WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

May 26, 2025 – 06:11 PM JST

PDB ID	:	9M5M / pdb_00009m5m
Title	:	Crystal structure of Plasmodium vivax aspartyl-tRNA synthetase (PvDRS)
Authors	:	Sharma, V.K.; Manickam, Y.; Bagale, S.; Pradeepkumar, P.I.; Sharma, A.
Deposited on	:	2025-03-06
Resolution	:	2.06 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

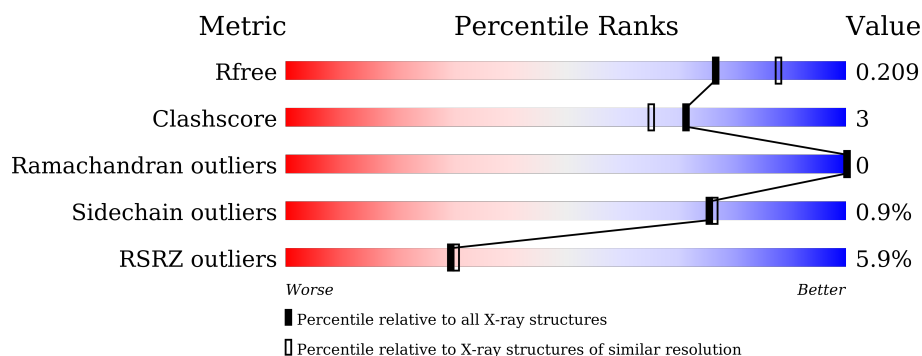|		
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.06 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	Percentile Ranks	Value
Rfree		0.209
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		0.9%
RSRZ outliers		5.9%

Worse — Better

▮ Percentile relative to all X-ray structures
◻ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	164625	3436 (2.08-2.04)
Clashscore	180529	3661 (2.08-2.04)
Ramachandran outliers	177936	3649 (2.08-2.04)
Sidechain outliers	177891	3649 (2.08-2.04)
RSRZ outliers	164620	3436 (2.08-2.04)

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 <=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	536	5% ▮ 86% 7% 7%
1	B	536	6% ▮ 85% 9% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8598 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 aspartate–tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			4058	2605	676	751	26			
1	B	501	Total	C	N	O	S	0	1	0
			4003	2569	658	749	27			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).
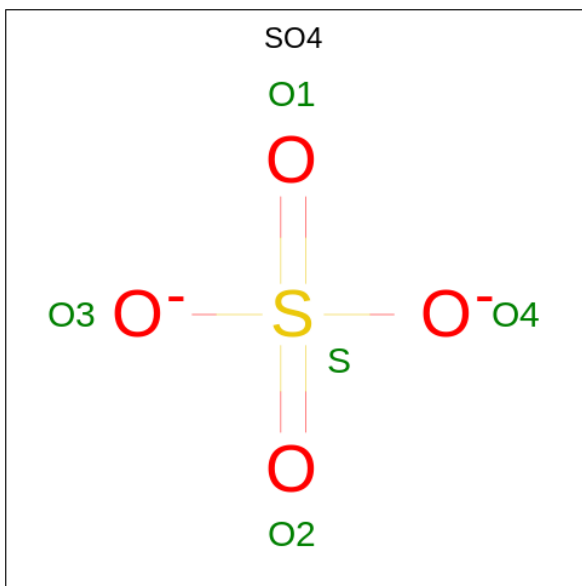
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).

EDO

O2

OH

C1

C2

HO

O1
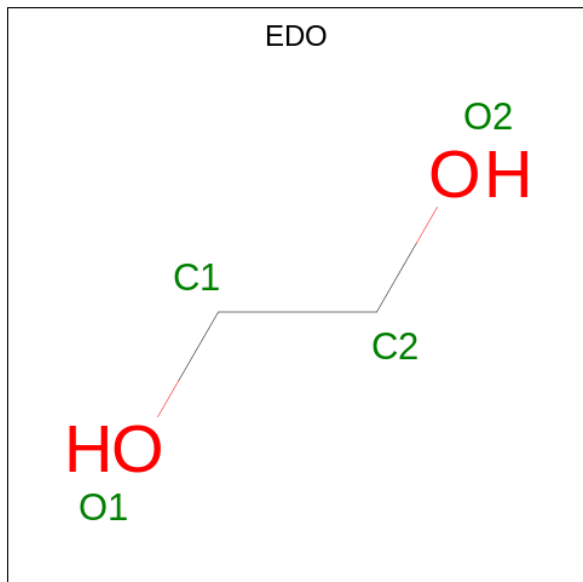
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	241	Total 250	O 250	0	9
4	B	251	Total 259	O 259	0	8

W O R L D W I D E
PDB
PROTEIN DATA BANK

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: aspartate–tRNA ligase

Chain A:

- Molecule 1: aspartate–tRNA ligase

Chain B:
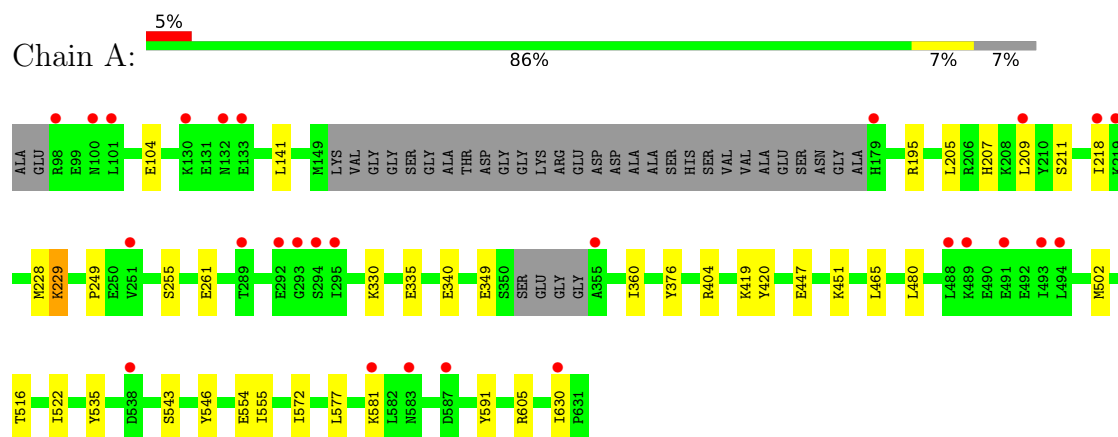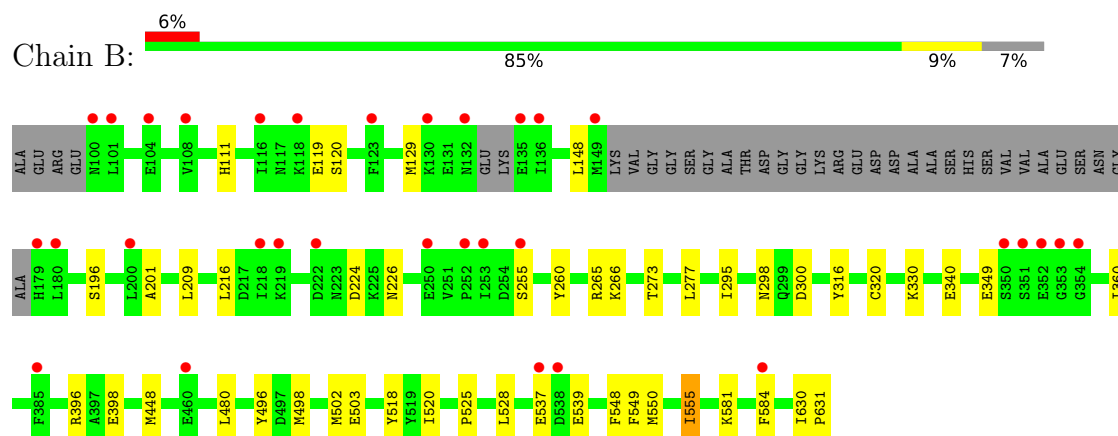
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	140.45Å 140.45Å 272.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	72.79 – 2.06 72.79 – 2.06	Depositor EDS
% Data completeness (in resolution range)	99.3 (72.79-2.06) 99.3 (72.79-2.06)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 2.07Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.183 , 0.211 0.183 , 0.209	Depositor DCC
R_{free} test set	4860 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	47.0	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 62.8	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8598	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, EDO

