



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:15 PM UTC

PDB ID : 7QQG / pdb_00007qqg
Title : Crystal structure of MYORG bound to 1-deoxygalactonojirimycin
Authors : Meek, R.W.; Davies, G.J.
Deposited on : 2022-01-07
Resolution : 2.43 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

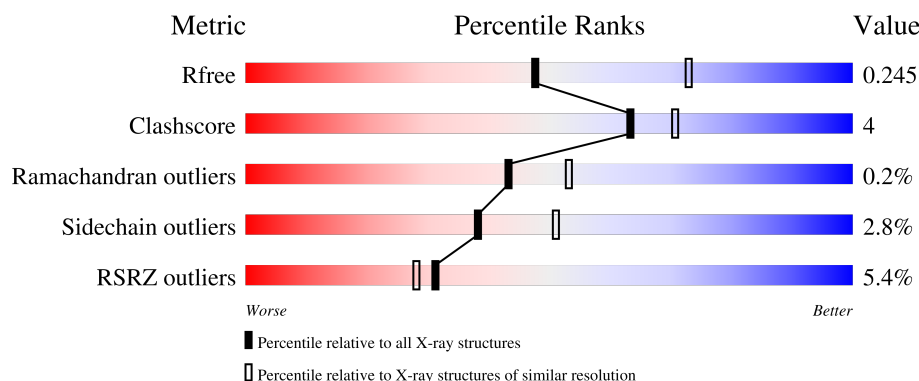
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



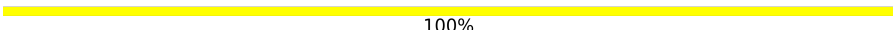
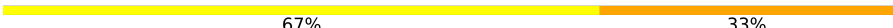
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	636	2% 87% 9% .
1	B	636	2% 86% 11% ..
1	C	636	5% 85% 11% ..
1	D	636	12% 69% 9% 22%
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	G	2	 50%50%
2	H	2	 100%
2	I	2	 50%50%
2	J	2	 50%50%
2	K	2	 100%
3	F	3	 67%33%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19500 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 Myogenesis-regulating glycosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	618	Total	C	N	O	S	0	0	0
			4973	3207	866	884	16			
1	B	623	Total	C	N	O	S	0	0	0
			5013	3234	874	889	16			
1	C	614	Total	C	N	O	S	0	0	0
			4913	3175	848	874	16			
1	D	496	Total	C	N	O	S	0	0	0
			3964	2575	672	707	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	GLY	-	expression tag	UNP Q6NSJ0
B	79	GLY	-	expression tag	UNP Q6NSJ0
C	79	GLY	-	expression tag	UNP Q6NSJ0
D	79	GLY	-	expression tag	UNP Q6NSJ0

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



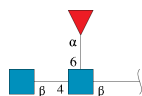
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

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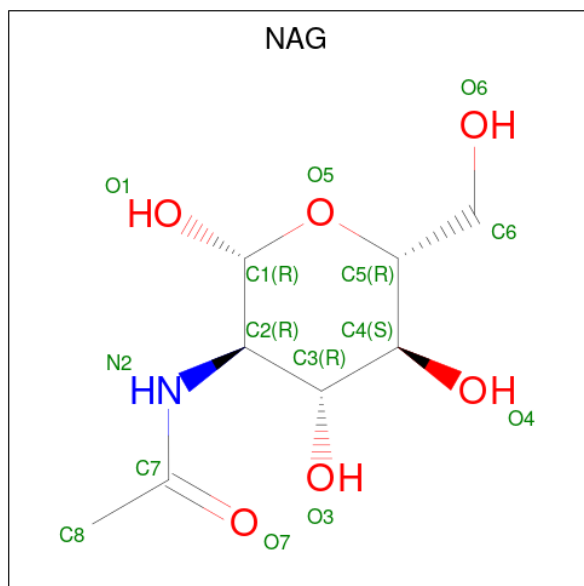
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



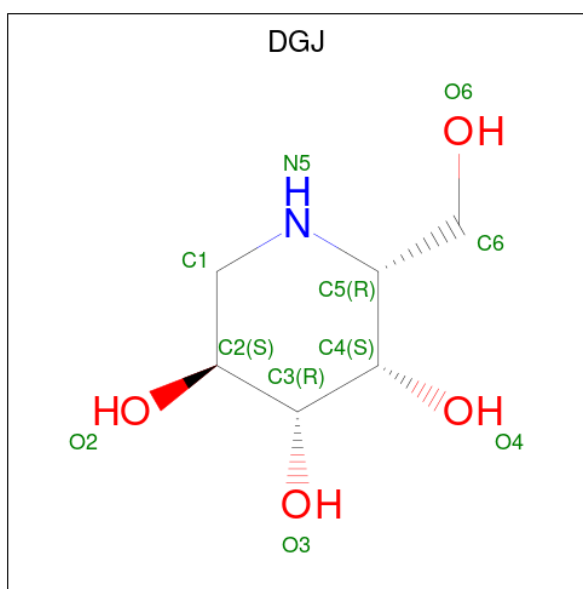
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 5 is (2R,3S,4R,5S)-2-(hydroxymethyl)piperidine-3,4,5-triol (CCD ID: DGJ) (formula: C₆H₁₃NO₄) (labeled as "Ligand of Interest" by depositor).



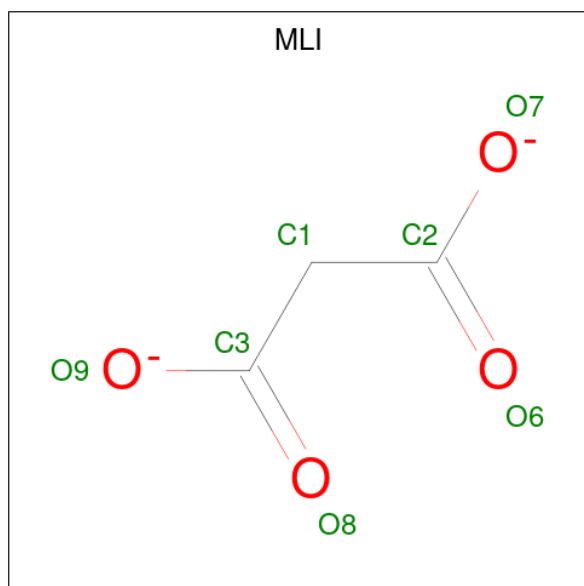
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			11	6	1	4		
5	B	1	Total	C	N	O	0	0
			11	6	1	4		
5	C	1	Total	C	N	O	0	0
			11	6	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 6 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	3	4		
6	B	1	Total	C	O	0	0
			7	3	4		

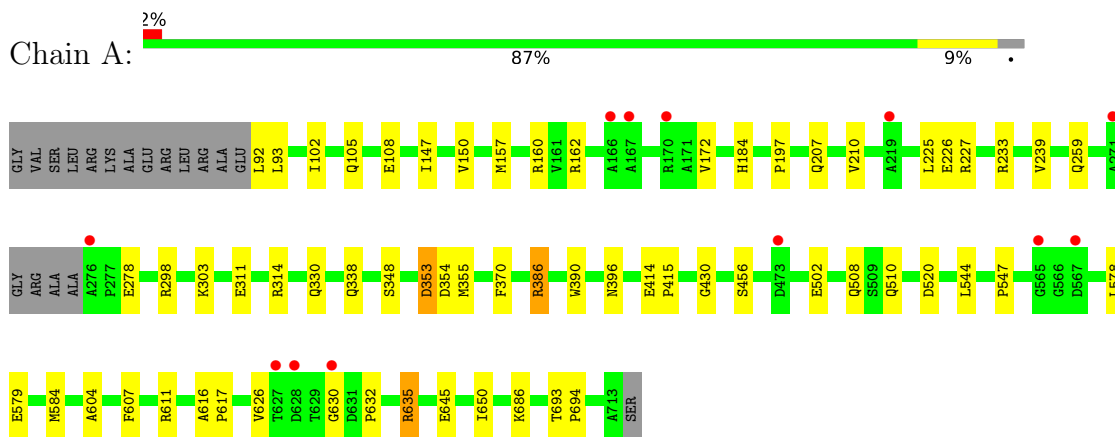
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	86	Total	O	0	0
			86	86		
7	B	91	Total	O	0	0
			91	91		
7	C	33	Total	O	0	0
			33	33		
7	D	23	Total	O	0	0
			23	23		

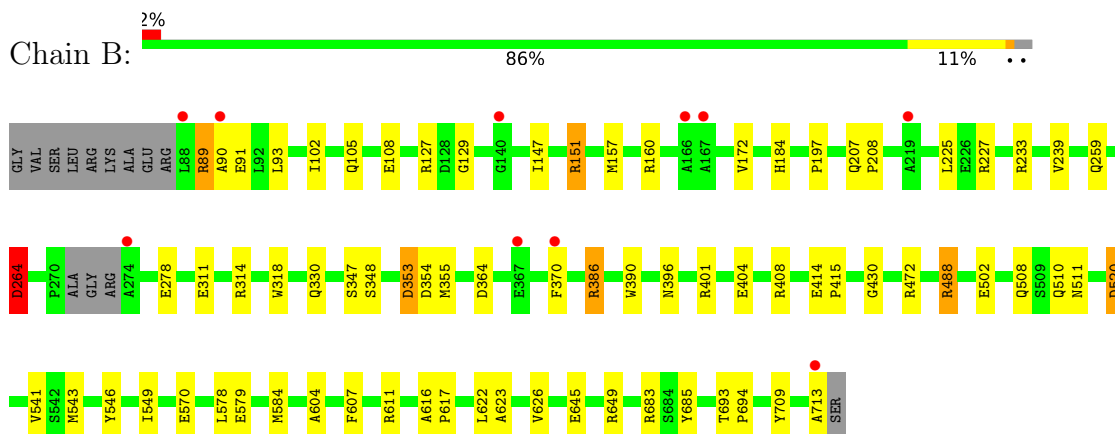
3 Residue-property plots [i](#)

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.

