



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:21 AM UTC

PDB ID : 9K34 / pdb_00009k34
Title : Human IgG1 Fc fragments, mutant (2CT1.9)
Authors : Kim, J.-S.; Kim, J.-W.
Deposited on : 2024-10-18
Resolution : 3.00 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

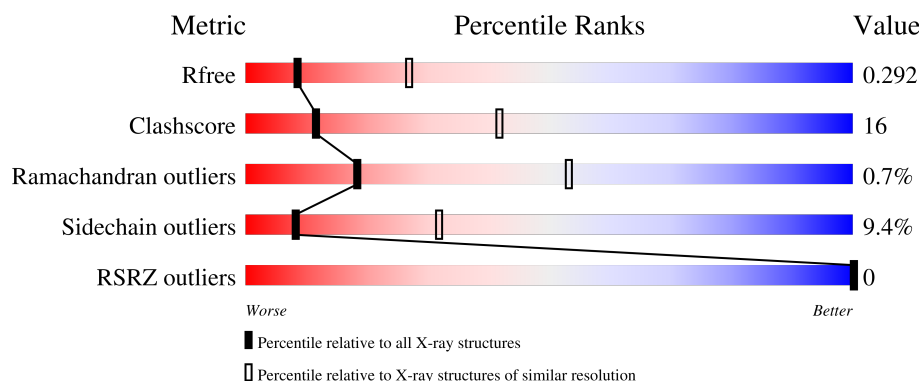
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	223	
1	B	223	
1	C	223	
1	D	223	
2	E	9	

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Mol	Chain	Length	Quality of chain
3	F	8	38% 62%
3	H	8	25% 38% 38%
4	G	10	10% 60% 30%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7397 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 Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1678	1073	285	314	6			
1	B	208	Total	C	N	O	S	0	0	0
			1686	1077	287	316	6			
1	C	206	Total	C	N	O	S	0	0	0
			1678	1073	285	314	6			
1	D	208	Total	C	N	O	S	0	0	0
			1686	1077	287	316	6			

There are 40 discrepancies between the modelled and reference sequences:

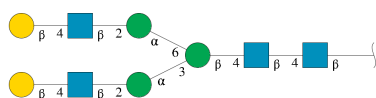
Chain	Residue	Modelled	Actual	Comment	Reference
A	137	ARG	ASP	conflict	UNP P0DOX5
A	139	TRP	LEU	conflict	UNP P0DOX5
A	140	ARG	THR	conflict	UNP P0DOX5
A	142	GLU	ASN	conflict	UNP P0DOX5
A	143	GLU	GLN	conflict	UNP P0DOX5
A	194	GLU	ASP	conflict	UNP P0DOX5
A	195	ALA	LYS	conflict	UNP P0DOX5
A	199	TRP	GLN	conflict	UNP P0DOX5
A	220	TRP	LYS	conflict	UNP P0DOX5
A	224	ARG	LEU	conflict	UNP P0DOX5
B	137	ARG	ASP	conflict	UNP P0DOX5
B	139	TRP	LEU	conflict	UNP P0DOX5
B	140	ARG	THR	conflict	UNP P0DOX5
B	142	GLU	ASN	conflict	UNP P0DOX5
B	143	GLU	GLN	conflict	UNP P0DOX5
B	194	GLU	ASP	conflict	UNP P0DOX5
B	195	ALA	LYS	conflict	UNP P0DOX5
B	199	TRP	GLN	conflict	UNP P0DOX5
B	220	TRP	LYS	conflict	UNP P0DOX5
B	224	ARG	LEU	conflict	UNP P0DOX5
C	137	ARG	ASP	conflict	UNP P0DOX5

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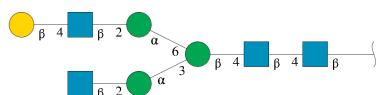
Chain	Residue	Modelled	Actual	Comment	Reference
C	139	TRP	LEU	conflict	UNP P0DOX5
C	140	ARG	THR	conflict	UNP P0DOX5
C	142	GLU	ASN	conflict	UNP P0DOX5
C	143	GLU	GLN	conflict	UNP P0DOX5
C	194	GLU	ASP	conflict	UNP P0DOX5
C	195	ALA	LYS	conflict	UNP P0DOX5
C	199	TRP	GLN	conflict	UNP P0DOX5
C	220	TRP	LYS	conflict	UNP P0DOX5
C	224	ARG	LEU	conflict	UNP P0DOX5
D	137	ARG	ASP	conflict	UNP P0DOX5
D	139	TRP	LEU	conflict	UNP P0DOX5
D	140	ARG	THR	conflict	UNP P0DOX5
D	142	GLU	ASN	conflict	UNP P0DOX5
D	143	GLU	GLN	conflict	UNP P0DOX5
D	194	GLU	ASP	conflict	UNP P0DOX5
D	195	ALA	LYS	conflict	UNP P0DOX5
D	199	TRP	GLN	conflict	UNP P0DOX5
D	220	TRP	LYS	conflict	UNP P0DOX5
D	224	ARG	LEU	conflict	UNP P0DOX5

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



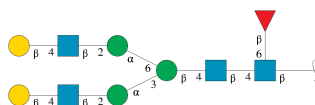
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	9	Total	C	N	O	0	0	0
			111	62	4	45			

- 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)-2-acetamido-2-deoxy-beta-D-glucopyranose.



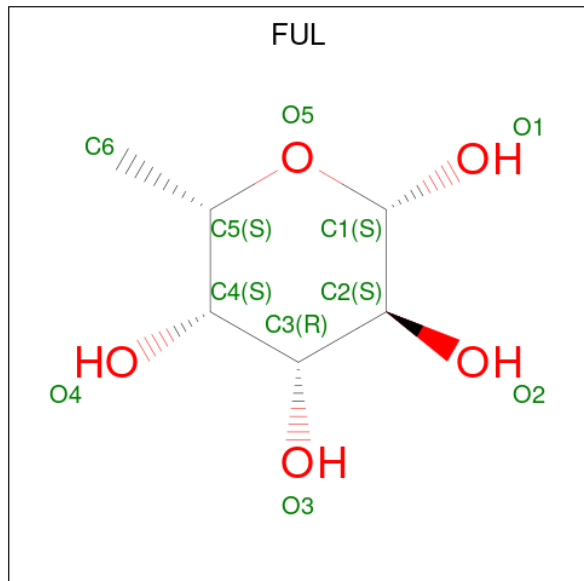
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	8	Total	C	N	O	0	0	0
			100	56	4	40			
3	H	8	Total	C	N	O	0	0	0
			100	56	4	40			

- Molecule 4 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	10	Total	C	N	O	0	0	0
			121	68	4	49			

- Molecule 5 is beta-L-fucopyranose (CCD ID: FUL) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		

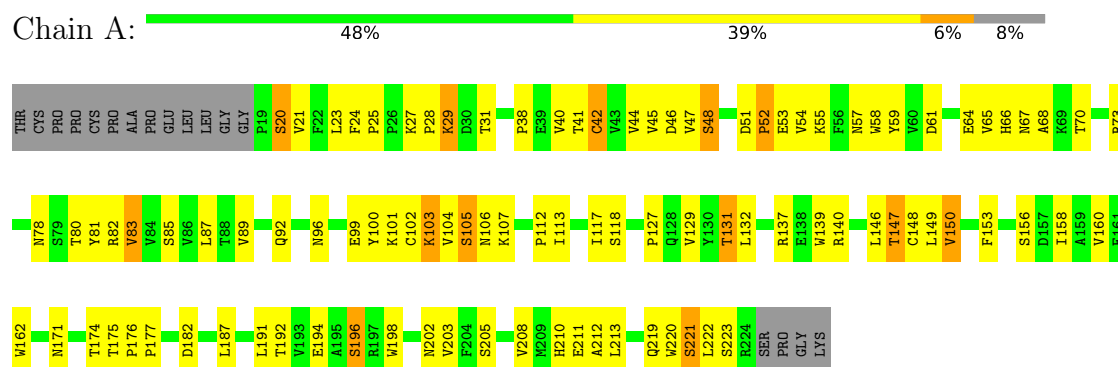
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	59	Total 59	O 59	0	0
6	B	54	Total 54	O 54	0	0
6	C	53	Total 53	O 53	0	0
6	D	61	Total 61	O 61	0	0

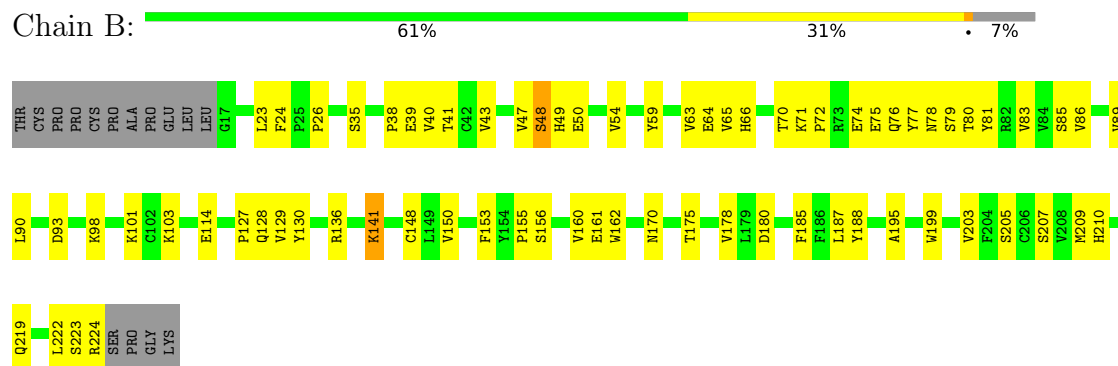
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

