Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 07:23 PM JST

PDB ID	:	7VT4
Title	:	Crystal structure of mutant E393Q of MtGlu5
Authors	:	Ye, T.J.; Ko, P.T.; Huang, K.F.; Wu, S.H.
Deposited on	:	2021-10-28
Resolution	:	1.93 Å(reported)

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

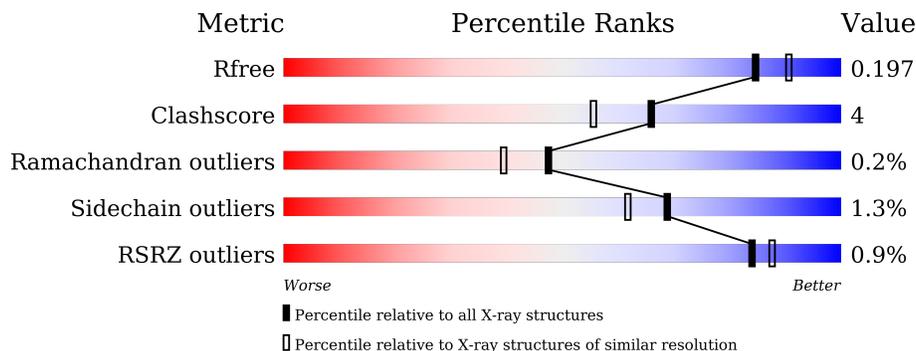|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.197
Clashscore		4
Ramachandran outliers		0.2%
Sidechain outliers		1.3%
RSRZ outliers		0.9%

Worse ← → *Better*

∎ Percentile relative to all X-ray structures

❘ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	468	.% 84% 10% 6%
1	B	468	87% 7% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8674 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 Endoglucanase H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total 3520	C 2239	N 646	O 632	S 3	0	0	0
1	B	437	Total 3513	C 2235	N 645	O 630	S 3	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A399DY85
A	393	GLN	GLU	engineered mutation	UNP A0A399DY85
A	456	LYS	-	expression tag	UNP A0A399DY85
A	457	LEU	-	expression tag	UNP A0A399DY85
A	458	ALA	-	expression tag	UNP A0A399DY85
A	459	ALA	-	expression tag	UNP A0A399DY85
A	460	ALA	-	expression tag	UNP A0A399DY85
A	461	LEU	-	expression tag	UNP A0A399DY85
A	462	GLU	-	expression tag	UNP A0A399DY85
A	463	HIS	-	expression tag	UNP A0A399DY85
A	464	HIS	-	expression tag	UNP A0A399DY85
A	465	HIS	-	expression tag	UNP A0A399DY85
A	466	HIS	-	expression tag	UNP A0A399DY85
A	467	HIS	-	expression tag	UNP A0A399DY85
A	468	HIS	-	expression tag	UNP A0A399DY85
B	1	MET	-	initiating methionine	UNP A0A399DY85
B	393	GLN	GLU	engineered mutation	UNP A0A399DY85
B	456	LYS	-	expression tag	UNP A0A399DY85
B	457	LEU	-	expression tag	UNP A0A399DY85
B	458	ALA	-	expression tag	UNP A0A399DY85
B	459	ALA	-	expression tag	UNP A0A399DY85
B	460	ALA	-	expression tag	UNP A0A399DY85
B	461	LEU	-	expression tag	UNP A0A399DY85
B	462	GLU	-	expression tag	UNP A0A399DY85
B	463	HIS	-	expression tag	UNP A0A399DY85

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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Chain	Residue	Modelled	Actual	Comment	Reference
B	464	HIS	-	expression tag	UNP A0A399DY85
B	465	HIS	-	expression tag	UNP A0A399DY85
B	466	HIS	-	expression tag	UNP A0A399DY85
B	467	HIS	-	expression tag	UNP A0A399DY85
B	468	HIS	-	expression tag	UNP A0A399DY85

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).

GOL
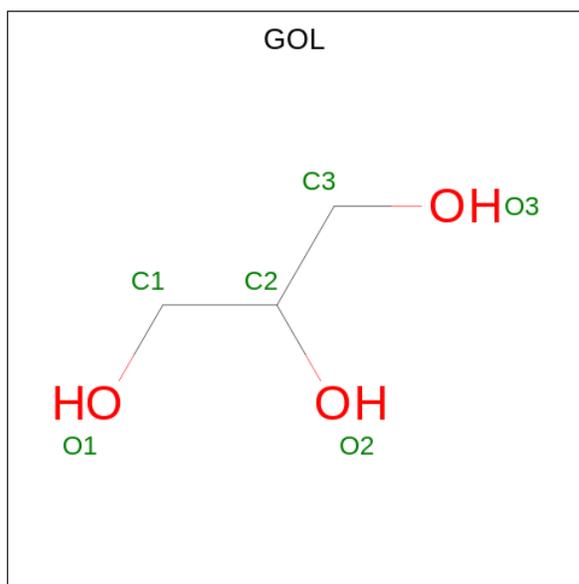
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).

SO4

O1

O

O3 O⁻ — S — O⁻ O4

S

O

O2
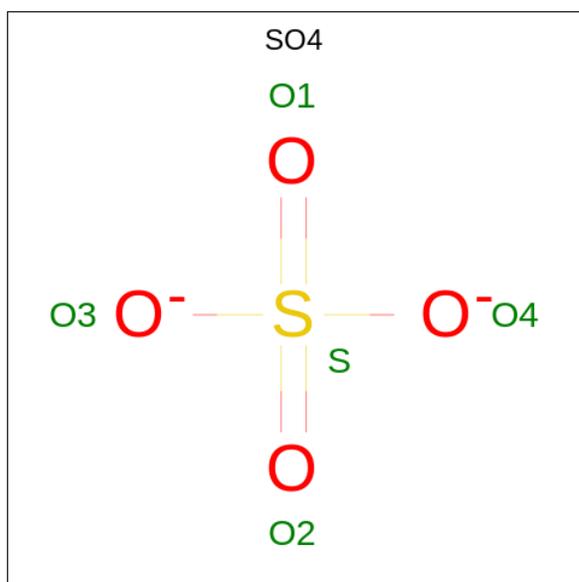
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	734	Total 734	O 734	0	0
4	B	806	Total 806	O 806	0	0

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: Endoglucanase H

Chain A:

• Molecule 1: Endoglucanase H

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.25Å 114.35Å 80.15Å 90.00° 103.23° 90.00°	Depositor
Resolution (Å)	26.97 – 1.93 26.97 – 1.93	Depositor EDS
% Data completeness (in resolution range)	89.5 (26.97-1.93) 89.5 (26.97-1.93)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.02 (at 1.93Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.158 , 0.197 0.158 , 0.197	Depositor DCC
R_{free} test set	4288 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	19.6	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 60.4	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8674	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.44	0/3624	0.58	0/4943
1	B	0.47	0/3617	0.60	0/4933
All	All	0.45	0/7241	0.59	0/9876

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 ⓘ

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	3520	0	3386	34	1
1	B	3513	0	3379	20	1
2	A	18	0	24	0	0
2	B	18	0	24	4	0
3	A	35	0	0	2	0
3	B	30	0	0	1	0
4	A	734	0	0	20	2
4	B	806	0	0	10	4
All	All	8674	0	6813	56	5

