



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2024 – 05:10 am GMT

PDB ID : 6GRE
Title : Crystal structure of the tandem DUF26 ectodomain from the Arabidopsis thaliana cysteine-rich receptor-like protein PDLP5.
Authors : Brandt, B.; Hothorn, M.
Deposited on : 2018-06-11
Resolution : 1.29 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

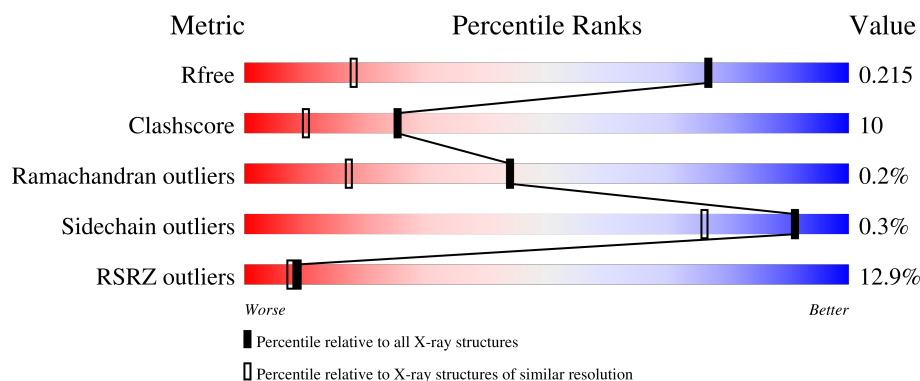
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.29 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}	164625	1387 (1.30-1.30)
Clashscore	180529	1497 (1.30-1.30)
Ramachandran outliers	177936	1455 (1.30-1.30)
Sidechain outliers	177891	1455 (1.30-1.30)
RSRZ outliers	164620	1384 (1.30-1.30)

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	228	<div> <div>12%</div> <div>78%</div> <div>12%</div> <div>10%</div> </div>
1	B	228	<div> <div>11%</div> <div>78%</div> <div>12%</div> <div>9%</div> </div>
2	C	2	<div> <div>50%</div> <div>50%</div> </div>
2	D	2	<div> <div>50%</div> <div>50%</div> </div>
2	E	2	<div> <div>50%</div> <div>50%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	A	307	-	-	X	-
8	AE3	B	310	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 3664 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 Cysteine-rich repeat secretory protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	16	0
			1599	991	264	326	18			
1	B	207	Total	C	N	O	S	0	16	0
			1602	994	264	327	17			

There are 24 discrepancies between the modelled and reference sequences:

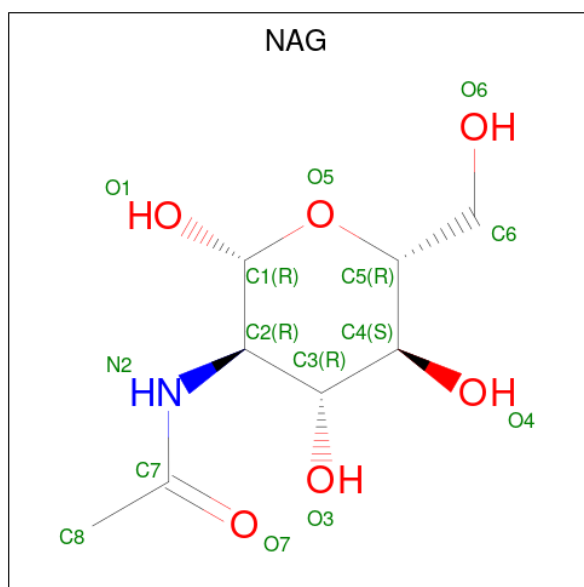
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	initiating methionine	UNP Q8GUJ2
A	25	GLY	-	expression tag	UNP Q8GUJ2
A	242	LEU	-	expression tag	UNP Q8GUJ2
A	243	GLU	-	expression tag	UNP Q8GUJ2
A	244	GLY	-	expression tag	UNP Q8GUJ2
A	245	SER	-	expression tag	UNP Q8GUJ2
A	246	GLU	-	expression tag	UNP Q8GUJ2
A	247	ASN	-	expression tag	UNP Q8GUJ2
A	248	LEU	-	expression tag	UNP Q8GUJ2
A	249	TYR	-	expression tag	UNP Q8GUJ2
A	250	PHE	-	expression tag	UNP Q8GUJ2
A	251	GLN	-	expression tag	UNP Q8GUJ2
B	24	MET	-	initiating methionine	UNP Q8GUJ2
B	25	GLY	-	expression tag	UNP Q8GUJ2
B	242	LEU	-	expression tag	UNP Q8GUJ2
B	243	GLU	-	expression tag	UNP Q8GUJ2
B	244	GLY	-	expression tag	UNP Q8GUJ2
B	245	SER	-	expression tag	UNP Q8GUJ2
B	246	GLU	-	expression tag	UNP Q8GUJ2
B	247	ASN	-	expression tag	UNP Q8GUJ2
B	248	LEU	-	expression tag	UNP Q8GUJ2
B	249	TYR	-	expression tag	UNP Q8GUJ2
B	250	PHE	-	expression tag	UNP Q8GUJ2
B	251	GLN	-	expression tag	UNP Q8GUJ2

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

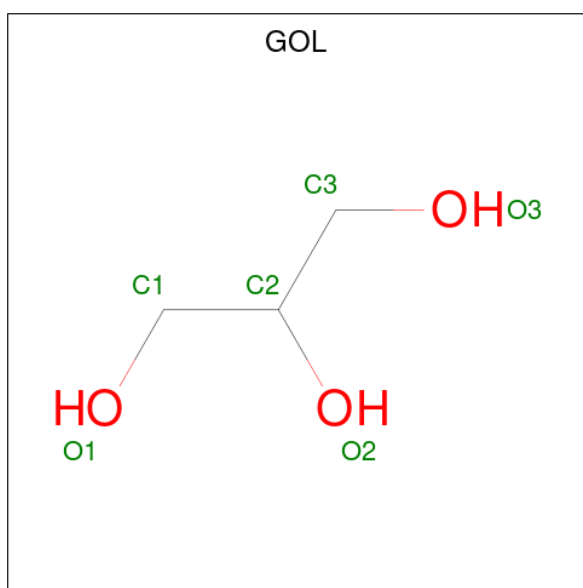
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Na	0	0
			1	1		
5	B	1	Total	Na	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

