



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 12:34 AM BST

PDB ID : 4LHU
Title : Crystal Structure of 9C2 TCR bound to CD1d
Authors : Uldrich, A.P.; Le Nours, J.; Pellicci, D.G.; Gras, S.; Rossjohn, J.; Godfrey, D.I.
Deposited on : 2013-07-01
Resolution : 2.87 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

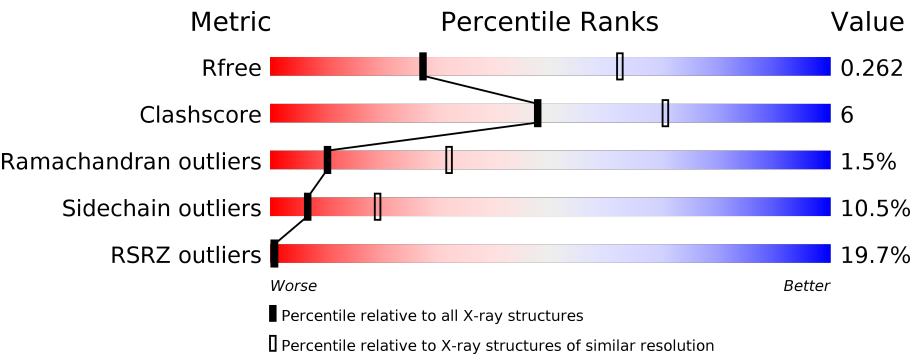
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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.



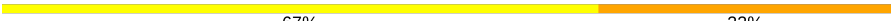
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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 on 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	278	<div><div>13%</div><div><div></div><div>78%</div><div>18%</div><div>••</div></div></div>
2	B	100	<div><div>10%</div><div><div></div><div>83%</div><div>13%</div><div>•</div></div></div>
3	D	236	<div><div>19%</div><div><div></div><div>69%</div><div>15%</div><div>•</div><div>14%</div></div></div>
4	G	251	<div><div>26%</div><div><div></div><div>70%</div><div>15%</div><div>5%</div><div>10%</div></div></div>
5	C	2	<div><div></div><div><div></div><div>100%</div></div></div>
5	E	2	<div><div></div><div><div></div><div>50%</div><div>50%</div></div></div>

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Mol	Chain	Length	Quality of chain
6	F	3	 67% 33%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 6749 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	272	Total	C	N	O	S	0	0	0
			2185	1397	382	399	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	278	HIS	-	expression tag	UNP P15813
A	279	HIS	-	expression tag	UNP P15813
A	280	HIS	-	expression tag	UNP P15813
A	281	HIS	-	expression tag	UNP P15813
A	282	HIS	-	expression tag	UNP P15813
A	283	HIS	-	expression tag	UNP P15813

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			

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 9C2 TCR delta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	202	Total	C	N	O	S	4	0	0
			1592	1015	269	301	7			

- Molecule 4 is a protein called 9C2 TCR gamma chain.

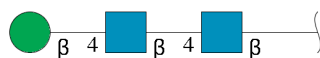
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	227	Total	C	N	O	S	4	0	0
			1847	1183	312	346	6			

- Molecule 5 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
5	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



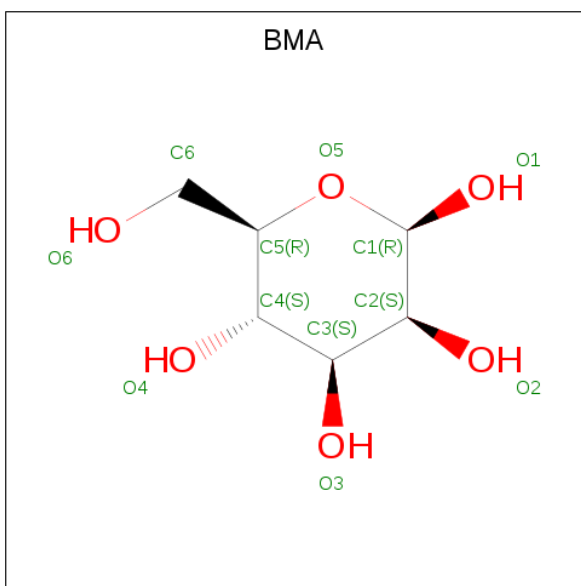
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).

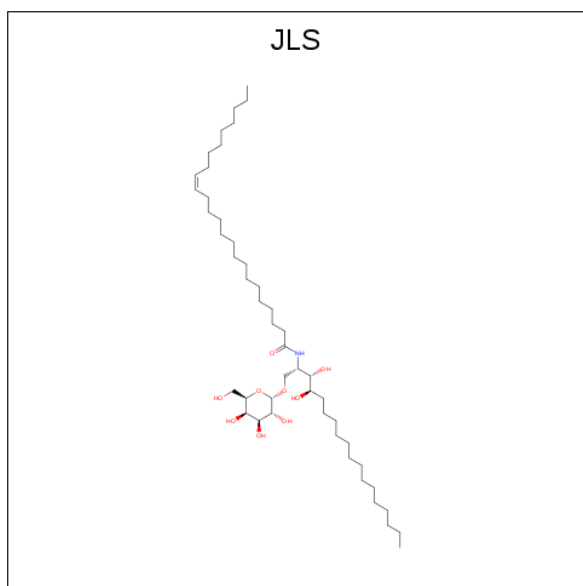


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 10 is (15Z)-N-[(2S,3S,4R)-1-(alpha-D-galactopyranosyloxy)-3,4-dihydroxyoctadecan-2-yl]tetracos-15-enamide (three-letter code: JLS) (formula: C₄₈H₉₃NO₉).



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

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	G	1	Total	Cl	0	0
			1	1		

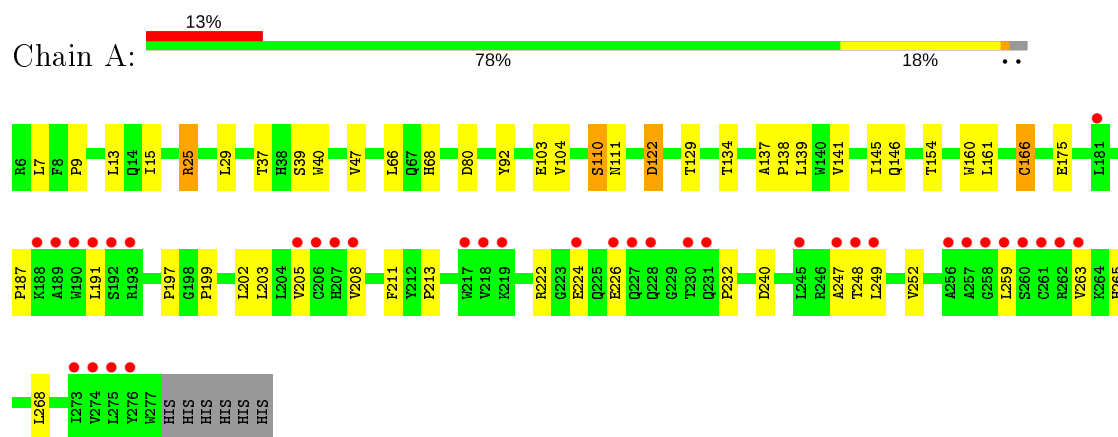
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	44	Total	O	0	0
			44	44		
12	B	6	Total	O	0	0
			6	6		
12	D	18	Total	O	0	0
			18	18		
12	G	41	Total	O	0	0
			41	41		

