



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 25, 2022 – 05:05 pm BST

PDB ID : 7ZCN
Title : Nitrite-bound MSOX movie series dataset 1 (0.8 MGy) of the copper nitrite reductase from Bradyrhizobium sp. ORS 375 (two-domain) - nitrite (start)
Authors : Rose, S.L.; Baba, S.; Okumura, H.; Antonyuk, S.V.; Sasaki, D.; Tosha, T.; Kumasaka, T.; Eady, R.R.; Yamamoto, M.; Hasnain, S.S.
Deposited on : 2022-03-28
Resolution : 1.19 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.29
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

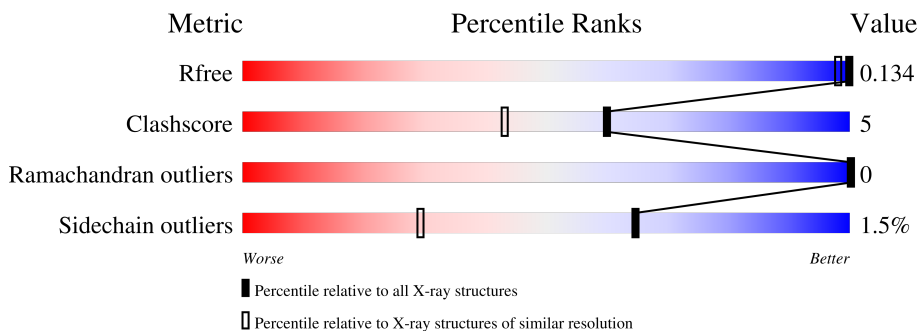
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.19 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	1223 (1.22-1.18)
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	350	89% (green), 8% (yellow), 3% (orange), 2% (red), 2% (grey)
2	E	2	100% (yellow)
2	F	2	100% (orange)

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FRU	F	2[A]	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3514 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.

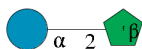
- Molecule 1 is a protein called Copper-containing nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	341	2814	1811	482	506	15	1	38	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP H0SLX7
A	342	GLU	-	expression tag	UNP H0SLX7
A	343	ASN	-	expression tag	UNP H0SLX7
A	344	LEU	-	expression tag	UNP H0SLX7
A	345	TYR	-	expression tag	UNP H0SLX7
A	346	PHE	-	expression tag	UNP H0SLX7
A	347	GLN	-	expression tag	UNP H0SLX7
A	348	GLY	-	expression tag	UNP H0SLX7
A	349	GLY	-	expression tag	UNP H0SLX7
A	350	SER	-	expression tag	UNP H0SLX7

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	E	2	23	12	11	0	2	0
2	F	2	23	12	11	0	2	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

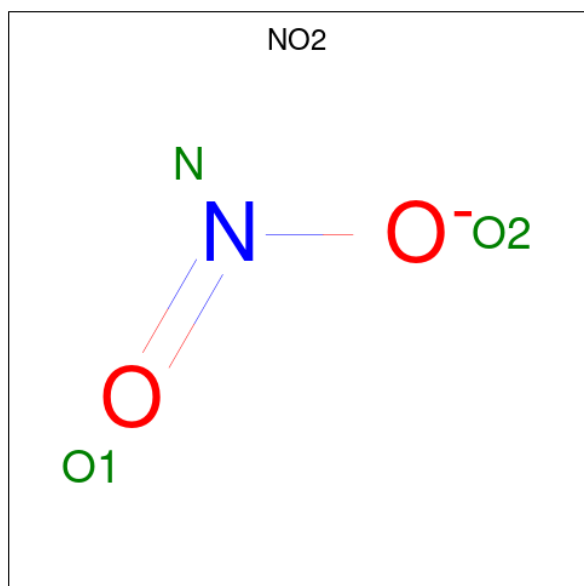


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	1
3	A	1	Total O S 5 4 1	0	1
3	A	1	Total O S 5 4 1	0	1
3	A	1	Total O S 5 4 1	0	1
3	A	1	Total O S 10 8 2	0	1
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	1

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is NITRITE ION (three-letter code: NO2) (formula: NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	N	O	0	1
			3	1	2		
5	A	1	Total	N	O	0	0
			3	1	2		
5	A	1	Total	N	O	0	1
			6	2	4		
5	A	1	Total	N	O	0	0
			3	1	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	1
6	A	1	Total C O 6 3 3	2	0
6	A	1	Total C O 12 6 6	0	1


- Molecule 7 is water.

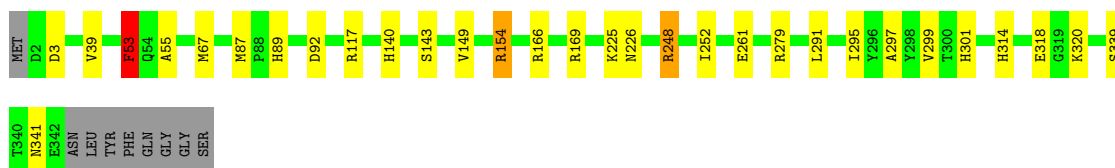
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	519	Total O 553 553	0	98

3 Residue-property plots [i](#)

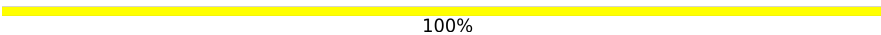
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: Copper-containing nitrite reductase

Chain A:  89% 8% ..



- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain E:  100%

GLC1
FRU2

- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain F:  100%

GLC1
FRU2

4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	106.72Å 106.72Å 106.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.47 – 1.19 75.47 – 1.19	Depositor EDS
% Data completeness (in resolution range)	99.8 (75.47-1.19) 99.8 (75.47-1.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 1.19Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.108 , 0.134 0.109 , 0.134	Depositor DCC
R_{free} test set	6414 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	12.8	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.027 for l,-k,h	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	3514	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: NO2, SO4, GLC, GOL, FRU, CU

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	0.78	2/2990 (0.1%)	1.02	19/4059 (0.5%)

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	318	GLU	CD-OE1	-7.19	1.17	1.25
1	A	117	ARG	CD-NE	-7.09	1.34	1.46

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	117	ARG	NE-CZ-NH1	-10.63	114.99	120.30
1	A	117	ARG	NE-CZ-NH2	9.69	125.14	120.30
1	A	154[A]	ARG	CG-CD-NE	-8.28	94.42	111.80
1	A	154[B]	ARG	CG-CD-NE	-8.28	94.42	111.80
1	A	169[A]	ARG	NE-CZ-NH2	-8.02	116.29	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	299	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	A	301	HIS	Peptide

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	2814	0	2845	21	0
2	E	23	0	20	0	0
2	F	23	0	21	7	0
3	A	60	0	0	1	0
4	A	2	0	0	0	0
5	A	15	0	0	1	0
6	A	24	0	31	0	0
7	A	553	0	0	3	0
All	All	3514	0	2917	27	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 5.

