



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:23 PM UTC

PDB ID : 8DIR / pdb_00008dir
Title : The complex structure between human IgG1 Fc and its high affinity receptor FcγRI H174R variant
Authors : Lu, J.; Sun, P.D.
Deposited on : 2022-06-29
Resolution : 2.30 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

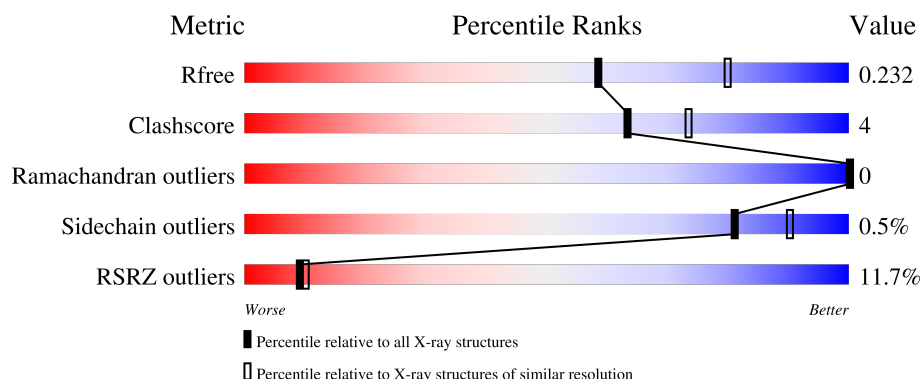
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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	4% 89% 8% .
1	B	219	5% 89% 9% .
2	C	277	22% 81% 14% 5%
3	D	9	56% 33% 11%
3	E	9	56% 44%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5962 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	C	N	O	S	0	0	0
			1712	1091	287	328	6			
1	A	215	Total	C	N	O	S	3	1	0
			1714	1092	287	329	6			

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

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

There are 27 discrepancies between the modelled and reference sequences:

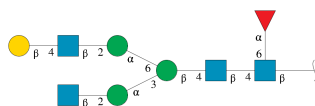
Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ALA	-	expression tag	UNP P12314
C	20	PRO	-	expression tag	UNP P12314
C	25	LYS	THR	conflict	UNP P12314
C	38	SER	THR	conflict	UNP P12314
C	46	PRO	LEU	conflict	UNP P12314
C	63	ILE	THR	conflict	UNP P12314
C	69	THR	SER	conflict	UNP P12314
C	71	HIS	ARG	conflict	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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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	C	N	O	0	0	0
			110	62	4	44			
3	E	9	Total	C	N	O	0	0	0
			110	62	4	44			

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Na	0	0
			2	2		
4	C	1	Total	Na	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	49	Total	O	0	0
			49	49		
5	A	110	Total	O	0	0
			110	110		

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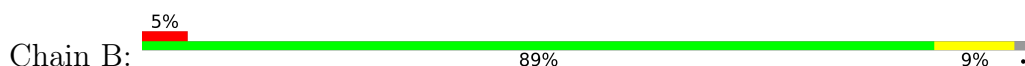
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	85	Total	O	0	0
			85	85		

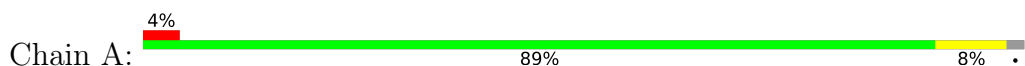
3 Residue-property plots [i](#)

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.

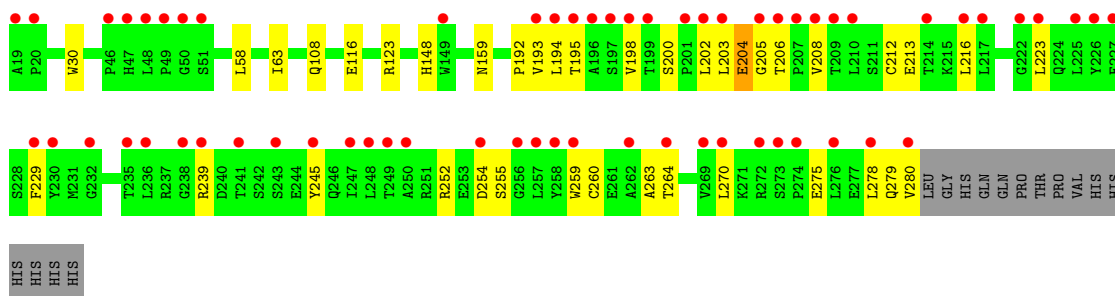
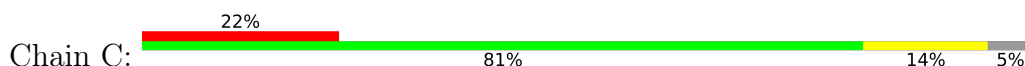
- Molecule 1: Ig gamma-1 Fc chain



- 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:  56% 44%

NAG1	NAG2	MAN3	MAN4	NAG5	GAL6	MAN7	NAG8	FUC9
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	204.29Å 89.28Å 56.03Å 90.00° 97.72° 90.00°	Depositor
Resolution (Å)	36.87 – 2.30 36.87 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (36.87-2.30) 99.7 (36.87-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.196 , 0.233 0.195 , 0.232	Depositor DCC
R_{free} test set	2191 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5962	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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: FUC, BMA, GAL, NAG, NA, 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	0.09	0/1765	0.31	0/2405
1	B	0.08	0/1760	0.27	0/2400
2	C	0.13	0/2121	0.45	3/2883 (0.1%)
All	All	0.11	0/5646	0.36	3/7688 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	204	GLU	CB-CA-C	11.66	130.29	109.64
2	C	204	GLU	N-CA-C	-11.17	95.72	110.24
2	C	205	GLY	N-CA-C	7.75	125.66	115.36

There are no chirality outliers.

