Full wwPDB X-ray Structure Validation Report ⓘ

Jul 27, 2022 – 10:17 am BST

PDB ID	:	7PR7
Title	:	Crystal structure of human heparanase in complex with covalent inhibitor VL166
Authors	:	Wu, L.; Armstrong, Z.; Davies, G.J.
Deposited on	:	2021-09-21
Resolution	:	1.52 Å(reported)

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

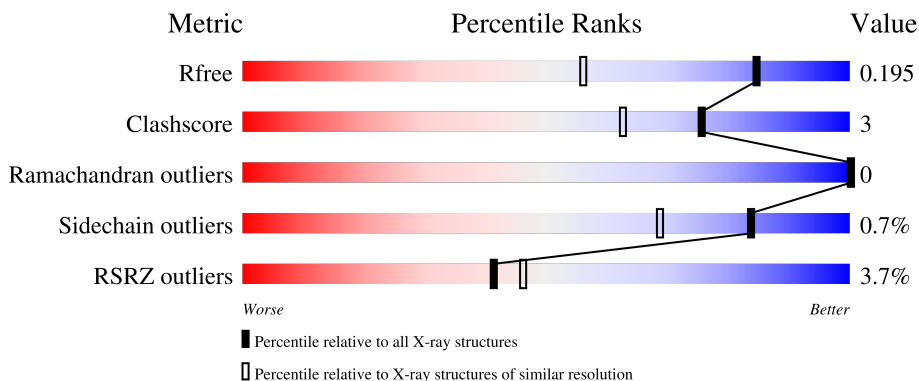|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 1.52 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	Percentile Ranks	Value
Rfree		0.195
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		0.7%
RSRZ outliers		3.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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 <=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	385	3% 93% 7%
2	B	74	5% 91% 9%
3	C	2	100%
4	D	2	50% 50%

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
6	EDO	A	605	-	X	-	-

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 7993 atoms, of which 3865 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 Heparanase 50 kDa subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	385	Total 6212	C 1993	H 3125	N 526	O 556	S 12	89	4	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	159	LYS	-	expression tag	UNP Q9Y251
A	307	ARG	LYS	variant	UNP Q9Y251

- Molecule 2 is a protein called Heparanase 8 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	74	Total 1204	C 388	H 609	N 97	O 110	14	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	2	Total 48	C 14	H 24	N 1	O 9	5	0	0

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-(2R,3S,5R,6R)-2,3,4,5,6-pentakis(oxidanyl)cyclohexane-1-carboxylic acid.
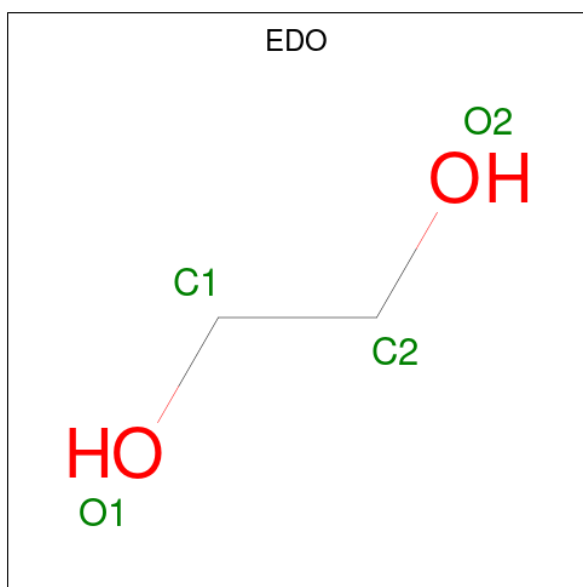
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	2	Total 50	C 15	H 23	N 1	O 11	6	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
5	A	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
5	A	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 1	Cl 1	0	0

- Molecule 8 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	276	Total 276	O 276	0	0
8	B	48	Total 48	O 48	0	0