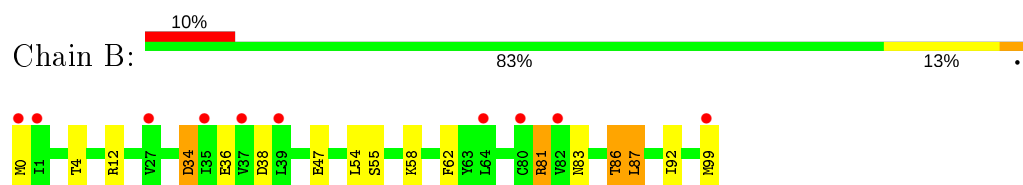
3 Residue-property plots [i](#)

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



	NAG1	NAG2	BMA3
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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	131.62Å 152.69Å 135.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.47 – 2.87 47.47 – 2.87	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.47-2.87) 99.1 (47.47-2.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.86Å)	Xtriage
Refinement program	BUSTER-TNT, BUSTER 2.10.0	Depositor
R, R_{free}	0.206 , 0.243 0.223 , 0.262	Depositor DCC
R_{free} test set	1579 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	75.9	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 85.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6749	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BMA, NAG, JLS, CL

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	0.43	0/2250	0.64	0/3063
2	B	0.40	0/859	0.61	0/1162
3	D	0.44	0/1627	0.64	0/2200
4	G	0.47	0/1896	0.65	1/2576 (0.0%)
All	All	0.44	0/6632	0.64	1/9001 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	103	ARG	C-N-CA	5.80	134.47	122.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2185	0	2121	22	0
2	B	836	0	805	8	0
3	D	1592	0	1600	14	0
4	G	1847	0	1830	43	0
5	C	28	0	25	0	0
5	E	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	39	0	34	1	0
7	A	14	0	13	0	0
8	A	11	0	10	0	0
9	A	1	0	0	0	0
10	A	58	0	93	3	0
11	G	1	0	0	0	0
12	A	44	0	0	0	0
12	B	6	0	0	0	0
12	D	18	0	0	0	0
12	G	41	0	0	0	0
All	All	6749	0	6556	78	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 6.

All (78) 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:G:170:TRP:CZ2	4:G:212:CYS:HB2	1.96	0.99
4:G:26:CYS:HG	4:G:98:CYS:HG	1.21	0.85
4:G:169:HIS:O	4:G:170:TRP:HB2	1.75	0.84
4:G:169:HIS:O	4:G:170:TRP:CB	2.30	0.79
4:G:170:TRP:CZ2	4:G:212:CYS:CB	2.65	0.79
4:G:170:TRP:CE2	4:G:212:CYS:HA	2.21	0.75
4:G:169:HIS:O	4:G:170:TRP:CD1	2.44	0.70
3:D:11:GLN:O	3:D:113:THR:HG22	1.93	0.68
1:A:122:ASP:HB3	1:A:134:THR:HG21	1.83	0.60
4:G:169:HIS:O	4:G:170:TRP:CG	2.55	0.59
4:G:171:GLN:HA	4:G:177:THR:O	2.03	0.59
3:D:9:GLN:HE21	3:D:110:GLY:HA3	1.68	0.59
1:A:205:VAL:HG21	2:B:99:MET:HG2	1.87	0.57
4:G:170:TRP:CZ2	4:G:212:CYS:SG	2.98	0.57
4:G:93:SER:HB3	4:G:123:VAL:HG22	1.88	0.56
4:G:134:PRO:HB2	4:G:158:LEU:HD22	1.89	0.55
4:G:169:HIS:HB2	4:G:213:ILE:CD1	2.37	0.55
4:G:170:TRP:NE1	4:G:212:CYS:HA	2.22	0.53
1:A:154:THR:HG21	10:A:308:JLS:H61	1.91	0.53
4:G:167:LYS:O	4:G:168:ILE:CG2	2.57	0.53
2:B:54:LEU:HD11	2:B:62:PHE:HB3	1.90	0.53
1:A:9:PRO:HB3	1:A:103:GLU:HB3	1.92	0.52
2:B:4:THR:HA	2:B:86:THR:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:170:TRP:CE2	4:G:212:CYS:CB	2.93	0.51
1:A:104:VAL:HG12	1:A:110:SER:HB2	1.91	0.51
3:D:37:ILE:HG21	3:D:77:VAL:HG21	1.93	0.51
3:D:175:TYR:HE2	4:G:182:GLN:HG2	1.75	0.51
4:G:167:LYS:O	4:G:168:ILE:HG23	2.11	0.51
4:G:170:TRP:C	4:G:171:GLN:HG2	2.31	0.50
1:A:232:PRO:HA	1:A:247:ALA:HA	1.94	0.50
1:A:68:HIS:HE1	3:D:103:ASN:OD1	1.95	0.50
4:G:37:HIS:HD2	4:G:49:ARG:HE	1.58	0.50
2:B:81:ARG:HB3	2:B:92:ILE:HG22	1.94	0.49
3:D:194:GLN:HA	3:D:199:THR:HA	1.95	0.49
4:G:170:TRP:CE2	4:G:212:CYS:CA	2.95	0.49
3:D:104:THR:O	4:G:49:ARG:NH2	2.47	0.48
4:G:167:LYS:C	4:G:168:ILE:HG23	2.34	0.48
1:A:208:VAL:HG21	1:A:263:VAL:HG11	1.96	0.47
1:A:213:PRO:HD2	1:A:265:HIS:HE1	1.78	0.47
4:G:154:TYR:HE2	4:G:199:LEU:HD23	1.79	0.47
4:G:206:LEU:HD22	4:G:232:ILE:HB	1.97	0.47
2:B:36:GLU:HB2	2:B:83:ASN:HB3	1.96	0.47
1:A:160:TRP:CD1	3:D:34:SER:HB3	2.50	0.47
1:A:80:ASP:OD2	10:A:308:JLS:H57	2.15	0.47
4:G:203:GLU:HA	4:G:206:LEU:HD12	1.96	0.46
1:A:141:VAL:O	1:A:145:ILE:HG12	2.16	0.46
4:G:89:ILE:O	4:G:123:VAL:HG21	2.15	0.46
1:A:25:ARG:HB2	5:E:1:NAG:H82	1.98	0.46
1:A:213:PRO:HD2	1:A:265:HIS:CE1	2.51	0.45
4:G:170:TRP:NE1	4:G:212:CYS:SG	2.90	0.45
3:D:175:TYR:CE2	4:G:182:GLN:HG2	2.52	0.44
4:G:168:ILE:C	4:G:169:HIS:CG	2.90	0.44
4:G:169:HIS:HB2	4:G:170:TRP:H	1.52	0.44
1:A:161:LEU:O	1:A:166:CYS:HB2	2.17	0.44
4:G:102:ASP:OD2	4:G:104:GLY:HA2	2.17	0.44
4:G:104:GLY:HA3	4:G:112:LYS:HE2	2.00	0.44
1:A:240:ASP:HB2	2:B:12:ARG:HE	1.83	0.44
4:G:141:PRO:HB2	4:G:232:ILE:HG12	1.99	0.44
3:D:170:SER:HB3	3:D:175:TYR:HA	1.99	0.44
4:G:42:GLN:HB2	4:G:45:LYS:HD2	2.00	0.43
4:G:170:TRP:HZ2	4:G:212:CYS:SG	2.40	0.43
1:A:205:VAL:HG22	1:A:248:THR:HG22	2.01	0.43
4:G:138:ILE:HD11	6:F:1:NAG:H4	2.01	0.43
3:D:24:LEU:HD12	3:D:79:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:160:LYS:H	4:G:160:LYS:HZ2	1.67	0.43
1:A:197:PRO:HG3	1:A:203:LEU:HD23	2.01	0.42
4:G:126:LYS:HB3	4:G:128:LEU:HD12	2.00	0.42
3:D:18:VAL:HG23	3:D:118:GLU:O	2.19	0.42
3:D:106:LYS:HB3	4:G:49:ARG:CZ	2.49	0.42
3:D:133:LYS:HB3	3:D:138:VAL:HG23	2.02	0.42
4:G:143:ILE:HG13	4:G:143:ILE:H	1.75	0.42
4:G:106:PRO:HD2	4:G:112:LYS:NZ	2.35	0.42
1:A:29:LEU:HD11	2:B:55:SER:HB2	2.01	0.41
2:B:83:ASN:HA	2:B:87:LEU:HD11	2.00	0.41
1:A:47:VAL:HG11	10:A:308:JLS:H29	2.03	0.41
1:A:137:ALA:C	1:A:139:LEU:H	2.24	0.41
4:G:104:GLY:H	4:G:107:LYS:HA	1.86	0.41
1:A:187:PRO:HB3	1:A:211:PHE:HB3	2.04	0.40

