Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2023 – 08:12 PM JST

PDB ID	:	8GUL
Title	:	Chitin-active AA10 LPMO (GbpA) complexed with Cu(II) from Vibrio campbellii
Authors	:	Zhou, Y.; Robinson, R.C.; Suginta, W.
Deposited on	:	2022-09-12
Resolution	:	2.44 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:

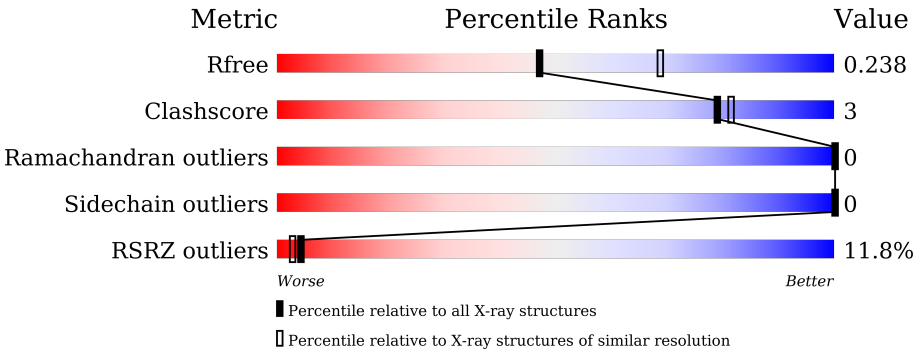
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.44 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}	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	464	8% 92% 8%
1	B	464	13% 72% 6% 22%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6624 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.

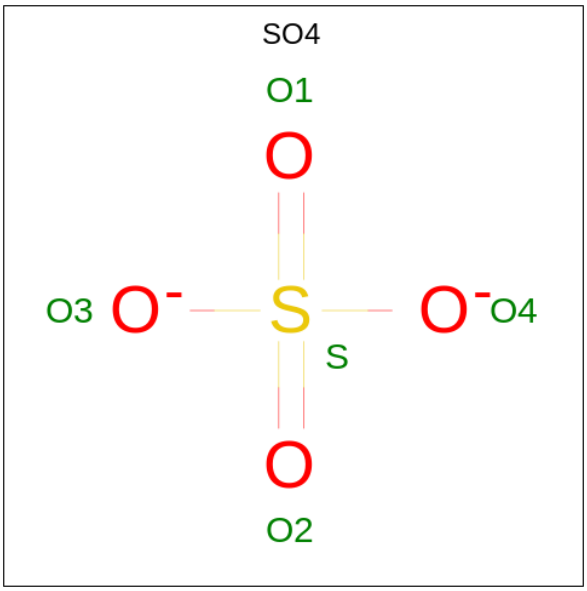
- Molecule 1 is a protein called GlcNAc-binding protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3607	2260	601	734	12			
1	B	361	Total	C	N	O	S	0	0	0
			2801	1744	481	566	10			

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		

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



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

- Molecule 4 is water.

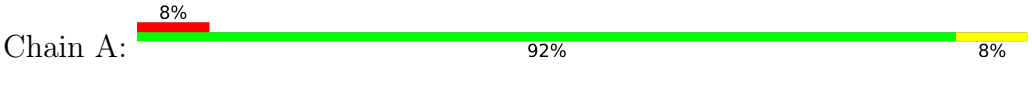
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	101	Total O 101 101	0	0
4	B	108	Total O 108 108	0	0

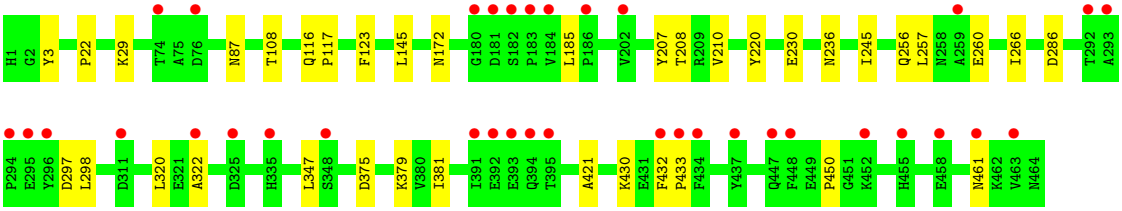
3 Residue-property plots (i)

