



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 05:23 AM BST

PDB ID : 4UTC
Title : Crystal structure of dengue 2 virus envelope glycoprotein
Authors : Kikuti, C.; Rouvinski, A.; Guardado-Calvo, P.; Barba-Spaeth, G.; Duquerroy, S.; Vaney, M.C.; Rey, F.A.
Deposited on : 2014-07-18
Resolution : 3.08 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 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	:	2.13.1
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)	:	2.13.1

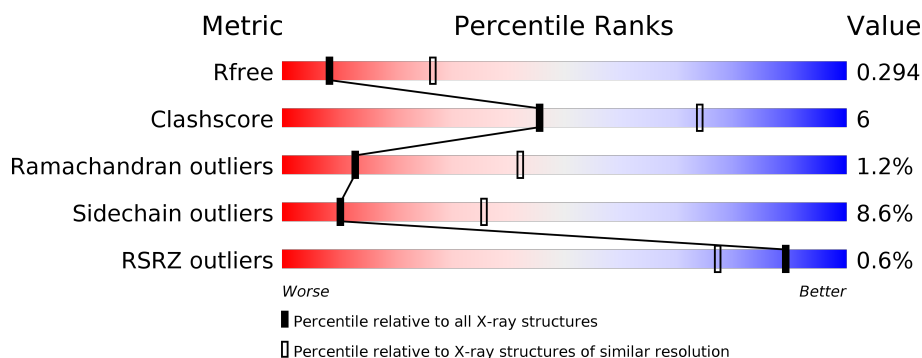
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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	422	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 72%, green 19%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 72% 19% • 7% </div> </div>
1	B	422	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 72%, yellow 18%, orange 8%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 72% 18% • 8% </div> </div>
2	C	3	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 33%, orange 67%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 33% 67% </div> </div>
3	D	2	<div> <div style="width: 100%; height: 10px; background: yellow;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 100% </div> </div>
3	F	2	<div> <div style="width: 100%; height: 10px; background: yellow;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 100% </div> </div>
4	E	6	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 50%, orange 50%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 50% 50% </div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6243 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 ENVELOPE GLYCOPROTEIN E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			3035	1912	521	578	24			
1	B	390	Total	C	N	O	S	0	0	0
			3037	1914	523	576	24			

There are 64 discrepancies between the modelled and reference sequences:

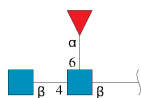
Chain	Residue	Modelled	Actual	Comment	Reference
A	392	LEU	-	expression tag	UNP Q68Y26
A	393	ARG	-	expression tag	UNP Q68Y26
A	394	PRO	-	expression tag	UNP Q68Y26
A	395	LEU	-	expression tag	UNP Q68Y26
A	396	GLU	-	expression tag	UNP Q68Y26
A	397	SER	-	expression tag	UNP Q68Y26
A	398	ARG	-	expression tag	UNP Q68Y26
A	399	GLY	-	expression tag	UNP Q68Y26
A	400	PRO	-	expression tag	UNP Q68Y26
A	401	PHE	-	expression tag	UNP Q68Y26
A	402	GLU	-	expression tag	UNP Q68Y26
A	403	GLY	-	expression tag	UNP Q68Y26
A	404	LYS	-	expression tag	UNP Q68Y26
A	405	PRO	-	expression tag	UNP Q68Y26
A	406	ILE	-	expression tag	UNP Q68Y26
A	407	PRO	-	expression tag	UNP Q68Y26
A	408	ASN	-	expression tag	UNP Q68Y26
A	409	PRO	-	expression tag	UNP Q68Y26
A	410	LEU	-	expression tag	UNP Q68Y26
A	411	LEU	-	expression tag	UNP Q68Y26
A	412	GLY	-	expression tag	UNP Q68Y26
A	413	LEU	-	expression tag	UNP Q68Y26
A	414	ASP	-	expression tag	UNP Q68Y26
A	415	SER	-	expression tag	UNP Q68Y26
A	416	THR	-	expression tag	UNP Q68Y26

Continued on next page...

Continued from previous page...

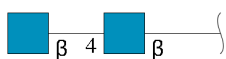
Chain	Residue	Modelled	Actual	Comment	Reference
A	417	ARG	-	expression tag	UNP Q68Y26
A	418	THR	-	expression tag	UNP Q68Y26
A	419	GLY	-	expression tag	UNP Q68Y26
A	420	HIS	-	expression tag	UNP Q68Y26
A	421	HIS	-	expression tag	UNP Q68Y26
A	422	HIS	-	expression tag	UNP Q68Y26
A	118	LYS	MET	conflict	UNP Q68Y26
B	392	LEU	-	expression tag	UNP Q68Y26
B	393	ARG	-	expression tag	UNP Q68Y26
B	394	PRO	-	expression tag	UNP Q68Y26
B	395	LEU	-	expression tag	UNP Q68Y26
B	396	GLU	-	expression tag	UNP Q68Y26
B	397	SER	-	expression tag	UNP Q68Y26
B	398	ARG	-	expression tag	UNP Q68Y26
B	399	GLY	-	expression tag	UNP Q68Y26
B	400	PRO	-	expression tag	UNP Q68Y26
B	401	PHE	-	expression tag	UNP Q68Y26
B	402	GLU	-	expression tag	UNP Q68Y26
B	403	GLY	-	expression tag	UNP Q68Y26
B	404	LYS	-	expression tag	UNP Q68Y26
B	405	PRO	-	expression tag	UNP Q68Y26
B	406	ILE	-	expression tag	UNP Q68Y26
B	407	PRO	-	expression tag	UNP Q68Y26
B	408	ASN	-	expression tag	UNP Q68Y26
B	409	PRO	-	expression tag	UNP Q68Y26
B	410	LEU	-	expression tag	UNP Q68Y26
B	411	LEU	-	expression tag	UNP Q68Y26
B	412	GLY	-	expression tag	UNP Q68Y26
B	413	LEU	-	expression tag	UNP Q68Y26
B	414	ASP	-	expression tag	UNP Q68Y26
B	415	SER	-	expression tag	UNP Q68Y26
B	416	THR	-	expression tag	UNP Q68Y26
B	417	ARG	-	expression tag	UNP Q68Y26
B	418	THR	-	expression tag	UNP Q68Y26
B	419	GLY	-	expression tag	UNP Q68Y26
B	420	HIS	-	expression tag	UNP Q68Y26
B	421	HIS	-	expression tag	UNP Q68Y26
B	422	HIS	-	expression tag	UNP Q68Y26
B	118	LYS	MET	conflict	UNP Q68Y26

