



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:56 PM UTC

PDB ID : 9N8N / pdb_00009n8n
Title : Tandem antigen chimera of Pfs230 and Pfs48/45 bound by potent mAbs
Authors : Ivanochko, D.; Semesi, A.; Julien, J.P.
Deposited on : 2025-02-09
Resolution : 2.22 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

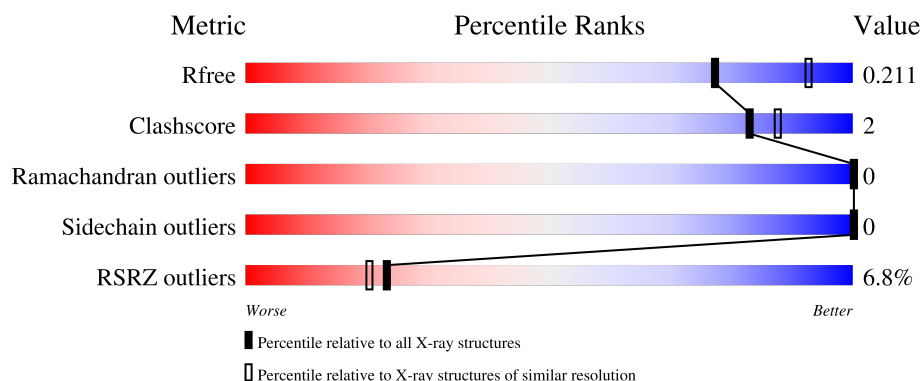
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	227	4% 90% 6% .
2	B	215	99% .
3	E	214	3% 94% . .
4	F	230	2% 90% 6% .
5	I	324	18% 84% 11% 5%

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Mol	Chain	Length	Quality of chain
6	C	3	 100%

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
14	CAC	F	302	-	X	-	-
14	CAC	F	304	-	X	-	-

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 9630 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 RUPA-39 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1626	1035	268	317	6			

- Molecule 2 is a protein called RUPA-39 Kappa chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1640	1024	280	331	5			

- Molecule 3 is a protein called RUPA-44 Kappa chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	209	Total	C	N	O	S	0	0	0
			1615	1016	269	325	5			

- Molecule 4 is a protein called RUPA-44 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	222	Total	C	N	O	S	0	0	0
			1658	1057	274	322	5			

- Molecule 5 is a protein called Gametocyte surface protein P230,Gametocyte surface protein P45/48.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	308	Total	C	N	O	S	0	0	0
			2437	1554	378	494	11			

There are 22 discrepancies between the modelled and reference sequences:

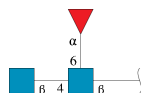
Chain	Residue	Modelled	Actual	Comment	Reference
I	34	GLN	ASN	conflict	UNP P68874

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Chain	Residue	Modelled	Actual	Comment	Reference
I	174	VAL	-	linker	UNP P68874
I	175	TYR	-	linker	UNP P68874
I	176	VAL	-	linker	UNP P68874
I	177	GLU	-	linker	UNP P68874
I	178	PRO	-	linker	UNP P68874
I	179	TYR	-	linker	UNP P68874
I	180	GLY	-	linker	UNP P68874
I	181	LYS	-	linker	UNP P68874
I	186	GLN	ASN	conflict	UNP Q8I6T1
I	195	TYR	HIS	conflict	UNP Q8I6T1
I	284	LEU	GLY	conflict	UNP Q8I6T1
I	289	VAL	ILE	conflict	UNP Q8I6T1
I	316	GLY	-	expression tag	UNP Q8I6T1
I	317	THR	-	expression tag	UNP Q8I6T1
I	318	LYS	-	expression tag	UNP Q8I6T1
I	319	HIS	-	expression tag	UNP Q8I6T1
I	320	HIS	-	expression tag	UNP Q8I6T1
I	321	HIS	-	expression tag	UNP Q8I6T1
I	322	HIS	-	expression tag	UNP Q8I6T1
I	323	HIS	-	expression tag	UNP Q8I6T1
I	324	HIS	-	expression tag	UNP Q8I6T1

- Molecule 6 is an oligosaccharide called 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
6	C	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



