



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:33 PM UTC

PDB ID : 9QR8 / pdb_00009qr8
Title : Gliadin degrading prolyl endopeptidase Celiacase (neprosin C334V)
Authors : Rodriguez-Banqueri, A.; Eckhard, U.; Gomis-Ruth, F.X.
Deposited on : 2025-04-03
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

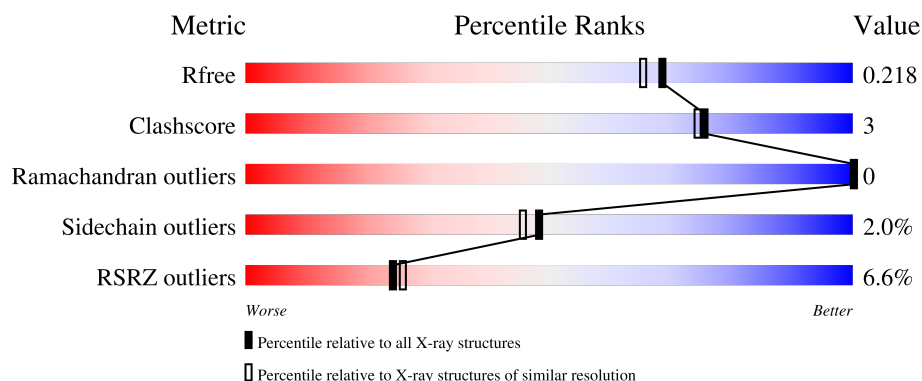
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	367	5% 64% 6% 30%
2	B	2	100%
3	C	3	100%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 2280 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 Protein neprosin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			1979	1260	326	387	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	initiating methionine	UNP C0HLV2
A	24	VAL	-	expression tag	UNP C0HLV2
A	334	VAL	CYS	engineered mutation	UNP C0HLV2
A	401	ALA	-	expression tag	UNP C0HLV2
A	402	ILE	-	expression tag	UNP C0HLV2
A	403	ALA	-	expression tag	UNP C0HLV2
A	404	HIS	-	expression tag	UNP C0HLV2
A	405	HIS	-	expression tag	UNP C0HLV2
A	406	HIS	-	expression tag	UNP C0HLV2
A	407	HIS	-	expression tag	UNP C0HLV2
A	408	HIS	-	expression tag	UNP C0HLV2
A	409	HIS	-	expression tag	UNP C0HLV2

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



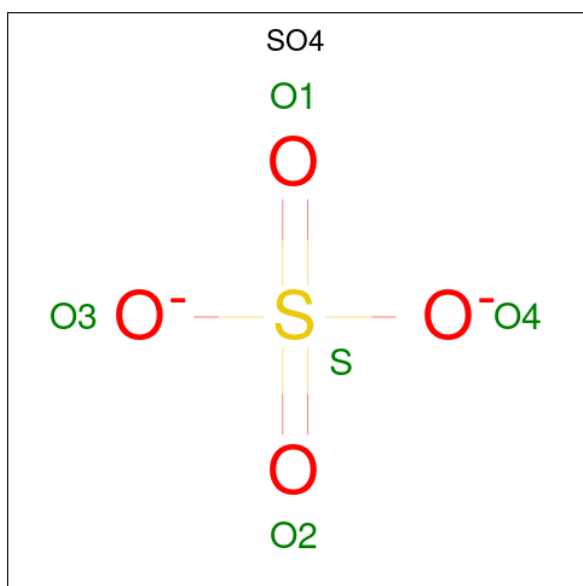
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

