



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 11:21 AM EDT

PDB ID : 6EG0
Title : Crystal structure of Dpr4 Ig1-Ig2 in complex with DIP-Eta Ig1-Ig3
Authors : Cosmanescu, F.; Shapiro, L.
Deposited on : 2018-08-17
Resolution : 2.90 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

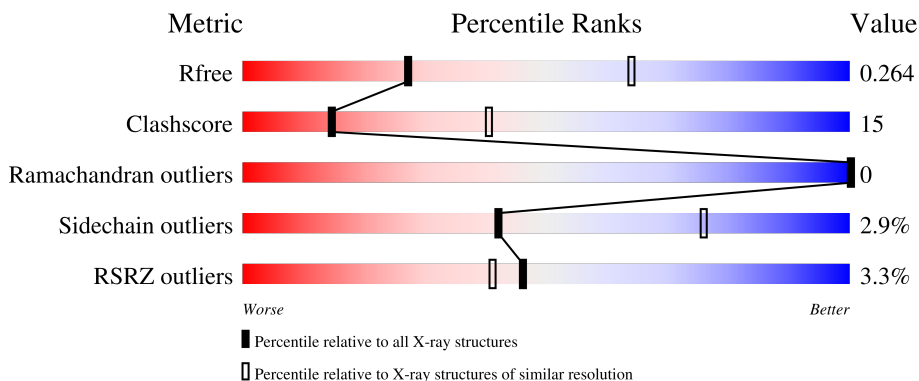
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	220	 4% 61% 29% 9%
2	B	314	 3% 68% 29% ..
3	C	3	 33% 33% 33%
4	D	4	 75% 25%
5	E	5	 60% 40%

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Mol	Chain	Length	Quality of chain
6	F	8	 75% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	2	-	-	-	X
3	FUC	C	3	-	-	-	X
5	MAN	E	4	-	-	-	X
7	NAG	B	406	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 4352 atoms, of which 32 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 Defective proboscis extension response 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	201	1573	978	287	302	6	0	1	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	247	HIS	-	expression tag	UNP Q59DX6
A	248	HIS	-	expression tag	UNP Q59DX6
A	249	HIS	-	expression tag	UNP Q59DX6
A	250	HIS	-	expression tag	UNP Q59DX6
A	251	HIS	-	expression tag	UNP Q59DX6

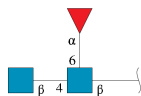
- Molecule 2 is a protein called Dpr-interacting protein eta, isoform B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	309	2414	1521	425	452	16	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

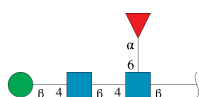
Chain	Residue	Modelled	Actual	Comment	Reference
B	339	HIS	-	expression tag	UNP Q9VMN9
B	340	HIS	-	expression tag	UNP Q9VMN9
B	341	HIS	-	expression tag	UNP Q9VMN9
B	342	HIS	-	expression tag	UNP Q9VMN9
B	343	HIS	-	expression tag	UNP Q9VMN9
B	344	HIS	-	expression tag	UNP Q9VMN9

- 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.



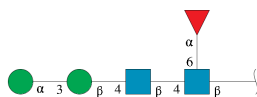
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	3	38	22	2	14	0	0	0

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



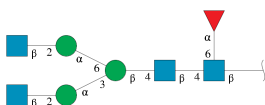
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	4	49	28	2	19	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	E	5	60	34	2	24	0	0	0

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



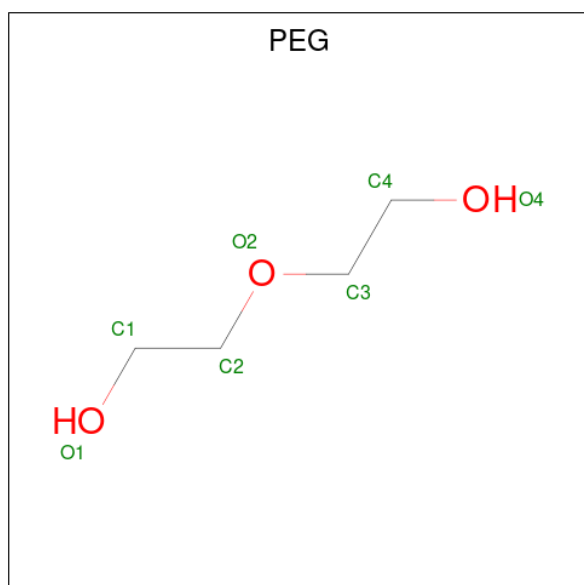
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	F	8	99	56	4	39	0	0	0

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



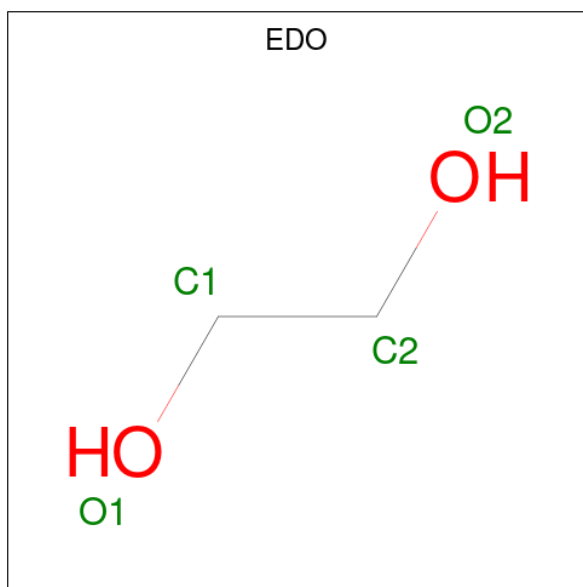
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	B	1	14	8	1	5	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



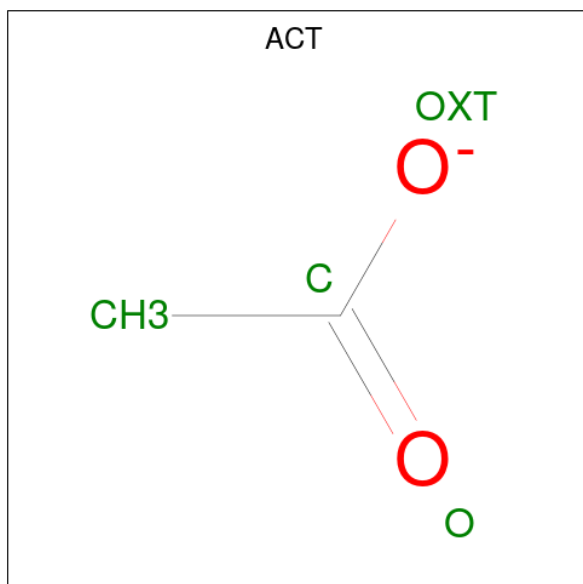
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	H	O	0	0
			17	4	10	3		
8	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 10 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂⁻).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	H	O	0	0
			7	2	3	2		
10	B	1	Total	C	H	O	0	0
			7	2	3	2		