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.
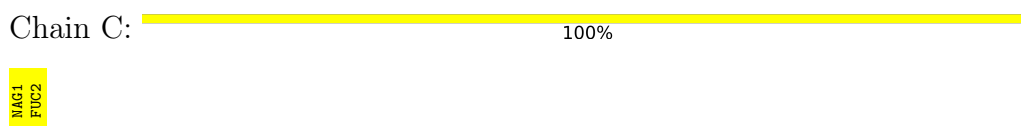
• Molecule 1: Heparanase 50 kDa subunit

Chain A:
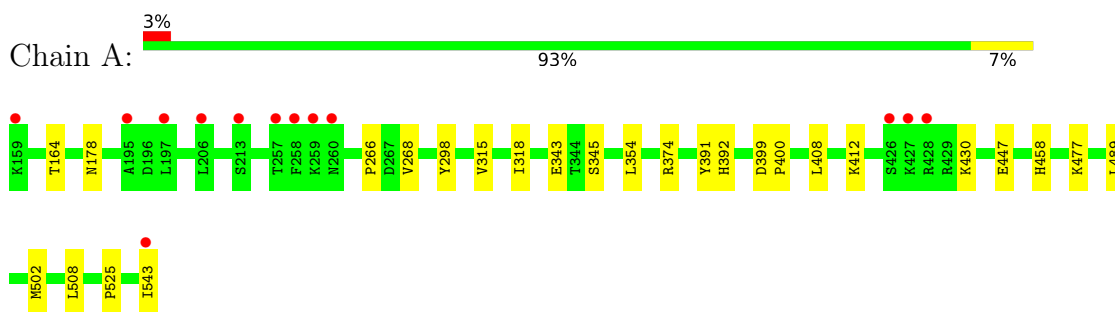
• Molecule 2: Heparanase 8 kDa subunit

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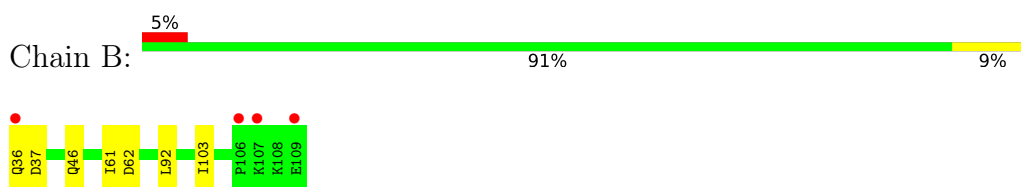
• Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 4: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-(2R,3S,5R,6R)-2,3,4,5,6-pentakis (oxidanyl)cyclohexane-1-carboxylic acid

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	46.40Å 71.01Å 79.23Å 90.00° 95.14° 90.00°	Depositor
Resolution (Å)	46.26 – 1.52 46.21 – 1.52	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.26-1.52) 97.8 (46.21-1.52)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 1.52Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.166 , 0.188 0.175 , 0.195	Depositor DCC
R_{free} test set	3872 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	7993	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \|L\| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 8I4, CL, NDG, EDO, NAG, FUC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.76	1/3162 (0.0%)	0.87	1/4276 (0.0%)
2	B	0.75	0/609	0.86	0/826
All	All	0.76	1/3771 (0.0%)	0.87	1/5102 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	343	GLU	CD-OE2	11.41	1.38	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	ARG	NE-CZ-NH2	-9.90	115.35	120.30

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	3087	3125	3111	17	0
2	B	595	609	604	8	0
3	C	24	24	22	0	0
4	D	27	23	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	42	42	39	0	0
6	A	28	42	41	5	0
7	A	1	0	0	0	0
8	A	276	0	0	1	0
8	B	48	0	0	4	0
All	All	4128	3865	3829	24	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 3.