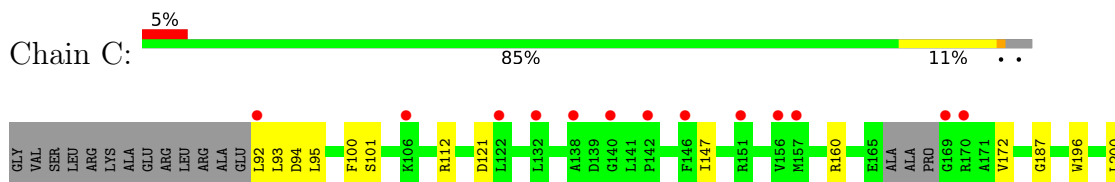
- Molecule 1: Myogenesis-regulating glycosidase

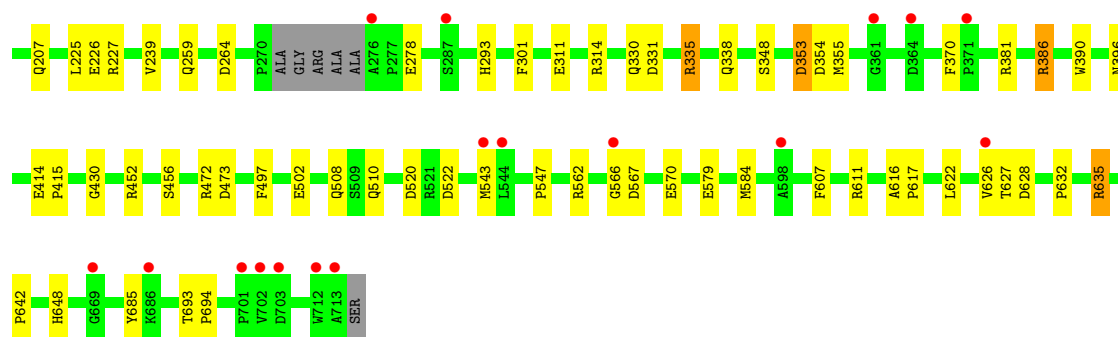


- Molecule 1: Myogenesis-regulating glycosidase

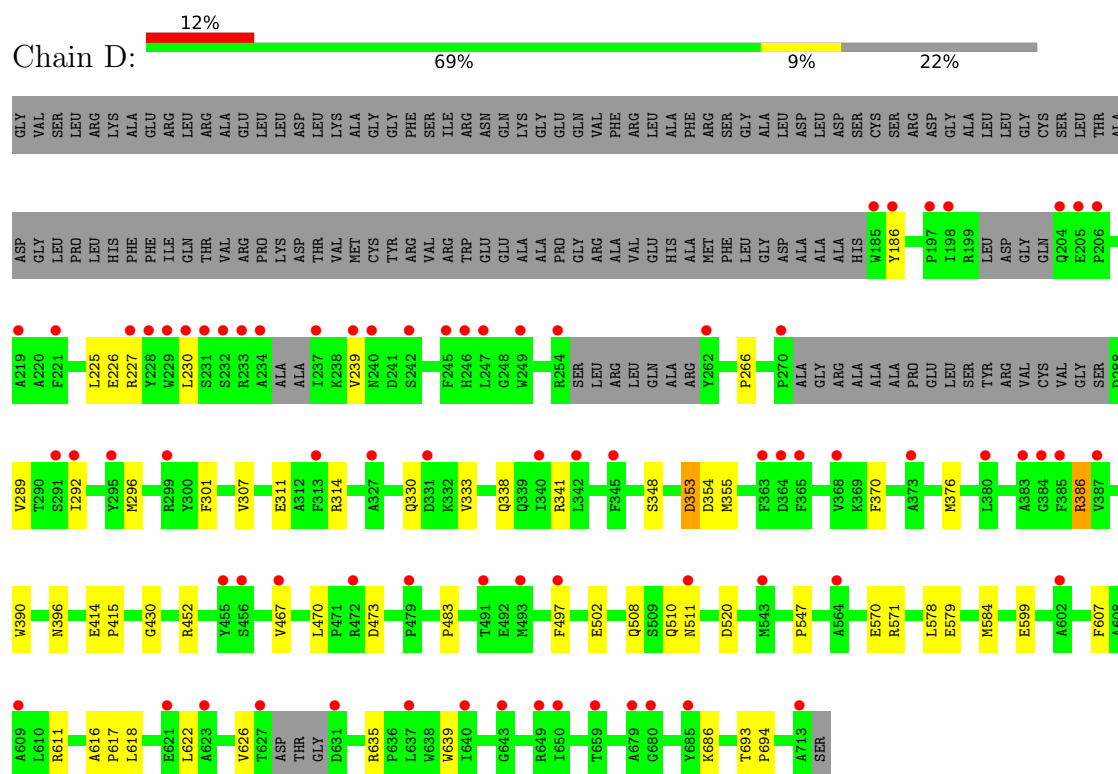


- Molecule 1: Myogenesis-regulating glycosidase

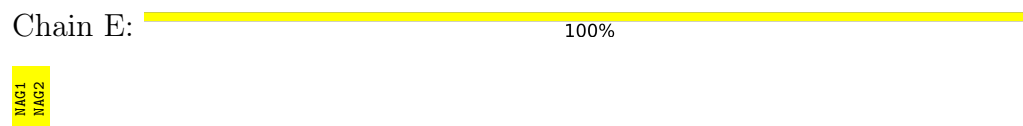




• Molecule 1: Myogenesis-regulating glycosidase



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



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



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

Chain H:  100%

MAG1
MAG2

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

Chain I:  50% 50%

MAG1
MAG2

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

Chain J:  50% 50%

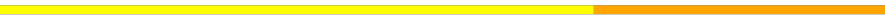
MAG1
MAG2

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

Chain K:  100%

MAG1
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  67% 33%

MAG1
MAG2
FUC3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.11Å 78.88Å 176.22Å 80.78° 80.21° 62.64°	Depositor
Resolution (Å)	69.75 – 2.43 69.75 – 2.43	Depositor EDS
% Data completeness (in resolution range)	98.1 (69.75-2.43) 96.9 (69.75-2.43)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.224 , 0.250 (Not available) , 0.245	Depositor DCC
R_{free} test set	6102 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19500	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DGJ, FUC, NAG, MLI

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	0.99	0/5129	1.29	0/6988
1	B	0.99	0/5169	1.30	4/7040 (0.1%)
1	C	0.98	0/5067	1.30	5/6907 (0.1%)
1	D	0.97	0/4097	1.32	2/5602 (0.0%)
All	All	0.98	0/19462	1.30	11/26537 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	264	ASP	CA-CB-CG	7.07	119.67	112.60
1	C	566	GLY	CA-C-N	5.52	127.61	120.44
1	C	566	GLY	C-N-CA	5.52	127.61	120.44
1	B	570	GLU	CA-C-N	5.50	127.58	120.44
1	B	570	GLU	C-N-CA	5.50	127.58	120.44
1	C	567	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	364	ASP	CA-CB-CG	5.21	117.81	112.60
1	D	570	GLU	CA-C-N	5.10	127.07	120.44
1	D	570	GLU	C-N-CA	5.10	127.07	120.44
1	C	570	GLU	CA-C-N	5.04	127.00	120.44
1	C	570	GLU	C-N-CA	5.04	127.00	120.44

