



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:36 AM UTC

PDB ID : 4WO4 / pdb_00004wo4
Title : The molecular bases of Delta/Alpha beta T cell-mediated antigen recognition.
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de Boer, R.; Lim, R.T.; McPherson, K.; Besra, G.; Howell, A.R.; Moretta, L.;
McCluskey, J.; Heemskerk, M.H.M.; Gras, S.; Rossjohn, J.; Godfrey, D.I.
Deposited on : 2014-10-15
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

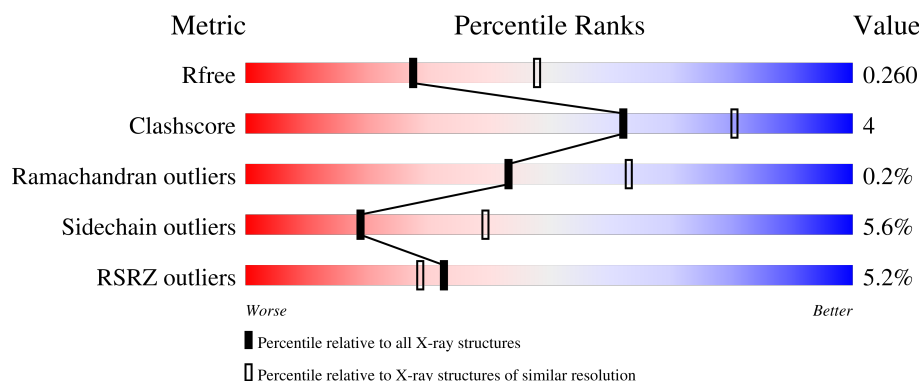
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



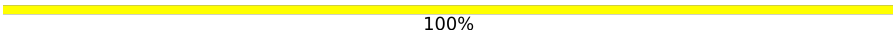
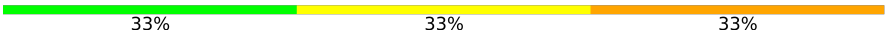
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	274	4% 85% 14% .
2	B	100	13% 83% 14% ..
3	C	207	3% 81% 15% .
4	D	245	5% 87% 11% ..

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Mol	Chain	Length	Quality of chain
5	E	4	 25% 75%
6	F	2	 100%
7	G	3	 33% 33% 33%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6806 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 Antigen-presenting glycoprotein CD1d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2170	1390	381	392	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	278	PRO	-	expression tag	UNP P15813
A	279	ARG	-	expression tag	UNP P15813

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			797	508	136	151	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769

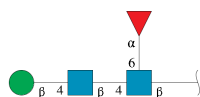
- Molecule 3 is a protein called TCR variable DELTA 1 CHAIN and TCR constant Alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	200	Total	C	N	O	S	0	2	0
			1576	1000	259	307	10			

- Molecule 4 is a protein called TCR variable BETA 2 (TRVB20) chain and TCR constant BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	3	0
			1885	1195	327	355	8			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



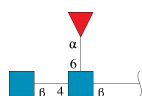
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



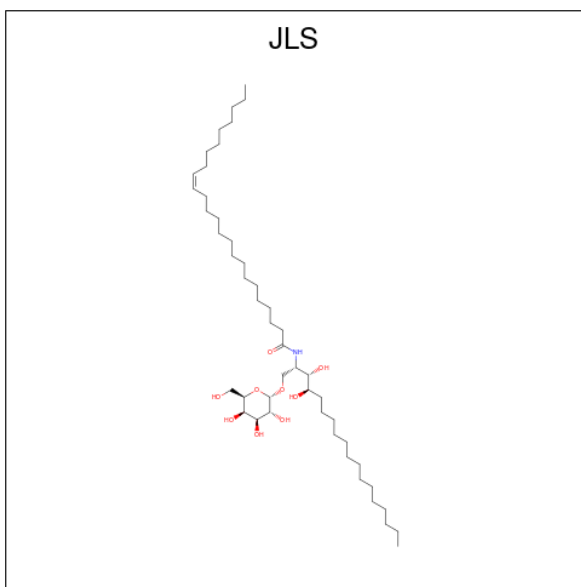
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 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
7	G	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 8 is (15Z)-N-[(2S,3S,4R)-1-(alpha-D-galactopyranosyloxy)-3,4-dihydroxyoctadecan-2-yl]tetracos-15-enamide (CCD ID: JLS) (formula: C₄₈H₉₃NO₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			58	48	1	9		

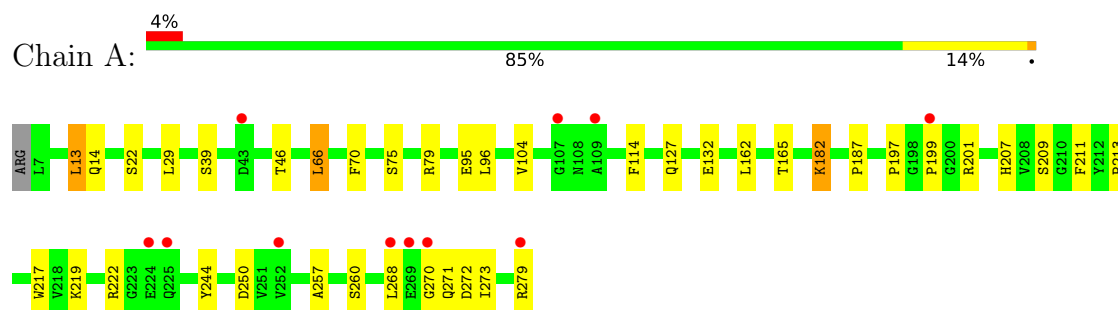
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	70	Total	O	0	0
			70	70		
9	B	15	Total	O	0	0
			15	15		
9	C	61	Total	O	0	0
			61	61		
9	D	59	Total	O	0	0
			59	59		

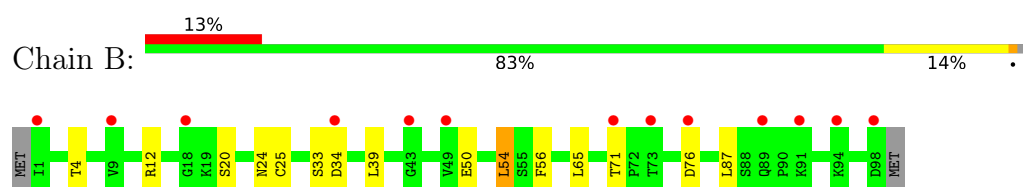
3 Residue-property plots [i](#)

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.