- Molecule 2 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.



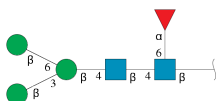
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 3 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
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-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
4	E	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	O	0	0
			3	3		
5	B	3	Total	O	0	0
			3	3		

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.

Chain A:

Sequence logo for Chain A. The y-axis lists amino acids, and the x-axis shows positions M1 to L135. The color scale at the top indicates conservation percentage: 72% (green), 19% (yellow), and 7% (grey).

Position	Conservation (%)	Most Frequent Amino Acid(s)
M1	72%	GLY
S16	72%	GLY
S19	72%	GLY
W20	72%	GLY
V24	72%	GLY
A35	72%	GLY
K36	72%	GLY
H37	72%	GLY
K38	72%	GLY
L41	72%	GLY
K47	72%	GLY
P83	72%	GLY
A54	72%	GLY
T55	72%	GLY
L56	72%	GLY
K64	72%	GLY
L65	72%	GLY
E71	72%	GLY
C74	72%	GLY
Q77	72%	GLY
L82	72%	GLY
N83	72%	GLY
E94	72%	GLY
K88	72%	GLY
S95	72%	GLY
R99	72%	GLY
G102	72%	GLY
C105	72%	GLY
T120	72%	GLY
C121	72%	GLY
K122	72%	GLY
M125	72%	GLY
K128	72%	GLY
I129	72%	GLY
V130	72%	GLY
Q131	72%	GLY
P132	72%	GLY
L135	72%	GLY
T138	72%	GLY
E147	72%	GLY
E148	72%	GLY
H149	72%	GLY
A150	72%	GLY
I164	72%	GLY
P166	72%	GLY
Q167	72%	GLY
T176	72%	GLY
T182	72%	GLY
T189	72%	GLY
GLY	72%	GLY
LEU	72%	GLY
D192	72%	GLY
F193	72%	GLY
N194	72%	GLY
L198	72%	GLY
M201	72%	GLY
W206	72%	GLY
L207	72%	GLY
V208	72%	GLY
H209	72%	GLY
F213	72%	GLY
L216	72%	GLY
L221	72%	GLY
P222	72%	GLY
G223	72%	GLY
S229	72%	GLY
N230	72%	GLY
V238	72%	GLY
T239	72%	GLY
F240	72%	GLY
K241	72%	GLY
D249	72%	GLY
V250	72%	GLY
V251	72%	GLY
V252	72%	GLY
L253	72%	GLY
I270	72%	GLY
L277	72%	GLY
L278	72%	GLY
LEU	72%	GLY
GLY	72%	GLY
L279	72%	GLY
ASP	72%	GLY

Chain B:

Amino Acid	Count
ARG	1322
THR	823
GLY	1335
HIS	836
HIS	837
HIS	838
HIS	1339
HIS	1340
D341	1342
E343	1344
K344	1345
E345	1346
E346	1351
L351	1352
P356	1357
V365	1369
A369	1376
S376	1377
I378	1379
V380	1381
G381	1387
L387	1388
K388	1389
I390	1391
K391	1392
L392	1395
GLU	1396
SER	1397
ARG	1398
GLY	1399
PRO	1400
PHE	1401
GLU	1402
GLY	1403
LYS	1404
PRO	1405
ILE	1406
PRO	1407
ASN	1408
PRO	1409
LEU	1410
LEU	1411
GLY	1412
LEU	1413
ASP	1414
ASP	1415
SER	1416
THR	1417
MI	1464
T165	1465
T176	1466
T180	1467
R188	1468
G190	1469
L191	1470
D192	1471
F193	1472
M194	1473
E195	1474
L207	1475
V208	1476
H209	1477
G223	1478
T226	1479
K234	1480
V238	1481
T239	1482
K247	1483
Q248	1484
D249	1485
V250	1486
V251	1487
V252	1488
L253	1489
Q271	1490
M272	1491
N276	1492
L277	1493
T280	1494
L283	1495
R286	1496
L287	1497
K288	1498
PRO	1499
ASN	1500
PRO	1501
LEU	1502
LEU	1503
GLY	1504
LEU	1505
ASP	1506
ASP	1507
SER	1508
THR	1509
MI	1564
G14	1565
VAL	1566
SER	1567
GLY	1568
GLY	1569
SER	1570
W20	1571
L41	1572
K47	1573
T48	1574
E49	1575
A50	1576
K51	1577
Q52	1578
T55	1579
K64	1580
L65	1581
C74	1582
Q77	1583
E84	1584
I91	1585
S95	1586
R99	1587
G102	1588
C105	1589
C116	1590
T120	1591
C121	1592
K122	1593
P132	1594
E133	1595
M134	1596
L135	1597
E136	1598
Y137	1599
T138	1600
I139	1601
S145	1602
G146	1603
E147	1604
E148	1605

