



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:17 PM UTC

PDB ID : 6YTB / pdb_00006ytb
Title : GLYCOSYLATED KNOB/DUMMY-HOLE/DUMMY FC FRAGMENT
Authors : Kuglstatter, A.; Leibrock, L.; Benz, J.
Deposited on : 2020-04-24
Resolution : 1.65 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

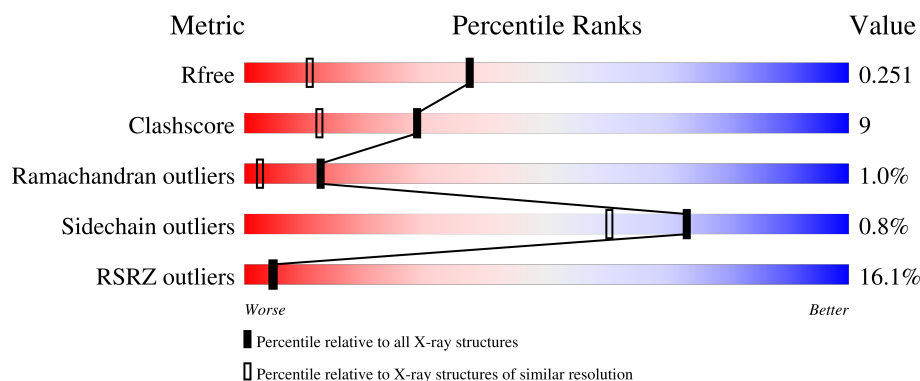
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	245	20% 69% 16% • 13%
2	B	245	8% 73% 13% •• 13%
3	C	8	25% 50% 25%
3	D	8	25% 75%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3873 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	207	Total	C	N	O	S	0	8	0
			1718	1099	286	326	7			

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 Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	209	Total	C	N	O	S	0	8	0
			1730	1104	290	329	7			

There are 17 discrepancies between the modelled and reference sequences:

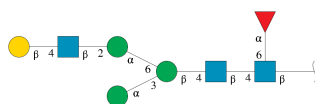
Chain	Residue	Modelled	Actual	Comment	Reference
B	357	LYS	GLU	engineered mutation	UNP P0DOX5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	366	SER	THR	engineered mutation	UNP P0DOX5
B	368	ALA	LEU	engineered mutation	UNP P0DOX5
B	407	VAL	TYR	engineered mutation	UNP P0DOX5
B	448	GLY	-	expression tag	UNP P0DOX5
B	449	GLY	-	expression tag	UNP P0DOX5
B	450	GLY	-	expression tag	UNP P0DOX5
B	451	GLY	-	expression tag	UNP P0DOX5
B	452	SER	-	expression tag	UNP P0DOX5
B	453	HIS	-	expression tag	UNP P0DOX5
B	454	HIS	-	expression tag	UNP P0DOX5
B	455	HIS	-	expression tag	UNP P0DOX5
B	456	HIS	-	expression tag	UNP P0DOX5
B	457	HIS	-	expression tag	UNP P0DOX5
B	458	HIS	-	expression tag	UNP P0DOX5
B	459	HIS	-	expression tag	UNP P0DOX5
B	460	HIS	-	expression tag	UNP P0DOX5

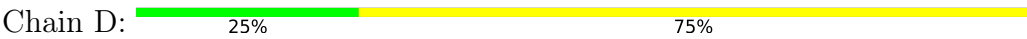
- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	0	0	0
			96	54	3	39			
3	D	8	Total	C	N	O	0	0	0
			96	54	3	39			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	93	Total	O	0	0
			93	93		
4	B	140	Total	O	0	0
			140	140		



MAG1
MAG2
BKA3
MAN4
MAG5
GAL6
MAN7
FUC8

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.16Å 75.22Å 149.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.70 – 1.65 46.70 – 1.66	Depositor EDS
% Data completeness (in resolution range)	91.4 (46.70-1.65) 91.5 (46.70-1.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.65Å)	Xtriage
Refinement program	PHENIX dev_3893	Depositor
R, R_{free}	0.216 , 0.249 0.219 , 0.251	Depositor DCC
R_{free} test set	3023 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3873	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.47	2/1771 (0.1%)	0.83	6/2405 (0.2%)
2	B	0.46	1/1783 (0.1%)	0.78	5/2421 (0.2%)
All	All	0.47	3/3554 (0.1%)	0.80	11/4826 (0.2%)