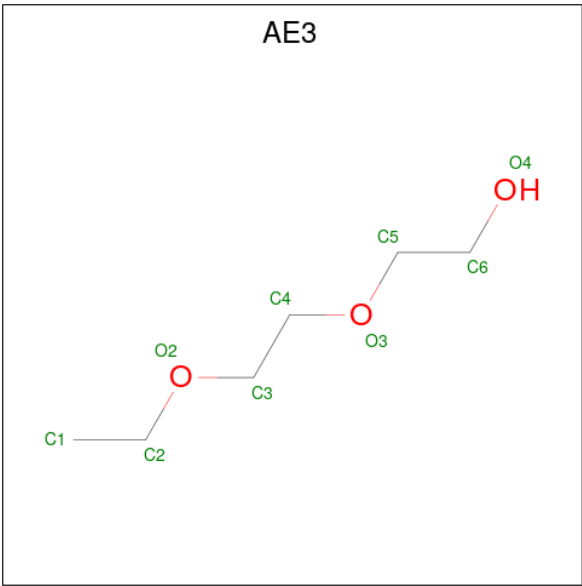
- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is 2-(2-ETHOXYETHOXY)ETHANOL (three-letter code: AE3) (formula:

C₆H₁₄O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			9	6	3		

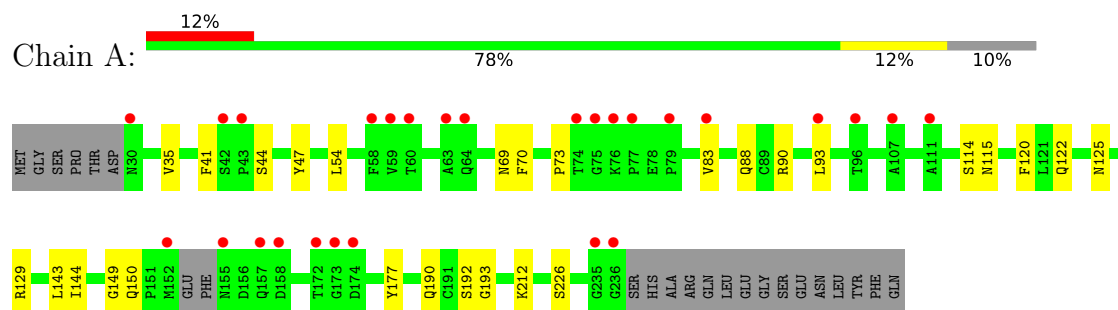
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	148	Total	O	0	0
			148	148		
9	B	162	Total	O	0	0
			162	162		

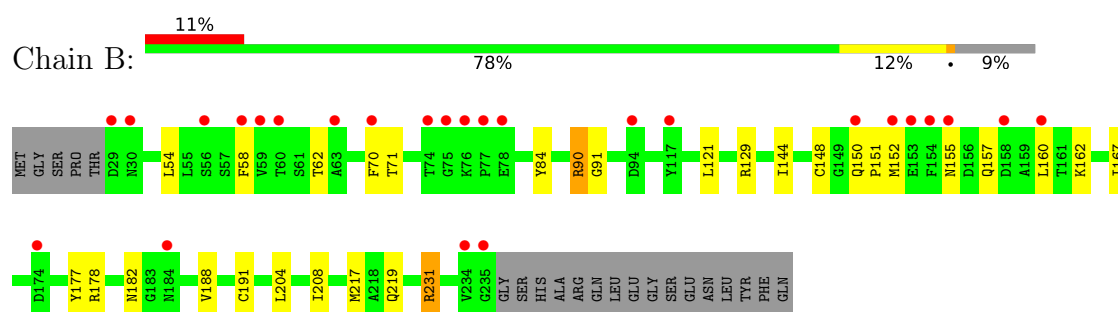
3 Residue-property plots [i](#)

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: Cysteine-rich repeat secretory protein 2



- Molecule 1: Cysteine-rich repeat secretory protein 2



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



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



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

Chain E:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.76Å 47.97Å 62.19Å 97.70° 102.72° 99.86°	Depositor
Resolution (Å)	37.77 – 1.29 37.77 – 1.29	Depositor EDS
% Data completeness (in resolution range)	94.6 (37.77-1.29) 94.6 (37.77-1.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 1.29Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.186 , 0.210 0.196 , 0.215	Depositor DCC
R_{free} test set	5440 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3664	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AE3, EDO, GOL, SO4, NAG, NA

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	0.55	0/1663	0.74	0/2249
1	B	0.60	0/1672	0.81	3/2265 (0.1%)
All	All	0.58	0/3335	0.78	3/4514 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	178	ARG	NE-CZ-NH1	-7.32	116.64	120.30
1	B	129	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	B	231	ARG	NE-CZ-NH1	5.23	122.92	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	90[A]	ARG	Sidechain
1	B	90[B]	ARG	Sidechain

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	1599	0	1546	34	0
1	B	1602	0	1564	28	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
3	A	14	0	13	0	0
4	A	16	0	24	5	0
4	B	12	0	18	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	B	6	0	8	1	0
8	B	9	0	14	13	0
9	A	148	0	0	4	0
9	B	162	0	0	3	0
All	All	3664	0	3262	63	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 10.