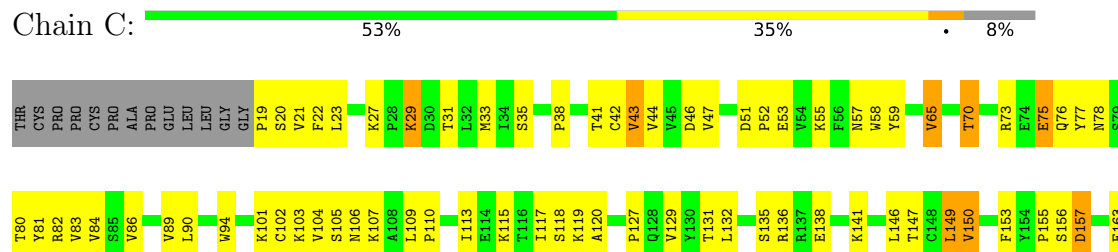
- Molecule 1: Immunoglobulin gamma-1 heavy chain



- Molecule 1: Immunoglobulin gamma-1 heavy chain



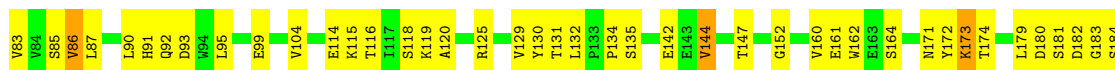
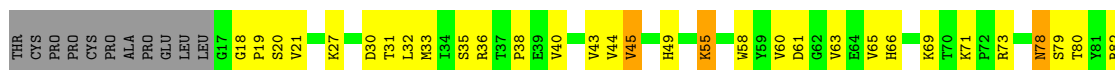
- Molecule 1: Immunoglobulin gamma-1 heavy chain





- Molecule 1: Immunoglobulin gamma-1 heavy chain

Chain D: 56% 34% 7%



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

Chain E: 11% 89%



- 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

Chain F: 38% 62%



- 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

Chain H: 25% 38% 38%



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

ta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranos
e

Chain G:  10% 60% 30%

MAG1
MAG2
BMA3
MAN4
NAG5
GAL6
MAN7
NAG8
GAL9
FUL10

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.99Å 101.63Å 146.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.99 – 3.00 14.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.2 (14.99-3.00) 95.4 (14.99-3.00)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.214 , 0.279 0.227 , 0.292	Depositor DCC
R_{free} test set	1120 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	63.2	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 63.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7397	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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

5.1 Standard geometry

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

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	0.26	0/1730	0.44	0/2359
1	B	0.27	0/1738	0.46	0/2370
1	C	0.24	0/1730	0.51	2/2359 (0.1%)
1	D	0.24	0/1738	0.47	0/2370
All	All	0.25	0/6936	0.47	2/9458 (0.0%)

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
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	70	THR	CA-C-N	-5.01	117.87	122.28
1	C	70	THR	C-N-CA	-5.01	117.87	122.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	LYS	Peptide
1	C	65	VAL	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	1678	0	1633	70	0
1	B	1686	0	1636	47	0
1	C	1678	0	1633	57	0
1	D	1686	0	1638	51	0
2	E	111	0	94	1	0
3	F	100	0	85	3	0
3	H	100	0	85	3	0
4	G	121	0	103	4	0
5	A	10	0	10	0	0
6	A	59	0	0	2	0
6	B	54	0	0	0	0
6	C	53	0	0	4	0
6	D	61	0	0	2	0
All	All	7397	0	6917	226	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 16.

