



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:10 AM UTC

PDB ID : 6YXH / pdb_00006yxh
Title : Cryogenic human alkaline ceramidase 3 (ACER3) at 2.6 Å resolution determined by Serial Crystallography (SSX) using CrystalDirect
Authors : Healey, R.D.; Basu, S.; Humm, A.S.; Leyrat, C.; Dupeux, F.; Pica, A.; Granier, S.; Marquez, J.A.
Deposited on : 2020-05-01
Resolution : 2.60 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

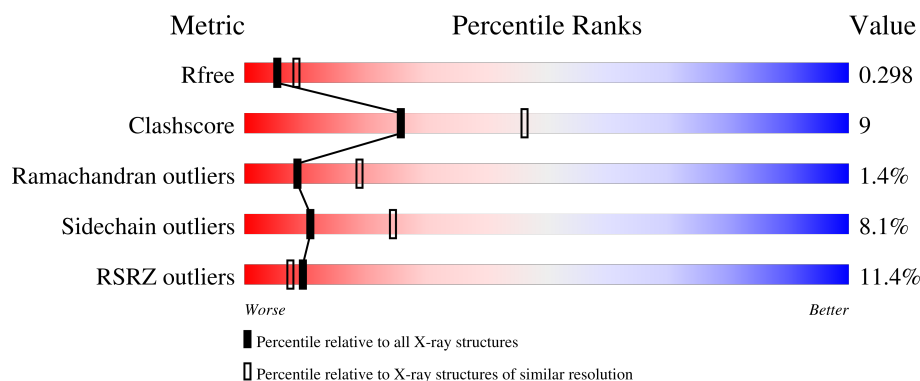
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	350	11% 71% 25% .

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
6	MG	A	411	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 2951 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 Alkaline ceramidase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	350	2855	1878	456	503	18	18	0	0

There are 107 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PHE	-	expression tag	UNP Q9NUN7
A	245	ALA	-	expression tag	UNP Q9NUN7
A	246	ASP	-	expression tag	UNP Q9NUN7
A	247	LEU	-	expression tag	UNP Q9NUN7
A	248	GLU	-	expression tag	UNP Q9NUN7
A	249	ASP	-	expression tag	UNP Q9NUN7
A	250	ASN	-	expression tag	UNP Q9NUN7
A	251	TRP	-	expression tag	UNP Q9NUN7
A	252	GLU	-	expression tag	UNP Q9NUN7
A	253	THR	-	expression tag	UNP Q9NUN7
A	254	LEU	-	expression tag	UNP Q9NUN7
A	255	ASN	-	expression tag	UNP Q9NUN7
A	256	ASP	-	expression tag	UNP Q9NUN7
A	257	ASN	-	expression tag	UNP Q9NUN7
A	258	LEU	-	expression tag	UNP Q9NUN7
A	259	LYS	-	expression tag	UNP Q9NUN7
A	260	VAL	-	expression tag	UNP Q9NUN7
A	261	ILE	-	expression tag	UNP Q9NUN7
A	262	GLU	-	expression tag	UNP Q9NUN7
A	263	LYS	-	expression tag	UNP Q9NUN7
A	264	ALA	-	expression tag	UNP Q9NUN7
A	265	ASP	-	expression tag	UNP Q9NUN7
A	266	ASN	-	expression tag	UNP Q9NUN7
A	267	ALA	-	expression tag	UNP Q9NUN7
A	268	ALA	-	expression tag	UNP Q9NUN7
A	269	GLN	-	expression tag	UNP Q9NUN7
A	270	VAL	-	expression tag	UNP Q9NUN7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	271	LYS	-	expression tag	UNP Q9NUN7
A	272	ASP	-	expression tag	UNP Q9NUN7
A	273	ALA	-	expression tag	UNP Q9NUN7
A	274	LEU	-	expression tag	UNP Q9NUN7
A	275	THR	-	expression tag	UNP Q9NUN7
A	276	LYS	-	expression tag	UNP Q9NUN7
A	277	MET	-	expression tag	UNP Q9NUN7
A	278	ARG	-	expression tag	UNP Q9NUN7
A	279	ALA	-	expression tag	UNP Q9NUN7
A	280	ALA	-	expression tag	UNP Q9NUN7
A	281	ALA	-	expression tag	UNP Q9NUN7
A	282	LEU	-	expression tag	UNP Q9NUN7
A	283	ASP	-	expression tag	UNP Q9NUN7
A	284	ALA	-	expression tag	UNP Q9NUN7
A	285	GLN	-	expression tag	UNP Q9NUN7
A	286	LYS	-	expression tag	UNP Q9NUN7
A	287	ALA	-	expression tag	UNP Q9NUN7
A	288	THR	-	expression tag	UNP Q9NUN7
A	289	PRO	-	expression tag	UNP Q9NUN7
A	290	PRO	-	expression tag	UNP Q9NUN7
A	291	LYS	-	expression tag	UNP Q9NUN7
A	292	LEU	-	expression tag	UNP Q9NUN7
A	293	GLU	-	expression tag	UNP Q9NUN7
A	294	ASP	-	expression tag	UNP Q9NUN7
A	295	LYS	-	expression tag	UNP Q9NUN7
A	296	SER	-	expression tag	UNP Q9NUN7
A	297	PRO	-	expression tag	UNP Q9NUN7
A	298	ASP	-	expression tag	UNP Q9NUN7
A	299	SER	-	expression tag	UNP Q9NUN7
A	300	PRO	-	expression tag	UNP Q9NUN7
A	301	GLU	-	expression tag	UNP Q9NUN7
A	302	MET	-	expression tag	UNP Q9NUN7
A	303	LYS	-	expression tag	UNP Q9NUN7
A	304	ASP	-	expression tag	UNP Q9NUN7
A	305	PHE	-	expression tag	UNP Q9NUN7
A	306	ARG	-	expression tag	UNP Q9NUN7
A	307	HIS	-	expression tag	UNP Q9NUN7
A	308	GLY	-	expression tag	UNP Q9NUN7
A	309	PHE	-	expression tag	UNP Q9NUN7
A	310	ASP	-	expression tag	UNP Q9NUN7
A	311	ILE	-	expression tag	UNP Q9NUN7
A	312	LEU	-	expression tag	UNP Q9NUN7

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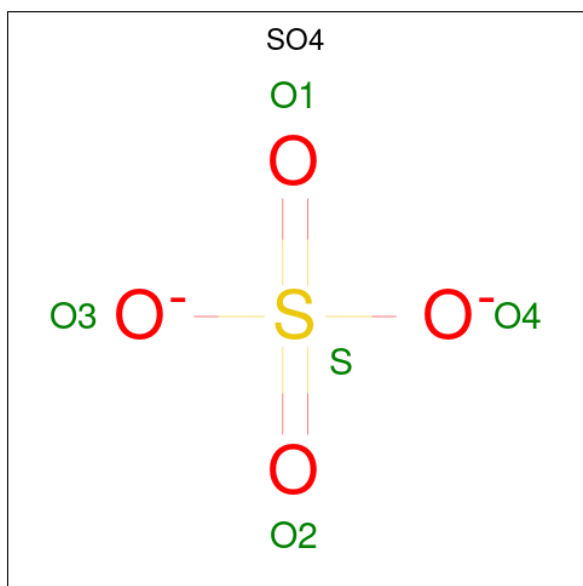
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Chain	Residue	Modelled	Actual	Comment	Reference
A	313	VAL	-	expression tag	UNP Q9NUN7
A	314	GLY	-	expression tag	UNP Q9NUN7
A	315	GLN	-	expression tag	UNP Q9NUN7
A	316	ILE	-	expression tag	UNP Q9NUN7
A	317	ASP	-	expression tag	UNP Q9NUN7
A	318	ASP	-	expression tag	UNP Q9NUN7
A	319	ALA	-	expression tag	UNP Q9NUN7
A	320	LEU	-	expression tag	UNP Q9NUN7
A	321	LYS	-	expression tag	UNP Q9NUN7
A	322	LEU	-	expression tag	UNP Q9NUN7
A	323	ALA	-	expression tag	UNP Q9NUN7
A	324	ASN	-	expression tag	UNP Q9NUN7
A	325	GLU	-	expression tag	UNP Q9NUN7
A	326	GLY	-	expression tag	UNP Q9NUN7
A	327	LYS	-	expression tag	UNP Q9NUN7
A	328	VAL	-	expression tag	UNP Q9NUN7
A	329	LYS	-	expression tag	UNP Q9NUN7
A	330	GLU	-	expression tag	UNP Q9NUN7
A	331	ALA	-	expression tag	UNP Q9NUN7
A	332	GLN	-	expression tag	UNP Q9NUN7
A	333	ALA	-	expression tag	UNP Q9NUN7
A	334	ALA	-	expression tag	UNP Q9NUN7
A	335	ALA	-	expression tag	UNP Q9NUN7
A	336	GLU	-	expression tag	UNP Q9NUN7
A	337	GLN	-	expression tag	UNP Q9NUN7
A	338	LEU	-	expression tag	UNP Q9NUN7
A	339	LYS	-	expression tag	UNP Q9NUN7
A	340	THR	-	expression tag	UNP Q9NUN7
A	341	THR	-	expression tag	UNP Q9NUN7
A	342	ARG	-	expression tag	UNP Q9NUN7
A	343	ASN	-	expression tag	UNP Q9NUN7
A	344	ALA	-	expression tag	UNP Q9NUN7
A	345	TYR	-	expression tag	UNP Q9NUN7
A	346	ILE	-	expression tag	UNP Q9NUN7
A	347	GLN	-	expression tag	UNP Q9NUN7
A	348	LYS	-	expression tag	UNP Q9NUN7
A	349	TYR	-	expression tag	UNP Q9NUN7
A	350	LEU	-	expression tag	UNP Q9NUN7

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

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



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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Na	0	0
			2	2		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total 2	Mg 2	0	0

