



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2026 – 01:15 pm BST

PDB ID : 9IGM / pdb_00009igm
Title : Structure of the 4-CHRD domain of human Chordin in complex with a Heparin Oligosaccharide
Authors : Snee, M.
Deposited on : 2025-02-19
Resolution : 2.92 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 : 1.8.4, CSD as541be (2020)
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

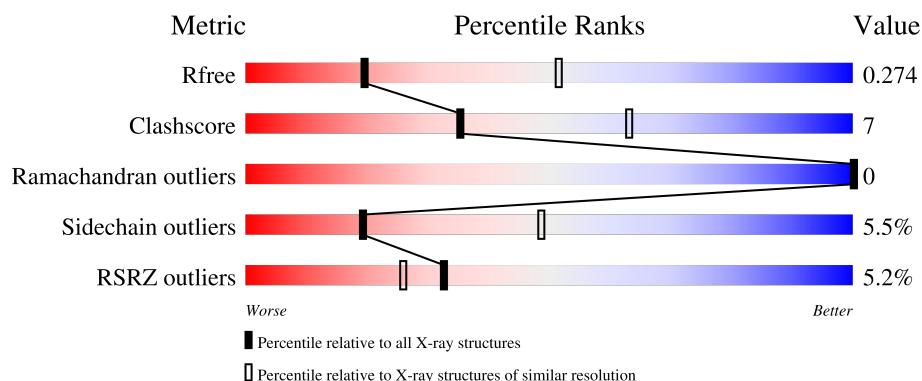
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	501	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>..</div> </div> </div>
2	X	5	<div> <div>60%</div> <div>40%</div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3860 atoms, of which 51 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.

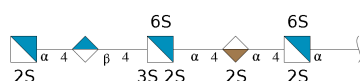
- Molecule 1 is a protein called Chordin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	480	3610	2283	663	650	14	0	2	0

There are 17 discrepancies between the modelled and reference sequences:

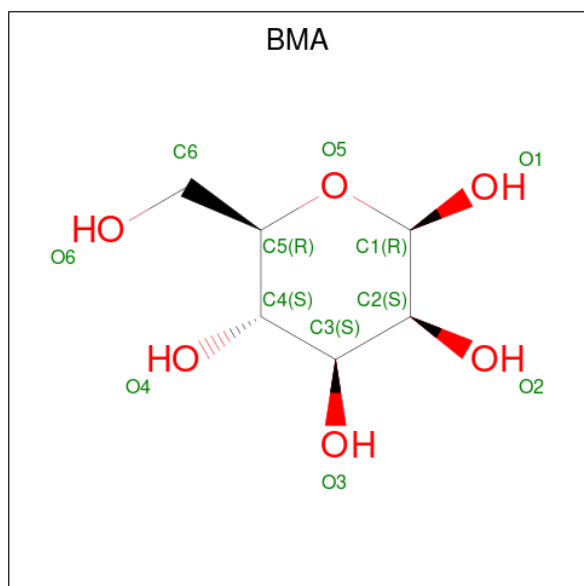
Chain	Residue	Modelled	Actual	Comment	Reference
A	164	ALA	-	expression tag	UNP Q9H2X0
A	165	PRO	-	expression tag	UNP Q9H2X0
A	166	LEU	-	expression tag	UNP Q9H2X0
A	167	ALA	-	expression tag	UNP Q9H2X0
A	630	LEU	MET	variant	UNP Q9H2X0
A	653	LEU	-	expression tag	UNP Q9H2X0
A	654	VAL	-	expression tag	UNP Q9H2X0
A	655	PRO	-	expression tag	UNP Q9H2X0
A	656	ARG	-	expression tag	UNP Q9H2X0
A	657	GLY	-	expression tag	UNP Q9H2X0
A	658	SER	-	expression tag	UNP Q9H2X0
A	659	HIS	-	expression tag	UNP Q9H2X0
A	660	HIS	-	expression tag	UNP Q9H2X0
A	661	HIS	-	expression tag	UNP Q9H2X0
A	662	HIS	-	expression tag	UNP Q9H2X0
A	663	HIS	-	expression tag	UNP Q9H2X0
A	664	HIS	-	expression tag	UNP Q9H2X0