All (226) 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:132:LEU:HB2	1:A:147:THR:HG23	1.61	0.83
1:C:127:PRO:HB3	1:C:153:PHE:HB3	1.62	0.81
1:D:152:GLY:HA2	1:D:184:SER:HB2	1.64	0.80
1:D:21:VAL:HG21	1:D:104:VAL:HG21	1.64	0.79
1:B:127:PRO:HB3	1:B:153:PHE:HB3	1.66	0.77
1:D:69:LYS:HB3	1:D:86:VAL:HG13	1.69	0.75
1:C:129:VAL:HG22	1:C:150:VAL:HG13	1.70	0.73
1:A:104:VAL:HG22	1:A:113:ILE:H	1.52	0.73
1:C:77:TYR:HD1	1:C:78:ASN:H	1.37	0.73
1:A:105:SER:OG	1:A:106:ASN:N	2.20	0.72
1:C:59:TYR:HB2	1:C:101:LYS:HB2	1.71	0.71
1:D:129:VAL:HG21	1:D:208:VAL:HG21	1.73	0.71
1:B:54:VAL:HG21	1:B:83:VAL:HG11	1.72	0.70
1:C:76:GLN:HB3	1:C:81:TYR:HA	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:THR:HG22	1:B:178:VAL:HG21	1.73	0.69
1:A:99:GLU:HG2	1:A:118:SER:HB2	1.76	0.68
1:A:73:ARG:HG2	1:A:83:VAL:HG22	1.74	0.67
1:A:78:ASN:ND2	6:A:402:HOH:O	2.28	0.67
1:A:46:ASP:OD1	1:A:78:ASN:ND2	2.28	0.67
1:D:66:HIS:O	6:D:301:HOH:O	2.13	0.66
1:C:29:LYS:NZ	6:C:302:HOH:O	2.21	0.66
1:B:49:HIS:NE2	1:B:75:GLU:OE1	2.30	0.65
1:C:163:GLU:OE2	6:C:301:HOH:O	2.13	0.65
1:D:173:LYS:NZ	6:D:303:HOH:O	2.29	0.65
1:C:23:LEU:HD23	1:C:117:ILE:HB	1.78	0.64
1:B:41:THR:HG23	1:B:86:VAL:HG22	1.79	0.64
1:D:90:LEU:HD23	1:D:92:GLN:HE21	1.63	0.64
1:A:127:PRO:HB3	1:A:153:PHE:HB3	1.79	0.64
1:B:150:VAL:HB	1:B:187:LEU:HG	1.80	0.64
1:C:47:VAL:HG12	1:C:52:PRO:HA	1.81	0.63
1:C:127:PRO:HB2	1:C:150:VAL:HG12	1.80	0.63
1:B:41:THR:HG21	3:F:5:NAG:H61	1.81	0.63
1:C:22:PHE:HD1	4:G:6:GAL:H62	1.64	0.62
1:D:78:ASN:HB2	1:D:80:THR:HG23	1.80	0.62
1:D:40:VAL:HG23	1:D:87:LEU:HB3	1.81	0.62
1:A:129:VAL:HG13	1:A:220:TRP:CD1	2.35	0.62
1:A:54:VAL:HG22	1:A:105:SER:HB2	1.81	0.61
3:H:7:MAN:H2	3:H:8:NAG:H83	1.82	0.61
1:A:205:SER:HB3	1:A:221:SER:HA	1.81	0.61
1:C:146:LEU:HD12	1:C:191:LEU:HD23	1.83	0.60
1:D:134:PRO:HG3	1:D:144:VAL:HG13	1.84	0.60
1:D:73:ARG:HG3	1:D:83:VAL:HG22	1.84	0.59
6:C:343:HOH:O	4:G:5:NAG:O7	2.16	0.59
1:A:104:VAL:HG21	1:A:112:PRO:HA	1.85	0.59
1:D:45:VAL:HG23	1:D:82:ARG:HG3	1.84	0.59
1:D:164:SER:HB2	1:D:204:PHE:CD2	2.37	0.59
1:C:77:TYR:HD1	1:C:78:ASN:N	2.01	0.58
1:A:38:PRO:HB2	1:A:89:VAL:HB	1.86	0.58
1:C:19:PRO:HA	1:C:46:ASP:HB2	1.86	0.58
1:A:54:VAL:HA	1:A:105:SER:HA	1.86	0.58
1:D:208:VAL:HG23	1:D:218:THR:HG23	1.86	0.58
1:C:75:GLU:HA	1:C:81:TYR:HE1	1.69	0.57
1:C:209:MET:HG2	1:C:217:TYR:HE1	1.68	0.57
1:D:31:THR:HG22	1:D:32:LEU:H	1.71	0.56
1:D:203:VAL:HA	1:D:223:SER:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ARG:HA	1:B:224:ARG:NE	2.21	0.56
3:F:7:MAN:H2	3:F:8:NAG:H83	1.87	0.55
1:C:175:THR:HG23	1:C:188:TYR:O	2.07	0.55
1:D:21:VAL:HG22	1:D:44:VAL:HG13	1.88	0.55
1:A:57:ASN:HB2	1:A:103:LYS:HD2	1.88	0.55
1:D:179:LEU:HD21	1:D:183:GLY:HA2	1.88	0.55
1:A:59:TYR:HD1	1:A:64:GLU:HA	1.72	0.55
1:A:198:TRP:CZ3	1:A:223:SER:HA	2.42	0.54
1:A:46:ASP:HA	1:A:80:THR:HG21	1.89	0.54
1:A:28:PRO:HD2	1:A:29:LYS:NZ	2.23	0.54
1:D:30:ASP:OD1	1:D:36:ARG:NH2	2.34	0.54
1:A:160:VAL:HG22	1:A:208:VAL:HG22	1.89	0.54
1:C:73:ARG:NH2	6:C:303:HOH:O	2.26	0.54
1:C:209:MET:HG2	1:C:217:TYR:CE1	2.43	0.53
1:C:27:LYS:HE2	4:G:9:GAL:H2	1.90	0.53
1:D:31:THR:O	1:D:33:MET:N	2.38	0.53
1:B:59:TYR:HB2	1:B:101:LYS:HB3	1.90	0.53
1:C:109:LEU:HD22	1:C:113:ILE:HD12	1.91	0.53
1:A:23:LEU:HD23	1:A:117:ILE:HB	1.90	0.53
1:B:65:VAL:HG12	1:B:66:HIS:H	1.73	0.53
1:B:161:GLU:HG3	1:B:207:SER:HB2	1.90	0.53
1:D:95:LEU:HA	1:D:119:LYS:HE2	1.91	0.53
1:D:142:GLU:H	1:D:142:GLU:CD	2.16	0.53
1:B:160:VAL:HG21	1:B:187:LEU:HD11	1.89	0.53
1:B:155:PRO:HD2	1:B:210:HIS:HE1	1.74	0.53
1:A:139:TRP:O	1:A:140:ARG:HB2	2.09	0.52
1:C:131:THR:HB	1:C:222:LEU:HG	1.91	0.52
1:C:138:GLU:HA	1:C:141:LYS:HG2	1.90	0.52
1:D:99:GLU:HA	1:D:118:SER:HB3	1.92	0.52
1:D:119:LYS:HG2	1:D:120:ALA:H	1.73	0.52
1:A:210:HIS:CD2	1:A:212:ALA:H	2.27	0.52
1:B:78:ASN:HB2	1:B:80:THR:OG1	2.10	0.52
1:D:49:HIS:NE2	1:D:79:SER:HA	2.25	0.52
1:C:47:VAL:CG1	1:C:52:PRO:HA	2.40	0.51
1:A:66:HIS:C	1:A:68:ALA:H	2.19	0.51
1:A:140:ARG:NH2	6:A:401:HOH:O	2.20	0.51
1:A:205:SER:HB2	1:A:219:GLN:HE21	1.74	0.51
1:D:218:THR:OG1	1:D:219:GLN:N	2.42	0.51
1:A:160:VAL:HB	1:A:174:THR:HG21	1.92	0.51
1:B:136:ARG:HH11	1:B:136:ARG:HG2	1.76	0.51
1:C:31:THR:HG21	1:C:94:TRP:HD1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:PRO:HB2	1:C:89:VAL:HG22	1.94	0.50
1:A:44:VAL:O	1:A:82:ARG:HA	2.12	0.50
1:B:128:GLN:HG2	1:B:130:TYR:CE1	2.47	0.50
1:D:60:VAL:HG23	1:D:65:VAL:HG21	1.93	0.50
1:A:42:CYS:HB2	1:A:58:TRP:CZ2	2.47	0.50
1:C:115:LYS:HE3	4:G:6:GAL:H4	1.93	0.50
1:C:174:THR:HG23	1:C:189:SER:HB2	1.94	0.50
1:A:21:VAL:HG11	1:A:113:ILE:HD12	1.93	0.50
1:B:155:PRO:HD2	1:B:210:HIS:CE1	2.46	0.50
1:C:75:GLU:HA	1:C:81:TYR:CE1	2.46	0.50
1:A:59:TYR:HB2	1:A:101:LYS:HB2	1.94	0.50
1:C:47:VAL:HB	1:C:81:TYR:HB3	1.92	0.50
1:A:45:VAL:O	1:A:47:VAL:HG23	2.12	0.49
1:A:70:THR:HA	1:A:85:SER:HA	1.92	0.49
1:B:23:LEU:HD12	1:B:24:PHE:H	1.78	0.49
1:D:131:THR:C	1:D:132:LEU:HD23	2.37	0.49
1:A:147:THR:HB	1:B:188:TYR:OH	2.12	0.49
1:B:70:THR:HA	1:B:85:SER:HA	1.94	0.49
1:B:48:SER:HB2	1:B:50:GLU:HG2	1.95	0.49
1:A:194:GLU:OE1	1:A:196:SER:OG	2.30	0.49
1:C:106:ASN:HB3	1:C:109:LEU:HD23	1.94	0.49
1:D:162:TRP:HE1	1:D:189:SER:HB3	1.78	0.49
1:C:77:TYR:O	1:C:80:THR:OG1	2.30	0.48
1:A:129:VAL:HG13	1:A:220:TRP:HD1	1.79	0.48
1:C:53:GLU:OE2	1:C:107:LYS:HG3	2.13	0.48
1:D:114:GLU:O	1:D:115:LYS:HG2	2.13	0.48
1:C:149:LEU:HB2	1:C:188:TYR:CE2	2.49	0.48
1:A:127:PRO:HB2	1:A:150:VAL:HG23	1.95	0.47
1:C:55:LYS:O	1:C:104:VAL:HA	2.15	0.47
3:H:7:MAN:H2	3:H:8:NAG:H2	1.62	0.47
1:A:59:TYR:O	1:A:100:TYR:HA	2.15	0.47
1:B:224:ARG:HA	1:B:224:ARG:CZ	2.45	0.47
1:D:134:PRO:HG3	1:D:144:VAL:CG1	2.45	0.46
1:A:158:ILE:HG13	1:A:210:HIS:HB2	1.96	0.46
1:D:58:TRP:CE3	1:D:87:LEU:HD22	2.51	0.46
1:A:78:ASN:C	1:A:80:THR:H	2.22	0.46
1:A:205:SER:CB	1:A:219:GLN:HE21	2.28	0.46
1:B:59:TYR:HA	1:B:64:GLU:HA	1.98	0.46
1:B:195:ALA:O	1:B:199:TRP:CD1	2.69	0.46
1:B:205:SER:OG	1:B:219:GLN:HG2	2.15	0.46
1:B:26:PRO:HB3	1:B:39:GLU:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:GLN:HG2	1:B:130:TYR:CZ	2.50	0.46
1:D:38:PRO:HD3	1:D:91:HIS:NE2	2.31	0.46
1:B:103:LYS:HG3	1:B:114:GLU:HG2	1.97	0.46
1:C:27:LYS:HA	1:C:27:LYS:HD3	1.55	0.46
3:F:1:NAG:H4	3:F:2:NAG:HN2	1.81	0.46
1:A:146:LEU:HB2	1:A:191:LEU:HB3	1.98	0.46
1:B:38:PRO:HB2	1:B:89:VAL:HG23	1.98	0.46
1:B:90:LEU:HD12	1:B:93:ASP:OD2	2.15	0.46
1:B:71:LYS:HB3	1:B:72:PRO:HD2	1.98	0.45
1:B:209:MET:HE2	1:B:209:MET:HB3	1.57	0.45
1:C:77:TYR:CD1	1:C:78:ASN:N	2.83	0.45
1:C:141:LYS:HA	1:C:141:LYS:HD3	1.71	0.45
1:A:66:HIS:O	1:A:68:ALA:N	2.49	0.45
1:C:57:ASN:HB2	1:C:103:LYS:HB3	1.98	0.45
1:D:61:ASP:OD1	1:D:99:GLU:HG3	2.16	0.45
1:D:71:LYS:HD3	1:D:71:LYS:N	2.31	0.45
1:A:89:VAL:HG13	1:A:100:TYR:OH	2.17	0.45
1:B:48:SER:HB2	1:B:50:GLU:H	1.81	0.45
1:C:21:VAL:HG21	1:C:104:VAL:HG21	1.98	0.45
1:D:129:VAL:HB	1:D:220:TRP:CE3	2.52	0.45
1:A:52:PRO:HB2	1:A:53:GLU:H	1.64	0.45
1:C:51:ASP:HB3	1:C:53:GLU:OE2	2.17	0.45
1:B:148:CYS:HB2	1:B:162:TRP:CZ2	2.52	0.45
1:B:77:TYR:C	1:B:79:SER:H	2.25	0.44
1:A:182:ASP:OD1	1:A:182:ASP:N	2.38	0.44
1:B:47:VAL:CG2	1:B:81:TYR:HB2	2.47	0.44
1:A:53:GLU:HG2	1:A:55:LYS:NZ	2.33	0.44
1:B:74:GLU:OE1	1:B:76:GLN:NE2	2.51	0.44
1:A:137:ARG:NH1	1:B:129:VAL:O	2.51	0.44
1:C:51:ASP:O	1:C:106:ASN:ND2	2.47	0.44
1:A:65:VAL:HG12	1:A:66:HIS:O	2.18	0.43
1:A:27:LYS:HD3	1:A:27:LYS:HA	1.67	0.43
1:A:131:THR:HB	1:A:222:LEU:HD13	1.99	0.43
1:A:160:VAL:HG21	1:A:187:LEU:HD11	2.00	0.43
1:D:171:ASN:O	1:D:191:LEU:HD12	2.17	0.43
1:D:90:LEU:O	1:D:93:ASP:N	2.51	0.43
1:A:48:SER:CB	1:A:81:TYR:HB2	2.49	0.43
1:A:92:GLN:O	1:A:96:ASN:ND2	2.51	0.43
1:A:106:ASN:HB3	1:A:107:LYS:H	1.62	0.43
1:A:20:SER:H	1:A:47:VAL:CG2	2.31	0.43
1:C:55:LYS:HB3	1:C:105:SER:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:LYS:HD2	1:D:55:LYS:HA	1.66	0.43
1:C:193:VAL:HG21	1:C:204:PHE:CZ	2.54	0.43
1:A:78:ASN:O	1:A:80:THR:HG23	2.18	0.42
1:D:58:TRP:HB3	1:D:65:VAL:HG23	2.01	0.42
1:D:125:ARG:HD2	1:D:125:ARG:HA	1.72	0.42
1:B:93:ASP:HB3	1:B:98:LYS:HD2	2.01	0.42
1:C:23:LEU:HD11	1:C:58:TRP:CH2	2.55	0.42
1:D:27:LYS:O	1:D:30:ASP:HB2	2.19	0.42
1:D:31:THR:C	1:D:33:MET:H	2.24	0.42
1:A:171:ASN:ND2	1:A:192:THR:HB	2.35	0.42
1:A:208:VAL:HG12	1:A:213:LEU:HD11	2.02	0.42
1:C:43:VAL:HB	1:C:84:VAL:HG12	2.00	0.42
1:D:182:ASP:HB2	1:D:184:SER:OG	2.20	0.42
1:A:24:PHE:HA	1:A:25:PRO:HD3	1.85	0.42
1:B:224:ARG:HH11	1:B:224:ARG:HG2	1.84	0.42
1:A:202:ASN:OD1	1:A:202:ASN:N	2.52	0.42
1:B:153:PHE:CE2	1:B:185:PHE:HB2	2.55	0.41
1:C:44:VAL:O	1:C:82:ARG:HA	2.21	0.41
1:D:45:VAL:HG21	3:H:1:NAG:O4	2.19	0.41
1:C:29:LYS:HB2	1:C:29:LYS:HE2	1.80	0.41
1:A:127:PRO:HG2	1:A:213:LEU:HD21	2.00	0.41
1:B:141:LYS:HA	1:B:141:LYS:HD2	1.71	0.41
1:C:127:PRO:CB	1:C:153:PHE:HB3	2.42	0.41
1:C:135:SER:HB2	1:D:130:TYR:HB3	2.03	0.41
1:A:20:SER:H	1:A:47:VAL:HG22	1.85	0.41
1:A:40:VAL:HG23	1:A:87:LEU:HB3	2.01	0.41
1:A:41:THR:HG21	2:E:8:NAG:H61	2.01	0.41
1:C:136:ARG:H	1:C:136:ARG:HG2	1.73	0.41
1:D:179:LEU:HD23	1:D:180:ASP:O	2.20	0.41
1:B:23:LEU:HD12	1:B:24:PHE:N	2.35	0.41
1:D:161:GLU:HG3	1:D:172:TYR:OH	2.20	0.41
1:C:70:THR:HA	1:C:86:VAL:O	2.20	0.41
1:B:222:LEU:HD12	1:B:222:LEU:HA	1.92	0.41
1:B:65:VAL:HG12	1:B:66:HIS:N	2.35	0.41
1:C:43:VAL:HA	1:C:84:VAL:HA	2.03	0.41
1:D:18:GLY:N	1:D:19:PRO:HD2	2.36	0.41
1:D:60:VAL:O	1:D:63:VAL:HG22	2.20	0.41
1:B:136:ARG:HG2	1:B:136:ARG:NH1	2.36	0.41
1:C:42:CYS:HB2	1:C:58:TRP:CH2	2.56	0.41
1:A:203:VAL:HA	1:A:223:SER:HB3	2.02	0.40
1:C:155:PRO:HB2	1:C:157:ASP:OD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:LYS:HA	1:D:27:LYS:HD3	1.67	0.40
1:A:162:TRP:CD2	1:A:191:LEU:HB2	2.56	0.40
1:A:176:PRO:HA	1:A:177:PRO:HD3	2.00	0.40
1:C:42:CYS:HG	1:C:102:CYS:HG	1.67	0.40
1:A:104:VAL:HG22	1:A:113:ILE:HG12	2.04	0.40
1:B:59:TYR:CD1	1:B:64:GLU:HB3	2.57	0.40
1:C:33:MET:HG3	1:C:217:TYR:OH	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	204/223 (92%)	187 (92%)	14 (7%)	3 (2%)	8	35
1	B	206/223 (92%)	192 (93%)	14 (7%)	0	100	100
1	C	204/223 (92%)	183 (90%)	18 (9%)	3 (2%)	8	35
1	D	206/223 (92%)	187 (91%)	19 (9%)	0	100	100
All	All	820/892 (92%)	749 (91%)	65 (8%)	6 (1%)	18	53