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: GlcNAc-binding protein A

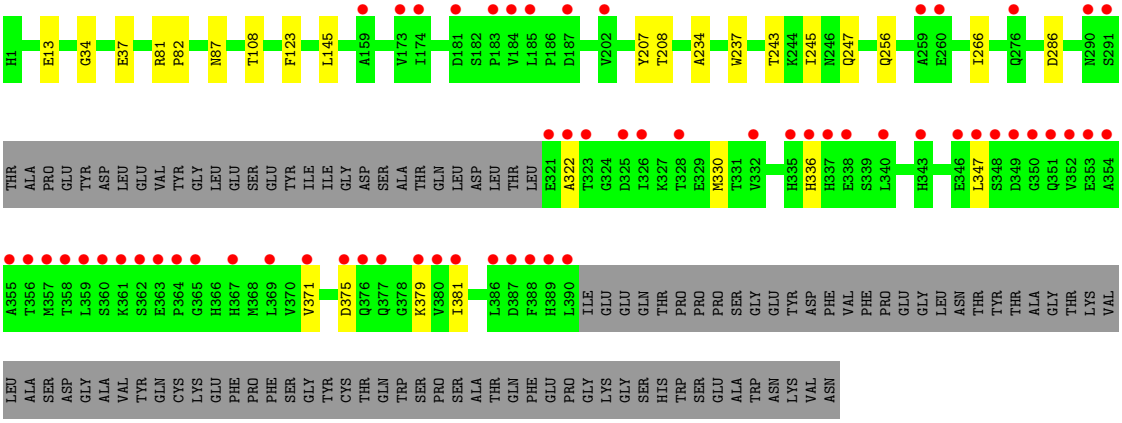
Chain A:





• Molecule 1: GlcNAc-binding protein A

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	113.43Å 113.43Å 213.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.78 – 2.44 29.78 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.78-2.44) 99.0 (29.78-2.44)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.204 , 0.240 0.203 , 0.238	Depositor DCC
R_{free} test set	2598 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	52.0	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6624	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU, 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	0.25	0/3700	0.46	0/5048
1	B	0.24	0/2866	0.47	0/3903
All	All	0.25	0/6566	0.46	0/8951

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	3607	0	3364	21	0
1	B	2801	0	2633	15	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	B	5	0	0	0	0
4	A	101	0	0	0	0
4	B	108	0	0	0	0
All	All	6624	0	5997	35	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (35) 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:B:81:ARG:HD3	1:B:82:PRO:HD2	1.61	0.80
1:A:210:VAL:HG21	1:A:220:TYR:HB2	1.68	0.75
1:A:322:ALA:HB2	1:A:347:LEU:HD23	1.71	0.72
1:A:208:THR:HG21	1:A:245:ILE:HD11	1.81	0.62
1:A:3:TYR:HA	1:A:172:ASN:HD21	1.65	0.60
1:B:13:GLU:OE1	1:B:81:ARG:NH1	2.38	0.56
1:A:256:GLN:HG3	1:A:266:ILE:HD13	1.88	0.56
1:B:375:ASP:HB3	1:B:381:ILE:HD11	1.89	0.54
1:B:87:ASN:HB3	1:B:145:LEU:HD11	1.88	0.54
1:A:22:PRO:HA	1:A:29:LYS:HG3	1.93	0.50
1:A:87:ASN:HB3	1:A:145:LEU:HD11	1.94	0.49
1:A:3:TYR:HA	1:A:172:ASN:ND2	2.27	0.48
1:A:260:GLU:OE2	1:B:336:HIS:ND1	2.45	0.48
1:B:330:MET:HG2	1:B:371:VAL:HG22	1.95	0.47
1:A:375:ASP:HB3	1:A:381:ILE:HD11	1.96	0.47
1:B:322:ALA:HB2	1:B:347:LEU:HD23	1.96	0.47
1:A:207:TYR:CZ	1:A:286:ASP:HB3	2.49	0.47
1:A:108:THR:HA	1:A:123:PHE:HA	1.97	0.47
1:B:208:THR:HG21	1:B:245:ILE:HD11	1.97	0.46
1:B:207:TYR:CZ	1:B:286:ASP:HB3	2.50	0.46
1:B:243:THR:O	1:B:247:GLN:HG3	2.16	0.46
1:A:297:ASP:OD1	1:A:298:LEU:N	2.49	0.46
1:B:375:ASP:OD1	1:B:379:LYS:N	2.45	0.45
1:A:116:GLN:HG3	1:A:117:PRO:HD2	1.99	0.45
1:B:256:GLN:HG3	1:B:266:ILE:HD13	1.99	0.45
1:B:234:ALA:HA	1:B:237:TRP:NE1	2.32	0.44
1:A:430:LYS:HD3	1:A:461:ASN:OD1	2.18	0.44
1:A:298:LEU:HD11	1:A:320:LEU:HB3	1.99	0.43
1:A:230:GLU:O	1:A:236:ASN:ND2	2.39	0.43
1:A:379:LYS:HB3	1:A:379:LYS:HE3	1.84	0.42
1:B:108:THR:HA	1:B:123:PHE:HA	2.01	0.42
1:A:185:LEU:HD12	1:A:257:LEU:HD21	2.01	0.42
1:B:34:GLY:O	1:B:37:GLU:HG2	2.20	0.41
1:A:421:ALA:HB2	1:A:450:PRO:HB2	2.04	0.40
1:A:432:PHE:HA	1:A:433:PRO:HA	1.86	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	462/464 (100%)	441 (96%)	21 (4%)	0	100	100
1	B	357/464 (77%)	341 (96%)	16 (4%)	0	100	100
All	All	819/928 (88%)	782 (96%)	37 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	392/392 (100%)	392 (100%)	0	100	100
1	B	305/392 (78%)	305 (100%)	0	100	100
All	All	697/784 (89%)	697 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	172	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	B	502	-	4,4,4	0.14	0	6,6,6	0.06	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

