



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:32 PM UTC

PDB ID : 8V58 / pdb_00008v58
Title : Complex of murine cathepsin K with bound heparan sulfate 12mer
Authors : Pedersen, L.C.; Xu, D.; Krahn, J.M.
Deposited on : 2023-11-30
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

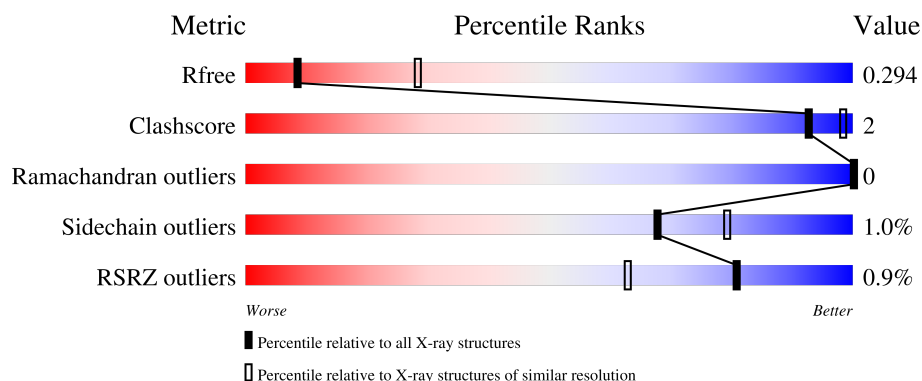
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	217	95%
1	B	217	2% 92% 6%
2	C	8	12% 88%
3	D	9	11% 89%

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
3	SGN	D	1	-	-	-	X

2 Entry composition [i](#)

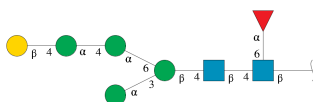
There are 6 unique types of molecules in this entry. The entry contains 6509 atoms, of which 3087 are hydrogens and 0 are deuteriums.

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 Cathepsin K.

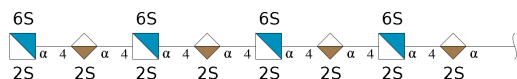
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	215	Total	C	H	N	O	S	0	0	0
			3123	1008	1510	279	314	12			
1	B	215	Total	C	H	N	O	S	0	0	0
			2967	974	1411	262	308	12			

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-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
2	C	8	Total	C	H	N	O	0	0	0
			180	52	87	2	39			

- Molecule 3 is an oligosaccharide called 2-deoxy-6-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-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-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-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid.



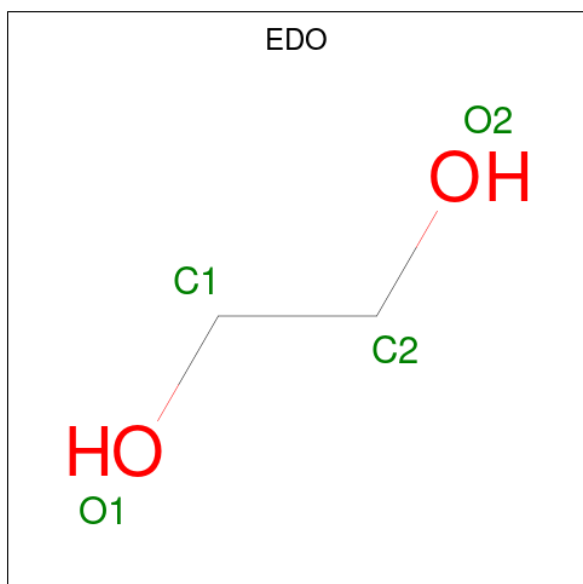
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	9	Total	C	H	N	O	S	0	0	1
			201	48	60	4	77	12			

- 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	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			10	2	6	2		

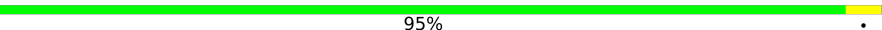
- Molecule 6 is water.

