Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2020 – 01:12 PM BST

PDB ID	:	6YT7
Title	:	GLYCOSYLATED KNOB/DUMMY-HOLE FC FRAGMENT
Authors	:	Kuglstatter, A.; Leibrock, L.; Benz, J.
Deposited on	:	2020-04-24
Resolution	:	1.55 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

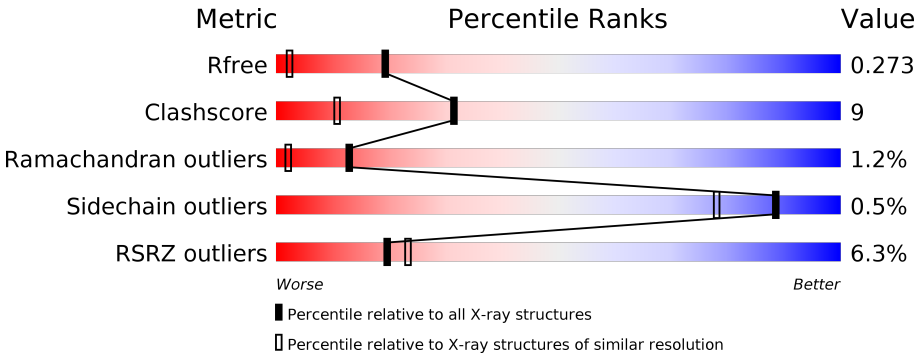
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 1.55 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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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 <=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	245	7%, 64%, 20%, ·, 13%
2	B	232	4%, 77%, 11%, · ·, 8%
3	C	8	25%, 50%, 25%
3	D	8	38%, 50%, 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3835 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 Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	7	0
			1718	1097	286	327	8			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	366	TRP	THR	engineered mutation	UNP P0DOX5
A	370	GLU	LYS	engineered mutation	UNP P0DOX5
A	448	GLY	-	expression tag	UNP P0DOX5
A	449	GLY	-	expression tag	UNP P0DOX5
A	450	GLY	-	expression tag	UNP P0DOX5
A	451	GLY	-	expression tag	UNP P0DOX5
A	452	SER	-	expression tag	UNP P0DOX5
A	453	HIS	-	expression tag	UNP P0DOX5
A	454	HIS	-	expression tag	UNP P0DOX5
A	455	HIS	-	expression tag	UNP P0DOX5
A	456	HIS	-	expression tag	UNP P0DOX5
A	457	HIS	-	expression tag	UNP P0DOX5
A	458	HIS	-	expression tag	UNP P0DOX5
A	459	HIS	-	expression tag	UNP P0DOX5
A	460	HIS	-	expression tag	UNP P0DOX5

- Molecule 2 is a protein called Ig gamma-1 chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	208	Total	C	N	O	S	0	8	0
			1720	1096	288	328	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	349	CYS	TYR	engineered mutation	UNP P01857

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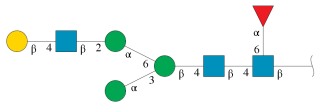
Chain	Residue	Modelled	Actual	Comment	Reference
B	366	SER	THR	engineered mutation	UNP P01857
B	368	ALA	LEU	engineered mutation	UNP P01857
B	407	VAL	TYR	engineered mutation	UNP P01857

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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
3	C	8	Total C N O 96 54 3 39	0	0	0
3	D	8	Total C N O 96 54 3 39	0	0	0

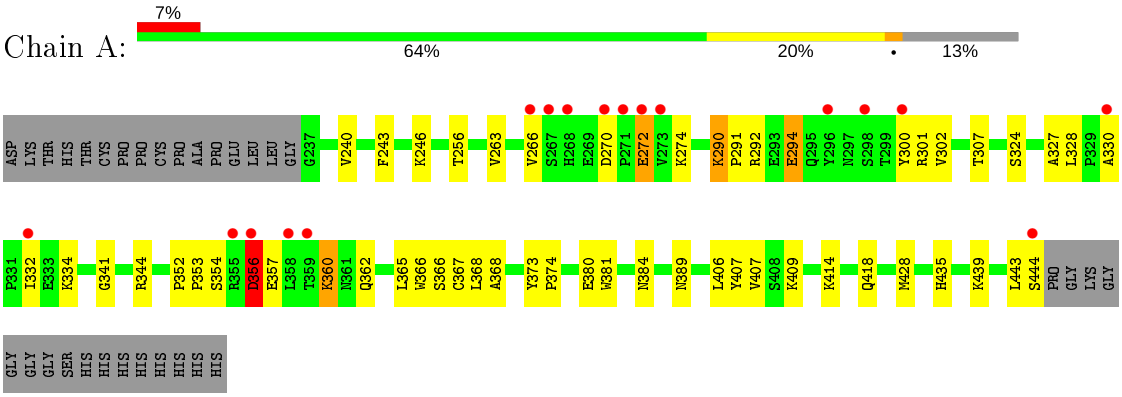
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	85	Total O 85 85	0	0
4	B	120	Total O 120 120	0	0