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	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	358	LEU	CA-C	-7.75	1.42	1.52
2	B	443	LEU	CG-CD2	-7.56	1.27	1.52
1	A	360	LYS	CE-NZ	6.77	1.69	1.49

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	LYS	CG-CD-CE	-11.48	84.90	111.30
2	B	443	LEU	CD1-CG-CD2	-9.28	90.39	110.80
2	B	443	LEU	CB-CG-CD2	8.76	136.99	110.70
1	A	360	LYS	CB-CG-CD	6.95	127.28	111.30
1	A	360	LYS	CD-CE-NZ	-6.12	92.31	111.90
1	A	360	LYS	CA-CB-CG	6.08	126.27	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	THR	CA-C-N	-6.08	109.92	121.54
1	A	359	THR	C-N-CA	-6.08	109.92	121.54
2	B	365	LEU	CB-CG-CD1	5.83	128.18	110.70
2	B	273	VAL	CG1-CB-CG2	5.28	122.42	110.80
2	B	419	GLN	CA-CB-CG	5.01	124.13	114.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	272	GLU	Sidechain
1	A	355	ARG	Peptide
2	B	389	ASN	Peptide

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	1718	0	1678	34	0
2	B	1730	0	1690	22	0
3	C	96	0	82	3	0
3	D	96	0	82	0	0
4	A	93	0	0	4	2
4	B	140	0	0	4	2
All	All	3873	0	3532	54	2

