



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:06 PM UTC

PDB ID : 2DW1 / pdb_00002dw1
Title : Crystal structure of VAP2 from Crotalus atrox venom (Form 2-2 crystal)
Authors : Takeda, S.; Igarashi, T.; Araki, S.
Deposited on : 2006-08-02
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

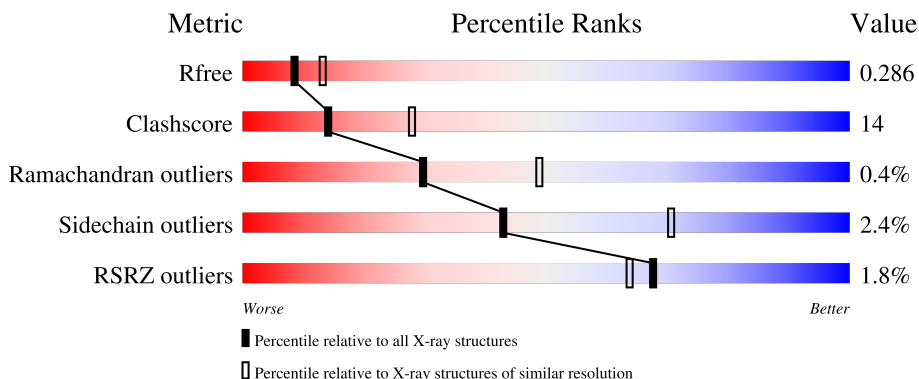
1 Overall quality at a glance

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	419	% 75% 22% ..
1	B	419	3% 68% 30% ..
2	C	3	33% 67%
3	D	4	25% 50% 25%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6801 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.

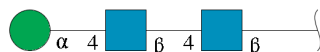
- Molecule 1 is a protein called Catrocollastatin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	S	0	0	0
			3219	1990	545	637	47			
1	B	415	Total	C	N	O	S	0	0	0
			3219	1990	545	637	47			

There are 2 discrepancies between the modelled and reference sequences:

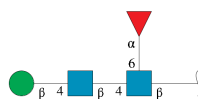
Chain	Residue	Modelled	Actual	Comment	Reference
A	203	VAL	PHE	SEE REMARK 999	UNP Q90282
B	203	VAL	PHE	SEE REMARK 999	UNP Q90282

- Molecule 2 is an oligosaccharide called alpha-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	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 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
3	D	4	Total	C	N	O	0	0	0
			49	28	2	19			

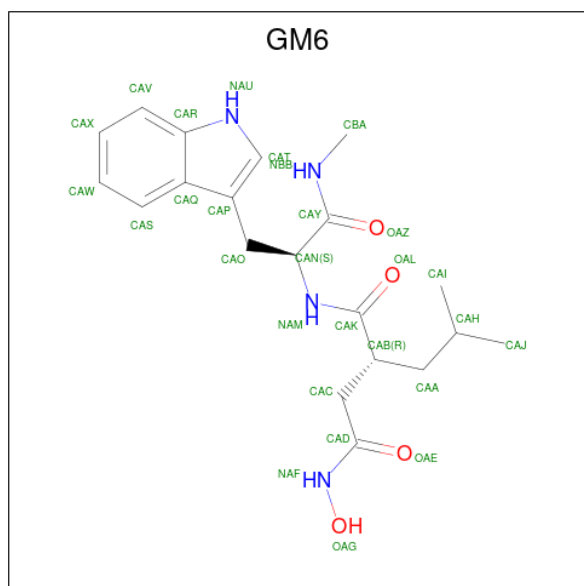
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Ca	0	0
			3	3		
4	B	3	Total	Ca	0	0
			3	3		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		

- Molecule 6 is 3-(N-HYDROXYCARBOXAMIDO)-2-ISOBUTYLPROPANOYL-TRP-MET HYLAMIDE (CCD ID: GM6) (formula: C₂₀H₂₈N₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			28	20	4	4		
6	B	1	Total	C	N	O	0	0
			28	20	4	4		

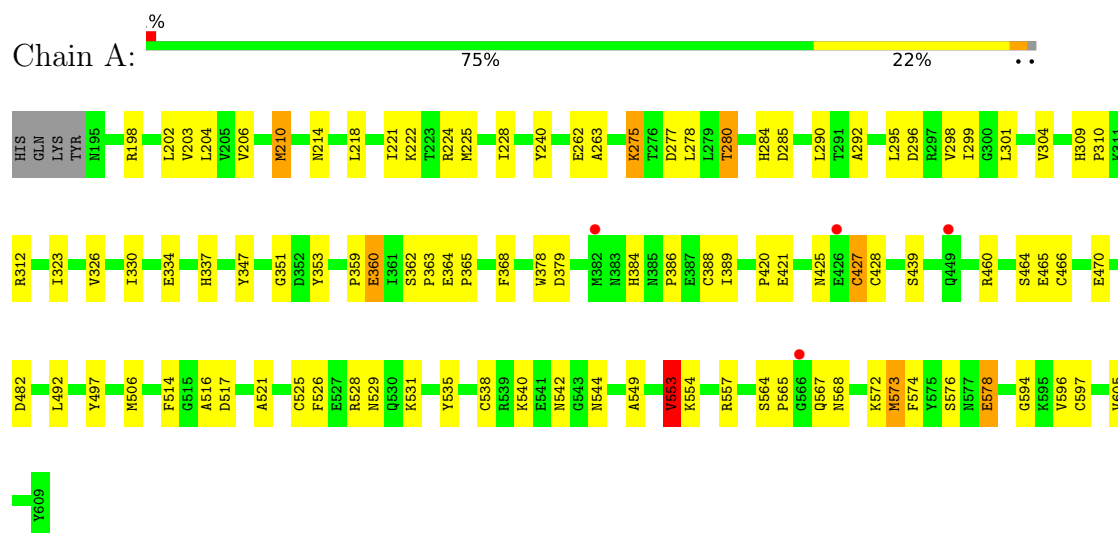
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	121	Total 121	O 121	0	0
7	B	90	Total 90	O 90	0	0

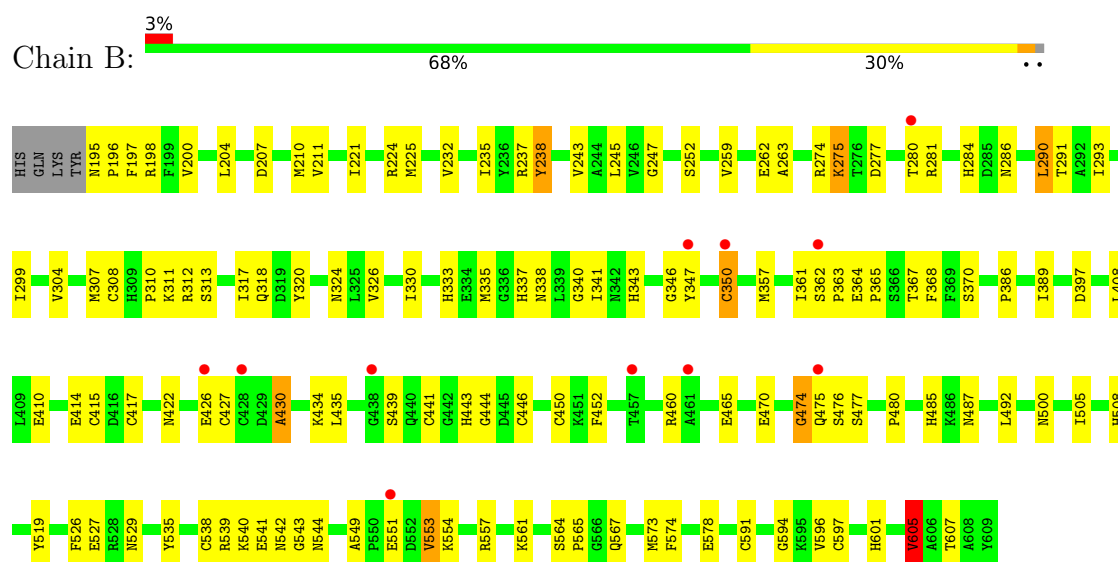
3 Residue-property plots

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: Catrocollastatin



• Molecule 1: Catrocollastatin



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

Chain C:  33% 67%

MAG1
MAG2
MAN3

- Molecule 3: 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 D:  25% 50% 25%