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 (56) 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:351:ARG:NH1	4:A:604:HOH:O	2.14	0.78
1:A:383:GLU:HG2	4:A:1117:HOH:O	1.89	0.72
1:A:15:THR:N	4:A:609:HOH:O	2.23	0.70
1:B:16:GLY:O	4:B:601:HOH:O	2.10	0.68
1:A:178:SER:O	4:A:602:HOH:O	2.12	0.67
1:A:174:GLU:OE1	4:A:603:HOH:O	2.13	0.67
1:B:16:GLY:N	4:B:606:HOH:O	2.29	0.66
1:A:286:ARG:NH1	4:A:613:HOH:O	2.28	0.66
1:A:287:LEU:HD22	1:A:334:LEU:HD11	1.78	0.66
1:B:152:GLY:HA2	2:B:503:GOL:H12	1.78	0.65
1:B:302:ARG:NH1	4:B:604:HOH:O	2.27	0.65
1:B:153:ARG:NH1	4:B:607:HOH:O	2.30	0.65
1:A:301:CYS:HB2	4:A:741:HOH:O	1.97	0.64
1:A:379:GLN:NE2	4:A:615:HOH:O	2.32	0.62
1:A:383:GLU:OE1	4:A:605:HOH:O	2.16	0.61
1:A:49:GLU:OE1	1:A:98:ARG:NH1	2.34	0.61
1:B:329:SER:OG	3:B:509:SO4:O2	2.19	0.60
1:A:238:ASN:OD1	4:A:606:HOH:O	2.17	0.59
1:B:351:ARG:NH2	4:B:613:HOH:O	2.35	0.59
2:B:503:GOL:O1	4:B:602:HOH:O	2.17	0.59
1:B:193:ARG:NH2	4:B:617:HOH:O	2.37	0.57
1:A:36:GLU:HB3	1:A:66:PRO:HB2	1.86	0.57
1:B:287:LEU:HD22	1:B:334:LEU:HD11	1.87	0.56
1:B:129:ARG:NH1	4:B:618:HOH:O	2.37	0.56
1:B:36:GLU:HB3	1:B:66:PRO:HB2	1.87	0.56
1:A:15:THR:OG1	4:A:601:HOH:O	2.05	0.55
1:A:444:THR:O	1:A:448:LYS:HG2	2.08	0.54
1:A:351:ARG:NH1	4:A:624:HOH:O	2.40	0.53
1:B:282:GLU:OE1	1:B:330:ARG:NH2	2.42	0.53
1:A:266:TYR:CG	1:A:338:ASN:HB2	2.44	0.52
1:A:254:ARG:NH2	3:A:510:SO4:O2	2.44	0.52
1:B:20:GLU:OE2	1:B:23:ARG:NH1	2.44	0.50
1:A:328:PRO:HD3	4:A:741:HOH:O	2.12	0.50
1:A:369:ASN:HB2	4:A:630:HOH:O	2.11	0.50
1:B:152:GLY:CA	2:B:503:GOL:H12	2.43	0.48
3:A:505:SO4:O4	4:A:607:HOH:O	2.20	0.48
1:A:371:ILE:HG22	1:A:415:GLU:HG3	1.97	0.47
1:A:56:ARG:NE	4:A:623:HOH:O	2.46	0.46
1:A:391:VAL:HG21	1:A:416:LEU:HD22	1.97	0.46
1:B:39:TRP:CE2	1:B:42:ALA:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ALA:HB1	1:A:348:ARG:HG2	1.99	0.44
1:B:380:ARG:HD2	4:B:1246:HOH:O	2.18	0.43
1:A:427:GLU:HG2	1:A:432:PHE:HB2	2.01	0.43
1:B:212:TYR:H	2:B:501:GOL:H12	1.83	0.43
1:A:290:ARG:CZ	1:A:351:ARG:HD2	2.49	0.42
1:A:369:ASN:ND2	4:A:636:HOH:O	2.46	0.42
1:A:39:TRP:CE2	1:A:42:ALA:HB2	2.55	0.42
1:B:266:TYR:CG	1:B:338:ASN:HB2	2.54	0.42
1:A:208:THR:HA	1:A:390:PHE:O	2.19	0.42
1:A:367:GLN:OE1	4:A:608:HOH:O	2.22	0.42
1:B:444:THR:O	1:B:448:LYS:HG2	2.20	0.41
1:A:368:GLN:HB3	4:A:892:HOH:O	2.19	0.41
1:A:106:ASN:HB3	1:A:145:GLU:HB3	2.03	0.41
1:B:441:GLN:NE2	4:B:649:HOH:O	2.54	0.41
1:A:257:PHE:HA	1:A:261:ALA:O	2.21	0.40
1:A:20:GLU:HG2	4:A:640:HOH:O	2.22	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:THR:O	1:B:379:GLN:NE2[1_556]	1.96	0.24
4:A:1210:HOH:O	4:B:1204:HOH:O[1_556]	2.12	0.08
4:B:604:HOH:O	4:B:626:HOH:O[2_645]	2.13	0.07
4:A:1117:HOH:O	4:B:991:HOH:O[1_556]	2.15	0.05
4:B:735:HOH:O	4:B:1042:HOH:O[2_655]	2.18	0.02

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	436/468 (93%)	423 (97%)	12 (3%)	1 (0%)	47	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	435/468 (93%)	422 (97%)	12 (3%)	1 (0%)	47	39
All	All	871/936 (93%)	845 (97%)	24 (3%)	2 (0%)	47	39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	VAL
1	B	186	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	357/382 (94%)	353 (99%)	4 (1%)	73	67
1	B	356/382 (93%)	351 (99%)	5 (1%)	67	58
All	All	713/764 (93%)	704 (99%)	9 (1%)	69	62

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ARG
1	A	86	PHE
1	A	110	TYR
1	A	274	TYR
1	B	86	PHE
1	B	110	TYR
1	B	219	HIS
1	B	254	ARG
1	B	286	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

19 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	SO4	B	509	-	4,4,4	0.13	0	6,6,6	0.21	0
3	SO4	A	510	-	4,4,4	0.13	0	6,6,6	0.09	0
3	SO4	A	504	-	4,4,4	0.12	0	6,6,6	0.27	0
2	GOL	B	501	-	5,5,5	0.93	0	5,5,5	1.16	0
3	SO4	B	505	-	4,4,4	0.15	0	6,6,6	0.13	0
3	SO4	B	508	-	4,4,4	0.13	0	6,6,6	0.12	0
3	SO4	B	507	-	4,4,4	0.13	0	6,6,6	0.17	0
2	GOL	A	502	-	5,5,5	0.82	0	5,5,5	1.08	0
2	GOL	A	501	-	5,5,5	0.87	0	5,5,5	1.06	0
3	SO4	A	506	-	4,4,4	0.13	0	6,6,6	0.05	0
3	SO4	A	508	-	4,4,4	0.12	0	6,6,6	0.09	0
3	SO4	B	506	-	4,4,4	0.13	0	6,6,6	0.12	0
3	SO4	B	504	-	4,4,4	0.19	0	6,6,6	0.32	0
3	SO4	A	505	-	4,4,4	0.16	0	6,6,6	0.14	0
2	GOL	A	503	-	5,5,5	0.85	0	5,5,5	0.94	0
2	GOL	B	503	-	5,5,5	0.78	0	5,5,5	0.94	0
3	SO4	A	509	-	4,4,4	0.16	0	6,6,6	0.10	0
3	SO4	A	507	-	4,4,4	0.10	0	6,6,6	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	GOL	B	502	-	5,5,5	0.87	0	5,5,5	1.00	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
2	GOL	A	503	-	-	2/4/4/4	-
2	GOL	A	502	-	-	2/4/4/4	-
2	GOL	B	503	-	-	0/4/4/4	-
2	GOL	A	501	-	-	3/4/4/4	-
2	GOL	B	502	-	-	4/4/4/4	-
2	GOL	B	501	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GOL	O1-C1-C2-C3
2	A	502	GOL	C1-C2-C3-O3
2	A	502	GOL	O2-C2-C3-O3
2	B	502	GOL	O1-C1-C2-C3
2	B	502	GOL	C1-C2-C3-O3
2	B	502	GOL	O2-C2-C3-O3
2	A	501	GOL	C1-C2-C3-O3
2	A	503	GOL	C1-C2-C3-O3
2	B	501	GOL	O1-C1-C2-C3
2	B	501	GOL	C1-C2-C3-O3
2	A	501	GOL	O1-C1-C2-O2
2	B	501	GOL	O2-C2-C3-O3
2	B	502	GOL	O1-C1-C2-O2
2	A	503	GOL	O2-C2-C3-O3
2	B	501	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	509	SO4	1	0
3	A	510	SO4	1	0
2	B	501	GOL	1	0
3	A	505	SO4	1	0
2	B	503	GOL	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SO4 B 509