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

3 Residue-property plots [i](#)

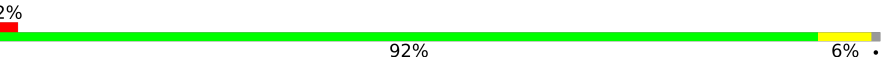
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

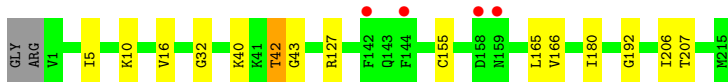
- Molecule 1: Cathepsin K

Chain A:  95%

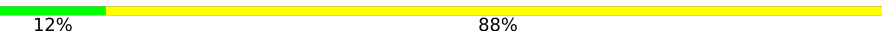


- Molecule 1: Cathepsin K

Chain B:  2% 92% 6%

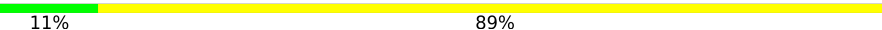


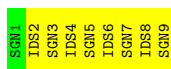
- Molecule 2: beta-D-galactopyranose-(1-4)-alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  12% 88%



- Molecule 3: 2-deoxy-6-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-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-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-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid

Chain D:  11% 89%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	111.89Å 111.89Å 116.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.87 – 3.10 19.87 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.87-3.10) 97.5 (19.87-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 3.09Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.236 , 0.293 0.237 , 0.294	Depositor DCC
R_{free} test set	691 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	92.5	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,l,k 0.016 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6509	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: BMA, GAL, FUC, MAN, IDS, NAG, EDO, SGN

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	0.40	0/1648	0.65	0/2233
1	B	0.30	0/1589	0.61	1/2160 (0.0%)
All	All	0.35	0/3237	0.63	1/4393 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	42	THR	N-CA-C	-5.32	99.46	110.80

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	1613	1510	1512	3	0
1	B	1556	1411	1419	7	0
2	C	93	87	79	0	0
3	D	141	60	45	0	0
4	B	14	13	13	0	0
5	B	4	6	6	0	0
6	B	1	0	0	0	0
All	All	3422	3087	3074	10	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 2.

All (10) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ILE:HG23	1:B:207:THR:HG23	1.81	0.62
1:B:32:GLY:HA3	1:B:165:LEU:HD22	1.87	0.56
1:B:40:LYS:NZ	1:B:127:ARG:O	2.41	0.54
1:B:42:THR:HG22	1:B:43:GLY:H	1.72	0.53
1:A:206:ILE:HG23	1:A:207:THR:HG23	1.92	0.52
1:B:166:VAL:HG22	1:B:180:ILE:CD1	2.42	0.50
1:A:32:GLY:HA3	1:A:165:LEU:HD22	1.92	0.50
1:B:16:VAL:HG21	1:B:192:GLY:HA3	1.97	0.47
1:A:134:SER:HB3	1:A:160:VAL:HG21	1.98	0.44
1:B:5:ILE:HD11	1:B:10:LYS:HD2	1.99	0.44

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	213/217 (98%)	203 (95%)	10 (5%)	0	100	100
1	B	213/217 (98%)	202 (95%)	11 (5%)	0	100	100
All	All	426/434 (98%)	405 (95%)	21 (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	163/172 (95%)	161 (99%)	2 (1%)	63	78
1	B	151/172 (88%)	150 (99%)	1 (1%)	76	82
All	All	314/344 (91%)	311 (99%)	3 (1%)	68	79

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

Mol	Chain	Res	Type
1	A	123	ARG
1	A	153	GLU
1	B	155	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	143	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 ⓘ