All (24) 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:298[B]:TYR:CE1	1:A:345[B]:SER:OG	1.72	1.43
1:A:298[B]:TYR:HE1	1:A:345[B]:SER:OG	1.12	1.11
1:A:298[B]:TYR:CD1	1:A:345[B]:SER:OG	2.34	0.79
2:B:46[B]:GLN:NE2	8:B:201:HOH:O	2.00	0.79
1:A:489:LEU:HG	6:A:605:EDO:H11	1.71	0.72
2:B:61:ILE:HG12	2:B:92:LEU:HD11	1.79	0.65
1:A:315:VAL:O	1:A:318:ILE:HG12	2.00	0.62
2:B:37:ASP:N	8:B:202:HOH:O	2.14	0.60
1:A:502[A]:MET:SD	1:A:508:LEU:HD23	2.45	0.57
1:A:400:PRO:HD3	1:A:502[B]:MET:HE2	1.88	0.56
1:A:447:GLU:HB3	1:A:543:ILE:O	2.06	0.55
1:A:430:LYS:HE3	1:A:458:HIS:CE1	2.42	0.55
1:A:399:ASP:HB3	6:A:606:EDO:C1	2.39	0.53
2:B:62:ASP:HB2	4:D:2:NDG:H8C3	1.91	0.52
1:A:525:PRO:HG3	6:A:609:EDO:H11	1.90	0.52
1:A:164:THR:HA	2:B:103:ILE:O	2.10	0.51
2:B:37:ASP:CA	8:B:202:HOH:O	2.59	0.48
2:B:37:ASP:HA	8:B:202:HOH:O	2.15	0.45
1:A:477:LYS:HZ1	6:A:609:EDO:H12	1.82	0.44
2:B:36:GLN:O	2:B:36:GLN:HG2	2.19	0.43
1:A:408:LEU:O	1:A:412:LYS:HG2	2.20	0.41
1:A:266:PRO:HG2	1:A:268:VAL:HG13	2.02	0.41
1:A:477:LYS:NZ	6:A:609:EDO:H21	2.36	0.41
1:A:178:ASN:ND2	8:A:704:HOH:O	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	387/385 (100%)	377 (97%)	10 (3%)	0	100	100
2	B	73/74 (99%)	73 (100%)	0	0	100	100
All	All	460/459 (100%)	450 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	338/335 (101%)	335 (99%)	3 (1%)	78	60
2	B	67/66 (102%)	67 (100%)	0	100	100
All	All	405/401 (101%)	402 (99%)	3 (1%)	84	69

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

Mol	Chain	Res	Type
1	A	354	LEU
1	A	391	TYR
1	A	392	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	472	ASN

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 ⓘ

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	NAG	C	1	1,3	14,14,15	0.88	0	17,19,21	1.81	3 (17%)
3	FUC	C	2	3	10,10,11	1.18	1 (10%)	14,14,16	1.59	4 (28%)
4	8I4	D	1	4,1	13,13,14	1.42	4 (30%)	17,19,21	1.67	6 (35%)
4	NDG	D	2	4	14,14,15	1.10	1 (7%)	17,19,21	1.35	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
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	FUC	C	2	3	-	-	0/1/1/1
4	8I4	D	1	4,1	-	2/4/24/28	0/1/1/1
4	NDG	D	2	4	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	8I4	C1-C2	2.45	1.57	1.52
4	D	2	NDG	O5-C5	-2.36	1.38	1.43
3	C	2	FUC	O5-C5	2.24	1.48	1.43
4	D	1	8I4	O3-C3	2.12	1.48	1.43
4	D	1	8I4	O6A-C6	2.03	1.28	1.22
4	D	1	8I4	O6B-C6	-2.03	1.23	1.30

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1	NAG	O5-C1-C2	-5.65	102.36	111.29
4	D	1	8I4	O6B-C6-O6A	-3.05	117.16	124.09
3	C	2	FUC	C6-C5-C4	-2.88	107.75	113.07
4	D	1	8I4	O4-C4-C5	-2.84	103.47	109.68
3	C	1	NAG	C1-O5-C5	2.70	115.85	112.19
3	C	2	FUC	O4-C4-C3	-2.57	104.40	110.35
4	D	1	8I4	O6B-C6-C5	2.46	121.30	114.01
3	C	1	NAG	O5-C5-C6	2.41	110.99	107.20
3	C	2	FUC	O5-C5-C6	2.41	112.50	107.33
4	D	1	8I4	O7-C7-C1	-2.36	104.10	109.94
4	D	1	8I4	C1-C2-C3	-2.24	107.43	110.69
4	D	2	NDG	C1-O5-C5	2.21	115.19	112.19
4	D	2	NDG	O4-C4-C3	-2.16	105.35	110.35
3	C	2	FUC	O3-C3-C4	-2.14	105.41	110.35
4	D	2	NDG	O4-C4-C5	2.11	114.55	109.30
4	D	1	8I4	O4-C4-C3	2.03	115.04	110.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	8I4	C4-C5-C6-O6A
4	D	1	8I4	C4-C5-C6-O6B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2	NDG	1	0