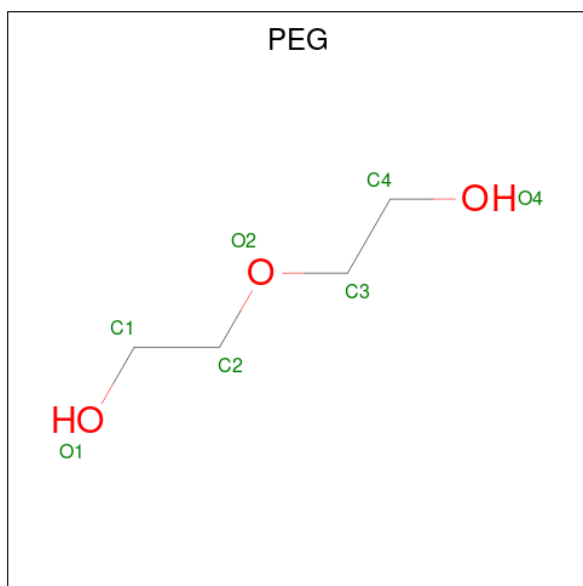
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Cl	0	0
			2	2		

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



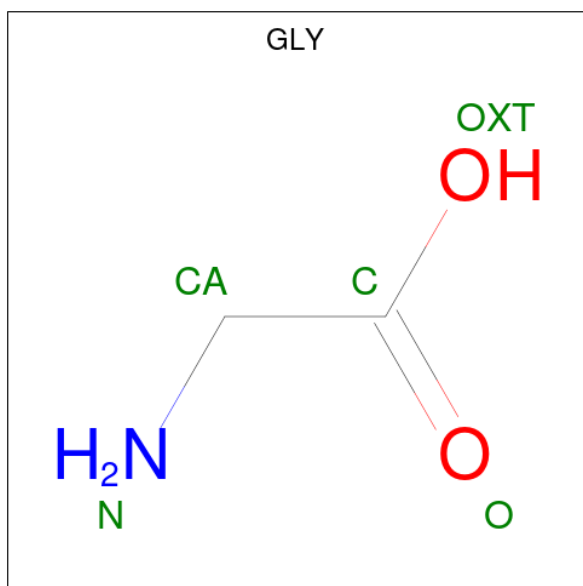
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 9 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			5	2	1	2		
9	A	1	Total	C	N	O	0	0
			5	2	1	2		
9	A	1	Total	C	N	O	0	0
			5	2	1	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			5	2	1	2		
9	A	1	Total	C	N	O	0	0
			5	2	1	2		

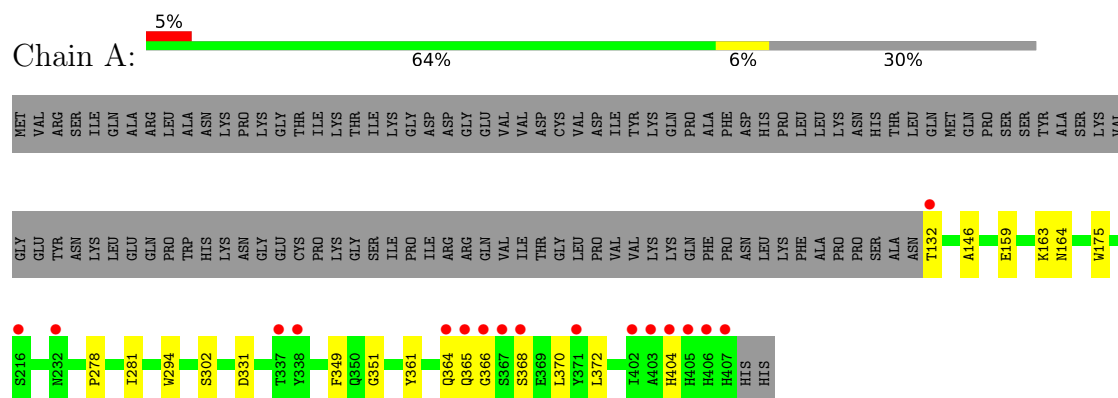
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	185	Total	O	0	0
			185	185		