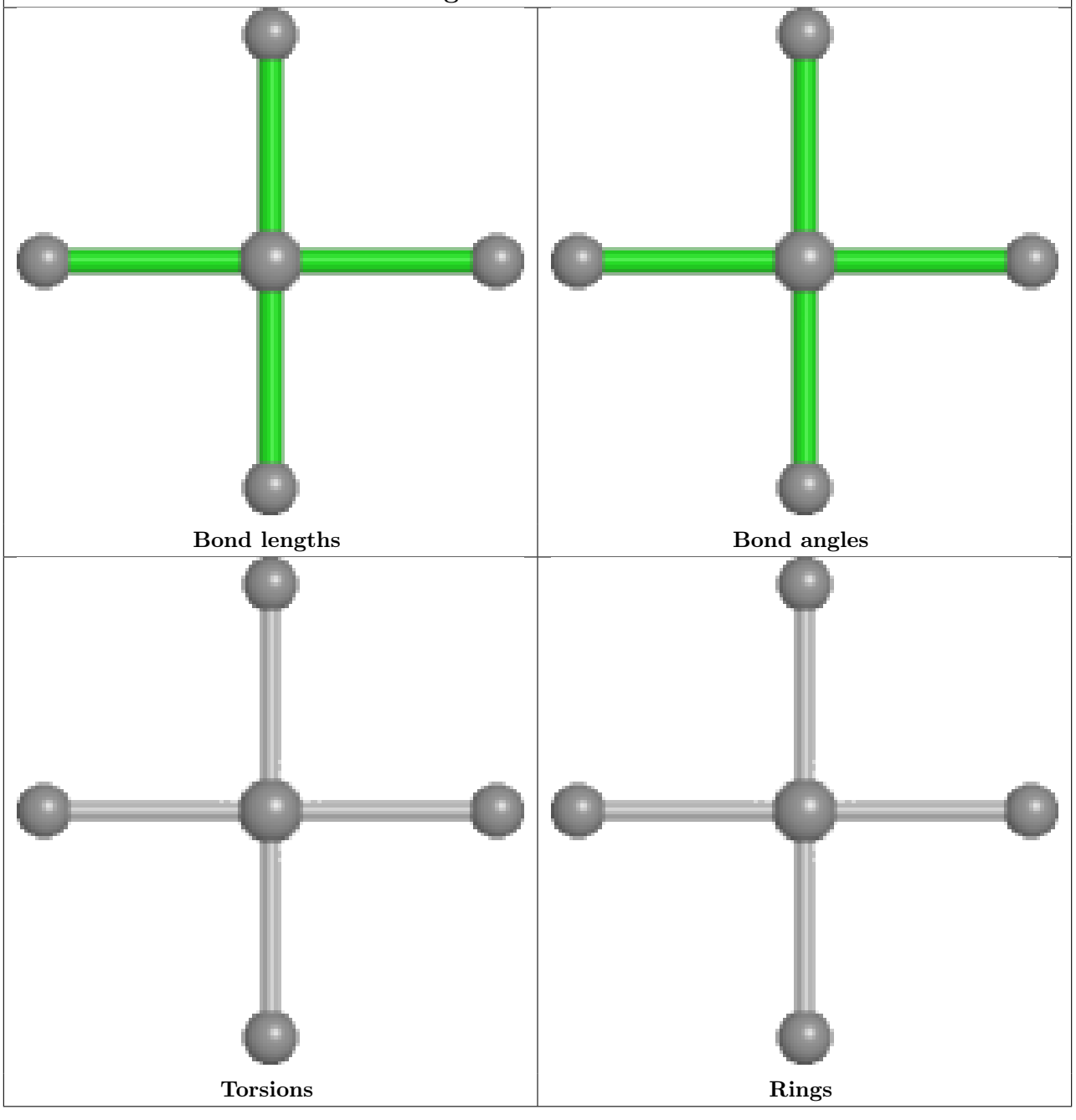
There are no ring outliers.