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	0.50	0/4147	0.58	2/5591 (0.0%)
1	B	0.55	0/4094	0.63	5/5531 (0.1%)
All	All	0.52	0/8241	0.61	7/11122 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	209	LEU	CB-CA-C	-6.25	100.00	110.56
1	B	298	ASN	N-CA-C	6.11	118.66	110.35
1	B	196	SER	N-CA-C	5.89	118.71	108.76
1	B	539	GLU	CA-C-N	5.78	125.64	119.28
1	B	539	GLU	C-N-CA	5.78	125.64	119.28
1	A	419	LYS	N-CA-C	5.43	117.00	111.14
1	B	111	HIS	N-CA-C	5.24	117.90	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4058	0	3947	28	0
1	B	4003	0	3824	32	0

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	15	0	0	0	0
2	B	5	0	0	0	0
3	A	4	0	6	1	0
3	B	4	0	6	1	0
4	A	250	0	0	2	0
4	B	259	0	0	2	0
All	All	8598	0	7783	51	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 3.

All (51) 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:360:ILE:HG22	1:B:360:ILE:HG22	1.36	1.02
1:A:360:ILE:HG22	1:B:360:ILE:CG2	2.12	0.77
1:B:349:GLU:HG2	1:B:581:LYS:HB3	1.75	0.68
1:B:525:PRO:HG2	1:B:528:LEU:HD12	1.76	0.68
1:B:201:ALA:HB3	1:B:216:LEU:HB3	1.76	0.67
1:A:360:ILE:CG2	1:B:360:ILE:HG22	2.22	0.67
1:A:349:GLU:HG2	1:A:581:LYS:HB3	1.78	0.66
1:A:255:SER:O	3:A:702:EDO:H21	2.08	0.53
1:A:141:LEU:HB2	1:A:207:HIS:HB3	1.90	0.53
1:A:572:ILE:HG23	1:A:577:LEU:HB2	1.90	0.53
1:B:480:LEU:HD13	1:B:502:MET:HG3	1.91	0.52
1:B:224:ASP:OD2	1:B:226:ASN:N	2.43	0.51
1:A:229:LYS:NZ	4:A:807:HOH:O	2.44	0.50
1:A:376:TYR:OH	1:B:631:PRO:OXT	2.20	0.50
1:A:229:LYS:NZ	1:A:229:LYS:HB2	2.27	0.49
1:B:316:TYR:CZ	1:B:320[A]:CYS:SG	3.07	0.47
1:A:522:ILE:HG22	1:A:546:TYR:HB3	1.96	0.47
1:B:129:MET:HE2	1:B:129:MET:HB2	1.78	0.47
1:A:591:TYR:HA	1:B:273:THR:HG23	1.96	0.47
1:B:120:SER:HA	1:B:266:LYS:HG2	1.96	0.47
1:A:195:ARG:NH2	4:A:811:HOH:O	2.47	0.47
1:B:630:ILE:HD13	4:B:846:HOH:O	2.14	0.47
1:A:404:ARG:NH2	1:A:605:ARG:NH2	2.63	0.46
1:A:404:ARG:NH2	1:A:605:ARG:HH22	2.14	0.45
1:A:447:GLU:HG2	1:A:451:LYS:HE3	1.97	0.45
1:B:119:GLU:O	1:B:266:LYS:HE3	2.16	0.45
1:A:465:LEU:HG	1:A:516:THR:HB	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:TYR:CE1	1:B:129:MET:HG2	2.53	0.44
1:B:550:MET:SD	1:B:555:ILE:HD13	2.58	0.44
1:A:535:TYR:HA	1:A:543:SER:HA	2.01	0.43
1:B:209:LEU:HD11	1:B:448:MET:HG2	2.00	0.43
1:B:520:ILE:HG12	1:B:548:PHE:CD1	2.53	0.43
1:A:229:LYS:NZ	1:A:229:LYS:CB	2.82	0.43
1:A:630:ILE:HD13	1:B:584:PHE:CZ	2.54	0.43
1:B:209:LEU:H	1:B:209:LEU:HD23	1.84	0.43
1:A:340:GLU:OE2	1:B:330:LYS:NZ	2.52	0.42
1:B:265:ARG:O	1:B:266:LYS:HG3	2.19	0.42
1:A:205:LEU:O	1:A:211:SER:HA	2.20	0.42
1:A:480:LEU:HD13	1:A:502:MET:HG3	2.01	0.42
1:B:396:ARG:NE	1:B:398:GLU:OE2	2.53	0.42
1:A:218:ILE:HG23	1:A:228:MET:HE2	2.01	0.42
1:A:330:LYS:NZ	1:B:340:GLU:OE1	2.52	0.41
1:B:349:GLU:HG2	1:B:581:LYS:CB	2.47	0.41
1:B:498:MET:HE3	1:B:503:GLU:HG2	2.02	0.41
1:A:249:PRO:HD3	1:A:261:GLU:HG3	2.01	0.41
1:B:496:TYR:CE2	1:B:498:MET:HA	2.55	0.41
1:B:295:ILE:HA	4:B:943:HOH:O	2.20	0.41
1:B:518:TYR:HA	1:B:549:PHE:O	2.21	0.40
1:A:335:GLU:O	1:A:335:GLU:HG3	2.21	0.40
1:B:148:LEU:HD13	1:B:260:TYR:CG	2.57	0.40
1:B:255:SER:O	3:B:702:EDO:H21	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	A	495/536 (92%)	482 (97%)	13 (3%)	0	100	100

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	496/536 (92%)	485 (98%)	11 (2%)	0	100	100
All	All	991/1072 (92%)	967 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	440/485 (91%)	436 (99%)	4 (1%)	75	76
1	B	426/485 (88%)	422 (99%)	4 (1%)	75	76
All	All	866/970 (89%)	858 (99%)	8 (1%)	75	76

