



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 16, 2026 – 04:25 pm BST

PDB ID : 9IBF / pdb_00009ibf
Title : Crystal structure of hFcgammaRI-FAb complex
Authors : Feitsma, L.J.; Janssen, B.J.C.
Deposited on : 2025-02-12
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

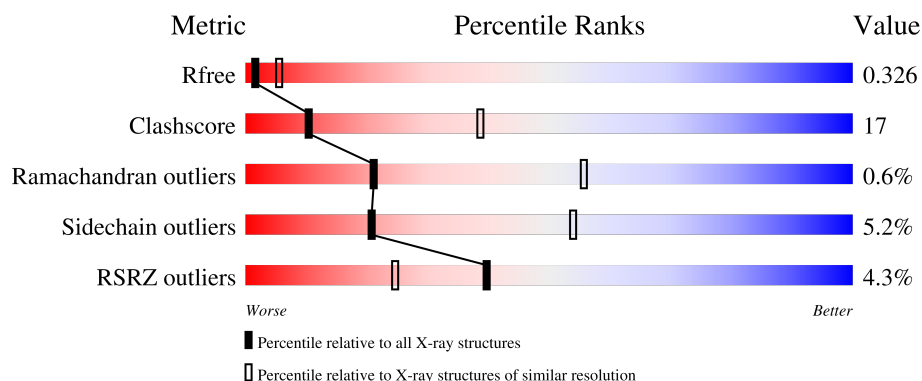
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	280	
1	B	280	
2	H	223	
2	I	223	
3	L	220	

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Mol	Chain	Length	Quality of chain
3	M	220	
4	C	2	
4	D	2	
4	E	2	
5	F	3	

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
8	EPE	L	301	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11029 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 High affinity immunoglobulin gamma Fc receptor I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2082	1321	360	392	9			
1	B	265	Total	C	N	O	S	0	0	0
			2090	1325	361	395	9			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	PRO	THR	engineered mutation	UNP P12314
A	25	LYS	THR	engineered mutation	UNP P12314
A	38	SER	THR	engineered mutation	UNP P12314
A	46	PRO	LEU	engineered mutation	UNP P12314
A	63	ILE	THR	engineered mutation	UNP P12314
A	69	THR	SER	engineered mutation	UNP P12314
A	71	HIS	ARG	engineered mutation	UNP P12314
A	77	GLU	VAL	engineered mutation	UNP P12314
A	78	ASP	ASN	engineered mutation	UNP P12314
A	100	VAL	ILE	engineered mutation	UNP P12314
A	114	LEU	PHE	engineered mutation	UNP P12314
A	160	MET	ILE	engineered mutation	UNP P12314
A	163	SER	ASN	engineered mutation	UNP P12314
A	195	THR	ASN	engineered mutation	UNP P12314
A	206	THR	ASN	engineered mutation	UNP P12314
A	207	PRO	LEU	engineered mutation	UNP P12314
A	240	ASP	ASN	engineered mutation	UNP P12314
A	283	HIS	LEU	engineered mutation	UNP P12314
A	285	GLN	LEU	engineered mutation	UNP P12314
A	290	HIS	-	expression tag	UNP P12314
A	291	HIS	-	expression tag	UNP P12314
A	292	HIS	-	expression tag	UNP P12314
A	293	HIS	-	expression tag	UNP P12314
A	294	HIS	-	expression tag	UNP P12314
A	295	HIS	-	expression tag	UNP P12314

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Chain	Residue	Modelled	Actual	Comment	Reference
B	20	PRO	THR	engineered mutation	UNP P12314
B	25	LYS	THR	engineered mutation	UNP P12314
B	38	SER	THR	engineered mutation	UNP P12314
B	46	PRO	LEU	engineered mutation	UNP P12314
B	63	ILE	THR	engineered mutation	UNP P12314
B	69	THR	SER	engineered mutation	UNP P12314
B	71	HIS	ARG	engineered mutation	UNP P12314
B	77	GLU	VAL	engineered mutation	UNP P12314
B	78	ASP	ASN	engineered mutation	UNP P12314
B	100	VAL	ILE	engineered mutation	UNP P12314
B	114	LEU	PHE	engineered mutation	UNP P12314
B	160	MET	ILE	engineered mutation	UNP P12314
B	163	SER	ASN	engineered mutation	UNP P12314
B	195	THR	ASN	engineered mutation	UNP P12314
B	206	THR	ASN	engineered mutation	UNP P12314
B	207	PRO	LEU	engineered mutation	UNP P12314
B	240	ASP	ASN	engineered mutation	UNP P12314
B	283	HIS	LEU	engineered mutation	UNP P12314
B	285	GLN	LEU	engineered mutation	UNP P12314
B	290	HIS	-	expression tag	UNP P12314
B	291	HIS	-	expression tag	UNP P12314
B	292	HIS	-	expression tag	UNP P12314
B	293	HIS	-	expression tag	UNP P12314
B	294	HIS	-	expression tag	UNP P12314
B	295	HIS	-	expression tag	UNP P12314

- Molecule 2 is a protein called Antibody Heavy chain FAb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	223	Total	C	N	O	S	0	0	0
			1666	1051	277	330	8			
2	I	223	Total	C	N	O	S	0	0	0
			1666	1051	277	330	8			

- Molecule 3 is a protein called Antibody Light chain FAb.

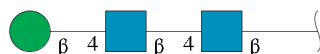
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	220	Total	C	N	O	S	0	0	0
			1677	1041	277	352	7			
3	M	220	Total	C	N	O	S	0	0	0
			1677	1041	277	352	7			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



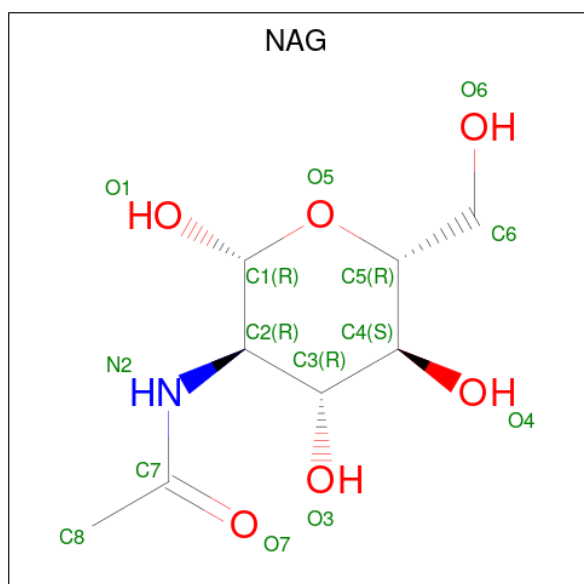
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called 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
5	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