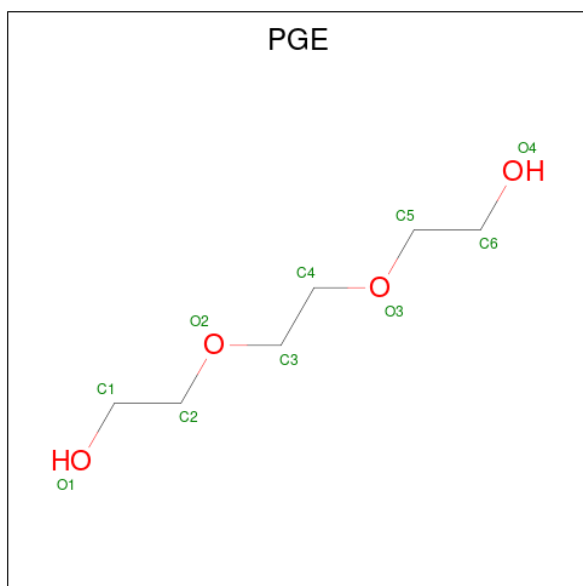
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	F	1	Total	C	O	0	0
			4	2	2		
7	F	1	Total	C	O	0	0
			4	2	2		
7	F	1	Total	C	O	0	0
			4	2	2		
7	I	1	Total	C	O	0	0
			4	2	2		
7	I	1	Total	C	O	0	0
			4	2	2		
7	I	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

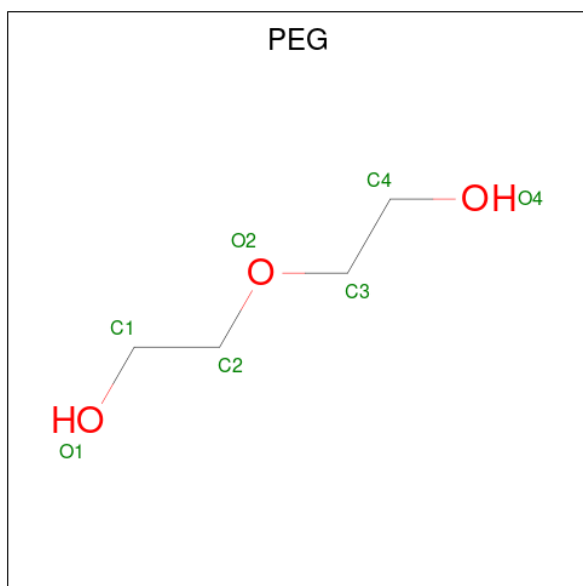
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Cl	0	0
			1	1		

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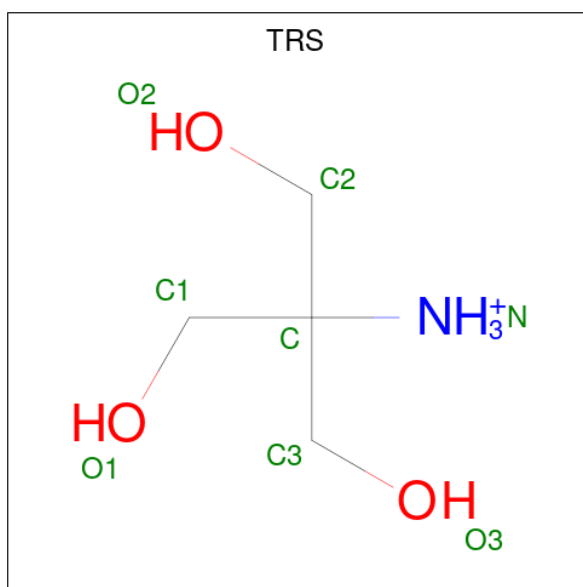
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	2	Total	Cl	0	0
			2	2		

- Molecule 10 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



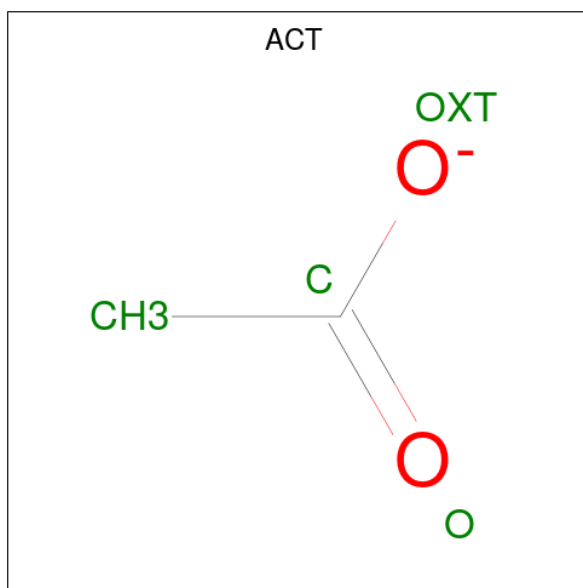
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			7	4	3		
10	B	1	Total	C	O	0	0
			7	4	3		
10	B	1	Total	C	O	0	0
			7	4	3		
10	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 11 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 12 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

