WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 15, 2023 – 02:43 PM EDT

PDB ID	:	8DIN
Title	:	The complex structure between human IgG1 Fc and its high affinity receptor FcgRI H174R variant
Authors	:	Lu, J.; Sun, P.D.
Deposited on	:	2022-06-29
Resolution	:	2.50 Å(reported)

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

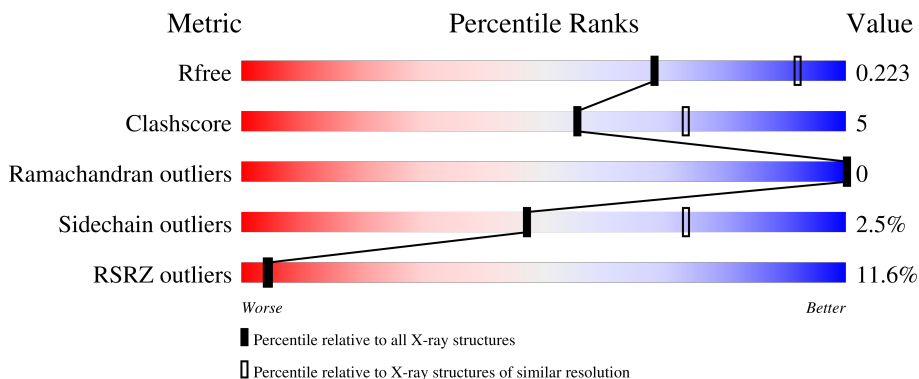|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.50 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		0.223
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		2.5%
RSRZ outliers		11.6%

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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	219	2% / 90% / 6% ··
1	B	219	4% / 91% / 7% ·
2	C	277	25% / 74% / 17% ·· 5%
3	D	9	44% / 56%
3	E	9	22% / 78%

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
3	NAG	D	8	-	-	-	X

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 5839 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 Ig gamma-1 Fc chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	215	Total 1712	C 1091	N 287	O 328	S 6	0	0	0
1	A	214	Total 1710	C 1090	N 286	O 328	S 6	3	1	0

- Molecule 2 is a protein called High affinity immunoglobulin gamma Fc receptor I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	262	Total 2069	C 1312	N 359	O 389	S 9	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ALA	-	expression tag	UNP P12314
C	20	PRO	-	expression tag	UNP P12314
C	25	LYS	THR	conflict	UNP P12314
C	38	SER	THR	conflict	UNP P12314
C	46	PRO	LEU	conflict	UNP P12314
C	63	ILE	THR	conflict	UNP P12314
C	69	THR	SER	conflict	UNP P12314
C	71	HIS	ARG	conflict	UNP P12314
C	77	GLU	VAL	conflict	UNP P12314
C	78	ASP	ASN	conflict	UNP P12314
C	100	VAL	ILE	conflict	UNP P12314
C	114	LEU	PHE	conflict	UNP P12314
C	160	MET	ILE	conflict	UNP P12314
C	163	SER	ASN	conflict	UNP P12314
C	174	ARG	HIS	conflict	UNP P12314
C	195	THR	ASN	conflict	UNP P12314
C	206	THR	ASN	conflict	UNP P12314
C	207	PRO	LEU	conflict	UNP P12314

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W O R L D W I D E
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Chain	Residue	Modelled	Actual	Comment	Reference
C	240	ASP	ASN	conflict	UNP P12314
C	283	HIS	LEU	conflict	UNP P12314
C	285	GLN	LEU	conflict	UNP P12314
C	290	HIS	-	expression tag	UNP P12314
C	291	HIS	-	expression tag	UNP P12314
C	292	HIS	-	expression tag	UNP P12314
C	293	HIS	-	expression tag	UNP P12314
C	294	HIS	-	expression tag	UNP P12314
C	295	HIS	-	expression tag	UNP P12314

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.
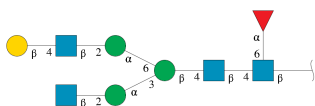
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	9	Total 110	C 62	N 4	O 44	0	0	0
3	E	9	Total 110	C 62	N 4	O 44	0	0	0