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 A 510

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 A 504

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 B 505

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 B 508

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 B 507

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL A 502

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 A 506

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 A 508

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 B 506

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 B 504

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 A 505

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL A 503

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL B 503

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 A 509

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 A 507

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL B 502

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	438/468 (93%)	-0.37	6 (1%)	75	80	10, 22, 49, 81	0
1	B	437/468 (93%)	-0.53	2 (0%)	91	93	6, 17, 38, 60	0
All	All	875/936 (93%)	-0.45	8 (0%)	84	87	6, 20, 45, 81	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	357	PRO	3.0
1	A	304	ASP	2.7
1	A	356	GLY	2.4
1	B	358	GLY	2.2
1	A	303	ARG	2.2
1	A	315	GLY	2.2
1	A	259	GLY	2.1
1	A	56	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	B	503	6/6	0.74	0.26	52,53,54,57	0
3	SO4	A	510	5/5	0.75	0.21	110,110,110,111	0
3	SO4	A	509	5/5	0.82	0.24	103,103,104,104	0
3	SO4	B	509	5/5	0.83	0.25	65,71,72,76	0
3	SO4	A	508	5/5	0.84	0.23	111,111,111,112	0
3	SO4	B	508	5/5	0.87	0.27	95,96,96,96	0
2	GOL	A	502	6/6	0.88	0.13	49,54,55,56	0
3	SO4	A	505	5/5	0.88	0.13	81,82,83,83	0
3	SO4	A	506	5/5	0.88	0.21	70,71,72,73	0
2	GOL	B	501	6/6	0.88	0.12	18,31,32,41	0
3	SO4	B	507	5/5	0.89	0.16	65,65,67,69	0
2	GOL	B	502	6/6	0.92	0.15	52,55,59,60	0
2	GOL	A	503	6/6	0.92	0.14	52,57,58,61	0
3	SO4	B	505	5/5	0.93	0.12	70,71,72,72	0
2	GOL	A	501	6/6	0.93	0.11	20,28,30,33	0
3	SO4	A	507	5/5	0.97	0.11	56,56,57,57	0
