



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 02:29 PM UTC

PDB ID : 7Y1U / pdb_00007y1u
Title : Crystal structure of isocitrate dehydrogenase from *Campylobacter corcagiensis*
Authors : Bian, M.J.; Cheng, Q.P.; Wang, P.; Zhu, G.P.
Deposited on : 2022-06-08
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

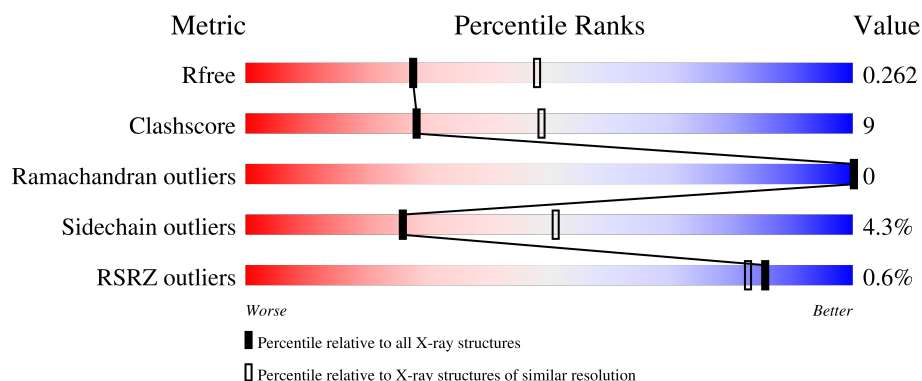
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	723	

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
5	PG4	A	808	-	-	X	-

2 Entry composition [i](#)

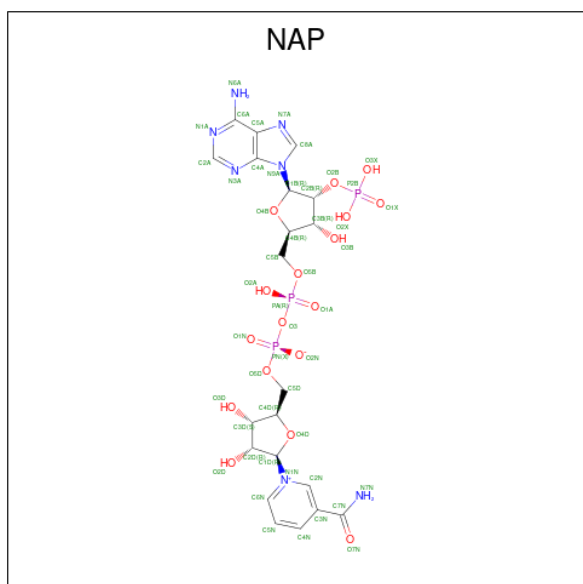
There are 7 unique types of molecules in this entry. The entry contains 5975 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Isocitrate dehydrogenase [NADP].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	723	Total	C	N	O	S	0	1	0
			5714	3643	952	1100	19			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).

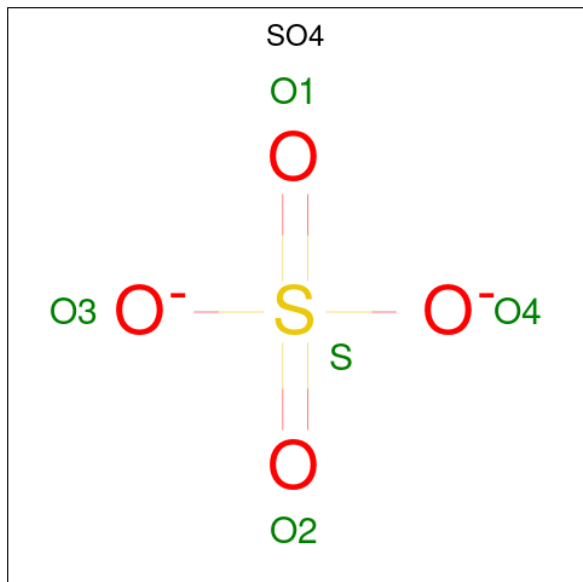


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		

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



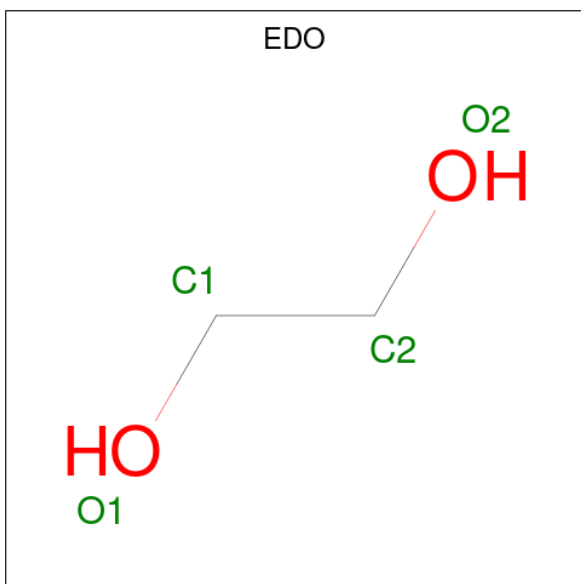
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

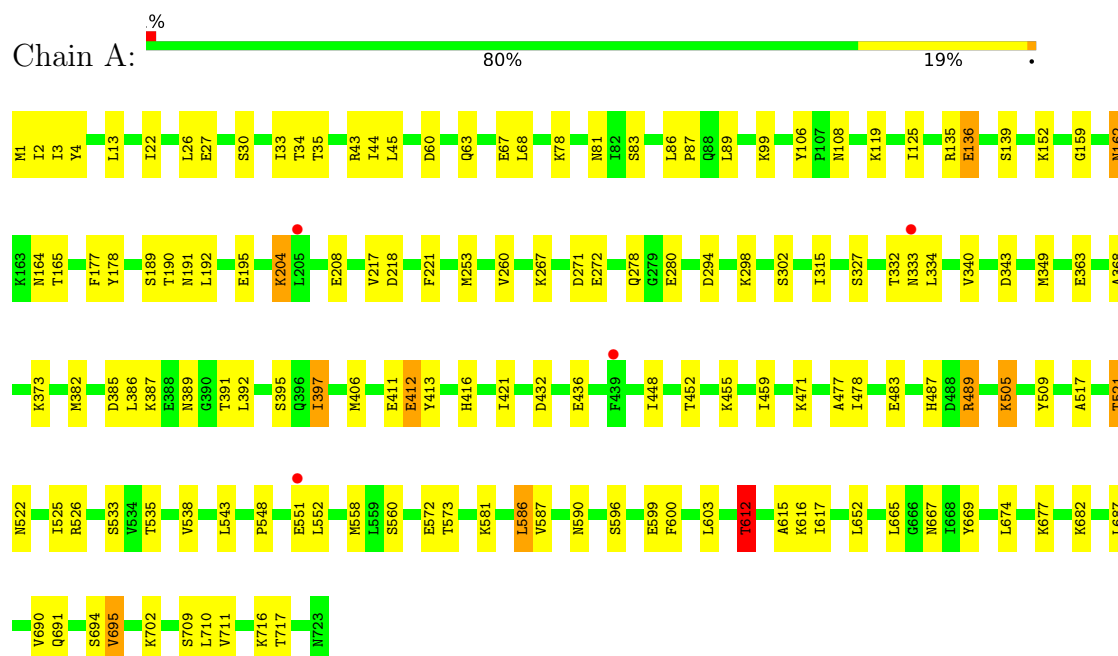
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	149	Total	O	0	0
			149	149		

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: Isocitrate dehydrogenase [NADP]



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.50Å 92.69Å 147.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.93 – 2.50 48.93 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.93-2.50) 99.9 (48.93-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.188 , 0.259 0.198 , 0.262	Depositor DCC
R_{free} test set	1548 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5975	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, MN, PG4, NAP, 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	1.11	2/5818 (0.0%)	1.47	9/7842 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	LEU	C-O	7.16	1.32	1.24
1	A	533	SER	C-O	5.21	1.30	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	ASP	CA-CB-CG	5.95	118.55	112.60
1	A	136	GLU	N-CA-C	-5.66	104.56	112.25
1	A	136	GLU	CB-CA-C	5.64	118.98	111.14
1	A	177	PHE	CA-C-N	5.42	127.49	120.44
1	A	177	PHE	C-N-CA	5.42	127.49	120.44
1	A	278	GLN	CA-C-N	5.33	125.87	120.00
1	A	278	GLN	C-N-CA	5.33	125.87	120.00
1	A	363	GLU	CB-CA-C	5.13	118.20	109.84
1	A	612	THR	CB-CA-C	5.03	120.00	109.68

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	5714	0	5789	103	0
2	A	48	0	25	2	0
3	A	1	0	0	0	0
4	A	25	0	0	0	0
5	A	26	0	36	10	0
6	A	12	0	18	1	0
7	A	149	0	0	2	0
All	All	5975	0	5868	104	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 9.