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	GLU
1	A	229	LYS
1	A	554	GLU
1	A	555	ILE
1	B	277	LEU
1	B	300	ASP
1	B	537	GLU
1	B	555	ILE

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

Mol	Chain	Res	Type
1	A	299	GLN
1	A	401	ASN
1	B	401	ASN
1	B	405	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	SO4	A	701	-	4,4,4	0.66	0	6,6,6	0.24	0
2	SO4	A	703	-	4,4,4	0.61	0	6,6,6	0.11	0
3	EDO	B	702	-	3,3,3	0.29	0	2,2,2	0.22	0
2	SO4	B	701	-	4,4,4	0.27	0	6,6,6	0.25	0
2	SO4	A	704	-	4,4,4	0.59	0	6,6,6	0.14	0
3	EDO	A	702	-	3,3,3	0.33	0	2,2,2	0.25	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	EDO	A	702	-	-	0/1/1/1	-
3	EDO	B	702	-	-	0/1/1/1	-

There are no bond length outliers.

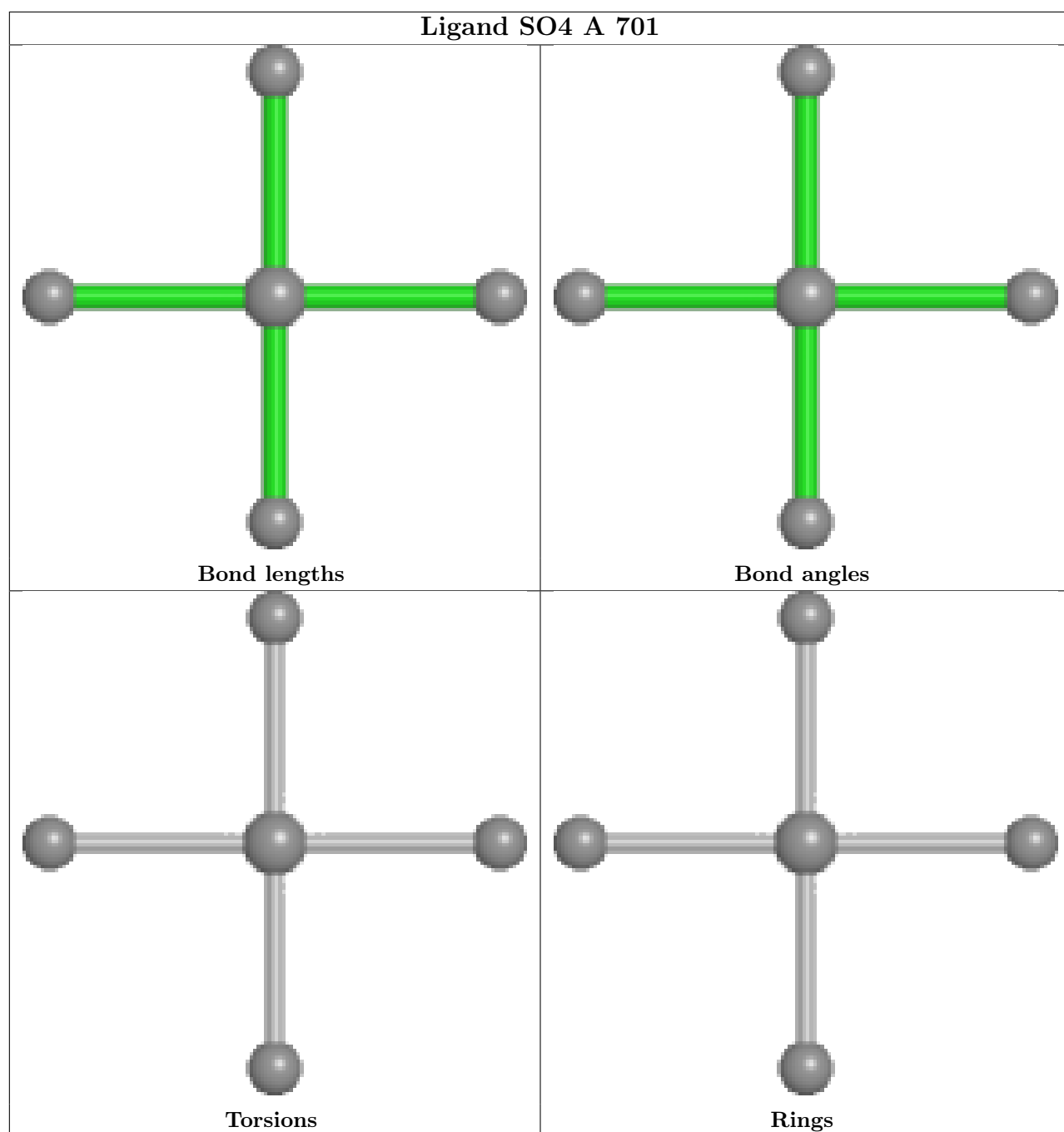There are no bond angle outliers.