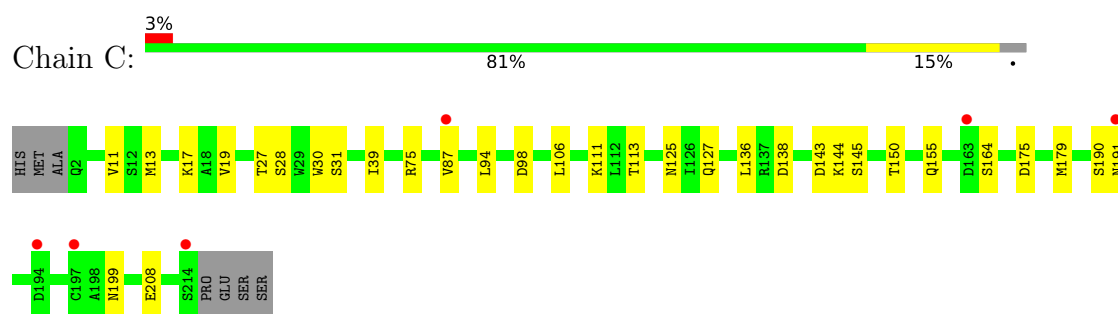
- Molecule 1: Antigen-presenting glycoprotein CD1d



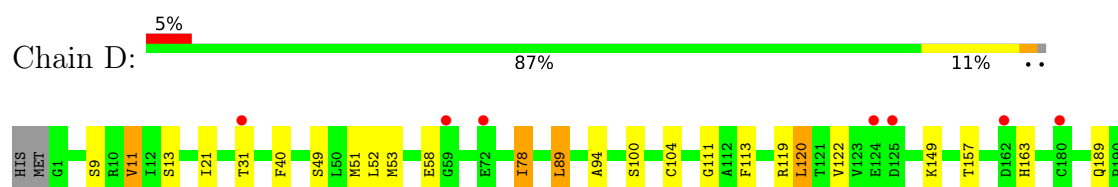
- Molecule 2: Beta-2-microglobulin

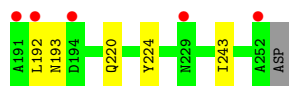


- Molecule 3: TCR variable DELTA 1 CHAIN and TCR constant Alpha



- Molecule 4: TCR variable BETA 2 (TRVB20) chain and TCR constant BETA





- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 25% 75%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 33% 33% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.93Å 79.25Å 189.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.60 – 2.50 36.60 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (36.60-2.50) 99.8 (36.60-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.194 , 0.237 (Not available) , 0.260	Depositor DCC
R_{free} test set	2113 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6806	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: BMA, FUC, JLS, NAG

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	0.84	0/2236	1.20	9/3047 (0.3%)
2	B	0.83	0/820	1.18	2/1115 (0.2%)
3	C	0.85	0/1614	1.21	9/2188 (0.4%)
4	D	0.86	0/1944	1.11	1/2646 (0.0%)
All	All	0.85	0/6614	1.17	21/8996 (0.2%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	175	ASP	CA-CB-CG	7.73	120.33	112.60
3	C	199	ASN	CA-C-N	6.59	130.71	120.82
3	C	199	ASN	C-N-CA	6.59	130.71	120.82
1	A	213	PRO	CA-C-N	6.08	127.69	120.09
1	A	213	PRO	C-N-CA	6.08	127.69	120.09
3	C	190	SER	CA-C-N	5.98	130.84	120.68
3	C	190	SER	C-N-CA	5.98	130.84	120.68
2	B	87	LEU	CA-C-N	5.94	128.24	120.28
2	B	87	LEU	C-N-CA	5.94	128.24	120.28
3	C	191	ASN	CA-C-N	5.45	128.45	120.71
3	C	191	ASN	C-N-CA	5.45	128.45	120.71
4	D	113	PHE	CA-CB-CG	5.36	119.16	113.80
1	A	75	SER	CA-C-N	5.35	127.45	120.28
1	A	75	SER	C-N-CA	5.35	127.45	120.28
1	A	182	LYS	CA-C-N	5.33	128.27	120.71
1	A	182	LYS	C-N-CA	5.33	128.27	120.71
3	C	150	THR	CA-C-N	5.33	130.12	122.40
3	C	150	THR	C-N-CA	5.33	130.12	122.40
1	A	79	ARG	CA-C-N	5.19	127.19	120.44
1	A	79	ARG	C-N-CA	5.19	127.19	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	ILE	N-CA-CB	5.05	116.61	110.95

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	2170	0	2093	16	1
2	B	797	0	740	5	0
3	C	1576	0	1527	19	1
4	D	1885	0	1821	16	0
5	E	49	0	43	0	0
6	F	28	0	25	0	0
7	G	38	0	34	1	0
8	A	58	0	93	3	0
9	A	70	0	0	0	0
9	B	15	0	0	0	0
9	C	61	0	0	0	0
9	D	59	0	0	0	0
All	All	6806	0	6376	53	1

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 4.