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	270/278 (97%)	250 (93%)	17 (6%)	3 (1%)	14	40
2	B	98/100 (98%)	95 (97%)	2 (2%)	1 (1%)	15	42
3	D	200/236 (85%)	181 (90%)	15 (8%)	4 (2%)	7	25
4	G	225/251 (90%)	204 (91%)	17 (8%)	4 (2%)	8	27
All	All	793/865 (92%)	730 (92%)	51 (6%)	12 (2%)	10	32

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	PRO

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Mol	Chain	Res	Type
4	G	170	TRP
2	B	34	ASP
3	D	124	HIS
3	D	144	GLU
3	D	196	ASP
4	G	125	ASP
4	G	169	HIS
4	G	107	LYS
3	D	168	VAL
1	A	138	PRO
1	A	252	VAL

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	238/244 (98%)	214 (90%)	24 (10%)	7	21
2	B	95/95 (100%)	87 (92%)	8 (8%)	11	30
3	D	180/210 (86%)	160 (89%)	20 (11%)	6	17
4	G	208/228 (91%)	184 (88%)	24 (12%)	5	15
All	All	721/777 (93%)	645 (90%)	76 (10%)	7	19

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	13	LEU
1	A	15	ILE
1	A	25	ARG
1	A	37	THR
1	A	39	SER
1	A	40	TRP
1	A	66	LEU
1	A	92	TYR
1	A	110	SER

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Mol	Chain	Res	Type
1	A	111	ASN
1	A	122	ASP
1	A	129	THR
1	A	146	GLN
1	A	166	CYS
1	A	175	GLU
1	A	191	LEU
1	A	202	LEU
1	A	222	ARG
1	A	224	GLU
1	A	226	GLU
1	A	249	LEU
1	A	259	LEU
1	A	268	LEU
2	B	0	MET
2	B	34	ASP
2	B	38	ASP
2	B	47	GLU
2	B	58	LYS
2	B	81	ARG
2	B	86	THR
2	B	87	LEU
3	D	5	GLN
3	D	11	GLN
3	D	14	VAL
3	D	15	SER
3	D	25	ASN
3	D	34	SER
3	D	53	ARG
3	D	56	SER
3	D	72	LYS
3	D	77	VAL
3	D	96	LEU
3	D	120	ARG
3	D	122	GLN
3	D	136	THR
3	D	141	LEU
3	D	162	GLU
3	D	168	VAL
3	D	176	ASN
3	D	180	LEU
3	D	198	LYS

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Mol	Chain	Res	Type
4	G	26	CYS
4	G	48	GLN
4	G	49	ARG
4	G	51	LEU
4	G	58	SER
4	G	90	GLU
4	G	100	THR
4	G	112	LYS
4	G	127	GLN
4	G	128	LEU
4	G	154	TYR
4	G	155	LEU
4	G	156	CYS
4	G	160	LYS
4	G	169	HIS
4	G	171	GLN
4	G	178	ILE
4	G	182	GLN
4	G	188	LYS
4	G	194	MET
4	G	209	GLU
4	G	211	ARG
4	G	213	ILE
4	G	232	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
1	A	184	GLN
1	A	238	ASN
3	D	9	GLN
3	D	60	ASN
3	D	85	GLN
3	D	122	GLN
4	G	37	HIS
4	G	48	GLN
4	G	169	HIS

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 ⓘ

7 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	C	1	1,5	14,14,15	1.98	3 (21%)	17,19,21	2.22	6 (35%)
5	NAG	C	2	5	14,14,15	1.85	3 (21%)	17,19,21	1.81	4 (23%)
5	NAG	E	1	1,5	14,14,15	1.89	5 (35%)	17,19,21	1.97	5 (29%)
5	NAG	E	2	5	14,14,15	1.91	3 (21%)	17,19,21	1.70	3 (17%)
6	NAG	F	1	3,6	14,14,15	1.89	3 (21%)	17,19,21	2.43	8 (47%)
6	NAG	F	2	6	14,14,15	1.90	2 (14%)	17,19,21	2.12	6 (35%)
6	BMA	F	3	6	11,11,12	1.90	4 (36%)	15,15,17	1.48	2 (13%)