There are no chirality outliers.
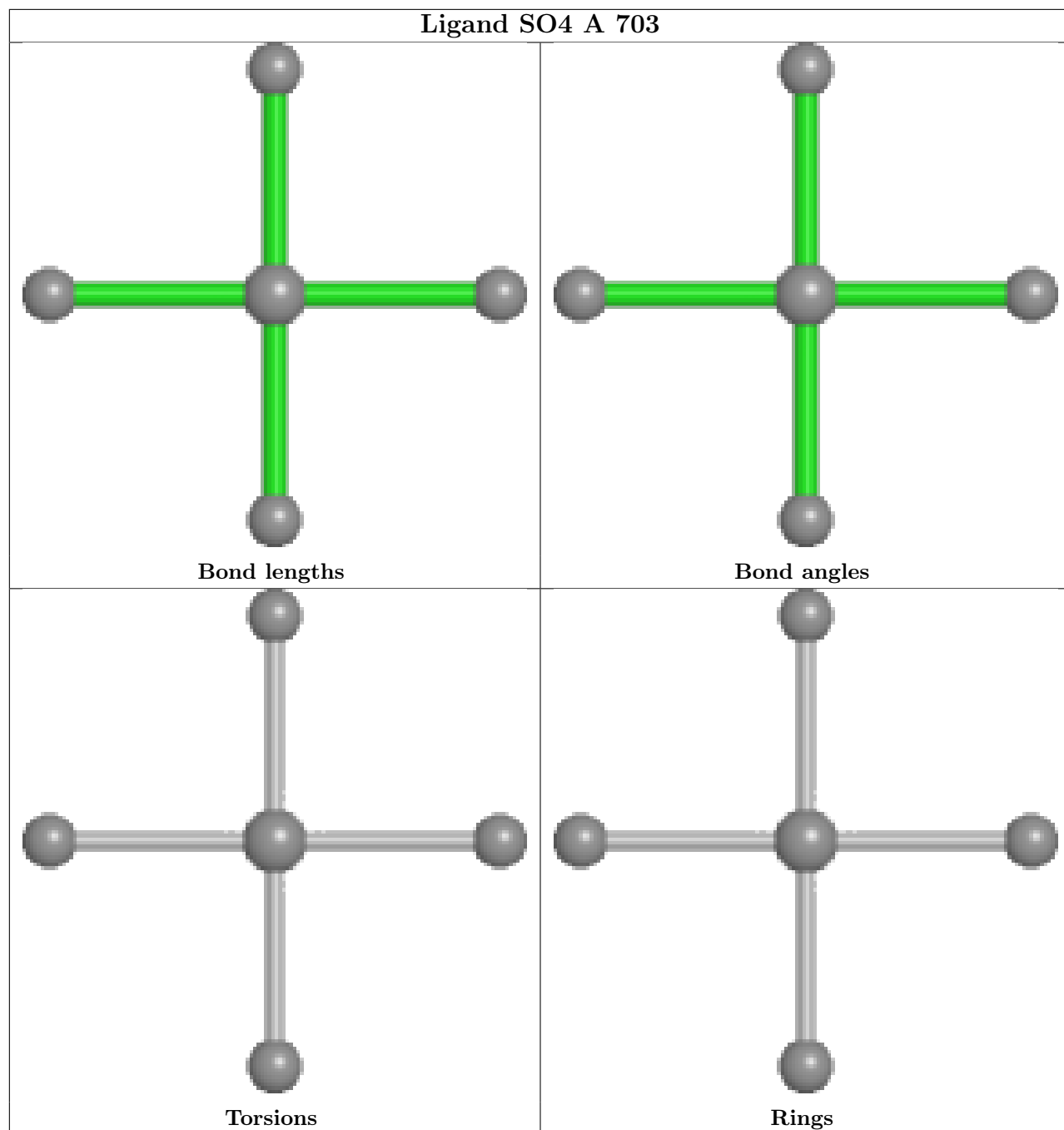
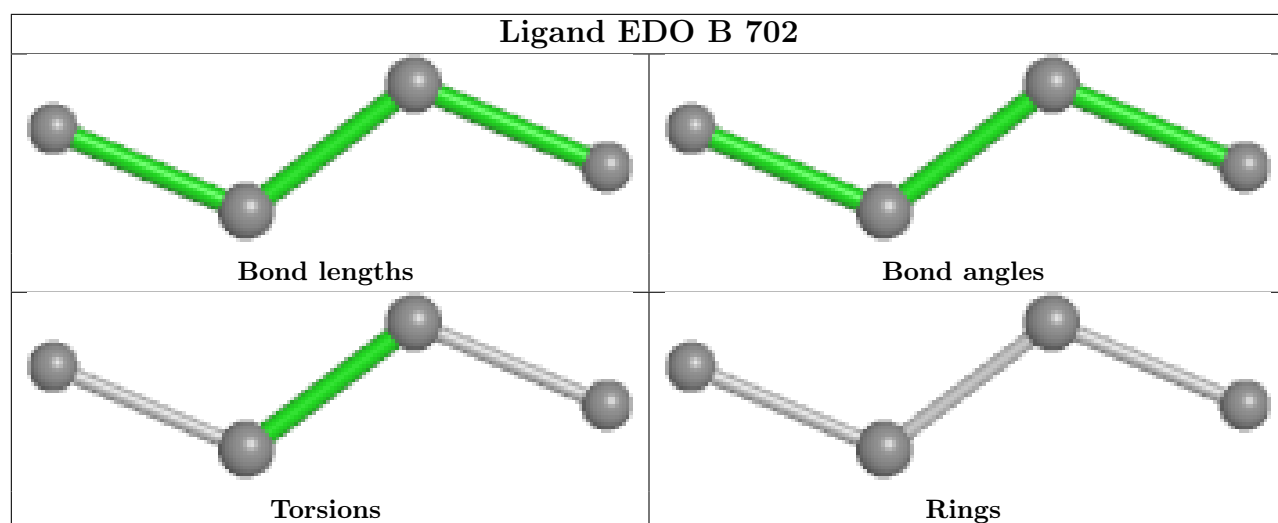There are no torsion outliers.

There are no ring outliers.
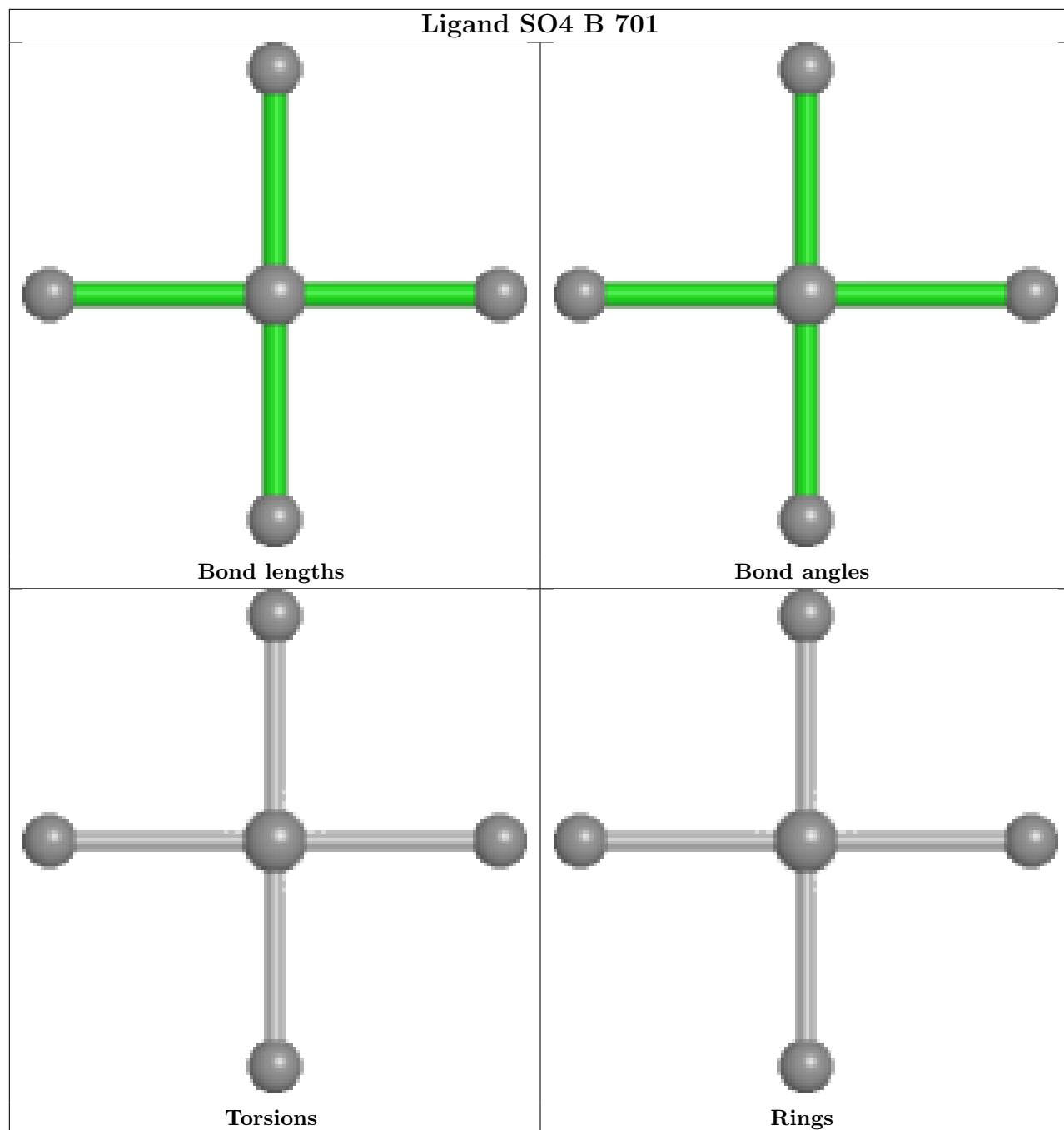
2 monomers are involved in 2 short contacts:

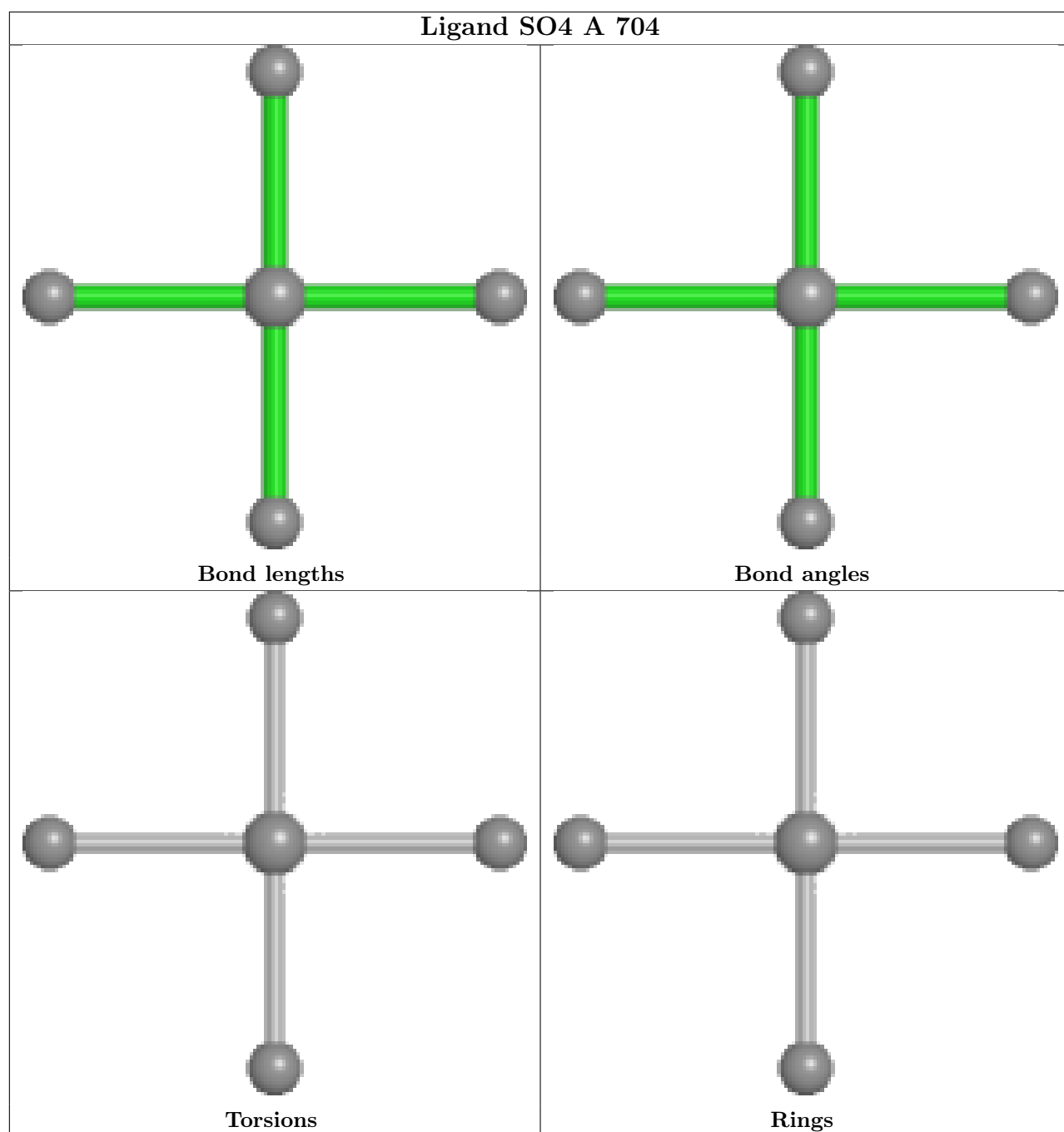| Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	EDO	1	0
3	A	702	EDO	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.
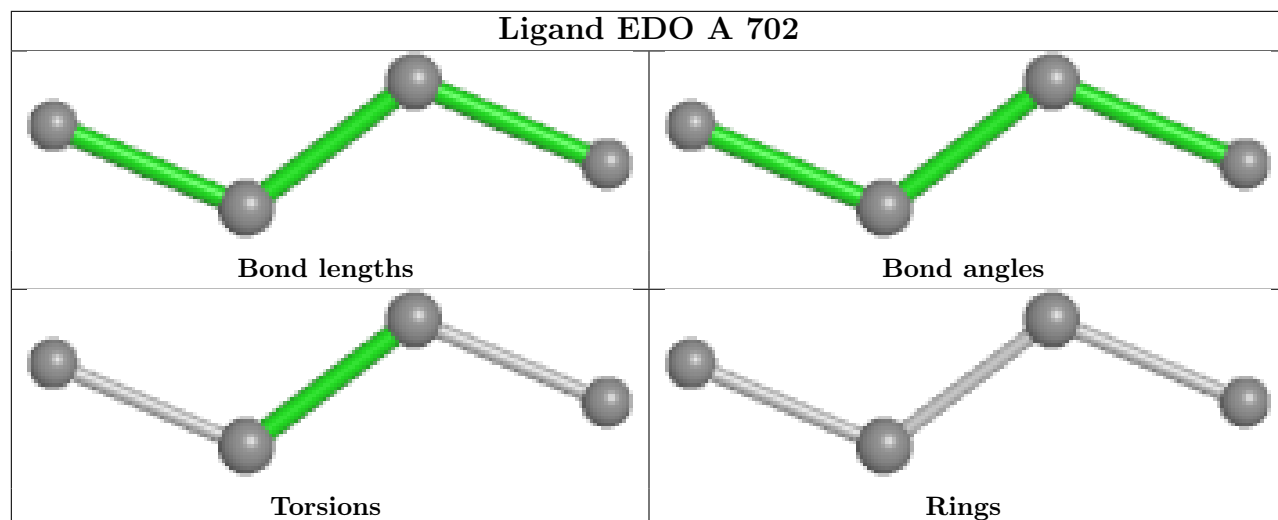
Ligand SO4 A 701