All (63) 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:47:TYR:CE1	1:A:83[B]:VAL:HG12	2.03	0.93
1:B:71[A]:THR:HG21	9:B:512:HOH:O	1.75	0.86
1:B:148:CYS:O	8:B:310:AE3:H6C1	1.82	0.80
1:A:47:TYR:CZ	1:A:83[B]:VAL:HG12	2.19	0.77
1:A:73:PRO:HG3	9:A:505:HOH:O	1.86	0.74
1:B:152[A]:MET:SD	1:B:219:GLN:HG2	2.31	0.69
1:A:88[A]:GLN:HE22	1:A:192:SER:HA	1.60	0.67
1:B:148:CYS:O	8:B:310:AE3:C6	2.45	0.65
1:A:120[A]:PHE:CD2	1:A:129:ARG:HD2	2.35	0.61
1:B:151:PRO:HD3	8:B:310:AE3:H4C2	1.81	0.61
1:B:162:LYS:HG2	1:B:182[A]:ASN:ND2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:VAL:CG2	8:B:310:AE3:H5C1	2.33	0.58
1:A:88[A]:GLN:HE22	1:A:193:GLY:H	1.52	0.57
1:B:191[A]:CYS:SG	1:B:204:LEU:HG	2.45	0.57
1:A:88[A]:GLN:HE22	1:A:193:GLY:N	2.02	0.57
1:A:120[A]:PHE:HE1	1:A:122:GLN:HB2	1.70	0.56
4:A:307:EDO:H21	1:B:144[B]:ILE:HG23	1.87	0.55
1:B:167:ILE:HG22	1:B:208:ILE:HG23	1.88	0.55
1:B:71[A]:THR:HG22	1:B:84:TYR:CD2	2.41	0.55
1:B:58:PHE:O	1:B:62:THR:HG23	2.07	0.55
1:A:44:SER:HA	9:A:441:HOH:O	2.07	0.54
1:A:88[A]:GLN:NE2	1:A:193:GLY:H	2.05	0.54
1:A:226:SER:OG	8:B:310:AE3:H1C1	2.09	0.53
1:A:120[A]:PHE:HD2	1:A:129:ARG:HD2	1.72	0.53
1:A:144:ILE:HD11	8:B:310:AE3:H1C3	1.91	0.52
1:B:71[A]:THR:HG22	1:B:84:TYR:HD2	1.75	0.52
1:A:120[A]:PHE:HD2	1:A:129:ARG:CD	2.23	0.52
1:B:157:GLN:HG3	9:B:407:HOH:O	2.10	0.51
1:A:212:LYS:HD2	9:A:452:HOH:O	2.10	0.51
1:A:190:GLN:NE2	9:A:402:HOH:O	2.43	0.50
1:B:71[A]:THR:HG23	9:B:415:HOH:O	2.10	0.50
1:B:155:ASN:CG	1:B:155:ASN:O	2.49	0.48
1:A:41:PHE:CZ	1:A:115:ASN:HA	2.48	0.48
1:B:157:GLN:NE2	1:B:160:LEU:HD22	2.28	0.48
1:A:144:ILE:HG23	8:B:310:AE3:H6C2	1.96	0.48
1:A:150:GLN:N	4:A:307:EDO:H11	2.29	0.48
1:A:143[B]:LEU:HD23	1:A:144:ILE:C	2.35	0.47
1:A:35:VAL:HG11	8:B:310:AE3:H3C2	1.95	0.47
4:A:307:EDO:C2	1:B:144[B]:ILE:HD12	2.45	0.46
1:B:150:GLN:HA	8:B:310:AE3:C4	2.46	0.46
1:B:188[B]:VAL:HG13	1:B:231:ARG:HG2	1.98	0.46
1:A:149:GLY:C	4:A:307:EDO:H11	2.37	0.45
1:B:90[B]:ARG:HG2	1:B:177:TYR:CE1	2.51	0.45
1:A:35:VAL:HG22	8:B:310:AE3:H5C1	1.97	0.45
1:A:120[A]:PHE:HD2	1:A:129:ARG:CG	2.30	0.45
1:B:157:GLN:NE2	1:B:160:LEU:CD2	2.80	0.45
1:A:90:ARG:HG2	1:A:177:TYR:CE1	2.53	0.44
1:A:54:LEU:CD1	1:A:70[A]:PHE:HB2	2.48	0.43
1:A:93:LEU:HD11	1:A:125:ASN:HB3	1.99	0.43
1:B:157:GLN:HE21	1:B:160:LEU:HD23	1.82	0.43
8:B:310:AE3:H1C3	8:B:310:AE3:H3C1	1.10	0.43
1:A:88[A]:GLN:NE2	1:A:192:SER:HA	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:LEU:CD1	1:B:70:PHE:HB2	2.49	0.42
1:A:69:ASN:O	1:A:70[B]:PHE:CD1	2.72	0.42
1:A:120[A]:PHE:CE2	1:A:129:ARG:HD2	2.55	0.42
1:B:144[A]:ILE:CD1	7:B:308:GOL:O3	2.68	0.41
4:A:307:EDO:H21	1:B:144[B]:ILE:HD12	2.02	0.41
1:B:91:GLY:HA3	4:B:307:EDO:H12	2.02	0.41
1:B:160:LEU:HD13	1:B:217:MET:HG2	2.03	0.41
1:A:35:VAL:HG11	8:B:310:AE3:H4C1	2.02	0.41
1:A:35:VAL:HG21	8:B:310:AE3:H5C1	2.03	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	219/228 (96%)	216 (99%)	2 (1%)	1 (0%)	25	6
1	B	221/228 (97%)	217 (98%)	4 (2%)	0	100	100
All	All	440/456 (96%)	433 (98%)	6 (1%)	1 (0%)	44	17