MAG1
MAG2
EMJ3
FUC4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.67Å 118.18Å 138.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.50) 98.7 (50.00-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.48Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.227 , 0.286 0.231 , 0.286	Depositor DCC
R_{free} test set	1656 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 29.2	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	0.94	EDS
Total number of atoms	6801	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 68.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.1288e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CA, MAN, FUC, GM6, BMA, ZN

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	0.39	0/3291	0.93	7/4453 (0.2%)
1	B	0.38	0/3291	0.92	9/4453 (0.2%)
All	All	0.39	0/6582	0.92	16/8906 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	485	HIS	N-CA-C	-7.79	100.47	110.53
1	A	368	PHE	N-CA-C	6.58	120.19	109.59
1	B	427	CYS	N-CA-C	-6.38	105.42	113.72
1	A	549	ALA	N-CA-C	-6.06	101.72	110.08
1	B	549	ALA	N-CA-C	-6.00	101.56	110.20
1	B	578	GLU	N-CA-C	-5.99	104.83	111.36
1	B	474	GLY	N-CA-C	-5.68	101.83	112.22
1	B	397	ASP	N-CA-C	-5.65	106.38	113.72
1	A	379	ASP	N-CA-C	-5.39	105.32	111.14
1	A	202	LEU	N-CA-C	5.36	118.55	109.76
1	B	350	CYS	N-CA-C	-5.35	105.02	112.30
1	A	578	GLU	N-CA-C	-5.30	105.67	111.82
1	B	605	VAL	CB-CA-C	-5.29	105.11	112.04
1	A	428	CYS	N-CA-C	5.29	118.02	109.40
1	B	197	PHE	N-CA-C	5.09	117.27	110.35
1	A	553	VAL	N-CA-C	5.03	117.34	111.05

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	3219	0	2986	76	0
1	B	3219	0	2986	102	0
2	C	39	0	34	3	0
3	D	49	0	43	3	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	28	0	28	1	0
6	B	28	0	27	2	0
7	A	121	0	0	1	0
7	B	90	0	0	5	0
All	All	6801	0	6104	181	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 14.