There are no planarity outliers.

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	1714	0	1684	12	0
1	B	1712	0	1680	10	0
2	C	2069	0	2041	23	0
3	D	110	0	94	1	0
3	E	110	0	94	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
4	C	1	0	0	0	0
5	A	110	0	0	3	0
5	B	49	0	0	0	0
5	C	85	0	0	0	0
All	All	5962	0	5593	45	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 4.

All (45) 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:346:PRO:HB3	1:A:372:PHE:HB3	1.71	0.72
2:C:202:LEU:HD21	2:C:206:THR:HB	1.74	0.70
2:C:263:ALA:HB2	2:C:270:LEU:HD23	1.78	0.66
2:C:239:ARG:NH2	2:C:264:THR:O	2.29	0.66
2:C:116:GLU:HG2	2:C:159:ASN:HA	1.82	0.62
2:C:252:ARG:HB3	2:C:280:VAL:HB	1.85	0.59
1:B:292:ARG:HG2	1:B:302:VAL:HG12	1.86	0.58
2:C:255:SER:OG	2:C:278:LEU:O	2.23	0.57
1:B:443:LEU:HD23	1:B:445:PRO:HD2	1.86	0.56
2:C:198:VAL:HG21	2:C:208:VAL:HG12	1.88	0.55
2:C:203:LEU:O	2:C:204:GLU:C	2.50	0.54
1:A:276:ASN:HB2	1:A:322:LYS:HB3	1.91	0.52
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.45	0.51
2:C:58:LEU:HB2	2:C:63:ILE:HD11	1.93	0.51
1:A:368:LEU:HD13	1:A:407:TYR:CZ	2.46	0.51
2:C:194:LEU:HD13	2:C:260:CYS:HB2	1.92	0.51
2:C:30:TRP:HB3	2:C:108:GLN:HB3	1.93	0.50
1:B:243:PHE:HE1	3:D:3:BMA:H62	1.76	0.49
2:C:192:PRO:HB2	2:C:212:CYS:SG	2.54	0.47
1:A:274:LYS:NZ	5:A:709:HOH:O	2.48	0.47
1:B:368:LEU:HD13	1:B:407:TYR:CZ	2.49	0.47
2:C:193:VAL:HG13	2:C:213:GLU:HB2	1.96	0.47
5:A:753:HOH:O	2:C:148:HIS:HE1	1.98	0.46
2:C:195:THR:HG23	2:C:213:GLU:HG3	1.97	0.46
1:B:270:ASP:CG	1:B:326:LYS:HD2	2.40	0.46
2:C:108:GLN:OE1	2:C:123:ARG:HD3	2.17	0.45
1:A:444:SER:O	1:A:444:SER:OG	2.27	0.45
1:A:443:LEU:HD22	1:A:445:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:216:LEU:HD11	2:C:223:LEU:HD22	1.98	0.44
2:C:229:PHE:CG	2:C:245:TYR:HB2	2.52	0.44
1:A:259:VAL:HG23	1:A:306:LEU:HB3	1.99	0.44
1:A:248:LYS:HE3	1:A:255:ARG:CZ	2.48	0.44
1:B:444:SER:HB2	1:B:445:PRO:HD3	2.00	0.43
1:A:322:LYS:NZ	5:A:712:HOH:O	2.52	0.43
2:C:200:SER:OG	2:C:279:GLN:HB3	2.20	0.42
1:B:351:LEU:HB2	1:B:366:THR:HB	2.02	0.42
1:B:294:GLU:HG2	1:B:300:TYR:CE1	2.54	0.42
1:A:351:LEU:HB2	1:A:366:THR:HB	2.02	0.41
2:C:202:LEU:HD23	2:C:280:VAL:HG13	2.02	0.41
1:B:344:ARG:CZ	1:B:403:SER:HB3	2.50	0.41
2:C:259:TRP:NE1	2:C:275:GLU:HG3	2.36	0.41
1:A:234:LEU:HD13	1:A:234:LEU:HA	1.61	0.40
1:B:328:LEU:HD13	1:B:332:ILE:HG13	2.03	0.40
2:C:252:ARG:CZ	2:C:279:GLN:HG3	2.52	0.40
2:C:254:ASP:OD1	2:C:254:ASP:N	2.53	0.40

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	214/219 (98%)	211 (99%)	3 (1%)	0	100	100
1	B	213/219 (97%)	211 (99%)	2 (1%)	0	100	100
2	C	260/277 (94%)	249 (96%)	11 (4%)	0	100	100
All	All	687/715 (96%)	671 (98%)	16 (2%)	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%)	199 (100%)	1 (0%)	81	90
1	B	199/202 (98%)	197 (99%)	2 (1%)	68	82
2	C	231/245 (94%)	231 (100%)	0	100	100
All	All	630/649 (97%)	627 (100%)	3 (0%)	81	90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	242	LEU
1	B	363	VAL
1	A	234	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	418	GLN
1	A	285	HIS
1	A	311	GLN
1	A	315	ASN
2	C	55	GLN
2	C	148	HIS

