



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2020 – 02:32 PM BST

PDB ID : 7CBK
Title : Structure of Human Neutrophil Elastase Ecotin complex
Authors : Jobichen, C.; Sivaraman, J.
Deposited on : 2020-06-12
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

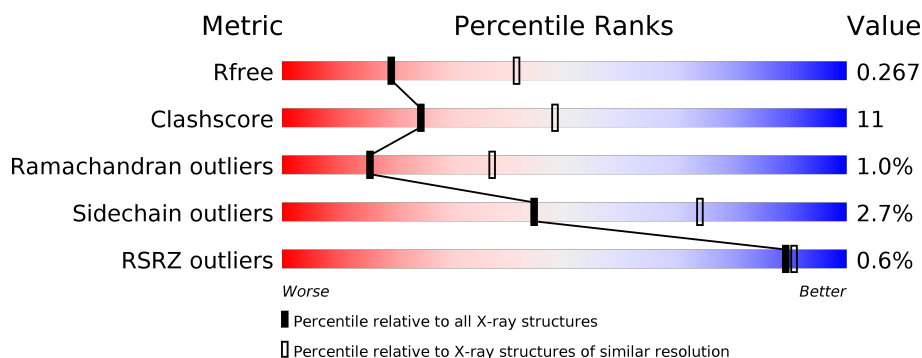
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	162	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 16%, green 64%, grey 19%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 64% 16% • 19% </div> </div>
1	C	162	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 61%, yellow 19%, orange 1%, grey 19%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 61% 19% • 19% </div> </div>
2	B	267	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 21%, green 60%, grey 18%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 60% 21% • 18% </div> </div>
2	D	267	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 67%, yellow 14%, orange 1%, grey 18%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 67% 14% • 18% </div> </div>
3	E	3	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 33%, yellow 67%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 33% 67% </div> </div>
3	F	3	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 33%, yellow 67%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 33% 67% </div> </div>

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Mol	Chain	Length	Quality of chain
3	G	3	 67% 33%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5656 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 Ecotin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	132	Total	C	N	O	S	0	0	0
			1041	665	174	196	6			
1	C	132	Total	C	N	O	S	0	0	0
			1041	666	173	196	6			

- Molecule 2 is a protein called Neutrophil elastase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	218	Total	C	N	O	S	0	0	0
			1627	1021	313	282	11			
2	B	218	Total	C	N	O	S	0	0	0
			1623	1019	312	281	11			

- Molecule 3 is an oligosaccharide called 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	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	F	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	G	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

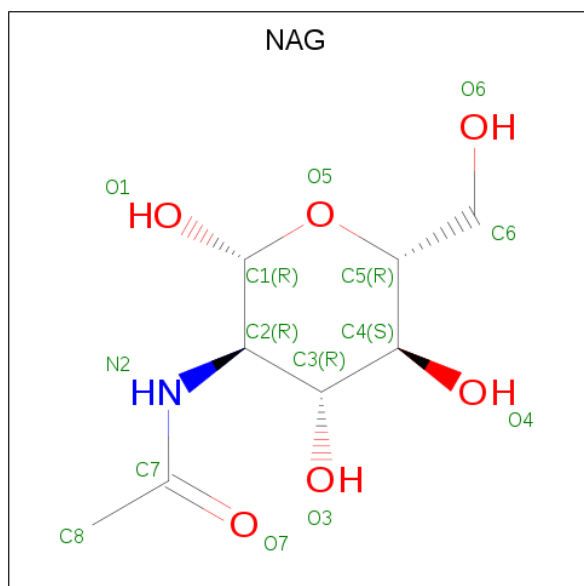


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

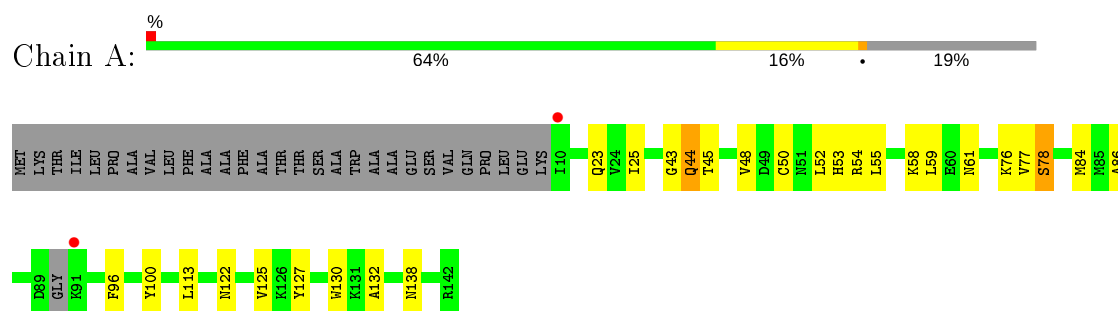
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	25	Total	O	0	0
			25	25		
8	C	18	Total	O	0	0
			18	18		
8	D	71	Total	O	0	0
			71	71		
8	B	65	Total	O	0	0
			65	65		

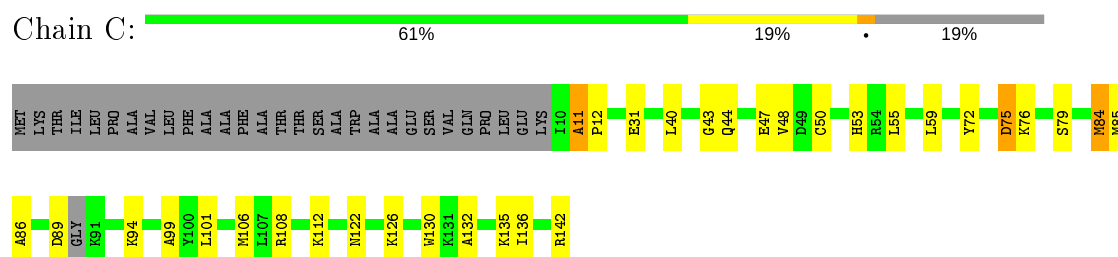
3 Residue-property plots [i](#)

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.