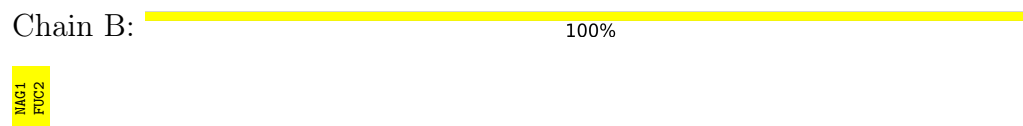
3 Residue-property plots [i](#)

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: Protein neprosin



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



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.01Å 39.58Å 64.64Å 90.00° 108.11° 90.00°	Depositor
Resolution (Å)	61.44 – 1.90 61.44 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.4 (61.44-1.90) 96.4 (61.44-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.210 , 0.258 (Not available) , 0.218	Depositor DCC
R_{free} test set	529 reflections (2.33%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2280	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.93% 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: PEG, TRS, GOL, FUC, SO4, BMA, NAG, CL

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	0.32	0/2046	0.53	0/2804

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	1979	0	1780	12	0
2	B	24	0	22	0	0
3	C	39	0	34	0	0
4	A	5	0	0	0	0
5	A	2	0	0	0	0
6	A	8	0	12	1	0
7	A	7	0	10	0	0
8	A	6	0	8	1	0
9	A	25	0	10	1	0
10	A	185	0	0	1	0
All	All	2280	0	1876	12	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 (12) 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:331:ASP:OD1	10:A:601:HOH:O	2.07	0.73
1:A:365:GLN:NE2	1:A:366:GLY:O	2.25	0.60
1:A:361:TYR:HB2	1:A:372:LEU:HD11	1.92	0.51
1:A:146:ALA:HB2	9:A:510:GLY:HA2	1.94	0.48
1:A:164:ASN:OD1	1:A:302:SER:HB3	2.13	0.48
1:A:278:PRO:O	1:A:281:ILE:HG12	2.15	0.47
1:A:351:GLY:HA3	1:A:361:TYR:OH	2.14	0.47
1:A:163:LYS:HE3	1:A:164:ASN:OD1	2.18	0.44
1:A:159:GLU:OE2	8:A:506:GOL:H11	2.20	0.42
1:A:294:TRP:CZ3	1:A:349:PHE:HE1	2.38	0.41
1:A:365:GLN:HB2	1:A:370:LEU:HD13	2.03	0.41
1:A:175:TRP:HE1	6:A:504:TRS:C1	2.34	0.41

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	254/367 (69%)	247 (97%)	7 (3%)	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	202/302 (67%)	198 (98%)	4 (2%)	48 46

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	THR
1	A	364	GLN
1	A	368	SER
1	A	404	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	133	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 ⓘ

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	NAG	B	1	1,2	14,14,15	0.51	0	17,19,21	0.78	1 (5%)
2	FUC	B	2	2	10,10,11	0.96	0	14,14,16	1.09	2 (14%)
3	NAG	C	1	3,1	14,14,15	0.66	1 (7%)	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	2	3	14,14,15	0.74	1 (7%)	17,19,21	0.64	0
3	BMA	C	3	3	11,11,12	0.73	0	15,15,17	1.34	1 (6%)

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	B	1	1,2	-	2/6/23/26	0/1/1/1
2	FUC	B	2	2	-	-	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	NAG	O5-C1	-2.26	1.39	1.43
3	C	2	NAG	C1-C2	2.03	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	BMA	C1-O5-C5	4.01	117.56	112.19
2	B	2	FUC	C1-O5-C5	2.68	119.30	112.97
2	B	1	NAG	C1-O5-C5	2.30	115.28	112.19
2	B	2	FUC	C1-C2-C3	2.01	112.58	109.64

There are no chirality outliers.