- Molecule 2 is an oligosaccharide called 2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-3,6-di-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	X	5	Total	C	H	N	O	S	0	0	0
			137	30	51	3	46	7			

- Molecule 3 is beta-D-mannopyranose (CCD ID: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
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	3	Total	Ca	0	0
			3	3		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		

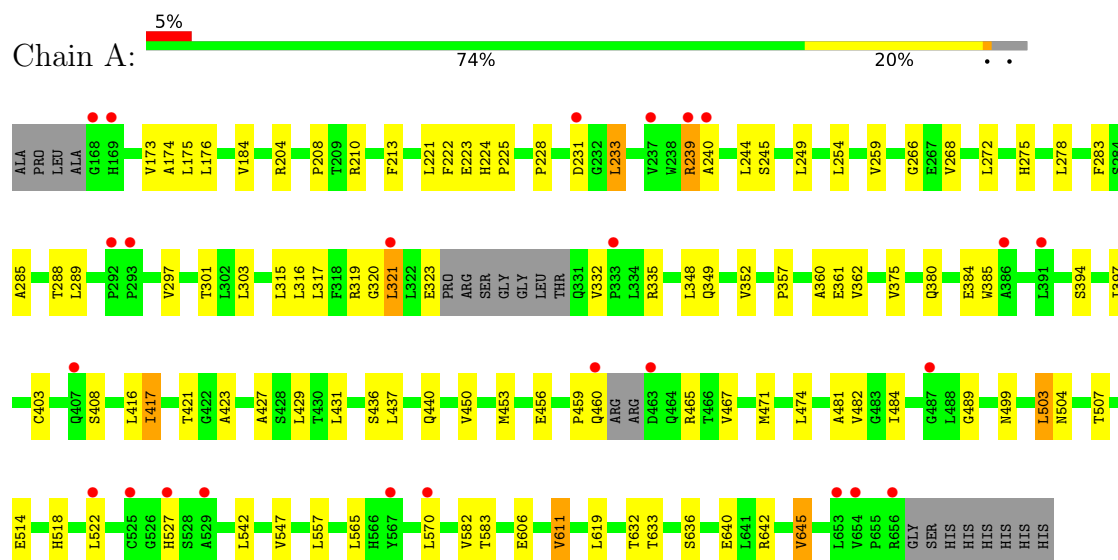
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	27	Total	O	0	0
			27	27		

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: Chordin



• Molecule 2: 2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-2-deoxy-3,6-di-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	172.77Å 172.77Å 129.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	74.81 – 2.92 74.81 – 2.92	Depositor EDS
% Data completeness (in resolution range)	99.9 (74.81-2.92) 92.1 (74.81-2.92)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.61 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.239 , 0.274 0.241 , 0.274	Depositor DCC
R_{free} test set	1300 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	101.6	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 85.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3860	wwPDB-VP
Average B, all atoms (Å ²)	132.0	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SO4, CA, SUS, BDP, IDS, BMA, SGN, GNS