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 (54) 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:360:LYS:CE	1:A:360:LYS:NZ	1.69	1.52
1:A:360:LYS:HZ2	1:A:360:LYS:HG3	1.06	1.11
1:A:360:LYS:NZ	1:A:360:LYS:HG3	1.67	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:LYS:NZ	4:B:601:HOH:O	1.89	0.95
1:A:360:LYS:NZ	1:A:360:LYS:CG	2.36	0.88
1:A:360:LYS:HZ2	1:A:360:LYS:CG	1.89	0.86
1:A:360:LYS:NZ	1:A:360:LYS:CD	2.38	0.85
1:A:352:PRO:O	4:A:601:HOH:O	1.95	0.84
1:A:360:LYS:O	1:A:414:LYS:HE2	1.92	0.69
1:A:366[A]:TRP:CH2	1:A:409:LYS:HD3	2.29	0.68
1:A:256:THR:HG23	4:A:652:HOH:O	1.93	0.67
1:A:380:GLU:OE2	4:A:602:HOH:O	2.14	0.66
1:A:272:GLU:O	1:A:325:ASN:ND2	2.31	0.64
1:A:246:LYS:NZ	3:C:6:GAL:O4	2.18	0.63
1:A:355:ARG:HA	1:A:358:LEU:HD23	1.82	0.61
2:B:415:SER:O	2:B:419:GLN:HG2	2.02	0.59
1:A:368[A]:LEU:HD13	1:A:407[A]:TYR:CZ	2.37	0.59
2:B:288:LYS:O	4:B:601:HOH:O	2.17	0.57
2:B:365:LEU:HD12	2:B:441:LEU:CD2	2.35	0.56
1:A:296:TYR:C	1:A:298:SER:H	2.17	0.53
2:B:351:LEU:HB2	2:B:366[A]:SER:HB2	1.91	0.52
2:B:365:LEU:HD11	2:B:417:TRP:CZ3	2.46	0.51
1:A:373[A]:TYR:CG	1:A:374:PRO:HA	2.47	0.50
2:B:360:LYS:O	2:B:361:ASN:CB	2.60	0.50
2:B:416:ARG:O	2:B:419:GLN:HB2	2.12	0.49
1:A:243:PHE:CG	3:C:5:NAG:H5	2.47	0.49
1:A:353:PRO:HA	4:A:601:HOH:O	2.12	0.48
2:B:358:LEU:O	2:B:414:LYS:HD3	2.14	0.48
2:B:288:LYS:HB2	4:B:601:HOH:O	2.12	0.48
2:B:353:PRO:HA	4:B:607:HOH:O	2.14	0.48
1:A:240:VAL:HG22	1:A:263:VAL:HG22	1.95	0.48
2:B:414:LYS:HD2	2:B:418:GLN:NE2	2.31	0.46
1:A:292:ARG:CB	1:A:302:VAL:HG22	2.45	0.46
1:A:367:CYS:HB2	1:A:381:TRP:CZ2	2.51	0.46
2:B:357[A]:LYS:HD2	2:B:360:LYS:HG3	1.97	0.45
1:A:248:LYS:O	1:A:252[B]:MET:HG3	2.17	0.45
1:A:296:TYR:C	1:A:298:SER:N	2.74	0.45
2:B:311:GLN:HG3	2:B:315:ASN:ND2	2.32	0.45
1:A:266:VAL:O	1:A:300:TYR:HB2	2.17	0.45
1:A:406:LEU:C	1:A:406:LEU:HD12	2.42	0.44
2:B:353:PRO:HD3	2:B:365:LEU:HD13	2.00	0.44
2:B:414:LYS:HB3	2:B:414:LYS:HE2	1.70	0.44
2:B:443:LEU:HD13	2:B:444:SER:N	2.33	0.43
1:A:414:LYS:HE3	1:A:414:LYS:HB3	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:PHE:CE1	3:C:2:NAG:H4	2.54	0.42
1:A:414:LYS:O	1:A:418:GLN:HG3	2.19	0.42
1:A:366[A]:TRP:CH2	2:B:368[A]:ALA:HB1	2.55	0.42
1:A:407[A]:TYR:CE2	2:B:407[A]:VAL:HG11	2.56	0.41
2:B:406:LEU:HD12	2:B:406:LEU:C	2.45	0.41
2:B:252[B]:MET:HE3	2:B:428:MET:HG2	2.02	0.41
1:A:274:LYS:HB3	1:A:324:SER:HB2	2.03	0.41
1:A:292:ARG:HB2	1:A:302:VAL:HG22	2.02	0.41
1:A:311:GLN:HG3	1:A:315:ASN:ND2	2.36	0.41
2:B:357[A]:LYS:O	2:B:360:LYS:HB2	2.21	0.40

All (2) 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:602:HOH:O	4:B:702:HOH:O[3_555]	2.00	0.20
4:A:644:HOH:O	4:B:640:HOH:O[3_555]	2.05	0.15

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%)	24	10
2	B	205/245 (84%)	200 (98%)	2 (1%)	3 (2%)	8	1
All	All	408/490 (83%)	395 (97%)	9 (2%)	4 (1%)	12	2

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	356	ASP
2	B	361	ASN

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Mol	Chain	Res	Type
2	B	419	GLN
2	B	296	TYR

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	200/223 (90%)	200 (100%)	0	100	100
2	B	202/223 (91%)	199 (98%)	3 (2%)	57	37
All	All	402/446 (90%)	399 (99%)	3 (1%)	73	64

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	370[A]	LYS
2	B	370[B]	GLU
2	B	443	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	A	418	GLN
1	A	433	HIS
1	A	434	ASN
2	B	285	HIS
2	B	361	ASN
2	B	433	HIS
2	B	435	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 ⓘ

