



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:55 PM UTC

PDB ID : 4MR9 / pdb_00004mr9
Title : Crystal structure of the extracellular domain of human GABA(B) receptor bound to the antagonist SCH50911
Authors : Geng, Y.; Bush, M.; Mosyak, L.; Wang, F.; Fan, Q.R.
Deposited on : 2013-09-17
Resolution : 2.35 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

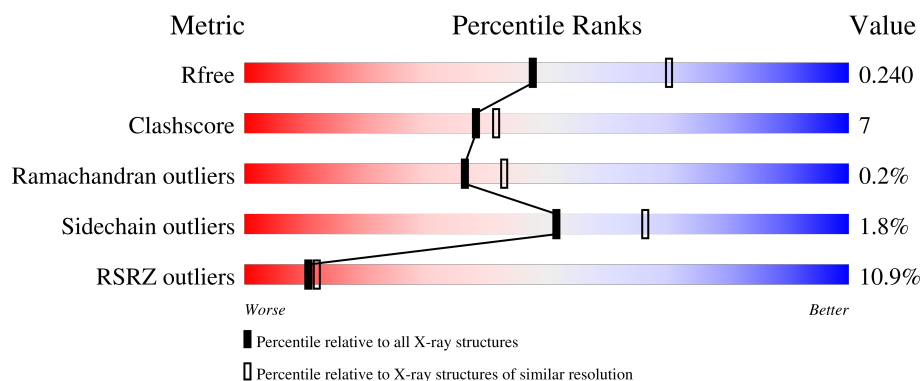
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	420	16% 78% 16% • •
2	B	433	5% 85% 7% • 7%
3	C	4	100%
4	D	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	D	1	-	-	X	-
6	NAG	A	502	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6831 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 Gamma-aminobutyric acid type B receptor subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3271	2090	551	616	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	460	ASP	-	expression tag	UNP Q9UBS5
A	461	TYR	-	expression tag	UNP Q9UBS5
A	462	LYS	-	expression tag	UNP Q9UBS5
A	463	ASP	-	expression tag	UNP Q9UBS5
A	464	ASP	-	expression tag	UNP Q9UBS5
A	465	ASP	-	expression tag	UNP Q9UBS5
A	466	ASP	-	expression tag	UNP Q9UBS5
A	467	LYS	-	expression tag	UNP Q9UBS5

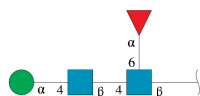
- Molecule 2 is a protein called Gamma-aminobutyric acid type B receptor subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	403	Total	C	N	O	S	0	0	0
			3214	2052	543	604	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	467	ASP	-	expression tag	UNP O75899
B	468	TYR	-	expression tag	UNP O75899
B	469	LYS	-	expression tag	UNP O75899
B	470	ASP	-	expression tag	UNP O75899
B	471	ASP	-	expression tag	UNP O75899
B	472	ASP	-	expression tag	UNP O75899
B	473	ASP	-	expression tag	UNP O75899
B	474	LYS	-	expression tag	UNP O75899

- Molecule 3 is an oligosaccharide called alpha-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.



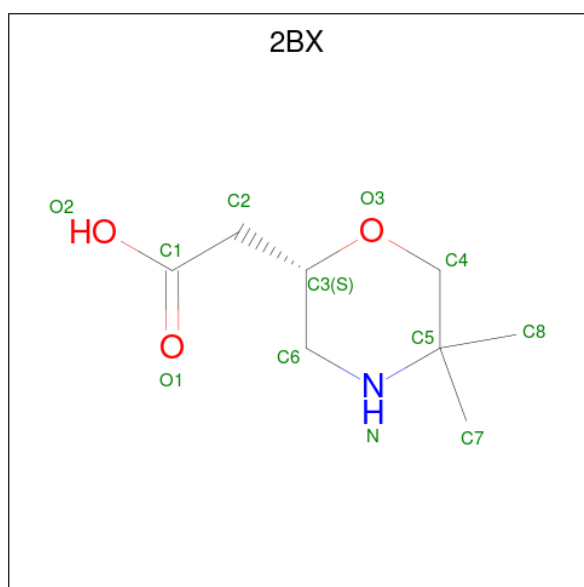
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



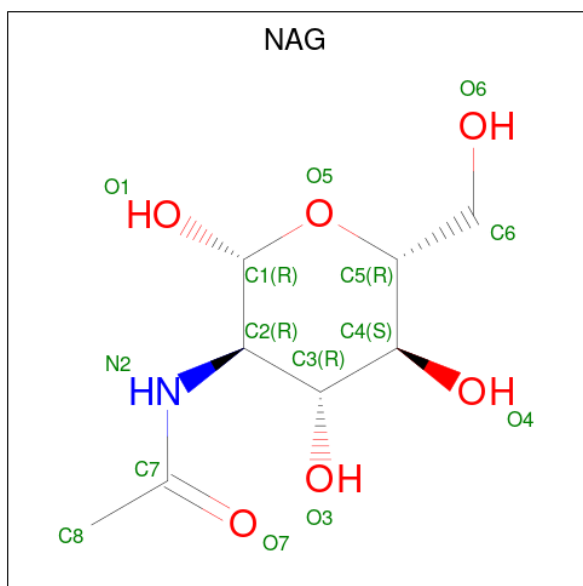
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 5 is [(2S)-5,5-dimethylmorpholin-2-yl]acetic acid (CCD ID: 2BX) (formula: C₈H₁₅NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			12	8	1	3		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