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	SER

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	186/188 (99%)	186 (100%)	0	100	100
1	B	187/188 (100%)	186 (100%)	1 (0%)	86	67
All	All	373/376 (99%)	372 (100%)	1 (0%)	91	76

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	121	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	190	GLN
1	B	146	ASN
1	B	157	GLN
1	B	219	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	2,1	14,14,15	0.48	0	17,19,21	0.78	0
2	NAG	C	2	2	14,14,15	0.29	0	17,19,21	1.05	1 (5%)
2	NAG	D	1	2,1	14,14,15	0.50	0	17,19,21	0.90	0
2	NAG	D	2	2	14,14,15	0.38	0	17,19,21	1.16	3 (17%)
2	NAG	E	1	2,1	14,14,15	0.50	0	17,19,21	1.08	0
2	NAG	E	2	2	14,14,15	0.38	0	17,19,21	0.75	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
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	O5-C5-C6	3.06	112.00	107.20
2	D	2	NAG	O5-C5-C6	2.58	111.25	107.20
2	D	2	NAG	O5-C5-C4	-2.17	105.55	110.83
2	D	2	NAG	C4-C3-C2	2.09	114.08	111.02
2	E	2	NAG	O5-C5-C6	2.04	110.39	107.20

There are no chirality outliers.

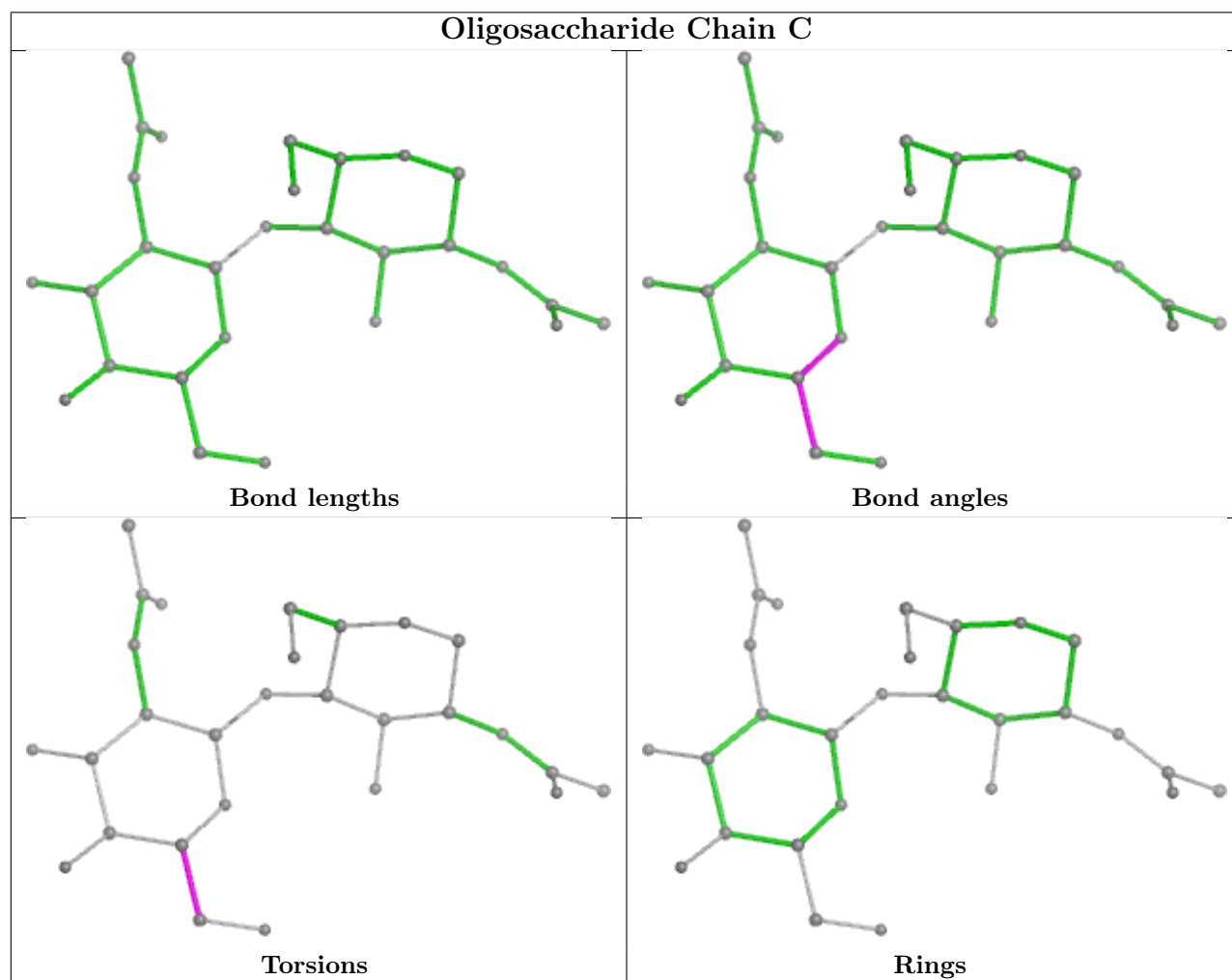
All (3) torsion outliers are listed below:

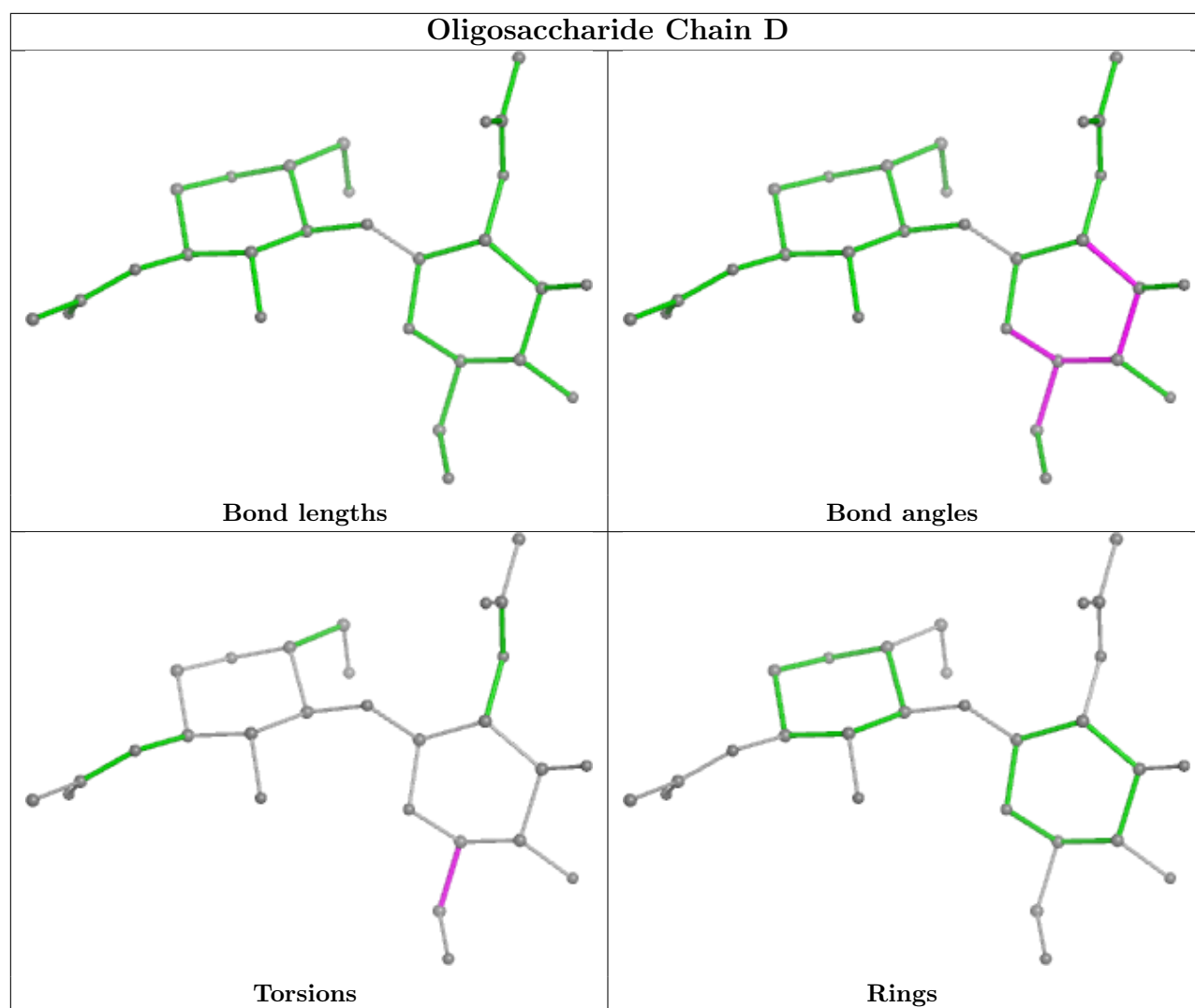
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6

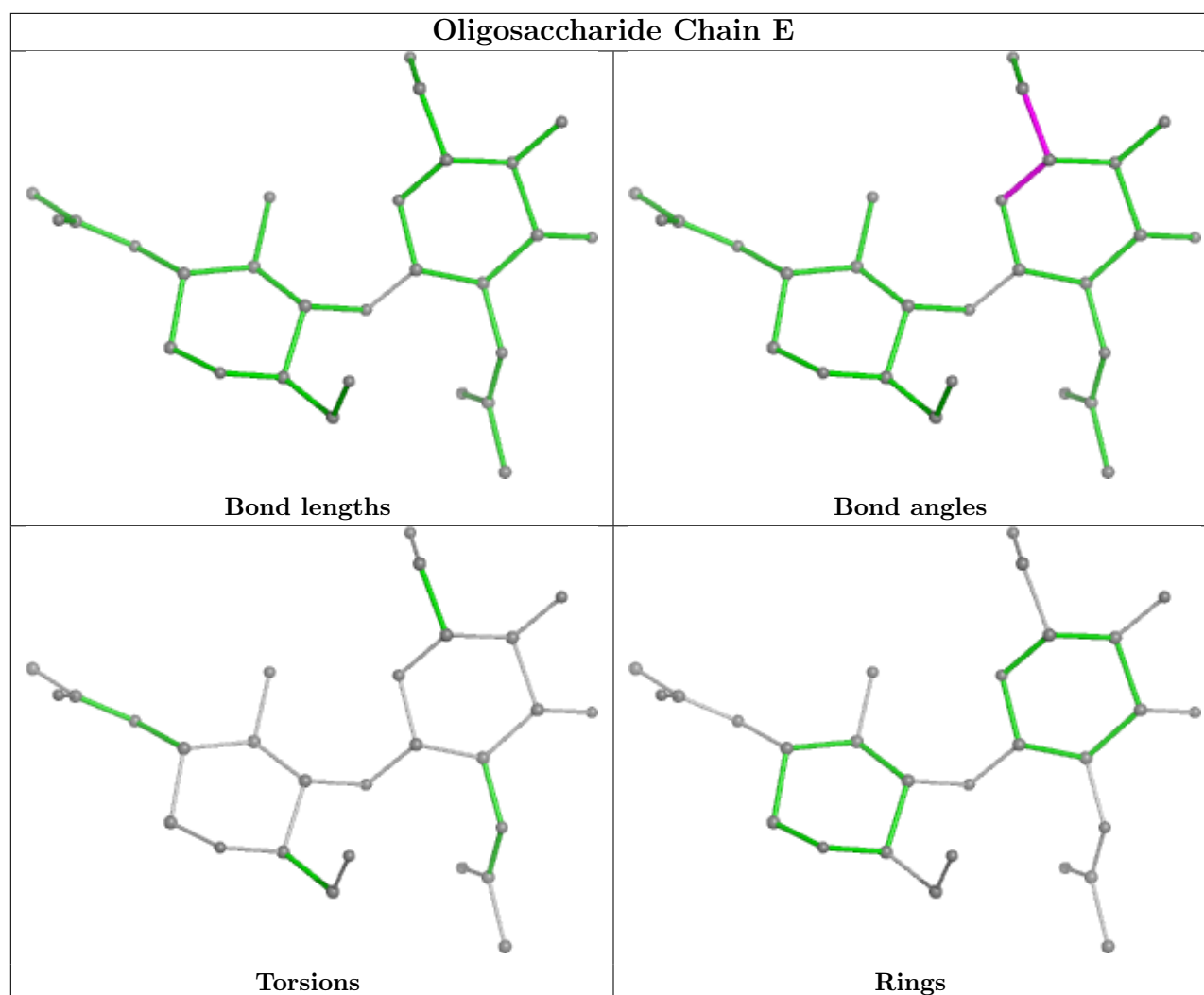
There are no ring outliers.

