



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2025 – 11:54 PM EDT

PDB ID : 6WBJ / pdb_00006wbj
Title : High resolution crystal structure of mRECK(CC4) in fusion with engineered MBP
Authors : Chang, T.H.; Hsieh, F.L.; Gabelli, S.B.; Nathans, J.
Deposited on : 2020-03-26
Resolution : 1.65 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

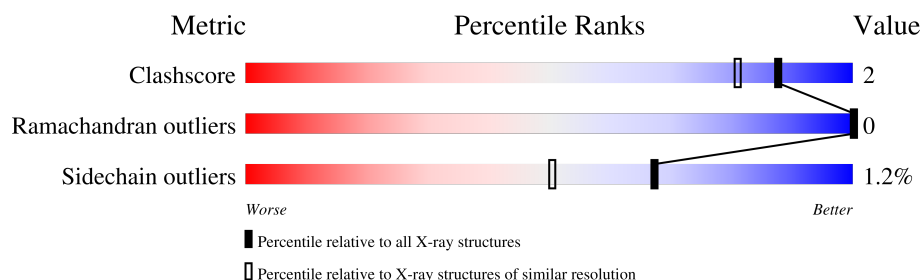
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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))
Clashscore	180529	2515 (1.66-1.66)
Ramachandran outliers	177936	2475 (1.66-1.66)
Sidechain outliers	177891	2475 (1.66-1.66)

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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	447	
2	B	2	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7290 atoms, of which 3373 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 Maltodextrin-binding protein, Reversion-inducing cysteine-rich protein with Kazal motifs fusion.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	432	Total	C	H	N	O	S	0	9	0
			6721	2164	3344	556	642	15			

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A376KDN7
A	2	ALA	-	expression tag	UNP A0A376KDN7
A	3	LYS	-	expression tag	UNP A0A376KDN7
A	4	THR	-	expression tag	UNP A0A376KDN7
A	84	ALA	ASP	engineered mutation	UNP A0A376KDN7
A	85	ALA	LYS	engineered mutation	UNP A0A376KDN7
A	174	ALA	GLU	engineered mutation	UNP A0A376KDN7
A	175	ALA	ASN	engineered mutation	UNP A0A376KDN7
A	217	HIS	ALA	engineered mutation	UNP A0A376KDN7
A	221	HIS	LYS	engineered mutation	UNP A0A376KDN7
A	241	ALA	LYS	engineered mutation	UNP A0A376KDN7
A	314	VAL	ALA	engineered mutation	UNP A0A376KDN7
A	319	VAL	ILE	engineered mutation	UNP A0A376KDN7
A	364	ALA	LYS	engineered mutation	UNP A0A376KDN7
A	365	ALA	ASP	engineered mutation	UNP A0A376KDN7
A	369	ASN	-	linker	UNP A0A376KDN7
A	370	ALA	-	linker	UNP A0A376KDN7
A	371	ALA	-	linker	UNP A0A376KDN7
A	372	ALA	-	linker	UNP A0A376KDN7
A	438	GLY	-	expression tag	UNP Q9Z0J1
A	439	THR	-	expression tag	UNP Q9Z0J1
A	440	HIS	-	expression tag	UNP Q9Z0J1
A	441	HIS	-	expression tag	UNP Q9Z0J1
A	442	HIS	-	expression tag	UNP Q9Z0J1
A	443	HIS	-	expression tag	UNP Q9Z0J1
A	444	HIS	-	expression tag	UNP Q9Z0J1

Continued on next page...

Continued from previous page...

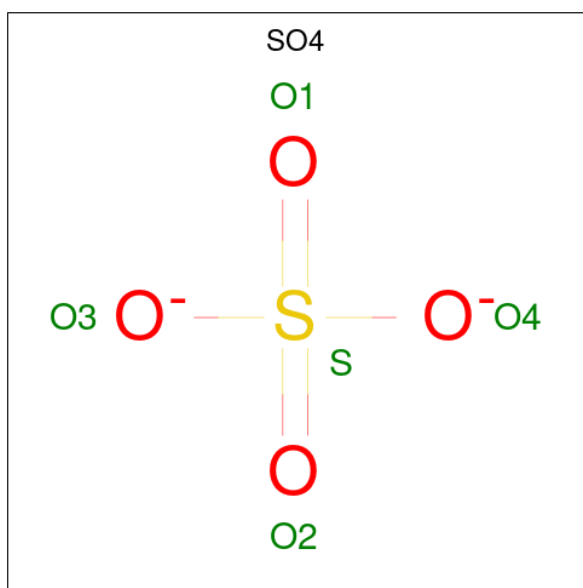
Chain	Residue	Modelled	Actual	Comment	Reference
A	445	HIS	-	expression tag	UNP Q9Z0J1
A	446	HIS	-	expression tag	UNP Q9Z0J1
A	447	HIS	-	expression tag	UNP Q9Z0J1

