



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 11, 2025 – 02:08 pm BST

PDB ID : 9QWJ / pdb_00009qwj
Title : Crystal structure of S2c TCR in complex with CD1c
Authors : Karuppiah, V.
Deposited on : 2025-04-14
Resolution : 2.04 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 Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

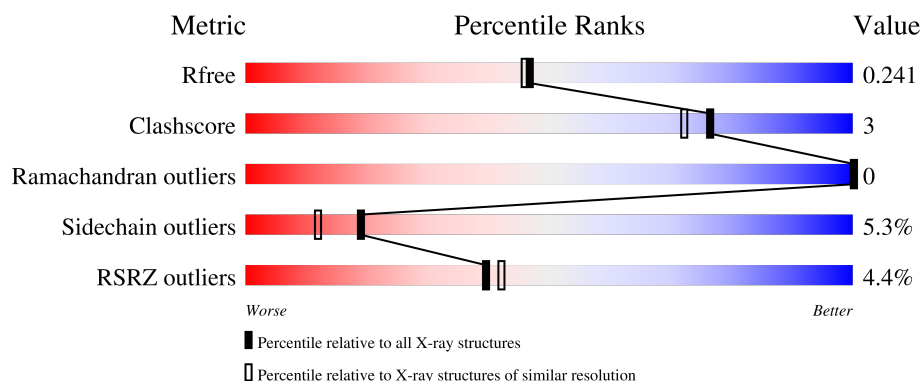
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

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	B	442	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>9%</div> <div>15%</div> </div> </div>
1	N	442	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>7%</div> <div>17%</div> </div> </div>
2	D	199	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>7%</div> </div> </div>
2	T	199	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>5%</div> </div> </div>
3	E	246	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	U	246	<div><div></div><div>2%</div><div>90%</div><div>8% ..</div></div>
4	C	2	<div><div></div><div>100%</div></div>
4	F	2	<div><div></div><div>50%</div><div>50%</div></div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 13571 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 Beta-2-microglobulin,T-cell surface glycoprotein CD1c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	374	Total	C	N	O	S	0	0	0
			3017	1929	516	562	10			
1	N	367	Total	C	N	O	S	0	0	0
			2969	1902	509	548	10			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	MET	-	initiating methionine	UNP P61769
B	-17	TYR	-	expression tag	UNP P61769
B	-16	ARG	-	expression tag	UNP P61769
B	-15	MET	-	expression tag	UNP P61769
B	-14	GLN	-	expression tag	UNP P61769
B	-13	LEU	-	expression tag	UNP P61769
B	-12	LEU	-	expression tag	UNP P61769
B	-11	SER	-	expression tag	UNP P61769
B	-10	CYS	-	expression tag	UNP P61769
B	-9	ILE	-	expression tag	UNP P61769
B	-8	ALA	-	expression tag	UNP P61769
B	-7	LEU	-	expression tag	UNP P61769
B	-6	SER	-	expression tag	UNP P61769
B	-5	LEU	-	expression tag	UNP P61769
B	-4	ALA	-	expression tag	UNP P61769
B	-3	LEU	-	expression tag	UNP P61769
B	-2	VAL	-	expression tag	UNP P61769
B	-1	THR	-	expression tag	UNP P61769
B	0	ASN	-	expression tag	UNP P61769
B	1	SER	-	expression tag	UNP P61769
B	100	ILE	-	linker	UNP P61769
B	101	GLY	-	linker	UNP P61769
B	102	GLY	-	linker	UNP P61769
B	103	GLY	-	linker	UNP P61769
B	104	GLY	-	linker	UNP P61769

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Chain	Residue	Modelled	Actual	Comment	Reference
B	105	SER	-	linker	UNP P61769
B	106	GLY	-	linker	UNP P61769
B	107	GLY	-	linker	UNP P61769
B	108	GLY	-	linker	UNP P61769
B	109	GLY	-	linker	UNP P61769
B	110	SER	-	linker	UNP P61769
B	111	GLY	-	linker	UNP P61769
B	112	GLY	-	linker	UNP P61769
B	113	GLY	-	linker	UNP P61769
B	114	GLY	-	linker	UNP P61769
B	115	SER	-	linker	UNP P61769
B	390	SER	-	expression tag	UNP P29017
B	391	LEU	-	expression tag	UNP P29017
B	392	SER	-	expression tag	UNP P29017
B	393	THR	-	expression tag	UNP P29017
B	394	PRO	-	expression tag	UNP P29017
B	395	PRO	-	expression tag	UNP P29017
B	396	THR	-	expression tag	UNP P29017
B	397	PRO	-	expression tag	UNP P29017
B	398	SER	-	expression tag	UNP P29017
B	399	THR	-	expression tag	UNP P29017
B	400	PRO	-	expression tag	UNP P29017
B	401	PRO	-	expression tag	UNP P29017
B	402	THR	-	expression tag	UNP P29017
B	403	GLY	-	expression tag	UNP P29017
B	404	LEU	-	expression tag	UNP P29017
B	405	ASN	-	expression tag	UNP P29017
B	406	ASP	-	expression tag	UNP P29017
B	407	ILE	-	expression tag	UNP P29017
B	408	PHE	-	expression tag	UNP P29017
B	409	GLU	-	expression tag	UNP P29017
B	410	ALA	-	expression tag	UNP P29017
B	411	GLN	-	expression tag	UNP P29017
B	412	LYS	-	expression tag	UNP P29017
B	413	ILE	-	expression tag	UNP P29017
B	414	GLU	-	expression tag	UNP P29017
B	415	TRP	-	expression tag	UNP P29017
B	416	HIS	-	expression tag	UNP P29017
B	417	GLU	-	expression tag	UNP P29017
B	418	HIS	-	expression tag	UNP P29017
B	419	HIS	-	expression tag	UNP P29017
B	420	HIS	-	expression tag	UNP P29017

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Chain	Residue	Modelled	Actual	Comment	Reference
B	421	HIS	-	expression tag	UNP P29017
B	422	HIS	-	expression tag	UNP P29017
B	423	HIS	-	expression tag	UNP P29017
N	-18	MET	-	initiating methionine	UNP P61769
N	-17	TYR	-	expression tag	UNP P61769
N	-16	ARG	-	expression tag	UNP P61769
N	-15	MET	-	expression tag	UNP P61769
N	-14	GLN	-	expression tag	UNP P61769
N	-13	LEU	-	expression tag	UNP P61769
N	-12	LEU	-	expression tag	UNP P61769
N	-11	SER	-	expression tag	UNP P61769
N	-10	CYS	-	expression tag	UNP P61769
N	-9	ILE	-	expression tag	UNP P61769
N	-8	ALA	-	expression tag	UNP P61769
N	-7	LEU	-	expression tag	UNP P61769
N	-6	SER	-	expression tag	UNP P61769
N	-5	LEU	-	expression tag	UNP P61769
N	-4	ALA	-	expression tag	UNP P61769
N	-3	LEU	-	expression tag	UNP P61769
N	-2	VAL	-	expression tag	UNP P61769
N	-1	THR	-	expression tag	UNP P61769
N	0	ASN	-	expression tag	UNP P61769
N	1	SER	-	expression tag	UNP P61769
N	100	ILE	-	linker	UNP P61769
N	101	GLY	-	linker	UNP P61769
N	102	GLY	-	linker	UNP P61769
N	103	GLY	-	linker	UNP P61769
N	104	GLY	-	linker	UNP P61769
N	105	SER	-	linker	UNP P61769
N	106	GLY	-	linker	UNP P61769
N	107	GLY	-	linker	UNP P61769
N	108	GLY	-	linker	UNP P61769
N	109	GLY	-	linker	UNP P61769
N	110	SER	-	linker	UNP P61769
N	111	GLY	-	linker	UNP P61769
N	112	GLY	-	linker	UNP P61769
N	113	GLY	-	linker	UNP P61769
N	114	GLY	-	linker	UNP P61769
N	115	SER	-	linker	UNP P61769
N	390	SER	-	expression tag	UNP P29017
N	391	LEU	-	expression tag	UNP P29017
N	392	SER	-	expression tag	UNP P29017