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	119	LYS
1	C	120	ALA
1	A	52	PRO
1	A	67	ASN
1	C	110	PRO
1	A	105	SER

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	192/205 (94%)	174 (91%)	18 (9%)	8	32
1	B	192/205 (94%)	180 (94%)	12 (6%)	16	48
1	C	192/205 (94%)	169 (88%)	23 (12%)	5	22
1	D	192/205 (94%)	173 (90%)	19 (10%)	7	30
All	All	768/820 (94%)	696 (91%)	72 (9%)	8	32

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	SER
1	A	29	LYS
1	A	31	THR
1	A	42	CYS
1	A	48	SER
1	A	51	ASP
1	A	61	ASP
1	A	83	VAL
1	A	102	CYS
1	A	131	THR
1	A	147	THR
1	A	148	CYS
1	A	149	LEU
1	A	150	VAL
1	A	156	SER
1	A	196	SER
1	A	211	GLU
1	A	221	SER
1	B	35	SER
1	B	40	VAL
1	B	43	VAL
1	B	48	SER
1	B	63	VAL
1	B	141	LYS

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Mol	Chain	Res	Type
1	B	156	SER
1	B	170	ASN
1	B	175	THR
1	B	180	ASP
1	B	203	VAL
1	B	223	SER
1	C	20	SER
1	C	29	LYS
1	C	35	SER
1	C	41	THR
1	C	43	VAL
1	C	65	VAL
1	C	75	GLU
1	C	83	VAL
1	C	90	LEU
1	C	118	SER
1	C	132	LEU
1	C	147	THR
1	C	149	LEU
1	C	150	VAL
1	C	156	SER
1	C	157	ASP
1	C	173	LYS
1	C	174	THR
1	C	196	SER
1	C	203	VAL
1	C	207	SER
1	C	221	SER
1	C	223	SER
1	D	20	SER
1	D	35	SER
1	D	43	VAL
1	D	45	VAL
1	D	55	LYS
1	D	78	ASN
1	D	85	SER
1	D	86	VAL
1	D	116	THR
1	D	135	SER
1	D	144	VAL
1	D	147	THR
1	D	160	VAL

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Mol	Chain	Res	Type
1	D	173	LYS
1	D	174	THR
1	D	181	SER
1	D	189	SER
1	D	218	THR
1	D	222	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	219	GLN
1	B	123	GLN
1	B	219	GLN
1	C	219	GLN
1	D	92	GLN
1	D	200	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 ⓘ

35 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	NAG	E	1	2	14,14,15	0.62	1 (7%)	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	2	2	14,14,15	0.36	0	17,19,21	0.78	0
2	BMA	E	3	2	11,11,12	0.77	0	15,15,17	1.27	2 (13%)
2	MAN	E	4	2	11,11,12	1.22	1 (9%)	15,15,17	1.53	1 (6%)
2	NAG	E	5	2	14,14,15	0.91	1 (7%)	17,19,21	0.98	2 (11%)
2	GAL	E	6	2	11,11,12	1.40	2 (18%)	15,15,17	1.09	1 (6%)
2	MAN	E	7	2	11,11,12	1.01	1 (9%)	15,15,17	1.11	2 (13%)
2	NAG	E	8	2	14,14,15	0.36	0	17,19,21	0.61	0
2	GAL	E	9	2	11,11,12	1.62	4 (36%)	15,15,17	1.00	1 (6%)
3	NAG	F	1	3	14,14,15	0.70	1 (7%)	17,19,21	1.06	1 (5%)
3	NAG	F	2	3	14,14,15	0.40	0	17,19,21	1.32	1 (5%)
3	BMA	F	3	3	11,11,12	1.10	1 (9%)	15,15,17	1.16	2 (13%)
3	MAN	F	4	3	11,11,12	0.95	1 (9%)	15,15,17	0.97	1 (6%)
3	NAG	F	5	3	14,14,15	0.80	1 (7%)	17,19,21	0.79	0
3	GAL	F	6	3	11,11,12	1.15	1 (9%)	15,15,17	0.94	0
3	MAN	F	7	3	11,11,12	1.07	1 (9%)	15,15,17	1.24	2 (13%)
3	NAG	F	8	3	14,14,15	1.27	2 (14%)	17,19,21	1.19	1 (5%)
4	NAG	G	1	4	14,14,15	0.49	0	17,19,21	0.59	0
4	FUL	G	10	4	10,10,11	1.87	3 (30%)	14,14,16	1.98	2 (14%)
4	NAG	G	2	4	14,14,15	0.58	1 (7%)	17,19,21	0.49	0
4	BMA	G	3	4	11,11,12	1.10	1 (9%)	15,15,17	1.64	4 (26%)
4	MAN	G	4	4	11,11,12	1.31	2 (18%)	15,15,17	1.02	1 (6%)
4	NAG	G	5	4	14,14,15	1.04	1 (7%)	17,19,21	1.39	3 (17%)
4	GAL	G	6	4	11,11,12	1.11	1 (9%)	15,15,17	1.10	1 (6%)
4	MAN	G	7	4	11,11,12	1.43	3 (27%)	15,15,17	2.04	3 (20%)
4	NAG	G	8	4	14,14,15	0.42	0	17,19,21	1.04	1 (5%)
4	GAL	G	9	4	11,11,12	1.67	2 (18%)	15,15,17	0.97	0
3	NAG	H	1	3	14,14,15	0.64	0	17,19,21	0.91	1 (5%)
3	NAG	H	2	3	14,14,15	0.45	0	17,19,21	0.45	0
3	BMA	H	3	3	11,11,12	1.07	1 (9%)	15,15,17	0.79	0
3	MAN	H	4	3	11,11,12	1.09	0	15,15,17	1.50	2 (13%)
3	NAG	H	5	3	14,14,15	0.22	0	17,19,21	0.52	0
3	GAL	H	6	3	11,11,12	1.26	1 (9%)	15,15,17	1.19	0
3	MAN	H	7	3	11,11,12	0.72	0	15,15,17	1.34	2 (13%)
3	NAG	H	8	3	14,14,15	1.08	1 (7%)	17,19,21	1.11	1 (5%)