All (104) 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:411:GLU:HA	1:A:452:THR:CG2	1.95	0.96
1:A:411:GLU:HA	1:A:452:THR:HG21	1.46	0.93
1:A:517:ALA:O	1:A:521:THR:HG23	1.70	0.91
1:A:581:LYS:NZ	5:A:808:PG4:H52	1.90	0.86
1:A:581:LYS:HZ3	5:A:808:PG4:H52	1.43	0.84
1:A:22:ILE:HD12	1:A:603:LEU:HD22	1.61	0.81
1:A:581:LYS:NZ	5:A:808:PG4:H81	1.99	0.78
1:A:391:THR:HB	7:A:1022:HOH:O	1.83	0.77
1:A:333:ASN:CG	1:A:340:VAL:HG21	2.13	0.73
1:A:4:TYR:O	1:A:35:THR:HA	1.90	0.71
1:A:551:GLU:HG3	1:A:552:LEU:HG	1.73	0.70
1:A:483:GLU:O	1:A:489:ARG:NH1	2.24	0.69
1:A:333:ASN:OD1	1:A:340:VAL:HG21	1.94	0.68
1:A:581:LYS:HZ2	5:A:808:PG4:H81	1.60	0.66
1:A:165:THR:O	1:A:387:LYS:HE2	1.98	0.64
1:A:253:MET:HE2	1:A:413:TYR:CE1	2.33	0.64
1:A:522:ASN:O	1:A:526:ARG:HG3	2.00	0.62
1:A:162:ASN:ND2	1:A:164:ASN:HB2	2.16	0.60
1:A:333:ASN:OD1	1:A:340:VAL:CG2	2.49	0.60
1:A:108:ASN:O	1:A:119:LYS:NZ	2.35	0.60
1:A:682:LYS:HE3	1:A:717:THR:HG21	1.84	0.60
1:A:106:TYR:OH	5:A:809:PG4:H21	2.01	0.60
1:A:1:MET:HE3	1:A:34:THR:OG1	2.02	0.59
1:A:260:VAL:HG21	1:A:421:ILE:HD11	1.82	0.59
1:A:382:MET:HE3	1:A:386:LEU:HG	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LEU:HD13	1:A:586:LEU:HD22	1.84	0.59
1:A:600:PHE:CD1	1:A:652:LEU:HD22	2.38	0.59
1:A:411:GLU:CA	1:A:452:THR:CG2	2.78	0.58
1:A:600:PHE:CE1	1:A:652:LEU:HD22	2.38	0.57
1:A:596:SER:HA	1:A:599:GLU:OE2	2.04	0.57
1:A:581:LYS:HZ3	5:A:808:PG4:H81	1.70	0.56
1:A:272:GLU:HB2	1:A:315:ILE:HD11	1.89	0.55
1:A:22:ILE:HD12	1:A:603:LEU:CD2	2.33	0.55
1:A:1:MET:CE	1:A:34:THR:OG1	2.55	0.54
1:A:581:LYS:HZ1	5:A:808:PG4:H42	1.73	0.54
1:A:695:VAL:HG13	1:A:711:VAL:HG21	1.88	0.54
1:A:382:MET:HE2	1:A:386:LEU:HD11	1.90	0.54
1:A:86:LEU:HB3	1:A:87:PRO:HD3	1.91	0.53
1:A:78:LYS:O	1:A:572:GLU:HA	2.08	0.53
1:A:99:LYS:NZ	1:A:702:LYS:O	2.42	0.53
1:A:581:LYS:NZ	5:A:808:PG4:H12	2.24	0.53
1:A:382:MET:HE1	1:A:392:LEU:CD1	2.38	0.53
1:A:221:PHE:HA	1:A:448:ILE:O	2.08	0.52
1:A:382:MET:HE1	1:A:392:LEU:HD11	1.91	0.52
1:A:612:THR:HG22	1:A:615:ALA:H	1.76	0.51
1:A:695:VAL:CG1	1:A:711:VAL:HG21	2.40	0.51
1:A:139:SER:HB2	1:A:406:MET:HE2	1.93	0.50
1:A:280:GLU:OE2	1:A:302:SER:OG	2.23	0.50
1:A:135:ARG:HD3	1:A:406:MET:SD	2.52	0.49
1:A:162:ASN:HD21	1:A:164:ASN:HB2	1.75	0.49
1:A:551:GLU:CG	1:A:552:LEU:HG	2.42	0.49
1:A:1:MET:HE1	1:A:34:THR:HG23	1.94	0.49
1:A:421:ILE:CD1	5:A:809:PG4:H82	2.43	0.49
1:A:162:ASN:C	1:A:162:ASN:HD22	2.21	0.48
1:A:477:ALA:O	1:A:509:TYR:HA	2.13	0.48
1:A:343:ASP:OD1	1:A:343:ASP:N	2.47	0.48
1:A:411:GLU:HA	1:A:452:THR:HG23	1.89	0.48
1:A:332:THR:C	1:A:334:LEU:H	2.22	0.48
1:A:81:ASN:O	2:A:801:NAP:H2N	2.14	0.47
1:A:411:GLU:CA	1:A:452:THR:HG23	2.44	0.47
1:A:136:GLU:HG3	7:A:985:HOH:O	2.14	0.47
1:A:253:MET:O	1:A:416:HIS:CE1	2.69	0.46
1:A:253:MET:HE2	1:A:413:TYR:CZ	2.51	0.46
1:A:43:ARG:NH2	1:A:125:ILE:O	2.49	0.46
1:A:560:SER:HB3	1:A:572:GLU:HB2	1.98	0.46
1:A:294:ASP:O	1:A:298:LYS:HG3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ASP:OD1	1:A:389:ASN:ND2	2.48	0.45
1:A:478:ILE:HD12	1:A:521:THR:HG22	1.97	0.45
1:A:83:SER:HB2	6:A:812:EDO:H22	1.98	0.45
1:A:349:MET:CE	1:A:368:ALA:HB2	2.47	0.45
1:A:411:GLU:OE2	1:A:487:HIS:NE2	2.30	0.45
1:A:587:VAL:O	1:A:694:SER:HA	2.16	0.45
1:A:152:LYS:HA	1:A:395:SER:HA	1.99	0.44
1:A:471:LYS:NZ	1:A:505:LYS:O	2.50	0.44
1:A:412:GLU:HG3	1:A:538:VAL:HG21	1.99	0.44
1:A:432:ASP:OD1	1:A:436:GLU:N	2.51	0.44
1:A:548:PRO:HG3	1:A:558:MET:HE2	2.00	0.44
1:A:3:ILE:HD13	1:A:68:LEU:CD2	2.48	0.43
1:A:178:TYR:CD1	1:A:373:LYS:HD2	2.52	0.43
1:A:253:MET:HE2	1:A:413:TYR:CD1	2.53	0.43
1:A:397:ILE:HA	1:A:525:ILE:O	2.18	0.43
1:A:581:LYS:HZ1	5:A:808:PG4:H12	1.82	0.43
1:A:63:GLN:OE1	1:A:67:GLU:OE2	2.37	0.43
1:A:159:GLY:O	1:A:391:THR:HG21	2.19	0.43
1:A:217:VAL:HA	1:A:452:THR:O	2.19	0.43
1:A:687:LEU:O	1:A:690:VAL:HG22	2.18	0.43
1:A:455:LYS:O	1:A:459:ILE:HG13	2.20	0.42
1:A:617:ILE:HG21	1:A:665:LEU:HD13	2.00	0.42
1:A:548:PRO:HA	1:A:551:GLU:HG2	2.00	0.42
1:A:195:GLU:HA	1:A:204:LYS:O	2.19	0.42
1:A:162:ASN:HD22	1:A:164:ASN:N	2.18	0.42
1:A:535:THR:HG21	1:A:543:LEU:HD12	2.02	0.41
1:A:44:ILE:HD11	1:A:89:LEU:HD12	2.03	0.41
1:A:60:ASP:CG	1:A:63:GLN:HB2	2.45	0.41
1:A:382:MET:CE	1:A:386:LEU:HG	2.48	0.41
1:A:139:SER:HB2	1:A:406:MET:CE	2.51	0.41
1:A:332:THR:C	1:A:334:LEU:N	2.79	0.41
1:A:2:ILE:O	1:A:33:ILE:HA	2.20	0.40
1:A:333:ASN:OD1	1:A:340:VAL:HB	2.21	0.40
1:A:573:THR:HB	1:A:599:GLU:HG3	2.04	0.40
1:A:590:ASN:O	1:A:691:GLN:HG2	2.21	0.40
1:A:616:LYS:HE3	1:A:616:LYS:HB2	1.83	0.40
2:A:801:NAP:O1X	2:A:801:NAP:O3B	2.39	0.40
1:A:665:LEU:HD23	1:A:669:TYR:HE2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	722/723 (100%)	691 (96%)	31 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	627/626 (100%)	600 (96%)	27 (4%)	26	51

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	27	GLU
1	A	30	SER
1	A	162	ASN
1	A	189	SER
1	A	190	THR
1	A	191	ASN
1	A	192	LEU
1	A	204	LYS
1	A	208	GLU
1	A	218	ASP
1	A	267	LYS
1	A	327	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	397	ILE
1	A	412	GLU
1	A	489	ARG
1	A	505	LYS
1	A	521	THR
1	A	586	LEU
1	A	612	THR
1	A	667	ASN
1	A	674	LEU
1	A	677	LYS
1	A	695	VAL
1	A	709	SER
1	A	710	LEU
1	A	716	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	162	ASN
1	A	210	ASN
1	A	416	HIS
1	A	490	ASN
1	A	647	ASN
1	A	684	ASN

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

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PG4	A	808	-	12,12,12	0.15	0	11,11,11	0.12	0
2	NAP	A	801	-	50,52,52	4.63	31 (62%)	71,80,80	2.21	27 (38%)
6	EDO	A	811	-	3,3,3	0.10	0	2,2,2	0.06	0
5	PG4	A	809	-	12,12,12	0.15	0	11,11,11	0.12	0
4	SO4	A	807	-	4,4,4	0.30	0	6,6,6	0.16	0
4	SO4	A	803	-	4,4,4	0.43	0	6,6,6	0.15	0
4	SO4	A	805	-	4,4,4	0.33	0	6,6,6	0.28	0
6	EDO	A	810	-	3,3,3	0.23	0	2,2,2	0.12	0
4	SO4	A	806	-	4,4,4	0.29	0	6,6,6	0.24	0
6	EDO	A	812	-	3,3,3	0.27	0	2,2,2	0.47	0
4	SO4	A	804	-	4,4,4	0.45	0	6,6,6	0.14	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
5	PG4	A	808	-	-	9/10/10/10	-
2	NAP	A	801	-	-	5/35/67/67	0/5/5/5
6	EDO	A	811	-	-	1/1/1/1	-
5	PG4	A	809	-	-	6/10/10/10	-
6	EDO	A	810	-	-	1/1/1/1	-
6	EDO	A	812	-	-	1/1/1/1	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	NAP	O4D-C1D	11.40	1.55	1.40
2	A	801	NAP	C2N-N1N	10.83	1.46	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	NAP	O4D-C4D	-8.58	1.25	1.45
2	A	801	NAP	C3B-C4B	-8.39	1.31	1.53
2	A	801	NAP	C2B-C1B	-8.34	1.32	1.53
2	A	801	NAP	C2N-C3N	8.08	1.51	1.39
2	A	801	NAP	C4A-N3A	8.07	1.49	1.34
2	A	801	NAP	C2D-C3D	-7.95	1.31	1.53
2	A	801	NAP	C6A-N6A	6.41	1.50	1.34
2	A	801	NAP	C5N-C4N	5.91	1.49	1.38
2	A	801	NAP	C6N-C5N	5.54	1.50	1.38
2	A	801	NAP	O4B-C1B	5.47	1.54	1.42
2	A	801	NAP	C7N-N7N	5.00	1.42	1.33
2	A	801	NAP	C2A-N3A	4.96	1.42	1.33
2	A	801	NAP	C3D-C4D	4.80	1.65	1.53
2	A	801	NAP	C6N-N1N	4.56	1.45	1.35
2	A	801	NAP	C2A-N1A	4.54	1.42	1.33
2	A	801	NAP	O4B-C4B	4.21	1.54	1.45
2	A	801	NAP	C5A-C6A	4.18	1.52	1.41
2	A	801	NAP	C4N-C3N	3.73	1.45	1.39
2	A	801	NAP	C3B-C2B	3.71	1.61	1.53
2	A	801	NAP	O3B-C3B	3.59	1.51	1.43
2	A	801	NAP	C6A-N1A	3.29	1.45	1.35
2	A	801	NAP	PN-O3	3.22	1.63	1.59
2	A	801	NAP	O7N-C7N	-3.21	1.18	1.24
2	A	801	NAP	O2D-C2D	2.95	1.50	1.43
2	A	801	NAP	O5B-C5B	-2.51	1.35	1.44
2	A	801	NAP	C5A-N7A	-2.41	1.34	1.39
2	A	801	NAP	C8A-N7A	2.33	1.36	1.31
2	A	801	NAP	P2B-O2B	2.11	1.63	1.59
2	A	801	NAP	PN-O5D	2.05	1.67	1.59