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Chain	Residue	Modelled	Actual	Comment	Reference
N	393	THR	-	expression tag	UNP P29017
N	394	PRO	-	expression tag	UNP P29017
N	395	PRO	-	expression tag	UNP P29017
N	396	THR	-	expression tag	UNP P29017
N	397	PRO	-	expression tag	UNP P29017
N	398	SER	-	expression tag	UNP P29017
N	399	THR	-	expression tag	UNP P29017
N	400	PRO	-	expression tag	UNP P29017
N	401	PRO	-	expression tag	UNP P29017
N	402	THR	-	expression tag	UNP P29017
N	403	GLY	-	expression tag	UNP P29017
N	404	LEU	-	expression tag	UNP P29017
N	405	ASN	-	expression tag	UNP P29017
N	406	ASP	-	expression tag	UNP P29017
N	407	ILE	-	expression tag	UNP P29017
N	408	PHE	-	expression tag	UNP P29017
N	409	GLU	-	expression tag	UNP P29017
N	410	ALA	-	expression tag	UNP P29017
N	411	GLN	-	expression tag	UNP P29017
N	412	LYS	-	expression tag	UNP P29017
N	413	ILE	-	expression tag	UNP P29017
N	414	GLU	-	expression tag	UNP P29017
N	415	TRP	-	expression tag	UNP P29017
N	416	HIS	-	expression tag	UNP P29017
N	417	GLU	-	expression tag	UNP P29017
N	418	HIS	-	expression tag	UNP P29017
N	419	HIS	-	expression tag	UNP P29017
N	420	HIS	-	expression tag	UNP P29017
N	421	HIS	-	expression tag	UNP P29017
N	422	HIS	-	expression tag	UNP P29017
N	423	HIS	-	expression tag	UNP P29017

- Molecule 2 is a protein called TCR alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	186	Total	C	N	O	S	0	1	0
			1450	915	231	296	8			
2	T	189	Total	C	N	O	S	0	0	0
			1465	922	235	300	8			

- Molecule 3 is a protein called TCR beta.

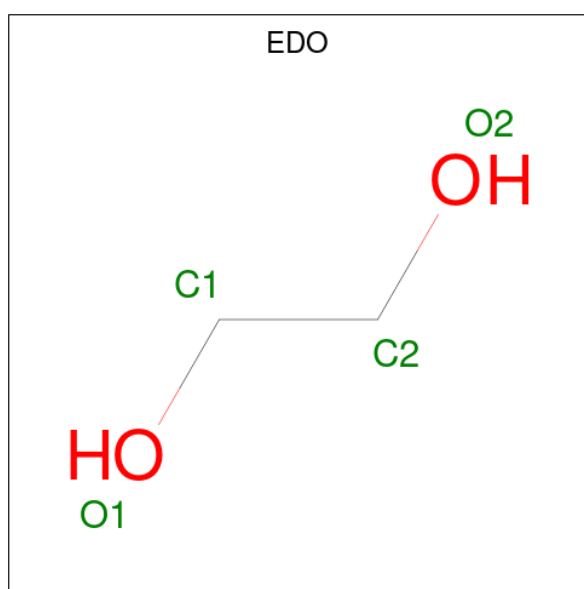
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	244	Total	C	N	O	S	0	0	0
			1961	1227	354	374	6			
3	U	244	Total	C	N	O	S	0	0	0
			1961	1227	354	374	6			

- Molecule 4 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
4	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



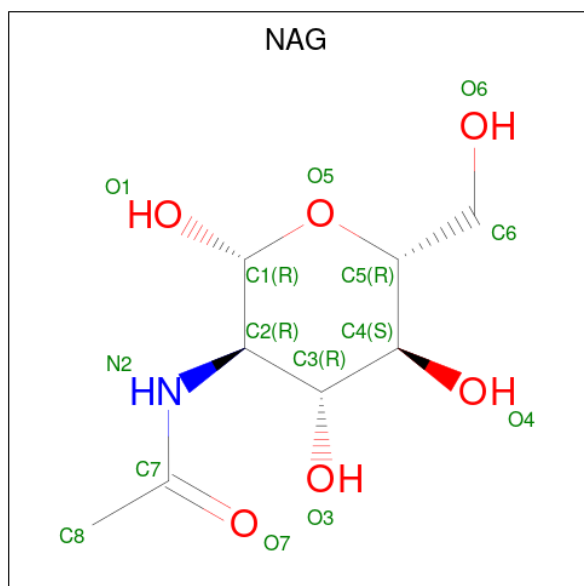
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

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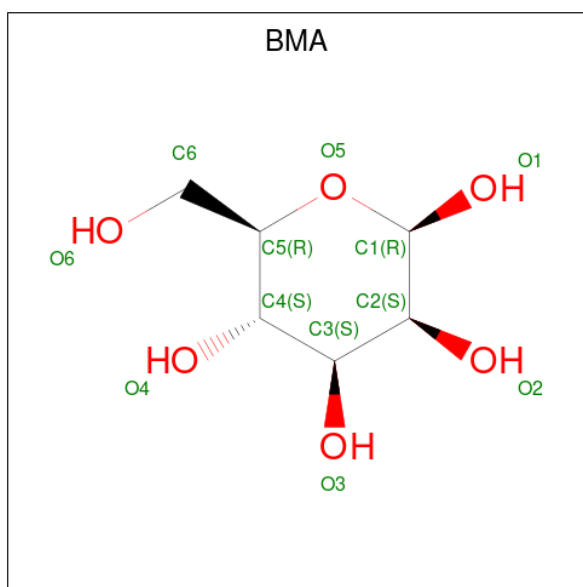
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			4	2	2		
5	N	1	Total	C	O	0	0
			4	2	2		
5	N	1	Total	C	O	0	0
			4	2	2		
5	T	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



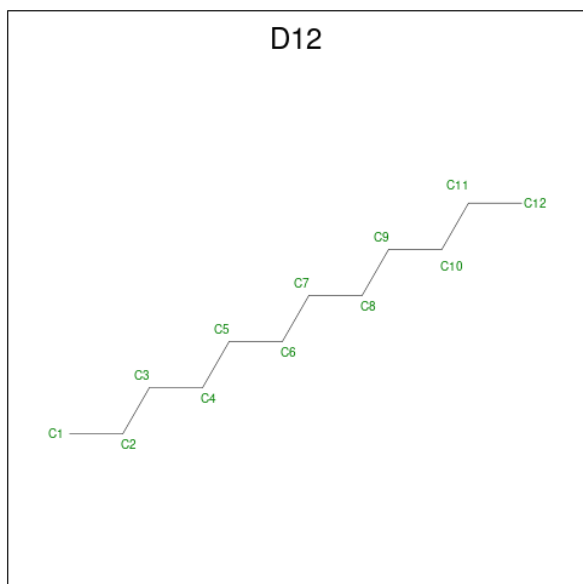
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	N	1	Total	C	N	O	0	0
			14	8	1	5		
6	N	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is beta-D-mannopyranose (CCD ID: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			11	6	5		
7	N	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is DODECANE (CCD ID: D12) (formula: $C_{12}H_{26}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	C	0	0
			12	12		