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	0.13	0/3690	0.30	0/5020

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3610	0	3672	55	0
2	X	86	51	35	2	0
3	A	22	0	20	0	0
4	A	56	0	48	0	0
5	A	3	0	0	0	0
6	A	5	0	0	0	0
7	A	27	0	0	1	0
All	All	3809	51	3775	56	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 (56) 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:239[A]:ARG:HD3	1:A:240:ALA:H	1.39	0.86
1:A:421:THR:HG23	1:A:423:ALA:H	1.55	0.70
1:A:557:LEU:HD12	1:A:645:VAL:HG21	1.78	0.65
1:A:453:MET:HG3	1:A:471:MET:HB2	1.79	0.64
1:A:176:LEU:HB3	1:A:268:VAL:HB	1.78	0.64
1:A:315:LEU:HD23	1:A:360:ALA:HB2	1.82	0.62
1:A:259:VAL:HG12	1:A:266:GLY:HA2	1.81	0.61
1:A:429:LEU:HD23	1:A:437:LEU:HD21	1.83	0.60
1:A:474:LEU:HB2	1:A:481:ALA:HB2	1.84	0.60
1:A:565:LEU:HB3	1:A:611:VAL:HG23	1.84	0.59
1:A:239[A]:ARG:HD3	1:A:240:ALA:N	2.15	0.57
1:A:174:ALA:HB2	1:A:272:LEU:HD23	1.89	0.55
1:A:208:PRO:HG2	1:A:228:PRO:HG3	1.89	0.55
1:A:283:PHE:HB2	1:A:303:LEU:HB2	1.87	0.54
1:A:408:SER:HB3	1:A:427:ALA:HB3	1.89	0.54
1:A:221:LEU:HD21	1:A:245:SER:HB3	1.90	0.53
1:A:289:LEU:HD23	1:A:289:LEU:H	1.73	0.53
1:A:375:VAL:HG11	1:A:489:GLY:HA2	1.91	0.52
1:A:249:LEU:HD13	1:A:254:LEU:HD23	1.93	0.51
1:A:297:VAL:HA	1:A:320:GLY:HA3	1.92	0.50
1:A:301:THR:HB	1:A:316:LEU:HD13	1.95	0.49
1:A:175:LEU:O	1:A:319:ARG:NH1	2.46	0.48
1:A:285:ALA:HB2	1:A:397:ILE:HA	1.96	0.48
1:A:440:GLN:HG2	1:A:482:VAL:HG12	1.94	0.48
1:A:583:THR:OG1	1:A:632:THR:OG1	2.31	0.47
1:A:335:ARG:NH2	1:A:384:GLU:OE2	2.47	0.47
1:A:450:VAL:HA	1:A:507:THR:HG22	1.96	0.47
1:A:204:ARG:HD3	1:A:288:THR:HG21	1.96	0.47
1:A:317:LEU:HD22	1:A:357:PRO:HB2	1.96	0.47
1:A:210:ARG:HD3	1:A:225:PRO:HA	1.97	0.46
1:A:224:HIS:CE1	7:A:801:HOH:O	2.68	0.46
1:A:527:HIS:NE2	2:X:3:SUS:O6S	2.46	0.46
1:A:459:PRO:HG3	1:A:465:ARG:HB2	1.98	0.46
1:A:456:GLU:HG2	1:A:467:VAL:HG22	1.99	0.45
1:A:361:GLU:HG3	1:A:362:VAL:H	1.81	0.45
1:A:175:LEU:HD13	1:A:319:ARG:HD3	1.99	0.45
1:A:173:VAL:HB	1:A:278:LEU:HD11	1.99	0.44
1:A:233:LEU:HD21	1:A:403:CYS:SG	2.58	0.44
1:A:436:SER:HB3	1:A:484:ILE:HD11	1.98	0.44
1:A:210:ARG:HD2	1:A:223:GLU:HG2	1.99	0.44
1:A:421:THR:HG21	1:A:514:GLU:HG2	2.00	0.43
1:A:636:SER:HB2	1:A:640:GLU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:PHE:HB2	1:A:222:PHE:HB3	2.00	0.42
1:A:522:LEU:HD13	1:A:570:LEU:HD21	2.01	0.42
1:A:275:HIS:CE1	1:A:315:LEU:HG	2.54	0.42
1:A:321:LEU:HD21	1:A:385:TRP:HB2	2.02	0.42
1:A:499:ASN:O	1:A:518[A]:HIS:NE2	2.30	0.41
2:X:3:SUS:H6	2:X:4:BDP:O5	2.19	0.41
1:A:380:GLN:HE21	1:A:394:SER:HB2	1.85	0.41
1:A:471:MET:HE1	1:A:503:LEU:HD11	2.01	0.41
1:A:224:HIS:ND1	1:A:225:PRO:HD2	2.36	0.41
1:A:335:ARG:HA	1:A:349:GLN:HG2	2.03	0.41
1:A:417:ILE:H	1:A:417:ILE:HG13	1.74	0.41
1:A:453:MET:HA	1:A:504:ASN:O	2.20	0.41
1:A:633:THR:OG1	1:A:640:GLU:OE1	2.36	0.40
1:A:542:LEU:O	1:A:642:ARG:HD3	2.22	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	476/501 (95%)	451 (95%)	25 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	383/401 (96%)	361 (94%)	22 (6%)	18 48

