



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:12 AM UTC

PDB ID : 4I9X / pdb_00004i9x
Title : Crystal structure of human cytomegalovirus glycoprotein UL141 targeting the death receptor TRAIL-R2
Authors : Nemcovicova, I.; Zajonc, D.M.
Deposited on : 2012-12-05
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

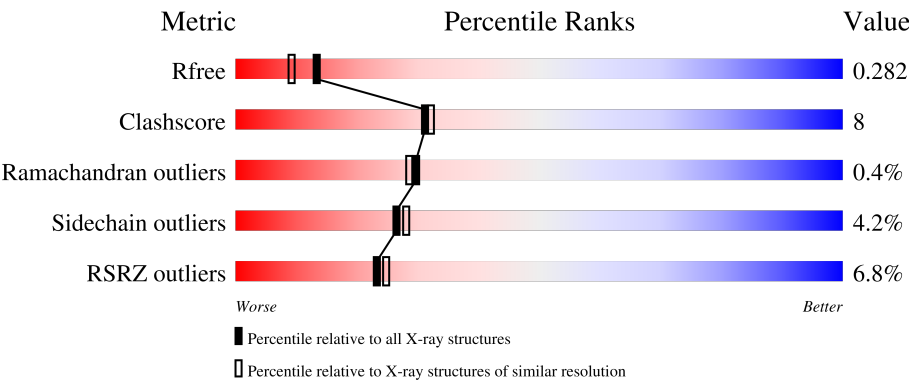
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



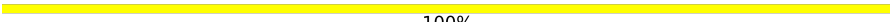
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	215	4% 69% 17% • 13%
1	B	215	7% 69% 15% • 13%
2	C	127	4% 70% 12% • 17%
2	D	127	8% 70% 14% • 15%
3	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	F	2	 100%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4933 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 Protein UL141.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	187	Total	C	N	O	S	Se	0	0	0
			1500	959	261	270	4	6			
1	B	188	Total	C	N	O	S	Se	0	0	0
			1506	963	263	270	4	6			

- Molecule 2 is a protein called Tumor necrosis factor receptor superfamily member 10B.

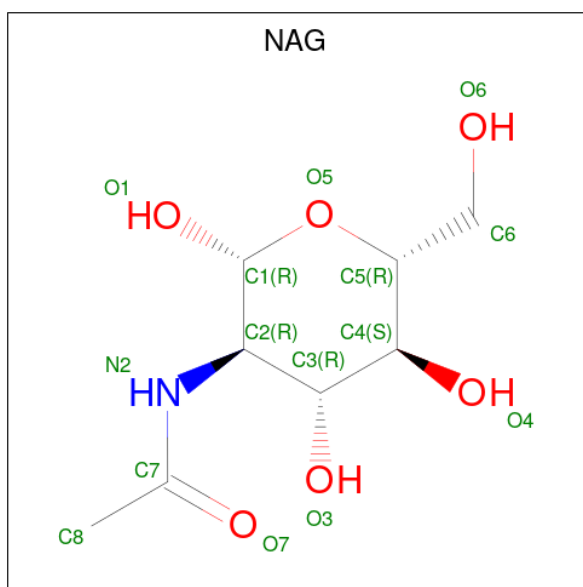
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	105	Total	C	N	O	S	Se	0	1	0
			801	479	144	162	14	2			
2	D	108	Total	C	N	O	S	Se	0	0	0
			812	486	147	163	14	2			

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



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		
5	D	2	Total	Ca	0	0
			2	2		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Na	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	79	Total	O	0	0
			79	79		
7	B	74	Total	O	0	0
			74	74		

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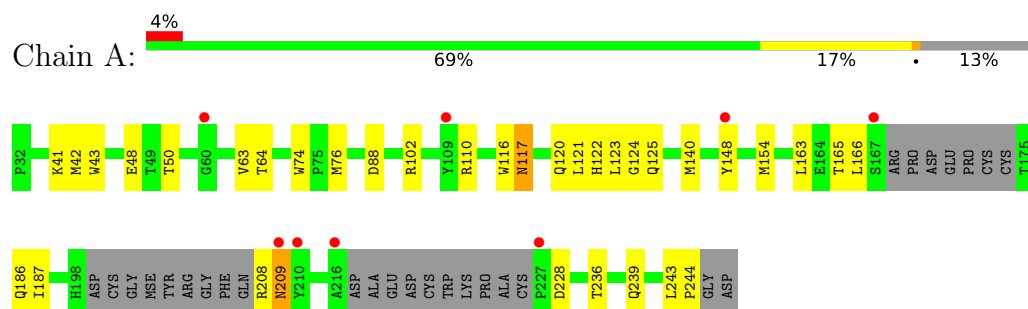
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	40	Total	O	0	0
			40	40		
7	D	46	Total	O	0	0
			46	46		