No monomer is involved in short contacts.

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 502



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, 95^{th} 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	464/464 (100%)	0.26	36 (7%)	13	10	47, 68, 118, 166	0
1	B	361/464 (77%)	0.65	61 (16%)	1	1	38, 62, 140, 163	0
All	All	825/928 (88%)	0.43	97 (11%)	4	3	38, 65, 130, 166	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	347	LEU	6.9
1	A	437	TYR	6.9
1	B	357	MET	6.8
1	B	336	HIS	6.1
1	B	364	PRO	5.6
1	B	359	LEU	5.6
1	B	352	VAL	5.6
1	B	326	ILE	5.4
1	B	259	ALA	5.4
1	A	181	ASP	5.3
1	B	349	ASP	5.2
1	B	355	ALA	5.2
1	B	328	THR	5.1
1	B	388	PHE	5.0
1	B	343	HIS	4.8
1	B	184	VAL	4.8
1	B	365	GLY	4.7
1	B	356	THR	4.7
1	B	354	ALA	4.3
1	B	350	GLY	4.2
1	B	362	SER	4.2
1	A	458	GLU	4.2
1	B	291	SER	4.1
1	B	376	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	363	GLU	4.0
1	B	353	GLU	4.0
1	B	181	ASP	4.0
1	B	321	GLU	3.9
1	A	335	HIS	3.9
1	A	294	PRO	3.9
1	B	367	HIS	3.8
1	A	432	PHE	3.8
1	A	448	PHE	3.8
1	B	387	ASP	3.7
1	B	386	LEU	3.7
1	A	293	ALA	3.6
1	A	434	PHE	3.6
1	B	337	HIS	3.6
1	B	338	GLU	3.5
1	A	322	ALA	3.5
1	B	390	LEU	3.5
1	A	182	SER	3.5
1	A	296	TYR	3.5
1	B	183	PRO	3.4
1	B	325	ASP	3.4
1	B	389	HIS	3.4
1	A	394	GLN	3.4
1	B	380	VAL	3.4
1	B	323	THR	3.3
1	B	361	LYS	3.3
1	A	180	GLY	3.3
1	B	173	VAL	3.2
1	B	322	ALA	3.2
1	B	351	GLN	3.1
1	B	348	SER	3.1
1	B	335	HIS	2.9
1	B	358	THR	2.9
1	B	185	LEU	2.9
1	A	393	GLU	2.9
1	B	202	VAL	2.8
1	A	325	ASP	2.8
1	A	461	ASN	2.8
1	B	379	LYS	2.7
1	B	346	GLU	2.7
1	A	455	HIS	2.7
1	B	377	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	186	PRO	2.6
1	A	447	GLN	2.6
1	A	184	VAL	2.6
1	B	369	LEU	2.6
1	B	381	ILE	2.5
1	A	392	GLU	2.5
1	B	340	LEU	2.5
1	A	183	PRO	2.5
1	A	202	VAL	2.4
1	A	292	THR	2.4
1	B	187	ASP	2.4
1	A	295	GLU	2.4
1	B	290	ASN	2.3
1	A	76	ASP	2.3
1	B	375	ASP	2.3
1	B	332	VAL	2.3
1	A	433	PRO	2.3
1	A	259	ALA	2.3
1	A	74	THR	2.2
1	A	395	THR	2.2
1	B	360	SER	2.2
1	B	159	ALA	2.2
1	B	174	ILE	2.2
1	A	452	LYS	2.1
1	A	311	ASP	2.1
1	B	276	GLN	2.1
1	B	260	GLU	2.1
1	A	348	SER	2.1
1	A	463	VAL	2.0
1	B	371	VAL	2.0
1	A	391	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 monosaccharides in this entry.