All (181) 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:204:LEU:HD13	1:A:225:MET:HE3	1.35	1.08
1:B:204:LEU:HD13	1:B:225:MET:HE3	1.43	1.00
1:B:210:MET:HE2	1:B:290:LEU:HD23	1.45	0.97
1:B:529:ASN:HD21	1:B:557:ARG:HB3	1.39	0.87
3:D:1:NAG:H61	3:D:4:FUC:O2	1.80	0.81
1:B:195:ASN:HB2	1:B:196:PRO:HD2	1.63	0.80
1:A:309:HIS:HD2	1:A:312:ARG:H	1.29	0.80
1:A:204:LEU:CD1	1:A:225:MET:HE3	2.11	0.80
1:A:526:PHE:HB3	1:A:553:VAL:HG13	1.65	0.79
2:C:1:NAG:H62	2:C:2:NAG:O5	1.83	0.79
1:A:529:ASN:HD21	1:A:557:ARG:HB3	1.47	0.78
1:B:225:MET:HE1	1:B:290:LEU:HD22	1.67	0.76
1:B:542:ASN:HB2	1:B:544:ASN:ND2	2.01	0.75
1:B:363:PRO:C	1:B:365:PRO:HD3	2.13	0.74
1:B:286:ASN:HB2	1:B:307:MET:HE1	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ARG:HD2	1:A:389:ILE:HG13	1.69	0.73
1:B:259:VAL:HG12	1:B:293:ILE:HD13	1.71	0.72
1:A:567:GLN:HG3	1:A:568:ASN:H	1.55	0.72
1:A:364:GLU:O	1:A:364:GLU:HG2	1.90	0.71
1:A:210:MET:HE2	1:A:290:LEU:HB3	1.74	0.69
1:A:204:LEU:HD13	1:A:225:MET:CE	2.20	0.69
1:A:594:GLY:O	1:A:605:VAL:HG23	1.93	0.69
1:B:307:MET:HE3	1:B:308:CYS:H	1.58	0.68
1:B:439:SER:CB	1:B:450:CYS:HB3	2.24	0.68
1:B:299:ILE:HG12	6:B:1:GM6:OAL	1.92	0.67
1:B:224:ARG:HE	1:B:324:ASN:ND2	1.93	0.67
1:B:526:PHE:O	1:B:553:VAL:HG22	1.95	0.66
1:A:309:HIS:CD2	1:A:312:ARG:H	2.11	0.65
1:A:206:VAL:HG13	1:A:210:MET:HE3	1.78	0.65
1:B:596:VAL:HG21	7:B:810:HOH:O	1.98	0.64
1:B:237:ARG:NH2	1:B:422:ASN:HB3	2.14	0.62
1:A:225:MET:HE1	1:A:290:LEU:HD13	1.80	0.62
1:A:363:PRO:C	1:A:365:PRO:HD3	2.25	0.61
1:B:259:VAL:HG12	1:B:293:ILE:CD1	2.29	0.61
1:B:415:CYS:SG	1:B:435:LEU:HD23	2.39	0.61
1:A:384:HIS:O	1:A:386:PRO:HD3	2.03	0.59
1:B:362:SER:O	1:B:365:PRO:HG3	2.03	0.59
1:B:439:SER:HB3	1:B:450:CYS:HB3	1.84	0.59
1:A:521:ALA:HB1	1:A:525:CYS:SG	2.43	0.58
1:A:594:GLY:C	1:A:605:VAL:HG23	2.28	0.58
1:B:198:ARG:HD2	1:B:389:ILE:HG13	1.85	0.58
1:A:299:ILE:HG12	6:A:2:GM6:OAL	2.04	0.58
1:B:539:ARG:HH11	1:B:539:ARG:HG2	1.68	0.58
1:A:203:VAL:HG11	1:A:278:LEU:HD21	1.85	0.57
1:A:225:MET:HE1	1:A:290:LEU:CD1	2.34	0.57
1:B:200:VAL:HG11	1:B:335:MET:CE	2.34	0.57
1:B:470:GLU:HB3	1:B:480:PRO:HG2	1.87	0.57
1:B:551:GLU:HG2	7:B:835:HOH:O	2.05	0.56
1:B:235:ILE:HG12	1:B:367:THR:HB	1.88	0.56
1:A:514:PHE:CD2	1:A:572:LYS:HD3	2.41	0.56
1:B:225:MET:CE	1:B:290:LEU:HD22	2.35	0.56
1:B:487:ASN:HD21	1:B:500:ASN:H	1.52	0.55
1:A:351:GLY:C	1:A:353:TYR:H	2.13	0.55
1:B:326:VAL:O	1:B:330:ILE:HG12	2.06	0.55
1:B:368:PHE:HA	7:B:891:HOH:O	2.08	0.54
1:B:540:LYS:HA	1:B:544:ASN:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:ASP:O	1:B:280:THR:HG22	2.07	0.54
1:A:362:SER:O	1:A:365:PRO:HG3	2.08	0.53
1:A:425:ASN:C	1:A:425:ASN:HD22	2.17	0.53
1:B:542:ASN:HB2	1:B:544:ASN:HD21	1.72	0.53
1:A:526:PHE:CB	1:A:553:VAL:HG13	2.37	0.53
1:B:281:ARG:HH11	1:B:281:ARG:HG3	1.74	0.53
1:B:307:MET:HE3	1:B:313:SER:OG	2.08	0.53
1:B:386:PRO:O	1:B:389:ILE:HG12	2.09	0.53
1:A:224:ARG:O	1:A:228:ILE:HG13	2.09	0.52
1:B:535:TYR:CD1	1:B:573:MET:HE2	2.44	0.52
1:A:285:ASP:HB3	1:A:388:CYS:SG	2.50	0.52
1:A:421:GLU:OE2	1:A:421:GLU:N	2.40	0.52
1:B:487:ASN:ND2	1:B:500:ASN:H	2.08	0.52
1:B:211:VAL:HG21	1:B:252:SER:HA	1.93	0.51
1:B:317:ILE:HG23	1:B:330:ILE:CG2	2.41	0.51
1:A:347:TYR:O	2:C:1:NAG:H3	2.10	0.51
1:B:304:VAL:HA	1:B:337:HIS:O	2.11	0.50
1:A:535:TYR:CD1	1:A:573:MET:HE2	2.45	0.50
1:B:408:LEU:O	1:B:410:GLU:HG3	2.11	0.50
1:A:278:LEU:HG	1:A:284:HIS:CE1	2.46	0.50
1:A:574:PHE:C	1:A:574:PHE:CD1	2.90	0.50
1:A:263:ALA:HB1	1:A:301:LEU:HD22	1.94	0.50
1:B:541:GLU:C	1:B:543:GLY:H	2.20	0.50
1:B:574:PHE:C	1:B:574:PHE:CD2	2.89	0.49
1:A:225:MET:HE1	1:A:290:LEU:HD22	1.94	0.49
1:B:317:ILE:HG23	1:B:330:ILE:HG21	1.94	0.49
1:B:291:THR:OG1	1:B:293:ILE:HG12	2.12	0.49
1:B:200:VAL:HG11	1:B:335:MET:HE3	1.95	0.48
1:B:347:TYR:CD2	3:D:2:NAG:H4	2.49	0.48
1:B:607:THR:HG22	1:B:607:THR:O	2.12	0.48
1:B:274:ARG:HH21	1:B:284:HIS:CD2	2.32	0.48
1:B:475:GLN:HE21	1:B:475:GLN:HA	1.79	0.48
1:A:240:TYR:HB2	1:A:378:TRP:HZ2	1.77	0.48
1:B:439:SER:HB2	1:B:450:CYS:HB3	1.93	0.48
1:B:474:GLY:C	1:B:476:SER:H	2.22	0.48
1:A:210:MET:HG2	1:A:292:ALA:HB2	1.96	0.47
1:A:427:CYS:HB3	1:A:439:SER:HB2	1.95	0.47
1:B:307:MET:O	1:B:308:CYS:HB2	2.14	0.47
1:B:221:ILE:O	1:B:225:MET:HG2	2.15	0.47
1:A:564:SER:HB2	1:A:565:PRO:HD2	1.95	0.47
1:B:460:ARG:NH1	1:B:470:GLU:HG2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:PHE:CG	1:A:572:LYS:HD3	2.50	0.47
1:B:245:LEU:HD11	1:B:247:GLY:O	2.14	0.47
1:B:318:GLN:C	1:B:320:TYR:H	2.22	0.47
1:A:567:GLN:HG3	1:A:568:ASN:N	2.24	0.47
1:A:225:MET:HE1	1:A:290:LEU:CD2	2.45	0.46
1:A:596:VAL:CG1	1:A:597:CYS:N	2.78	0.46
1:B:341:ILE:HG21	1:B:357:MET:HG3	1.97	0.46
1:A:240:TYR:HB2	1:A:378:TRP:CZ2	2.51	0.46
1:A:516:ALA:HB1	7:A:921:HOH:O	2.15	0.46
1:B:350:CYS:HB3	1:B:370:SER:HA	1.96	0.46
1:A:573:MET:SD	1:A:573:MET:C	2.99	0.46
1:B:237:ARG:HA	7:B:874:HOH:O	2.14	0.46
1:A:364:GLU:N	1:A:365:PRO:HD3	2.30	0.46
1:B:422:ASN:HD22	1:B:422:ASN:N	2.12	0.46
1:A:465:GLU:CD	1:A:492:LEU:H	2.23	0.45
1:A:277:ASP:O	1:A:280:THR:HB	2.16	0.45
1:A:334:GLU:HA	1:A:334:GLU:OE1	2.15	0.45
1:B:460:ARG:HH12	1:B:470:GLU:HG2	1.80	0.45
1:B:361:ILE:HG12	1:B:362:SER:H	1.82	0.45
1:B:364:GLU:N	1:B:365:PRO:HD3	2.32	0.45
1:A:540:LYS:HA	1:A:544:ASN:O	2.15	0.45
1:B:475:GLN:HA	1:B:475:GLN:NE2	2.31	0.45
1:B:554:LYS:HB2	7:B:887:HOH:O	2.18	0.44
1:B:343:HIS:HA	1:B:357:MET:O	2.17	0.44
1:A:304:VAL:HA	1:A:337:HIS:O	2.18	0.44
1:A:516:ALA:O	1:A:517:ASP:HB2	2.18	0.44
1:A:528:ARG:HA	1:A:531:LYS:HE3	1.99	0.44
1:A:567:GLN:CG	1:A:568:ASN:H	2.28	0.43
1:B:505:ILE:HD11	1:B:508:HIS:CD2	2.52	0.43
1:B:607:THR:O	1:B:607:THR:CG2	2.65	0.43
1:A:576:SER:C	1:A:578:GLU:H	2.25	0.43
1:B:281:ARG:HG3	1:B:281:ARG:NH1	2.34	0.43
1:B:591:CYS:HB3	1:B:597:CYS:SG	2.59	0.43
1:B:597:CYS:HA	1:B:601:HIS:O	2.18	0.43
1:A:295:LEU:HB2	1:A:298:VAL:O	2.19	0.43
1:B:363:PRO:O	1:B:365:PRO:HD3	2.18	0.43
1:B:238:TYR:CD1	1:B:238:TYR:C	2.96	0.43
1:B:539:ARG:HG2	1:B:539:ARG:NH1	2.33	0.43
1:A:535:TYR:CG	1:A:573:MET:HE2	2.54	0.43
1:B:275:LYS:CG	1:B:310:PRO:HB2	2.48	0.43
1:B:594:GLY:O	1:B:605:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:SER:HB2	1:B:565:PRO:HD2	2.01	0.43
1:A:460:ARG:NH1	1:A:482:ASP:HA	2.34	0.42
1:B:195:ASN:HB2	1:B:196:PRO:CD	2.43	0.42
1:B:446:CYS:HB2	1:B:477:SER:C	2.43	0.42
1:B:311:LYS:HG3	1:B:312:ARG:N	2.34	0.42
1:B:414:GLU:OE2	1:B:434:LYS:HD2	2.19	0.42
1:B:474:GLY:C	1:B:476:SER:N	2.78	0.42
1:B:207:ASP:OD1	1:B:291:THR:HA	2.20	0.42
1:B:443:HIS:ND1	1:B:444:GLY:N	2.67	0.42
1:A:218:LEU:O	1:A:222:LYS:HG3	2.18	0.42
1:B:232:VAL:HG12	1:B:243:VAL:HG21	2.02	0.42
1:B:527:GLU:HA	1:B:553:VAL:HG21	2.01	0.42
1:A:326:VAL:O	1:A:330:ILE:HG12	2.20	0.42
1:A:275:LYS:HG2	1:A:310:PRO:HB2	2.02	0.42
1:B:417:CYS:SG	1:B:430:ALA:HB2	2.59	0.42
1:B:441:CYS:HB3	1:B:452:PHE:HE2	1.84	0.42
1:B:333:HIS:CE1	6:B:1:GM6:HAI2	2.55	0.41
1:B:475:GLN:O	1:B:475:GLN:HG3	2.20	0.41
1:A:497:TYR:CZ	1:A:605:VAL:HG21	2.55	0.41
1:B:318:GLN:C	1:B:320:TYR:N	2.78	0.41
1:B:465:GLU:CD	1:B:492:LEU:H	2.28	0.41
1:B:326:VAL:HG13	1:B:361:ILE:CD1	2.50	0.41
1:A:347:TYR:CE2	2:C:2:NAG:H3	2.55	0.41
1:B:338:ASN:C	1:B:340:GLY:H	2.29	0.41
1:B:210:MET:HE2	1:B:290:LEU:CD2	2.33	0.41
1:A:359:PRO:HG2	1:A:360:GLU:OE2	2.20	0.41
1:A:542:ASN:N	1:A:542:ASN:ND2	2.69	0.41
1:B:237:ARG:HH11	1:B:237:ARG:HG2	1.86	0.41
1:B:361:ILE:HG12	1:B:362:SER:N	2.36	0.41
1:B:519:TYR:O	1:B:561:LYS:N	2.37	0.41
1:A:542:ASN:N	1:A:542:ASN:HD22	2.19	0.41
1:B:262:GLU:O	1:B:263:ALA:C	2.64	0.41
1:A:323:ILE:HB	1:A:326:VAL:HG23	2.03	0.40
1:A:506:MET:HE1	1:A:554:LYS:HB3	2.04	0.40
1:B:335:MET:O	1:B:338:ASN:HB2	2.21	0.40
1:A:386:PRO:O	1:A:389:ILE:HG12	2.22	0.40
1:A:420:PRO:HG2	1:A:421:GLU:CD	2.47	0.40
1:A:351:GLY:C	1:A:353:TYR:N	2.79	0.40
1:A:460:ARG:HD2	1:A:470:GLU:OE2	2.20	0.40
1:A:517:ASP:CB	1:A:564:SER:HA	2.51	0.40
3:D:1:NAG:C6	3:D:4:FUC:O2	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:SER:C	1:A:466:CYS:N	2.79	0.40
1:A:214:ASN:HB2	1:A:221:ILE:HD11	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	413/419 (99%)	390 (94%)	22 (5%)	1 (0%)	43	63
1	B	413/419 (99%)	374 (91%)	37 (9%)	2 (0%)	24	43
All	All	826/838 (99%)	764 (92%)	59 (7%)	3 (0%)	30	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	ASP
1	B	346	GLY
1	B	430	ALA