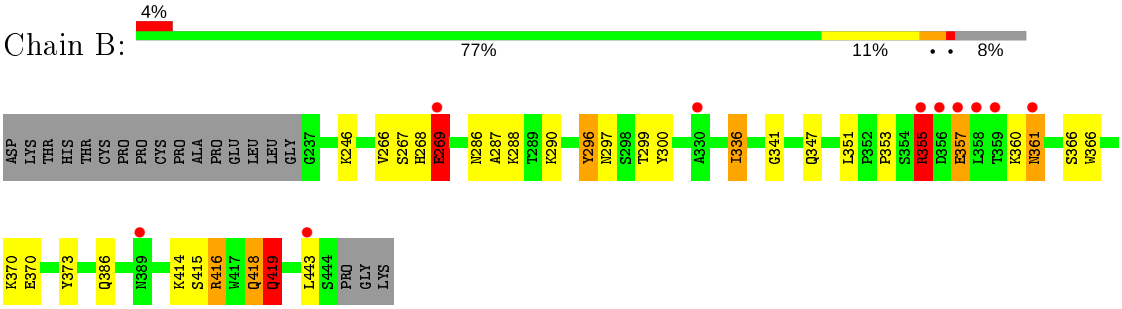
3 Residue-property plots (i)

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.

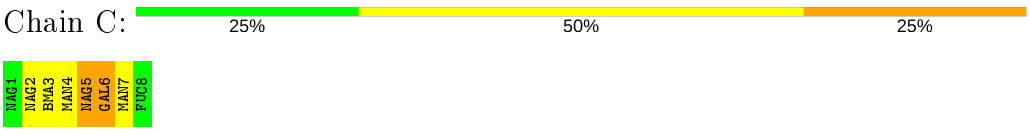
• Molecule 1: Immunoglobulin gamma-1 heavy chain



• Molecule 2: Ig gamma-1 chain C region



• Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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



• Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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 D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	49.02Å 75.10Å 149.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.11 – 1.55 74.72 – 1.55	Depositor EDS
% Data completeness (in resolution range)	79.0 (67.11-1.55) 79.1 (74.72-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 1.55Å)	Xtriage
Refinement program	PHENIX dev_3893	Depositor
R, R_{free}	0.234 , 0.273 0.234 , 0.273	Depositor DCC
R_{free} test set	3215 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	26.9	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3835	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MAN, GAL, 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	0/1768	1.06	9/2402 (0.4%)
2	B	0.67	2/1772 (0.1%)	1.79	22/2406 (0.9%)
All	All	0.60	2/3540 (0.1%)	1.47	31/4808 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	6
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	416	ARG	CB-CG	-8.17	1.30	1.52
2	B	416	ARG	CG-CD	-5.53	1.38	1.51

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	269	GLU	OE1-CD-OE2	-42.66	72.11	123.30
2	B	357	GLU	OE1-CD-OE2	-31.71	85.24	123.30
2	B	269	GLU	CG-CD-OE1	23.45	165.21	118.30
1	A	356	ASP	CB-CG-OD1	22.85	138.87	118.30
2	B	443	LEU	CB-CG-CD2	-21.54	74.38	111.00
1	A	356	ASP	CB-CG-OD2	-20.66	99.71	118.30
2	B	443	LEU	CB-CG-CD1	20.06	145.10	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	357	GLU	CG-CD-OE1	19.40	157.11	118.30
2	B	419	GLN	CG-CD-OE1	18.62	158.84	121.60
2	B	419	GLN	CG-CD-NE2	-17.29	75.19	116.70
2	B	357	GLU	CG-CD-OE2	-12.95	92.41	118.30
2	B	269	GLU	CG-CD-OE2	-12.03	94.25	118.30
2	B	355	ARG	CD-NE-CZ	11.18	139.25	123.60
2	B	355	ARG	NE-CZ-NH2	-10.17	115.21	120.30
1	A	356	ASP	OD1-CG-OD2	-10.09	104.14	123.30
2	B	419	GLN	OE1-CD-NE2	-9.54	99.95	121.90
1	A	418	GLN	CA-CB-CG	9.40	134.08	113.40
2	B	336	ILE	CG1-CB-CG2	-8.97	91.66	111.40
2	B	443	LEU	CD1-CG-CD2	-8.02	86.43	110.50
2	B	416	ARG	NE-CZ-NH2	-7.95	116.33	120.30
2	B	416	ARG	CG-CD-NE	-7.03	97.03	111.80
2	B	296	TYR	CB-CG-CD1	-6.92	116.85	121.00
1	A	294	GLU	OE1-CD-OE2	-6.65	115.32	123.30
1	A	360	LYS	CB-CG-CD	-6.43	94.88	111.60
2	B	419	GLN	CA-CB-CG	-6.38	99.36	113.40
2	B	416	ARG	NE-CZ-NH1	-6.23	117.19	120.30
1	A	272	GLU	N-CA-CB	-6.20	99.44	110.60
2	B	296	TYR	CB-CG-CD2	6.14	124.69	121.00
1	A	290	LYS	CD-CE-NZ	5.52	124.40	111.70
1	A	272	GLU	CB-CA-C	5.18	120.76	110.40
2	B	419	GLN	CB-CG-CD	5.10	124.87	111.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	294	GLU	Sidechain
1	A	356	ASP	Sidechain
2	B	268	HIS	Peptide
2	B	355	ARG	Sidechain
2	B	357	GLU	Sidechain
2	B	416	ARG	Sidechain
2	B	418	GLN	Peptide
2	B	419	GLN	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1718	0	1670	38	1
2	B	1720	0	1675	20	0
3	C	96	0	82	2	0
3	D	96	0	82	1	1
4	A	85	0	0	9	2
4	B	120	0	0	4	2
All	All	3835	0	3509	58	3

