



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:17 AM UTC

PDB ID : 8CWJ / pdb_00008cwj
Title : Fab arms of antibodies 4C12-B12 and CR3022 bound to pangolin receptor binding domain (pRBD)
Authors : Langley, D.B.; Christ, D.
Deposited on : 2022-05-19
Resolution : 2.45 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

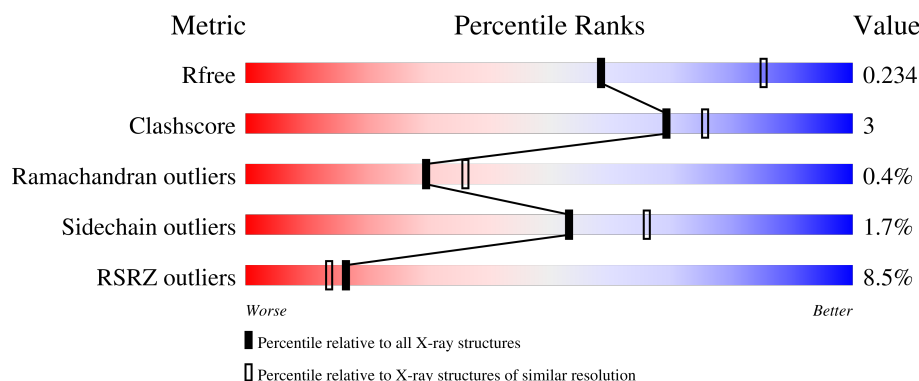
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	230	9% 83% 11% • 5%
1	H	230	9% 84% 10% • 6%
2	B	220	20% 82% 15% • •
2	L	220	3% 93% 6%
3	G	204	2% 89% 7% •

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Mol	Chain	Length	Quality of chain
3	I	204	2% 91% 6% •
4	J	230	9% 83% 10% 7%
4	U	230	10% 87% 7% 7%
5	K	215	5% 94% 5%
5	V	215	11% 89% 9% ••
6	C	3	67% 33%
6	D	3	67% 33%
6	E	3	67% 33%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 16808 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 Heavy chain of CR3022 antibody Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	217	Total	C	N	O	S	0	1	0
			1601	1016	259	318	8			
1	A	218	Total	C	N	O	S	0	7	0
			1662	1057	269	327	9			

- Molecule 2 is a protein called Light chain of CR3022 antibody Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	220	Total	C	N	O	S	0	1	0
			1705	1068	281	351	5			
2	B	218	Total	C	N	O	S	0	0	0
			1652	1035	272	341	4			

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	197	Total	C	N	O	S	0	1	0
			1555	994	259	294	8			
3	I	197	Total	C	N	O	S	0	1	0
			1552	994	259	291	8			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	420	GLY	ASP	conflict	UNP A0A7D6TQ96
G	529	GLY	-	expression tag	UNP A0A7D6TQ96
G	530	SER	-	expression tag	UNP A0A7D6TQ96
G	531	HIS	-	expression tag	UNP A0A7D6TQ96
G	532	HIS	-	expression tag	UNP A0A7D6TQ96
G	533	HIS	-	expression tag	UNP A0A7D6TQ96
G	534	HIS	-	expression tag	UNP A0A7D6TQ96
G	535	HIS	-	expression tag	UNP A0A7D6TQ96

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Chain	Residue	Modelled	Actual	Comment	Reference
G	536	HIS	-	expression tag	UNP A0A7D6TQ96
I	420	GLY	ASP	conflict	UNP A0A7D6TQ96
I	529	GLY	-	expression tag	UNP A0A7D6TQ96
I	530	SER	-	expression tag	UNP A0A7D6TQ96
I	531	HIS	-	expression tag	UNP A0A7D6TQ96
I	532	HIS	-	expression tag	UNP A0A7D6TQ96
I	533	HIS	-	expression tag	UNP A0A7D6TQ96
I	534	HIS	-	expression tag	UNP A0A7D6TQ96
I	535	HIS	-	expression tag	UNP A0A7D6TQ96
I	536	HIS	-	expression tag	UNP A0A7D6TQ96

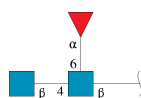
- Molecule 4 is a protein called Heavy chain of 4C12-B12 antibody Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	213	Total	C	N	O	S	0	2	0
			1600	1005	268	321	6			
4	U	214	Total	C	N	O	S	0	3	0
			1607	1010	269	322	6			

- Molecule 5 is a protein called Light chain of 4C12-B12 antibody Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	214	Total	C	N	O	S	0	4	0
			1668	1039	278	344	7			
5	V	213	Total	C	N	O	S	0	0	0
			1615	1009	269	331	6			

- 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			
6	D	3	Total	C	N	O	0	0	0
			38	22	2	14			
6	E	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



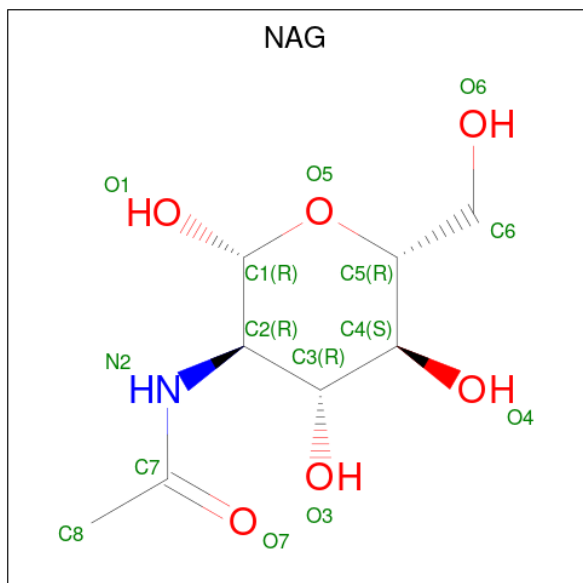
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	H	1	Total	C	O	0	0
			6	3	3		
7	G	1	Total	C	O	0	0
			6	3	3		
7	G	1	Total	C	O	0	0
			6	3	3		
7	I	1	Total	C	O	0	0
			6	3	3		
7	I	1	Total	C	O	0	0
			6	3	3		
7	I	1	Total	C	O	0	0
			6	3	3		
7	I	1	Total	C	O	0	0
			6	3	3		
7	J	1	Total	C	O	0	0
			6	3	3		
7	J	1	Total	C	O	0	0
			6	3	3		
7	K	1	Total	C	O	0	0
			6	3	3		
7	U	1	Total	C	O	0	0
			6	3	3		
7	V	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	G	3	Total	Cl	0	0
			3	3		
9	I	4	Total	Cl	0	0
			4	4		
9	J	1	Total	Cl	0	0
			1	1		
9	K	1	Total	Cl	0	0
			1	1		
9	U	1	Total	Cl	0	0
			1	1		