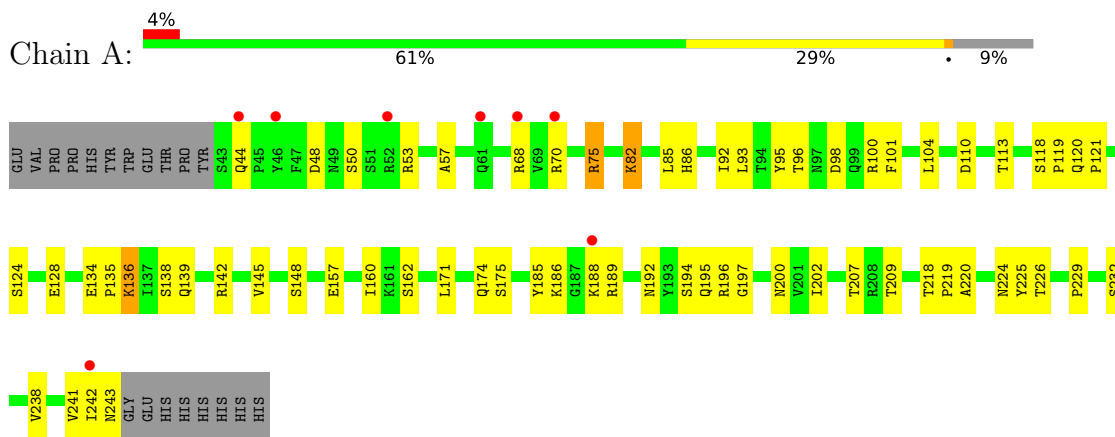
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	5	Total	O	0	0
			5	5		
11	B	42	Total	O	0	0
			42	42		

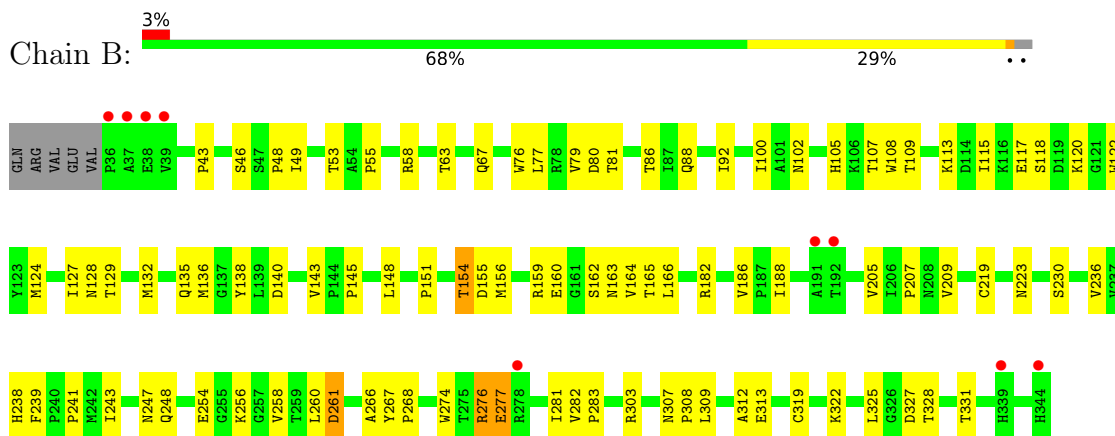
3 Residue-property plots [i](#)

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.

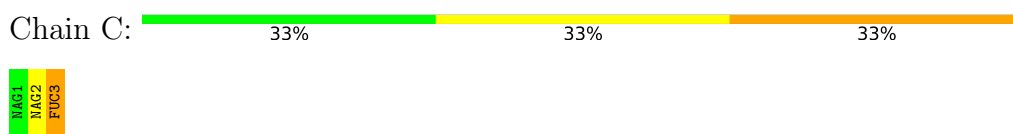
- Molecule 1: Defective proboscis extension response 4




- Molecule 2: Dpr-interacting protein eta, isoform B



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



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

Chain D:  75% 25%

MAG1
MAG2
BMA3
FUC4

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  60% 40%

MAG1
MAG2
BMA3
MAN4
FUC5

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

Chain F:  75% 25%

MAG1
MAG2
BMA3
MAN4
MAG5
MAG7
FUC8

4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	94.29Å 94.29Å 212.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 2.90 19.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.99-2.90) 99.4 (19.99-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.88Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.221 , 0.264 0.221 , 0.264	Depositor DCC
R_{free} test set	1233 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	64.0	Xtrriage
Anisotropy	0.504	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4352	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: ACT, MAN, BMA, NAG, PEG, FUC, EDO

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	0.24	0/1606	0.45	0/2178
2	B	0.24	0/2475	0.45	0/3371
All	All	0.24	0/4081	0.45	0/5549

There are no bond length outliers.

There are no bond angle outliers.

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	1573	0	1564	59	0
2	B	2414	0	2400	77	0
3	C	38	0	34	1	0
4	D	49	0	43	3	0
5	E	60	0	52	2	0
6	F	99	0	85	0	0
7	B	14	0	13	0	0
8	B	14	20	20	0	0
9	B	4	6	6	0	0
10	B	8	6	6	0	0
11	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	B	42	0	0	2	0
All	All	4320	32	4223	130	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 15.