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 9.

All (58) 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:B:286:ASN:O	2:B:288:LYS:NZ	1.90	1.03
2:B:347[A]:GLN:OE1	4:B:601:HOH:O	1.89	0.89
1:A:357:GLU:HG2	1:A:360:LYS:HE2	1.55	0.88
1:A:360:LYS:HE3	1:A:362:GLN:O	1.82	0.79
1:A:389:ASN:ND2	4:A:604:HOH:O	2.17	0.78
1:A:357:GLU:CG	1:A:360:LYS:HE2	2.13	0.77
1:A:380:GLU:OE2	4:A:601:HOH:O	2.03	0.75
2:B:297:ASN:OD1	2:B:299:THR:HG22	1.86	0.75
2:B:290:LYS:NZ	4:B:602:HOH:O	2.09	0.73
1:A:274:LYS:HB3	1:A:324:SER:HB2	1.75	0.68
1:A:380:GLU:OE1	4:A:602:HOH:O	2.12	0.68
1:A:352:PRO:O	4:A:603:HOH:O	2.13	0.66
2:B:267:SER:OG	2:B:269:GLU:HB2	1.94	0.66
1:A:366[A]:TRP:CH2	1:A:409:LYS:HD3	2.32	0.64
1:A:292:ARG:HB3	1:A:302:VAL:HG22	1.80	0.63
2:B:290:LYS:HD3	2:B:290:LYS:N	2.15	0.62
1:A:360:LYS:O	1:A:414:LYS:NZ	2.27	0.61
2:B:360:LYS:O	2:B:361:ASN:HB2	2.01	0.60
2:B:287:ALA:C	2:B:288:LYS:HD2	2.23	0.59
1:A:246:LYS:NZ	3:C:6:GAL:O4	2.22	0.57
2:B:415:SER:O	2:B:419:GLN:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:LYS:N	2:B:288:LYS:HD2	2.22	0.55
2:B:353:PRO:HA	4:B:605:HOH:O	2.06	0.55
1:A:368[A]:LEU:HD13	1:A:407[A]:TYR:CZ	2.42	0.54
2:B:246:LYS:HG2	3:D:6:GAL:O4	2.09	0.53
1:A:344:ARG:NE	4:A:608:HOH:O	2.41	0.53
1:A:243:PHE:CG	3:C:5:NAG:H5	2.43	0.53
2:B:414:LYS:O	2:B:418:GLN:HG2	2.10	0.51
1:A:307:THR:HG23	4:A:675:HOH:O	2.10	0.51
1:A:353:PRO:HA	4:A:603:HOH:O	2.11	0.51
1:A:439:LYS:HE2	4:A:629:HOH:O	2.11	0.50
1:A:328:LEU:HD21	1:A:332:ILE:HG13	1.94	0.48
1:A:240:VAL:O	1:A:334:LYS:NZ	2.47	0.48
2:B:269:GLU:OE2	2:B:269:GLU:N	2.47	0.48
2:B:414:LYS:HB3	2:B:414:LYS:HE2	1.62	0.48
1:A:353:PRO:HD3	1:A:365:LEU:HD23	1.96	0.47
1:A:443:LEU:HD12	1:A:444:SER:N	2.31	0.46
2:B:386:GLN:NE2	4:B:603:HOH:O	2.26	0.46
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.50	0.46
1:A:290:LYS:HB3	1:A:291:PRO:HD2	1.98	0.45
1:A:354:SER:OG	1:A:356:ASP:HB2	2.16	0.45
2:B:351:LEU:HB2	2:B:366[A]:SER:HB2	1.99	0.45
1:A:428:MET:HA	1:A:435:HIS:O	2.17	0.45
2:B:341:GLY:HA3	2:B:373:TYR:HE2	1.82	0.44
1:A:373[A]:TYR:CG	1:A:374:PRO:HA	2.53	0.44
1:A:292:ARG:NH2	1:A:300:TYR:CZ	2.86	0.43
2:B:336:ILE:HG21	2:B:336:ILE:HD13	1.78	0.43
1:A:270:ASP:OD2	1:A:327:ALA:HB2	2.18	0.43
1:A:272:GLU:H	1:A:272:GLU:HG2	1.26	0.43
1:A:341:GLY:HA3	1:A:373[A]:TYR:CE2	2.54	0.43
1:A:292:ARG:CB	1:A:302:VAL:HG22	2.45	0.43
1:A:328:LEU:HG	1:A:330:ALA:O	2.19	0.43
2:B:266:VAL:HB	2:B:300:TYR:HB2	2.01	0.42
1:A:256:THR:HB	4:A:675:HOH:O	2.19	0.42
1:A:266:VAL:HB	1:A:300:TYR:HB2	2.02	0.42
1:A:353:PRO:HD3	1:A:365:LEU:CD2	2.50	0.42
1:A:406:LEU:HD12	1:A:406:LEU:C	2.41	0.41
1:A:263:VAL:O	1:A:301:ARG:HA	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:601:HOH:O	4:B:665:HOH:O[3_555]	2.02	0.18
1:A:384:ASN:ND2	3:D:5:NAG:O3[3_555]	2.13	0.07
4:A:656:HOH:O	4:B:674:HOH:O[1_455]	2.14	0.06