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

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings
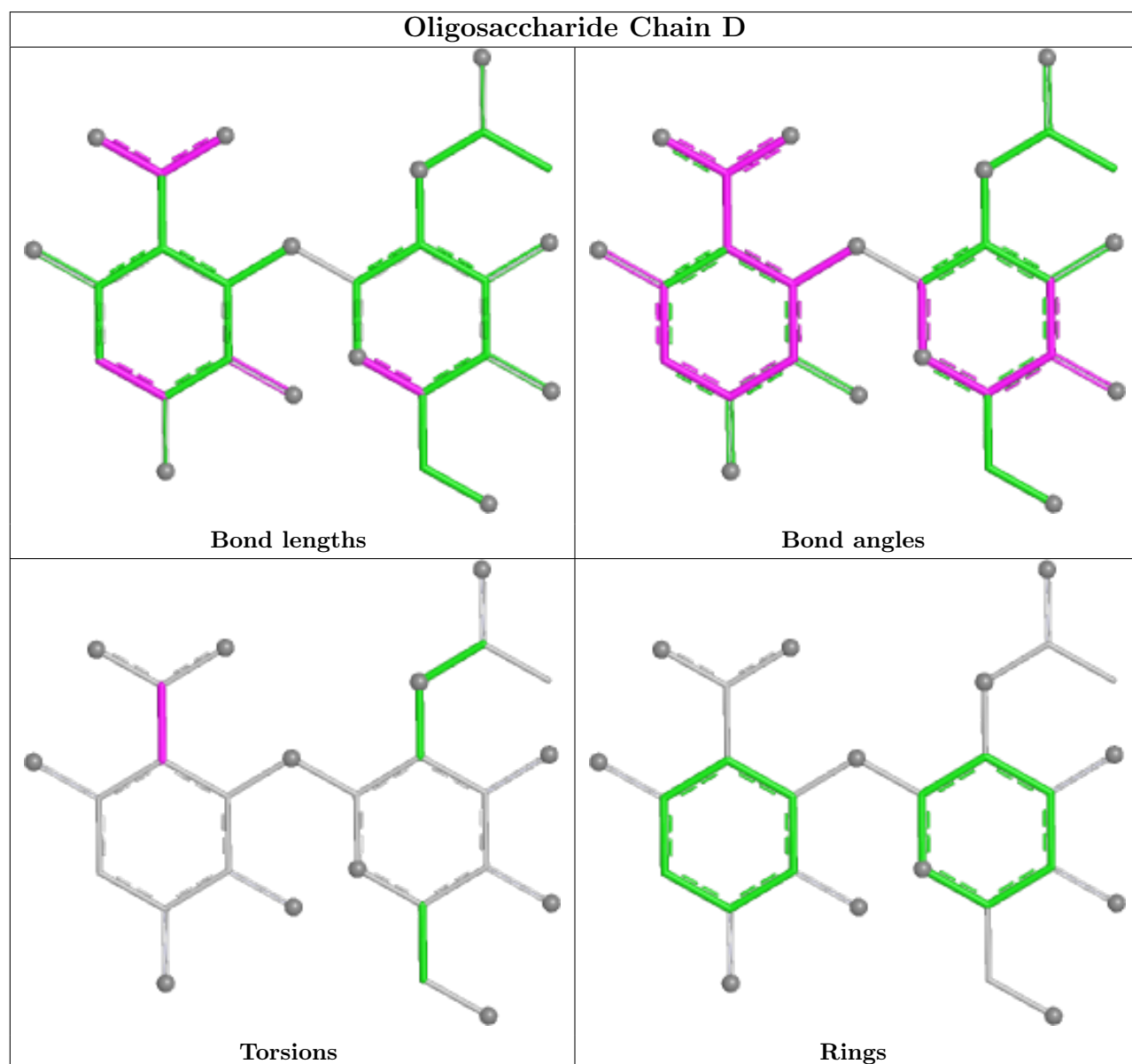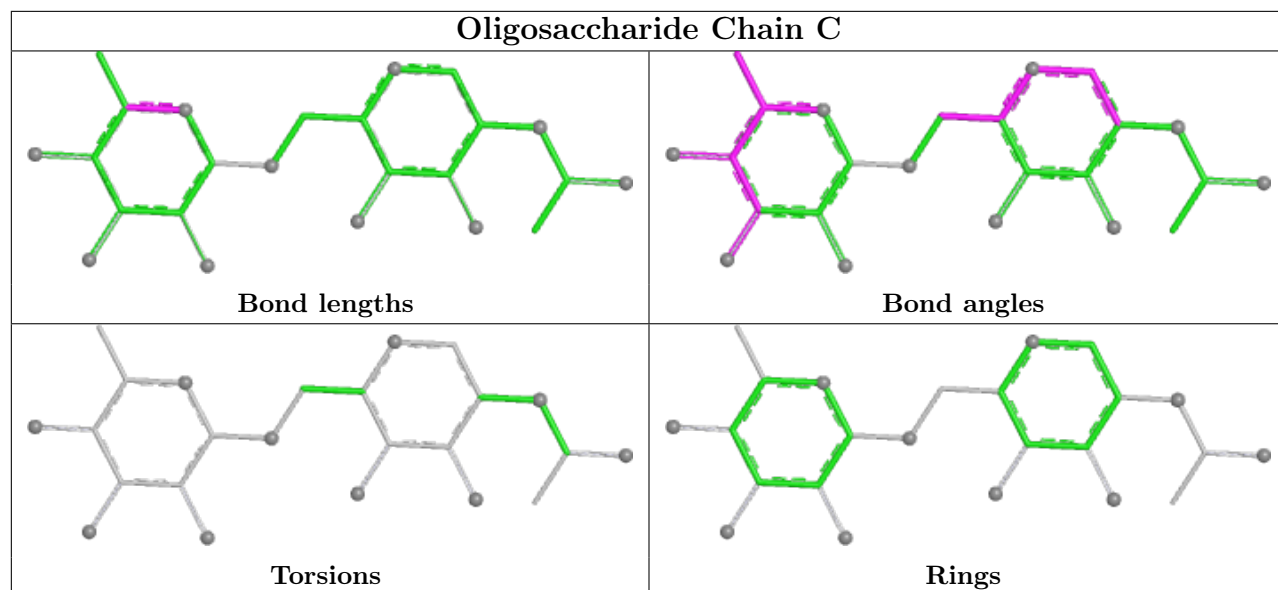
5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	$\#|Z| > 2$
6	EDO	A	608	-	3,3,3	0.47	0	2,2,2	0.08	0
6	EDO	A	610	-	3,3,3	0.29	0	2,2,2	0.26	0
5	NAG	A	603	1	14,14,15	0.66	0	17,19,21	1.41	1 (5%)
6	EDO	A	606	-	3,3,3	0.20	0	2,2,2	0.44	0
6	EDO	A	605	-	3,3,3	1.27	1 (33%)	2,2,2	2.02	1 (50%)
5	NAG	A	602	1	14,14,15	1.00	1 (7%)	17,19,21	1.57	3 (17%)
6	EDO	A	607	-	3,3,3	0.17	0	2,2,2	0.40	0
6	EDO	A	609	-	3,3,3	0.30	0	2,2,2	0.59	0
5	NAG	A	601	1	14,14,15	0.87	1 (7%)	17,19,21	1.84	3 (17%)
6	EDO	A	604	-	3,3,3	0.50	0	2,2,2	0.44	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