All (130) 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:157:GLU:HG3	1:A:238:VAL:HG13	1.65	0.79
1:A:219:PRO:HA	1:A:241:VAL:HG21	1.64	0.78
1:A:188:LYS:HE2	4:D:4:FUC:H63	1.67	0.75
1:A:120:GLN:O	1:A:145:VAL:HG11	1.87	0.74
1:A:229:PRO:HG2	1:A:232:SER:HB2	1.72	0.72
2:B:77:LEU:HD13	2:B:124:MET:HE3	1.71	0.72
1:A:82:LYS:HD3	1:A:128:GLU:HB2	1.72	0.70
2:B:241:PRO:HA	2:B:266:ALA:HB2	1.74	0.69
1:A:186:LYS:HD3	1:A:225:TYR:CE1	2.30	0.67
2:B:80:ASP:OD1	2:B:81:THR:N	2.30	0.64
1:A:171:LEU:CD2	1:A:209:THR:HG22	2.28	0.63
1:A:207:THR:O	1:A:209:THR:HG23	1.99	0.63
1:A:192:ASN:O	1:A:195:GLN:HG2	2.00	0.61
2:B:258:VAL:HG12	2:B:309:LEU:HD21	1.82	0.61
1:A:188:LYS:HG2	4:D:4:FUC:O4	2.00	0.61
2:B:63:THR:HG22	2:B:109:THR:OG1	1.99	0.61
2:B:63:THR:HG22	2:B:109:THR:HG23	1.81	0.61
2:B:238:HIS:HB3	2:B:325:LEU:HD11	1.82	0.61
2:B:261:ASP:OD1	2:B:303:ARG:HG2	2.02	0.60
3:C:2:NAG:H5	3:C:3:FUC:H61	1.83	0.60
2:B:46:SER:OG	2:B:67:GLN:HG3	2.03	0.59
2:B:53:THR:HG22	2:B:140:ASP:HB3	1.85	0.59
1:A:192:ASN:ND2	1:A:194:SER:OG	2.38	0.57
2:B:154:THR:HG23	2:B:155:ASP:H	1.70	0.57
1:A:95:TYR:CZ	2:B:128:ASN:HB3	2.39	0.56
1:A:200:ASN:OD1	1:A:202:ILE:HD11	2.05	0.56
1:A:120:GLN:HB3	1:A:121:PRO:HD2	1.86	0.56
2:B:276:ARG:NH2	2:B:312:ALA:O	2.38	0.56
1:A:92:ILE:CD1	1:A:93:LEU:HD22	2.36	0.56
2:B:182:ARG:HB2	2:B:186:VAL:O	2.06	0.56
2:B:113:LYS:HE2	11:B:537:HOH:O	2.04	0.55
2:B:88[B]:GLN:HA	2:B:88[B]:GLN:OE1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:THR:HG23	1:A:220:ALA:H	1.73	0.54
1:A:185:TYR:HB2	1:A:226:THR:HB	1.89	0.54
1:A:136:LYS:HE2	1:A:138:SER:HB3	1.89	0.53
1:A:160:ILE:CD1	1:A:241:VAL:HG12	2.38	0.53
2:B:63:THR:HG22	2:B:109:THR:CG2	2.39	0.53
2:B:138:TYR:CD1	5:E:1:NAG:H62	2.45	0.52
1:A:86:HIS:ND1	2:B:132:MET:HG3	2.25	0.52
1:A:57:ALA:O	1:A:145:VAL:HA	2.10	0.52
2:B:239:PHE:CE2	2:B:266:ALA:HA	2.45	0.52
1:A:219:PRO:HA	1:A:241:VAL:CG2	2.35	0.52
1:A:162:SER:OG	1:A:243:ASN:HB2	2.10	0.51
2:B:205:VAL:HG12	2:B:207:PRO:HD3	1.93	0.51
2:B:165:THR:HG22	2:B:205:VAL:HG22	1.92	0.51
1:A:85:LEU:HG	2:B:124:MET:HE1	1.92	0.51
2:B:276:ARG:HH22	2:B:313:GLU:HA	1.76	0.51
1:A:95:TYR:CE1	2:B:128:ASN:HB3	2.46	0.50
1:A:148:SER:HA	1:A:174:GLN:HB2	1.93	0.50
2:B:117:GLU:O	2:B:120:LYS:HG2	2.10	0.50
2:B:281:ILE:H	2:B:281:ILE:HD12	1.76	0.50
1:A:53:ARG:CZ	1:A:139:GLN:HG3	2.42	0.50
2:B:267:TYR:HA	2:B:268:PRO:C	2.31	0.50
2:B:219:CYS:O	2:B:230:SER:HA	2.12	0.50
2:B:156:MET:HG3	2:B:166:LEU:CD2	2.41	0.50
1:A:82:LYS:HD3	1:A:128:GLU:CB	2.38	0.50
1:A:86:HIS:HD1	2:B:132:MET:HG3	1.77	0.49
1:A:68:ARG:HA	1:A:110:ASP:O	2.12	0.49
2:B:127:ILE:HG22	2:B:129:THR:HG23	1.94	0.49
1:A:48:ASP:OD1	1:A:70:ARG:NH2	2.45	0.48
2:B:165:THR:CG2	2:B:205:VAL:HG22	2.44	0.48
2:B:55:PRO:HG2	2:B:58:ARG:HG3	1.96	0.48
2:B:79:VAL:HG21	2:B:136:MET:CE	2.43	0.48
1:A:218:THR:OG1	1:A:219:PRO:HD2	2.13	0.48
2:B:236:VAL:HG13	2:B:267:TYR:CE2	2.49	0.48
1:A:171:LEU:HD22	1:A:209:THR:HG22	1.95	0.47
2:B:164:VAL:HG12	2:B:209:VAL:CG2	2.45	0.47
2:B:86:THR:OG1	2:B:100:ILE:HD12	2.15	0.47
1:A:224:ASN:HA	1:A:238:VAL:HA	1.96	0.47
2:B:282:VAL:HG13	2:B:283:PRO:HD2	1.97	0.47
1:A:121:PRO:HA	1:A:145:VAL:HG13	1.97	0.46
2:B:105:HIS:ND1	11:B:503:HOH:O	2.36	0.46
2:B:274:TRP:CZ3	2:B:319:CYS:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:THR:HG21	1:A:101:PHE:HB2	1.98	0.46
1:A:160:ILE:HD12	1:A:160:ILE:O	2.15	0.46
2:B:102:ASN:HD22	2:B:105:HIS:H	1.63	0.46
2:B:260:LEU:HD12	2:B:260:LEU:N	2.31	0.46
2:B:55:PRO:HG2	2:B:58:ARG:CG	2.45	0.46
2:B:102:ASN:HB3	2:B:108:TRP:CE3	2.51	0.46
2:B:79:VAL:HG21	2:B:136:MET:HE3	1.96	0.46
2:B:102:ASN:HA	2:B:107:THR:O	2.16	0.45
2:B:138:TYR:CG	5:E:1:NAG:H62	2.51	0.45
2:B:159:ARG:NH1	2:B:160:GLU:O	2.49	0.45
1:A:75:ARG:N	1:A:75:ARG:HD3	2.32	0.45
2:B:48:PRO:HA	2:B:135:GLN:OE1	2.16	0.45
1:A:82:LYS:NZ	1:A:82:LYS:HB3	2.31	0.45
2:B:256:LYS:O	2:B:309:LEU:HD23	2.17	0.45
1:A:218:THR:HG23	1:A:220:ALA:N	2.31	0.45
2:B:92:ILE:HD12	2:B:92:ILE:N	2.32	0.44
2:B:248:GLN:HG3	2:B:331:THR:O	2.18	0.44
2:B:281:ILE:HD12	2:B:281:ILE:N	2.33	0.44
1:A:118:SER:N	1:A:119:PRO:HD3	2.33	0.44
2:B:122:TRP:HB3	2:B:136:MET:CE	2.48	0.44
1:A:175:SER:HB3	1:A:232:SER:OG	2.18	0.43
1:A:242:ILE:HG22	1:A:243:ASN:N	2.33	0.43
2:B:127:ILE:CG2	2:B:129:THR:HG23	2.49	0.43
2:B:148:LEU:HB2	2:B:151:PRO:HG2	2.00	0.43
2:B:117:GLU:OE2	2:B:143:VAL:HG21	2.18	0.43
1:A:50:SER:O	1:A:68:ARG:NH1	2.51	0.43
1:A:44:GLN:OE1	1:A:44:GLN:N	2.52	0.42
1:A:82:LYS:HE2	1:A:128:GLU:OE1	2.20	0.42
2:B:243:ILE:HG12	2:B:328:THR:HG23	2.01	0.42
1:A:95:TYR:O	2:B:128:ASN:HB2	2.19	0.42
2:B:122:TRP:HB3	2:B:136:MET:HE3	1.99	0.42
2:B:322:LYS:CB	2:B:327:ASP:HB3	2.49	0.42
2:B:182:ARG:HG3	2:B:188:ILE:CG1	2.50	0.42
1:A:44:GLN:O	1:A:44:GLN:HG2	2.18	0.42
1:A:98:ASP:O	1:A:100:ARG:N	2.52	0.42
1:A:202:ILE:HD12	1:A:202:ILE:N	2.34	0.42
2:B:241:PRO:CA	2:B:266:ALA:HB2	2.45	0.42
1:A:157:GLU:HG3	1:A:238:VAL:CG1	2.41	0.42
2:B:162:SER:O	2:B:209:VAL:HG23	2.20	0.41
2:B:276:ARG:HD3	2:B:277:GLU:HB2	2.03	0.41
1:A:92:ILE:HD12	1:A:93:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:SER:OG	1:A:145:VAL:HG12	2.21	0.41
1:A:134:GLU:HA	1:A:135:PRO:HA	1.91	0.41
2:B:164:VAL:HG12	2:B:209:VAL:HG21	2.03	0.41
2:B:182:ARG:HG3	2:B:188:ILE:HG12	2.03	0.41
2:B:58:ARG:O	2:B:115:ILE:HG12	2.20	0.41
2:B:145:PRO:HD3	2:B:223:ASN:OD1	2.21	0.41
2:B:63:THR:CG2	2:B:109:THR:HG23	2.49	0.41
1:A:136:LYS:NZ	2:B:81:THR:O	2.53	0.40
2:B:49:ILE:HD13	2:B:76:TRP:CH2	2.56	0.40
2:B:307:ASN:HA	2:B:308:PRO:HA	1.86	0.40
2:B:307:ASN:OD1	2:B:308:PRO:HA	2.22	0.40
1:A:188:LYS:HE2	4:D:4:FUC:C6	2.45	0.40
2:B:43:PRO:HA	2:B:67:GLN:O	2.22	0.40
1:A:104:LEU:HB2	1:A:113:THR:HB	2.02	0.40
1:A:196:ARG:NH1	1:A:197:GLY:O	2.54	0.40
2:B:63:THR:HG22	2:B:109:THR:CB	2.52	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	200/220 (91%)	188 (94%)	12 (6%)	0	100	100
2	B	308/314 (98%)	291 (94%)	17 (6%)	0	100	100
All	All	508/534 (95%)	479 (94%)	29 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/196 (91%)	174 (97%)	5 (3%)	43	76
2	B	272/276 (99%)	264 (97%)	8 (3%)	42	76
All	All	451/472 (96%)	438 (97%)	13 (3%)	42	76