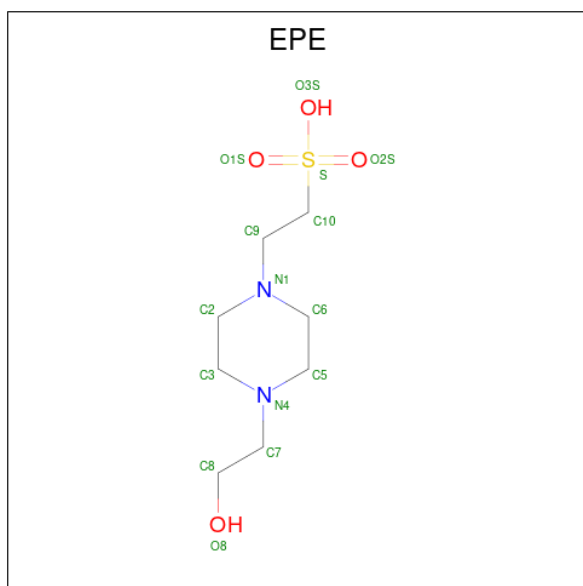


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Cl	0	0
			2	2		
7	B	1	Total	Cl	0	0
			1	1		
7	H	1	Total	Cl	0	0
			1	1		
7	I	1	Total	Cl	0	0
			1	1		

- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).

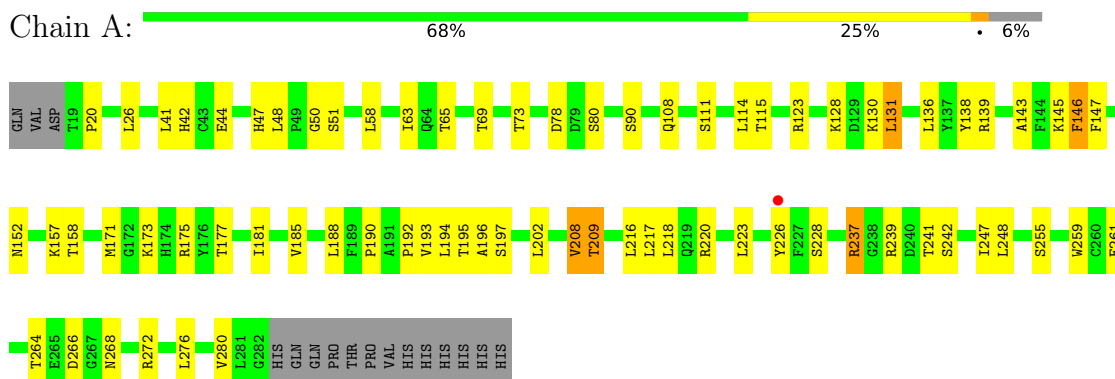


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	L	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

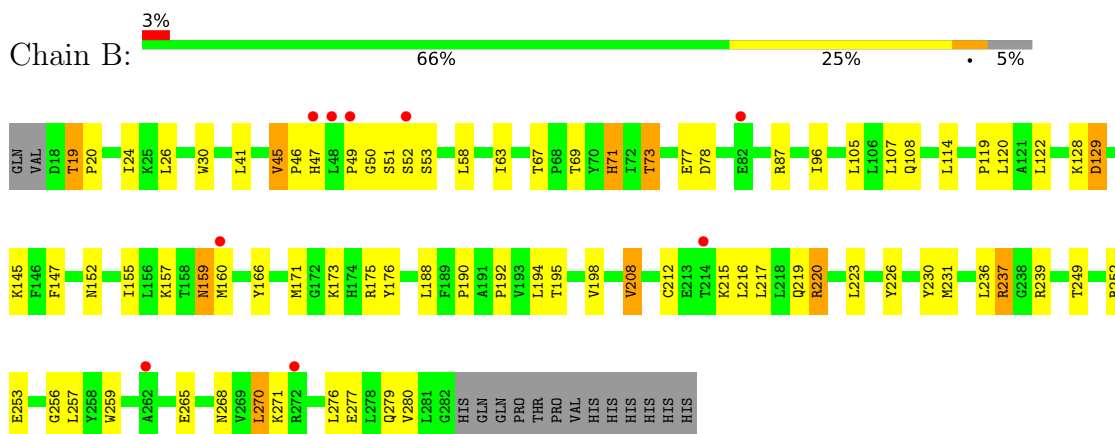
3 Residue-property plots

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.

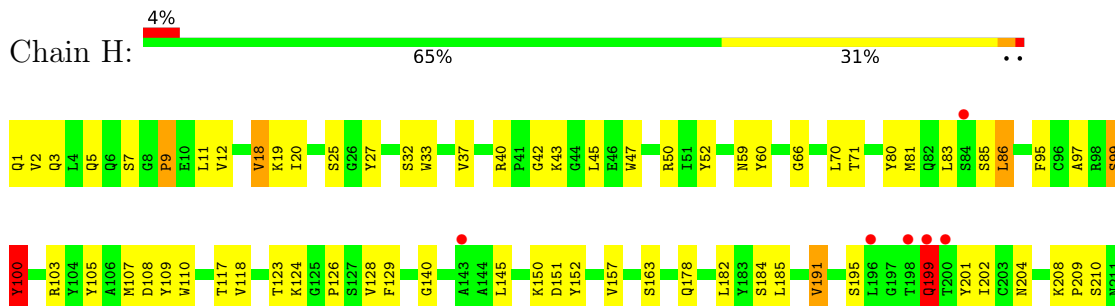
- Molecule 1: High affinity immunoglobulin gamma Fc receptor I