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 A 703

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO B 702

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 B 701

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 A 704

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO A 702

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	501/536 (93%)	0.14	27 (5%)	32	34	37, 53, 90, 122	0
1	B	501/536 (93%)	0.23	32 (6%)	27	28	30, 55, 106, 129	6 (1%)
All	All	1002/1072 (93%)	0.18	59 (5%)	29	30	30, 54, 101, 129	6 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	353	GLY	6.3
1	B	351	SER	5.7
1	B	100	ASN	5.5
1	B	179	HIS	4.7
1	A	493	ILE	4.4
1	B	352	GLU	4.2
1	B	130	LYS	3.9
1	A	355	ALA	3.7
1	A	494	LEU	3.6
1	B	200	LEU	3.4
1	B	101	LEU	3.3
1	A	133	GLU	3.3
1	B	253	ILE	3.3
1	A	491	GLU	3.2
1	A	219	LYS	3.2
1	B	538	ASP	3.1
1	B	218	ILE	3.1
1	B	354	GLY	3.0
1	A	100	ASN	3.0
1	A	130	LYS	3.0
1	A	98	ARG	3.0
1	B	350	SER	2.9
1	A	132	ASN	2.9
1	A	293	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	136	ILE	2.9
1	B	250	GLU	2.8
1	B	132	ASN	2.8
1	B	118	LYS	2.8
1	A	292	GLU	2.7
1	B	123	PHE	2.5
1	A	489	LYS	2.5
1	B	219	LYS	2.5
1	B	584	PHE	2.4
1	A	538	ASP	2.4
1	A	251	VAL	2.4
1	B	255	SER	2.4
1	A	179	HIS	2.3
1	A	294	SER	2.3
1	A	587	ASP	2.3
1	B	135	GLU	2.3
1	A	101	LEU	2.3
1	B	252	PRO	2.3
1	A	295	ILE	2.3
1	B	149	MET	2.3
1	B	222	ASP	2.2
1	A	488	LEU	2.2
1	B	180	LEU	2.2
1	B	108	VAL	2.2
1	B	460	GLU	2.1
1	A	630	ILE	2.1
1	B	537	GLU	2.1
1	B	385	PHE	2.1
1	A	581	LYS	2.1
1	A	209	LEU	2.1
1	B	116	ILE	2.1
1	A	583	ASN	2.0
1	B	104	GLU	2.0
1	A	289	THR	2.0
1	A	218	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	SO4	B	701	5/5	0.70	0.24	66,73,82,83	5
2	SO4	A	704	5/5	0.74	0.17	67,76,77,84	5
2	SO4	A	701	5/5	0.78	0.18	64,71,80,81	5
3	EDO	B	702	4/4	0.82	0.19	71,74,77,80	0
3	EDO	A	702	4/4	0.83	0.21	62,65,66,68	0
2	SO4	A	703	5/5	0.85	0.10	72,73,78,79	5