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	203/245 (83%)	195 (96%)	7 (3%)	1 (0%)	29 9
2	B	204/232 (88%)	197 (97%)	3 (2%)	4 (2%)	7 1
All	All	407/477 (85%)	392 (96%)	10 (2%)	5 (1%)	13 2

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	356	ASP
2	B	269	GLU
2	B	419	GLN
2	B	361	ASN
2	B	296	TYR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	200/223 (90%)	200 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	201/214 (94%)	199 (99%)	2 (1%)	76 57
All	All	401/437 (92%)	399 (100%)	2 (0%)	88 78

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	355	ARG
2	B	370[A]	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	386	GLN
1	A	389	ASN
1	A	421	ASN
2	B	419	GLN
2	B	421	ASN

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)

16 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	1,3	14,14,15	0.52	0	17,19,21	0.76	0
3	NAG	C	2	3	14,14,15	0.30	0	17,19,21	0.65	1 (5%)
3	BMA	C	3	3	11,11,12	0.98	1 (9%)	15,15,17	1.17	2 (13%)
3	MAN	C	4	3	11,11,12	1.05	0	15,15,17	1.51	3 (20%)
3	NAG	C	5	3	14,14,15	0.75	1 (7%)	17,19,21	0.71	0
3	GAL	C	6	3	11,11,12	1.09	1 (9%)	15,15,17	1.30	2 (13%)
3	MAN	C	7	3	11,11,12	1.39	1 (9%)	15,15,17	1.17	2 (13%)
3	FUC	C	8	3	10,10,11	0.63	0	14,14,16	0.71	0
3	NAG	D	1	3,2	14,14,15	0.34	0	17,19,21	0.59	0
3	NAG	D	2	3	14,14,15	0.31	0	17,19,21	0.67	0
3	BMA	D	3	3	11,11,12	0.68	0	15,15,17	0.77	0
3	MAN	D	4	3	11,11,12	1.00	1 (9%)	15,15,17	1.25	2 (13%)
3	NAG	D	5	3	14,14,15	0.49	0	17,19,21	0.60	0
3	GAL	D	6	3	11,11,12	1.25	1 (9%)	15,15,17	1.23	2 (13%)
3	MAN	D	7	3	11,11,12	1.34	1 (9%)	15,15,17	1.03	0
3	FUC	D	8	3	10,10,11	1.26	2 (20%)	14,14,16	0.81	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	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	NAG	C	5	3	-	0/6/23/26	0/1/1/1
3	GAL	C	6	3	-	0/2/19/22	0/1/1/1
3	MAN	C	7	3	-	0/2/19/22	0/1/1/1
3	FUC	C	8	3	-	-	0/1/1/1
3	NAG	D	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	NAG	D	5	3	-	0/6/23/26	0/1/1/1
3	GAL	D	6	3	-	0/2/19/22	0/1/1/1
3	MAN	D	7	3	-	0/2/19/22	0/1/1/1
3	FUC	D	8	3	-	-	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	BMA	C1-C2	3.06	1.59	1.52
3	C	6	GAL	C1-C2	3.03	1.59	1.52
3	D	6	GAL	C1-C2	3.00	1.59	1.52
3	C	7	MAN	O5-C1	-2.80	1.39	1.43
3	D	7	MAN	O5-C1	-2.73	1.39	1.43
3	D	8	FUC	C2-C3	2.68	1.56	1.52
3	D	4	MAN	O2-C2	-2.26	1.38	1.43
3	D	8	FUC	O5-C5	2.16	1.48	1.43
3	C	5	NAG	O5-C1	-2.05	1.40	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	4	MAN	C1-O5-C5	3.59	117.06	112.19
3	D	4	MAN	O2-C2-C3	-3.51	103.10	110.14
3	C	4	MAN	O2-C2-C3	-3.49	103.16	110.14
3	D	4	MAN	C1-O5-C5	2.60	115.72	112.19
3	D	6	GAL	O3-C3-C4	-2.60	104.34	110.35
3	C	3	BMA	C1-O5-C5	2.58	115.69	112.19
3	C	6	GAL	O2-C2-C3	-2.45	105.24	110.14
3	C	3	BMA	O2-C2-C3	-2.41	105.30	110.14
3	C	7	MAN	C3-C4-C5	2.35	114.43	110.24
3	D	6	GAL	C1-C2-C3	2.34	112.55	109.67
3	C	7	MAN	C2-C3-C4	2.26	114.80	110.89
3	C	2	NAG	C1-O5-C5	2.21	115.19	112.19
3	C	6	GAL	O5-C1-C2	2.13	114.06	110.77
3	C	4	MAN	C3-C4-C5	2.00	113.81	110.24