All (53) 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:270:GLY:O	1:A:271:GLN:OE1	1.85	0.94
3:C:13[B]:MET:HE2	3:C:94:LEU:HD12	1.65	0.77
3:C:13[B]:MET:HE1	3:C:17:LYS:CB	2.17	0.74
3:C:39:ILE:HG21	3:C:87:VAL:HG11	1.71	0.71
3:C:13[B]:MET:CE	3:C:94:LEU:HD12	2.21	0.69
1:A:207:HIS:HD2	1:A:244:TYR:OH	1.77	0.67
3:C:27:THR:HB	3:C:106:LEU:HD21	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:ILE:HG21	3:C:87:VAL:HG21	1.76	0.67
3:C:179:MET:HE1	4:D:149:LYS:HE3	1.77	0.67
4:D:11:VAL:HG13	4:D:120:LEU:HD23	1.79	0.64
1:A:70:PHE:HB2	8:A:310:JLS:H41	1.81	0.63
3:C:13[B]:MET:HE1	3:C:17:LYS:HB3	1.80	0.62
4:D:31:THR:HG22	4:D:31:THR:O	1.99	0.61
3:C:87:VAL:HG13	3:C:87:VAL:O	2.02	0.59
1:A:197:PRO:HG2	1:A:250:ASP:OD1	2.03	0.58
1:A:187:PRO:HB3	1:A:211:PHE:HB3	1.86	0.58
3:C:13[B]:MET:HE1	3:C:17:LYS:HB2	1.87	0.55
1:A:268:LEU:CD1	1:A:272:ASP:HA	2.37	0.55
1:A:222:ARG:NH2	1:A:257:ALA:O	2.40	0.54
1:A:114:PHE:HB2	1:A:162:LEU:HD11	1.90	0.54
1:A:270:GLY:O	1:A:271:GLN:CD	2.50	0.54
1:A:268:LEU:HD13	1:A:272:ASP:HA	1.90	0.54
4:D:21:ILE:HD12	4:D:89:LEU:HD23	1.90	0.53
4:D:78:ILE:HD13	4:D:89:LEU:HD12	1.90	0.53
2:B:20:SER:HA	2:B:71:THR:HG22	1.91	0.52
3:C:11:VAL:HG11	3:C:19:VAL:HG21	1.92	0.51
3:C:75:ARG:NH2	3:C:98:ASP:OD2	2.45	0.50
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.94	0.50
4:D:220:GLN:HG3	4:D:243:ILE:HG23	1.93	0.50
3:C:13[B]:MET:HE2	3:C:94:LEU:CD1	2.37	0.49
2:B:33:SER:HB2	2:B:54:LEU:HD11	1.94	0.49
1:A:268:LEU:HD13	1:A:271:GLN:O	2.14	0.48
3:C:75:ARG:HH22	3:C:98:ASP:CG	2.22	0.47
4:D:163:HIS:HB3	4:D:224:TYR:HB2	1.97	0.47
1:A:13:LEU:HG	2:B:56:PHE:CZ	2.50	0.47
3:C:144:LYS:HE2	4:D:157:THR:HG21	1.97	0.46
1:A:127:GLN:HB2	1:A:132:GLU:HG3	1.98	0.46
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.96	0.46
8:A:310:JLS:H43	8:A:310:JLS:H14	1.97	0.46
1:A:14:GLN:HB2	8:A:310:JLS:H21	1.98	0.45
1:A:66:LEU:HD11	1:A:165:THR:HG21	1.97	0.45
3:C:13[B]:MET:HE3	3:C:13[B]:MET:HB3	1.63	0.44
4:D:94:ALA:HB1	4:D:122:VAL:HG21	1.99	0.44
4:D:189:GLN:HB3	4:D:192:LEU:HD13	1.99	0.44
4:D:49:SER:HB3	4:D:51:MET:HE2	2.00	0.44
3:C:111:LYS:HE2	4:D:52:LEU:HD21	2.01	0.42
3:C:11:VAL:HG11	3:C:19:VAL:CG2	2.50	0.41
4:D:31:THR:O	4:D:31:THR:CG2	2.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:40:PHE:O	4:D:104:CYS:HA	2.21	0.41
1:A:217:TRP:CZ2	1:A:219:LYS:HG3	2.55	0.41
3:C:30:TRP:HE3	7:G:3:FUC:H63	1.85	0.40
4:D:53:MET:HE1	4:D:89:LEU:HD11	2.03	0.40
4:D:31:THR:HG23	4:D:58:GLU:HB3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ARG:NH1	3:C:143:ASP:O[2_154]	2.08	0.12

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	271/274 (99%)	261 (96%)	9 (3%)	1 (0%)	30	49
2	B	96/100 (96%)	93 (97%)	3 (3%)	0	100	100
3	C	200/207 (97%)	194 (97%)	6 (3%)	0	100	100
4	D	243/245 (99%)	238 (98%)	4 (2%)	1 (0%)	30	49
All	All	810/826 (98%)	786 (97%)	22 (3%)	2 (0%)	43	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	PRO
4	D	111	GLY

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	233/240 (97%)	220 (94%)	13 (6%)	19	39
2	B	87/95 (92%)	81 (93%)	6 (7%)	14	30
3	C	178/185 (96%)	166 (93%)	12 (7%)	15	31
4	D	206/212 (97%)	196 (95%)	10 (5%)	22	45
All	All	704/732 (96%)	663 (94%)	41 (6%)	19	38

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	22	SER
1	A	29	LEU
1	A	39	SER
1	A	46	THR
1	A	66	LEU
1	A	95	GLU
1	A	96	LEU
1	A	104	VAL
1	A	182	LYS
1	A	201	ARG
1	A	209	SER
1	A	260	SER
2	B	4	THR
2	B	12	ARG
2	B	34	ASP
2	B	50	GLU
2	B	54	LEU
2	B	76	ASP
3	C	28	SER
3	C	31	SER
3	C	113	THR
3	C	125	ASN
3	C	127	GLN

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Mol	Chain	Res	Type
3	C	136	LEU
3	C	138	ASP
3	C	145[A]	SER
3	C	145[B]	SER
3	C	155	GLN
3	C	164	SER
3	C	208	GLU
4	D	9	SER
4	D	11	VAL
4	D	13[A]	SER
4	D	13[B]	SER
4	D	78	ILE
4	D	89	LEU
4	D	100	SER
4	D	119	ARG
4	D	120	LEU
4	D	193	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	111	ASN
1	A	127	GLN
1	A	184	GLN
1	A	207	HIS
1	A	227	GLN
2	B	13	HIS
2	B	17	ASN
2	B	42	ASN
3	C	44	GLN
3	C	157	ASN
3	C	191	ASN
3	C	203	ASN
4	D	44	GLN
4	D	48	GLN
4	D	128	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	$\# Z > 2$
5	NAG	E	1	1,5	14,14,15	0.54	0	17,19,21	0.88	0
5	NAG	E	2	5	14,14,15	0.61	0	17,19,21	1.57	2 (11%)
5	BMA	E	3	5	11,11,12	0.59	0	15,15,17	0.93	1 (6%)
5	FUC	E	4	5	10,10,11	0.91	0	14,14,16	1.35	2 (14%)
6	NAG	F	1	1,6	14,14,15	0.73	0	17,19,21	1.88	2 (11%)
6	NAG	F	2	6	14,14,15	0.78	0	17,19,21	1.42	2 (11%)
7	NAG	G	1	7,1	14,14,15	0.52	0	17,19,21	0.97	0
7	NAG	G	2	7	14,14,15	0.52	0	17,19,21	1.02	1 (5%)
7	FUC	G	3	7	10,10,11	0.85	0	14,14,16	1.68	3 (21%)

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	NAG	E	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
5	FUC	E	4	5	-	-	0/1/1/1
6	NAG	F	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
7	NAG	G	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	G	2	7	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FUC	G	3	7	-	-	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	1	NAG	C1-O5-C5	5.48	119.54	112.19
5	E	2	NAG	C4-C3-C2	4.87	118.16	111.02
7	G	3	FUC	C1-C2-C3	4.53	116.24	109.64
6	F	2	NAG	C4-C3-C2	4.28	117.29	111.02
5	E	2	NAG	C3-C4-C5	3.10	115.84	110.23
7	G	3	FUC	C2-C3-C4	3.06	116.24	110.86
5	E	4	FUC	C1-C2-C3	2.45	113.21	109.64
7	G	2	NAG	C4-C3-C2	2.43	114.58	111.02
6	F	1	NAG	O5-C1-C2	2.29	114.84	111.29
7	G	3	FUC	O5-C5-C6	2.24	112.26	107.40
6	F	2	NAG	O5-C5-C6	2.04	111.63	107.66
5	E	4	FUC	C1-O5-C5	2.03	117.75	112.97
5	E	3	BMA	C2-C3-C4	2.02	114.41	110.86

There are no chirality outliers.