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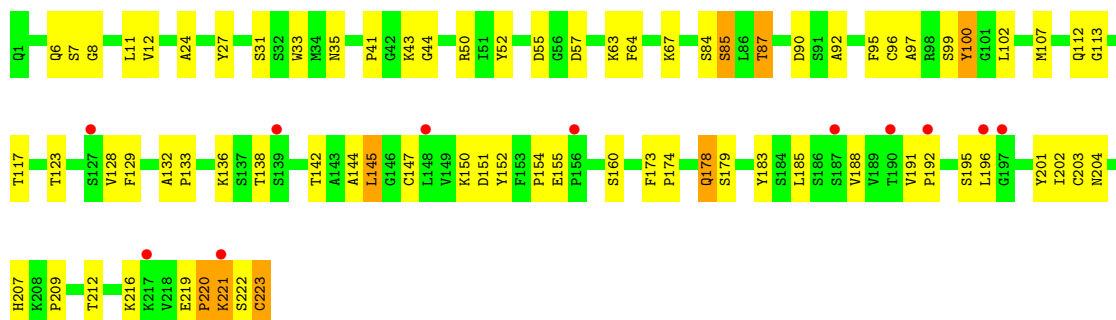


- Molecule 2: Antibody Heavy chain FAb





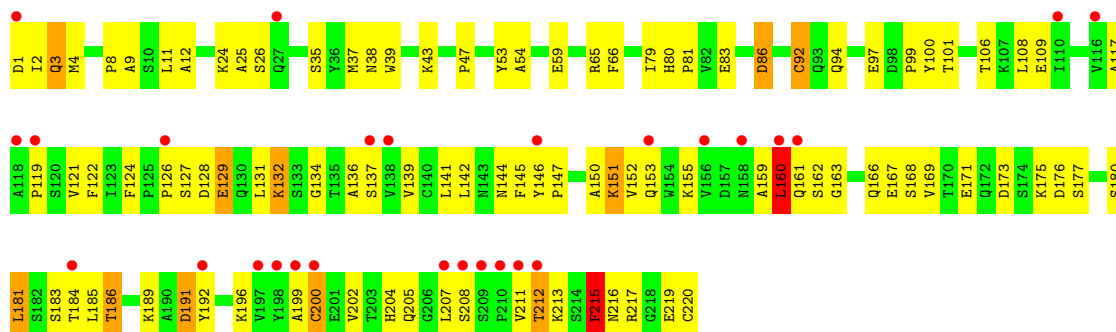
• Molecule 2: Antibody Heavy chain FAB



• Molecule 3: Antibody Light chain FAB



• Molecule 3: Antibody Light chain FAB



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50% 50%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.72Å 126.49Å 141.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.70 – 3.20 57.70 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (57.70-3.20) 99.9 (57.70-3.20)	Depositor EDS
R_{merge}	0.95	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.259 , 0.314 0.269 , 0.326	Depositor DCC
R_{free} test set	2083 reflections (5.67%)	wwPDB-VP
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 84.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	11029	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.2605e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: BMA, CL, EPE, NAG

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	0.61	0/2135	1.12	9/2903 (0.3%)
1	B	0.62	0/2143	1.09	7/2914 (0.2%)
2	H	0.61	0/1708	1.11	9/2320 (0.4%)
2	I	0.60	0/1708	1.13	6/2320 (0.3%)
3	L	0.59	0/1713	1.09	7/2325 (0.3%)
3	M	0.60	0/1713	1.20	16/2325 (0.7%)
All	All	0.61	0/11120	1.12	54/15107 (0.4%)

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	B	0	2
All	All	0	3

There are no bond length outliers.

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	191	VAL	N-CA-CB	-8.91	102.10	111.64
3	L	59	GLU	CB-CG-CD	8.68	127.36	112.60
2	H	219	GLU	CB-CA-C	8.49	120.48	108.68
1	A	130	LYS	CB-CA-C	8.31	125.82	110.11
3	M	3	GLN	N-CA-CB	8.15	123.40	110.85

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	ARG	Sidechain
1	B	220	ARG	Sidechain
1	B	237	ARG	Sidechain

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	2082	0	2048	51	0
1	B	2090	0	2051	69	0
2	H	1666	0	1633	66	0
2	I	1666	0	1633	64	0
3	L	1677	0	1592	64	0
3	M	1677	0	1592	85	0
4	C	28	0	25	4	0
4	D	28	0	25	2	0
4	E	28	0	25	1	0
5	F	39	0	34	0	0
6	A	14	0	13	0	0
6	B	14	0	13	3	0
7	A	2	0	0	1	0
7	B	1	0	0	0	0
7	H	1	0	0	0	0
7	I	1	0	0	0	0
8	L	15	0	18	7	0
All	All	11029	0	10702	370	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 17.

The worst 5 of 370 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)
3:L:137:SER:HB3	3:L:186:THR:HG22	1.37	1.07
3:M:142:LEU:HD21	3:M:202:VAL:HG21	1.31	1.07
2:I:6:GLN:NE2	2:I:96:CYS:H	1.53	1.06
2:H:123:THR:HG22	2:H:210:SER:OG	1.55	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:20:ILE:HD11	2:H:81:MET:HE2	1.43	0.99

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	262/280 (94%)	253 (97%)	9 (3%)	0	100	100
1	B	263/280 (94%)	255 (97%)	6 (2%)	2 (1%)	16	50
2	H	221/223 (99%)	207 (94%)	11 (5%)	3 (1%)	9	39
2	I	221/223 (99%)	203 (92%)	18 (8%)	0	100	100
3	L	218/220 (99%)	205 (94%)	12 (6%)	1 (0%)	24	59
3	M	218/220 (99%)	195 (89%)	21 (10%)	2 (1%)	14	47
All	All	1403/1446 (97%)	1318 (94%)	77 (6%)	8 (1%)	21	56

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	19	THR
1	B	51	SER
2	H	140	GLY
2	H	222	SER
3	L	112	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	233/249 (94%)	224 (96%)	9 (4%)	28	62
1	B	234/249 (94%)	225 (96%)	9 (4%)	29	62
2	H	187/187 (100%)	179 (96%)	8 (4%)	26	59
2	I	187/187 (100%)	176 (94%)	11 (6%)	18	50
3	L	189/189 (100%)	175 (93%)	14 (7%)	13	43
3	M	189/189 (100%)	177 (94%)	12 (6%)	16	48
All	All	1219/1250 (98%)	1156 (95%)	63 (5%)	21	54

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	59	GLU
3	M	160	LEU
3	L	140	CYS
3	M	129	GLU
3	M	211	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	204	ASN
3	M	130	GLN
3	L	164	ASN
3	M	204	HIS
2	I	207	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 i