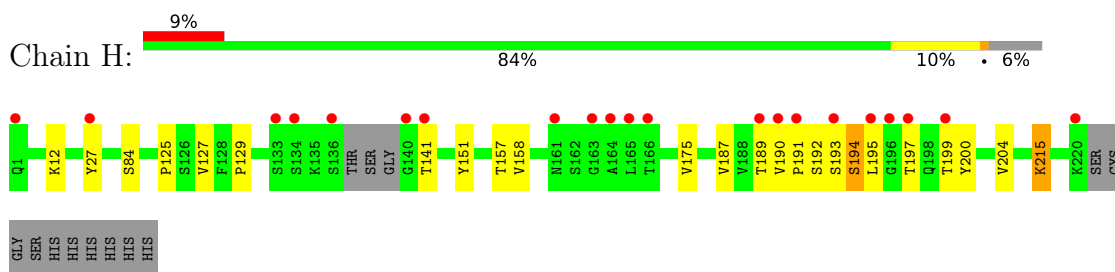
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	H	50	Total 50	O 50	0	0
10	L	18	Total 18	O 18	0	0
10	G	58	Total 58	O 58	0	0
10	A	49	Total 49	O 49	0	0
10	B	6	Total 6	O 6	0	0
10	I	43	Total 43	O 43	0	0
10	J	44	Total 44	O 44	0	0
10	K	29	Total 29	O 29	0	0
10	U	44	Total 44	O 44	0	0
10	V	22	Total 22	O 22	0	0

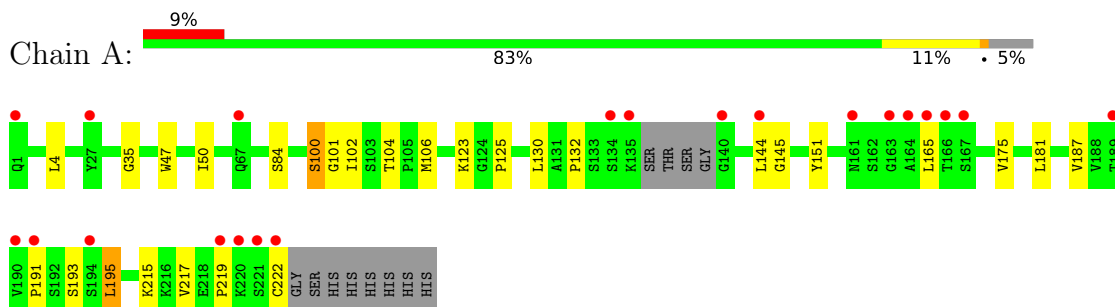
3 Residue-property plots [i](#)

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.

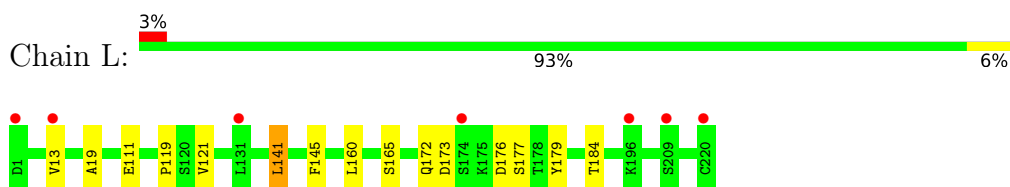
- Molecule 1: Heavy chain of CR3022 antibody Fab



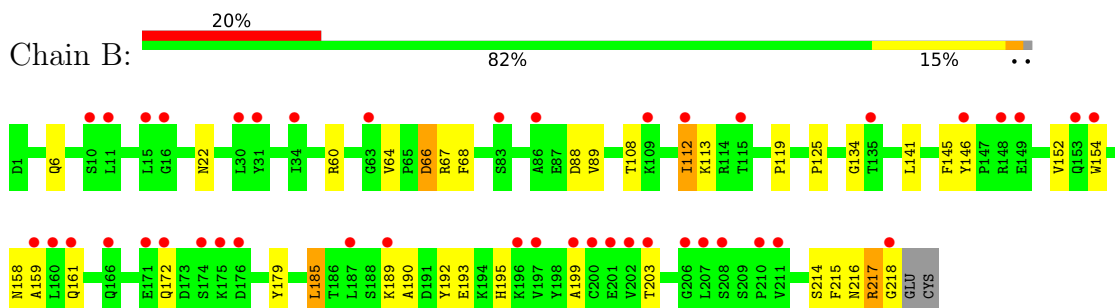
- Molecule 1: Heavy chain of CR3022 antibody Fab



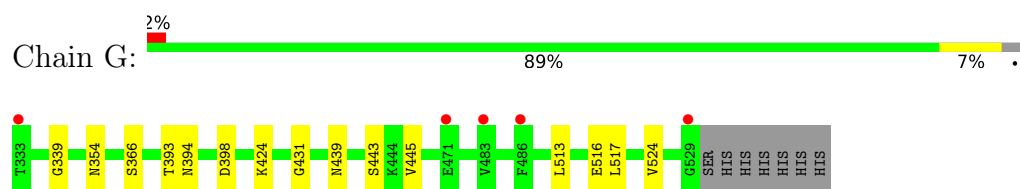
- Molecule 2: Light chain of CR3022 antibody Fab



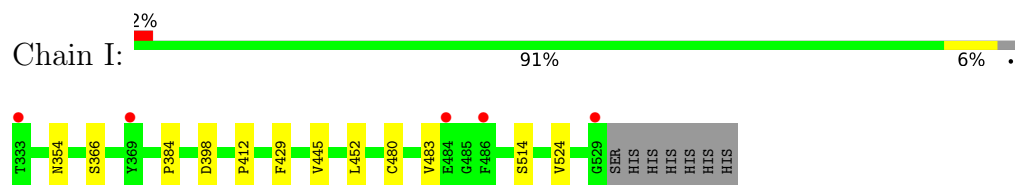
- Molecule 2: Light chain of CR3022 antibody Fab