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	3,1	14,14,15	0.28	0	17,19,21	0.66	0
3	NAG	C	2	3	14,14,15	0.33	0	17,19,21	0.50	0
3	BMA	C	3	3	11,11,12	1.16	1 (9%)	15,15,17	1.24	2 (13%)
3	MAN	C	4	3	11,11,12	1.07	0	15,15,17	1.59	2 (13%)
3	NAG	C	5	3	14,14,15	0.84	1 (7%)	17,19,21	0.66	0
3	GAL	C	6	3	11,11,12	1.28	2 (18%)	15,15,17	1.42	2 (13%)
3	MAN	C	7	3	11,11,12	1.29	3 (27%)	15,15,17	1.12	1 (6%)
3	FUC	C	8	3	10,10,11	0.82	0	14,14,16	0.84	0
3	NAG	D	1	3,2	14,14,15	0.55	0	17,19,21	0.61	0
3	NAG	D	2	3	14,14,15	0.65	1 (7%)	17,19,21	0.71	0
3	BMA	D	3	3	11,11,12	0.84	1 (9%)	15,15,17	0.77	0
3	MAN	D	4	3	11,11,12	0.91	1 (9%)	15,15,17	1.49	2 (13%)
3	NAG	D	5	3	14,14,15	0.50	0	17,19,21	0.46	0
3	GAL	D	6	3	11,11,12	1.39	2 (18%)	15,15,17	1.12	2 (13%)
3	MAN	D	7	3	11,11,12	1.17	1 (9%)	15,15,17	0.79	0
3	FUC	D	8	3	10,10,11	0.99	1 (10%)	14,14,16	0.71	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	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	1/2/19/22	0/1/1/1
3	NAG	C	5	3	-	1/6/23/26	0/1/1/1
3	GAL	C	6	3	-	0/2/19/22	0/1/1/1
3	MAN	C	7	3	-	2/2/19/22	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	-	2/2/19/22	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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	BMA	C1-C2	3.38	1.60	1.52
3	C	6	GAL	C1-C2	3.20	1.59	1.52
3	D	6	GAL	C1-C2	3.03	1.59	1.52
3	D	6	GAL	O2-C2	2.78	1.49	1.43
3	C	7	MAN	C1-C2	2.71	1.58	1.52
3	D	7	MAN	O5-C1	-2.55	1.39	1.43
3	D	3	BMA	O5-C1	-2.52	1.39	1.43
3	D	4	MAN	O5-C5	2.48	1.48	1.43
3	C	5	NAG	O5-C1	-2.40	1.39	1.43
3	D	8	FUC	C2-C3	2.31	1.56	1.52
3	D	2	NAG	O5-C1	-2.25	1.39	1.43
3	C	7	MAN	O5-C1	-2.19	1.40	1.43
3	C	7	MAN	C2-C3	2.06	1.55	1.52
3	C	6	GAL	C2-C3	2.05	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	MAN	C1-O5-C5	4.48	118.19	112.19
3	C	4	MAN	C1-O5-C5	4.33	117.99	112.19
3	C	4	MAN	O2-C2-C3	-3.34	103.23	110.15
3	C	6	GAL	C1-O5-C5	3.13	116.38	112.19
3	D	4	MAN	O2-C2-C3	-3.05	103.84	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	BMA	C1-O5-C5	2.78	115.92	112.19
3	C	3	BMA	O2-C2-C3	-2.66	104.65	110.15
3	C	7	MAN	O2-C2-C3	-2.55	104.86	110.15
3	D	6	GAL	C1-C2-C3	2.18	112.82	109.64
3	D	6	GAL	O2-C2-C1	2.10	114.03	109.22
3	C	6	GAL	C1-C2-C3	2.07	112.66	109.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