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	VAL
1	A	231	ASP
1	A	233	LEU
1	A	239[A]	ARG
1	A	239[B]	ARG
1	A	244	LEU
1	A	321	LEU
1	A	323	GLU
1	A	332	VAL
1	A	348	LEU
1	A	352	VAL
1	A	416	LEU
1	A	417	ILE
1	A	431	LEU
1	A	460	GLN
1	A	503	LEU
1	A	547	VAL
1	A	582	VAL
1	A	606	GLU
1	A	611	VAL
1	A	619	LEU
1	A	645	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	440	GLN
1	A	460	GLN
1	A	621	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 ⓘ

5 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	SGN	X	1	2	19,20,20	0.58	0	24,31,31	1.61	3 (12%)
2	IDS	X	2	2	16,16,17	0.96	1 (6%)	17,24,26	1.68	3 (17%)
2	SUS	X	3	2	22,23,24	1.01	1 (4%)	24,36,38	1.56	3 (12%)
2	BDP	X	4	2	12,12,13	0.58	0	14,17,19	1.71	3 (21%)
2	GNS	X	5	2	14,15,16	0.65	0	17,22,24	1.41	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SGN	X	1	2	-	2/11/31/31	0/1/1/1
2	IDS	X	2	2	-	2/9/26/29	0/1/1/1
2	SUS	X	3	2	-	3/16/33/36	0/1/1/1
2	BDP	X	4	2	-	0/4/21/24	0/1/1/1
2	GNS	X	5	2	-	3/7/24/27	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	3	SUS	C3-C2	3.84	1.57	1.52
2	X	2	IDS	O2-C2	-2.72	1.43	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	3	SUS	O4-C4-C3	-4.19	98.83	109.94
2	X	1	SGN	O4-C4-C3	-4.09	100.89	110.35
2	X	2	IDS	C2-O2-S	4.02	123.16	117.91
2	X	4	BDP	O4-C4-C3	-3.70	101.79	110.35
2	X	1	SGN	C1-C2-N2	3.58	114.94	110.67
2	X	3	SUS	O5-C1-C2	-3.30	106.07	111.29
2	X	2	IDS	O5-C5-C6	3.29	117.12	106.31
2	X	5	GNS	O5-C1-C2	-3.20	106.23	111.29
2	X	3	SUS	C3-O3-S3	3.11	124.88	118.88
2	X	4	BDP	O2-C2-C1	3.07	115.44	109.15
2	X	1	SGN	O1S-S1-N2	-2.99	103.42	108.87
2	X	2	IDS	O4-C4-C3	-2.94	103.56	110.35
2	X	5	GNS	C4-C3-C2	2.89	115.26	111.02
2	X	4	BDP	O5-C1-C2	-2.84	106.38	110.77
2	X	5	GNS	O4-C4-C3	-2.02	105.68	110.35

There are no chirality outliers.