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	NAP	N3A-C2A-N1A	-5.67	120.00	128.58
2	A	801	NAP	C5B-C4B-C3B	-5.25	96.31	115.21
2	A	801	NAP	C5N-C4N-C3N	-4.12	116.31	120.36
2	A	801	NAP	C6N-N1N-C2N	-3.97	118.50	121.88
2	A	801	NAP	C2B-C1B-N9A	-3.67	107.71	113.75
2	A	801	NAP	C4D-O4D-C1D	-3.65	106.58	109.92
2	A	801	NAP	N9A-C8A-N7A	-3.62	108.80	113.94
2	A	801	NAP	O2N-PN-O3	-3.55	97.68	107.27
2	A	801	NAP	O3-PA-O1A	3.55	121.38	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	NAP	O2B-C2B-C3B	-3.49	99.14	111.68
2	A	801	NAP	O5B-PA-O1A	3.46	122.65	108.94
2	A	801	NAP	O7N-C7N-C3N	3.44	123.81	119.60
2	A	801	NAP	C5A-C4A-N3A	-3.30	122.17	126.72
2	A	801	NAP	C3N-C7N-N7N	-3.17	113.83	117.74
2	A	801	NAP	C3B-C2B-C1B	3.15	108.84	102.81
2	A	801	NAP	C2A-N3A-C4A	2.98	119.10	111.83
2	A	801	NAP	O3B-C3B-C2B	2.94	119.42	111.19
2	A	801	NAP	C6N-C5N-C4N	2.86	123.57	119.45
2	A	801	NAP	O3D-C3D-C4D	-2.76	103.17	111.08
2	A	801	NAP	C5A-N7A-C8A	2.38	107.18	103.45
2	A	801	NAP	O4B-C4B-C3B	2.34	109.79	105.15
2	A	801	NAP	C5A-C4A-N9A	2.28	108.30	105.81
2	A	801	NAP	C4B-O4B-C1B	-2.26	104.47	109.47
2	A	801	NAP	O2A-PA-O3	-2.24	101.22	107.27
2	A	801	NAP	O3-PN-O1N	2.18	117.26	110.70
2	A	801	NAP	C2N-C3N-C4N	2.13	120.73	118.26
2	A	801	NAP	C4A-C5A-N7A	-2.05	108.24	110.58

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	NAP	C5B-O5B-PA-O2A
2	A	801	NAP	C5B-O5B-PA-O3
2	A	801	NAP	O4D-C1D-N1N-C2N
2	A	801	NAP	O4D-C1D-N1N-C6N
5	A	808	PG4	O2-C3-C4-O3
5	A	808	PG4	O3-C5-C6-O4
5	A	808	PG4	O4-C7-C8-O5
5	A	809	PG4	O3-C5-C6-O4
6	A	810	EDO	O1-C1-C2-O2
6	A	812	EDO	O1-C1-C2-O2
5	A	809	PG4	O2-C3-C4-O3
5	A	809	PG4	C1-C2-O2-C3
5	A	809	PG4	C5-C6-O4-C7
5	A	808	PG4	C4-C3-O2-C2
5	A	808	PG4	C1-C2-O2-C3
5	A	808	PG4	C3-C4-O3-C5
5	A	808	PG4	C5-C6-O4-C7
5	A	808	PG4	C8-C7-O4-C6
5	A	808	PG4	C6-C5-O3-C4

Continued on next page...

Continued from previous page...

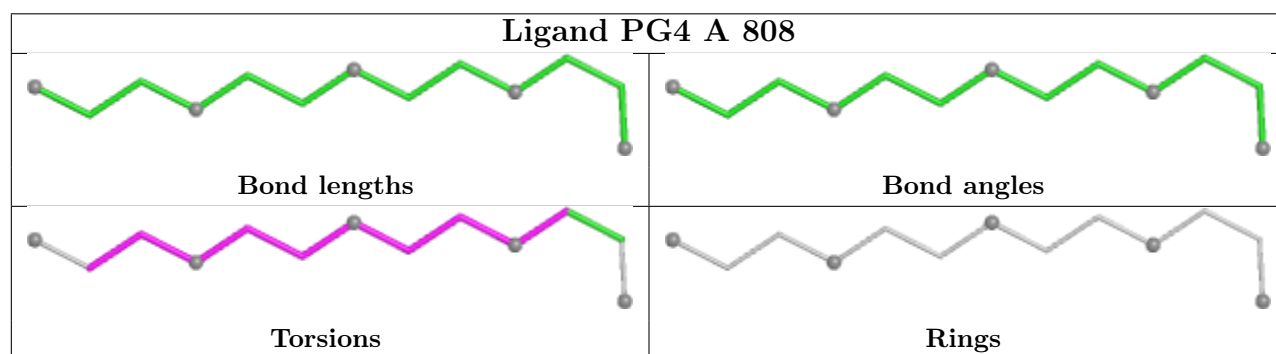
Mol	Chain	Res	Type	Atoms
2	A	801	NAP	C2D-C1D-N1N-C2N
5	A	809	PG4	C6-C5-O3-C4
6	A	811	EDO	O1-C1-C2-O2
5	A	809	PG4	C3-C4-O3-C5

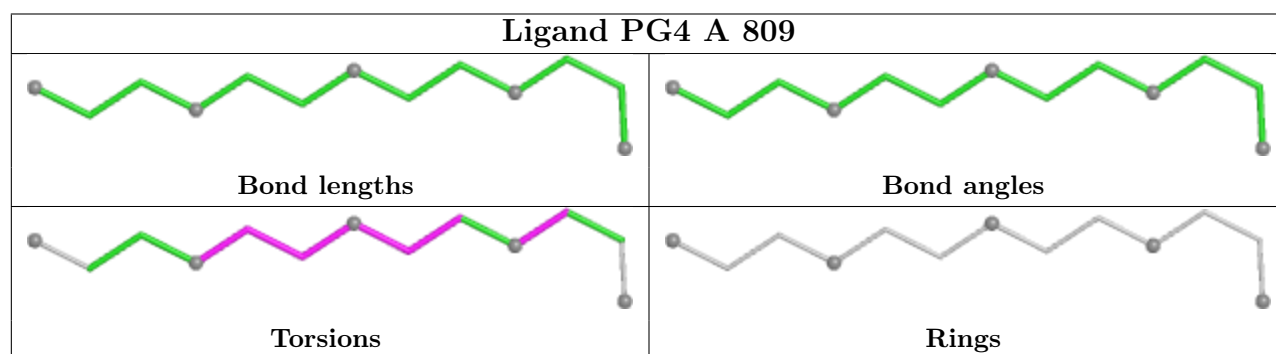
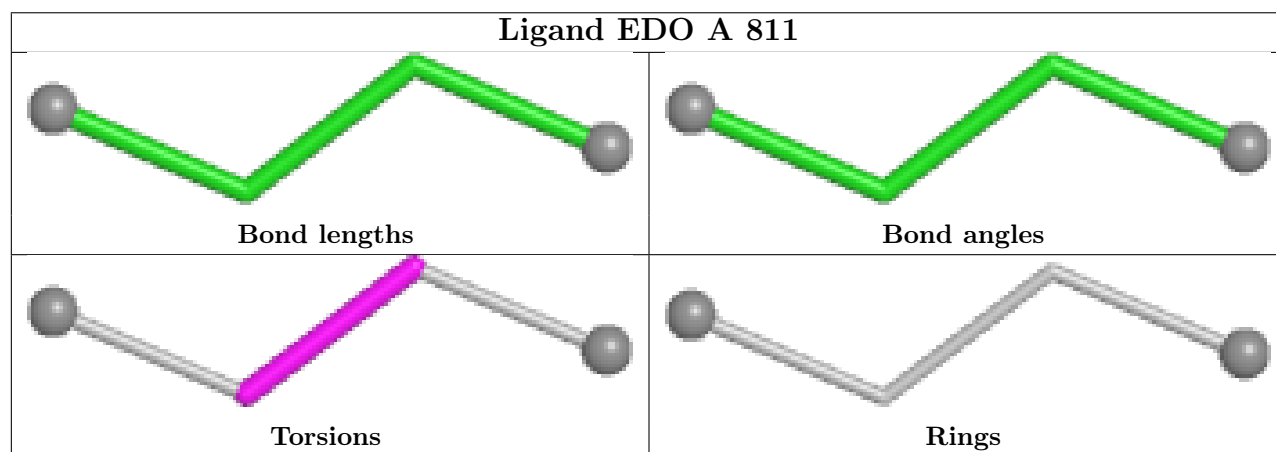
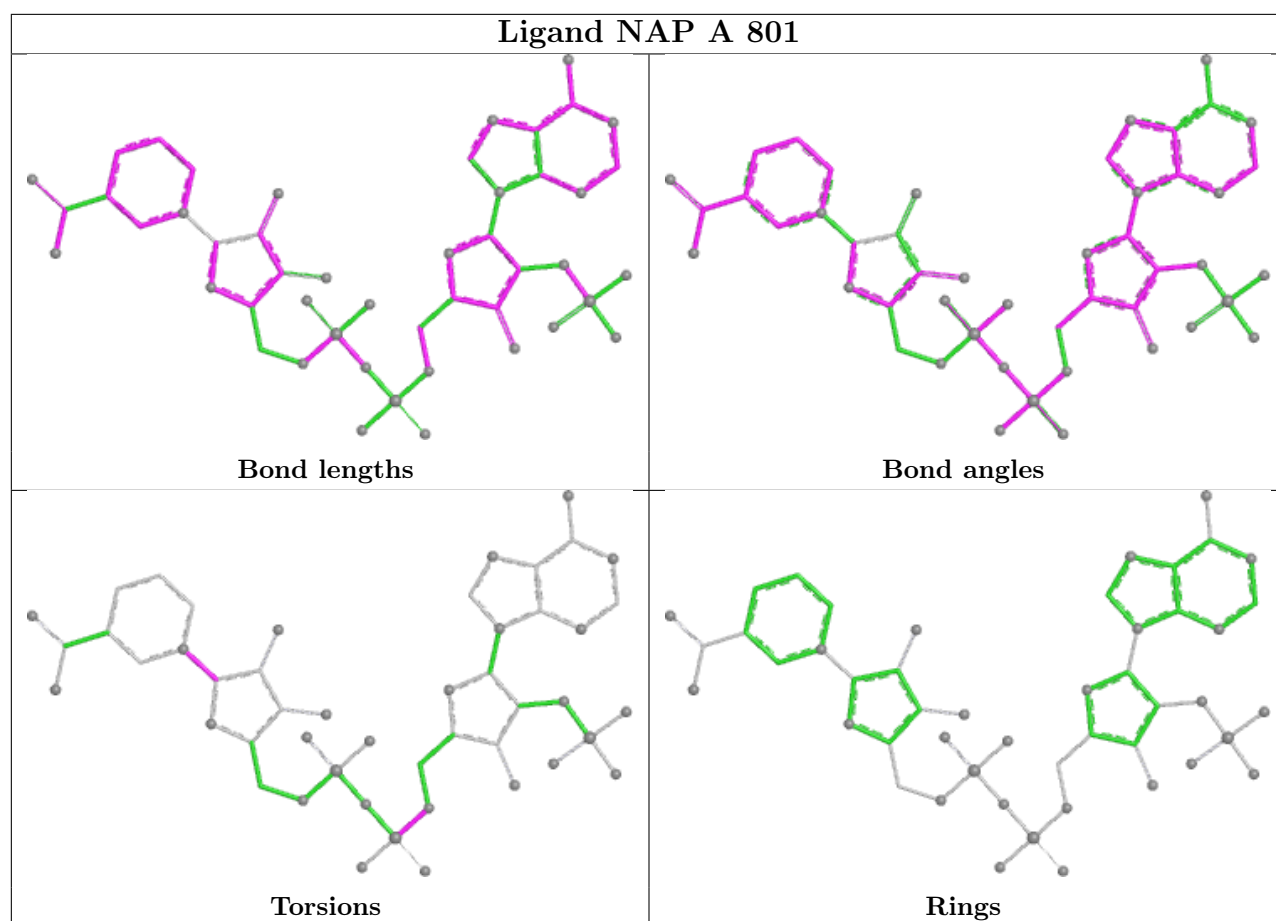
There are no ring outliers.