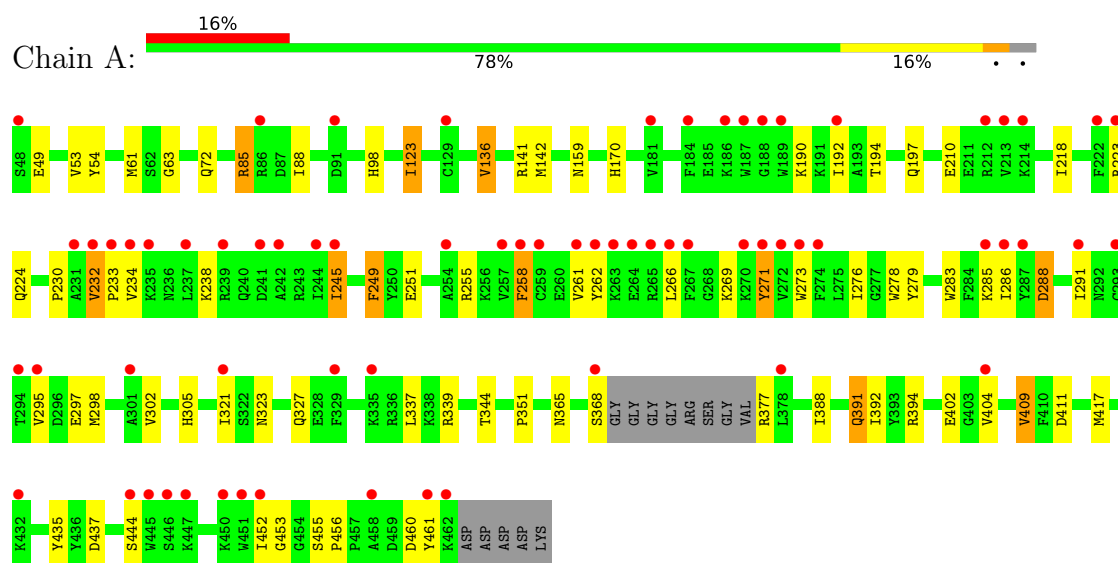
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	113	Total	O	0	0
			113	113		
7	B	134	Total	O	0	0
			134	134		

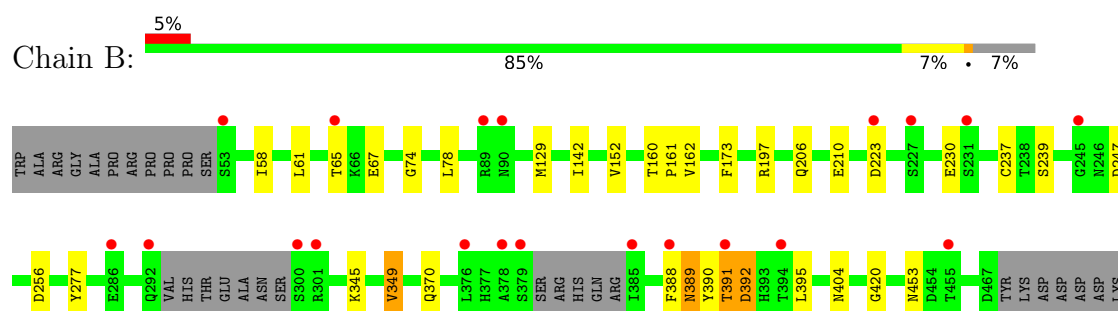
3 Residue-property plots

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.

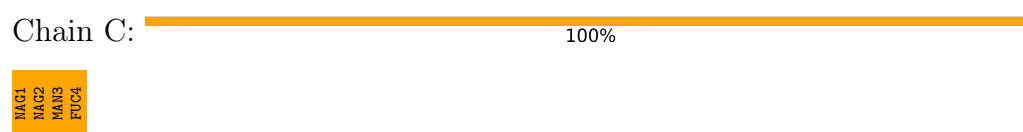
- Molecule 1: Gamma-aminobutyric acid type B receptor subunit 1



- Molecule 2: Gamma-aminobutyric acid type B receptor subunit 2



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

Chain D:

100%

RMS1
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.50Å 113.07Å 73.22Å 90.00° 96.96° 90.00°	Depositor
Resolution (Å)	72.68 – 2.35 72.68 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.5 (72.68-2.35) 99.5 (72.68-2.35)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.34Å)	Xtriage
Refinement program	BUSTER-TNT, BUSTER	Depositor
R, R_{free}	0.207 , 0.229 0.216 , 0.240	Depositor DCC
R_{free} test set	2347 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	54.8	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.5	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	6831	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: NAG, MAN, FUC, 2BX

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	0.85	2/3354 (0.1%)	1.38	22/4547 (0.5%)
2	B	0.87	0/3287	1.34	7/4449 (0.2%)
All	All	0.86	2/6641 (0.0%)	1.36	29/8996 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	232	VAL	CA-CB	5.33	1.57	1.54
1	A	170	HIS	CG-CD2	5.25	1.41	1.35