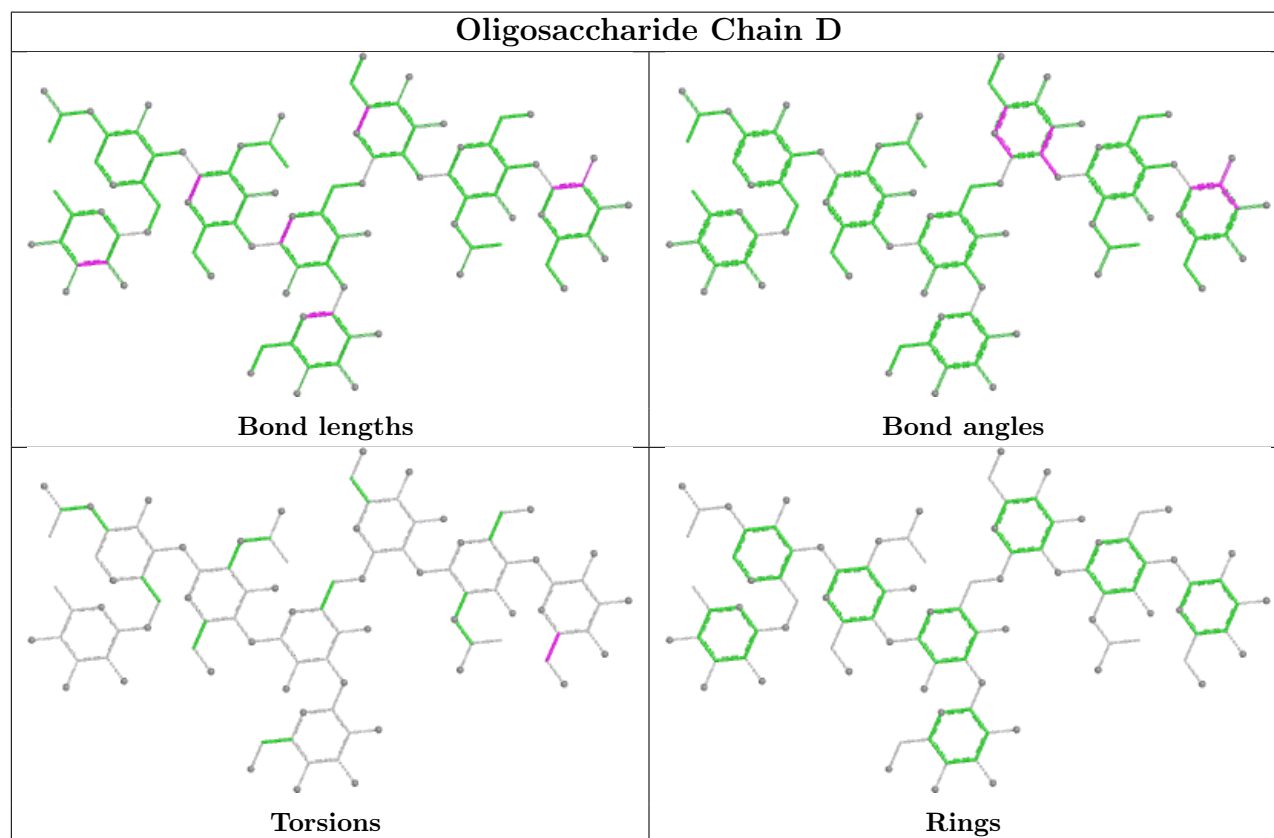
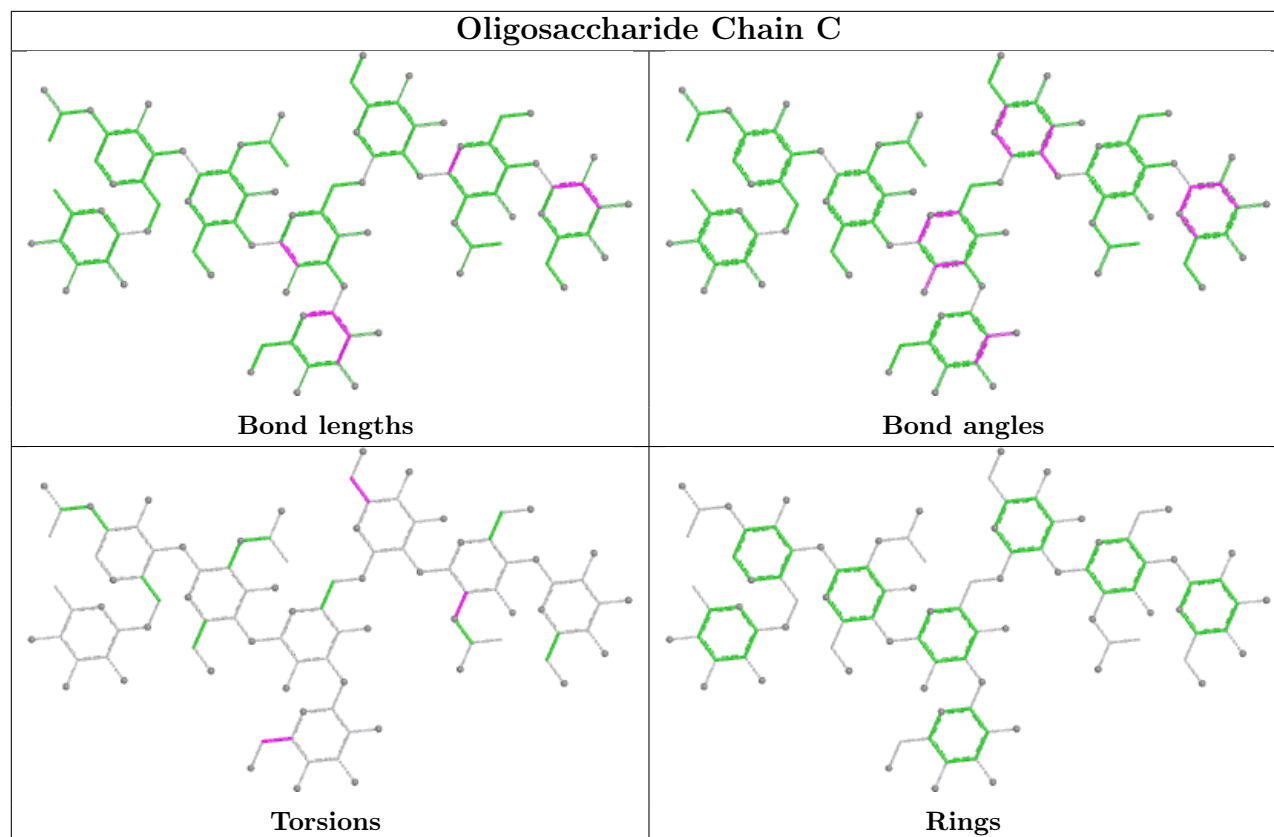
Mol	Chain	Res	Type	Atoms
3	D	6	GAL	O5-C5-C6-O6
3	C	7	MAN	O5-C5-C6-O6
3	D	6	GAL	C4-C5-C6-O6
3	C	7	MAN	C4-C5-C6-O6
3	C	4	MAN	C4-C5-C6-O6
3	C	5	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	5	NAG	1	0
3	C	2	NAG	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.