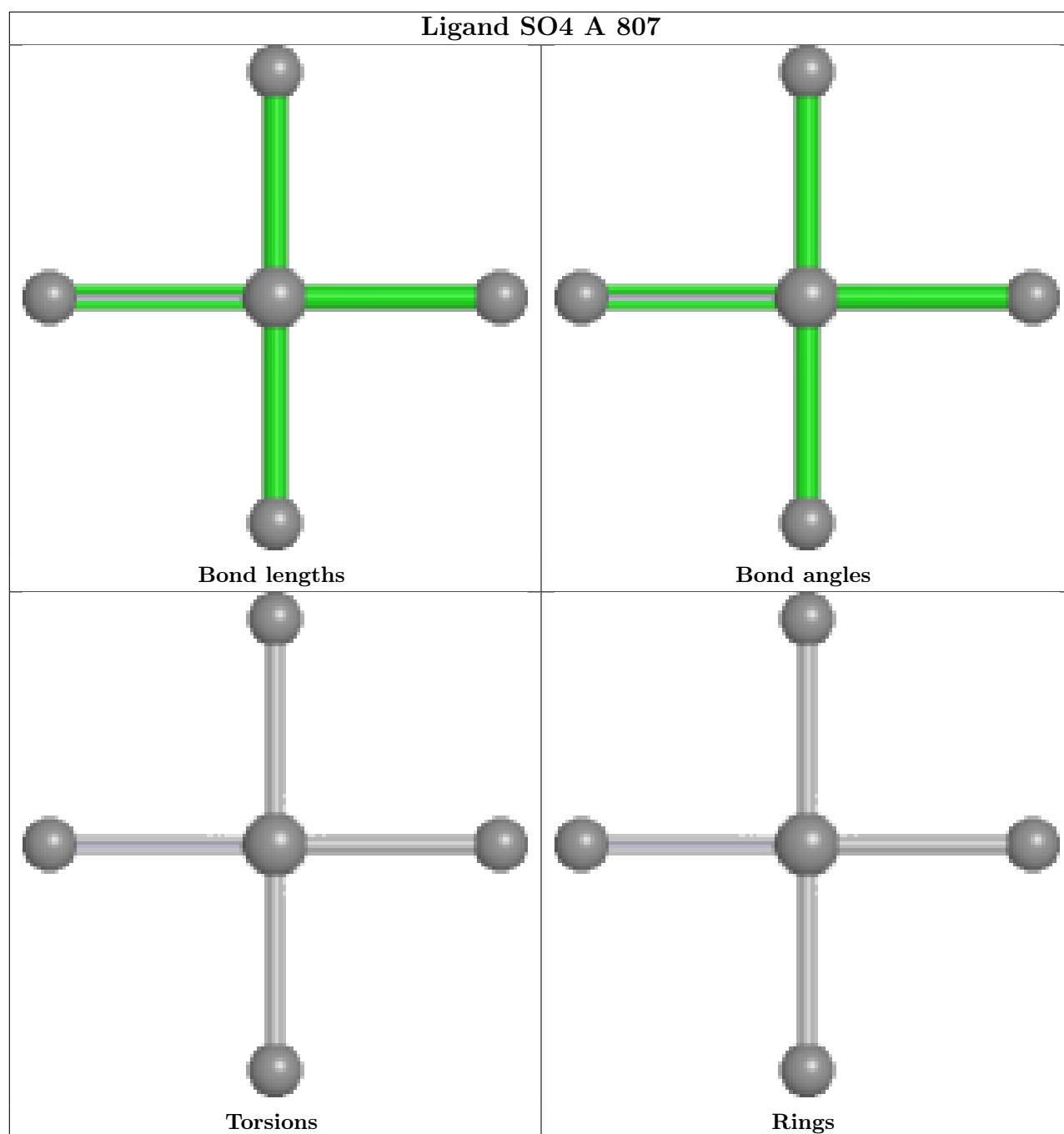
4 monomers are involved in 13 short contacts:

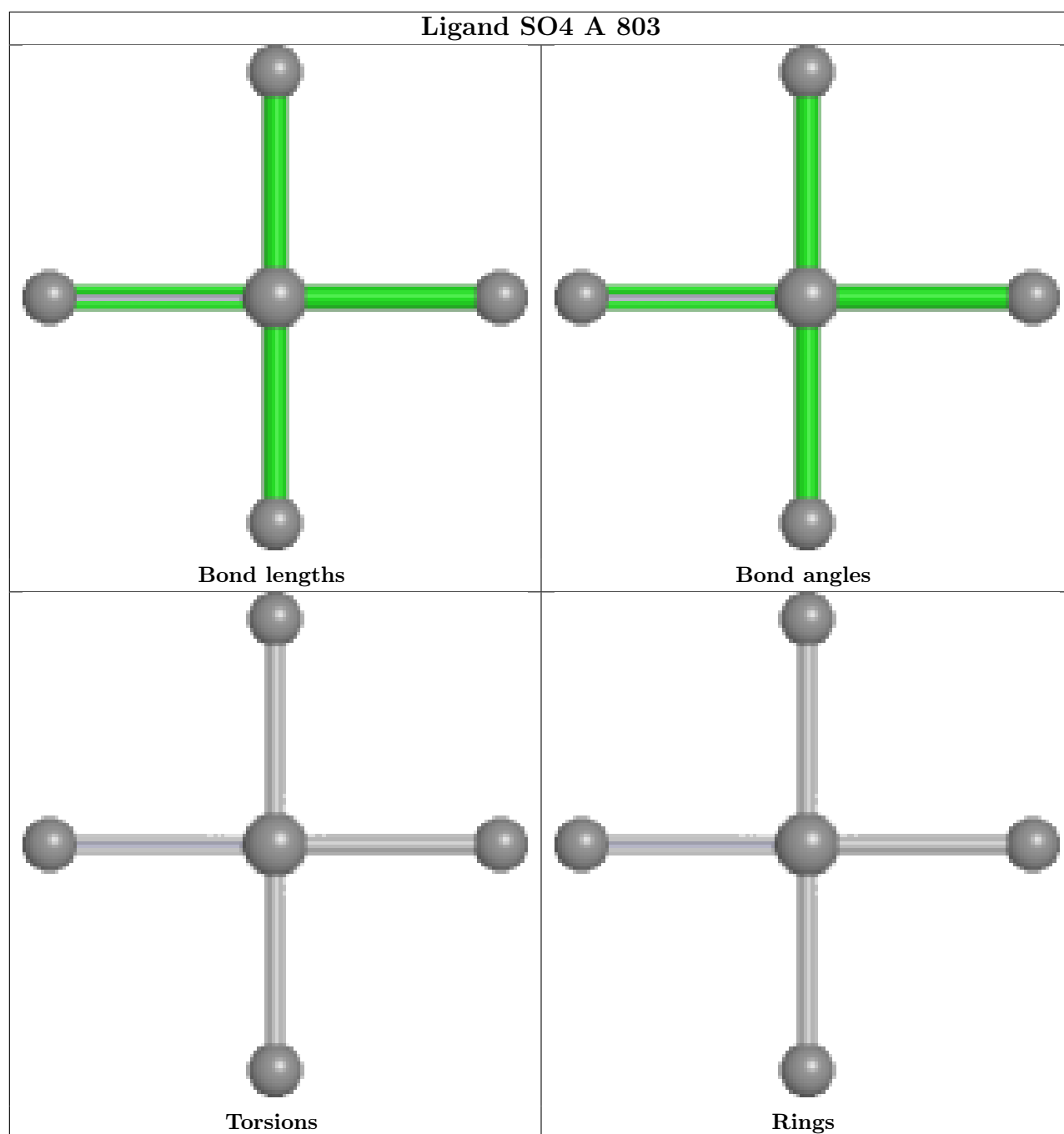
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	808	PG4	8	0
2	A	801	NAP	2	0
5	A	809	PG4	2	0
6	A	812	EDO	1	0

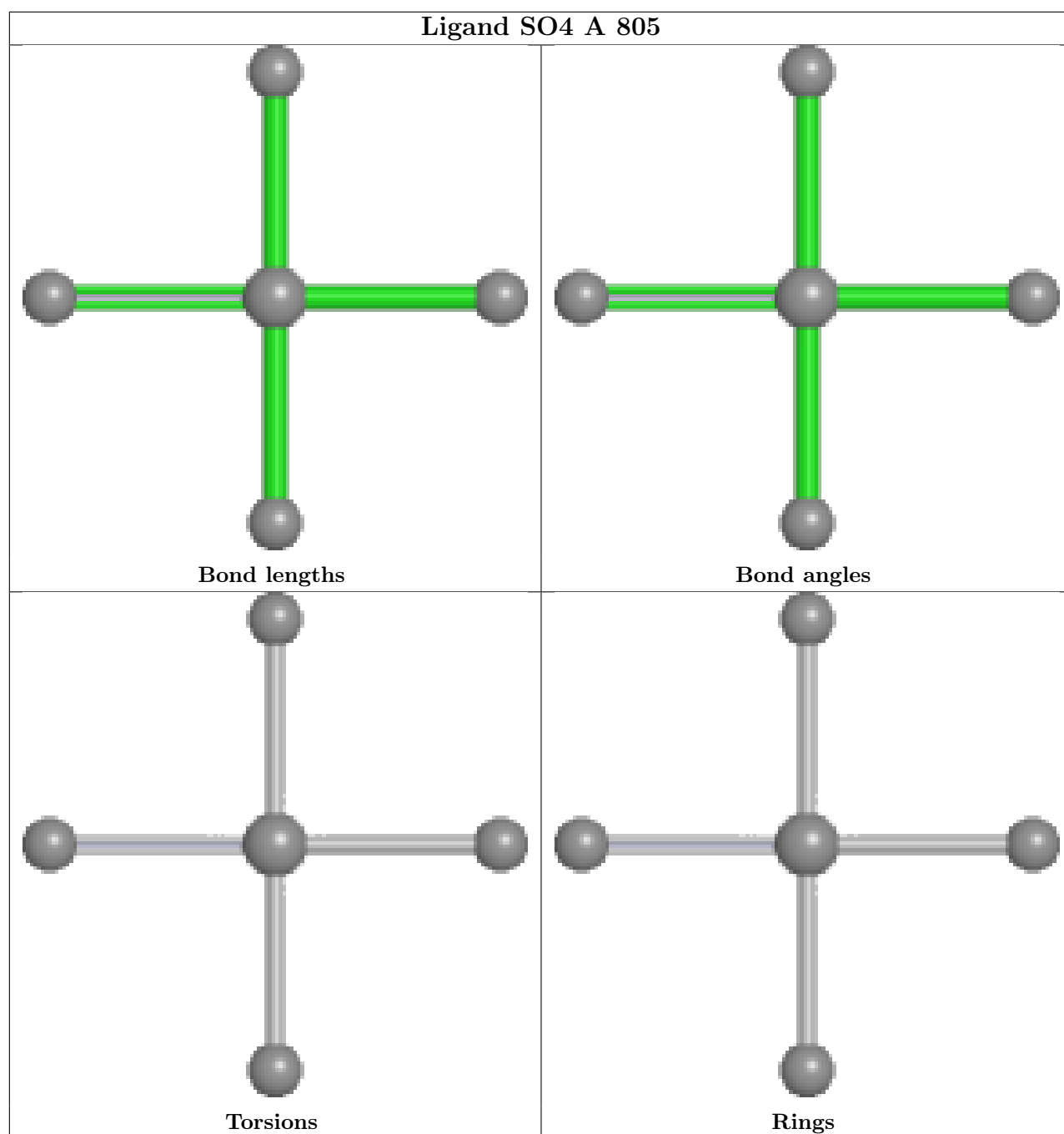
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