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	HIS	ND1-CE1-NE2	8.48	116.88	108.40
1	A	288	ASP	CA-CB-CG	8.10	120.70	112.60
1	A	271	TYR	N-CA-C	7.80	122.14	109.59
1	A	245	ILE	N-CA-C	6.83	117.73	107.75
1	A	460	ASP	CA-C-N	6.79	129.71	120.54
1	A	460	ASP	C-N-CA	6.79	129.71	120.54
1	A	232	VAL	N-CA-CB	6.67	115.66	110.45
2	B	389	ASN	N-CA-C	-6.65	99.64	109.81
1	A	63	GLY	CA-C-N	6.58	127.43	119.99
1	A	63	GLY	C-N-CA	6.58	127.43	119.99
1	A	49	GLU	CB-CG-CD	6.52	123.68	112.60
1	A	238	LYS	CA-C-N	6.51	129.33	120.54
1	A	238	LYS	C-N-CA	6.51	129.33	120.54
1	A	54	TYR	N-CA-C	6.42	119.93	109.59
1	A	136	VAL	N-CA-CB	6.27	119.98	110.58
2	B	237	CYS	N-CA-C	6.19	118.83	111.33
1	A	411	ASP	CA-CB-CG	6.00	118.60	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	TYR	N-CA-C	5.92	118.21	111.11
2	B	349	VAL	N-CA-CB	5.75	117.21	110.82
1	A	453	GLY	N-CA-C	-5.64	99.82	113.18
1	A	437	ASP	CA-C-N	5.53	127.96	120.38
1	A	437	ASP	C-N-CA	5.53	127.96	120.38
1	A	258	PHE	CA-CB-CG	-5.37	108.43	113.80
2	B	256	ASP	CA-C-N	5.33	127.74	120.54
2	B	256	ASP	C-N-CA	5.33	127.74	120.54
2	B	392	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	437	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	159	ASN	CA-CB-CG	5.13	117.73	112.60
2	B	277	TYR	N-CA-C	5.07	117.67	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	3271	0	3195	56	0
2	B	3214	0	3162	19	0
3	C	49	0	46	8	0
4	D	24	0	23	7	0
5	A	12	0	14	0	0
6	A	14	0	13	7	0
7	A	113	0	0	2	0
7	B	134	0	0	1	0
All	All	6831	0	6453	83	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 7.