All (10) torsion outliers are listed below:

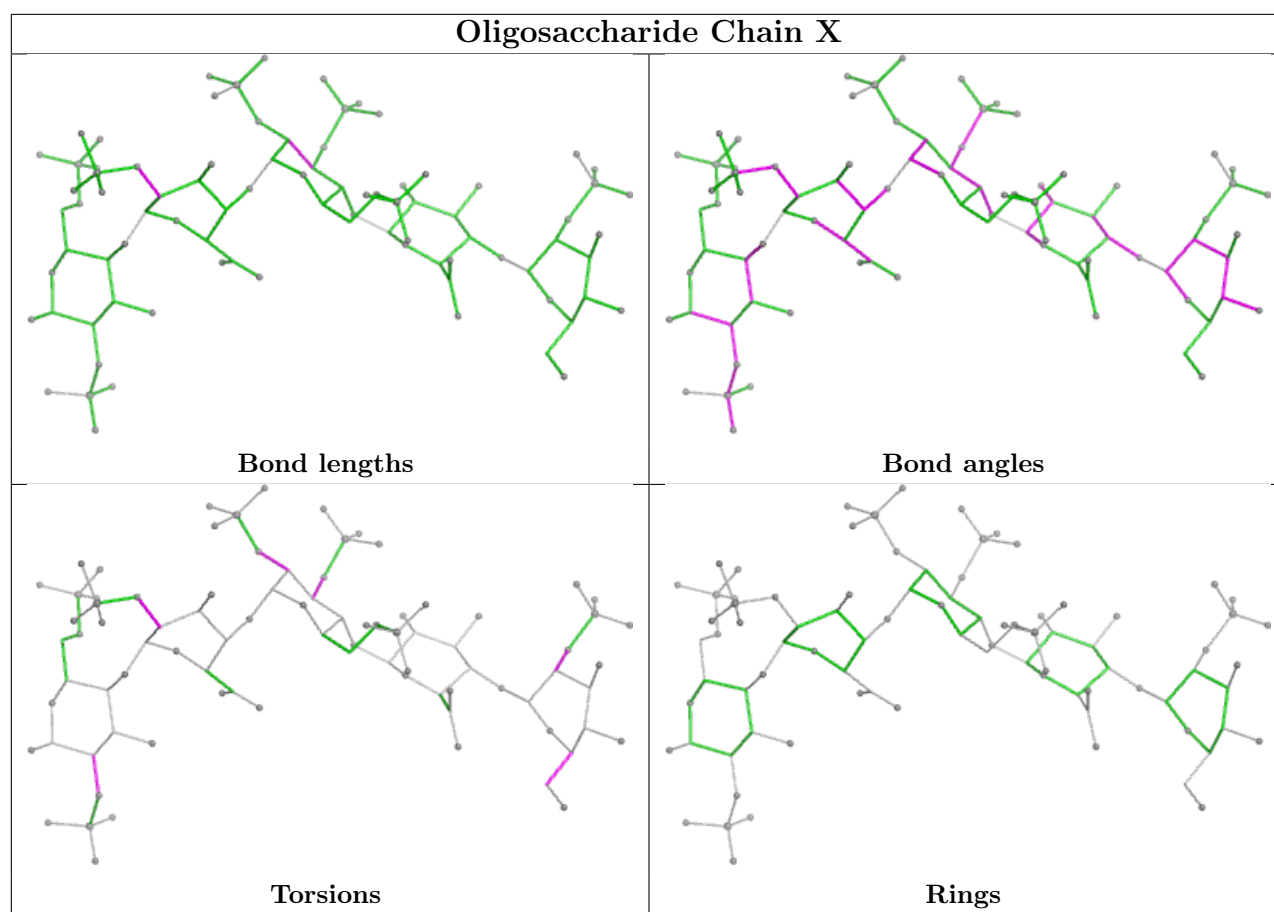
Mol	Chain	Res	Type	Atoms
2	X	1	SGN	C1-C2-N2-S1
2	X	1	SGN	C3-C2-N2-S1
2	X	3	SUS	C2-C3-O3-S3
2	X	3	SUS	C4-C3-O3-S3
2	X	5	GNS	C1-C2-N2-S1
2	X	5	GNS	C3-C2-N2-S1
2	X	5	GNS	O5-C5-C6-O6
2	X	2	IDS	C1-C2-O2-S
2	X	3	SUS	C1-C2-N2-S1
2	X	2	IDS	C3-C2-O2-S