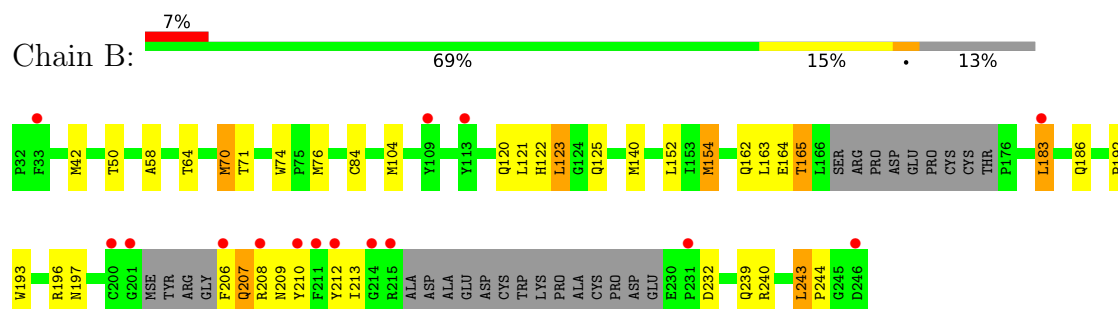
3 Residue-property plots

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

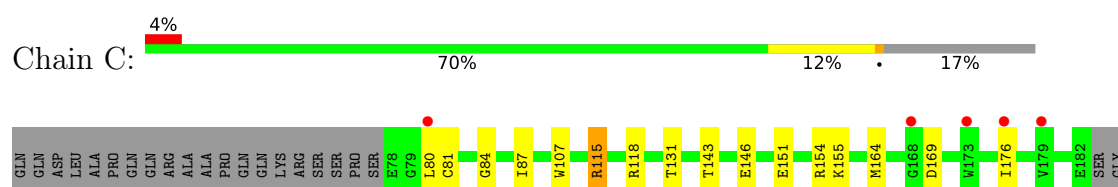
• Molecule 1: Protein UL141



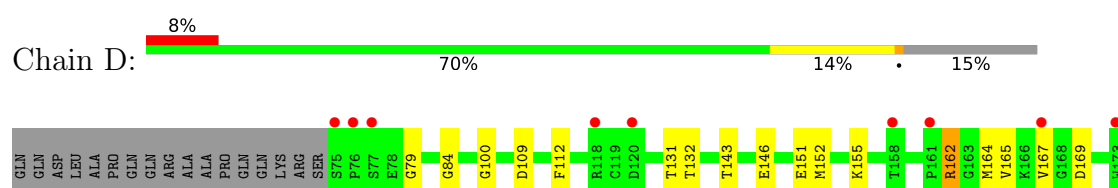
• Molecule 1: Protein UL141

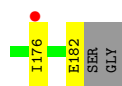


• Molecule 2: Tumor necrosis factor receptor superfamily member 10B



• Molecule 2: Tumor necrosis factor receptor superfamily member 10B





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

Chain E:  50% 50%



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

Chain F:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.92Å 97.04Å 141.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.83 – 2.10 19.83 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.83-2.10) 99.5 (19.83-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.6.0104	Depositor
R, R_{free}	0.223 , 0.274 0.227 , 0.282	Depositor DCC
R_{free} test set	999 reflections (1.81%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4933	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: NA, NAG, CA