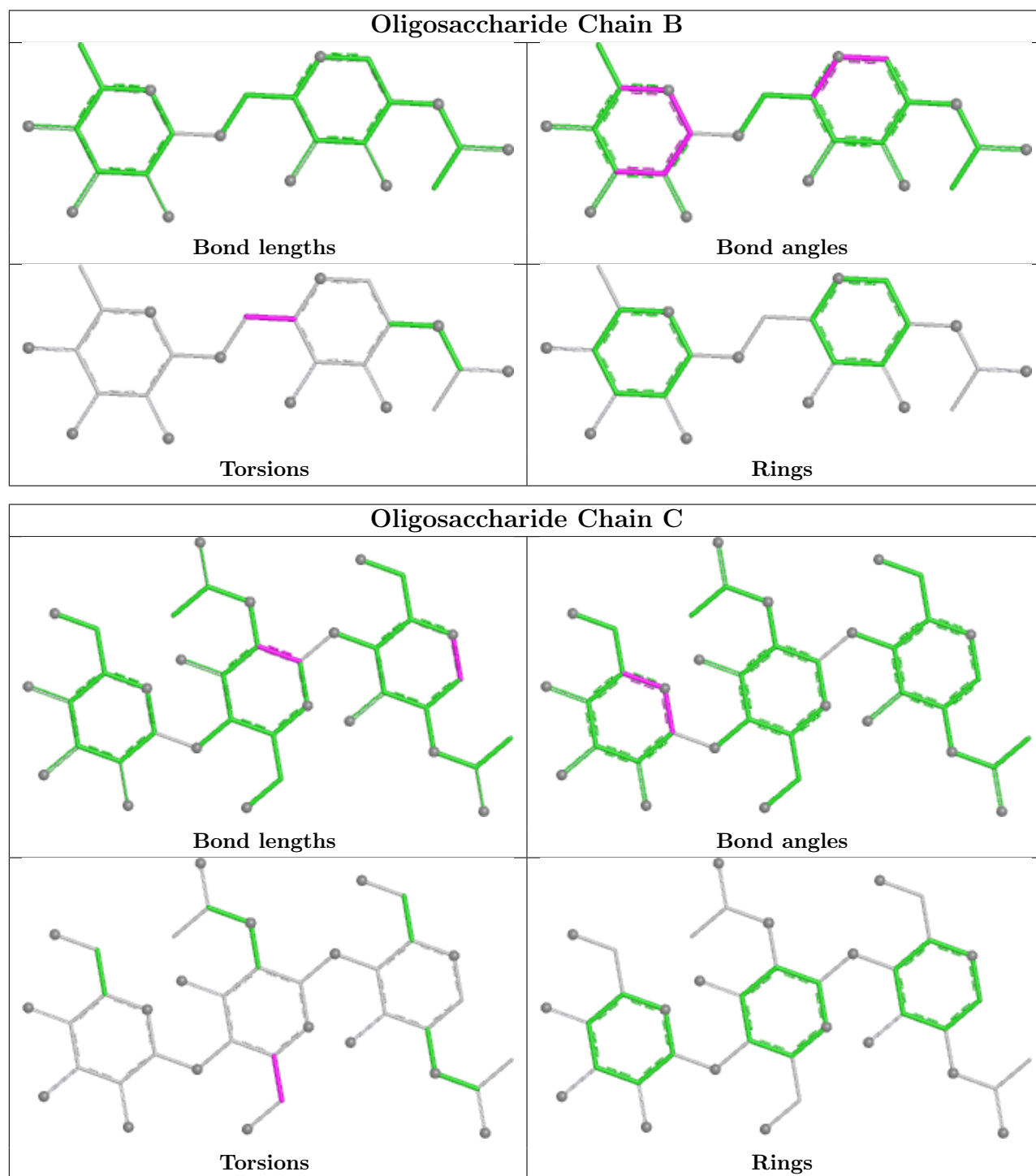
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6

There are no ring outliers.