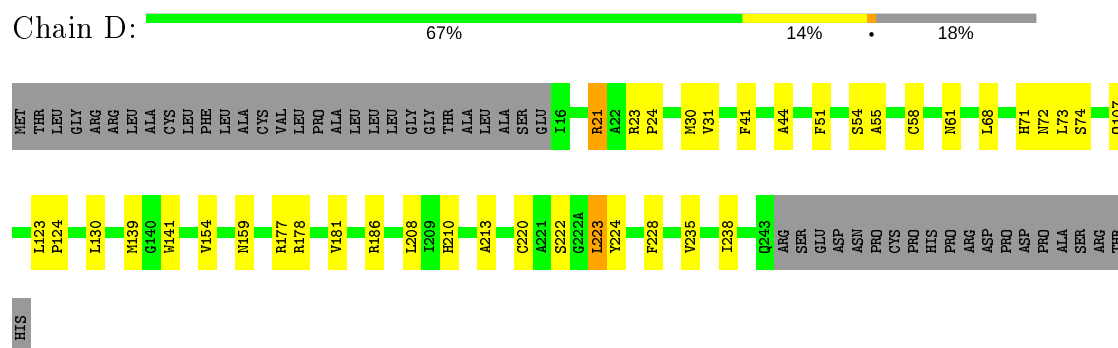
- Molecule 1: Ecotin



- Molecule 1: Ecotin

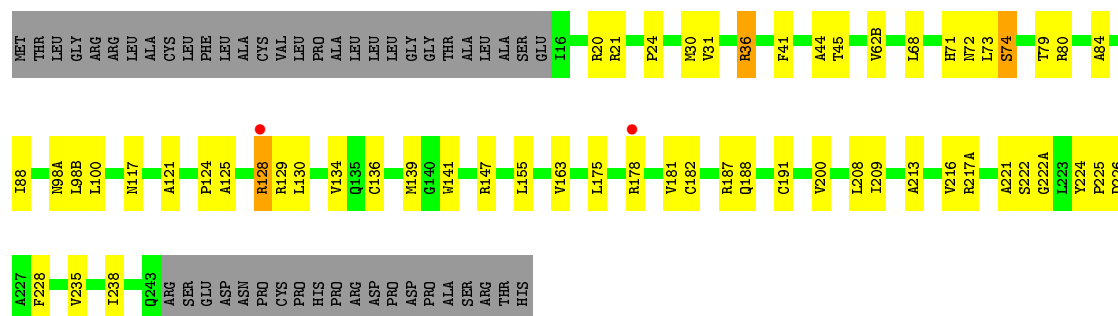


- Molecule 2: Neutrophil elastase



- Molecule 2: Neutrophil elastase





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

Chain E: 33% 67%



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

Chain F: 33% 67%



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

Chain G: 67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.19 Å 165.10 Å 64.00 Å 90.00° 108.75° 90.00°	Depositor
Resolution (Å)	24.43 – 2.70 40.74 – 2.67	Depositor EDS
% Data completeness (in resolution range)	95.7 (24.43-2.70) 94.4 (40.74-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 2.69 Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.199 , 0.266 0.203 , 0.267	Depositor DCC
R_{free} test set	2003 reflections (8.45%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.053 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5656	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% 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: FUC, GOL, MG, NAG, SO4

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	0.50	1/1061 (0.1%)	0.65	0/1435
1	C	0.47	1/1061 (0.1%)	0.68	1/1437 (0.1%)
2	B	0.49	0/1653	0.69	2/2248 (0.1%)
2	D	0.51	0/1657	0.66	0/2253
All	All	0.49	2/5432 (0.0%)	0.67	3/7373 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	50	CYS	CB-SG	-6.71	1.70	1.82
1	A	50	CYS	CB-SG	-6.57	1.71	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	187	ARG	CG-CD-NE	6.53	125.51	111.80
2	B	128	ARG	N-CA-CB	-5.42	100.85	110.60
1	C	84	MET	CG-SD-CE	5.07	108.32	100.20

There are no chirality outliers.

There are no planarity outliers.

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	1041	0	1034	20	0
1	C	1041	0	1037	19	0
2	B	1623	0	1626	55	0
2	D	1627	0	1633	36	0
3	E	38	0	34	0	0
3	F	38	0	34	5	0
3	G	38	0	34	0	0
4	D	6	0	8	2	0
5	B	5	0	0	0	0
5	D	5	0	0	0	0
6	D	1	0	0	0	0
7	B	14	0	13	2	0
8	A	25	0	0	0	0
8	B	65	0	0	3	0
8	C	18	0	0	2	0
8	D	71	0	0	0	0
All	All	5656	0	5453	119	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 11.

