



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:37 PM UTC

PDB ID : 9RM3 / pdb_00009rm3
Title : Crystal structure of human CD22 Ig domains 1-3 in complex with modified sialoside 17
Authors : Ereno-Orbea, J.; Sicard, T.; Julien, J.-P.
Deposited on : 2025-06-17
Resolution : 2.86 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

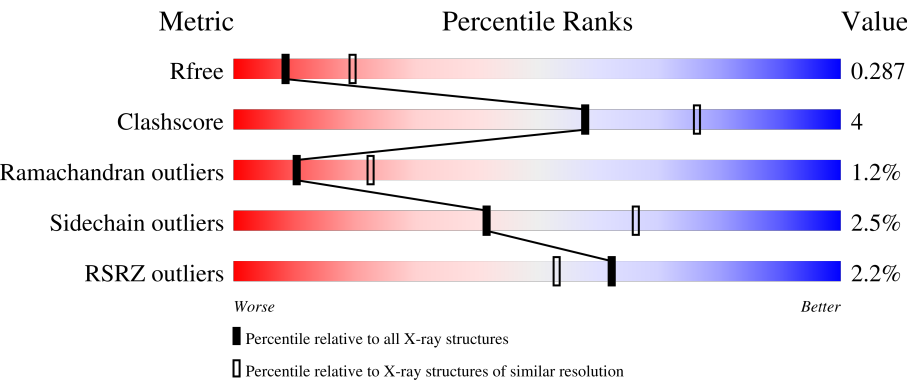
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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.



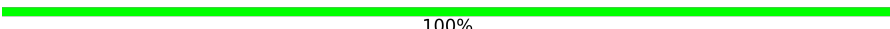
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	324	% 79% 13% 7%
1	B	324	% 81% 9% 10%
1	C	324	% 75% 14% 10%
1	D	324	5% 68% 15% • 15%
2	E	3	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	3	 33% 67%
2	K	3	 100%
2	N	3	 67% 33%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9650 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 B-cell receptor CD22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	0	0
			2387	1510	404	460	13			
1	B	293	Total	C	N	O	S	0	0	0
			2335	1477	396	449	13			
1	C	291	Total	C	N	O	S	0	0	0
			2318	1471	391	443	13			
1	D	276	Total	C	N	O	S	0	0	0
			2189	1388	367	421	13			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLU	-	expression tag	UNP P20273
A	18	THR	-	expression tag	UNP P20273
A	19	GLY	-	expression tag	UNP P20273
A	67	ALA	ASN	engineered mutation	UNP P20273
A	112	ALA	ASN	engineered mutation	UNP P20273
A	135	ALA	ASN	engineered mutation	UNP P20273
A	164	ALA	ASN	engineered mutation	UNP P20273
A	231	ALA	ASN	engineered mutation	UNP P20273
A	331	GLY	-	expression tag	UNP P20273
A	332	GLY	-	expression tag	UNP P20273
A	333	THR	-	expression tag	UNP P20273
A	334	LYS	-	expression tag	UNP P20273
A	335	HIS	-	expression tag	UNP P20273
A	336	HIS	-	expression tag	UNP P20273
A	337	HIS	-	expression tag	UNP P20273
A	338	HIS	-	expression tag	UNP P20273
A	339	HIS	-	expression tag	UNP P20273
A	340	HIS	-	expression tag	UNP P20273
B	17	GLU	-	expression tag	UNP P20273
B	18	THR	-	expression tag	UNP P20273
B	19	GLY	-	expression tag	UNP P20273

Continued on next page...

Continued from previous page...

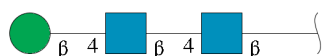
Chain	Residue	Modelled	Actual	Comment	Reference
B	67	ALA	ASN	engineered mutation	UNP P20273
B	112	ALA	ASN	engineered mutation	UNP P20273
B	135	ALA	ASN	engineered mutation	UNP P20273
B	164	ALA	ASN	engineered mutation	UNP P20273
B	231	ALA	ASN	engineered mutation	UNP P20273
B	331	GLY	-	expression tag	UNP P20273
B	332	GLY	-	expression tag	UNP P20273
B	333	THR	-	expression tag	UNP P20273
B	334	LYS	-	expression tag	UNP P20273
B	335	HIS	-	expression tag	UNP P20273
B	336	HIS	-	expression tag	UNP P20273
B	337	HIS	-	expression tag	UNP P20273
B	338	HIS	-	expression tag	UNP P20273
B	339	HIS	-	expression tag	UNP P20273
B	340	HIS	-	expression tag	UNP P20273
C	17	GLU	-	expression tag	UNP P20273
C	18	THR	-	expression tag	UNP P20273
C	19	GLY	-	expression tag	UNP P20273
C	67	ALA	ASN	engineered mutation	UNP P20273
C	112	ALA	ASN	engineered mutation	UNP P20273
C	135	ALA	ASN	engineered mutation	UNP P20273
C	164	ALA	ASN	engineered mutation	UNP P20273
C	231	ALA	ASN	engineered mutation	UNP P20273
C	331	GLY	-	expression tag	UNP P20273
C	332	GLY	-	expression tag	UNP P20273
C	333	THR	-	expression tag	UNP P20273
C	334	LYS	-	expression tag	UNP P20273
C	335	HIS	-	expression tag	UNP P20273
C	336	HIS	-	expression tag	UNP P20273
C	337	HIS	-	expression tag	UNP P20273
C	338	HIS	-	expression tag	UNP P20273
C	339	HIS	-	expression tag	UNP P20273
C	340	HIS	-	expression tag	UNP P20273
D	17	GLU	-	expression tag	UNP P20273
D	18	THR	-	expression tag	UNP P20273
D	19	GLY	-	expression tag	UNP P20273
D	67	ALA	ASN	engineered mutation	UNP P20273
D	112	ALA	ASN	engineered mutation	UNP P20273
D	135	ALA	ASN	engineered mutation	UNP P20273
D	164	ALA	ASN	engineered mutation	UNP P20273
D	231	ALA	ASN	engineered mutation	UNP P20273
D	331	GLY	-	expression tag	UNP P20273

Continued on next page...

Continued from previous page...

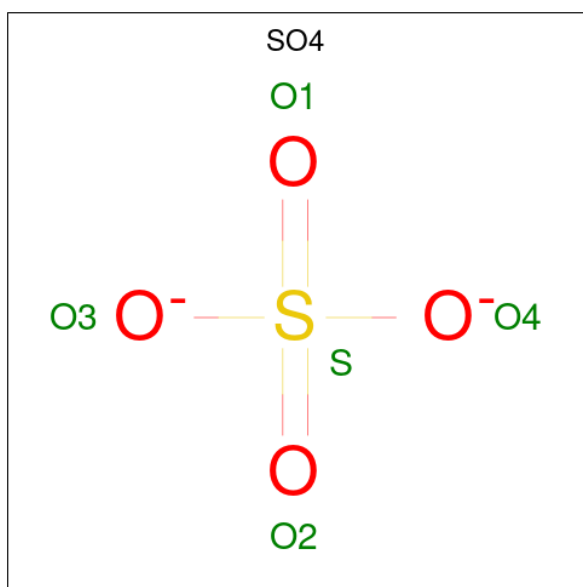
Chain	Residue	Modelled	Actual	Comment	Reference
D	332	GLY	-	expression tag	UNP P20273
D	333	THR	-	expression tag	UNP P20273
D	334	LYS	-	expression tag	UNP P20273
D	335	HIS	-	expression tag	UNP P20273
D	336	HIS	-	expression tag	UNP P20273
D	337	HIS	-	expression tag	UNP P20273
D	338	HIS	-	expression tag	UNP P20273
D	339	HIS	-	expression tag	UNP P20273
D	340	HIS	-	expression tag	UNP P20273

- Molecule 2 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.



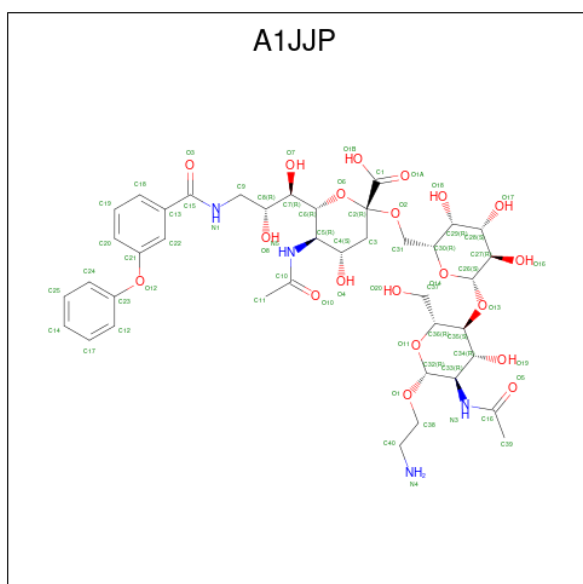
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 is (2R,4S,5R,6R)-5-acetamido-2-[[[(2R,3R,4S,5R,6S)-6-[(2R,3S,4R,5R,6R)-5-acetamido-6-(2-azanylethoxy)-2-(hydroxymethyl)-4-oxidanyl-oxan-3-yl]oxy-3,4,5-tris(oxidanyl)oxan-2-yl]methoxy]-6-[(1R,2R)-1,2-bis(oxidanyl)-3-[(3-phenoxyphenyl)carbonylamino]propyl]-4-oxidanyl-oxane-2-carboxylic acid (CCD ID: A1JJP) (formula: C₄₀H₅₆N₄O₂₀) (labeled as "Ligand of Interest" by depositor).