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	C	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1
5	NAG	E	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
6	NAG	F	1	3,6	-	1/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	F	3	6	-	2/2/19/22	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1	NAG	O5-C1	5.03	1.51	1.43
5	E	2	NAG	O5-C1	4.89	1.51	1.43
6	F	2	NAG	O5-C1	4.82	1.51	1.43
6	F	1	NAG	O5-C1	4.69	1.51	1.43
6	F	3	BMA	C4-C3	-4.62	1.40	1.52
5	C	2	NAG	O5-C1	4.47	1.50	1.43
5	E	1	NAG	O5-C1	4.08	1.50	1.43
5	C	1	NAG	C7-N2	3.23	1.45	1.34
6	F	2	NAG	C7-N2	3.22	1.45	1.34
5	E	2	NAG	C7-N2	3.21	1.45	1.34
6	F	1	NAG	C7-N2	3.16	1.45	1.34
5	C	2	NAG	C7-N2	3.06	1.44	1.34
5	E	1	NAG	C7-N2	2.71	1.43	1.34
5	E	1	NAG	C1-C2	-2.64	1.48	1.52
5	E	1	NAG	C3-C2	-2.62	1.46	1.52
6	F	3	BMA	C2-C3	-2.60	1.48	1.52
6	F	3	BMA	O5-C1	-2.31	1.40	1.43
5	E	1	NAG	C4-C3	-2.21	1.46	1.52
5	C	1	NAG	C3-C2	-2.16	1.47	1.52
5	C	2	NAG	C4-C3	-2.10	1.47	1.52
6	F	1	NAG	C4-C3	-2.08	1.47	1.52
5	E	2	NAG	C4-C3	-2.05	1.47	1.52
6	F	3	BMA	O5-C5	2.04	1.47	1.43

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	1	NAG	C4-C3-C2	6.21	120.12	111.02
6	F	1	NAG	O5-C5-C6	5.13	115.25	107.20
5	C	1	NAG	O5-C5-C6	5.03	115.09	107.20
5	E	2	NAG	O5-C5-C6	4.81	114.75	107.20
5	C	1	NAG	C1-O5-C5	4.50	118.28	112.19
5	C	2	NAG	C4-C3-C2	4.42	117.50	111.02
5	E	1	NAG	C1-O5-C5	4.15	117.82	112.19
5	E	1	NAG	C1-C2-N2	-4.03	103.60	110.49
6	F	2	NAG	C4-C3-C2	3.79	116.58	111.02
6	F	2	NAG	C3-C4-C5	3.59	116.65	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1	NAG	C4-C3-C2	3.57	116.25	111.02
5	C	2	NAG	O5-C5-C6	3.53	112.74	107.20
6	F	2	NAG	C1-O5-C5	3.25	116.60	112.19
6	F	3	BMA	C2-C3-C4	3.08	116.22	110.89
6	F	2	NAG	O5-C5-C6	2.93	111.80	107.20
5	E	1	NAG	O5-C5-C6	2.87	111.70	107.20
6	F	2	NAG	O5-C1-C2	2.69	115.54	111.29
5	C	1	NAG	O5-C1-C2	2.65	115.48	111.29
6	F	2	NAG	O4-C4-C5	2.44	115.35	109.30
6	F	1	NAG	C3-C4-C5	2.43	114.57	110.24
5	E	2	NAG	C1-C2-N2	-2.41	106.38	110.49
6	F	1	NAG	O5-C1-C2	2.38	115.04	111.29
5	C	2	NAG	C3-C4-C5	2.36	114.45	110.24
5	E	1	NAG	O5-C5-C4	2.34	116.53	110.83
5	C	2	NAG	C1-C2-N2	-2.33	106.50	110.49
6	F	1	NAG	C1-C2-N2	-2.32	106.53	110.49
6	F	1	NAG	O6-C6-C5	2.21	118.88	111.29
6	F	3	BMA	O4-C4-C3	-2.17	105.32	110.35
5	E	2	NAG	C1-O5-C5	2.17	115.13	112.19
5	C	1	NAG	O6-C6-C5	2.13	118.61	111.29
5	E	1	NAG	O3-C3-C2	-2.12	105.09	109.47
6	F	1	NAG	O4-C4-C3	-2.08	105.53	110.35
6	F	1	NAG	C8-C7-N2	2.06	119.59	116.10
5	C	1	NAG	C8-C7-N2	2.02	119.52	116.10

There are no chirality outliers.

All (10) torsion outliers are listed below:

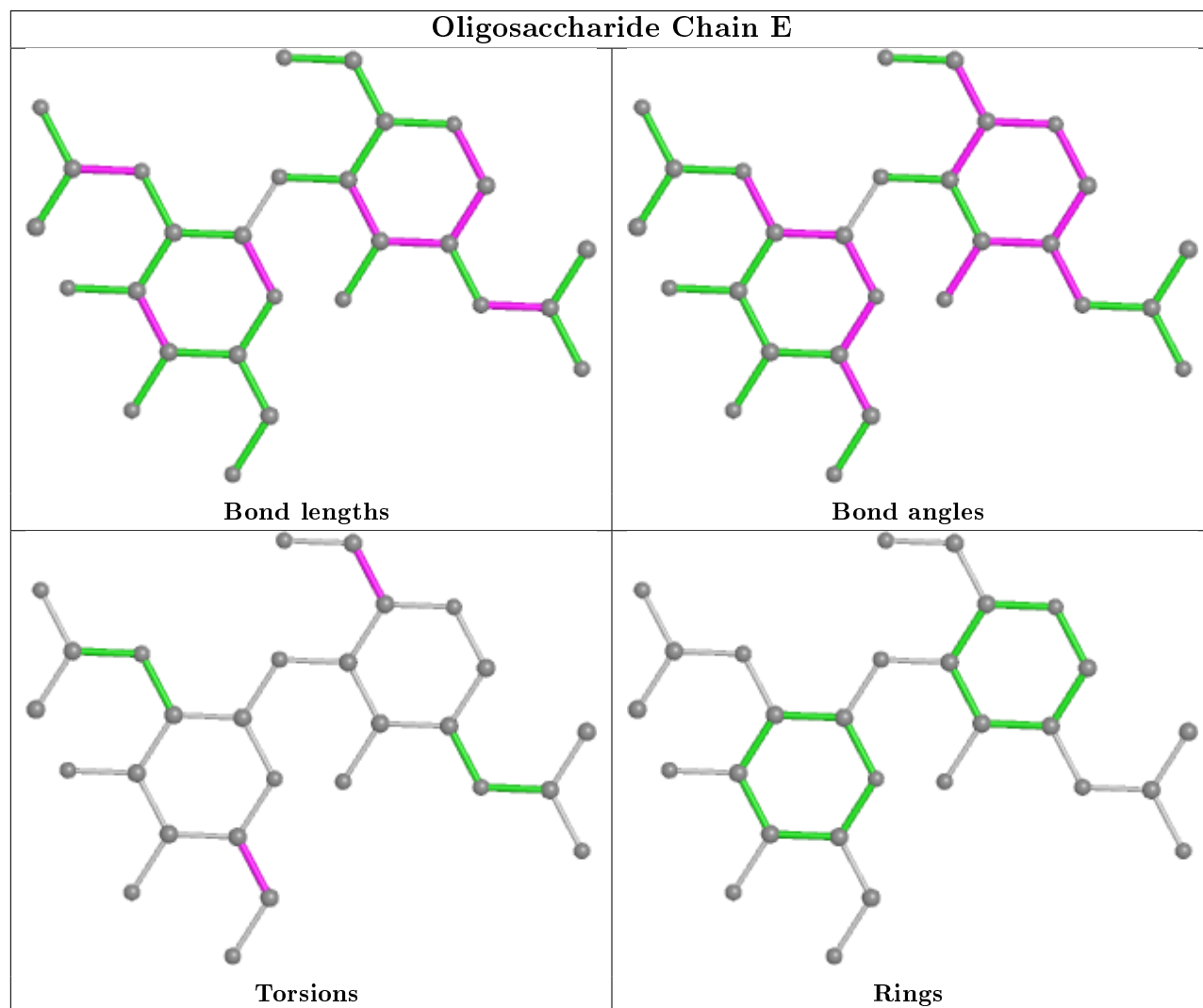
Mol	Chain	Res	Type	Atoms
5	C	1	NAG	O5-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
6	F	3	BMA	C4-C5-C6-O6
6	F	2	NAG	C4-C5-C6-O6
5	C	1	NAG	C4-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
6	F	3	BMA	O5-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6
6	F	1	NAG	O5-C5-C6-O6