All (83) 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:365:ASN:HD21	6:A:502:NAG:C1	1.17	1.58
1:A:323:ASN:HD21	3:C:1:NAG:C1	1.10	1.57
2:B:404:ASN:HD21	4:D:1:NAG:C1	0.89	1.50
1:A:368:SER:O	1:A:377:ARG:N	1.74	1.17
1:A:288:ASP:HB3	1:A:291:ILE:HD12	1.46	0.95
1:A:365:ASN:HD21	6:A:502:NAG:C2	1.79	0.95
3:C:1:NAG:C6	3:C:4:FUC:C1	2.56	0.84
1:A:288:ASP:HB3	1:A:291:ILE:CD1	2.10	0.81
1:A:365:ASN:CG	6:A:502:NAG:C1	2.54	0.80
2:B:404:ASN:HD22	4:D:1:NAG:H83	1.47	0.80
1:A:141:ARG:HH11	1:A:142:MET:HE3	1.54	0.73
3:C:2:NAG:C4	3:C:3:MAN:C1	2.66	0.72
3:C:1:NAG:C4	3:C:2:NAG:C1	2.68	0.72
1:A:224:GLN:HB3	1:A:233:PRO:HB3	1.71	0.72
2:B:404:ASN:ND2	4:D:1:NAG:C2	2.53	0.70
3:C:3:MAN:C1	3:C:3:MAN:O6	2.39	0.70
4:D:1:NAG:HO6	4:D:2:FUC:C1	2.04	0.70
1:A:262:TYR:CZ	1:A:297:GLU:OE1	2.46	0.69
3:C:2:NAG:HO4	3:C:3:MAN:C1	2.04	0.69
3:C:1:NAG:HO6	3:C:4:FUC:C1	2.07	0.68
1:A:88:ILE:CD1	6:A:502:NAG:H82	2.24	0.67
1:A:210:GLU:OE2	1:A:223:ARG:CZ	2.44	0.66
2:B:453:ASN:HA	7:B:644:HOH:O	2.00	0.62
1:A:88:ILE:HD13	6:A:502:NAG:H82	1.81	0.62
1:A:85:ARG:NH2	1:A:321:ILE:O	2.33	0.61
1:A:321:ILE:HG12	1:A:402:GLU:O	2.01	0.61
1:A:262:TYR:CE1	1:A:297:GLU:OE1	2.55	0.60
1:A:283:TRP:HA	1:A:286:ILE:HD12	1.84	0.58
1:A:323:ASN:ND2	3:C:1:NAG:C2	2.65	0.58
4:D:1:NAG:C6	4:D:2:FUC:C1	2.80	0.58
1:A:302:VAL:O	1:A:305:HIS:HD2	1.88	0.57
1:A:276:ILE:HD11	1:A:279:TYR:CE1	2.40	0.56
1:A:339:ARG:HD2	7:A:667:HOH:O	2.05	0.56
2:B:129:MET:HB2	2:B:152:VAL:O	2.06	0.56
1:A:266:LEU:CD2	1:A:273:TRP:HZ2	2.19	0.55
1:A:351:PRO:HB3	1:A:404:VAL:HG23	1.89	0.55
2:B:389:ASN:C	2:B:391:THR:H	2.15	0.55
2:B:58:ILE:HD12	2:B:129:MET:HG2	1.88	0.54
1:A:266:LEU:HD23	1:A:273:TRP:HZ2	1.72	0.54
1:A:365:ASN:OD1	6:A:502:NAG:C1	2.55	0.54
2:B:65:THR:HG22	2:B:67:GLU:H	1.73	0.54
1:A:388:ILE:O	1:A:392:ILE:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:404:ASN:CG	4:D:1:NAG:C1	2.69	0.52
2:B:206:GLN:HE21	2:B:210:GLU:HG2	1.75	0.51
1:A:291:ILE:HG21	1:A:298:MET:HE1	1.94	0.49
1:A:409:VAL:HG23	1:A:417:MET:HB2	1.95	0.49
2:B:61:LEU:HD13	2:B:142:ILE:HD13	1.95	0.49
1:A:53:VAL:HG13	1:A:123:ILE:HG12	1.95	0.48
1:A:276:ILE:HD13	1:A:278:TRP:CE2	2.48	0.48
1:A:455:SER:HB3	1:A:456:PRO:HD2	1.94	0.48
1:A:455:SER:CB	1:A:456:PRO:HD2	2.44	0.48
1:A:337:LEU:HD22	1:A:344:THR:HG21	1.96	0.47
2:B:404:ASN:HD22	4:D:1:NAG:C8	2.20	0.47
1:A:194:THR:OG1	1:A:223:ARG:HG2	2.14	0.47
2:B:230:GLU:HB3	2:B:239:SER:HB3	1.96	0.47
1:A:266:LEU:HD12	1:A:271:TYR:CE1	2.50	0.47
1:A:266:LEU:O	1:A:266:LEU:HG	2.15	0.46
1:A:302:VAL:O	1:A:305:HIS:CD2	2.67	0.46
1:A:288:ASP:O	1:A:291:ILE:HB	2.15	0.46
1:A:262:TYR:CE2	1:A:297:GLU:OE1	2.68	0.46
1:A:190:LYS:HA	1:A:218:ILE:HG12	1.99	0.45
1:A:391:GLN:HE21	1:A:394:ARG:HH22	1.64	0.45
1:A:197:GLN:HB2	1:A:249:PHE:HB3	1.99	0.45
1:A:327:GLN:H	1:A:327:GLN:CD	2.24	0.45
1:A:285:LYS:HA	1:A:295:VAL:HG13	1.99	0.45
2:B:74:GLY:O	2:B:78:LEU:HG	2.16	0.45
1:A:230:PRO:O	1:A:234:VAL:HG23	2.17	0.45
1:A:98:HIS:HD2	7:A:663:HOH:O	2.00	0.44
2:B:197:ARG:NH2	2:B:247:ASP:O	2.50	0.44
2:B:173:PHE:CD2	2:B:420:GLY:HA2	2.53	0.44
1:A:269:LYS:HG3	1:A:452:ILE:HB	2.01	0.42
1:A:435:TYR:HB2	1:A:444:SER:HB2	2.01	0.42
1:A:61:MET:CE	1:A:72:GLN:HE21	2.32	0.42
1:A:269:LYS:HE2	1:A:452:ILE:HG22	2.02	0.42
1:A:251:GLU:OE2	1:A:255:ARG:NH2	2.52	0.42
2:B:388:PHE:HB2	2:B:395:LEU:HD23	2.02	0.41
2:B:388:PHE:HD1	2:B:392:ASP:HB3	1.85	0.41
1:A:258:PHE:HA	1:A:261:VAL:HB	2.03	0.41
1:A:298:MET:O	1:A:302:VAL:HG22	2.21	0.41
1:A:232:VAL:HG22	1:A:233:PRO:HD3	2.03	0.41
2:B:160:THR:HA	2:B:161:PRO:HD3	1.94	0.41
1:A:365:ASN:ND2	6:A:502:NAG:C2	2.60	0.40
1:A:61:MET:CE	1:A:72:GLN:NE2	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	403/420 (96%)	390 (97%)	13 (3%)	0	100	100
2	B	397/433 (92%)	381 (96%)	14 (4%)	2 (0%)	24	27
All	All	800/853 (94%)	771 (96%)	27 (3%)	2 (0%)	36	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	390	TYR
2	B	223	ASP

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	354/362 (98%)	346 (98%)	8 (2%)	44	58
2	B	349/375 (93%)	344 (99%)	5 (1%)	59	73
All	All	703/737 (95%)	690 (98%)	13 (2%)	51	66

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

Mol	Chain	Res	Type
1	A	85	ARG

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Mol	Chain	Res	Type
1	A	123	ILE
1	A	136	VAL
1	A	192	ILE
1	A	245	ILE
1	A	249	PHE
1	A	391	GLN
1	A	409	VAL
2	B	162	VAL
2	B	345	LYS
2	B	349	VAL
2	B	370	GLN
2	B	391	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	98	HIS
1	A	161	GLN
1	A	197	GLN
1	A	240	GLN
1	A	305	HIS
1	A	323	ASN
1	A	365	ASN
1	A	391	GLN
1	A	397	ASN
1	A	407	HIS
2	B	90	ASN
2	B	206	GLN
2	B	254	GLN
2	B	337	GLN
2	B	404	ASN
2	B	459	GLN