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	H	O	0	0	0
			44	12	21	11			

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

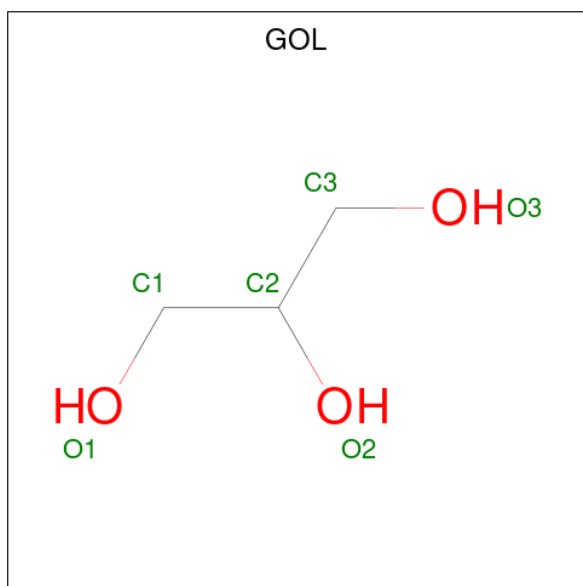


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



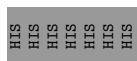
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	504	Total	O	0	0
			504	504		

Note EDS failed to run properly.

- Molecule 1: Maltodextrin-binding protein, Reversion-inducing cysteine-rich protein with Kazal motifs fusion



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	80.40Å 110.22Å 57.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.82 – 1.65	Depositor
% Data completeness (in resolution range)	99.6 (57.82-1.65)	Depositor
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 1.65Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.156 , 0.177	Depositor
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.376	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7290	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% 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: SO4, GLC, ZN, 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	0.45	3/3486 (0.1%)	0.57	0/4739

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	433	GLU	CD-OE2	-8.23	1.16	1.25
1	A	433	GLU	CD-OE1	-7.30	1.17	1.25
1	A	417	CYS	CB-SG	-5.21	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	401	MET	Mainchain

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	3377	3344	3344	13	1
2	B	23	21	21	0	0
3	A	5	0	0	0	0
4	A	2	0	0	0	0
5	A	6	8	8	0	0
6	A	504	0	0	2	0
All	All	3917	3373	3373	13	1

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 2.

All (13) 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:374:MET:HE3	6:A:1011:HOH:O	1.95	0.65
1:A:36:LYS:HD2	1:A:37:VAL:N	2.22	0.54
1:A:376:ASN:OD1	1:A:378:THR:OG1	2.24	0.52
1:A:70:GLY:HA3	1:A:334:ASN:O	2.11	0.50
1:A:36:LYS:HD2	1:A:37:VAL:H	1.75	0.50
1:A:398:ARG:HA	1:A:401:MET:HE2	1.96	0.47
1:A:140:GLU:OE1	1:A:144:LYS:NZ	2.33	0.47
1:A:64:TRP:CD1	1:A:68:ARG:HG3	2.50	0.47
1:A:402[A]:SER:OG	1:A:404:LYS:HD2	2.17	0.45
1:A:231:PRO:HA	1:A:234:TRP:CE2	2.52	0.44
1:A:159[B]:THR:HG23	6:A:618:HOH:O	2.17	0.44
1:A:397:LYS:O	1:A:401:MET:HG3	2.19	0.43
1:A:197:LEU:HD11	1:A:206:MET:CE	2.51	0.41

All (1) 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:315:LYS:HZ2	1:A:435:SER:O[1_556]	1.57	0.03

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	439/447 (98%)	433 (99%)	6 (1%)	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	354/358 (99%)	349 (99%)	5 (1%)	62	43

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	258[A]	LYS
1	A	258[B]	LYS
1	A	260	PHE
1	A	375	ARG

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

5.3.3 RNA [i](#)

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 ⓘ

2 monosaccharides 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	$\# Z > 2$
2	GLC	B	1	2	12,12,12	0.39	0	17,17,17	0.53	0
2	GLC	B	2	2	11,11,12	0.49	0	15,15,17	0.91	1 (6%)

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	GLC	B	1	2	-	0/2/22/22	0/1/1/1
2	GLC	B	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	GLC	C1-O5-C5	2.52	115.56	112.19