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

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Mg 1	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	26	Total 26	O 26	0	0
5	A	52	Total 52	O 52	0	0
5	C	49	Total 49	O 49	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.
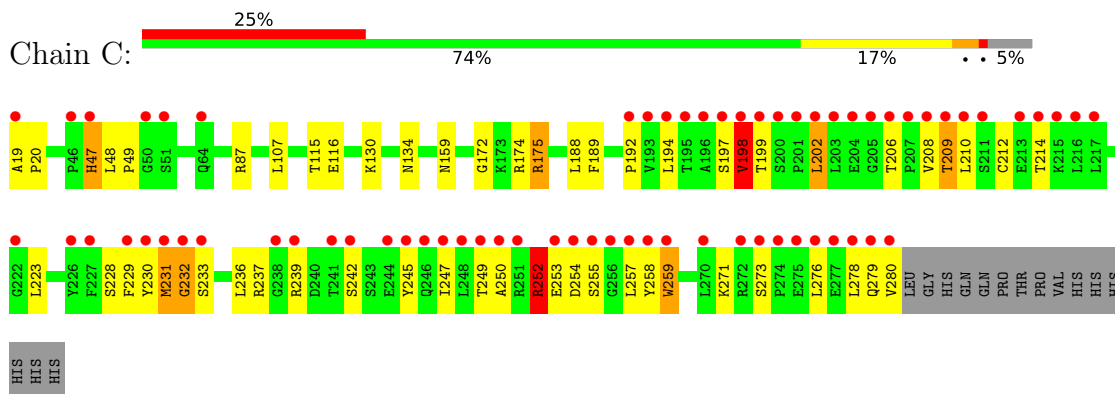
- Molecule 1: Ig gamma-1 Fc chain
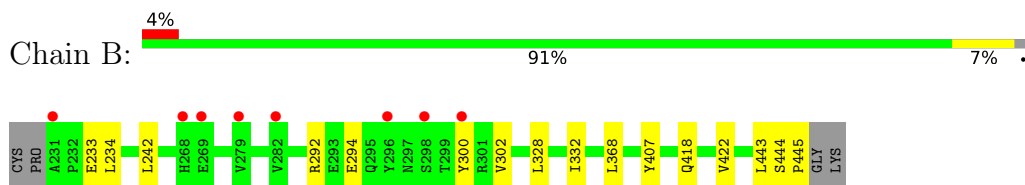
- Molecule 1: Ig gamma-1 Fc chain
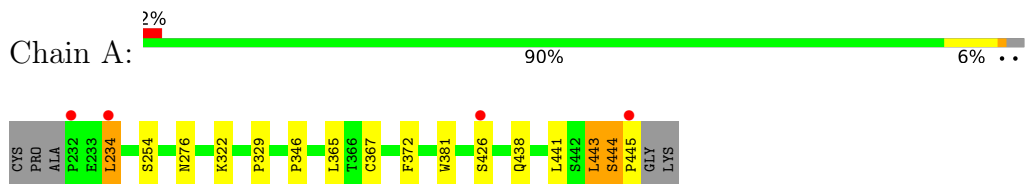
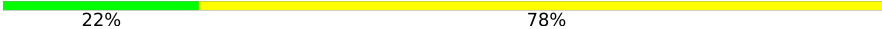- Molecule 2: High affinity immunoglobulin gamma Fc receptor I

- Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose
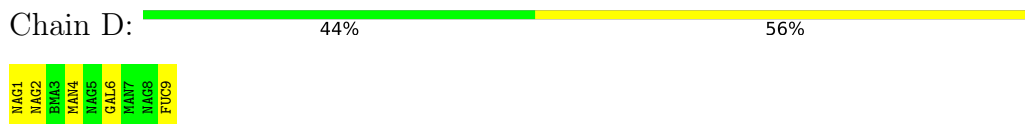
• Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

22% 78%

NAG1 NAG2 BMA3 MAN4 NAG5 GAL6 MAN7 NAG8 FUC9

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	204.00Å 88.80Å 55.92Å 90.00° 98.05° 90.00°	Depositor
Resolution (Å)	36.77 – 2.50 36.77 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.0 (36.77-2.50) 96.6 (36.77-2.29)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.177 , 0.223 0.178 , 0.223	Depositor DCC
R_{free} test set	2133 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	51.3	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.1	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	0.96	EDS
Total number of atoms	5839	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, FUC, MG, GAL, BMA, MAN

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	0.33	0/1761	0.62	1/2400 (0.0%)
1	B	0.30	0/1760	0.51	0/2400
2	C	0.37	1/2121 (0.0%)	0.80	5/2883 (0.2%)
All	All	0.34	1/5642 (0.0%)	0.66	6/7683 (0.1%)