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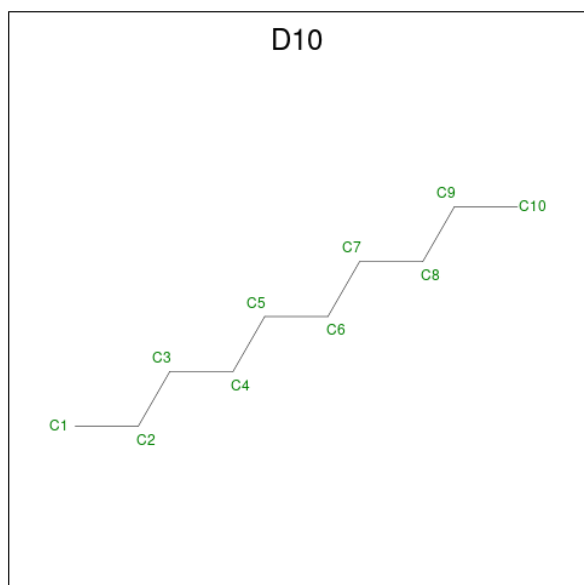
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C 12 12	0	0

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total Ca 1 1	0	0
9	T	2	Total Ca 2 2	0	0

- Molecule 10 is DECANE (CCD ID: D10) (formula: C₁₀H₂₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	N	1	Total C 10 10	0	0
10	N	1	Total C 10 10	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	141	Total O 141 141	0	0

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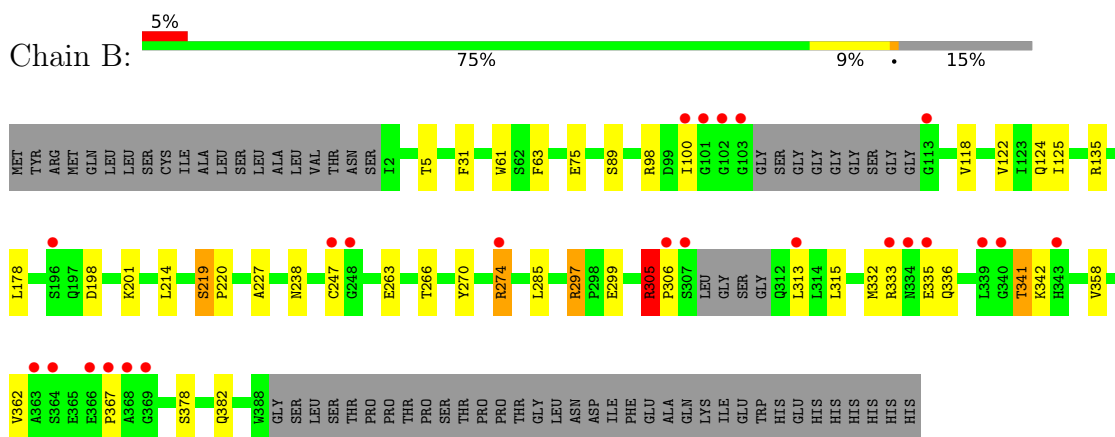
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	55	Total 55	O 55	0	0
11	E	86	Total 86	O 86	0	0
11	N	101	Total 101	O 101	0	0
11	T	63	Total 63	O 63	0	0
11	U	65	Total 65	O 65	0	0

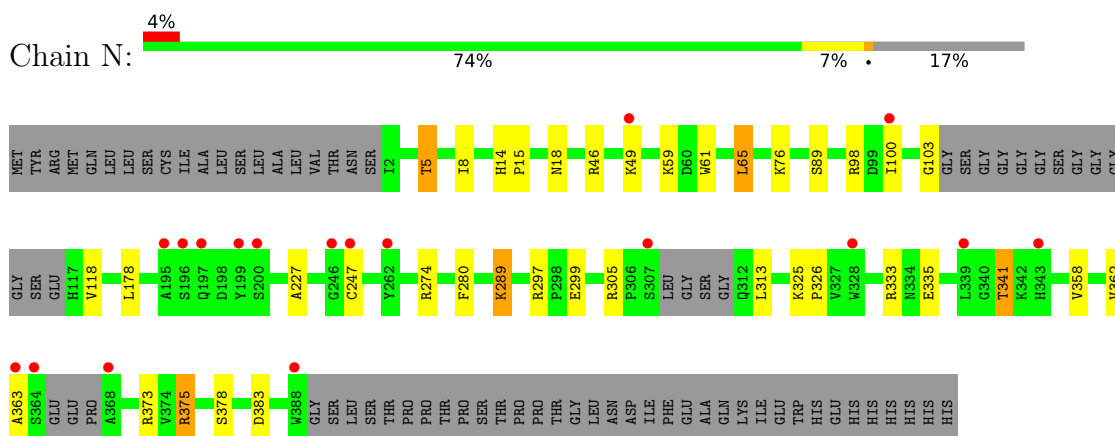
3 Residue-property plots [i](#)

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.

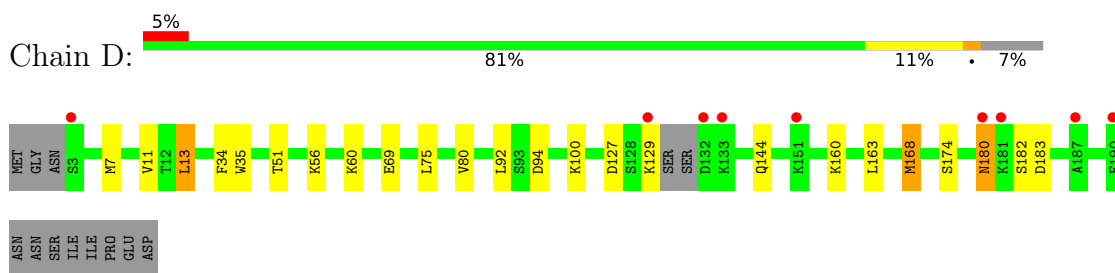
- Molecule 1: Beta-2-microglobulin,T-cell surface glycoprotein CD1c




- Molecule 1: Beta-2-microglobulin,T-cell surface glycoprotein CD1c

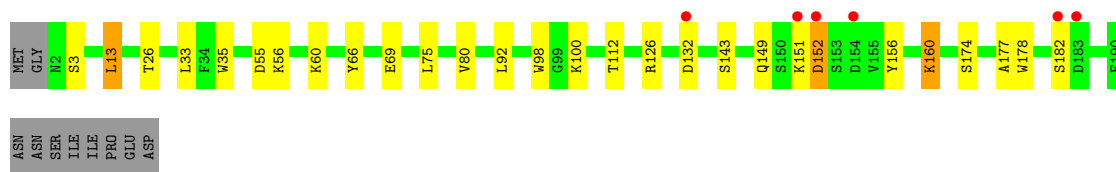


- Molecule 2: TCR alpha




- Molecule 2: TCR alpha

Chain T:  3% 81% 13% 5%




- Molecule 3: TCR beta

Chain E:  3% 89% 9%



- Molecule 3: TCR beta

Chain U:  2% 90% 8%



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

Chain C:  100%



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

Chain F:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.37Å 122.07Å 108.70Å 90.00° 110.03° 90.00°	Depositor
Resolution (Å)	67.03 – 2.04 67.03 – 2.04	Depositor EDS
% Data completeness (in resolution range)	100.0 (67.03-2.04) 100.0 (67.03-2.04)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.200 , 0.235 0.208 , 0.241	Depositor DCC
R_{free} test set	6481 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13571	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.70% 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: NAG, BMA, EDO, D10, D12, CA