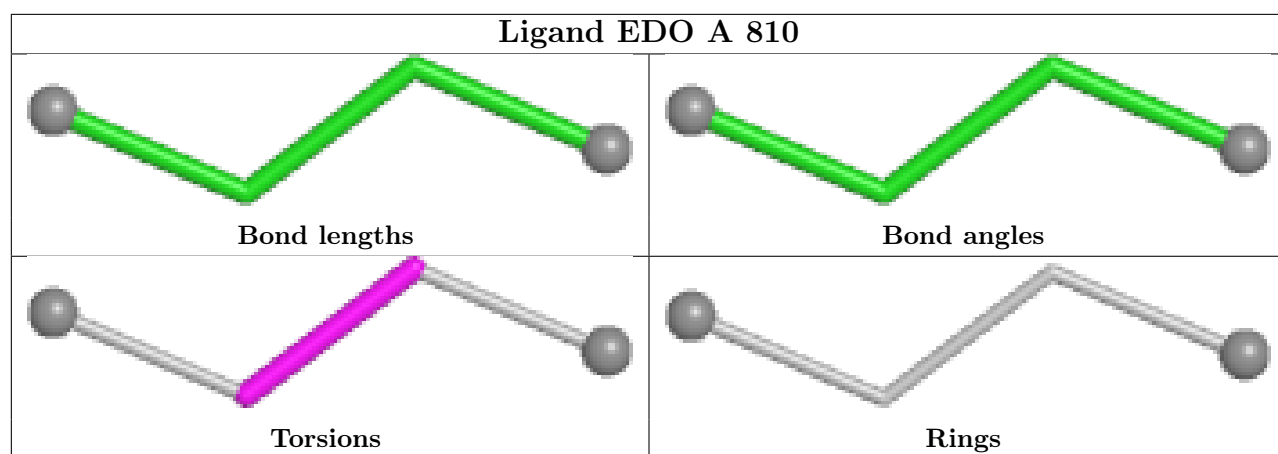


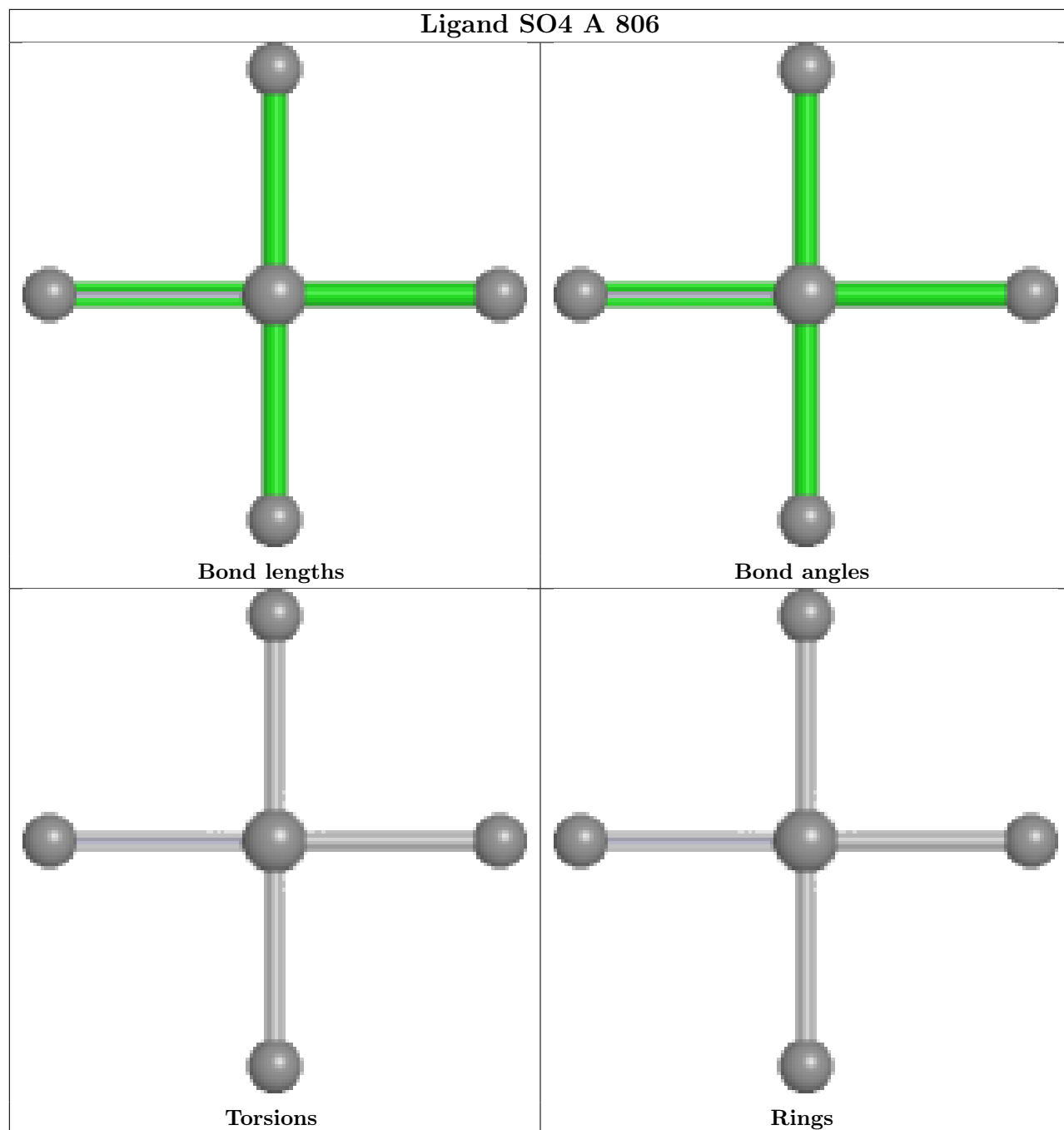


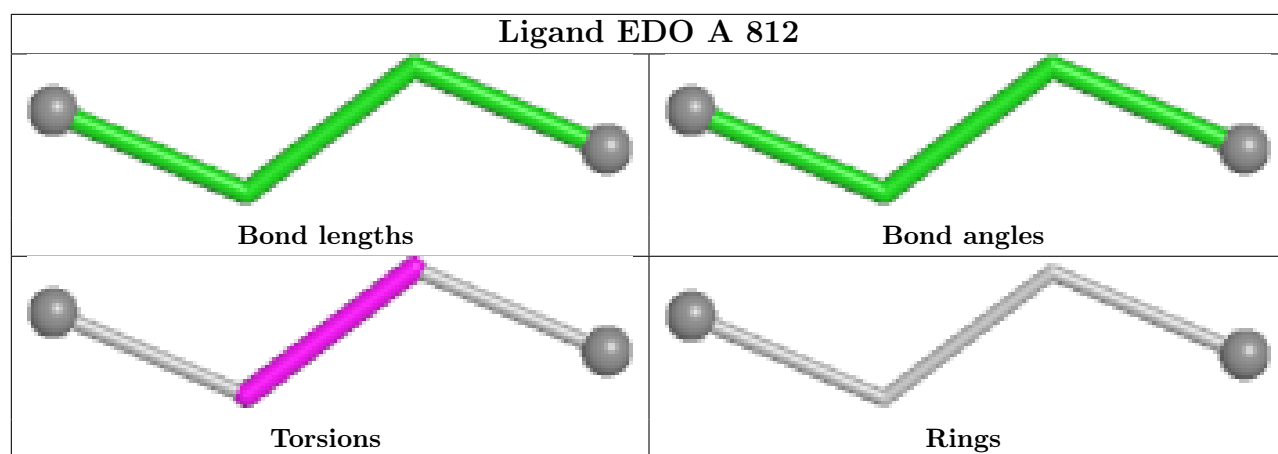


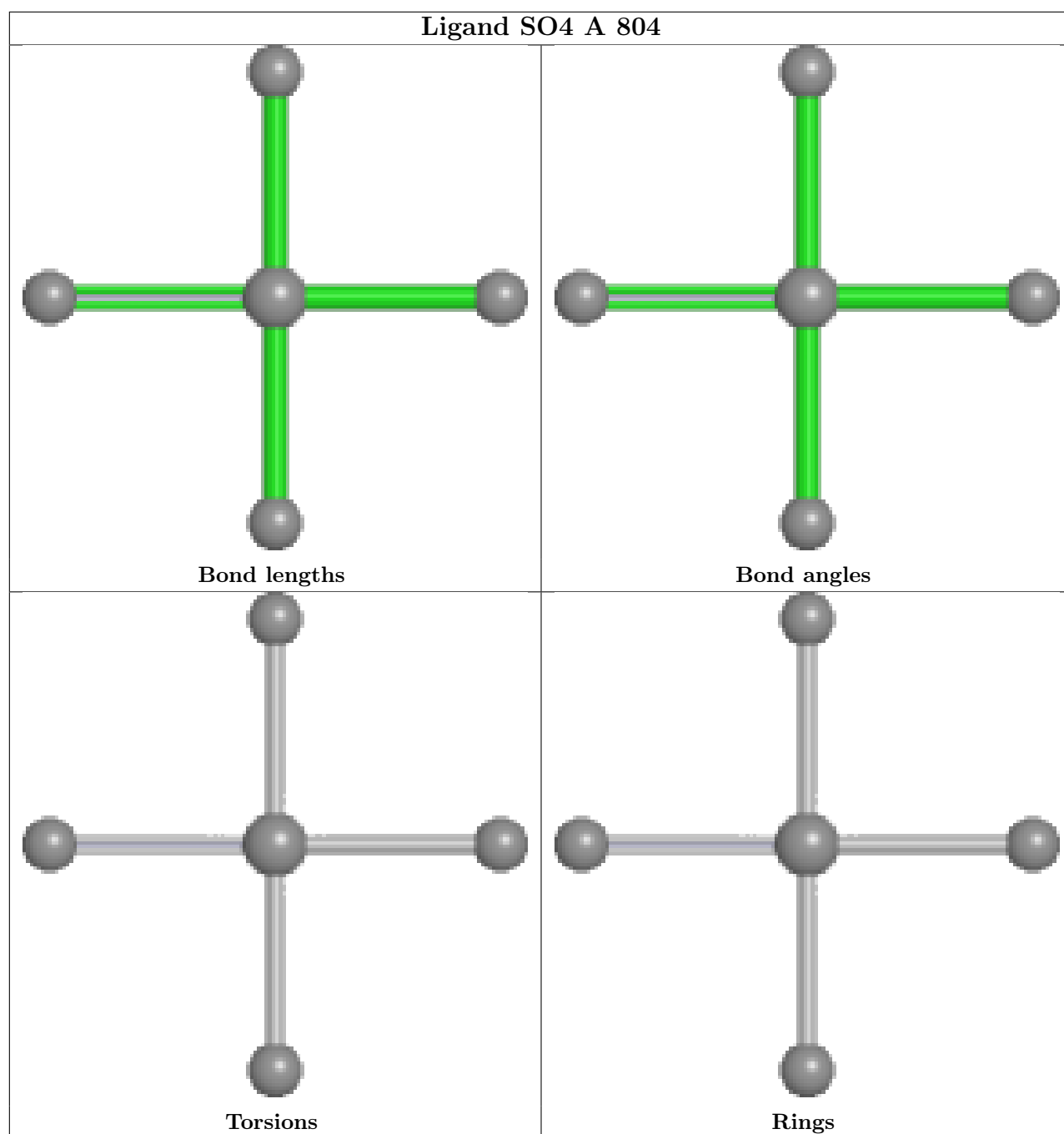












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	723/723 (100%)	-0.11	4 (0%) 85 83	26, 47, 73, 106	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	333	ASN	4.0
1	A	551	GLU	3.5
1	A	205	LEU	2.1
1	A	439	PHE	2.1

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
5	PG4	A	809	13/13	0.81	0.18	59,67,78,85	0
4	SO4	A	805	5/5	0.86	0.12	65,72,83,98	0
4	SO4	A	807	5/5	0.87	0.12	80,83,86,88	0

Continued on next page...

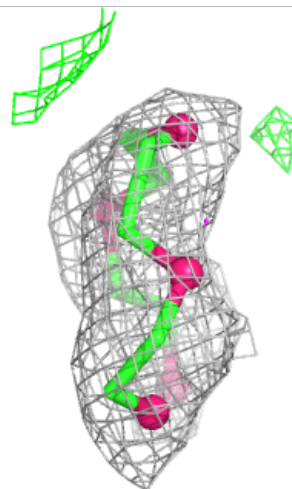
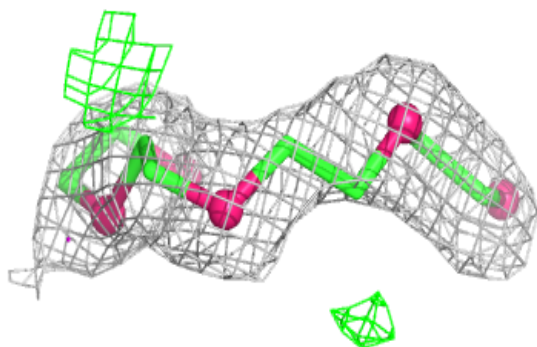
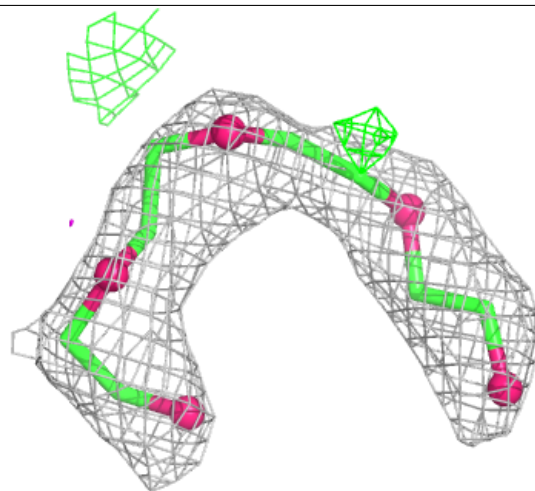
