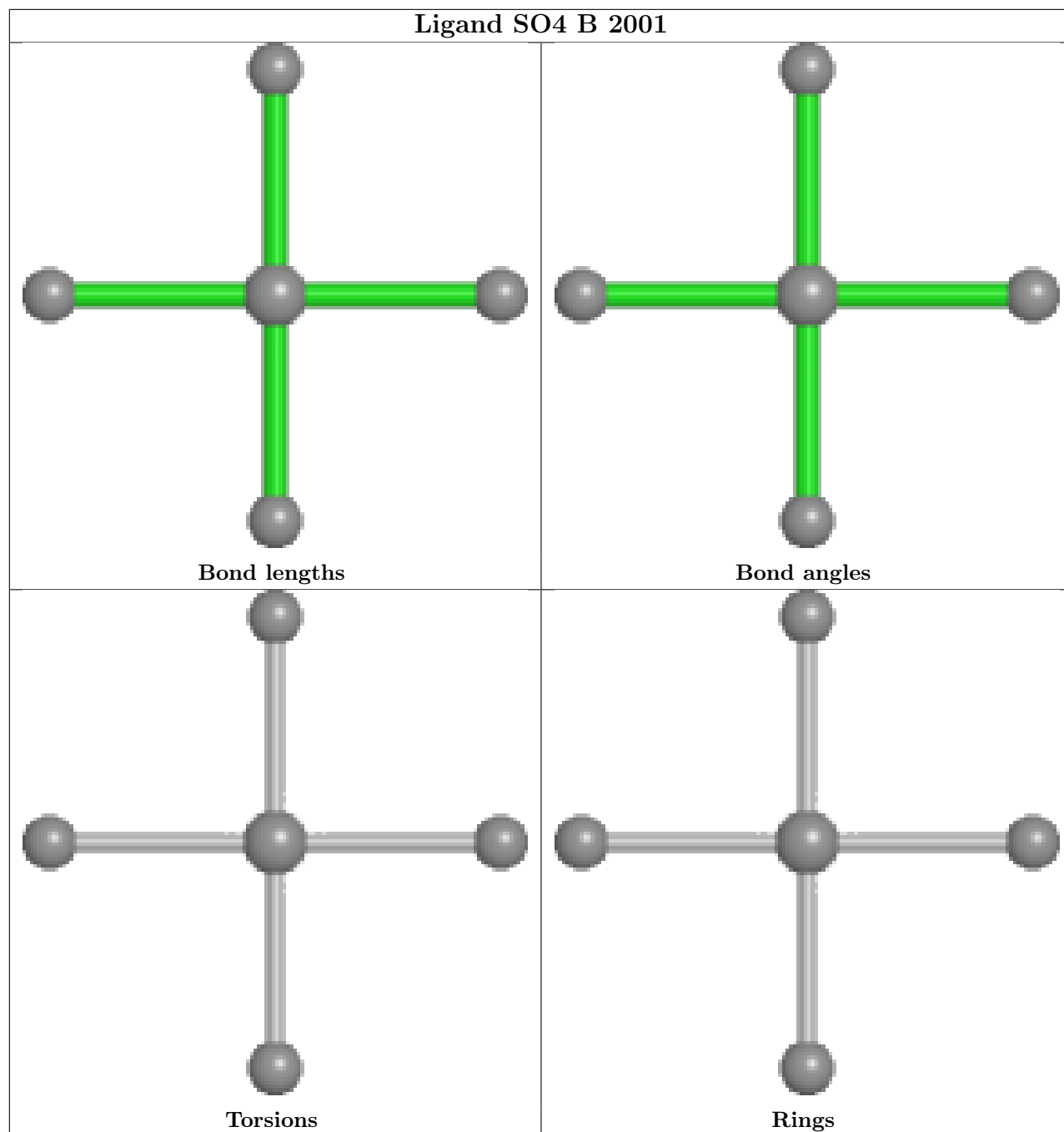












5.7 Other polymers [i](#)

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	714/793 (90%)	-0.07	28 (3%) 39 16	44, 85, 156, 194	0
1	B	731/793 (92%)	-0.17	11 (1%) 73 46	46, 83, 144, 204	0
2	C	12/15 (80%)	-0.02	0 100 100	73, 80, 146, 156	0
2	D	10/15 (66%)	-0.06	0 100 100	74, 101, 142, 158	0
All	All	1467/1616 (90%)	-0.12	39 (2%) 54 26	44, 85, 151, 204	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1452	LEU	4.7
1	A	1504	LEU	3.9
1	A	1525	TYR	3.7
1	B	1218	LEU	3.5
1	B	1103	LEU	3.2
1	A	1502	ASP	3.2
1	A	1130	TYR	3.2
1	A	1507	ARG	3.1
1	A	1468	ALA	3.0
1	A	1508	GLN	3.0
1	B	1462	ASP	3.0
1	B	1524	THR	2.8
1	A	1498	GLN	2.7
1	A	1503	GLU	2.7
1	B	1217	PRO	2.6
1	A	1506	ARG	2.6
1	A	1217	PRO	2.6
1	B	1385	PRO	2.6
1	A	1218	LEU	2.6