All (12) torsion outliers are listed below:

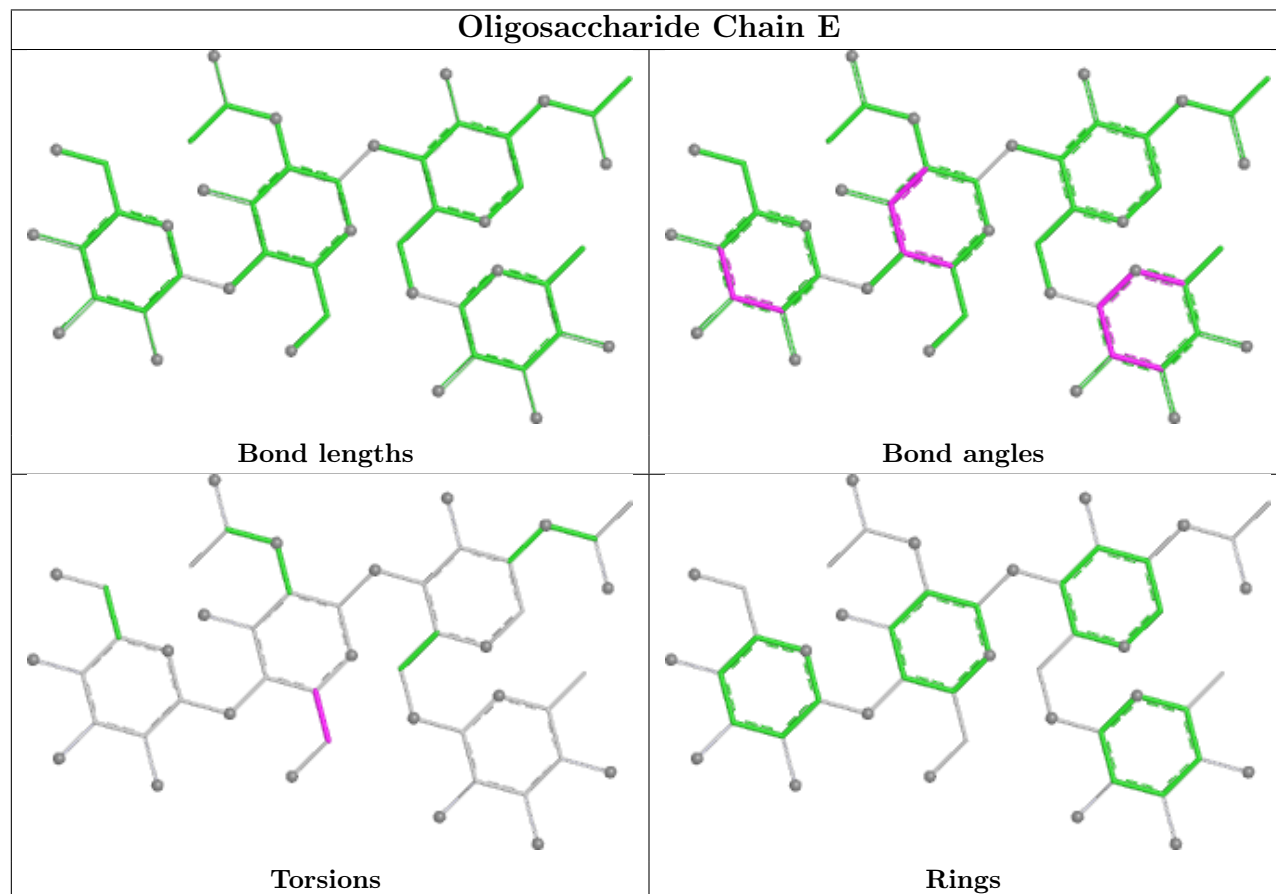
Mol	Chain	Res	Type	Atoms
6	F	1	NAG	C8-C7-N2-C2
6	F	1	NAG	O7-C7-N2-C2
6	F	2	NAG	O5-C5-C6-O6
7	G	2	NAG	C4-C5-C6-O6
6	F	1	NAG	C4-C5-C6-O6
7	G	1	NAG	C8-C7-N2-C2
7	G	2	NAG	O5-C5-C6-O6
7	G	1	NAG	O7-C7-N2-C2
6	F	1	NAG	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
6	F	2	NAG	C4-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6