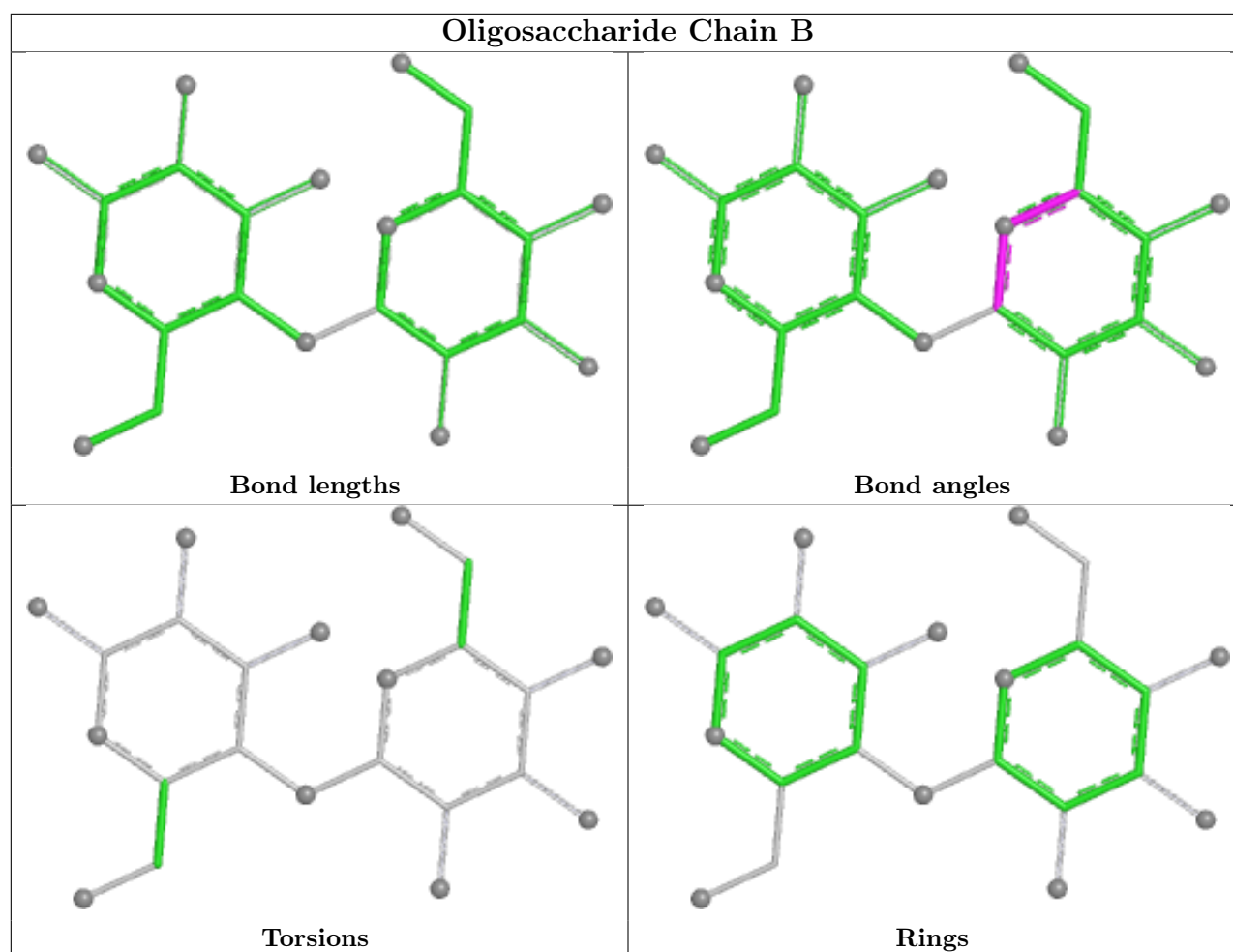
There are no chirality outliers.

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 oligosaccharide.



5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	502	-	4,4,4	0.26	0	6,6,6	0.24	0
5	GOL	A	505	-	5,5,5	0.52	0	5,5,5	0.75	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	505	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

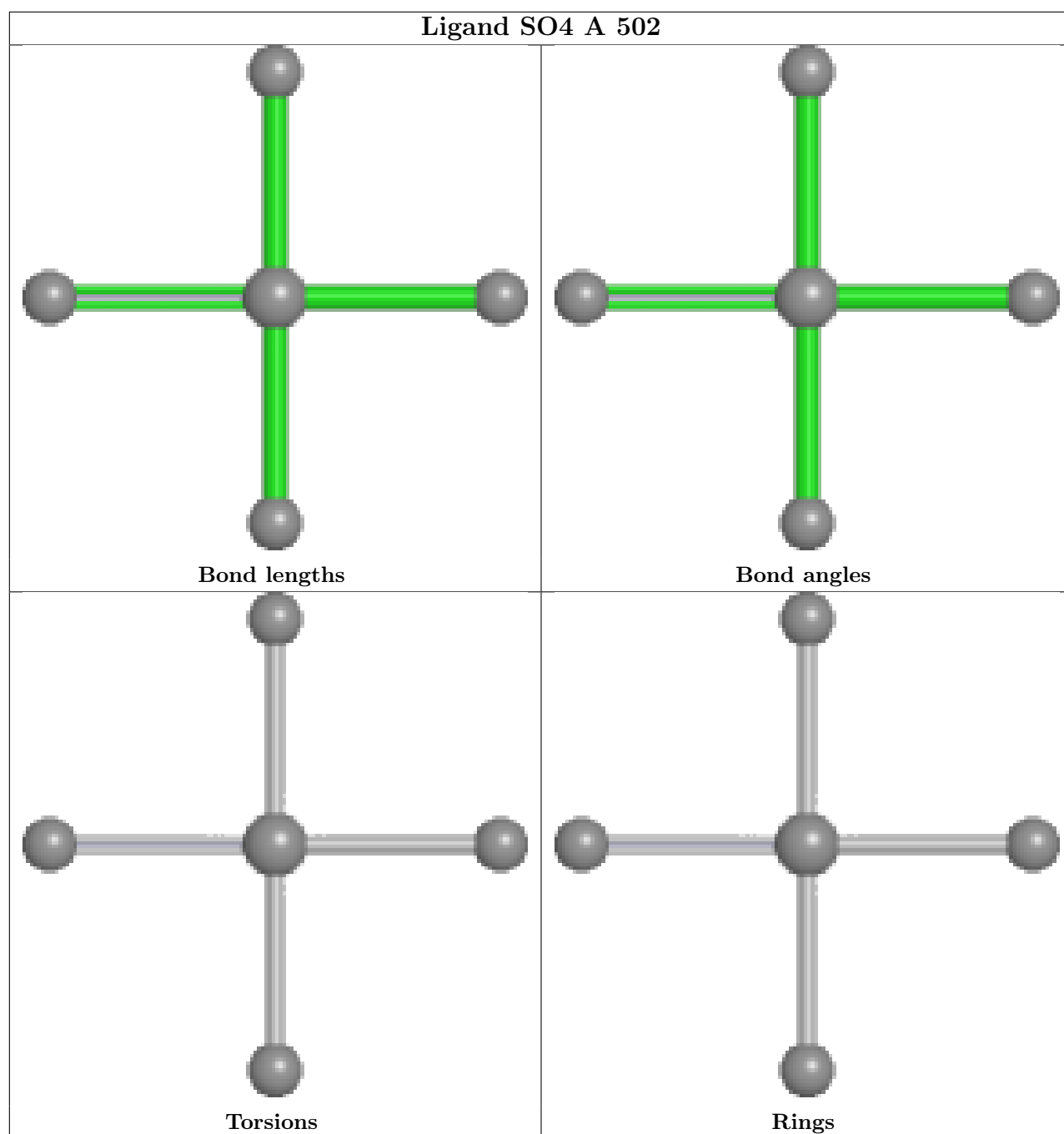
All (2) torsion outliers are listed below:

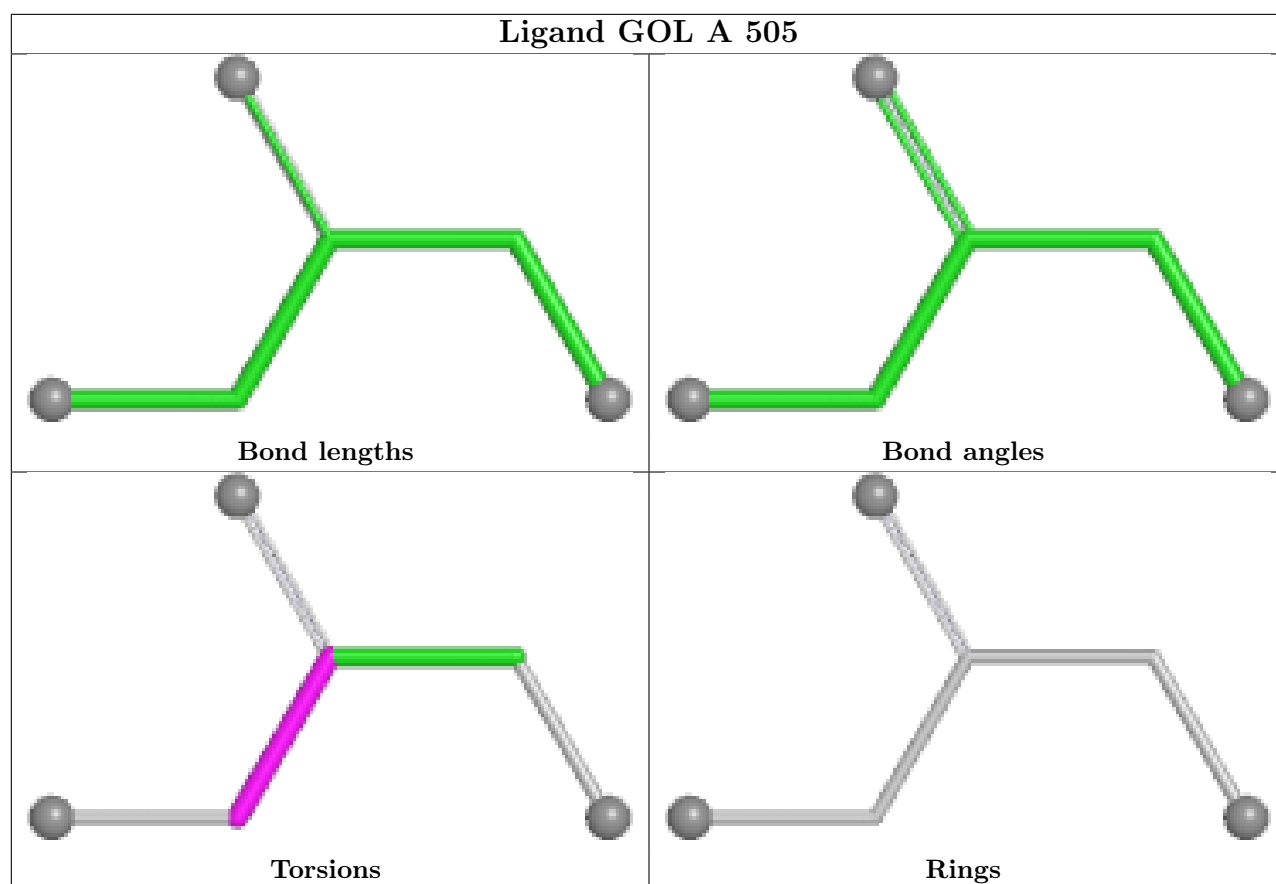
Mol	Chain	Res	Type	Atoms
5	A	505	GOL	C1-C2-C3-O3
5	A	505	GOL	O2-C2-C3-O3