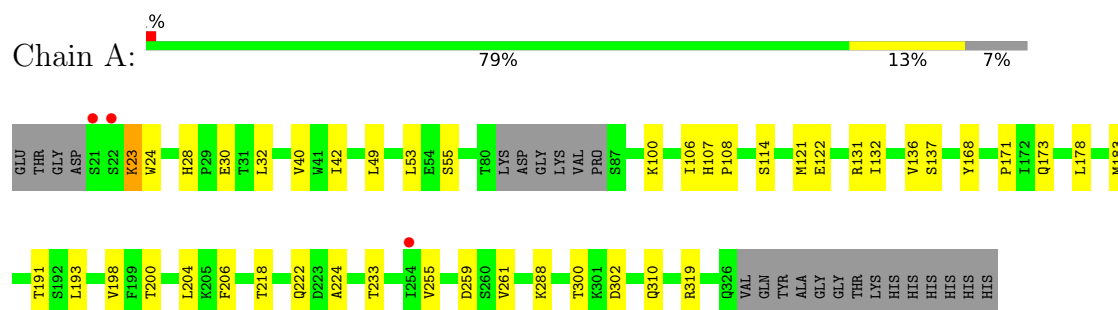


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			58	34	4	20		
4	B	1	Total	C	N	O	0	0
			64	40	4	20		
4	C	1	Total	C	N	O	0	0
			64	40	4	20		
4	D	1	Total	C	N	O	0	0
			64	40	4	20		

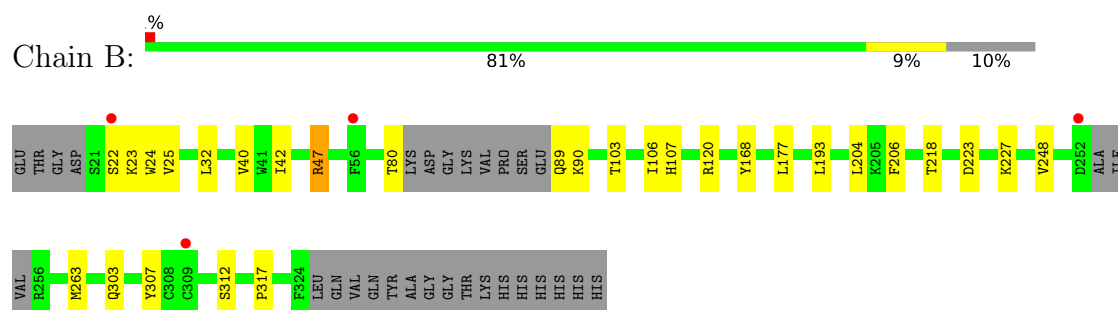
3 Residue-property plots

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.

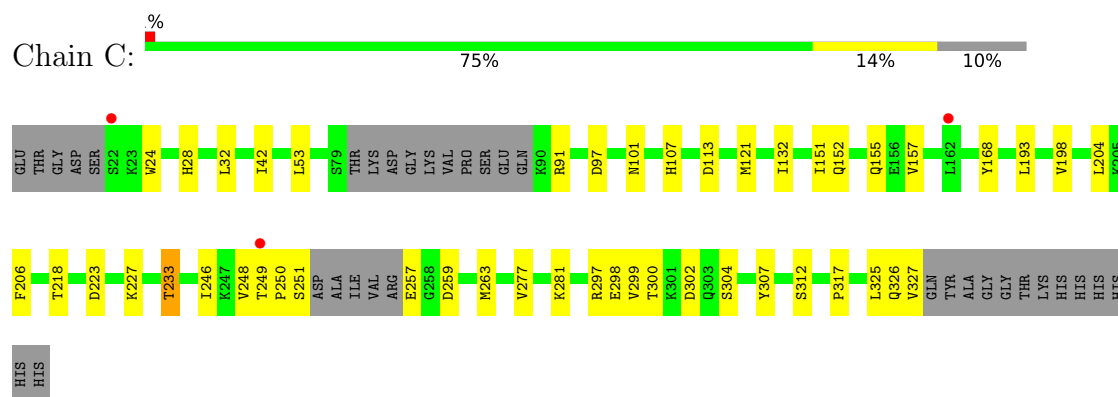
• Molecule 1: B-cell receptor CD22



• Molecule 1: B-cell receptor CD22

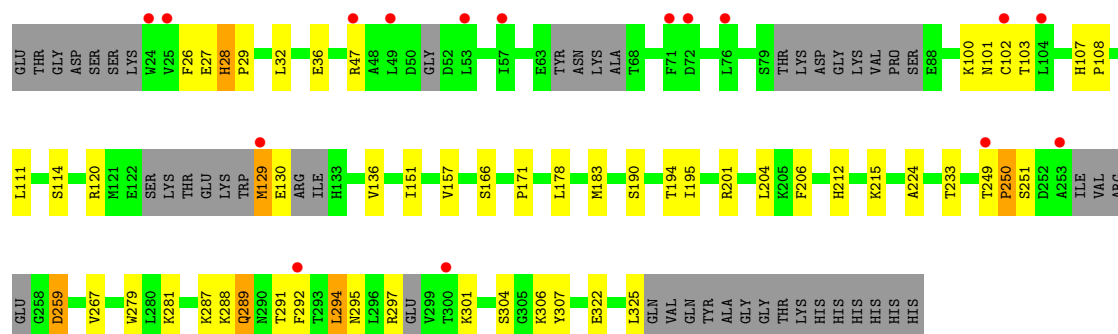


• Molecule 1: B-cell receptor CD22



• Molecule 1: B-cell receptor CD22





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

Chain E: 100%



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

Chain H: 33% 67%



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

Chain K: 100%



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

Chain N: 67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	97.26Å 114.08Å 155.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.20 – 2.86 49.20 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.20-2.86) 99.7 (49.20-2.86)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.242 , 0.289 0.247 , 0.287	Depositor DCC
R_{free} test set	2000 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	85.3	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9650	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.02% 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: NAG, BMA, SO4, A1JJP

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	0.14	0/2444	0.31	0/3317
1	B	0.12	0/2391	0.31	0/3243
1	C	0.11	0/2374	0.30	0/3221
1	D	0.18	0/2238	0.36	0/3034
All	All	0.14	0/9447	0.32	0/12815

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2387	0	2332	24	0
1	B	2335	0	2276	15	0
1	C	2318	0	2267	21	0
1	D	2189	0	2124	26	0
2	E	39	0	34	0	0
2	H	39	0	34	1	0
2	K	39	0	34	0	0
2	N	39	0	34	0	0
3	A	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	1	0
3	C	5	0	0	0	0
4	A	58	0	0	0	0
4	B	64	0	0	0	0
4	C	64	0	0	0	0
4	D	64	0	0	0	0
All	All	9650	0	9135	84	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 4.