9 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
4	NAG	C	1	4,1	14,14,15	0.42	0	17,19,21	1.12	2 (11%)
4	NAG	C	2	4	14,14,15	0.36	0	17,19,21	0.90	0
4	NAG	D	1	4,1	14,14,15	0.44	0	17,19,21	1.59	4 (23%)
4	NAG	D	2	4	14,14,15	0.33	0	17,19,21	1.26	1 (5%)
4	NAG	E	1	4,1	14,14,15	0.43	0	17,19,21	0.92	1 (5%)
4	NAG	E	2	4	14,14,15	0.33	0	17,19,21	0.78	0
5	NAG	F	1	5,1	14,14,15	0.39	0	17,19,21	1.26	2 (11%)
5	NAG	F	2	5	14,14,15	0.47	0	17,19,21	1.47	2 (11%)
5	BMA	F	3	5	11,11,12	0.80	1 (9%)	15,15,17	2.45	3 (20%)

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
4	NAG	C	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	C	2	4	-	2/6/23/26	0/1/1/1
4	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	4/6/23/26	0/1/1/1
5	NAG	F	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	BMA	F	3	5	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	3	BMA	C2-C3	2.20	1.55	1.52

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	3	BMA	C1-C2-C3	7.57	118.97	109.67
5	F	2	NAG	C1-O5-C5	5.07	119.06	112.19
4	D	1	NAG	C2-N2-C7	4.87	129.83	122.90
4	D	2	NAG	C2-N2-C7	4.69	129.59	122.90
5	F	3	BMA	C1-O5-C5	4.04	117.67	112.19

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

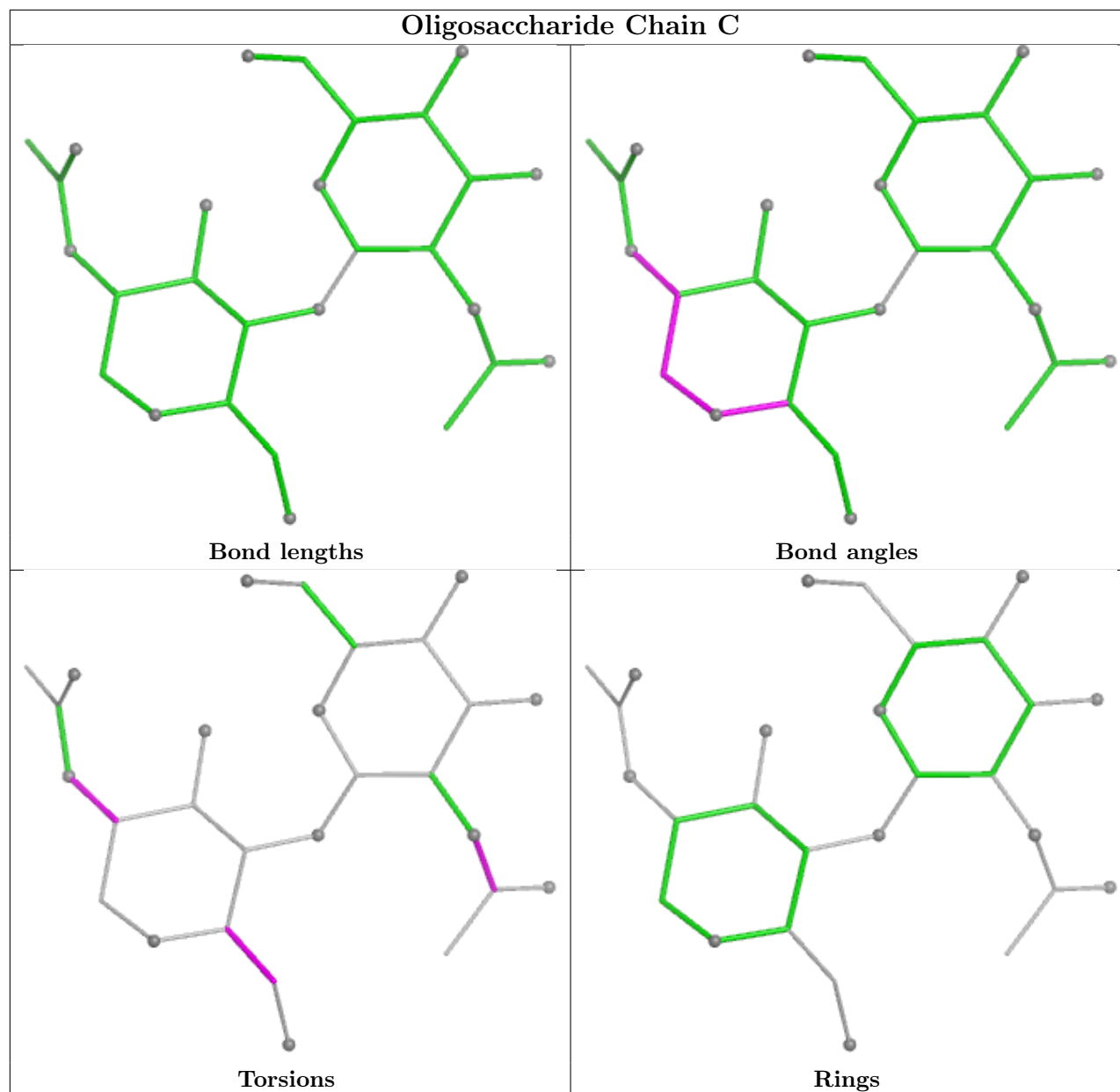
Mol	Chain	Res	Type	Atoms
4	C	2	NAG	C8-C7-N2-C2
4	C	2	NAG	O7-C7-N2-C2
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	E	1	NAG	C8-C7-N2-C2