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 ⓘ

6 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	1.20	1 (7%)	17,19,21	3.30	9 (52%)
3	NAG	C	2	3	14,14,15	1.03	0	17,19,21	2.91	8 (47%)
3	MAN	C	3	3	11,11,12	1.25	1 (9%)	15,15,17	2.54	5 (33%)
3	FUC	C	4	3	10,10,11	1.42	2 (20%)	14,14,16	2.40	3 (21%)
4	NAG	D	1	4,2	14,14,15	1.43	2 (14%)	17,19,21	3.52	9 (52%)
4	FUC	D	2	4	10,10,11	1.00	0	14,14,16	1.60	1 (7%)

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	-	4/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	MAN	C	3	3	-	2/2/19/22	1/1/1/1
3	FUC	C	4	3	-	-	0/1/1/1
4	NAG	D	1	4,2	-	2/6/23/26	0/1/1/1
4	FUC	D	2	4	-	-	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	NAG	O5-C1	-2.76	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	NAG	C7-N2	2.59	1.42	1.34
4	D	1	NAG	C8-C7	2.33	1.55	1.50
3	C	4	FUC	O2-C2	2.32	1.48	1.43
3	C	3	MAN	O5-C1	2.21	1.47	1.43
3	C	4	FUC	C4-C5	2.02	1.57	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	NAG	C1-O5-C5	-7.87	101.64	112.19
3	C	1	NAG	O5-C1-C2	7.70	123.21	111.29
4	D	1	NAG	C1-C2-N2	6.76	121.08	110.43
3	C	4	FUC	O5-C1-C2	6.45	126.17	110.79
3	C	2	NAG	C3-C4-C5	6.44	121.92	110.23
4	D	1	NAG	C4-C3-C2	-6.08	102.11	111.02
3	C	1	NAG	O4-C4-C3	-6.04	96.14	110.38
3	C	3	MAN	C1-C2-C3	-5.35	101.85	109.64
3	C	2	NAG	O4-C4-C3	-5.28	97.92	110.38
3	C	3	MAN	O3-C3-C2	-4.96	99.94	110.05
3	C	2	NAG	C4-C3-C2	-4.62	104.24	111.02
4	D	2	FUC	O5-C1-C2	4.34	121.14	110.79
3	C	4	FUC	O2-C2-C1	4.12	118.65	109.22
3	C	1	NAG	C4-C3-C2	-3.92	105.27	111.02
3	C	1	NAG	C1-O5-C5	3.80	117.28	112.19
3	C	1	NAG	O6-C6-C5	-3.74	98.61	111.33
3	C	1	NAG	O5-C5-C6	-3.71	100.44	107.66
3	C	3	MAN	C6-C5-C4	-3.67	104.01	113.02
3	C	2	NAG	O4-C4-C5	-3.62	100.42	109.32
4	D	1	NAG	O6-C6-C5	-3.61	99.03	111.33
4	D	1	NAG	O5-C5-C4	-3.57	102.15	110.83
3	C	3	MAN	O5-C1-C2	3.33	118.73	110.79
4	D	1	NAG	C3-C4-C5	3.30	116.21	110.23
3	C	2	NAG	C1-O5-C5	-3.07	108.07	112.19
3	C	4	FUC	O5-C5-C6	-3.01	100.88	107.40
3	C	2	NAG	C8-C7-N2	-2.90	111.31	116.12
3	C	1	NAG	C6-C5-C4	-2.85	106.02	113.02
3	C	1	NAG	O5-C5-C4	2.83	117.72	110.83
3	C	2	NAG	C1-C2-N2	2.59	114.51	110.43
4	D	1	NAG	O4-C4-C5	-2.56	103.02	109.32
4	D	1	NAG	C8-C7-N2	2.46	120.19	116.12
4	D	1	NAG	O4-C4-C3	-2.29	104.98	110.38
3	C	1	NAG	C3-C4-C5	2.28	114.37	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	O5-C1-C2	2.20	114.70	111.29
3	C	3	MAN	C2-C3-C4	2.08	114.52	110.86