All (84) 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:D:26:PHE:CG	1:D:130:GLU:HG3	2.24	0.72
1:D:29:PRO:HG2	1:D:32:LEU:HD11	1.75	0.68
1:C:248:VAL:HG23	1:C:263:MET:HG2	1.75	0.68
1:B:32:LEU:HD22	1:B:42:ILE:HG12	1.76	0.67
1:D:101:ASN:OD1	1:D:103:THR:N	2.22	0.67
1:A:255:VAL:HG13	1:A:259:ASP:HB2	1.83	0.61
1:B:120:ARG:NE	3:B:501:SO4:O2	2.34	0.61
1:A:49:LEU:HA	1:B:47:ARG:HG3	1.84	0.58
1:A:171:PRO:HG2	1:A:224:ALA:HB2	1.85	0.58
1:D:27:GLU:HG2	1:D:195:ILE:HD12	1.86	0.58
1:D:259:ASP:OD1	1:D:259:ASP:N	2.38	0.56
1:D:28:HIS:HD1	1:D:28:HIS:C	2.13	0.56
1:B:103:THR:OG1	2:H:1:NAG:O7	2.23	0.56
1:D:120:ARG:HH11	1:D:129:MET:HG3	1.72	0.55
1:A:300:THR:OG1	1:A:302:ASP:OD1	2.25	0.55
1:B:312:SER:HA	1:B:317:PRO:HA	1.90	0.54
1:D:190:SER:OG	1:D:201:ARG:NH1	2.41	0.54
1:A:255:VAL:HG21	1:A:261:VAL:HG22	1.90	0.54
1:C:32:LEU:HD22	1:C:42:ILE:HG12	1.89	0.54
1:C:249:THR:O	1:C:251:SER:N	2.42	0.53
1:C:304:SER:HB2	1:C:327:VAL:H	1.73	0.53
1:D:279:TRP:CD2	1:D:294:LEU:HB2	2.44	0.52
1:A:178:LEU:HB2	1:A:183:MET:HE2	1.90	0.52
1:D:130:GLU:HA	1:D:130:GLU:OE1	2.09	0.52
1:B:204:LEU:HD23	1:B:206:PHE:HB2	1.91	0.52
1:A:53:LEU:HD11	1:A:121:MET:HE3	1.92	0.51
1:B:107:HIS:O	1:B:107:HIS:ND1	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:THR:HG23	1:A:233:THR:HG22	1.93	0.50
1:B:248:VAL:HG23	1:B:263:MET:HG2	1.93	0.50
1:A:193:LEU:HD12	1:A:198:VAL:HG22	1.94	0.49
1:C:107:HIS:ND1	1:C:107:HIS:O	2.45	0.49
1:C:281:LYS:HD3	1:C:307:TYR:CZ	2.47	0.49
1:C:204:LEU:HD23	1:C:206:PHE:HB2	1.95	0.49
1:C:91:ARG:NH1	1:C:113:ASP:OD2	2.40	0.49
1:A:204:LEU:HD23	1:A:206:PHE:HB2	1.95	0.48
1:C:53:LEU:HD11	1:C:121:MET:HE3	1.95	0.48
1:C:168:TYR:CZ	1:C:193:LEU:HD23	2.49	0.48
1:D:204:LEU:HD23	1:D:206:PHE:HB2	1.95	0.48
1:A:168:TYR:CZ	1:A:193:LEU:HD23	2.50	0.47
1:B:177:LEU:HB2	1:B:218:THR:HB	1.97	0.47
1:D:101:ASN:OD1	1:D:101:ASN:C	2.57	0.47
1:B:303:GLN:O	1:B:307:TYR:OH	2.26	0.47
1:A:55:SER:HB3	1:A:122:GLU:HB2	1.97	0.47
1:A:23:LYS:H	1:A:49:LEU:HD12	1.80	0.46
1:D:171:PRO:HG2	1:D:224:ALA:HB2	1.97	0.46
1:D:28:HIS:C	1:D:28:HIS:ND1	2.73	0.46
1:D:281:LYS:HD3	1:D:307:TYR:CE2	2.50	0.46
1:B:223:ASP:OD1	1:B:227:LYS:N	2.48	0.46
1:A:28:HIS:CE1	1:A:132:ILE:HG12	2.51	0.46
1:D:289:GLN:HG2	1:D:294:LEU:HD23	1.98	0.45
1:A:32:LEU:HD13	1:A:42:ILE:HG23	1.99	0.45
1:C:28:HIS:CE1	1:C:132:ILE:HG12	2.52	0.45
1:C:24:TRP:HZ3	1:C:121:MET:HE2	1.82	0.44
1:C:257:GLU:HB3	1:C:327:VAL:HG13	1.99	0.44
1:A:24:TRP:HZ3	1:A:121:MET:HE2	1.83	0.44
1:D:178:LEU:HB2	1:D:183:MET:HE3	1.99	0.44
1:D:291:THR:OG1	1:D:292:PHE:N	2.51	0.44
1:D:212:HIS:HA	1:D:215:LYS:HG3	2.01	0.43
1:C:151:ILE:HG23	1:C:157:VAL:HG11	2.00	0.43
1:C:300:THR:OG1	1:C:302:ASP:OD1	2.36	0.42
1:D:249:THR:HB	1:D:250:PRO:HD2	1.99	0.42
1:C:152:GLN:NE2	1:C:155:GLN:OE1	2.52	0.42
1:D:151:ILE:HG23	1:D:157:VAL:HG11	2.02	0.42
1:D:36:GLU:OE1	1:D:111:LEU:N	2.51	0.42
1:A:49:LEU:HD21	1:B:25:VAL:HG11	2.02	0.41
1:D:107:HIS:HA	1:D:108:PRO:HA	1.86	0.41
1:B:40:VAL:HG12	1:B:106:ILE:HB	2.01	0.41
1:A:288:LYS:HA	1:A:288:LYS:HE2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:GLN:HG3	1:A:222:GLN:HB2	2.02	0.41
1:B:168:TYR:CZ	1:B:193:LEU:HD23	2.55	0.41
1:C:223:ASP:OD1	1:C:227:LYS:N	2.52	0.41
1:D:114:SER:HB2	1:D:136:VAL:HB	2.01	0.41
1:D:304:SER:HB2	1:D:325:LEU:HB2	2.03	0.41
1:B:22:SER:O	1:B:23:LYS:HG3	2.21	0.41
1:C:312:SER:HA	1:C:317:PRO:HA	2.02	0.41
1:A:107:HIS:HA	1:A:108:PRO:HA	1.83	0.40
1:A:191:THR:HG22	1:A:200:THR:HG23	2.03	0.40
1:A:310:GLN:OE1	1:A:319:ARG:NH2	2.46	0.40
1:C:97:ASP:OD1	1:C:101:ASN:N	2.52	0.40
1:C:218:THR:HG23	1:C:233:THR:HG22	2.03	0.40
1:D:306:LYS:HB3	1:D:322:GLU:HB3	2.02	0.40
1:A:40:VAL:HG12	1:A:106:ILE:HB	2.03	0.40
1:A:114:SER:HB2	1:A:136:VAL:HB	2.02	0.40
1:C:193:LEU:HD12	1:C:198:VAL:HG22	2.03	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	296/324 (91%)	283 (96%)	13 (4%)	0	100	100
1	B	287/324 (89%)	265 (92%)	20 (7%)	2 (1%)	18	35
1	C	285/324 (88%)	261 (92%)	19 (7%)	5 (2%)	6	15
1	D	262/324 (81%)	239 (91%)	17 (6%)	6 (2%)	5	11
All	All	1130/1296 (87%)	1048 (93%)	69 (6%)	13 (1%)	10	22

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	250	PRO
1	D	297	ARG
1	C	297	ARG
1	B	24	TRP
1	C	299	VAL
1	C	326	GLN
1	B	90	LYS
1	C	325	LEU
1	D	251	SER
1	D	287	LYS
1	D	166	SER
1	D	301	LYS
1	C	250	PRO

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	273/292 (94%)	268 (98%)	5 (2%)	51	73
1	B	267/292 (91%)	264 (99%)	3 (1%)	65	81
1	C	265/292 (91%)	260 (98%)	5 (2%)	50	72
1	D	251/292 (86%)	238 (95%)	13 (5%)	21	43
All	All	1056/1168 (90%)	1030 (98%)	26 (2%)	42	66

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	30	GLU
1	A	100	LYS
1	A	131	ARG
1	A	137	SER
1	B	47	ARG
1	B	80	THR
1	B	89	GLN
1	C	233	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	246	ILE
1	C	259	ASP
1	C	277	VAL
1	C	298	GLU
1	D	28	HIS
1	D	47	ARG
1	D	100	LYS
1	D	102	CYS
1	D	129	MET
1	D	194	THR
1	D	233	THR
1	D	259	ASP
1	D	267	VAL
1	D	288	LYS
1	D	289	GLN
1	D	294	LEU
1	D	295	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	HIS
1	B	146	GLN
1	B	240	HIS
1	C	110	HIS
1	C	152	GLN
1	C	310	GLN
1	D	213	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 ⓘ

12 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	$\# Z > 2$
2	NAG	E	1	2,1	14,14,15	0.28	0	17,19,21	0.53	0
2	NAG	E	2	2	14,14,15	0.28	0	17,19,21	0.45	0
2	BMA	E	3	2	11,11,12	0.66	0	15,15,17	0.85	0
2	NAG	H	1	2,1	14,14,15	0.32	0	17,19,21	0.67	0
2	NAG	H	2	2	14,14,15	0.30	0	17,19,21	0.58	0
2	BMA	H	3	2	11,11,12	0.79	1 (9%)	15,15,17	0.76	0
2	NAG	K	1	2,1	14,14,15	0.27	0	17,19,21	0.48	0
2	NAG	K	2	2	14,14,15	0.24	0	17,19,21	0.52	0
2	BMA	K	3	2	11,11,12	0.68	0	15,15,17	0.70	0
2	NAG	N	1	2,1	14,14,15	0.44	0	17,19,21	0.43	0
2	NAG	N	2	2	14,14,15	0.43	0	17,19,21	0.61	0
2	BMA	N	3	2	11,11,12	0.86	1 (9%)	15,15,17	1.01	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	BMA	H	3	2	-	1/2/19/22	0/1/1/1
2	NAG	K	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	BMA	K	3	2	-	0/2/19/22	0/1/1/1
2	NAG	N	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	BMA	N	3	2	-	1/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	3	BMA	C1-C2	2.20	1.57	1.52
2	H	3	BMA	C1-C2	2.11	1.57	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	3	BMA	C1-O5-C5	2.32	115.30	112.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