Of 17 monosaccharides modelled in this entry, 16 were used 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
2	NAG	C	1	2,1	14,14,15	0.66	0	17,19,21	0.75	0
2	NAG	C	2	2	14,14,15	1.05	1 (7%)	17,19,21	1.11	1 (5%)
2	BMA	C	3	2	11,11,12	1.46	2 (18%)	15,15,17	1.87	2 (13%)
2	MAN	C	4	2	11,11,12	1.45	2 (18%)	15,15,17	1.82	4 (26%)
2	MAN	C	5	2	11,11,12	0.74	0	15,15,17	1.19	2 (13%)
2	GAL	C	6	2	11,11,12	1.16	2 (18%)	15,15,17	1.10	0
2	MAN	C	7	2	11,11,12	0.99	1 (9%)	15,15,17	2.44	4 (26%)
2	FUC	C	8	2	10,10,11	1.35	2 (20%)	14,14,16	1.48	4 (28%)
3	IDS	D	2	3	16,16,17	0.99	1 (6%)	16,24,26	1.31	3 (18%)
3	SGN	D	3	3	19,19,20	0.94	1 (5%)	23,29,31	2.04	4 (17%)
3	IDS	D	4	3	16,16,17	1.08	1 (6%)	16,24,26	1.67	4 (25%)
3	SGN	D	5	3	19,19,20	0.90	0	23,29,31	2.54	6 (26%)
3	IDS	D	6	3	16,16,17	0.92	0	16,24,26	2.03	4 (25%)
3	SGN	D	7	3	19,19,20	1.05	2 (10%)	23,29,31	2.04	5 (21%)
3	IDS	D	8	3	16,16,17	0.86	0	16,24,26	1.81	3 (18%)
3	SGN	D	9	3	19,19,20	0.80	0	23,29,31	1.51	3 (13%)

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	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	1/1/1/1
2	MAN	C	4	2	-	1/2/19/22	0/1/1/1
2	MAN	C	5	2	-	1/2/19/22	1/1/1/1
2	GAL	C	6	2	-	0/2/19/22	0/1/1/1
2	MAN	C	7	2	-	2/2/19/22	0/1/1/1
2	FUC	C	8	2	-	-	0/1/1/1
3	IDS	D	2	3	-	0/9/26/29	0/1/1/1
3	SGN	D	3	3	-	2/11/28/31	0/1/1/1
3	IDS	D	4	3	-	3/9/26/29	0/1/1/1
3	SGN	D	5	3	-	6/11/28/31	0/1/1/1
3	IDS	D	6	3	-	1/9/26/29	0/1/1/1
3	SGN	D	7	3	-	3/11/28/31	0/1/1/1
3	IDS	D	8	3	-	5/9/26/29	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SGN	D	9	3	-	2/11/28/31	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	O5-C1	-3.73	1.37	1.43
2	C	3	BMA	C4-C5	3.14	1.59	1.53
2	C	4	MAN	C1-C2	2.86	1.59	1.52
2	C	8	FUC	C1-C2	2.56	1.58	1.52
2	C	6	GAL	O5-C1	-2.52	1.39	1.43
3	D	2	IDS	O2-S	-2.44	1.50	1.57
2	C	6	GAL	C4-C5	2.41	1.58	1.53
2	C	3	BMA	O5-C5	2.32	1.47	1.43
2	C	4	MAN	C4-C5	2.29	1.57	1.53
2	C	7	MAN	C1-C2	2.23	1.57	1.52
2	C	8	FUC	C4-C3	2.21	1.58	1.52
3	D	7	SGN	S1-N2	2.09	1.62	1.59
3	D	7	SGN	O2S-S1	2.06	1.44	1.42
3	D	4	IDS	O4-C4	2.01	1.47	1.43
3	D	3	SGN	O2S-S1	2.01	1.44	1.42