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	0.21	0	17,19,21	0.62	0
3	NAG	D	2	3	14,14,15	0.31	0	17,19,21	0.55	0
3	BMA	D	3	3	11,11,12	0.37	0	15,15,17	0.92	1 (6%)
3	MAN	D	4	3	11,11,12	0.61	0	15,15,17	1.10	2 (13%)
3	NAG	D	5	3	14,14,15	0.57	0	17,19,21	0.77	0
3	GAL	D	6	3	11,11,12	0.54	0	15,15,17	0.80	0
3	MAN	D	7	3	11,11,12	0.60	0	15,15,17	0.91	1 (6%)
3	NAG	D	8	3	14,14,15	0.34	0	17,19,21	0.52	0
3	FUC	D	9	3	10,10,11	1.12	1 (10%)	14,14,16	1.84	3 (21%)
3	NAG	E	1	1,3	14,14,15	0.38	0	17,19,21	0.60	0
3	NAG	E	2	3	14,14,15	0.37	0	17,19,21	0.53	0
3	BMA	E	3	3	11,11,12	0.51	0	15,15,17	0.91	1 (6%)
3	MAN	E	4	3	11,11,12	0.51	0	15,15,17	1.14	2 (13%)
3	NAG	E	5	3	14,14,15	0.61	1 (7%)	17,19,21	0.44	0
3	GAL	E	6	3	11,11,12	0.52	0	15,15,17	0.80	0
3	MAN	E	7	3	11,11,12	0.52	0	15,15,17	1.10	2 (13%)
3	NAG	E	8	3	14,14,15	0.49	0	17,19,21	0.53	0
3	FUC	E	9	3	10,10,11	0.52	0	14,14,16	0.82	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	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	5	3	-	3/6/23/26	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	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1
3	MAN	E	4	3	-	1/2/19/22	0/1/1/1
3	NAG	E	5	3	-	1/6/23/26	0/1/1/1
3	GAL	E	6	3	-	0/2/19/22	0/1/1/1
3	MAN	E	7	3	-	2/2/19/22	0/1/1/1
3	NAG	E	8	3	-	0/6/23/26	0/1/1/1
3	FUC	E	9	3	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	9	FUC	C4-C5	2.30	1.57	1.52
3	E	5	NAG	O5-C1	-2.13	1.40	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	9	FUC	O5-C5-C4	4.65	117.93	109.55
3	D	9	FUC	C3-C4-C5	3.20	114.68	109.81
3	D	9	FUC	C1-O5-C5	3.20	120.50	112.97
3	E	7	MAN	C1-O5-C5	3.17	116.44	112.19
3	E	4	MAN	C1-O5-C5	3.09	116.33	112.19
3	D	4	MAN	C1-O5-C5	3.05	116.28	112.19
3	E	3	BMA	C1-O5-C5	2.56	115.62	112.19
3	E	4	MAN	O2-C2-C3	-2.53	104.91	110.15
3	D	3	BMA	C1-O5-C5	2.47	115.49	112.19
3	D	7	MAN	C1-O5-C5	2.43	115.45	112.19
3	D	4	MAN	O2-C2-C3	-2.23	105.53	110.15
3	E	7	MAN	O2-C2-C3	-2.12	105.76	110.15

There are no chirality outliers.

All (14) torsion outliers are listed below:

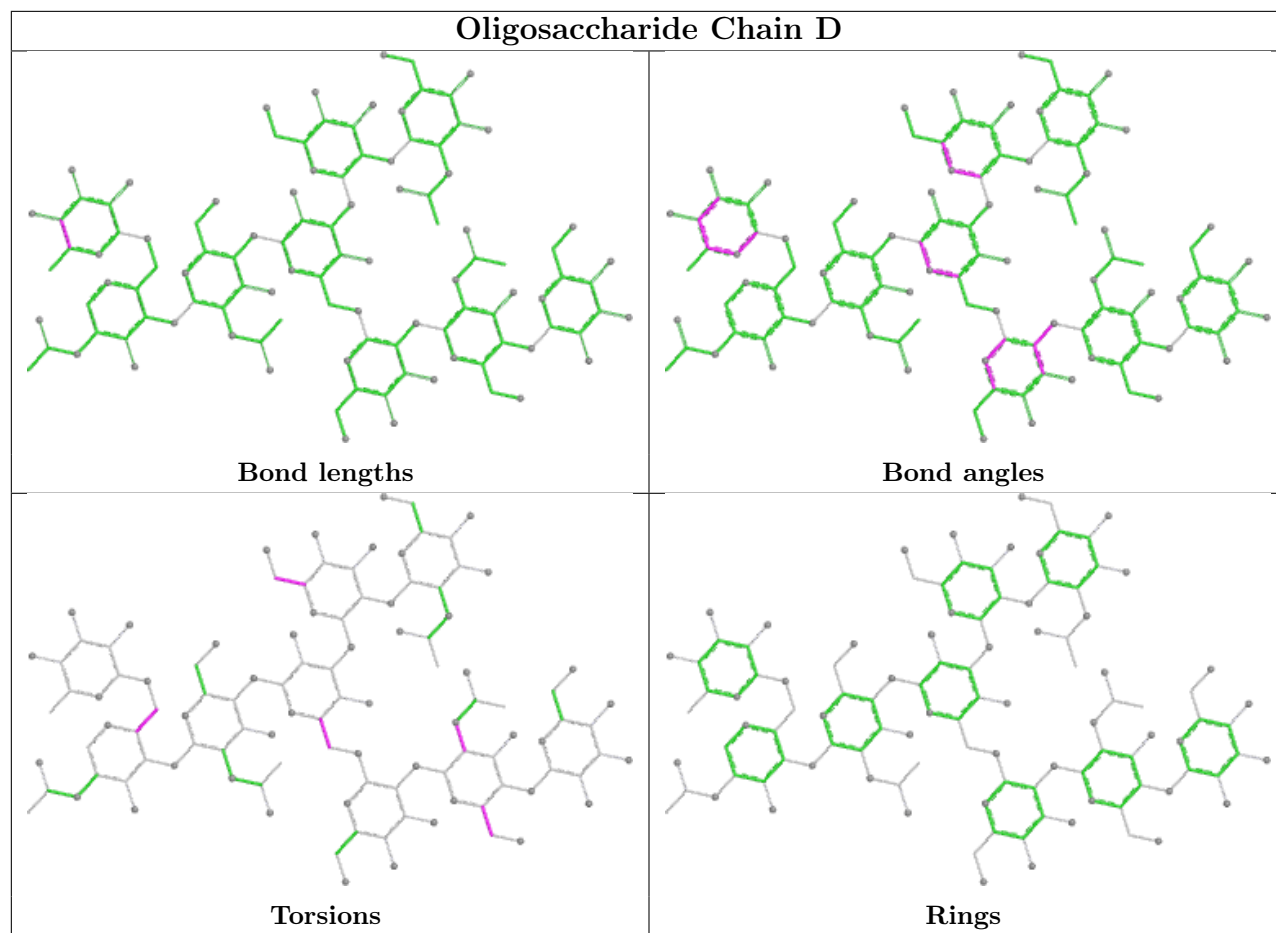
Mol	Chain	Res	Type	Atoms
3	D	7	MAN	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
3	D	5	NAG	O5-C5-C6-O6
3	D	5	NAG	C4-C5-C6-O6
3	E	7	MAN	C4-C5-C6-O6
3	D	7	MAN	C4-C5-C6-O6
3	E	7	MAN	O5-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
3	D	5	NAG	C1-C2-N2-C7
3	E	5	NAG	C1-C2-N2-C7
3	E	4	MAN	O5-C5-C6-O6