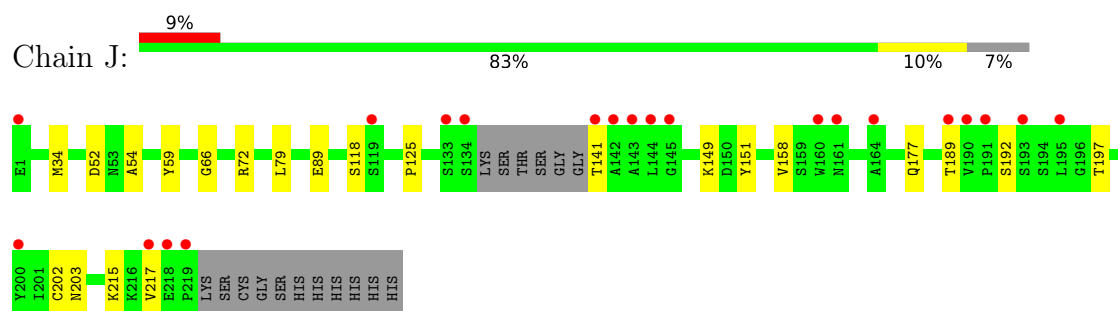
- Molecule 3: Spike glycoprotein



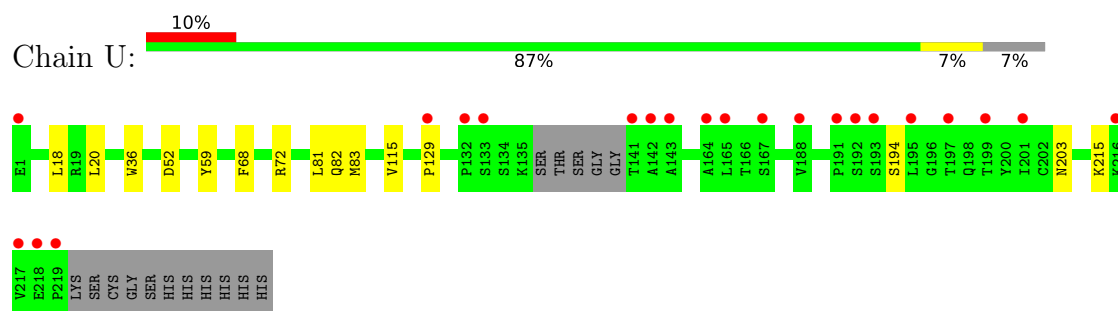
- Molecule 3: Spike glycoprotein



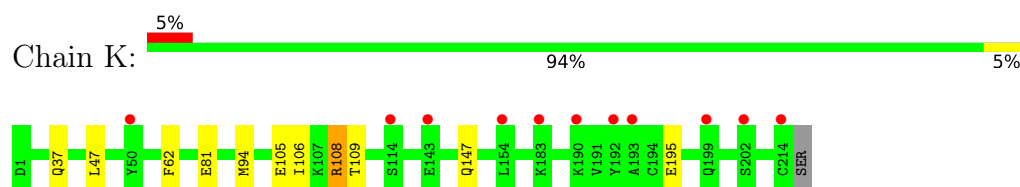
- Molecule 4: Heavy chain of 4C12-B12 antibody Fab



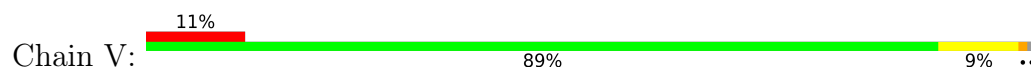
- Molecule 4: Heavy chain of 4C12-B12 antibody Fab

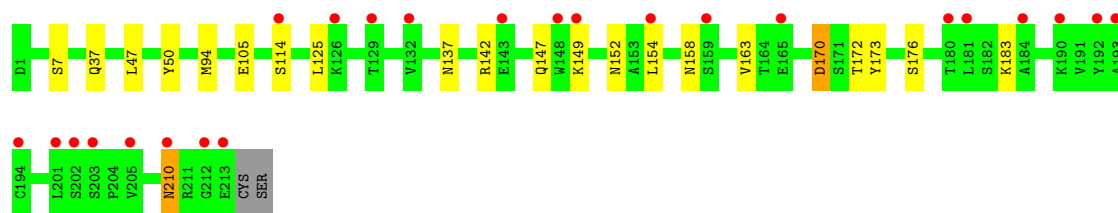


- Molecule 5: Light chain of 4C12-B12 antibody Fab



- Molecule 5: Light chain of 4C12-B12 antibody Fab





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

Chain C: 67% 33%



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

Chain D: 67% 33%



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

Chain E: 67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.43Å 144.10Å 168.84Å 90.00° 117.51° 90.00°	Depositor
Resolution (Å)	48.69 – 2.45 48.69 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.69-2.45) 99.9 (48.69-2.45)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.11.1	Depositor
R, R_{free}	0.196 , 0.230 0.202 , 0.234	Depositor DCC
R_{free} test set	6037 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.006 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16808	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: FUC, NAG, CL, GOL

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	0.12	0/1703	0.38	0/2323
1	H	0.13	0/1642	0.41	0/2242
2	B	0.11	0/1690	0.36	0/2310
2	L	0.11	0/1743	0.35	0/2374
3	G	0.14	0/1599	0.37	0/2179
3	I	0.12	0/1596	0.35	0/2175
4	J	0.13	0/1638	0.38	0/2234
4	U	0.12	0/1645	0.37	0/2245
5	K	0.12	0/1702	0.35	0/2312
5	V	0.11	0/1649	0.33	0/2244
All	All	0.12	0/16607	0.36	0/22638

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

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	1662	0	1624	15	0
1	H	1601	0	1546	15	0
2	B	1652	0	1538	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1705	0	1624	9	0
3	G	1555	0	1459	9	0
3	I	1552	0	1459	7	0
4	J	1600	0	1531	13	0
4	U	1607	0	1534	8	0
5	K	1668	0	1595	7	0
5	V	1615	0	1542	16	0
6	C	38	0	34	1	0
6	D	38	0	34	1	0
6	E	38	0	34	0	0
7	G	12	0	16	0	0
7	H	6	0	8	0	0
7	I	30	0	40	0	0
7	J	12	0	16	1	0
7	K	6	0	8	1	0
7	U	6	0	8	0	0
7	V	18	0	24	3	0
8	G	14	0	13	2	0
9	G	3	0	0	0	0
9	I	4	0	0	0	0
9	J	1	0	0	0	0
9	K	1	0	0	0	0
9	U	1	0	0	0	0
10	A	49	0	0	0	0
10	B	6	0	0	0	0
10	G	58	0	0	1	0
10	H	50	0	0	1	0
10	I	43	0	0	0	0
10	J	44	0	0	0	0
10	K	29	0	0	0	0
10	L	18	0	0	0	0
10	U	44	0	0	0	0
10	V	22	0	0	0	0
All	All	16808	0	15687	111	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 111 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)
4:J:141:THR:N	4:J:192:SER:HG	1.90	0.68
4:U:52:ASP:O	4:U:72:ARG:NH2	2.27	0.68
2:B:119:PRO:HB3	2:B:145:PHE:HB3	1.78	0.65
4:J:66:GLY:H	7:J:302:GOL:H12	1.64	0.63
1:H:129:PRO:HD3	1:H:215:LYS:HE3	1.82	0.60