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

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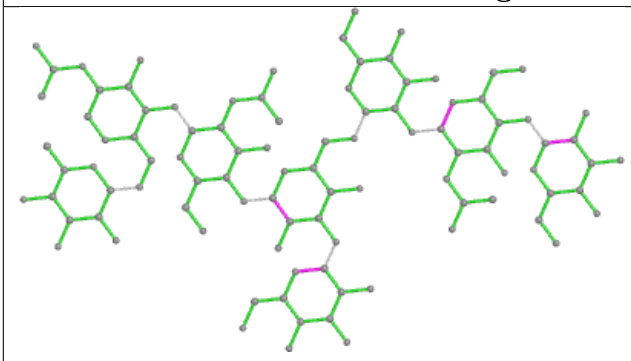
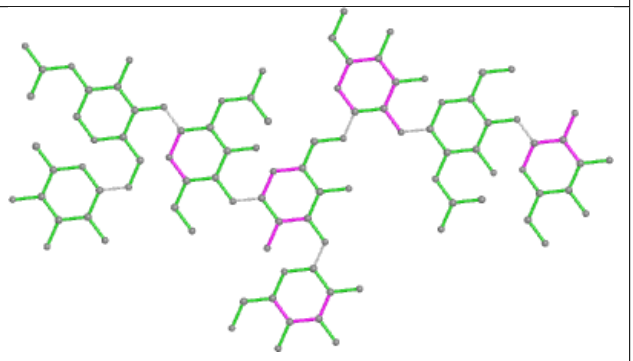
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	6	GAL	1	0
3	C	6	GAL	1	0