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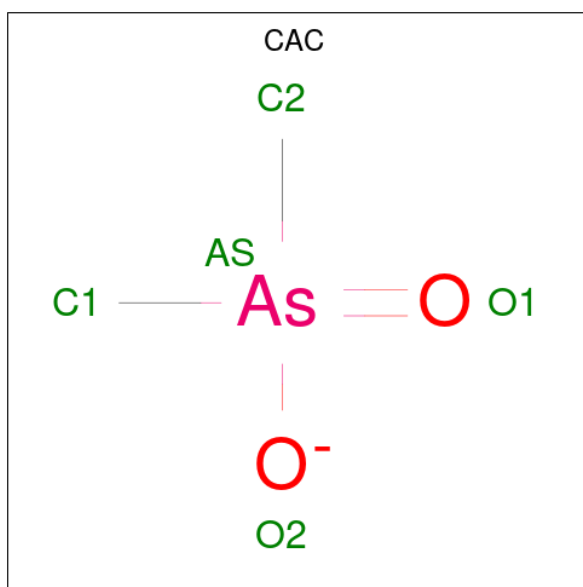
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	E	1	Total	C	O	0	0
			4	2	2		
12	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 13 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total	Ca	0	0
			1	1		
13	E	1	Total	Ca	0	0
			1	1		

- Molecule 14 is CACODYLATE ION (CCD ID: CAC) (formula: C₂H₆AsO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	F	1	Total	As	C	O	0	0
			5	1	2	2		
14	F	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	94	Total	O	0	0
			94	94		

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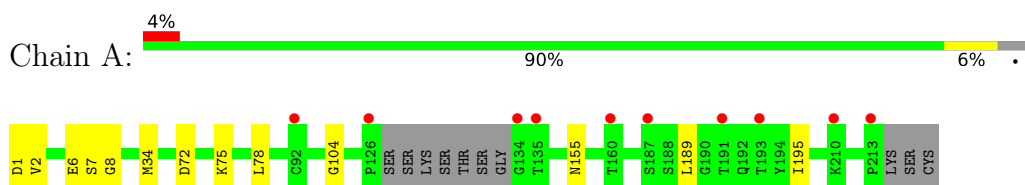
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	B	76	Total 76	O 76	0	0
15	E	103	Total 103	O 103	0	0
15	F	116	Total 116	O 116	0	0
15	I	62	Total 62	O 62	0	0

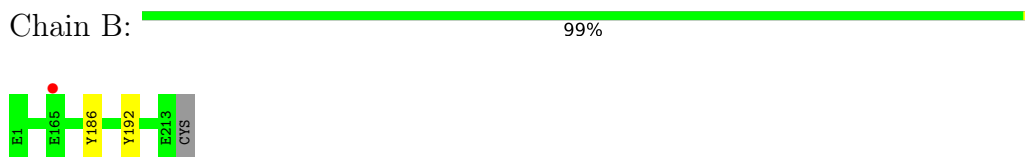
3 Residue-property plots [i](#)

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.