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

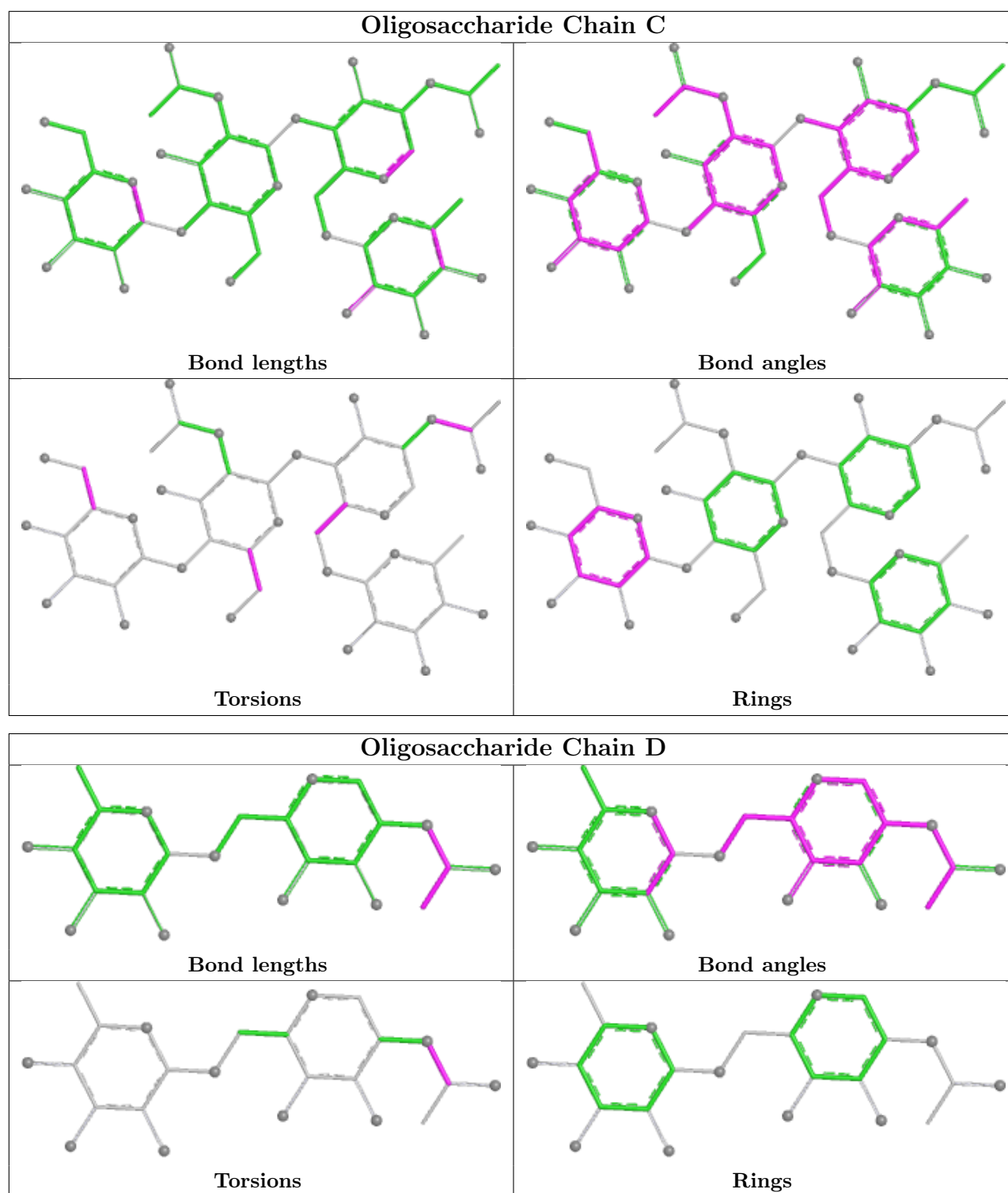
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	3	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3	MAN	3	0
4	D	2	FUC	2	0
3	C	1	NAG	5	0
3	C	2	NAG	3	0
4	D	1	NAG	7	0
3	C	4	FUC	2	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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	2BX	A	501	-	9,12,12	0.54	0	11,17,17	2.49	3 (27%)
6	NAG	A	502	1	14,14,15	1.03	0	17,19,21	2.53	5 (29%)

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
5	2BX	A	501	-	-	0/4/16/16	0/1/1/1
6	NAG	A	502	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	2BX	C6-N-C5	6.96	123.01	114.31
6	A	502	NAG	C1-O5-C5	-6.02	104.12	112.19
6	A	502	NAG	C2-N2-C7	-5.99	114.88	122.90
6	A	502	NAG	C1-C2-N2	4.05	116.81	110.43
5	A	501	2BX	O2-C1-O1	-2.91	115.86	123.33
6	A	502	NAG	O5-C5-C4	-2.39	105.01	110.83
5	A	501	2BX	C4-O3-C3	2.16	115.36	112.23
6	A	502	NAG	O5-C1-C2	2.04	114.45	111.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	502	NAG	7	0