6	EDO	A	608	-	-	1/1/1/1	-
6	EDO	A	610	-	-	0/1/1/1	-
5	NAG	A	603	1	-	0/6/23/26	0/1/1/1
6	EDO	A	606	-	-	0/1/1/1	-
6	EDO	A	605	-	-	1/1/1/1	-
5	NAG	A	602	1	-	2/6/23/26	0/1/1/1
6	EDO	A	607	-	-	1/1/1/1	-
6	EDO	A	609	-	-	1/1/1/1	-
5	NAG	A	601	1	-	2/6/23/26	0/1/1/1
6	EDO	A	604	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	NAG	C1-C2	2.41	1.55	1.52
5	A	601	NAG	C1-C2	2.19	1.55	1.52
6	A	605	EDO	O1-C1	-2.18	1.30	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	601	NAG	C1-O5-C5	3.92	117.50	112.19
5	A	601	NAG	O5-C5-C6	3.90	113.31	107.20
5	A	603	NAG	C1-O5-C5	3.56	117.02	112.19
5	A	601	NAG	C2-N2-C7	3.49	127.88	122.90
5	A	602	NAG	O3-C3-C2	3.27	116.24	109.47
5	A	602	NAG	C4-C3-C2	-3.14	106.42	111.02
6	A	605	EDO	O2-C2-C1	2.65	130.97	111.91
5	A	602	NAG	C3-C4-C5	-2.19	106.33	110.24