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	NAG	E	1	2	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	2/2/19/22	1/1/1/1
2	NAG	E	5	2	-	4/6/23/26	0/1/1/1
2	GAL	E	6	2	-	1/2/19/22	0/1/1/1
2	MAN	E	7	2	-	2/2/19/22	0/1/1/1
2	NAG	E	8	2	-	4/6/23/26	0/1/1/1
2	GAL	E	9	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	3	-	3/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
3	MAN	F	4	3	-	2/2/19/22	0/1/1/1
3	NAG	F	5	3	-	4/6/23/26	0/1/1/1
3	GAL	F	6	3	-	0/2/19/22	0/1/1/1
3	MAN	F	7	3	-	1/2/19/22	0/1/1/1
3	NAG	F	8	3	-	3/6/23/26	0/1/1/1
4	NAG	G	1	4	-	2/6/23/26	0/1/1/1
4	FUL	G	10	4	-	-	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	0/1/1/1
4	MAN	G	4	4	-	2/2/19/22	0/1/1/1
4	NAG	G	5	4	-	1/6/23/26	0/1/1/1
4	GAL	G	6	4	-	2/2/19/22	0/1/1/1
4	MAN	G	7	4	-	0/2/19/22	0/1/1/1
4	NAG	G	8	4	-	4/6/23/26	0/1/1/1
4	GAL	G	9	4	-	0/2/19/22	0/1/1/1
3	NAG	H	1	3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	BMA	H	3	3	-	0/2/19/22	0/1/1/1
3	MAN	H	4	3	-	0/2/19/22	0/1/1/1
3	NAG	H	5	3	-	2/6/23/26	0/1/1/1
3	GAL	H	6	3	-	1/2/19/22	0/1/1/1
3	MAN	H	7	3	-	2/2/19/22	0/1/1/1
3	NAG	H	8	3	-	4/6/23/26	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	10	FUL	O5-C1	4.34	1.51	1.43
3	F	8	NAG	O5-C1	4.14	1.50	1.43
2	E	4	MAN	O5-C5	3.64	1.50	1.43
3	H	8	NAG	O5-C1	3.59	1.49	1.43
4	G	5	NAG	O5-C1	-3.47	1.37	1.43
4	G	9	GAL	C2-C3	3.26	1.57	1.52
2	E	5	NAG	O5-C1	-3.15	1.38	1.43
2	E	6	GAL	C4-C3	3.11	1.60	1.52
3	F	3	BMA	O5-C5	2.97	1.49	1.43
4	G	7	MAN	O5-C5	2.92	1.49	1.43
2	E	9	GAL	C1-C2	2.91	1.59	1.52
4	G	3	BMA	C2-C3	2.76	1.56	1.52
3	F	5	NAG	C1-C2	2.69	1.56	1.52
4	G	4	MAN	O5-C1	-2.68	1.39	1.43
4	G	10	FUL	O5-C5	2.61	1.48	1.43
3	F	4	MAN	O5-C1	-2.50	1.39	1.43
4	G	7	MAN	C1-C2	2.49	1.58	1.52
3	F	6	GAL	C1-C2	2.46	1.58	1.52
2	E	9	GAL	O5-C5	2.43	1.48	1.43
3	F	1	NAG	O5-C1	-2.40	1.39	1.43
3	H	6	GAL	C4-C5	2.38	1.58	1.53
4	G	10	FUL	C2-C3	-2.34	1.48	1.52
2	E	6	GAL	C4-C5	2.33	1.58	1.53
3	F	8	NAG	C1-C2	2.25	1.55	1.52
2	E	9	GAL	C4-C5	2.25	1.57	1.53
4	G	6	GAL	C1-C2	2.19	1.57	1.52
3	H	3	BMA	C4-C3	2.17	1.58	1.52
4	G	7	MAN	O5-C1	2.12	1.47	1.43
4	G	9	GAL	C4-C3	2.10	1.57	1.52
4	G	4	MAN	C1-C2	2.10	1.57	1.52
3	F	7	MAN	O5-C5	2.07	1.47	1.43
2	E	9	GAL	C4-C3	2.06	1.57	1.52
2	E	1	NAG	C1-C2	2.06	1.55	1.52
2	E	7	MAN	C1-C2	2.03	1.57	1.52
4	G	2	NAG	C1-C2	2.03	1.55	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	7	MAN	C1-O5-C5	6.36	120.71	112.19
2	E	4	MAN	C1-O5-C5	5.15	119.08	112.19
4	G	10	FUL	C3-C4-C5	5.02	117.44	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	8	NAG	C1-O5-C5	4.69	118.47	112.19
4	G	10	FUL	O5-C5-C4	4.37	117.41	109.55
3	H	8	NAG	C1-O5-C5	4.29	117.93	112.19
3	H	4	MAN	O2-C2-C3	-4.24	101.37	110.15
3	F	7	MAN	C1-O5-C5	3.94	117.47	112.19
3	H	7	MAN	C1-O5-C5	3.73	117.19	112.19
3	F	2	NAG	C3-C4-C5	3.70	116.94	110.23
4	G	5	NAG	C4-C3-C2	3.60	116.29	111.02
4	G	5	NAG	C3-C4-C5	3.54	116.64	110.23
4	G	8	NAG	C1-O5-C5	3.53	116.92	112.19
3	H	4	MAN	C1-O5-C5	3.43	116.78	112.19
3	H	1	NAG	C1-O5-C5	3.39	116.73	112.19
4	G	3	BMA	C2-C3-C4	3.33	116.71	110.86
2	E	3	BMA	C1-C2-C3	3.18	114.27	109.64
4	G	3	BMA	C1-C2-C3	3.09	114.14	109.64
3	F	1	NAG	C3-C4-C5	2.86	115.42	110.23
4	G	7	MAN	O2-C2-C3	-2.86	104.23	110.15
2	E	7	MAN	C1-O5-C5	2.80	115.94	112.19
2	E	5	NAG	C3-C4-C5	2.66	115.06	110.23
3	F	4	MAN	O2-C2-C3	-2.54	104.89	110.15
4	G	3	BMA	C3-C4-C5	2.45	114.68	110.23
2	E	5	NAG	C4-C3-C2	2.36	114.48	111.02
3	H	7	MAN	O2-C2-C3	-2.32	105.34	110.15
4	G	7	MAN	O5-C1-C2	2.31	116.31	110.79
2	E	6	GAL	O5-C1-C2	-2.30	105.30	110.79
3	F	3	BMA	C1-O5-C5	2.28	115.25	112.19
4	G	3	BMA	O3-C3-C4	-2.18	105.23	110.38
3	F	3	BMA	O5-C5-C6	2.17	111.89	107.66
4	G	5	NAG	C1-O5-C5	-2.16	109.30	112.19
4	G	4	MAN	O2-C2-C3	-2.14	105.71	110.15
3	F	7	MAN	O2-C2-C3	-2.12	105.75	110.15
2	E	7	MAN	O2-C2-C3	-2.12	105.75	110.15
4	G	6	GAL	O2-C2-C1	2.11	114.06	109.22
2	E	3	BMA	O2-C2-C3	-2.10	105.80	110.15
2	E	9	GAL	O2-C2-C1	2.06	113.95	109.22

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	5	NAG	O5-C5-C6-O6
3	F	4	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	H	7	MAN	O5-C5-C6-O6
3	H	8	NAG	O5-C5-C6-O6
3	H	7	MAN	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
3	F	4	MAN	C4-C5-C6-O6
2	E	4	MAN	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	E	5	NAG	C4-C5-C6-O6
4	G	6	GAL	O5-C5-C6-O6
4	G	4	MAN	C4-C5-C6-O6
3	H	8	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	5	NAG	C8-C7-N2-C2
2	E	5	NAG	O7-C7-N2-C2
2	E	8	NAG	C8-C7-N2-C2
2	E	8	NAG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	F	5	NAG	C8-C7-N2-C2
3	F	5	NAG	O7-C7-N2-C2
3	F	8	NAG	C8-C7-N2-C2
3	F	8	NAG	O7-C7-N2-C2
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
3	H	5	NAG	C8-C7-N2-C2
3	H	5	NAG	O7-C7-N2-C2
3	H	8	NAG	C8-C7-N2-C2
3	H	8	NAG	O7-C7-N2-C2
4	G	8	NAG	C8-C7-N2-C2
4	G	8	NAG	O7-C7-N2-C2
3	H	2	NAG	O5-C5-C6-O6
4	G	4	MAN	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
2	E	4	MAN	C4-C5-C6-O6
4	G	8	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	E	6	GAL	O5-C5-C6-O6
4	G	6	GAL	C4-C5-C6-O6
3	F	5	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
4	G	3	BMA	C4-C5-C6-O6
2	E	8	NAG	C4-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
2	E	7	MAN	C4-C5-C6-O6
3	H	6	GAL	O5-C5-C6-O6
2	E	8	NAG	O5-C5-C6-O6
3	F	7	MAN	C4-C5-C6-O6
3	F	8	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
4	G	5	NAG	C1-C2-N2-C7
4	G	8	NAG	C4-C5-C6-O6
2	E	7	MAN	O5-C5-C6-O6
3	F	5	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6