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	0.97	4/1535 (0.3%)	0.90	0/2080
1	B	1.00	7/1541 (0.5%)	0.93	1/2086 (0.0%)
2	C	0.89	2/815 (0.2%)	0.83	0/1101
2	D	1.00	3/828 (0.4%)	0.98	0/1121
All	All	0.97	16/4719 (0.3%)	0.91	1/6388 (0.0%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	154	MSE	SE-CE	-7.05	1.74	1.95
1	A	76	MSE	SE-CE	-6.41	1.76	1.95
1	A	140	MSE	SE-CE	-6.33	1.76	1.95
1	B	76	MSE	SE-CE	-6.12	1.77	1.95
1	B	140	MSE	SE-CE	-5.84	1.77	1.95
1	B	104	MSE	SE-CE	-5.75	1.78	1.95
1	A	154	MSE	SE-CE	-5.61	1.78	1.95
1	B	70	MSE	SE-CE	-5.41	1.79	1.95
1	A	140	MSE	CG-SE	-5.32	1.79	1.95
2	D	164	MSE	CG-SE	-5.29	1.79	1.95
2	D	152	MSE	SE-CE	-5.26	1.79	1.95
2	C	164	MSE	CG-SE	-5.26	1.79	1.95
2	D	164	MSE	SE-CE	-5.23	1.79	1.95
2	C	164	MSE	SE-CE	-5.11	1.80	1.95
1	B	76	MSE	CG-SE	-5.10	1.80	1.95
1	B	140	MSE	CG-SE	-5.07	1.80	1.95

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	ARG	N-CA-C	5.95	119.10	109.40

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	1500	0	1434	26	0
1	B	1506	0	1435	30	0
2	C	801	0	705	13	0
2	D	812	0	710	11	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
4	A	14	0	13	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	D	2	0	0	0	0
6	B	1	0	0	0	0
7	A	79	0	0	2	0
7	B	74	0	0	0	0
7	C	40	0	0	2	0
7	D	46	0	0	3	0
All	All	4933	0	4347	74	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 8.