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	221/230 (96%)	212 (96%)	8 (4%)	1 (0%)	24	29
1	H	214/230 (93%)	200 (94%)	11 (5%)	3 (1%)	9	8
2	B	216/220 (98%)	199 (92%)	14 (6%)	3 (1%)	9	8
2	L	219/220 (100%)	211 (96%)	8 (4%)	0	100	100
3	G	196/204 (96%)	190 (97%)	6 (3%)	0	100	100
3	I	196/204 (96%)	190 (97%)	6 (3%)	0	100	100
4	J	211/230 (92%)	207 (98%)	4 (2%)	0	100	100
4	U	213/230 (93%)	202 (95%)	10 (5%)	1 (0%)	24	29
5	K	216/215 (100%)	209 (97%)	7 (3%)	0	100	100
5	V	211/215 (98%)	201 (95%)	10 (5%)	0	100	100
All	All	2113/2198 (96%)	2021 (96%)	84 (4%)	8 (0%)	30	36

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	194	SER
1	H	192	SER
4	U	194	SER

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Mol	Chain	Res	Type
1	H	199	THR
2	B	159	ALA

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	187/194 (96%)	181 (97%)	6 (3%)	34	46
1	H	178/194 (92%)	175 (98%)	3 (2%)	53	66
2	B	182/195 (93%)	176 (97%)	6 (3%)	33	45
2	L	193/195 (99%)	191 (99%)	2 (1%)	68	77
3	G	169/176 (96%)	168 (99%)	1 (1%)	78	85
3	I	168/176 (96%)	166 (99%)	2 (1%)	63	74
4	J	177/192 (92%)	174 (98%)	3 (2%)	53	66
4	U	177/192 (92%)	176 (99%)	1 (1%)	78	85
5	K	189/188 (100%)	187 (99%)	2 (1%)	65	75
5	V	181/188 (96%)	177 (98%)	4 (2%)	45	59
All	All	1801/1890 (95%)	1771 (98%)	30 (2%)	53	66

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	152	VAL
5	V	170	ASP
2	B	203	THR
5	V	210	ASN
5	K	108	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	HIS

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Mol	Chain	Res	Type
4	U	82	GLN
2	B	43	GLN
4	U	84	ASN
3	I	414	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 ⓘ

9 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	6,3	14,14,15	0.25	0	17,19,21	0.76	1 (5%)
6	NAG	C	2	6	14,14,15	0.22	0	17,19,21	0.46	0
6	FUC	C	3	6	10,10,11	0.89	0	14,14,16	0.78	0
6	NAG	D	1	6,3	14,14,15	0.25	0	17,19,21	1.02	1 (5%)
6	NAG	D	2	6	14,14,15	0.29	0	17,19,21	0.48	0
6	FUC	D	3	6	10,10,11	0.77	0	14,14,16	0.72	0
6	NAG	E	1	6,3	14,14,15	0.35	0	17,19,21	0.60	0
6	NAG	E	2	6	14,14,15	0.35	0	17,19,21	0.46	0
6	FUC	E	3	6	10,10,11	1.03	1 (10%)	14,14,16	0.92	1 (7%)

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	6,3	-	4/6/23/26	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
6	NAG	D	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	D	2	6	-	2/6/23/26	0/1/1/1
6	FUC	D	3	6	-	-	0/1/1/1
6	NAG	E	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	E	2	6	-	1/6/23/26	0/1/1/1
6	FUC	E	3	6	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	3	FUC	O5-C1	-2.36	1.39	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1	NAG	C1-O5-C5	3.16	116.42	112.19
6	E	3	FUC	O2-C2-C1	2.16	114.16	109.22
6	C	1	NAG	C1-O5-C5	2.12	115.02	112.19