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	7	MAN	C1-O5-C5	7.55	122.30	112.19
2	C	3	BMA	C1-O5-C5	6.28	120.61	112.19
3	D	5	SGN	O1S-S1-O2S	-6.13	106.71	120.36
3	D	5	SGN	O6-C6-C5	6.03	118.31	107.57
3	D	7	SGN	O1S-S1-O2S	-6.01	107.00	120.36
3	D	6	IDS	O2-C2-C3	-5.99	98.58	106.95
3	D	3	SGN	O4-C4-C3	-5.89	96.49	110.38
3	D	3	SGN	O1S-S1-O2S	-5.06	109.10	120.36
3	D	9	SGN	O1S-S1-O2S	-4.93	109.40	120.36
3	D	5	SGN	C4-C3-C2	-4.82	103.96	111.02
3	D	8	IDS	O4-C4-C3	4.40	120.75	110.38
3	D	7	SGN	O6-C6-C5	4.28	115.19	107.57
3	D	5	SGN	O4-C4-C5	4.23	119.74	109.32
2	C	4	MAN	C1-O5-C5	3.98	117.52	112.19
2	C	2	NAG	C1-O5-C5	3.90	117.41	112.19
3	D	4	IDS	O3-C3-C2	-3.44	100.86	109.32
3	D	7	SGN	O4-C4-C3	3.42	118.44	110.38
3	D	5	SGN	C6-C5-C4	3.38	119.16	112.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	8	IDS	O2-C2-C3	3.29	111.55	106.95
3	D	4	IDS	O3S-S-O2	3.27	113.88	106.37
3	D	6	IDS	O4-C4-C5	3.19	117.05	109.76
3	D	2	IDS	O2-C2-C3	2.94	111.06	106.95
2	C	7	MAN	O5-C1-C2	2.92	117.75	110.79
3	D	6	IDS	O4-C4-C3	-2.79	103.80	110.38
2	C	4	MAN	O2-C2-C3	-2.75	104.46	110.15
3	D	8	IDS	O5-C5-C6	2.73	116.35	106.59
2	C	7	MAN	O2-C2-C3	-2.70	104.56	110.15
3	D	3	SGN	O6-C6-C5	2.61	112.23	107.57
2	C	8	FUC	O5-C5-C4	2.59	114.21	109.55
2	C	8	FUC	C1-O5-C5	2.59	119.07	112.97
2	C	4	MAN	O4-C4-C3	-2.57	104.32	110.38
2	C	8	FUC	C3-C4-C5	2.56	113.70	109.81
2	C	5	MAN	C1-O5-C5	2.56	115.62	112.19
3	D	5	SGN	O5-C5-C6	-2.52	102.14	107.59
3	D	4	IDS	C4-C3-C2	2.50	114.76	110.23
3	D	7	SGN	C4-C3-C2	-2.46	107.41	111.02
2	C	7	MAN	C1-C2-C3	2.42	113.17	109.64
3	D	6	IDS	O5-C5-C6	2.42	115.23	106.59
3	D	9	SGN	O5-C1-C2	-2.42	107.55	111.29
3	D	2	IDS	O5-C5-C6	2.40	115.14	106.59
3	D	7	SGN	O2S-S1-N2	2.36	112.84	108.88
2	C	5	MAN	O2-C2-C3	-2.28	105.42	110.15
3	D	9	SGN	C1-O5-C5	2.16	115.09	112.19
3	D	2	IDS	O6B-C6-C5	2.13	121.32	113.64
3	D	4	IDS	O2-C2-C3	2.07	109.85	106.95
2	C	8	FUC	C1-C2-C3	2.07	112.65	109.64
2	C	4	MAN	C6-C5-C4	2.06	118.09	113.02
2	C	3	BMA	C3-C4-C5	2.02	113.89	110.23
3	D	3	SGN	C6-C5-C4	2.01	116.29	112.07

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	3	SGN	C4-C5-C6-O6
3	D	3	SGN	O5-C5-C6-O6
3	D	4	IDS	C3-C2-O2-S
3	D	4	IDS	C4-C5-C6-O6A
3	D	4	IDS	C4-C5-C6-O6B
3	D	5	SGN	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