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
2	C	0	4
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	253	GLU	CA-C	5.07	1.66	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	198	VAL	C-N-CA	19.51	170.48	121.70
1	A	444	SER	C-N-CD	-12.97	92.07	120.60
2	C	232	GLY	N-CA-C	-11.43	84.54	113.10
2	C	199	THR	N-CA-C	11.24	141.34	111.00
2	C	107	LEU	CA-CB-CG	-6.10	101.26	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	444	SER	Peptide
2	C	198	VAL	Peptide
2	C	249	THR	Peptide
2	C	250	ALA	Peptide
2	C	252	ARG	Peptide

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	1710	0	1681	7	0
1	B	1712	0	1680	9	0
2	C	2069	0	2040	43	0
3	D	110	0	94	1	0
3	E	110	0	94	0	0
4	A	1	0	0	0	0
5	A	52	0	0	1	0
5	B	26	0	0	1	0
5	C	49	0	0	0	0
All	All	5839	0	5589	57	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 57 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:C:255:SER:HA	2:C:278:LEU:HD12	1.60	0.83
2:C:202:LEU:HD22	2:C:280:VAL:HG13	1.70	0.74
2:C:252:ARG:HB3	2:C:280:VAL:HB	1.69	0.74
2:C:202:LEU:HB3	2:C:280:VAL:HA	1.73	0.69
2:C:252:ARG:HG3	2:C:252:ARG:O	1.93	0.68

There are no symmetry-related clashes.

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	213/219 (97%)	210 (99%)	3 (1%)	0	100	100
1	B	213/219 (97%)	208 (98%)	5 (2%)	0	100	100
2	C	260/277 (94%)	250 (96%)	10 (4%)	0	100	100
All	All	686/715 (96%)	668 (97%)	18 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	200/202 (99%)	195 (98%)	5 (2%)	47	73
1	B	199/202 (98%)	198 (100%)	1 (0%)	88	96
2	C	231/245 (94%)	220 (95%)	11 (5%)	25	48
All	All	630/649 (97%)	613 (97%)	17 (3%)	47	71

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	252	ARG
2	C	259	TRP
2	C	48	LEU
2	C	175	ARG
2	C	198	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	419	GLN

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 ⓘ

18 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	$\#|Z| > 2$
3	NAG	D	1	1,3	14,14,15	0.24	0	17,19,21	0.72	1 (5%)
3	NAG	D	2	3	14,14,15	0.43	0	17,19,21	0.54	0
3	BMA	D	3	3	11,11,12	0.64	0	15,15,17	0.97	0
3	MAN	D	4	3	11,11,12	0.93	0	15,15,17	1.23	2 (13%)
3	NAG	D	5	3	14,14,15	0.51	0	17,19,21	0.80	0
3	GAL	D	6	3	11,11,12	0.74	1 (9%)	15,15,17	0.95	0
3	MAN	D	7	3	11,11,12	0.73	0	15,15,17	0.91	0
3	NAG	D	8	3	14,14,15	0.42	0	17,19,21	0.49	0
3	FUC	D	9	3	10,10,11	1.14	1 (10%)	14,14,16	1.95	3 (21%)
3	NAG	E	1	1,3	14,14,15	0.63	1 (7%)	17,19,21	0.86	1 (5%)
3	NAG	E	2	3	14,14,15	0.63	1 (7%)	17,19,21	0.66	0
3	BMA	E	3	3	11,11,12	0.83	0	15,15,17	1.21	1 (6%)
3	MAN	E	4	3	11,11,12	0.80	0	15,15,17	1.59	2 (13%)
3	NAG	E	5	3	14,14,15	0.40	0	17,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	GAL	E	6	3	11,11,12	0.93	1 (9%)	15,15,17	1.19	1 (6%)
3	MAN	E	7	3	11,11,12	0.63	0	15,15,17	1.09	1 (6%)
3	NAG	E	8	3	14,14,15	0.51	0	17,19,21	0.55	0
3	FUC	E	9	3	10,10,11	1.10	1 (10%)	14,14,16	0.95	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
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
3	MAN	D	4	3	-	1/2/19/22	0/1/1/1
3	NAG	D	5	3	-	2/6/23/26	0/1/1/1
3	GAL	D	6	3	-	0/2/19/22	0/1/1/1
3	MAN	D	7	3	-	2/2/19/22	0/1/1/1
3	NAG	D	8	3	-	0/6/23/26	0/1/1/1
3	FUC	D	9	3	-	-	0/1/1/1
3	NAG	E	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	1/2/19/22	0/1/1/1
3	NAG	E	5	3	-	0/6/23/26	0/1/1/1
3	GAL	E	6	3	-	2/2/19/22	0/1/1/1
3	MAN	E	7	3	-	2/2/19/22	0/1/1/1
3	NAG	E	8	3	-	2/6/23/26	0/1/1/1
3	FUC	E	9	3	-	-	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	6	GAL	C1-C2	2.74	1.58	1.52
3	D	9	FUC	C4-C5	2.27	1.57	1.52
3	E	2	NAG	O5-C1	-2.12	1.40	1.43
3	D	6	GAL	C1-C2	2.10	1.57	1.52
3	E	1	NAG	C1-C2	2.09	1.55	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	9	FUC	O5-C5-C4	4.66	117.88	109.52
3	E	4	MAN	C1-O5-C5	4.19	117.87	112.19
3	D	9	FUC	C1-O5-C5	3.69	121.13	112.78
3	D	9	FUC	C3-C4-C5	3.58	115.34	109.77
3	D	4	MAN	C1-O5-C5	3.57	117.03	112.19