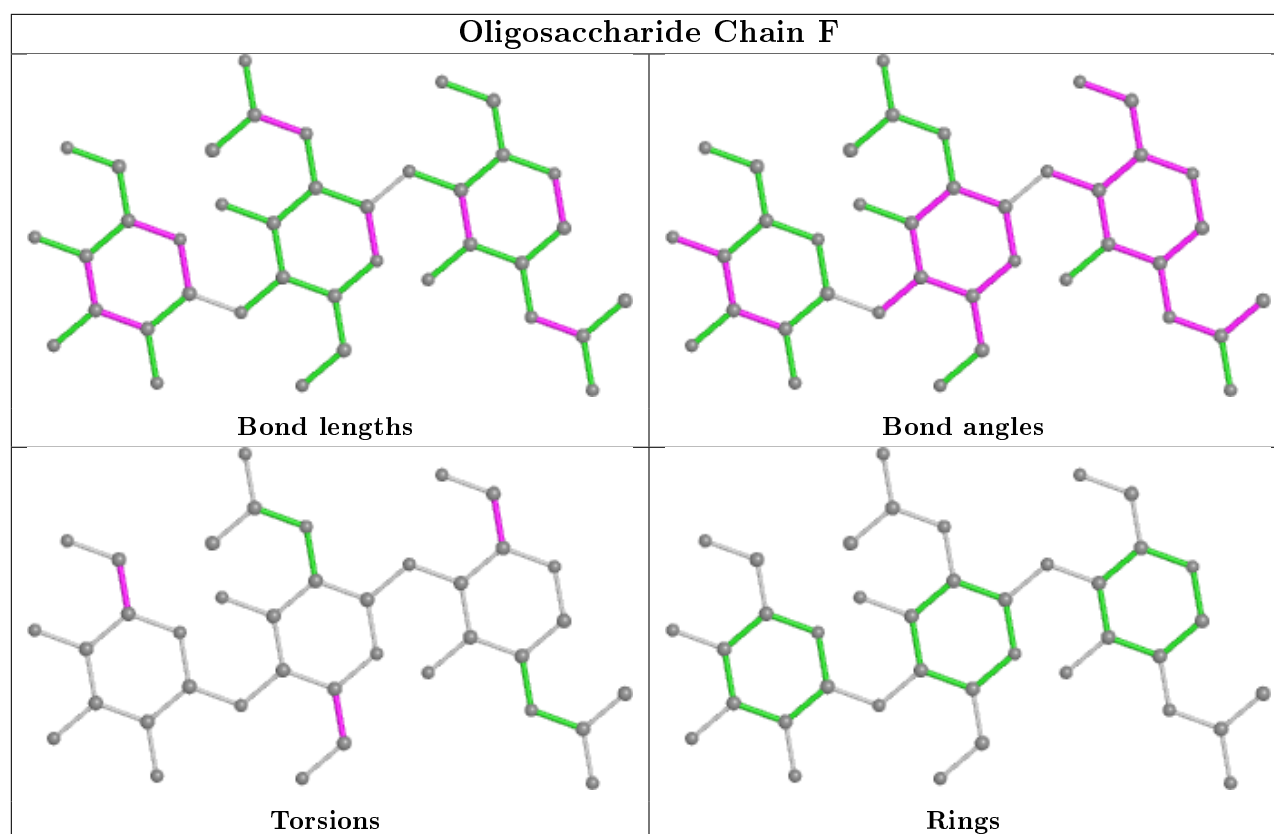
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	1	NAG	1	0
5	E	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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	NAG	A	301	1	14,14,15	1.99	3 (21%)	17,19,21	1.93	5 (29%)
8	BMA	A	306	-	11,11,12	1.91	4 (36%)	15,15,17	2.16	6 (40%)
10	JLS	A	308	-	58,58,58	0.43	1 (1%)	63,67,67	1.01	6 (9%)