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

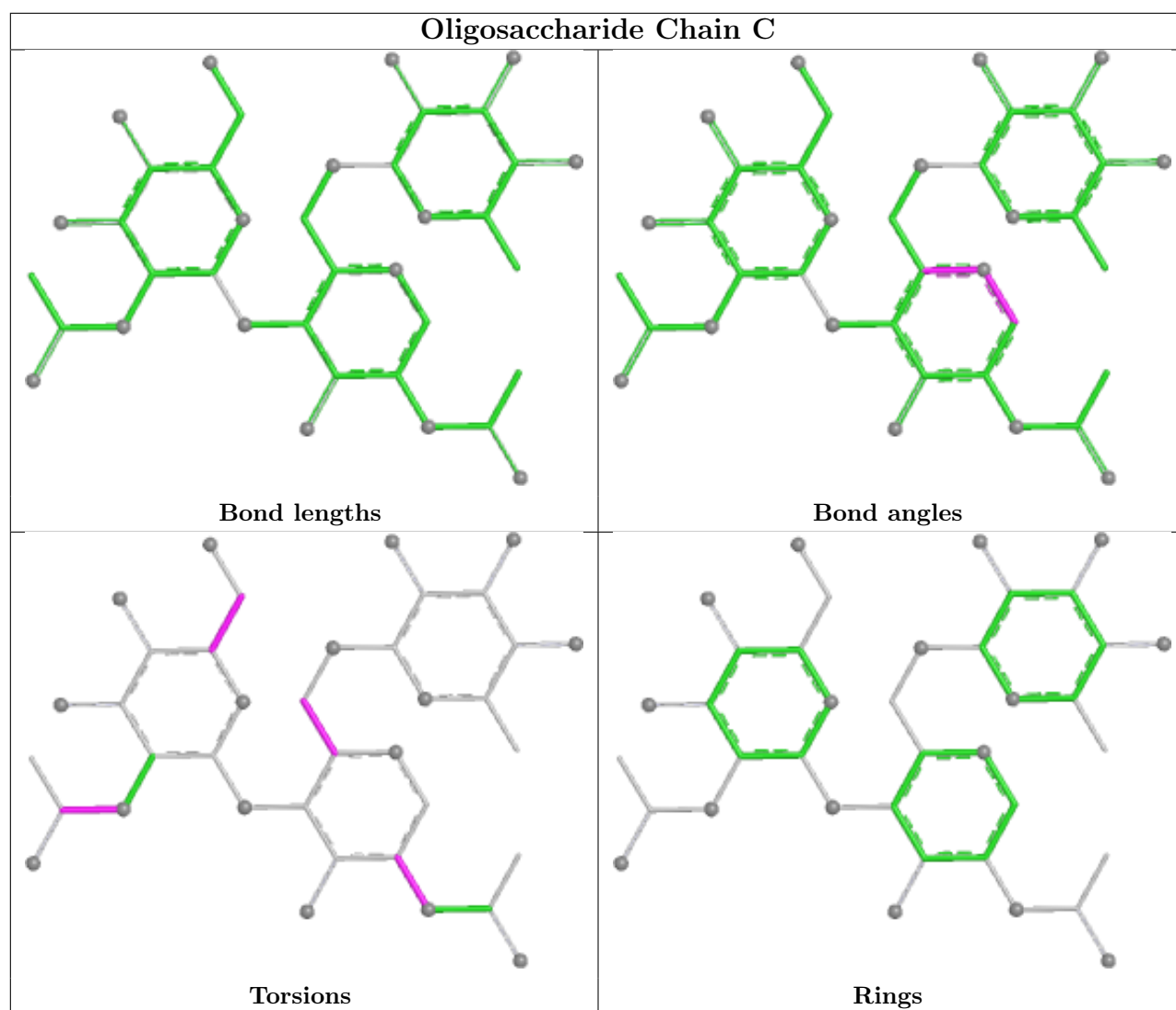
Mol	Chain	Res	Type	Atoms
6	D	2	NAG	O5-C5-C6-O6
6	D	2	NAG	C4-C5-C6-O6
6	C	2	NAG	C8-C7-N2-C2
6	C	2	NAG	O7-C7-N2-C2
6	C	1	NAG	O5-C5-C6-O6

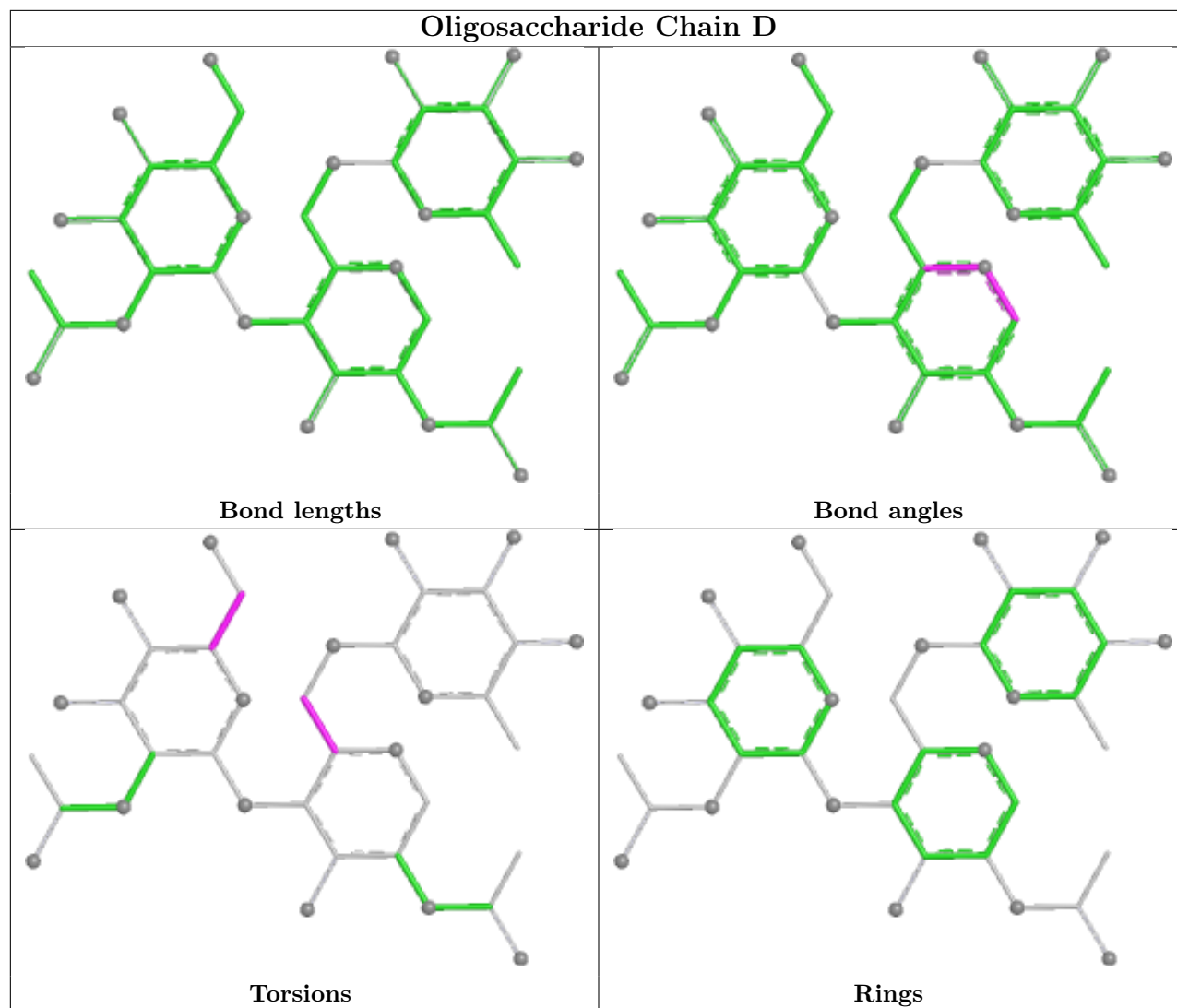
There are no ring outliers.