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

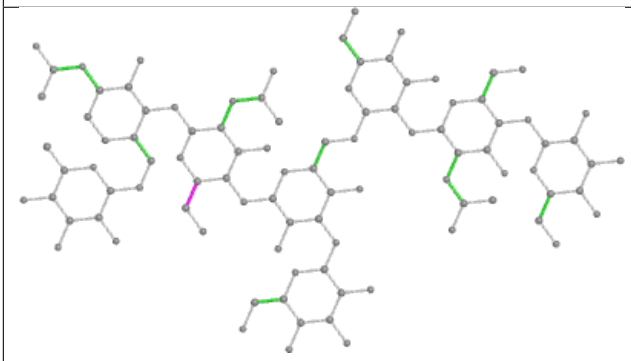
Oligosaccharide Chain C



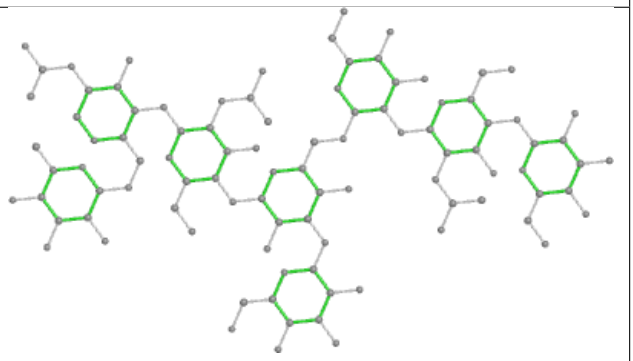
Bond lengths



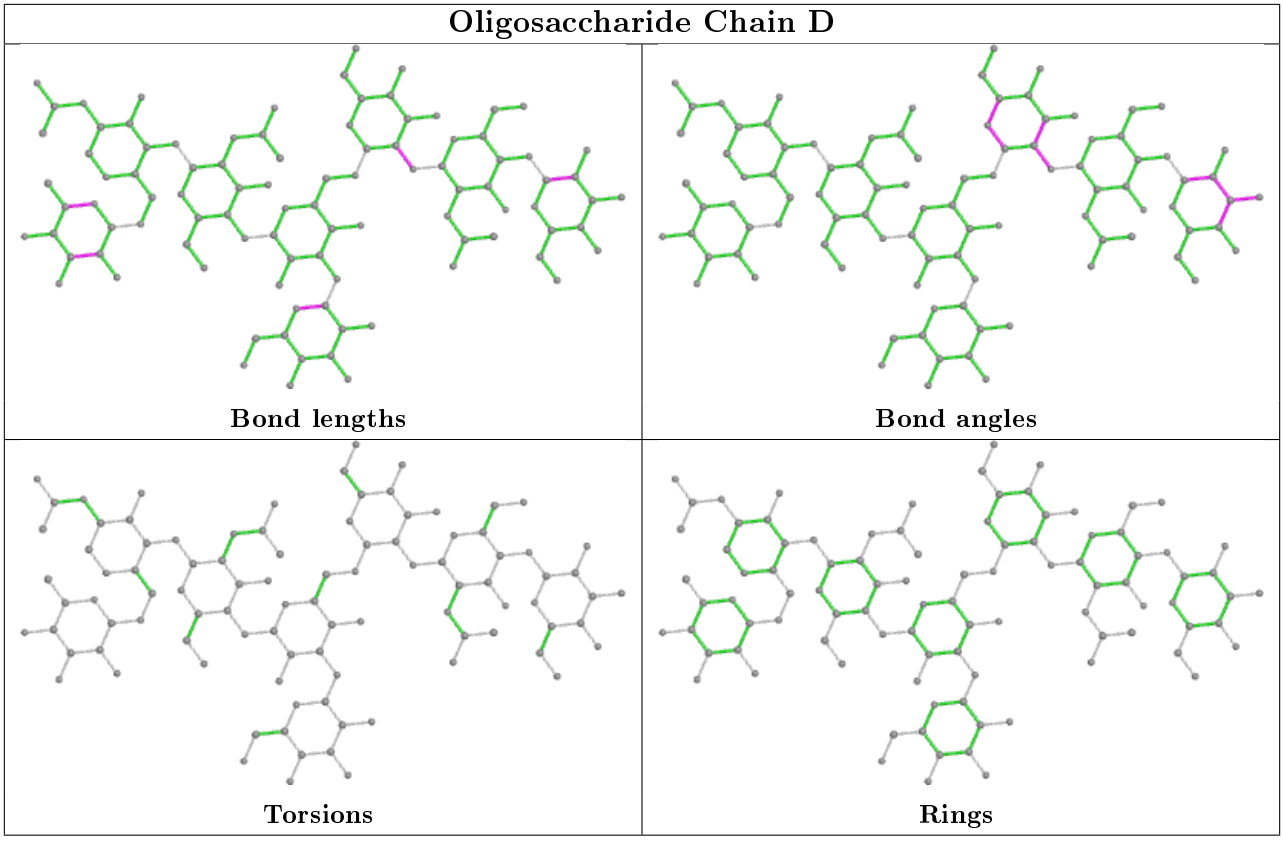
Bond angles



Torsions



Rings



5.6 Ligand geometry

There are no ligands in this entry.

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

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, 95^{th} 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	213/245 (86%)	0.59	17 (7%)	12	14	18, 33, 72, 82	10 (4%)
2	B	213/232 (91%)	0.40	10 (4%)	31	36	17, 31, 53, 81	10 (4%)
All	All	426/477 (89%)	0.50	27 (6%)	20	23	17, 32, 65, 82	20 (4%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	358	LEU	11.3
2	B	355	ARG	5.8
1	A	296	TYR	5.6
1	A	358	LEU	4.6
2	B	359	THR	4.5
1	A	330	ALA	4.2
1	A	355	ARG	4.1
1	A	273	VAL	3.7
1	A	356	ASP	3.7
2	B	269	GLU	3.4
1	A	359	THR	3.2
1	A	300	TYR	3.1
2	B	356	ASP	3.0
2	B	443	LEU	2.9
1	A	272	GLU	2.9
2	B	389	ASN	2.7
1	A	271	PRO	2.6
1	A	270	ASP	2.5
2	B	361	ASN	2.4
1	A	266	VAL	2.4
1	A	332	ILE	2.3
2	B	330	ALA	2.3
1	A	298	SER	2.2
1	A	444	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	357	GLU	2.2
1	A	268	HIS	2.0
1	A	267	SER	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)