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	NAG	A	301	1	-	1/6/23/26	0/1/1/1
8	BMA	A	306	-	-	2/2/19/22	0/1/1/1
10	JLS	A	308	-	-	28/56/76/76	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	301	NAG	O5-C1	5.45	1.52	1.43
8	A	306	BMA	C4-C3	-4.66	1.40	1.52
7	A	301	NAG	C7-N2	3.01	1.44	1.34
8	A	306	BMA	C2-C3	-2.56	1.48	1.52
8	A	306	BMA	O5-C1	-2.24	1.40	1.43
7	A	301	NAG	C4-C3	-2.22	1.46	1.52
8	A	306	BMA	O5-C5	2.10	1.47	1.43
10	A	308	JLS	O1A-C1A	2.05	1.43	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	301	NAG	O5-C5-C6	5.66	116.08	107.20
8	A	306	BMA	C2-C3-C4	4.55	118.76	110.89
8	A	306	BMA	C3-C4-C5	3.03	115.65	110.24
8	A	306	BMA	C1-C2-C3	2.85	113.17	109.67
10	A	308	JLS	CAC-CAB-CAA	-2.80	105.40	113.26
8	A	306	BMA	C1-O5-C5	2.71	115.86	112.19
8	A	306	BMA	O4-C4-C3	-2.68	104.14	110.35
7	A	301	NAG	C4-C3-C2	2.49	114.66	111.02
7	A	301	NAG	C1-O5-C5	2.44	115.50	112.19
10	A	308	JLS	OAA-CAA-CAB	-2.26	117.89	122.02
10	A	308	JLS	C6-C5-C4	-2.23	110.51	114.18
10	A	308	JLS	O5A-C5M-C6A	2.21	111.93	106.44
10	A	308	JLS	O4-C4-C3	2.19	114.43	109.10
8	A	306	BMA	O6-C6-C5	2.19	118.79	111.29
7	A	301	NAG	O6-C6-C5	2.18	118.78	111.29
10	A	308	JLS	C1A-O5A-C5M	2.14	117.88	113.69
7	A	301	NAG	C3-C4-C5	2.02	113.84	110.24

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	308	JLS	N2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
10	A	308	JLS	O3-C3-C4-C5
10	A	308	JLS	C3-C4-C5-C6
10	A	308	JLS	O4-C4-C5-C6
8	A	306	BMA	O5-C5-C6-O6
10	A	308	JLS	C5-C6-C7-C8
10	A	308	JLS	C12-C13-C14-C15
10	A	308	JLS	C9-C10-C11-C12
10	A	308	JLS	CAK-CAL-CAM-CAN
10	A	308	JLS	CAB-CAC-CAD-CAE
10	A	308	JLS	CAI-CAJ-CAK-CAL
10	A	308	JLS	C6-C7-C8-C9
10	A	308	JLS	C11-C12-C13-C14
10	A	308	JLS	CAF-CAG-CAH-CAI
10	A	308	JLS	CAJ-CAK-CAL-CAM
10	A	308	JLS	CAC-CAD-CAE-CAF
10	A	308	JLS	C15-C16-C17-C18
10	A	308	JLS	CAU-CAV-CAW-CAX
10	A	308	JLS	CAQ-CAR-CAS-CAT
7	A	301	NAG	O5-C5-C6-O6
10	A	308	JLS	CAE-CAF-CAG-CAH
10	A	308	JLS	CAG-CAH-CAI-CAJ
10	A	308	JLS	CAT-CAU-CAV-CAW
10	A	308	JLS	C10-C11-C12-C13
10	A	308	JLS	C14-C15-C16-C17
10	A	308	JLS	CAD-CAE-CAF-CAG
10	A	308	JLS	CAR-CAS-CAT-CAU
10	A	308	JLS	O3-C3-C4-O4
8	A	306	BMA	C4-C5-C6-O6
10	A	308	JLS	CAM-CAN-CAO-CAP
10	A	308	JLS	C2-C3-C4-C5

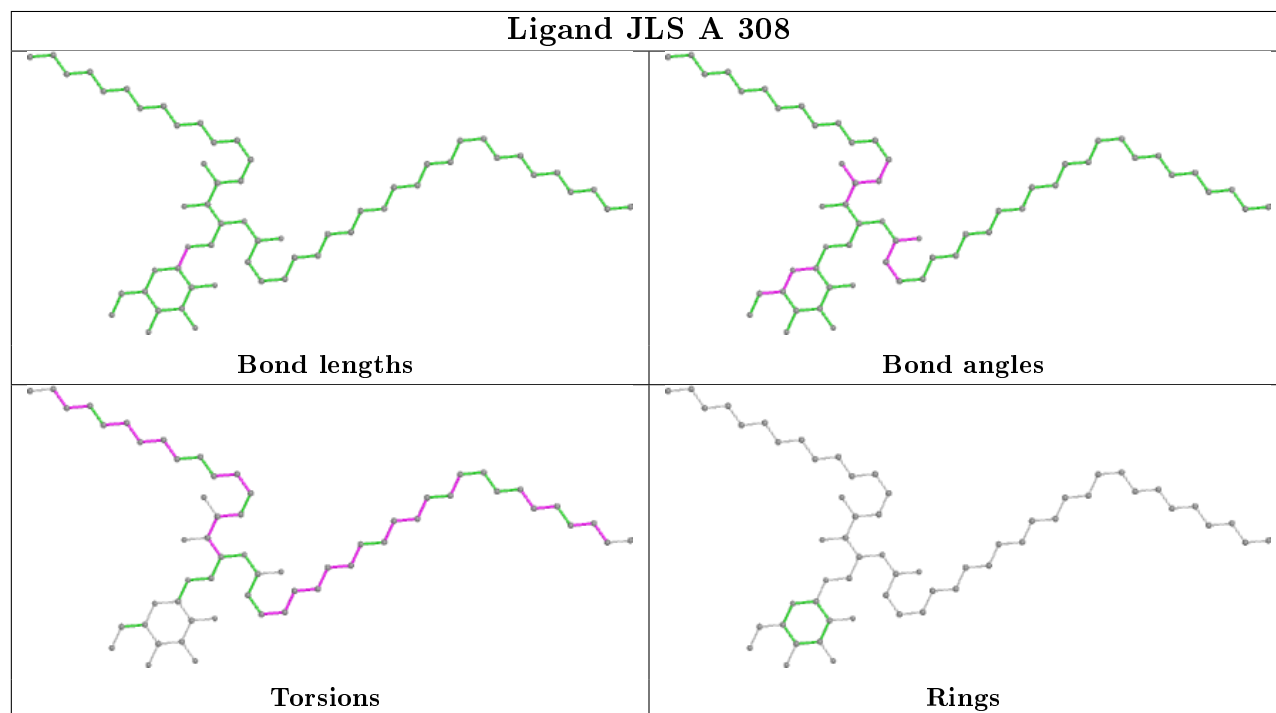
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	308	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	272/278 (97%)	0.69	36 (13%)	3 2	45, 88, 201, 212	0
2	B	100/100 (100%)	0.62	10 (10%)	7 5	74, 118, 154, 199	0
3	D	202/236 (85%)	1.36	46 (22%)	0 0	48, 109, 226, 240	2 (0%)
4	G	227/251 (90%)	1.74	66 (29%)	0 0	45, 105, 209, 227	1 (0%)
All	All	801/865 (92%)	1.15	158 (19%)	1 1	45, 104, 209, 240	3 (0%)