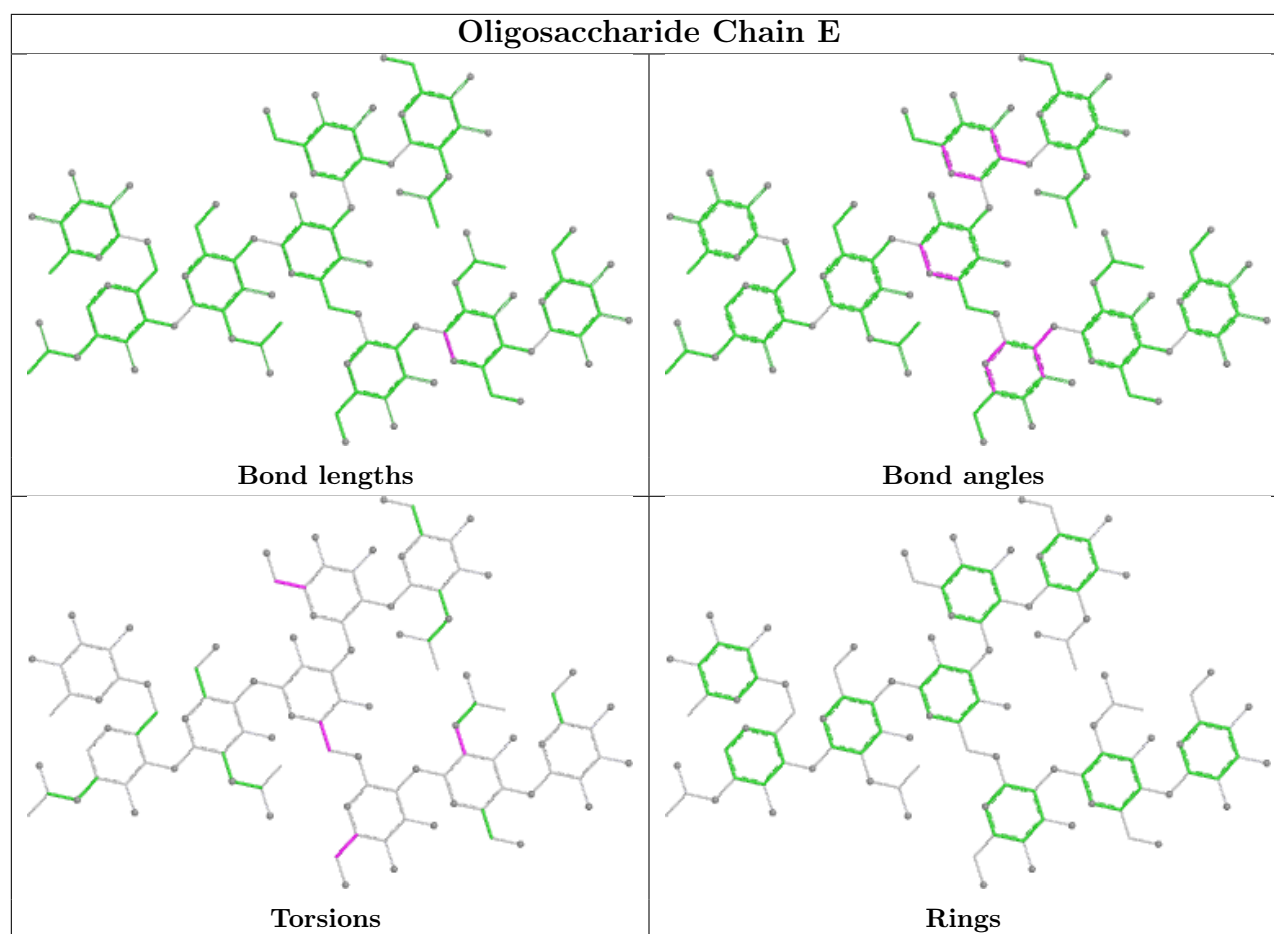
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3	BMA	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.