Chain C: 33% 67%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%



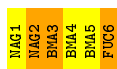
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%



- Molecule 4: beta-D-mannopyranose-(1-3)-[beta-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 E:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.46 Å 105.46 Å 165.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.08 45.37 – 3.08	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-3.08) 97.9 (45.37-3.08)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.06 Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.211 , 0.279 0.225 , 0.294	Depositor DCC
R_{free} test set	886 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	86.0	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 83.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6243	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.53	0/3095	0.76	0/4183
1	B	0.51	0/3098	0.77	1/4188 (0.0%)
All	All	0.52	0/6193	0.76	1/8371 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	SER	N-CA-C	-5.96	94.90	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3035	0	3021	35	0
1	B	3037	0	3032	37	0
2	C	38	0	34	5	0
3	D	28	0	25	0	0
3	F	28	0	25	0	0
4	E	71	0	61	6	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6243	0	6198	80	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 6.

The worst 5 of 80 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)
4:E:2:NAG:H3	4:E:6:FUC:H61	1.60	0.84
2:C:2:NAG:H3	2:C:3:FUC:H61	1.57	0.83
1:A:20:TRP:HA	1:A:287:LEU:O	1.82	0.79
1:B:195:GLU:HG2	1:B:209:HIS:CE1	2.20	0.76
1:A:239:THR:HB	1:A:251:VAL:HG23	1.76	0.66

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	385/422 (91%)	353 (92%)	29 (8%)	3 (1%)	19	52
1	B	386/422 (92%)	357 (92%)	23 (6%)	6 (2%)	9	35
All	All	771/844 (91%)	710 (92%)	52 (7%)	9 (1%)	13	42

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	345	ARG
1	A	176	THR
1	B	146	GLY
1	B	344	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	148	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	339/366 (93%)	312 (92%)	27 (8%)	12	38
1	B	339/366 (93%)	308 (91%)	31 (9%)	9	31
All	All	678/732 (93%)	620 (91%)	58 (9%)	10	36

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	390	ASN
1	B	134	ASN
1	B	351	LEU
1	B	49	GLU
1	B	84	GLU

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

Mol	Chain	Res	Type
1	A	200	GLN
1	A	282	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 ⓘ

13 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	C	1	1,2	14,14,15	0.39	0	17,19,21	0.87	0
2	NAG	C	2	2	14,14,15	0.24	0	17,19,21	0.71	1 (5%)
2	FUC	C	3	2	10,10,11	0.46	0	14,14,16	1.36	2 (14%)
3	NAG	D	1	1,3	14,14,15	0.27	0	17,19,21	1.08	1 (5%)
3	NAG	D	2	3	14,14,15	0.33	0	17,19,21	1.57	2 (11%)
4	NAG	E	1	1,4	14,14,15	0.42	0	17,19,21	0.79	0
4	NAG	E	2	4	14,14,15	0.29	0	17,19,21	0.97	2 (11%)
4	BMA	E	3	4	11,11,12	0.45	0	15,15,17	1.32	1 (6%)
4	BMA	E	4	4	11,11,12	0.52	0	15,15,17	1.03	1 (6%)
4	BMA	E	5	4	11,11,12	0.48	0	15,15,17	1.83	1 (6%)
4	FUC	E	6	4	10,10,11	0.52	0	14,14,16	1.41	3 (21%)
3	NAG	F	1	1,3	14,14,15	0.27	0	17,19,21	0.70	1 (5%)
3	NAG	F	2	3	14,14,15	0.34	0	17,19,21	1.61	2 (11%)

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

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

Continued on next page...

Continued from previous page...

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

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	5	BMA	C1-O5-C5	6.40	120.86	112.19
3	D	2	NAG	C1-O5-C5	5.37	119.47	112.19
3	F	2	NAG	C1-O5-C5	5.32	119.41	112.19
3	D	1	NAG	C1-O5-C5	4.08	117.72	112.19
4	E	6	FUC	C1-O5-C5	3.86	121.53	112.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	E	4	BMA	O5-C5-C6-O6