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	4973	0	4802	32	0
1	B	5013	0	4851	47	0
1	C	4913	0	4715	35	0
1	D	3964	0	3713	38	0
2	E	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
3	F	38	0	34	1	0
4	A	42	0	39	1	0
4	B	28	0	26	0	0
4	C	42	0	39	0	0
4	D	28	0	26	0	0
5	A	11	0	13	0	0
5	B	11	0	13	1	0
5	C	11	0	13	0	0
5	D	11	0	13	0	0
6	A	7	0	2	0	0
6	B	7	0	2	0	0
7	A	86	0	0	2	0
7	B	91	0	0	0	0
7	C	33	0	0	0	0
7	D	23	0	0	0	0
All	All	19500	0	18451	151	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 (151) 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:108:GLU:OE2	1:A:233:ARG:HD3	1.71	0.90
1:C:547:PRO:HG3	1:C:626:VAL:HG11	1.72	0.72
1:A:584:MET:O	1:A:611:ARG:NH2	2.22	0.72
1:D:584:MET:O	1:D:611:ARG:NH2	2.24	0.71
1:C:584:MET:O	1:C:611:ARG:NH2	2.23	0.70
1:B:584:MET:O	1:B:611:ARG:NH2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:LEU:HD11	1:D:289:VAL:CG2	2.22	0.69
1:C:93:LEU:HD11	1:C:100:PHE:HB2	1.73	0.68
1:C:187:GLY:N	1:C:543:MET:HE1	2.08	0.68
1:C:293:HIS:CE1	1:C:543:MET:HG2	2.32	0.65
1:D:330:GLN:HA	1:D:376:MET:HE1	1.78	0.65
1:A:303:LYS:HD2	1:A:630:GLY:HA2	1.78	0.65
1:A:314:ARG:HH22	3:F:3:FUC:H3	1.63	0.64
1:B:488:ARG:NH2	1:B:511:ASN:OD1	2.31	0.63
1:B:318:TRP:CD1	1:B:347:SER:HG	2.17	0.62
1:D:225:LEU:HD12	1:D:225:LEU:O	2.02	0.58
1:A:547:PRO:HG3	1:A:626:VAL:HG11	1.85	0.57
1:D:547:PRO:HG3	1:D:626:VAL:HG11	1.87	0.56
1:D:348:SER:O	1:D:386:ARG:NH1	2.39	0.56
1:C:353:ASP:HA	1:C:390:TRP:HB2	1.88	0.55
1:A:348:SER:O	1:A:386:ARG:NH1	2.39	0.55
1:B:127:ARG:HD2	1:B:129:GLY:O	2.06	0.55
1:C:93:LEU:HD12	1:C:94:ASP:N	2.22	0.55
1:B:348:SER:O	1:B:386:ARG:NH1	2.40	0.54
1:C:348:SER:O	1:C:386:ARG:NH1	2.41	0.54
1:D:353:ASP:HA	1:D:390:TRP:HB2	1.90	0.54
1:C:95:LEU:C	1:C:95:LEU:HD13	2.33	0.54
1:B:353:ASP:HA	1:B:390:TRP:HB2	1.91	0.53
1:B:622:LEU:O	1:B:626:VAL:HG13	2.07	0.53
1:D:330:GLN:HG3	1:D:376:MET:HE3	1.91	0.53
1:D:230:LEU:CD2	1:D:292:ILE:HD11	2.39	0.53
1:A:314:ARG:O	1:A:611:ARG:HD3	2.09	0.53
1:C:522:ASP:OD2	1:C:562:ARG:HD3	2.09	0.53
1:D:225:LEU:HD12	1:D:225:LEU:C	2.34	0.53
1:A:353:ASP:HA	1:A:390:TRP:HB2	1.91	0.52
1:D:227:ARG:HB3	1:D:239:VAL:HB	1.90	0.52
1:D:314:ARG:O	1:D:611:ARG:HD3	2.11	0.51
1:C:314:ARG:O	1:C:611:ARG:HD3	2.11	0.51
1:B:227:ARG:HB3	1:B:239:VAL:HB	1.93	0.51
1:B:546:TYR:O	1:B:549:ILE:HD11	2.11	0.51
1:B:108:GLU:OE1	1:B:233:ARG:NE	2.41	0.50
1:D:571:ARG:NH2	1:D:599:GLU:OE1	2.40	0.50
1:B:314:ARG:O	1:B:611:ARG:HD3	2.12	0.49
1:B:404:GLU:OE1	1:B:408:ARG:NH1	2.46	0.49
1:B:541:VAL:HG11	1:B:549:ILE:HD12	1.95	0.48
1:A:632:PRO:HG2	1:A:635:ARG:HG3	1.95	0.48
1:B:683:ARG:HG3	1:B:713:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:LYS:HD2	1:A:630:GLY:CA	2.44	0.47
1:B:623:ALA:O	1:B:626:VAL:HG22	2.14	0.47
1:C:632:PRO:HG2	1:C:635:ARG:HG3	1.95	0.47
1:D:508:GLN:HA	1:D:510:GLN:OE1	2.15	0.47
1:C:508:GLN:HA	1:C:510:GLN:OE1	2.14	0.47
1:B:520:ASP:OD1	5:B:803:DGJ:O2	2.22	0.47
1:C:616:ALA:HB3	1:C:617:PRO:HD3	1.97	0.47
1:C:227:ARG:HB3	1:C:239:VAL:HB	1.97	0.46
1:B:207:GLN:OE1	1:B:208:PRO:HD3	2.15	0.46
1:C:354:ASP:OD1	1:C:355:MET:HB2	2.15	0.46
1:B:508:GLN:HA	1:B:510:GLN:OE1	2.15	0.46
1:B:645:GLU:OE2	1:B:649:ARG:NH2	2.49	0.46
1:D:226:GLU:HG2	1:D:301:PHE:CE1	2.51	0.46
1:D:616:ALA:HB3	1:D:617:PRO:HD3	1.98	0.46
1:A:508:GLN:HA	1:A:510:GLN:OE1	2.15	0.46
1:B:89:ARG:O	1:B:127:ARG:NH2	2.48	0.46
1:D:467:VAL:HG23	1:D:470:LEU:HD22	1.98	0.46
1:A:303:LYS:CE	1:A:630:GLY:HA3	2.46	0.46
1:B:207:GLN:OE1	1:B:207:GLN:HA	2.16	0.46
1:B:354:ASP:OD1	1:B:355:MET:HB2	2.16	0.46
1:C:693:THR:HA	1:C:694:PRO:C	2.41	0.46
1:D:354:ASP:OD1	1:D:355:MET:HB2	2.16	0.46
1:C:93:LEU:HD12	1:C:101:SER:O	2.15	0.45
1:C:226:GLU:HG2	1:C:301:PHE:CE1	2.51	0.45
1:D:635:ARG:HH11	1:D:639:TRP:NE1	2.13	0.45
1:B:616:ALA:HB3	1:B:617:PRO:HD3	1.99	0.45
1:A:354:ASP:OD1	1:A:355:MET:HB2	2.16	0.45
1:A:693:THR:HA	1:A:694:PRO:C	2.41	0.45
1:D:266:PRO:HB2	1:D:483:PRO:HG3	1.97	0.45
1:B:685:TYR:HB3	1:B:709:TYR:CZ	2.52	0.45
1:D:330:GLN:HB2	1:D:370:PHE:HA	1.98	0.45
1:A:227:ARG:HB3	1:A:239:VAL:HB	1.99	0.45
1:A:616:ALA:HB3	1:A:617:PRO:HD3	1.97	0.45
1:C:331:ASP:OD2	1:C:335:ARG:HD2	2.17	0.45
1:B:311:GLU:OE1	1:B:386:ARG:NH2	2.49	0.44
1:B:693:THR:HA	1:B:694:PRO:C	2.42	0.44
1:C:311:GLU:OE1	1:C:386:ARG:NH2	2.50	0.44
1:C:396:ASN:HA	1:C:430:GLY:HA3	1.99	0.44
1:A:311:GLU:OE1	1:A:386:ARG:NH2	2.50	0.44
1:A:330:GLN:HB2	1:A:370:PHE:HA	2.00	0.44
1:A:414:GLU:HB2	1:A:415:PRO:CD	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:693:THR:HA	1:D:694:PRO:C	2.42	0.44
1:D:333:VAL:HB	1:D:376:MET:CE	2.48	0.44
1:D:452:ARG:HD2	1:D:497:PHE:CD1	2.53	0.44
1:B:93:LEU:HD12	1:B:102:ILE:HG12	2.00	0.44
1:C:579:GLU:HG2	1:C:607:PHE:CZ	2.53	0.44
1:C:330:GLN:HB2	1:C:370:PHE:HA	2.00	0.44
1:D:467:VAL:HG21	1:D:483:PRO:HB2	1.99	0.44
1:D:579:GLU:HG2	1:D:607:PHE:CZ	2.52	0.44
1:D:396:ASN:HA	1:D:430:GLY:HA3	2.00	0.43
1:D:414:GLU:HB2	1:D:415:PRO:CD	2.47	0.43
1:B:172:VAL:O	1:B:259:GLN:HA	2.18	0.43
1:B:579:GLU:HG2	1:B:607:PHE:CZ	2.53	0.43
1:C:147:ILE:HA	1:C:160:ARG:O	2.18	0.43
1:A:579:GLU:HG2	1:A:607:PHE:CZ	2.54	0.43
1:B:151:ARG:HH11	1:B:151:ARG:CG	2.31	0.43
1:B:330:GLN:HB2	1:B:370:PHE:HA	2.01	0.43
1:B:396:ASN:HA	1:B:430:GLY:HA3	2.01	0.43
1:D:311:GLU:OE1	1:D:386:ARG:NH2	2.51	0.43
1:C:452:ARG:HD2	1:C:497:PHE:CD1	2.54	0.43
1:A:172:VAL:O	1:A:259:GLN:HA	2.19	0.43
1:B:318:TRP:HD1	1:B:347:SER:HG	1.60	0.43
1:C:414:GLU:HB2	1:C:415:PRO:CD	2.49	0.43
1:A:226:GLU:HB2	1:A:544:LEU:HD22	2.01	0.43
1:A:578:LEU:HD11	1:A:604:ALA:HB2	2.00	0.43
1:A:396:ASN:HA	1:A:430:GLY:HA3	2.00	0.42
1:B:147:ILE:HA	1:B:160:ARG:O	2.18	0.42
1:B:184:HIS:HB3	1:B:197:PRO:CG	2.49	0.42
1:B:318:TRP:HD1	1:B:347:SER:OG	2.03	0.42
1:C:622:LEU:O	1:C:626:VAL:HG23	2.19	0.42
1:B:414:GLU:HB2	1:B:415:PRO:CD	2.49	0.42
1:B:541:VAL:HG12	1:B:549:ILE:CD1	2.50	0.42
1:B:401:ARG:NE	1:B:404:GLU:OE2	2.53	0.42
1:B:541:VAL:HG12	1:B:549:ILE:HD11	2.01	0.42
1:B:90:ALA:HB3	1:B:93:LEU:HD22	2.01	0.42
1:B:90:ALA:O	1:B:93:LEU:HB3	2.20	0.42
1:C:172:VAL:O	1:C:259:GLN:HA	2.20	0.42
1:C:93:LEU:CD1	1:C:101:SER:O	2.66	0.42
1:A:147:ILE:HA	1:A:160:ARG:O	2.18	0.42
1:A:93:LEU:HD12	1:A:102:ILE:HG12	2.01	0.42
1:A:150:VAL:O	1:A:157:MET:HE3	2.19	0.42
1:C:93:LEU:HD23	1:C:147:ILE:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:642:PRO:O	1:C:648:HIS:NE2	2.53	0.42
1:B:91:GLU:HG2	1:B:157:MET:HE3	2.01	0.41
1:D:452:ARG:HD2	1:D:497:PHE:CE1	2.55	0.41
1:A:162:ARG:HH21	4:A:801:NAG:H2	1.85	0.41
1:B:543:MET:HB2	1:B:543:MET:HE2	1.72	0.41
1:D:333:VAL:HB	1:D:376:MET:HE1	2.02	0.41
1:B:264:ASP:HA	1:B:472:ARG:NH1	2.35	0.41
1:C:628:ASP:OD1	1:D:307:VAL:HG12	2.20	0.41
1:D:354:ASP:HA	1:D:355:MET:HA	1.88	0.41
1:A:210:VAL:HG12	7:A:931:HOH:O	2.21	0.41
1:D:186:TYR:CD2	1:D:230:LEU:HD12	2.56	0.41
1:D:622:LEU:O	1:D:626:VAL:HG23	2.21	0.41
1:A:184:HIS:HB3	1:A:197:PRO:CG	2.51	0.40
1:B:541:VAL:CG1	1:B:549:ILE:CD1	2.99	0.40
1:A:414:GLU:HB2	1:A:415:PRO:HD2	2.04	0.40
1:A:632:PRO:HD3	7:A:943:HOH:O	2.21	0.40
1:C:414:GLU:HB2	1:C:415:PRO:HD2	2.04	0.40
1:D:225:LEU:C	1:D:225:LEU:CD1	2.94	0.40
1:D:414:GLU:HB2	1:D:415:PRO:HD2	2.04	0.40
1:B:578:LEU:HD11	1:B:604:ALA:HB2	2.04	0.40
1:C:196:TRP:CZ3	1:C:543:MET:HE2	2.57	0.40
1:D:578:LEU:HD23	1:D:578:LEU:C	2.47	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	614/636 (96%)	586 (95%)	27 (4%)	1 (0%)	43 53
1	B	619/636 (97%)	592 (96%)	26 (4%)	1 (0%)	43 53
1	C	608/636 (96%)	579 (95%)	28 (5%)	1 (0%)	43 53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	484/636 (76%)	455 (94%)	28 (6%)	1 (0%)	43	53
All	All	2325/2544 (91%)	2212 (95%)	109 (5%)	4 (0%)	43	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	520	ASP
1	B	520	ASP
1	C	520	ASP
1	D	520	ASP

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	517/533 (97%)	502 (97%)	15 (3%)	37	49
1	B	519/533 (97%)	509 (98%)	10 (2%)	50	63
1	C	507/533 (95%)	487 (96%)	20 (4%)	28	40
1	D	402/533 (75%)	392 (98%)	10 (2%)	42	54
All	All	1945/2132 (91%)	1890 (97%)	55 (3%)	38	51

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	LEU
1	A	105	GLN
1	A	207	GLN
1	A	225	LEU
1	A	278	GLU
1	A	298	ARG
1	A	338	GLN
1	A	353	ASP
1	A	386	ARG
1	A	456	SER

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Mol	Chain	Res	Type
1	A	502	GLU
1	A	635	ARG
1	A	645	GLU
1	A	650	ILE
1	A	686	LYS
1	B	89	ARG
1	B	105	GLN
1	B	151	ARG
1	B	225	LEU
1	B	264	ASP
1	B	278	GLU
1	B	353	ASP
1	B	386	ARG
1	B	488	ARG
1	B	502	GLU
1	C	92	LEU
1	C	112	ARG
1	C	121	ASP
1	C	200	LEU
1	C	207	GLN
1	C	225	LEU
1	C	264	ASP
1	C	278	GLU
1	C	335	ARG
1	C	338	GLN
1	C	353	ASP
1	C	381	ARG
1	C	386	ARG
1	C	456	SER
1	C	472	ARG
1	C	473	ASP
1	C	502	GLU
1	C	627	THR
1	C	635	ARG
1	C	685	TYR
1	D	296	MET
1	D	338	GLN
1	D	341	ARG
1	D	353	ASP
1	D	386	ARG
1	D	473	ASP
1	D	502	GLU

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Mol	Chain	Res	Type
1	D	511	ASN
1	D	618	LEU
1	D	686	LYS

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

Mol	Chain	Res	Type
1	A	105	GLN
1	A	195	HIS
1	A	207	GLN
1	A	344	HIS
1	B	344	HIS
1	B	447	HIS
1	C	207	GLN
1	C	338	GLN
1	C	344	HIS
1	D	344	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 ⓘ