All (119) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:159:ASN:HD21	3:F:1:NAG:C1	1.15	1.59
2:D:159:ASN:ND2	3:F:1:NAG:C1	1.85	1.35
2:B:129:ARG:HD3	2:B:178:ARG:HH22	1.25	1.02
2:D:159:ASN:CG	3:F:1:NAG:C1	2.33	0.95
2:B:129:ARG:CD	2:B:178:ARG:HH22	1.80	0.92
1:A:84:MET:HE3	2:B:191:CYS:HA	1.57	0.86
2:D:159:ASN:OD1	3:F:1:NAG:C1	2.24	0.86
2:B:129:ARG:HH11	2:B:178:ARG:NH1	1.76	0.84
2:B:129:ARG:HD3	2:B:178:ARG:NH2	1.93	0.82
1:A:86:ALA:HB3	2:B:41:PHE:HA	1.66	0.78
2:B:129:ARG:CD	2:B:178:ARG:NH2	2.48	0.77
1:A:76:LYS:O	1:A:78:SER:N	2.19	0.74
2:B:147:ARG:HE	2:B:221:ALA:HB3	1.56	0.70
2:B:129:ARG:NH1	2:B:178:ARG:NH1	2.42	0.67
1:C:11:ALA:HB3	1:C:12:PRO:HD3	1.76	0.65
2:B:31:VAL:HB	2:B:44:ALA:HB3	1.79	0.64
2:B:221:ALA:O	2:B:222(A):GLY:N	2.33	0.60
1:C:48:VAL:HB	1:C:53:HIS:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:ARG:NH2	8:B:404:HOH:O	2.33	0.59
2:D:178:ARG:HB2	4:D:307:GOL:H11	1.84	0.58
2:B:121:ALA:HB1	2:B:209:ILE:HD13	1.86	0.58
2:B:129:ARG:HD2	2:B:178:ARG:HH22	1.68	0.57
2:B:129:ARG:NH1	2:B:178:ARG:CZ	2.69	0.56
1:A:84:MET:HE2	2:B:216:VAL:HG11	1.88	0.55
1:C:43:GLY:HA2	1:C:55:LEU:HD22	1.88	0.55
1:A:43:GLY:HA2	1:A:55:LEU:HD22	1.89	0.55
2:B:30:MET:HG2	2:B:155:LEU:HD21	1.88	0.54
2:B:147:ARG:HH21	2:B:221:ALA:HB3	1.72	0.54
1:A:45:THR:HG22	1:A:96:PHE:HD1	1.72	0.54
2:D:30:MET:HB2	2:D:139:MET:HE1	1.90	0.54
2:D:181:VAL:HG13	2:D:228:PHE:HB2	1.90	0.53
2:D:31:VAL:HB	2:D:44:ALA:HB3	1.89	0.53
2:B:30:MET:HB2	2:B:139:MET:HE1	1.89	0.53
2:B:147:ARG:NH2	2:B:188:GLN:OE1	2.41	0.53
2:D:222:SER:OG	2:D:223:LEU:O	2.17	0.53
1:A:52:LEU:HD11	2:B:98(B):LEU:HD11	1.90	0.53
2:D:159:ASN:OD1	3:F:1:NAG:C2	2.57	0.53
1:C:47:GLU:OE1	1:C:94:LYS:HG3	2.09	0.53
2:B:181:VAL:HG13	2:B:228:PHE:HB2	1.90	0.52
2:D:73:LEU:HD11	2:D:141:TRP:CE2	2.45	0.52
1:C:79:SER:O	8:C:201:HOH:O	2.18	0.52
2:B:98(A):ASN:HB3	2:B:100:LEU:CD1	2.40	0.51
2:D:235:VAL:HA	2:D:238:ILE:HD12	1.91	0.51
2:B:72:ASN:O	2:B:80:ARG:NH2	2.44	0.51
1:A:48:VAL:HB	1:A:53:HIS:NE2	2.25	0.51
2:B:129:ARG:HH12	2:B:178:ARG:HB3	1.77	0.50
1:C:85:MET:O	2:D:41:PHE:O	2.30	0.50
1:A:54:ARG:HD2	1:A:100:TYR:HB2	1.94	0.50
1:A:84:MET:HE3	2:B:191:CYS:CA	2.36	0.49
2:B:84:ALA:HB2	7:B:304:NAG:H83	1.94	0.49
2:D:73:LEU:HD13	2:D:141:TRP:NE1	2.27	0.49
1:A:132:ALA:HB2	1:C:130:TRP:CZ2	2.48	0.49
2:B:72:ASN:OD1	2:B:74:SER:HB3	2.13	0.48
1:C:85:MET:SD	2:D:58:CYS:HA	2.53	0.48
2:B:129:ARG:HH11	2:B:178:ARG:CZ	2.25	0.48
2:D:73:LEU:HD22	2:D:141:TRP:CG	2.48	0.48
2:D:24:PRO:HA	2:D:71:HIS:CE1	2.49	0.48
1:A:23:GLN:OE1	1:A:125:VAL:HG23	2.14	0.47
2:D:73:LEU:CD2	2:D:141:TRP:CG	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:TRP:CZ2	1:C:132:ALA:HB2	2.49	0.47
1:A:44:GLN:NE2	1:A:122:ASN:HB3	2.30	0.47
2:D:71:HIS:CE1	2:D:154:VAL:HG13	2.50	0.47
2:D:73:LEU:HD22	2:D:141:TRP:CD1	2.50	0.47
2:B:30:MET:SD	2:B:139:MET:HE2	2.54	0.47
1:C:59:LEU:HD11	1:C:72:TYR:HB3	1.96	0.47
2:D:177:ARG:HG2	4:D:307:GOL:H32	1.97	0.47
1:A:84:MET:HE2	2:B:216:VAL:CG1	2.45	0.47
2:B:124:PRO:HA	2:B:208:LEU:HD13	1.96	0.46
2:B:31:VAL:HG13	2:B:68:LEU:HD23	1.98	0.46
1:C:126:LYS:NZ	8:C:205:HOH:O	2.49	0.46
2:D:130:LEU:HD21	2:D:210:HIS:CE1	2.50	0.46
2:B:141:TRP:CE2	2:B:155:LEU:HD13	2.51	0.46
2:B:45:THR:HG21	2:B:209:ILE:HG12	1.98	0.46
2:B:24:PRO:HA	2:B:71:HIS:CE1	2.50	0.46
1:A:138:ASN:OD1	1:C:126:LYS:HG2	2.16	0.46
2:B:20:ARG:NH1	8:B:410:HOH:O	2.49	0.46
7:B:304:NAG:H82	7:B:304:NAG:O3	2.16	0.45
2:D:31:VAL:HG13	2:D:68:LEU:HD23	1.98	0.45
2:B:129:ARG:HH11	2:B:178:ARG:HH12	1.59	0.45
2:B:98(A):ASN:HB3	2:B:100:LEU:HD11	1.98	0.45
2:D:124:PRO:HA	2:D:208:LEU:HD13	1.99	0.45
1:C:89:ASP:OD1	1:C:89:ASP:N	2.50	0.45
2:D:30:MET:SD	2:D:139:MET:HE2	2.57	0.44
2:B:62(B):VAL:HG11	2:B:88:ILE:HD11	2.00	0.44
1:C:44:GLN:NE2	1:C:122:ASN:HB3	2.32	0.44
2:B:182:CYS:HB3	2:B:225:PRO:HB2	2.00	0.44
2:D:73:LEU:CD1	2:D:141:TRP:CE2	3.01	0.44
2:D:23:ARG:HD3	2:D:23:ARG:HA	1.91	0.44
2:D:71:HIS:NE2	2:D:154:VAL:HG13	2.33	0.43
2:D:51:PHE:CE1	2:D:107:GLN:HG3	2.53	0.43
2:B:182:CYS:HA	2:B:226:ASP:O	2.18	0.43
1:A:44:GLN:HE21	1:A:122:ASN:HB3	1.84	0.43
1:A:25:ILE:HG12	1:A:127:TYR:CD1	2.53	0.43
2:B:73:LEU:HD22	2:B:141:TRP:CG	2.54	0.43
2:B:235:VAL:HA	2:B:238:ILE:HD12	2.01	0.42
2:D:213:ALA:HA	2:D:228:PHE:CD2	2.54	0.42
1:C:135:LYS:HD2	1:C:136:ILE:H	1.84	0.42
2:D:123:LEU:HA	2:D:123:LEU:HD23	1.83	0.42
2:D:72:ASN:OD1	2:D:74:SER:HB2	2.19	0.42
2:B:213:ALA:HA	2:B:228:PHE:CD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:LEU:HD23	1:C:40:LEU:HA	1.83	0.42
1:C:75:ASP:HB3	1:C:76:LYS:HD2	2.01	0.42
2:D:223:LEU:H	2:D:223:LEU:HD12	1.84	0.42
2:D:54:SER:OG	2:D:55:ALA:N	2.53	0.42
1:C:99:ALA:O	1:C:101:LEU:HD22	2.19	0.41
2:B:141:TRP:CD2	2:B:155:LEU:HD13	2.56	0.41
1:A:113:LEU:HD23	1:A:113:LEU:HA	1.83	0.41
2:B:130:LEU:HD22	2:B:134:VAL:HG11	2.01	0.41
2:B:175:LEU:O	2:B:217(A):ARG:NH2	2.54	0.41
1:A:58:LYS:HG3	1:A:59:LEU:N	2.36	0.41
2:B:136:CYS:HB3	2:B:200:VAL:O	2.21	0.41
2:B:79:THR:HB	2:B:117:ASN:ND2	2.36	0.41
2:B:134:VAL:O	2:B:163:VAL:HG23	2.21	0.40
2:B:125:ALA:HB3	2:B:128:ARG:HG3	2.04	0.40
2:B:147:ARG:NH2	2:B:188:GLN:HB3	2.36	0.40
2:B:188:GLN:NE2	8:B:414:HOH:O	2.54	0.40
1:C:84:MET:HE2	2:D:220:CYS:SG	2.61	0.40
2:D:21:ARG:HH21	2:D:23:ARG:NH2	2.20	0.40
2:B:98(A):ASN:HB3	2:B:100:LEU:HD12	2.03	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	128/162 (79%)	120 (94%)	7 (6%)	1 (1%)	19	43
1	C	128/162 (79%)	119 (93%)	6 (5%)	3 (2%)	6	16
2	B	216/267 (81%)	205 (95%)	9 (4%)	2 (1%)	17	40
2	D	216/267 (81%)	204 (94%)	11 (5%)	1 (0%)	29	54
All	All	688/858 (80%)	648 (94%)	33 (5%)	7 (1%)	15	37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	11	ALA
2	B	222	SER
1	C	86	ALA
1	A	77	VAL
2	D	224	TYR
2	B	224	TYR
1	C	31	GLU