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, 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	202/245 (82%)	1.06	48 (23%) 2 2	15, 35, 82, 92	3 (1%)
2	B	204/245 (83%)	0.56	17 (8%) 17 19	15, 31, 52, 84	3 (1%)
All	All	406/490 (82%)	0.81	65 (16%) 4 5	15, 32, 74, 92	6 (1%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	358	LEU	5.6
1	A	273	VAL	4.9
1	A	358	LEU	4.8
1	A	300	TYR	4.3
1	A	329	PRO	4.2
1	A	330	ALA	4.1
1	A	296	TYR	4.1
2	B	445	PRO	4.0
1	A	360	LYS	4.0
2	B	359	THR	3.9
1	A	299	THR	3.8
1	A	263	VAL	3.7
1	A	356	ASP	3.7
1	A	266	VAL	3.5
1	A	271	PRO	3.5
1	A	332	ILE	3.4
1	A	243	PHE	3.4
1	A	264	VAL	3.3
1	A	443	LEU	3.3
1	A	267	SER	3.1
1	A	326	LYS	3.1
1	A	295	GLN	3.1
2	B	356	ASP	3.1
1	A	297	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	359	THR	3.0
1	A	272	GLU	3.0
1	A	327	ALA	2.9
1	A	291	PRO	2.9
1	A	240	VAL	2.8
1	A	328	LEU	2.8
2	B	361	ASN	2.8
1	A	302	VAL	2.8
2	B	444	SER	2.8
1	A	298	SER	2.8
1	A	270	ASP	2.7
1	A	265	ASP	2.7
2	B	355	ARG	2.7
2	B	389	ASN	2.6
1	A	237	GLY	2.6
2	B	443	LEU	2.6
2	B	330	ALA	2.6
1	A	292	ARG	2.6
1	A	361	ASN	2.5
1	A	268	HIS	2.5
1	A	241	PHE	2.5
1	A	323	VAL	2.4
2	B	291	PRO	2.4
1	A	354	SER	2.4
2	B	418	GLN	2.4
2	B	413	ASP	2.4
1	A	239	SER	2.3
1	A	289	THR	2.3
1	A	276	ASN	2.3
1	A	331	PRO	2.2
1	A	294	GLU	2.2
1	A	303	VAL	2.2
1	A	384	ASN	2.2
1	A	256	THR	2.2
2	B	365	LEU	2.2
1	A	355	ARG	2.1
2	B	360	LYS	2.1
1	A	274	LYS	2.1
2	B	290	LYS	2.1
1	A	325	ASN	2.0
2	B	273	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