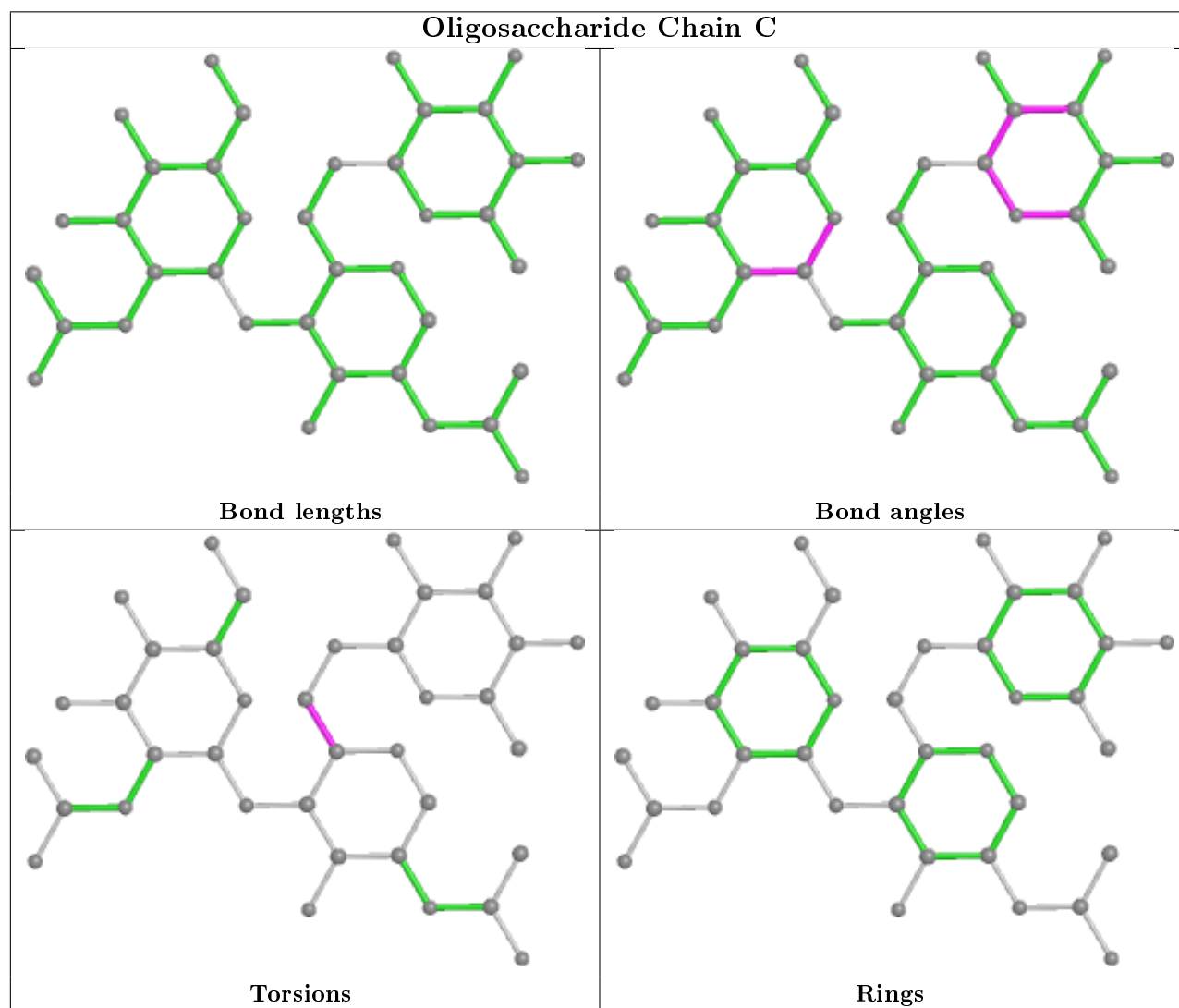
All (1) ring outliers are listed below:

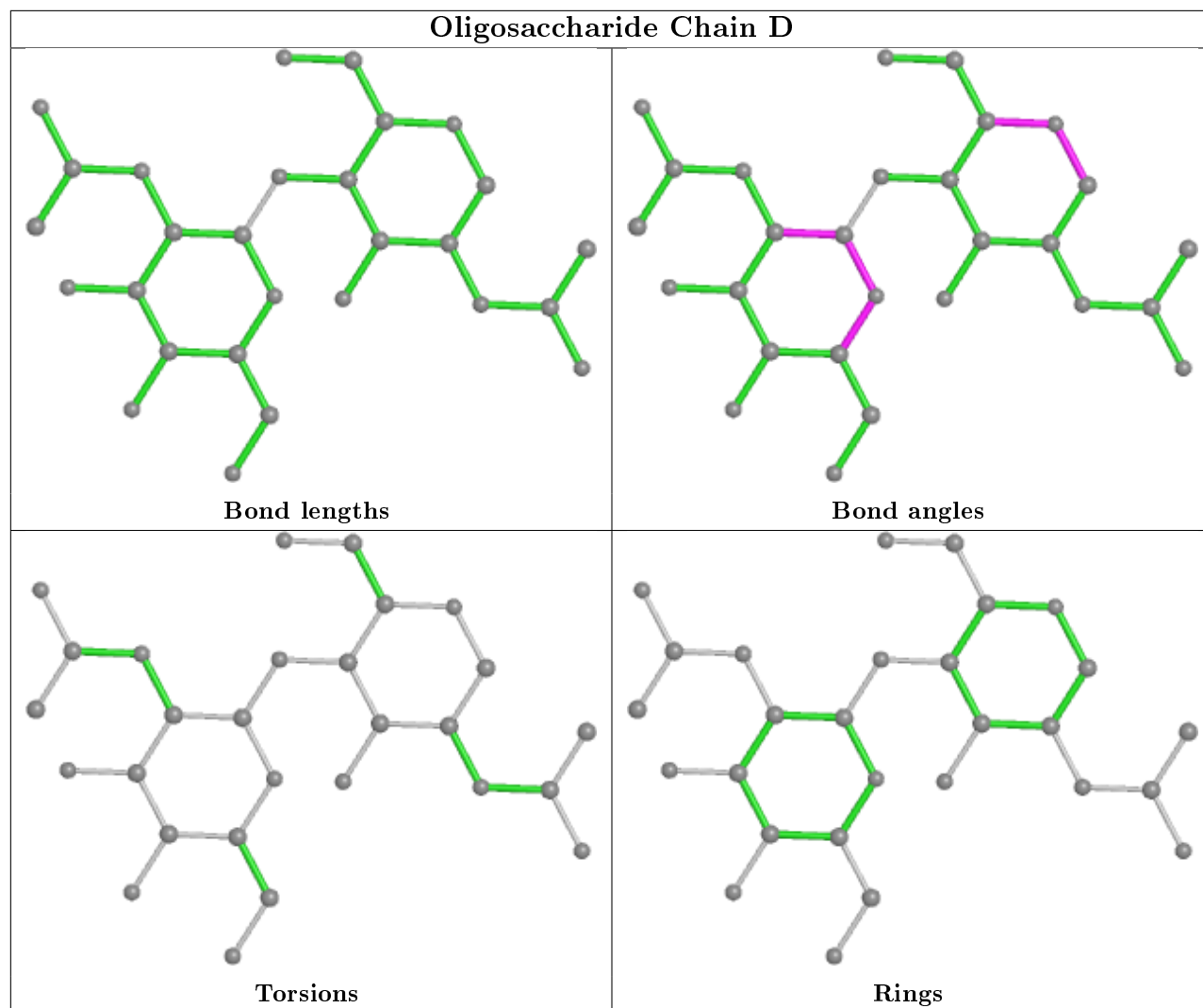
Mol	Chain	Res	Type	Atoms
4	E	5	BMA	C1-C2-C3-C4-C5-O5