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.
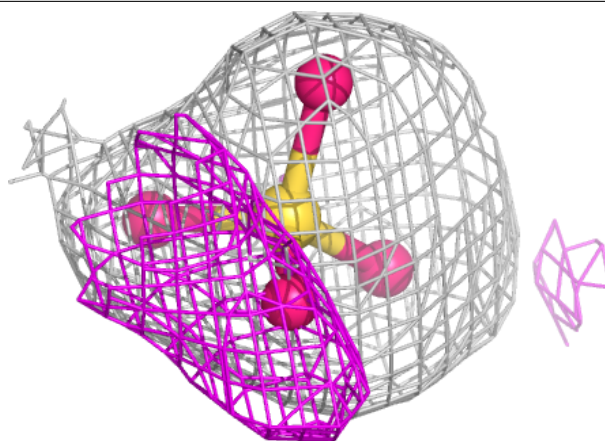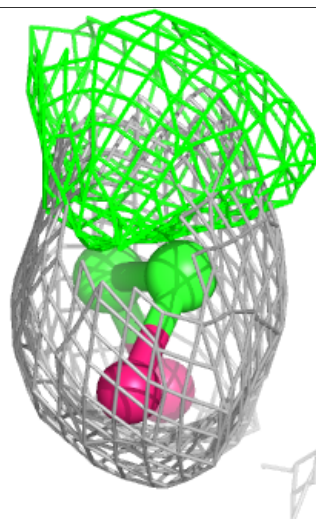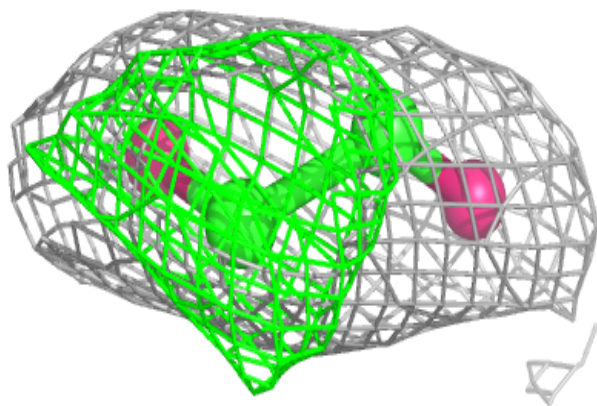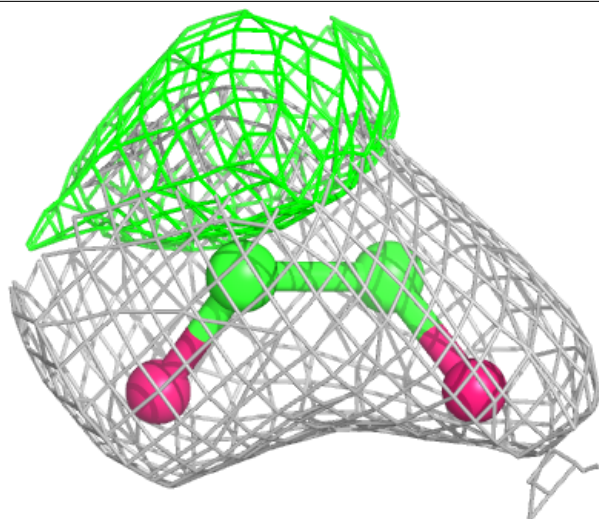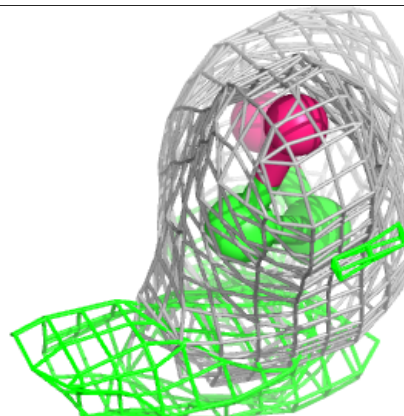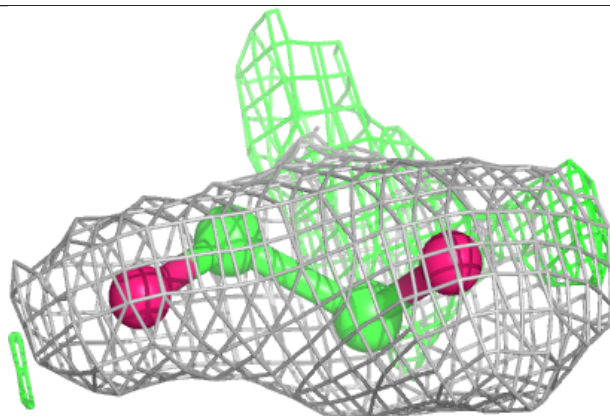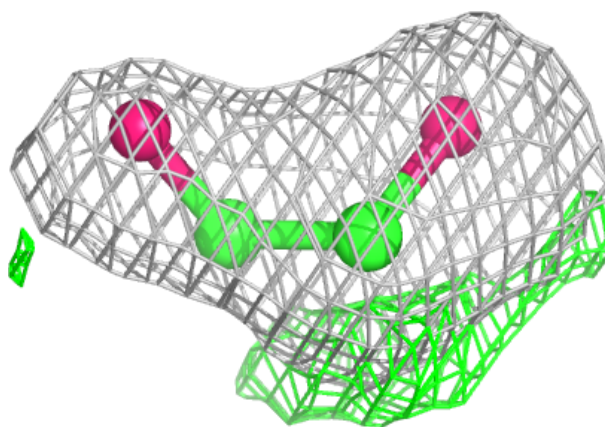
Electron density around SO4 B 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
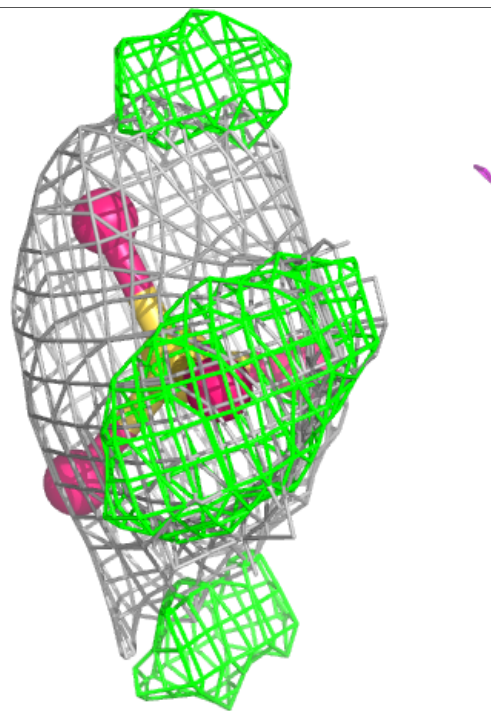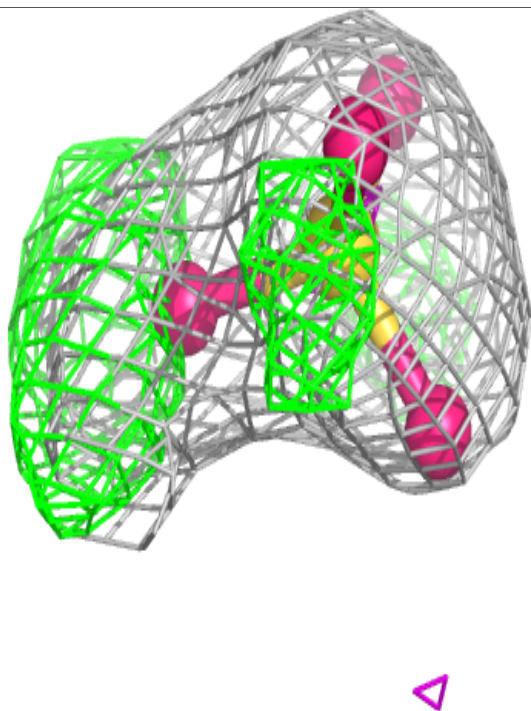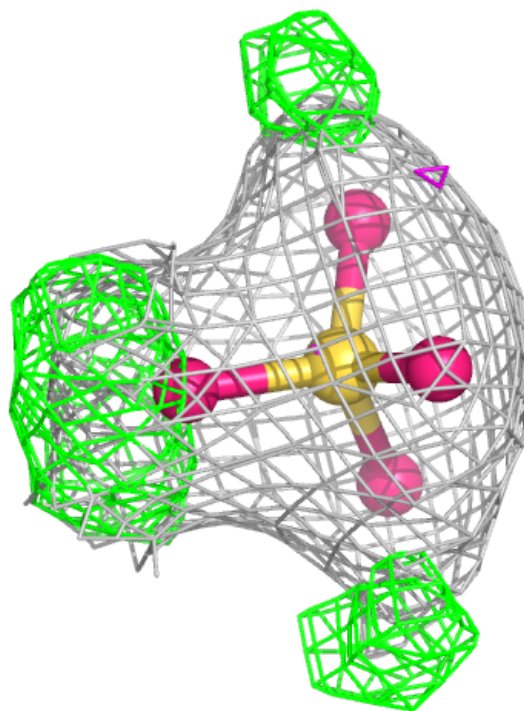
Electron density around SO4 A 704:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