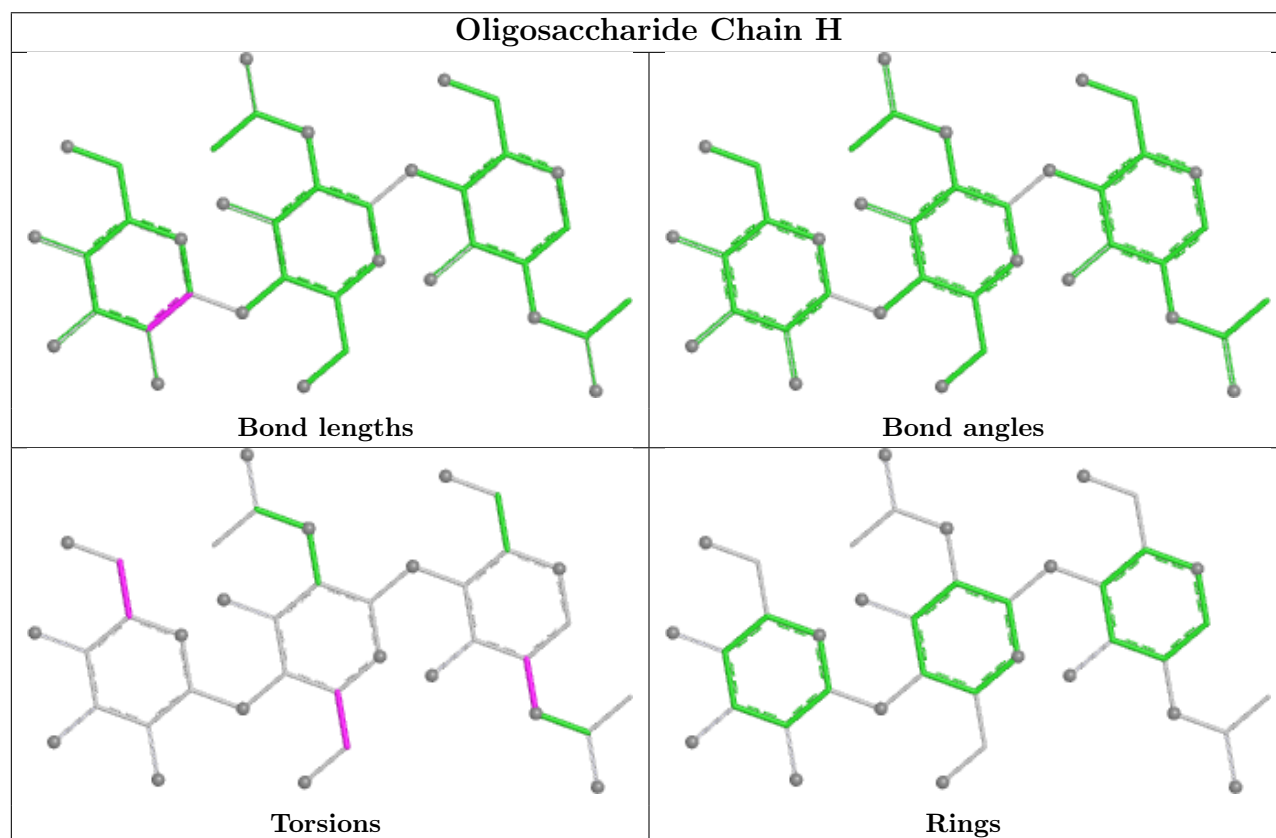
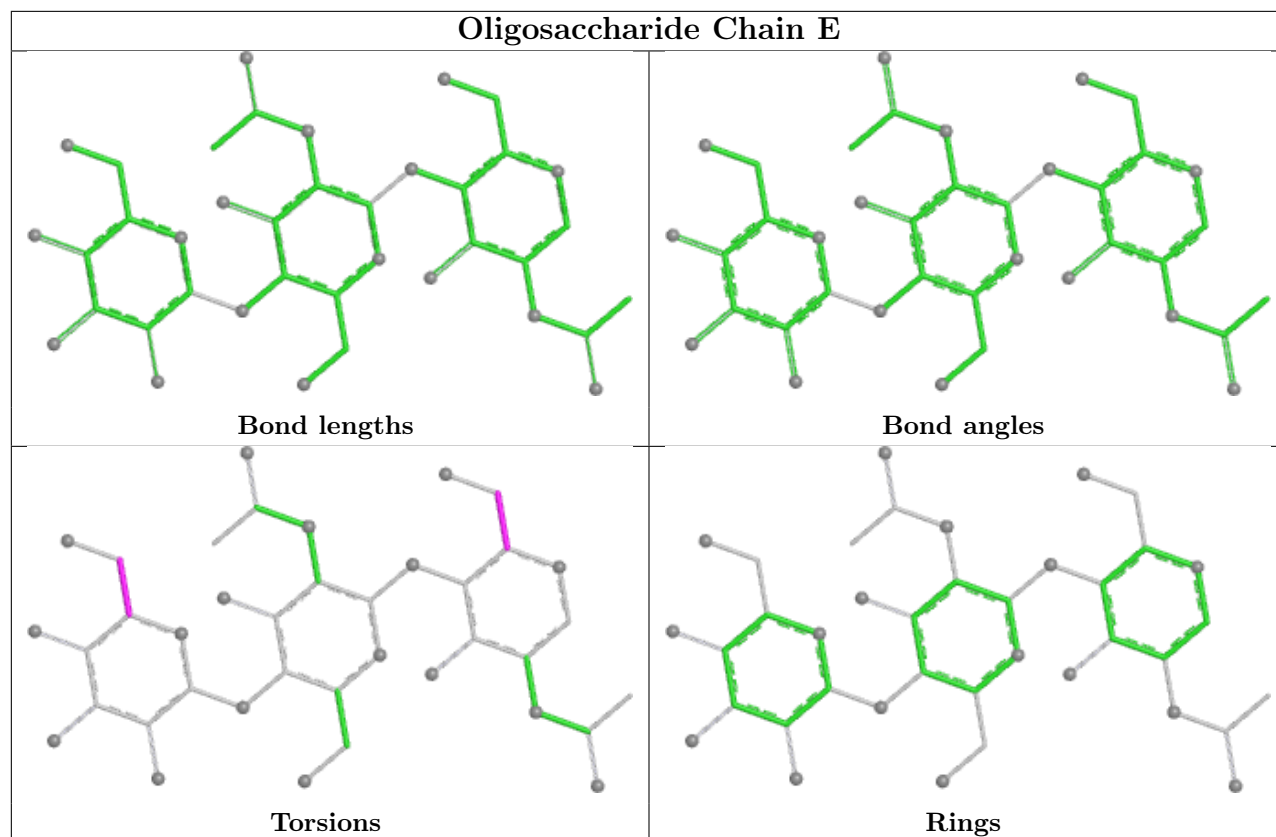
Mol	Chain	Res	Type	Atoms
2	K	2	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
2	E	3	BMA	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
2	N	3	BMA	O5-C5-C6-O6
2	H	3	BMA	O5-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	H	1	NAG	C3-C2-N2-C7
2	N	1	NAG	O5-C5-C6-O6
2	H	1	NAG	C1-C2-N2-C7

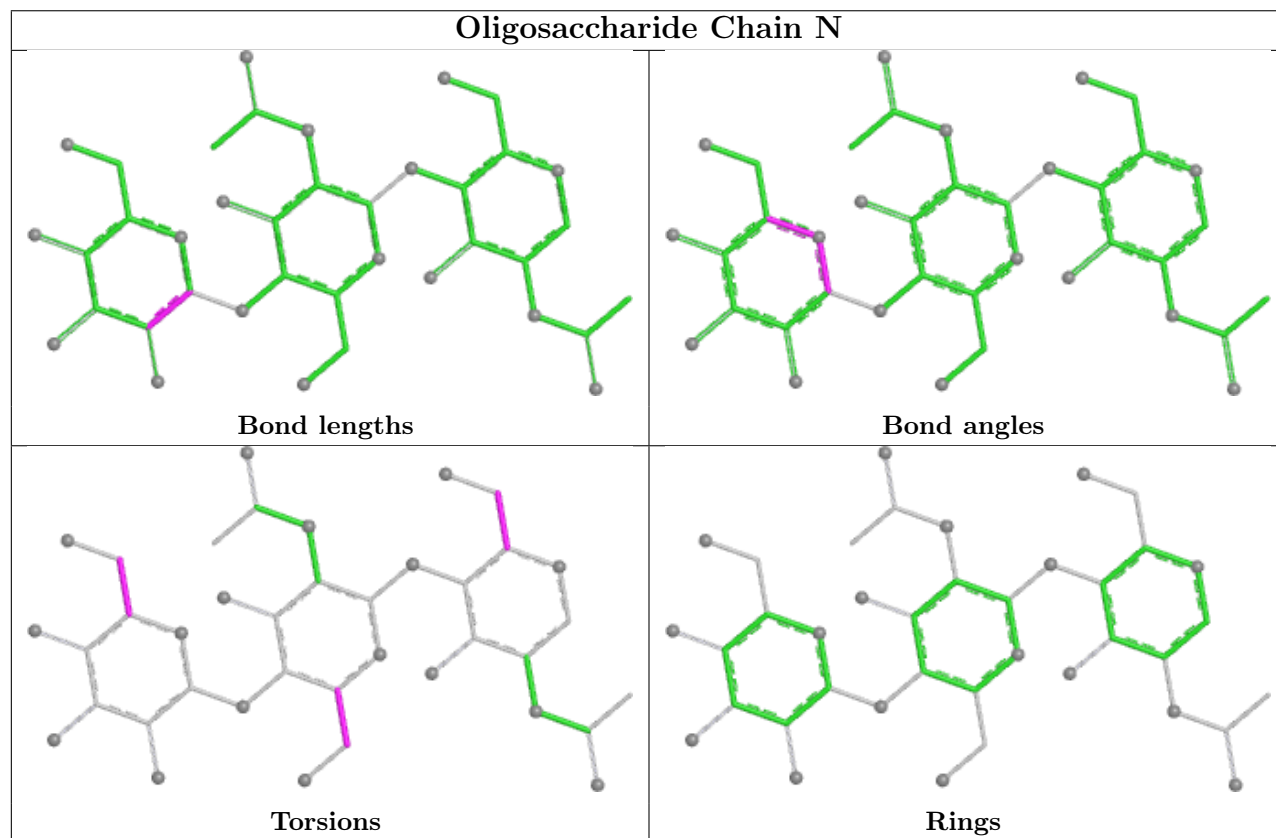
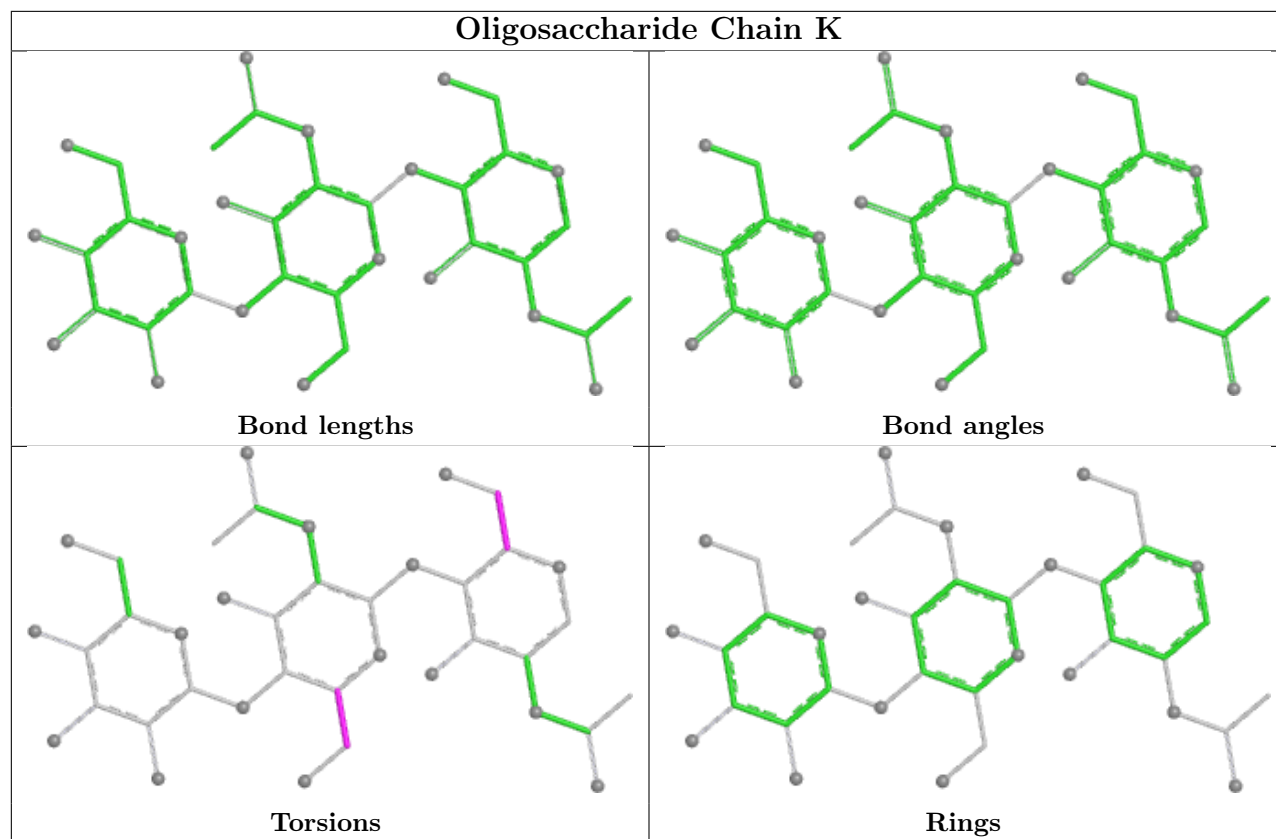
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	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