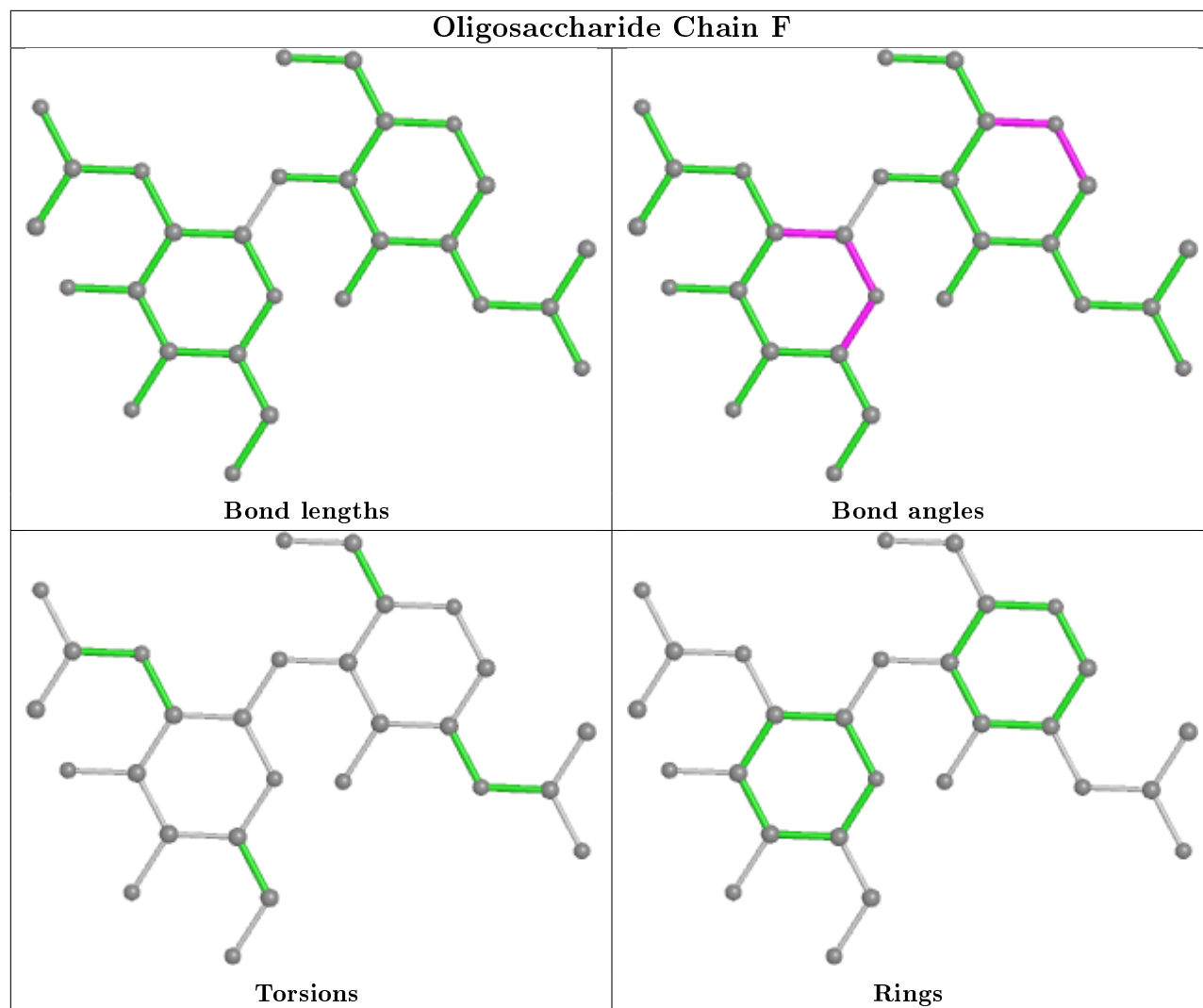
7 monomers are involved in 11 short contacts:

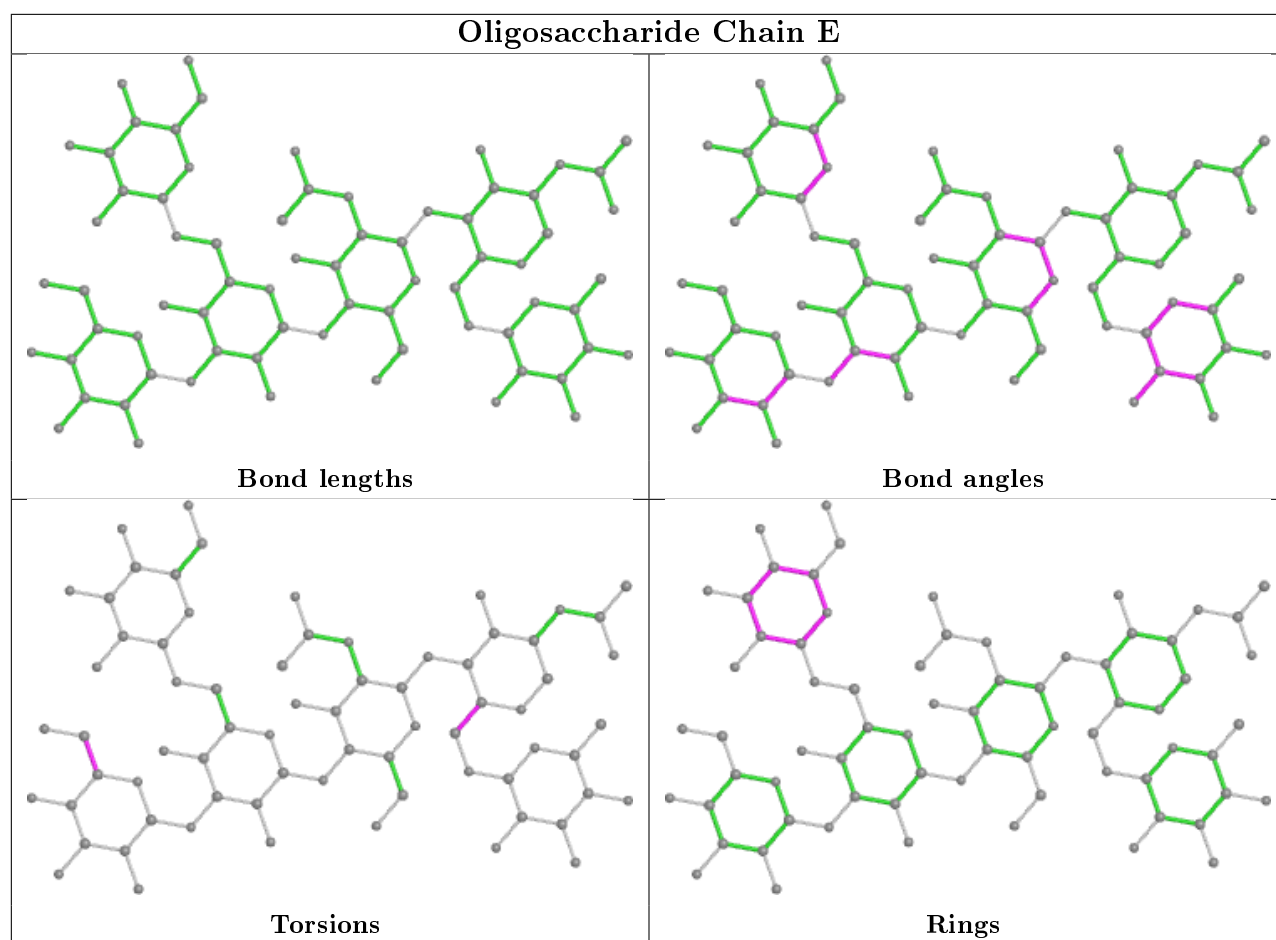
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	6	FUC	1	0
2	C	3	FUC	2	0
2	C	1	NAG	3	0
4	E	2	NAG	5	0
4	E	3	BMA	2	0
4	E	1	NAG	3	0
2	C	2	NAG	3	0

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](#)

There are no ligands in this entry.

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	391/422 (92%)	-0.03	4 (1%) 82 66	46, 78, 125, 147	0
1	B	390/422 (92%)	0.09	1 (0%) 94 87	40, 86, 118, 134	0
All	All	781/844 (92%)	0.03	5 (0%) 89 77	40, 82, 121, 147	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	135	LEU	4.5
1	B	378	ILE	3.1
1	A	189	THR	2.8
1	A	395	LEU	2.1
1	A	277	LEU	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.