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	ARG
1	A	82	LYS
1	A	136	LYS
1	A	142	ARG
1	A	189	ARG
2	B	118	SER
2	B	154	THR
2	B	163	ASN
2	B	247	ASN
2	B	254	GLU
2	B	261	ASP
2	B	276	ARG
2	B	277	GLU

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	61	GLN
1	A	102	GLN
1	A	120	GLN
1	A	192	ASN
1	A	243	ASN
2	B	89	ASN
2	B	105	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

20 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	C	1	3,1	14,14,15	0.34	0	17,19,21	0.41	0
3	NAG	C	2	3	14,14,15	0.18	0	17,19,21	0.40	0
3	FUC	C	3	3	10,10,11	0.73	0	14,14,16	1.04	1 (7%)
4	NAG	D	1	4,1	14,14,15	0.30	0	17,19,21	0.59	0
4	NAG	D	2	4	14,14,15	0.23	0	17,19,21	0.40	0
4	BMA	D	3	4	11,11,12	0.54	0	15,15,17	0.80	0
4	FUC	D	4	4	10,10,11	0.68	0	14,14,16	0.72	0
5	NAG	E	1	5,2	14,14,15	0.27	0	17,19,21	0.48	0
5	NAG	E	2	5	14,14,15	0.20	0	17,19,21	0.41	0
5	BMA	E	3	5	11,11,12	0.48	0	15,15,17	0.80	0
5	MAN	E	4	5	11,11,12	0.66	0	15,15,17	0.92	1 (6%)
5	FUC	E	5	5	10,10,11	0.67	0	14,14,16	0.80	0
6	NAG	F	1	6,2	14,14,15	0.33	0	17,19,21	0.51	0
6	NAG	F	2	6	14,14,15	0.31	0	17,19,21	0.39	0
6	BMA	F	3	6	11,11,12	0.43	0	15,15,17	0.95	0
6	MAN	F	4	6	11,11,12	0.71	0	15,15,17	1.04	2 (13%)
6	NAG	F	5	6	14,14,15	0.29	0	17,19,21	0.38	0
6	MAN	F	6	6	11,11,12	0.62	0	15,15,17	1.17	2 (13%)
6	NAG	F	7	6	14,14,15	0.15	0	17,19,21	0.62	0
6	FUC	F	8	6	10,10,11	0.68	0	14,14,16	0.77	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	6	MAN	O2-C2-C3	-3.05	104.03	110.14
6	F	6	MAN	C1-O5-C5	2.66	115.80	112.19
6	F	4	MAN	O2-C2-C3	-2.65	104.82	110.14
5	E	4	MAN	O2-C2-C3	-2.23	105.66	110.14
6	F	4	MAN	C1-O5-C5	2.17	115.14	112.19
3	C	3	FUC	C1-O5-C5	2.05	117.43	112.78