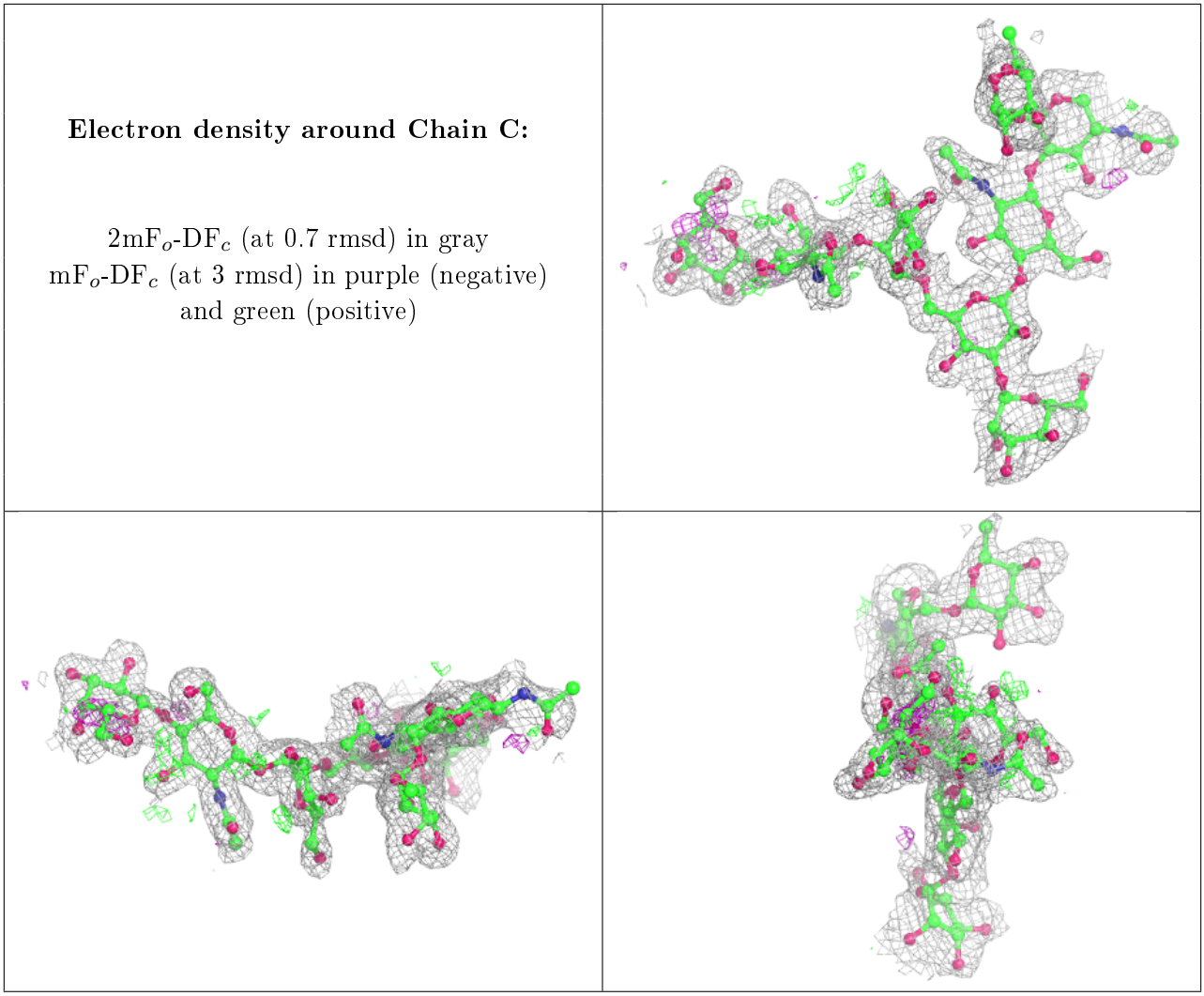
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	MAN	C	7	11/12	0.58	0.18	66,69,72,74	0
3	NAG	C	2	14/15	0.73	0.14	49,55,59,63	0
3	FUC	D	8	10/11	0.75	0.17	39,43,47,49	0
3	FUC	C	8	10/11	0.76	0.26	61,67,70,70	0
3	NAG	C	5	14/15	0.79	0.16	38,42,44,46	0
3	NAG	C	1	14/15	0.79	0.14	61,63,70,73	0
3	NAG	D	5	14/15	0.79	0.15	33,44,48,49	0
3	BMA	C	3	11/12	0.80	0.09	41,46,54,54	0
3	GAL	C	6	11/12	0.81	0.20	34,38,45,46	0
3	GAL	D	6	11/12	0.82	0.25	37,43,56,59	0
3	MAN	D	7	11/12	0.85	0.16	50,57,59,62	0
3	MAN	D	4	11/12	0.86	0.11	33,40,45,46	0
3	MAN	C	4	11/12	0.88	0.15	37,45,50,54	0
3	NAG	D	2	14/15	0.88	0.09	32,39,43,44	0
3	BMA	D	3	11/12	0.89	0.09	36,39,44,44	0
3	NAG	D	1	14/15	0.90	0.08	33,38,45,48	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.

