



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:12 AM UTC

PDB ID : 8SM8 / pdb_00008sm8
Title : Air-oxidized A. ca TruffO expressed from M9 minimal medium supplemented with Fe
Authors : Liu, C.; Rittle, J.
Deposited on : 2023-04-25
Resolution : 2.00 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

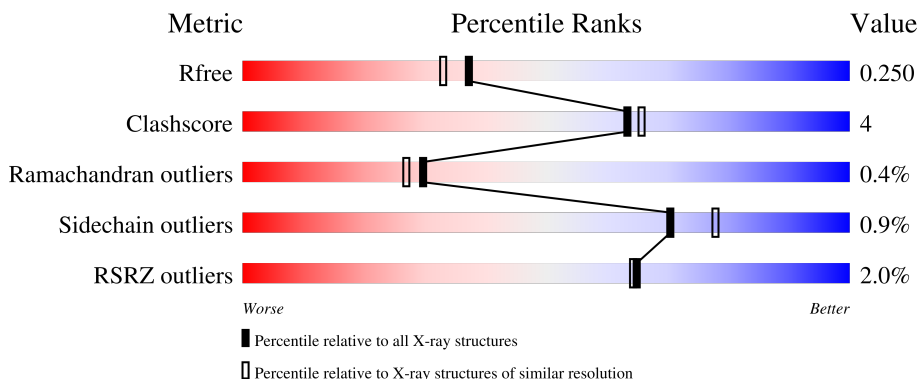
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	388	
1	D	388	
1	G	388	
1	J	388	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11818 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 Putative amidohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	344	Total	C	N	O	S	0	1	0
			2763	1773	472	504	14			
1	A	344	Total	C	N	O	S	0	2	0
			2771	1778	475	504	14			
1	D	343	Total	C	N	O	S	0	0	0
			2748	1764	469	501	14			
1	J	345	Total	C	N	O	S	0	1	0
			2770	1781	473	501	15			

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-30	MET	-	initiating methionine	UNP B6JH23
G	-29	GLY	-	expression tag	UNP B6JH23
G	-28	SER	-	expression tag	UNP B6JH23
G	-27	SER	-	expression tag	UNP B6JH23
G	-26	HIS	-	expression tag	UNP B6JH23
G	-25	HIS	-	expression tag	UNP B6JH23
G	-24	HIS	-	expression tag	UNP B6JH23
G	-23	HIS	-	expression tag	UNP B6JH23
G	-22	HIS	-	expression tag	UNP B6JH23
G	-21	HIS	-	expression tag	UNP B6JH23
G	-20	SER	-	expression tag	UNP B6JH23
G	-19	SER	-	expression tag	UNP B6JH23
G	-18	GLY	-	expression tag	UNP B6JH23
G	-17	LEU	-	expression tag	UNP B6JH23
G	-16	VAL	-	expression tag	UNP B6JH23
G	-15	PRO	-	expression tag	UNP B6JH23
G	-14	ARG	-	expression tag	UNP B6JH23
G	-13	GLY	-	expression tag	UNP B6JH23
G	-12	SER	-	expression tag	UNP B6JH23
G	-11	HIS	-	expression tag	UNP B6JH23
G	-10	MET	-	expression tag	UNP B6JH23

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-9	GLY	-	expression tag	UNP B6JH23
G	-8	GLU	-	expression tag	UNP B6JH23
G	-7	ASN	-	expression tag	UNP B6JH23
G	-6	LEU	-	expression tag	UNP B6JH23
G	-5	TYR	-	expression tag	UNP B6JH23
G	-4	PHE	-	expression tag	UNP B6JH23
G	-3	GLN	-	expression tag	UNP B6JH23
G	-2	SER	-	expression tag	UNP B6JH23
G	-1	GLY	-	expression tag	UNP B6JH23
G	0	GLY	-	expression tag	UNP B6JH23
A	-30	MET	-	initiating methionine	UNP B6JH23
A	-29	GLY	-	expression tag	UNP B6JH23
A	-28	SER	-	expression tag	UNP B6JH23
A	-27	SER	-	expression tag	UNP B6JH23
A	-26	HIS	-	expression tag	UNP B6JH23
A	-25	HIS	-	expression tag	UNP B6JH23
A	-24	HIS	-	expression tag	UNP B6JH23
A	-23	HIS	-	expression tag	UNP B6JH23
A	-22	HIS	-	expression tag	UNP B6JH23
A	-21	HIS	-	expression tag	UNP B6JH23
A	-20	SER	-	expression tag	UNP B6JH23
A	-19	SER	-	expression tag	UNP B6JH23
A	-18	GLY	-	expression tag	UNP B6JH23
A	-17	LEU	-	expression tag	UNP B6JH23
A	-16	VAL	-	expression tag	UNP B6JH23
A	-15	PRO	-	expression tag	UNP B6JH23
A	-14	ARG	-	expression tag	UNP B6JH23
A	-13	GLY	-	expression tag	UNP B6JH23
A	-12	SER	-	expression tag	UNP B6JH23
A	-11	HIS	-	expression tag	UNP B6JH23
A	-10	MET	-	expression tag	UNP B6JH23
A	-9	GLY	-	expression tag	UNP B6JH23
A	-8	GLU	-	expression tag	UNP B6JH23
A	-7	ASN	-	expression tag	UNP B6JH23
A	-6	LEU	-	expression tag	UNP B6JH23
A	-5	TYR	-	expression tag	UNP B6JH23
A	-4	PHE	-	expression tag	UNP B6JH23
A	-3	GLN	-	expression tag	UNP B6JH23
A	-2	SER	-	expression tag	UNP B6JH23
A	-1	GLY	-	expression tag	UNP B6JH23
A	0	GLY	-	expression tag	UNP B6JH23
D	-30	MET	-	initiating methionine	UNP B6JH23

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-29	GLY	-	expression tag	UNP B6JH23
D	-28	SER	-	expression tag	UNP B6JH23
D	-27	SER	-	expression tag	UNP B6JH23
D	-26	HIS	-	expression tag	UNP B6JH23
D	-25	HIS	-	expression tag	UNP B6JH23
D	-24	HIS	-	expression tag	UNP B6JH23
D	-23	HIS	-	expression tag	UNP B6JH23
D	-22	HIS	-	expression tag	UNP B6JH23
D	-21	HIS	-	expression tag	UNP B6JH23
D	-20	SER	-	expression tag	UNP B6JH23
D	-19	SER	-	expression tag	UNP B6JH23
D	-18	GLY	-	expression tag	UNP B6JH23
D	-17	LEU	-	expression tag	UNP B6JH23
D	-16	VAL	-	expression tag	UNP B6JH23
D	-15	PRO	-	expression tag	UNP B6JH23
D	-14	ARG	-	expression tag	UNP B6JH23
D	-13	GLY	-	expression tag	UNP B6JH23
D	-12	SER	-	expression tag	UNP B6JH23
D	-11	HIS	-	expression tag	UNP B6JH23
D	-10	MET	-	expression tag	UNP B6JH23
D	-9	GLY	-	expression tag	UNP B6JH23
D	-8	GLU	-	expression tag	UNP B6JH23
D	-7	ASN	-	expression tag	UNP B6JH23
D	-6	LEU	-	expression tag	UNP B6JH23
D	-5	TYR	-	expression tag	UNP B6JH23
D	-4	PHE	-	expression tag	UNP B6JH23
D	-3	GLN	-	expression tag	UNP B6JH23
D	-2	SER	-	expression tag	UNP B6JH23
D	-1	GLY	-	expression tag	UNP B6JH23
D	0	GLY	-	expression tag	UNP B6JH23
J	-30	MET	-	initiating methionine	UNP B6JH23
J	-29	GLY	-	expression tag	UNP B6JH23
J	-28	SER	-	expression tag	UNP B6JH23
J	-27	SER	-	expression tag	UNP B6JH23
J	-26	HIS	-	expression tag	UNP B6JH23
J	-25	HIS	-	expression tag	UNP B6JH23
J	-24	HIS	-	expression tag	UNP B6JH23
J	-23	HIS	-	expression tag	UNP B6JH23
J	-22	HIS	-	expression tag	UNP B6JH23
J	-21	HIS	-	expression tag	UNP B6JH23
J	-20	SER	-	expression tag	UNP B6JH23
J	-19	SER	-	expression tag	UNP B6JH23

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-18	GLY	-	expression tag	UNP B6JH23
J	-17	LEU	-	expression tag	UNP B6JH23
J	-16	VAL	-	expression tag	UNP B6JH23
J	-15	PRO	-	expression tag	UNP B6JH23
J	-14	ARG	-	expression tag	UNP B6JH23
J	-13	GLY	-	expression tag	UNP B6JH23
J	-12	SER	-	expression tag	UNP B6JH23
J	-11	HIS	-	expression tag	UNP B6JH23
J	-10	MET	-	expression tag	UNP B6JH23
J	-9	GLY	-	expression tag	UNP B6JH23
J	-8	GLU	-	expression tag	UNP B6JH23
J	-7	ASN	-	expression tag	UNP B6JH23
J	-6	LEU	-	expression tag	UNP B6JH23
J	-5	TYR	-	expression tag	UNP B6JH23
J	-4	PHE	-	expression tag	UNP B6JH23
J	-3	GLN	-	expression tag	UNP B6JH23
J	-2	SER	-	expression tag	UNP B6JH23
J	-1	GLY	-	expression tag	UNP B6JH23
J	0	GLY	-	expression tag	UNP B6JH23

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Fe 2 2	0	0
2	A	2	Total Fe 2 2	0	0
2	D	2	Total Fe 2 2	0	0
2	J	2	Total Fe 2 2	0	0

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



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

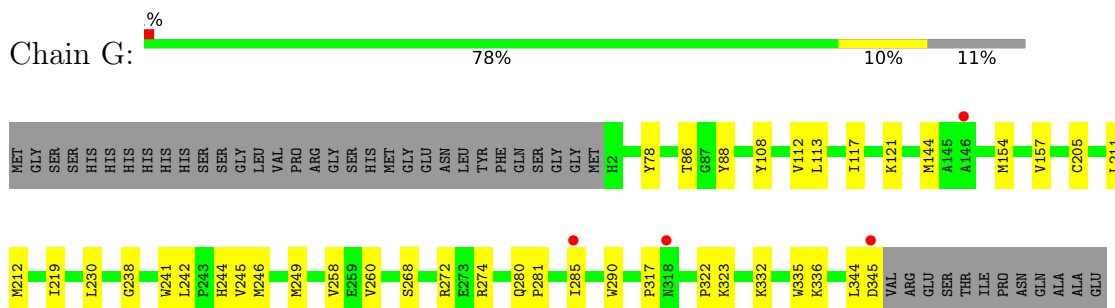
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	220	Total	O	0	0
			220	220		
5	A	193	Total	O	0	0
			193	193		
5	D	151	Total	O	0	0
			151	151		
5	J	172	Total	O	0	0
			172	172		

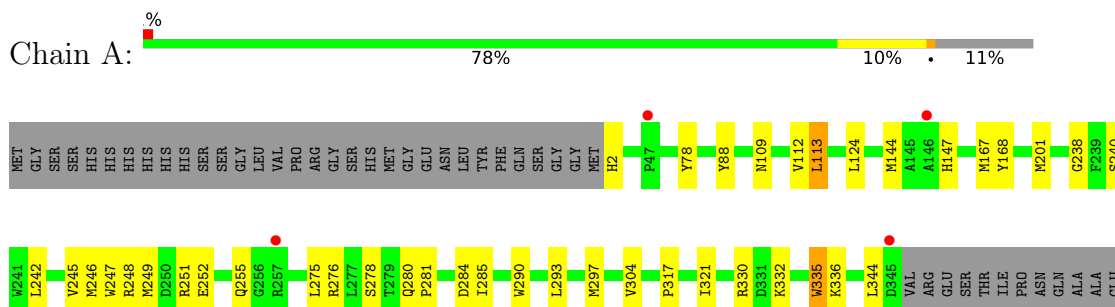
3 Residue-property plots

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.