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

EDS failed to run properly - this section is therefore empty.

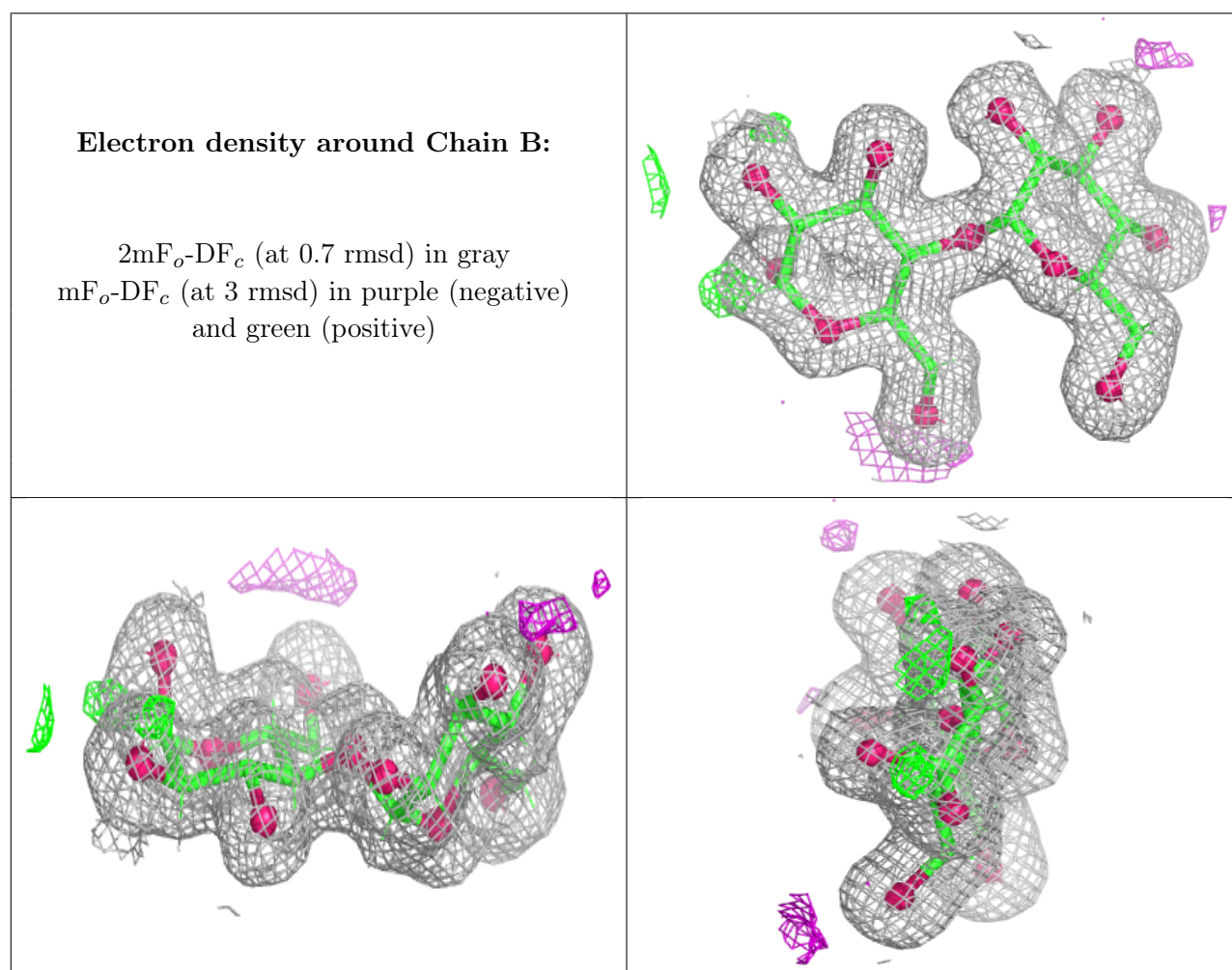
6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