5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	215/219 (98%)	-0.08	8 (3%) 45 48	25, 42, 68, 152	1 (0%)
1	B	215/219 (98%)	0.41	11 (5%) 33 35	34, 55, 95, 122	0
2	C	262/277 (94%)	0.86	62 (23%) 2 2	27, 48, 165, 189	0
All	All	692/715 (96%)	0.43	81 (11%) 9 10	25, 49, 152, 189	1 (0%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	270	LEU	5.0
2	C	227	PHE	4.9
1	A	232	PRO	4.8
2	C	51	SER	4.7
2	C	257	LEU	4.6
2	C	48	LEU	4.6
2	C	203	LEU	4.4
2	C	193	VAL	4.4
2	C	247	ILE	4.3
1	A	234	LEU	4.3
2	C	274	PRO	4.1
2	C	226	TYR	4.0
2	C	47	HIS	3.9
2	C	222	GLY	3.9
2	C	259	TRP	3.9
2	C	238	GLY	3.8
2	C	269	VAL	3.8
2	C	205	GLY	3.7
2	C	245	TYR	3.7
1	B	445	PRO	3.7
2	C	258	TYR	3.6
2	C	49	PRO	3.6
2	C	217	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
2	C	280	VAL	3.4
2	C	216	LEU	3.3
2	C	248	LEU	3.3
2	C	201	PRO	3.3
1	B	231	ALA	3.2
2	C	208	VAL	3.3
2	C	250	ALA	3.1
2	C	198	VAL	3.1
2	C	225	LEU	3.1
2	C	278	LEU	3.1
2	C	209	THR	3.1
2	C	241	THR	3.1
1	A	445	PRO	3.0
1	B	296	TYR	3.0
2	C	46	PRO	3.0
2	C	206	THR	2.9
2	C	230	TYR	2.9
1	B	291	PRO	2.9
2	C	196	ALA	2.9
1	B	300	TYR	2.8
2	C	20	PRO	2.7
2	C	207	PRO	2.7
2	C	239	ARG	2.7
2	C	149	TRP	2.7
2	C	194	LEU	2.7
2	C	199	THR	2.6
2	C	264	THR	2.6
1	A	444	SER	2.6
1	A	233	GLU	2.5
2	C	202	LEU	2.5
1	B	299	THR	2.5
2	C	223	LEU	2.5
2	C	232	GLY	2.5
2	C	214	THR	2.5
2	C	235	THR	2.4
1	B	298	SER	2.4
2	C	210	LEU	2.4
2	C	50	GLY	2.4
2	C	256	GLY	2.4
2	C	272	ARG	2.3
2	C	276	LEU	2.3
1	A	446	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	282	VAL	2.3
2	C	229	PHE	2.3
1	B	336	ILE	2.3
2	C	249	THR	2.2
2	C	254	ASP	2.2
1	B	444	SER	2.2
2	C	243	SER	2.1
2	C	273	SER	2.1
2	C	236	LEU	2.1
2	C	19	ALA	2.1
2	C	197	SER	2.1
2	C	195	THR	2.1
2	C	262	ALA	2.0
1	B	280	ASP	2.0
1	A	443	LEU	2.0
1	B	340	LYS	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](#)

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.

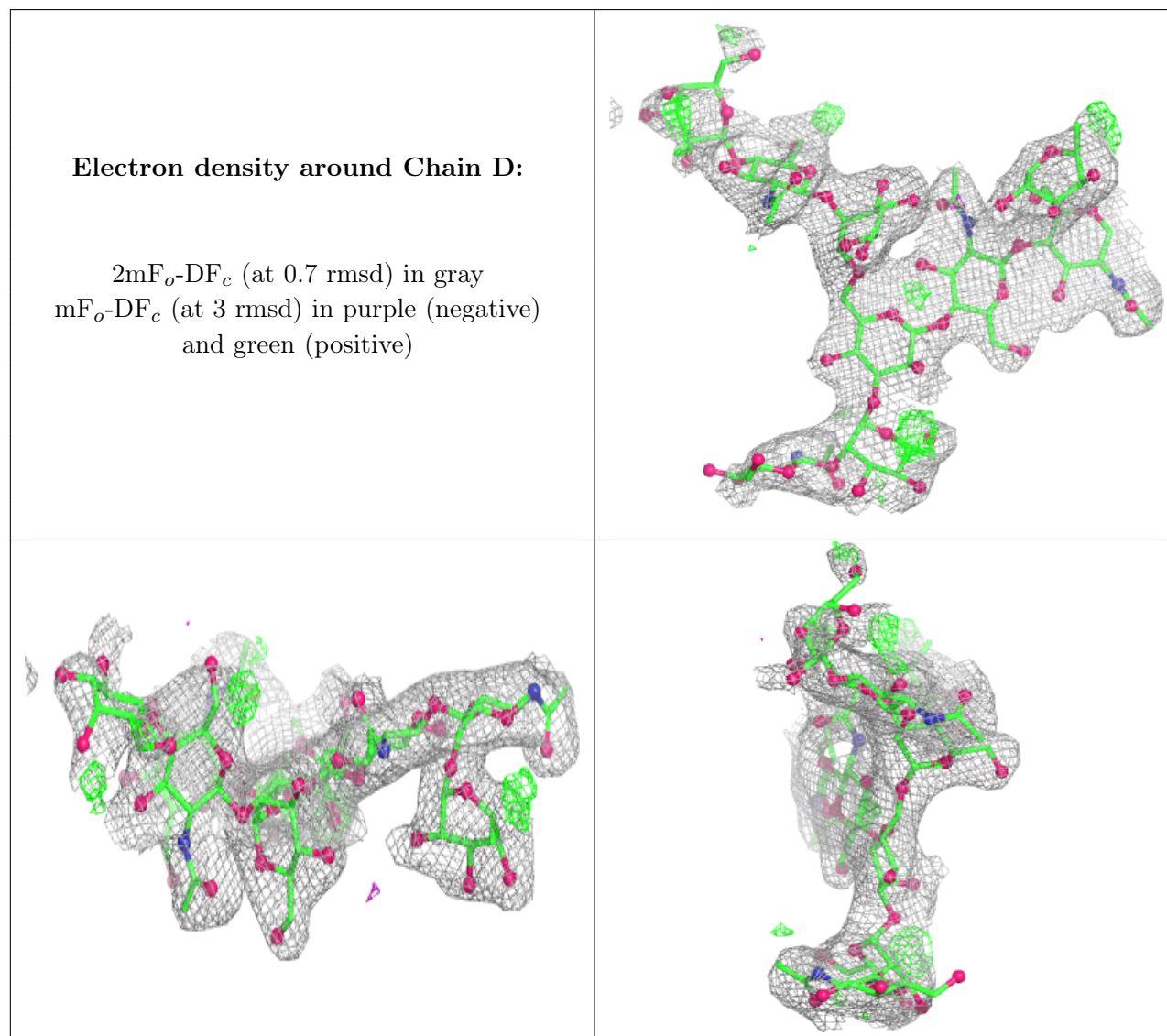
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	D	8	14/15	0.51	0.17	97,120,132,133	0
3	NAG	E	8	14/15	0.60	0.16	83,109,129,131	0
3	FUC	D	9	10/11	0.63	0.15	94,101,106,112	0
3	GAL	D	6	11/12	0.68	0.27	120,133,155,156	0
3	MAN	D	7	11/12	0.75	0.13	79,92,110,112	0
3	NAG	D	5	14/15	0.83	0.15	61,74,92,98	0
3	GAL	E	6	11/12	0.85	0.22	52,71,79,79	0
3	MAN	E	7	11/12	0.86	0.11	49,67,76,82	0
3	MAN	D	4	11/12	0.90	0.08	59,68,77,83	0
3	BMA	D	3	11/12	0.91	0.10	59,67,79,85	0
3	NAG	E	5	14/15	0.92	0.09	37,47,56,56	0
3	NAG	D	1	14/15	0.92	0.09	69,81,89,89	0