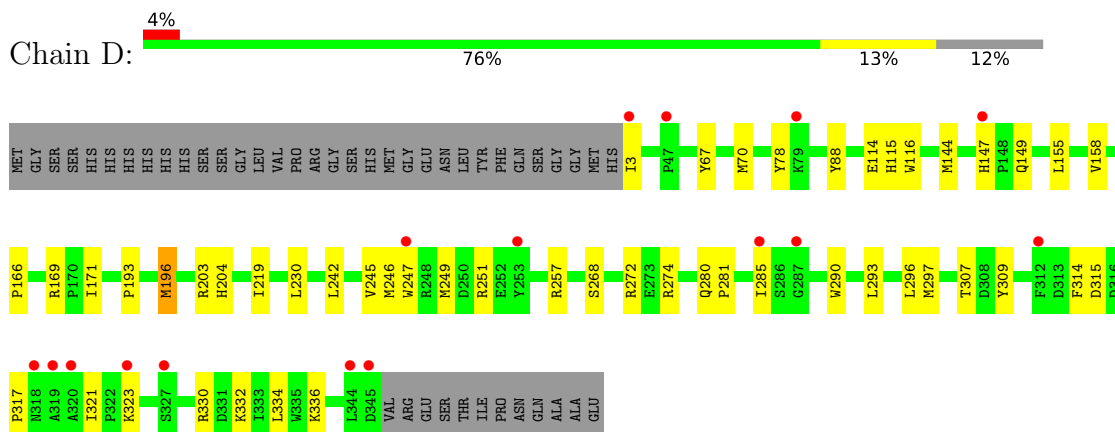
- Molecule 1: Putative amidohydrolase



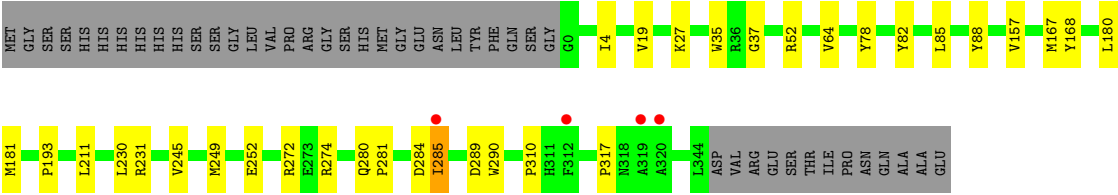
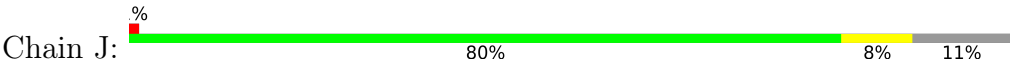
- Molecule 1: Putative amidohydrolase



- Molecule 1: Putative amidohydrolase



- Molecule 1: Putative amidohydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.93Å 154.82Å 74.95Å 90.00° 104.93° 90.00°	Depositor
Resolution (Å)	77.41 – 2.00 77.41 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.3 (77.41-2.00) 86.3 (77.41-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.74 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.192 , 0.252 0.193 , 0.250	Depositor DCC
R_{free} test set	1995 reflections (2.11%)	wwPDB-VP
Wilson B-factor (Å ²)	14.0	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.9	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	11818	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/2861	0.60	0/3888
1	D	0.38	0/2831	0.57	0/3848
1	G	0.41	0/2850	0.61	0/3874
1	J	0.40	0/2858	0.59	0/3883
All	All	0.40	0/11400	0.59	0/15493

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2771	0	2684	22	0
1	D	2748	0	2660	27	0
1	G	2763	0	2671	24	0
1	J	2770	0	2687	22	0
2	A	2	0	0	0	0
2	D	2	0	0	0	0
2	G	2	0	0	0	0
2	J	2	0	0	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	5	0	0	1	0
3	G	5	0	0	0	0
3	J	5	0	0	0	0
4	A	2	0	0	0	0
5	A	193	0	0	1	0
5	D	151	0	0	0	0
5	G	220	0	0	2	0
5	J	172	0	0	1	0
All	All	11818	0	10702	88	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 4.

All (88) 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:251:ARG:HG3	1:A:255:GLN:NE2	2.15	0.61
1:A:245:VAL:HG12	1:A:249:MET:HE2	1.83	0.60
1:D:219:ILE:HB	1:D:249:MET:HE1	1.83	0.59
1:A:280:GLN:HG2	1:A:281:PRO:HA	1.85	0.58
1:J:52:ARG:HG2	1:J:310:PRO:O	2.03	0.58
1:G:205:CYS:SG	1:A:252:GLU:HG3	2.44	0.58
1:G:219:ILE:HD12	1:G:249:MET:HE1	1.87	0.56
1:G:245:VAL:HG12	1:G:249:MET:HE2	1.87	0.56
1:G:78:TYR:CE1	1:G:317:PRO:HD2	2.41	0.56
1:G:113:LEU:HD22	1:G:144:MET:HE1	1.87	0.55
1:D:321:ILE:O	1:D:330:ARG:NH1	2.39	0.54
1:J:4:ILE:HG12	1:J:82:TYR:HB2	1.89	0.54
1:J:19:VAL:HG13	1:J:27:LYS:HG2	1.90	0.54
1:G:285:ILE:HD11	1:A:247:TRP:CE3	2.43	0.54
1:G:258:VAL:HG12	5:G:636:HOH:O	2.09	0.52
1:A:275:LEU:O	1:A:276:ARG:HD3	2.10	0.52
1:G:280:GLN:HG2	1:G:281:PRO:HA	1.92	0.52
1:D:280:GLN:HG2	1:D:281:PRO:HA	1.92	0.51
1:A:113:LEU:HD11	1:A:147:HIS:CD2	2.45	0.51
1:A:167:MET:HE2	1:A:168:TYR:CE1	2.45	0.51
1:J:285:ILE:HG23	1:J:290:TRP:NE1	2.27	0.50
1:D:114:GLU:HG2	1:D:115:HIS:CE1	2.47	0.49
1:G:157:VAL:HG21	1:G:211:LEU:HD23	1.93	0.49
1:D:3:ILE:HG12	1:D:334:LEU:HD22	1.94	0.49
1:D:155:LEU:HD21	1:D:171:ILE:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:LYS:HA	1:D:336:LYS:HB3	1.95	0.49
1:D:196:MET:HG2	1:D:203:ARG:HG3	1.94	0.49
1:G:238:GLY:HA2	5:G:541:HOH:O	2.13	0.48
1:J:280:GLN:HG2	1:J:281:PRO:HA	1.96	0.48
1:G:260:VAL:HG21	1:A:201:MET:HE3	1.94	0.47
1:A:109:ASN:HB3	1:A:144:MET:HE2	1.95	0.47
1:D:247:TRP:HH2	1:D:296:LEU:HD22	1.80	0.47
1:G:244:HIS:HB2	1:A:240:SER:OG	2.15	0.47
1:A:332:LYS:HA	1:A:336:LYS:HB3	1.97	0.47
1:J:285:ILE:HG13	1:J:289:ASP:HB2	1.97	0.47
1:J:230:LEU:O	1:J:274:ARG:HD2	2.15	0.46
1:G:336:LYS:HB3	1:G:336:LYS:HE2	1.69	0.46
1:J:78:TYR:CG	1:J:317:PRO:HG2	2.51	0.46
1:D:166:PRO:O	1:D:169:ARG:HG3	2.15	0.46
1:J:245:VAL:HG12	1:J:249:MET:HE2	1.97	0.46
1:G:86:THR:HB	1:G:154:MET:HE3	1.98	0.46
1:D:70:MET:HG3	1:D:309:TYR:CE2	2.51	0.46
1:A:278:SER:HA	1:A:304:VAL:O	2.16	0.46
1:D:193:PRO:HA	1:J:193:PRO:HA	1.98	0.46
1:D:147:HIS:CE1	1:D:149:GLN:HB2	2.51	0.45
1:D:204:HIS:ND1	1:J:252:GLU:OE2	2.50	0.45
1:J:180:LEU:C	1:J:181:MET:HE2	2.42	0.45
1:G:230:LEU:O	1:G:274:ARG:HD2	2.17	0.45
1:G:335:TRP:CZ3	1:G:336:LYS:HG2	2.53	0.44
1:D:67:TYR:HA	1:D:116:TRP:CZ3	2.53	0.44
1:G:112:VAL:HG12	1:G:117:ILE:HD12	1.98	0.44
1:A:2:HIS:HB2	1:A:335:TRP:CG	2.53	0.44
1:A:285:ILE:HG13	1:A:290:TRP:CD1	2.52	0.44
1:D:242:LEU:O	1:D:246:MET:HG3	2.18	0.44
1:D:204:HIS:NE2	3:D:403:SO4:O3	2.42	0.44
1:G:108:TYR:CE2	1:G:112:VAL:HG21	2.53	0.43
1:G:344:LEU:O	1:G:345:ASP:HB2	2.18	0.43
1:D:230:LEU:O	1:D:274:ARG:HD2	2.19	0.43
1:G:212:MET:HE2	1:G:241:TRP:CG	2.52	0.43
1:A:238:GLY:HA2	5:A:526:HOH:O	2.19	0.43
1:D:285:ILE:HG23	1:D:290:TRP:NE1	2.34	0.43
1:J:85:LEU:HD23	1:J:85:LEU:HA	1.86	0.43
1:G:290:TRP:CD1	1:G:322:PRO:HG2	2.53	0.43
1:J:285:ILE:HG23	1:J:290:TRP:HE1	1.84	0.43
1:D:251:ARG:NH1	1:J:284:ASP:OD2	2.52	0.42
1:G:242:LEU:HG	1:G:246:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:TYR:CE1	1:A:317:PRO:HD2	2.54	0.42
1:D:78:TYR:CE1	1:D:317:PRO:HD2	2.54	0.42
1:J:157:VAL:HG21	1:J:211:LEU:HD23	2.02	0.42
1:A:248:ARG:O	1:A:252:GLU:HG2	2.20	0.41
1:D:307:THR:HB	1:D:314:PHE:CD2	2.55	0.41
1:J:167:MET:HE3	1:J:168:TYR:CZ	2.55	0.41
1:D:245:VAL:O	1:D:249:MET:HG3	2.20	0.41
1:D:307:THR:HB	1:D:314:PHE:CE2	2.54	0.41
1:A:321:ILE:O	1:A:330:ARG:NH1	2.50	0.41
1:D:144:MET:HE3	1:D:144:MET:HB3	1.89	0.41
1:J:181:MET:SD	1:J:231:ARG:NH1	2.93	0.41
1:A:124:LEU:HD11	1:A:344:LEU:HD11	2.02	0.41
1:G:268:SER:O	1:G:272:ARG:HG3	2.21	0.41
1:A:293:LEU:O	1:A:297:MET:HG3	2.20	0.41
1:D:293:LEU:O	1:D:297:MET:HG3	2.21	0.41
1:J:180:LEU:O	1:J:181:MET:HE2	2.21	0.41
1:A:242:LEU:O	1:A:246:MET:HG3	2.19	0.41
1:J:272:ARG:HD2	5:J:597:HOH:O	2.21	0.41
1:J:230:LEU:HD12	1:J:230:LEU:HA	1.97	0.40
1:G:332:LYS:HA	1:G:336:LYS:HB2	2.02	0.40
1:D:268:SER:O	1:D:272:ARG:HG3	2.21	0.40
1:J:35:TRP:CH2	1:J:37:GLY:HA2	2.56	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	344/388 (89%)	333 (97%)	9 (3%)	2 (1%)	21	17
1	D	341/388 (88%)	330 (97%)	9 (3%)	2 (1%)	21	17
1	G	343/388 (88%)	334 (97%)	8 (2%)	1 (0%)	36	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	344/388 (89%)	333 (97%)	10 (3%)	1 (0%)	36	35
All	All	1372/1552 (88%)	1330 (97%)	36 (3%)	6 (0%)	30	27