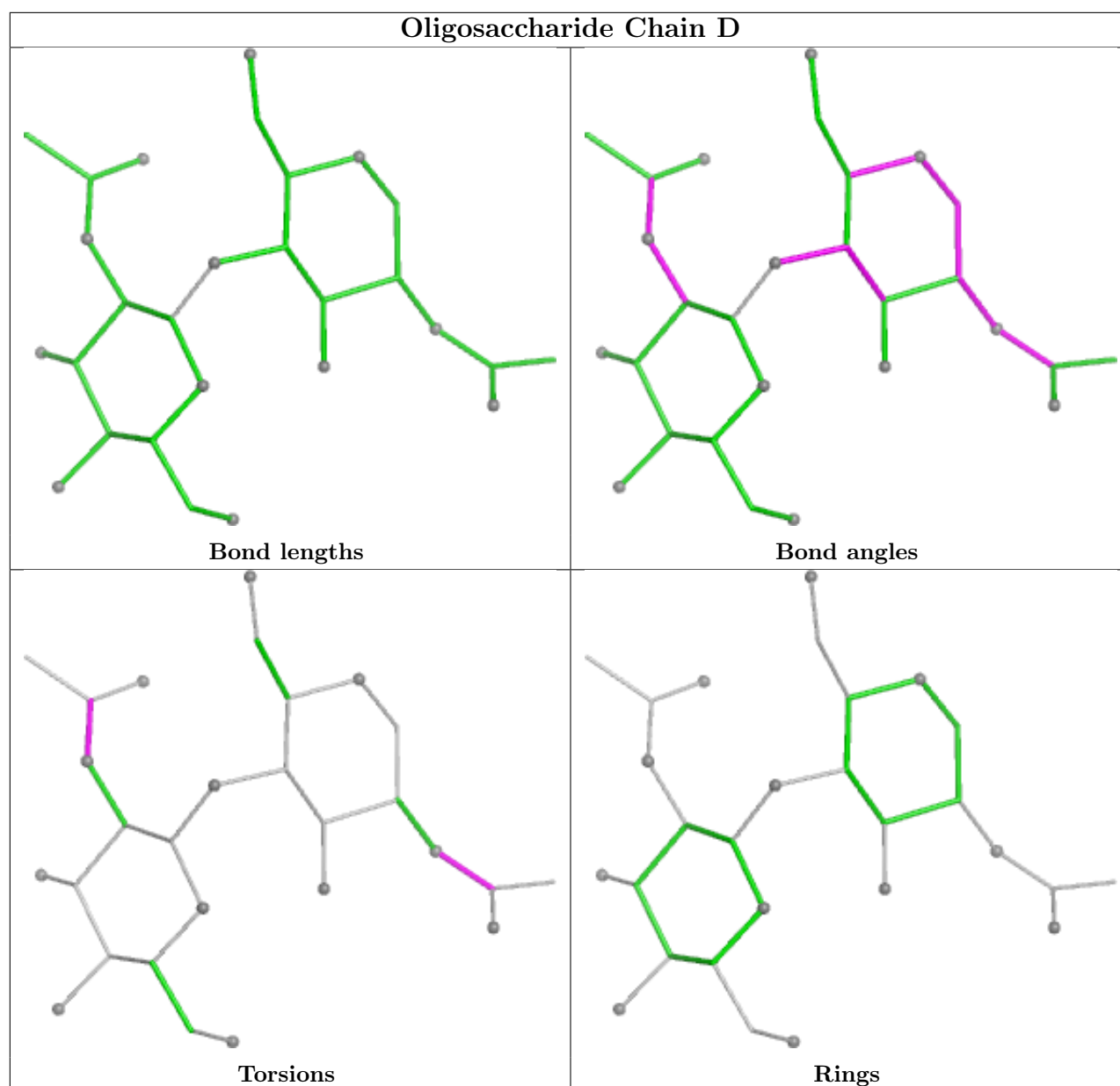
There are no ring outliers.

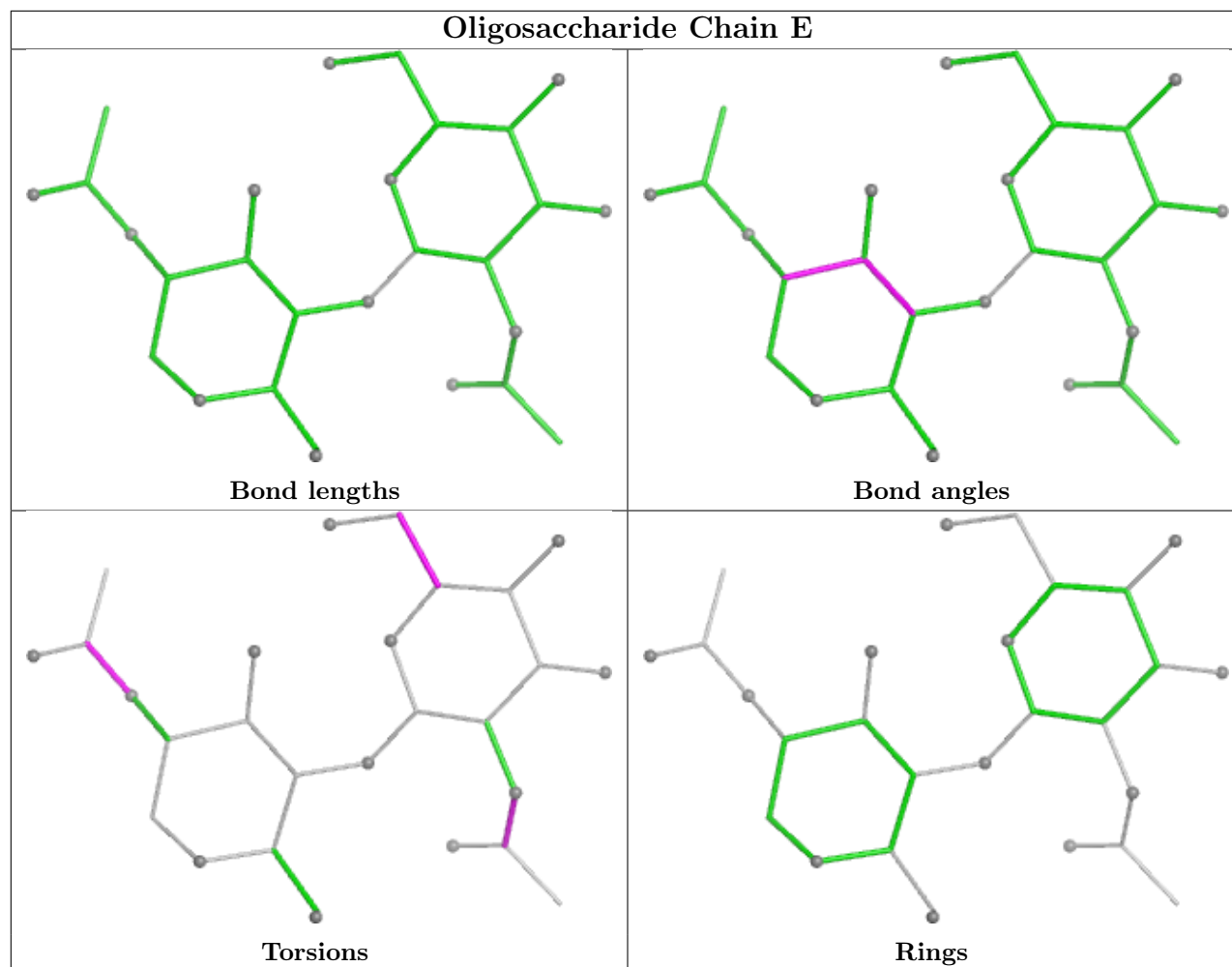
5 monomers are involved in 7 short contacts:

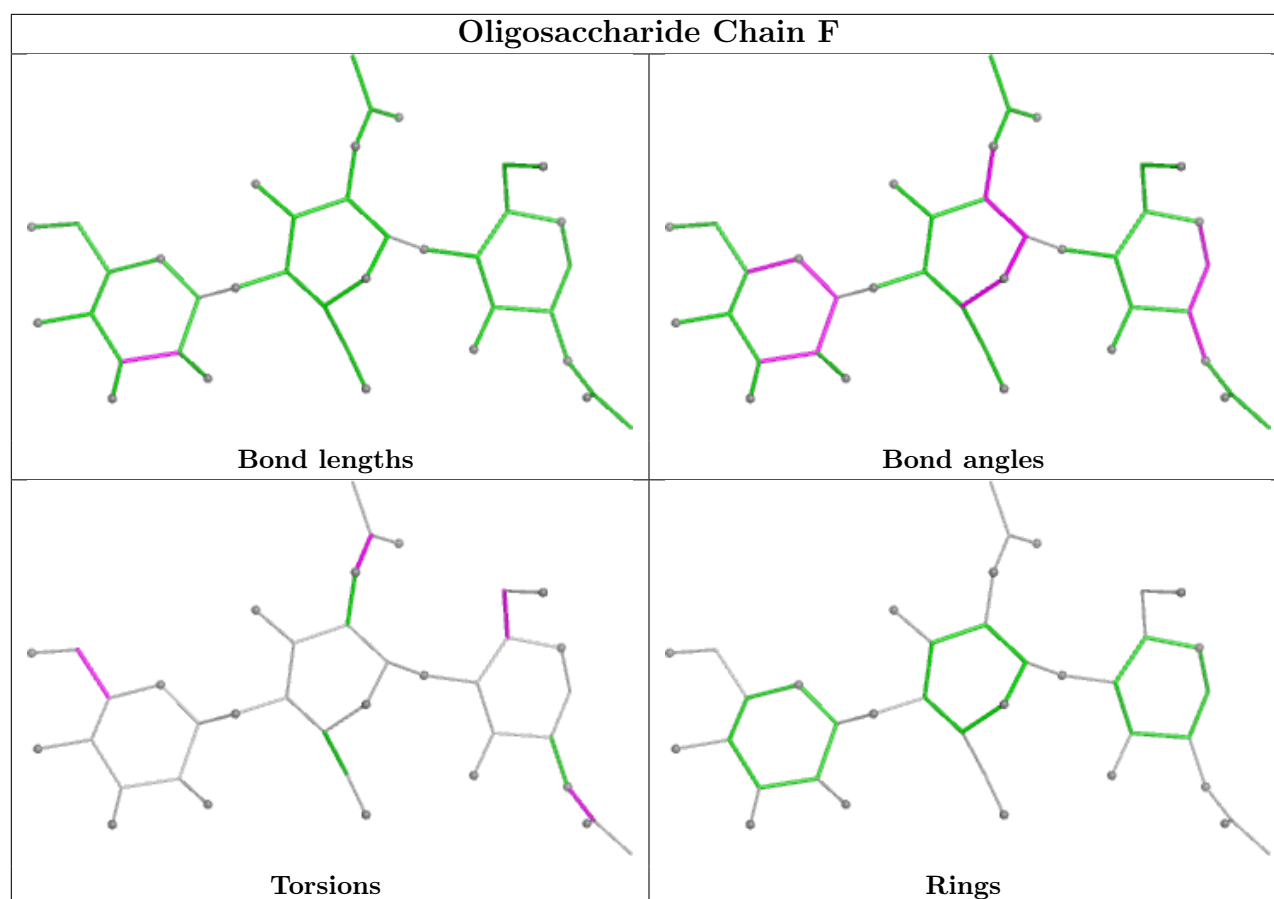
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2	NAG	2	0
4	E	1	NAG	1	0
4	D	2	NAG	1	0
4	C	1	NAG	3	0
4	D	1	NAG	2	0

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 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	A	301	1	14,14,15	0.40	0	17,19,21	1.60	2 (11%)
6	NAG	B	301	1	14,14,15	0.27	0	17,19,21	0.83	1 (5%)
8	EPE	L	301	-	15,15,15	0.57	1 (6%)	18,20,20	0.95	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
6	NAG	A	301	1	-	4/6/23/26	0/1/1/1
6	NAG	B	301	1	-	3/6/23/26	0/1/1/1
8	EPE	L	301	-	-	1/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	301	EPE	O3S-S	2.00	1.54	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	301	NAG	C2-N2-C7	4.88	129.85	122.90
8	L	301	EPE	O3S-S-C10	-2.85	101.16	105.77
6	A	301	NAG	C1-C2-N2	-2.75	105.78	110.49
6	B	301	NAG	C1-C2-N2	2.05	113.99	110.49

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	301	NAG	C8-C7-N2-C2
6	A	301	NAG	O7-C7-N2-C2
6	B	301	NAG	C8-C7-N2-C2
6	B	301	NAG	O7-C7-N2-C2
6	A	301	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	301	NAG	3	0
8	L	301	EPE	7	0

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 [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	264/280 (94%)	0.46	1 (0%) 88 79	16, 59, 91, 144	0
1	B	265/280 (94%)	0.52	9 (3%) 48 30	30, 62, 90, 130	0
2	H	223/223 (100%)	0.48	8 (3%) 46 28	23, 59, 116, 167	0
2	I	223/223 (100%)	0.65	11 (4%) 35 22	28, 79, 134, 189	0
3	L	220/220 (100%)	0.33	5 (2%) 61 41	19, 66, 103, 152	0
3	M	220/220 (100%)	0.88	27 (12%) 8 6	34, 99, 159, 198	0
All	All	1415/1446 (97%)	0.55	61 (4%) 40 24	16, 66, 131, 198	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	158	ASN	4.2
2	H	196	LEU	3.9
3	M	208	SER	3.8
2	H	200	THR	3.7
3	M	118	ALA	3.5