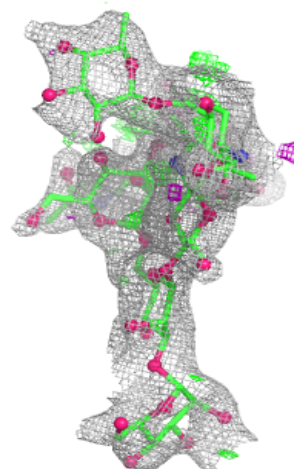
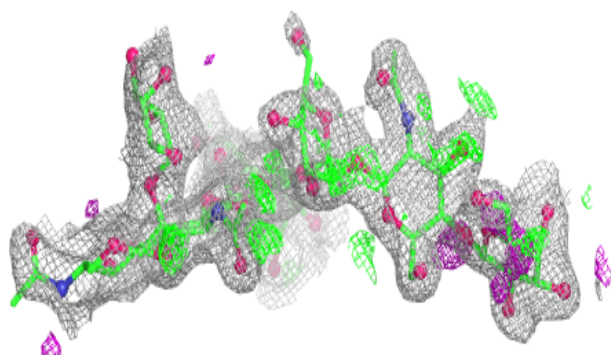
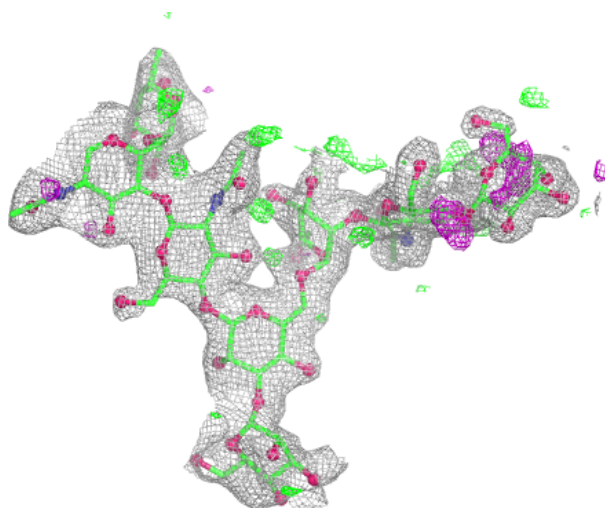
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