1	A	1473	ALA	2.5
1	A	1495	MET	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1474	LYS	2.5
1	A	1491	ARG	2.5
1	A	1524	THR	2.5
1	B	1521	SER	2.4
1	A	1462	ASP	2.4
1	A	1490	ASP	2.4
1	A	1500	GLU	2.3
1	A	1248	ALA	2.2
1	B	1453	SER	2.2
1	A	1471	ILE	2.2
1	A	1129	GLY	2.2
1	A	1488	SER	2.2
1	A	1499	ARG	2.2
1	A	1215	GLU	2.2
1	B	1219	ASN	2.2
1	A	1497	LEU	2.1
1	B	1858	GLN	2.0
1	B	1455	ASN	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.

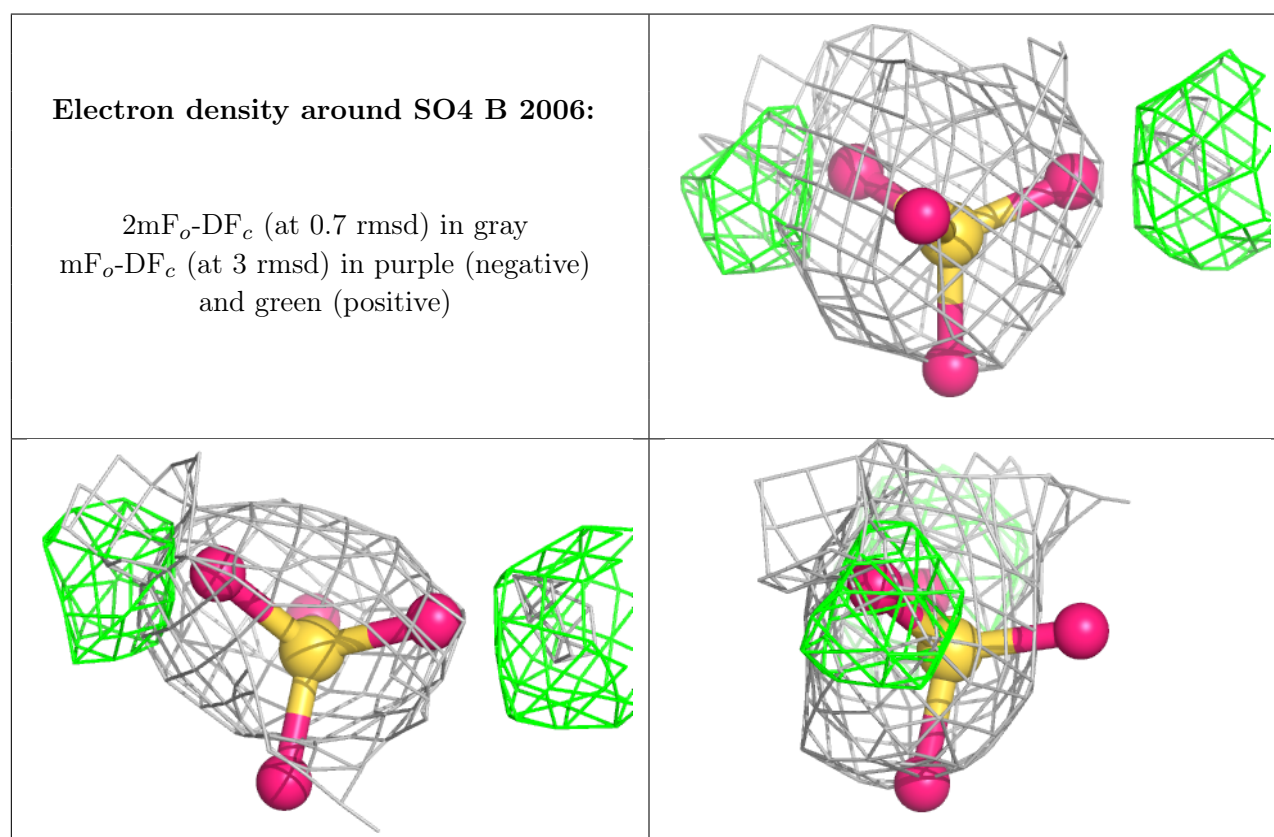
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	B	2006	5/5	0.78	0.37	59,60,63,65	5
4	SO4	B	2004	5/5	0.82	0.17	106,115,124,145	0
3	ADP	A	2001	27/27	0.85	0.27	71,122,141,145	0
4	SO4	B	2005	5/5	0.90	0.11	117,122,141,146	0
4	SO4	A	2003	5/5	0.91	0.17	88,91,94,104	5

Continued on next page...