3	SO4	B	506	5/5	0.98	0.10	41,43,45,47	0
3	SO4	B	504	5/5	0.99	0.04	19,22,23,30	0
3	SO4	A	504	5/5	0.99	0.08	31,36,39,42	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 GOL B 503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
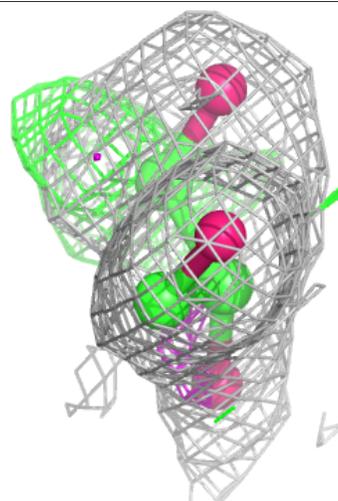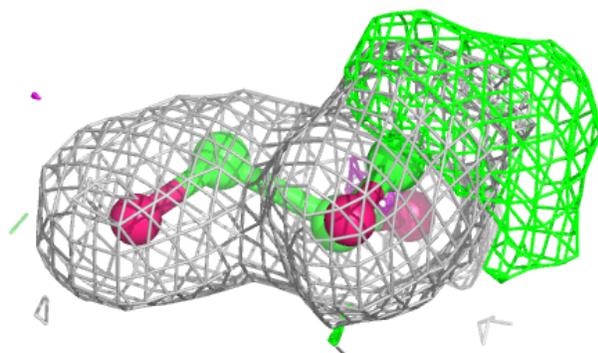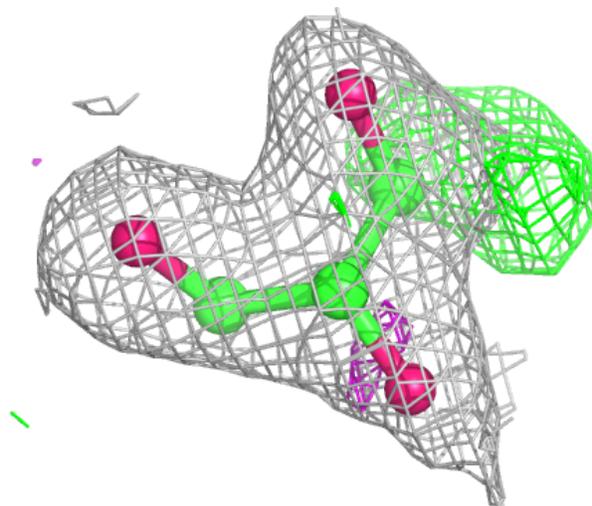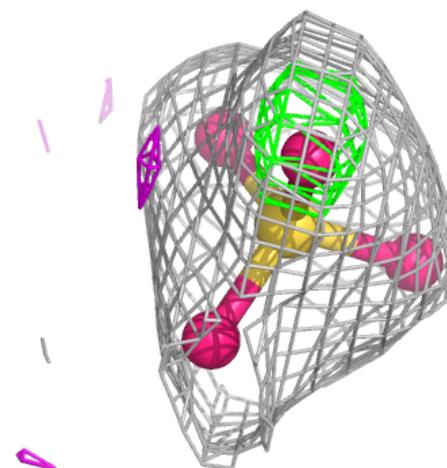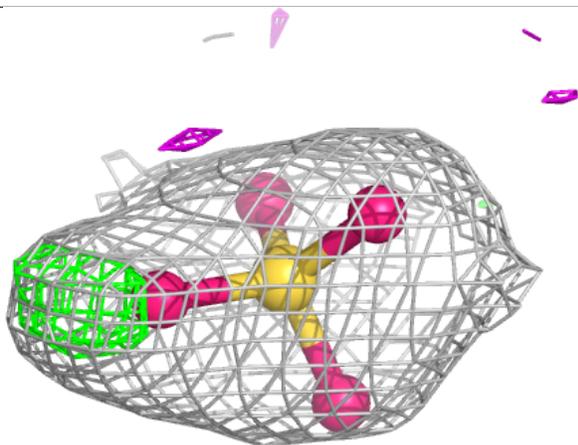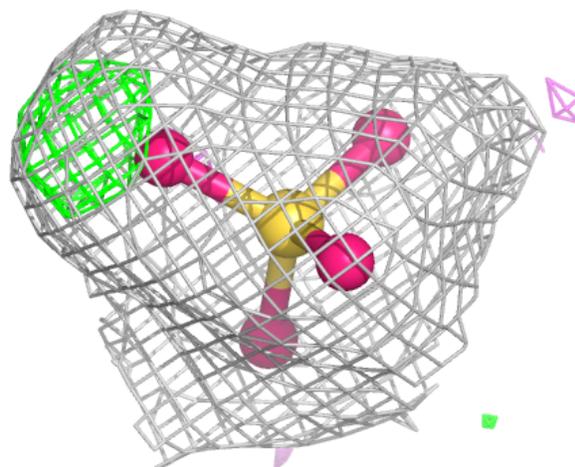and green (positive)
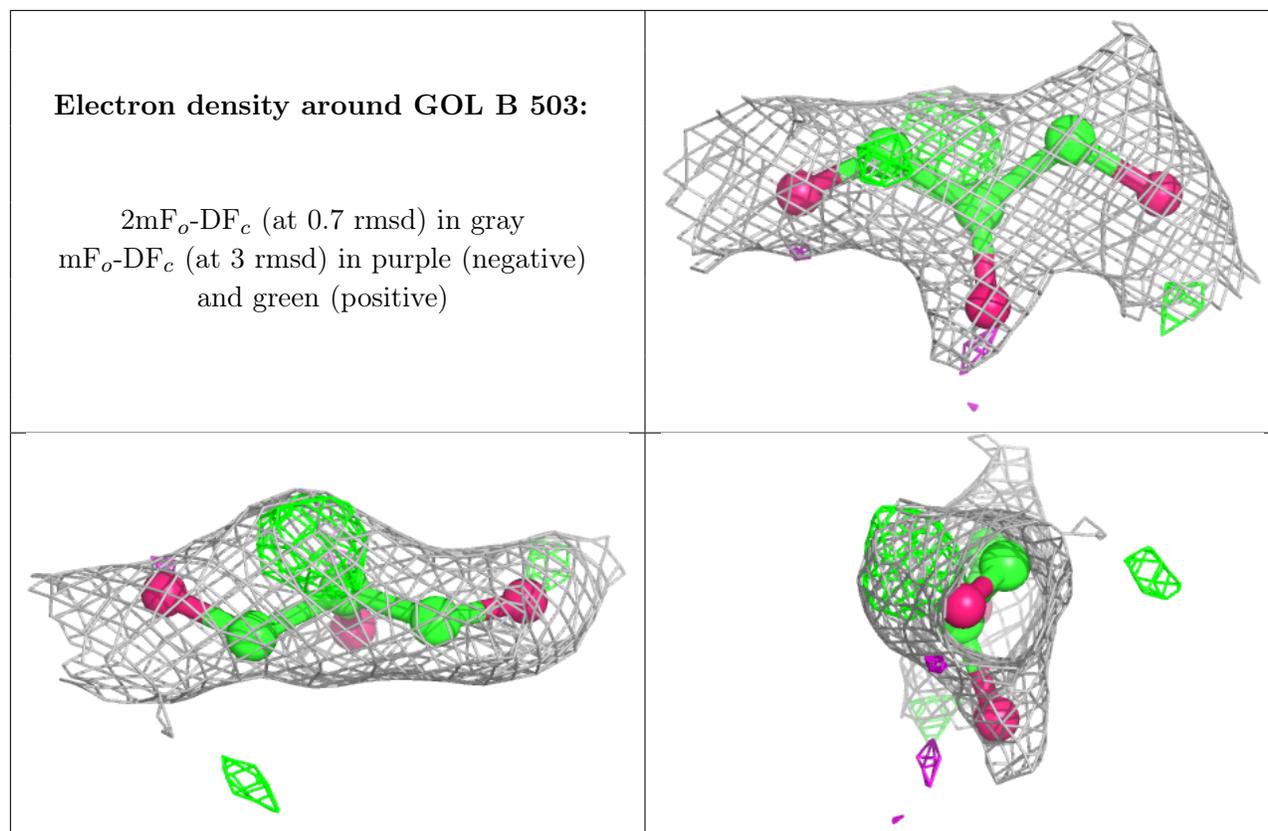
Electron density around SO4 A 510:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
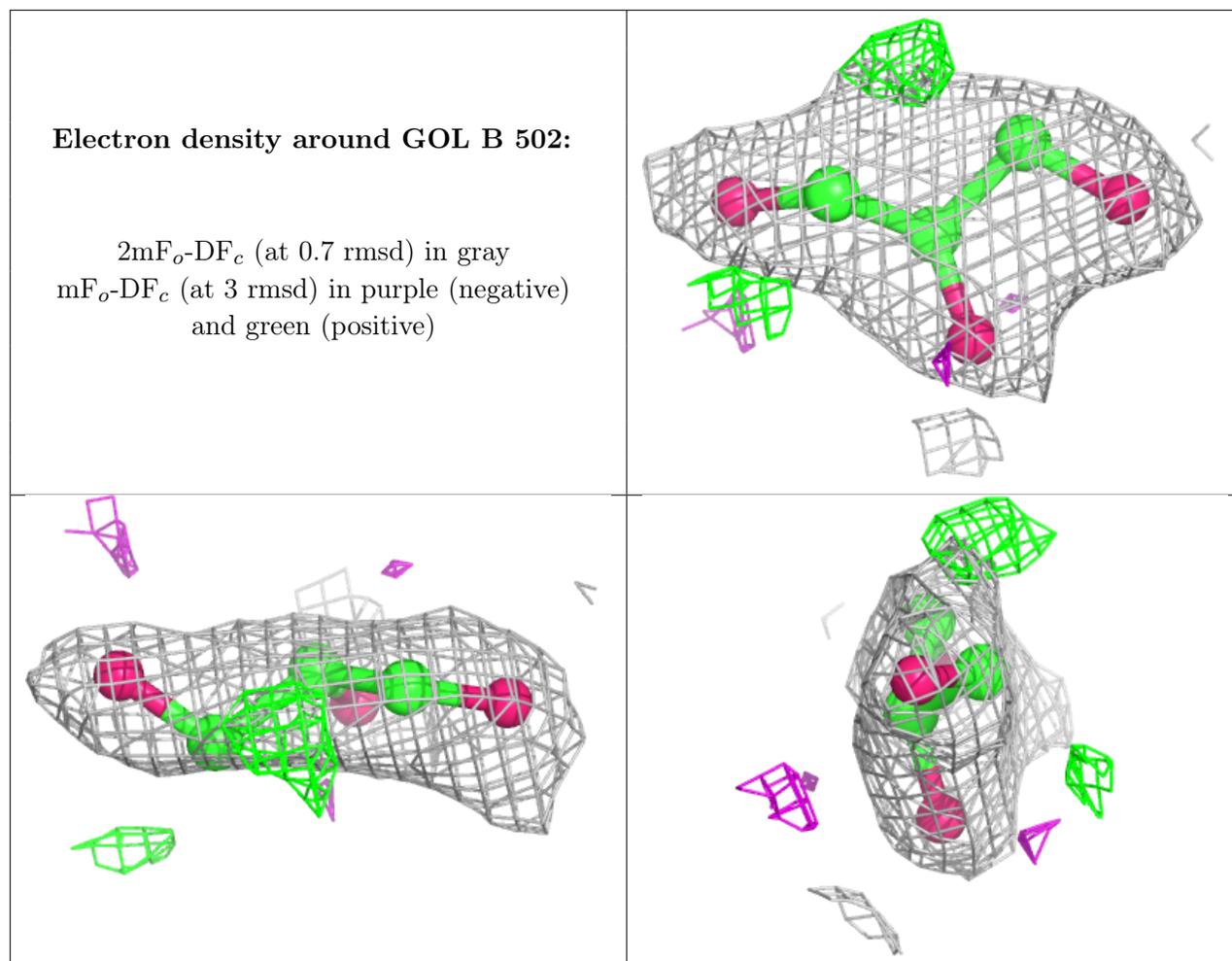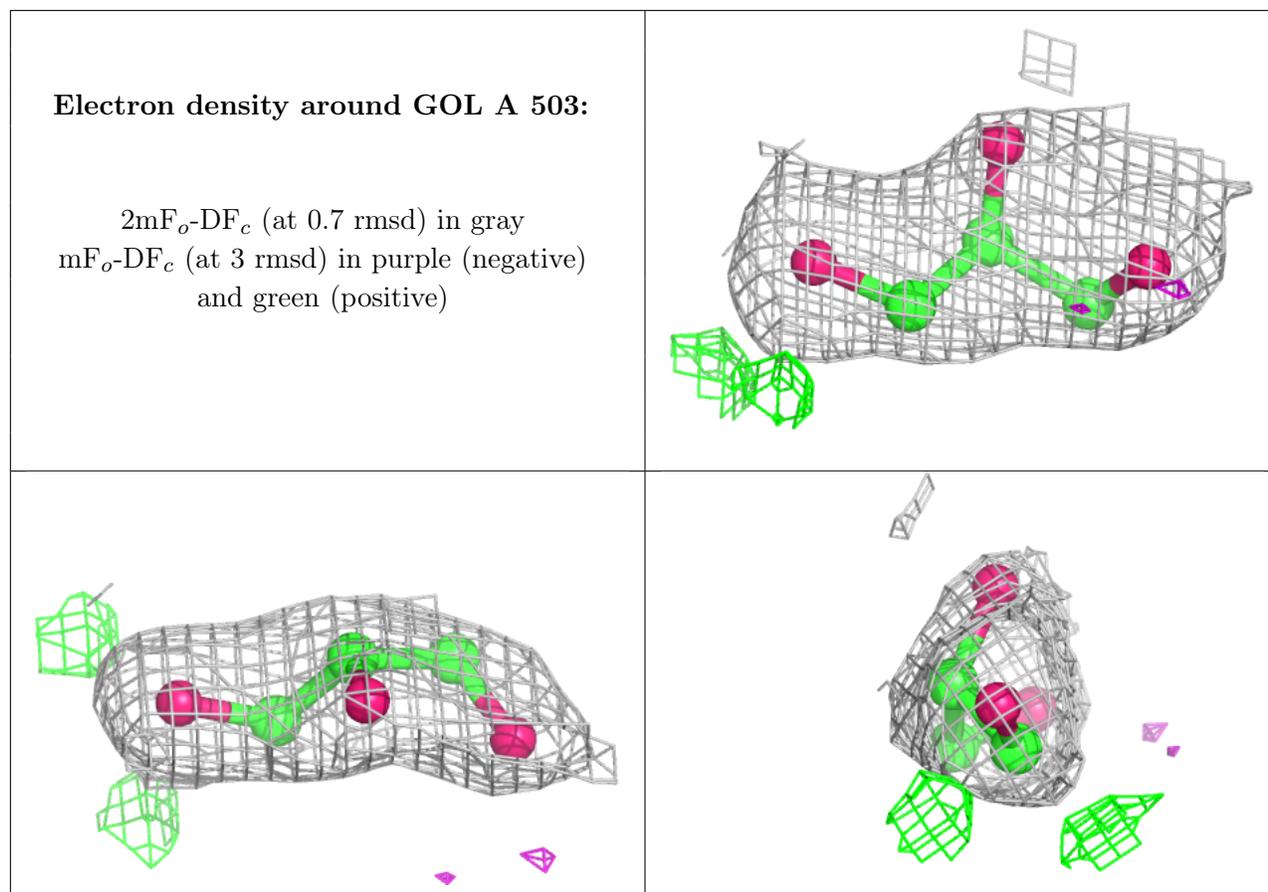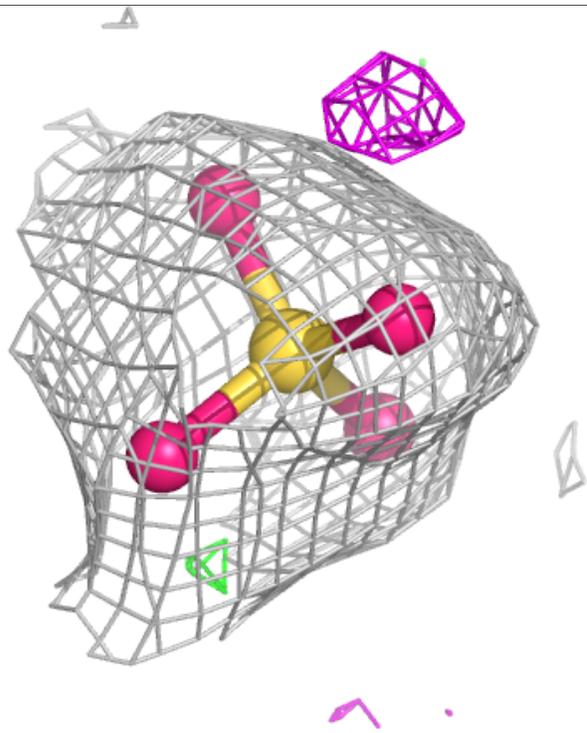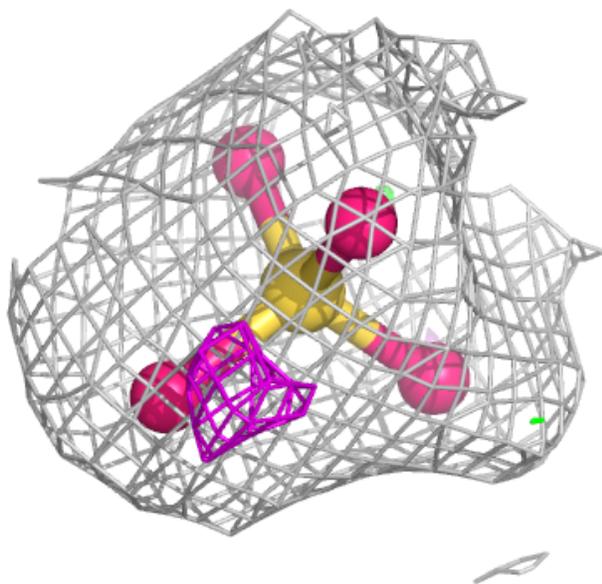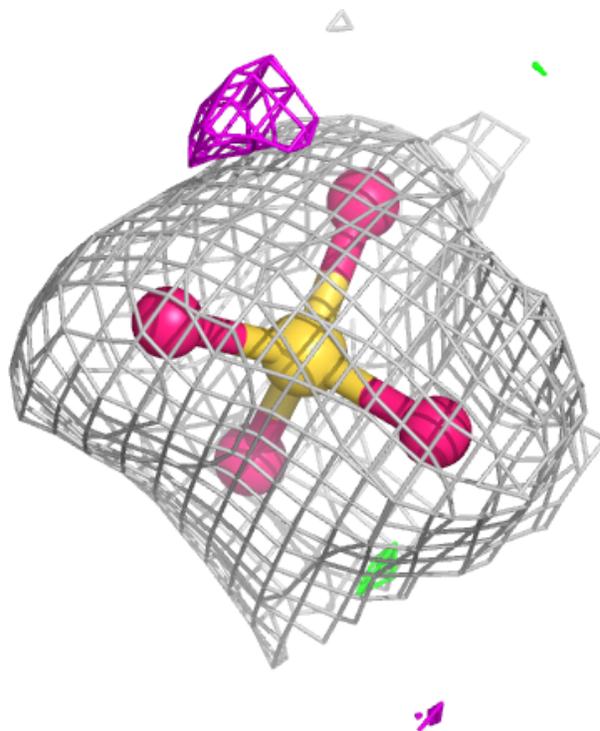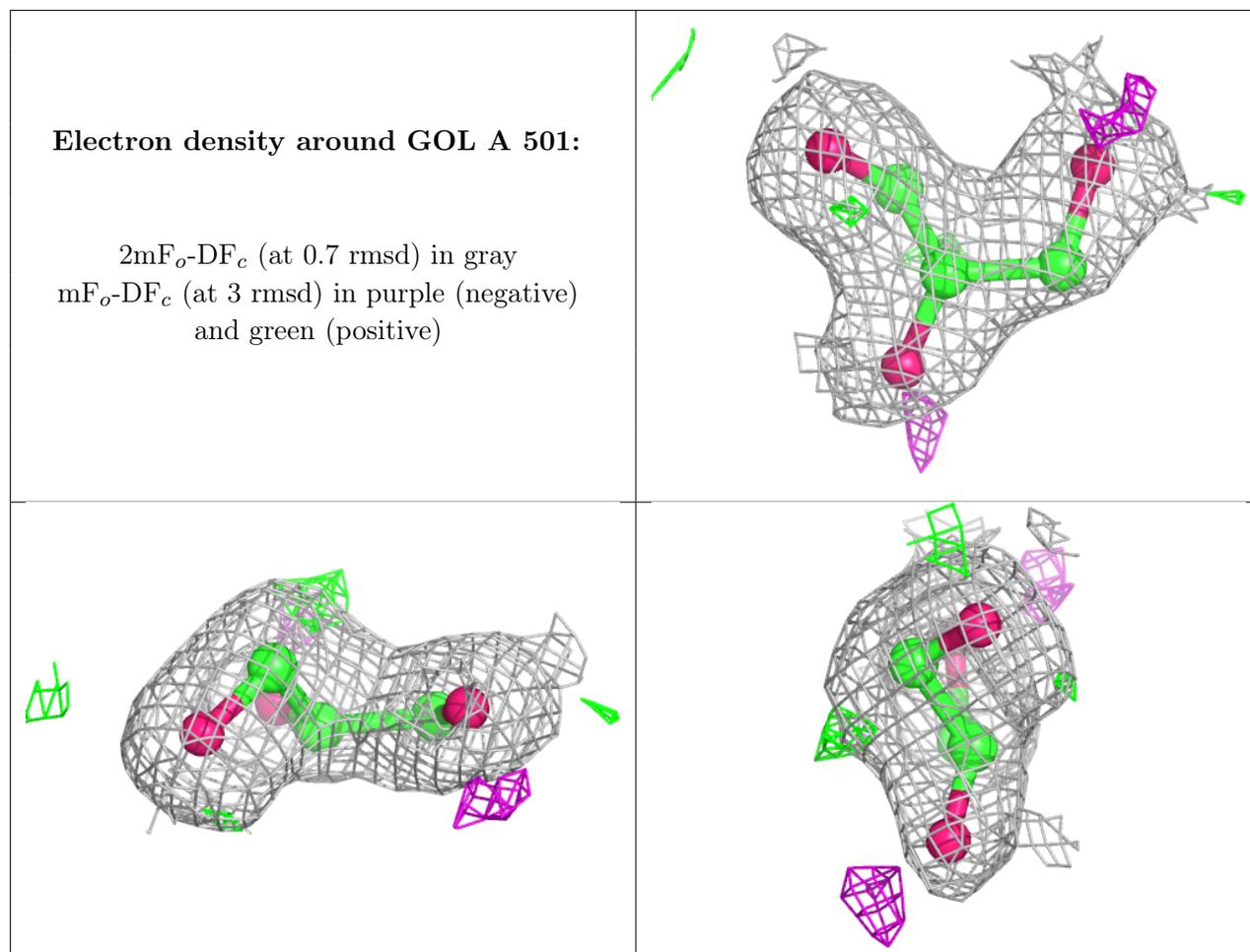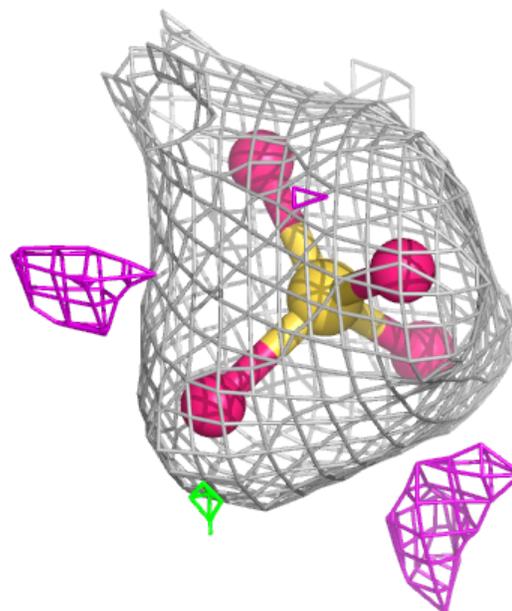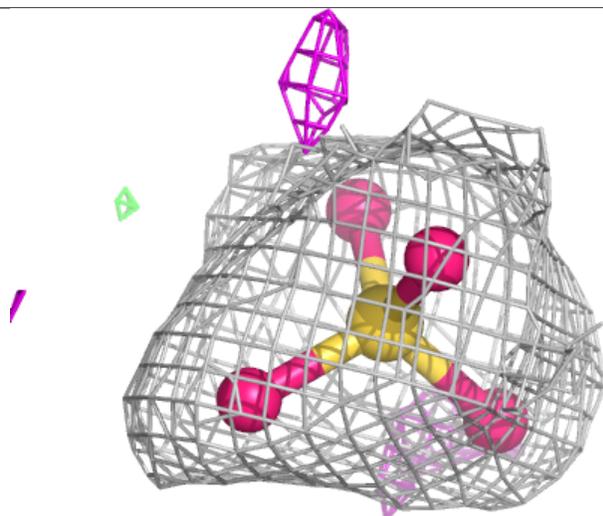and green (positive)