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	88	TYR
1	D	88	TYR
1	A	88	TYR
1	J	88	TYR
1	A	335	TRP
1	D	158	VAL

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	295/329 (90%)	292 (99%)	3 (1%)	68	75
1	D	292/329 (89%)	288 (99%)	4 (1%)	59	66
1	G	294/329 (89%)	292 (99%)	2 (1%)	76	82
1	J	294/329 (89%)	292 (99%)	2 (1%)	76	82
All	All	1175/1316 (89%)	1164 (99%)	11 (1%)	70	78

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	121	LYS
1	G	323	LYS
1	A	112	VAL
1	A	113	LEU
1	A	284	ASP
1	D	196	MET
1	D	257	ARG
1	D	315	ASP

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Mol	Chain	Res	Type
1	D	323	LYS
1	J	64	VAL
1	J	285	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	130	ASN
1	G	229	ASN
1	A	128	GLN
1	A	255	GLN
1	A	318	ASN
1	D	49	ASN
1	D	221	ASN
1	D	229	ASN
1	J	32	ASN
1	J	49	ASN
1	J	318	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 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	D	403	2	4,4,4	0.22	0	6,6,6	0.36	0
3	SO4	A	403	2	4,4,4	0.33	0	6,6,6	0.64	0
3	SO4	G	403	2	4,4,4	0.42	0	6,6,6	0.30	0
3	SO4	J	403	2	4,4,4	0.27	0	6,6,6	0.30	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

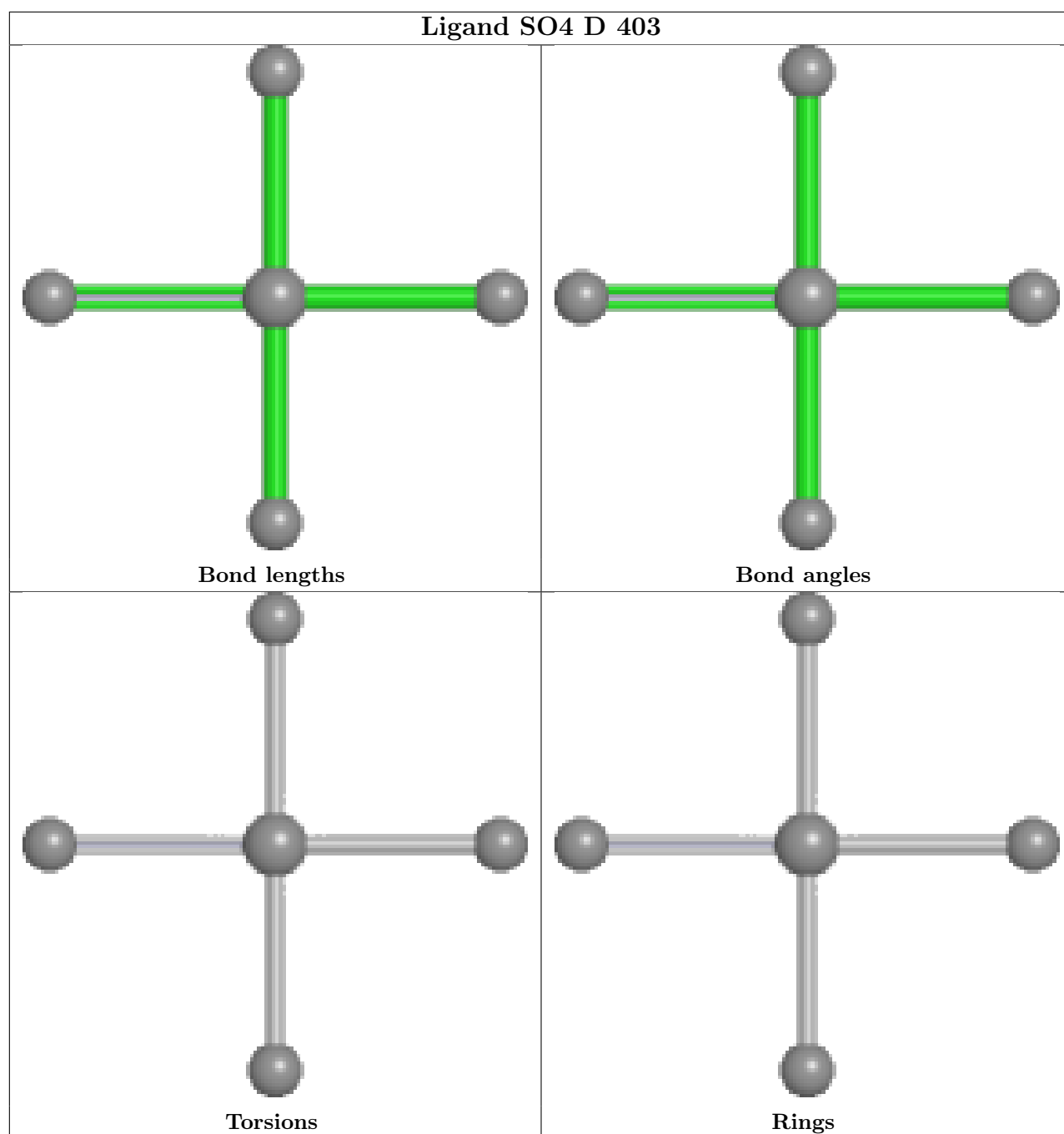
There are no torsion outliers.

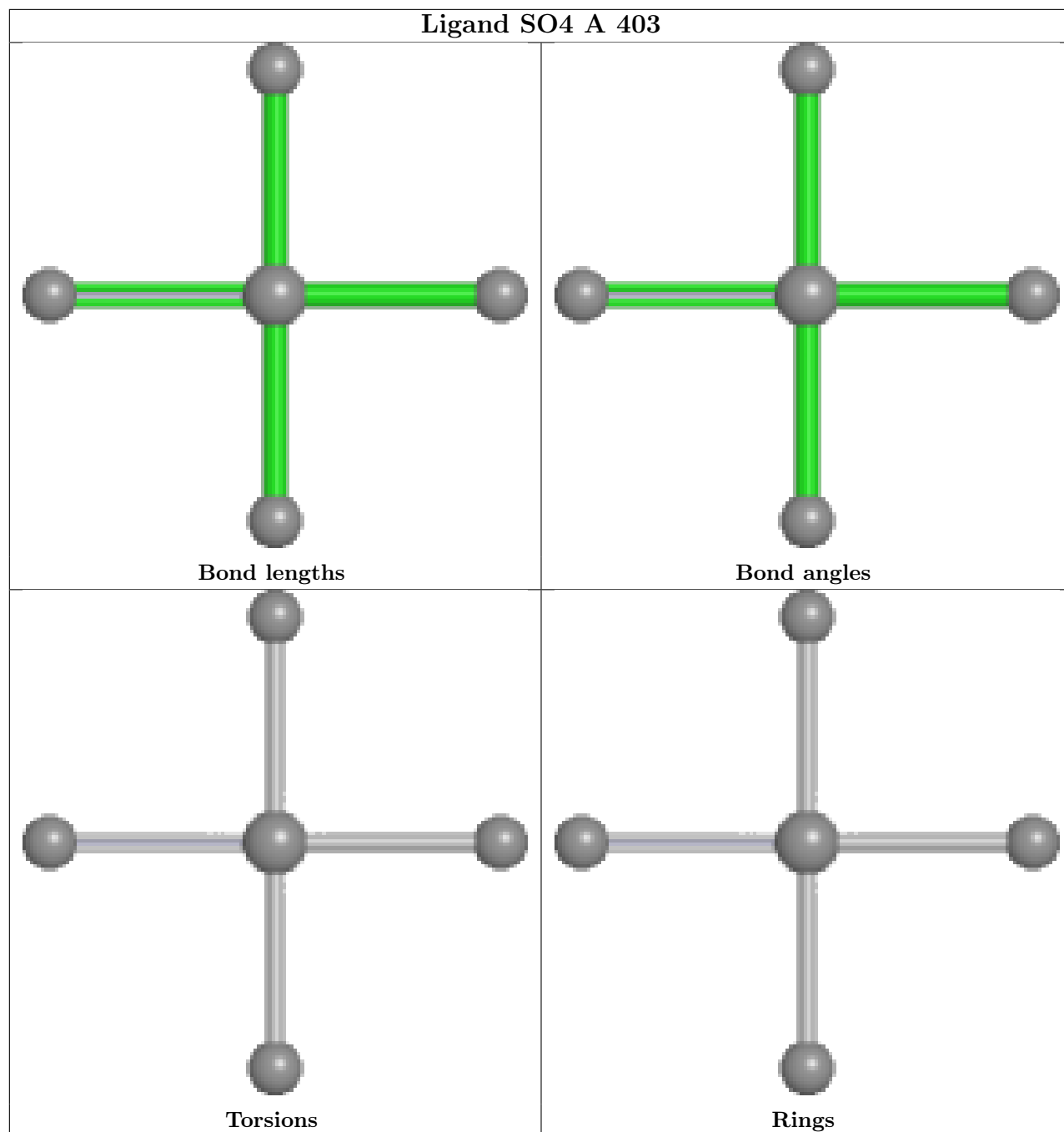
There are no ring outliers.