15 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	1,2	14,14,15	0.53	0	17,19,21	1.38	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	2	2	14,14,15	0.47	0	17,19,21	1.95	5 (29%)
3	NAG	F	1	1,3	14,14,15	0.42	0	17,19,21	1.26	2 (11%)
3	NAG	F	2	3	14,14,15	0.54	0	17,19,21	1.34	2 (11%)
3	FUC	F	3	3	10,10,11	0.87	1 (10%)	14,14,16	1.49	4 (28%)
2	NAG	G	1	1,2	14,14,15	0.52	0	17,19,21	0.99	0
2	NAG	G	2	2	14,14,15	0.80	0	17,19,21	1.16	2 (11%)
2	NAG	H	1	1,2	14,14,15	0.44	0	17,19,21	1.27	2 (11%)
2	NAG	H	2	2	14,14,15	0.67	0	17,19,21	1.12	1 (5%)
2	NAG	I	1	1,2	14,14,15	0.37	0	17,19,21	1.17	1 (5%)
2	NAG	I	2	2	14,14,15	0.42	0	17,19,21	1.08	0
2	NAG	J	1	1,2	14,14,15	0.50	0	17,19,21	0.85	0
2	NAG	J	2	2	14,14,15	0.25	0	17,19,21	0.97	1 (5%)
2	NAG	K	1	1,2	14,14,15	0.54	0	17,19,21	1.36	2 (11%)
2	NAG	K	2	2	14,14,15	0.41	0	17,19,21	0.97	1 (5%)

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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	FUC	F	3	3	-	-	0/1/1/1
2	NAG	G	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3	FUC	C2-C3	2.04	1.55	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C1-C2-N2	4.00	116.73	110.43
2	K	1	NAG	C1-C2-N2	-3.84	104.39	110.43
2	E	2	NAG	C4-C3-C2	-3.33	106.14	111.02
3	F	2	NAG	O5-C5-C6	3.17	113.84	107.66
3	F	1	NAG	C2-N2-C7	-3.04	118.83	122.90
2	E	1	NAG	C2-N2-C7	2.98	126.90	122.90
3	F	3	FUC	O2-C2-C3	2.81	115.97	110.15
2	E	2	NAG	O4-C4-C5	2.74	116.06	109.32
2	K	1	NAG	C4-C3-C2	2.65	114.90	111.02
3	F	1	NAG	O3-C3-C2	-2.61	103.98	109.40
2	E	2	NAG	C3-C4-C5	-2.59	105.53	110.23
2	G	2	NAG	C1-O5-C5	2.57	115.63	112.19
3	F	2	NAG	O5-C5-C4	-2.52	104.69	110.83
2	I	1	NAG	O5-C5-C6	2.42	112.37	107.66
2	G	2	NAG	C3-C4-C5	-2.41	105.87	110.23
2	E	2	NAG	C1-O5-C5	2.40	115.40	112.19
3	F	3	FUC	O3-C3-C2	2.38	114.91	110.05
2	H	1	NAG	O5-C1-C2	-2.34	107.67	111.29
2	H	2	NAG	C1-O5-C5	2.31	115.28	112.19
3	F	3	FUC	O3-C3-C4	-2.29	104.98	110.38
3	F	3	FUC	O5-C5-C6	2.21	112.19	107.40
2	E	1	NAG	O3-C3-C2	-2.19	104.86	109.40
2	K	2	NAG	C1-O5-C5	2.17	115.10	112.19
2	J	2	NAG	C1-O5-C5	2.10	115.00	112.19
2	H	1	NAG	O7-C7-N2	-2.04	118.38	121.98

There are no chirality outliers.

All (7) torsion outliers are listed below:

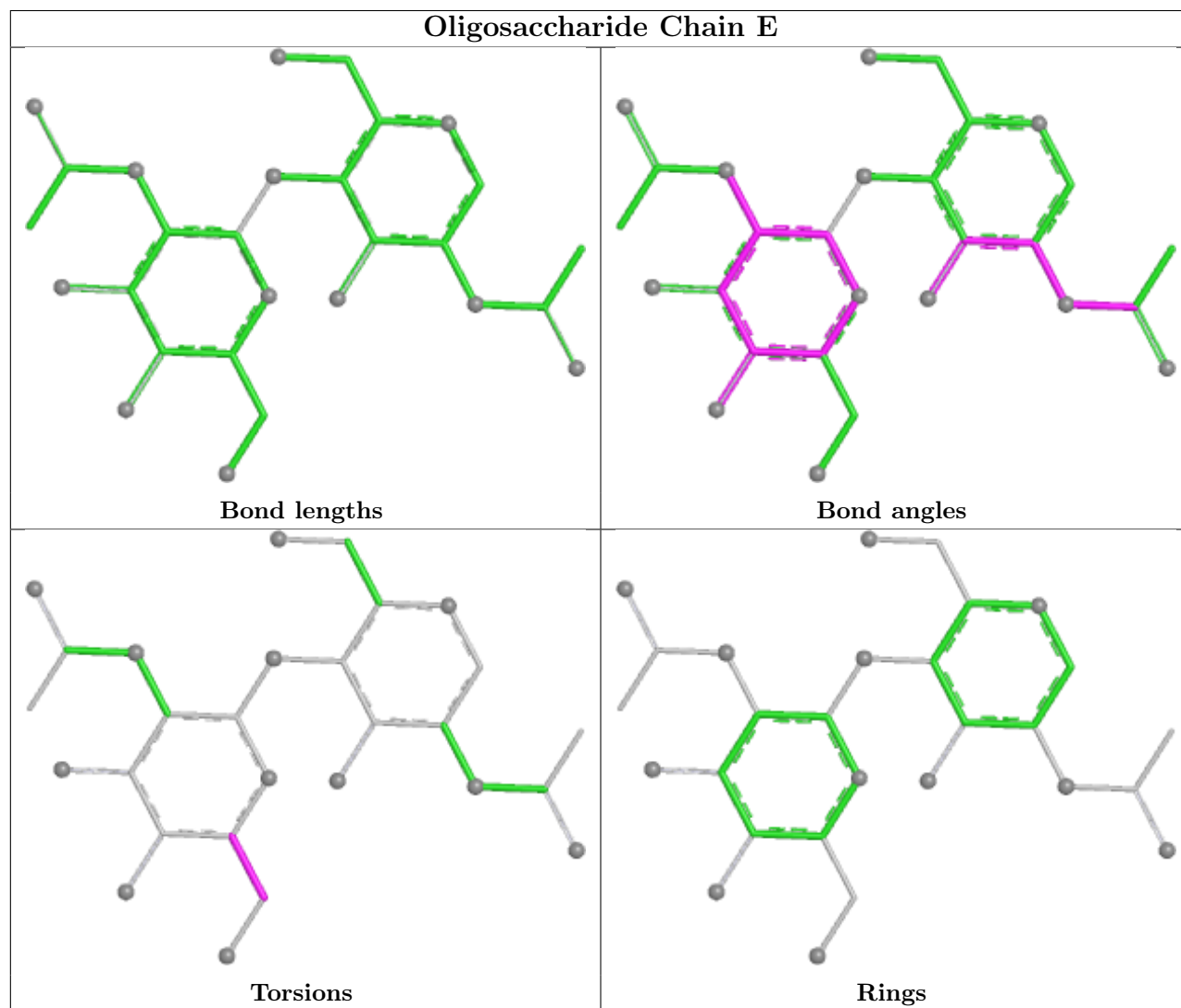
Mol	Chain	Res	Type	Atoms
2	J	2	NAG	O5-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	G	1	NAG	C1-C2-N2-C7
2	K	2	NAG	C4-C5-C6-O6

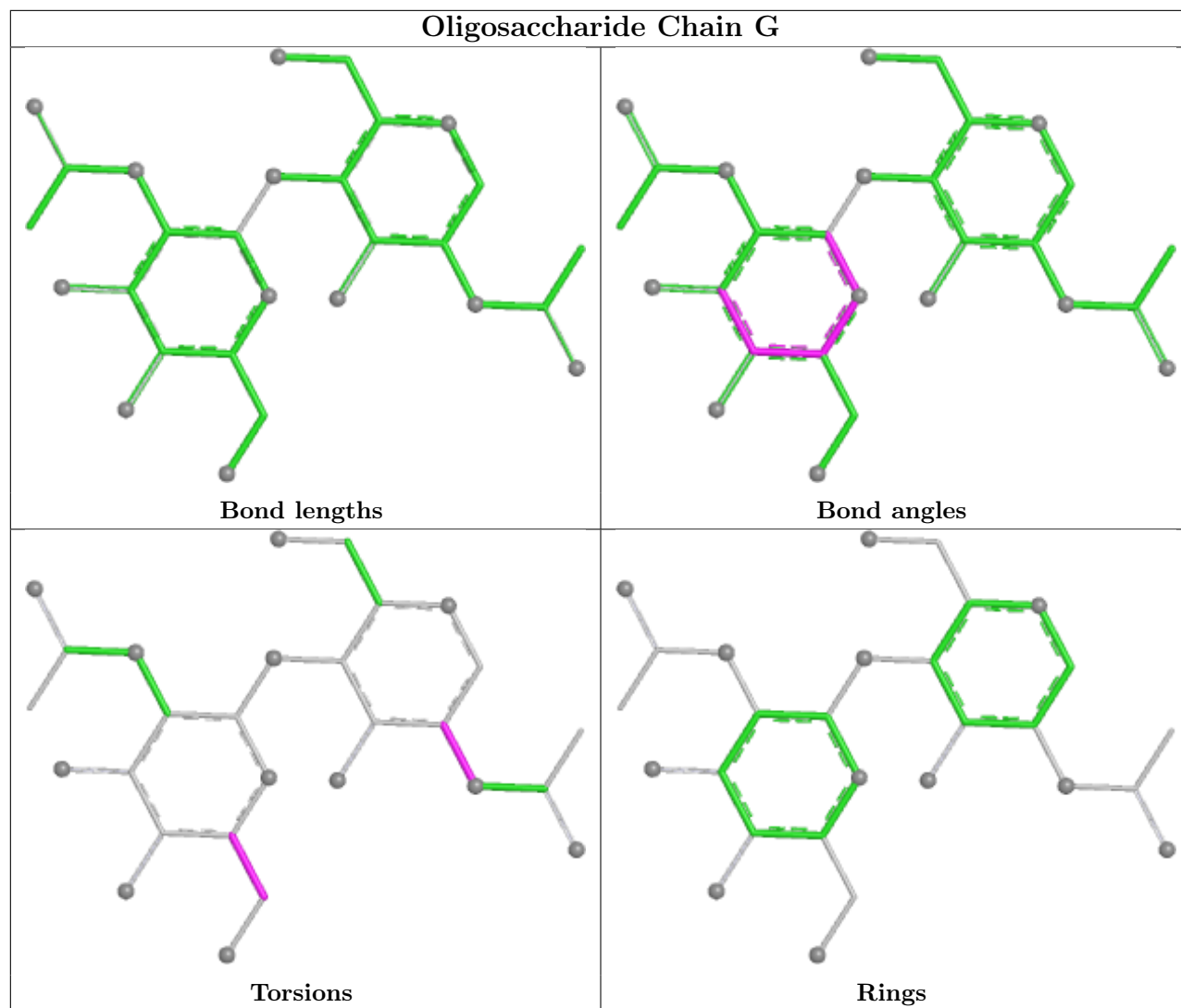
There are no ring outliers.