5.3.2 Protein sidechains [i](#)

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	361/365 (99%)	352 (98%)	9 (2%)	42	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	361/365 (99%)	353 (98%)	8 (2%)	45 73
All	All	722/730 (99%)	705 (98%)	17 (2%)	43 70

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210	MET
1	A	262	GLU
1	A	275	LYS
1	A	280	THR
1	A	360	GLU
1	A	427	CYS
1	A	538	CYS
1	A	553	VAL
1	A	573	MET
1	B	238	TYR
1	B	275	LYS
1	B	290	LEU
1	B	426	GLU
1	B	538	CYS
1	B	553	VAL
1	B	567	GLN
1	B	605	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	ASN
1	A	230	ASN
1	A	288	GLN
1	A	309	HIS
1	A	318	GLN
1	A	385	ASN
1	A	425	ASN
1	A	440	GLN
1	A	471	HIS
1	A	475	GLN
1	A	489	GLN
1	A	500	ASN
1	A	508	HIS
1	A	529	ASN

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Mol	Chain	Res	Type
1	A	542	ASN
1	A	569	ASN
1	A	599	ASN
1	B	288	GLN
1	B	324	ASN
1	B	342	ASN
1	B	385	ASN
1	B	475	GLN
1	B	487	ASN
1	B	494	ASN
1	B	500	ASN
1	B	502	ASN
1	B	508	HIS
1	B	529	ASN
1	B	542	ASN
1	B	544	ASN
1	B	563	ASN
1	B	567	GLN
1	B	568	ASN
1	B	581	HIS
1	B	599	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 ⓘ

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
2	NAG	C	1	1,2	14,14,15	0.83	0	17,19,21	1.47	4 (23%)
2	NAG	C	2	2	14,14,15	1.14	1 (7%)	17,19,21	1.30	4 (23%)
2	MAN	C	3	2	11,11,12	0.78	0	15,15,17	0.44	0
3	NAG	D	1	1,3	14,14,15	0.73	0	17,19,21	1.16	2 (11%)
3	NAG	D	2	3	14,14,15	0.60	0	17,19,21	0.69	0
3	BMA	D	3	3	11,11,12	0.65	0	15,15,17	0.38	0
3	FUC	D	4	3	10,10,11	0.70	0	14,14,16	0.80	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
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	MAN	C	3	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	-	3/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	FUC	D	4	3	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	C1-C2	3.50	1.57	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C4-C3-C2	-3.86	105.37	111.02
2	C	1	NAG	O4-C4-C5	2.71	116.00	109.32
3	D	1	NAG	C3-C4-C5	2.59	114.92	110.23
2	C	2	NAG	C1-O5-C5	2.34	115.33	112.19
2	C	2	NAG	C4-C3-C2	-2.29	107.66	111.02
2	C	2	NAG	C3-C4-C5	-2.26	106.14	110.23
2	C	2	NAG	C2-N2-C7	-2.25	119.88	122.90
2	C	1	NAG	C1-O5-C5	2.25	115.20	112.19
2	C	1	NAG	C2-N2-C7	-2.19	119.96	122.90
3	D	1	NAG	C2-N2-C7	-2.17	119.99	122.90

There are no chirality outliers.

All (13) torsion outliers are listed below:

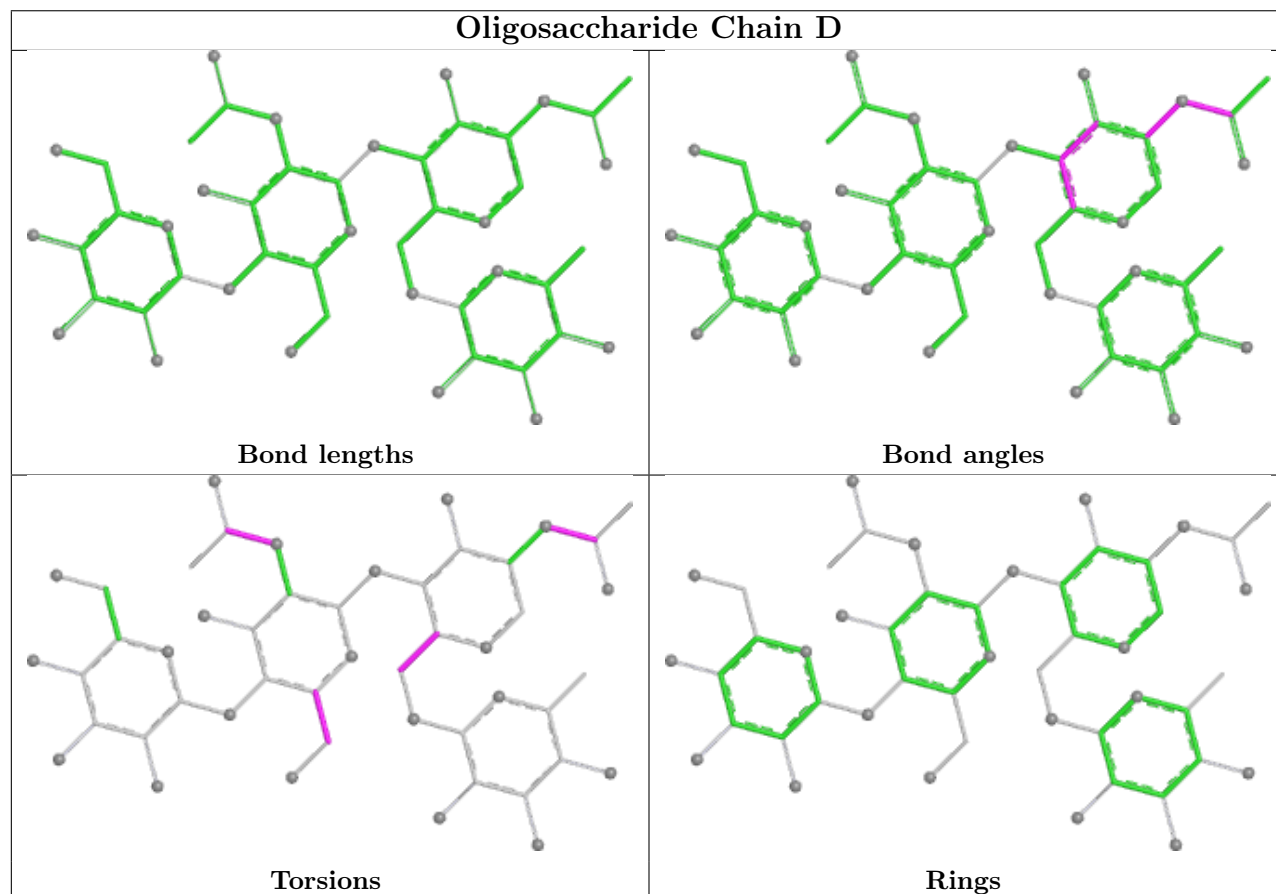
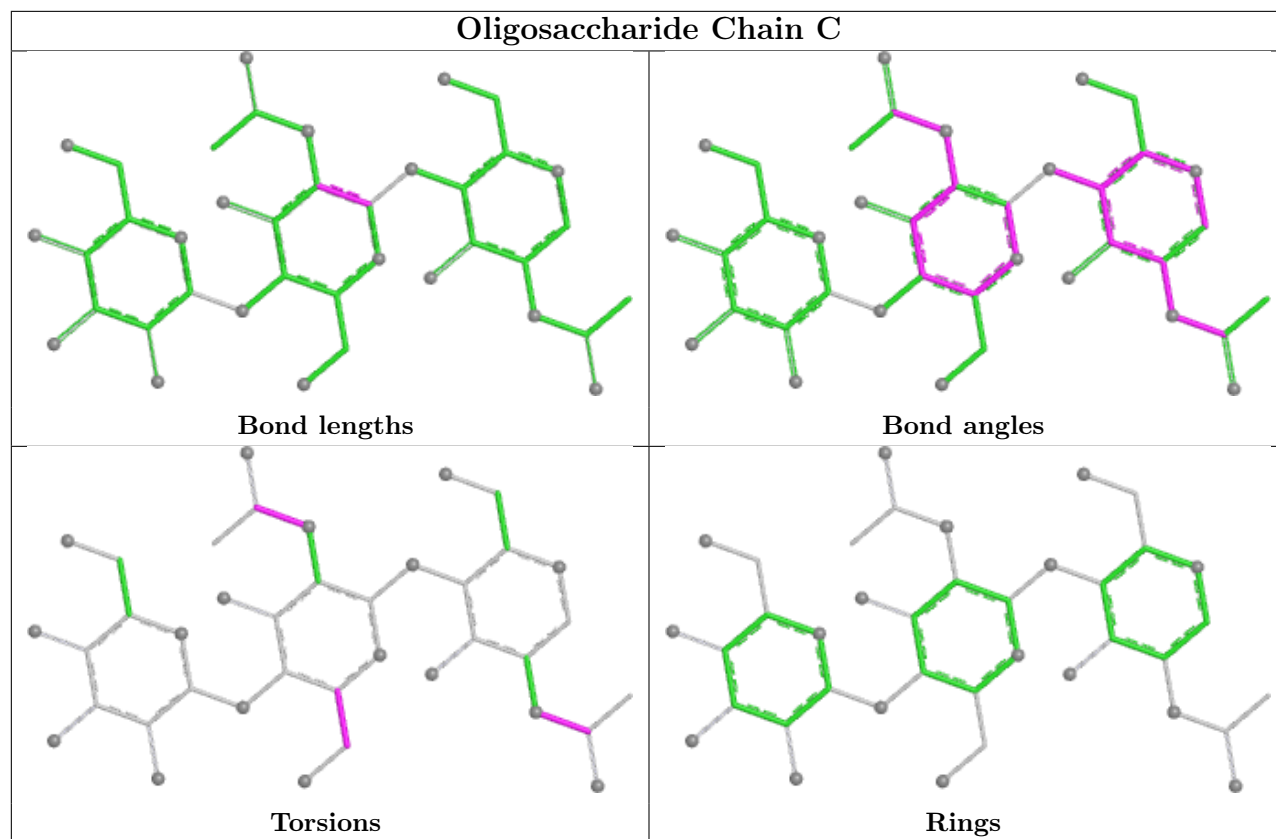
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	2	NAG	C8-C7-N2-C2
3	D	2	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
3	D	1	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	2	0
2	C	1	NAG	2	0
3	D	4	FUC	2	0
3	D	2	NAG	1	0
3	D	1	NAG	2	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

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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$
6	GM6	B	1	5	29,29,29	1.49	6 (20%)	37,39,39	1.21	4 (10%)
6	GM6	A	2	5	29,29,29	1.51	6 (20%)	37,39,39	1.20	4 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GM6	B	1	5	-	4/28/28/28	0/2/2/2
6	GM6	A	2	5	-	4/28/28/28	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2	GM6	CAQ-CAP	-3.26	1.38	1.44
6	B	1	GM6	CAQ-CAP	-2.89	1.39	1.44
6	B	1	GM6	CAO-CAP	2.50	1.55	1.50
6	B	1	GM6	CAS-CAQ	2.47	1.43	1.39
6	B	1	GM6	CAR-NAU	-2.45	1.33	1.37
6	A	2	GM6	CAO-CAP	2.41	1.54	1.50
6	A	2	GM6	CAX-CAV	2.38	1.43	1.38
6	A	2	GM6	CAR-NAU	-2.36	1.34	1.37
6	A	2	GM6	CAS-CAQ	2.33	1.43	1.39
6	A	2	GM6	CAW-CAX	2.14	1.42	1.38
6	B	1	GM6	CAX-CAV	2.13	1.42	1.38
6	B	1	GM6	CAW-CAX	2.00	1.42	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1	GM6	CAQ-CAR-NAU	-3.76	104.39	107.52
6	A	2	GM6	CAQ-CAR-NAU	-3.53	104.58	107.52
6	B	1	GM6	CAR-CAQ-CAP	2.28	109.47	107.17
6	A	2	GM6	CAR-CAQ-CAP	2.27	109.46	107.17
6	B	1	GM6	CAV-CAR-NAU	2.17	134.21	130.74
6	A	2	GM6	CAV-CAR-NAU	2.07	134.06	130.74
6	B	1	GM6	CBA-NBB-CAY	-2.02	118.69	122.21
6	A	2	GM6	CAN-CAO-CAP	-2.02	109.62	113.44

There are no chirality outliers.