All (74) 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:B:120:GLN:HE22	1:B:125:GLN:HE21	1.09	0.99
2:C:115:ARG:HG3	2:C:115:ARG:HH11	1.31	0.93
2:D:162:ARG:HG3	7:D:322:HOH:O	1.69	0.92
1:A:120:GLN:HE22	1:A:125:GLN:HE21	1.15	0.91
2:C:169:ASP:HA	2:C:176:ILE:HG22	1.57	0.86
1:B:120:GLN:NE2	1:B:125:GLN:HE21	1.75	0.85
1:A:120:GLN:HE21	1:A:122:HIS:H	1.26	0.82
1:B:120:GLN:HE22	1:B:125:GLN:NE2	1.79	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:162:ARG:HH11	2:D:162:ARG:HB3	1.45	0.80
1:B:120:GLN:HE21	1:B:122:HIS:H	1.30	0.78
1:B:243:LEU:HD23	1:B:244:PRO:HD2	1.67	0.74
1:B:206:PHE:HD2	1:B:207:GLN:H	1.33	0.74
1:A:120:GLN:NE2	1:A:125:GLN:HE21	1.87	0.71
1:A:42:MSE:HE1	1:A:74:TRP:HH2	1.56	0.70
1:A:116:TRP:C	1:A:117:ASN:HD22	1.99	0.70
2:C:115:ARG:HG3	2:C:115:ARG:NH1	2.05	0.70
1:B:84:CYS:HB3	1:B:232:ASP:OD1	1.92	0.70
1:A:186:GLN:HE21	1:A:244:PRO:HA	1.57	0.70
2:C:146[B]:GLU:O	2:C:151:GLU:HA	1.91	0.69
1:B:186:GLN:NE2	1:B:244:PRO:HB3	2.12	0.64
1:B:42:MSE:HE1	1:B:74:TRP:HH2	1.63	0.63
1:A:120:GLN:HE22	1:A:125:GLN:NE2	1.92	0.61
2:C:169:ASP:HB2	7:C:231:HOH:O	2.01	0.59
1:B:120:GLN:HE21	1:B:122:HIS:N	1.99	0.59
1:A:236:THR:HA	1:A:239:GLN:HE21	1.69	0.58
1:A:120:GLN:HE21	1:A:122:HIS:N	2.00	0.57
1:A:165:THR:HG22	1:A:209:ASN:HB2	1.87	0.57
1:B:192:PRO:HD2	1:B:193:TRP:CZ3	2.40	0.57
2:D:84:GLY:HA2	2:D:131:THR:O	2.05	0.56
1:A:176:PRO:HG2	1:A:243:LEU:HD22	1.88	0.56
1:A:165:THR:CG2	1:A:209:ASN:HB2	2.36	0.56
1:B:192:PRO:HD2	1:B:193:TRP:CE3	2.41	0.56
1:B:197:ASN:HD21	1:B:209:ASN:HB3	1.72	0.54
2:D:100:GLY:HA2	7:D:305:HOH:O	2.10	0.51
2:D:79:GLY:O	2:D:109:ASP:OD2	2.28	0.51
1:B:240:ARG:HG3	1:B:240:ARG:HH11	1.75	0.51
2:D:162:ARG:HB3	2:D:162:ARG:NH1	2.22	0.51
1:A:50:THR:HG22	1:B:50:THR:HG22	1.92	0.51
1:A:64:THR:HB	1:B:121:LEU:HB3	1.93	0.50
1:B:197:ASN:C	1:B:197:ASN:HD22	2.20	0.50
1:B:162:GLN:HB2	1:B:210:TYR:CE1	2.46	0.50
1:A:88:ASP:HB3	7:A:459:HOH:O	2.12	0.49
1:B:196:ARG:HB2	1:B:212:TYR:CZ	2.48	0.49
1:A:166:LEU:HD11	1:A:208:ARG:HH21	1.79	0.48
1:B:165:THR:HG22	1:B:209:ASN:HB2	1.96	0.48
1:B:42:MSE:HE1	1:B:74:TRP:CH2	2.46	0.48
2:D:162:ARG:NH1	7:D:344:HOH:O	2.46	0.47
1:A:117:ASN:HB3	7:A:413:HOH:O	2.15	0.47
1:B:152:LEU:HG	1:B:154:MSE:SE	2.65	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LEU:HD11	1:A:187:ILE:HG21	1.97	0.47
1:A:148:TYR:CD1	2:D:112:PHE:HB2	2.50	0.46
1:A:42:MSE:HE1	1:A:74:TRP:CH2	2.45	0.45
2:C:84:GLY:HA2	2:C:131:THR:O	2.17	0.45
1:A:124:GLY:C	1:A:125:GLN:NE2	2.75	0.44
2:C:146[B]:GLU:OE1	2:C:154:ARG:NE	2.51	0.44
2:C:81:CYS:O	2:C:107:TRP:HA	2.17	0.44
1:B:183:LEU:H	1:B:183:LEU:HD22	1.83	0.43
1:A:125:GLN:CD	1:A:125:GLN:N	2.76	0.43
1:B:70:MSE:O	1:B:71:THR:C	2.61	0.43
1:A:182:SER:O	1:A:183:LEU:C	2.61	0.43
2:D:143:THR:HG22	2:D:155:LYS:HA	2.01	0.43
2:D:146:GLU:O	2:D:151:GLU:HA	2.18	0.42
1:A:43:TRP:HZ2	2:D:151:GLU:HG3	1.84	0.42
2:C:143:THR:HG22	2:C:155:LYS:HA	2.00	0.42
1:B:162:GLN:HB2	1:B:210:TYR:HE1	1.84	0.42
1:B:58:ALA:HB2	1:B:213:ILE:HG22	2.02	0.42
1:B:164:GLU:OE2	1:B:210:TYR:HD1	2.03	0.42
2:C:80:LEU:HD23	2:C:87:ILE:CD1	2.50	0.41
1:A:63:VAL:HB	1:B:123:LEU:HD13	2.01	0.41
2:C:115:ARG:NH1	2:C:115:ARG:CG	2.78	0.41
2:C:118:ARG:HG3	7:C:230:HOH:O	2.21	0.41
1:A:121:LEU:HB3	1:B:64:THR:HB	2.03	0.41
1:B:206:PHE:O	1:B:207:GLN:CB	2.68	0.40
2:C:146[A]:GLU:O	2:C:151:GLU:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	179/215 (83%)	175 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	180/215 (84%)	168 (93%)	10 (6%)	2 (1%)	11	8
2	C	104/127 (82%)	100 (96%)	4 (4%)	0	100	100
2	D	106/127 (84%)	100 (94%)	6 (6%)	0	100	100
All	All	569/684 (83%)	543 (95%)	24 (4%)	2 (0%)	30	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	183	LEU
1	B	207	GLN

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	160/181 (88%)	152 (95%)	8 (5%)	22	22
1	B	159/181 (88%)	154 (97%)	5 (3%)	35	39
2	C	91/112 (81%)	90 (99%)	1 (1%)	65	74
2	D	92/112 (82%)	85 (92%)	7 (8%)	12	9
All	All	502/586 (86%)	481 (96%)	21 (4%)	26	28

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	48	GLU
1	A	102	ARG
1	A	110	ARG
1	A	117	ASN
1	A	123	LEU
1	A	209	ASN
1	A	228	ASP
1	B	123	LEU