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	O5-C5-C6-O6

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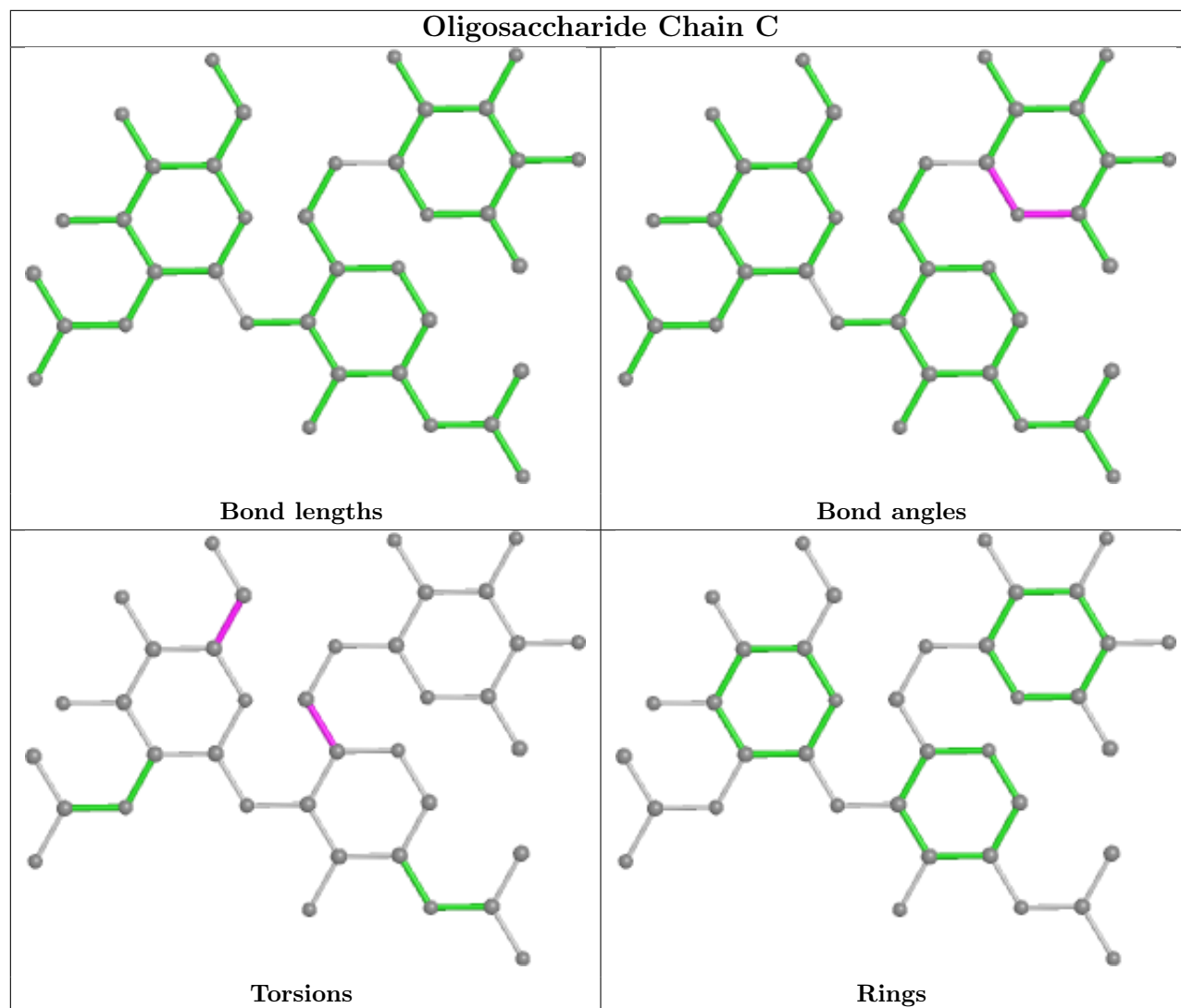
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C4-C5-C6-O6
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	D	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
4	D	1	NAG	C1-C2-N2-C7
6	F	6	MAN	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
4	D	1	NAG	C3-C2-N2-C7

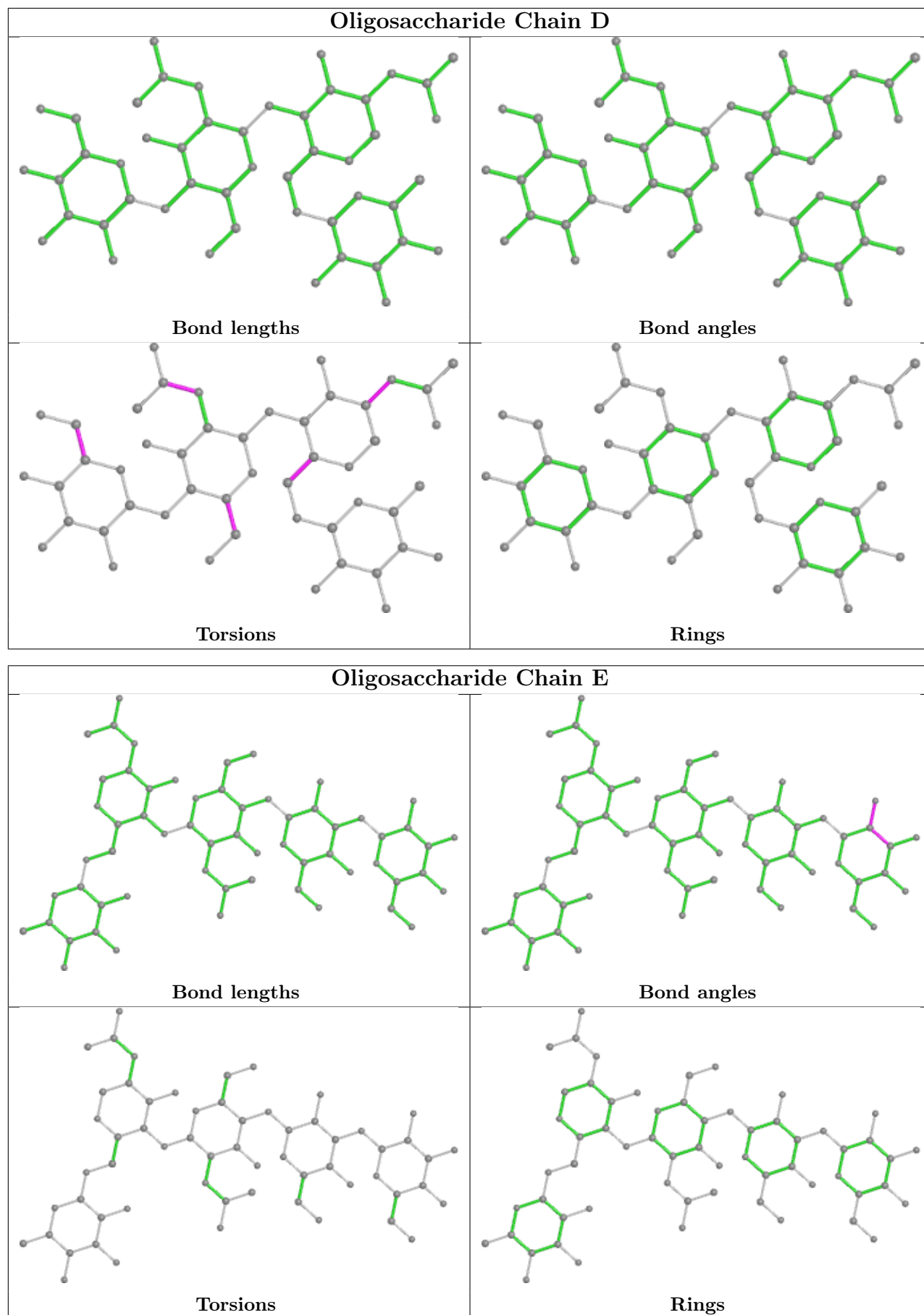
There are no ring outliers.