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	7	MAN	O5-C5-C6-O6
3	E	7	MAN	C4-C5-C6-O6
3	D	5	NAG	O5-C5-C6-O6
3	D	7	MAN	C4-C5-C6-O6
3	E	6	GAL	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	NAG	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 oligosaccharide.

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths　　　Bond angles

Torsions　　　Rings
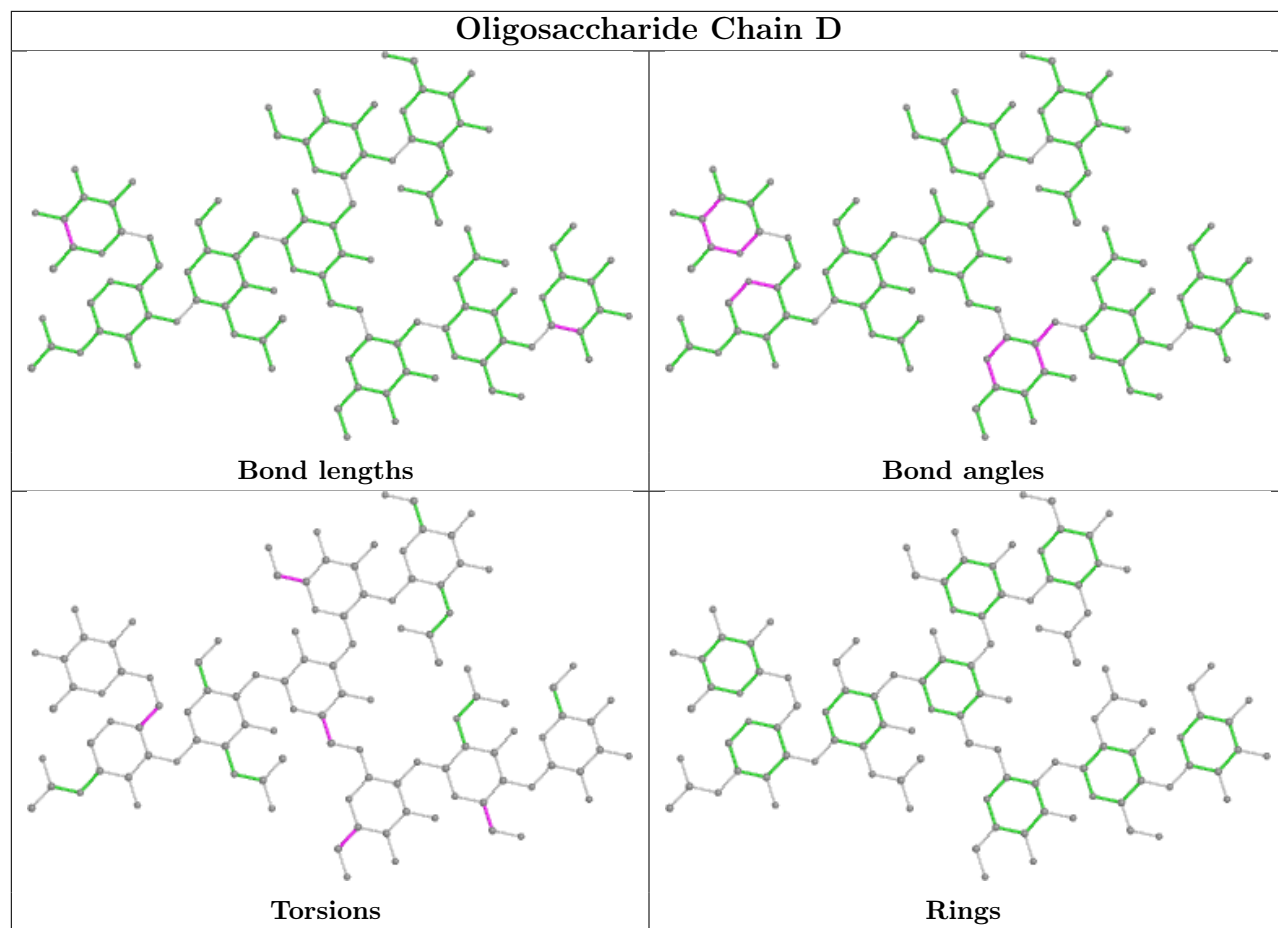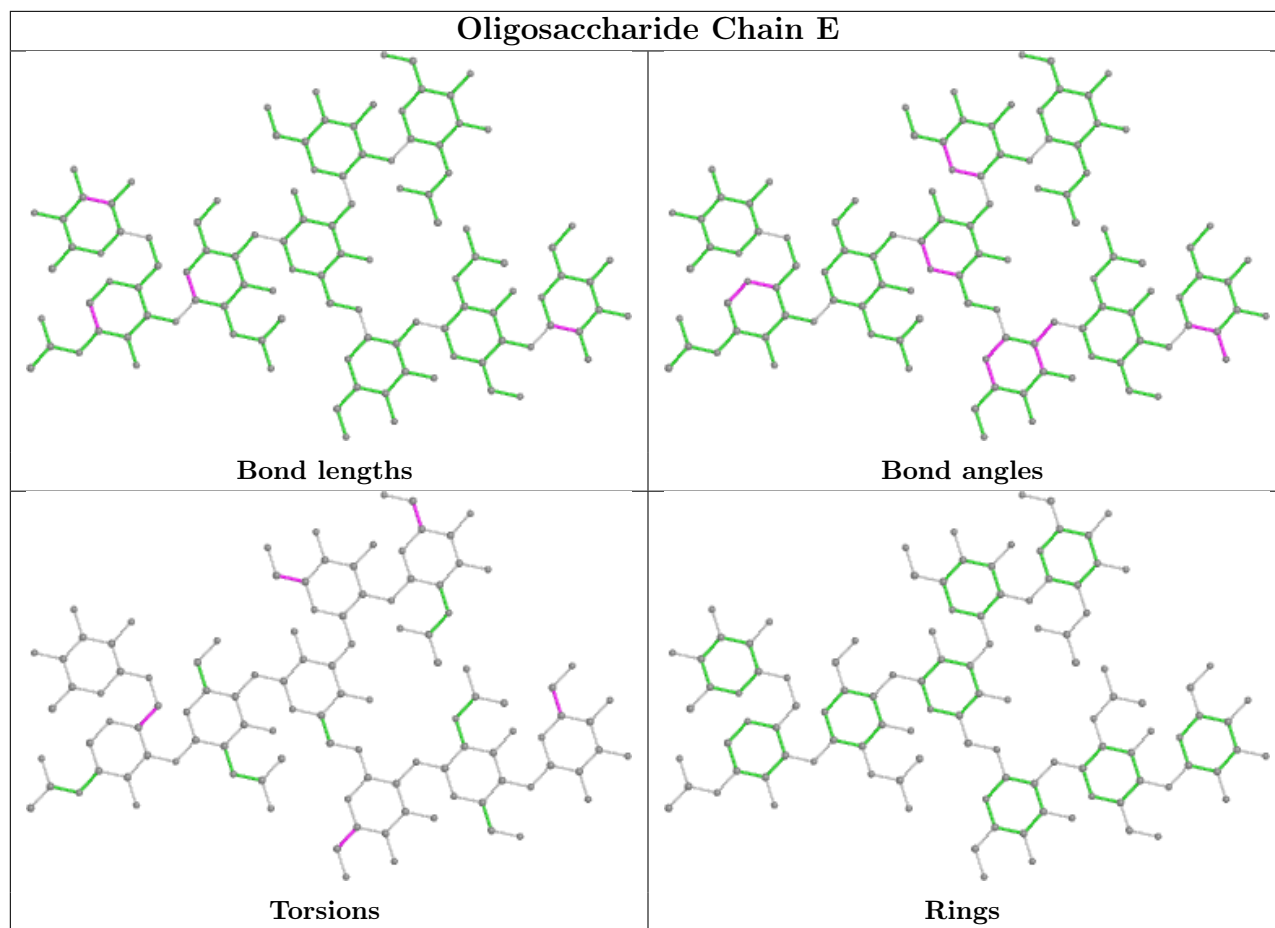
5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	214/219 (97%)	-0.02	4 (1%)	66	69	33, 49, 72, 139	0
1	B	215/219 (98%)	0.12	8 (3%)	41	45	39, 61, 107, 141	0
2	C	262/277 (94%)	1.68	68 (25%)	0	0	33, 55, 184, 259	0
All	All	691/715 (96%)	0.67	80 (11%)	4	4	33, 55, 159, 259	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	202	LEU	14.8
2	C	254	ASP	14.8
2	C	201	PRO	13.6
2	C	247	ILE	12.6
2	C	258	TYR	10.7