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 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	EDO	B	305	-	3,3,3	0.61	0	2,2,2	0.34	0
6	SO4	B	311	-	4,4,4	0.46	0	6,6,6	0.27	0
8	AE3	B	310	-	8,8,8	0.40	0	7,7,7	1.47	1 (14%)
4	EDO	A	304	-	3,3,3	0.46	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	A	309	-	4,4,4	0.45	0	6,6,6	0.18	0
4	EDO	B	307	-	3,3,3	0.44	0	2,2,2	0.20	0
4	EDO	A	307	-	3,3,3	0.34	0	2,2,2	0.23	0
4	EDO	A	306	-	3,3,3	0.34	0	2,2,2	0.50	0
4	EDO	A	305	-	3,3,3	0.29	0	2,2,2	0.50	0
7	GOL	B	308	-	5,5,5	0.16	0	5,5,5	0.75	0
4	EDO	B	306	-	3,3,3	0.41	0	2,2,2	0.39	0
3	NAG	A	303	1	14,14,15	0.50	0	17,19,21	0.95	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	EDO	B	305	-	-	0/1/1/1	-
8	AE3	B	310	-	-	5/6/6/6	-
4	EDO	A	304	-	-	0/1/1/1	-
4	EDO	B	307	-	-	1/1/1/1	-
4	EDO	A	307	-	-	0/1/1/1	-
4	EDO	A	306	-	-	1/1/1/1	-
4	EDO	A	305	-	-	0/1/1/1	-
7	GOL	B	308	-	-	0/4/4/4	-
4	EDO	B	306	-	-	1/1/1/1	-
3	NAG	A	303	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(°)
8	B	310	AE3	C2-O2-C3	-2.98	102.23	112.90

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	310	AE3	O2-C3-C4-O3
8	B	310	AE3	C1-C2-O2-C3
3	A	303	NAG	O5-C5-C6-O6
3	A	303	NAG	C4-C5-C6-O6
4	A	306	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
8	B	310	AE3	C4-C3-O2-C2
4	B	307	EDO	O1-C1-C2-O2
8	B	310	AE3	C3-C4-O3-C5
4	B	306	EDO	O1-C1-C2-O2
8	B	310	AE3	O3-C5-C6-O4

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	310	AE3	13	0
4	B	307	EDO	1	0
4	A	307	EDO	5	0
7	B	308	GOL	1	0

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	205/228 (89%)	0.80	27 (13%)	8 7	7, 21, 43, 75	16 (7%)
1	B	207/228 (90%)	0.81	26 (12%)	9 8	8, 19, 40, 66	16 (7%)
All	All	412/456 (90%)	0.81	53 (12%)	9 7	7, 20, 42, 75	32 (7%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	154	PHE	7.9
1	B	59	VAL	4.6
1	A	174	ASP	4.5
1	A	236	GLY	4.4
1	B	184[A]	ASN	4.1
1	A	43	PRO	4.1
1	B	76[A]	LYS	3.9
1	A	155	ASN	3.9
1	B	60	THR	3.7
1	B	155	ASN	3.6
1	B	152[A]	MET	3.4
1	A	74	THR	3.4
1	A	75	GLY	3.4
1	B	58	PHE	3.3
1	A	152	MET	3.3
1	B	75	GLY	3.2
1	B	160	LEU	3.0
1	A	173	GLY	3.0
1	A	158	ASP	3.0
1	B	74	THR	2.8
1	B	63	ALA	2.8
1	A	76	LYS	2.8
1	A	30	ASN	2.7
1	B	158[A]	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	83[A]	VAL	2.7
1	B	94	ASP	2.6
1	A	42	SER	2.6
1	B	29	ASP	2.5
1	A	59	VAL	2.5
1	A	157	GLN	2.5
1	B	234	VAL	2.5
1	B	235	GLY	2.4
1	B	70	PHE	2.4
1	A	60	THR	2.4
1	A	58	PHE	2.4
1	A	96	THR	2.3
1	A	107	ALA	2.3
1	B	78	GLU	2.3
1	A	63	ALA	2.2
1	B	77	PRO	2.2
1	A	77	PRO	2.2
1	A	172	THR	2.2
1	A	64	GLN	2.2
1	B	174	ASP	2.1
1	B	30	ASN	2.1
1	A	79	PRO	2.1
1	B	150	GLN	2.1
1	A	111	ALA	2.1
1	A	93	LEU	2.1
1	B	56	SER	2.1
1	A	235	GLY	2.1
1	B	117	TYR	2.0
1	B	153	GLU	2.0