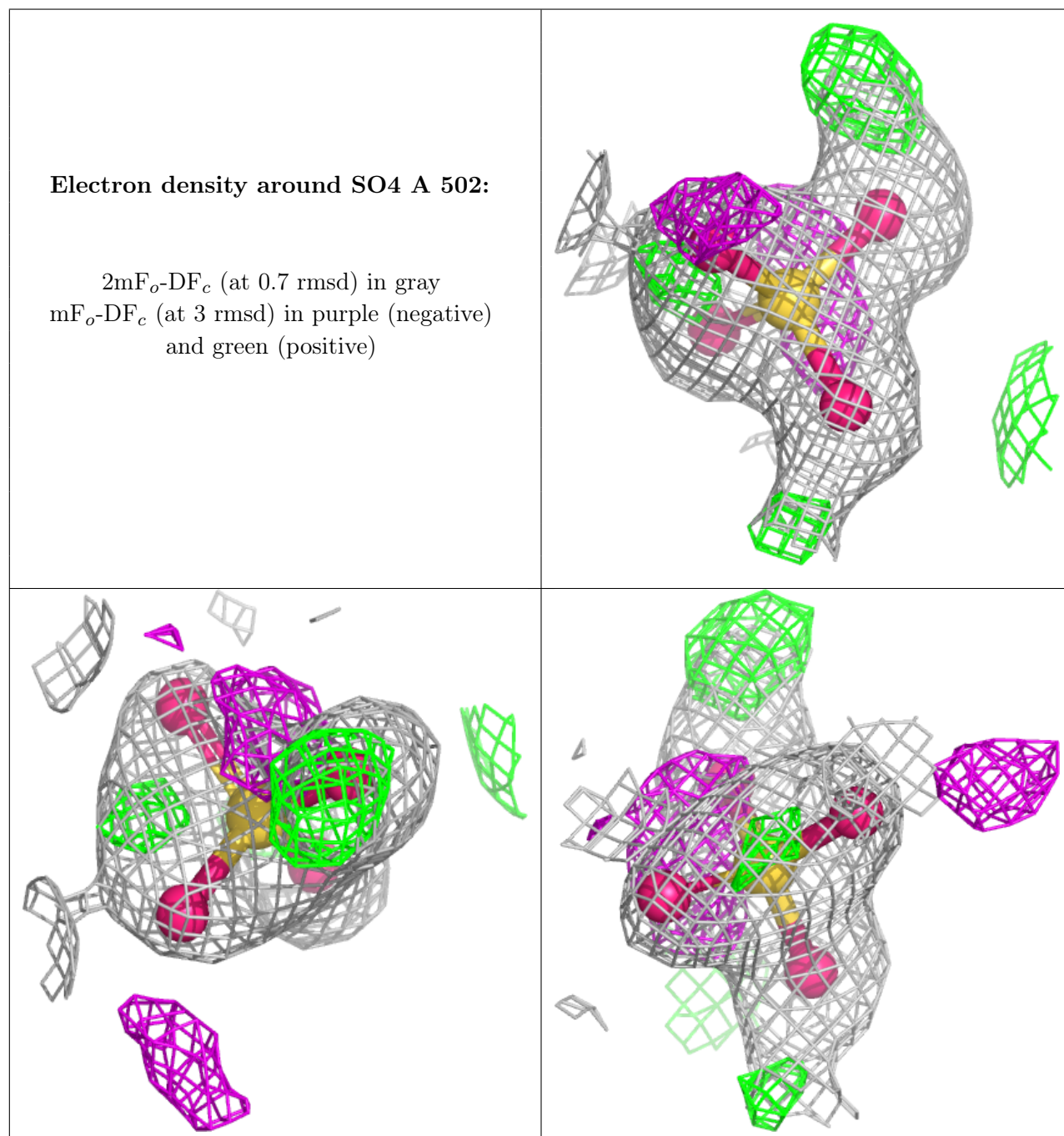
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands ⓘ