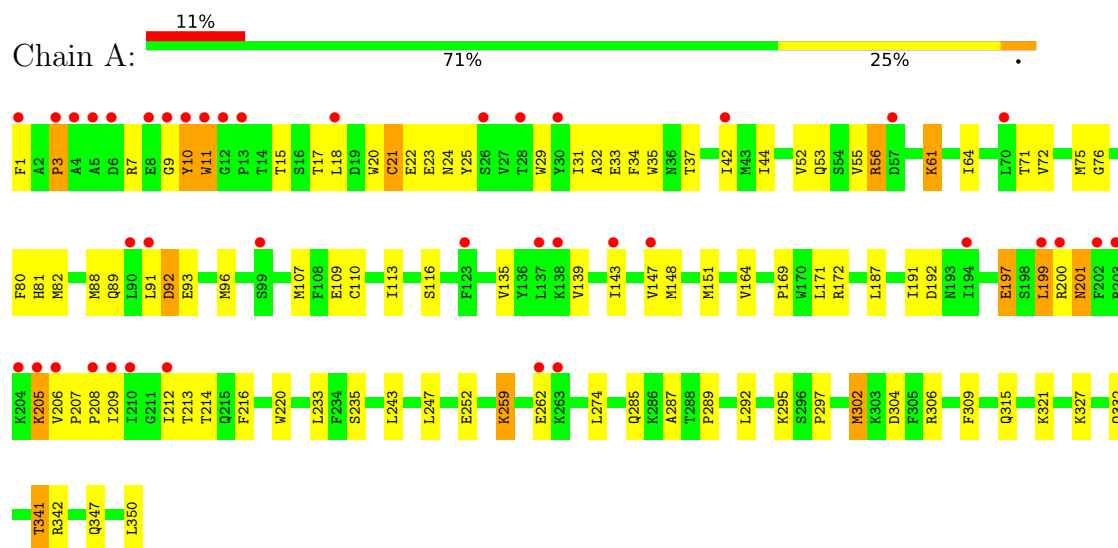
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	60	Total 60	O 60	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: Alkaline ceramidase 3



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	61.47Å 69.97Å 259.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.18 – 2.60 46.18 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.18-2.60) 100.0 (46.18-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.3 (6-FEB-2020)	Depositor
R, R_{free}	0.232 , 0.280 0.240 , 0.298	Depositor DCC
R_{free} test set	885 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	65.9	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2951	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.98% 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: SO4, CA, NA, ZN, MG

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	0.89	2/2935 (0.1%)	1.30	21/3990 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	302	MET	SD-CE	-5.14	1.66	1.79
1	A	347	GLN	CA-C	5.13	1.59	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	ILE	N-CA-C	-7.24	105.90	111.62
1	A	93	GLU	N-CA-C	6.22	117.73	111.07
1	A	201	ASN	CA-CB-CG	5.82	118.42	112.60
1	A	10	TYR	CA-C-N	5.75	132.53	121.54
1	A	10	TYR	C-N-CA	5.75	132.53	121.54
1	A	171	LEU	CA-C-N	5.70	127.84	120.44
1	A	171	LEU	C-N-CA	5.70	127.84	120.44
1	A	243	LEU	CA-C-N	5.65	128.73	120.71
1	A	243	LEU	C-N-CA	5.65	128.73	120.71
1	A	252	GLU	CA-C-N	5.62	127.74	120.44
1	A	252	GLU	C-N-CA	5.62	127.74	120.44
1	A	92	ASP	CA-C-N	5.46	127.55	120.44
1	A	92	ASP	C-N-CA	5.46	127.55	120.44
1	A	92	ASP	N-CA-C	-5.20	104.63	111.96
1	A	109	GLU	CA-C-N	5.20	128.91	120.60
1	A	109	GLU	C-N-CA	5.20	128.91	120.60
1	A	207	PRO	N-CA-C	5.11	116.93	110.70
1	A	274	LEU	CA-C-N	5.11	127.08	120.44
1	A	274	LEU	C-N-CA	5.11	127.08	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	LYS	CA-C-N	5.05	127.02	120.56
1	A	327	LYS	C-N-CA	5.05	127.02	120.56

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	2855	0	2858	54	0
2	A	1	0	0	0	0
3	A	30	0	0	1	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	2	0	0	0	0
7	A	60	0	0	1	0
All	All	2951	0	2858	54	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 (54) 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:315:GLN:OE1	1:A:341:THR:HG21	1.62	0.98
1:A:31:ILE:HG22	1:A:82:MET:HG3	1.52	0.90
1:A:148:MET:HA	1:A:148:MET:HE2	1.63	0.80
1:A:297:PRO:O	1:A:306:ARG:NH2	2.22	0.72
1:A:53:GLN:HA	1:A:56:ARG:HD3	1.72	0.71
1:A:205:LYS:HE2	1:A:208:PRO:HG3	1.76	0.68
1:A:32:ALA:O	1:A:81:HIS:O	2.14	0.66
1:A:197:GLU:HB2	1:A:199:LEU:HG	1.79	0.65
1:A:292:LEU:HB3	1:A:302:MET:HE1	1.79	0.64
1:A:259:LYS:HE2	1:A:262:GLU:OE1	1.98	0.62
1:A:164:VAL:HG21	1:A:172:ARG:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:MET:HA	1:A:107:MET:HE2	1.81	0.62
1:A:192:ASP:HB2	1:A:216:PHE:HB2	1.83	0.59
1:A:247:LEU:HD13	1:A:287:ALA:HB3	1.85	0.56
1:A:110:CYS:HB3	7:A:518:HOH:O	2.04	0.56
1:A:20:TRP:CD1	1:A:81:HIS:HE1	2.24	0.55
1:A:315:GLN:OE1	1:A:341:THR:CG2	2.47	0.55
1:A:209:ILE:HB	1:A:213:THR:HG23	1.90	0.54
1:A:35:TRP:NE1	1:A:212:ILE:HD12	2.23	0.54
1:A:31:ILE:CG2	1:A:82:MET:HG3	2.34	0.54
1:A:80:PHE:HB2	1:A:88:MET:O	2.08	0.53
1:A:17:THR:H	1:A:89:GLN:HE22	1.55	0.53
1:A:292:LEU:CB	1:A:302:MET:HE1	2.38	0.53
1:A:1:PHE:C	1:A:3:PRO:HD3	2.34	0.52
1:A:92:ASP:O	1:A:96:MET:HG3	2.09	0.52
1:A:72:VAL:HA	1:A:75:MET:HE2	1.92	0.51
1:A:10:TYR:HD2	1:A:29:TRP:O	1.94	0.51
1:A:20:TRP:CD1	1:A:81:HIS:CE1	2.99	0.51
1:A:187:LEU:O	1:A:191:ILE:HG12	2.10	0.50
1:A:76:GLY:HA3	1:A:91:LEU:O	2.11	0.50
1:A:55:VAL:HG12	1:A:64:ILE:HD13	1.94	0.49
1:A:7:ARG:HD3	1:A:23:GLU:HA	1.96	0.47
1:A:25:TYR:H	1:A:32:ALA:HA	1.78	0.47
1:A:292:LEU:HB3	1:A:302:MET:CE	2.42	0.47
1:A:31:ILE:HD11	1:A:34:PHE:CD1	2.49	0.47
1:A:113:ILE:HG23	1:A:116:SER:HB3	1.97	0.47
1:A:148:MET:HA	1:A:148:MET:CE	2.41	0.46
1:A:7:ARG:HD2	1:A:24:ASN:H	1.80	0.46
1:A:10:TYR:CD2	1:A:29:TRP:O	2.69	0.45
1:A:53:GLN:HG3	1:A:56:ARG:CZ	2.47	0.45
1:A:200:ARG:HD2	1:A:214:THR:HG21	1.99	0.44
1:A:107:MET:HE3	1:A:235:SER:HA	2.00	0.44
1:A:289:PRO:HG2	1:A:292:LEU:HD12	2.00	0.44
1:A:22:GLU:HB3	1:A:33:GLU:HG2	2.00	0.44
1:A:31:ILE:HD12	1:A:37:THR:HB	2.00	0.43
1:A:35:TRP:HE1	1:A:212:ILE:HD12	1.83	0.43
1:A:61:LYS:HE3	3:A:402:SO4:O2	2.20	0.42
1:A:23:GLU:CD	1:A:23:GLU:H	2.28	0.42
1:A:197:GLU:HG3	1:A:199:LEU:HD11	2.02	0.41
1:A:285:GLN:HG3	1:A:309:PHE:HB2	2.03	0.41
1:A:52:VAL:HA	1:A:55:VAL:HG22	2.03	0.41
1:A:350:LEU:HD13	1:A:350:LEU:HA	2.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:PRO:O	1:A:172:ARG:HB2	2.22	0.40
1:A:71:THR:O	1:A:75:MET:HG3	2.22	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	348/350 (99%)	327 (94%)	16 (5%)	5 (1%)	9	19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	GLY
1	A	11	TRP
1	A	205	LYS
1	A	3	PRO
1	A	21	CYS

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	308/308 (100%)	283 (92%)	25 (8%)	11	24

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	TRP
1	A	15	THR
1	A	18	LEU
1	A	21	CYS
1	A	42	ILE
1	A	56	ARG
1	A	61	LYS
1	A	135	VAL
1	A	139	VAL
1	A	143	ILE
1	A	147	VAL
1	A	151	MET
1	A	197	GLU
1	A	199	LEU
1	A	201	ASN
1	A	206	VAL
1	A	220	TRP
1	A	233	LEU
1	A	259	LYS
1	A	295	LYS
1	A	304	ASP
1	A	321	LYS
1	A	332	GLN
1	A	341	THR
1	A	342	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	146	GLN
1	A	190	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\# Z > 2$
3	SO4	A	406	-	4,4,4	0.25	0	6,6,6	0.24	0
3	SO4	A	404	-	4,4,4	0.41	0	6,6,6	0.22	0
3	SO4	A	405	-	4,4,4	0.41	0	6,6,6	0.14	0
3	SO4	A	402	6	4,4,4	0.50	0	6,6,6	0.32	0
3	SO4	A	407	-	4,4,4	0.47	0	6,6,6	0.27	0
3	SO4	A	403	-	4,4,4	0.34	0	6,6,6	0.14	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