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	407/420 (96%)	1.04	68 (16%) 4 4	41, 68, 112, 122	0
2	B	403/433 (93%)	0.52	20 (4%) 34 40	37, 61, 93, 135	0
All	All	810/853 (94%)	0.78	88 (10%) 10 12	37, 64, 107, 135	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	CYS	5.5
1	A	266	LEU	4.6
1	A	295	VAL	4.5
1	A	189	TRP	4.5
1	A	48	SER	4.1
1	A	212	ARG	3.8
2	B	388	PHE	3.8
2	B	245	GLY	3.6
1	A	258	PHE	3.6
1	A	461	TYR	3.5
1	A	458	ALA	3.5
2	B	379	SER	3.5
1	A	267	PHE	3.5
1	A	368	SER	3.4
2	B	300	SER	3.4
1	A	222	PHE	3.4
1	A	237	LEU	3.4
2	B	223	ASP	3.4
1	A	242	ALA	3.3
1	A	444	SER	3.3
2	B	385	ILE	3.2
1	A	233	PRO	3.2
2	B	378	ALA	3.1
1	A	293	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	294	THR	3.1
1	A	452	ILE	3.0
1	A	259	CYS	3.0
1	A	301	ALA	3.0
1	A	462	LYS	3.0
1	A	261	VAL	2.9
2	B	65	THR	2.9
1	A	321	ILE	2.9
1	A	262	TYR	2.9
1	A	232	VAL	2.9
2	B	376	LEU	2.8
2	B	286	GLU	2.8
1	A	404	VAL	2.8
2	B	292	GLN	2.8
1	A	272	VAL	2.8
1	A	91	ASP	2.7
1	A	291	ILE	2.7
1	A	254	ALA	2.6
2	B	227	SER	2.6
1	A	214	LYS	2.6
2	B	394	THR	2.6
1	A	213	VAL	2.5
1	A	235	LYS	2.5
1	A	223	ARG	2.5
1	A	239	ARG	2.5
1	A	257	VAL	2.5
1	A	271	TYR	2.5
1	A	450	LYS	2.5
1	A	244	ILE	2.4
2	B	231	SER	2.4
1	A	329	PHE	2.4
1	A	270	LYS	2.4
1	A	86	ARG	2.4
1	A	181	VAL	2.4
1	A	273	TRP	2.4
1	A	188	GLY	2.3
1	A	245	ILE	2.3
1	A	445	TRP	2.3
1	A	287	TYR	2.3
1	A	446	SER	2.3
1	A	378	LEU	2.2
2	B	53	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	447	LYS	2.2
1	A	274	PHE	2.2
2	B	89	ARG	2.2
1	A	263	LYS	2.2
1	A	187	TRP	2.2
2	B	391	THR	2.2
1	A	286	ILE	2.1
2	B	455	THR	2.1
1	A	265	ARG	2.1
1	A	184	PHE	2.1
2	B	301	ARG	2.1
1	A	231	ALA	2.1
1	A	264	GLU	2.1
2	B	90	ASN	2.1
1	A	234	VAL	2.1
1	A	432	LYS	2.0
1	A	192	ILE	2.0
1	A	186	LYS	2.0
1	A	285	LYS	2.0
1	A	451	TRP	2.0
1	A	241	ASP	2.0
1	A	335	LYS	2.0

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

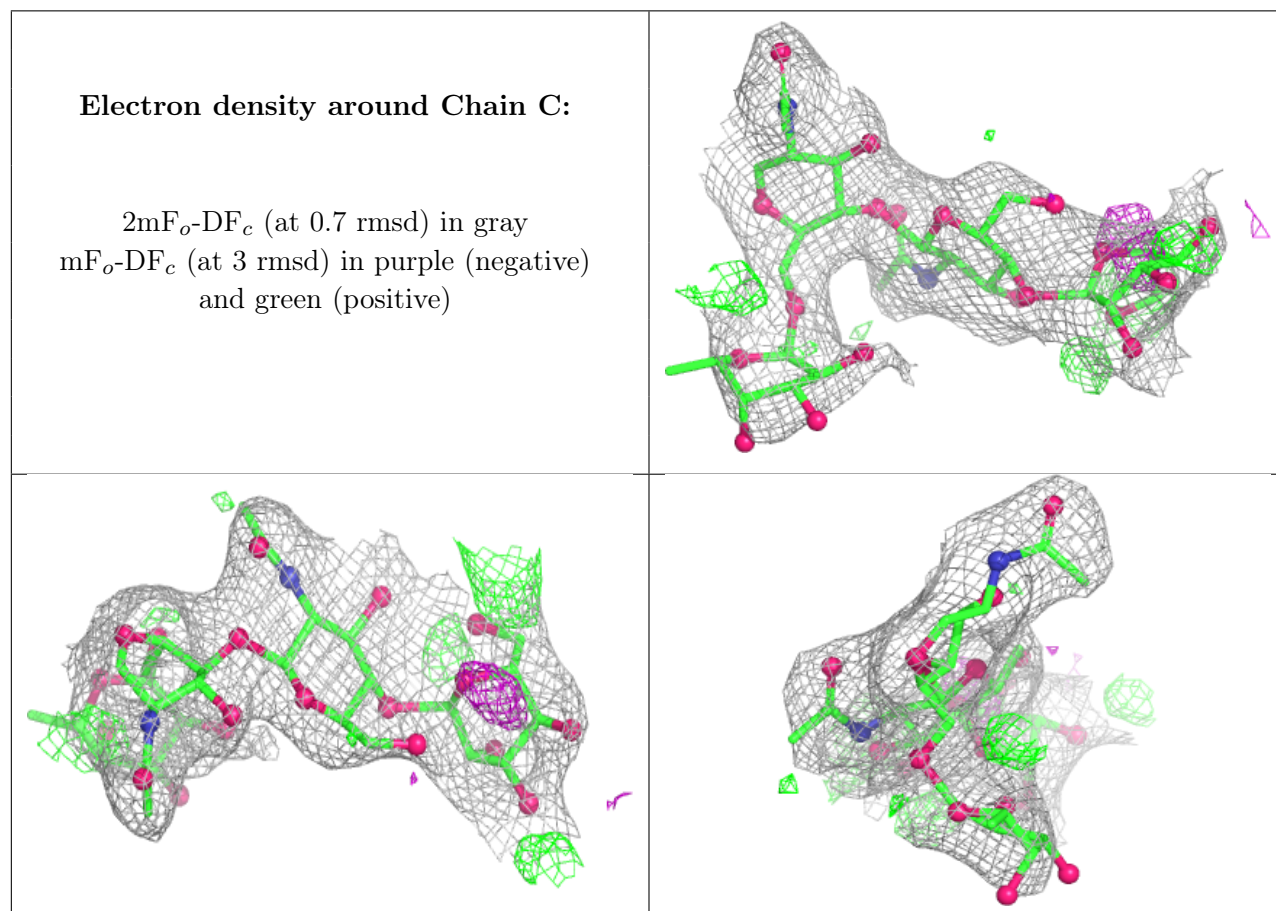
There are no non-standard protein/DNA/RNA residues in this entry.