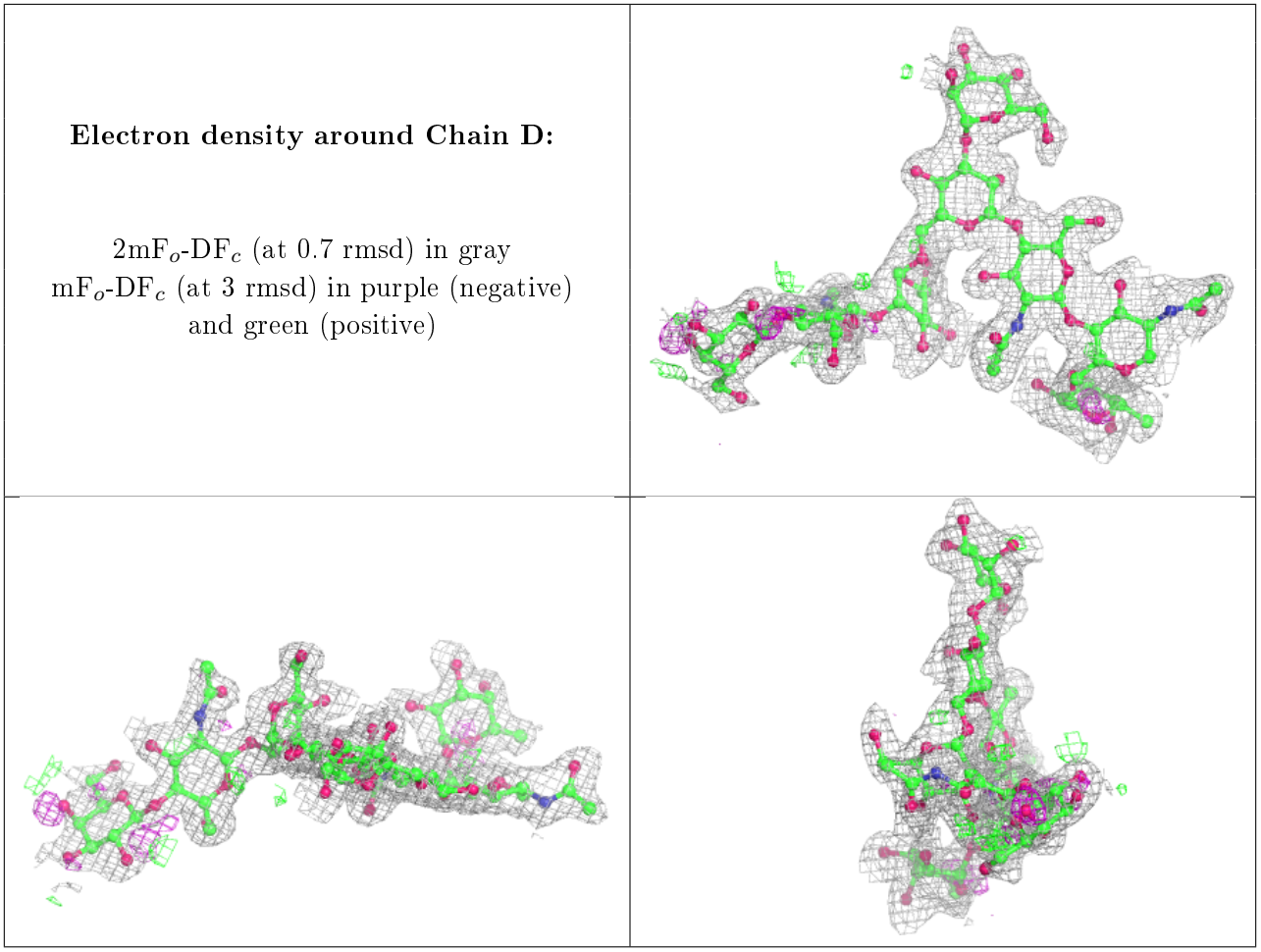
Electron density around Chain C:

$2mF_o$-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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.