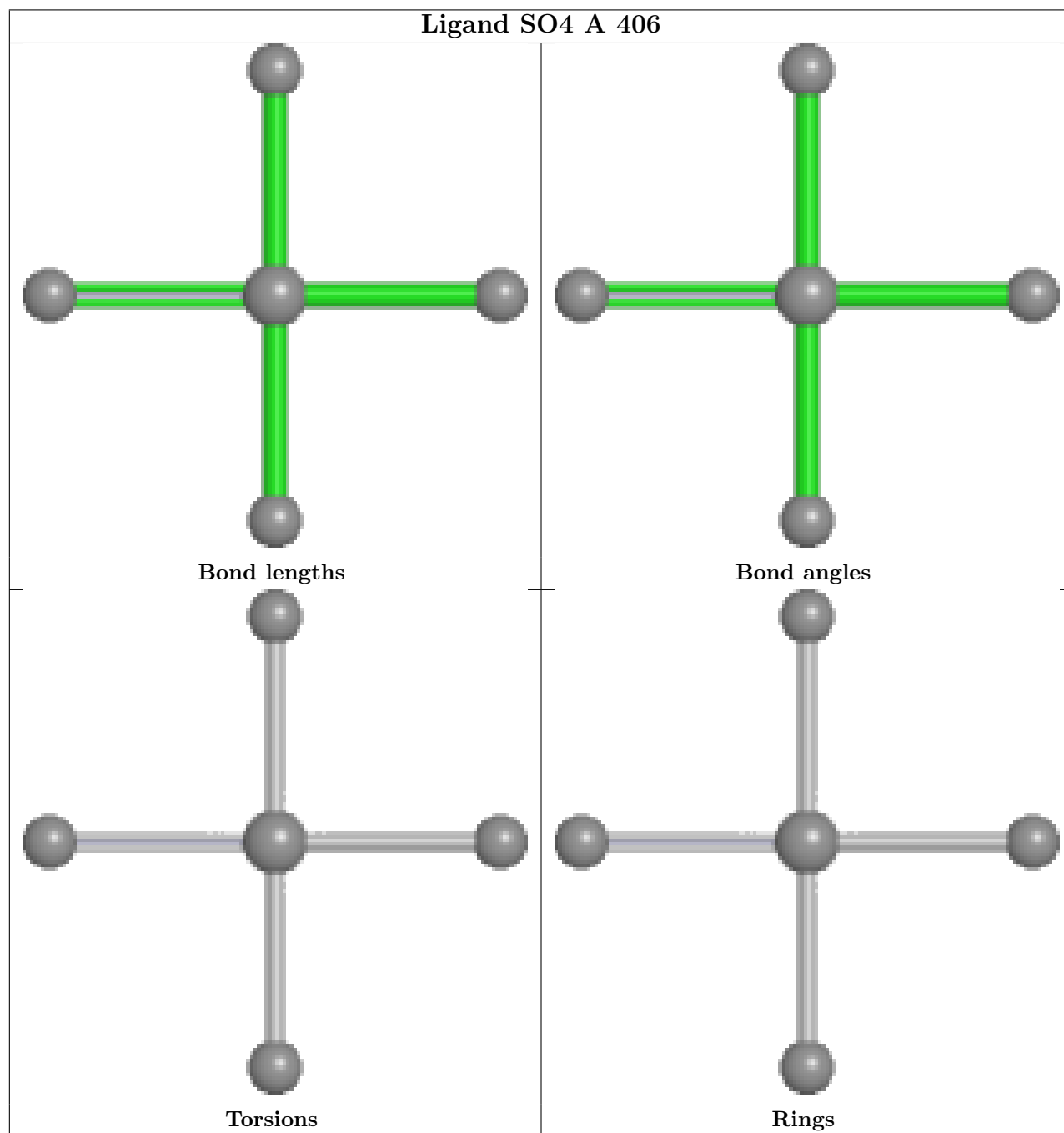
There are no ring outliers.

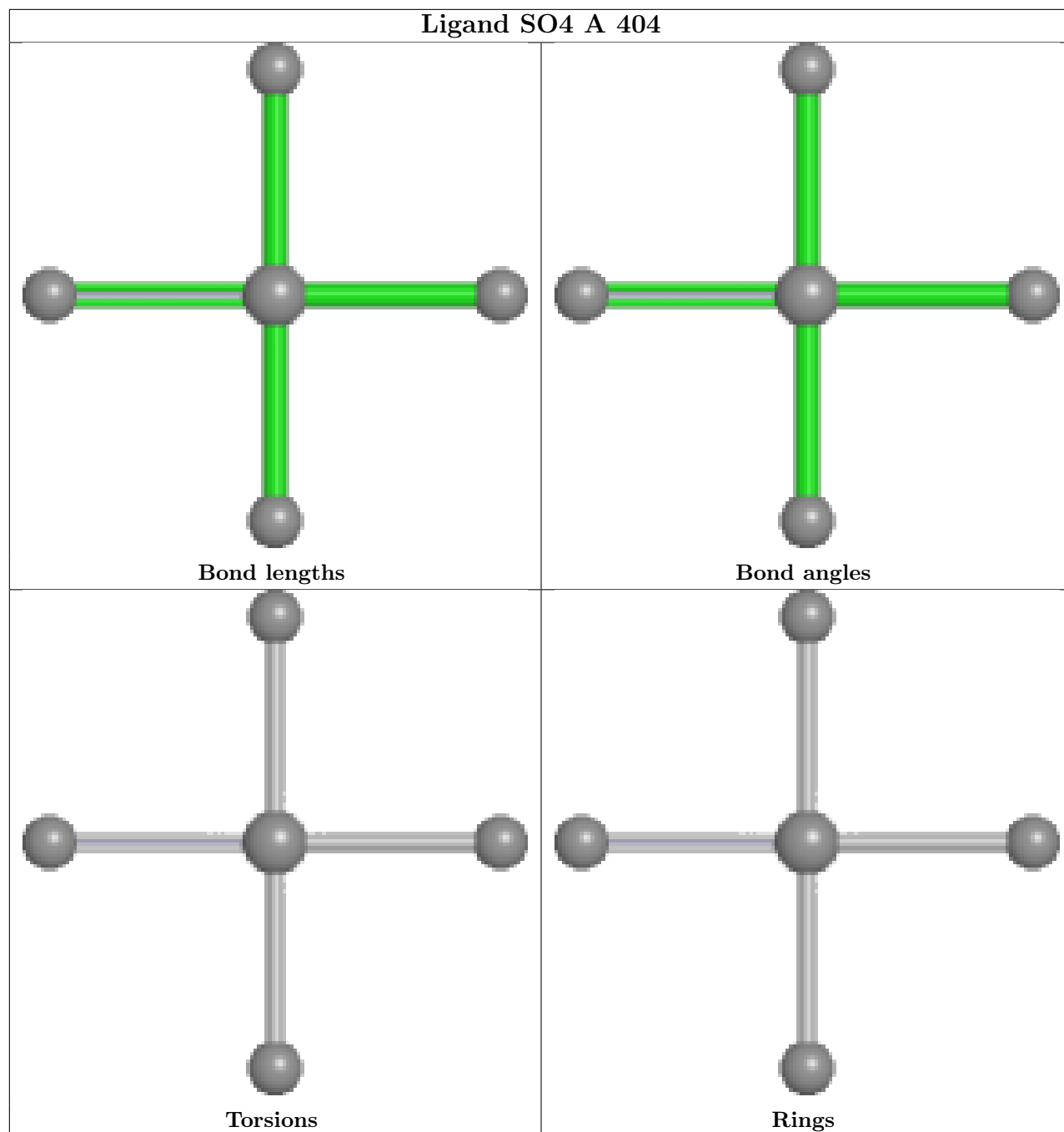
1 monomer is involved in 1 short contact:

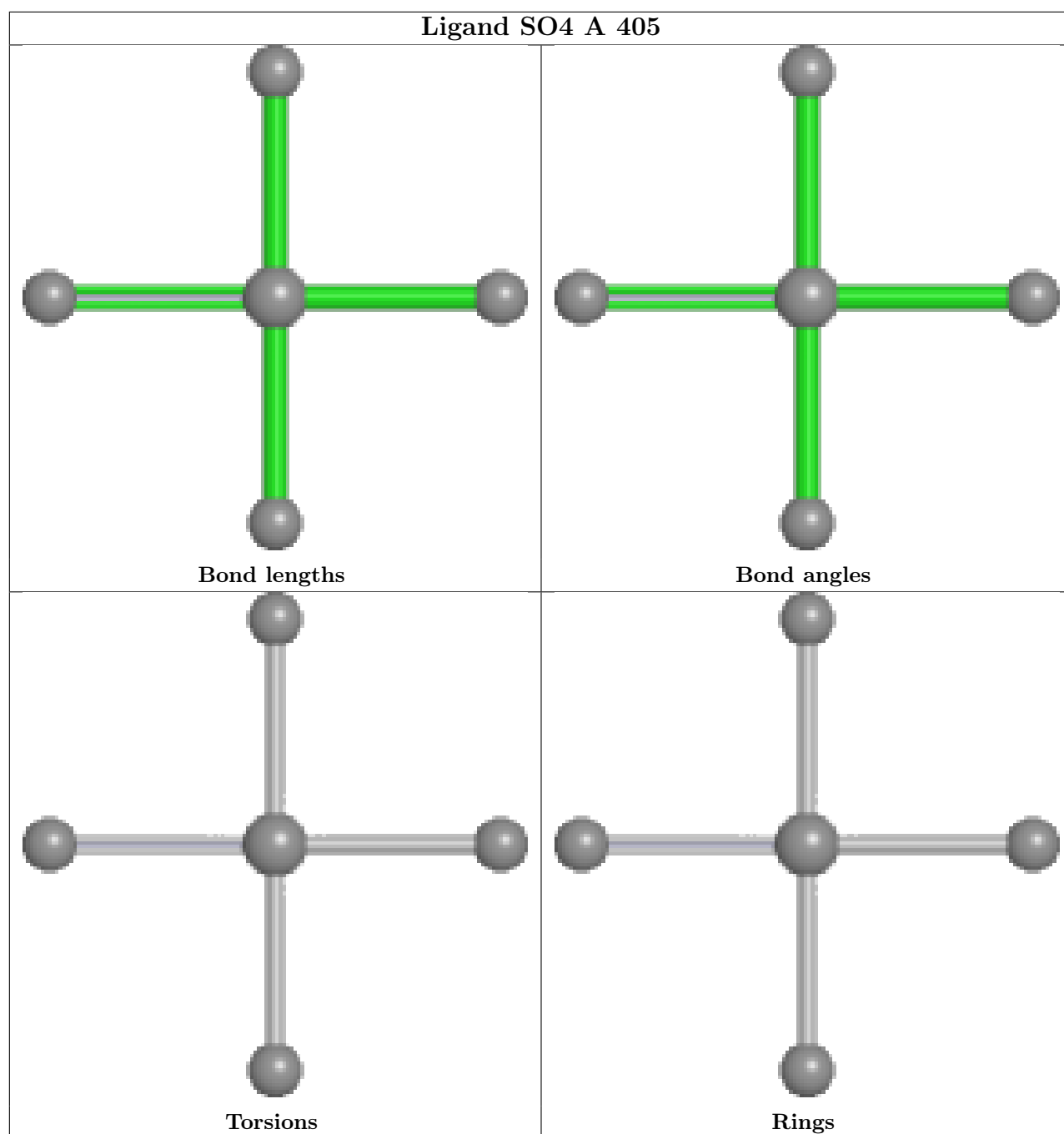
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	SO4	1	0