The worst 5 of 27 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)
2:F:2[A]:FRU:C3	2:F:2[A]:FRU:O3	1.67	1.40
2:F:1[A]:GLC:H3	2:F:2[A]:FRU:H11	1.46	0.94
1:A:154[B]:ARG:HD2	7:A:757:HOH:O	1.81	0.80
2:F:2[A]:FRU:O3	2:F:2[A]:FRU:H3	1.76	0.80
1:A:252:ILE:HD12	1:A:297:ALA:HB3	1.77	0.67

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	375/350 (107%)	368 (98%)	7 (2%)	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	310/284 (109%)	304 (98%)	6 (2%)	57 19

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	248	ARG
1	A	261[A]	GLU
1	A	261[B]	GLU
1	A	53[A]	PHE
1	A	3	ASP

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 [i](#)

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

5.5 Carbohydrates i

4 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	E	1[A]	2	11,11,12	1.84	1 (9%)	15,15,17	3.03	5 (33%)
2	FRU	E	2[A]	2	11,12,12	1.64	3 (27%)	10,18,18	3.31	5 (50%)
2	GLC	F	1[A]	2	11,11,12	3.35	6 (54%)	15,15,17	6.14	11 (73%)
2	FRU	F	2[A]	2	11,12,12	4.70	6 (54%)	10,18,18	4.70	7 (70%)

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	E	1[A]	2	-	0/2/19/22	0/1/1/1
2	FRU	E	2[A]	2	-	1/5/24/24	0/1/1/1
2	GLC	F	1[A]	2	-	1/2/19/22	0/1/1/1
2	FRU	F	2[A]	2	-	5/5/24/24	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2[A]	FRU	O3-C3	12.57	1.67	1.42
2	F	1[A]	GLC	C4-C5	7.63	1.69	1.53
2	F	2[A]	FRU	O4-C4	5.90	1.56	1.43
2	F	1[A]	GLC	O2-C2	5.14	1.54	1.43
2	F	2[A]	FRU	C4-C3	4.84	1.73	1.52

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1[A]	GLC	C1-C2-C3	-12.85	93.88	109.67
2	F	1[A]	GLC	C3-C4-C5	9.94	127.98	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2[A]	FRU	O4-C4-C3	9.15	139.57	112.15
2	F	2[A]	FRU	O3-C3-C4	9.12	144.83	113.32
2	F	1[A]	GLC	O2-C2-C3	8.19	126.54	110.14

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

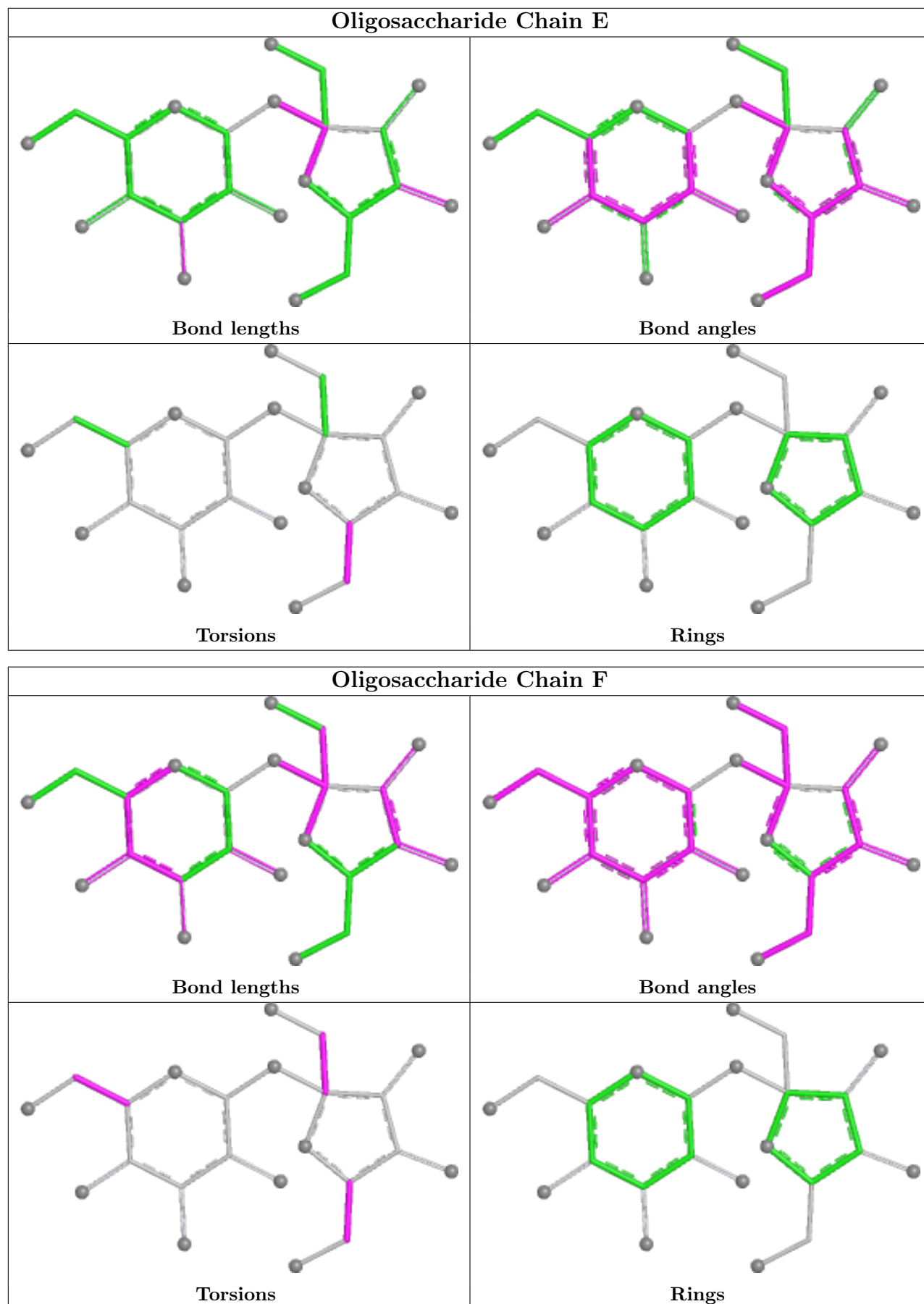
Mol	Chain	Res	Type	Atoms
2	F	2[A]	FRU	O1-C1-C2-C3
2	F	2[A]	FRU	O1-C1-C2-O2
2	F	2[A]	FRU	O1-C1-C2-O5
2	F	2[A]	FRU	O5-C5-C6-O6
2	F	2[A]	FRU	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1[A]	GLC	4	0
2	F	2[A]	FRU	6	0

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

Of 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 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
5	NO2	A	419[B]	-	1,2,2	1.11	0	0,1,1	-	-
6	GOL	A	410[A]	-	5,5,5	0.30	0	5,5,5	0.39	0
3	SO4	A	412[A]	-	4,4,4	0.50	0	6,6,6	0.45	0
6	GOL	A	410[B]	-	5,5,5	0.25	0	5,5,5	0.41	0
3	SO4	A	404[A]	-	4,4,4	0.17	0	6,6,6	0.46	0
6	GOL	A	409	-	5,5,5	1.91	1 (20%)	5,5,5	2.02	2 (40%)
3	SO4	A	413[A]	-	4,4,4	0.42	0	6,6,6	0.44	0
3	SO4	A	415	-	4,4,4	0.84	0	6,6,6	1.32	1 (16%)
6	GOL	A	408[A]	-	5,5,5	0.42	0	5,5,5	0.71	0
3	SO4	A	411[A]	-	4,4,4	0.38	0	6,6,6	0.51	0
3	SO4	A	414	-	4,4,4	0.99	0	6,6,6	0.41	0
3	SO4	A	413[B]	-	4,4,4	0.38	0	6,6,6	0.29	0
3	SO4	A	417[B]	-	4,4,4	0.21	0	6,6,6	0.41	0
3	SO4	A	402	-	4,4,4	0.80	0	6,6,6	0.45	0
5	NO2	A	418	-	1,2,2	3.91	1 (100%)	0,1,1	-	-
3	SO4	A	401	-	4,4,4	0.47	0	6,6,6	0.47	0
3	SO4	A	403[A]	-	4,4,4	0.38	0	6,6,6	0.35	0
5	NO2	A	420	-	1,2,2	1.18	0	0,1,1	-	-
5	NO2	A	419[A]	-	1,2,2	1.34	0	0,1,1	-	-
3	SO4	A	416	-	4,4,4	0.32	0	6,6,6	0.17	0
5	NO2	A	407[A]	4	1,2,2	0.06	0	0,1,1	-	-