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](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	SO4	A	501	-	4,4,4	0.27	0	6,6,6	0.27	0
9	GLY	A	509	-	4,4,4	1.16	1 (25%)	3,4,4	1.55	0
9	GLY	A	507	-	4,4,4	1.16	1 (25%)	3,4,4	1.48	0
8	GOL	A	506	-	5,5,5	1.01	0	5,5,5	0.87	0
7	PEG	A	505	-	6,6,6	0.13	0	5,5,5	0.11	0
9	GLY	A	510	-	4,4,4	1.15	1 (25%)	3,4,4	1.27	0
6	TRS	A	504	-	7,7,7	0.41	0	9,9,9	1.29	1 (11%)
9	GLY	A	511	-	4,4,4	1.09	1 (25%)	3,4,4	1.64	1 (33%)
9	GLY	A	508	-	4,4,4	1.14	1 (25%)	3,4,4	1.64	1 (33%)

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
9	GLY	A	509	-	-	2/2/2/2	-
9	GLY	A	507	-	-	2/2/2/2	-
8	GOL	A	506	-	-	2/4/4/4	-
7	PEG	A	505	-	-	2/4/4/4	-
9	GLY	A	510	-	-	2/2/2/2	-
6	TRS	A	504	-	-	6/9/9/9	-
9	GLY	A	511	-	-	0/2/2/2	-
9	GLY	A	508	-	-	1/2/2/2	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	509	GLY	OXT-C	-2.19	1.23	1.30
9	A	508	GLY	OXT-C	-2.15	1.23	1.30
9	A	507	GLY	OXT-C	-2.15	1.23	1.30
9	A	510	GLY	OXT-C	-2.07	1.24	1.30
9	A	511	GLY	OXT-C	-2.06	1.24	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	504	TRS	O3-C3-C	-2.66	103.46	110.88
9	A	508	GLY	OXT-C-O	-2.19	117.69	123.33
9	A	511	GLY	OXT-C-O	-2.07	118.00	123.33

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	504	TRS	C1-C-C2-O2
6	A	504	TRS	C3-C-C2-O2
6	A	504	TRS	N-C-C2-O2
8	A	506	GOL	C1-C2-C3-O3
9	A	510	GLY	O-C-CA-N
9	A	510	GLY	OXT-C-CA-N
9	A	509	GLY	O-C-CA-N
9	A	509	GLY	OXT-C-CA-N
8	A	506	GOL	O2-C2-C3-O3
9	A	507	GLY	O-C-CA-N
6	A	504	TRS	C2-C-C1-O1
9	A	507	GLY	OXT-C-CA-N
6	A	504	TRS	N-C-C1-O1
7	A	505	PEG	C1-C2-O2-C3
7	A	505	PEG	O2-C3-C4-O4
6	A	504	TRS	C3-C-C1-O1
9	A	508	GLY	OXT-C-CA-N

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	506	GOL	1	0
9	A	510	GLY	1	0
6	A	504	TRS	1	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 [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	256/367 (69%)	0.48	17 (6%) 24 26	22, 28, 48, 89	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	407	HIS	4.4
1	A	403	ALA	4.1
1	A	404	HIS	4.1
1	A	406	HIS	4.0
1	A	365	GLN	3.8
1	A	371	TYR	3.8
1	A	338	TYR	3.7
1	A	402	ILE	3.6
1	A	132	THR	3.5
1	A	366	GLY	3.3
1	A	368	SER	3.2
1	A	405	HIS	2.6
1	A	216	SER	2.6
1	A	337	THR	2.4
1	A	232	ASN	2.3
1	A	364	GLN	2.1
1	A	367	SER	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.