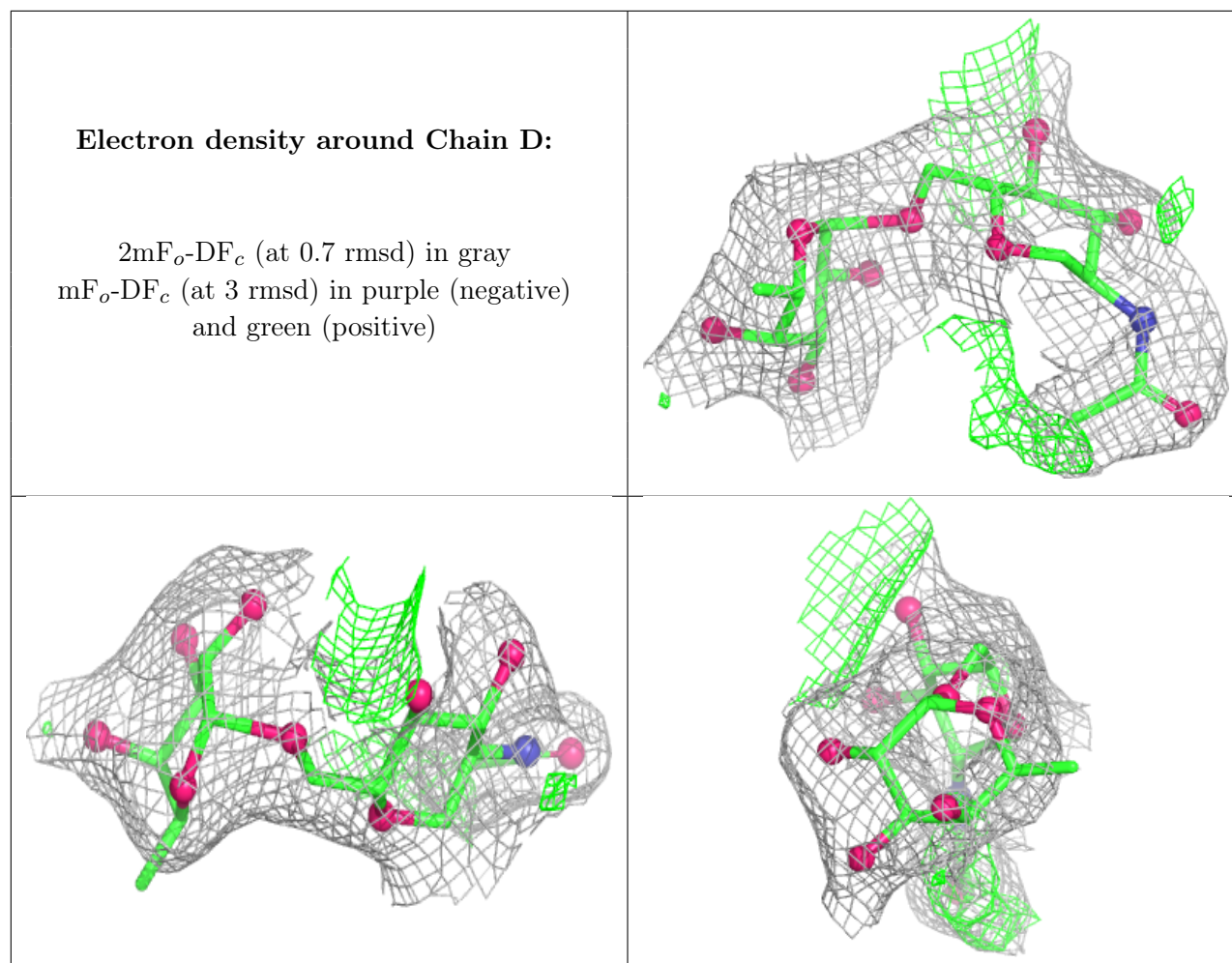
6.3 Carbohydrates [i](#)

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	MAN	C	3	11/12	0.68	0.19	98,100,101,102	0
3	FUC	C	4	10/11	0.71	0.18	101,102,103,104	0
4	NAG	D	1	14/15	0.74	0.16	78,82,85,85	0
3	NAG	C	2	14/15	0.83	0.14	86,90,92,93	0
3	NAG	C	1	14/15	0.86	0.11	80,83,85,86	0
4	FUC	D	2	10/11	0.90	0.15	84,85,86,86	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.





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
6	NAG	A	502	14/15	0.87	0.10	82,86,88,88	0
5	2BX	A	501	12/12	0.97	0.06	41,47,50,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.