All (8) torsion outliers are listed below:

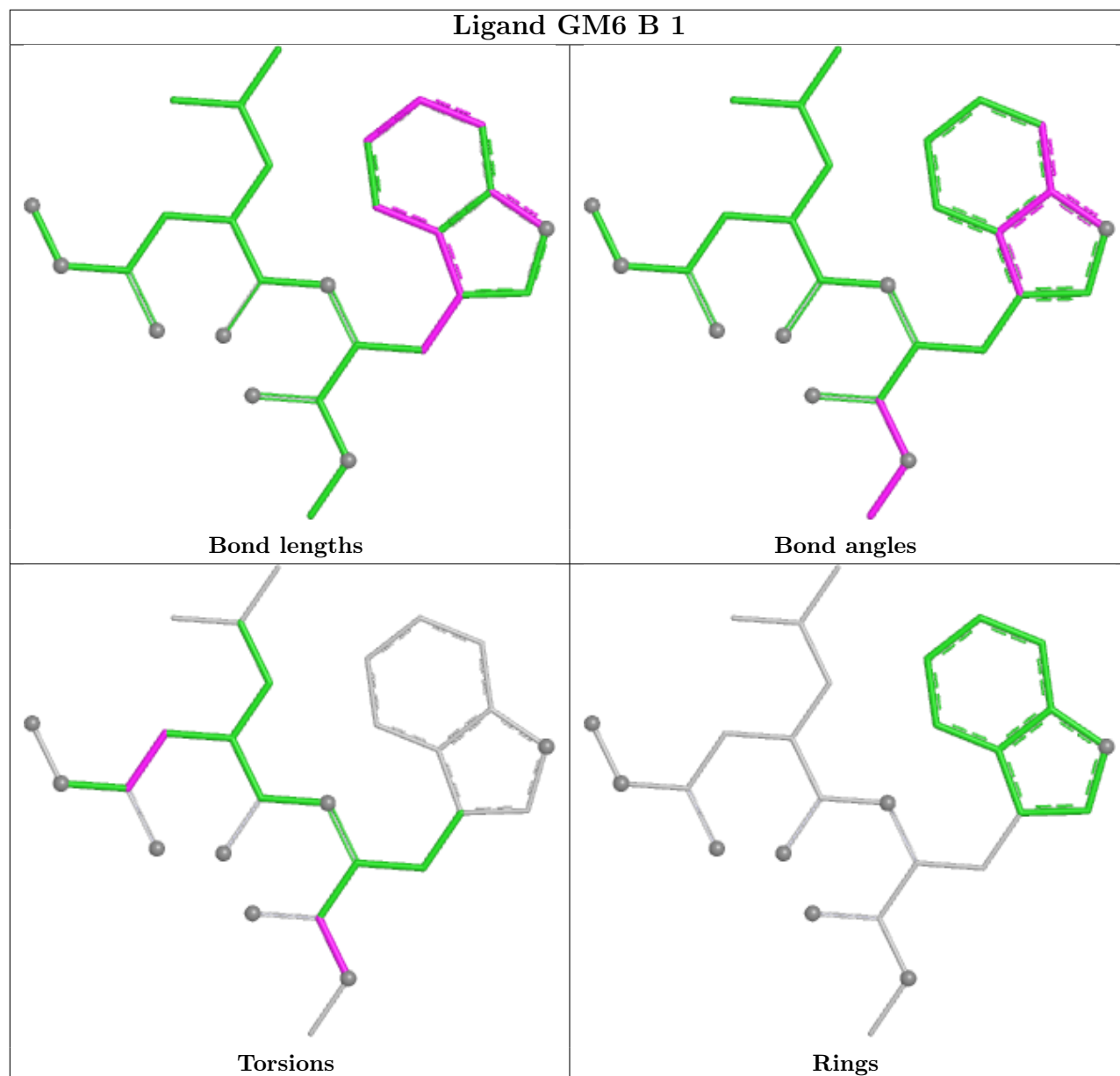
Mol	Chain	Res	Type	Atoms
6	B	1	GM6	CAN-CAY-NBB-CBA
6	B	1	GM6	OAZ-CAY-NBB-CBA
6	A	2	GM6	CAN-CAO-CAP-CAT
6	A	2	GM6	CAN-CAO-CAP-CAQ
6	B	1	GM6	CAB-CAC-CAD-OAE
6	A	2	GM6	CAB-CAC-CAD-OAE
6	B	1	GM6	CAB-CAC-CAD-NAF
6	A	2	GM6	CAB-CAC-CAD-NAF

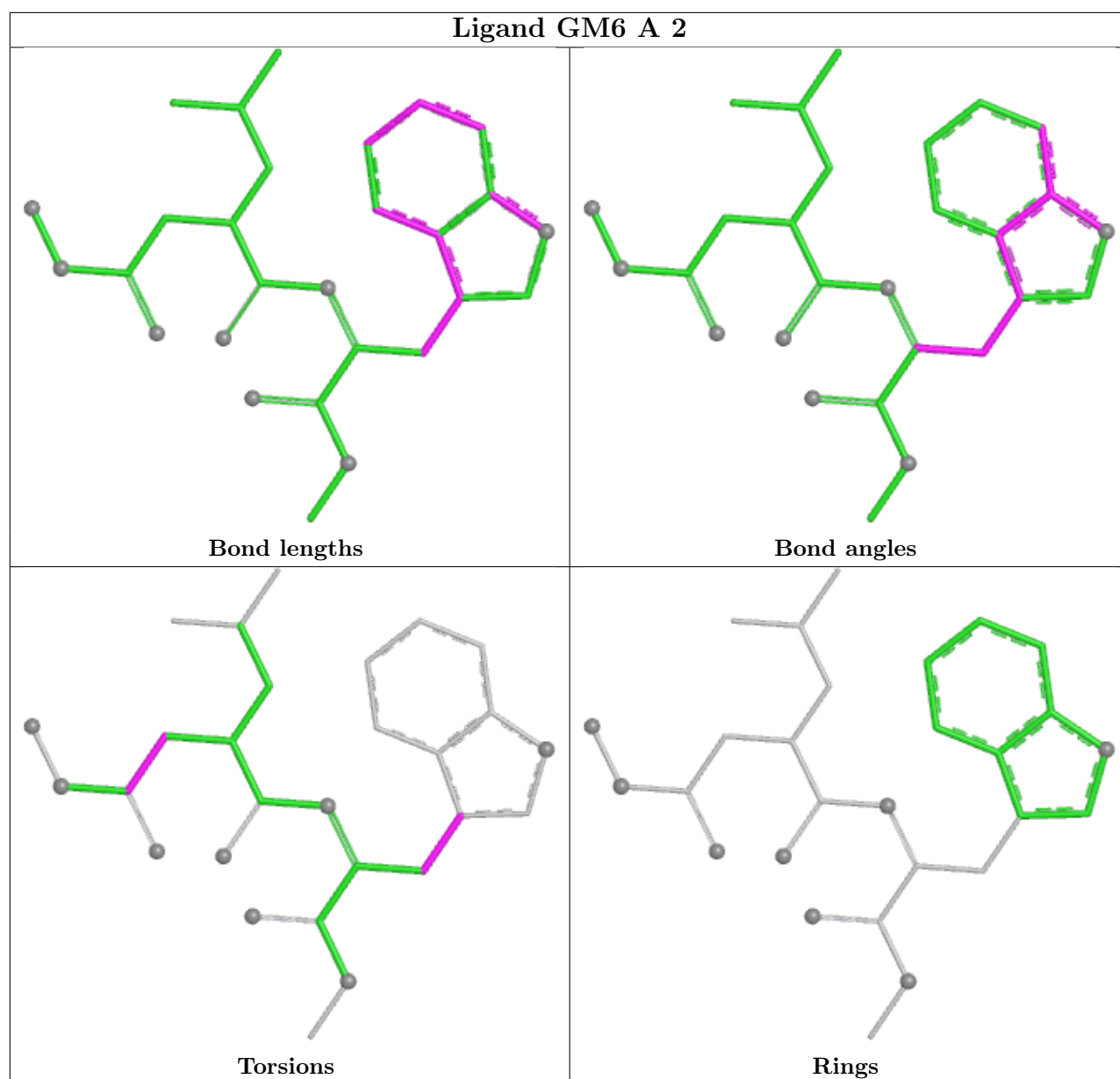
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1	GM6	2	0
6	A	2	GM6	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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	415/419 (99%)	-0.00	4 (0%) 79 76	13, 33, 59, 70	0
1	B	415/419 (99%)	0.28	11 (2%) 56 51	18, 39, 68, 83	0
All	All	830/838 (99%)	0.14	15 (1%) 67 64	13, 36, 65, 83	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	566	GLY	4.1
1	B	457	THR	3.5
1	B	475	GLN	3.5
1	B	347	TYR	3.3
1	A	426	GLU	3.2
1	B	428	CYS	2.5
1	B	461	ALA	2.3
1	A	382	MET	2.3
1	B	438	GLY	2.2
1	A	449	GLN	2.2
1	B	426	GLU	2.2
1	B	551	GLU	2.1
1	B	280	THR	2.1
1	B	350	CYS	2.1
1	B	362	SER	2.0