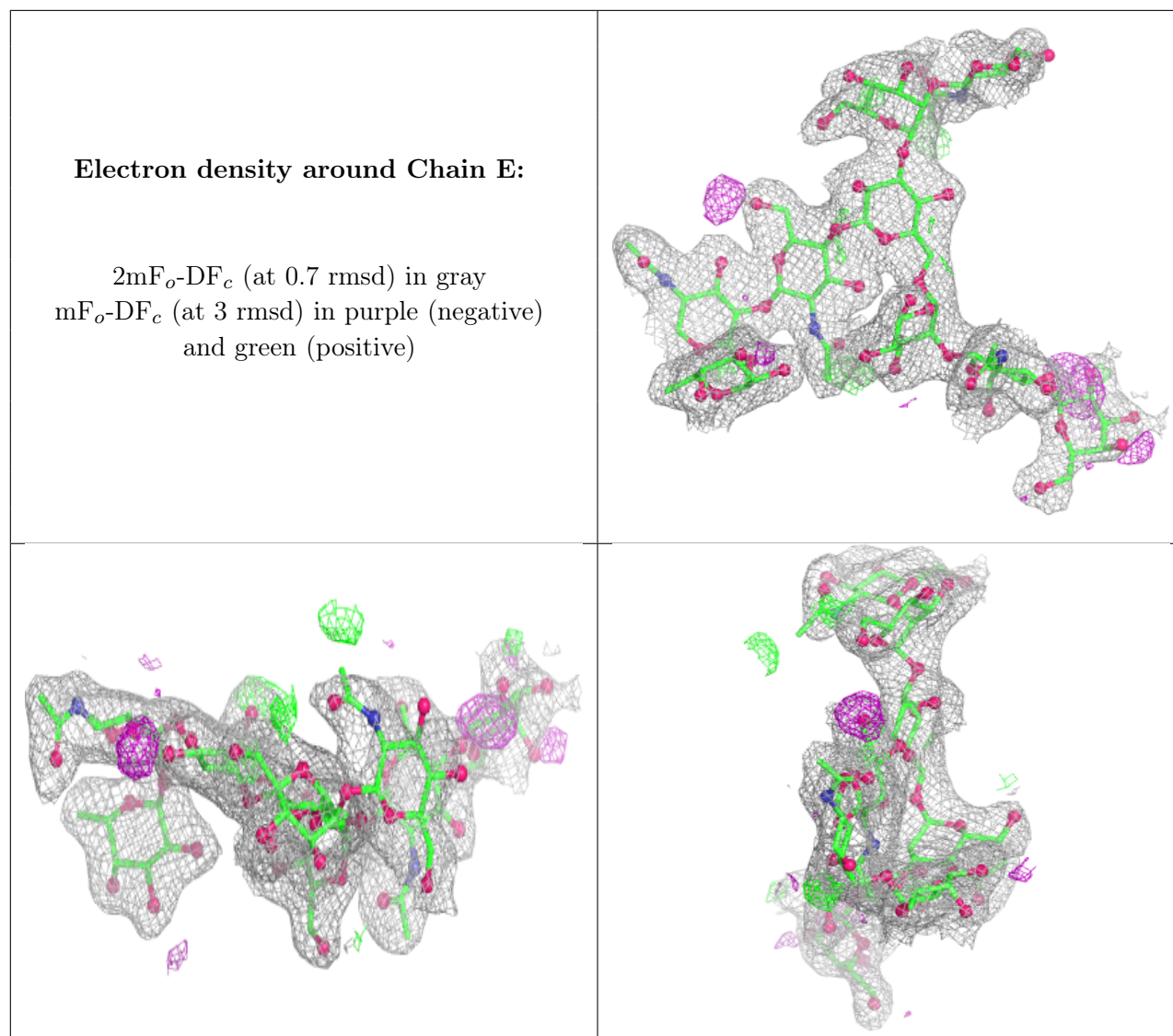
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	D	2	14/15	0.93	0.10	60,68,76,80	0
3	BMA	E	3	11/12	0.94	0.08	25,37,48,53	0
3	MAN	E	4	11/12	0.94	0.07	32,40,52,56	0
3	NAG	E	2	14/15	0.94	0.07	28,35,39,40	0
3	FUC	E	9	10/11	0.95	0.07	37,42,48,50	0
3	NAG	E	1	14/15	0.96	0.07	26,32,36,38	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.





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, 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.