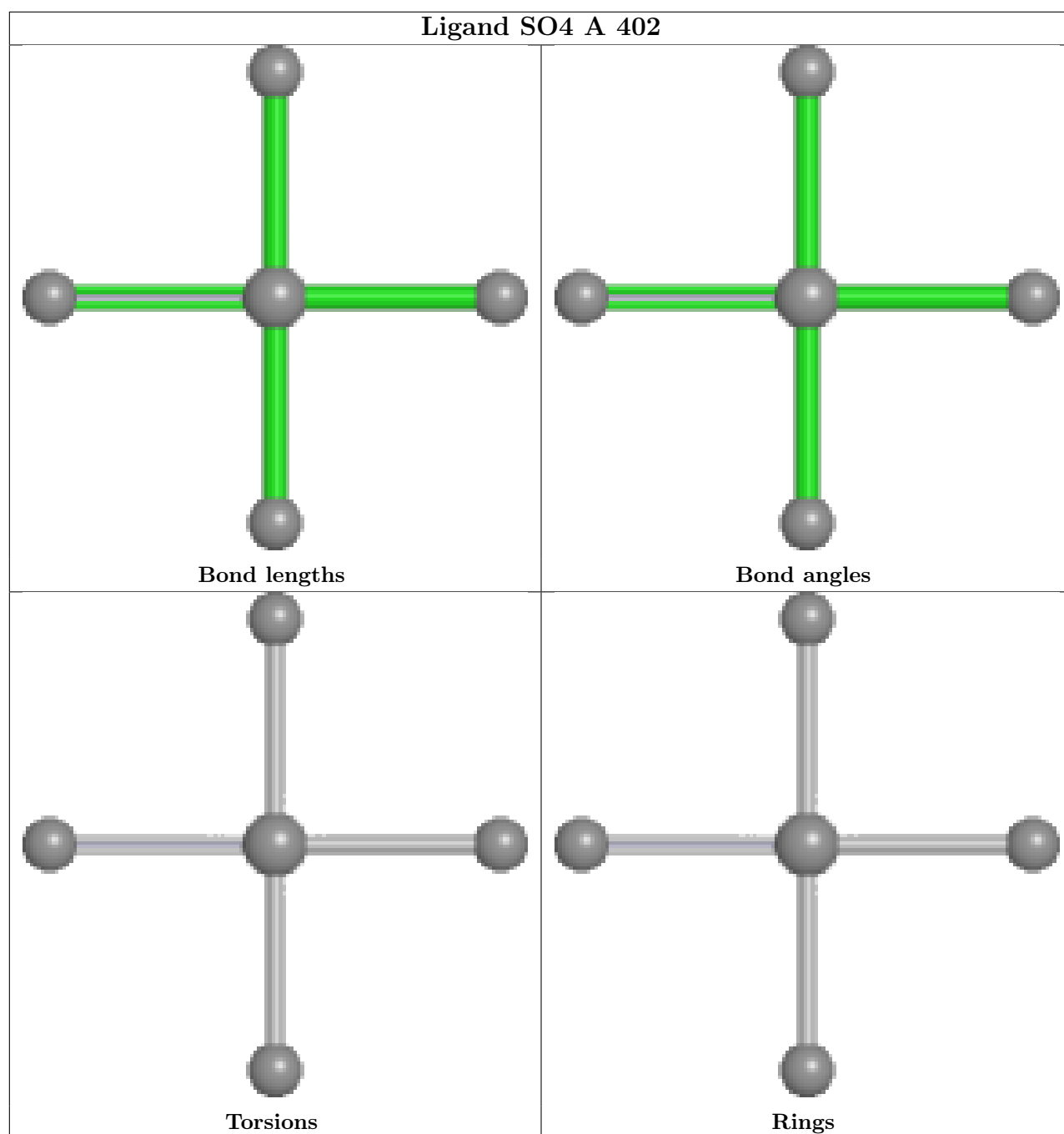
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

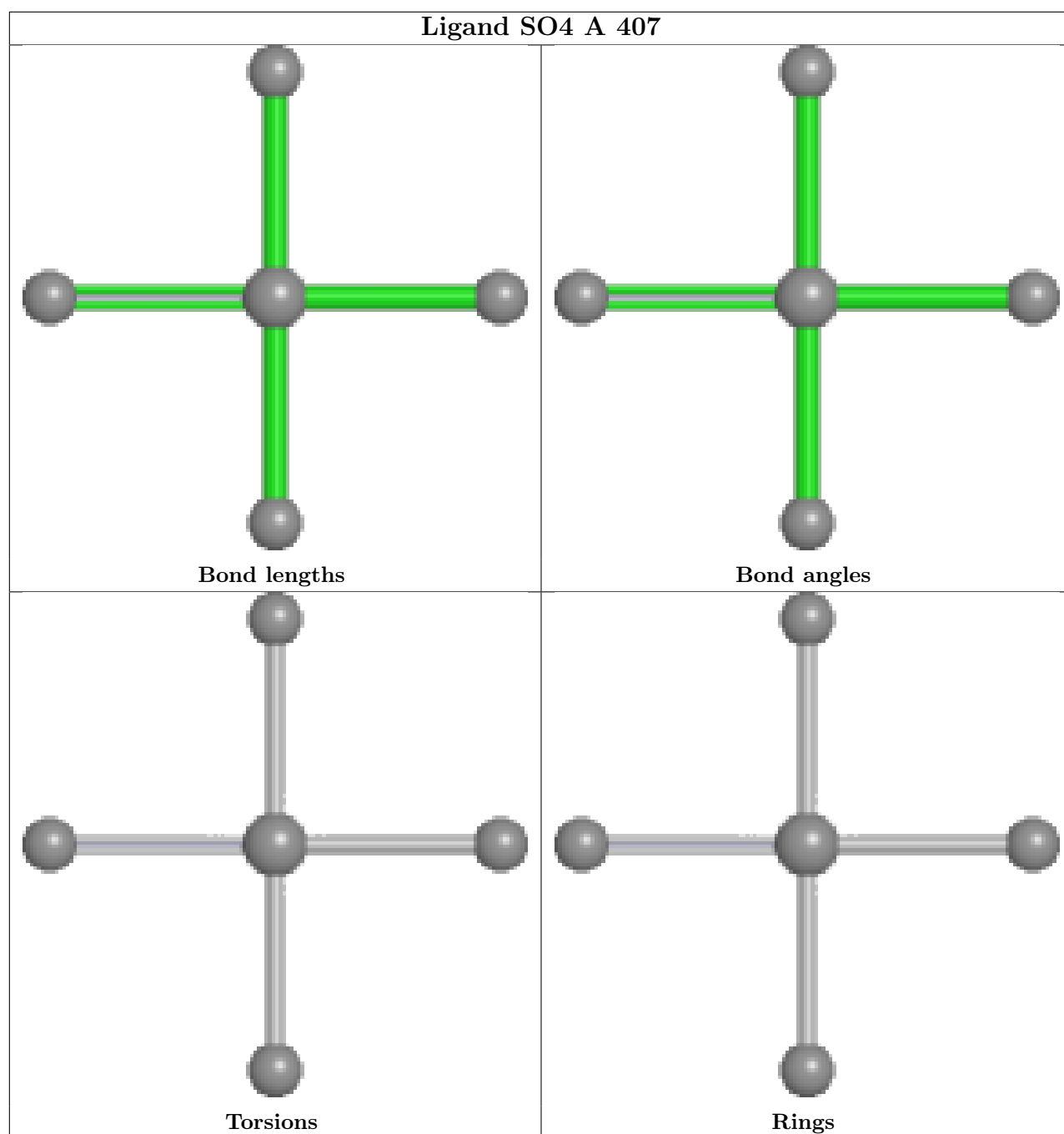
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