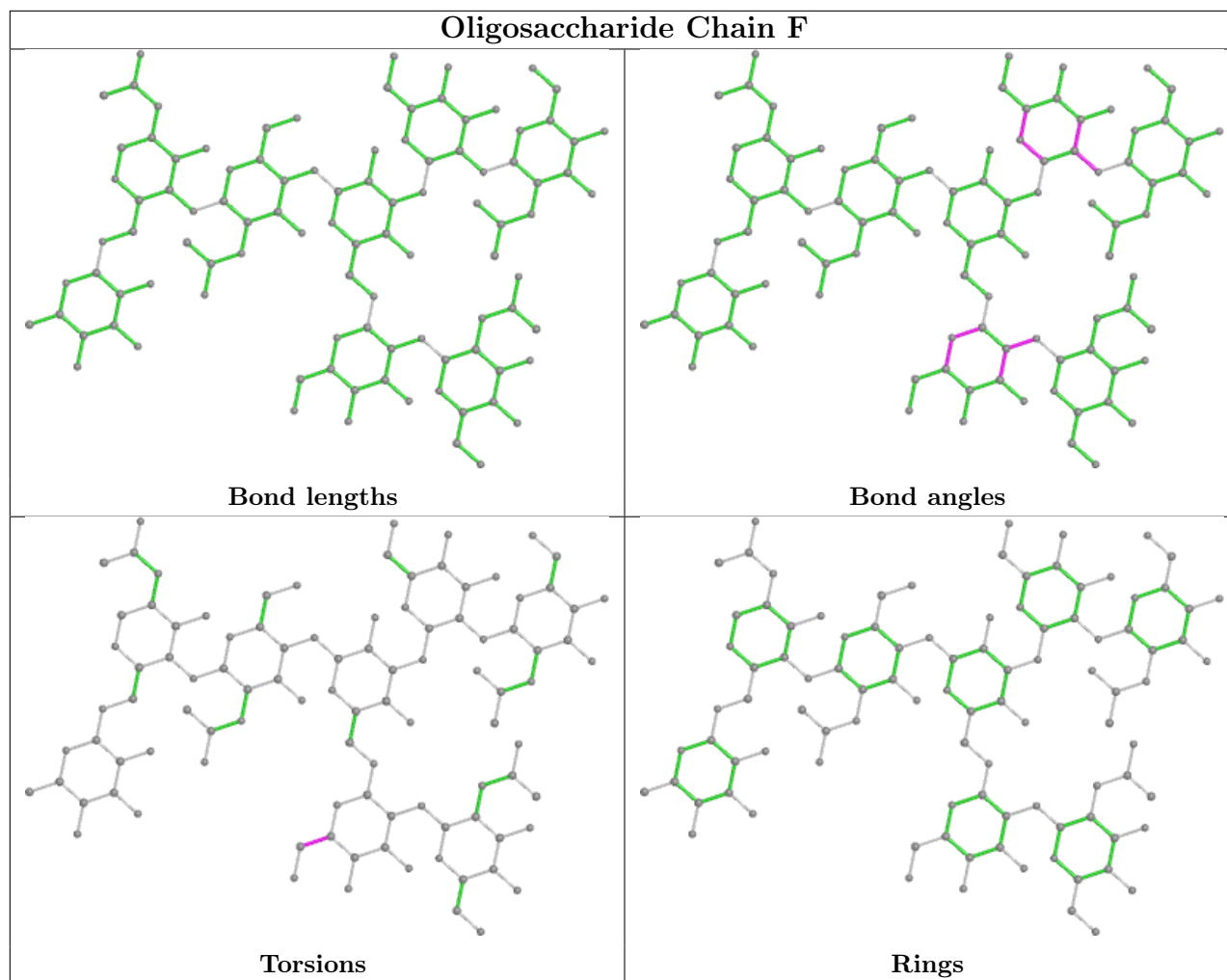
4 monomers are involved in 6 short contacts:

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

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







5.6 Ligand geometry [i](#)

6 ligands 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$
10	ACT	B	419	-	3,3,3	0.73	0	3,3,3	0.82	0
8	PEG	B	415	-	6,6,6	0.49	0	5,5,5	0.30	0
8	PEG	B	416	-	6,6,6	0.48	0	5,5,5	0.28	0
9	EDO	B	417	-	3,3,3	0.47	0	2,2,2	0.31	0
10	ACT	B	418	-	3,3,3	0.73	0	3,3,3	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	B	406	2	14,14,15	0.32	0	17,19,21	0.39	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
8	PEG	B	416	-	-	0/4/4/4	-
9	EDO	B	417	-	-	0/1/1/1	-
7	NAG	B	406	2	-	0/6/23/26	0/1/1/1
8	PEG	B	415	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	201/220 (91%)	0.04	8 (3%) 38 33	48, 82, 126, 148	0
2	B	309/314 (98%)	-0.31	9 (2%) 51 47	39, 54, 91, 149	0
All	All	510/534 (95%)	-0.17	17 (3%) 46 41	39, 62, 115, 149	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	39	VAL	4.1
2	B	191	ALA	4.1
1	A	46	TYR	3.9
2	B	37	ALA	3.7
1	A	44	GLN	3.4
1	A	242	ILE	3.1
2	B	339	HIS	2.7
2	B	192	THR	2.6
1	A	61	GLN	2.5
2	B	38	GLU	2.5
2	B	344	HIS	2.3
1	A	70	ARG	2.3
2	B	36	PRO	2.3
2	B	278	ARG	2.3
1	A	52	ARG	2.1
1	A	68	ARG	2.1
1	A	188	LYS	2.0