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	112/139 (81%)	109 (97%)	3 (3%)	44	74
1	C	113/139 (81%)	108 (96%)	5 (4%)	28	56
2	B	169/212 (80%)	166 (98%)	3 (2%)	59	83
2	D	170/212 (80%)	166 (98%)	4 (2%)	49	77
All	All	564/702 (80%)	549 (97%)	15 (3%)	44	74

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	61	ASN
1	A	78	SER
1	C	75	ASP
1	C	106	MET
1	C	108	ARG
1	C	112	LYS
1	C	142	ARG
2	D	21	ARG
2	D	61	ASN
2	D	186	ARG
2	D	223	LEU
2	B	21	ARG

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Mol	Chain	Res	Type
2	B	36	ARG
2	B	74	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	135	GLN
2	B	148	ASN

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 ⓘ

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	$\# Z > 2$
3	NAG	E	1	3,2	14,14,15	0.42	0	17,19,21	1.45	2 (11%)
3	NAG	E	2	3	14,14,15	0.39	0	17,19,21	0.51	0
3	FUC	E	3	3	10,10,11	0.75	0	14,14,16	1.92	3 (21%)
3	NAG	F	1	3	14,14,15	0.39	0	17,19,21	0.62	0
3	NAG	F	2	3	14,14,15	0.25	0	17,19,21	0.68	0
3	FUC	F	3	3	10,10,11	0.80	0	14,14,16	1.85	4 (28%)
3	NAG	G	1	3	14,14,15	0.31	0	17,19,21	0.67	0
3	NAG	G	2	3	14,14,15	0.53	0	17,19,21	0.47	0
3	FUC	G	3	3	10,10,11	0.96	1 (10%)	14,14,16	1.84	3 (21%)

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	E	1	3,2	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	FUC	E	3	3	-	-	0/1/1/1
3	NAG	F	1	3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	FUC	F	3	3	-	-	0/1/1/1
3	NAG	G	1	3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	FUC	G	3	3	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	3	FUC	O5-C5	2.00	1.47	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	C2-N2-C7	4.73	129.63	122.90
3	E	3	FUC	C1-O5-C5	4.38	122.70	112.78
3	G	3	FUC	C1-O5-C5	4.14	122.17	112.78
3	F	3	FUC	C1-O5-C5	4.02	121.88	112.78
3	F	3	FUC	O5-C1-C2	3.45	116.10	110.77
3	G	3	FUC	O5-C5-C4	3.39	115.61	109.52
3	E	3	FUC	O5-C1-C2	3.34	115.93	110.77
3	E	3	FUC	O5-C5-C4	3.32	115.48	109.52
3	G	3	FUC	O5-C1-C2	3.28	115.83	110.77
3	F	3	FUC	O5-C5-C4	2.68	114.32	109.52
3	E	1	NAG	C1-C2-N2	2.33	114.48	110.49
3	F	3	FUC	C1-C2-C3	2.13	112.28	109.67