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	806	5/5	0.89	0.09	59,63,82,83	0
6	EDO	A	810	4/4	0.89	0.12	43,44,46,49	0
6	EDO	A	811	4/4	0.91	0.16	54,56,56,59	0
5	PG4	A	808	13/13	0.92	0.09	43,47,50,51	0
3	MN	A	802	1/1	0.95	0.25	85,85,85,85	0
6	EDO	A	812	4/4	0.95	0.14	30,35,39,42	0
4	SO4	A	804	5/5	0.96	0.06	53,56,60,66	0
2	NAP	A	801	48/48	0.97	0.06	22,34,39,42	0
4	SO4	A	803	5/5	0.99	0.04	30,35,37,37	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.

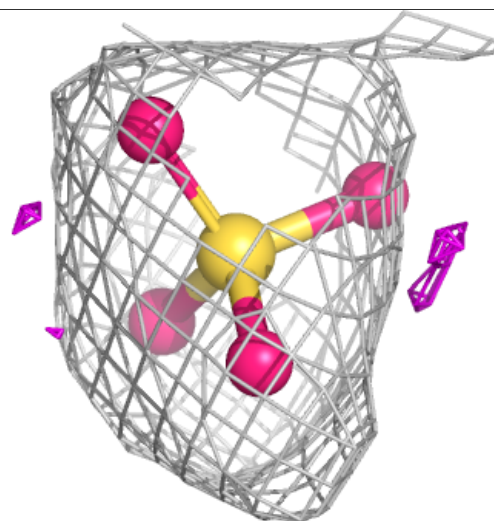
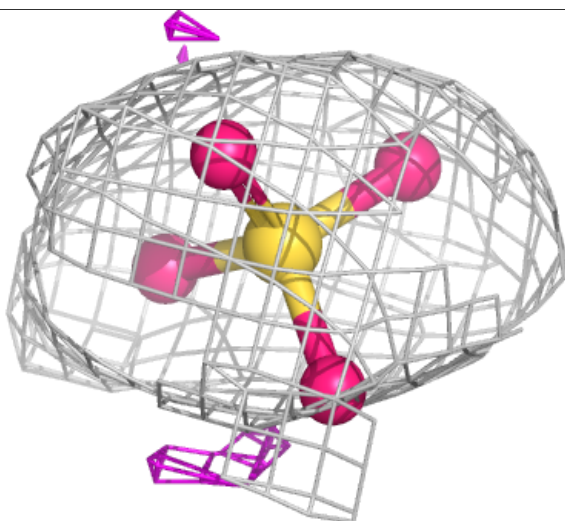
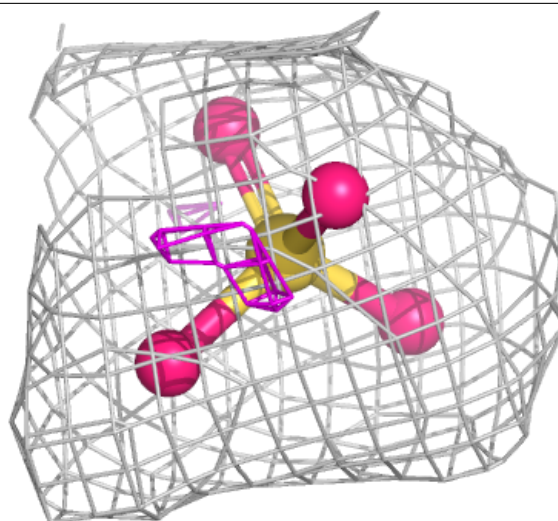
Electron density around PG4 A 809:

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



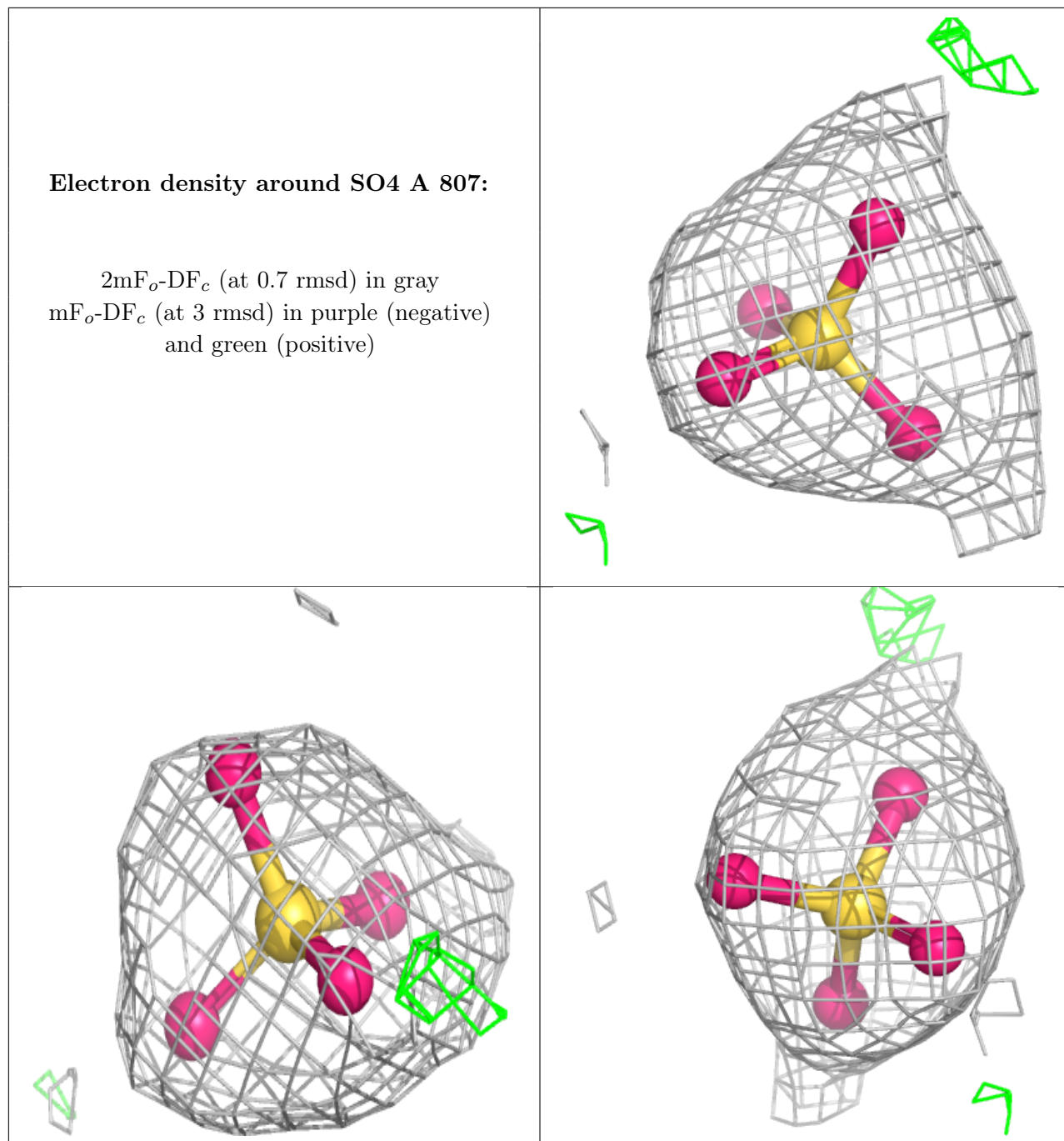
Electron density around SO4 A 805:

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



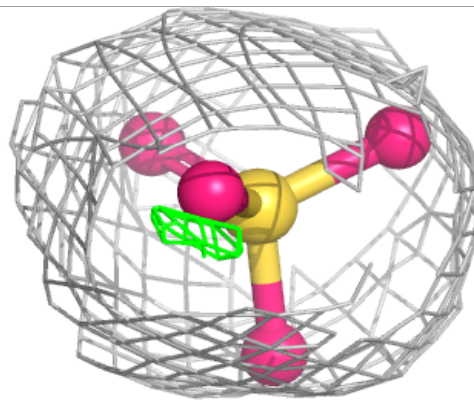
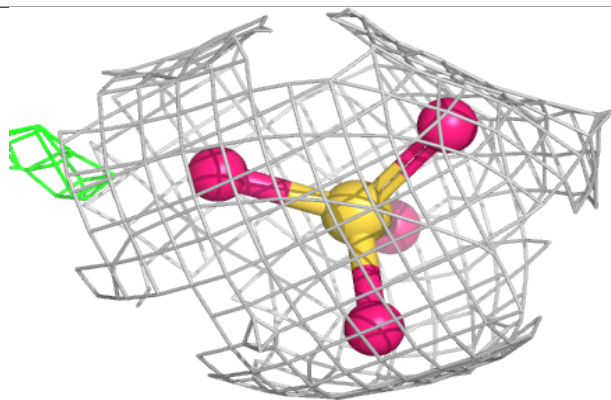
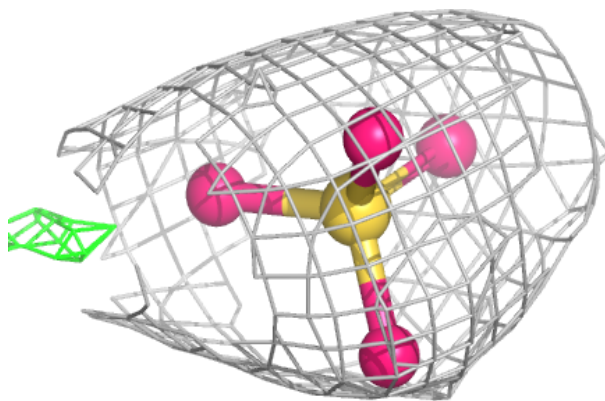
Electron density around SO4 A 807:

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

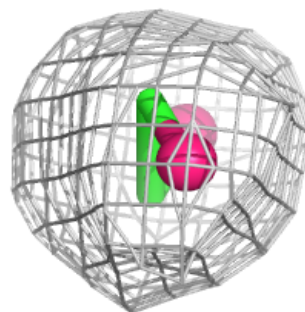
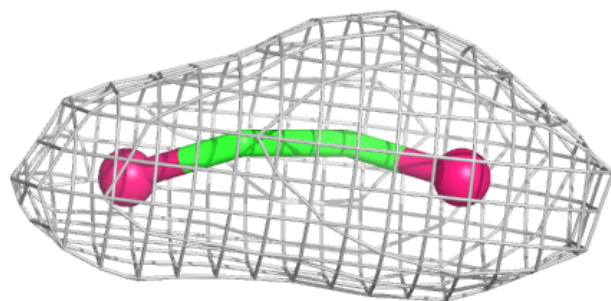
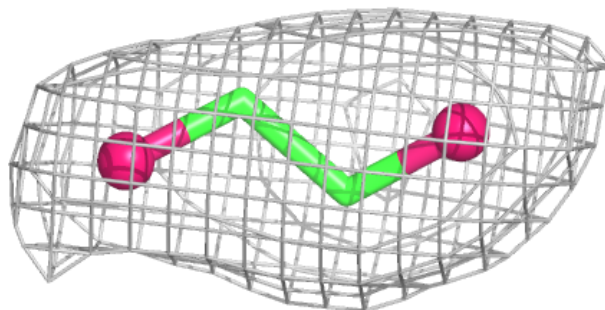


Electron density around SO4 A 806:

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

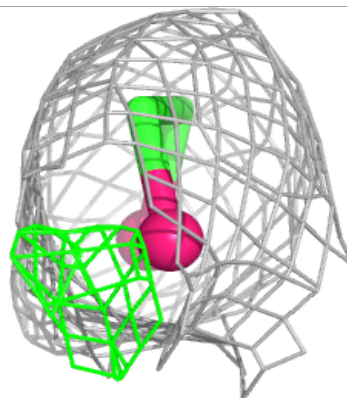
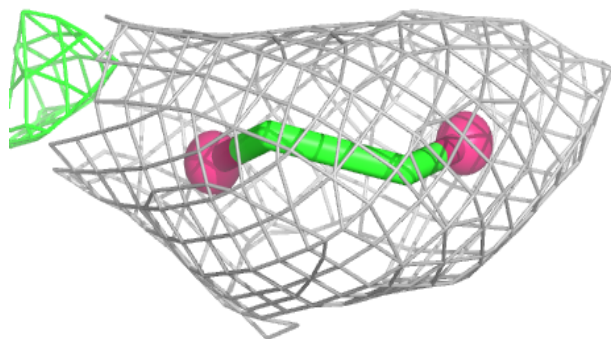
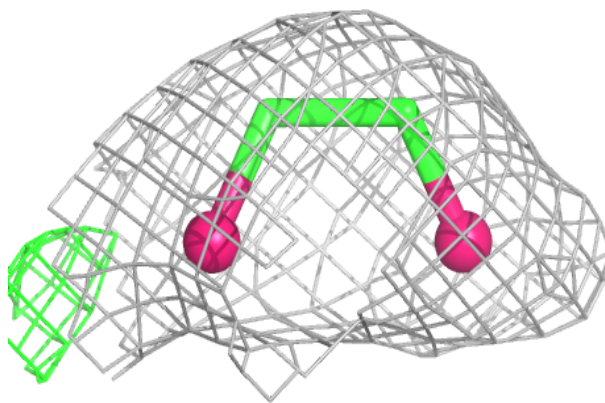
**Electron density around EDO A 810:**

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



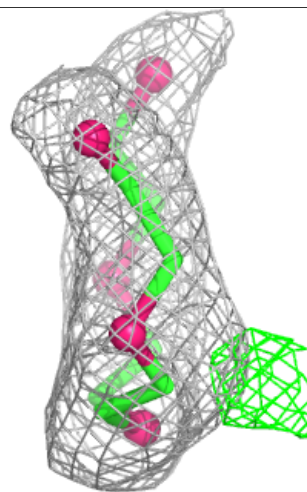
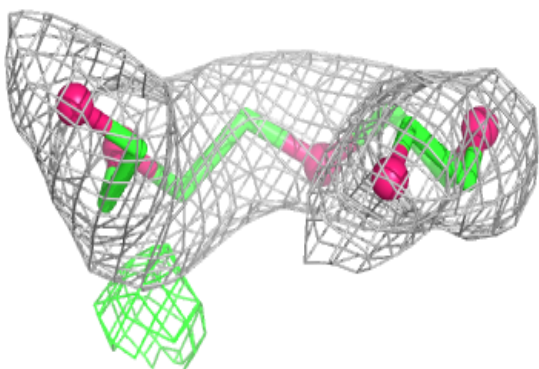
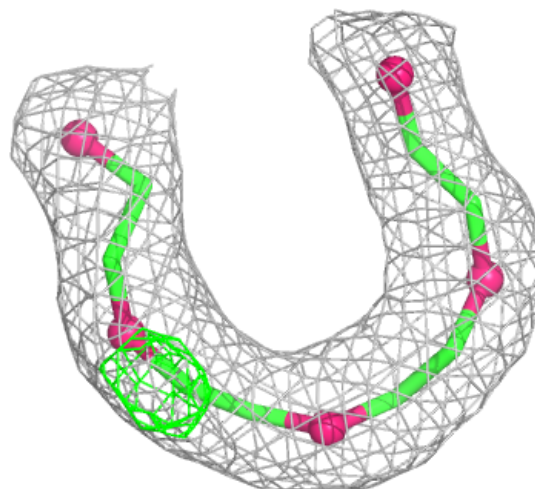
Electron density around EDO A 811:

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



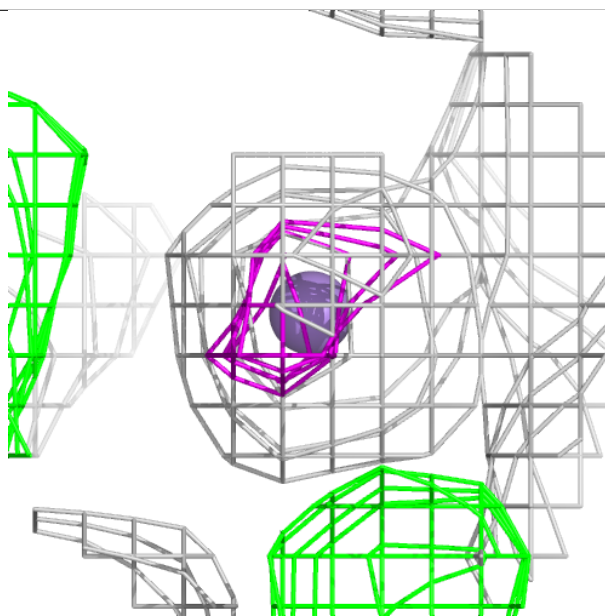
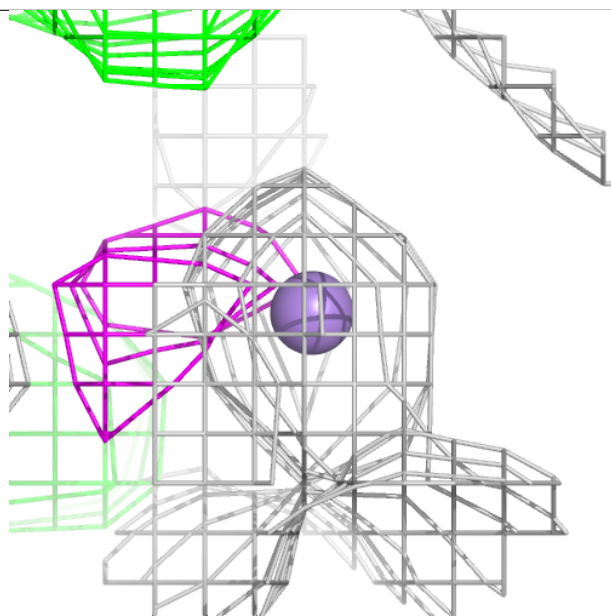
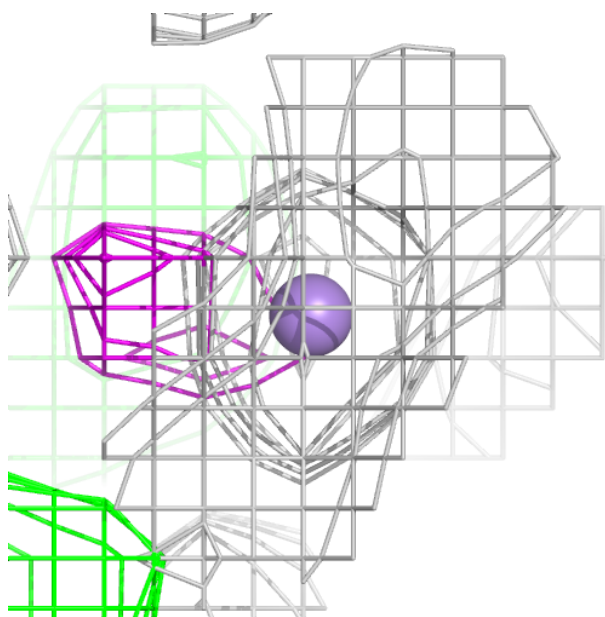
Electron density around PG4 A 808:

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



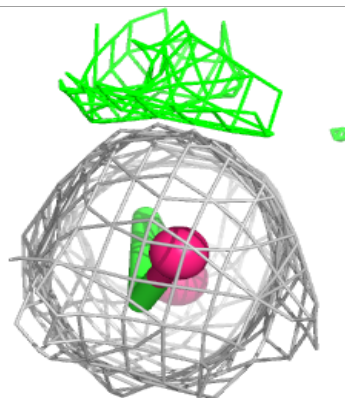
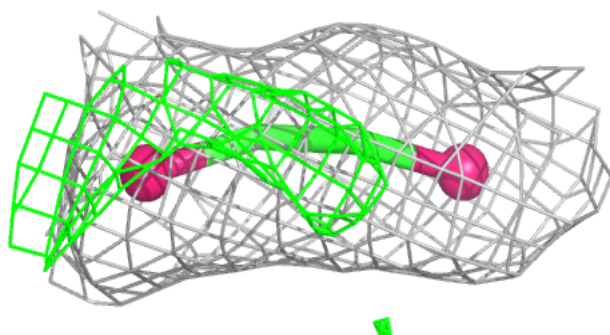
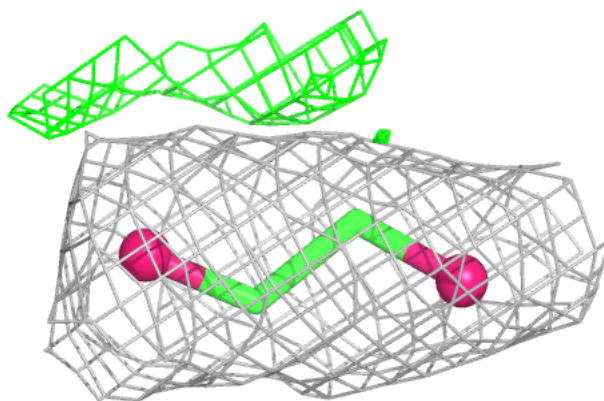
Electron density around MN A 802:

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



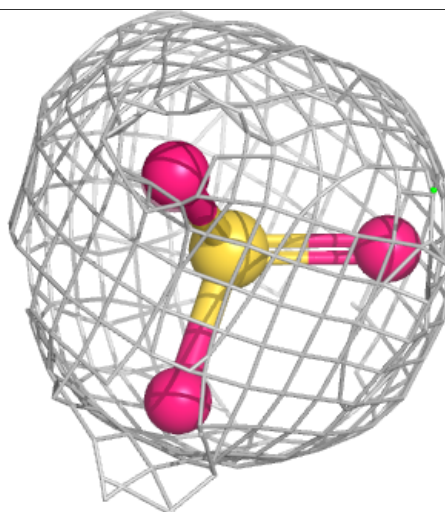
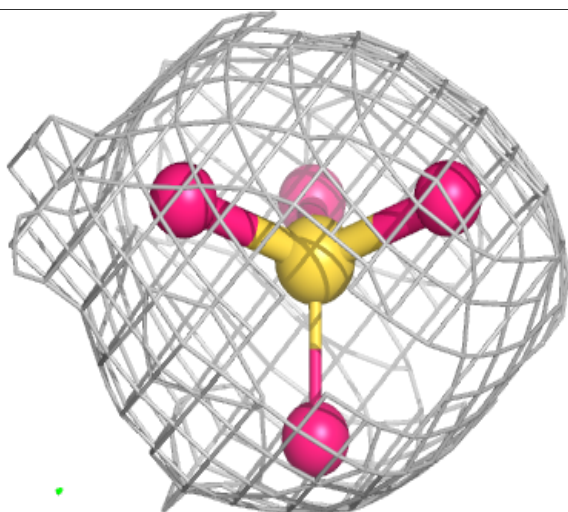
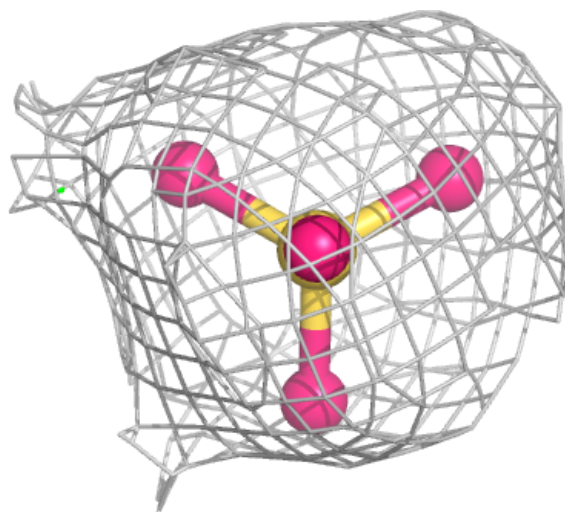
Electron density around EDO A 812:

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



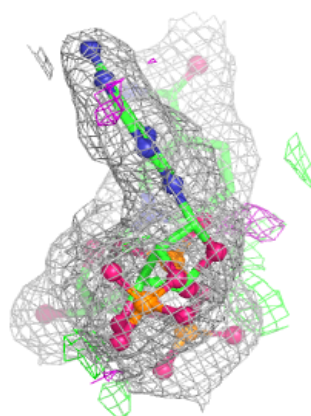
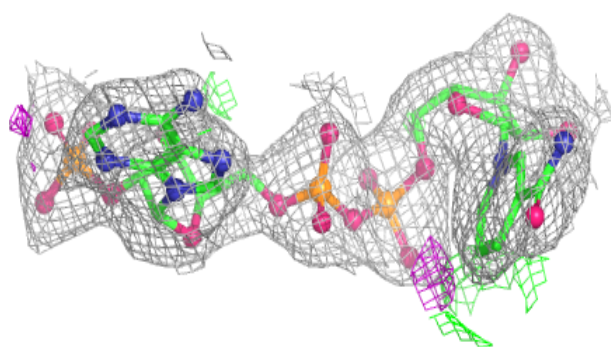
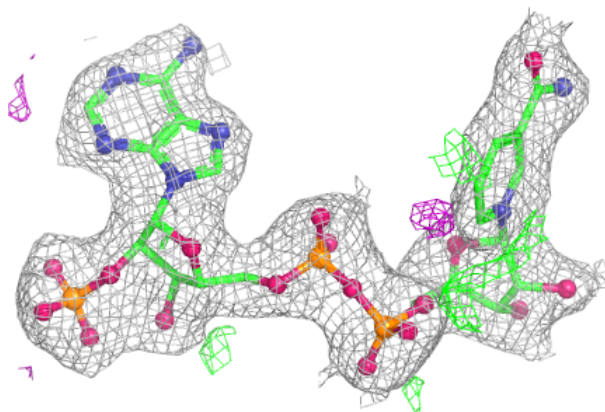
Electron density around SO4 A 804:

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



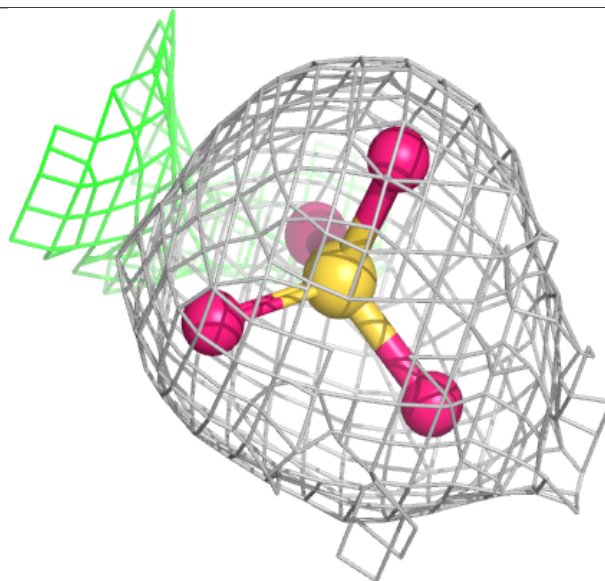
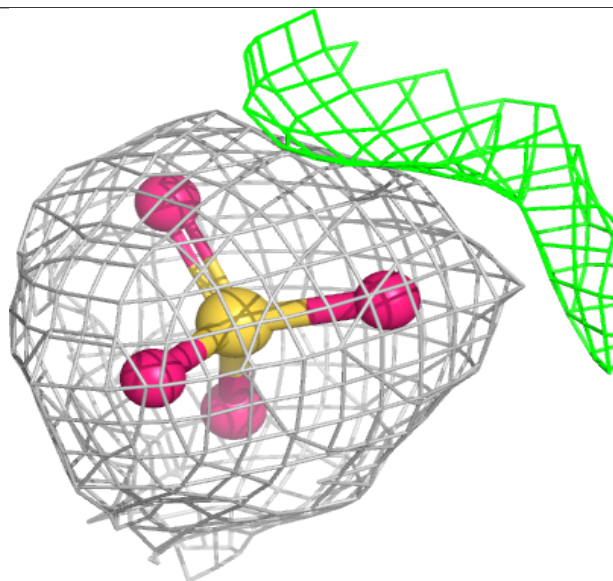
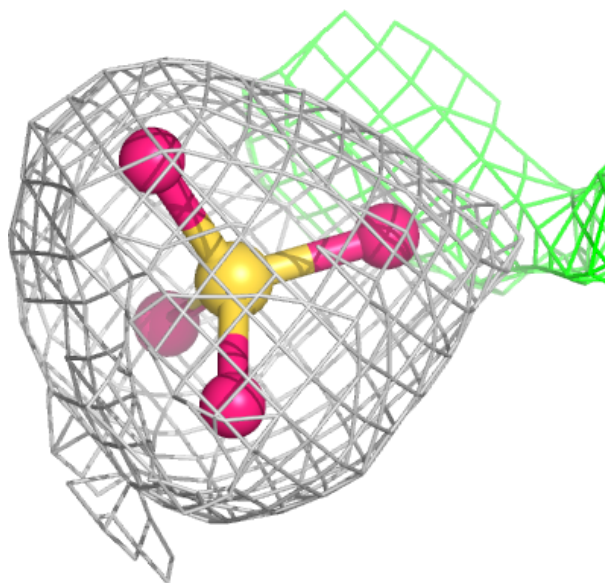
Electron density around NAP A 801:

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



Electron density around SO4 A 803:

$2mF_o-DF_c$ (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.