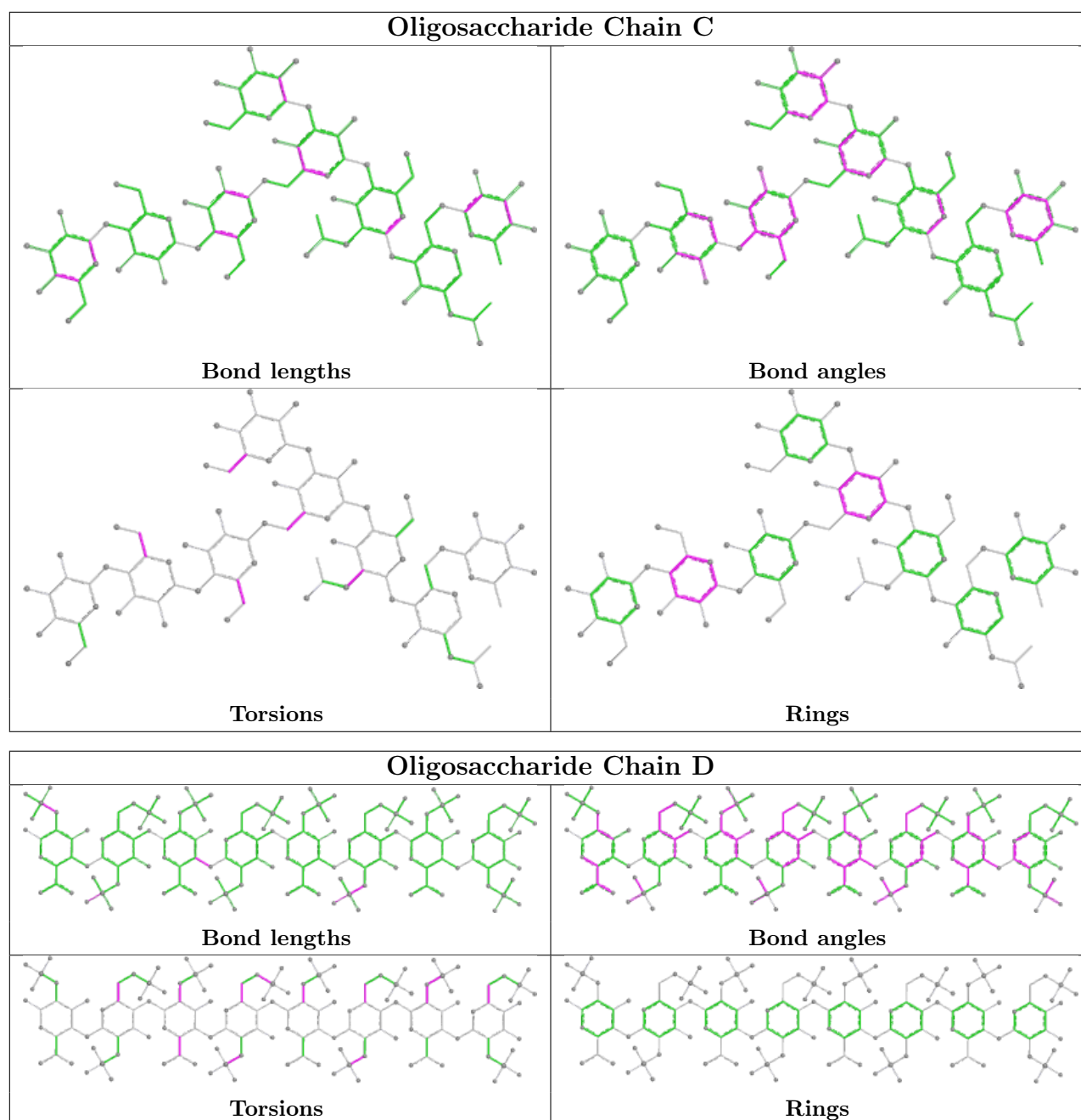
Mol	Chain	Res	Type	Atoms
3	D	5	SGN	O5-C5-C6-O6
3	D	6	IDS	C1-C2-O2-S
3	D	7	SGN	C4-C5-C6-O6
3	D	7	SGN	O5-C5-C6-O6
3	D	7	SGN	C2-N2-S1-O1S
3	D	8	IDS	C1-C2-O2-S
3	D	8	IDS	C3-C2-O2-S
3	D	9	SGN	C4-C5-C6-O6
3	D	9	SGN	O5-C5-C6-O6
2	C	7	MAN	C4-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
3	D	5	SGN	C6-O6-S2-O5S
3	D	8	IDS	C2-O2-S-O1S
2	C	4	MAN	O5-C5-C6-O6
3	D	8	IDS	C2-O2-S-O2S
3	D	8	IDS	C2-O2-S-O3S
2	C	5	MAN	O5-C5-C6-O6
3	D	5	SGN	C6-O6-S2-O4S
2	C	7	MAN	O5-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
3	D	5	SGN	C2-N2-S1-O1S
3	D	5	SGN	C6-O6-S2-O6S
2	C	2	NAG	C1-C2-N2-C7