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	X	4	BDP	1	0
2	X	3	SUS	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](#)

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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	704	4,3	14,14,15	0.39	0	17,19,21	0.62	0
3	BMA	A	702	4	11,11,12	0.28	0	15,15,17	0.61	0
4	NAG	A	703	1,4	14,14,15	0.41	0	17,19,21	0.48	0
3	BMA	A	701	4	11,11,12	0.31	0	15,15,17	0.52	0
6	SO4	A	710	-	4,4,4	0.41	0	6,6,6	0.05	0
4	NAG	A	705	1,4	14,14,15	0.38	0	17,19,21	0.78	0
4	NAG	A	706	4,3	14,14,15	0.38	0	17,19,21	0.51	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
4	NAG	A	704	4,3	-	2/6/23/26	0/1/1/1
3	BMA	A	702	4	-	0/2/19/22	0/1/1/1
4	NAG	A	703	1,4	-	0/6/23/26	0/1/1/1
3	BMA	A	701	4	-	0/2/19/22	0/1/1/1
4	NAG	A	705	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	706	4,3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	706	NAG	C8-C7-N2-C2
4	A	706	NAG	O7-C7-N2-C2
4	A	704	NAG	C8-C7-N2-C2
4	A	704	NAG	O7-C7-N2-C2
4	A	706	NAG	O5-C5-C6-O6
4	A	706	NAG	C4-C5-C6-O6

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	480/501 (95%)	0.50	25 (5%)	33 26	48, 124, 183, 211	2 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	529	ALA	3.8
1	A	463	ASP	3.5
1	A	237	VAL	3.3
1	A	391	LEU	3.2
1	A	239[A]	ARG	3.0
1	A	527	HIS	2.8
1	A	321	LEU	2.7
1	A	293	PRO	2.7
1	A	168	GLY	2.6
1	A	653	LEU	2.6
1	A	169	HIS	2.5
1	A	487	GLY	2.5
1	A	240	ALA	2.4
1	A	407	GLN	2.3
1	A	292	PRO	2.3
1	A	231	ASP	2.2
1	A	525	CYS	2.2
1	A	460	GLN	2.2
1	A	654	VAL	2.2
1	A	333	PRO	2.1
1	A	522	LEU	2.1
1	A	570	LEU	2.1
1	A	567	TYR	2.1
1	A	386	ALA	2.1
1	A	656	ARG	2.0