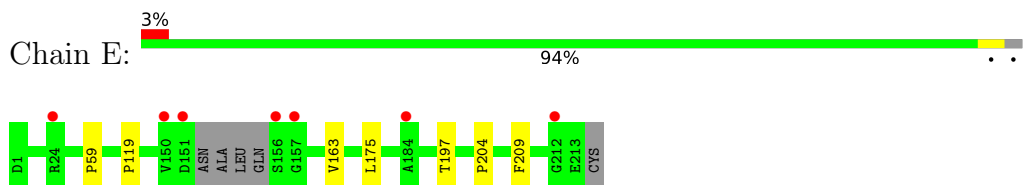
- Molecule 1: RUPA-39 heavy chain



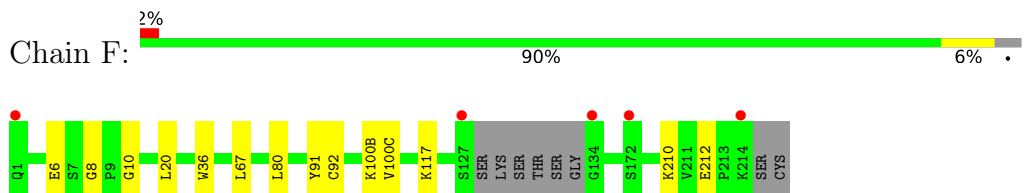
- Molecule 2: RUPA-39 Kappa chain



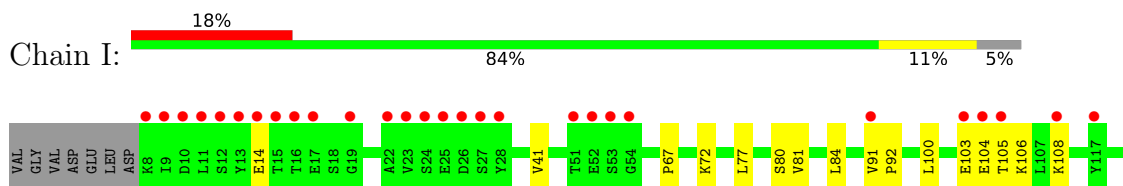
- Molecule 3: RUPA-44 Kappa chain

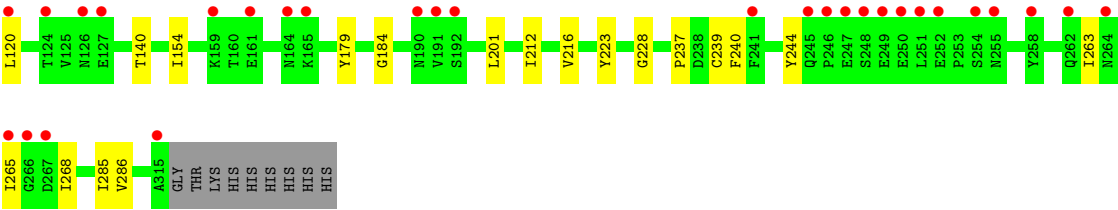


- Molecule 4: RUPA-44 heavy chain

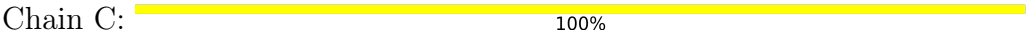


- Molecule 5: Gametocyte surface protein P230, Gametocyte surface protein P45/48





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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	227.99Å 80.49Å 137.73Å 90.00° 111.46° 90.00°	Depositor
Resolution (Å)	70.10 – 2.22 70.10 – 2.22	Depositor EDS
% Data completeness (in resolution range)	70.5 (70.10-2.22) 66.6 (70.10-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.174 , 0.210 0.176 , 0.211	Depositor DCC
R_{free} test set	1999 reflections (1.74%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 65.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9630	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: CL, PGE, PEG, ACT, FUC, CAC, TRS, CA, NAG, EDO

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	0.47	0/1665	0.67	0/2268
2	B	0.49	0/1678	0.70	0/2282
3	E	0.58	0/1652	0.78	0/2240
4	F	0.49	0/1703	0.70	0/2329
5	I	0.57	0/2486	0.80	0/3368
All	All	0.52	0/9184	0.74	0/12487

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	1626	0	1600	8	0
2	B	1640	0	1587	1	0
3	E	1615	0	1568	4	0
4	F	1658	0	1645	11	0
5	I	2437	0	2405	19	0
6	C	38	0	34	0	0
7	A	12	0	18	0	0
7	B	20	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	20	0	30	1	0
7	F	16	0	24	2	0
7	I	16	0	24	0	0
8	A	10	0	14	2	0
9	A	1	0	0	0	0
9	B	2	0	0	0	0
10	B	28	0	40	1	0
11	B	8	0	12	0	0
12	B	4	0	3	0	0
12	E	12	0	9	0	0
12	F	4	0	3	0	0
13	B	1	0	0	0	0
13	E	1	0	0	0	0
14	F	10	0	0	0	0
15	A	94	0	0	0	0
15	B	76	0	0	0	0
15	E	103	0	0	0	0
15	F	116	0	0	0	0
15	I	62	0	0	0	0
All	All	9630	0	9046	43	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.

The worst 5 of 43 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:34:MET:HB3	1:A:78:LEU:HD22	1.86	0.58
1:A:7:SER:HB2	8:A:304:PGE:H12	1.86	0.57
5:I:120:LEU:HB2	5:I:140:THR:HB	1.85	0.57
5:I:14:GLU:OE1	5:I:106:LYS:HD3	2.07	0.54
4:F:100(B):LYS:HG2	4:F:100(C):VAL:HG23	1.91	0.53

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	213/227 (94%)	209 (98%)	4 (2%)	0	100	100
2	B	212/215 (99%)	206 (97%)	6 (3%)	0	100	100
3	E	205/214 (96%)	198 (97%)	7 (3%)	0	100	100
4	F	218/230 (95%)	215 (99%)	3 (1%)	0	100	100
5	I	306/324 (94%)	284 (93%)	22 (7%)	0	100	100
All	All	1154/1210 (95%)	1112 (96%)	42 (4%)	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	182/191 (95%)	182 (100%)	0	100	100
2	B	185/186 (100%)	185 (100%)	0	100	100
3	E	184/188 (98%)	184 (100%)	0	100	100
4	F	190/197 (96%)	190 (100%)	0	100	100
5	I	287/301 (95%)	287 (100%)	0	100	100
All	All	1028/1063 (97%)	1028 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
5	I	34	GLN
5	I	35	ASN
3	E	160	GLN
3	E	199	GLN
4	F	77	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 ⓘ