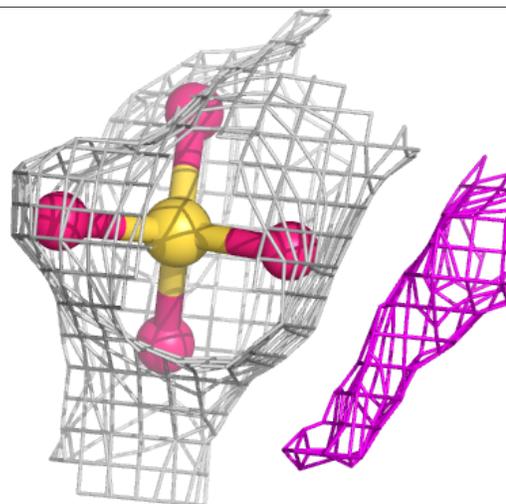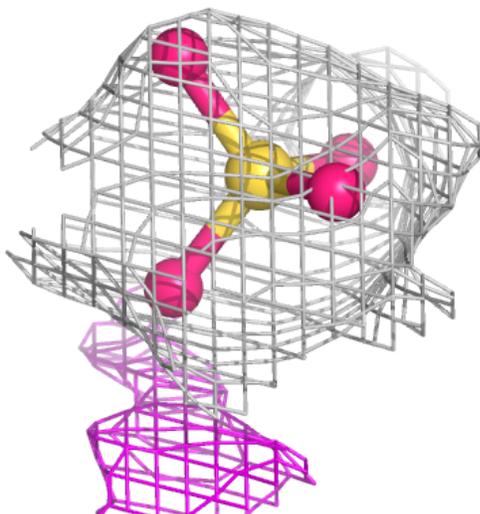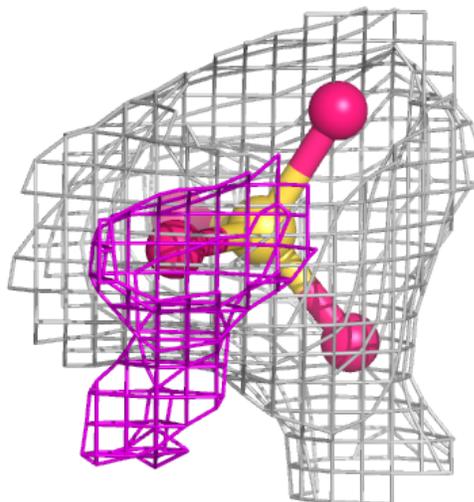
Electron density around SO4 A 509:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
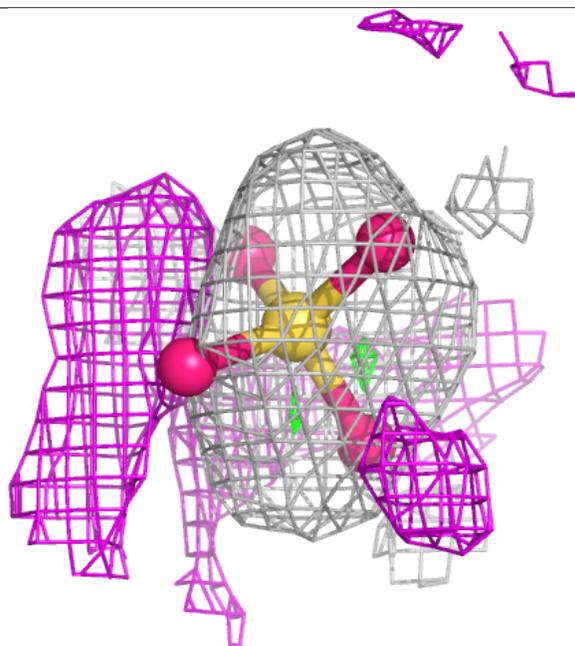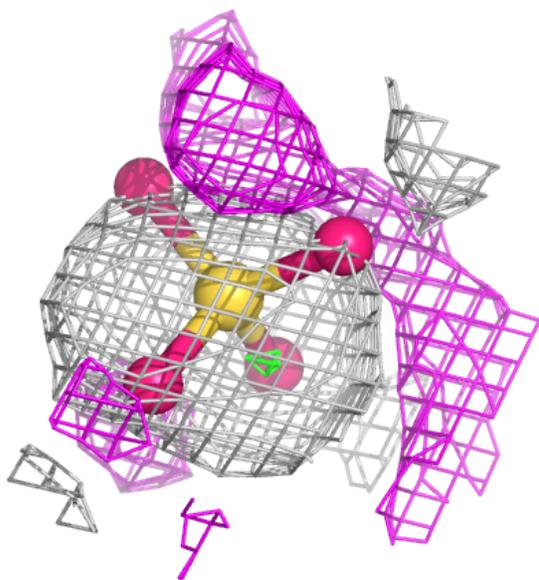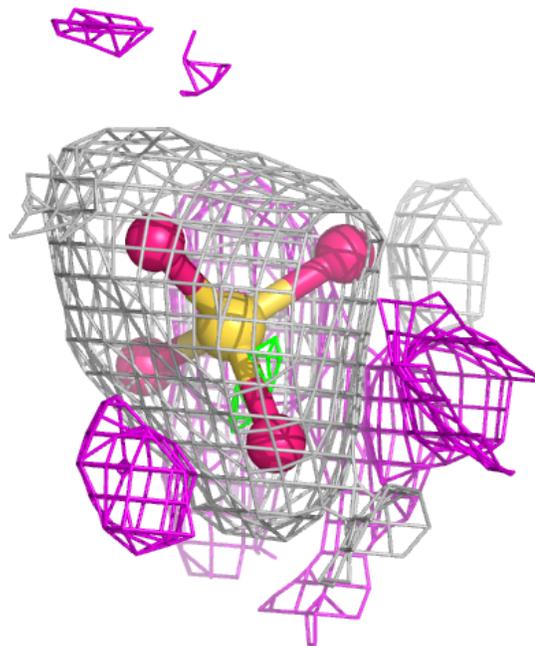
Electron density around SO4 B 509:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
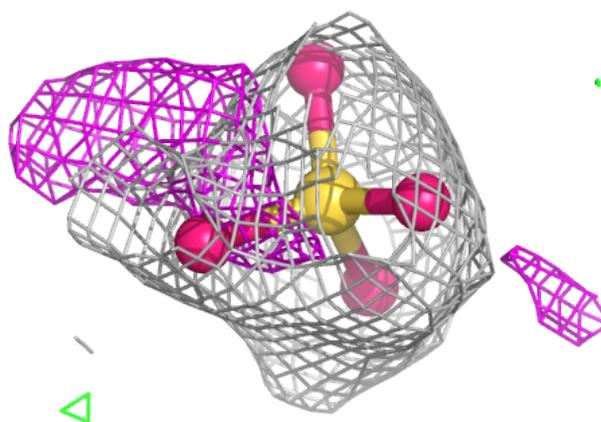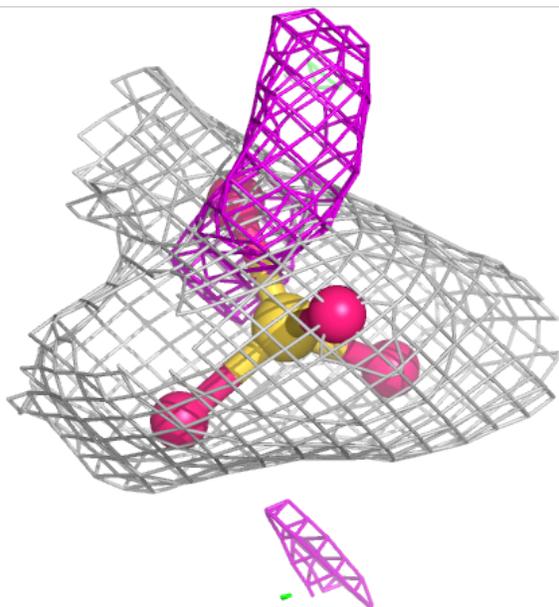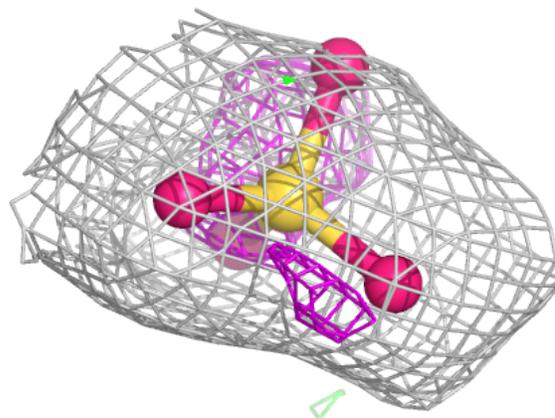
Electron density around SO4 A 508:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
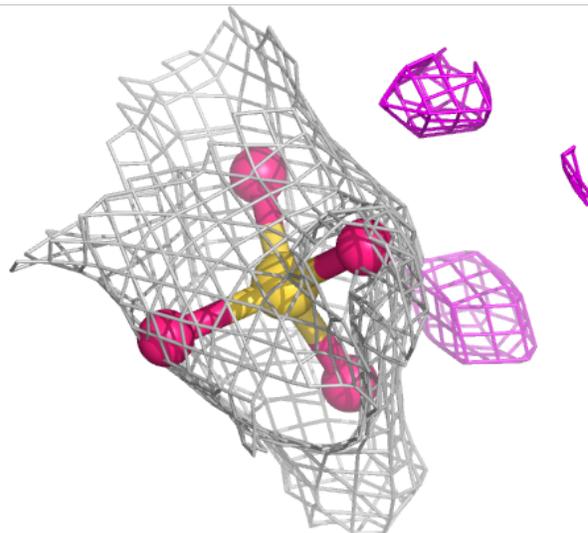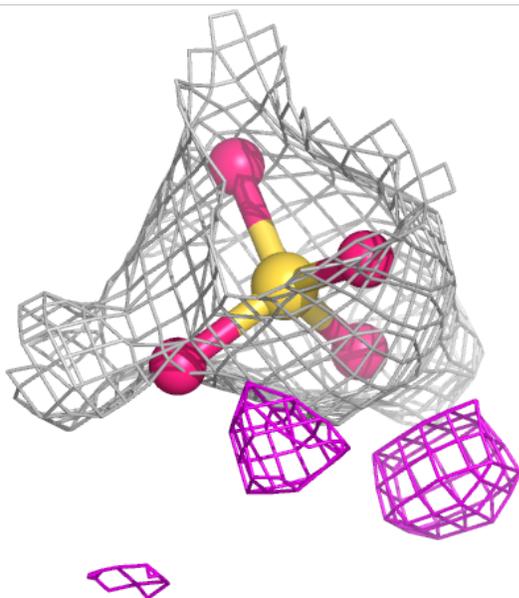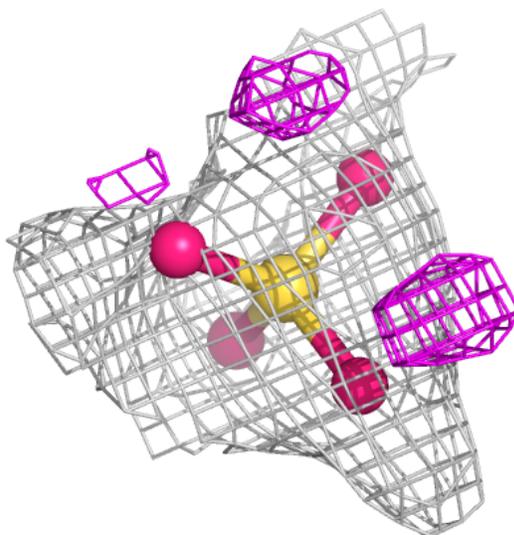
Electron density around SO4 B 508:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
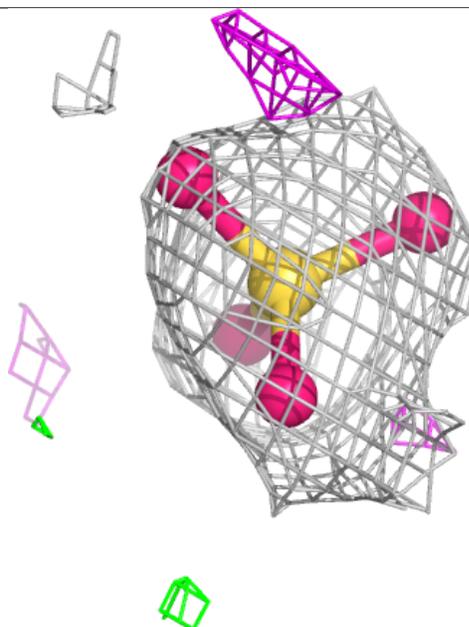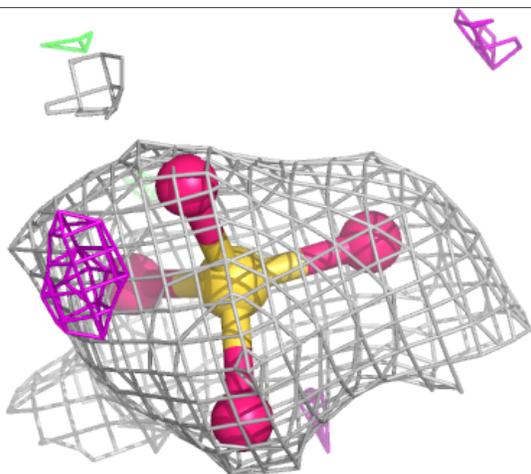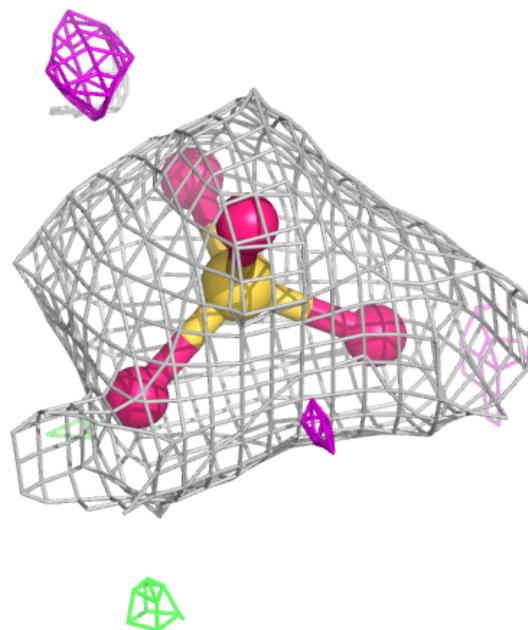
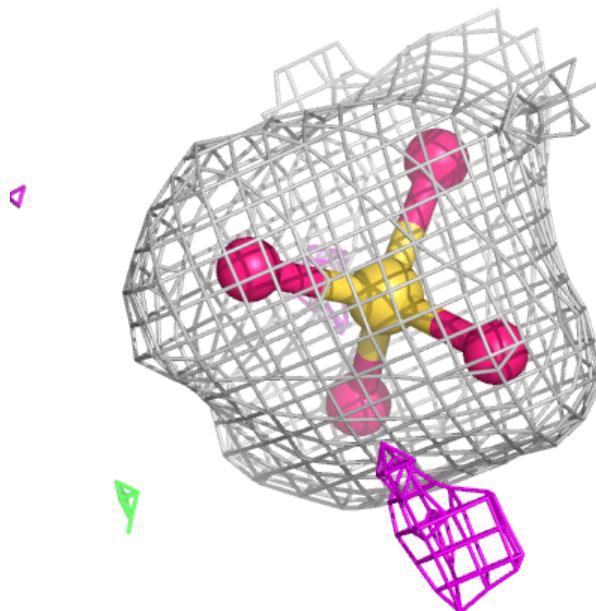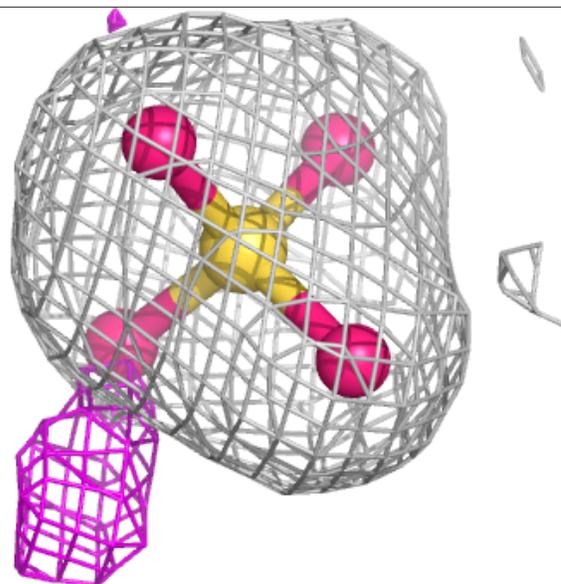**Electron density around GOL A 502:**