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

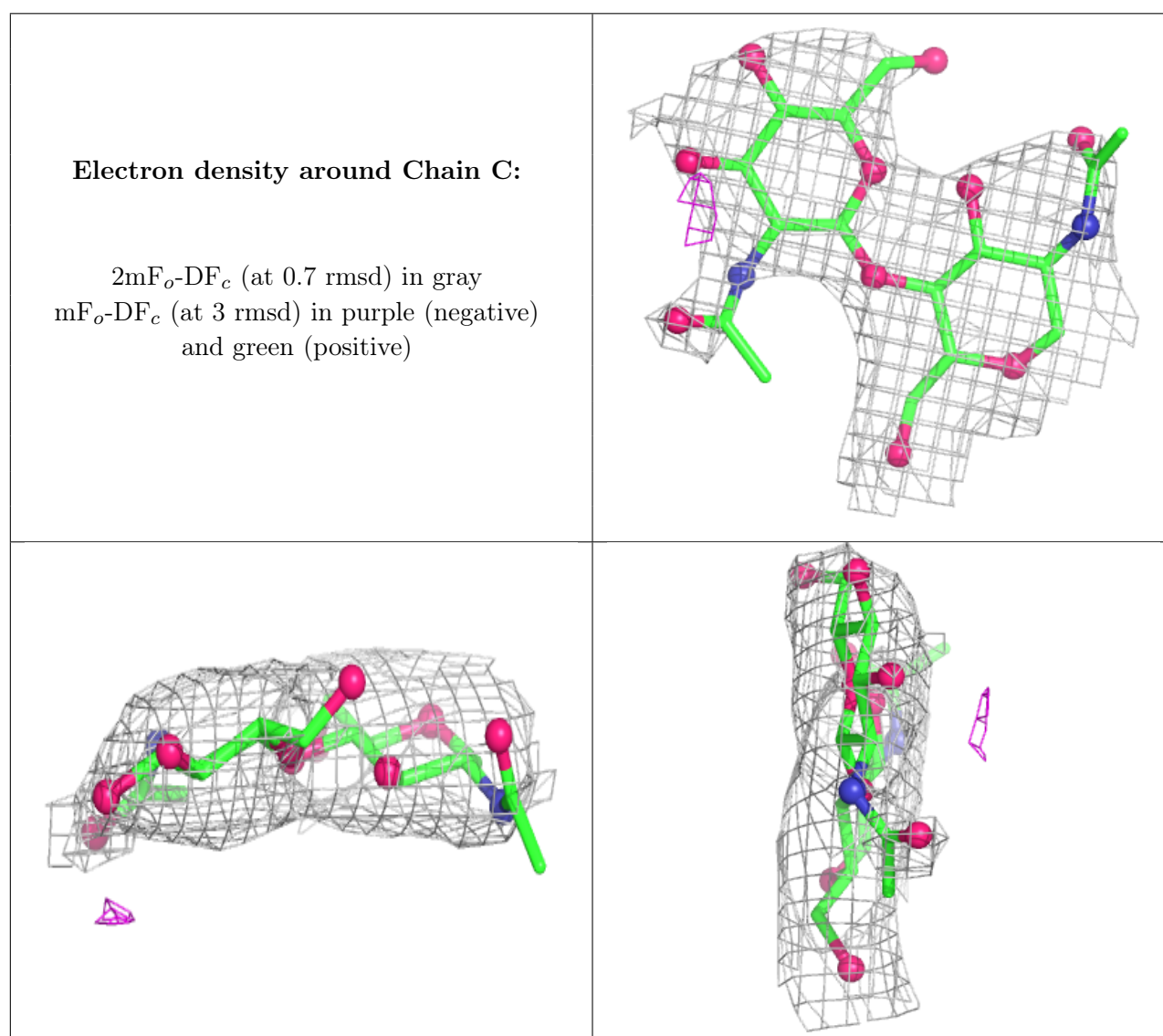
There are no non-standard protein/DNA/RNA residues in this entry.

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.

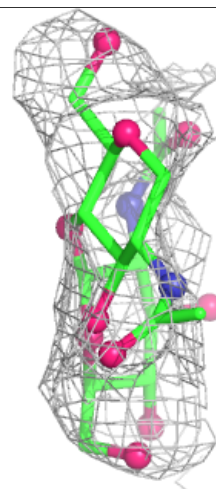
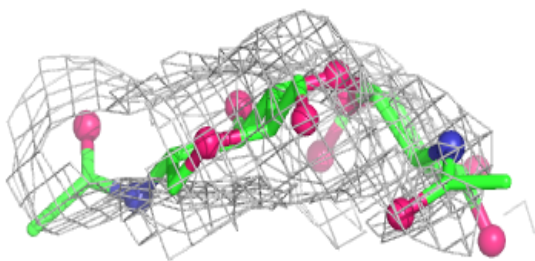
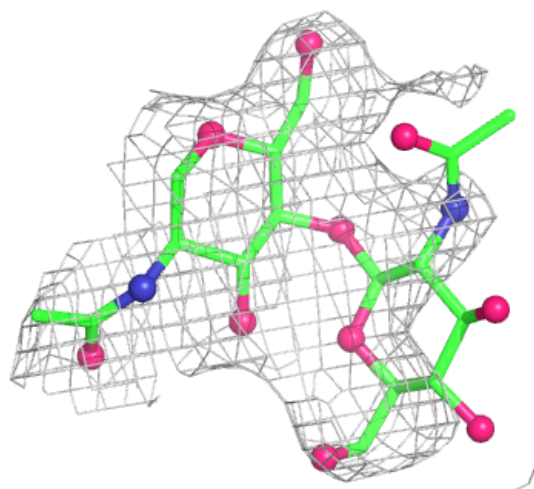
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	C	1	14/15	-	-	65,83,96,102	0
4	NAG	C	2	14/15	-	-	91,100,105,108	0
4	NAG	D	1	14/15	-	-	71,108,124,144	0
4	NAG	D	2	14/15	-	-	106,134,151,164	0
4	NAG	E	1	14/15	-	-	106,119,130,132	0
4	NAG	E	2	14/15	-	-	99,125,143,145	0
5	NAG	F	1	14/15	-	-	79,112,123,158	0
5	NAG	F	2	14/15	-	-	145,164,234,254	0
5	BMA	F	3	11/12	-	-	123,135,152,161	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.