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Mol	Chain	Res	Type
1	B	163	LEU
1	B	165	THR
1	B	239	GLN
1	B	243	LEU
2	C	115	ARG
2	D	132	THR
2	D	162	ARG
2	D	165	VAL
2	D	167	VAL
2	D	169	ASP
2	D	176	ILE
2	D	182	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	120	GLN
1	A	186	GLN
1	A	209	ASN
1	A	239	GLN
1	B	120	GLN
1	B	197	ASN
2	C	138	GLN
2	D	180	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](#)

4 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	1,3	14,14,15	0.54	0	17,19,21	0.94	0
3	NAG	E	2	3	14,14,15	0.71	0	17,19,21	1.42	2 (11%)
3	NAG	F	1	1,3	14,14,15	0.57	0	17,19,21	1.15	2 (11%)
3	NAG	F	2	3	14,14,15	0.68	0	17,19,21	1.15	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	C4-C3-C2	3.95	116.81	111.02
3	F	2	NAG	C4-C3-C2	3.45	116.08	111.02
3	F	1	NAG	C2-N2-C7	-2.84	119.10	122.90
3	E	2	NAG	C3-C4-C5	2.52	114.80	110.23
3	F	1	NAG	O5-C5-C6	2.27	112.08	107.66

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

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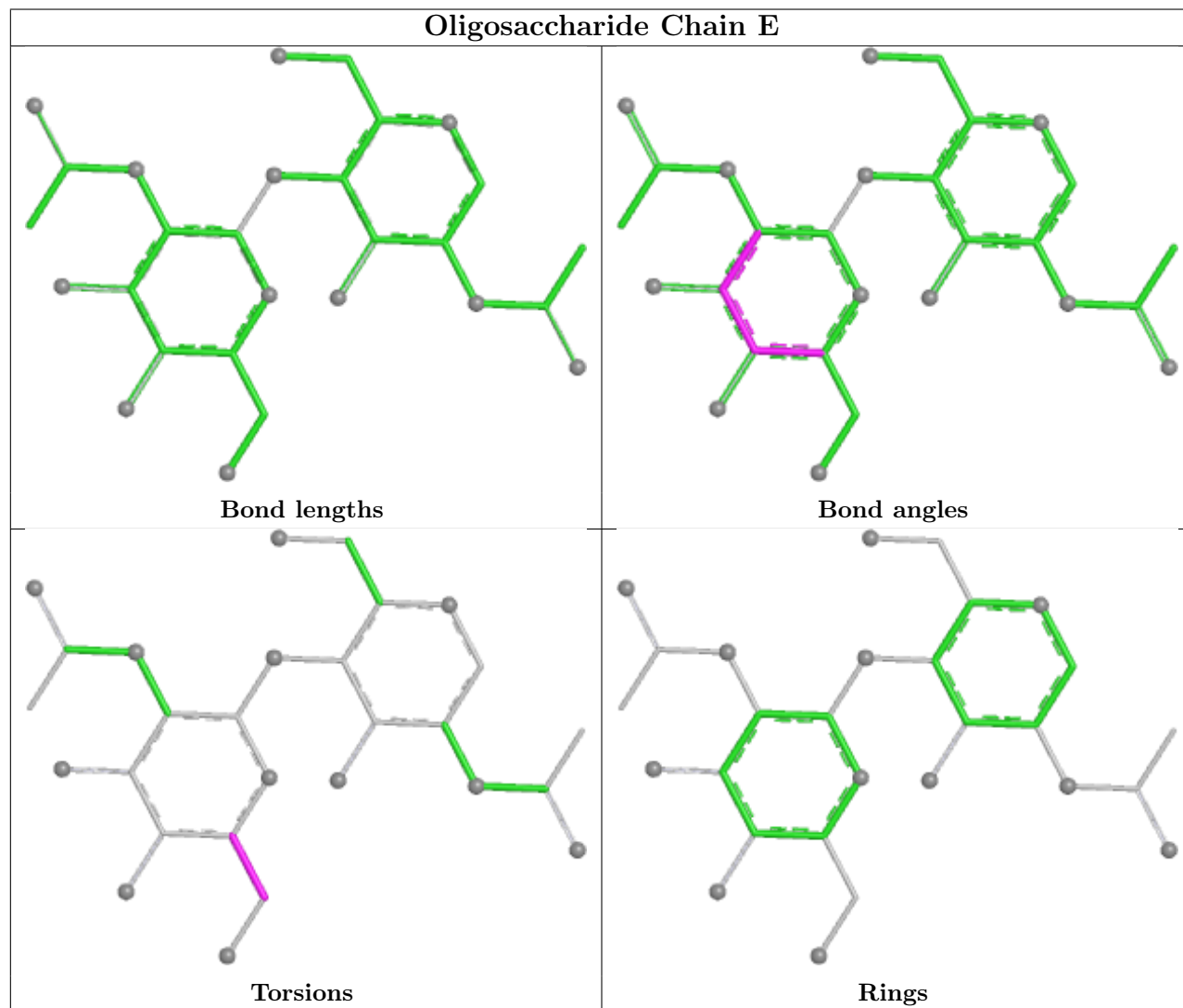
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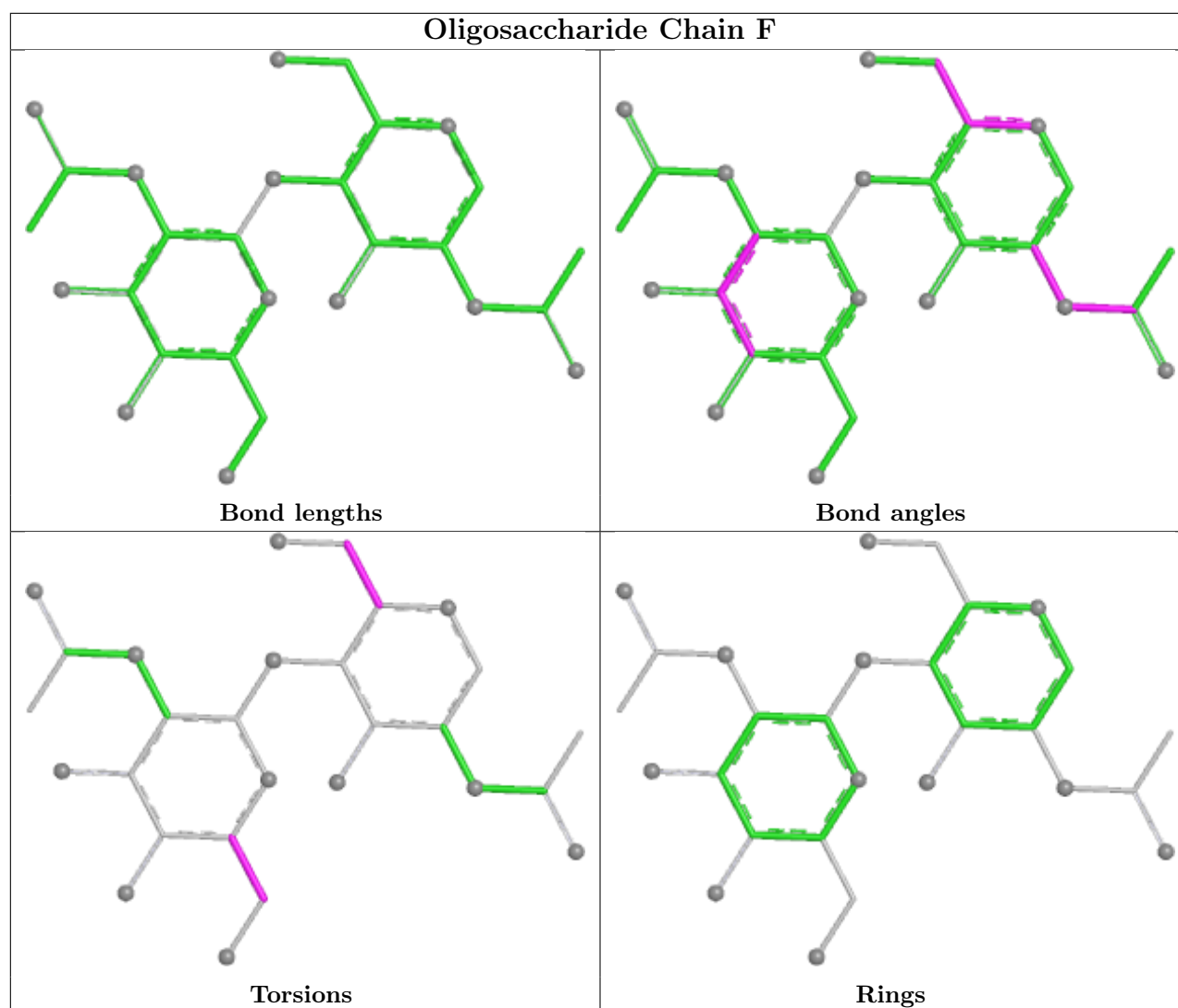
Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 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	$\# Z > 2$
4	NAG	A	303	1	14,14,15	0.62	0	17,19,21	1.65	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
4	NAG	A	303	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	303	NAG	C4-C3-C2	5.04	118.40	111.02
4	A	303	NAG	O5-C1-C2	-2.38	107.60	111.29