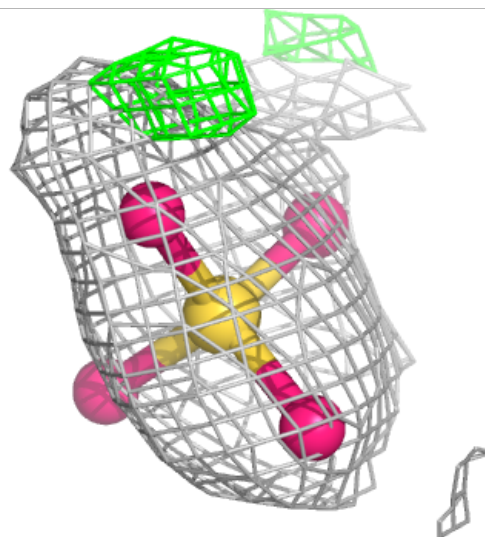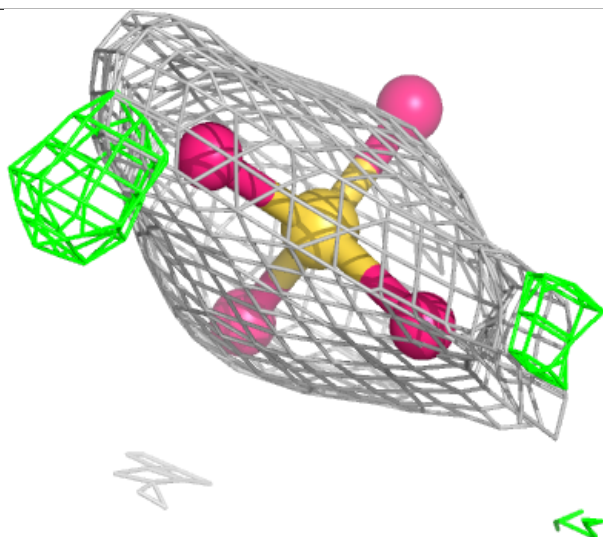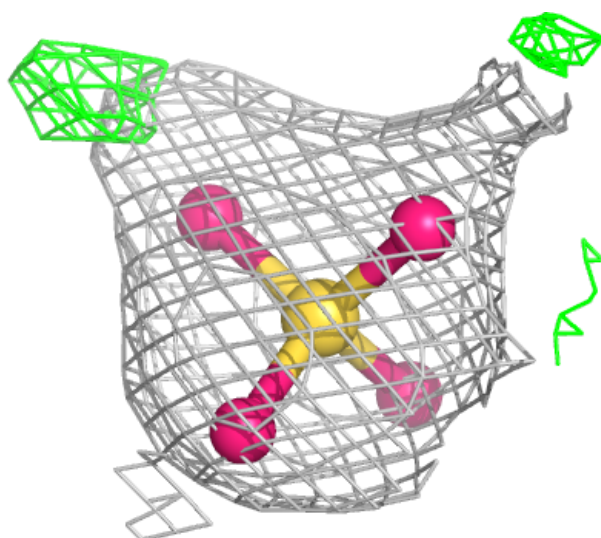
Electron density around SO4 A 701:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
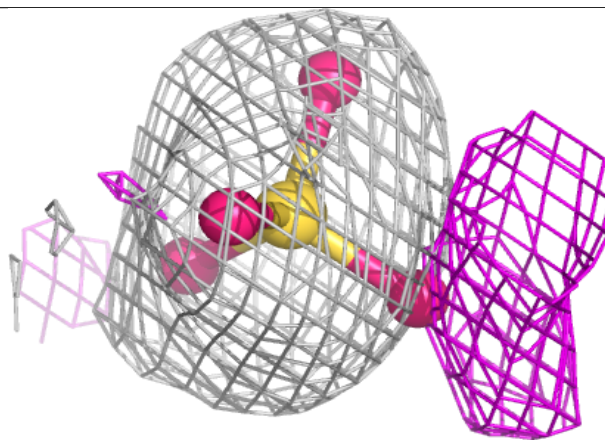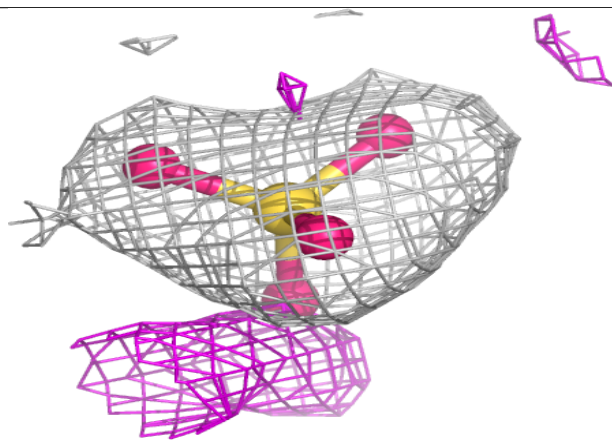
Electron density around EDO B 702:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
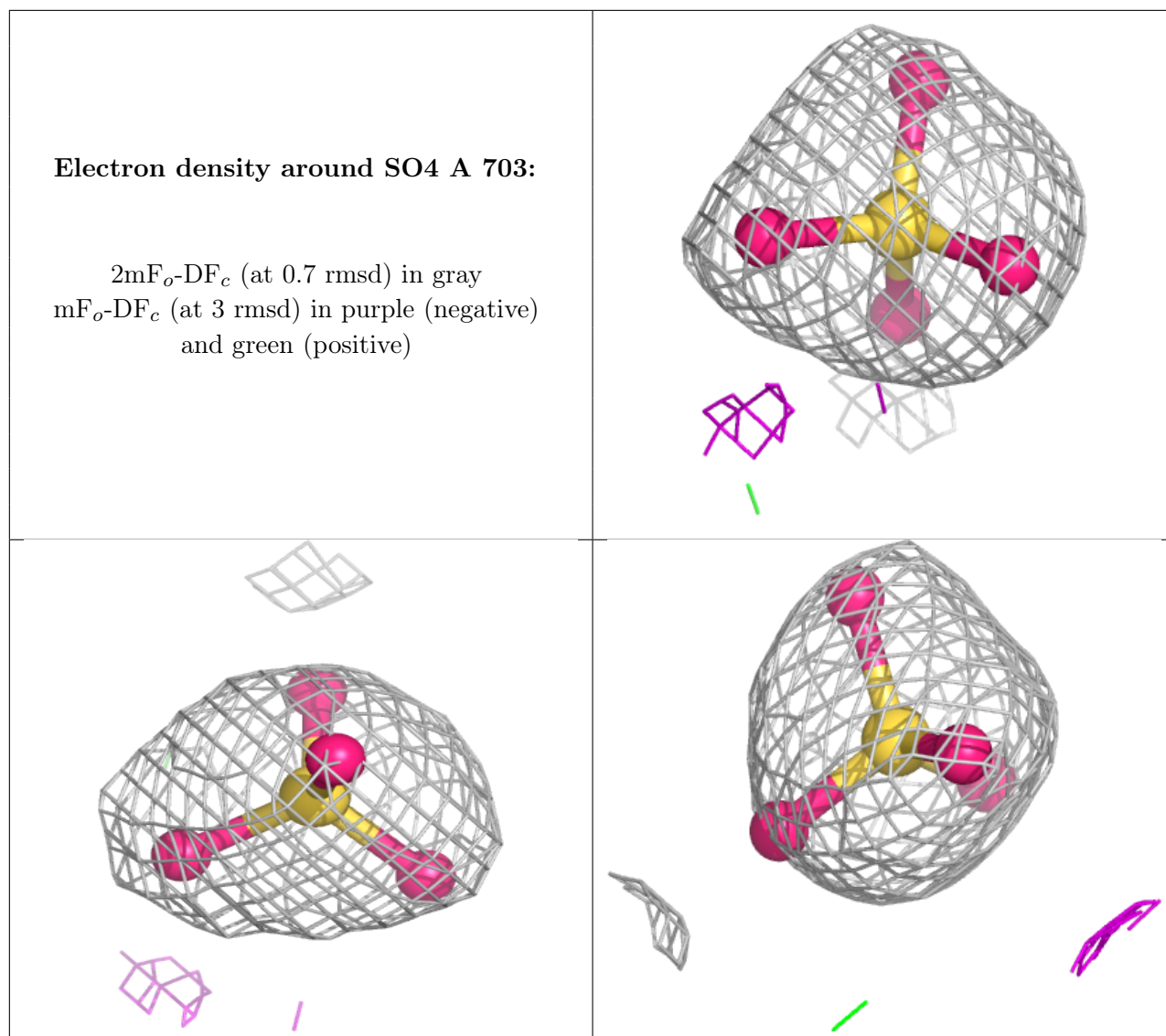and green (positive)

Electron density around EDO A 702:

$2mF_o$-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 703:

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

6.5   Other polymers ⓘ

There are no such residues in this entry.