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

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

6.3 Carbohydrates

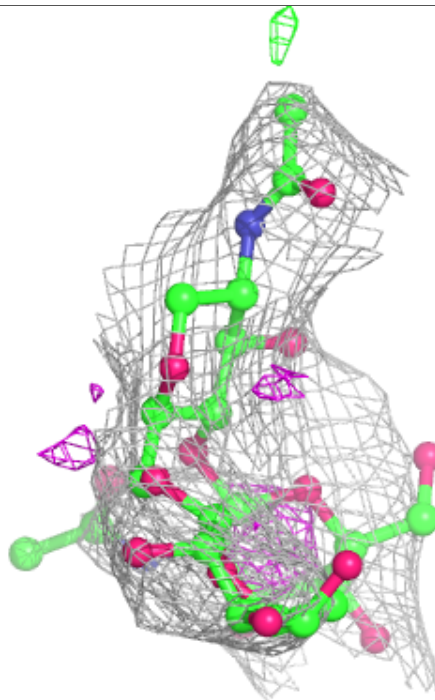
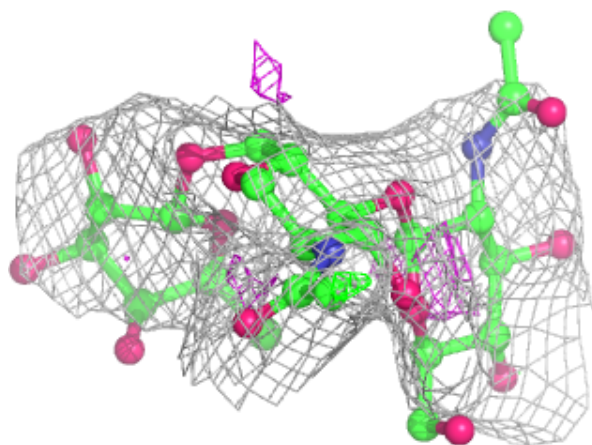
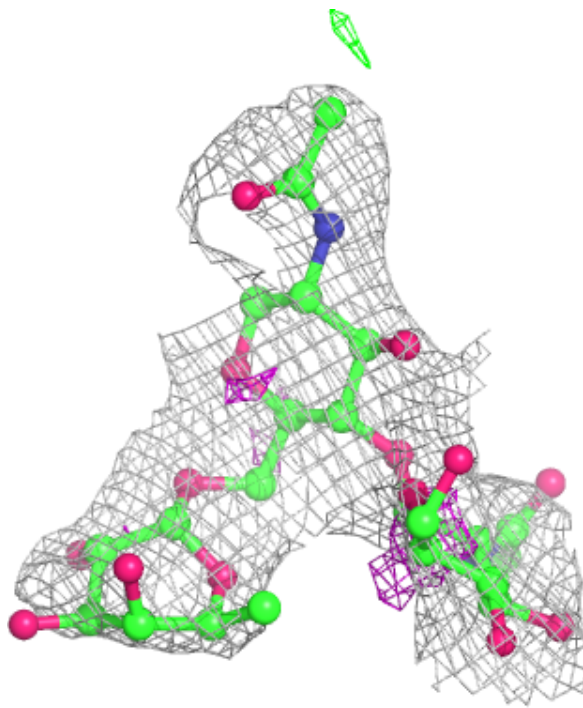
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MAN	E	4	11/12	0.73	0.48	130,157,169,172	0
3	NAG	C	2	14/15	0.75	0.48	120,134,151,152	0
5	BMA	E	3	11/12	0.78	0.32	116,144,158,167	0
3	FUC	C	3	10/11	0.78	0.47	104,136,149,149	0
4	BMA	D	3	11/12	0.85	0.37	134,159,164,170	0
6	NAG	F	5	14/15	0.86	0.40	111,132,140,147	0
6	NAG	F	7	14/15	0.87	0.41	94,122,135,136	0
4	FUC	D	4	10/11	0.88	0.22	116,124,137,138	0
3	NAG	C	1	14/15	0.89	0.26	70,115,125,125	0
4	NAG	D	1	14/15	0.90	0.21	104,118,134,136	0
6	MAN	F	4	11/12	0.90	0.25	100,122,135,140	0
4	NAG	D	2	14/15	0.91	0.33	116,131,147,147	0
6	BMA	F	3	11/12	0.92	0.14	89,101,111,114	0
5	FUC	E	5	10/11	0.92	0.18	72,87,96,106	0
6	MAN	F	6	11/12	0.93	0.21	84,97,109,117	0
5	NAG	E	2	14/15	0.94	0.28	55,100,119,147	0
6	NAG	F	2	14/15	0.95	0.12	50,75,83,97	0
5	NAG	E	1	14/15	0.95	0.15	53,75,83,84	0
6	NAG	F	1	14/15	0.96	0.12	43,54,67,71	0
6	FUC	F	8	10/11	0.98	0.16	48,57,76,79	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.

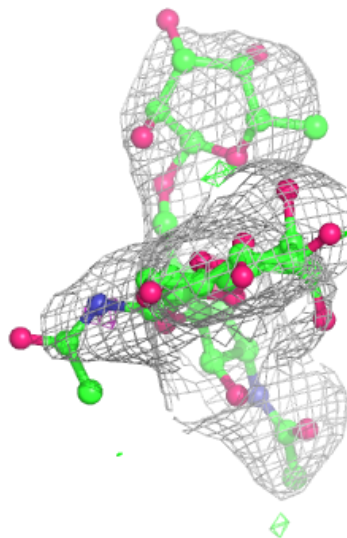
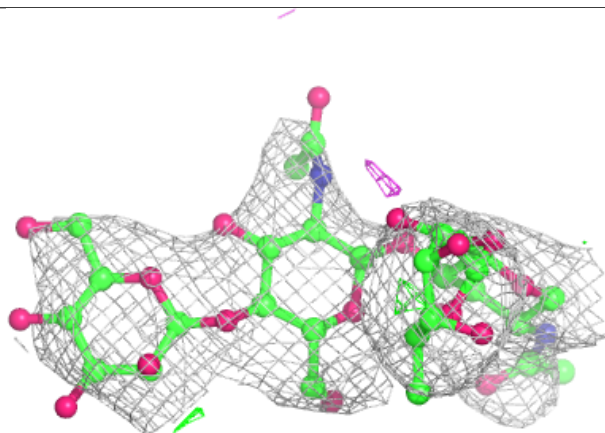
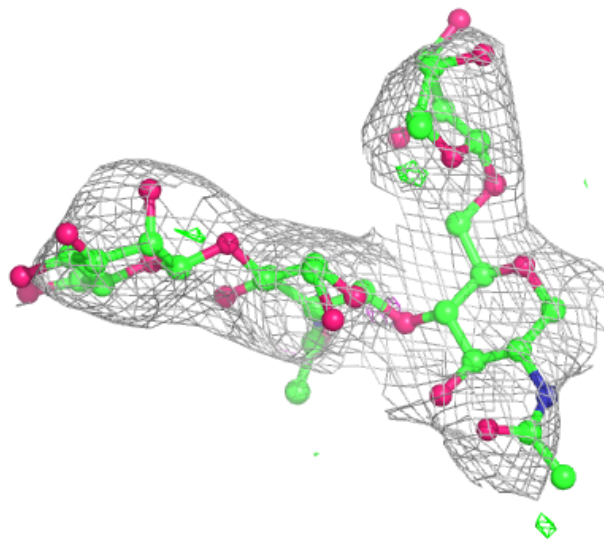
Electron density around Chain C:

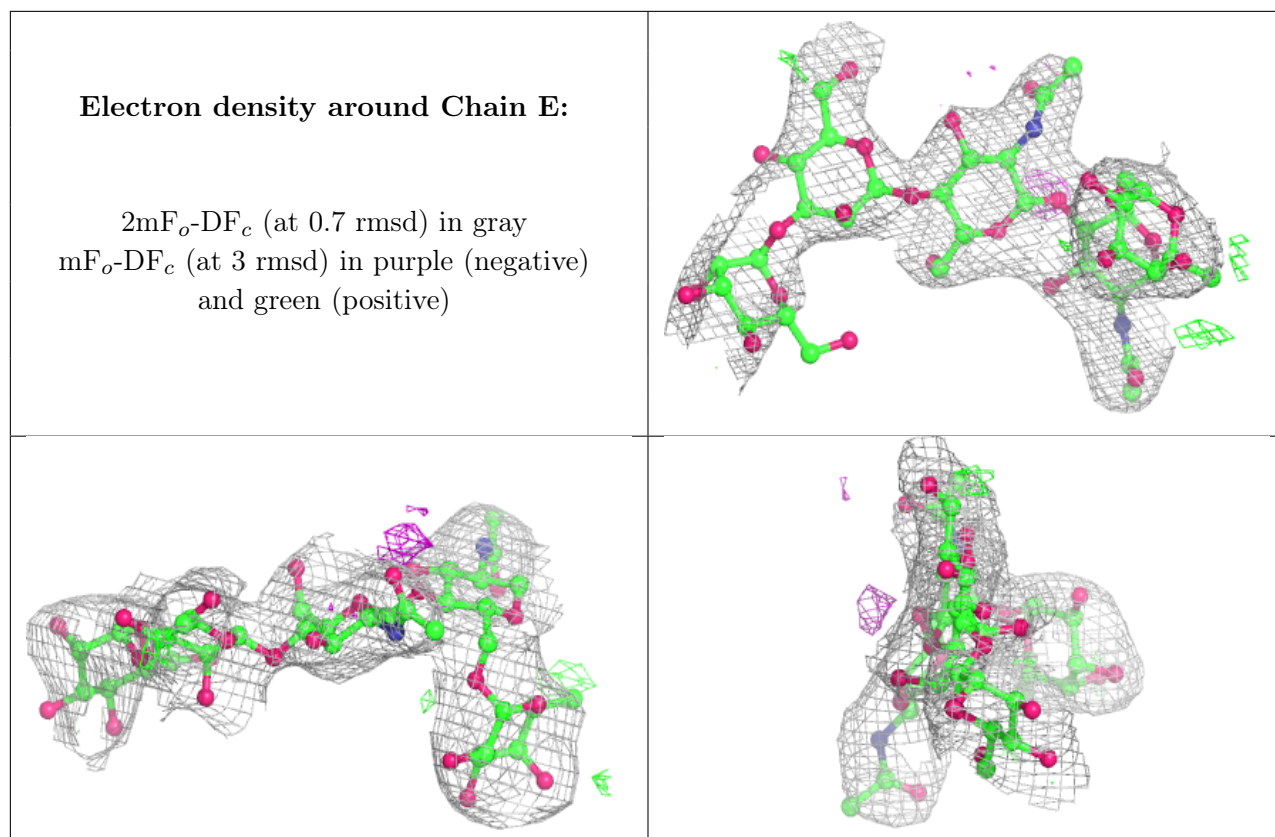
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

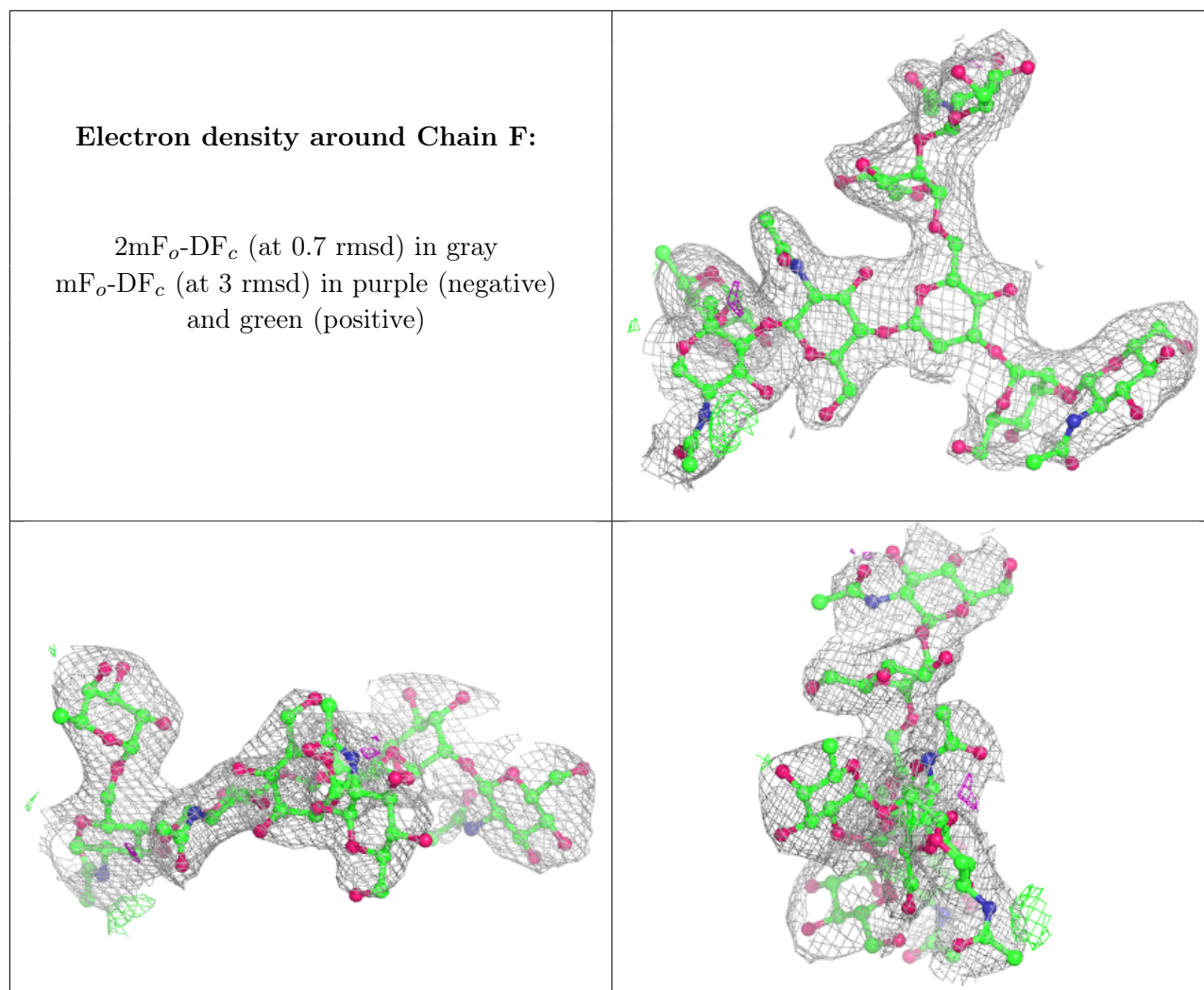


Electron density around Chain D:

$2mF_o-DF_c$ (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	406	14/15	0.71	0.46	106,130,148,152	0
8	PEG	B	415	7/7	0.85	0.36	77,95,120,120	0
9	EDO	B	417	4/4	0.86	0.53	70,84,95,111	0
8	PEG	B	416	7/7	0.90	0.17	67,86,119,119	0
10	ACT	B	419	4/4	0.93	0.34	75,86,104,104	0
10	ACT	B	418	4/4	0.94	0.23	67,75,80,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.