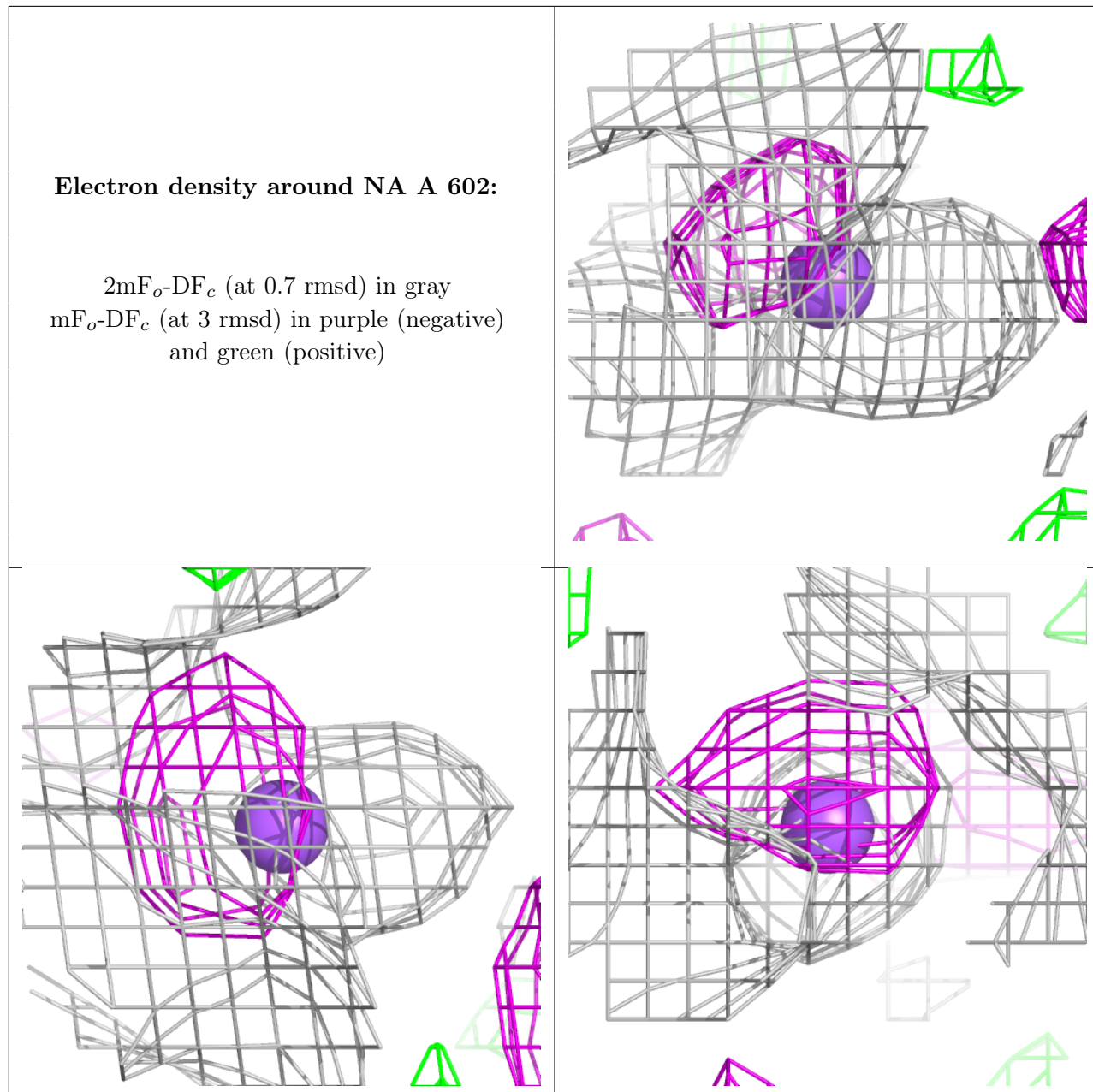
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NA	A	602	1/1	0.86	0.28	55,55,55,55	0
4	NA	C	301	1/1	0.92	0.11	53,53,53,53	0
4	NA	A	601	1/1	0.94	0.12	46,46,46,46	0

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.