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

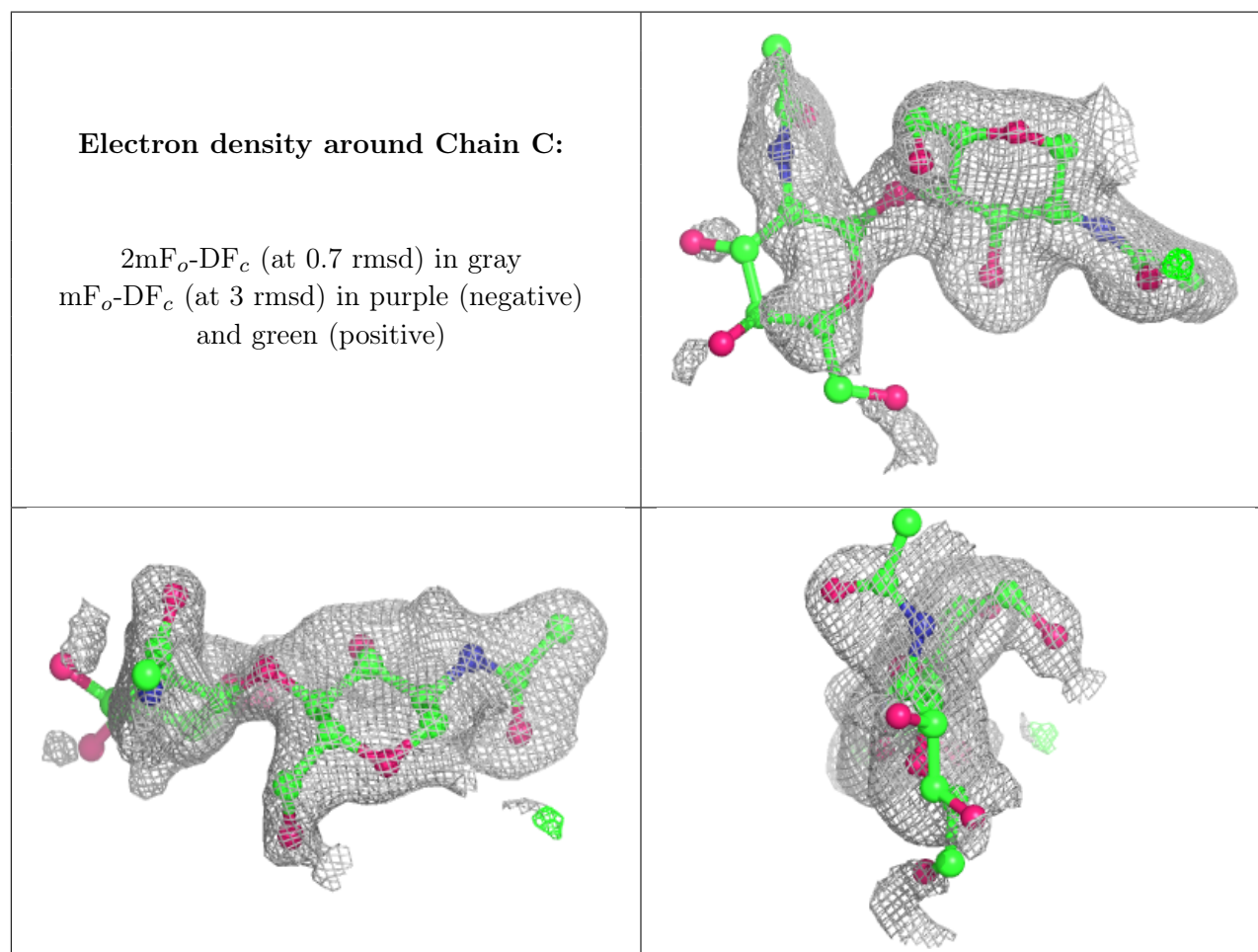
There are no non-standard protein/DNA/RNA residues in this entry.

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.

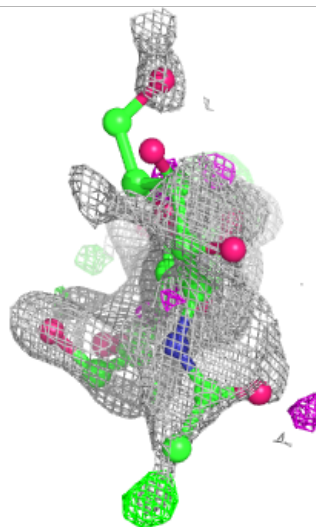
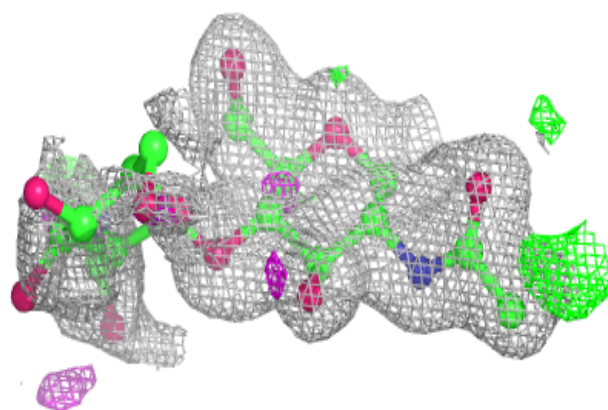
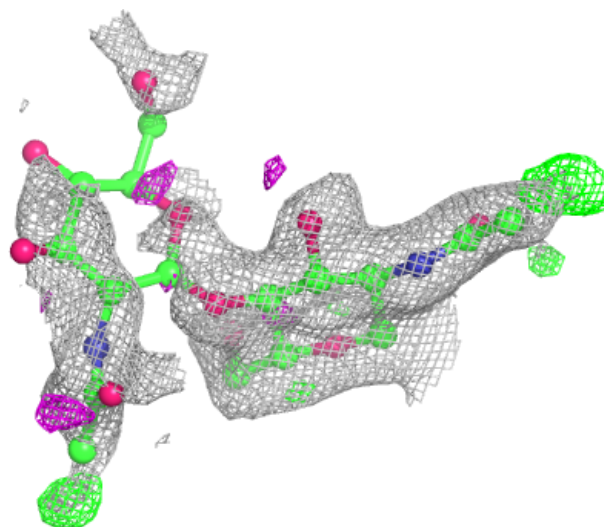
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	D	2	14/15	0.37	0.17	67,74,79,83	0
2	NAG	E	2	14/15	0.67	0.15	53,62,66,66	0
2	NAG	C	2	14/15	0.68	0.13	65,71,76,79	0
2	NAG	D	1	14/15	0.83	0.13	31,41,48,56	0
2	NAG	E	1	14/15	0.87	0.12	25,31,41,43	0
2	NAG	C	1	14/15	0.87	0.11	32,37,44,56	0