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	BMA	C1-C2-C3-C4-C5-O5
2	C	5	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

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



5.6 Ligand geometry [i](#)

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	EDO	B	402	-	3,3,3	0.47	0	2,2,2	0.31	0
4	NAG	B	401	1	14,14,15	0.32	0	17,19,21	0.93	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	402	-	-	1/1/1/1	-
4	NAG	B	401	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	NAG	C2-N2-C7	2.65	126.46	122.90

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	401	NAG	C8-C7-N2-C2
4	B	401	NAG	O7-C7-N2-C2
5	B	402	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	215/217 (99%)	-0.12	0	100 100	92, 108, 125, 137	0
1	B	215/217 (99%)	-0.04	4 (1%)	66 45	110, 139, 168, 178	0
All	All	430/434 (99%)	-0.08	4 (0%)	81 63	92, 121, 162, 178	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	144	PHE	2.5
1	B	159	ASN	2.4
1	B	158	ASP	2.1
1	B	142	PHE	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	SGN	D	1	1/20	-0.62	0.41	100,100,100,100	1
2	MAN	C	7	11/12	0.48	0.18	123,134,159,161	22
2	GAL	C	6	11/12	0.66	0.12	131,145,167,175	0
3	IDS	D	2	16/17	0.66	0.11	105,111,135,138	22
3	SGN	D	9	19/20	0.70	0.11	101,112,132,137	28

Continued on next page...

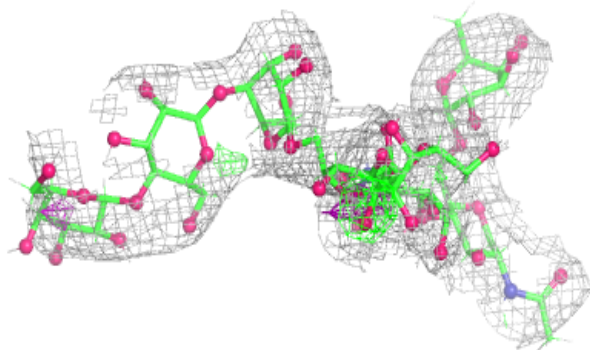
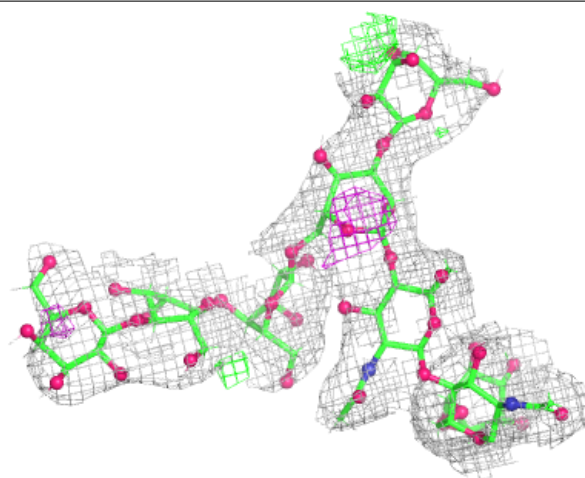
Continued from previous page...