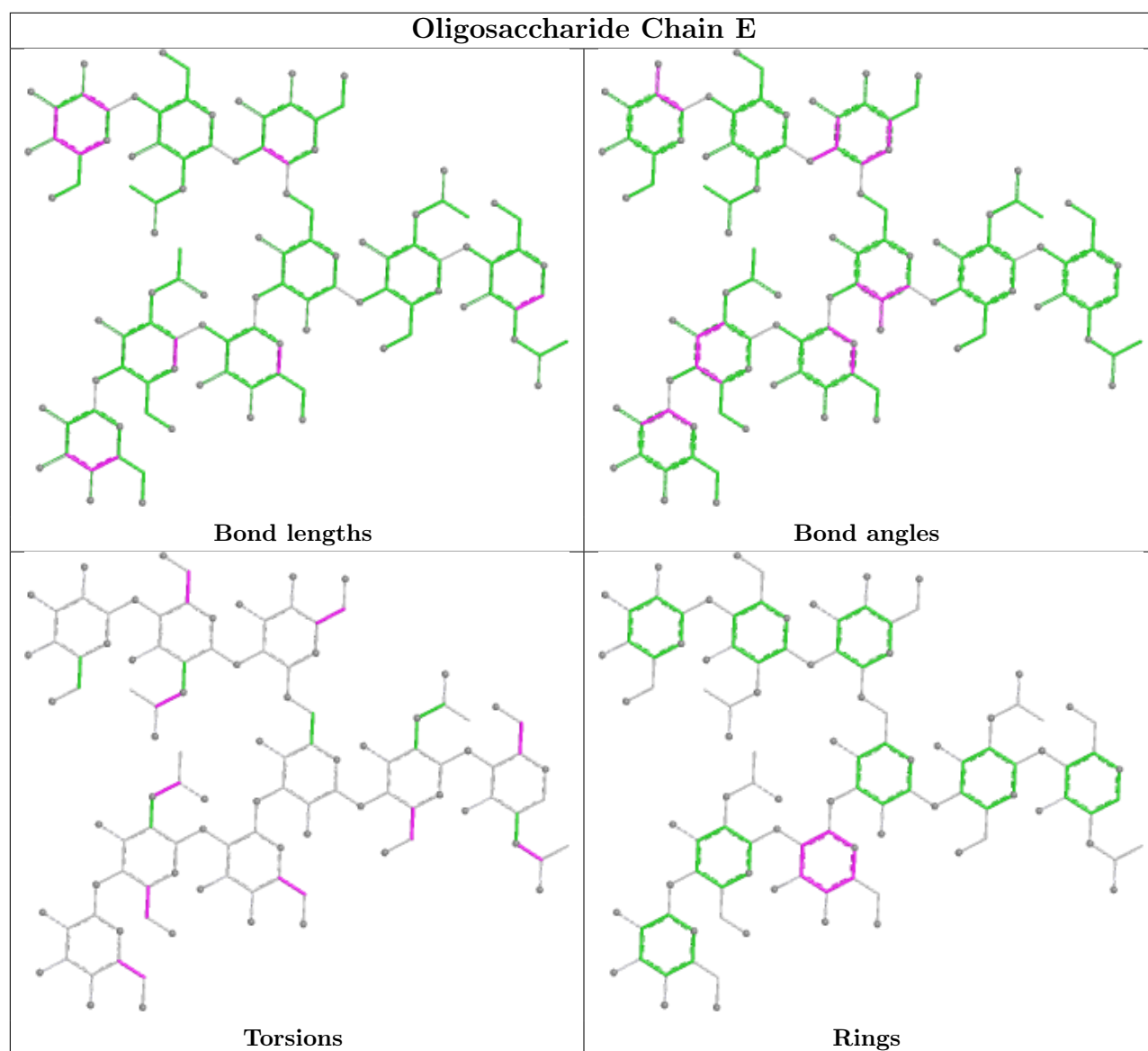
All (1) ring outliers are listed below:

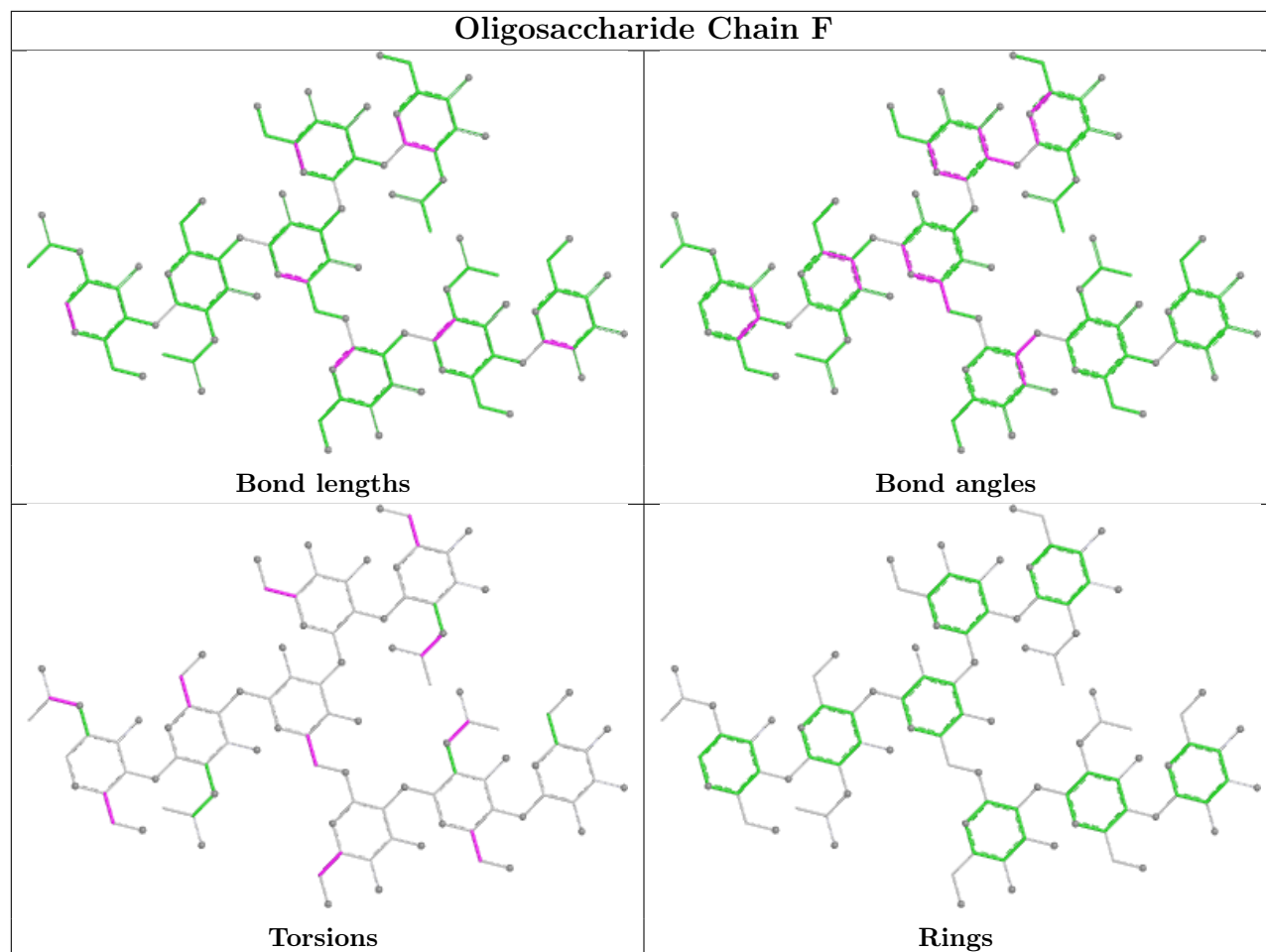
Mol	Chain	Res	Type	Atoms
2	E	4	MAN	C1-C2-C3-C4-C5-O5

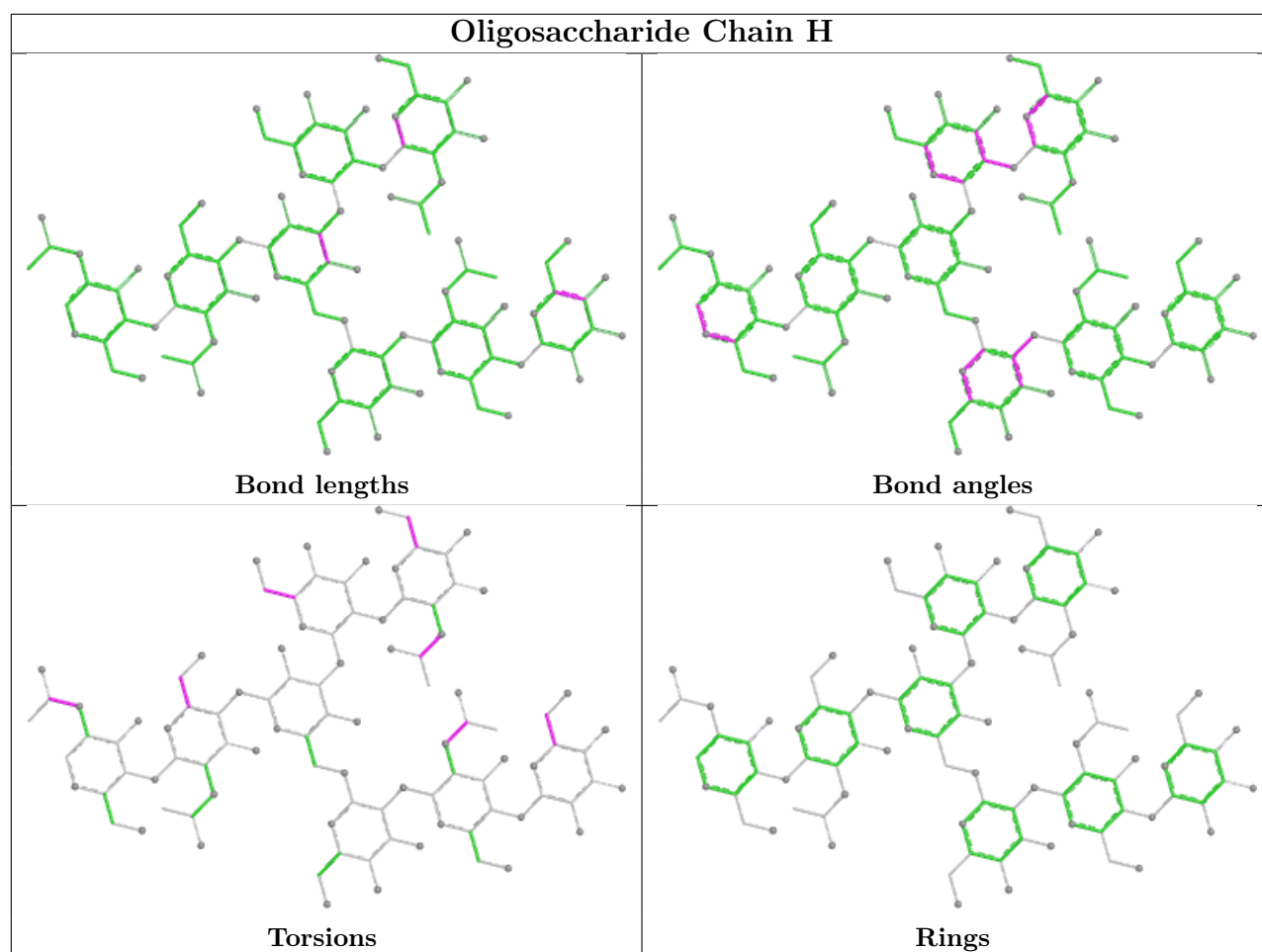
12 monomers are involved in 11 short contacts:

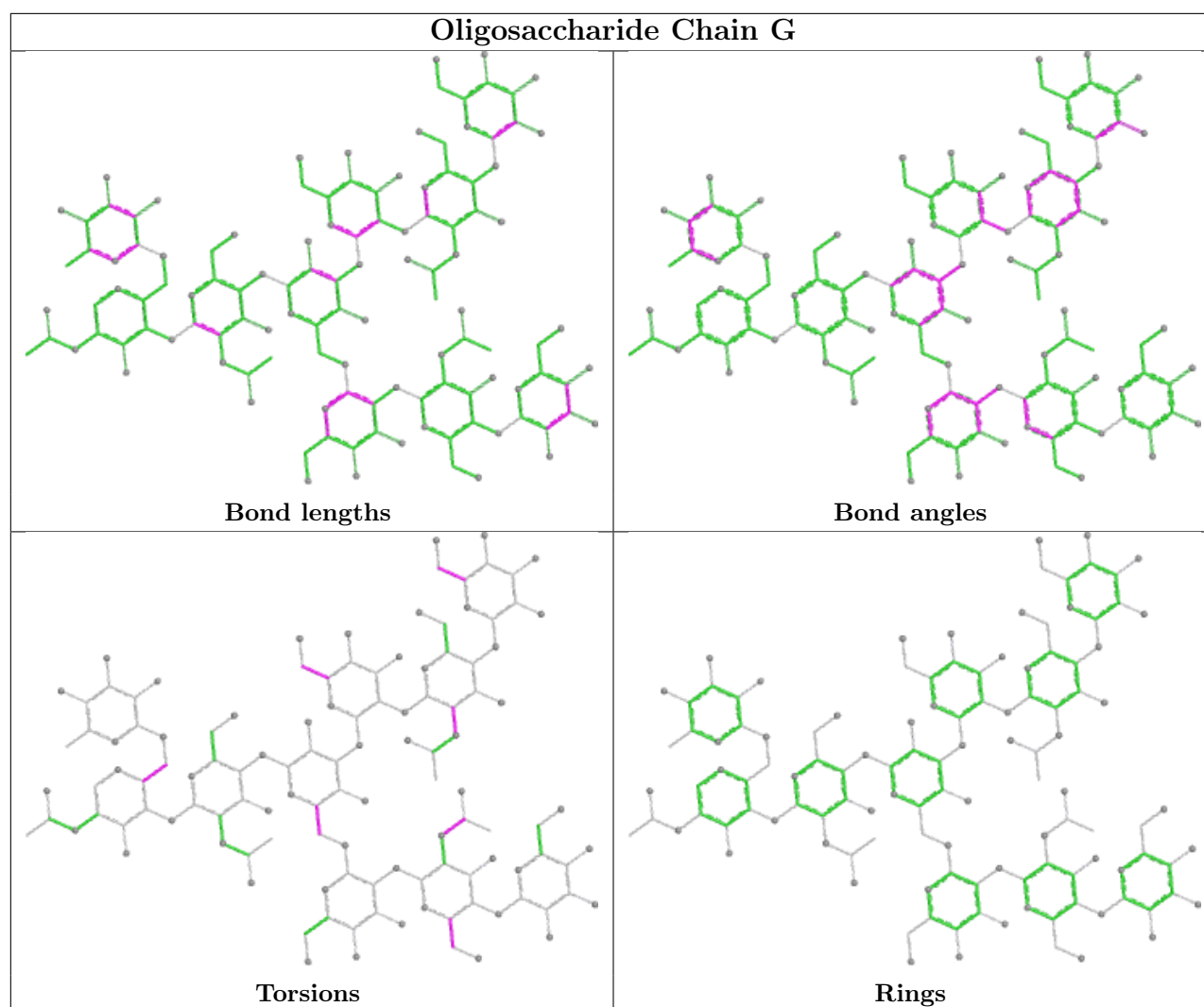
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	7	MAN	2	0
4	G	5	NAG	1	0
3	F	2	NAG	1	0
3	H	8	NAG	2	0
3	F	1	NAG	1	0
3	F	5	NAG	1	0
3	F	7	MAN	1	0
3	H	1	NAG	1	0
4	G	6	GAL	2	0
4	G	9	GAL	1	0
2	E	8	NAG	1	0
3	F	8	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
5	FUL	A	301	-	10,10,11	1.80	3 (30%)	14,14,16	1.51	2 (14%)

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	FUL	A	301	-	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	301	FUL	O5-C1	4.41	1.51	1.43
5	A	301	FUL	C2-C3	-2.11	1.49	1.52
5	A	301	FUL	O5-C5	2.09	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	301	FUL	C1-C2-C3	3.85	115.25	109.64
5	A	301	FUL	O5-C1-C2	2.15	115.92	110.79

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 [i](#)

There are no chain breaks in this entry.

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

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

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	206/223 (92%)	-0.53	0 100 100	30, 55, 101, 111	0
1	B	208/223 (93%)	-0.68	0 100 100	28, 53, 70, 75	0
1	C	206/223 (92%)	-0.62	0 100 100	32, 59, 90, 113	0
1	D	208/223 (93%)	-0.58	0 100 100	36, 64, 84, 92	0
All	All	828/892 (92%)	-0.60	0 100 100	28, 58, 89, 113	0

There are no RSRZ outliers to report.

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	F	1	14/15	0.34	0.16	66,86,94,95	0
2	NAG	E	1	14/15	0.43	0.15	98,110,115,115	0
3	NAG	F	8	14/15	0.54	0.11	118,124,126,127	0
3	MAN	F	7	11/12	0.61	0.15	100,117,121,123	0
3	GAL	F	6	11/12	0.61	0.16	81,93,103,108	0
4	FUL	G	10	10/11	0.61	0.12	110,116,122,125	0
3	GAL	H	6	11/12	0.62	0.19	79,96,100,102	0
3	NAG	F	5	14/15	0.63	0.16	71,88,95,99	0
3	NAG	H	8	14/15	0.64	0.09	113,124,130,133	0

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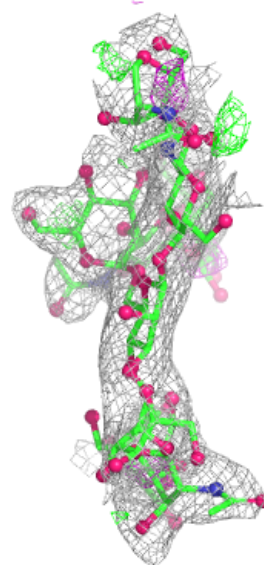
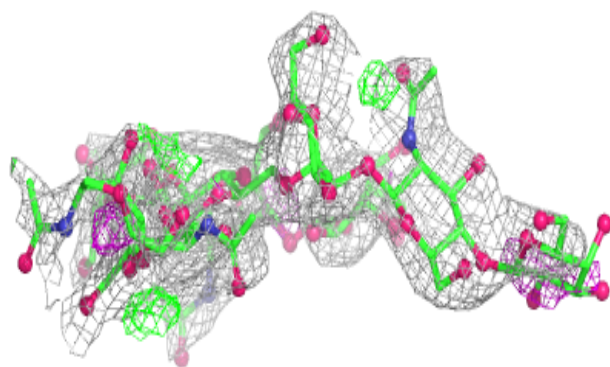
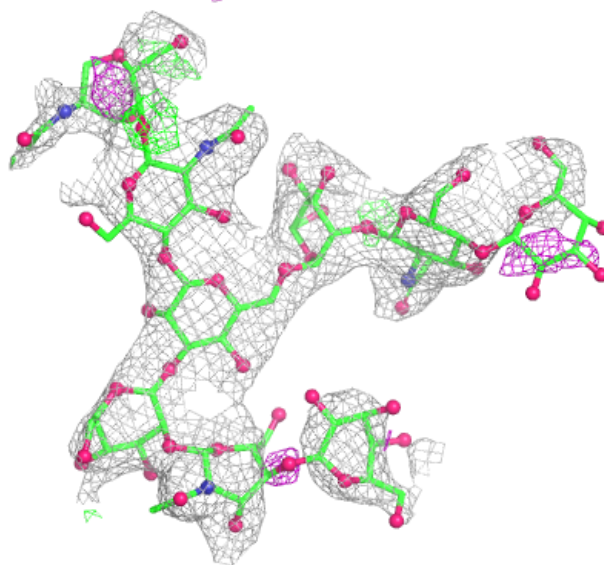
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	G	5	14/15	0.66	0.12	90,108,115,116	0
2	GAL	E	9	11/12	0.66	0.17	82,100,106,107	0
3	BMA	F	3	11/12	0.67	0.12	79,98,107,108	0
4	GAL	G	6	11/12	0.70	0.14	80,90,109,112	0
4	NAG	G	2	14/15	0.70	0.15	90,96,115,115	0
2	GAL	E	6	11/12	0.72	0.11	87,93,98,98	0
4	GAL	G	9	11/12	0.73	0.11	75,87,92,93	0
2	NAG	E	5	14/15	0.73	0.11	93,101,107,108	0
2	MAN	E	4	11/12	0.74	0.09	88,98,103,106	0
3	NAG	F	2	14/15	0.75	0.12	81,88,91,92	0
2	MAN	E	7	11/12	0.75	0.09	78,91,93,94	0
2	NAG	E	8	14/15	0.75	0.09	89,93,96,97	0
4	MAN	G	4	11/12	0.75	0.10	92,102,106,109	0
3	NAG	H	5	14/15	0.76	0.08	79,94,98,101	0
2	BMA	E	3	11/12	0.77	0.11	86,90,96,100	0
4	NAG	G	1	14/15	0.78	0.13	84,105,112,115	0
3	NAG	H	1	14/15	0.79	0.10	65,74,77,77	0
4	MAN	G	7	11/12	0.81	0.09	90,95,100,101	0
3	MAN	F	4	11/12	0.82	0.09	77,85,89,93	0
4	NAG	G	8	14/15	0.82	0.08	78,87,98,101	0
3	BMA	H	3	11/12	0.83	0.08	93,97,105,112	0
3	NAG	H	2	14/15	0.87	0.08	72,80,91,99	0
2	NAG	E	2	14/15	0.87	0.09	92,101,105,105	0
4	BMA	G	3	11/12	0.88	0.09	88,92,94,96	0
3	MAN	H	4	11/12	0.88	0.07	87,92,95,100	0
3	MAN	H	7	11/12	0.89	0.08	106,114,119,121	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.