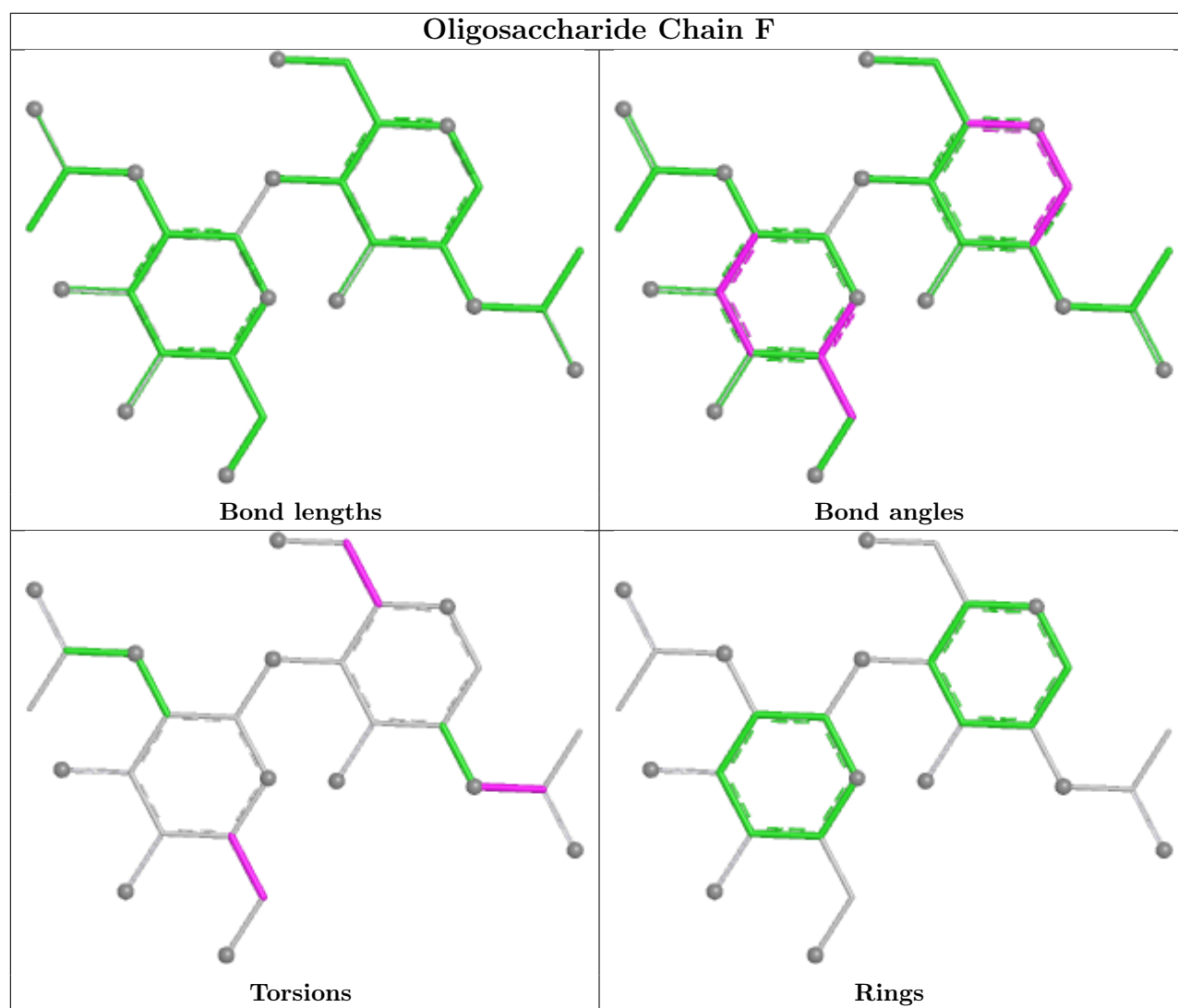
There are no ring outliers.

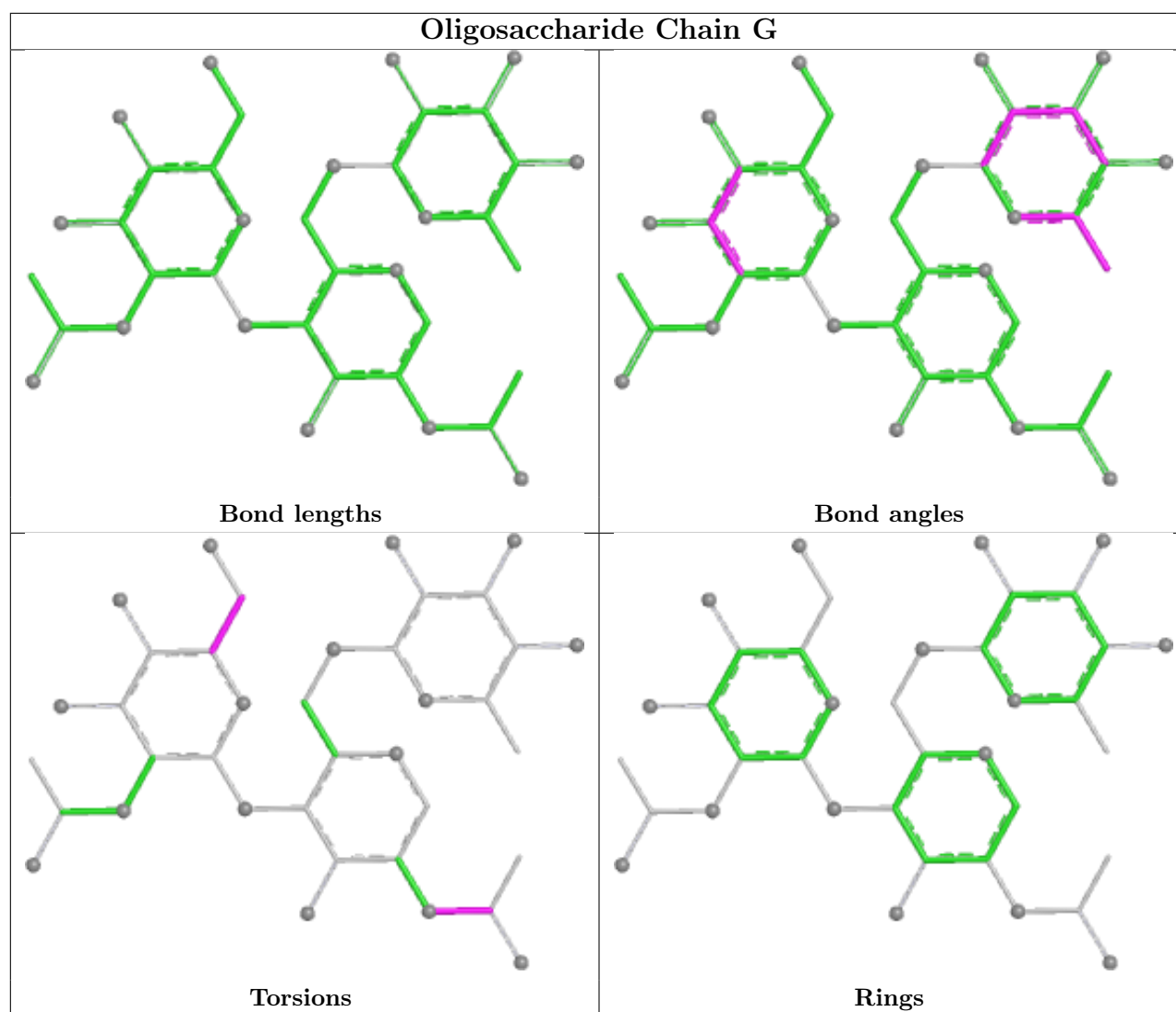
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	3	FUC	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](#)

1 ligand is 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	$\# Z > 2$
8	JLS	A	310	-	58,58,58	0.52	1 (1%)	64,67,67	1.18	5 (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
8	JLS	A	310	-	-	24/56/76/76	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	310	JLS	O1A-C1A	2.40	1.44	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	310	JLS	C6-C5-C4	-3.71	108.04	114.11
8	A	310	JLS	O4-C4-C3	3.47	117.38	109.25
8	A	310	JLS	C1-C2-C3	2.99	118.58	112.71
8	A	310	JLS	O3-C3-C4	-2.39	103.50	108.93
8	A	310	JLS	O3A-C3A-C2A	2.07	115.26	110.38