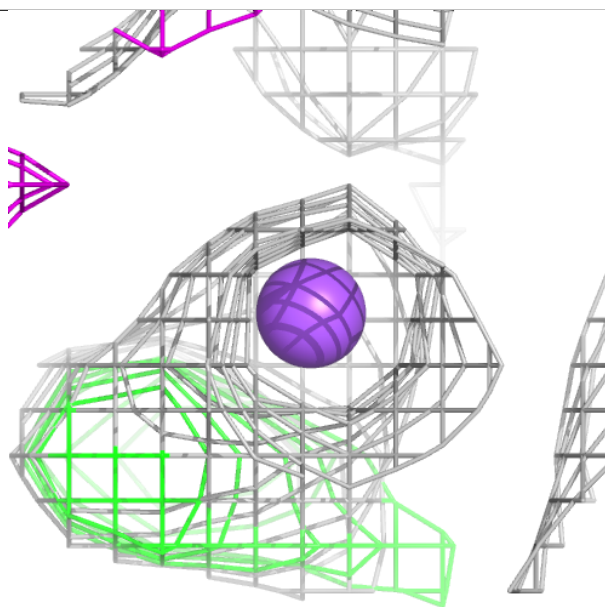
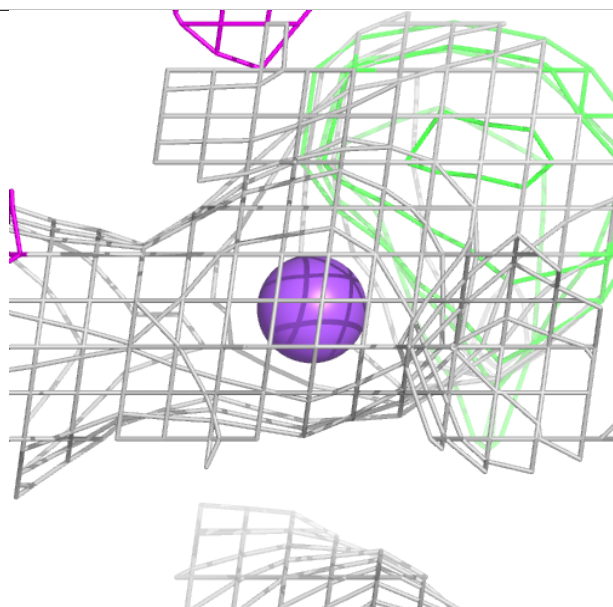
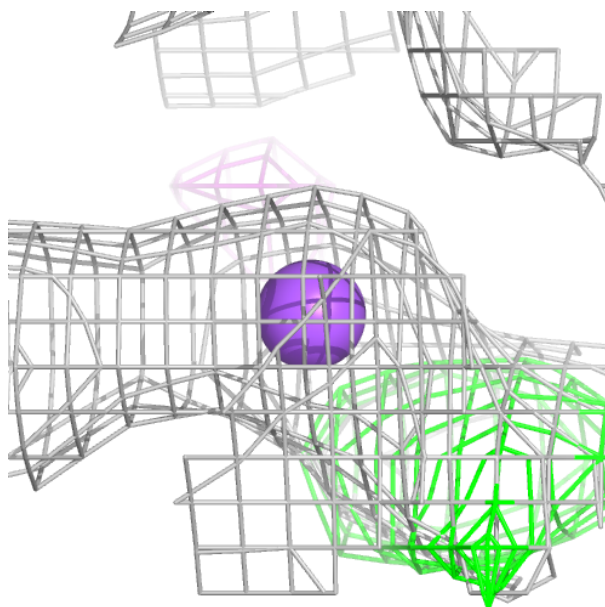
Electron density around NA A 602:

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



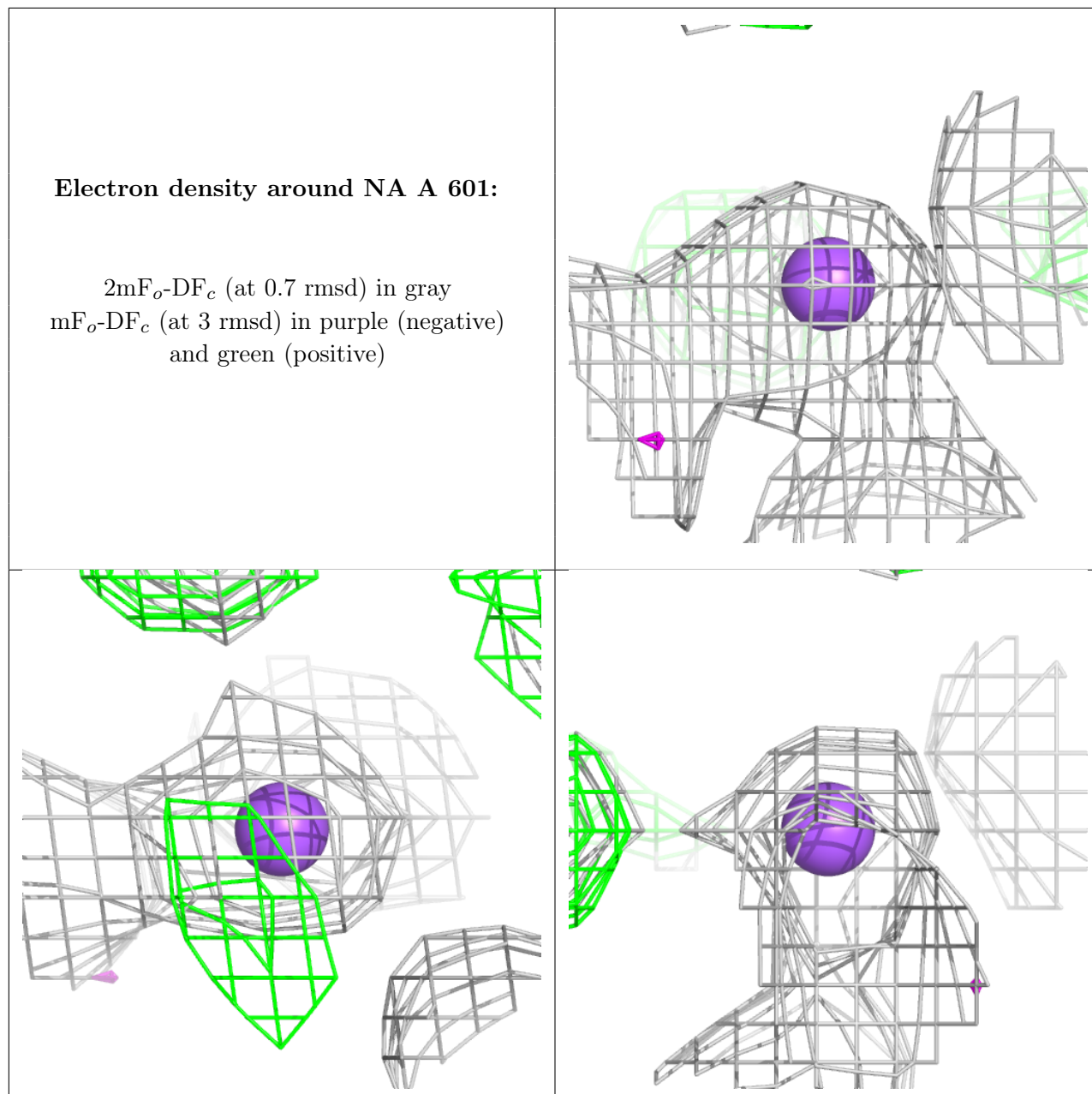
Electron density around NA C 301:

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



Electron density around NA A 601:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.