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	B	0.73	0/3105	1.13	4/4215 (0.1%)
1	N	0.68	0/3055	1.12	3/4146 (0.1%)
2	D	0.69	0/1484	1.18	5/2012 (0.2%)
2	T	0.70	0/1497	1.16	4/2031 (0.2%)
3	E	0.70	0/2012	1.13	4/2731 (0.1%)
3	U	0.69	0/2012	1.19	5/2731 (0.2%)
All	All	0.70	0/13165	1.15	25/17866 (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	6
1	N	0	4
2	T	0	1
3	E	0	7
3	U	0	3
All	All	0	21

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	60	LYS	CB-CA-C	-7.66	100.62	111.80
3	U	28	GLU	CB-CA-C	-7.30	102.60	109.83
2	D	127	ASP	CA-CB-CG	7.24	119.84	112.60
1	B	266	THR	CA-CB-OG1	-7.18	98.83	109.60
1	N	5	THR	CB-CA-C	6.98	118.71	108.87

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	135	ARG	Sidechain
1	B	274	ARG	Sidechain
1	B	297	ARG	Sidechain
1	B	305	ARG	Sidechain
1	B	98	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	B	3017	0	2862	13	0
1	N	2969	0	2826	13	0
2	D	1450	0	1370	11	0
2	T	1465	0	1383	10	0
3	E	1961	0	1866	9	0
3	U	1961	0	1866	10	0
4	C	28	0	24	0	0
4	F	28	0	24	0	0
5	B	8	0	12	0	0
5	D	4	0	6	0	0
5	E	4	0	6	0	0
5	N	8	0	12	0	0
5	T	4	0	6	0	0
6	B	56	0	52	9	0
6	N	28	0	26	4	0
7	B	11	0	10	0	0
7	N	11	0	10	0	0
8	B	24	0	52	0	0
9	D	1	0	0	0	0
9	T	2	0	0	0	0
10	N	20	0	44	0	0
11	B	141	0	0	0	0
11	D	55	0	0	0	0
11	E	86	0	0	0	0
11	N	101	0	0	0	0
11	T	63	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	U	65	0	0	0	0
All	All	13571	0	12457	71	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.

The worst 5 of 71 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)
6:B:902:NAG:O4	6:B:903:NAG:C1	2.01	1.09
6:N:902:NAG:O4	6:N:903:NAG:C1	1.99	1.08
6:B:902:NAG:HO4	6:B:903:NAG:C1	1.88	0.85
6:B:905:NAG:O4	6:B:906:NAG:C1	2.24	0.84
2:D:163:LEU:HB3	3:E:172:CYS:HB2	1.69	0.75

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	B	368/442 (83%)	349 (95%)	19 (5%)	0	100	100
1	N	359/442 (81%)	352 (98%)	7 (2%)	0	100	100
2	D	183/199 (92%)	175 (96%)	8 (4%)	0	100	100
2	T	187/199 (94%)	179 (96%)	8 (4%)	0	100	100
3	E	242/246 (98%)	234 (97%)	8 (3%)	0	100	100
3	U	242/246 (98%)	236 (98%)	6 (2%)	0	100	100
All	All	1581/1774 (89%)	1525 (96%)	56 (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	B	330/384 (86%)	312 (94%)	18 (6%)	18	11
1	N	325/384 (85%)	309 (95%)	16 (5%)	21	14
2	D	162/173 (94%)	151 (93%)	11 (7%)	13	7
2	T	164/173 (95%)	153 (93%)	11 (7%)	13	7
3	E	212/214 (99%)	202 (95%)	10 (5%)	22	16
3	U	212/214 (99%)	204 (96%)	8 (4%)	28	22
All	All	1405/1542 (91%)	1331 (95%)	74 (5%)	19	12

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	T	56	LYS
3	U	194	ARG
2	T	100	LYS
2	T	182	SER
2	D	129	LYS

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

Mol	Chain	Res	Type
1	B	9	GLN
1	B	336	GLN
2	D	95	GLN
3	E	84	GLN
3	E	108	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 ⓘ

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	$\# Z > 2$
4	NAG	C	1	4,1	14,14,15	0.39	0	17,19,21	1.10	2 (11%)
4	NAG	C	2	4	14,14,15	0.44	0	17,19,21	1.35	1 (5%)
4	NAG	F	1	4,1	14,14,15	0.67	1 (7%)	17,19,21	1.67	4 (23%)
4	NAG	F	2	4	14,14,15	0.40	0	17,19,21	0.94	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	NAG	C	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	C	2	4	-	2/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1	NAG	C1-C2	2.01	1.55	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2	NAG	C2-N2-C7	3.98	128.58	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	NAG	C4-C3-C2	3.81	116.60	111.02
4	F	1	NAG	O4-C4-C3	-3.60	102.03	110.35
4	C	1	NAG	C1-O5-C5	3.33	116.71	112.19
4	F	1	NAG	C2-N2-C7	-2.63	119.16	122.90

There are no chirality outliers.

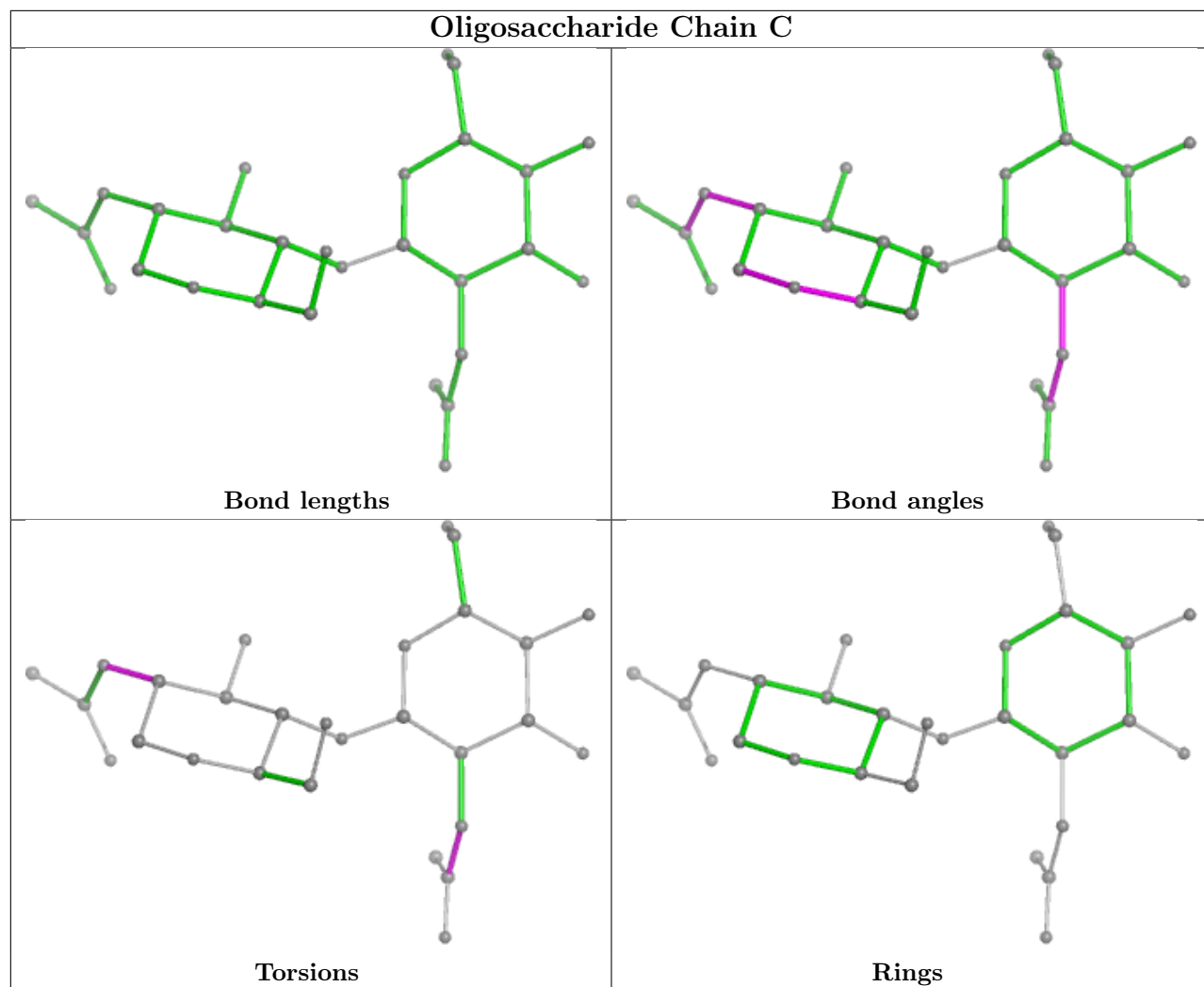
All (3) torsion outliers are listed below:

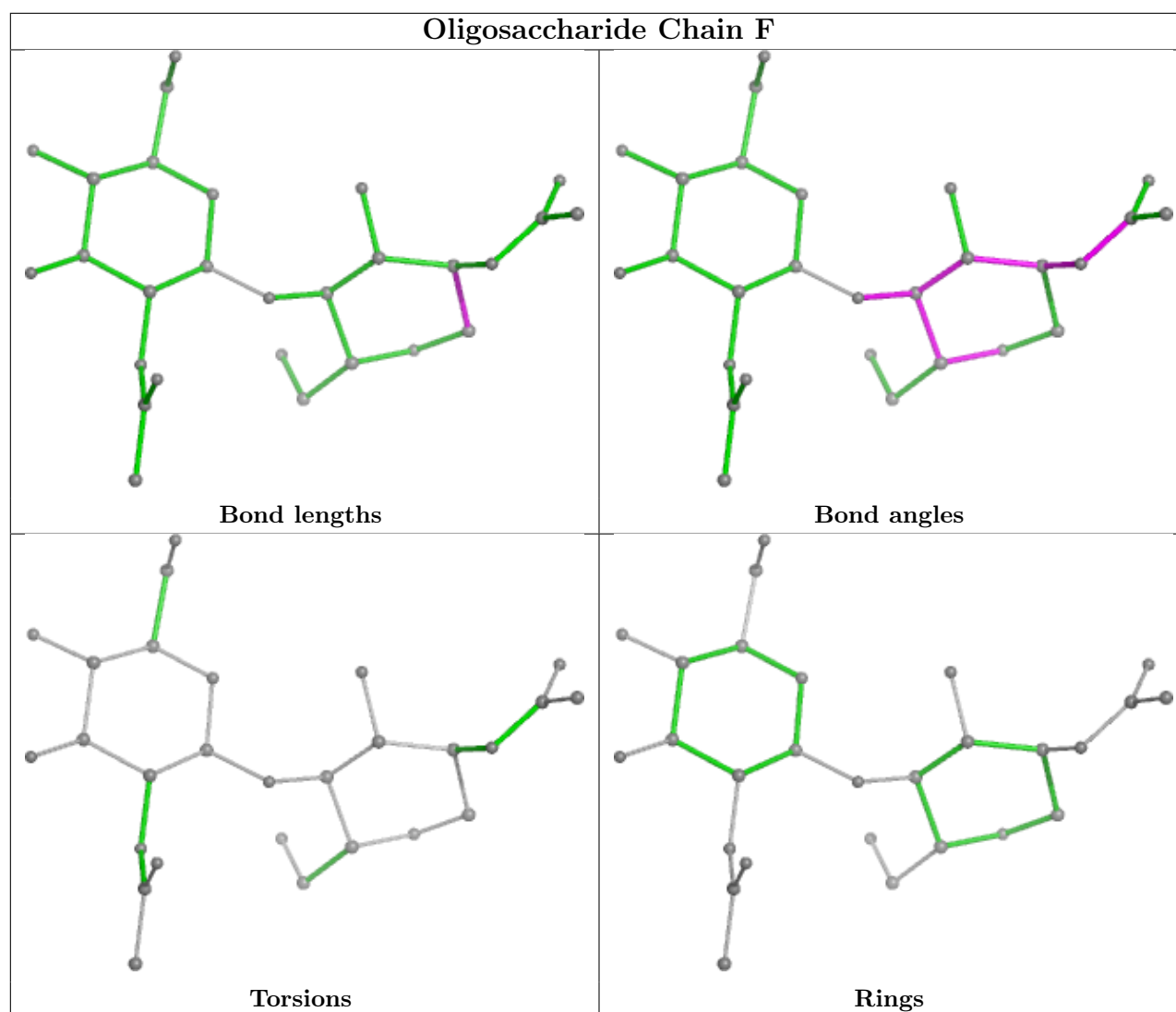
Mol	Chain	Res	Type	Atoms
4	C	2	NAG	C8-C7-N2-C2
4	C	2	NAG	O7-C7-N2-C2
4	C	1	NAG	C3-C2-N2-C7

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 22 ligands modelled in this entry, 3 are monoatomic - leaving 19 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	$\# Z > 2$
5	EDO	N	901	-	3,3,3	0.16	0	2,2,2	0.17	0
5	EDO	B	909	-	3,3,3	0.09	0	2,2,2	0.10	0
8	D12	B	907	-	11,11,11	0.58	0	10,10,10	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	D10	N	907	-	9,9,9	0.13	0	8,8,8	0.09	0
10	D10	N	906	-	9,9,9	0.47	0	8,8,8	0.66	0
5	EDO	T	201	-	3,3,3	0.25	0	2,2,2	0.29	0
6	NAG	B	906	-	14,14,15	0.51	0	17,19,21	1.07	1 (5%)
5	EDO	B	901	-	3,3,3	0.43	0	2,2,2	0.49	0
6	NAG	N	903	-	14,14,15	0.41	0	17,19,21	1.37	2 (11%)
5	EDO	N	905	-	3,3,3	0.19	0	2,2,2	0.29	0
6	NAG	N	902	1	14,14,15	0.44	0	17,19,21	1.10	2 (11%)
7	BMA	N	904	-	11,11,12	1.12	1 (9%)	15,15,17	1.11	1 (6%)
5	EDO	E	301	-	3,3,3	0.16	0	2,2,2	0.42	0
6	NAG	B	903	-	14,14,15	0.44	0	17,19,21	0.73	0
6	NAG	B	902	1	14,14,15	0.37	0	17,19,21	1.13	1 (5%)
8	D12	B	908	-	11,11,11	0.27	0	10,10,10	0.33	0
6	NAG	B	905	1	14,14,15	0.45	0	17,19,21	1.16	1 (5%)
5	EDO	D	201	-	3,3,3	0.29	0	2,2,2	0.49	0
7	BMA	B	904	-	11,11,12	0.94	0	15,15,17	1.08	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
5	EDO	N	901	-	-	0/1/1/1	-
5	EDO	B	909	-	-	0/1/1/1	-
8	D12	B	907	-	-	4/9/9/9	-
10	D10	N	907	-	-	1/7/7/7	-
10	D10	N	906	-	-	2/7/7/7	-
5	EDO	T	201	-	-	0/1/1/1	-
6	NAG	B	906	-	-	2/6/23/26	0/1/1/1
5	EDO	B	901	-	-	0/1/1/1	-
6	NAG	N	903	-	-	4/6/23/26	0/1/1/1
5	EDO	N	905	-	-	0/1/1/1	-
6	NAG	N	902	1	-	2/6/23/26	0/1/1/1
7	BMA	N	904	-	-	0/2/19/22	0/1/1/1
5	EDO	E	301	-	-	0/1/1/1	-
6	NAG	B	903	-	-	2/6/23/26	0/1/1/1
6	NAG	B	902	1	-	2/6/23/26	0/1/1/1
8	D12	B	908	-	-	4/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	905	1	-	2/6/23/26	0/1/1/1
5	EDO	D	201	-	-	0/1/1/1	-
7	BMA	B	904	-	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	904	BMA	C4-C5	2.05	1.57	1.53