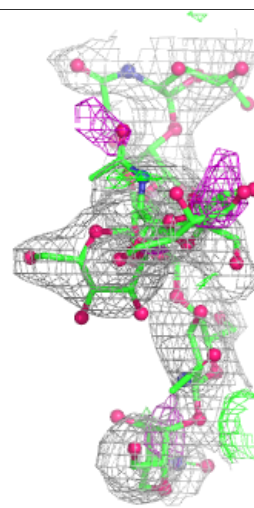
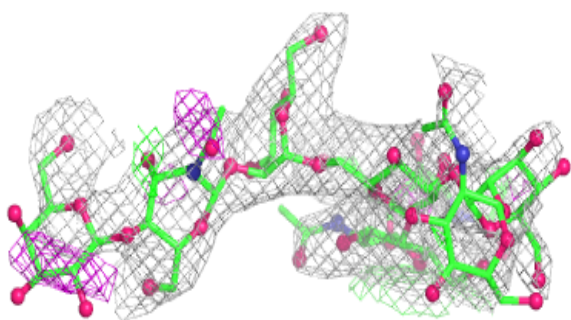
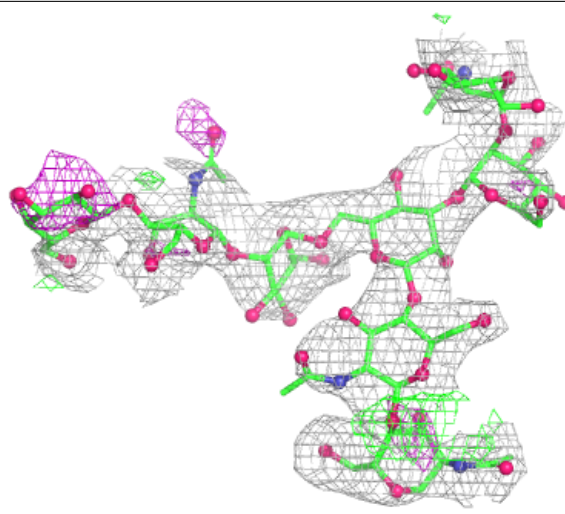
Electron density around Chain E:

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



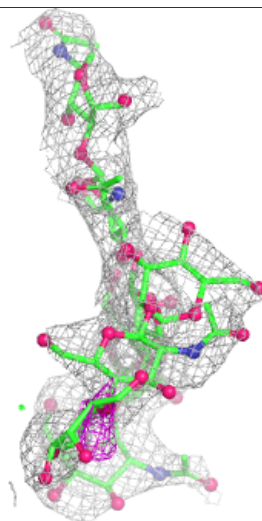
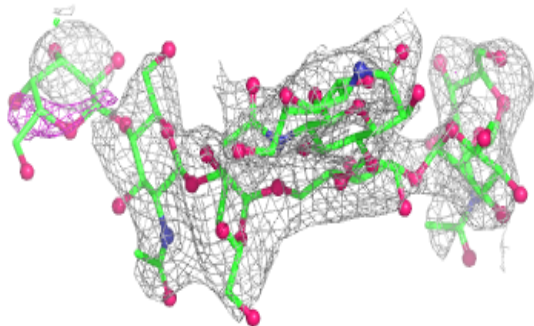
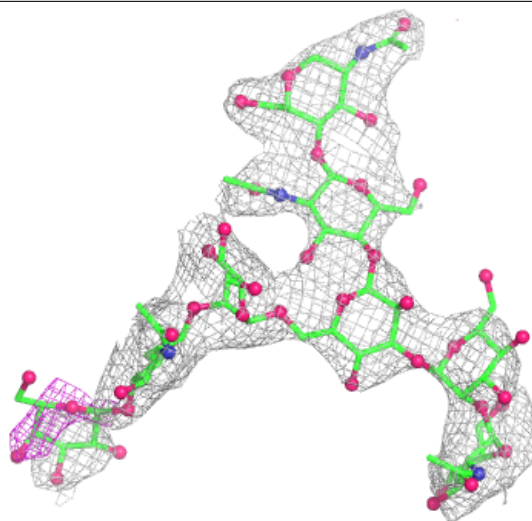
Electron density around Chain F:

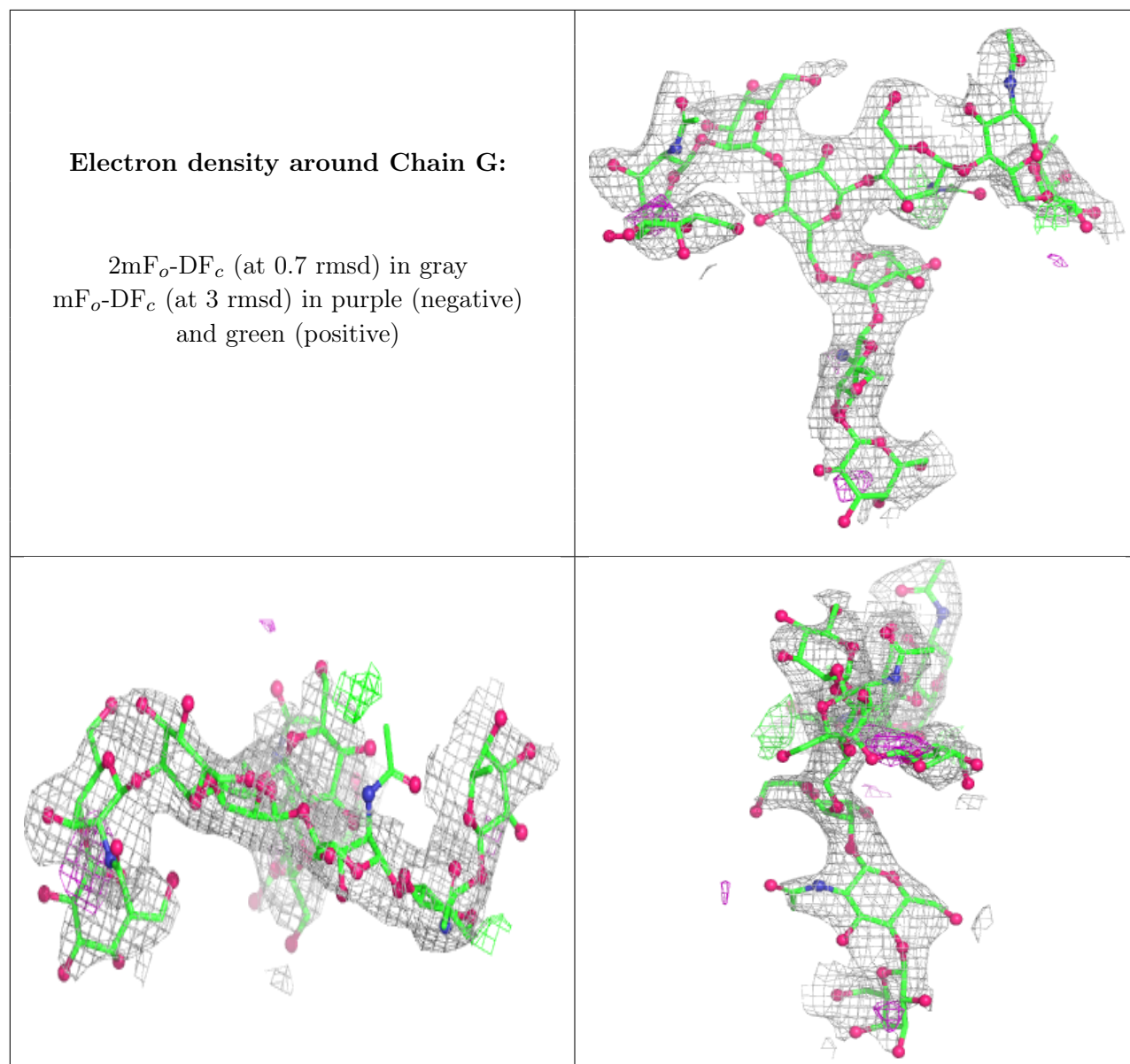
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

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





6.4 Ligands [i](#)

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
5	FUL	A	301	10/11	0.66	0.18	114,118,120,124	0

6.5 Other polymers [i](#)

There are no such residues in this entry.