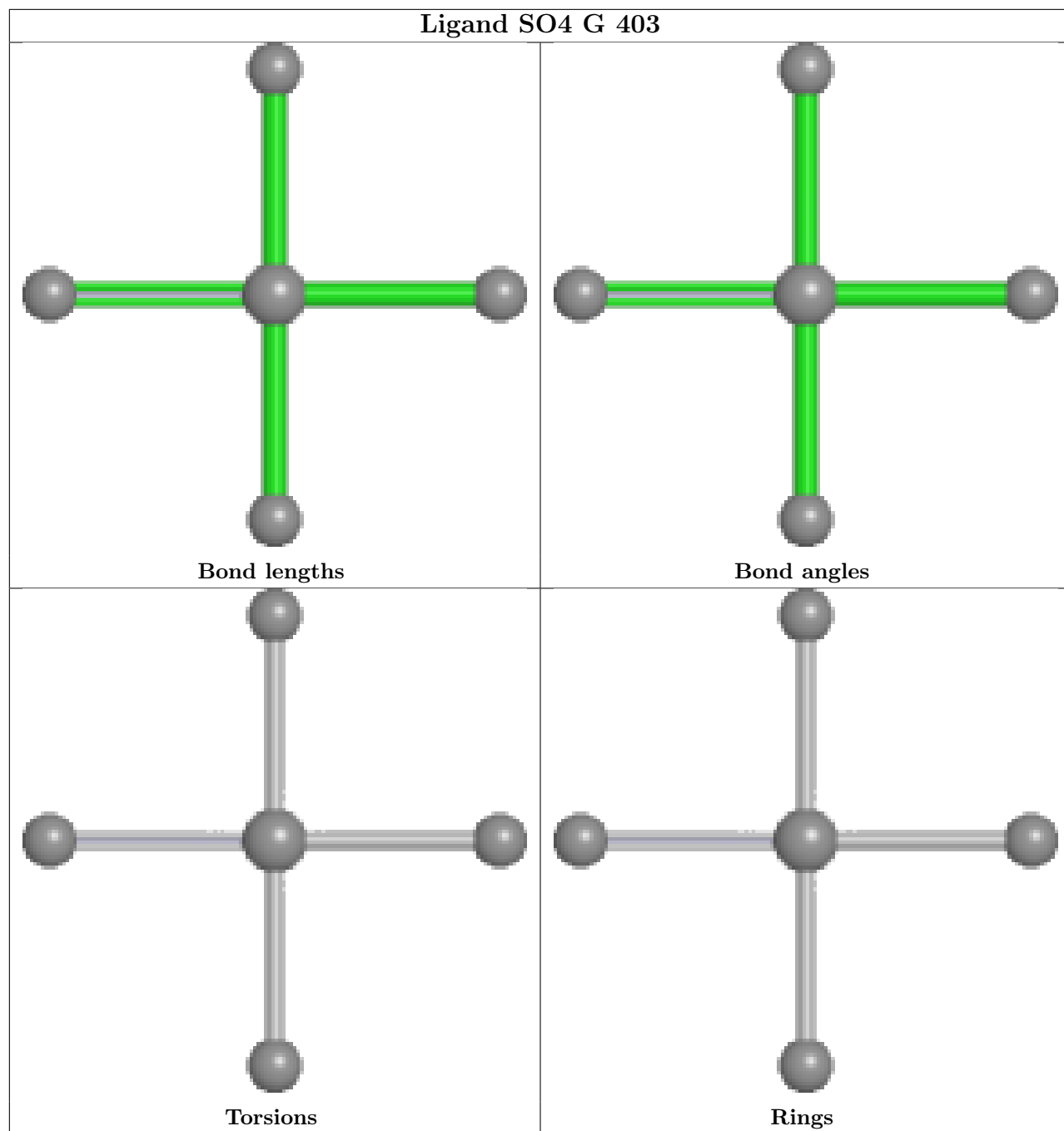
1 monomer is involved in 1 short contact:

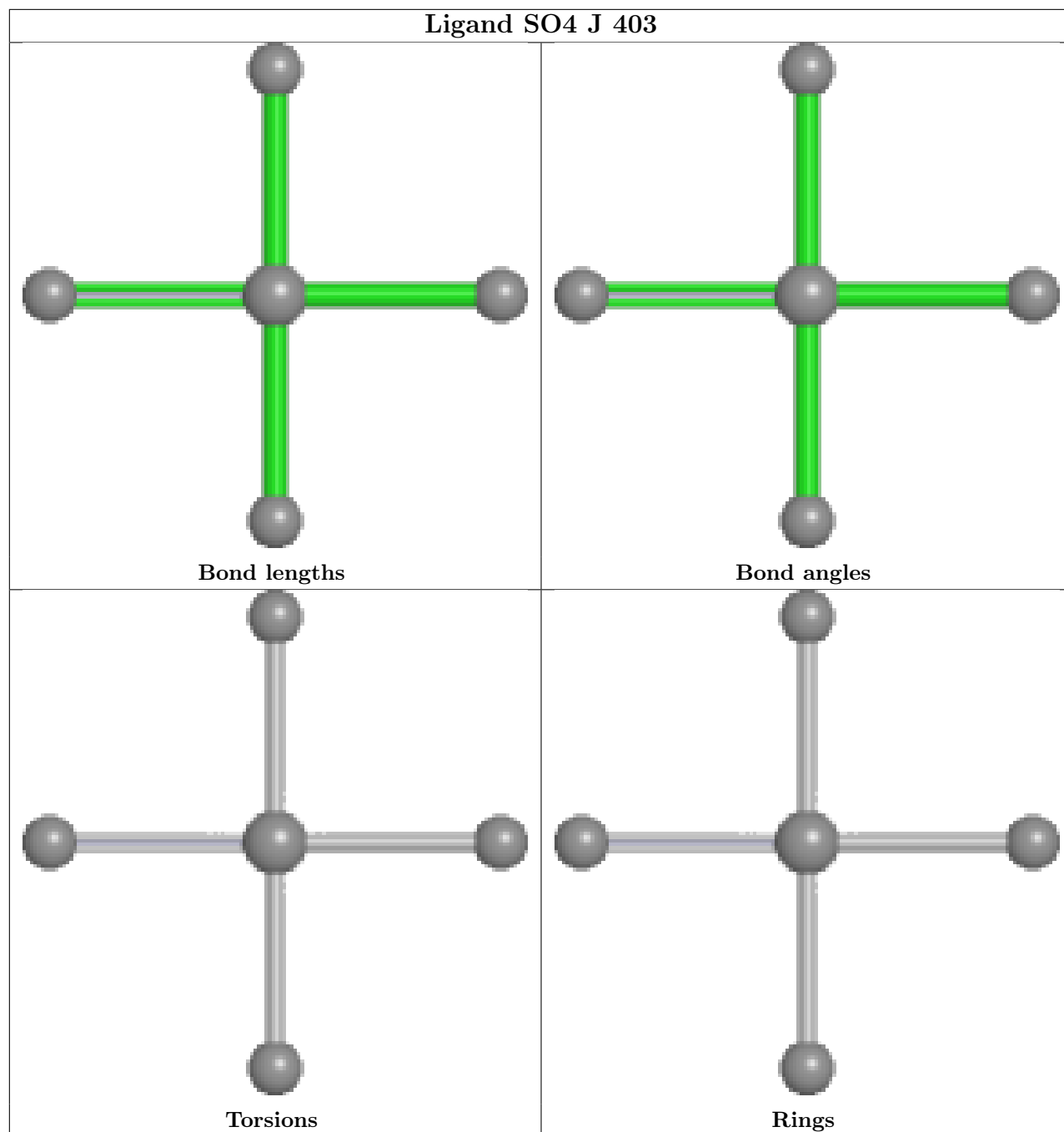
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	403	SO4	1	0

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	344/388 (88%)	0.02	4 (1%) 76 76	8, 16, 27, 61	2 (0%)
1	D	343/388 (88%)	0.48	16 (4%) 36 35	14, 23, 36, 71	0
1	G	344/388 (88%)	0.05	4 (1%) 76 76	10, 16, 27, 57	1 (0%)
1	J	345/388 (88%)	0.18	4 (1%) 76 76	11, 19, 30, 37	1 (0%)
All	All	1376/1552 (88%)	0.18	28 (2%) 65 64	8, 18, 32, 71	4 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	345	ASP	5.9
1	A	345	ASP	4.3
1	G	146	ALA	3.3
1	G	345	ASP	3.3
1	A	47	PRO	3.1
1	D	327	SER	3.1
1	D	79	LYS	3.1
1	A	146	ALA	3.0
1	D	3	ILE	3.0
1	D	320	ALA	2.8
1	G	318	ASN	2.7
1	J	320	ALA	2.5
1	D	253	TYR	2.5
1	D	344	LEU	2.5
1	D	319	ALA	2.5
1	J	319	ALA	2.4
1	D	247	TRP	2.4
1	D	47	PRO	2.4
1	D	318	ASN	2.3
1	D	287	GLY	2.3
1	D	147	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	312[A]	PHE	2.2
1	D	323	LYS	2.2
1	D	312	PHE	2.1
1	J	285	ILE	2.1
1	A	257	ARG	2.1
1	D	285	ILE	2.1
1	G	285	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.

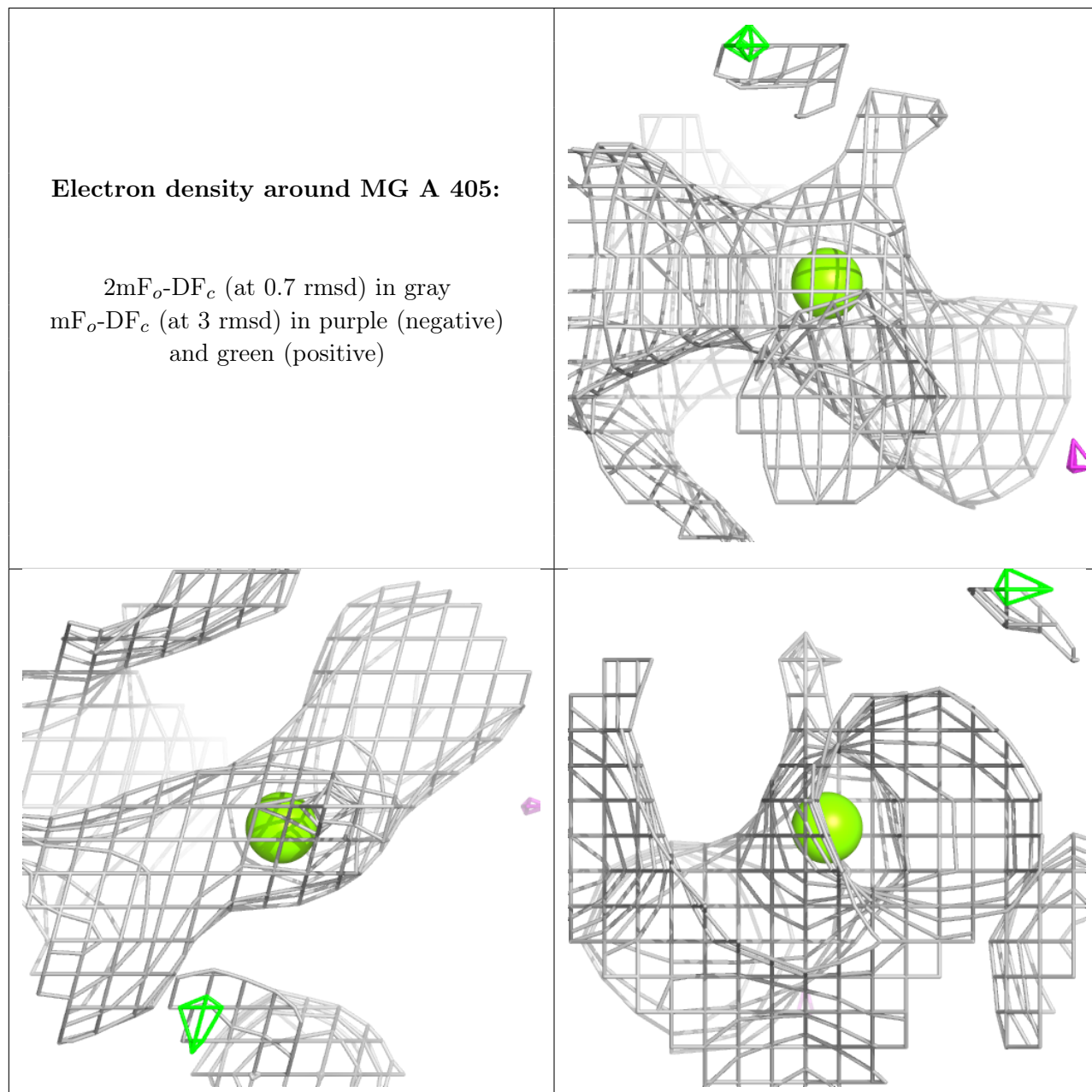
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	A	405	1/1	0.86	0.18	32,32,32,32	0
3	SO4	A	403	5/5	0.90	0.11	21,23,30,30	0
3	SO4	J	403	5/5	0.92	0.09	20,22,31,36	0
3	SO4	D	403	5/5	0.92	0.10	23,23,36,36	0
3	SO4	G	403	5/5	0.94	0.08	14,18,27,32	0
4	MG	A	404	1/1	0.95	0.04	26,26,26,26	0
2	FE	G	401	1/1	0.97	0.08	29,29,29,29	0
2	FE	D	401	1/1	0.97	0.07	35,35,35,35	0
2	FE	J	401	1/1	0.97	0.09	31,31,31,31	0
2	FE	G	402	1/1	0.98	0.11	24,24,24,24	0
2	FE	A	402	1/1	0.98	0.11	25,25,25,25	0
2	FE	J	402	1/1	0.98	0.12	30,30,30,30	0
2	FE	A	401	1/1	0.99	0.10	26,26,26,26	0
2	FE	D	402	1/1	0.99	0.14	28,28,28,28	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.