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

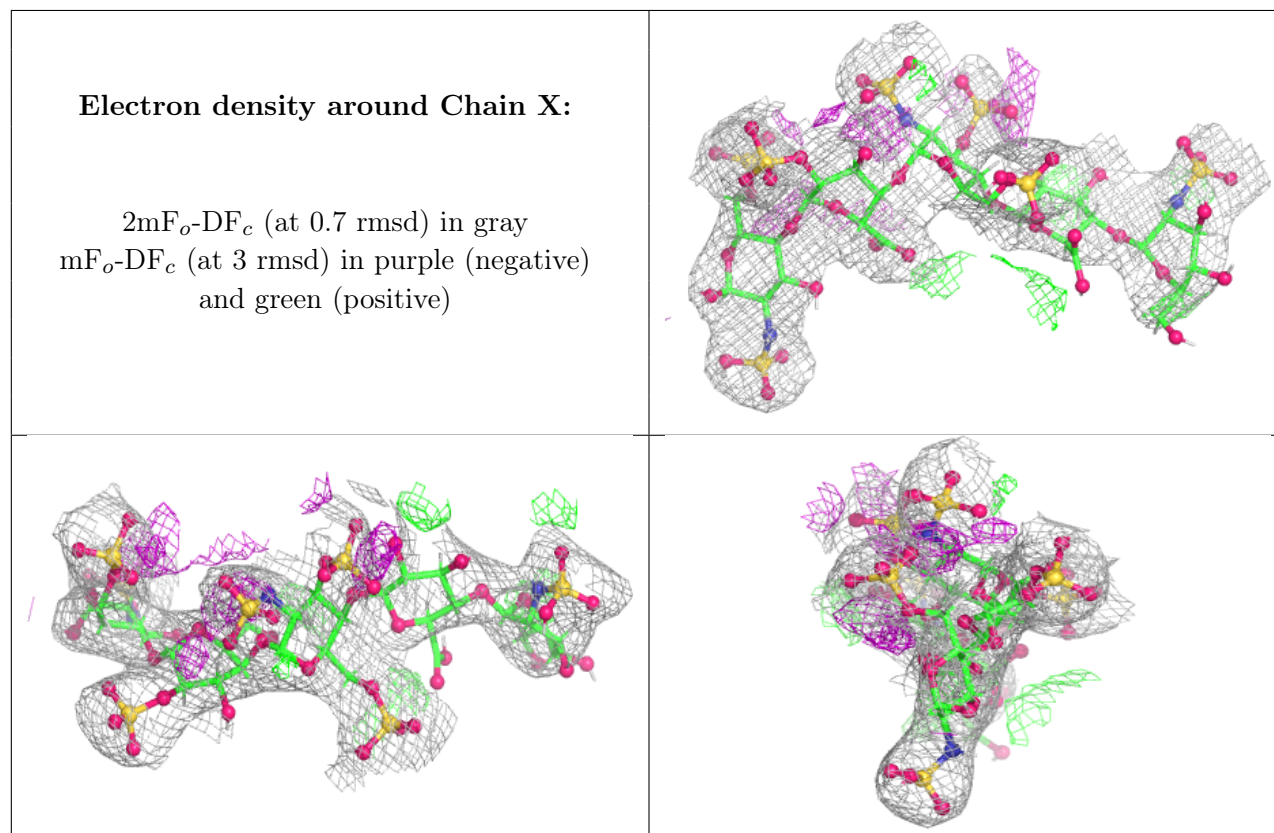
There are no non-standard protein/DNA/RNA residues in this entry.

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(\AA^2)	Q<0.9
2	SGN	X	1	20/20	-	-	99,141,170,172	32
2	IDS	X	2	16/17	-	-	104,129,147,162	24
2	SUS	X	3	23/24	-	-	119,147,178,192	34
2	BDP	X	4	12/13	-	-	147,177,197,224	20
2	GNS	X	5	15/16	-	-	129,195,231,239	27

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(Å ²)	Q<0.9
3	BMA	A	702	11/12	0.13	0.15	162,171,179,184	0
3	BMA	A	701	11/12	0.14	0.13	219,225,234,236	0
4	NAG	A	706	14/15	0.35	0.12	199,227,240,242	0
4	NAG	A	705	14/15	0.44	0.12	180,203,211,219	0
4	NAG	A	704	14/15	0.56	0.16	141,158,178,179	0
6	SO4	A	710	5/5	0.69	0.08	168,169,190,216	0
5	CA	A	709	1/1	0.87	0.23	154,154,154,154	0
5	CA	A	707	1/1	0.89	0.18	154,154,154,154	0
4	NAG	A	703	14/15	0.91	0.09	133,153,162,164	0
5	CA	A	708	1/1	0.92	0.16	154,154,154,154	0

6.5 Other polymers [i](#)

There are no such residues in this entry.