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

6.1 Protein, DNA and RNA chains

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	181/215 (84%)	0.20	9 (4%) 34 36	30, 45, 83, 99	0
1	B	182/215 (84%)	0.30	15 (8%) 17 18	28, 46, 84, 103	0
2	C	103/127 (81%)	0.37	5 (4%) 35 37	25, 53, 80, 101	1 (0%)
2	D	106/127 (83%)	0.57	10 (9%) 14 14	33, 51, 85, 109	1 (0%)
All	All	572/684 (83%)	0.33	39 (6%) 23 25	25, 48, 85, 109	2 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	201	GLY	3.8
1	A	227	PRO	3.8
1	B	206	PHE	3.7
2	D	75	SER	3.6
2	D	167	VAL	3.5
1	B	210	TYR	3.5
2	D	176	ILE	3.4
2	D	158	THR	3.4
2	C	173	TRP	3.2
1	B	33	PHE	3.2
2	D	173	TRP	3.1
1	A	209	ASN	2.9
2	D	161	PRO	2.9
1	A	109	TYR	2.9
1	B	200	CYS	2.9
1	B	246	ASP	2.8
2	D	77	SER	2.7
2	C	179	VAL	2.7
2	D	76	PRO	2.6
1	B	215	ARG	2.6
2	C	168	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	148	TYR	2.5
1	B	113	TYR	2.4
1	B	183	LEU	2.4
1	B	109	TYR	2.3
1	A	183	LEU	2.3
1	B	212	TYR	2.3
1	A	216	ALA	2.3
1	B	214	GLY	2.3
1	B	231	PRO	2.3
2	D	120	ASP	2.2
1	B	208	ARG	2.2
2	D	118	ARG	2.2
1	A	210	TYR	2.2
1	A	60	GLY	2.1
1	A	167	SER	2.1
2	C	176	ILE	2.1
1	B	211	PHE	2.1
2	C	80	LEU	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 [i](#)

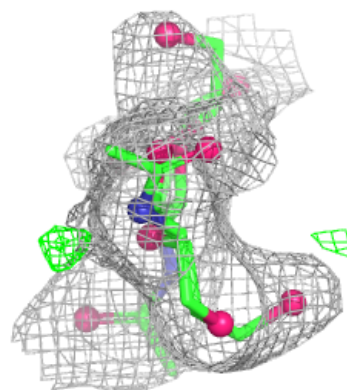
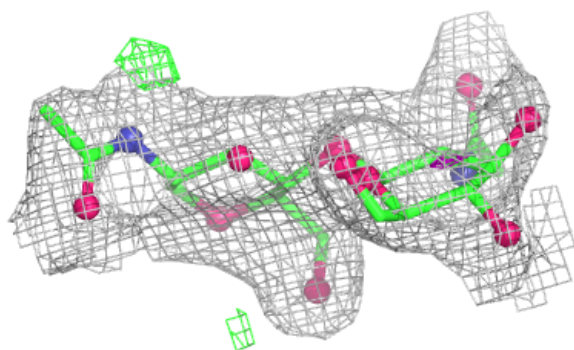
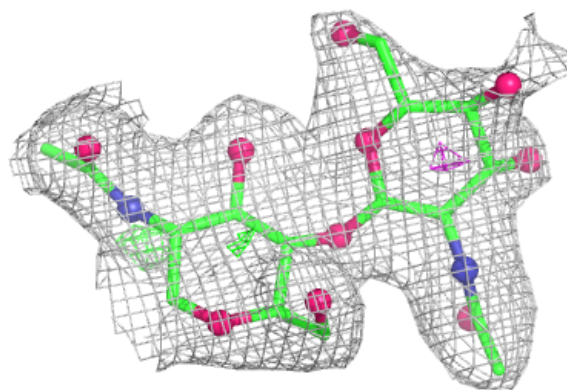
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