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6

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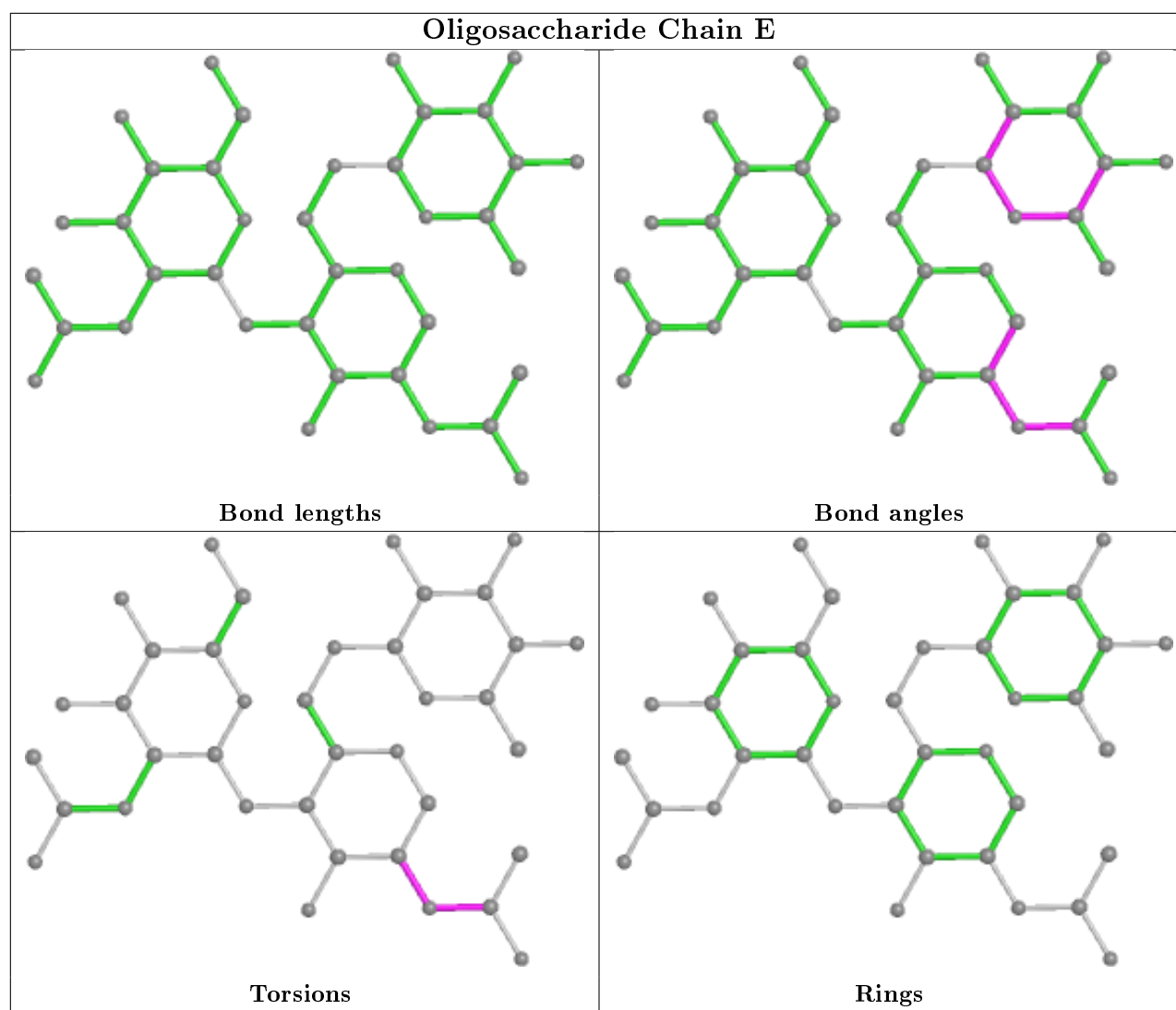
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	G	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C1-C2-N2-C7
3	E	1	NAG	C3-C2-N2-C7