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	177	ALA	15.2
3	D	180	LEU	15.1
4	G	228	ILE	11.2
3	D	165	PRO	11.0
3	D	178	VAL	10.9
4	G	230	PRO	9.9
4	G	227	ILE	9.6
3	D	192	SER	9.5
4	G	153	THR	8.9
4	G	234	THR	8.7
3	D	191	CYS	8.6
3	D	142	VAL	8.6
4	G	154	TYR	8.5
4	G	175	SER	8.4
4	G	235	ASP	8.4
4	G	152	GLY	8.3
3	D	166	ALA	8.2
3	D	179	LYS	8.1
3	D	167	ILE	8.0
4	G	174	LYS	7.9
4	G	140	LEU	7.4

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Mol	Chain	Res	Type	RSRZ
4	G	128	LEU	7.3
4	G	199	LEU	7.3
4	G	139	PHE	7.1
4	G	229	PHE	7.0
4	G	138	ILE	6.8
4	G	209	GLU	6.7
4	G	197	SER	6.7
4	G	142	SER	6.6
4	G	236	VAL	6.4
4	G	157	LEU	6.3
4	G	231	PRO	6.2
4	G	233	LYS	6.1
1	A	208	VAL	6.1
3	D	196	ASP	6.0
4	G	211	ARG	5.8
4	G	208	LYS	5.8
3	D	141	LEU	5.8
1	A	206	CYS	5.4
4	G	232	ILE	5.3
3	D	154	LEU	5.3
4	G	137	THR	5.3
3	D	193	VAL	5.3
4	G	145	GLU	5.2
4	G	207	ASP	5.2
2	B	99	MET	5.2
4	G	141	PRO	5.2
2	B	39	LEU	5.1
4	G	210	HIS	5.1
1	A	191	LEU	5.1
1	A	261	CYS	5.1
4	G	196	PHE	4.8
4	G	200	THR	4.8
4	G	126	LYS	4.8
1	A	256	ALA	4.8
4	G	151	ALA	4.7
3	D	168	VAL	4.6
3	D	201	HIS	4.6
3	D	190	THR	4.5
4	G	156	CYS	4.4
4	G	143	ILE	4.4
1	A	189	ALA	4.3
4	G	212	CYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	205	VAL	4.2
2	B	37	VAL	4.2
1	A	245	LEU	4.2
3	D	195	HIS	4.1
4	G	144	ALA	4.1
1	A	218	VAL	4.0
3	D	140	CYS	4.0
4	G	172	GLU	3.9
1	A	263	VAL	3.9
4	G	226	GLU	3.9
1	A	231	GLN	3.8
3	D	122	GLN	3.8
4	G	214	VAL	3.8
4	G	158	LEU	3.8
1	A	247	ALA	3.8
3	D	126	LYS	3.7
4	G	170	TRP	3.7
4	G	179	LEU	3.6
3	D	200	VAL	3.6
1	A	228	GLN	3.6
4	G	201	VAL	3.6
4	G	169	HIS	3.5
4	G	155	LEU	3.4
3	D	139	ALA	3.4
4	G	203	GLU	3.4
1	A	207	HIS	3.4
2	B	80	CYS	3.4
1	A	219	LYS	3.3
1	A	259	LEU	3.3
3	D	143	LYS	3.3
4	G	159	GLU	3.2
2	B	35	ILE	3.1
3	D	120	ARG	3.1
4	G	206	LEU	3.1
3	D	163	PHE	3.1
3	D	161	THR	3.1
1	A	249	LEU	3.1
4	G	136	PRO	3.1
3	D	138	VAL	3.0
3	D	146	TYR	3.0
1	A	217	TRP	3.0
1	A	273	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
3	D	205	PHE	2.9
4	G	202	PRO	2.9
3	D	176	ASN	2.9
3	D	131	VAL	2.9
1	A	260	SER	2.8
4	G	166	ILE	2.8
2	B	0	MET	2.8
4	G	204	GLU	2.8
4	G	171	GLN	2.8
1	A	248	THR	2.7
3	D	130	PHE	2.7
4	G	188	LYS	2.7
3	D	181	GLY	2.7
1	A	193	ARG	2.6
4	G	225	GLN	2.6
1	A	257	ALA	2.6
2	B	64	LEU	2.6
4	G	205	SER	2.6
2	B	27	VAL	2.6
1	A	190	TRP	2.6
3	D	175	TYR	2.6
3	D	147	PRO	2.6
1	A	274	VAL	2.5
3	D	133	LYS	2.5
1	A	262	ARG	2.5
3	D	145	PHE	2.4
4	G	132	VAL	2.4
3	D	174	LYS	2.4
3	D	160	ILE	2.4
4	G	173	LYS	2.4
3	D	77	VAL	2.4
4	G	213	ILE	2.3
3	D	169	ILE	2.3
4	G	198	TRP	2.3
2	B	82	VAL	2.3
3	D	189	VAL	2.2
3	D	125	THR	2.2
1	A	192	SER	2.2
3	D	186	SER	2.2
1	A	258	GLY	2.2
1	A	181	LEU	2.1
4	G	129	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	188	LYS	2.1
1	A	276	TYR	2.1
1	A	275	LEU	2.1
3	D	152	ILE	2.1
1	A	230	THR	2.1
4	G	146	THR	2.1
2	B	1	ILE	2.1
1	A	226	GLU	2.0
1	A	227	GLN	2.0
1	A	224	GLU	2.0
4	G	191	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](#)

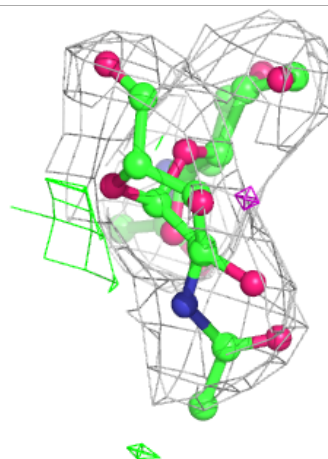
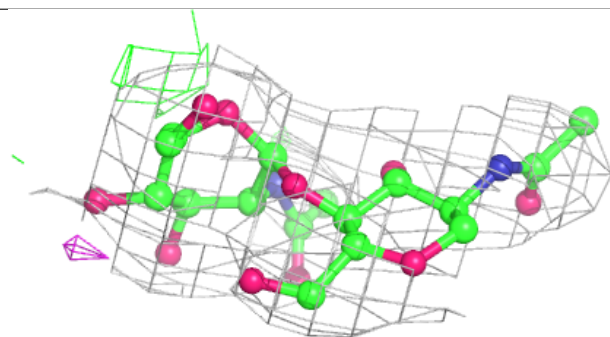
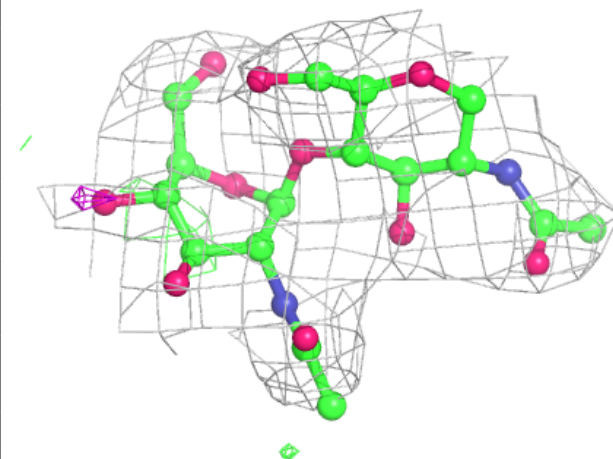
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