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	NAG	O5-C5-C6-O6
5	A	601	NAG	C4-C5-C6-O6
5	A	602	NAG	O5-C5-C6-O6
5	A	602	NAG	C4-C5-C6-O6
6	A	608	EDO	O1-C1-C2-O2
6	A	609	EDO	O1-C1-C2-O2
6	A	605	EDO	O1-C1-C2-O2
6	A	607	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	606	EDO	1	0
6	A	605	EDO	1	0
6	A	609	EDO	3	0

5.7 Other polymers ⓘ

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	385/385 (100%)	0.07	13 (3%)	45	50	20, 31, 54, 89	0
2	B	74/74 (100%)	0.25	4 (5%)	25	28	21, 31, 49, 80	0
All	All	459/459 (100%)	0.10	17 (3%)	41	46	20, 31, 54, 89	0

All (17) RSRZ outliers are listed below:

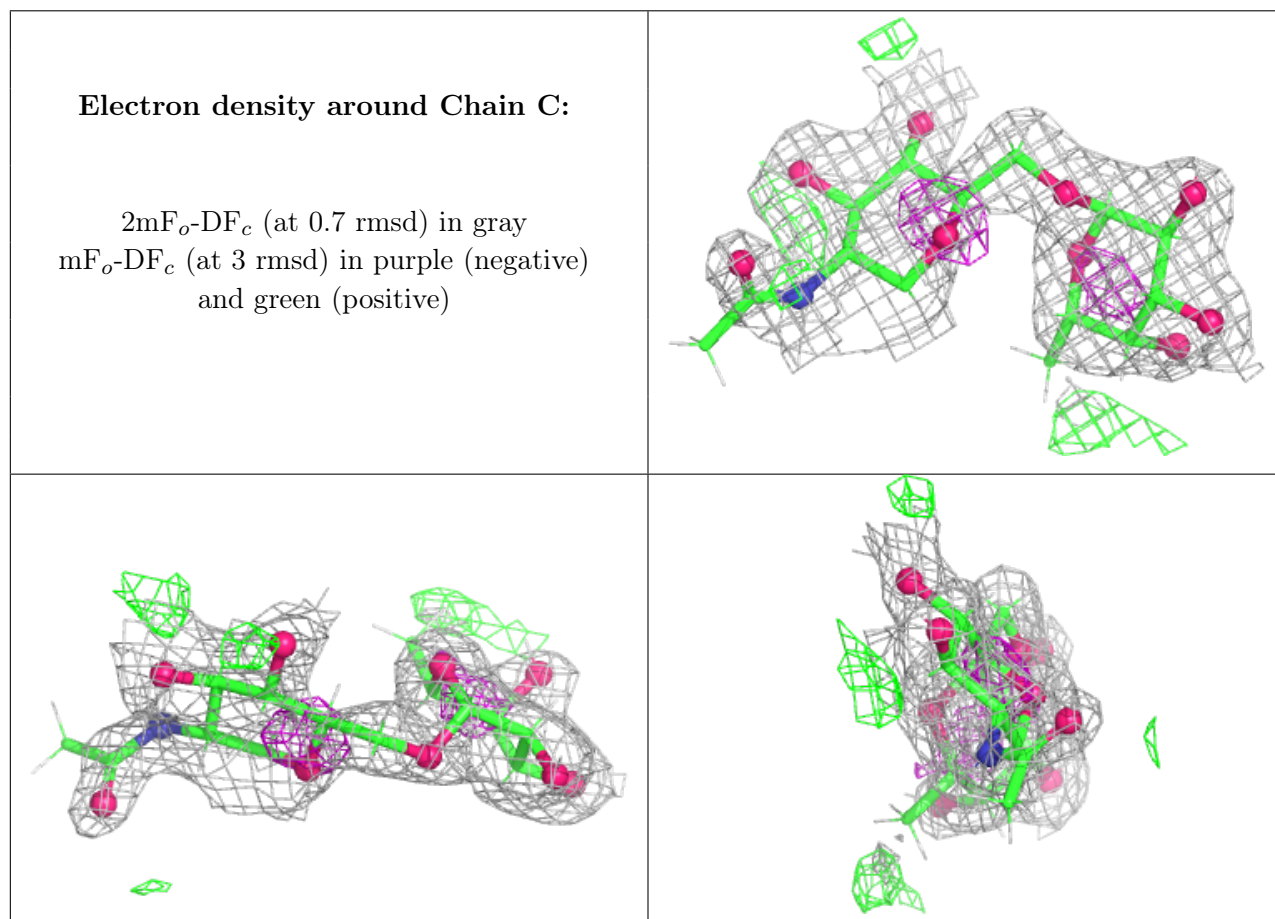| Mol	Chain	Res	Type	RSRZ
1	A	426	SER	7.4
1	A	258	PHE	6.0
2	B	36	GLN	5.0
1	A	427	LYS	4.8
1	A	428	ARG	4.3
1	A	197	LEU	4.2
1	A	257	THR	3.5
1	A	195	ALA	3.4
1	A	543	ILE	3.2
2	B	109	GLU	2.8
2	B	107	LYS	2.7
1	A	259	LYS	2.5
1	A	260	ASN	2.4
1	A	213	SER	2.3
1	A	159	LYS	2.2
1	A	206	LEU	2.2
2	B	106	PRO	2.0