6.4 Ligands (i)

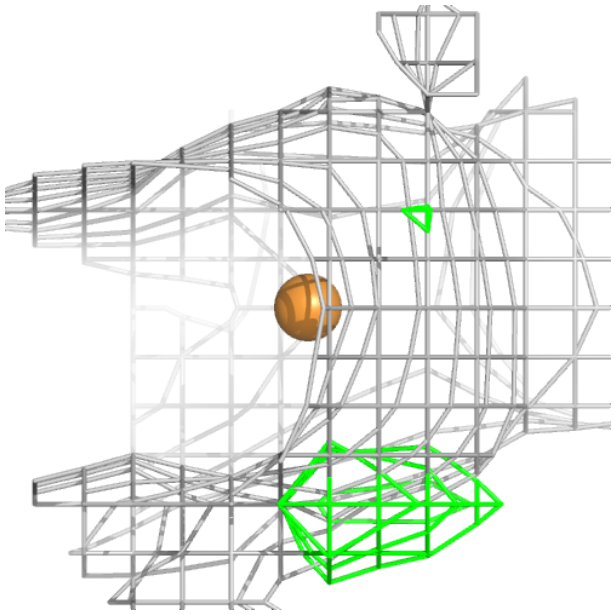
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

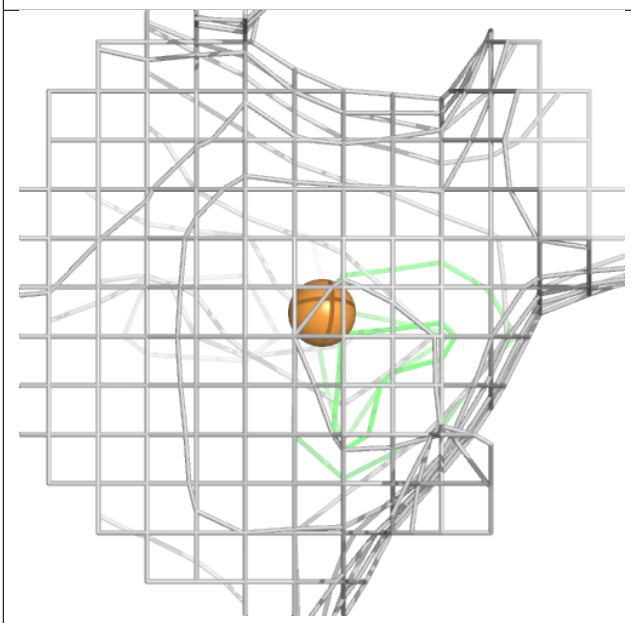
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CU	A	501	1/1	0.94	0.15	47,47,47,47	1
2	CU	B	501	1/1	0.96	0.12	48,48,48,48	1
3	SO4	B	502	5/5	0.98	0.11	68,69,83,84	0

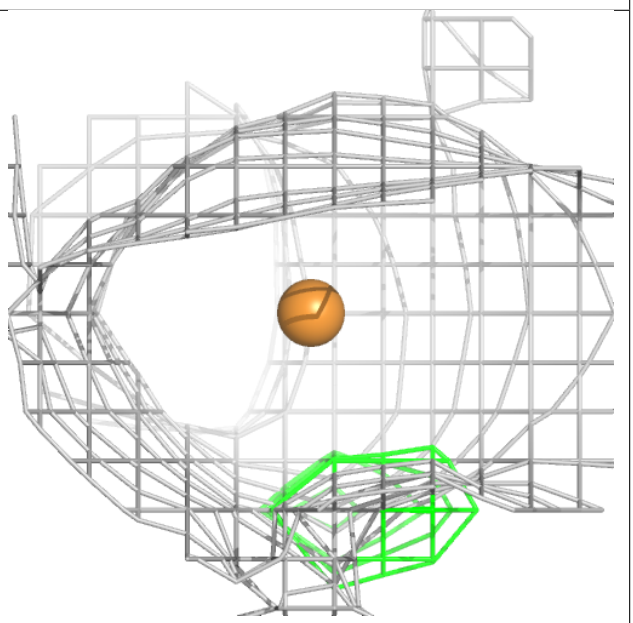
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CU 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)