Continued from previous page...

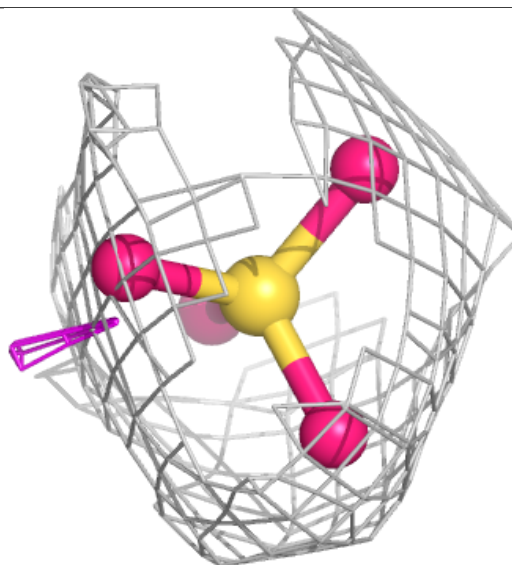
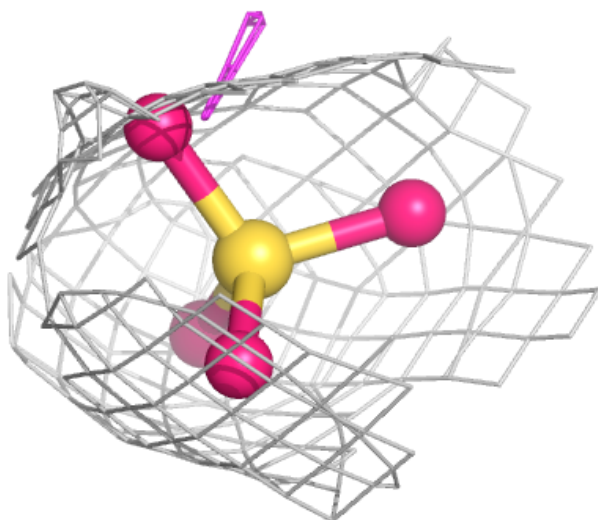
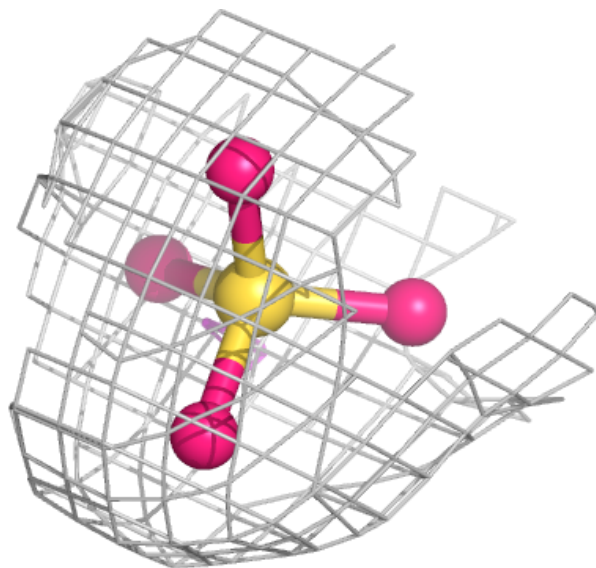
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	2004	5/5	0.94	0.14	101,118,128,144	0
4	SO4	B	2002	5/5	0.95	0.13	62,66,73,76	5
4	SO4	B	2003	5/5	0.96	0.21	67,81,98,103	0
4	SO4	A	2002	5/5	0.97	0.23	51,56,62,78	0
4	SO4	B	2001	5/5	0.99	0.16	57,62,70,71	0

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.