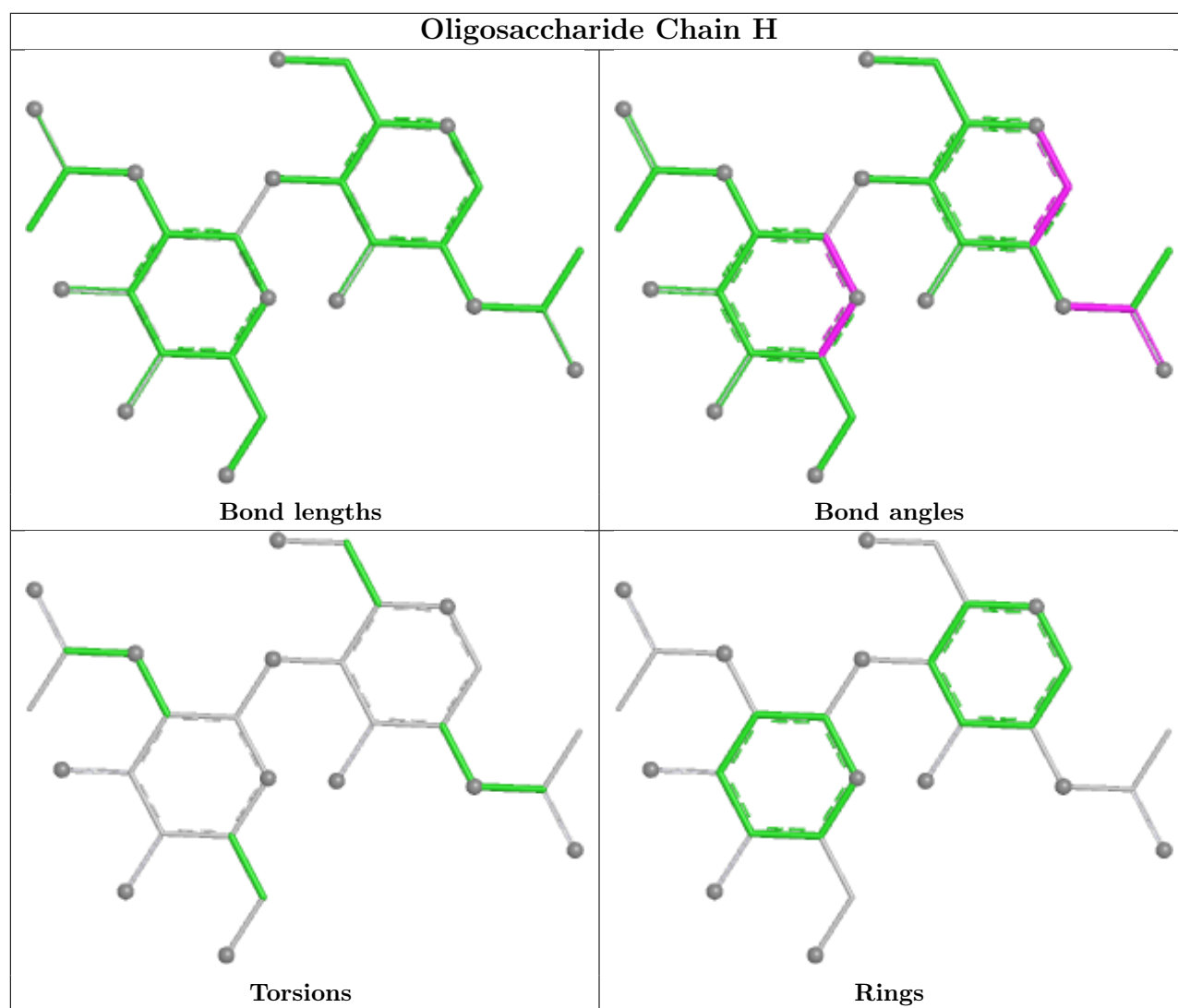
1 monomer is involved in 1 short contact:

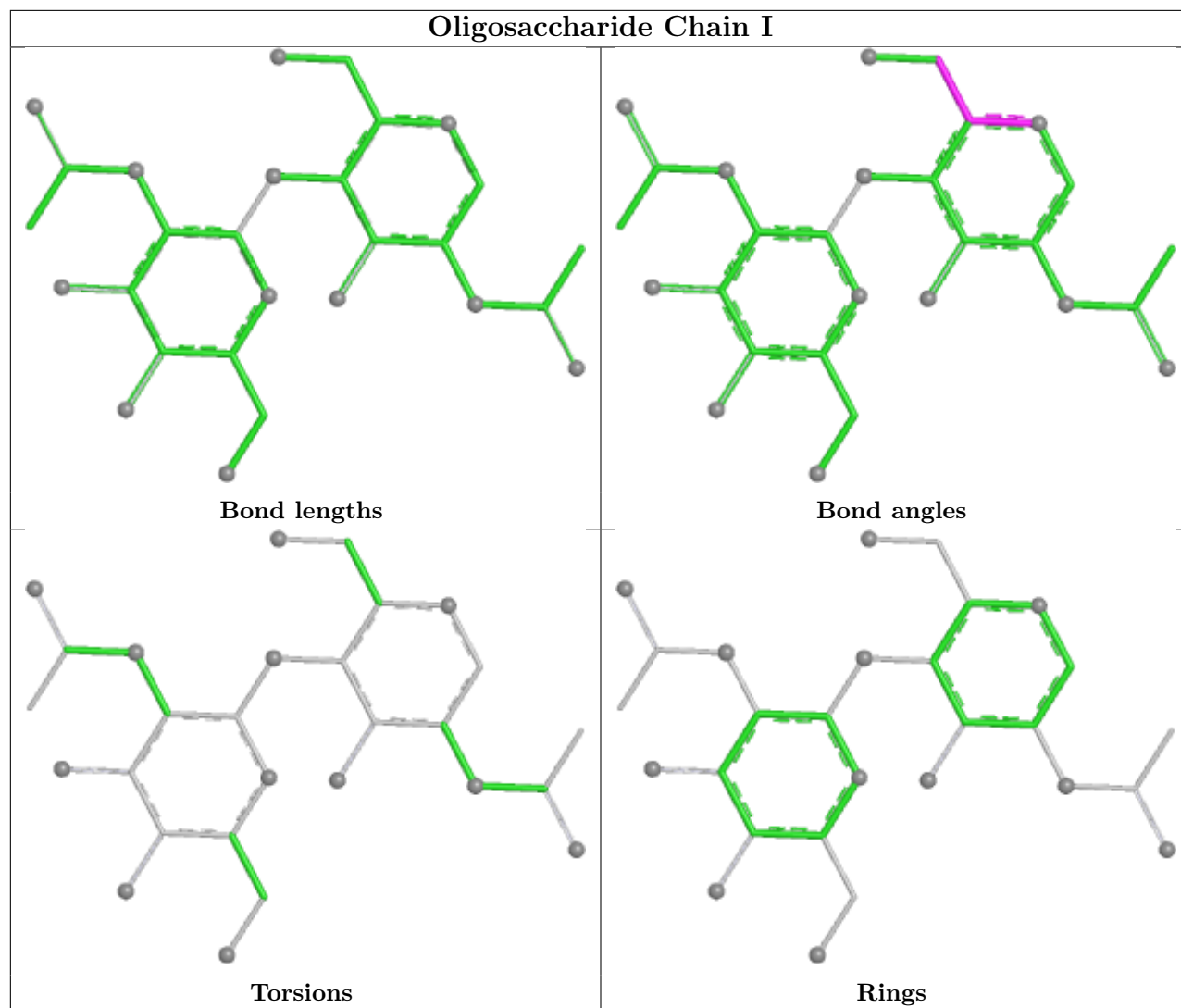
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	3	FUC	1	0

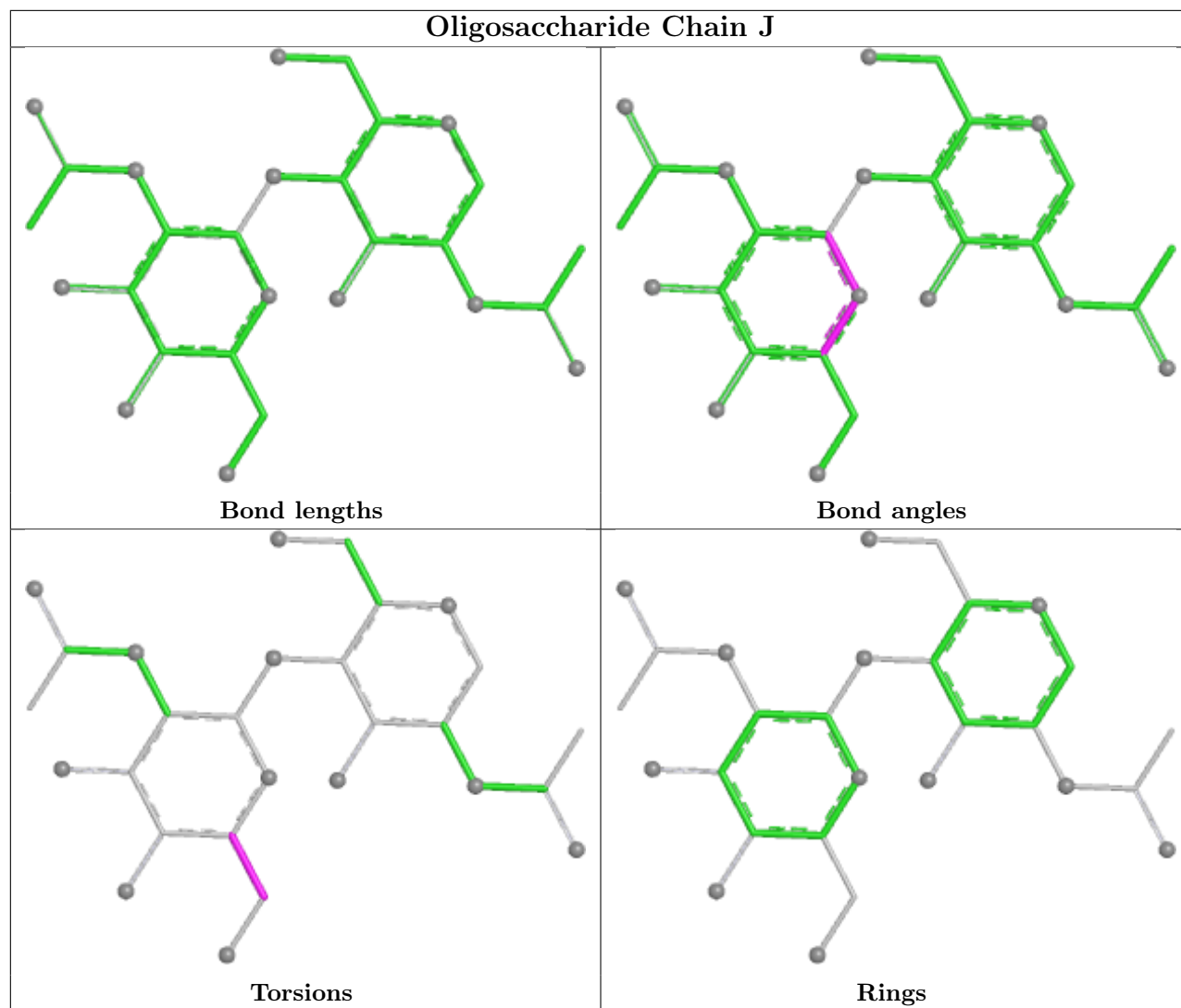
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