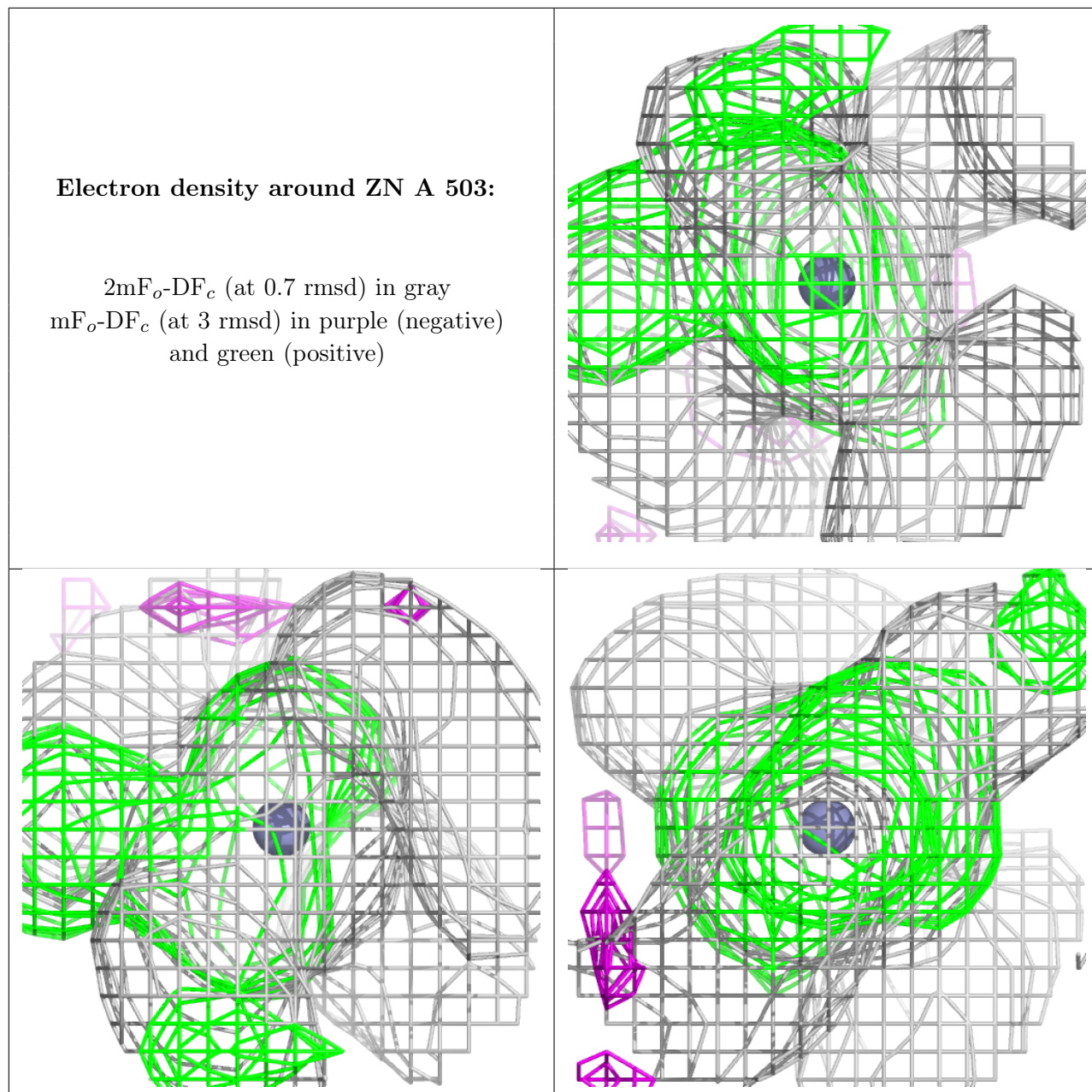
EDS failed to run properly - this section is therefore empty.

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.



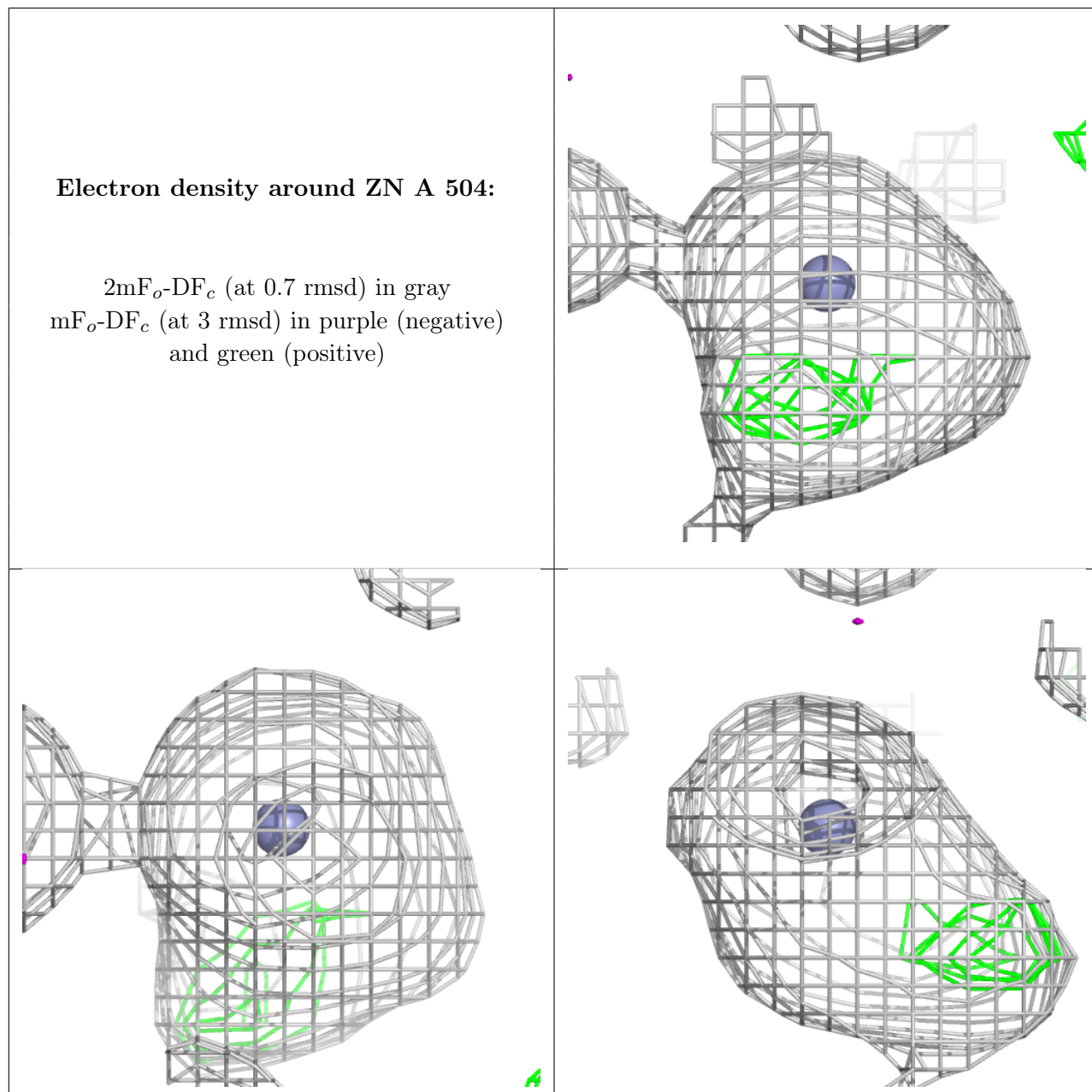
Electron density around ZN A 503:

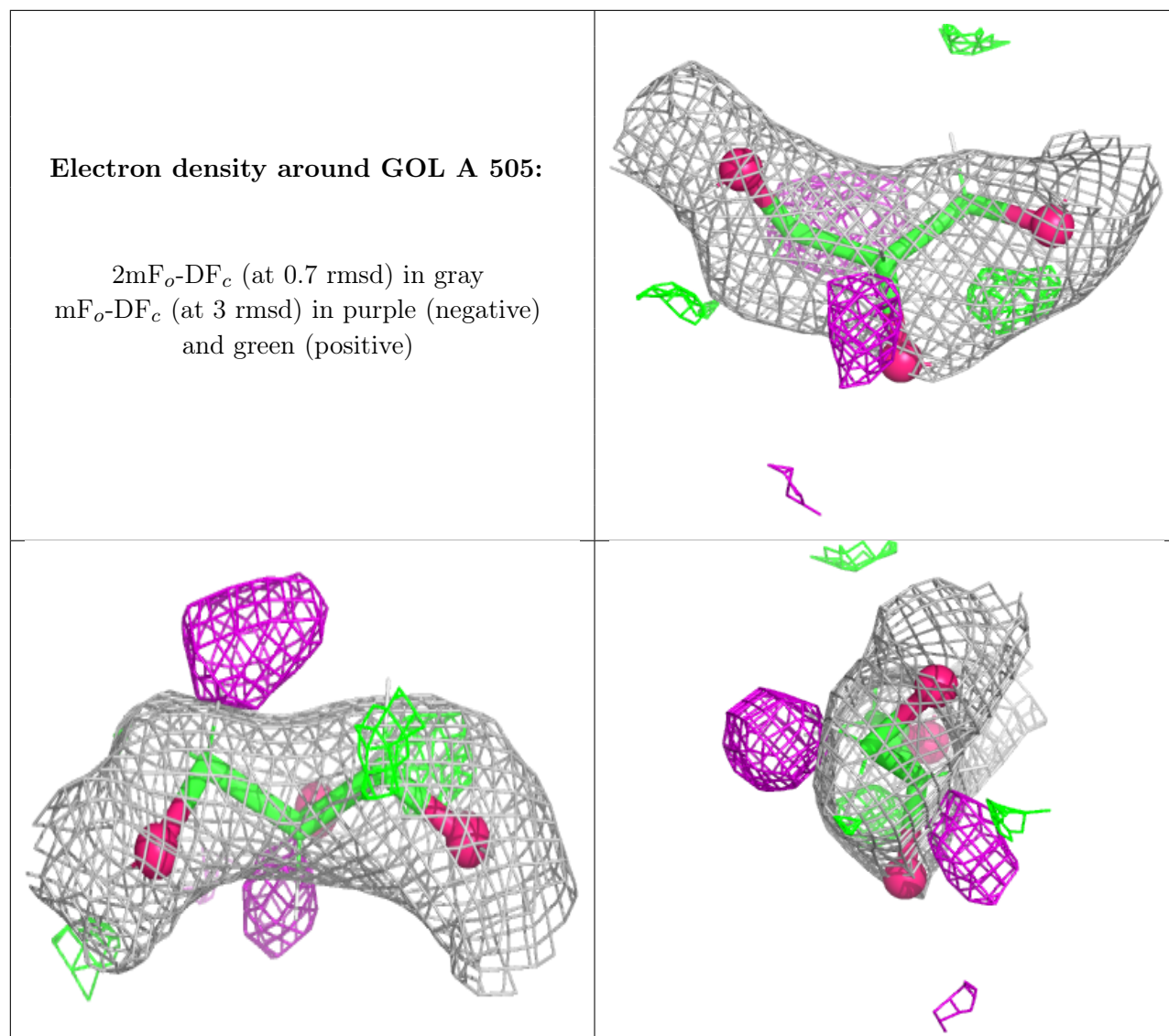
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN 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 [i](#)

EDS failed to run properly - this section is therefore empty.