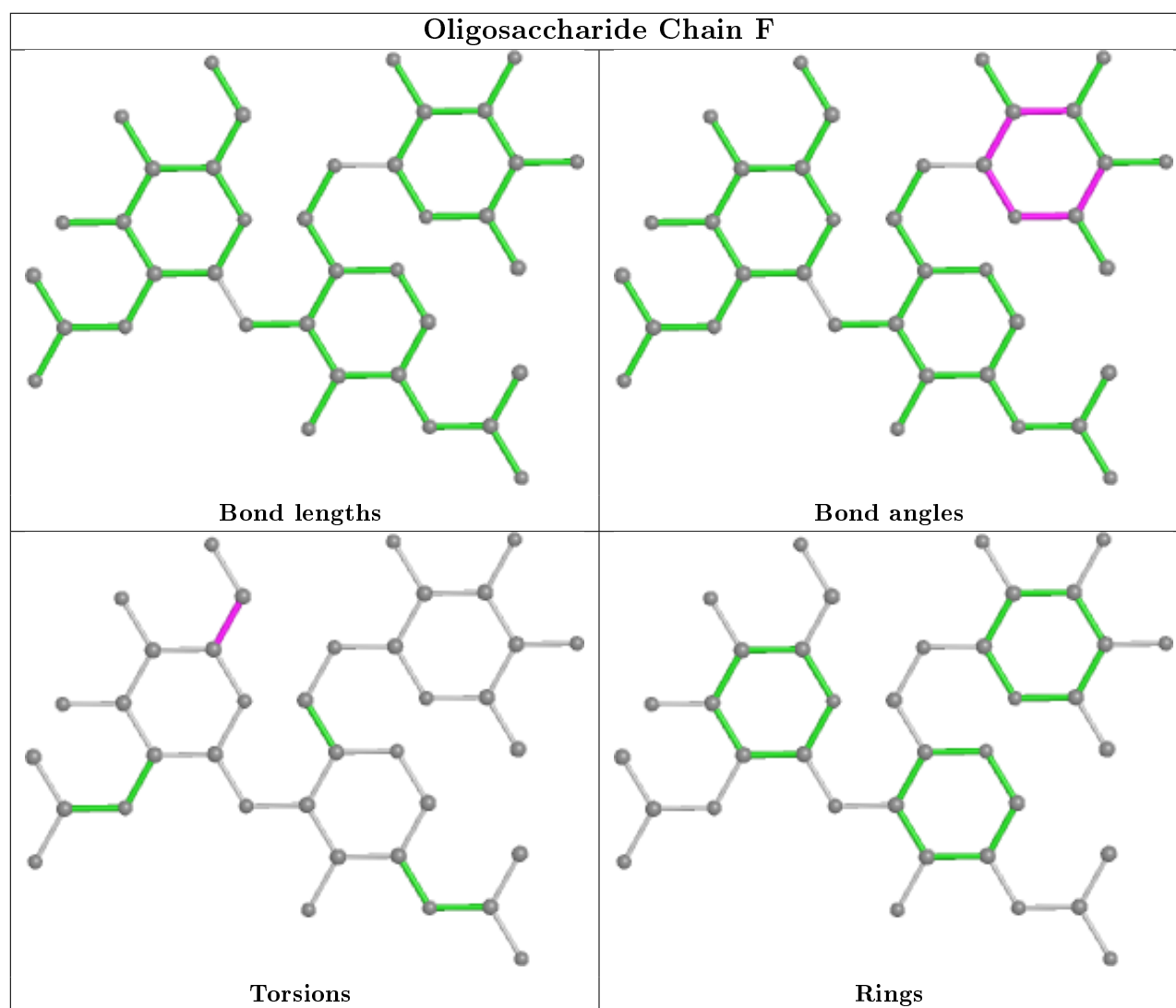
There are no ring outliers.

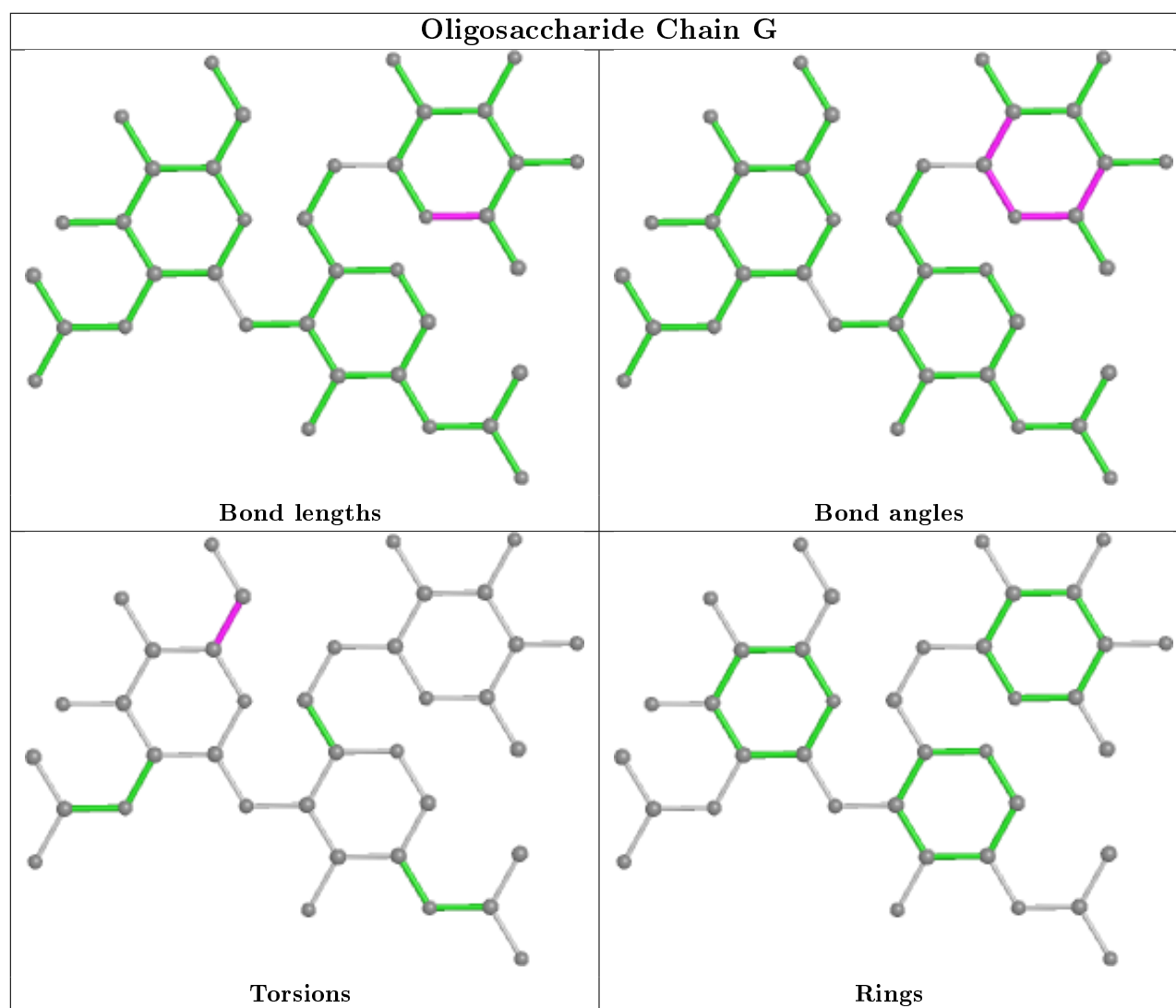
1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	5	0