3 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	$\# Z > 2$
6	NAG	C	1	4,6	14,14,15	0.44	0	17,19,21	0.85	1 (5%)
6	NAG	C	2	6	14,14,15	0.79	1 (7%)	17,19,21	0.76	1 (5%)
6	FUC	C	3	6	10,10,11	1.72	4 (40%)	14,14,16	0.80	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	NAG	C	1	4,6	-	2/6/23/26	0/1/1/1
6	NAG	C	2	6	-	4/6/23/26	0/1/1/1
6	FUC	C	3	6	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	3	FUC	C2-C3	3.18	1.57	1.52
6	C	3	FUC	O2-C2	2.29	1.48	1.43
6	C	3	FUC	O5-C5	2.16	1.47	1.43
6	C	3	FUC	C1-C2	2.13	1.57	1.52
6	C	2	NAG	C1-C2	2.10	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1	NAG	C1-O5-C5	2.58	115.65	112.19
6	C	2	NAG	C1-O5-C5	2.23	115.18	112.19

There are no chirality outliers.

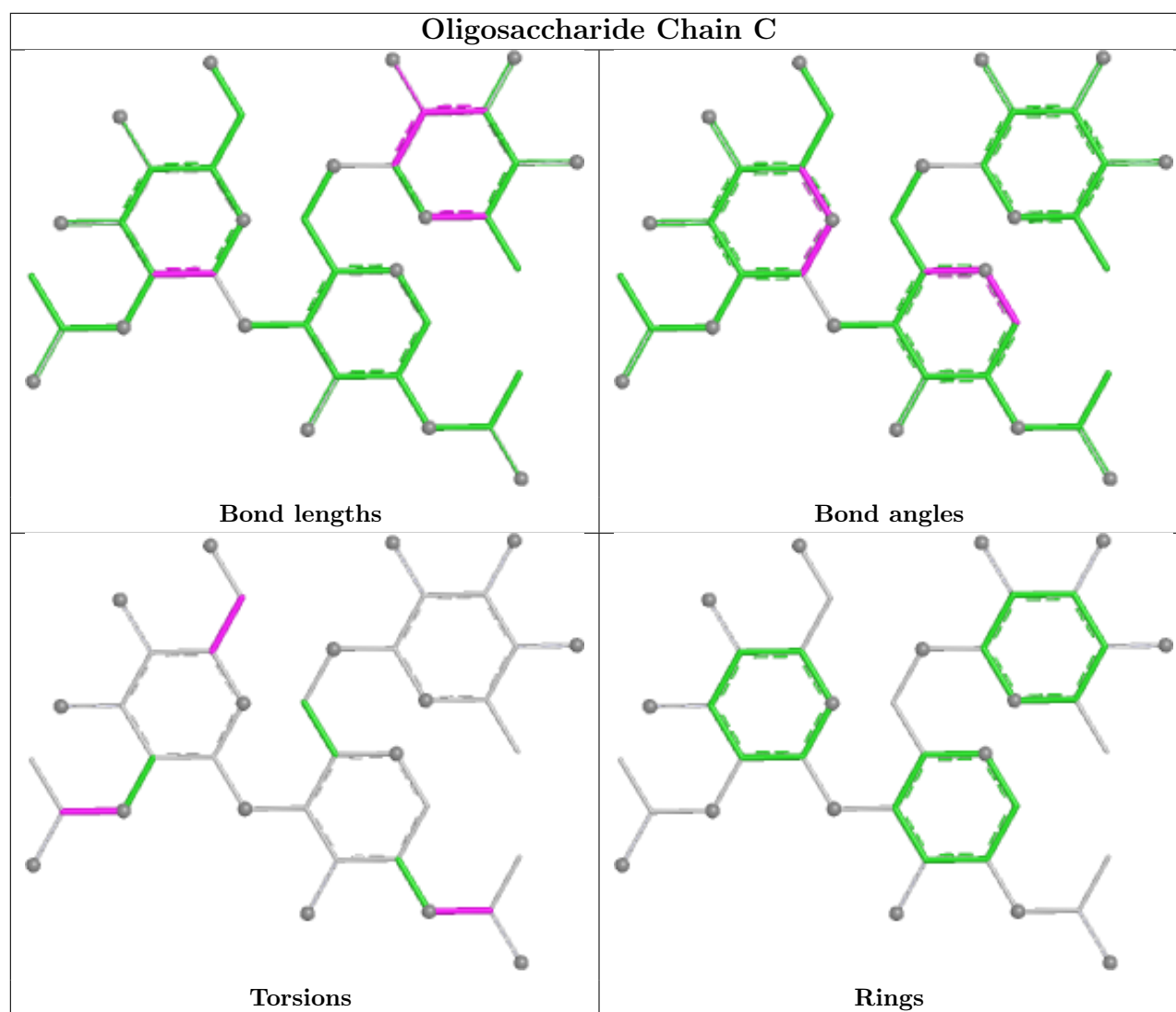
5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	2	NAG	O5-C5-C6-O6
6	C	1	NAG	C8-C7-N2-C2
6	C	1	NAG	O7-C7-N2-C2
6	C	2	NAG	C8-C7-N2-C2
6	C	2	NAG	O7-C7-N2-C2