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 ⓘ

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
3	NAG	D	8	14/15	0.64	0.42	90,118,132,135	0
3	GAL	D	6	11/12	0.65	0.32	121,135,145,146	0
3	GAL	E	6	11/12	0.78	0.37	61,84,94,96	0

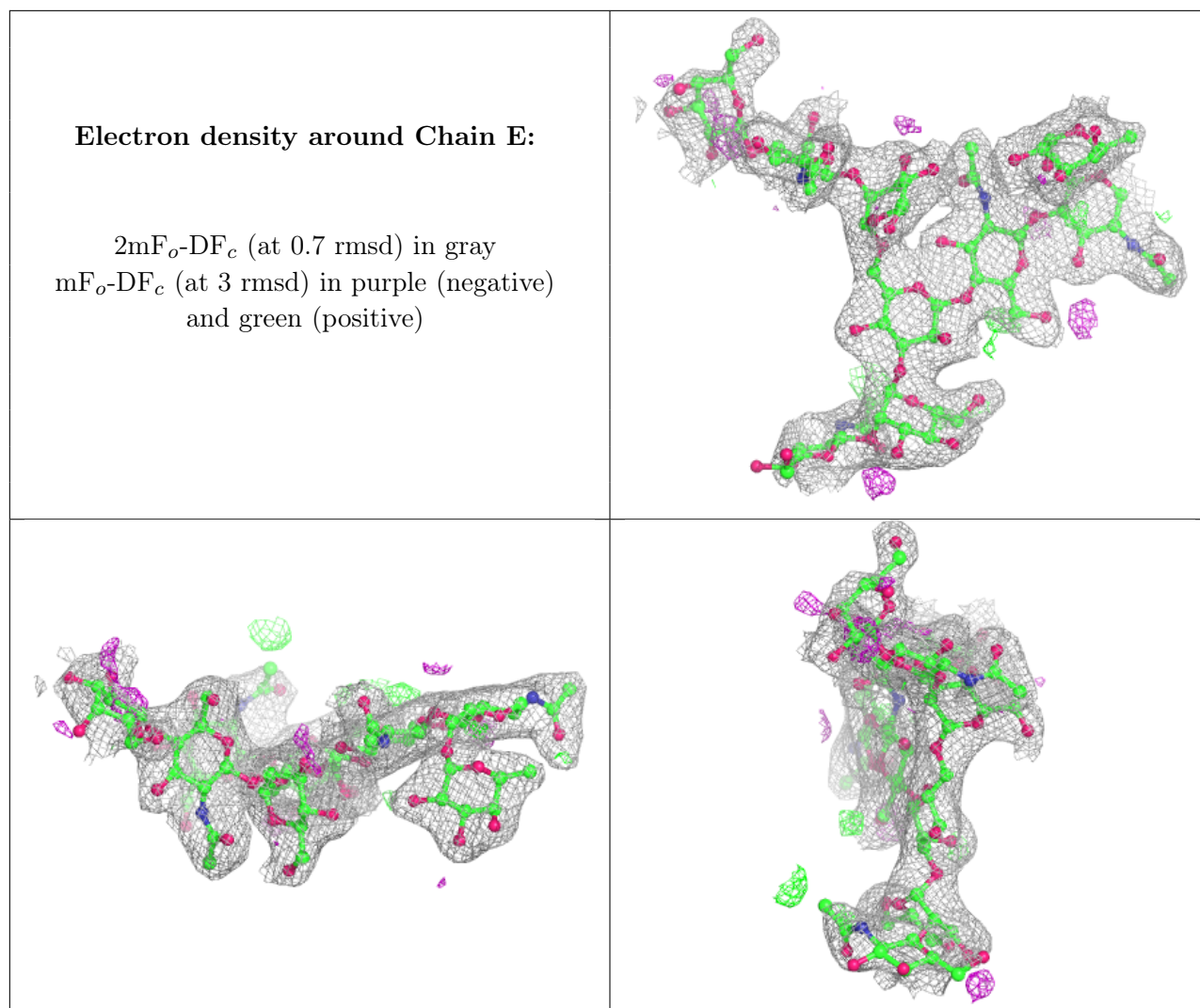*Continued on next page...*

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	E	8	14/15	0.84	0.32	80,106,123,131	0
3	NAG	D	5	14/15	0.85	0.14	75,86,98,110	0
3	FUC	D	9	10/11	0.89	0.29	99,109,117,117	0
3	MAN	D	4	11/12	0.89	0.20	72,81,96,101	0
3	NAG	D	1	14/15	0.89	0.25	75,89,95,103	0
3	MAN	D	7	11/12	0.91	0.12	83,99,109,117	0