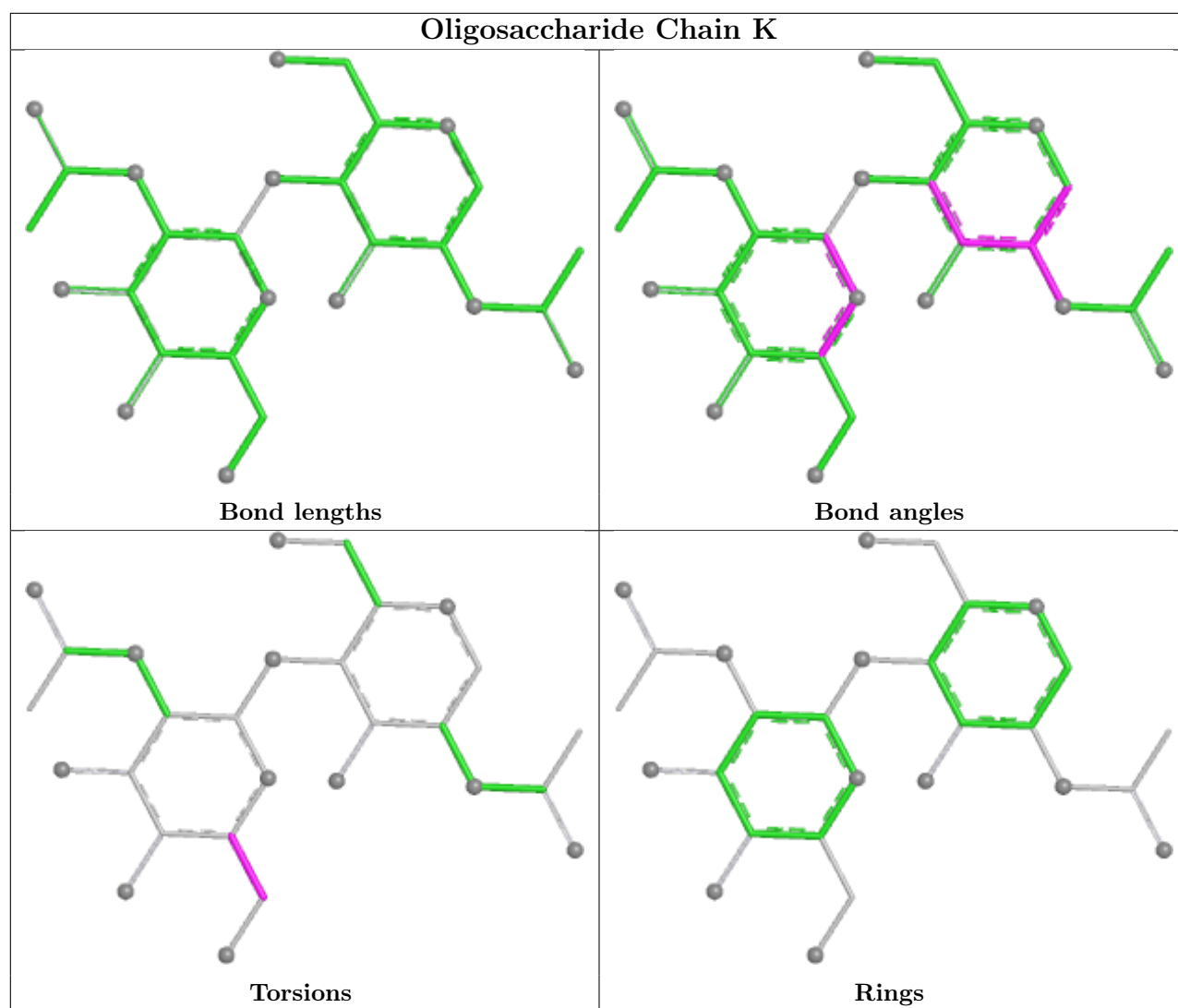


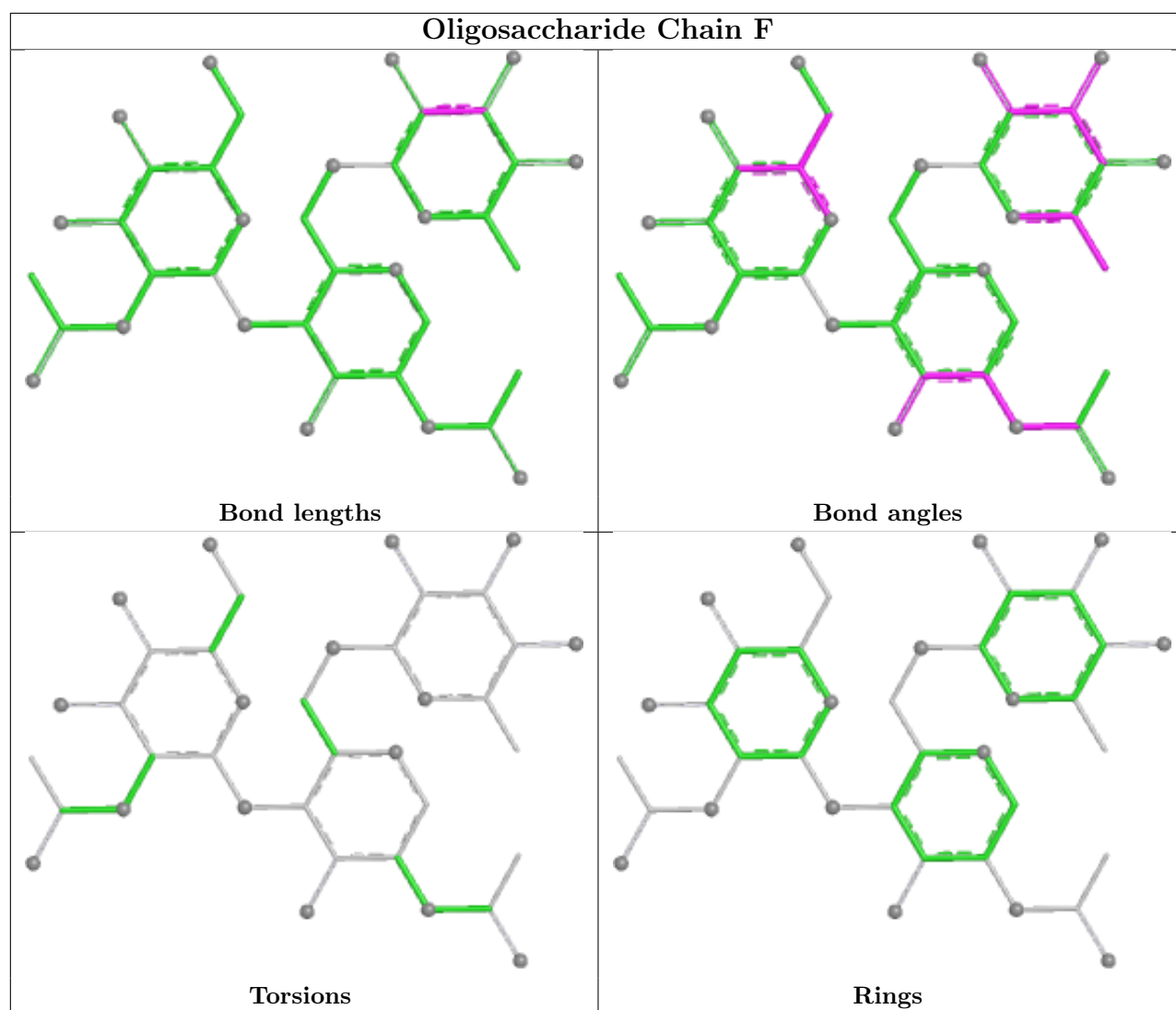












5.6 Ligand geometry [i](#)

16 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	$\# Z > 2$
4	NAG	D	1001	1	14,14,15	0.60	0	17,19,21	1.47	3 (17%)
6	MLI	B	804	-	6,6,6	1.28	0	7,7,7	1.58	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DGJ	B	803	-	11,11,11	1.51	3 (27%)	13,15,15	0.93	0
5	DGJ	A	803	-	11,11,11	1.46	3 (27%)	13,15,15	1.86	3 (23%)
4	NAG	A	805	1	14,14,15	0.56	0	17,19,21	1.00	0
6	MLI	A	804	-	6,6,6	1.83	2 (33%)	7,7,7	1.39	0
4	NAG	A	801	1	14,14,15	0.55	0	17,19,21	2.08	4 (23%)
4	NAG	B	801	1	14,14,15	0.59	0	17,19,21	1.21	3 (17%)
4	NAG	D	1002	1	14,14,15	0.61	0	17,19,21	1.65	2 (11%)
5	DGJ	C	804	-	11,11,11	1.92	3 (27%)	13,15,15	1.69	4 (30%)
5	DGJ	D	1000	-	11,11,11	1.52	1 (9%)	13,15,15	0.91	0
4	NAG	C	801	1	14,14,15	0.74	0	17,19,21	1.39	1 (5%)
4	NAG	C	802	1	14,14,15	0.33	0	17,19,21	1.36	3 (17%)
4	NAG	C	803	1	14,14,15	0.93	0	17,19,21	2.16	2 (11%)
4	NAG	B	802	1	14,14,15	0.48	0	17,19,21	1.08	1 (5%)
4	NAG	A	802	1	14,14,15	0.58	0	17,19,21	1.68	2 (11%)

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	NAG	D	1001	1	-	0/6/23/26	0/1/1/1
6	MLI	B	804	-	-	0/4/4/4	-
5	DGJ	B	803	-	-	0/2/19/19	0/1/1/1
5	DGJ	A	803	-	-	0/2/19/19	0/1/1/1
4	NAG	A	805	1	-	0/6/23/26	0/1/1/1
6	MLI	A	804	-	-	0/4/4/4	-
4	NAG	A	801	1	-	0/6/23/26	0/1/1/1
4	NAG	B	801	1	-	1/6/23/26	0/1/1/1
4	NAG	D	1002	1	-	1/6/23/26	0/1/1/1
5	DGJ	C	804	-	-	0/2/19/19	0/1/1/1
5	DGJ	D	1000	-	-	0/2/19/19	0/1/1/1
4	NAG	C	801	1	-	2/6/23/26	0/1/1/1
4	NAG	C	802	1	-	0/6/23/26	0/1/1/1
4	NAG	C	803	1	-	0/6/23/26	0/1/1/1
4	NAG	B	802	1	-	0/6/23/26	0/1/1/1
4	NAG	A	802	1	-	1/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1000	DGJ	C1-C2	4.11	1.56	1.52
5	C	804	DGJ	C1-C2	4.08	1.56	1.52
5	C	804	DGJ	C5-N5	3.10	1.52	1.47
5	B	803	DGJ	C1-N5	2.99	1.51	1.47
5	A	803	DGJ	C1-N5	2.83	1.51	1.47
5	B	803	DGJ	C5-N5	2.73	1.51	1.47
6	A	804	MLI	C1-C2	2.59	1.55	1.51
5	C	804	DGJ	C1-N5	2.57	1.50	1.47
5	B	803	DGJ	C1-C2	2.46	1.54	1.52
5	A	803	DGJ	C1-C2	2.43	1.54	1.52
6	A	804	MLI	C1-C3	2.31	1.54	1.51
5	A	803	DGJ	C5-N5	2.06	1.50	1.47