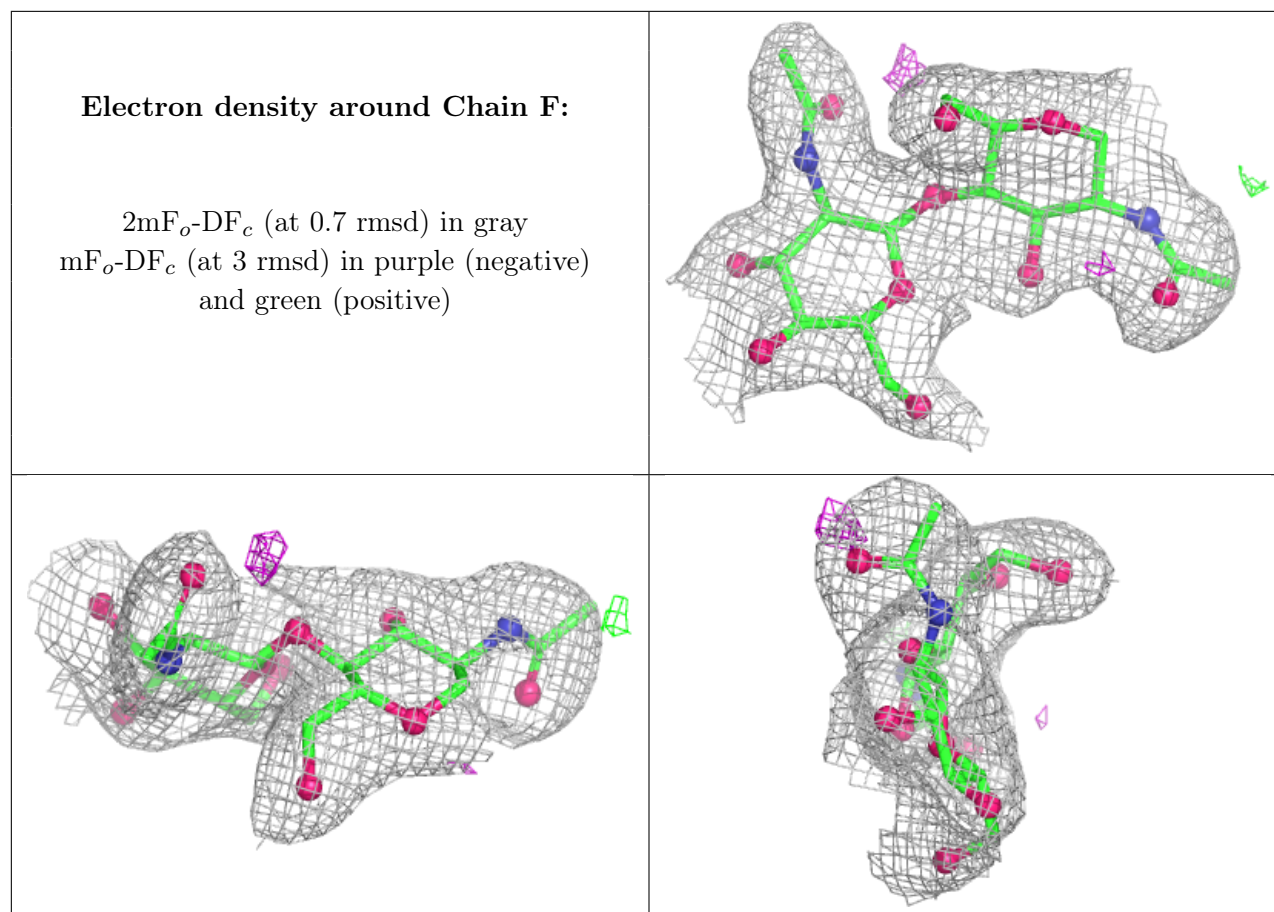
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	F	2	14/15	0.85	0.09	54,70,85,88	0
3	NAG	E	2	14/15	0.90	0.10	50,75,84,87	0
3	NAG	F	1	14/15	0.95	0.07	42,52,59,62	0
3	NAG	E	1	14/15	0.95	0.06	46,52,58,60	0

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)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	A	303	14/15	0.77	0.14	87,96,103,105	0
5	CA	D	201	1/1	0.90	0.29	74,74,74,74	0
5	CA	D	202	1/1	0.92	0.26	92,92,92,92	0
5	CA	A	304	1/1	0.93	0.49	93,93,93,93	0
6	NA	B	304	1/1	0.93	0.23	64,64,64,64	0
5	CA	B	303	1/1	0.94	0.32	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.