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







5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z > 2$
7	NAG	B	304	2	14,14,15	0.98	1 (7%)	17,19,21	0.59	0
5	SO4	D	308	-	4,4,4	0.11	0	6,6,6	0.34	0
5	SO4	B	305	-	4,4,4	0.20	0	6,6,6	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	D	307	-	5,5,5	0.90	0	5,5,5	0.96	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
7	NAG	B	304	2	-	2/6/23/26	0/1/1/1
4	GOL	D	307	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	304	NAG	C1-C2	3.50	1.57	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	307	GOL	O1-C1-C2-C3
7	B	304	NAG	C8-C7-N2-C2
7	B	304	NAG	O7-C7-N2-C2
4	D	307	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	304	NAG	2	0
4	D	307	GOL	2	0

5.7 Other polymers

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	132/162 (81%)	0.05	2 (1%) 73 76	31, 46, 87, 113	0
1	C	132/162 (81%)	0.17	0 100 100	28, 48, 75, 87	0
2	B	218/267 (81%)	-0.22	2 (0%) 84 85	20, 32, 57, 99	0
2	D	218/267 (81%)	-0.33	0 100 100	18, 27, 51, 86	0
All	All	700/858 (81%)	-0.13	4 (0%) 89 91	18, 37, 66, 113	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	128	ARG	3.2
2	B	178	ARG	3.1
1	A	91	LYS	2.9
1	A	10	ILE	2.1

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	E	2	14/15	0.75	0.25	77,80,82,84	0
3	NAG	G	2	14/15	0.82	0.26	90,93,94,95	0
3	NAG	F	2	14/15	0.88	0.19	65,67,67,67	0

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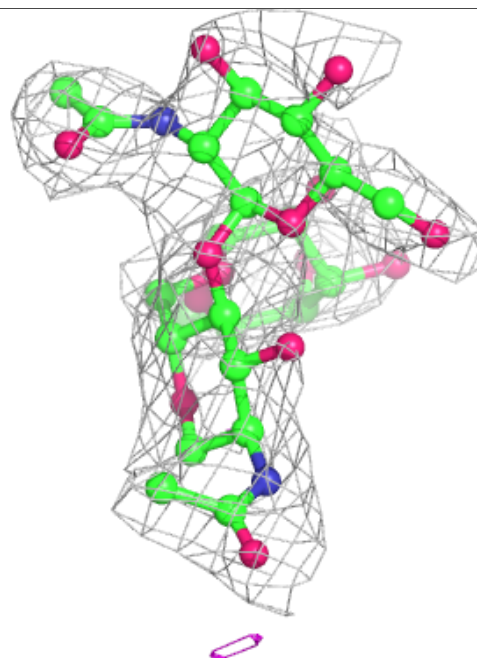
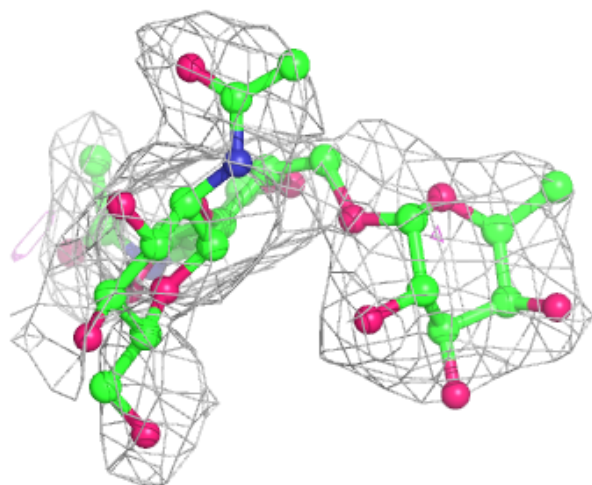
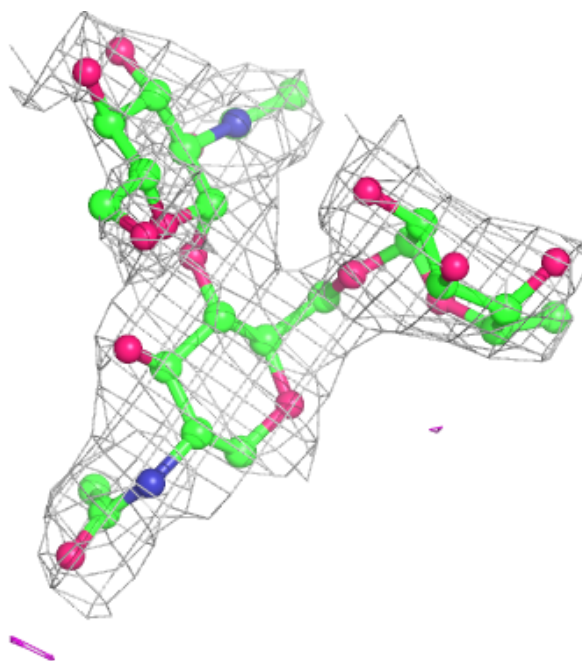
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	E	1	14/15	0.89	0.19	55,58,66,74	0
3	NAG	G	1	14/15	0.91	0.16	60,68,75,86	0
3	NAG	F	1	14/15	0.91	0.18	44,49,54,61	0
3	FUC	E	3	10/11	0.92	0.14	58,59,59,60	0
3	FUC	G	3	10/11	0.93	0.25	55,56,58,59	0
3	FUC	F	3	10/11	0.97	0.20	41,41,42,43	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.