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
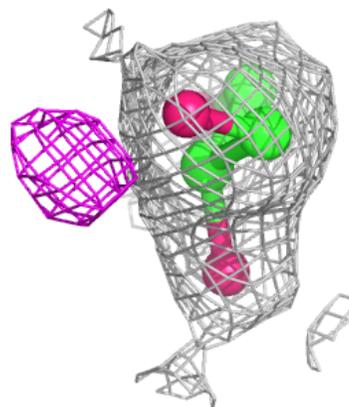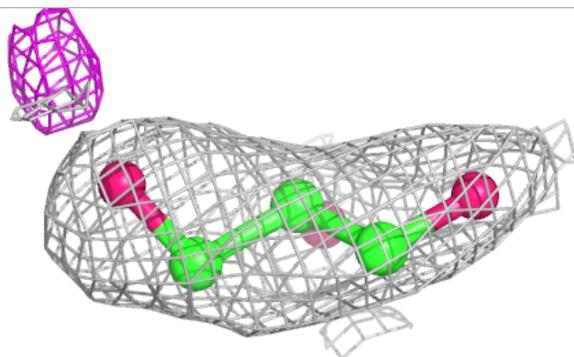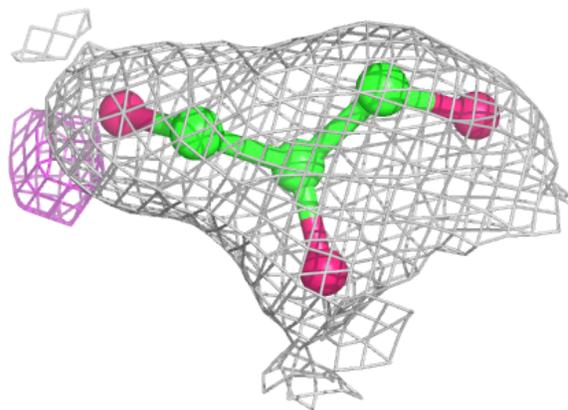
Electron density around SO4 A 505:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
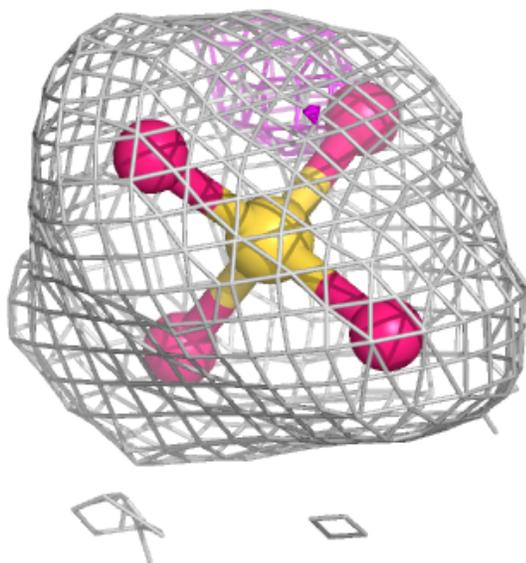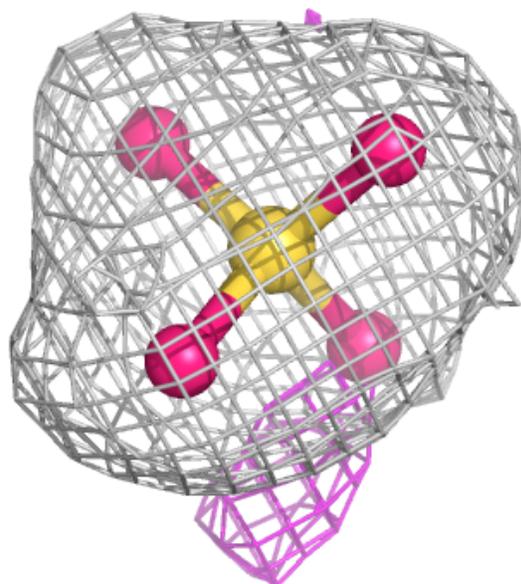and green (positive)
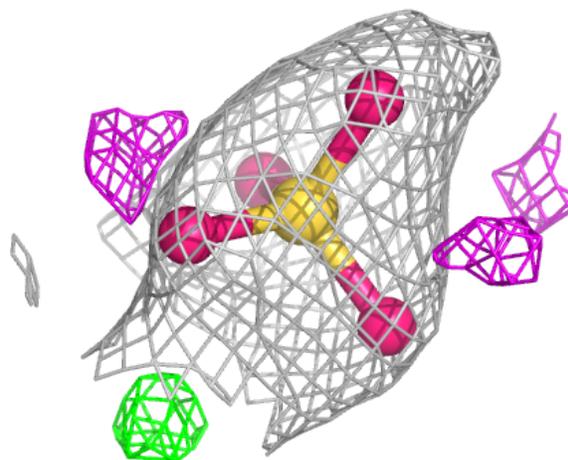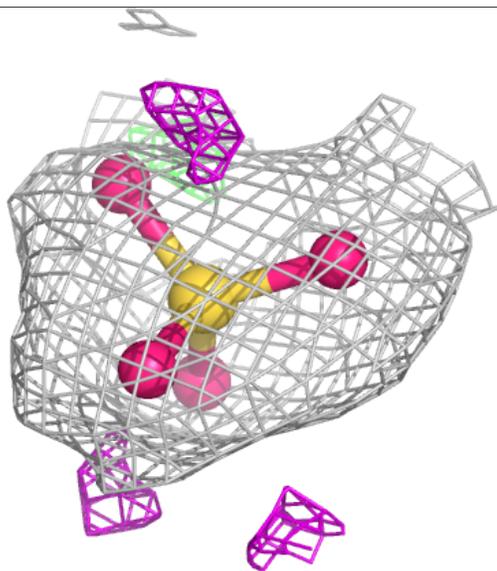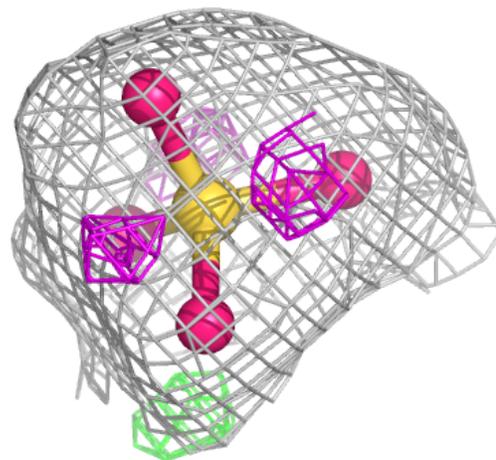
Electron density around SO4 A 506:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
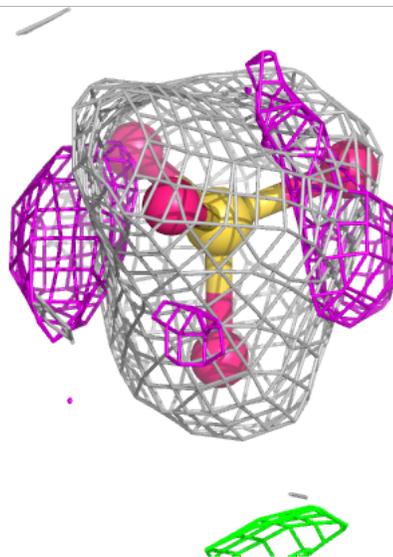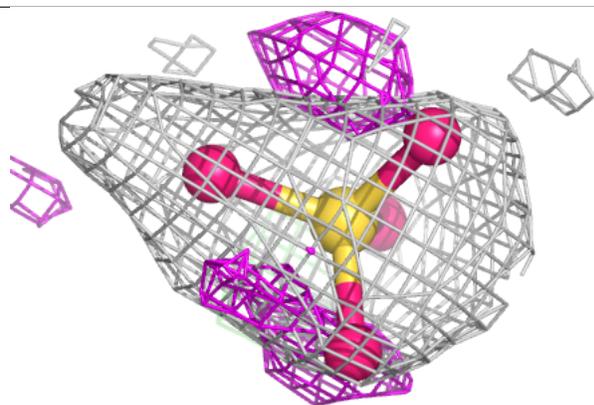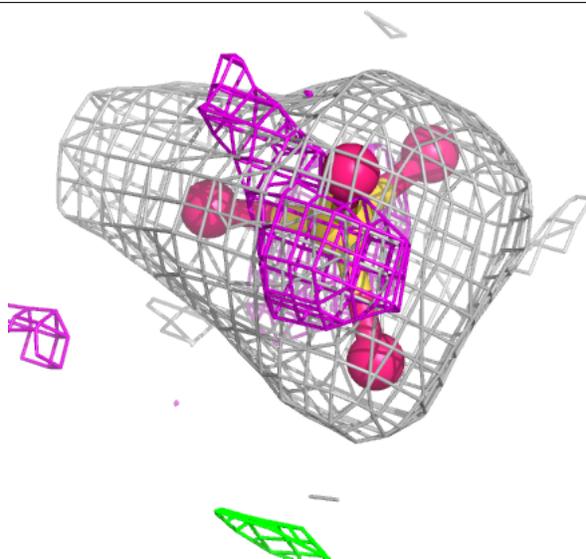
Electron density around GOL B 501:

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

Electron density around SO4 B 507:

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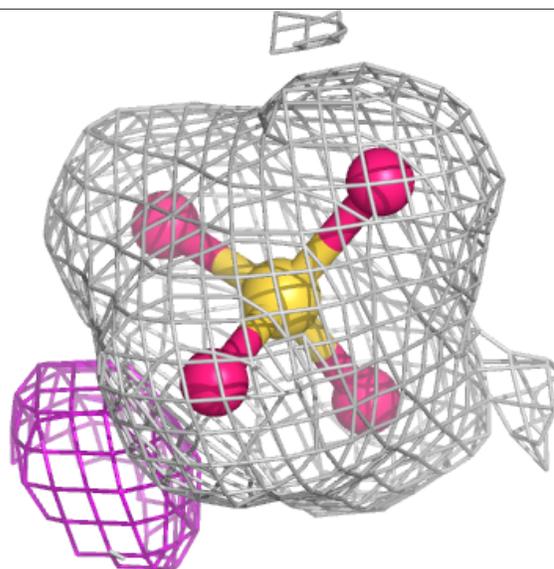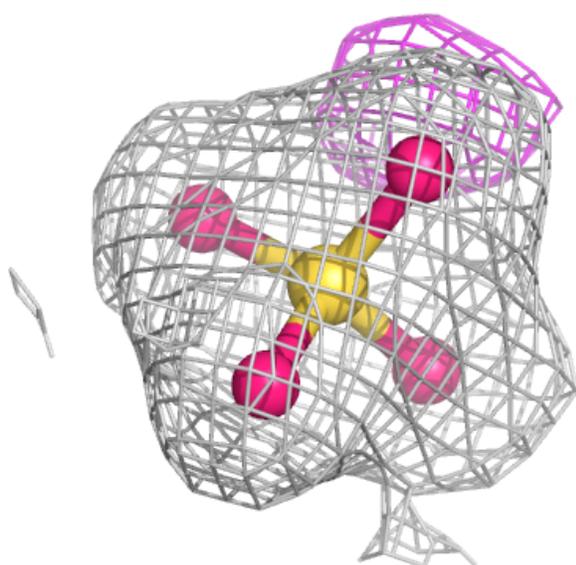and green (positive)

Electron density around GOL B 502:

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

Electron density around GOL A 503:

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

Electron density around SO4 B 505:

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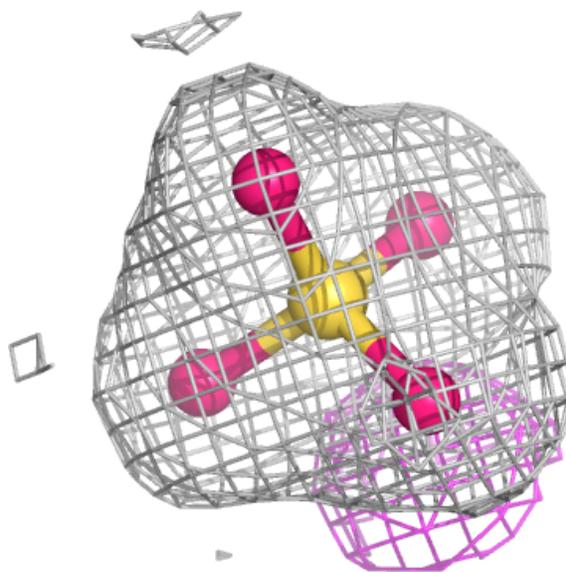$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around GOL A 501:

$2mF_o$-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 507:

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

Electron density around SO4 B 506:

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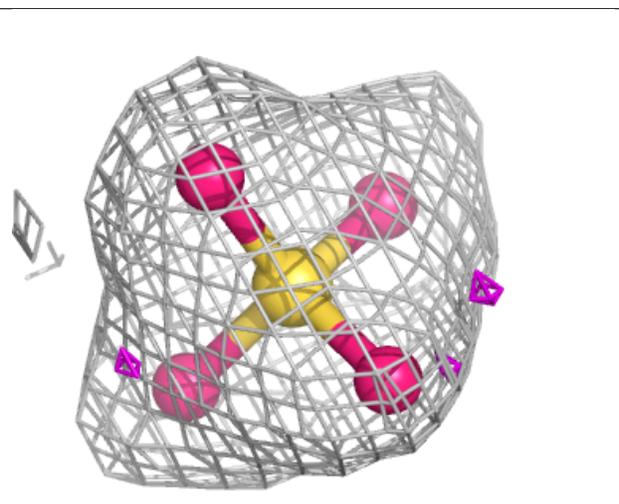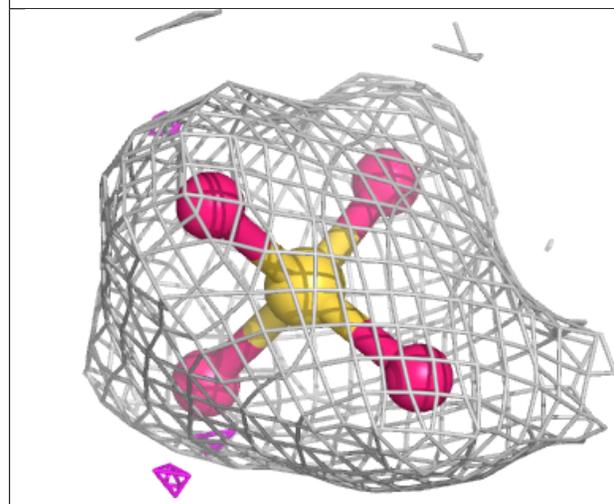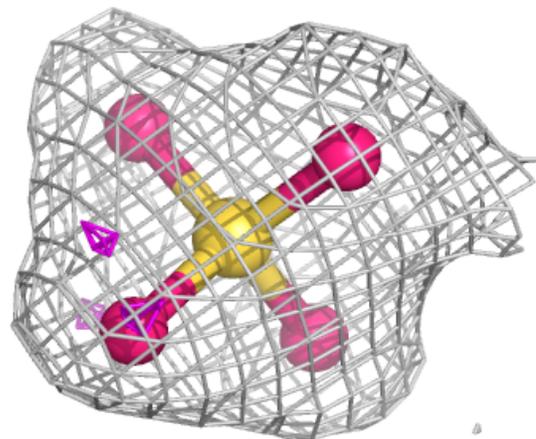mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around SO4 B 504:

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

Electron density around SO4 A 504:

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.