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
6	GOL	A	409	-	-	1/4/4/4	-
6	GOL	A	408[A]	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	410[A]	-	-	2/4/4/4	-
6	GOL	A	410[B]	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	409	GOL	C3-C2	-4.13	1.34	1.51
5	A	418	NO2	O1-N	3.91	1.42	1.22

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	409	GOL	O2-C2-C3	3.65	125.19	109.12
6	A	409	GOL	O2-C2-C1	2.09	118.31	109.12
3	A	415	SO4	O4-S-O2	-2.09	98.42	109.31

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	408[A]	GOL	O1-C1-C2-O2
6	A	408[A]	GOL	O1-C1-C2-C3
6	A	408[A]	GOL	C1-C2-C3-O3
6	A	409	GOL	O1-C1-C2-C3
6	A	410[A]	GOL	C1-C2-C3-O3

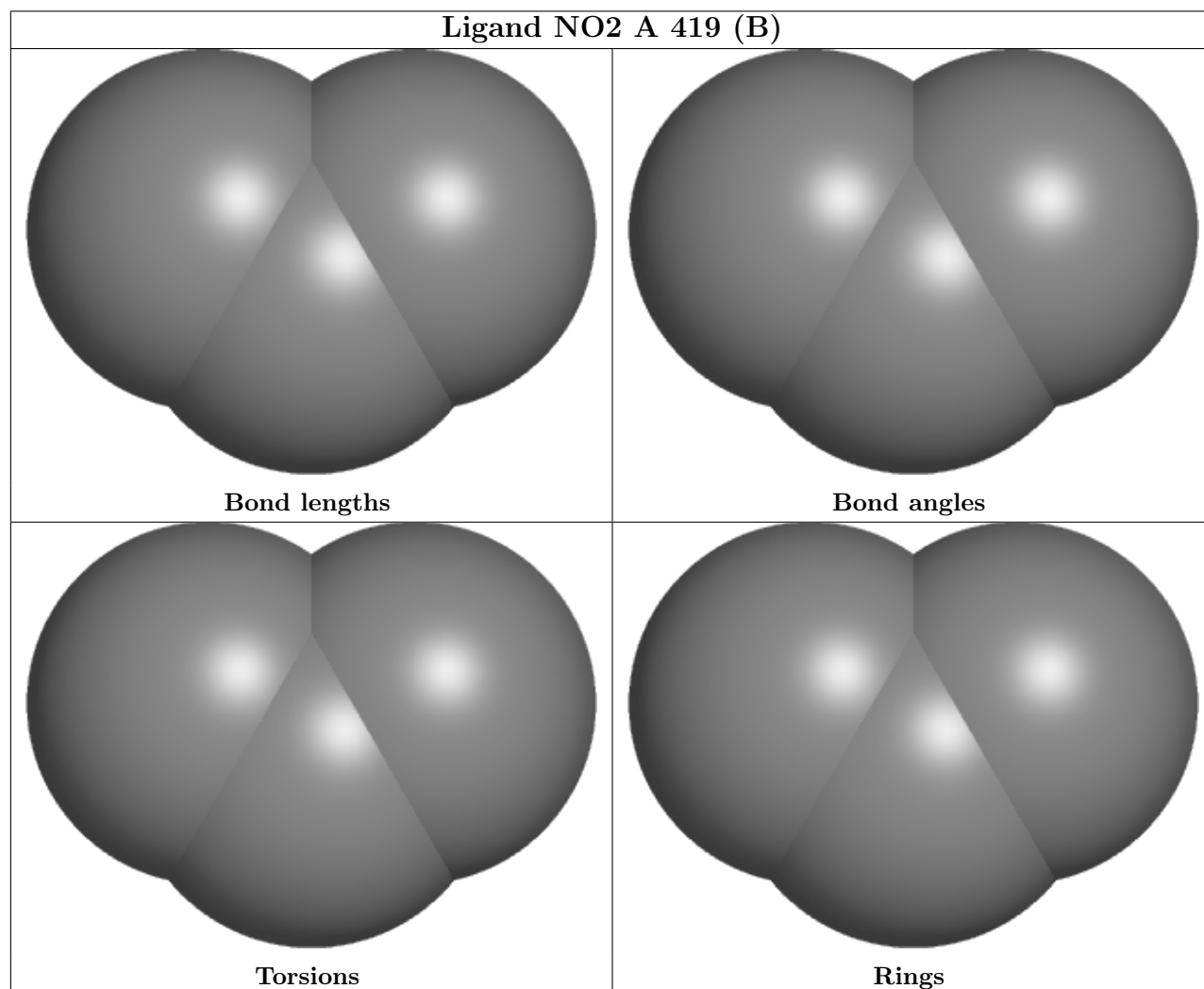
There are no ring outliers.

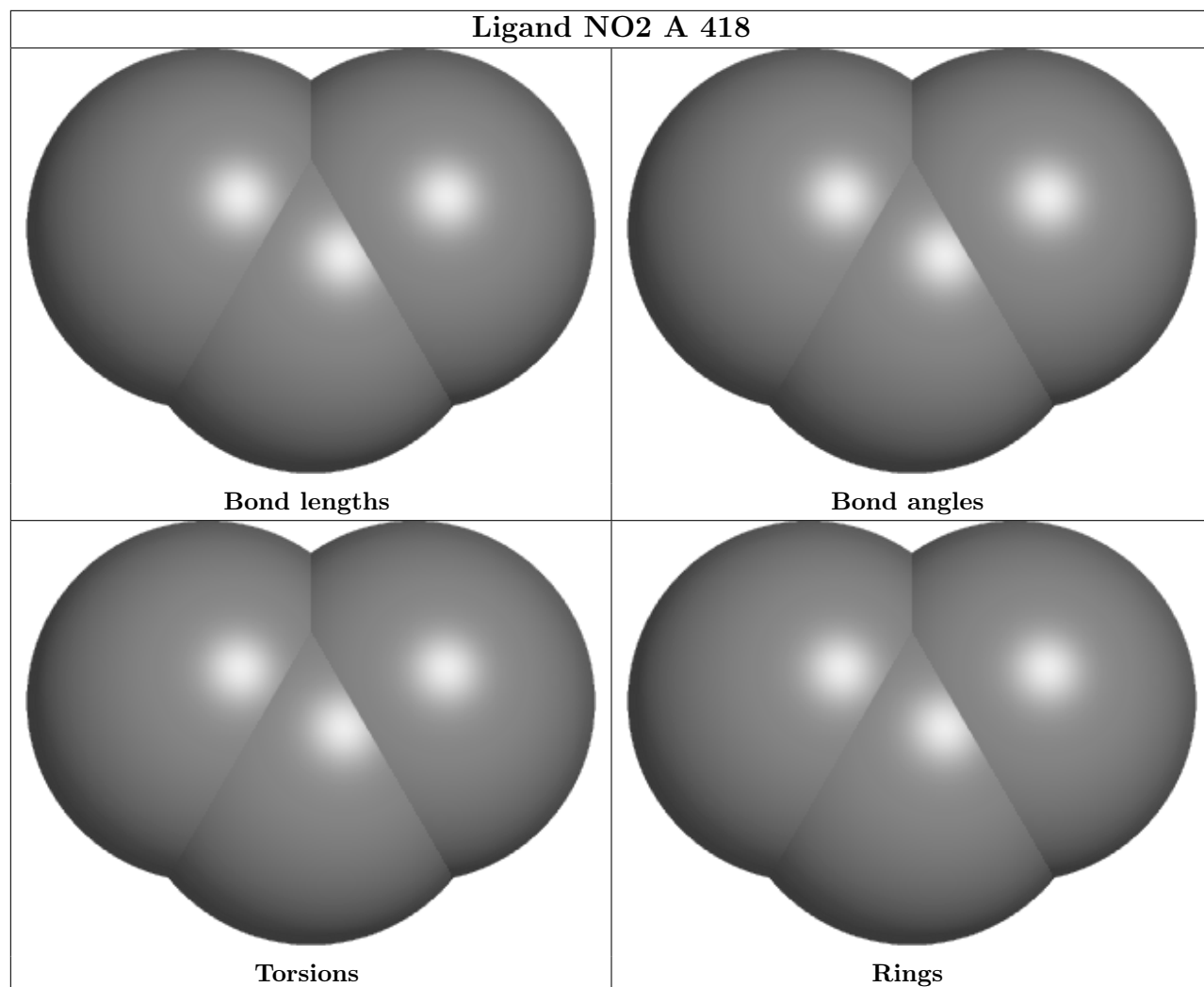
2 monomers are involved in 2 short contacts:

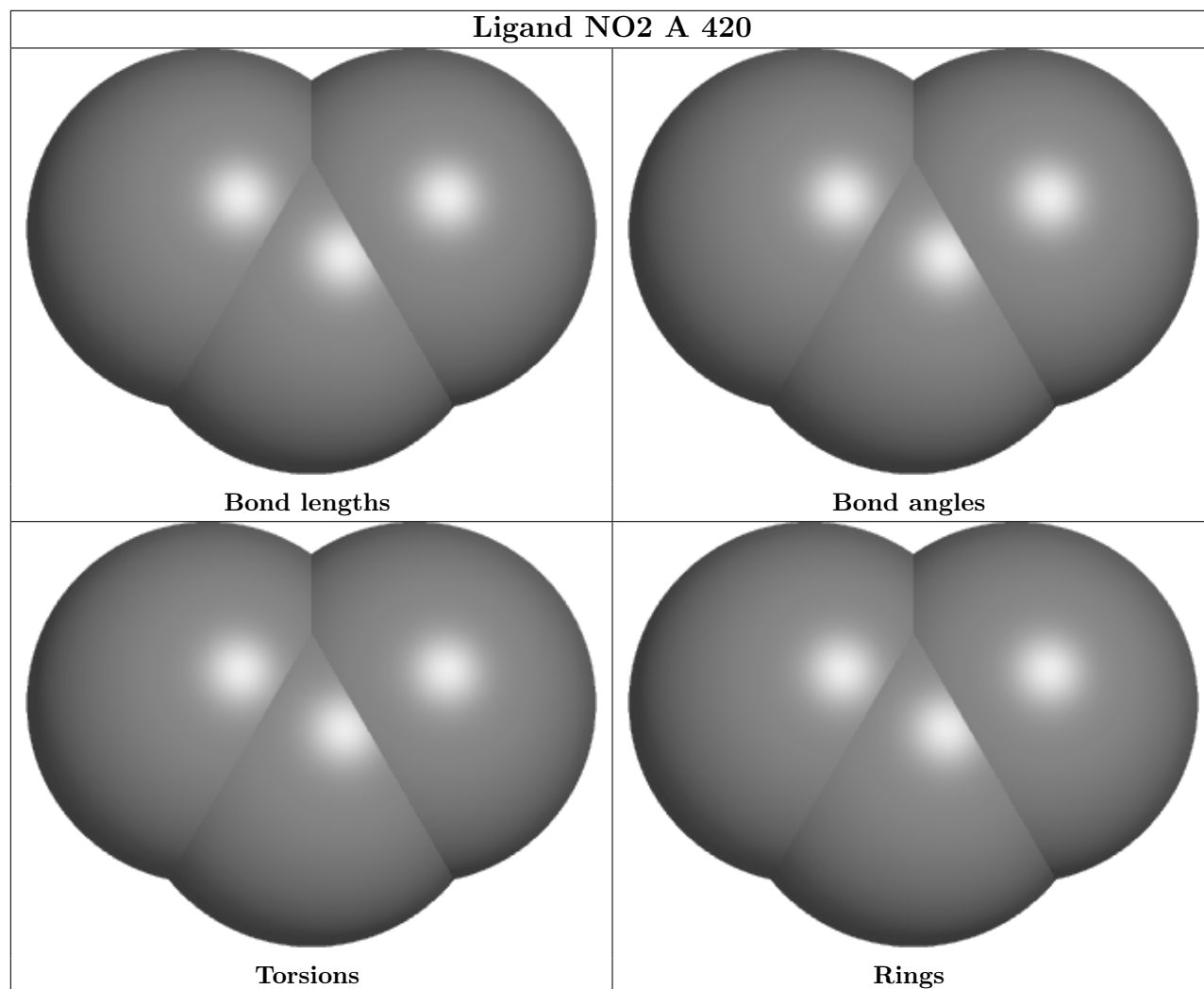
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	414	SO4	1	0
5	A	407[A]	NO2	1	0

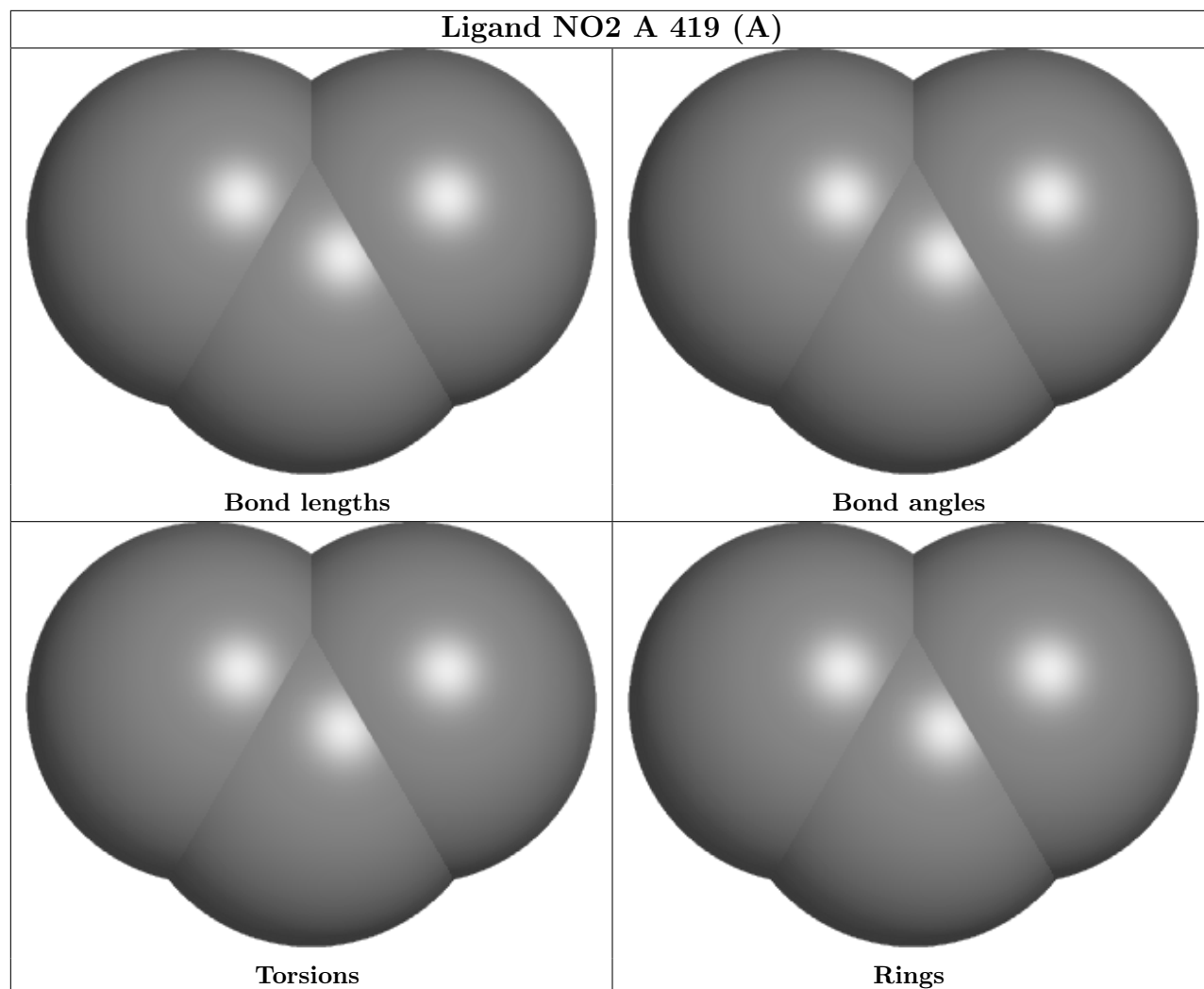
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