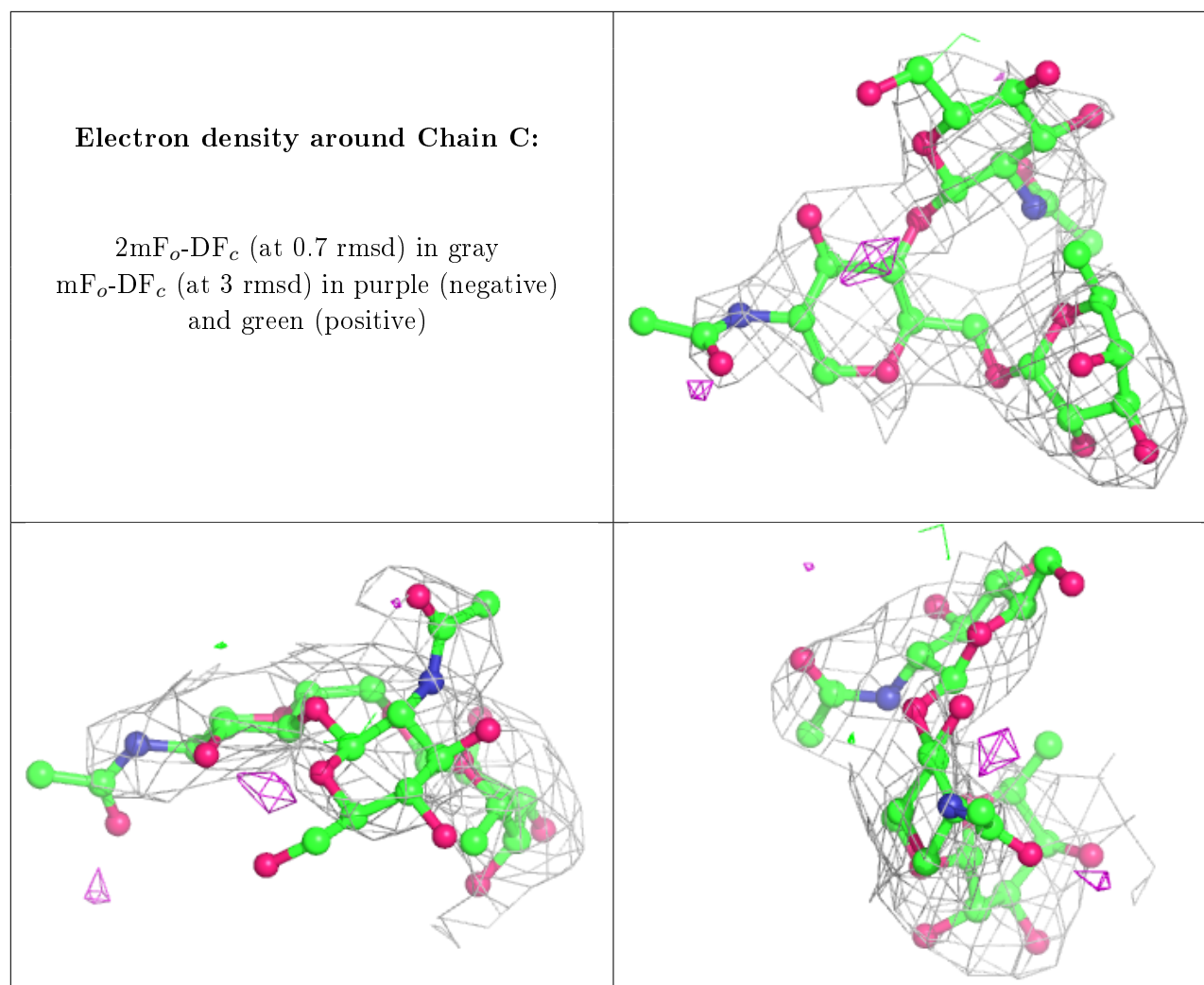
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	D	2	14/15	0.64	0.36	138,146,147,148	0
2	NAG	C	2	14/15	0.74	0.35	145,152,156,156	0
3	NAG	F	2	14/15	0.75	0.22	121,123,126,127	0
4	BMA	E	4	11/12	0.79	0.23	95,100,104,108	0

Continued on next page...

Continued from previous page...

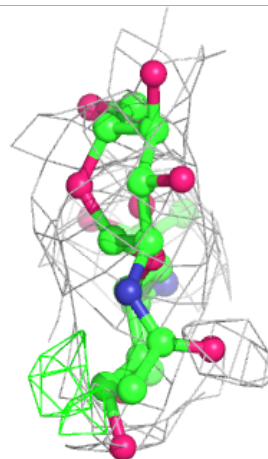
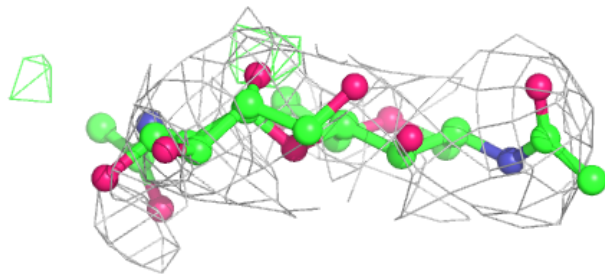
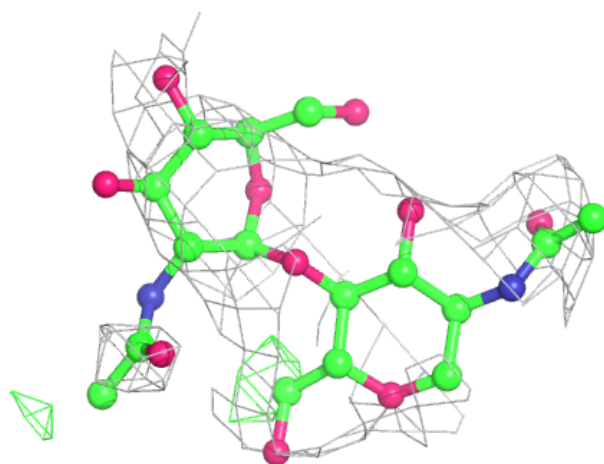
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FUC	C	3	10/11	0.80	0.24	123,125,126,127	0
2	NAG	C	1	14/15	0.82	0.38	129,136,140,145	0
4	BMA	E	3	11/12	0.84	0.20	92,94,101,102	0
3	NAG	F	1	14/15	0.84	0.26	100,106,113,115	0
3	NAG	D	1	14/15	0.87	0.15	113,119,126,132	0
4	FUC	E	6	10/11	0.93	0.20	61,69,72,73	0
4	NAG	E	2	14/15	0.93	0.19	83,86,88,89	0
4	NAG	E	1	14/15	0.94	0.18	75,81,88,90	0
4	BMA	E	5	11/12	0.96	0.12	92,93,96,98	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.