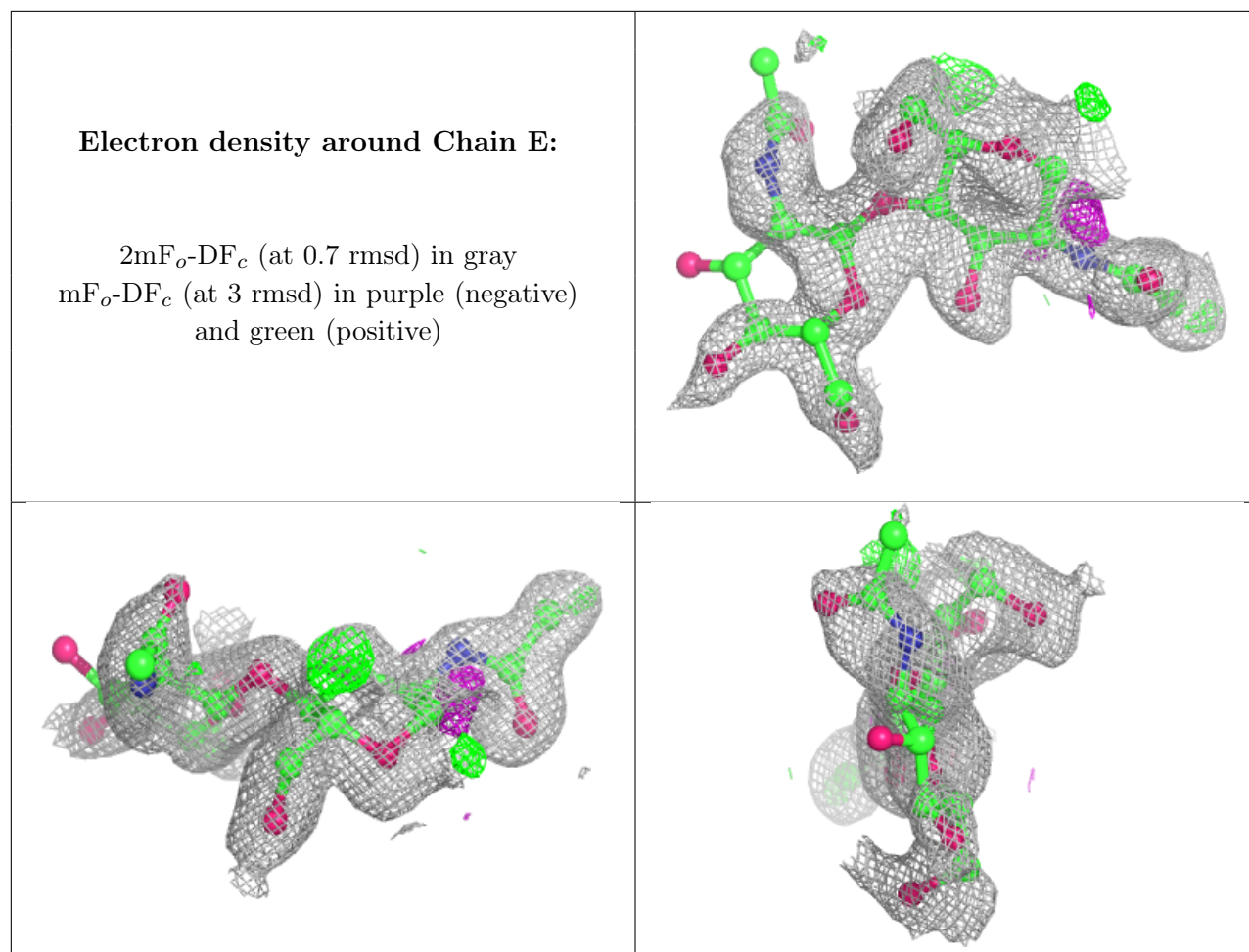
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain D:

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
3	NAG	A	303	14/15	0.71	0.16	31,45,54,55	0
4	EDO	A	304	4/4	0.75	0.20	37,39,40,46	0
4	EDO	B	306	4/4	0.78	0.17	41,43,43,43	0
6	SO4	B	311	5/5	0.80	0.13	48,50,59,63	0
4	EDO	A	306	4/4	0.84	0.15	37,37,39,40	0
6	SO4	A	309	5/5	0.87	0.10	46,52,55,57	0
5	NA	A	308	1/1	0.88	0.19	38,38,38,38	0
4	EDO	B	305	4/4	0.88	0.14	27,32,35,45	0
4	EDO	A	307	4/4	0.88	0.12	30,33,35,39	0
8	AE3	B	310	9/9	0.88	0.21	18,22,28,31	9
4	EDO	B	307	4/4	0.89	0.12	30,34,36,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	A	305	4/4	0.89	0.17	47,49,50,50	0
5	NA	B	309	1/1	0.89	0.21	39,39,39,39	0
7	GOL	B	308	6/6	0.92	0.09	21,28,29,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.