7 ligands 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	$\# Z > 2$
3	SO4	B	501	-	4,4,4	0.23	0	6,6,6	0.17	0
4	A1JJP	B	502	-	68,68,68	0.26	0	92,97,97	0.43	1 (1%)
4	A1JJP	C	601	-	68,68,68	0.26	0	92,97,97	0.51	2 (2%)
4	A1JJP	D	601	-	68,68,68	0.24	0	92,97,97	0.64	1 (1%)
3	SO4	C	602	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	A	501	-	4,4,4	0.23	0	6,6,6	0.11	0
4	A1JJP	A	502	-	61,61,68	0.30	0	83,88,97	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1JJP	B	502	-	-	7/51/109/109	0/5/5/5
4	A1JJP	C	601	-	-	8/51/109/109	0/5/5/5
4	A1JJP	D	601	-	-	14/51/109/109	0/5/5/5
4	A1JJP	A	502	-	-	5/47/105/109	0/4/4/5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	601	A1JJP	O6-C6-C5	-4.23	105.97	109.84
4	C	601	A1JJP	O1A-C1-C2	-2.79	115.37	123.79
4	B	502	A1JJP	O1A-C1-C2	-2.77	115.44	123.79
4	C	601	A1JJP	O6-C6-C5	-2.57	107.49	109.84

There are no chirality outliers.

All (34) torsion outliers are listed below:

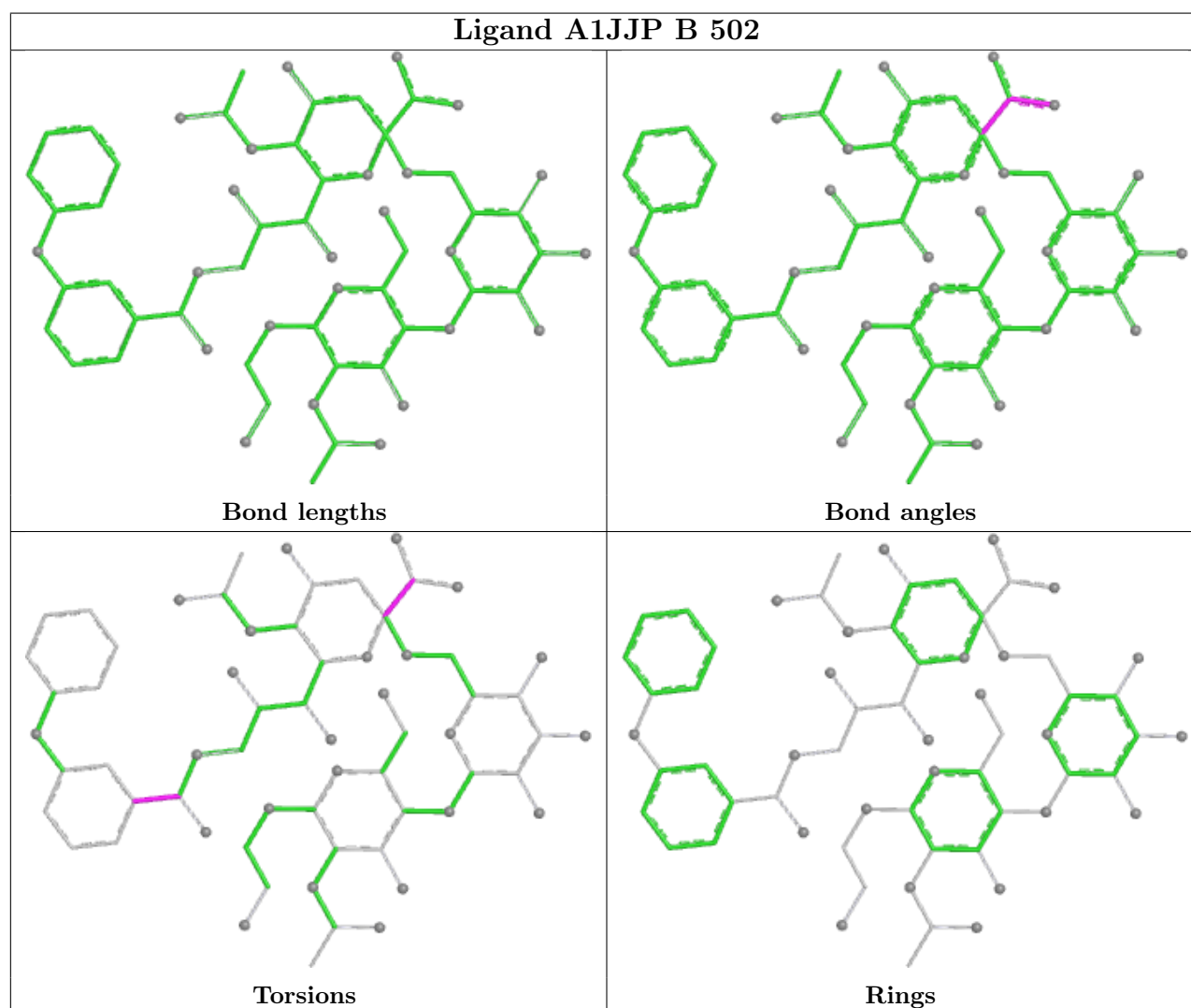
Mol	Chain	Res	Type	Atoms
4	A	502	A1JJP	O1B-C1-C2-O2
4	B	502	A1JJP	O1B-C1-C2-O2
4	C	601	A1JJP	O1B-C1-C2-O2
4	C	601	A1JJP	C33-C32-O1-C38
4	D	601	A1JJP	O1B-C1-C2-O2
4	D	601	A1JJP	C1-C2-O2-C31
4	D	601	A1JJP	C3-C2-O2-C31
4	D	601	A1JJP	O6-C2-O2-C31
4	D	601	A1JJP	C6-C7-C8-C9
4	D	601	A1JJP	C33-C32-O1-C38
4	D	601	A1JJP	C18-C13-C15-N1
4	C	601	A1JJP	C18-C13-C15-O3
4	C	601	A1JJP	C22-C13-C15-O3
4	D	601	A1JJP	C18-C13-C15-O3
4	D	601	A1JJP	C22-C13-C15-O3
4	C	601	A1JJP	C18-C13-C15-N1
4	C	601	A1JJP	C22-C13-C15-N1
4	D	601	A1JJP	C22-C13-C15-N1
4	D	601	A1JJP	O11-C32-O1-C38
4	C	601	A1JJP	O11-C32-O1-C38
4	B	502	A1JJP	C18-C13-C15-O3
4	B	502	A1JJP	C22-C13-C15-O3
4	D	601	A1JJP	C6-C7-C8-O8
4	B	502	A1JJP	C22-C13-C15-N1
4	B	502	A1JJP	C18-C13-C15-N1
4	D	601	A1JJP	O7-C7-C8-O8
4	A	502	A1JJP	C22-C13-C15-O3
4	A	502	A1JJP	C18-C13-C15-O3
4	B	502	A1JJP	O1A-C1-C2-O2
4	C	601	A1JJP	O1A-C1-C2-O2
4	A	502	A1JJP	C22-C13-C15-N1
4	A	502	A1JJP	C18-C13-C15-N1
4	D	601	A1JJP	O7-C7-C8-C9
4	B	502	A1JJP	O1A-C1-C2-C3

There are no ring outliers.