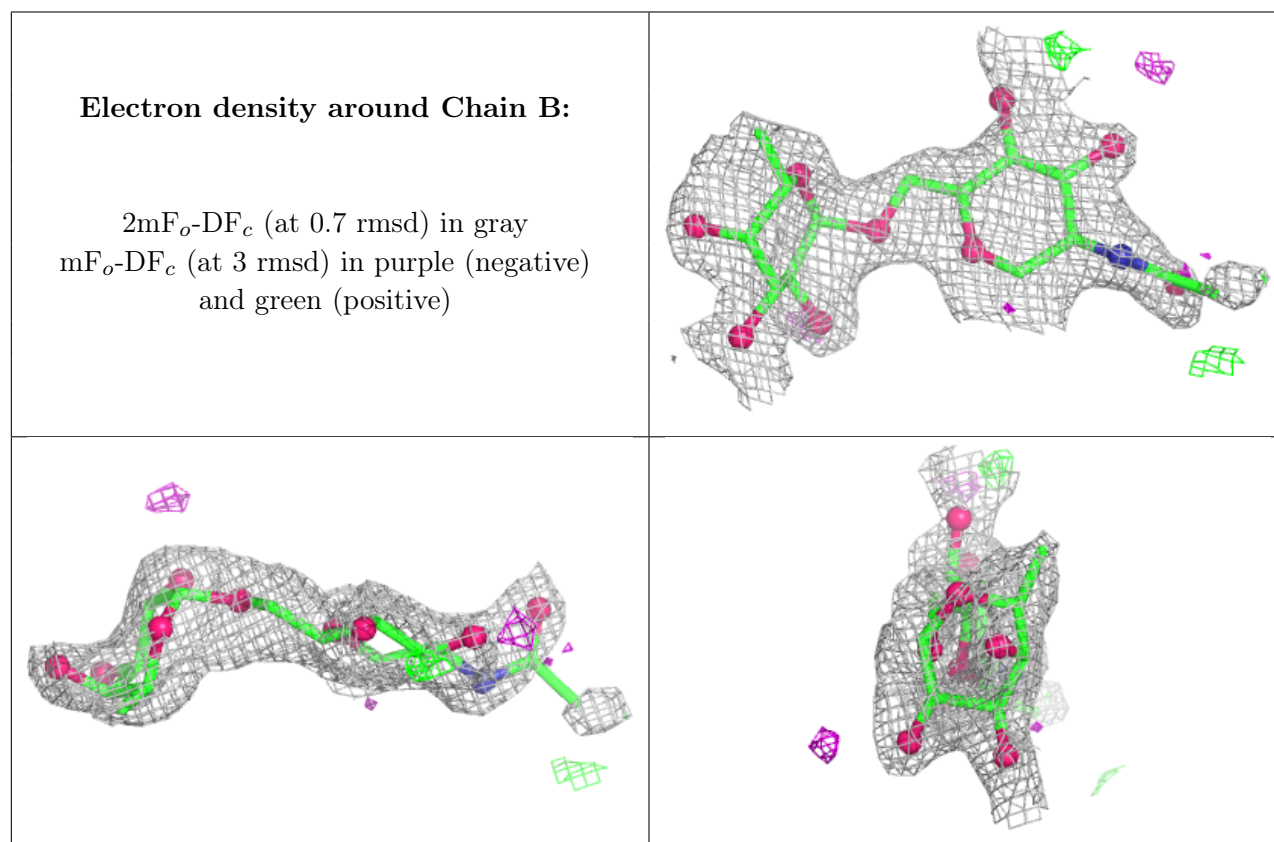
6.3 Carbohydrates [i](#)