3	MAN	E	7	11/12	0.92	0.12	61,73,84,94	0
3	BMA	D	3	11/12	0.95	0.12	66,73,88,91	0
3	NAG	E	1	14/15	0.95	0.16	32,36,44,46	0
3	NAG	E	5	14/15	0.95	0.10	41,52,59,60	0
3	NAG	D	2	14/15	0.96	0.15	65,74,87,94	0
3	BMA	E	3	11/12	0.96	0.12	35,43,54,57	0
3	FUC	E	9	10/11	0.96	0.11	33,45,48,51	0
3	MAN	E	4	11/12	0.97	0.13	37,46,59,60	0
3	NAG	E	2	14/15	0.98	0.11	32,37,46,50	0

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 D:

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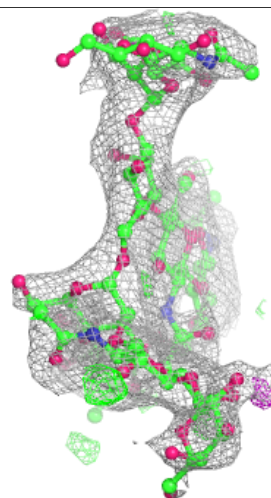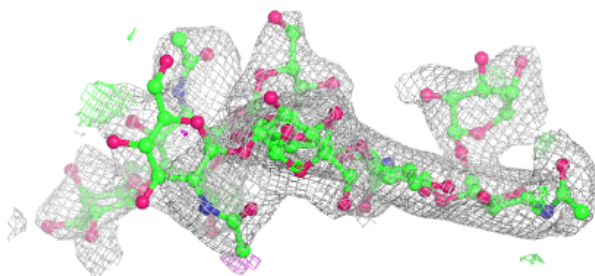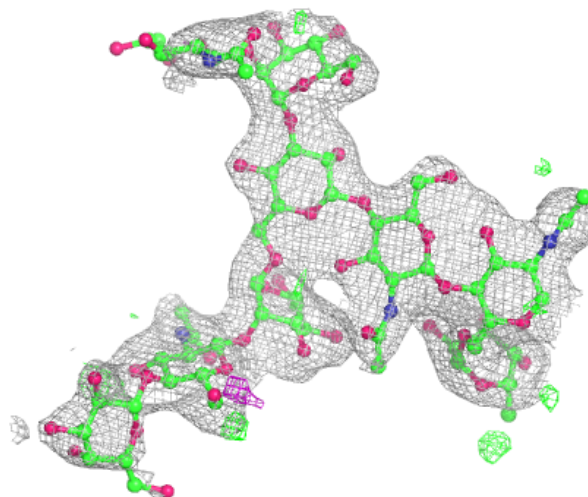
Electron density around Chain E:

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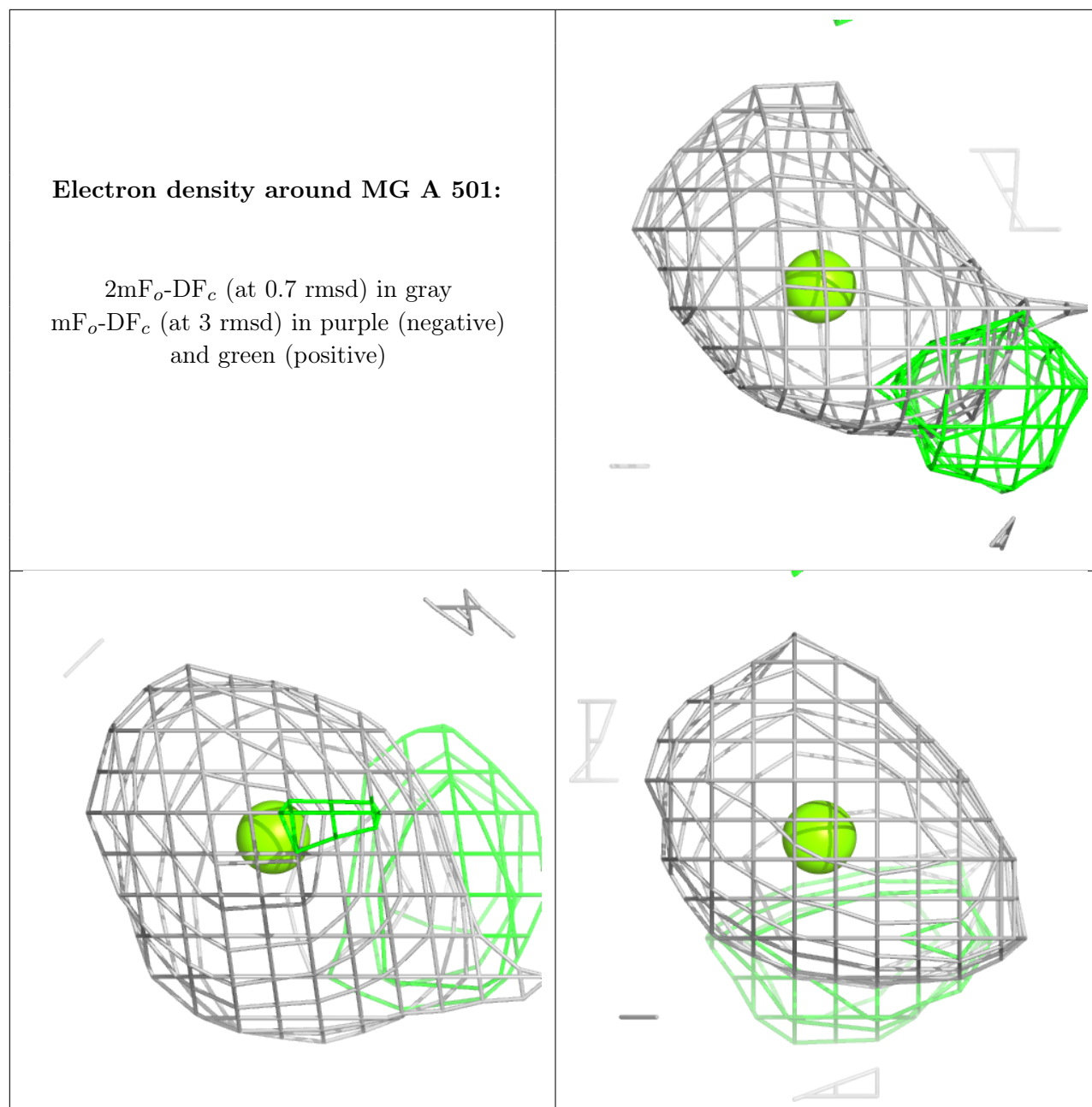mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

6.4 Ligands ⓘ

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
4	MG	A	501	1/1	0.92	0.22	67,67,67,67	0

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

Electron density around MG A 501:

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

6.5   Other polymers ⓘ

There are no such residues in this entry.