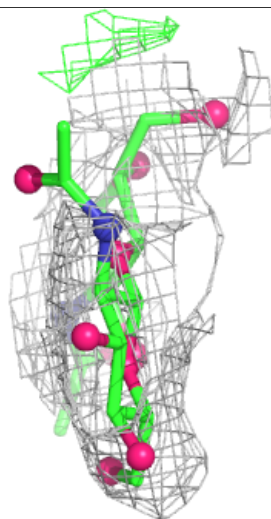
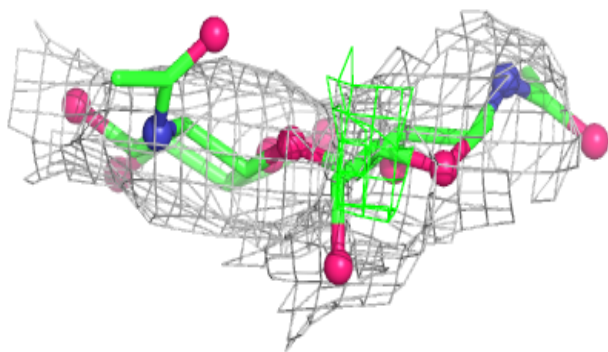
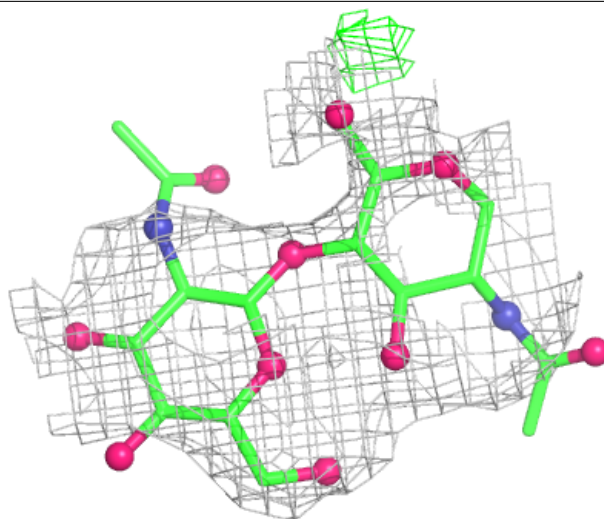
Electron density around Chain D:

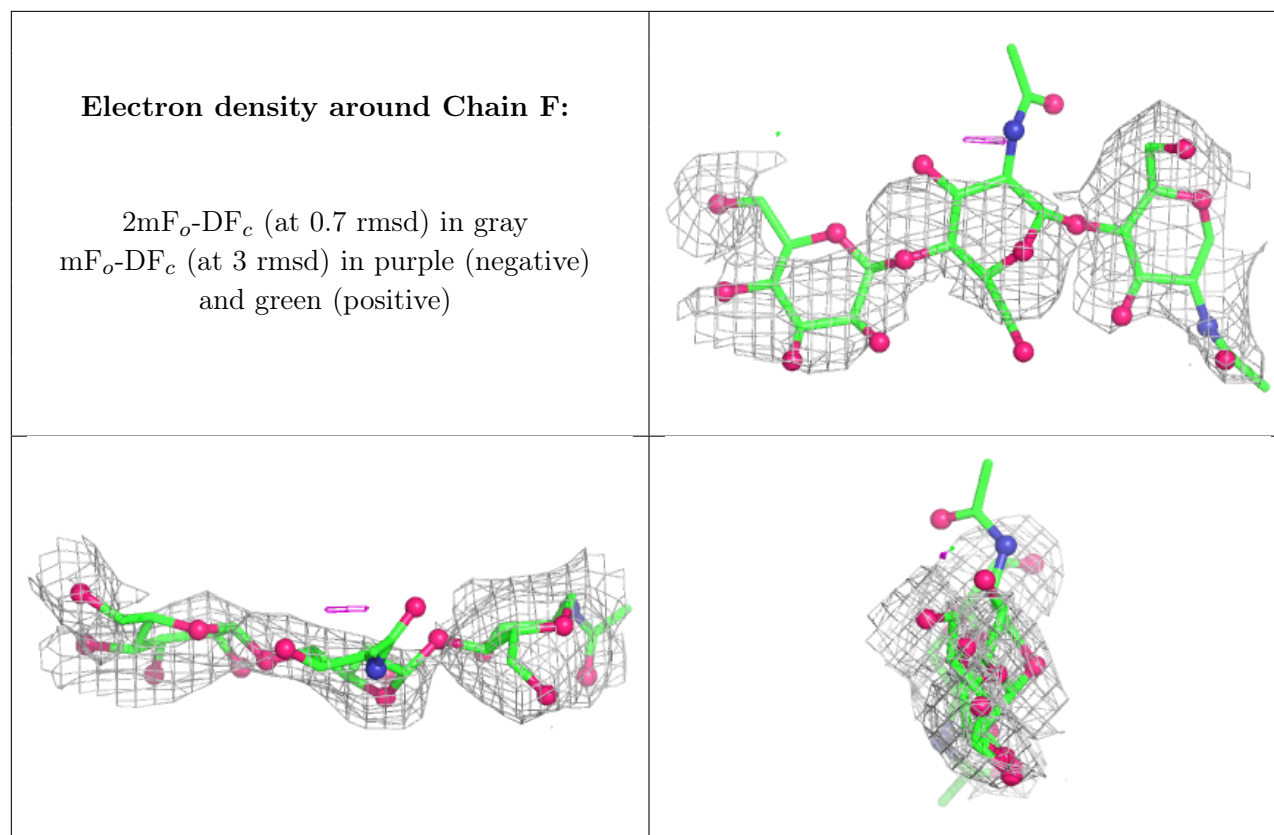
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 [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($\text{\AA}^2$)	Q<0.9
6	NAG	A	301	14/15	0.61	0.13	77,84,119,131	0
6	NAG	B	301	14/15	0.74	0.13	89,104,111,126	0
8	EPE	L	301	15/15	0.81	0.18	51,66,100,101	0
7	CL	A	303	1/1	0.95	0.06	45,45,45,45	0
7	CL	H	501	1/1	0.96	0.07	31,31,31,31	0
7	CL	B	302	1/1	0.97	0.07	54,54,54,54	0
7	CL	I	501	1/1	0.98	0.06	44,44,44,44	0
7	CL	A	302	1/1	0.98	0.07	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.