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 39 ligands modelled in this entry, 5 are monoatomic - leaving 34 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	$\# Z > 2$
7	EDO	E	304	-	3,3,3	0.61	0	2,2,2	0.19	0
12	ACT	B	311	-	3,3,3	2.52	1 (33%)	3,3,3	1.06	0
7	EDO	E	303	-	3,3,3	0.64	0	2,2,2	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	I	402	-	3,3,3	0.43	0	2,2,2	0.47	0
7	EDO	B	307	-	3,3,3	0.33	0	2,2,2	1.12	0
7	EDO	F	303	-	3,3,3	0.25	0	2,2,2	0.92	0
7	EDO	E	305	-	3,3,3	0.55	0	2,2,2	0.64	0
7	EDO	B	301	-	3,3,3	0.53	0	2,2,2	0.29	0
7	EDO	B	304	-	3,3,3	0.55	0	2,2,2	0.31	0
7	EDO	A	303	-	3,3,3	0.54	0	2,2,2	0.46	0
7	EDO	E	301	-	3,3,3	0.48	0	2,2,2	0.64	0
7	EDO	A	301	-	3,3,3	0.54	0	2,2,2	0.32	0
7	EDO	I	404	-	3,3,3	0.37	0	2,2,2	1.15	0
12	ACT	E	302	-	3,3,3	2.10	1 (33%)	3,3,3	1.19	0
7	EDO	E	306	-	3,3,3	0.63	0	2,2,2	0.56	0
14	CAC	F	304	-	2,4,4	3.37	2 (100%)	4,6,6	2.44	2 (50%)
7	EDO	A	302	-	3,3,3	0.65	0	2,2,2	0.33	0
8	PGE	A	304	-	9,9,9	0.13	0	8,8,8	0.12	0
7	EDO	I	403	-	3,3,3	0.57	0	2,2,2	0.26	0
10	PEG	B	309	-	6,6,6	0.29	0	5,5,5	0.13	0
10	PEG	B	310	-	6,6,6	0.18	0	5,5,5	0.15	0
7	EDO	B	306	-	3,3,3	0.41	0	2,2,2	0.73	0
10	PEG	B	303	-	6,6,6	0.24	0	5,5,5	0.12	0
12	ACT	E	308	-	3,3,3	1.12	0	3,3,3	0.83	0
10	PEG	B	305	-	6,6,6	0.38	0	5,5,5	0.15	0
7	EDO	B	302	-	3,3,3	0.52	0	2,2,2	0.46	0
7	EDO	F	306	-	3,3,3	0.47	0	2,2,2	0.92	0
14	CAC	F	302	-	2,4,4	3.31	2 (100%)	4,6,6	2.56	3 (75%)
12	ACT	F	301	-	3,3,3	2.63	1 (33%)	3,3,3	1.15	0
7	EDO	F	305	-	3,3,3	0.55	0	2,2,2	0.61	0
12	ACT	E	307	-	3,3,3	1.80	1 (33%)	3,3,3	1.32	0
7	EDO	I	401	-	3,3,3	0.59	0	2,2,2	0.33	0
11	TRS	B	308	-	7,7,7	0.14	0	9,9,9	0.22	0
7	EDO	F	307	-	3,3,3	0.63	0	2,2,2	0.34	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
7	EDO	E	304	-	-	0/1/1/1	-
7	EDO	E	303	-	-	1/1/1/1	-
7	EDO	I	402	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	B	307	-	-	1/1/1/1	-
7	EDO	F	303	-	-	1/1/1/1	-
7	EDO	E	305	-	-	0/1/1/1	-
7	EDO	B	301	-	-	0/1/1/1	-
7	EDO	B	304	-	-	0/1/1/1	-
7	EDO	A	303	-	-	1/1/1/1	-
7	EDO	E	301	-	-	1/1/1/1	-
7	EDO	A	301	-	-	0/1/1/1	-
7	EDO	I	404	-	-	0/1/1/1	-
7	EDO	E	306	-	-	0/1/1/1	-
7	EDO	A	302	-	-	0/1/1/1	-
8	PGE	A	304	-	-	0/7/7/7	-
7	EDO	I	403	-	-	1/1/1/1	-
10	PEG	B	309	-	-	1/4/4/4	-
10	PEG	B	310	-	-	2/4/4/4	-
7	EDO	B	306	-	-	1/1/1/1	-
10	PEG	B	303	-	-	3/4/4/4	-
10	PEG	B	305	-	-	2/4/4/4	-
7	EDO	B	302	-	-	0/1/1/1	-
7	EDO	F	306	-	-	1/1/1/1	-
7	EDO	F	305	-	-	1/1/1/1	-
7	EDO	I	401	-	-	1/1/1/1	-
11	TRS	B	308	-	-	0/9/9/9	-
7	EDO	F	307	-	-	1/1/1/1	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	301	ACT	CH3-C	4.45	1.66	1.49
12	B	311	ACT	CH3-C	4.07	1.65	1.49
14	F	304	CAC	AS-C1	3.59	1.98	1.90
14	F	302	CAC	AS-C1	3.55	1.98	1.90
12	E	302	ACT	CH3-C	3.26	1.61	1.49