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	803	NAG	C1-O5-C5	7.39	122.09	112.19
4	A	801	NAG	C3-C4-C5	-5.10	100.98	110.23
4	D	1002	NAG	C1-O5-C5	4.92	118.78	112.19
4	A	802	NAG	C1-O5-C5	4.52	118.24	112.19
4	C	801	NAG	C1-O5-C5	4.41	118.09	112.19
5	A	803	DGJ	C1-N5-C5	3.65	117.74	109.71
4	A	801	NAG	O4-C4-C5	3.57	118.11	109.32
5	A	803	DGJ	O2-C2-C3	3.50	117.40	110.15
4	D	1002	NAG	C1-C2-N2	-3.32	105.19	110.43
4	A	801	NAG	O3-C3-C2	3.26	116.18	109.40
4	C	803	NAG	C8-C7-N2	-3.23	110.76	116.12
5	C	804	DGJ	C1-N5-C5	3.15	116.64	109.71
4	D	1001	NAG	O3-C3-C2	-2.93	103.32	109.40
4	B	802	NAG	C1-O5-C5	2.78	115.91	112.19
4	C	802	NAG	C1-O5-C5	2.65	115.74	112.19
5	C	804	DGJ	C4-C5-N5	2.54	114.24	109.12
4	B	801	NAG	O4-C4-C5	2.45	115.35	109.32
4	C	802	NAG	O5-C1-C2	-2.42	107.55	111.29
4	B	801	NAG	C3-C4-C5	-2.42	105.85	110.23
4	D	1001	NAG	C4-C3-C2	2.41	114.55	111.02
5	C	804	DGJ	C3-C4-C5	2.39	114.52	111.02
6	B	804	MLI	O9-C3-C1	2.32	121.70	114.51
5	A	803	DGJ	O3-C3-C2	2.25	114.64	110.05
4	A	802	NAG	C4-C3-C2	-2.24	107.73	111.02
4	B	801	NAG	C1-O5-C5	2.21	115.15	112.19
4	C	802	NAG	C2-N2-C7	-2.15	120.02	122.90
5	C	804	DGJ	O4-C4-C3	-2.14	105.34	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	NAG	O5-C5-C4	-2.03	105.89	110.83
4	D	1001	NAG	C6-C5-C4	2.02	117.98	113.02

There are no chirality outliers.

All (5) torsion outliers are listed below:

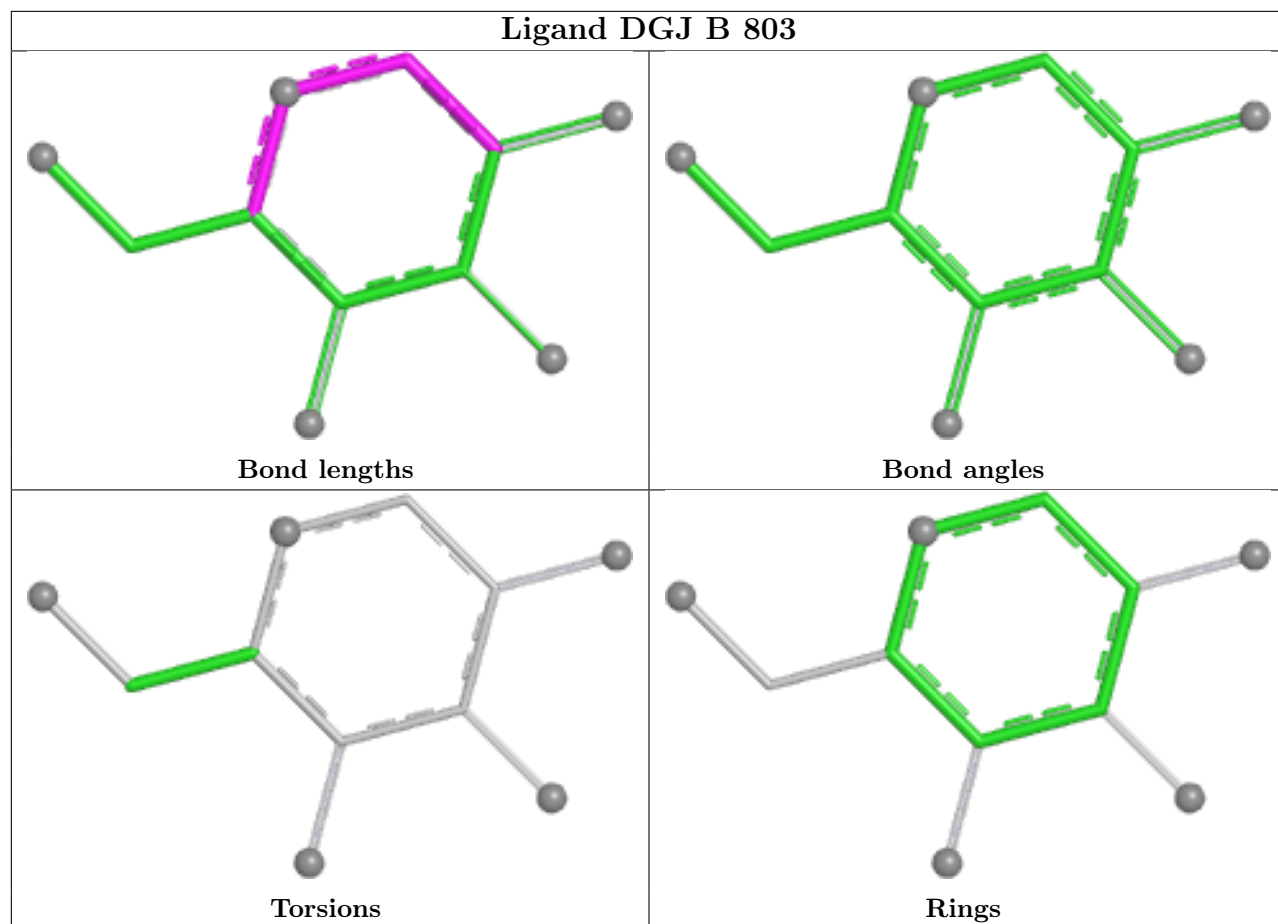
Mol	Chain	Res	Type	Atoms
4	C	801	NAG	O5-C5-C6-O6
4	C	801	NAG	C4-C5-C6-O6
4	D	1002	NAG	O5-C5-C6-O6
4	A	802	NAG	C8-C7-N2-C2
4	B	801	NAG	C4-C5-C6-O6

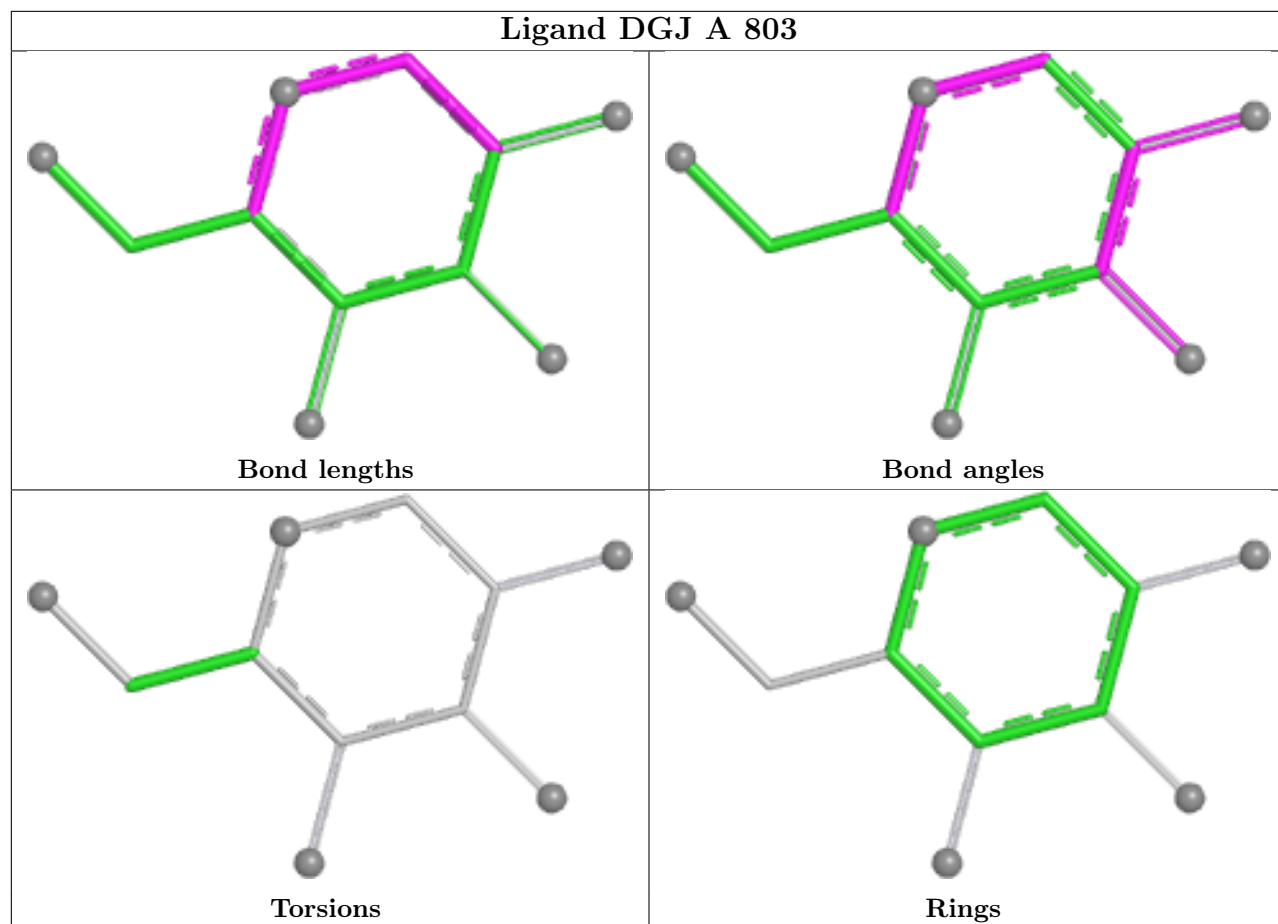
There are no ring outliers.