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	903	NAG	O5-C1-C2	3.86	117.38	111.29
6	B	902	NAG	O5-C1-C2	-2.74	106.97	111.29
7	B	904	BMA	C3-C4-C5	2.60	114.88	110.24
6	B	905	NAG	C4-C3-C2	-2.55	107.28	111.02
6	N	902	NAG	O5-C1-C2	-2.53	107.29	111.29

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	902	NAG	C8-C7-N2-C2
6	B	902	NAG	O7-C7-N2-C2
6	B	905	NAG	C8-C7-N2-C2
6	B	905	NAG	O7-C7-N2-C2
6	N	902	NAG	C8-C7-N2-C2

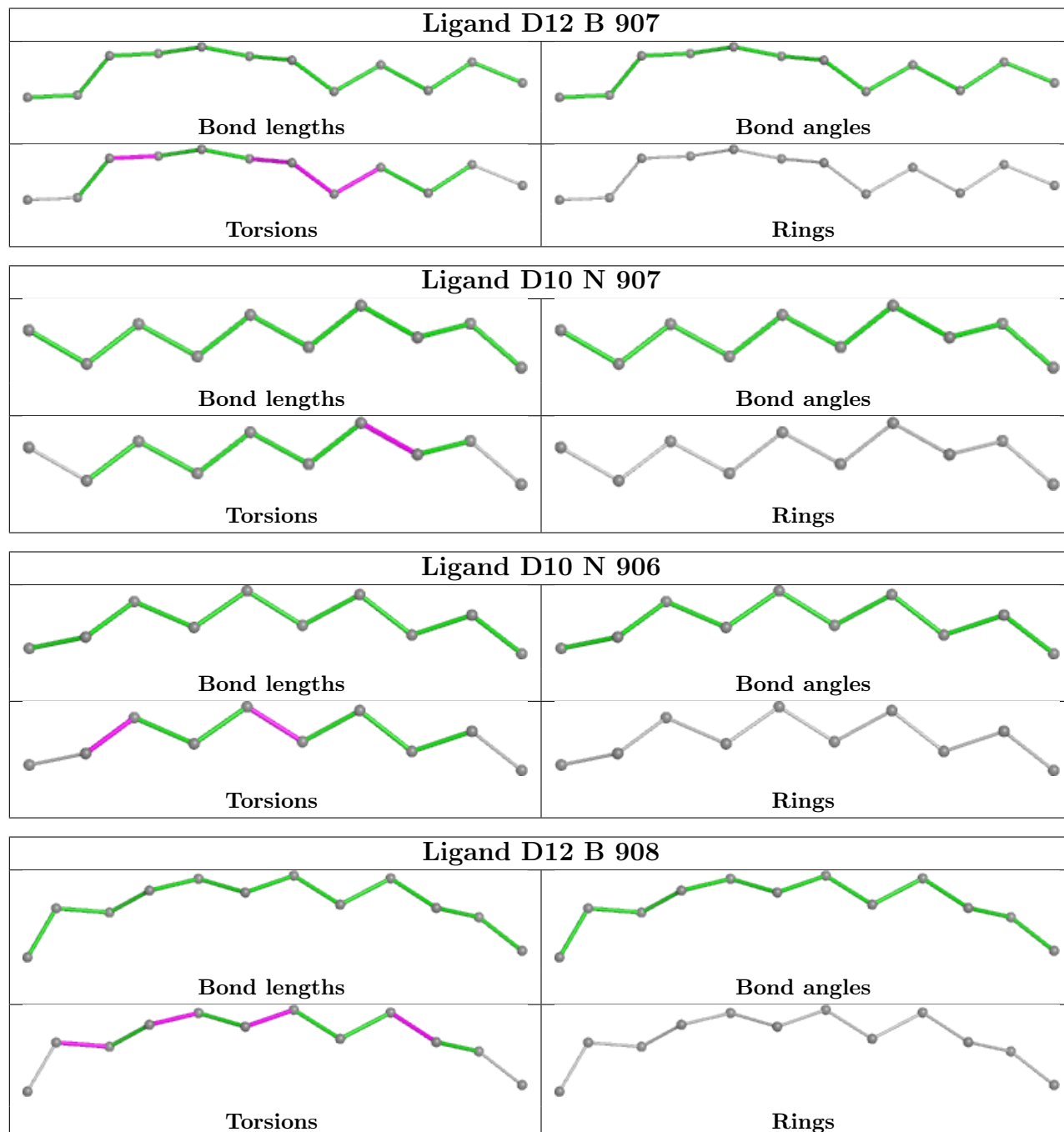
There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	906	NAG	4	0
6	N	903	NAG	3	0
6	N	902	NAG	4	0
6	B	903	NAG	3	0
6	B	902	NAG	3	0
6	B	905	NAG	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	B	374/442 (84%)	0.09	24 (6%) 27 28	24, 37, 79, 128	0
1	N	367/442 (83%)	0.24	18 (4%) 36 38	27, 41, 85, 107	0
2	D	186/199 (93%)	0.13	9 (4%) 36 39	22, 38, 77, 92	1 (0%)
2	T	189/199 (94%)	0.01	6 (3%) 50 52	24, 37, 70, 102	0
3	E	244/246 (99%)	-0.04	8 (3%) 49 51	25, 36, 67, 110	0
3	U	244/246 (99%)	0.03	5 (2%) 64 68	25, 37, 60, 86	0
All	All	1604/1774 (90%)	0.09	70 (4%) 39 42	22, 38, 76, 128	1 (0%)

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	247	CYS	6.2
1	B	101	GLY	5.5
1	B	103	GLY	5.3
3	E	98	THR	5.3
1	N	339	LEU	4.7