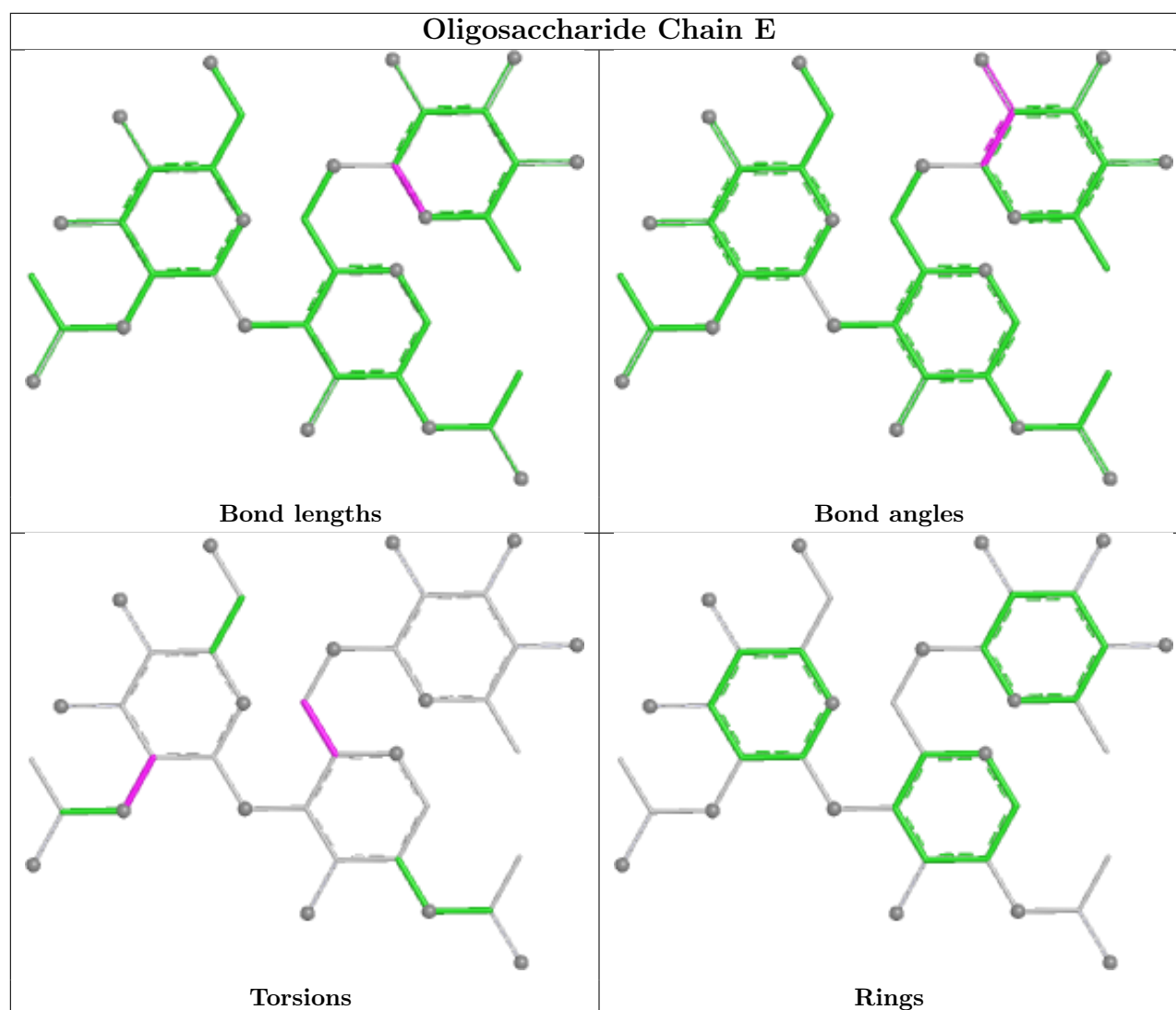
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1	NAG	1	0
6	C	1	NAG	1	0

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







5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 10 are monoatomic - leaving 16 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	GOL	K	301	-	5,5,5	0.36	0	5,5,5	0.45	0
8	NAG	G	602	3	14,14,15	1.02	2 (14%)	17,19,21	1.94	3 (17%)
7	GOL	I	602	-	5,5,5	0.38	0	5,5,5	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	U	301	-	5,5,5	0.38	0	5,5,5	0.36	0
7	GOL	I	603	-	5,5,5	0.38	0	5,5,5	0.32	0
7	GOL	G	601	-	5,5,5	0.38	0	5,5,5	0.31	0
7	GOL	H	301	-	5,5,5	0.37	0	5,5,5	0.34	0
7	GOL	J	302	-	5,5,5	0.34	0	5,5,5	0.42	0
7	GOL	V	301	-	5,5,5	0.38	0	5,5,5	0.37	0
7	GOL	I	604	-	5,5,5	0.38	0	5,5,5	0.34	0
7	GOL	J	301	-	5,5,5	0.36	0	5,5,5	0.35	0
7	GOL	I	601	-	5,5,5	0.38	0	5,5,5	0.35	0
7	GOL	G	603	-	5,5,5	0.38	0	5,5,5	0.34	0
7	GOL	V	302	-	5,5,5	0.36	0	5,5,5	0.46	0
7	GOL	V	303	-	5,5,5	0.35	0	5,5,5	0.36	0
7	GOL	I	605	-	5,5,5	0.37	0	5,5,5	0.25	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	GOL	K	301	-	-	0/4/4/4	-
8	NAG	G	602	3	-	2/6/23/26	0/1/1/1
7	GOL	I	602	-	-	0/4/4/4	-
7	GOL	U	301	-	-	0/4/4/4	-
7	GOL	I	603	-	-	2/4/4/4	-
7	GOL	G	601	-	-	2/4/4/4	-
7	GOL	H	301	-	-	2/4/4/4	-
7	GOL	J	302	-	-	2/4/4/4	-
7	GOL	V	301	-	-	0/4/4/4	-
7	GOL	I	604	-	-	1/4/4/4	-
7	GOL	J	301	-	-	0/4/4/4	-
7	GOL	I	601	-	-	4/4/4/4	-
7	GOL	G	603	-	-	2/4/4/4	-
7	GOL	V	302	-	-	0/4/4/4	-
7	GOL	V	303	-	-	2/4/4/4	-
7	GOL	I	605	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	602	NAG	O5-C1	2.60	1.48	1.43
8	G	602	NAG	C1-C2	-2.01	1.49	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	602	NAG	C1-O5-C5	6.23	120.53	112.19
8	G	602	NAG	C1-C2-N2	2.69	114.67	110.43
8	G	602	NAG	O5-C5-C4	2.21	116.20	110.83