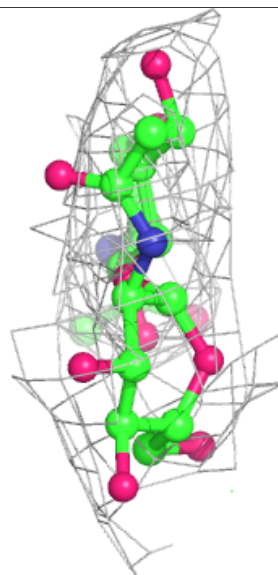
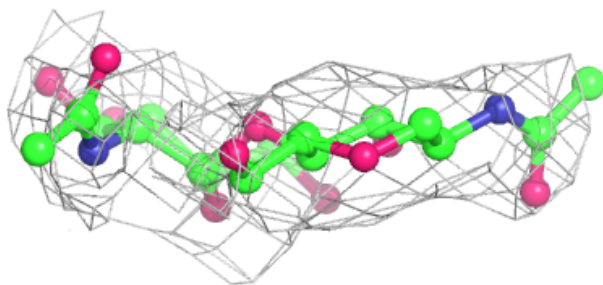
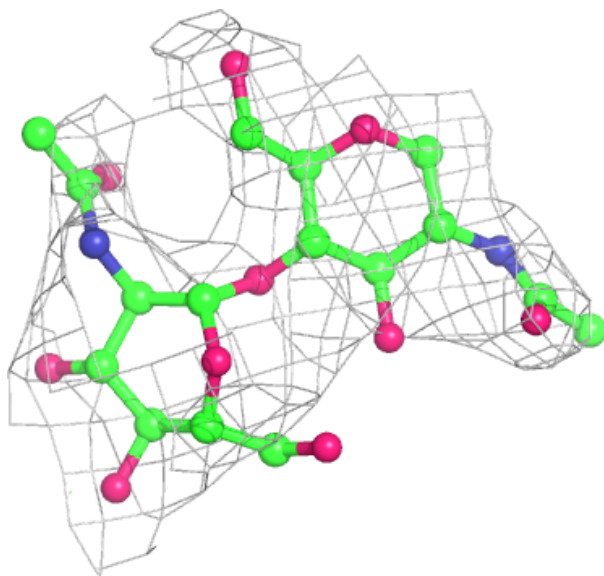
Electron density around Chain D:

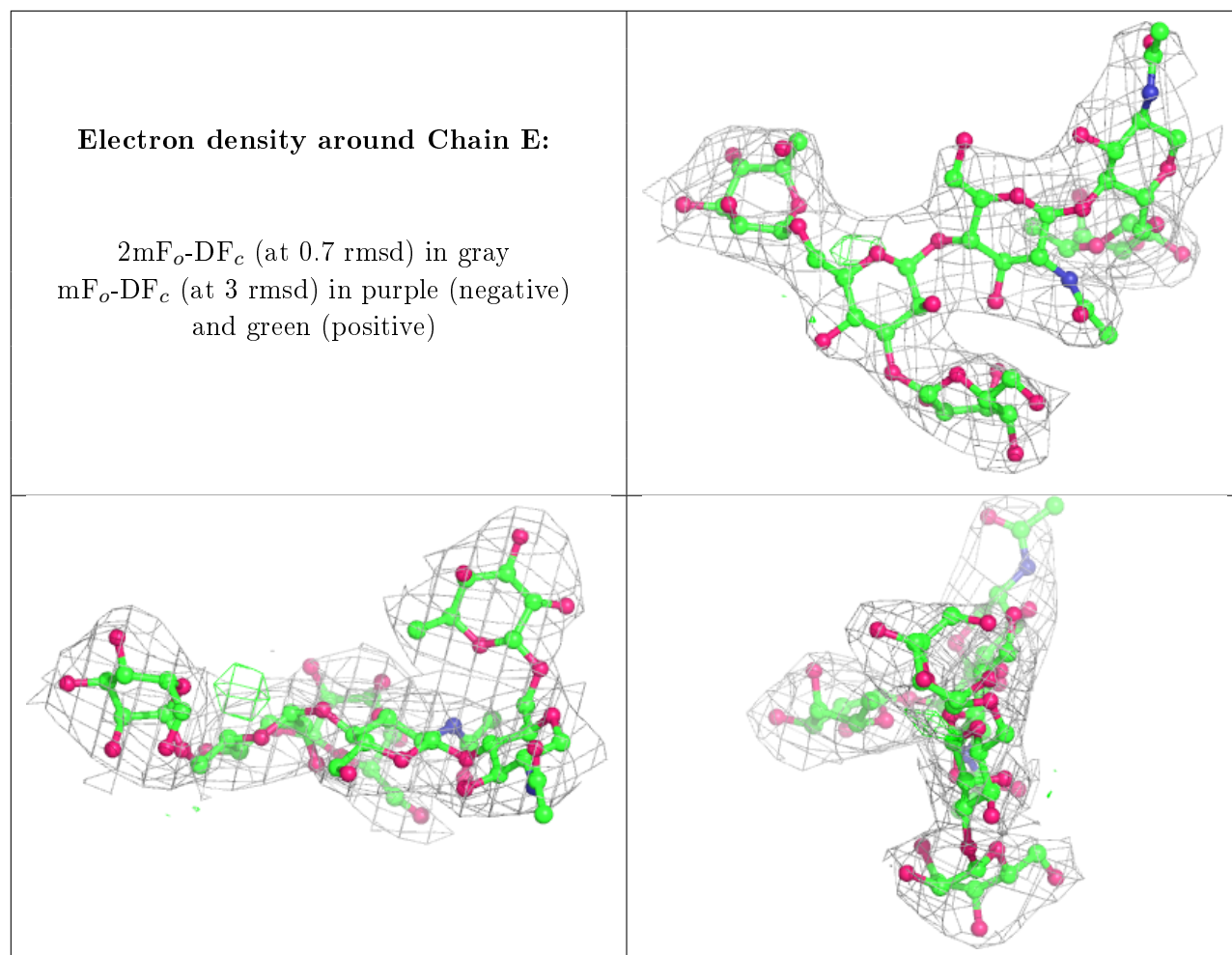
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.