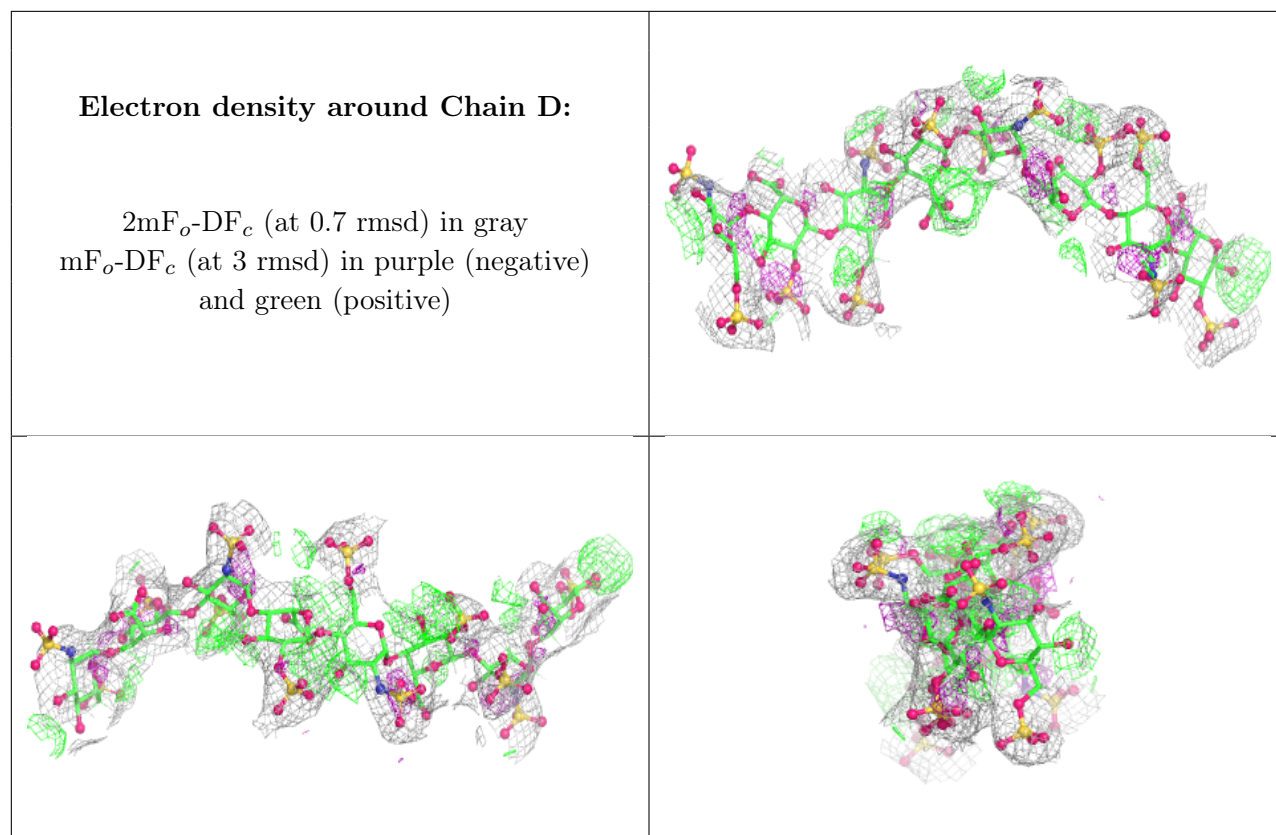
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	IDS	D	4	16/17	0.71	0.18	99,107,132,134	22
3	IDS	D	6	16/17	0.74	0.16	99,108,123,131	22
3	IDS	D	8	16/17	0.75	0.10	102,109,132,138	22
2	BMA	C	3	11/12	0.79	0.14	117,132,152,159	0
2	MAN	C	4	11/12	0.79	0.09	112,134,155,168	0
3	SGN	D	3	19/20	0.80	0.11	99,112,137,140	28
2	MAN	C	5	11/12	0.81	0.09	118,131,154,158	0
3	SGN	D	7	19/20	0.83	0.12	99,106,129,134	28
3	SGN	D	5	19/20	0.87	0.12	99,103,125,132	28
2	NAG	C	1	14/15	0.88	0.09	100,112,127,135	0
2	FUC	C	8	10/11	0.89	0.07	98,114,129,138	0
2	NAG	C	2	14/15	0.91	0.09	104,119,141,145	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](#)

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
5	EDO	B	402	4/4	0.66	0.22	100,121,133,141	0
4	NAG	B	401	14/15	0.68	0.09	117,137,163,165	0

6.5 Other polymers [i](#)

There are no such residues in this entry.