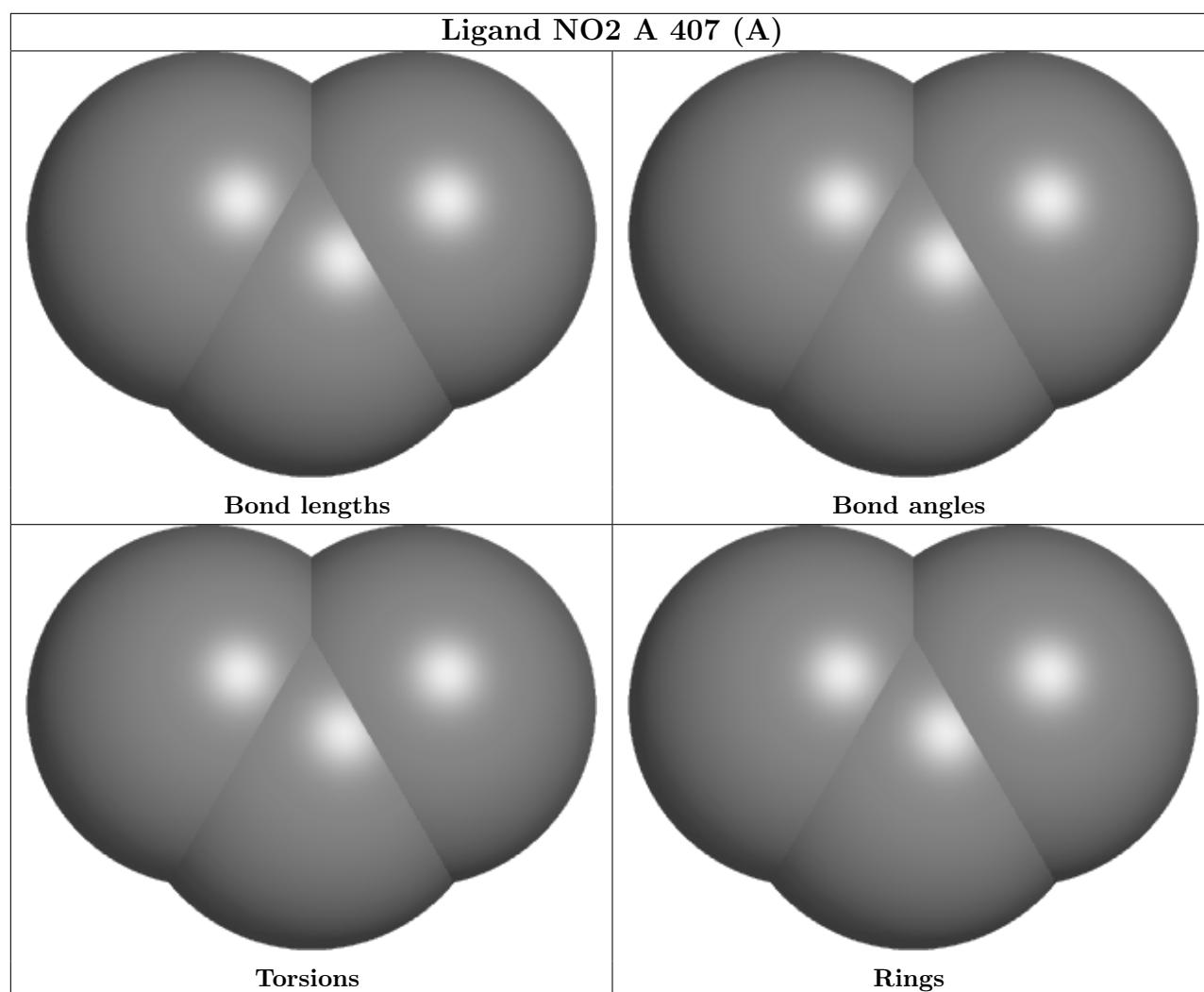
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

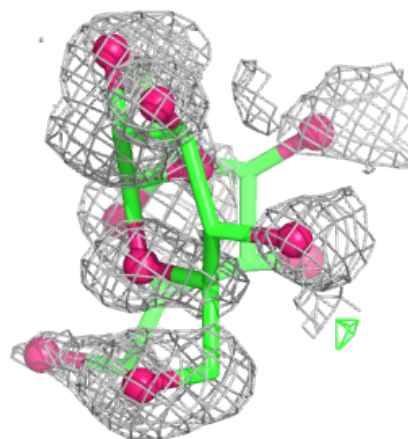
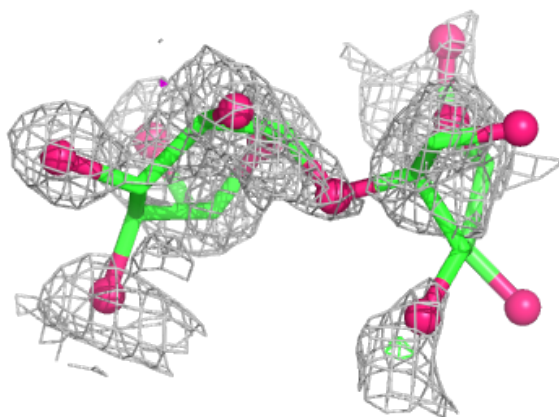
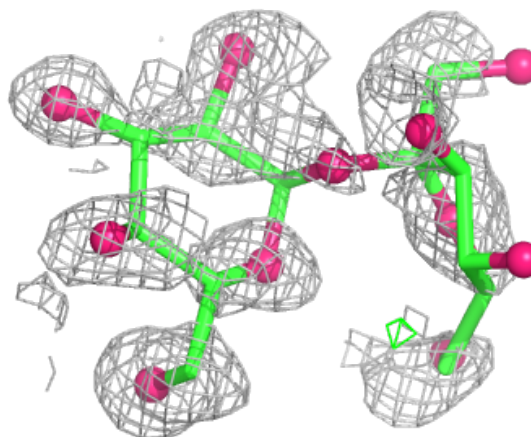
6.3 Carbohydrates