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

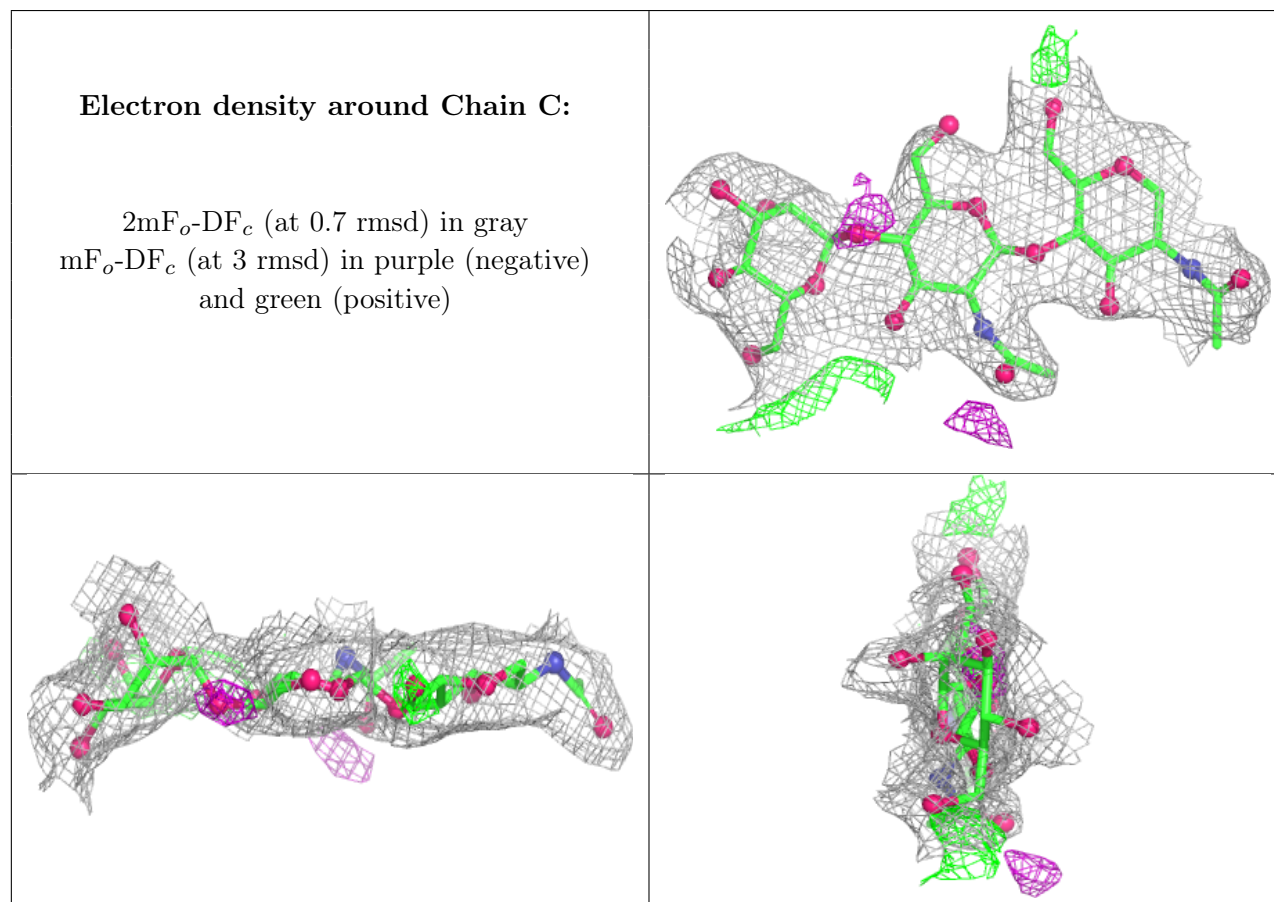
There are no non-standard protein/DNA/RNA residues in this entry.

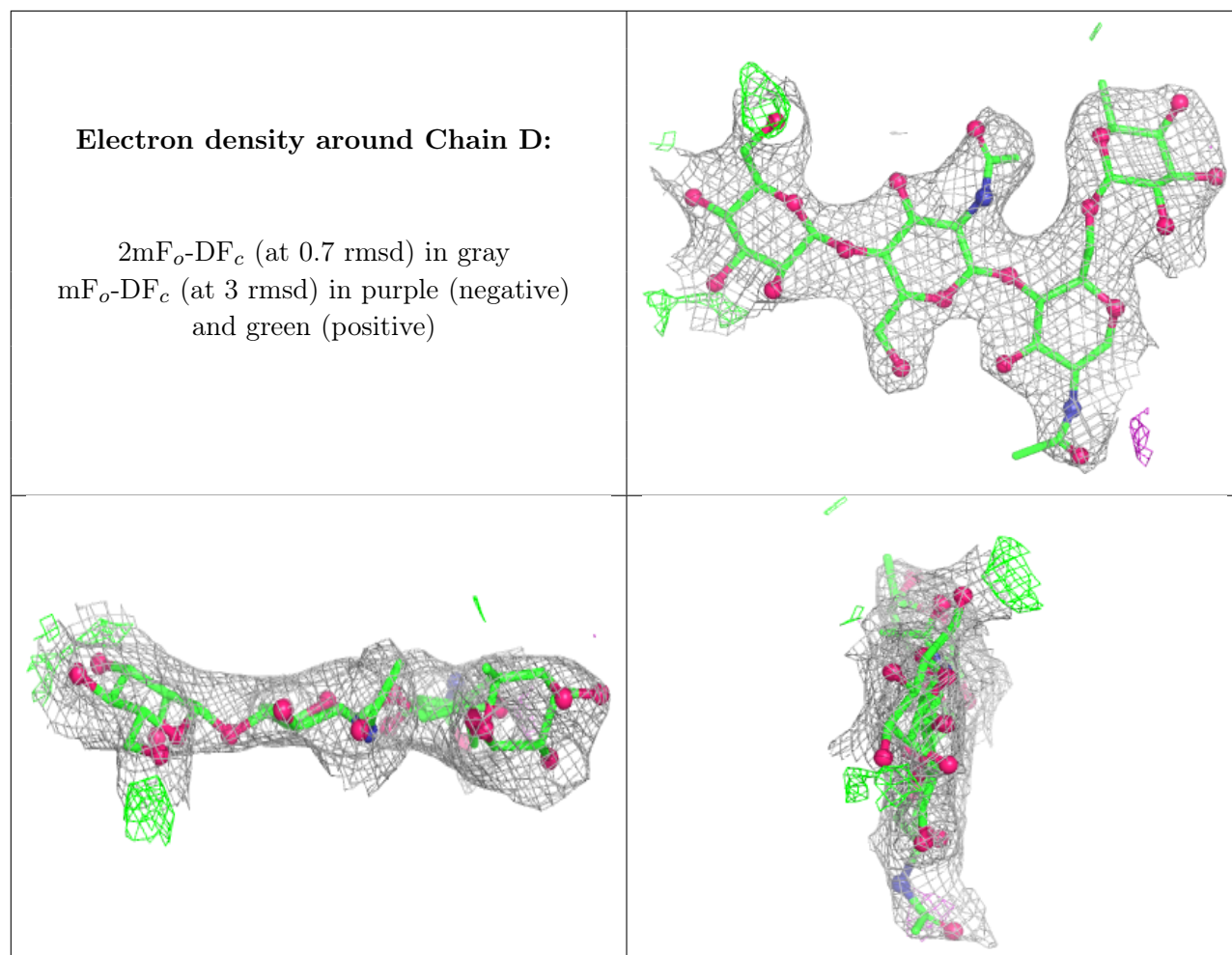
6.3 Carbohydrates ⓘ

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	MAN	C	3	11/12	0.31	0.16	103,104,106,106	0
3	BMA	D	3	11/12	0.41	0.18	77,79,80,81	0
2	NAG	C	2	14/15	0.51	0.16	85,90,93,100	0
3	NAG	D	2	14/15	0.71	0.13	67,71,73,76	0
3	FUC	D	4	10/11	0.72	0.14	61,62,63,63	0
2	NAG	C	1	14/15	0.77	0.12	58,61,67,77	0
3	NAG	D	1	14/15	0.82	0.12	59,63,66,66	0