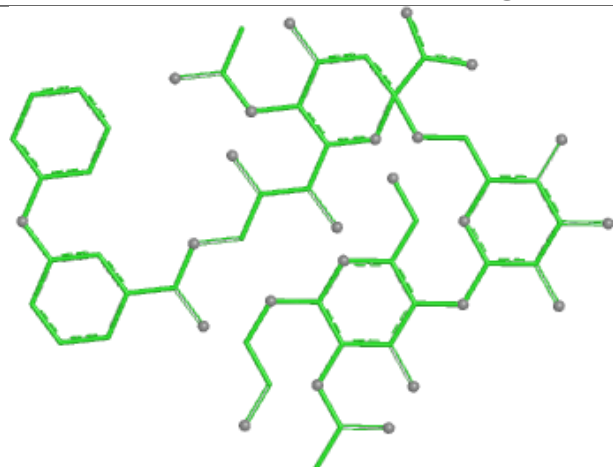
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	SO4	1	0

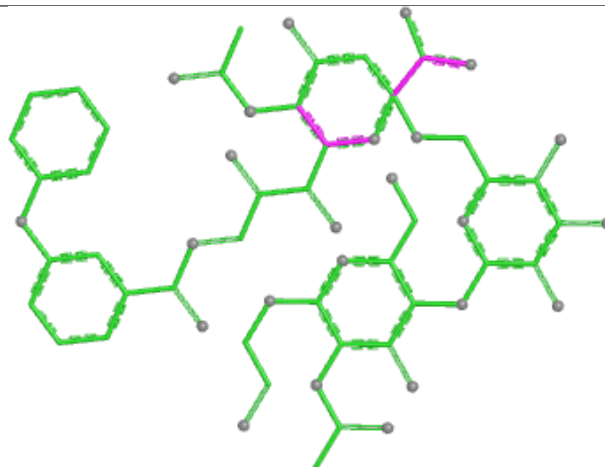
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