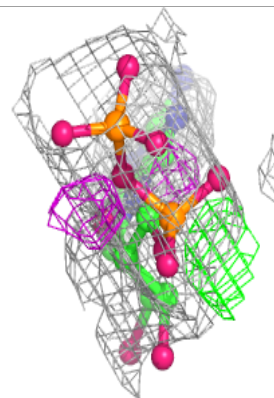
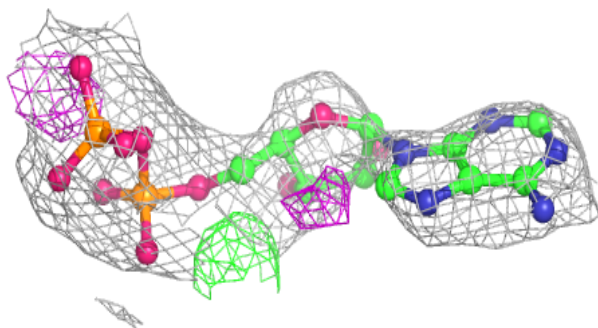
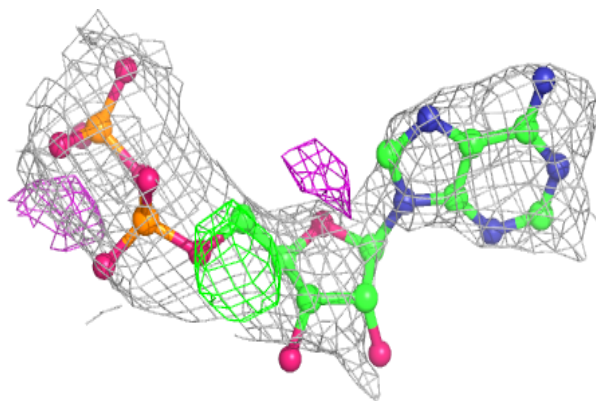
Electron density around SO4 B 2004:

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



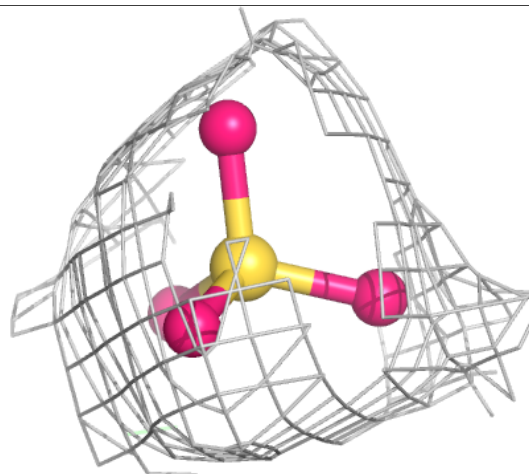
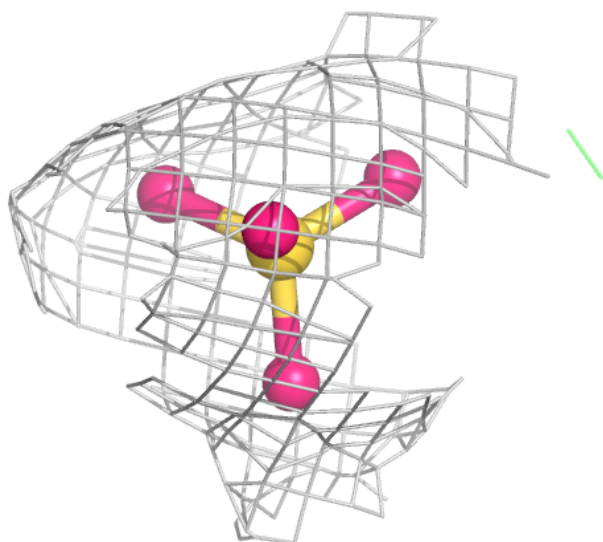
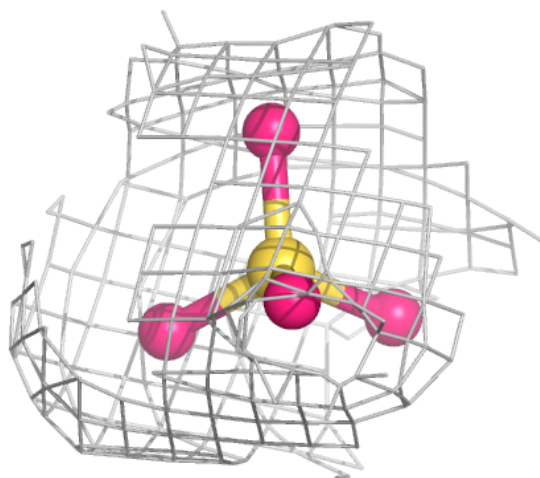
Electron density around ADP A 2001:

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



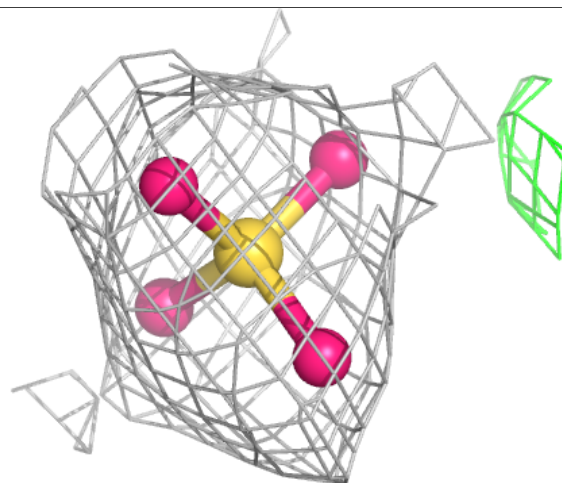
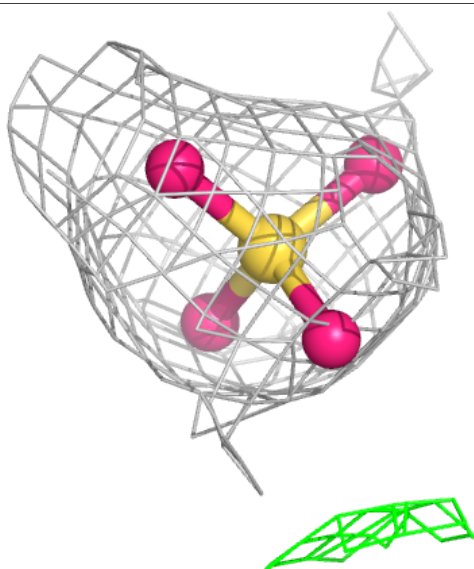
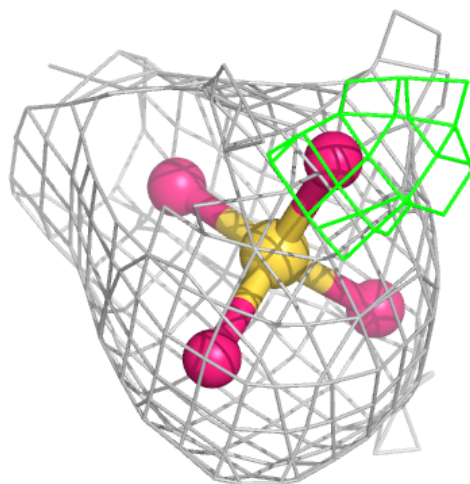
Electron density around SO4 B 2005:

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



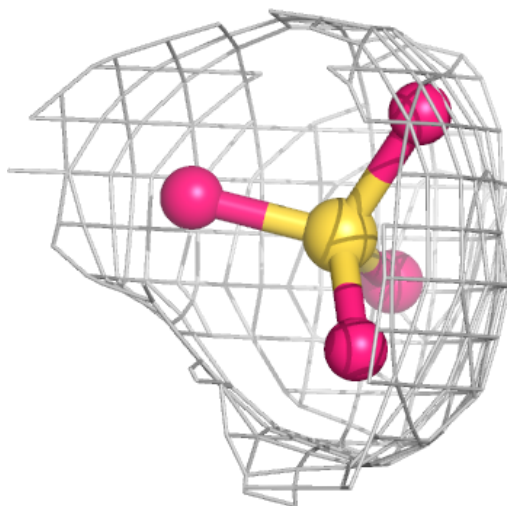
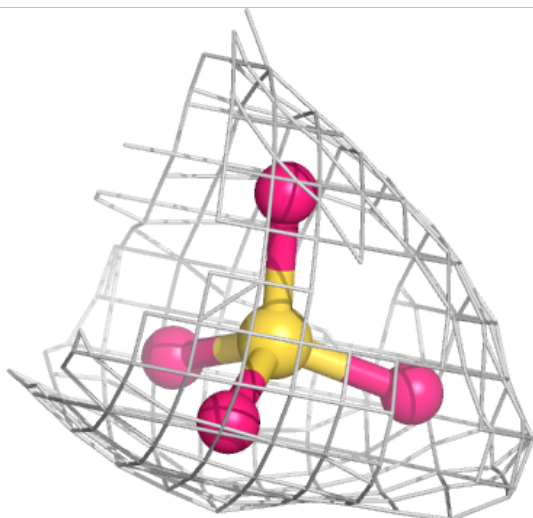
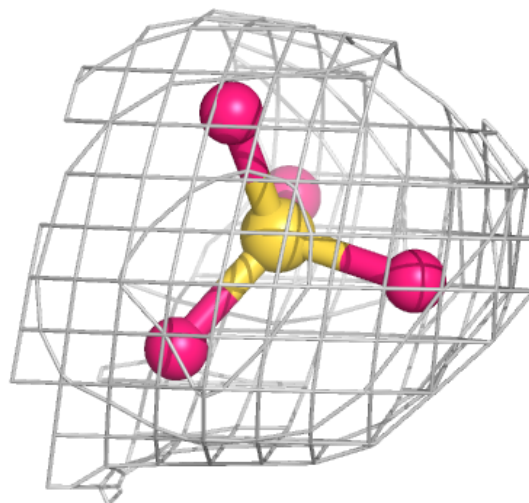
Electron density around SO4 A 2003:

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



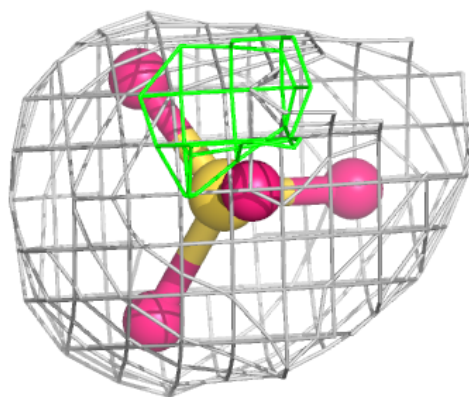
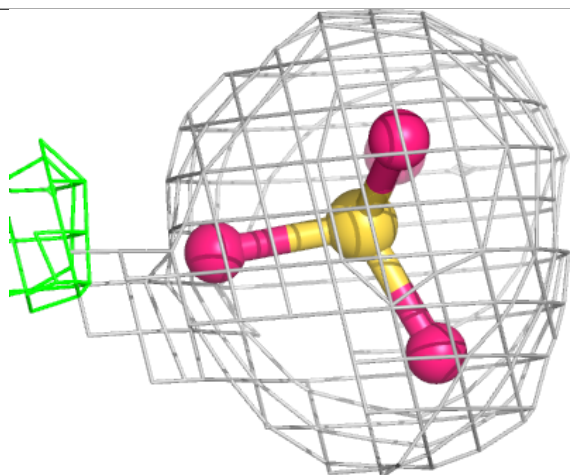
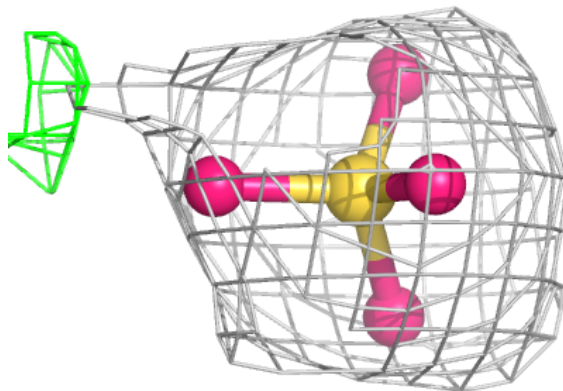
Electron density around SO4 A 2004:

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



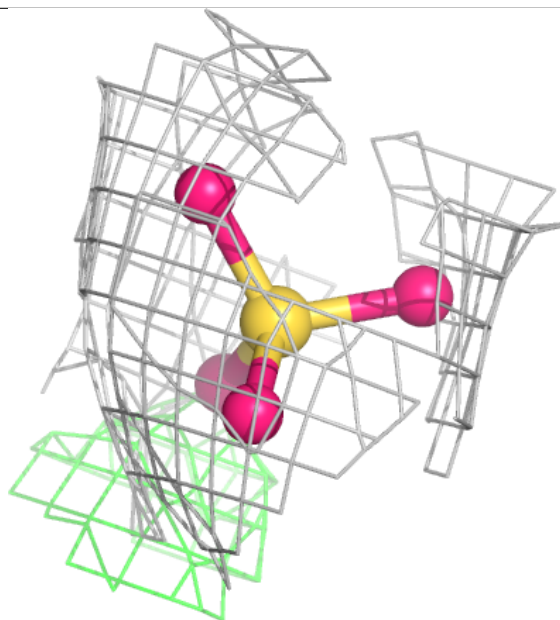
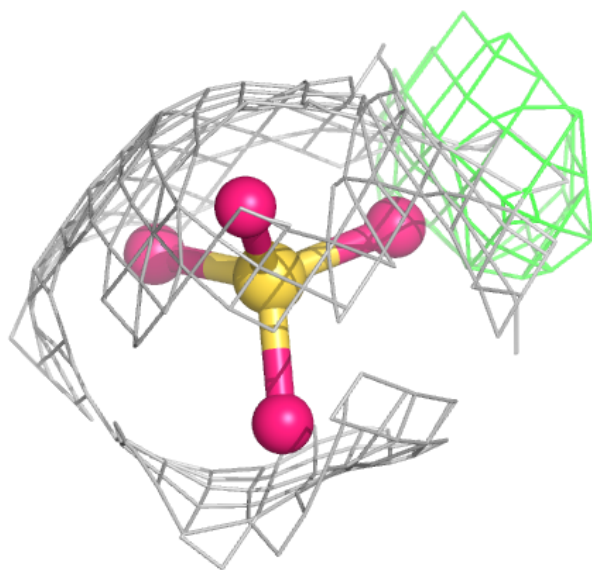
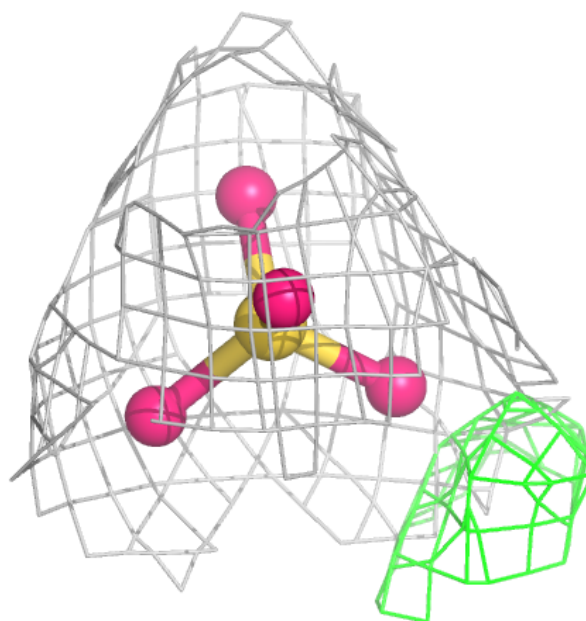
Electron density around SO4 B 2002:

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



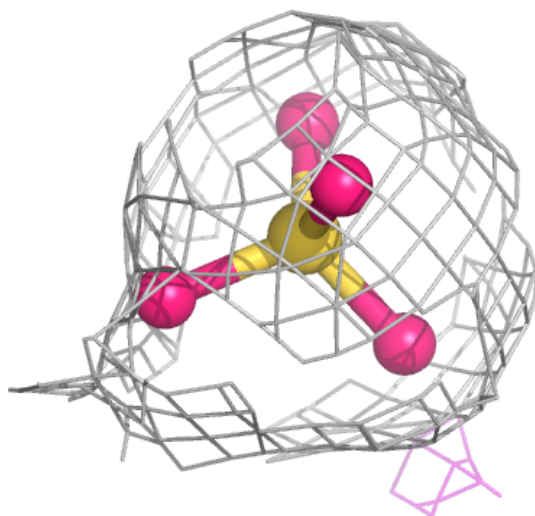
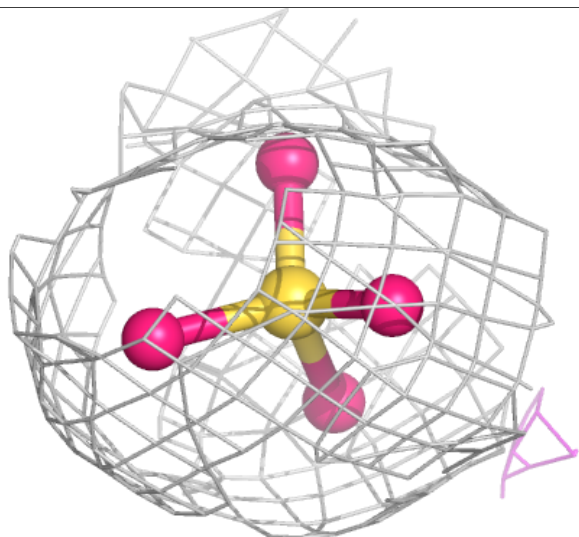
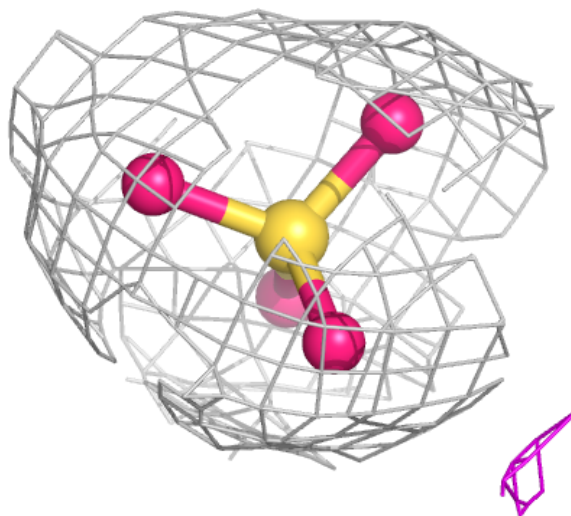
Electron density around SO4 B 2003:

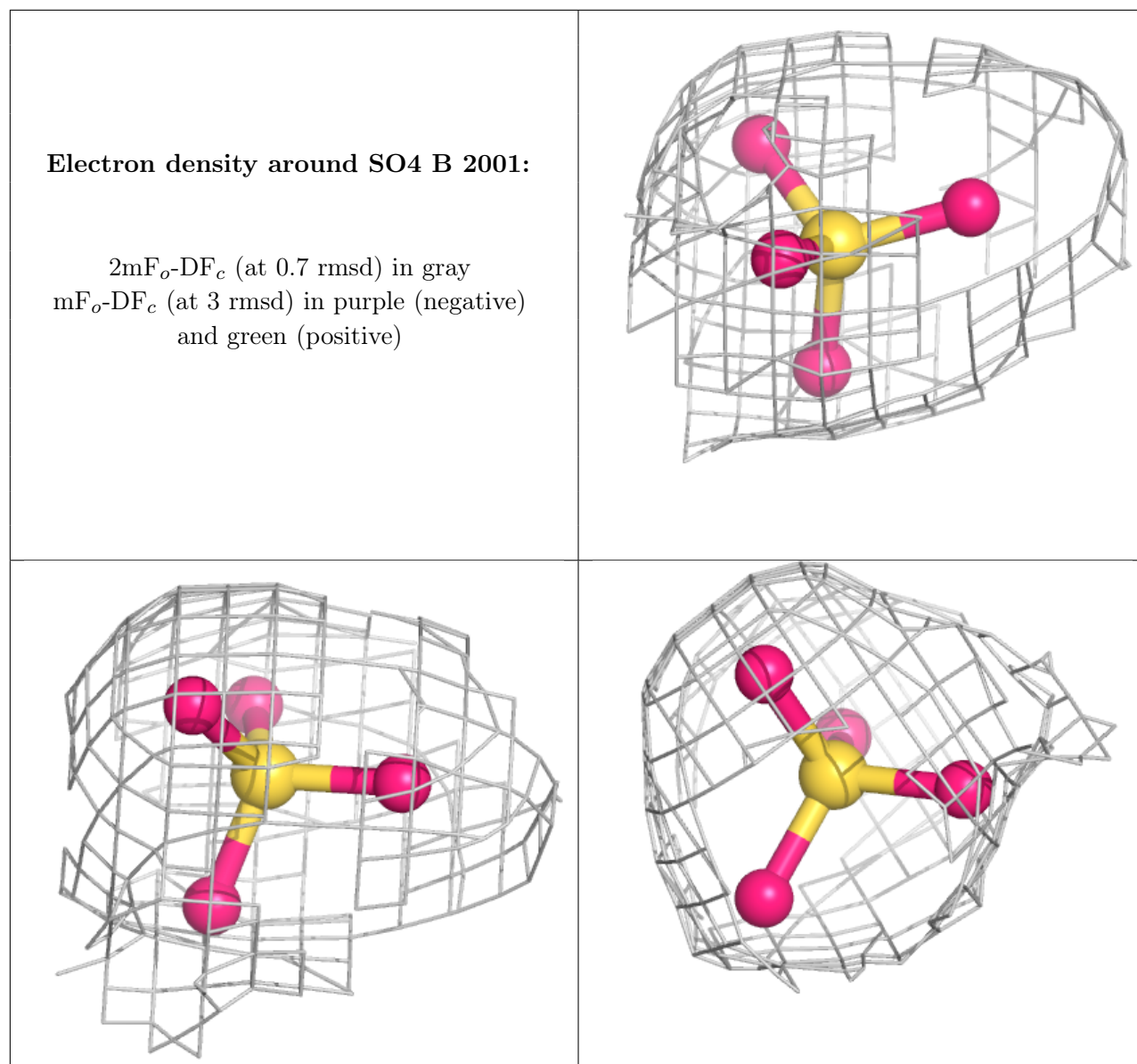
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SO4 A 2002:

$2mF_o-DF_c$ (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.