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	302	CAC	O1-AS-C2	-3.69	106.91	111.50
14	F	304	CAC	O2-AS-C2	3.49	114.30	105.84
14	F	304	CAC	O1-AS-C2	-2.69	108.16	111.50
14	F	302	CAC	O1-AS-C1	-2.63	108.22	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	302	CAC	O2-AS-C2	2.22	111.22	105.84

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	303	PEG	O1-C1-C2-O2
10	B	303	PEG	O2-C3-C4-O4
10	B	309	PEG	O1-C1-C2-O2
7	F	306	EDO	O1-C1-C2-O2
10	B	310	PEG	O2-C3-C4-O4

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	304	EDO	1	0
8	A	304	PGE	2	0
10	B	305	PEG	1	0
7	F	306	EDO	1	0
7	F	305	EDO	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 [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	217/227 (95%)	-0.06	10 (4%) 37 34	30, 51, 98, 126	0
2	B	214/215 (99%)	-0.03	1 (0%) 87 86	32, 53, 85, 105	0
3	E	209/214 (97%)	-0.14	7 (3%) 49 46	24, 46, 88, 104	0
4	F	222/230 (96%)	-0.29	5 (2%) 61 59	23, 45, 75, 100	0
5	I	308/324 (95%)	0.78	57 (18%) 3 2	30, 66, 116, 135	0
All	All	1170/1210 (96%)	0.11	80 (6%) 23 20	23, 52, 99, 135	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	I	315	ALA	7.5
5	I	251	LEU	6.3
5	I	105	THR	5.5
5	I	11	LEU	5.2
5	I	249	GLU	5.0

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.

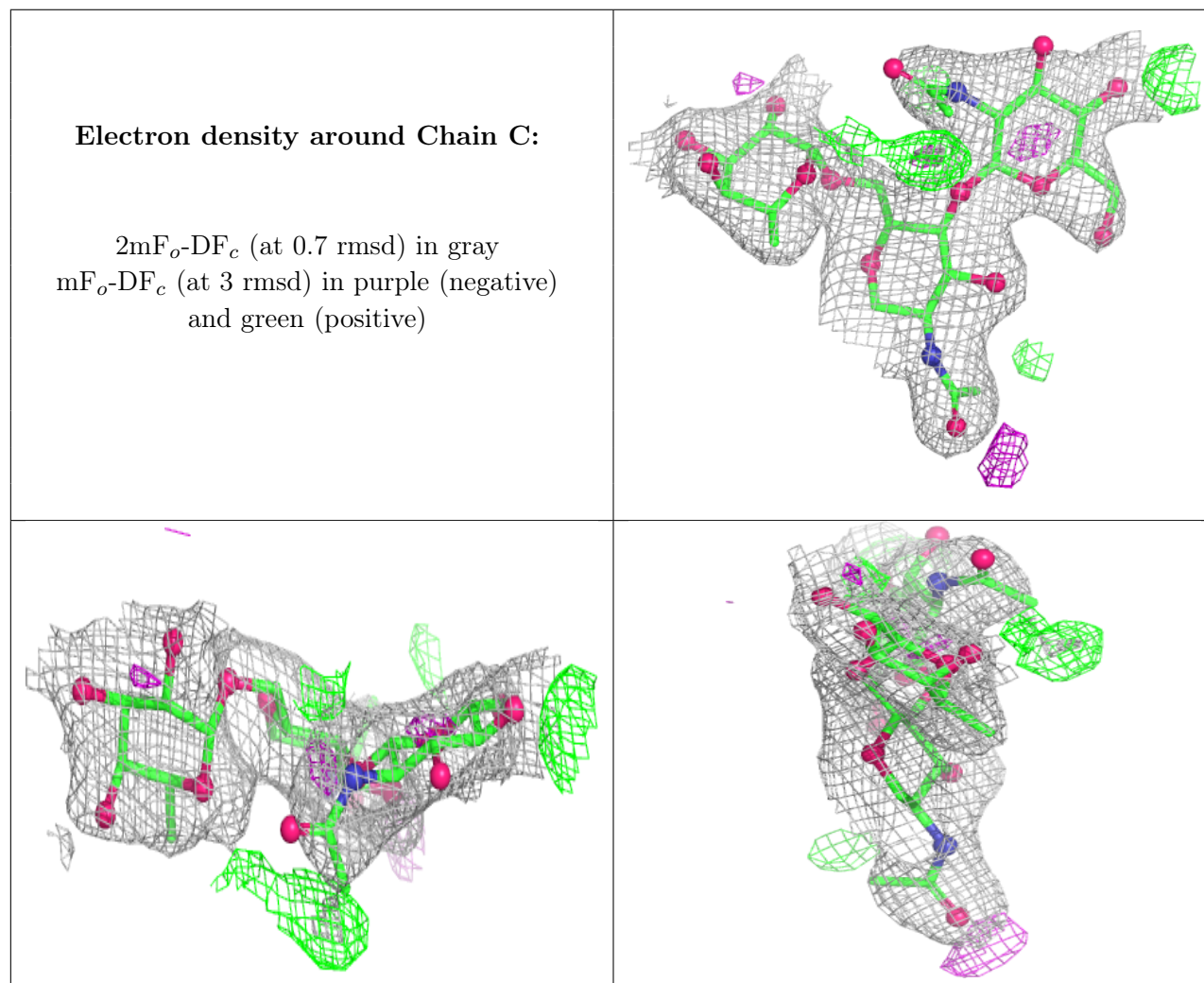
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	C	1	14/15	-	-	53,60,75,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	C	2	14/15	-	-	78,93,106,111	0
6	FUC	C	3	10/11	-	-	48,54,64,70	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 ⓘ