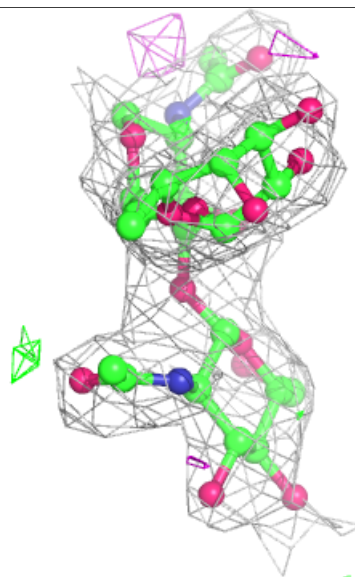
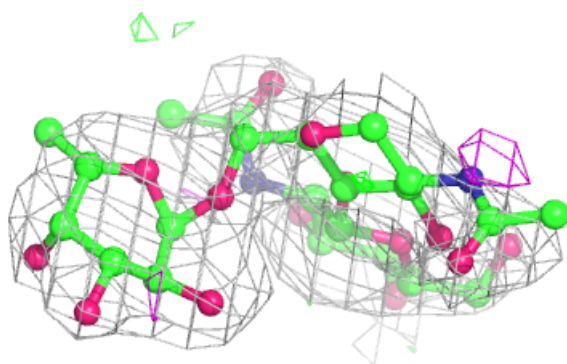
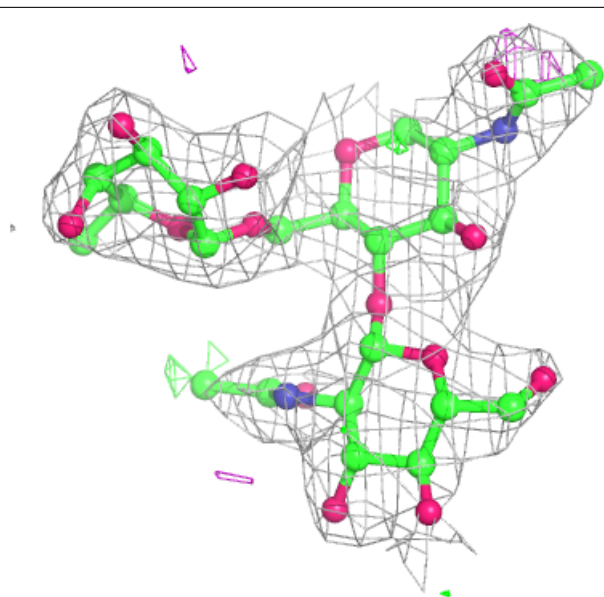
Electron density around Chain E:

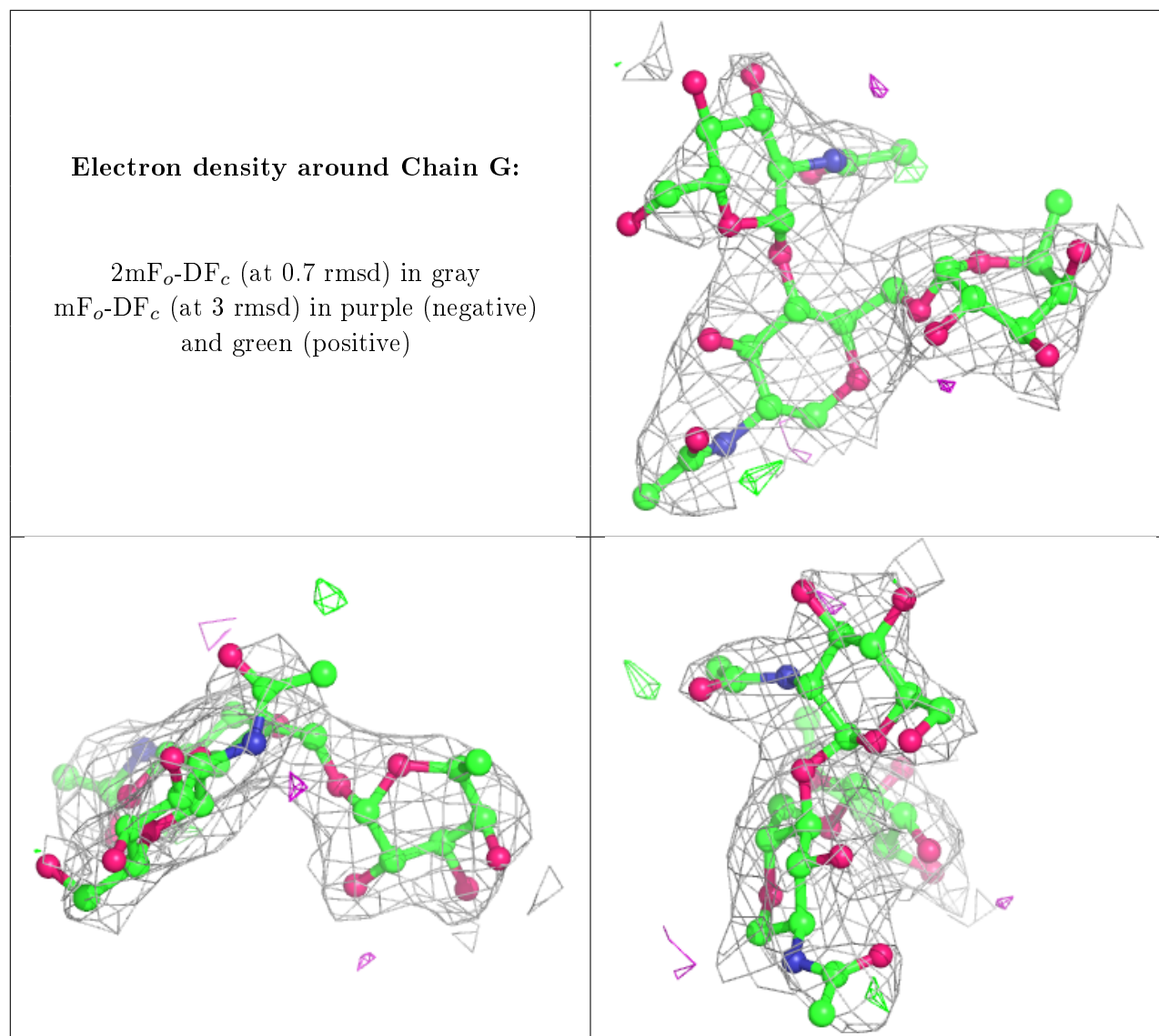
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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
7	NAG	B	304	14/15	0.67	0.36	92,94,98,99	0
4	GOL	D	307	6/6	0.93	0.15	37,38,38,39	0
5	SO4	B	305	5/5	0.98	0.11	30,31,31,32	0
6	MG	D	309	1/1	0.98	0.23	30,30,30,30	0
5	SO4	D	308	5/5	0.99	0.09	28,28,29,29	0

6.5 Other polymers

There are no such residues in this entry.