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

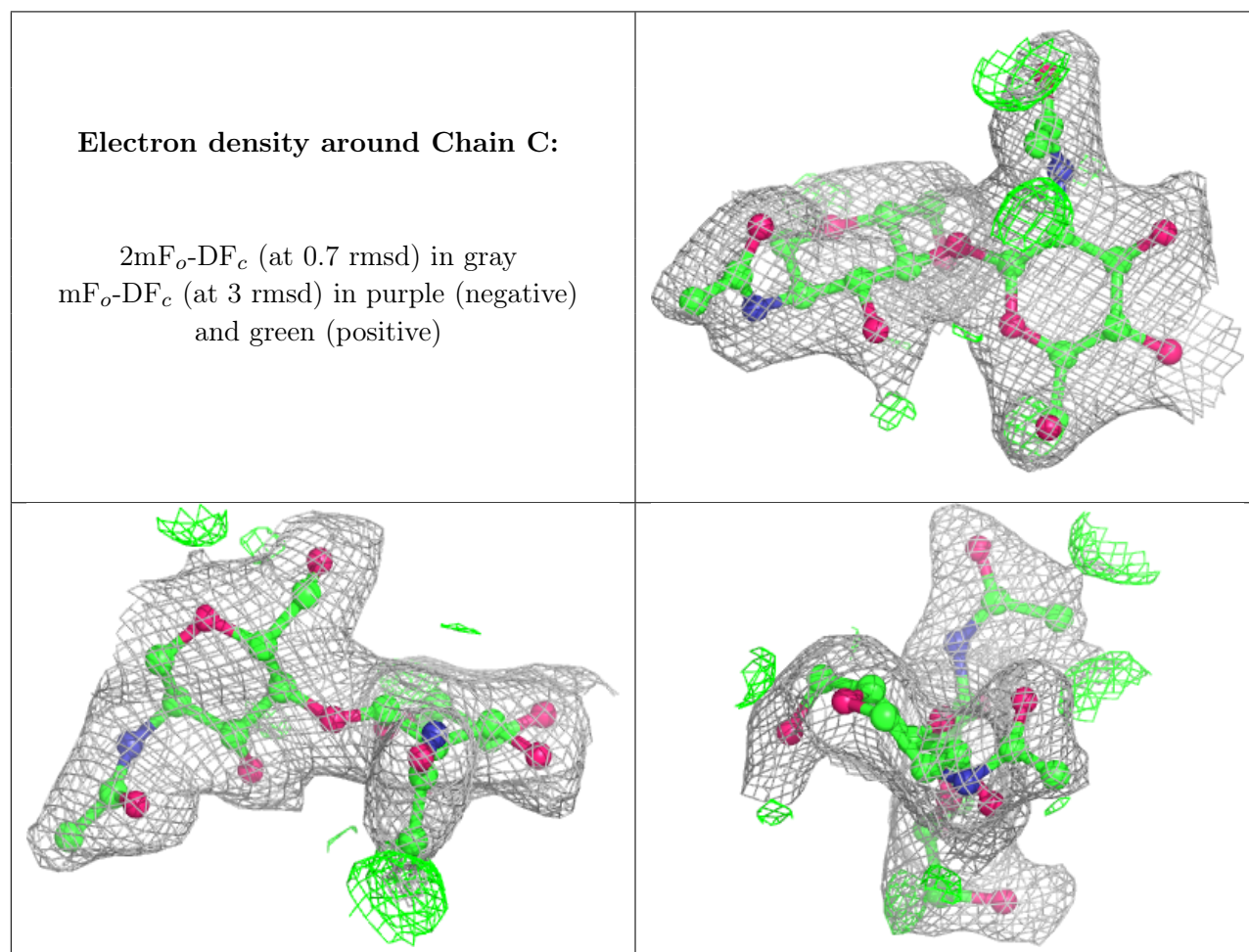
There are no non-standard protein/DNA/RNA residues in this entry.

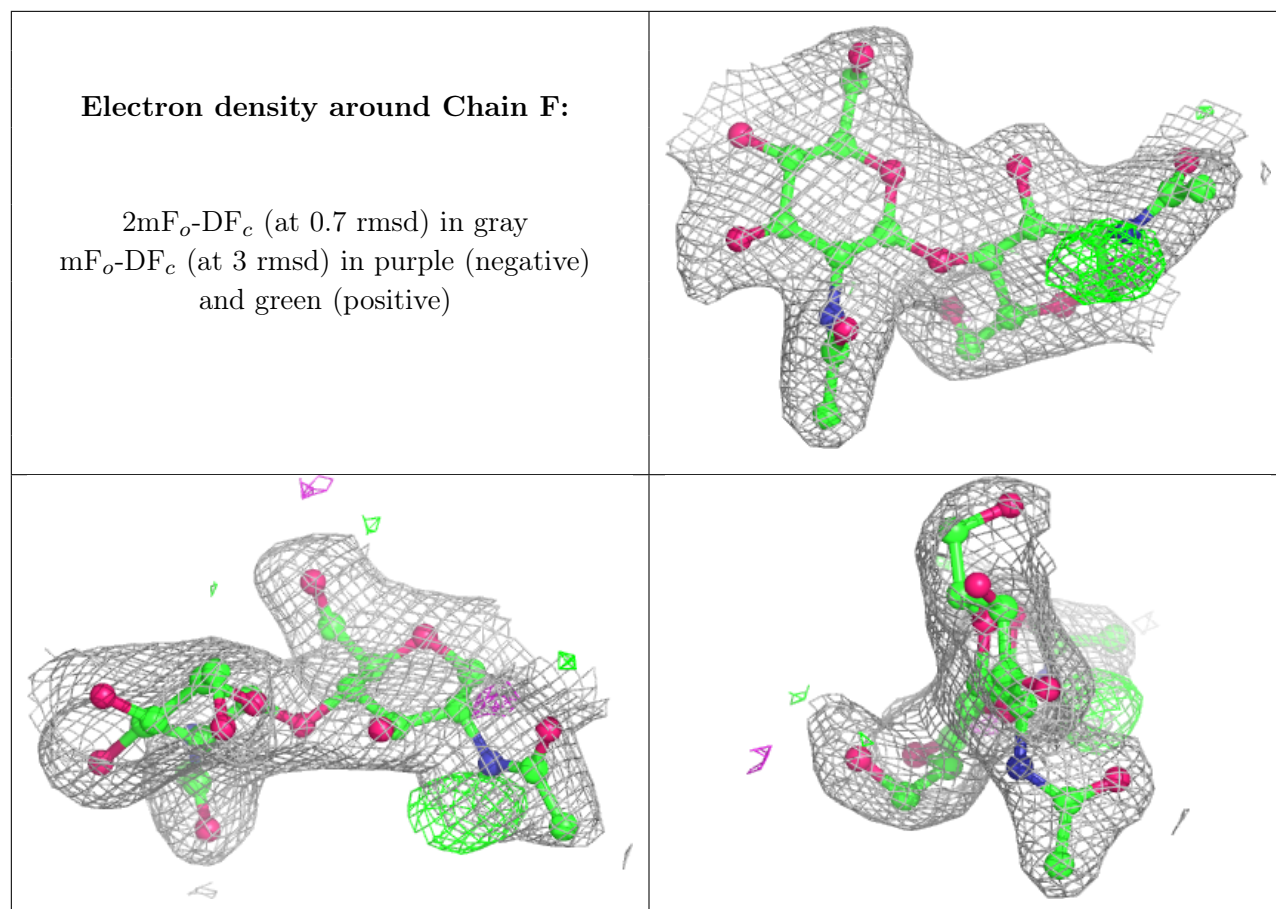
6.3 Carbohydrates [i](#)