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



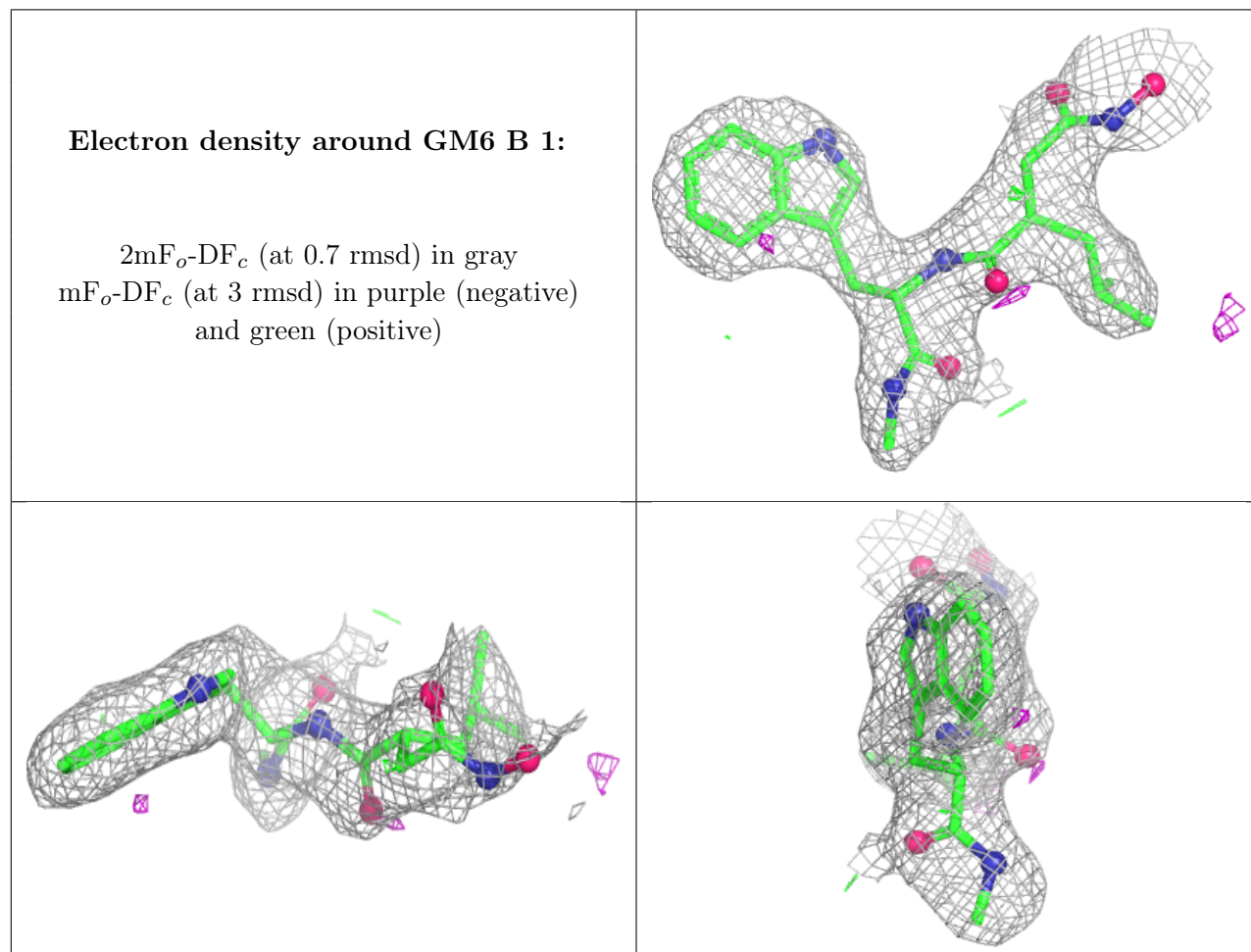


6.4 Ligands [i](#)

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

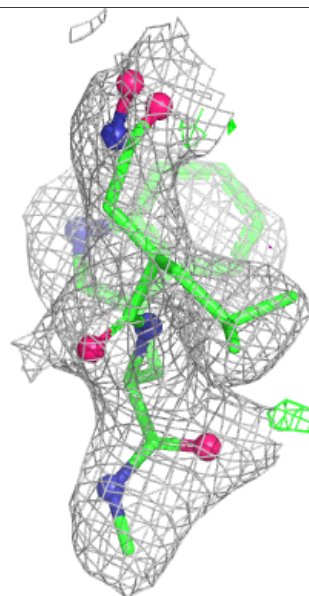
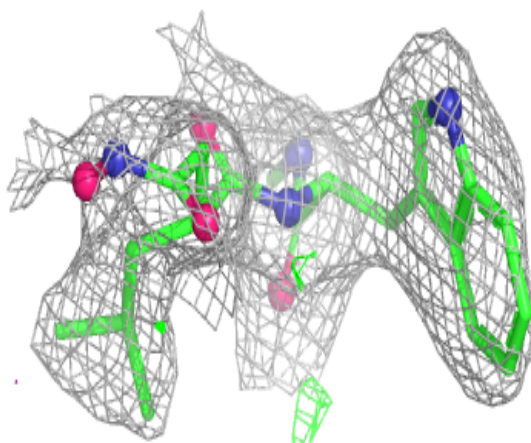
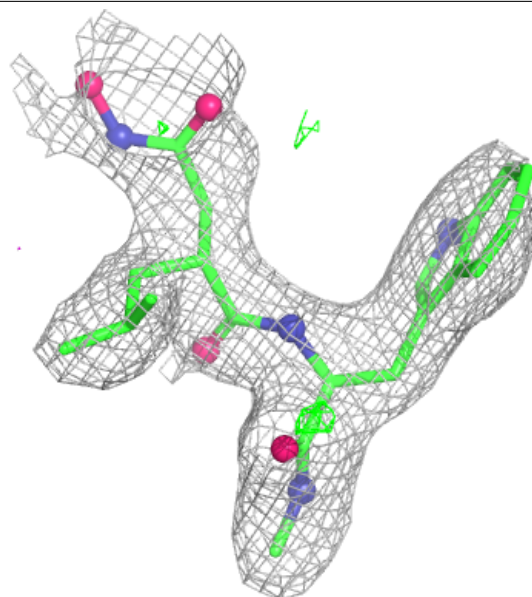
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GM6	B	1	28/28	0.91	0.11	31,36,45,55	0
6	GM6	A	2	28/28	0.94	0.10	16,34,46,49	0
4	CA	B	712	1/1	0.97	0.04	52,52,52,52	0
4	CA	B	711	1/1	0.98	0.03	43,43,43,43	0
4	CA	A	703	1/1	0.98	0.03	40,40,40,40	0
4	CA	B	713	1/1	0.99	0.04	42,42,42,42	0
5	ZN	A	700	1/1	0.99	0.03	22,22,22,22	0
5	ZN	B	700	1/1	0.99	0.02	29,29,29,29	0
4	CA	A	702	1/1	0.99	0.04	38,38,38,38	0
4	CA	A	701	1/1	0.99	0.03	35,35,35,35	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 GM6 A 2:

$2mF_o-DF_c$ (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.