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
7	EDO	E	304	4/4	0.73	0.27	68,69,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	E	303	4/4	0.75	0.19	68,70,75,77	0
12	ACT	F	301	4/4	0.76	0.17	37,68,71,75	0
10	PEG	B	309	7/7	0.77	0.27	61,67,88,108	0
7	EDO	A	301	4/4	0.80	0.21	70,78,81,82	0
7	EDO	I	403	4/4	0.82	0.17	68,72,75,84	0
12	ACT	E	302	4/4	0.83	0.20	56,64,69,75	0
8	PGE	A	304	10/10	0.83	0.22	59,73,88,99	0
12	ACT	B	311	4/4	0.84	0.15	50,70,73,76	0
7	EDO	E	306	4/4	0.84	0.20	48,57,58,63	0
7	EDO	A	303	4/4	0.84	0.21	60,63,71,80	0
10	PEG	B	310	7/7	0.85	0.20	68,74,82,84	0
12	ACT	E	308	4/4	0.86	0.16	65,67,80,83	0
7	EDO	A	302	4/4	0.86	0.20	49,62,67,71	0
9	CL	B	314	1/1	0.87	0.17	90,90,90,90	0
10	PEG	B	303	7/7	0.87	0.20	68,74,86,94	0
10	PEG	B	305	7/7	0.87	0.17	47,63,72,75	0
7	EDO	F	305	4/4	0.87	0.20	54,61,66,69	0
7	EDO	F	306	4/4	0.87	0.17	57,58,58,60	0
7	EDO	F	307	4/4	0.87	0.18	39,50,67,77	0
7	EDO	I	401	4/4	0.87	0.15	62,67,69,71	0
7	EDO	E	305	4/4	0.87	0.20	47,59,67,71	0
7	EDO	B	306	4/4	0.87	0.21	48,48,51,58	0
7	EDO	E	301	4/4	0.88	0.20	55,59,64,66	0
14	CAC	F	304	5/5	0.88	0.17	66,80,96,124	0
11	TRS	B	308	8/8	0.89	0.24	20,57,75,91	0
7	EDO	B	307	4/4	0.89	0.22	54,58,69,70	0
7	EDO	B	302	4/4	0.89	0.20	44,48,64,64	0
7	EDO	I	402	4/4	0.89	0.16	74,75,79,80	0
7	EDO	B	304	4/4	0.89	0.16	61,66,70,75	0
7	EDO	B	301	4/4	0.89	0.17	50,55,77,92	0
12	ACT	E	307	4/4	0.90	0.15	58,66,71,73	0
9	CL	B	313	1/1	0.92	0.17	83,83,83,83	0
14	CAC	F	302	5/5	0.93	0.16	80,84,89,102	0
9	CL	A	305	1/1	0.95	0.13	61,61,61,61	0
7	EDO	I	404	4/4	0.96	0.12	26,41,49,52	0
13	CA	B	312	1/1	0.96	0.12	79,79,79,79	0
7	EDO	F	303	4/4	0.97	0.08	40,41,51,52	0
13	CA	E	309	1/1	1.00	0.02	35,35,35,35	1

6.5 Other polymers ⓘ

There are no such residues in this entry.