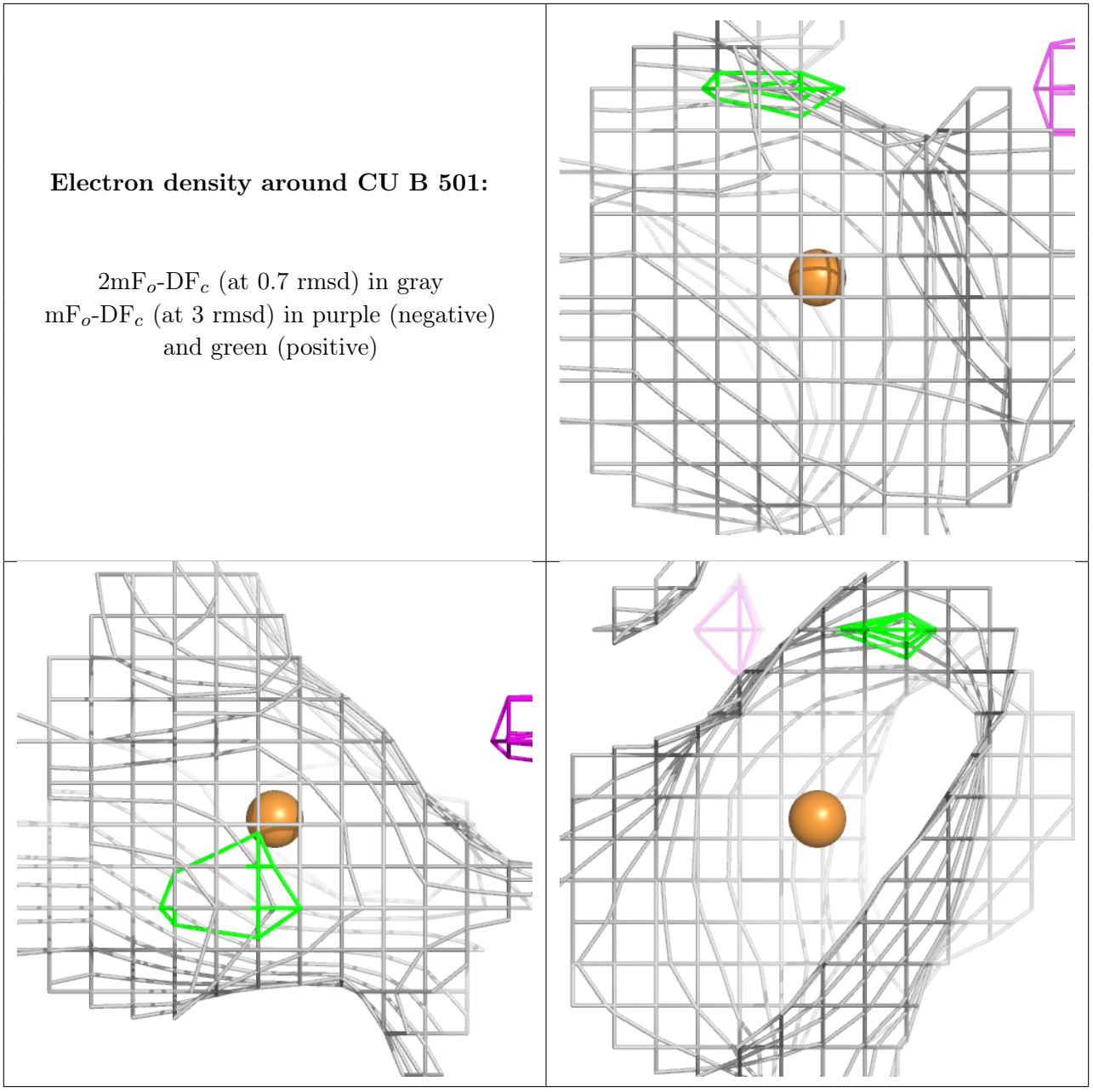






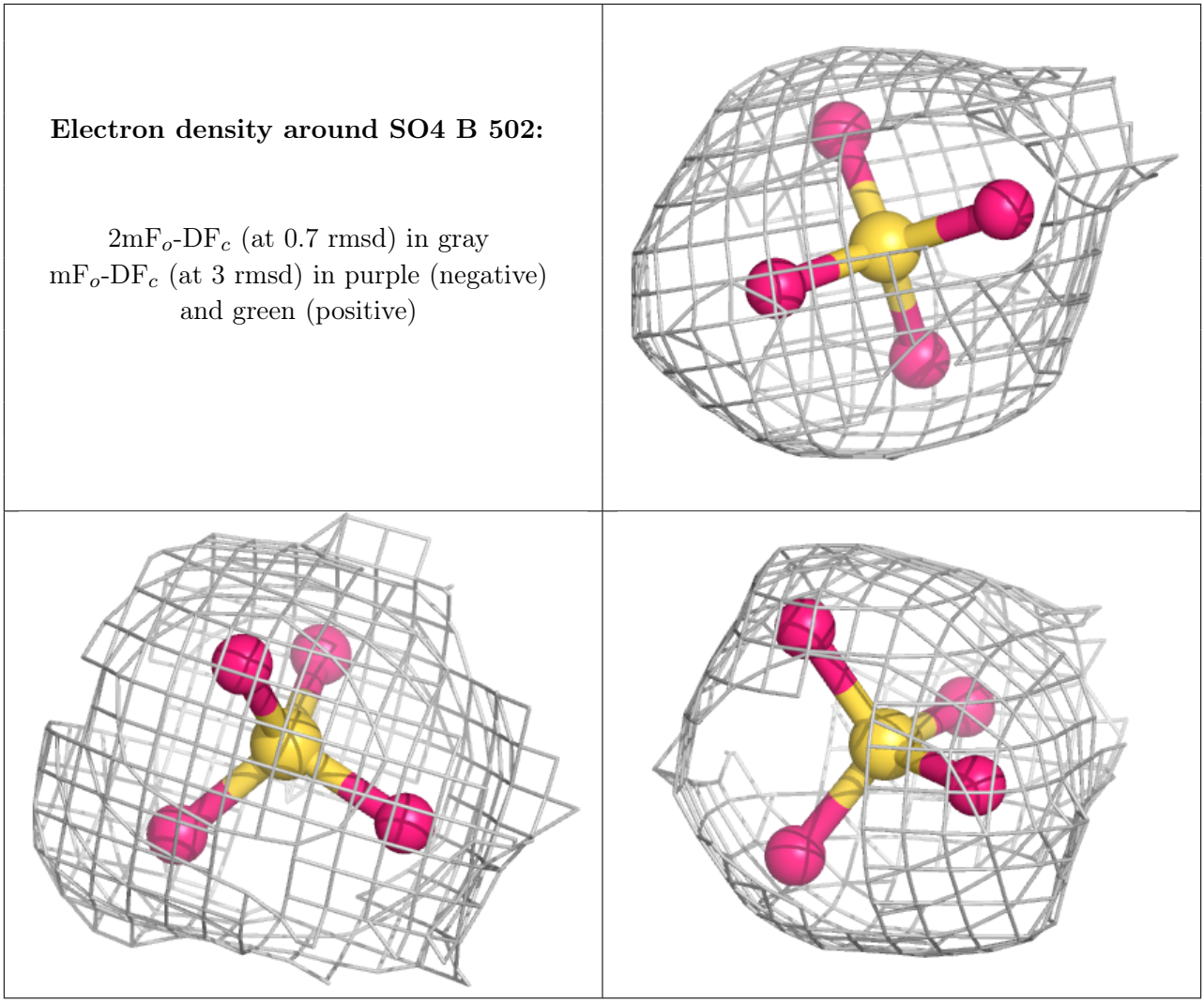
Electron density around CU B 501:

$2mF_o$-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 502:

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



6.5 Other polymers (i)

There are no such residues in this entry.