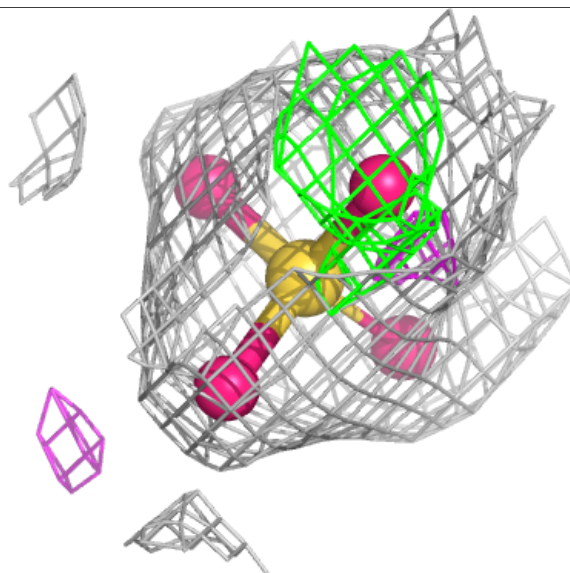
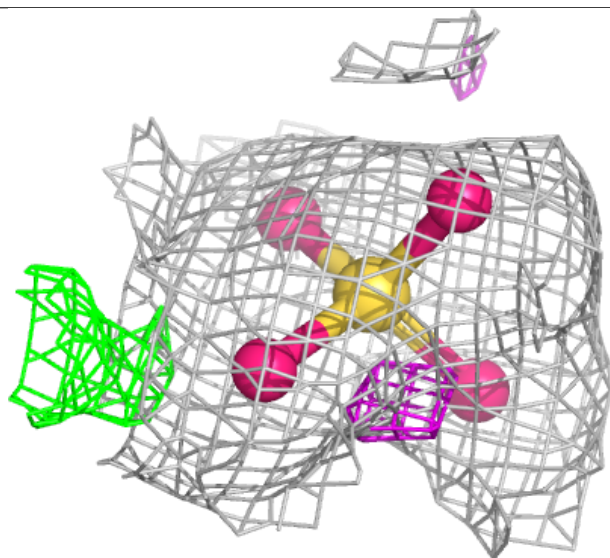
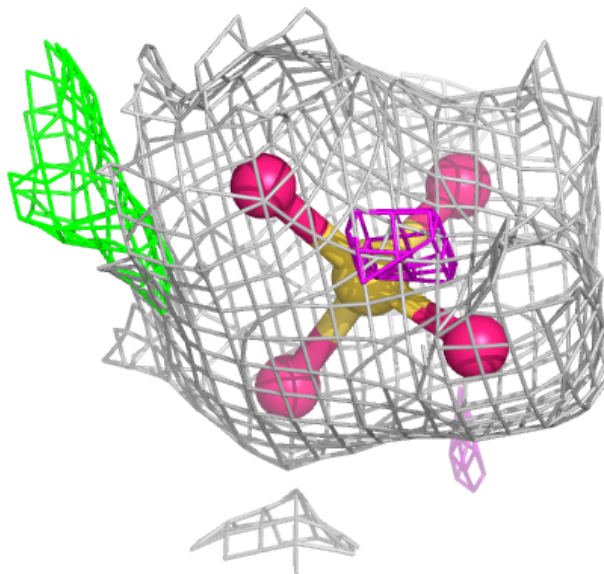
Electron density around MG A 405:

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



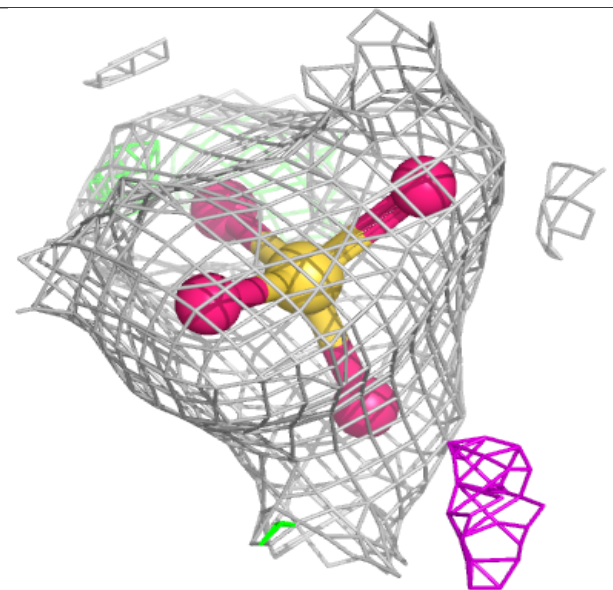
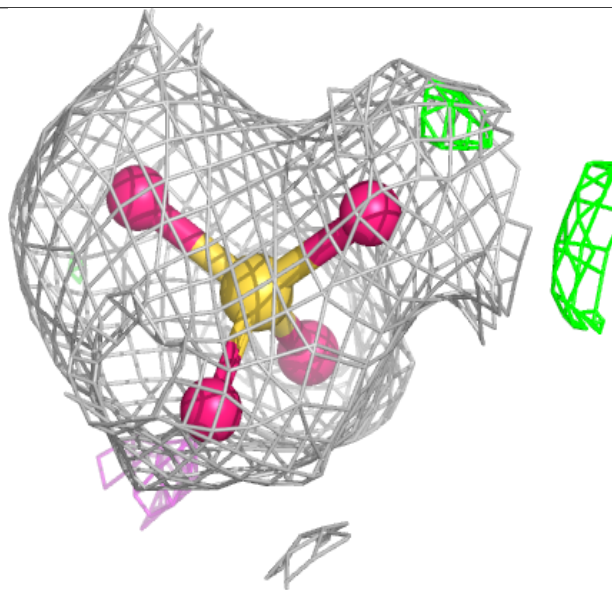
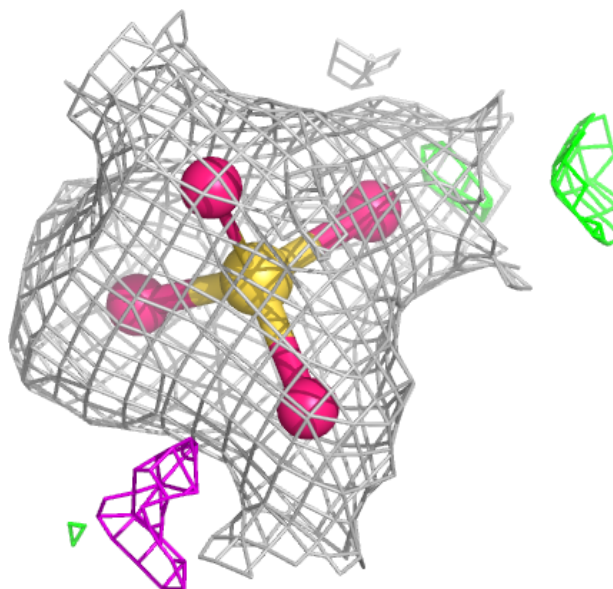
Electron density around SO4 A 403:

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



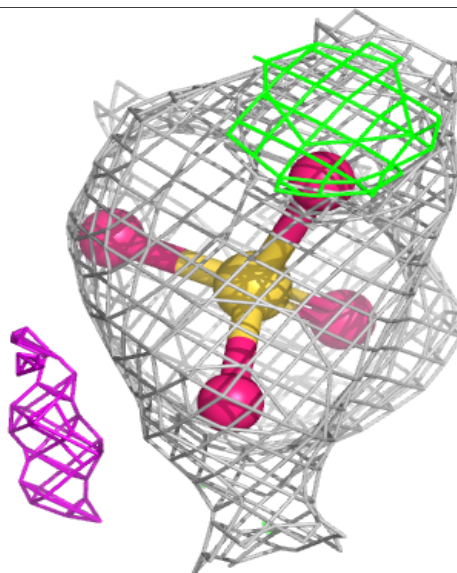
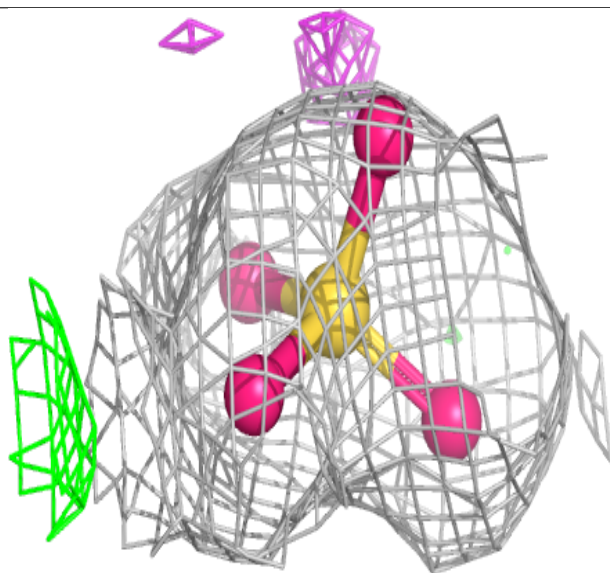
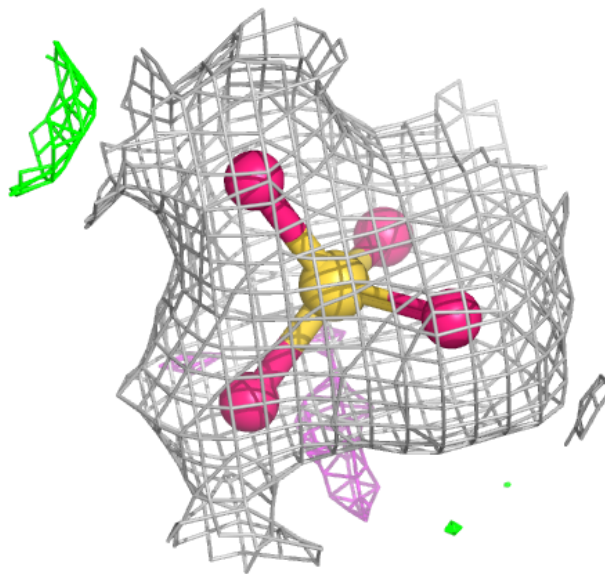
Electron density around SO4 J 403:

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



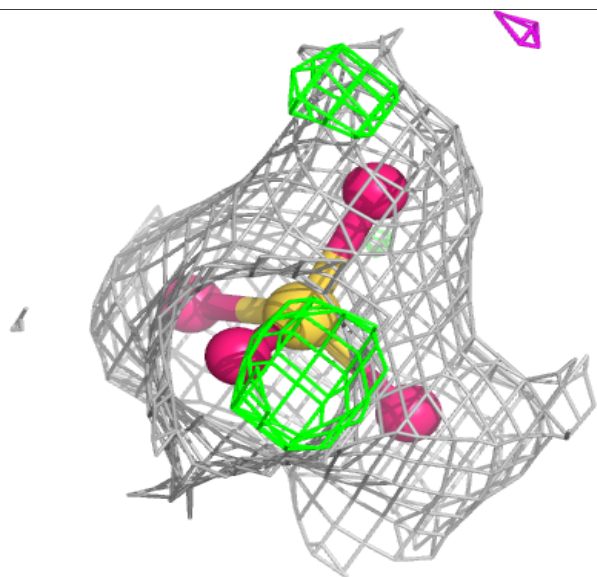
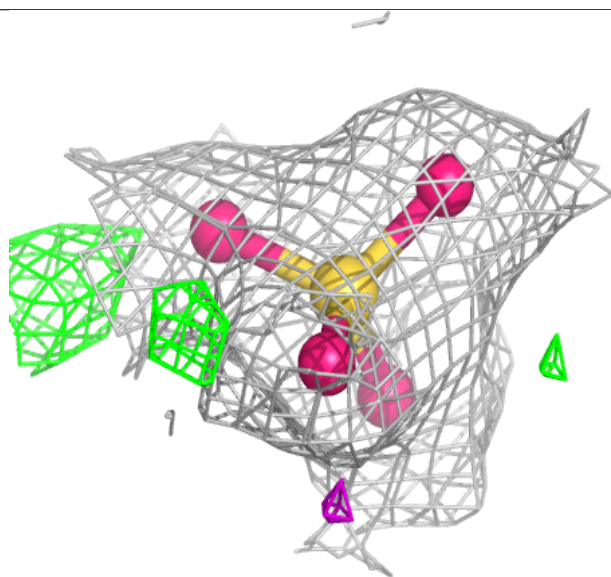
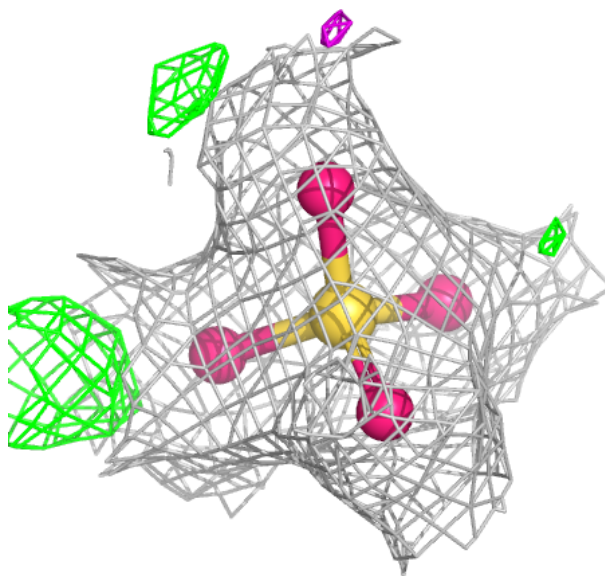
Electron density around SO4 D 403:

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



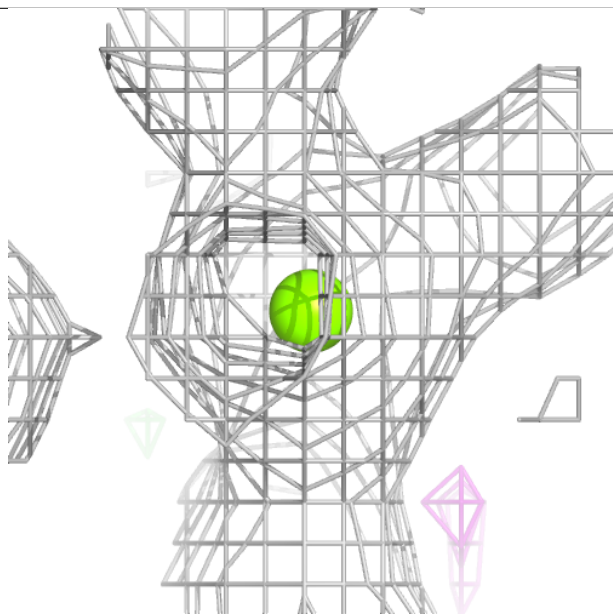
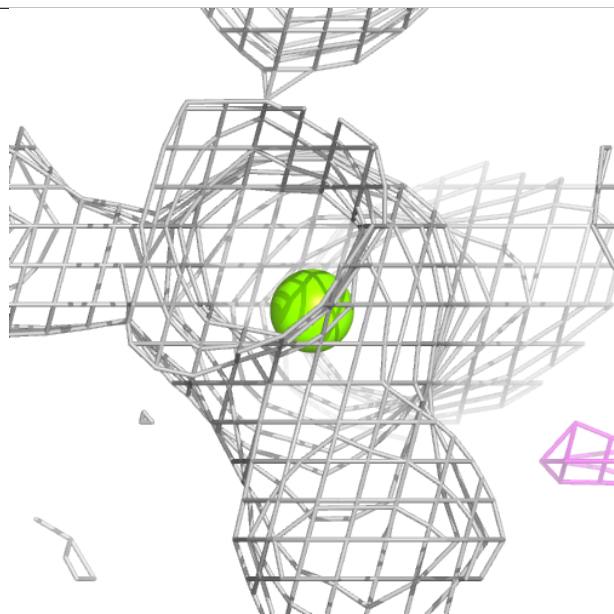
Electron density around SO4 G 403:

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



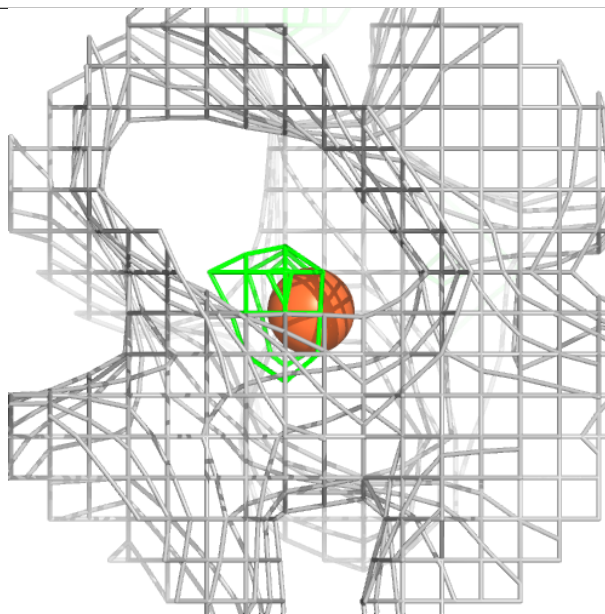
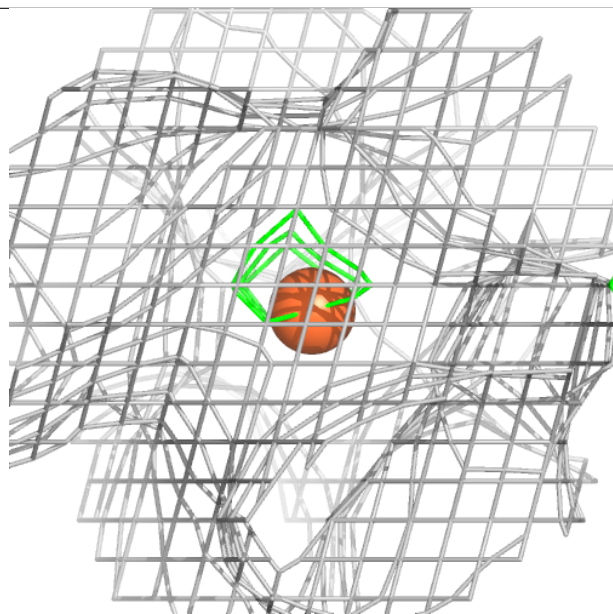
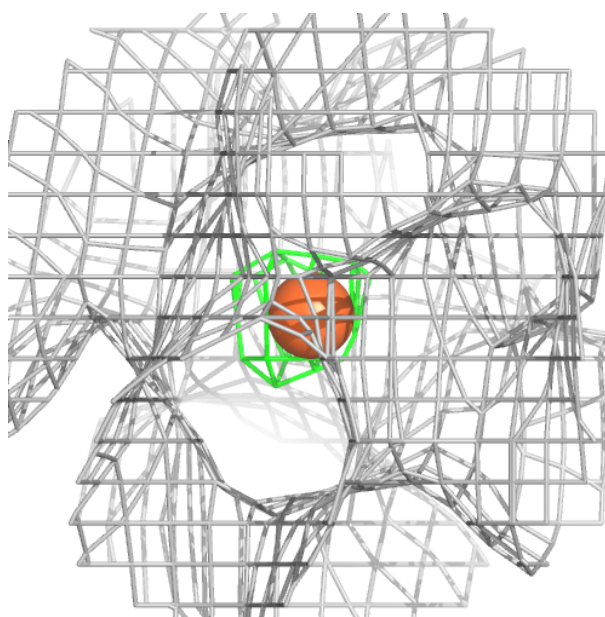
Electron density around MG A 404:

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



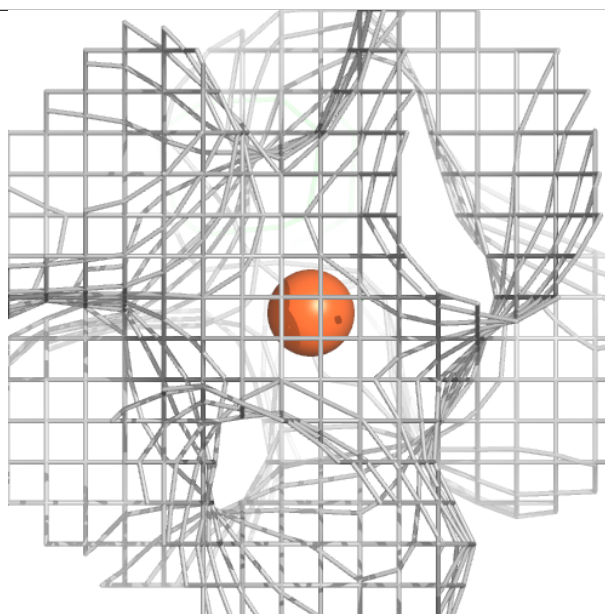
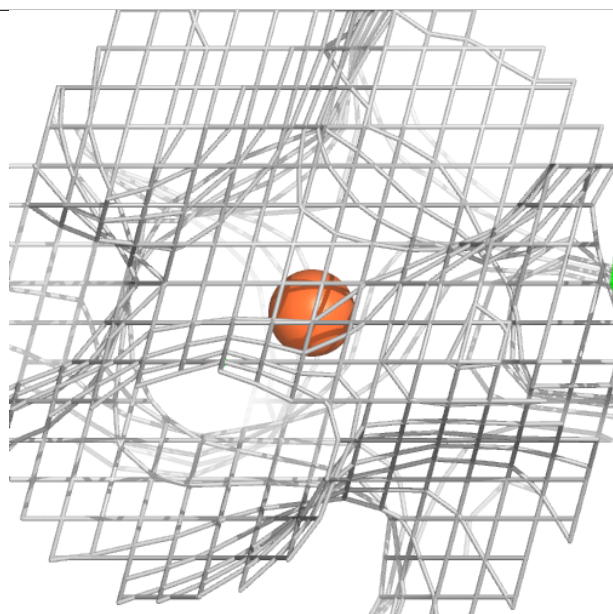
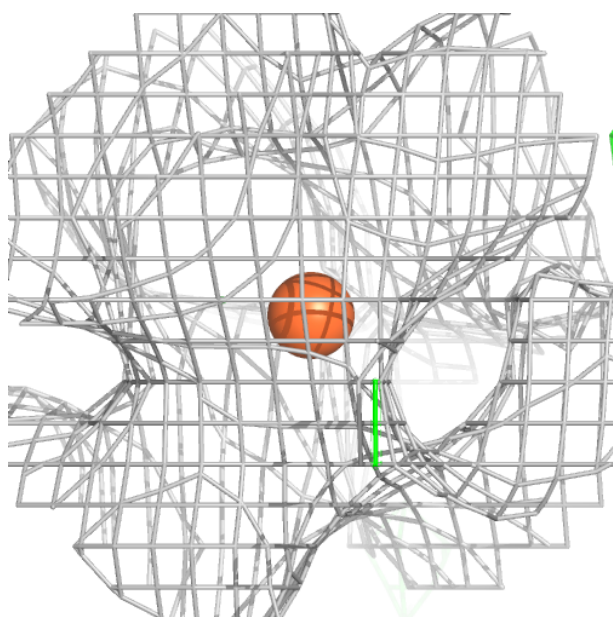
Electron density around FE G 401:

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and green (positive)



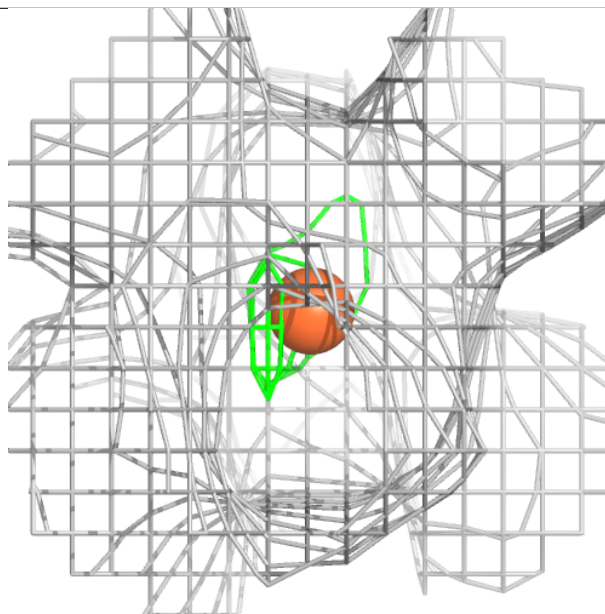
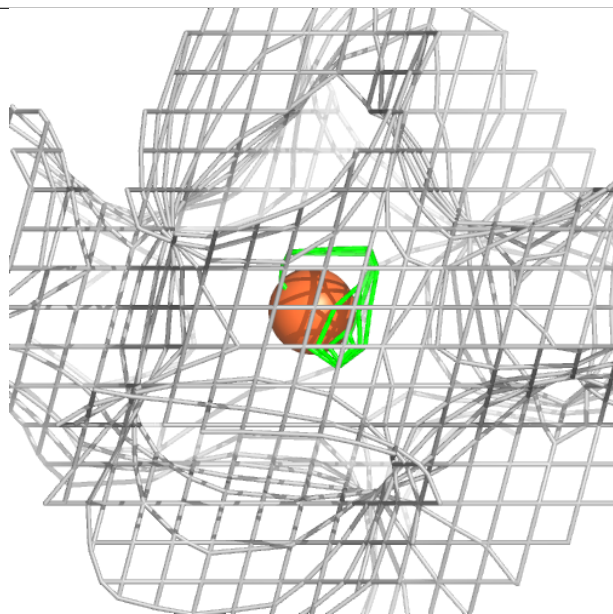
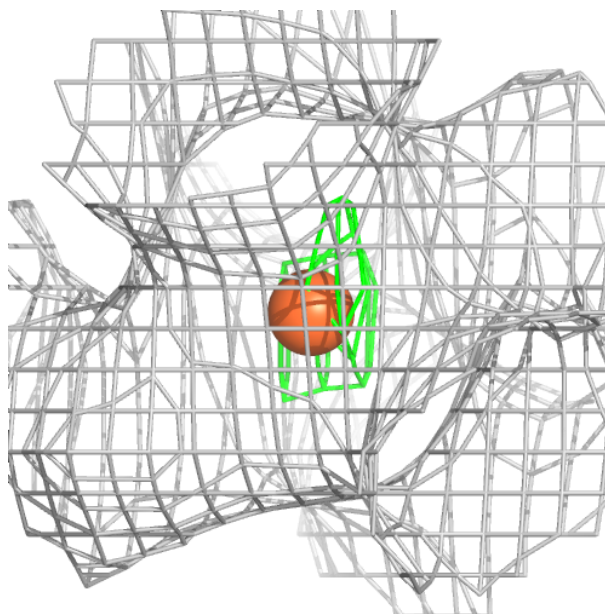
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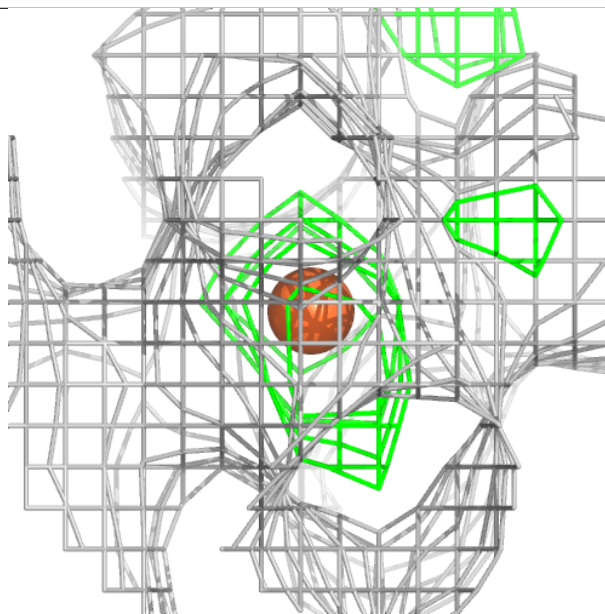
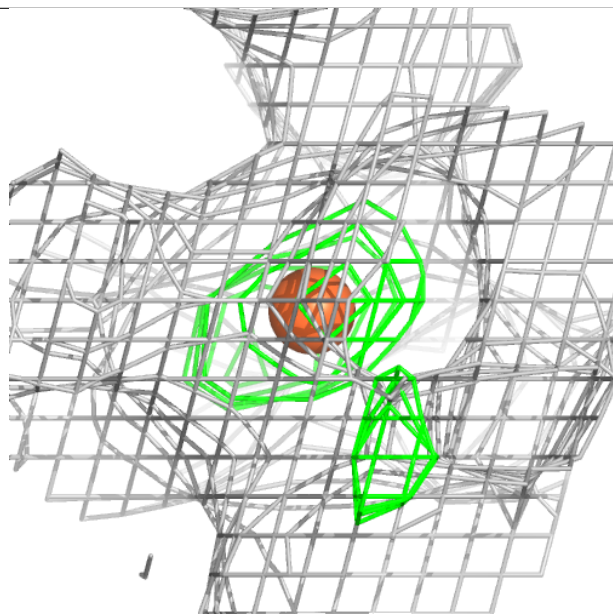
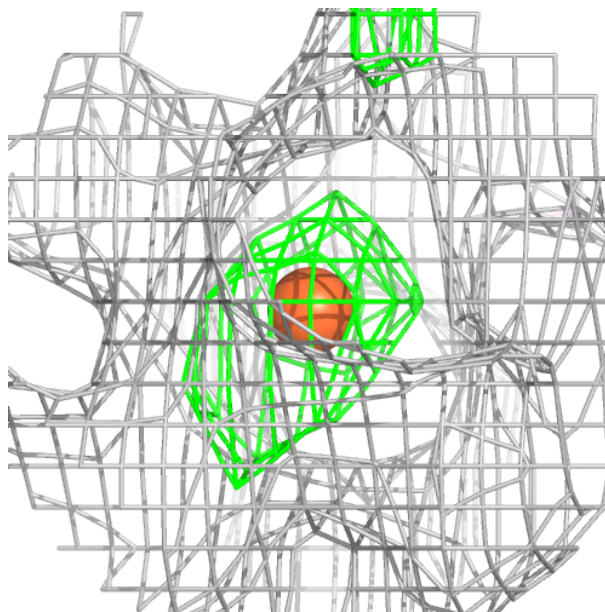
Electron density around FE J 401:

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and green (positive)



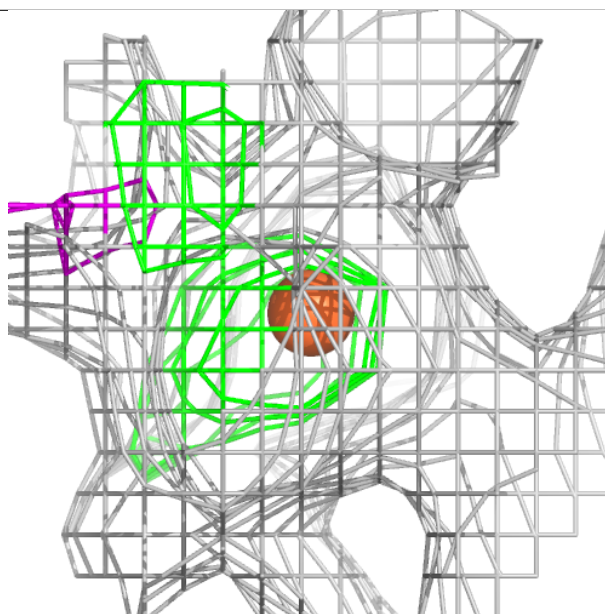
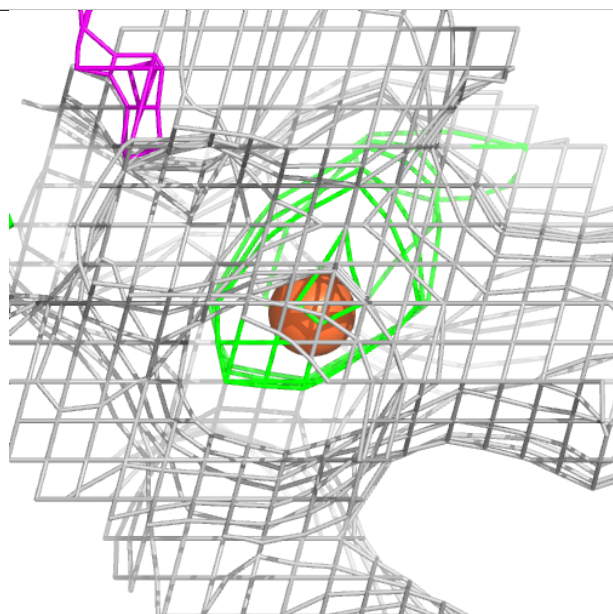
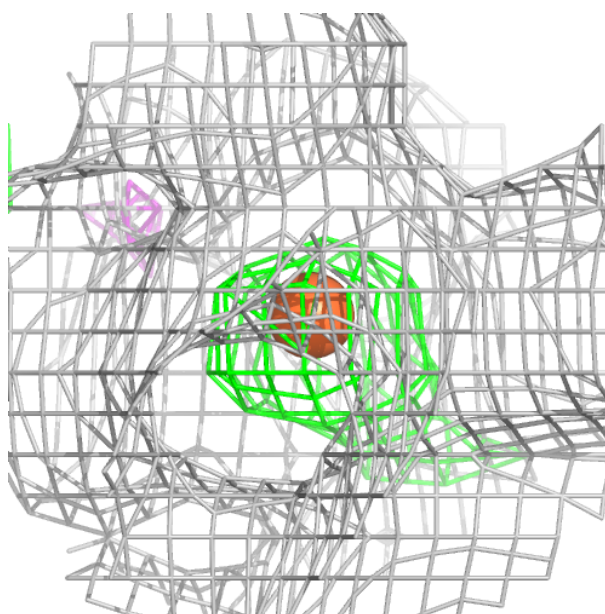
Electron density around FE G 402:

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



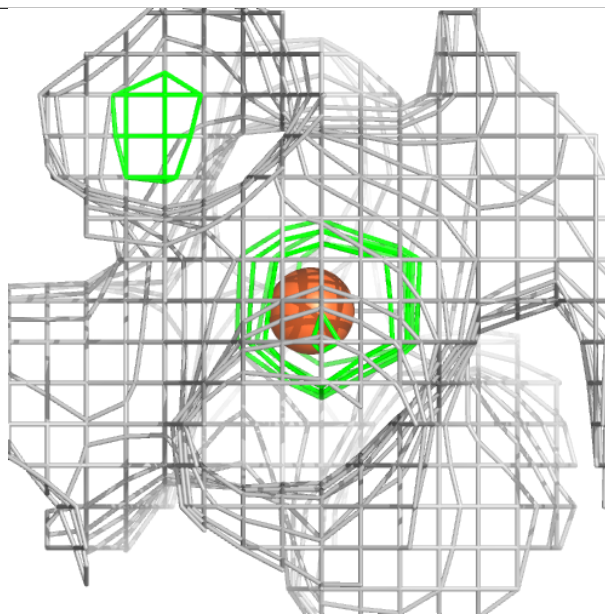
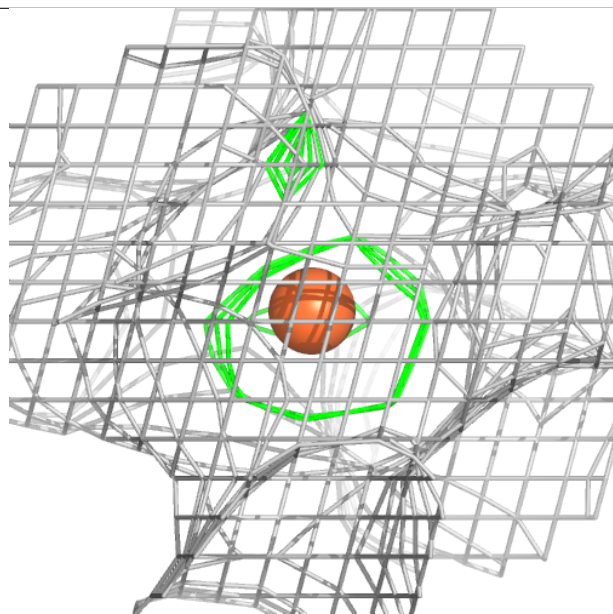
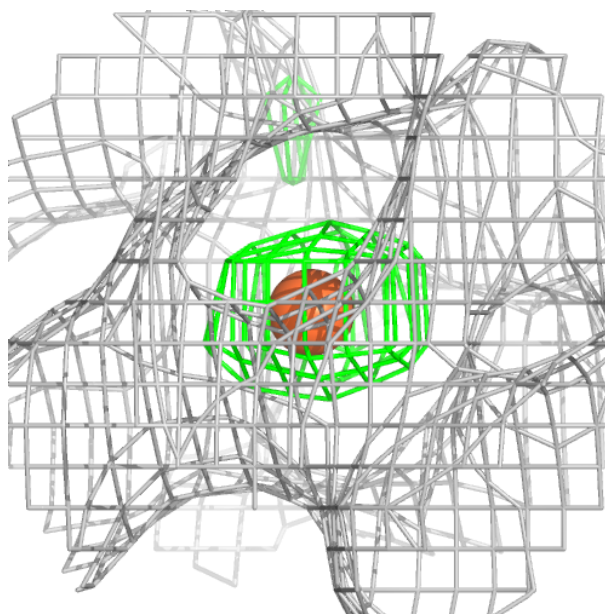
Electron density around FE A 402:

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



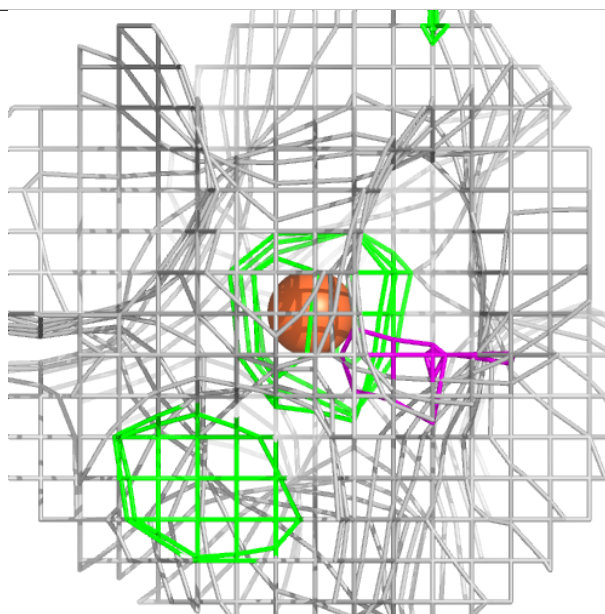
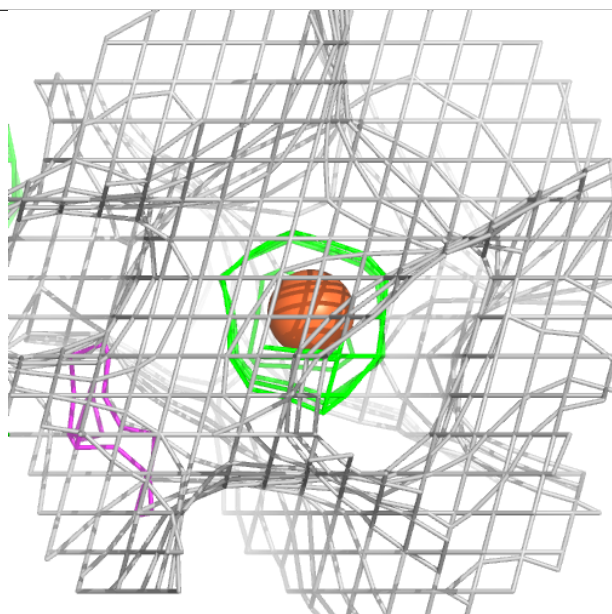
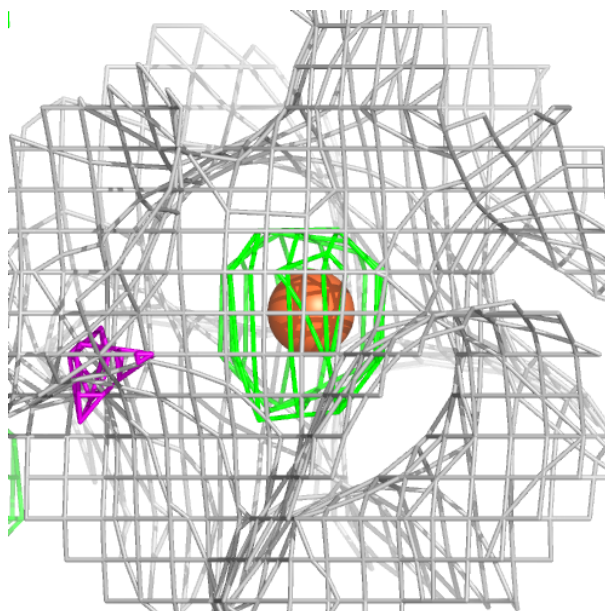
Electron density around FE J 402:

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



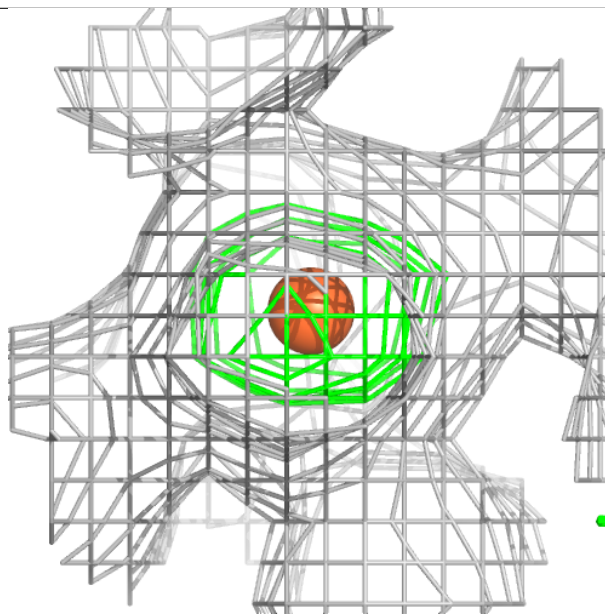
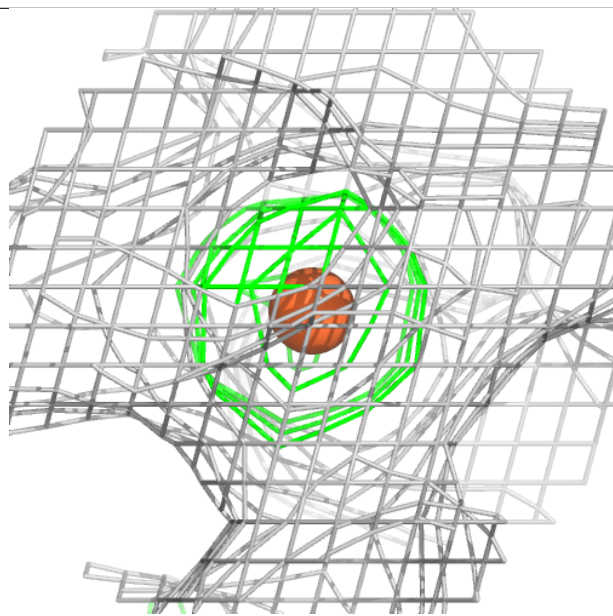
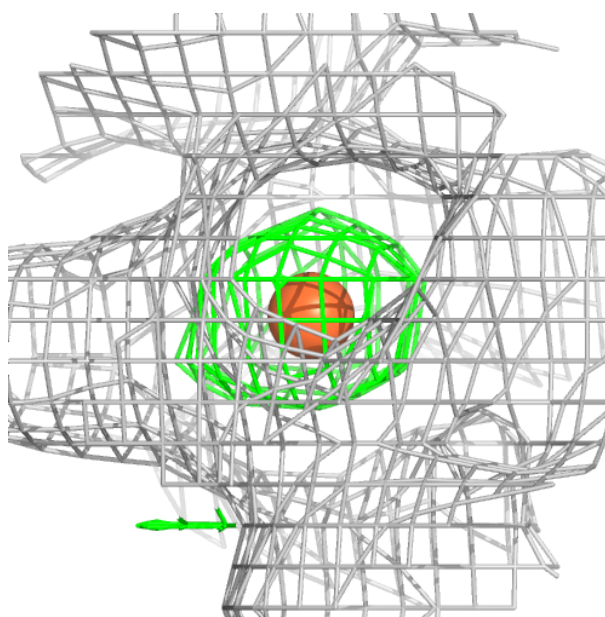
Electron density around FE A 401:

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



Electron density around FE D 402:

$2mF_o-DF_c$ (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.