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(\AA^2)	Q<0.9
4	NAG	C	1	14/15	-	-	35,38,45,47	0
4	NAG	C	2	14/15	-	-	41,48,52,59	0
4	NAG	F	1	14/15	-	-	42,46,55,70	0
4	NAG	F	2	14/15	-	-	34,47,55,55	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(\AA^2)	Q<0.9
6	NAG	B	906	14/15	0.62	0.16	64,85,97,98	0
7	BMA	B	904	11/12	0.70	0.13	62,74,83,84	0
6	NAG	N	903	14/15	0.76	0.13	70,87,91,92	0
6	NAG	B	903	14/15	0.77	0.12	60,83,93,99	0
7	BMA	N	904	11/12	0.79	0.12	52,62,68,76	0
6	NAG	N	902	14/15	0.82	0.12	58,63,68,77	0
6	NAG	B	905	14/15	0.82	0.13	48,54,60,66	0
10	D10	N	907	10/10	0.85	0.19	47,53,56,57	0
8	D12	B	907	12/12	0.86	0.19	43,49,58,59	0
10	D10	N	906	10/10	0.88	0.19	39,41,58,62	0
6	NAG	B	902	14/15	0.88	0.10	55,63,73,77	0
5	EDO	N	901	4/4	0.89	0.12	45,45,46,52	0
5	EDO	T	201	4/4	0.91	0.11	34,39,40,41	0

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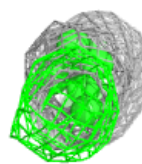
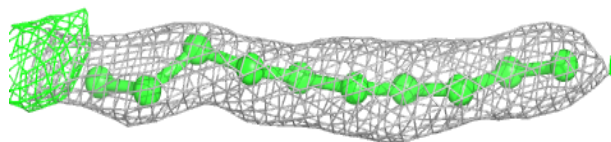
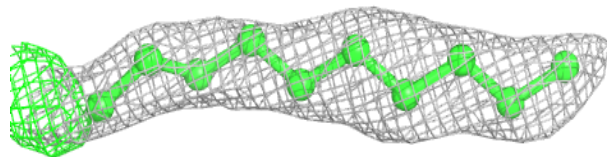
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	E	301	4/4	0.93	0.16	51,52,54,56	0
8	D12	B	908	12/12	0.93	0.11	35,37,45,46	0
5	EDO	D	201	4/4	0.95	0.09	37,45,46,46	0
5	EDO	B	901	4/4	0.95	0.08	44,45,48,53	0
5	EDO	N	905	4/4	0.96	0.07	37,39,43,43	0
5	EDO	B	909	4/4	0.97	0.07	37,41,43,44	0
9	CA	D	202	1/1	0.99	0.04	41,41,41,41	0
9	CA	T	203	1/1	0.99	0.05	43,43,43,43	0
9	CA	T	202	1/1	1.00	0.05	36,36,36,36	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

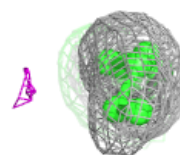
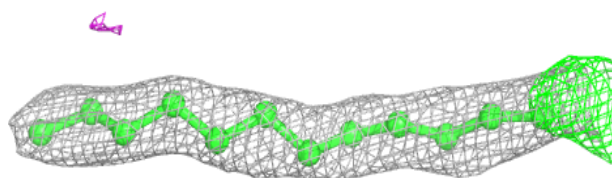
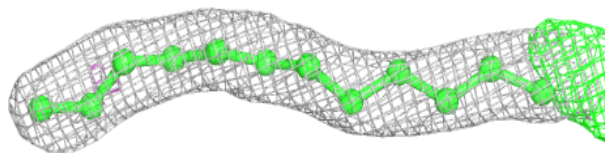
Electron density around D10 N 907:

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

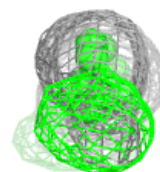
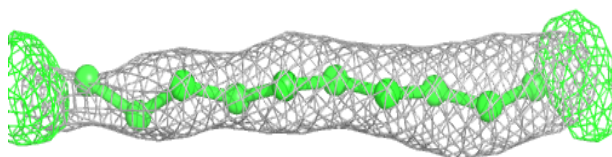
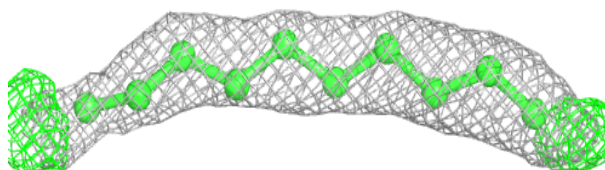


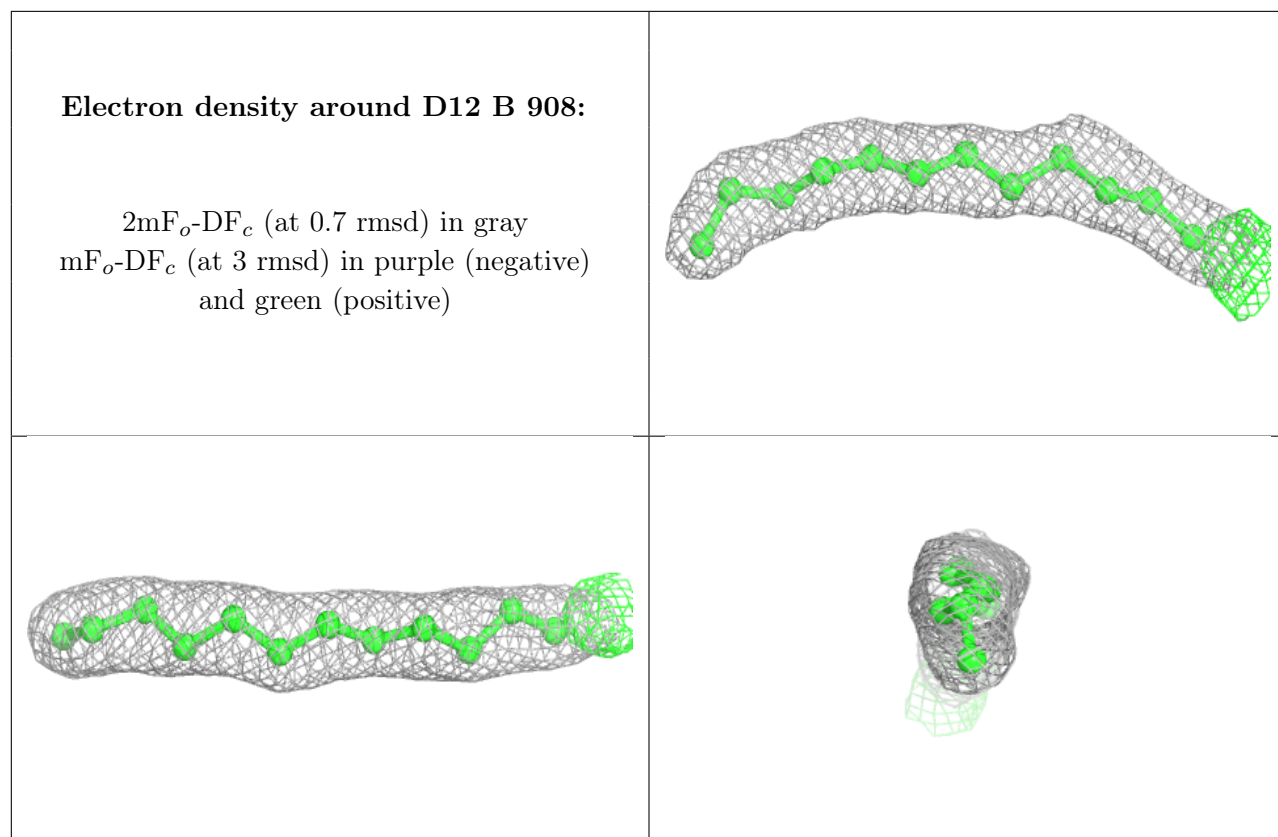
Electron density around D12 B 907:

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

**Electron density around D10 N 906:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.