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	310	JLS	C1-C2-C3-C4
8	A	310	JLS	N2-C2-C3-O3
8	A	310	JLS	N2-C2-C3-C4
8	A	310	JLS	C2-C3-C4-O4
8	A	310	JLS	C2-C3-C4-C5
8	A	310	JLS	O3-C3-C4-O4
8	A	310	JLS	O3-C3-C4-C5
8	A	310	JLS	O4-C4-C5-C6
8	A	310	JLS	CAJ-CAK-CAL-CAM
8	A	310	JLS	CAK-CAL-CAM-CAN
8	A	310	JLS	C11-C12-C13-C14
8	A	310	JLS	C14-C15-C16-C17
8	A	310	JLS	C11-C10-C9-C8
8	A	310	JLS	CAG-CAH-CAI-CAJ
8	A	310	JLS	C9-C10-C11-C12
8	A	310	JLS	CAL-CAM-CAN-CAO
8	A	310	JLS	CAH-CAI-CAJ-CAK
8	A	310	JLS	CAT-CAU-CAV-CAW

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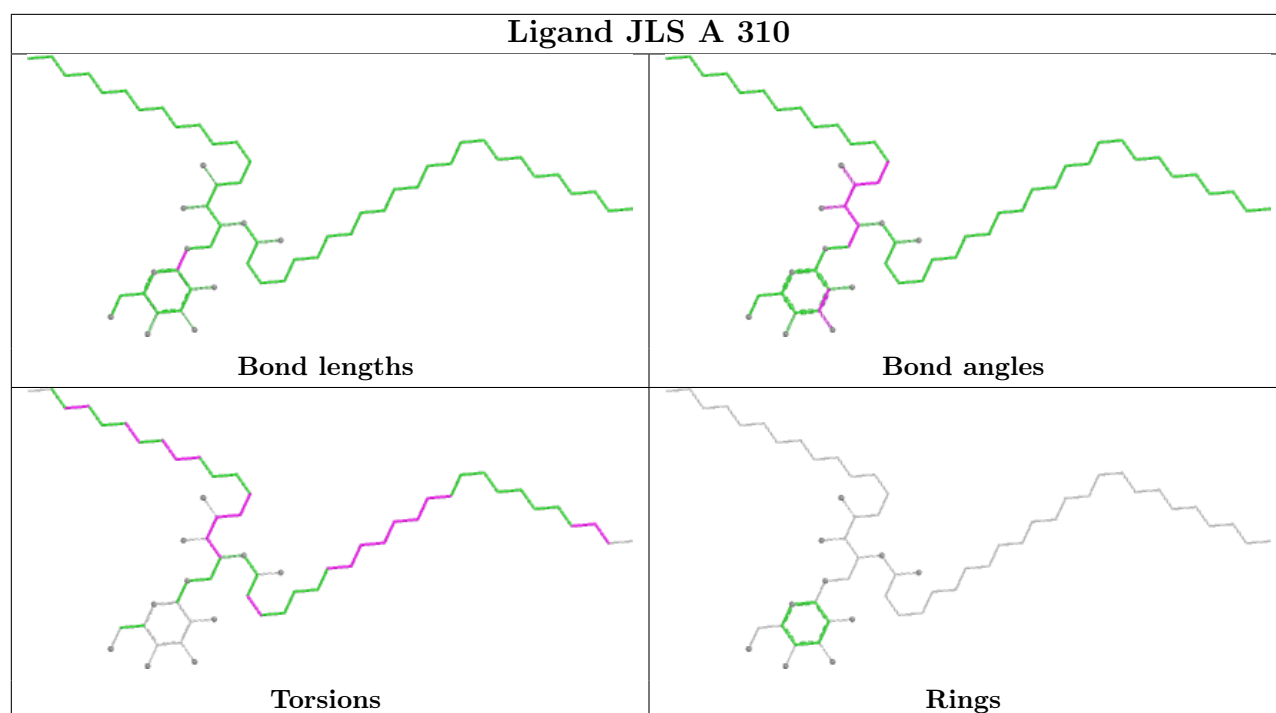
Mol	Chain	Res	Type	Atoms
8	A	310	JLS	C4-C5-C6-C7
8	A	310	JLS	CAA-CAB-CAC-CAD
8	A	310	JLS	CAF-CAG-CAH-CAI
8	A	310	JLS	CAU-CAV-CAW-CAX
8	A	310	JLS	CAI-CAJ-CAK-CAL
8	A	310	JLS	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	310	JLS	3	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

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	273/274 (99%)	0.31	11 (4%) 42 38	17, 38, 69, 89	0
2	B	98/100 (98%)	0.90	13 (13%) 7 6	19, 52, 80, 85	0
3	C	200/207 (96%)	0.04	6 (3%) 52 48	18, 33, 60, 83	2 (1%)
4	D	242/245 (98%)	0.20	12 (4%) 34 30	16, 35, 71, 93	3 (1%)
All	All	813/826 (98%)	0.28	42 (5%) 33 29	16, 38, 71, 93	5 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	GLY	6.1
4	D	162	ASP	3.9
4	D	229	ASN	3.8
4	D	194	ASP	3.4
1	A	268	LEU	3.3
2	B	1	ILE	3.3
3	C	214	SER	3.2
3	C	191	ASN	3.2
1	A	269	GLU	3.1
2	B	18	GLY	3.1
3	C	87	VAL	3.1
1	A	107	GLY	3.0
4	D	191	ALA	2.9
4	D	31	THR	2.8
4	D	252	ALA	2.8
1	A	199	PRO	2.7
3	C	197	CYS	2.7
2	B	89	GLN	2.6
4	D	180	CYS	2.6
2	B	98	ASP	2.5
1	A	279	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	109	ALA	2.5
2	B	73	THR	2.5
1	A	252	VAL	2.5
1	A	225	GLN	2.5
2	B	71	THR	2.4
2	B	94	LYS	2.4
3	C	163	ASP	2.4
4	D	72	GLU	2.2
2	B	43	GLY	2.2
4	D	192	LEU	2.2
4	D	59	GLY	2.1
2	B	34	ASP	2.1
4	D	125	ASP	2.1
2	B	49	VAL	2.1
1	A	224	GLU	2.1
2	B	91	LYS	2.1
1	A	43	ASP	2.1
2	B	76	ASP	2.1
2	B	9	VAL	2.0
4	D	124	GLU	2.0
3	C	194	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