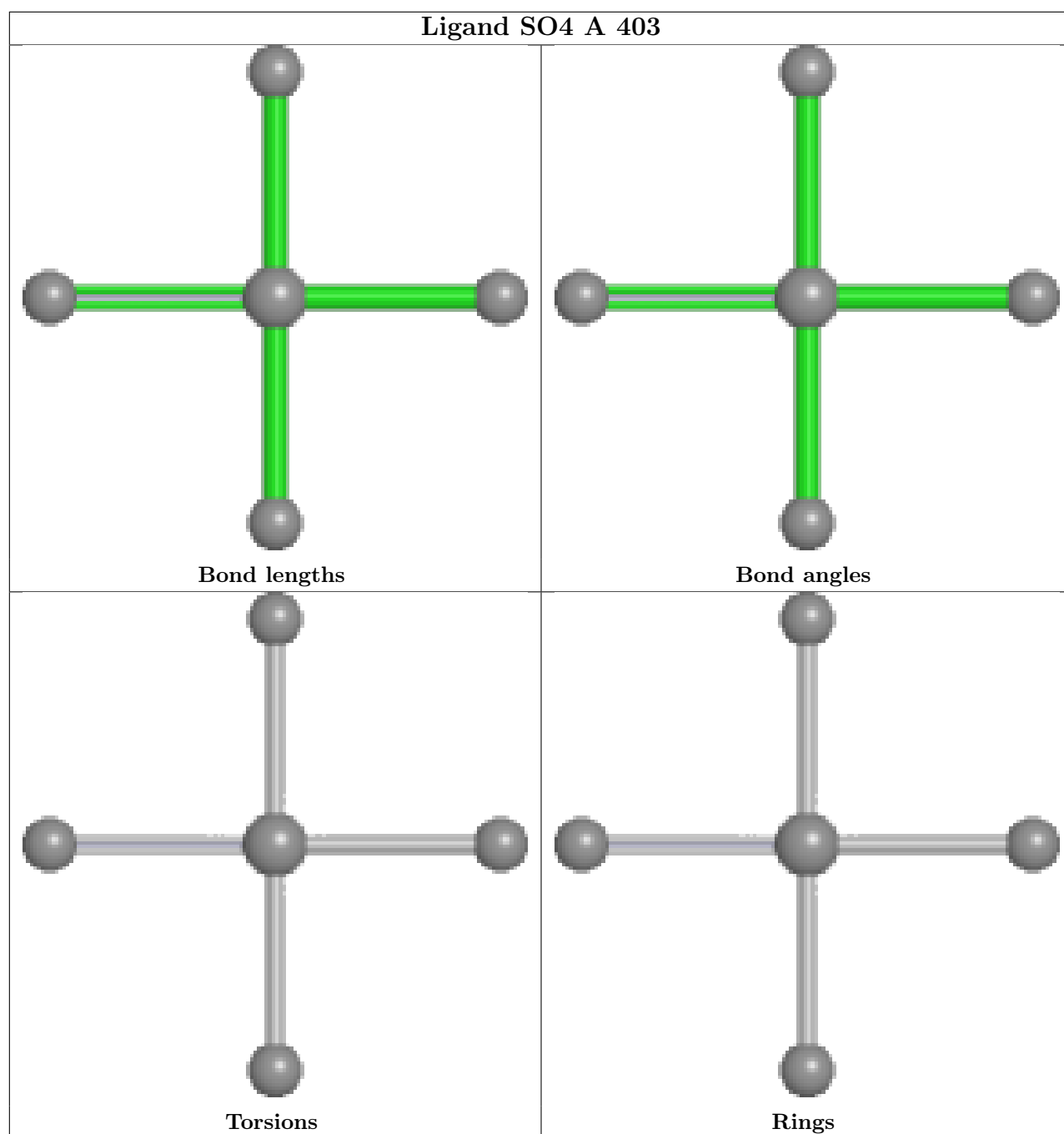












5.7 Other polymers [i](#)

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	350/350 (100%)	0.71	40 (11%) 10 7	34, 77, 135, 165	2 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	TYR	9.0
1	A	5	ALA	6.1
1	A	6	ASP	5.7
1	A	209	ILE	5.1
1	A	4	ALA	4.6
1	A	1	PHE	4.3
1	A	12	GLY	4.2
1	A	202	PHE	4.2
1	A	11	TRP	4.0
1	A	30	TYR	3.8
1	A	143	ILE	3.8
1	A	262	GLU	3.6
1	A	3	PRO	3.6
1	A	8	GLU	3.3
1	A	57	ASP	3.3
1	A	205	LYS	3.2
1	A	13	PRO	3.2
1	A	203	ARG	3.1
1	A	9	GLY	3.0
1	A	206	VAL	3.0
1	A	26	SER	2.8
1	A	194	ILE	2.6
1	A	210	ILE	2.6
1	A	263	LYS	2.6
1	A	28	THR	2.5
1	A	91	LEU	2.5
1	A	204	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	123	PHE	2.4
1	A	137	LEU	2.3
1	A	147	VAL	2.3
1	A	70	LEU	2.2
1	A	42	ILE	2.2
1	A	200	ARG	2.2
1	A	208	PRO	2.2
1	A	18	LEU	2.2
1	A	199	LEU	2.1
1	A	99	SER	2.1
1	A	90	LEU	2.1
1	A	138	LYS	2.0
1	A	212	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	A	411	1/1	0.50	0.59	73,73,73,73	1
3	SO4	A	406	5/5	0.65	0.14	138,139,139,139	0
3	SO4	A	407	5/5	0.78	0.11	114,114,114,114	0
4	NA	A	409	1/1	0.82	0.26	102,102,102,102	0
3	SO4	A	404	5/5	0.82	0.12	127,127,127,127	0
3	SO4	A	405	5/5	0.83	0.11	129,129,129,129	0
4	NA	A	408	1/1	0.86	0.16	66,66,66,66	0
3	SO4	A	403	5/5	0.87	0.10	133,133,133,133	0
3	SO4	A	402	5/5	0.88	0.12	96,97,97,97	0
6	MG	A	412	1/1	0.91	0.10	70,70,70,70	0

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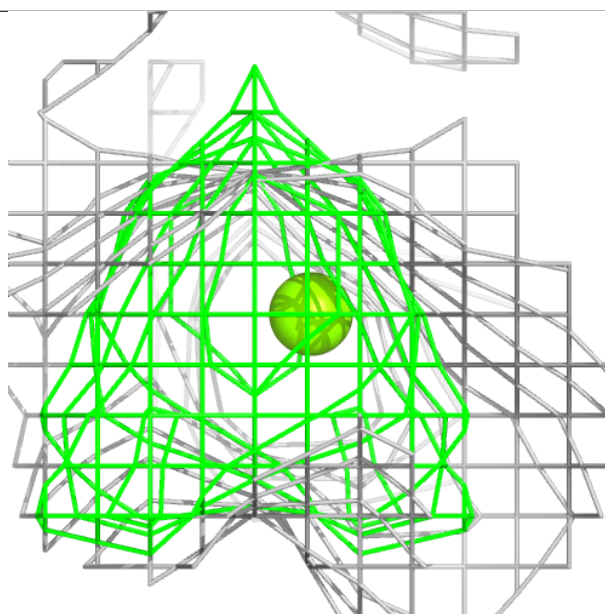
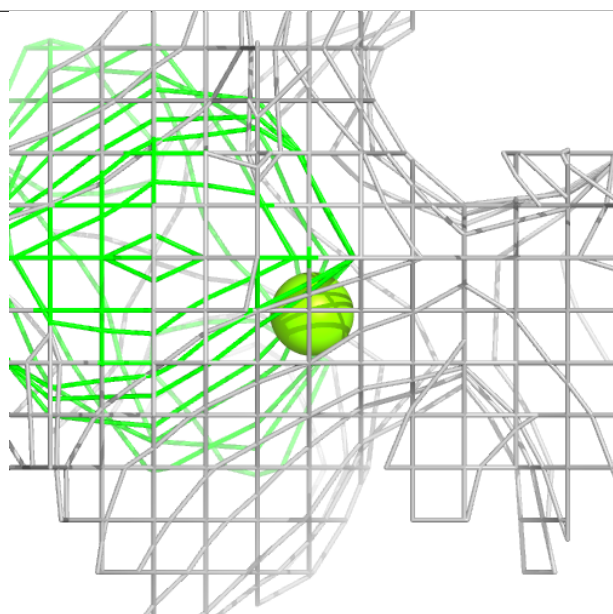
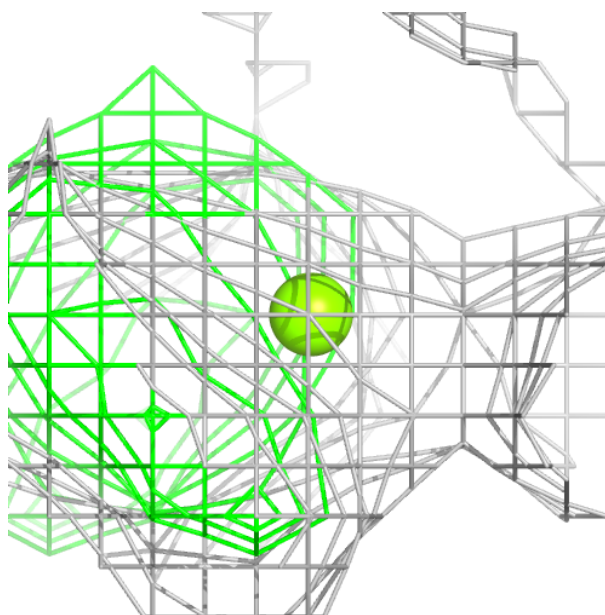
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	A	410	1/1	0.97	0.08	116,116,116,116	0
2	ZN	A	401	1/1	0.98	0.16	99,99,99,99	0

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.

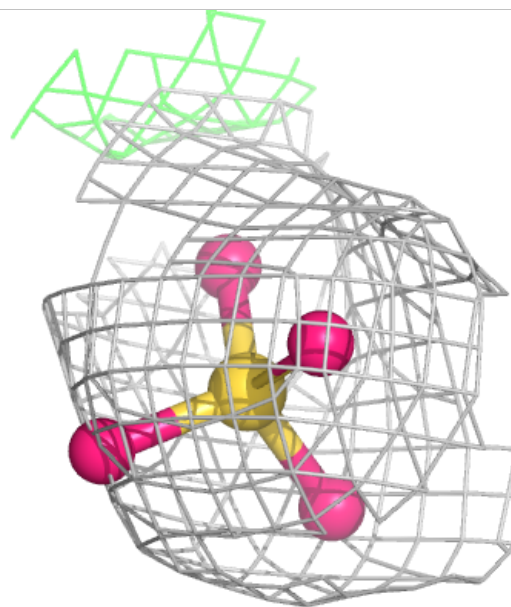
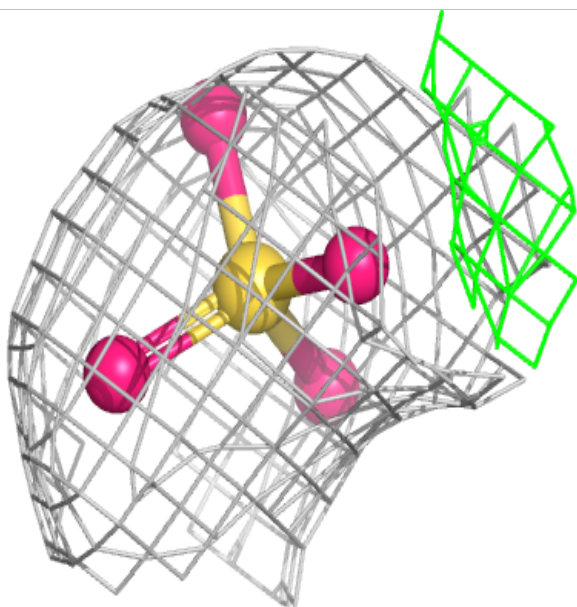
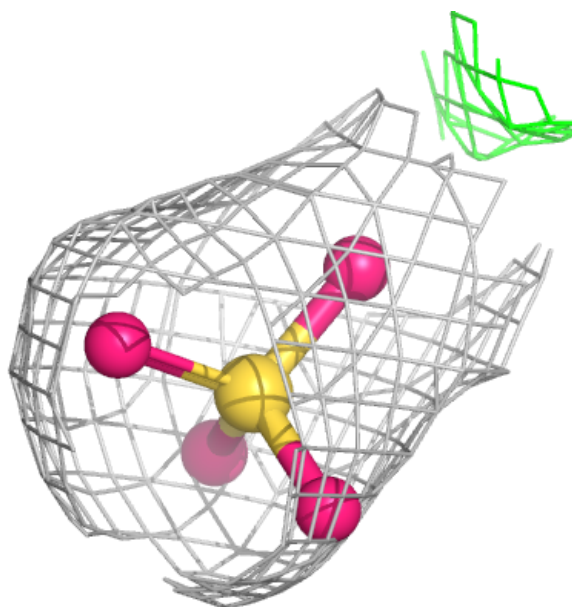
Electron density around MG A 411:

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



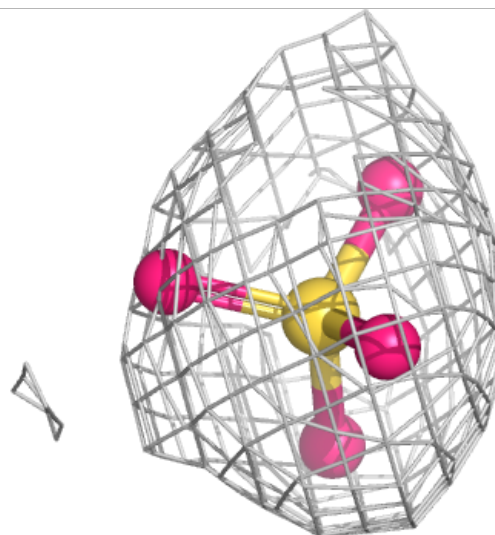
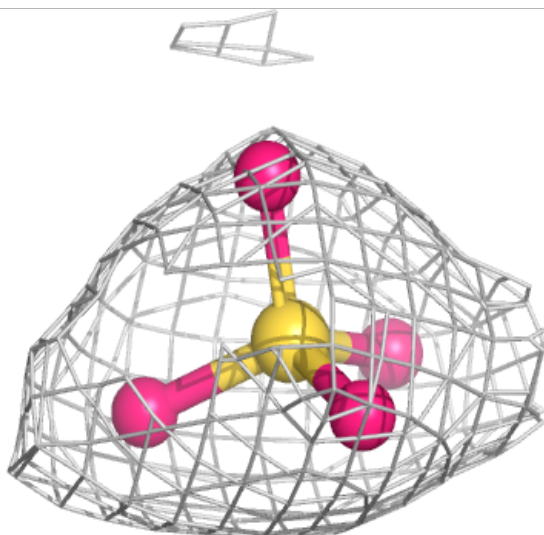
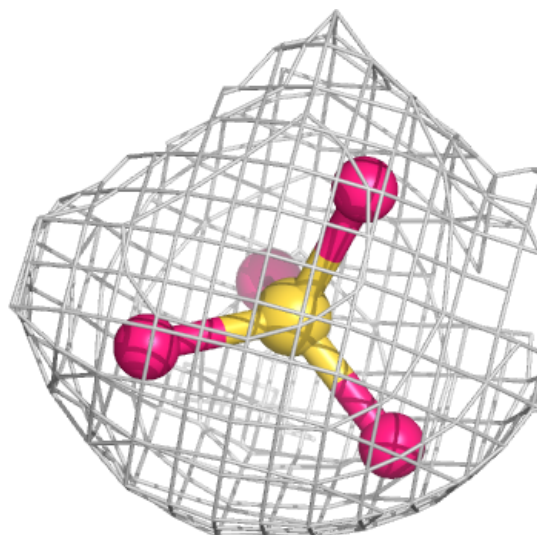
Electron density around SO4 A 406:

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



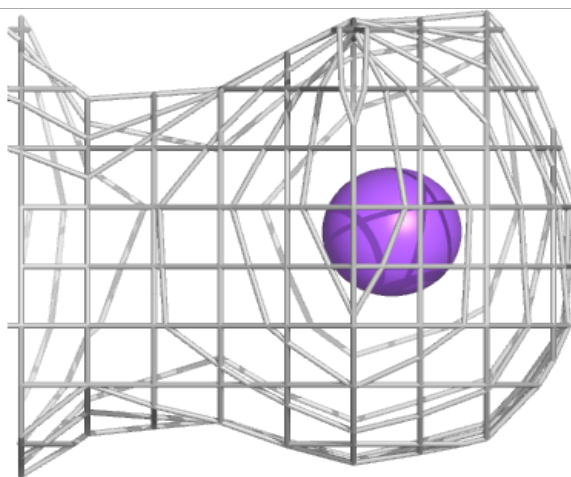
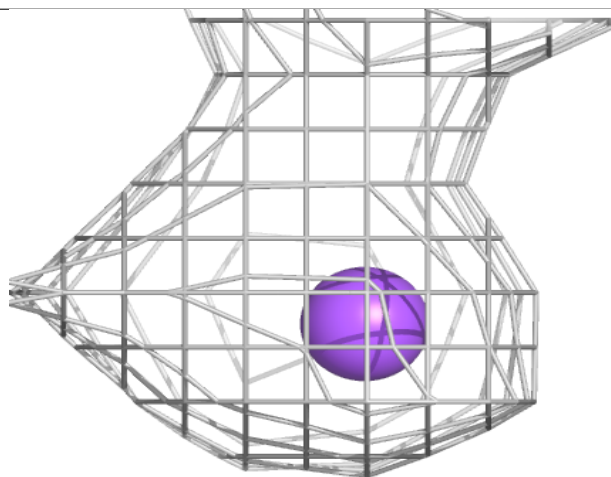
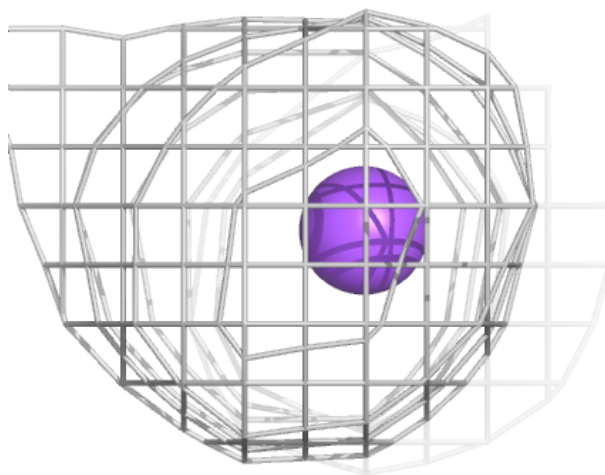
Electron density around SO4 A 407:

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



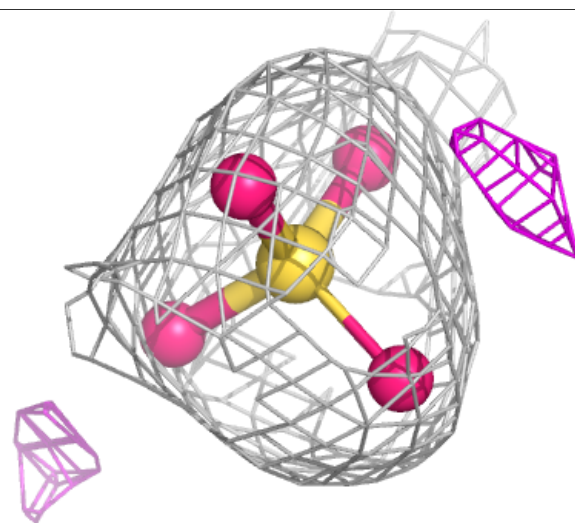
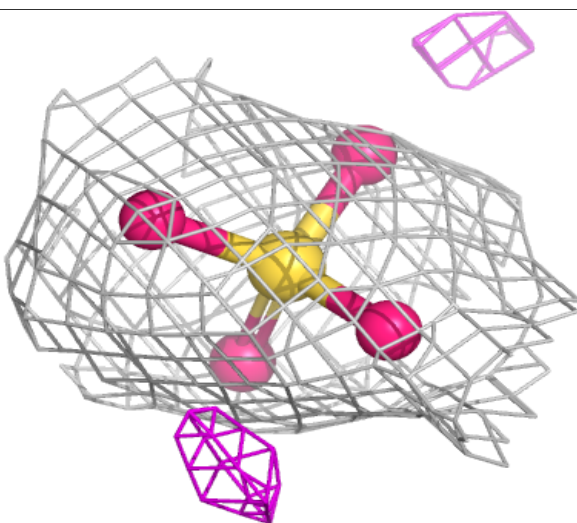
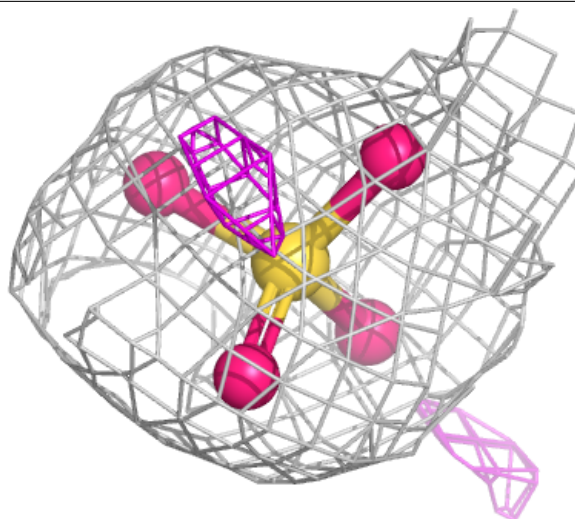
Electron density around NA A 409:

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



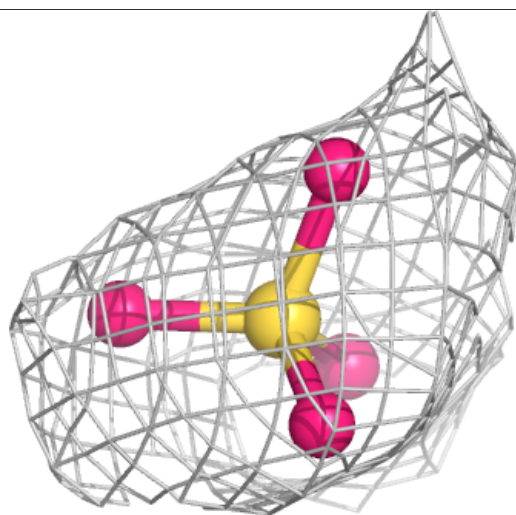
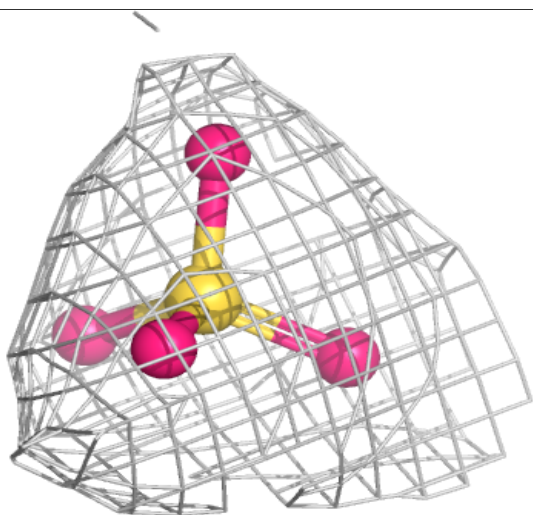
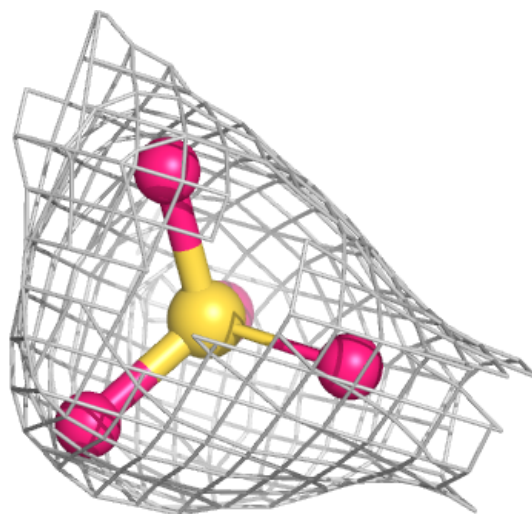
Electron density around SO4 A 404:

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



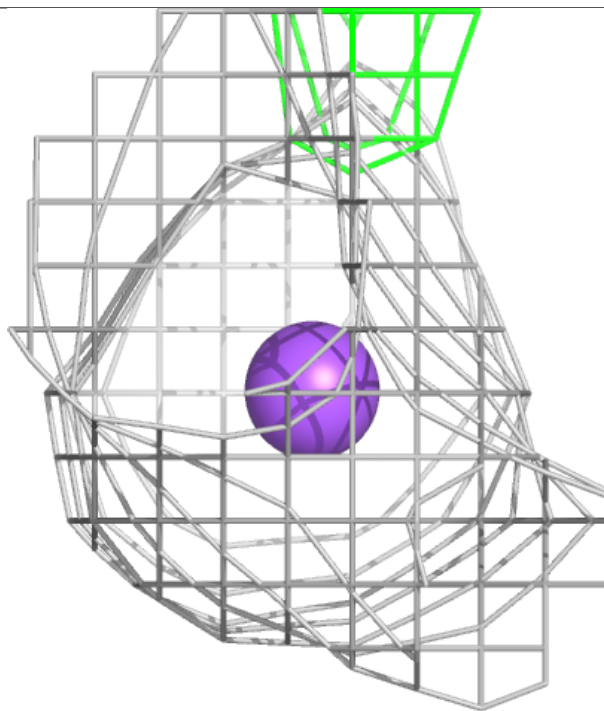
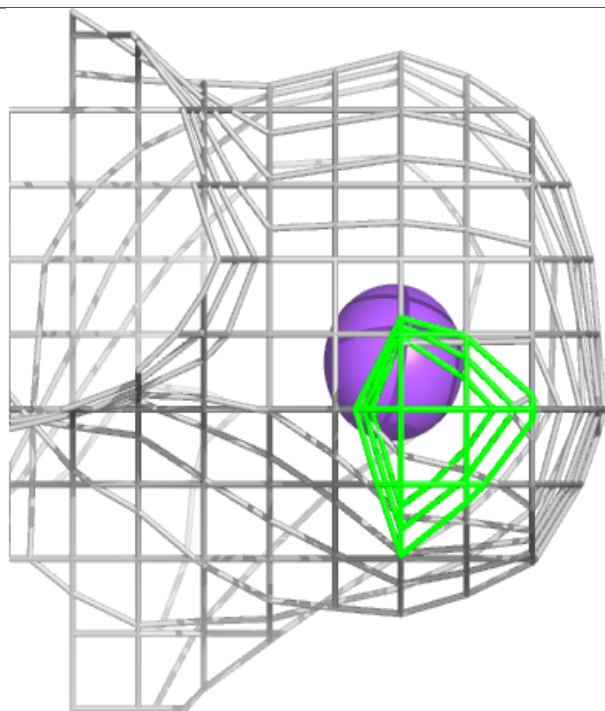
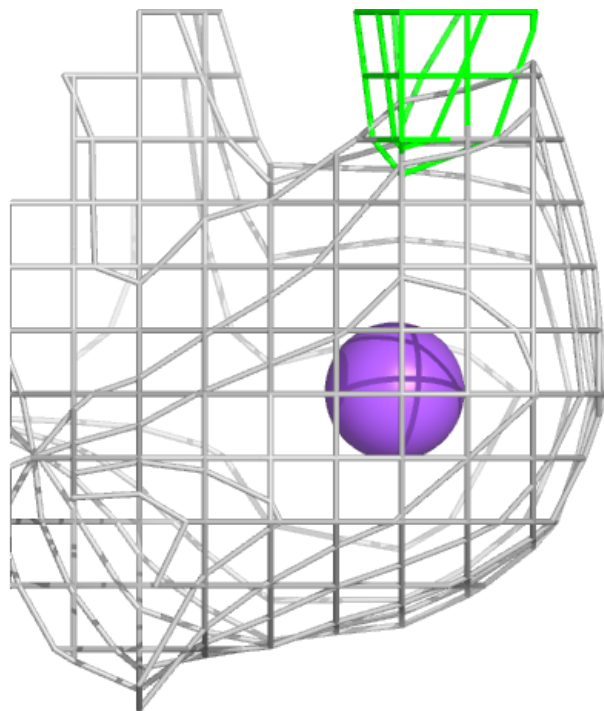
Electron density around SO4 A 405:

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



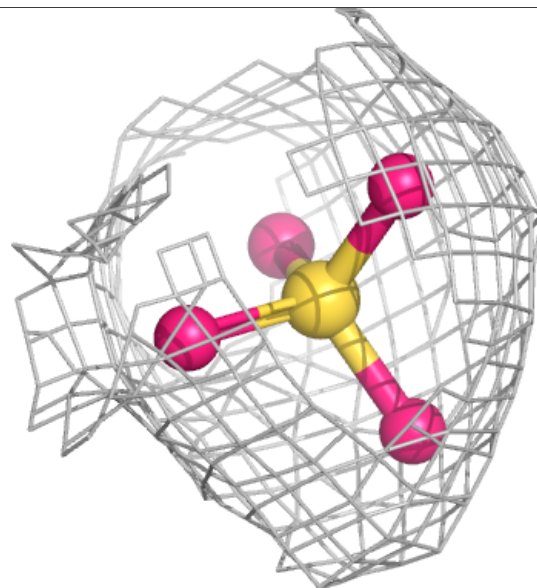
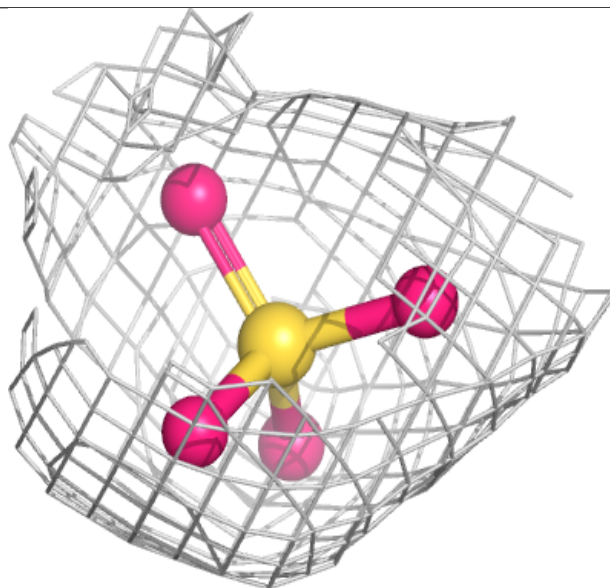
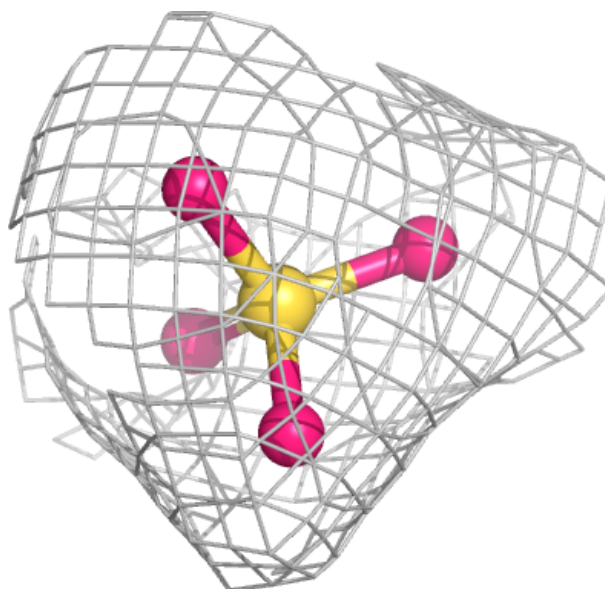
Electron density around NA A 408:

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and green (positive)



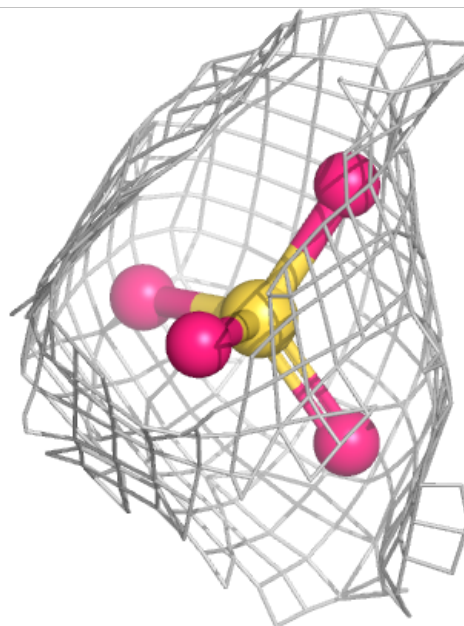
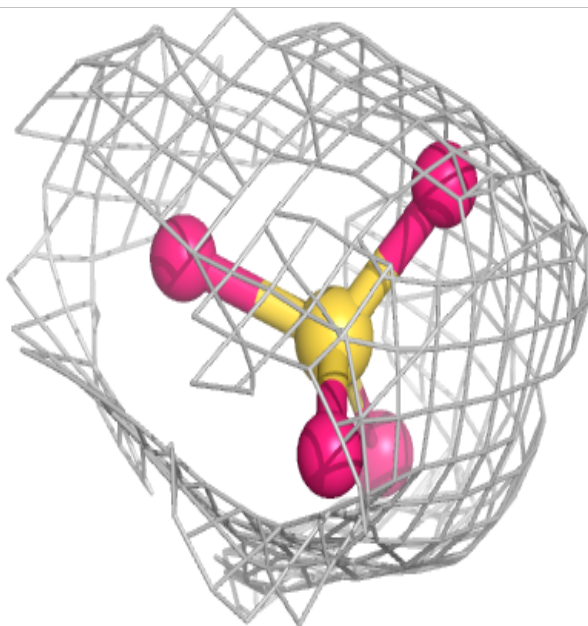
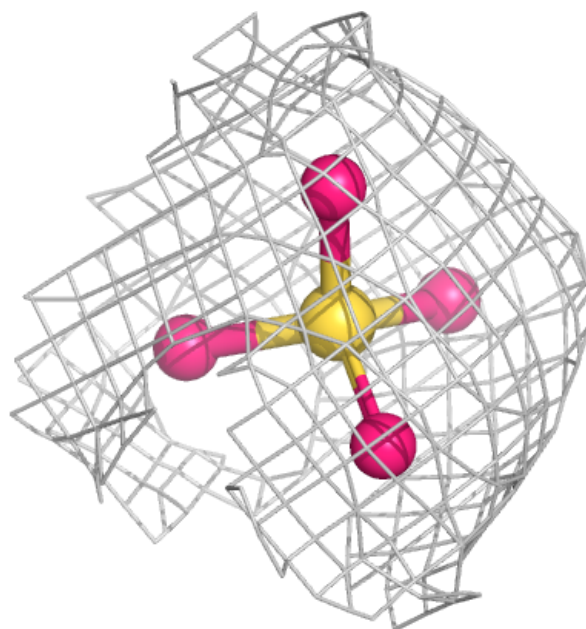
Electron density around SO4 A 403:

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and green (positive)



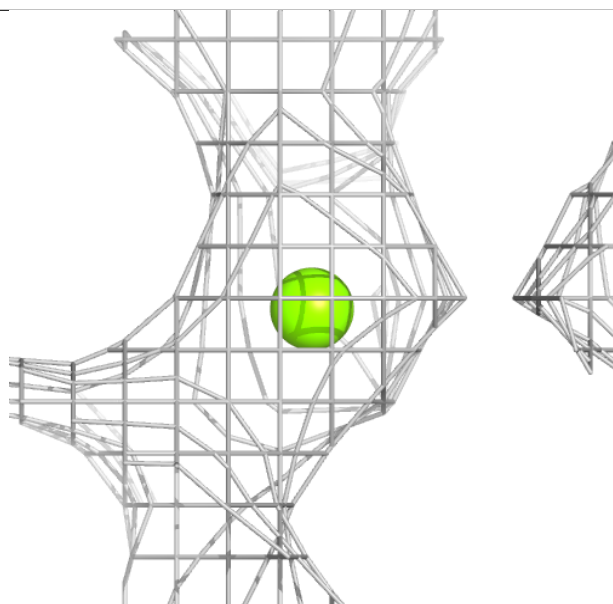
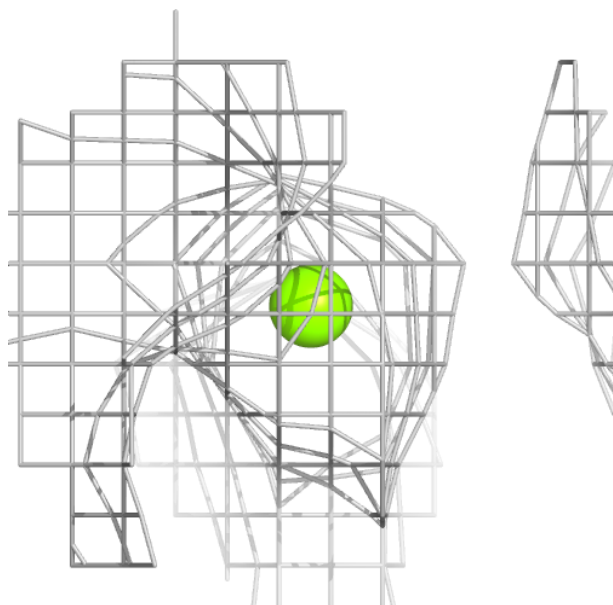
Electron density around SO4 A 402:

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and green (positive)



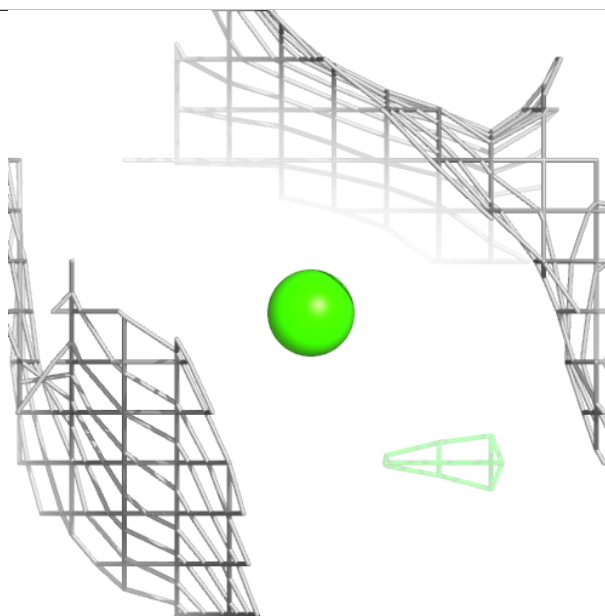
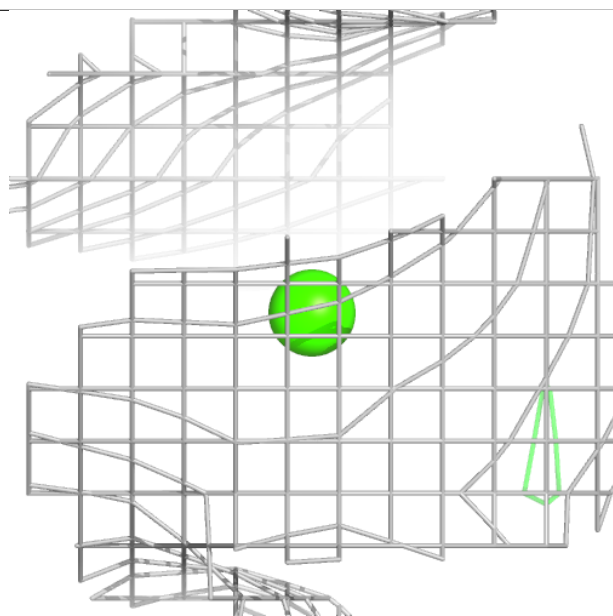
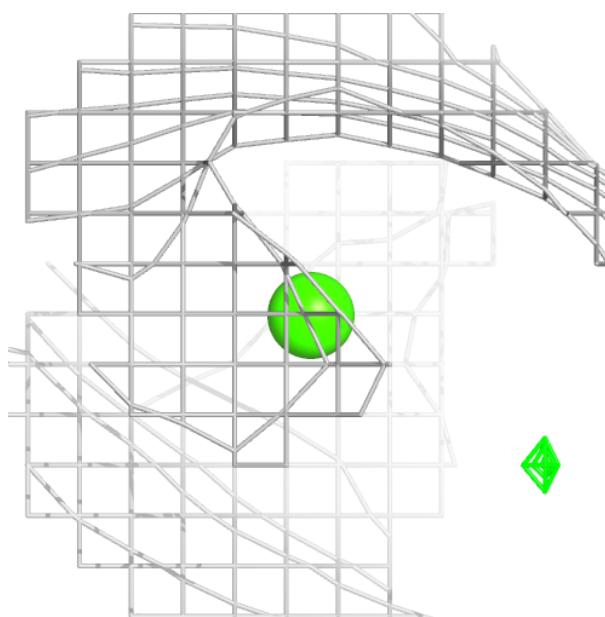
Electron density around MG A 412:

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and green (positive)



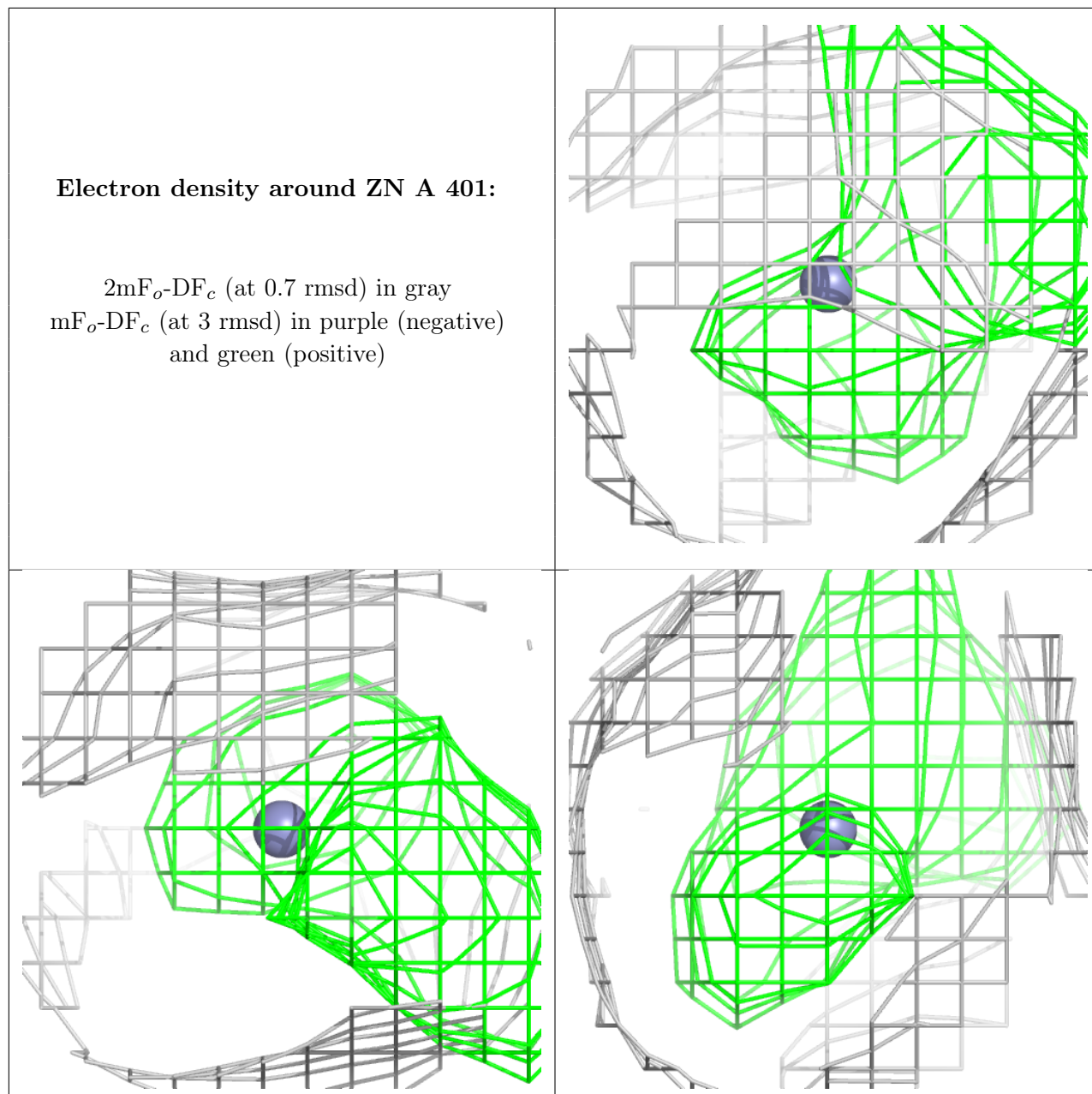
Electron density around CA A 410:

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and green (positive)



Electron density around ZN A 401:

$2mF_o-DF_c$ (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.