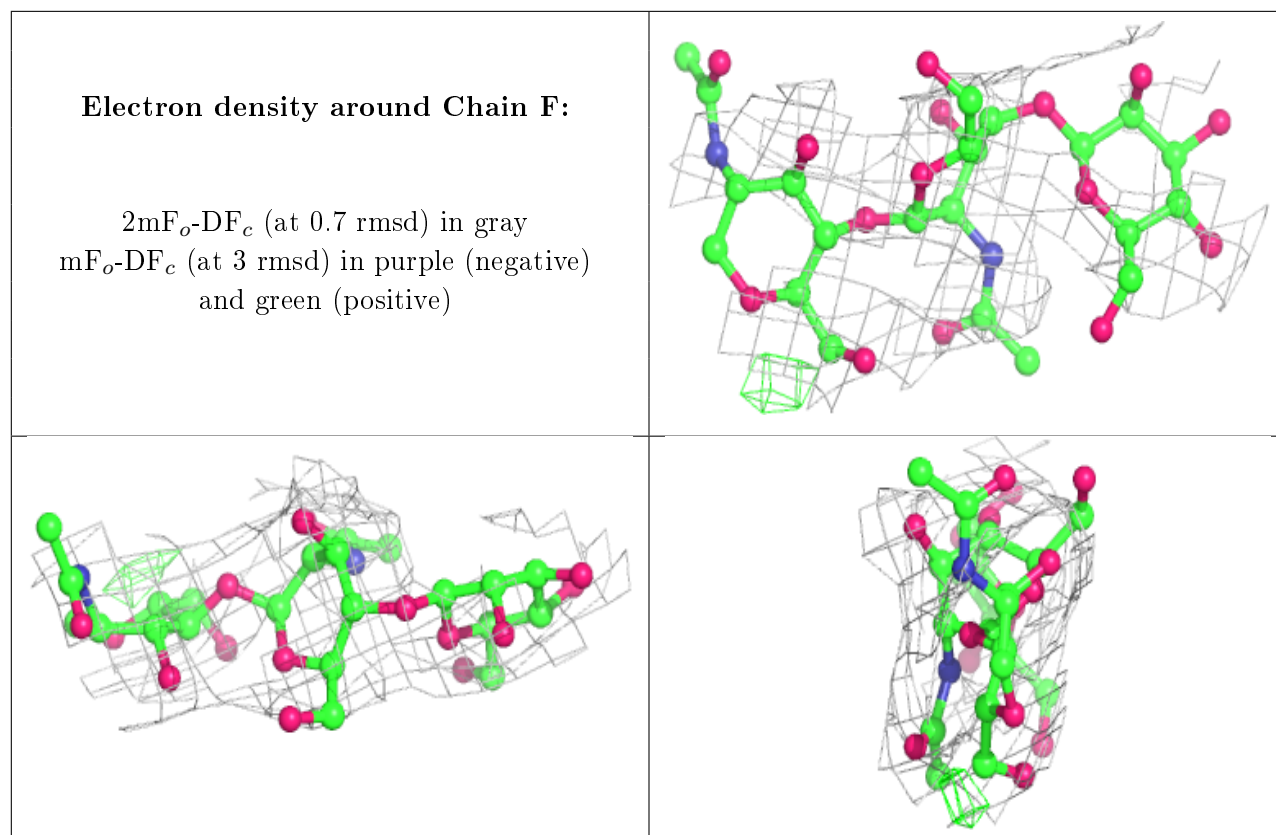
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	BMA	F	3	11/12	0.84	0.17	185,198,203,204	0
6	NAG	F	1	14/15	0.86	0.17	185,195,200,200	0
6	NAG	F	2	14/15	0.87	0.22	193,201,205,207	0
5	NAG	C	2	14/15	0.91	0.17	117,130,135,136	0
5	NAG	E	2	14/15	0.91	0.14	105,111,118,121	0
5	NAG	C	1	14/15	0.92	0.13	110,115,121,124	0
5	NAG	E	1	14/15	0.96	0.19	73,81,86,94	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 E:

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





6.4 Ligands [i](#)

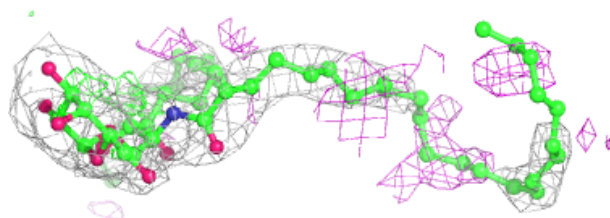
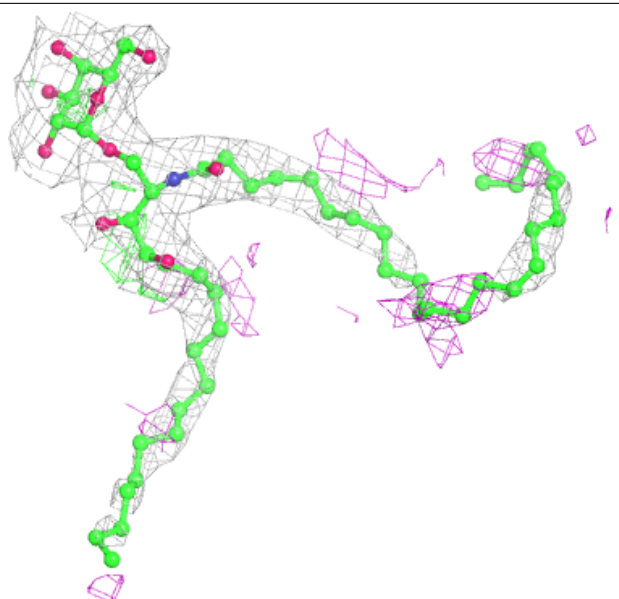
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	BMA	A	306	11/12	0.60	0.17	176,178,181,182	0
7	NAG	A	301	14/15	0.74	0.23	124,129,134,137	0
9	MG	A	307	1/1	0.83	0.35	80,80,80,80	0
10	JLS	A	308	58/58	0.94	0.45	47,63,84,85	0
11	CL	G	301	1/1	0.98	0.34	70,70,70,70	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 308:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.