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	601	GOL	O1-C1-C2-O2
7	I	605	GOL	O1-C1-C2-C3
7	V	303	GOL	O1-C1-C2-C3
8	G	602	NAG	C4-C5-C6-O6
8	G	602	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	K	301	GOL	1	0
8	G	602	NAG	2	0
7	J	302	GOL	1	0
7	V	301	GOL	1	0
7	V	302	GOL	2	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	218/230 (94%)	0.52	21 (9%)	13 10	26, 62, 103, 141	7 (3%)
1	H	217/230 (94%)	0.47	21 (9%)	13 10	42, 62, 126, 156	1 (0%)
2	B	218/220 (99%)	1.28	43 (19%)	3 2	52, 87, 130, 142	0
2	L	220/220 (100%)	0.58	7 (3%)	50 49	45, 76, 100, 125	1 (0%)
3	G	197/204 (96%)	0.08	5 (2%)	58 59	29, 49, 84, 114	1 (0%)
3	I	197/204 (96%)	0.21	5 (2%)	58 59	19, 51, 90, 124	1 (0%)
4	J	213/230 (92%)	0.42	21 (9%)	13 10	20, 56, 120, 145	2 (0%)
4	U	214/230 (93%)	0.63	22 (10%)	12 9	22, 63, 124, 151	3 (1%)
5	K	214/215 (99%)	0.51	11 (5%)	33 30	24, 65, 107, 133	4 (1%)
5	V	213/215 (99%)	0.78	24 (11%)	10 8	39, 74, 119, 145	0
All	All	2121/2198 (96%)	0.56	180 (8%)	16 14	19, 67, 118, 156	20 (0%)

The worst 5 of 180 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	140	GLY	5.2
5	V	213	GLU	4.8
1	H	193	SER	4.6
2	B	218	GLY	4.4
5	V	202	SER	4.4

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

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

6.3 Carbohydrates

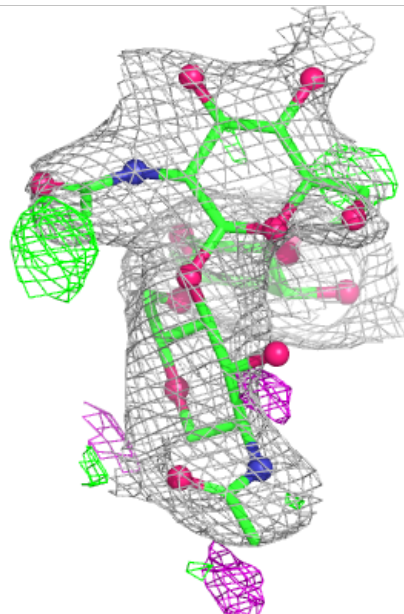
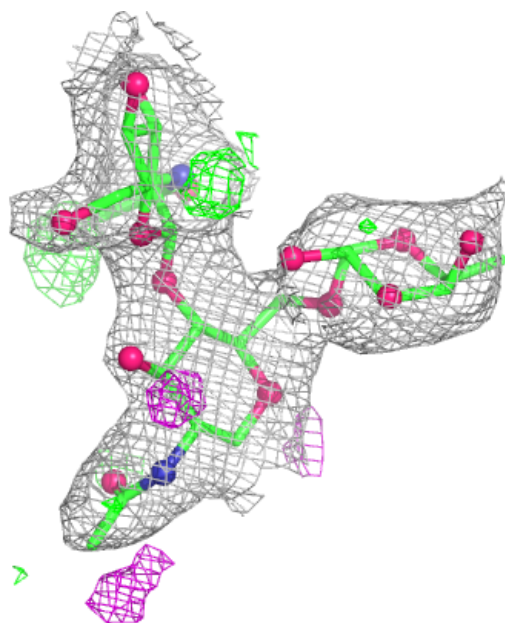
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	C	1	14/15	-	-	77,98,117,121	0
6	NAG	C	2	14/15	-	-	115,124,128,131	0
6	FUC	C	3	10/11	-	-	128,131,133,134	0
6	NAG	D	1	14/15	-	-	151,164,168,168	0
6	NAG	D	2	14/15	-	-	142,153,156,158	0
6	FUC	D	3	10/11	-	-	164,166,166,166	0
6	NAG	E	1	14/15	-	-	75,92,114,122	0
6	NAG	E	2	14/15	-	-	114,125,131,134	0
6	FUC	E	3	10/11	-	-	129,136,140,140	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.

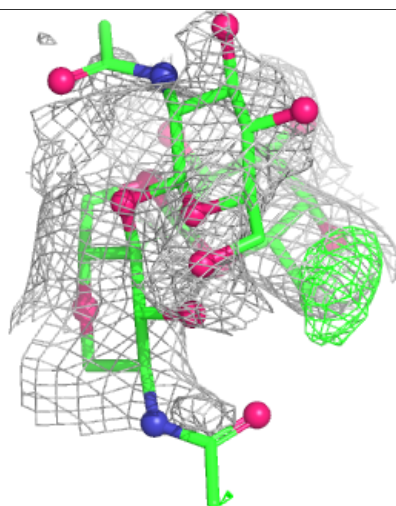
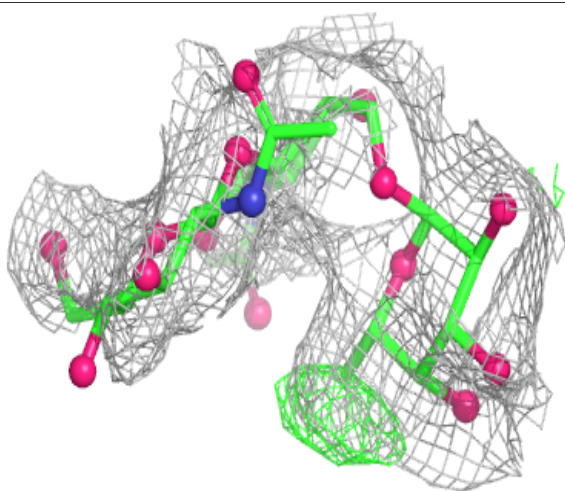
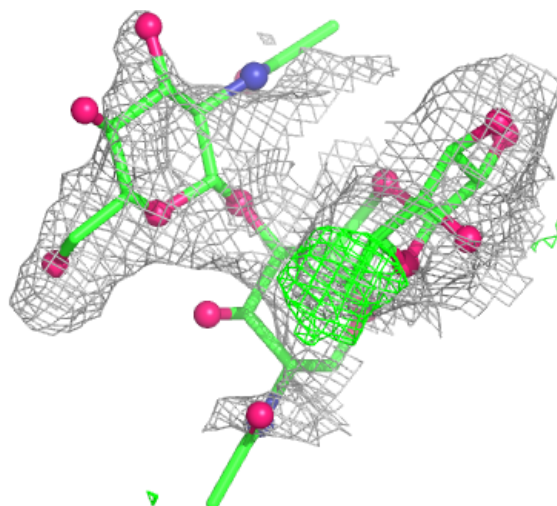
Electron density around Chain C:

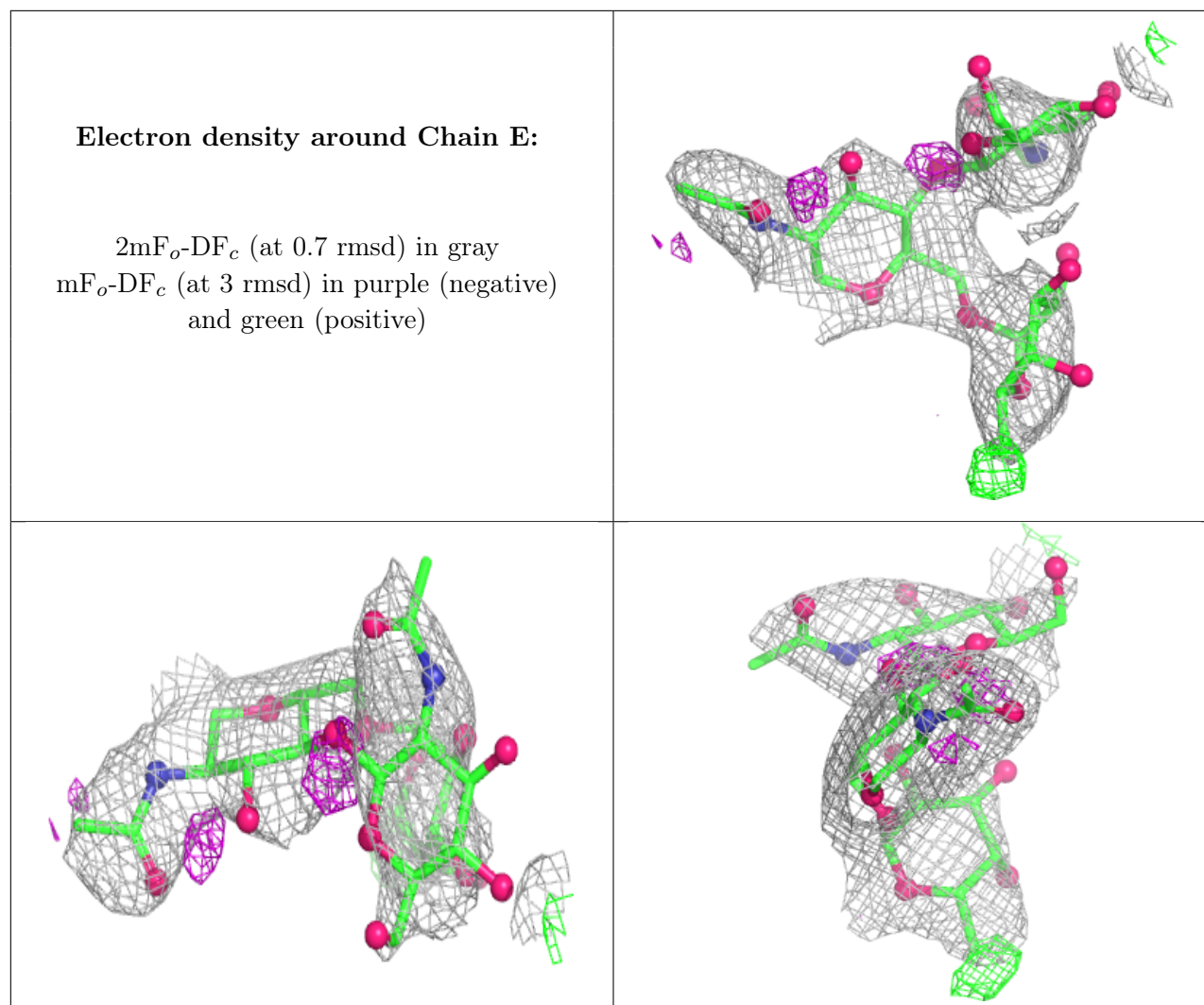
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain D:

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
7	GOL	J	301	6/6	0.66	0.26	82,84,86,86	0
8	NAG	G	602	14/15	0.71	0.17	126,135,139,140	0
9	CL	U	302	1/1	0.77	0.23	101,101,101,101	0
7	GOL	U	301	6/6	0.80	0.20	95,95,96,96	0
7	GOL	I	605	6/6	0.82	0.22	77,80,81,83	0
7	GOL	K	301	6/6	0.84	0.18	68,80,80,84	0
7	GOL	H	301	6/6	0.85	0.20	89,93,95,95	0
7	GOL	G	603	6/6	0.85	0.25	87,89,92,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	I	604	6/6	0.86	0.25	83,87,88,92	0
7	GOL	V	303	6/6	0.86	0.17	83,90,93,93	0
7	GOL	G	601	6/6	0.87	0.17	82,84,84,85	0
7	GOL	I	602	6/6	0.87	0.21	81,82,83,84	0
7	GOL	V	301	6/6	0.88	0.21	78,80,82,84	0
7	GOL	I	603	6/6	0.89	0.18	86,91,91,95	0
9	CL	I	607	1/1	0.90	0.24	96,96,96,96	0
7	GOL	I	601	6/6	0.90	0.19	71,77,81,84	0
9	CL	J	303	1/1	0.91	0.13	97,97,97,97	0
9	CL	I	609	1/1	0.91	0.17	87,87,87,87	0
9	CL	I	608	1/1	0.92	0.12	88,88,88,88	0
9	CL	G	604	1/1	0.92	0.14	97,97,97,97	0
9	CL	G	606	1/1	0.92	0.19	115,115,115,115	0
9	CL	K	302	1/1	0.92	0.14	105,105,105,105	0
7	GOL	V	302	6/6	0.92	0.16	72,82,84,85	0
7	GOL	J	302	6/6	0.93	0.12	67,80,82,83	0
9	CL	G	605	1/1	0.94	0.23	93,93,93,93	0
9	CL	I	606	1/1	0.94	0.14	91,91,91,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.