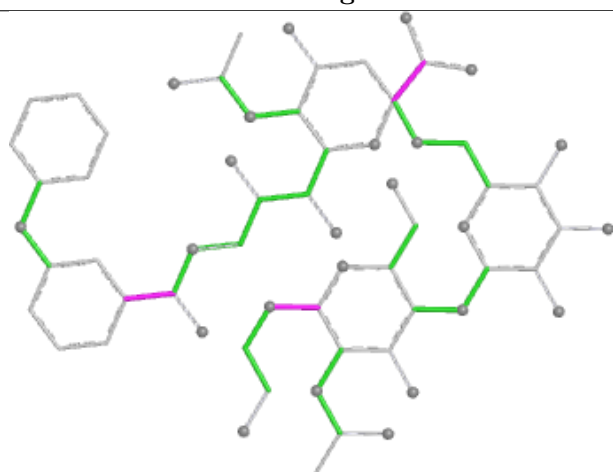
Ligand A1JJP C 601



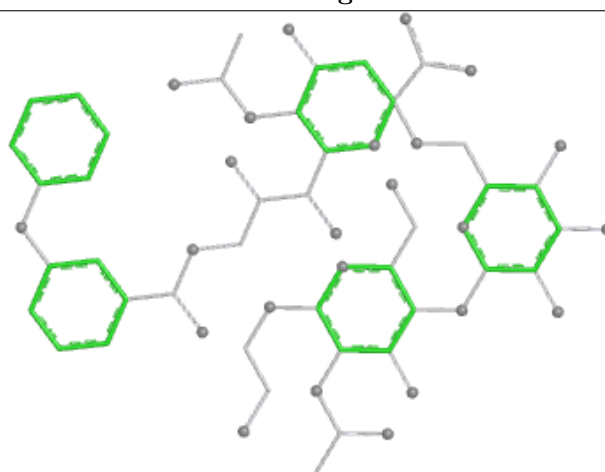
Bond lengths



Bond angles

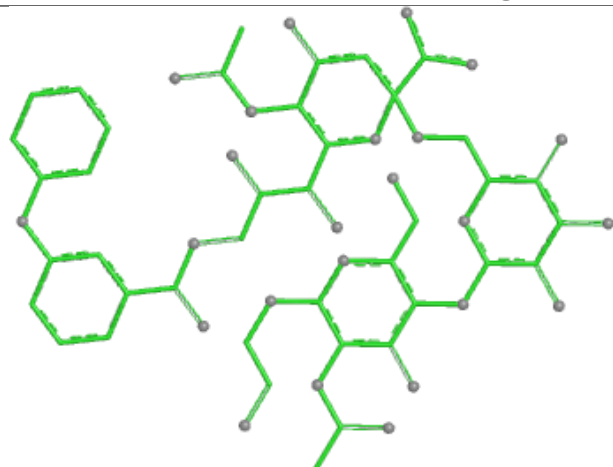


Torsions

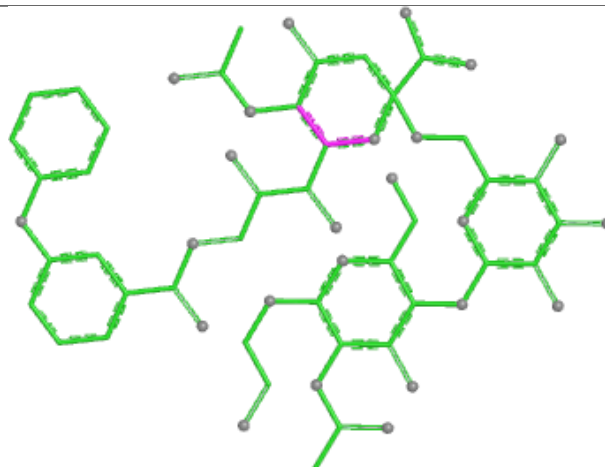


Rings

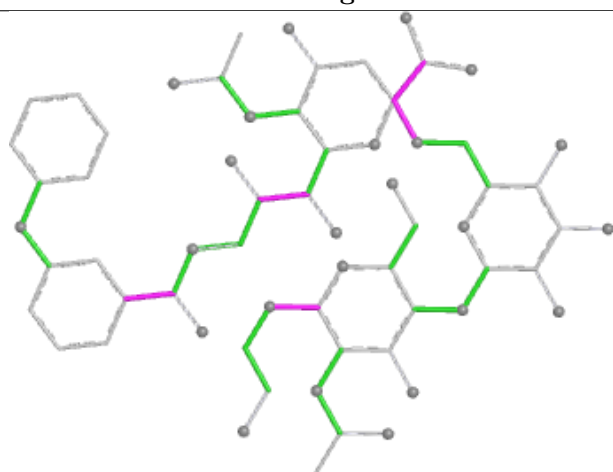
Ligand A1JJP D 601



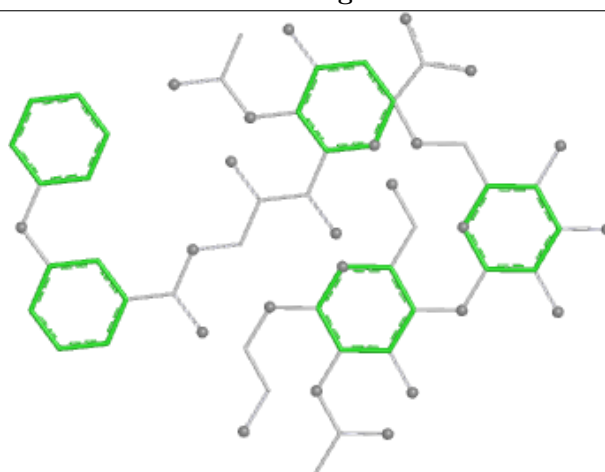
Bond lengths



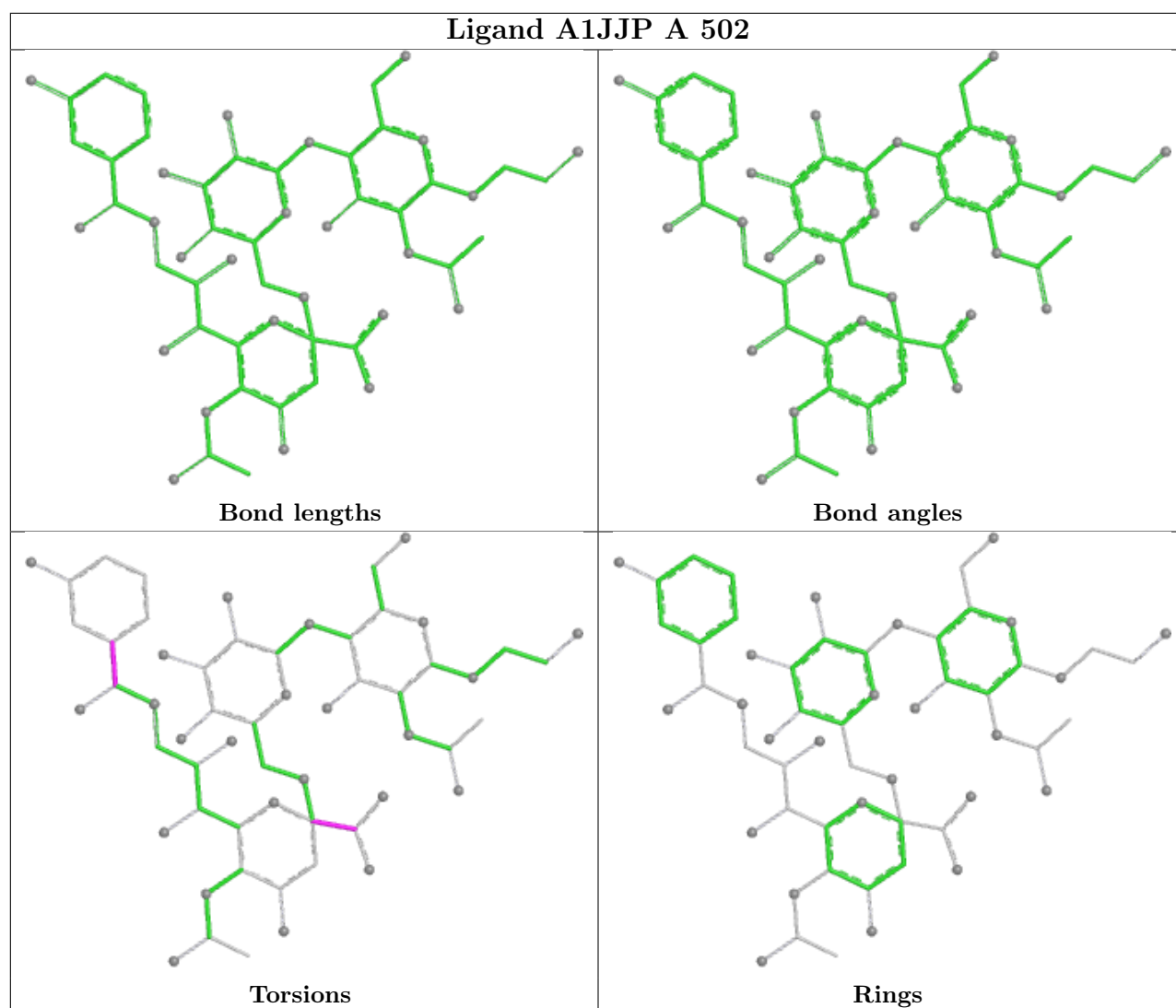
Bond angles



Torsions



Rings



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	300/324 (92%)	-0.23	3 (1%) 79 74	39, 63, 100, 142	0
1	B	293/324 (90%)	0.17	4 (1%) 73 67	58, 86, 131, 159	0
1	C	291/324 (89%)	-0.00	3 (1%) 79 74	60, 88, 124, 159	0
1	D	276/324 (85%)	0.39	16 (5%) 29 21	47, 91, 134, 152	0
All	All	1160/1296 (89%)	0.08	26 (2%) 62 53	39, 82, 128, 159	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	25	VAL	4.6
1	D	104	LEU	3.9
1	D	72	ASP	3.7
1	B	56	PHE	3.3
1	D	129	MET	2.9
1	D	49	LEU	2.9
1	D	102	CYS	2.9
1	D	292	PHE	2.8
1	D	300	THR	2.8
1	D	47	ARG	2.8
1	D	249	THR	2.7
1	B	309	CYS	2.7
1	B	252	ASP	2.7
1	B	22	SER	2.6
1	D	253	ALA	2.6
1	A	21	SER	2.6
1	A	254	ILE	2.5
1	D	57	ILE	2.5
1	D	24	TRP	2.4
1	C	249	THR	2.4
1	C	22	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	162	LEU	2.2
1	D	71	PHE	2.1
1	D	76	LEU	2.1
1	D	53	LEU	2.1
1	A	22	SER	2.1

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](#)

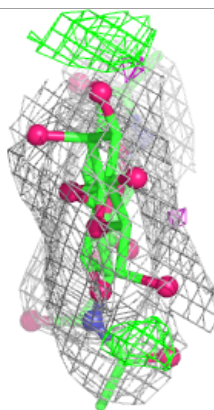
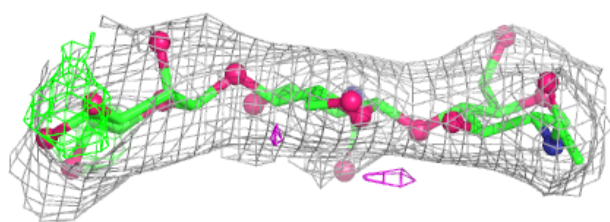
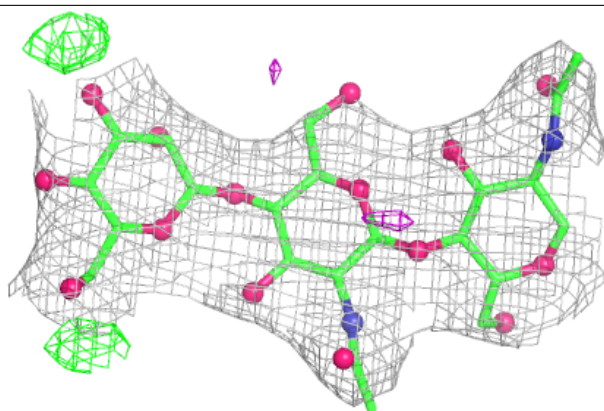
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	H	3	11/12	0.59	0.15	80,95,103,104	0
2	NAG	H	2	14/15	0.65	0.15	79,97,102,103	0
2	BMA	E	3	11/12	0.74	0.10	61,76,93,102	0
2	NAG	H	1	14/15	0.74	0.15	67,89,100,101	0
2	NAG	E	1	14/15	0.92	0.09	56,66,76,85	0
2	NAG	E	2	14/15	0.92	0.09	62,72,81,90	0
2	NAG	K	1	14/15	-	-	74,84,98,100	0
2	NAG	K	2	14/15	-	-	76,92,100,104	0
2	BMA	K	3	11/12	-	-	93,100,105,107	0
2	NAG	N	1	14/15	-	-	107,120,135,137	0
2	NAG	N	2	14/15	-	-	107,119,138,142	0
2	BMA	N	3	11/12	-	-	87,101,114,116	0

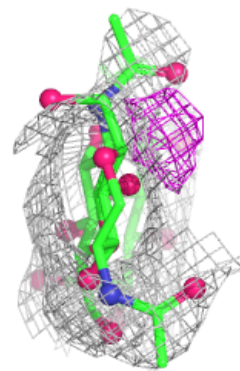
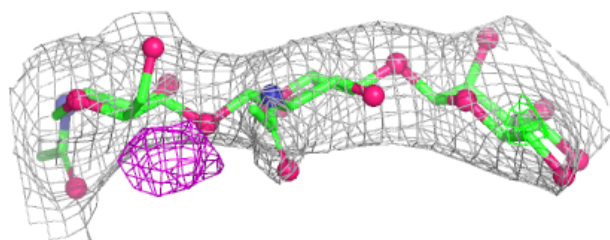
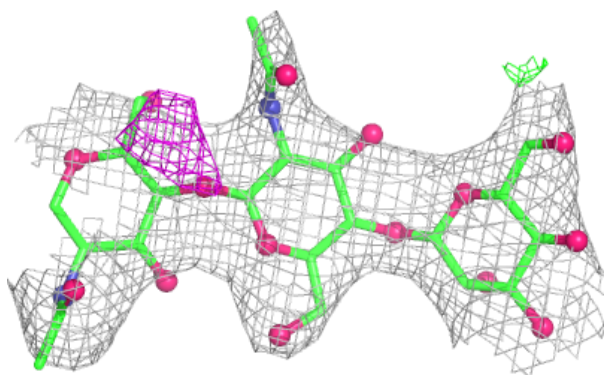
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

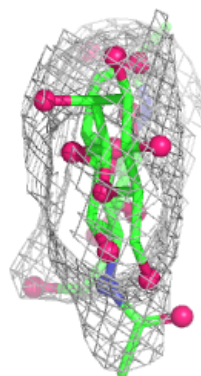
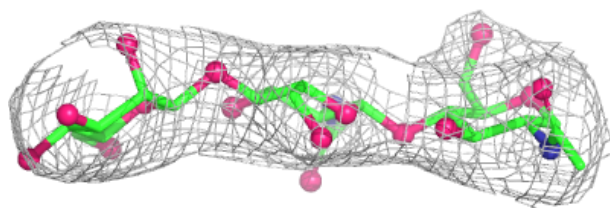
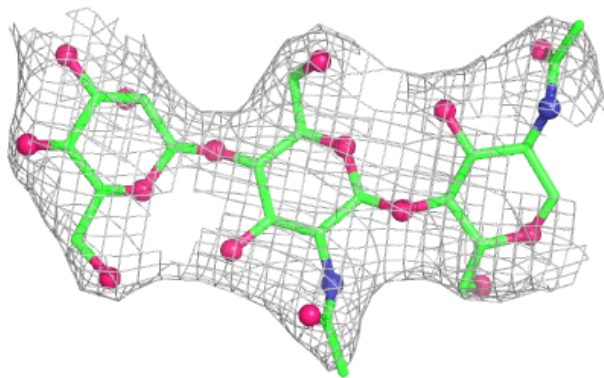
**Electron density around Chain H:**

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

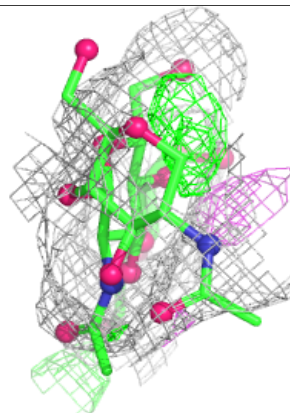
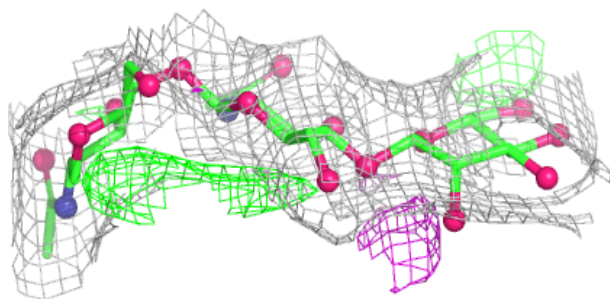
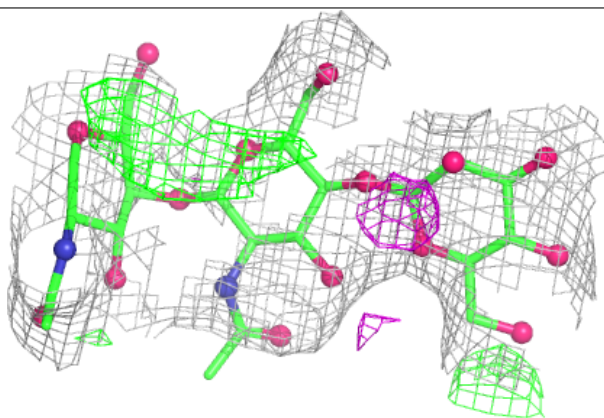


Electron density around Chain K:

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

**Electron density around Chain N:**

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

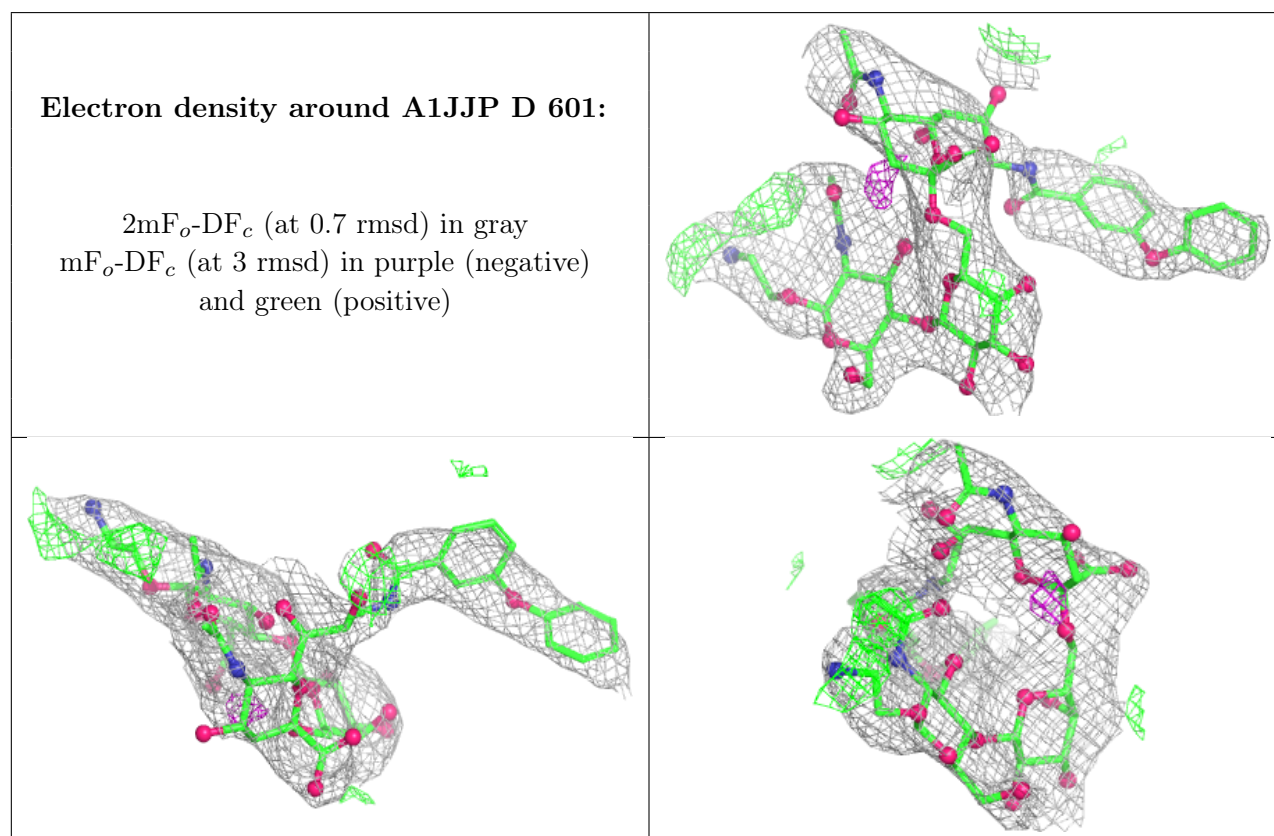


6.4 Ligands [i](#)

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.

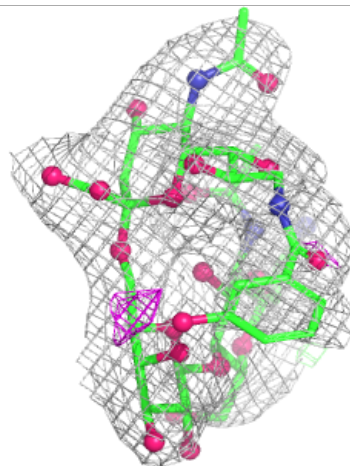
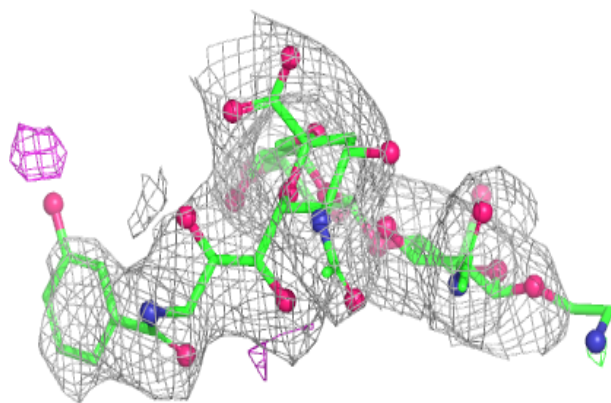
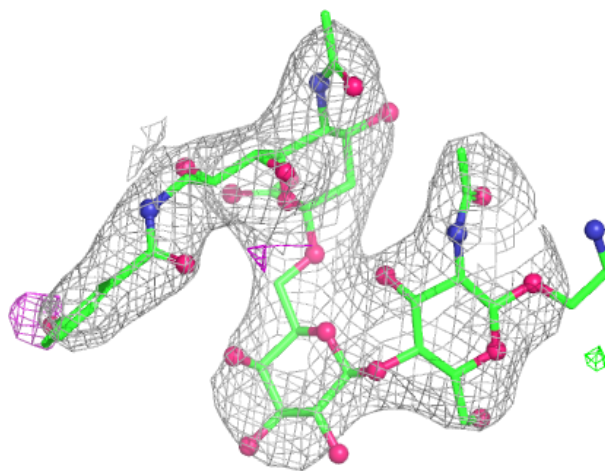
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	A1JJP	D	601	64/64	0.66	0.14	75,116,128,133	0
3	SO4	A	501	5/5	0.82	0.15	103,105,130,132	0
3	SO4	C	602	5/5	0.86	0.11	100,104,121,128	0
3	SO4	B	501	5/5	0.86	0.13	107,110,121,125	0
4	A1JJP	A	502	58/64	0.88	0.10	57,84,105,112	0
4	A1JJP	B	502	64/64	0.91	0.08	65,80,88,95	0
4	A1JJP	C	601	64/64	0.94	0.08	52,67,75,84	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.



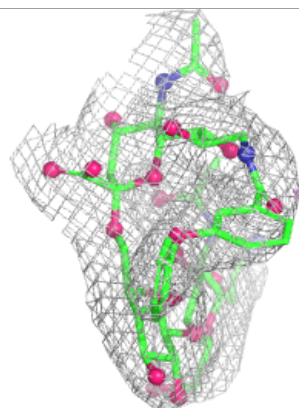
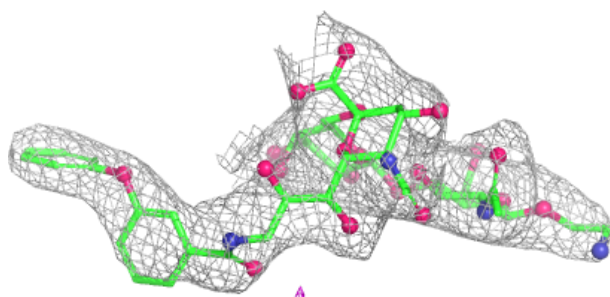
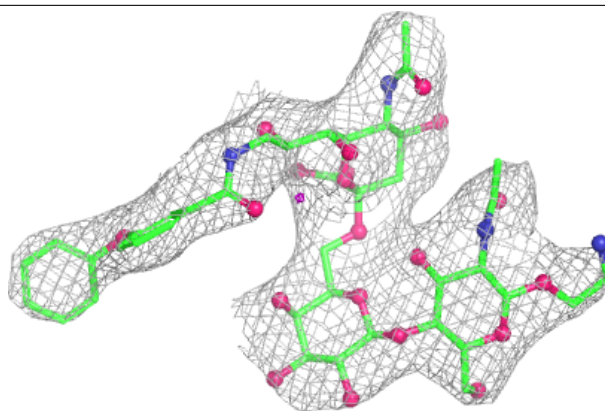
Electron density around A1JJP A 502:

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

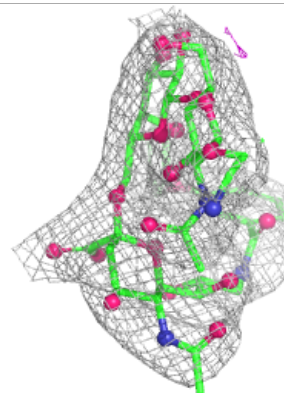
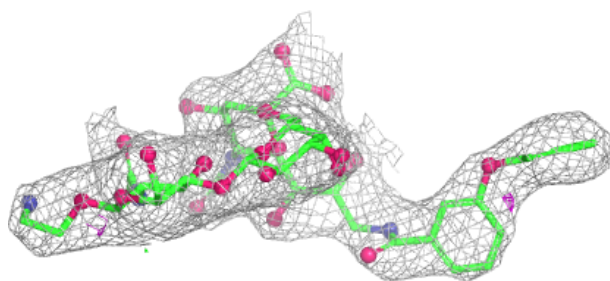
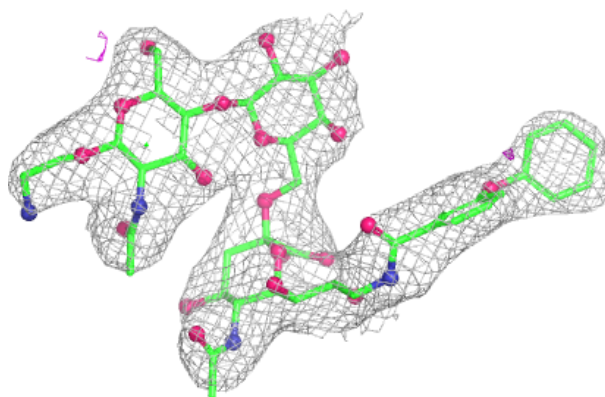


Electron density around A1JJP B 502:

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

**Electron density around A1JJP C 601:**

$2mF_o-DF_c$ (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.