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

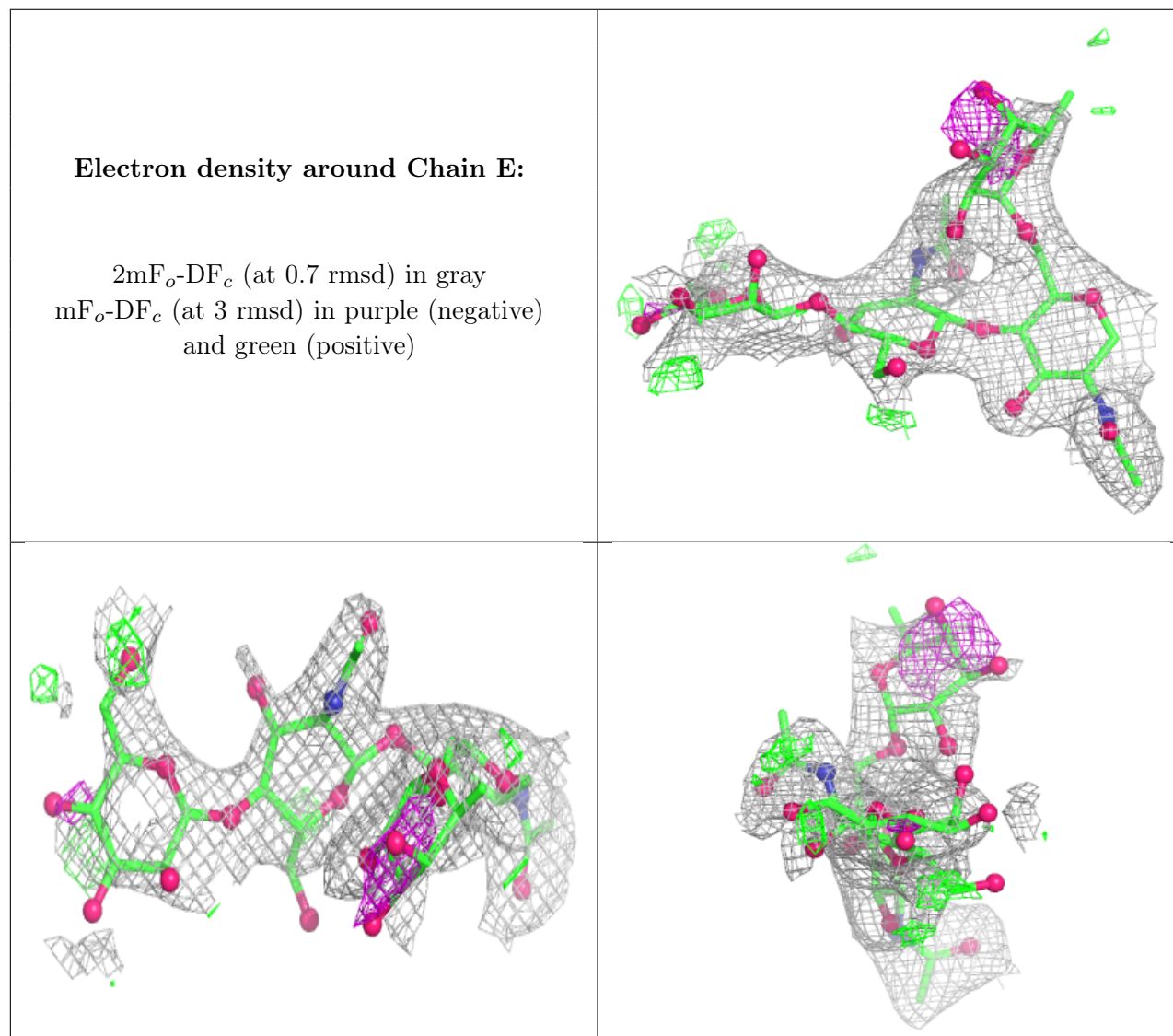
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BMA	E	3	11/12	0.15	0.21	91,93,93,93	0
5	FUC	E	4	10/11	0.60	0.23	63,66,67,67	0
6	NAG	F	2	14/15	0.62	0.20	80,84,89,89	0
7	FUC	G	3	10/11	0.70	0.24	76,78,78,78	0
5	NAG	E	2	14/15	0.72	0.15	72,78,86,88	0
7	NAG	G	2	14/15	0.81	0.16	73,77,80,80	0
7	NAG	G	1	14/15	0.85	0.14	60,65,72,72	0

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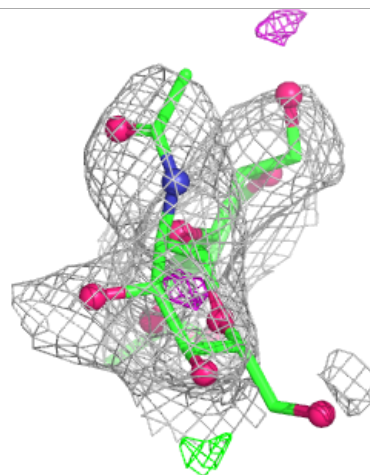
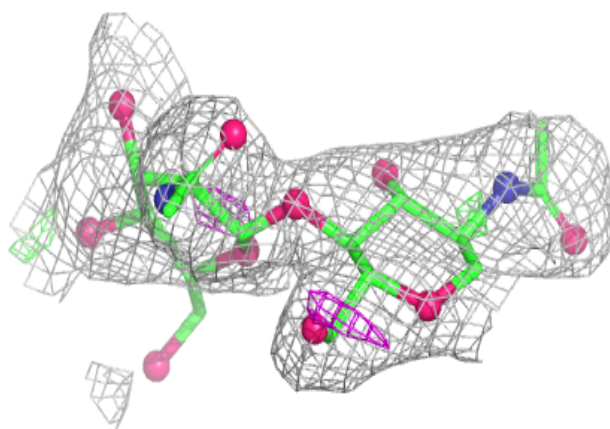
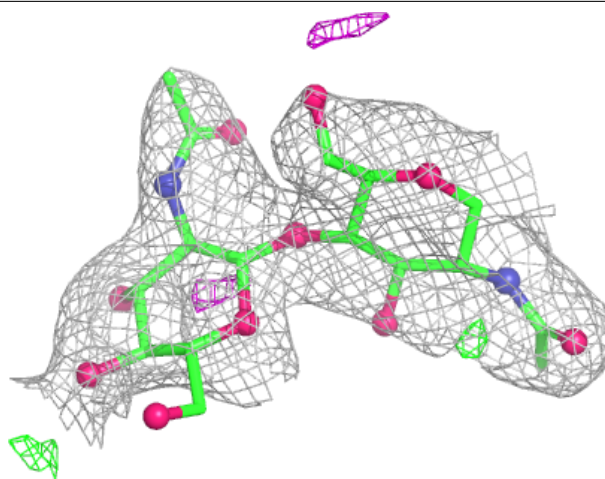
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	F	1	14/15	0.86	0.13	41,47,61,71	0
5	NAG	E	1	14/15	0.94	0.09	21,43,55,63	0