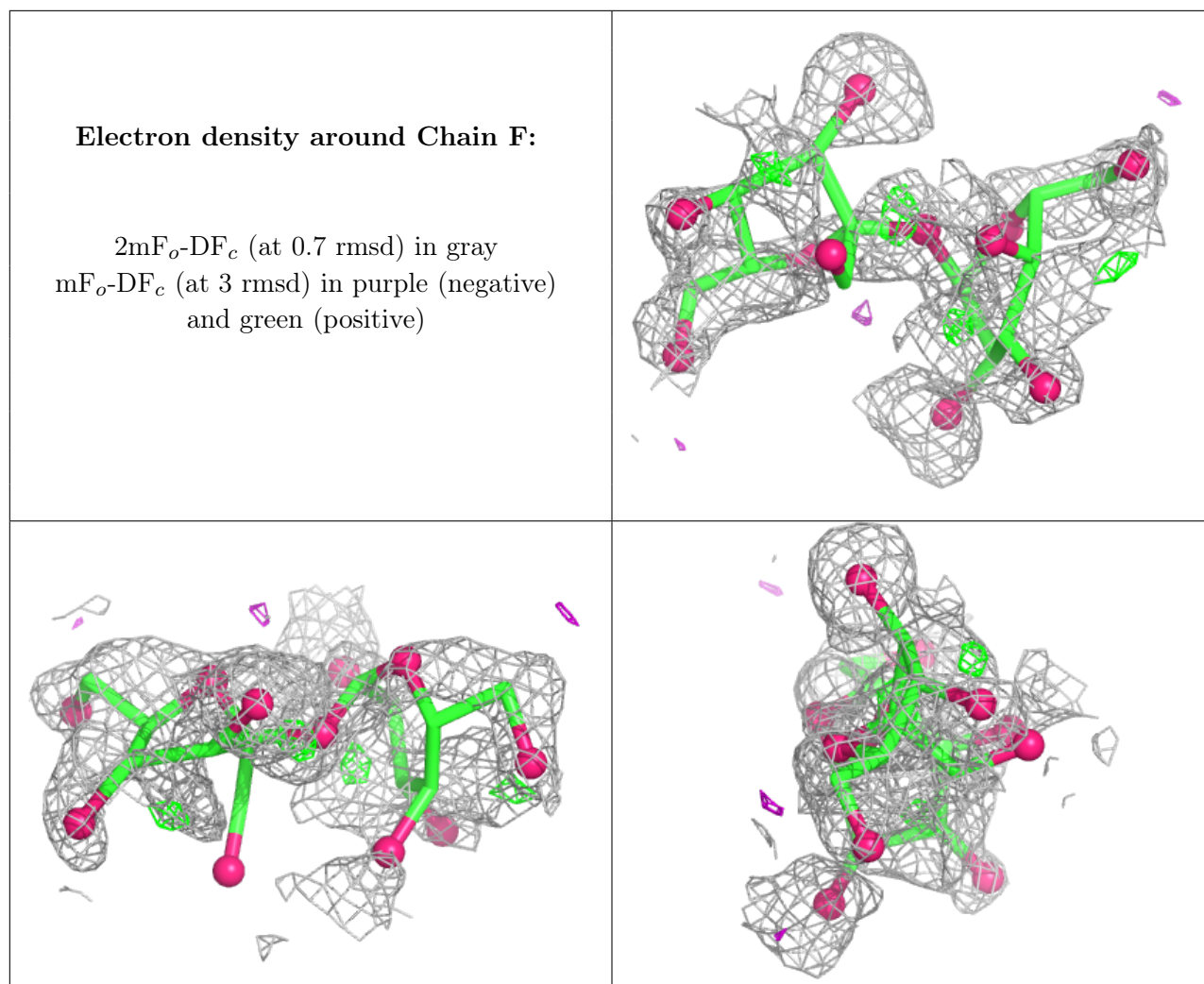
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

Electron density around Chain E:

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





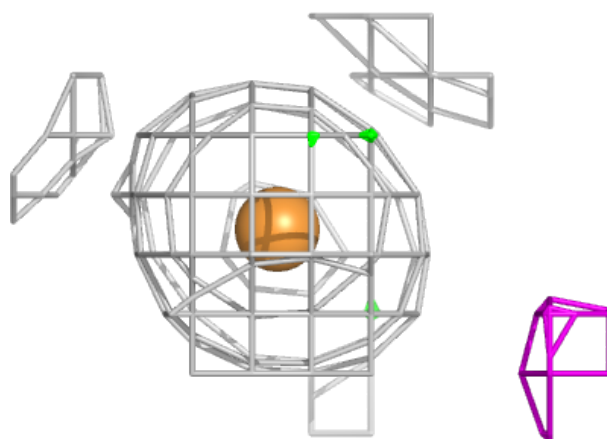
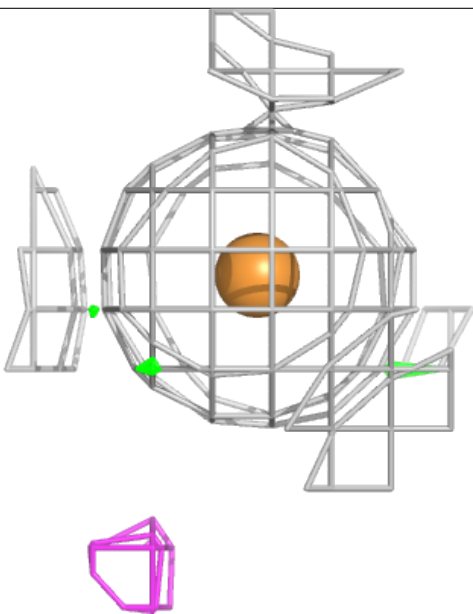
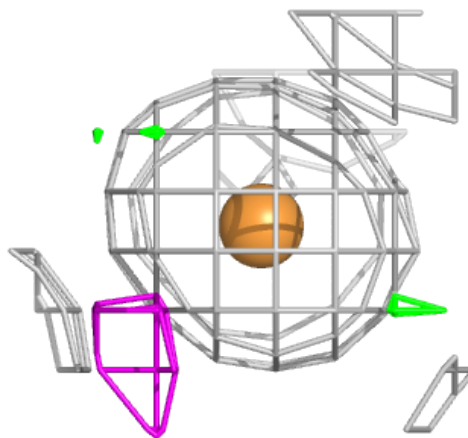
6.4 Ligands [i](#)

Unable to reproduce the depositor's R factor - 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.

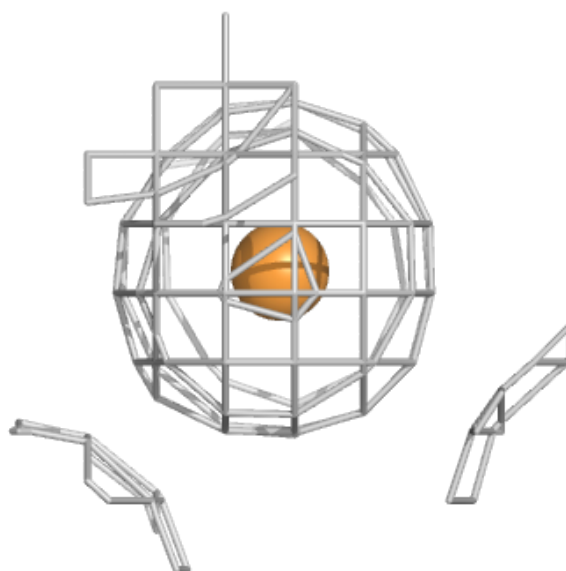
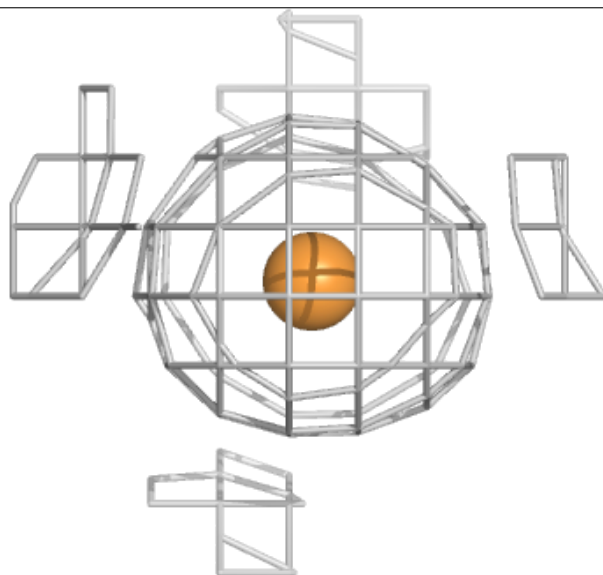
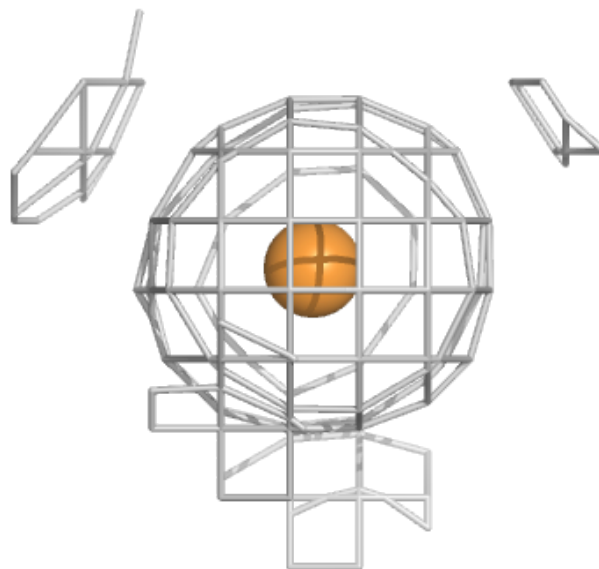
Electron density around CU A 405:

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



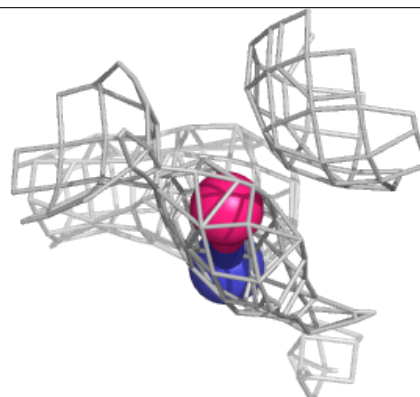
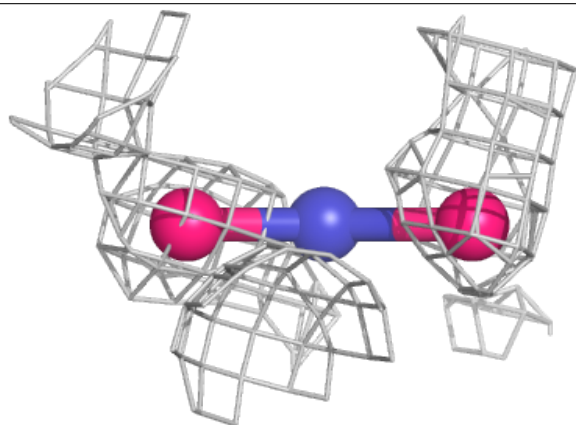
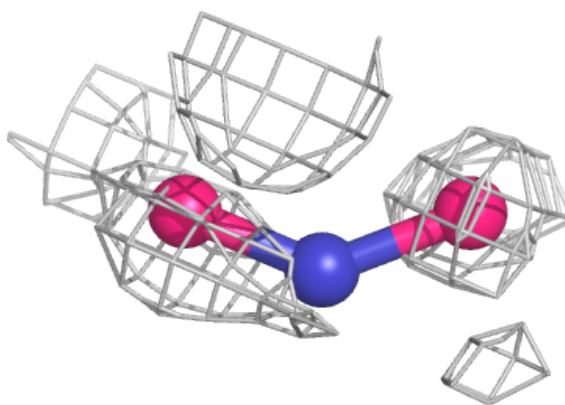
Electron density around CU A 406:

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

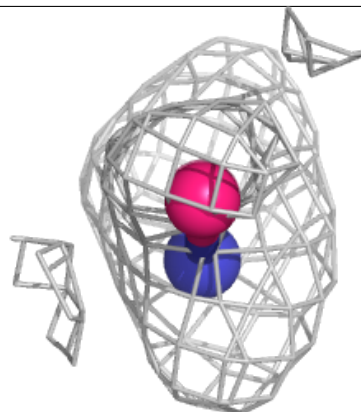
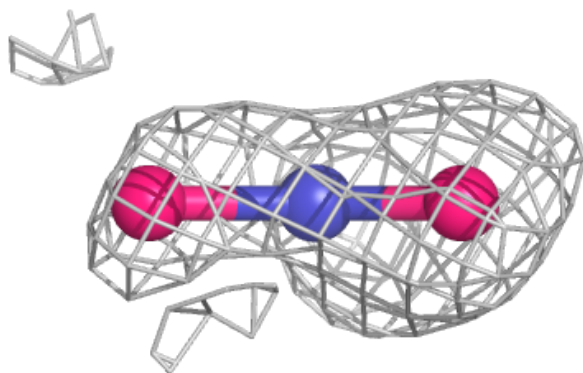
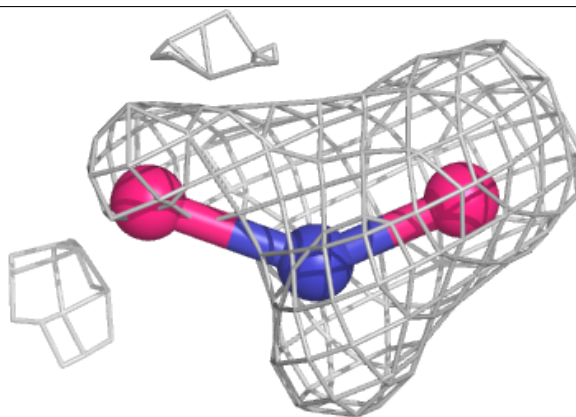


Electron density around NO2 A 407 (A):

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

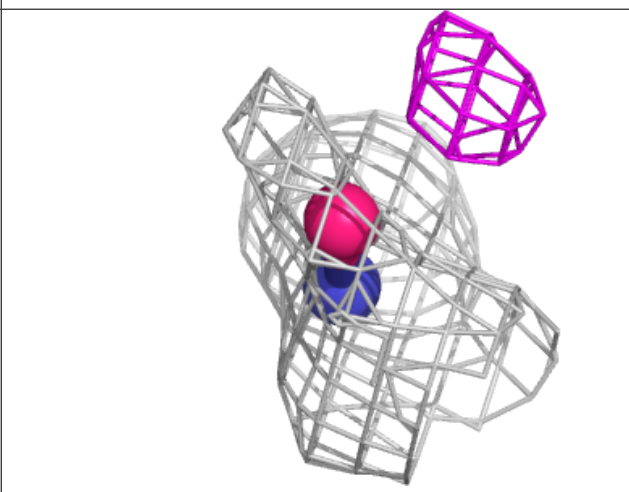
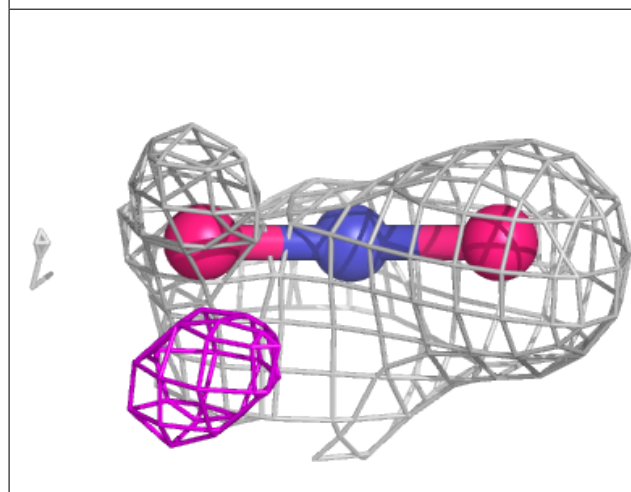
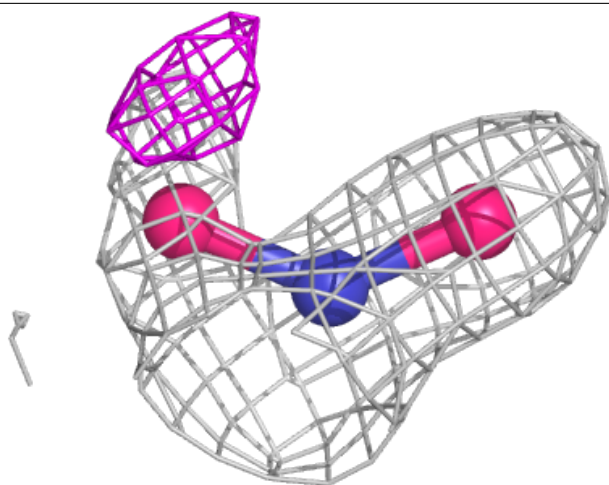
**Electron density around NO2 A 418:**