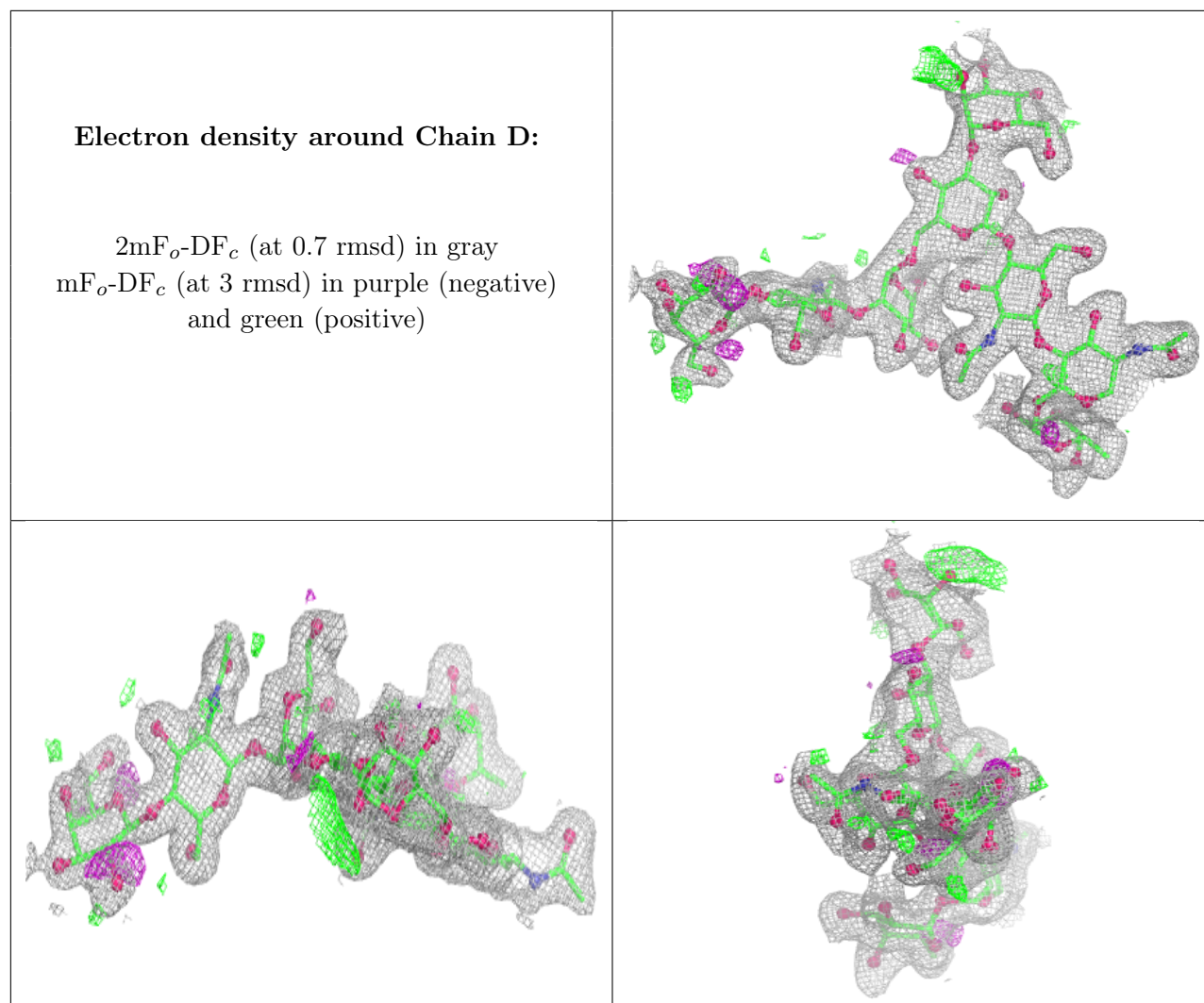
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	C	7	11/12	0.45	0.17	75,81,84,86	0
3	FUC	C	8	10/11	0.68	0.16	82,88,90,93	0
3	MAN	D	7	11/12	0.68	0.14	52,59,66,71	0
3	NAG	C	1	14/15	0.73	0.16	59,71,77,78	0
3	NAG	C	5	14/15	0.81	0.16	41,46,50,52	0
3	GAL	D	6	11/12	0.83	0.20	34,39,50,50	0
3	FUC	D	8	10/11	0.83	0.12	39,41,44,46	0
3	NAG	C	2	14/15	0.84	0.13	44,54,65,67	0
3	BMA	C	3	11/12	0.84	0.12	43,51,60,62	0
3	GAL	C	6	11/12	0.86	0.19	39,41,46,49	0
3	MAN	D	4	11/12	0.87	0.11	35,40,44,46	0
3	MAN	C	4	11/12	0.87	0.14	41,49,59,61	0
3	NAG	D	5	14/15	0.88	0.12	34,38,47,47	0
3	BMA	D	3	11/12	0.91	0.09	35,39,42,46	0
3	NAG	D	1	14/15	0.93	0.09	30,37,47,48	0
3	NAG	D	2	14/15	0.93	0.09	30,37,44,44	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)





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.