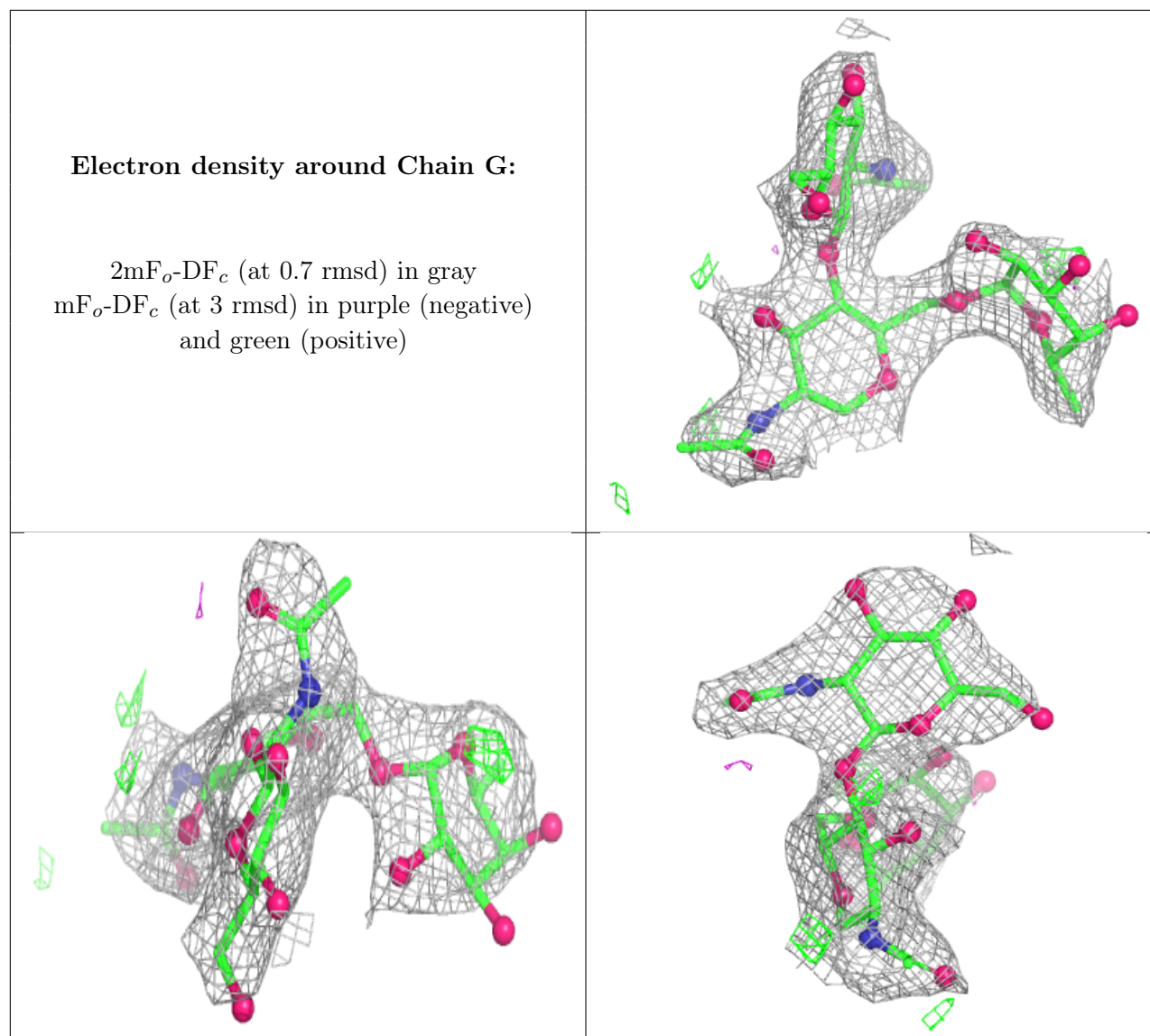
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain F:

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





6.4 Ligands [i](#)

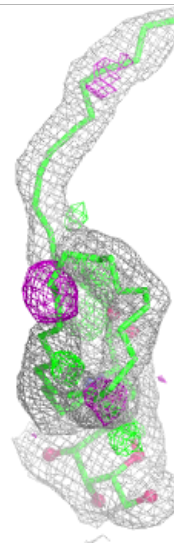
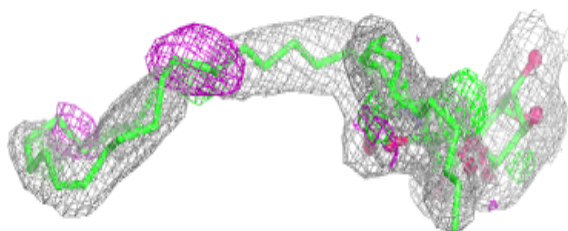
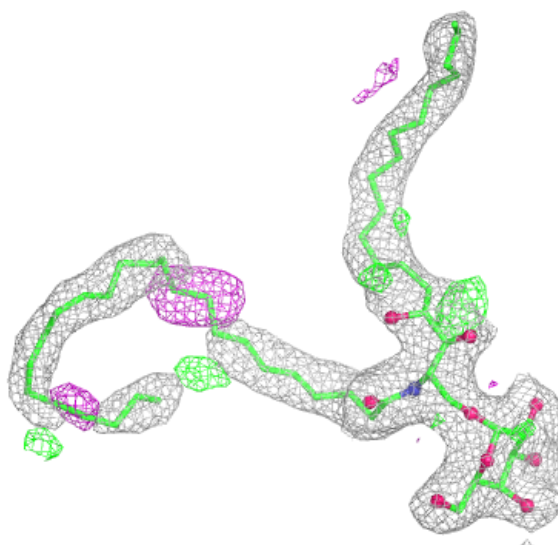
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	JLS	A	310	58/58	0.90	0.13	20,32,40,41	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 JLS A 310:

$2mF_o-DF_c$ (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.