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



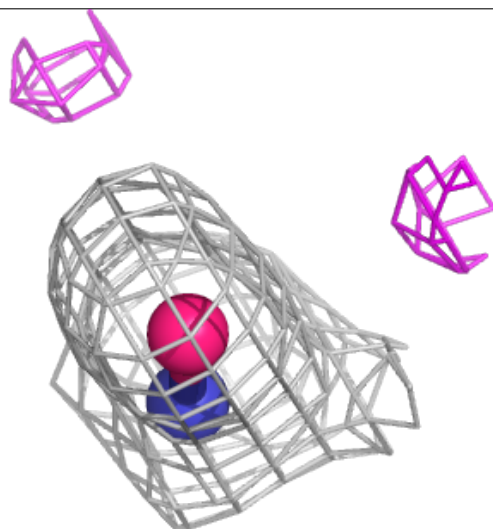
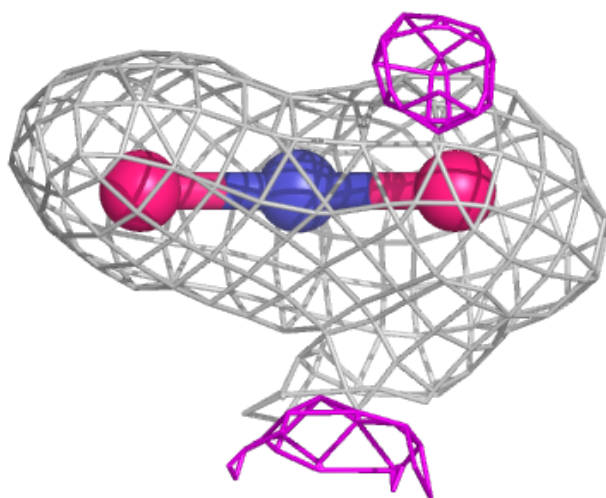
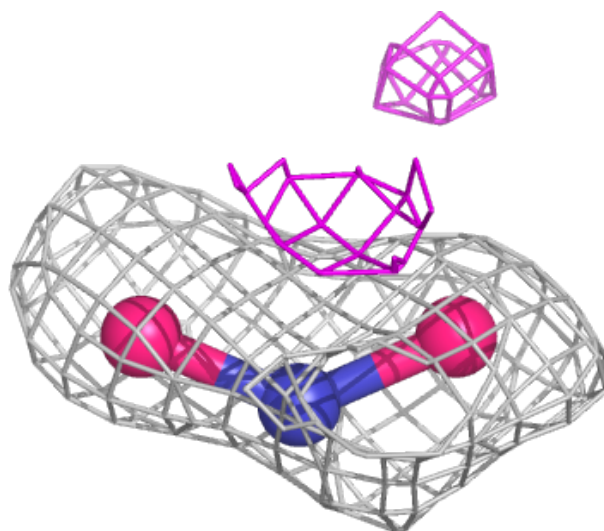
Electron density around NO2 A 419 (A):

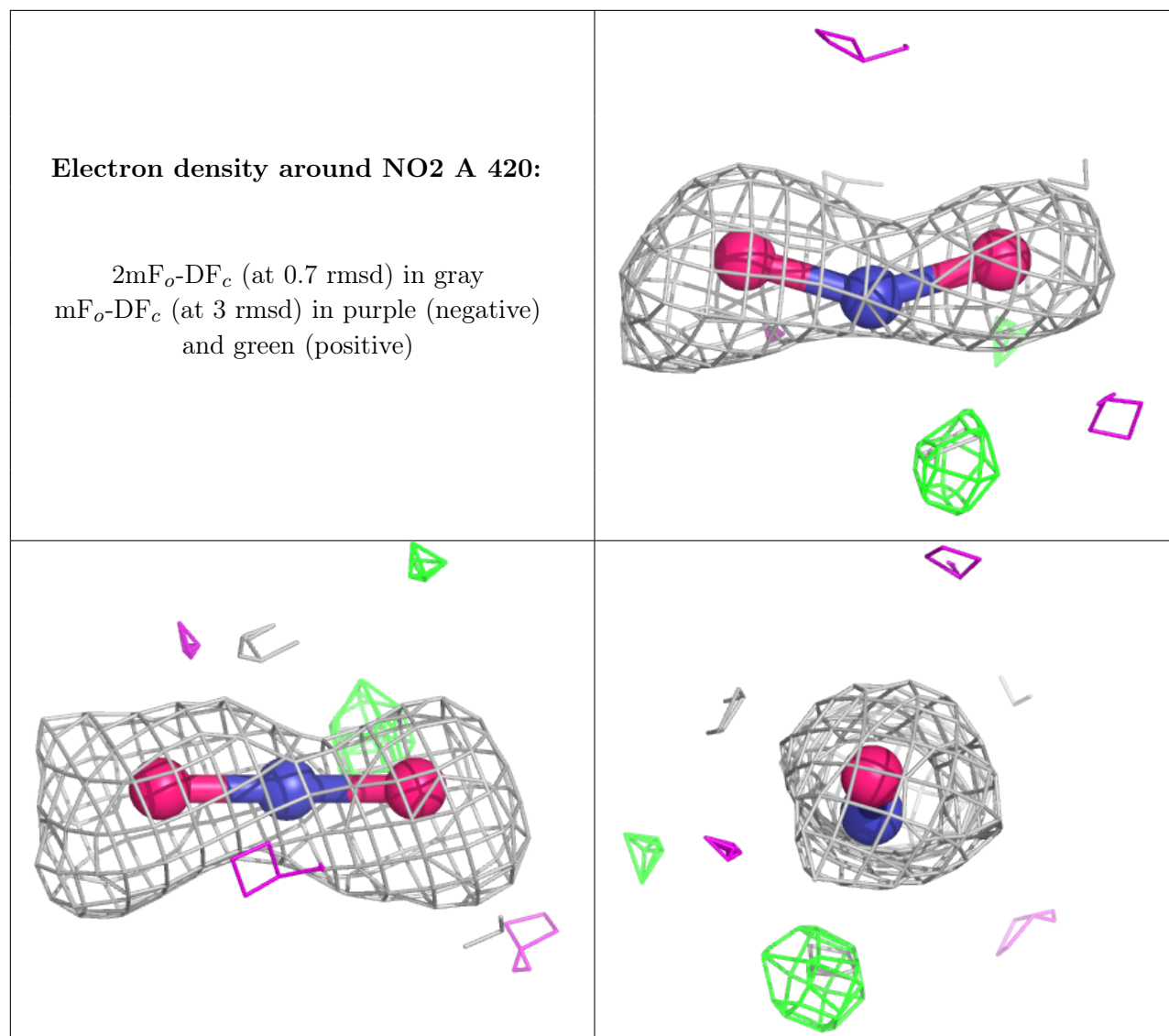
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NO2 A 419 (B):

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





6.5 Other polymers [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.