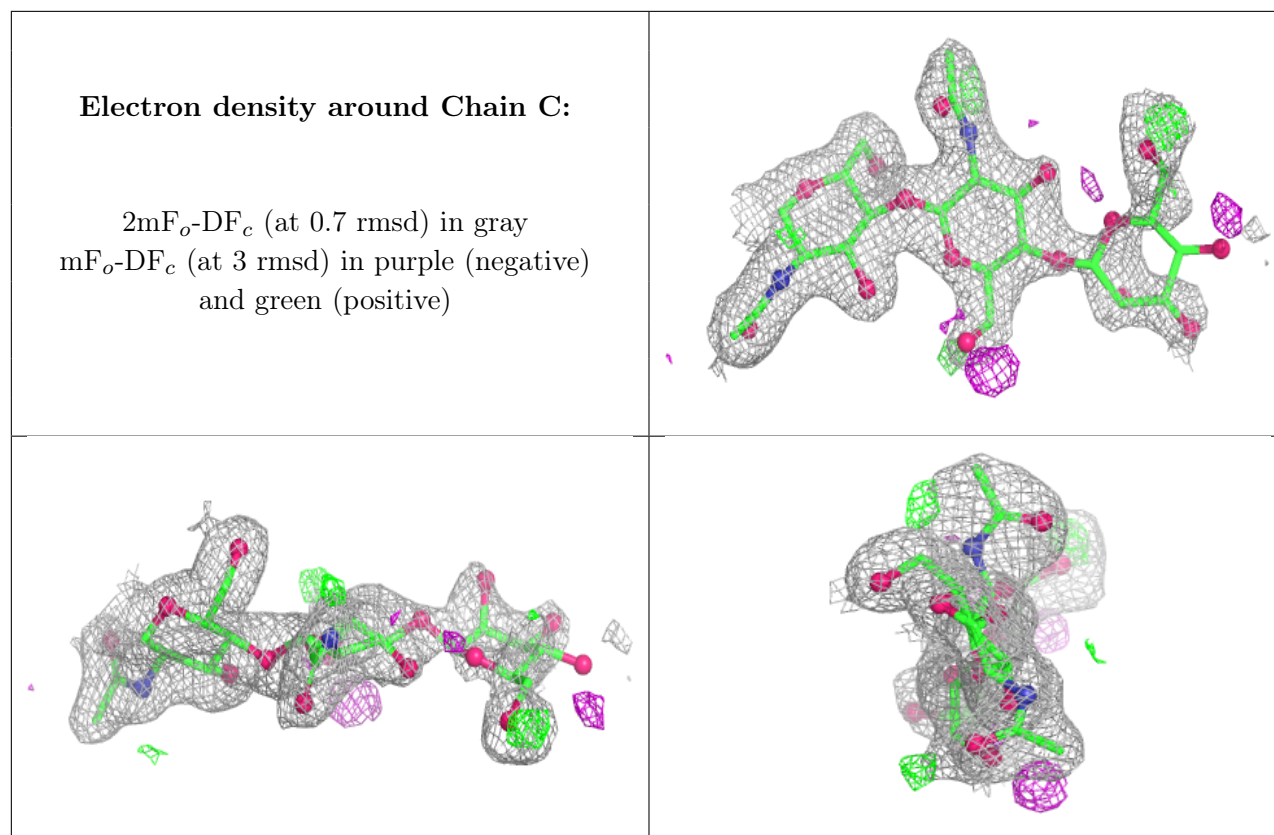
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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	BMA	C	3	11/12	0.38	0.21	77,83,90,94	0
2	NAG	B	1	14/15	0.71	0.17	59,63,67,71	0
2	FUC	B	2	10/11	0.74	0.16	51,60,64,67	0
3	NAG	C	2	14/15	0.80	0.15	41,47,62,71	0
3	NAG	C	1	14/15	0.95	0.08	25,29,34,38	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
8	GOL	A	506	6/6	0.71	0.17	48,51,52,53	0
9	GLY	A	511	5/5	0.71	0.16	58,58,62,63	0
9	GLY	A	509	5/5	0.73	0.18	61,68,77,78	0
6	TRS	A	504	8/8	0.78	0.16	31,40,44,47	0
4	SO4	A	501	5/5	0.80	0.13	60,71,80,87	0
9	GLY	A	507	5/5	0.81	0.15	41,46,52,57	0
9	GLY	A	508	5/5	0.82	0.13	44,45,52,57	0
7	PEG	A	505	7/7	0.85	0.14	40,44,51,55	0
9	GLY	A	510	5/5	0.87	0.17	49,51,56,57	0
5	CL	A	502	1/1	0.95	0.09	50,50,50,50	0
5	CL	A	503	1/1	0.96	0.09	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.