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

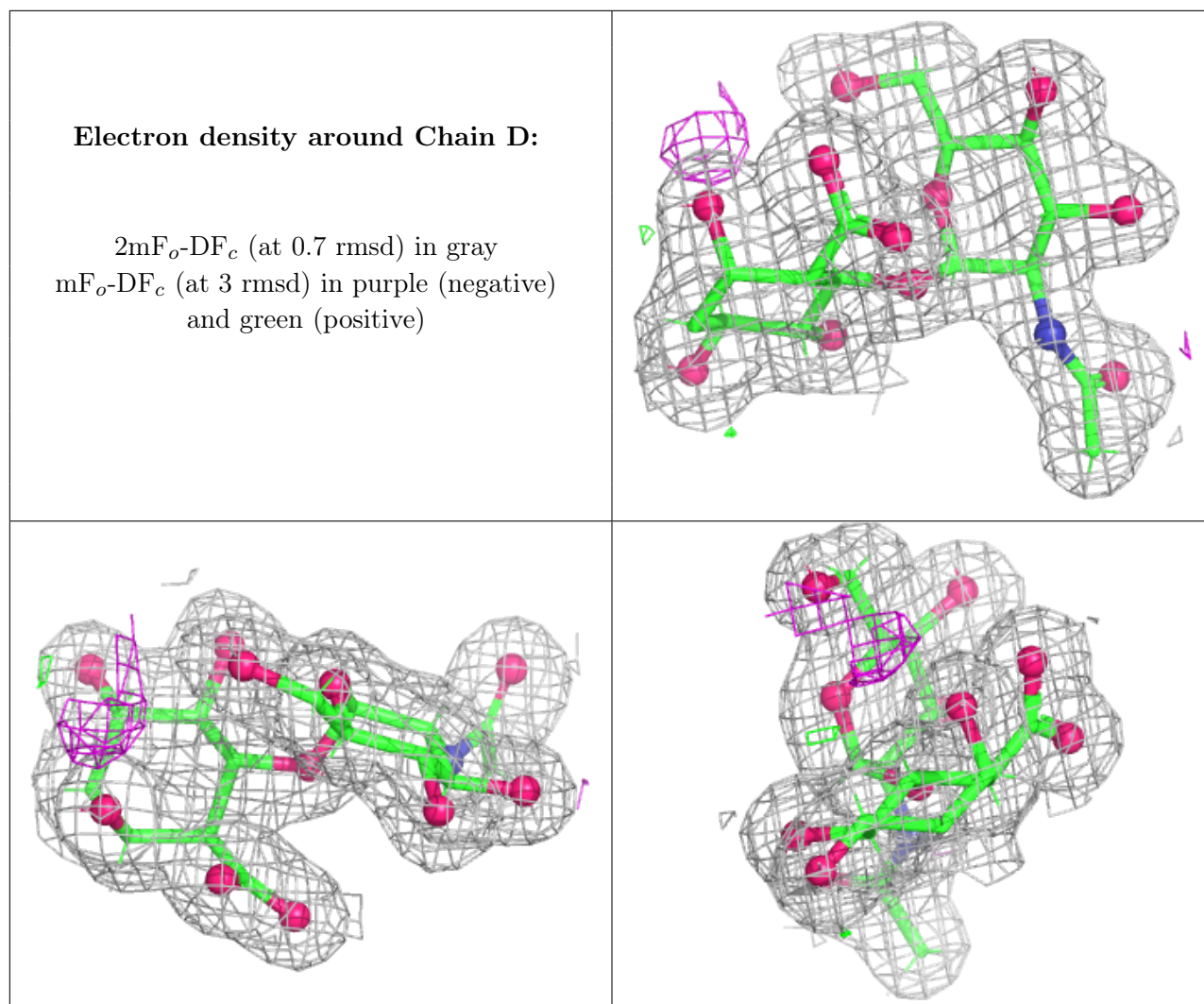There are no non-standard protein/DNA/RNA residues in this entry.

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	NAG	C	1	14/15	0.72	0.28	51,61,82,82	2
3	FUC	C	2	10/11	0.80	0.28	48,52,59,59	3
4	8I4	D	1	13/14	0.97	0.09	23,26,27,29	3
4	NDG	D	2	14/15	0.97	0.09	23,28,34,39	3

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

Electron density around Chain D:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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(Å^2)	Q<0.9
6	EDO	A	608	4/4	0.72	0.25	51,55,58,61	1
5	NAG	A	601	14/15	0.76	0.30	74,87,92,101	3
6	EDO	A	606	4/4	0.77	0.21	47,51,54,55	1
5	NAG	A	602	14/15	0.78	0.24	49,60,66,71	3
6	EDO	A	609	4/4	0.78	0.10	51,52,55,55	1
6	EDO	A	610	4/4	0.84	0.20	49,57,58,60	1
5	NAG	A	603	14/15	0.87	0.12	56,61,69,79	3
6	EDO	A	607	4/4	0.91	0.13	41,47,49,51	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	A	605	4/4	0.94	0.13	25,29,31,34	1
6	EDO	A	604	4/4	0.95	0.14	32,33,34,34	1
7	CL	A	611	1/1	0.96	0.08	41,41,41,41	0

6.5 Other polymers ⓘ

There are no such residues in this entry.