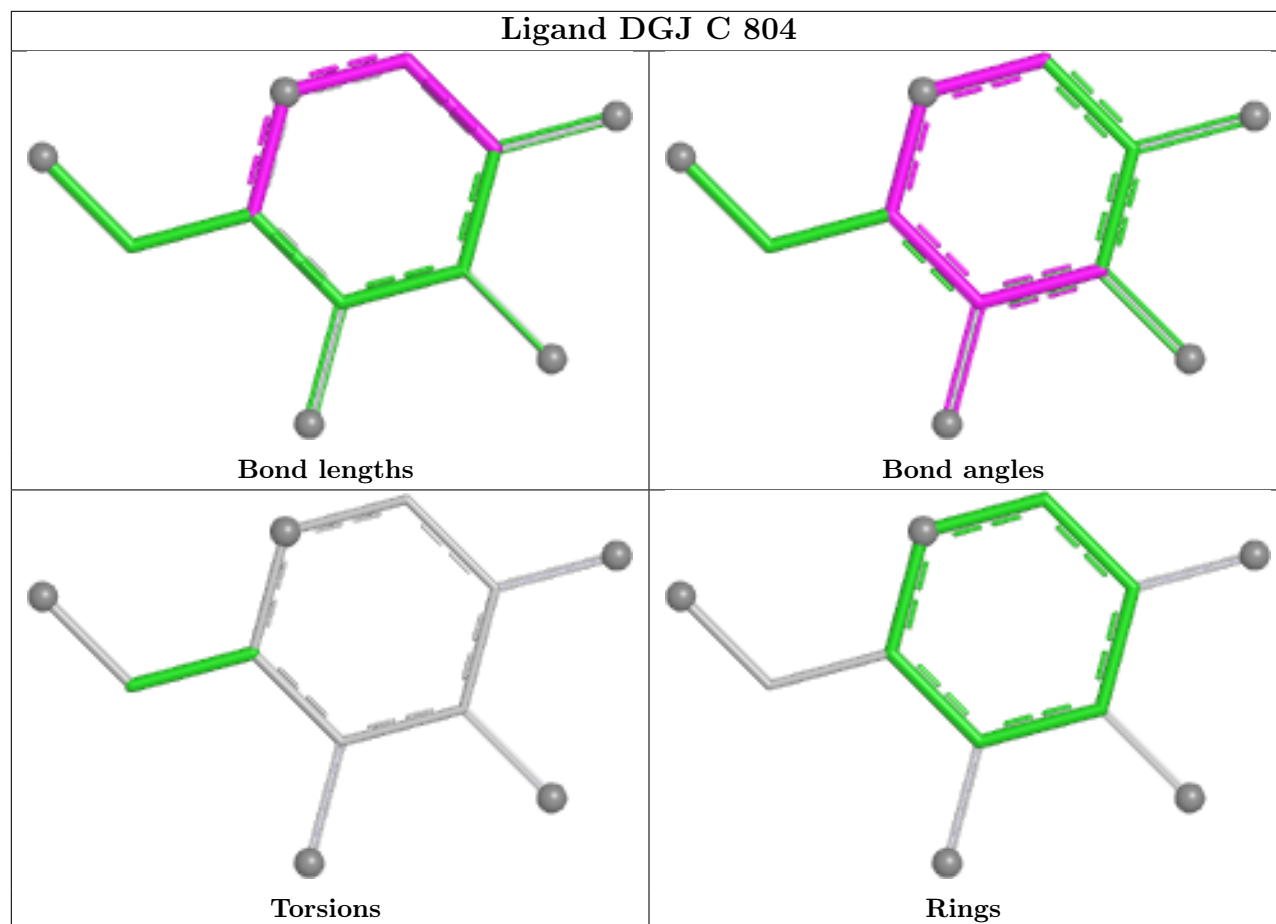
2 monomers are involved in 2 short contacts:

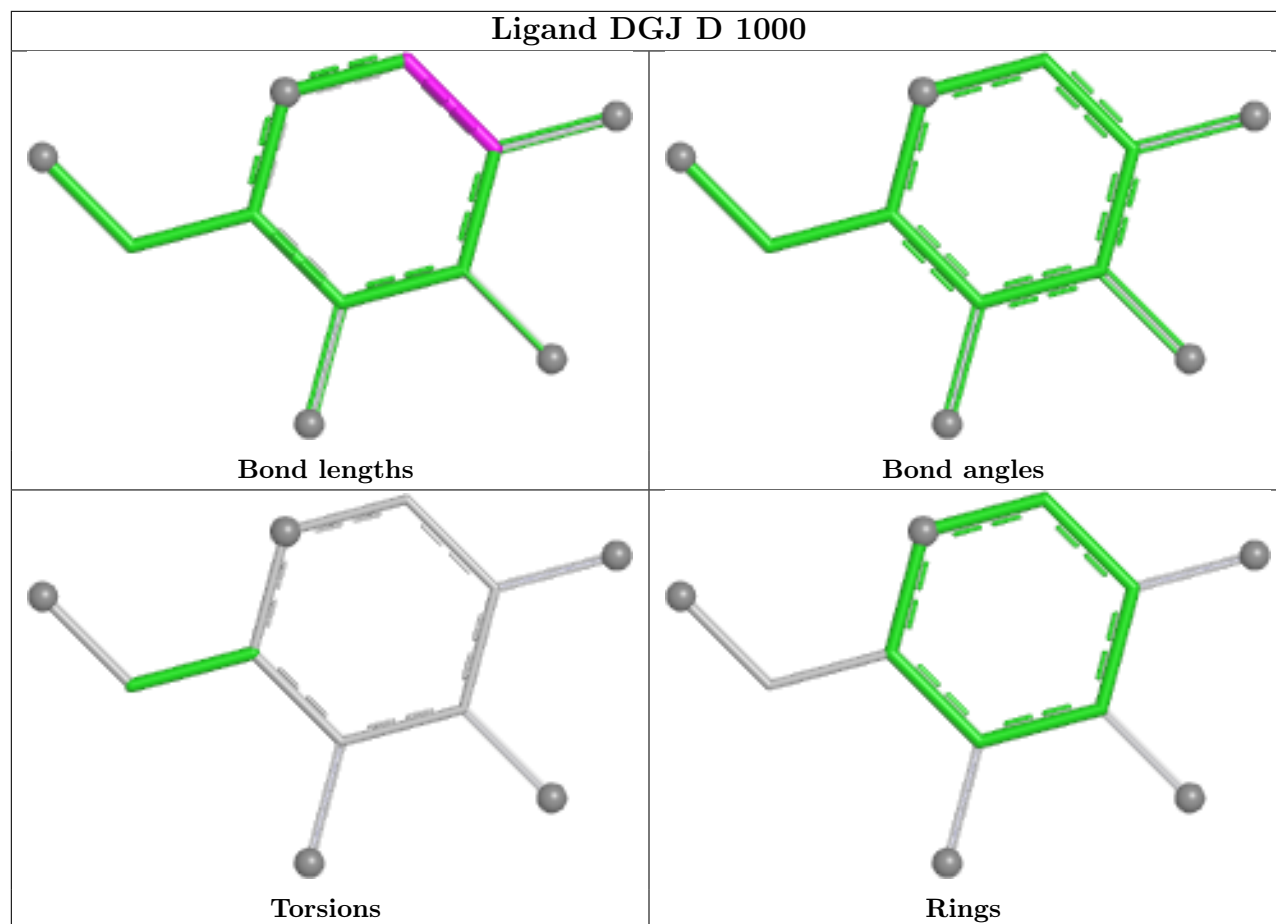
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	803	DGJ	1	0
4	A	801	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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	618/636 (97%)	0.08	12 (1%) 66 67	29, 45, 66, 95	0
1	B	623/636 (97%)	0.18	10 (1%) 70 72	32, 50, 72, 100	0
1	C	614/636 (96%)	0.73	30 (4%) 35 32	50, 70, 94, 110	0
1	D	496/636 (77%)	1.09	75 (15%) 5 4	52, 75, 101, 116	0
All	All	2351/2544 (92%)	0.49	127 (5%) 31 28	29, 60, 92, 116	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	242	SER	6.2
1	D	713	ALA	5.5
1	B	166	ALA	4.9
1	C	92	LEU	4.7
1	C	169	GLY	4.6
1	D	456	SER	4.6
1	D	342	LEU	4.4
1	D	205	GLU	4.4
1	D	270	PRO	4.1
1	D	627	THR	4.1
1	D	237	ILE	4.0
1	B	274	ALA	3.9
1	D	254	ARG	3.8
1	D	295	TYR	3.8
1	C	170	ARG	3.5
1	A	271	ALA	3.5
1	D	227	ARG	3.5
1	C	146	PHE	3.5
1	D	185	TRP	3.4
1	A	630	GLY	3.4
1	D	234	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	167	ALA	3.3
1	C	276	ALA	3.3
1	B	219	ALA	3.3
1	D	640	ILE	3.3
1	B	88	LEU	3.2
1	A	627	THR	3.0
1	D	233	ARG	3.0
1	D	623	ALA	3.0
1	D	249	TRP	2.9
1	D	385	PHE	2.9
1	D	467	VAL	2.9
1	C	626	VAL	2.9
1	D	228	TYR	2.9
1	D	384	GLY	2.9
1	C	122	LEU	2.9
1	C	371	PRO	2.8
1	D	219	ALA	2.8
1	D	543	MET	2.8
1	C	712	TRP	2.8
1	D	491	THR	2.8
1	D	197	PRO	2.8
1	A	276	ALA	2.8
1	D	327	ALA	2.8
1	A	170	ARG	2.8
1	C	132	LEU	2.7
1	D	245	PHE	2.7
1	A	219	ALA	2.7
1	D	292	ILE	2.7
1	D	246	HIS	2.7
1	C	701	PRO	2.7
1	D	239	VAL	2.6
1	D	240	ASN	2.6
1	B	713	ALA	2.6
1	D	186	TYR	2.6
1	D	479	PRO	2.6
1	D	643	GLY	2.6
1	D	680	GLY	2.6
1	D	493	MET	2.6
1	D	365	PHE	2.6
1	A	166	ALA	2.5
1	D	262	TYR	2.5
1	C	543	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	703	ASP	2.5
1	C	140	GLY	2.5
1	C	713	ALA	2.5
1	D	602	ALA	2.4
1	C	151	ARG	2.4
1	D	621	GLU	2.4
1	D	363	PHE	2.4
1	D	497	PHE	2.4
1	C	142	PRO	2.4
1	D	637	LEU	2.4
1	D	345	PHE	2.4
1	D	387	VAL	2.4
1	D	291	SER	2.3
1	A	565	GLY	2.3
1	C	669	GLY	2.3
1	D	650	ILE	2.3
1	D	472	ARG	2.3
1	A	567	ASP	2.3
1	C	364	ASP	2.3
1	D	206	PRO	2.3
1	D	679	ALA	2.3
1	B	370	PHE	2.3
1	B	90	ALA	2.2
1	D	609	ALA	2.2
1	C	361	GLY	2.2
1	C	157	MET	2.2
1	D	229	TRP	2.2
1	D	299	ARG	2.2
1	D	373	ALA	2.2
1	D	659	THR	2.2
1	C	106	LYS	2.2
1	C	287	SER	2.2
1	B	167	ALA	2.2
1	D	383	ALA	2.2
1	D	564	ALA	2.2
1	D	204	GLN	2.2
1	D	247	LEU	2.2
1	C	544	LEU	2.2
1	D	455	TYR	2.2
1	D	198	ILE	2.2
1	D	231	SER	2.2
1	D	232	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	156	VAL	2.1
1	D	313	PHE	2.1
1	A	473	ASP	2.1
1	C	686	LYS	2.1
1	D	368	VAL	2.1
1	C	566	GLY	2.1
1	D	331	ASP	2.1
1	C	138	ALA	2.1
1	C	598	ALA	2.1
1	D	380	LEU	2.1
1	D	511	ASN	2.1
1	B	367	GLU	2.1
1	D	631	ASP	2.1
1	D	685	TYR	2.1
1	C	702	VAL	2.0
1	D	221	PHE	2.0
1	D	230	LEU	2.0
1	B	140	GLY	2.0
1	D	340	ILE	2.0
1	A	628	ASP	2.0
1	D	364	ASP	2.0
1	D	649	ARG	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.

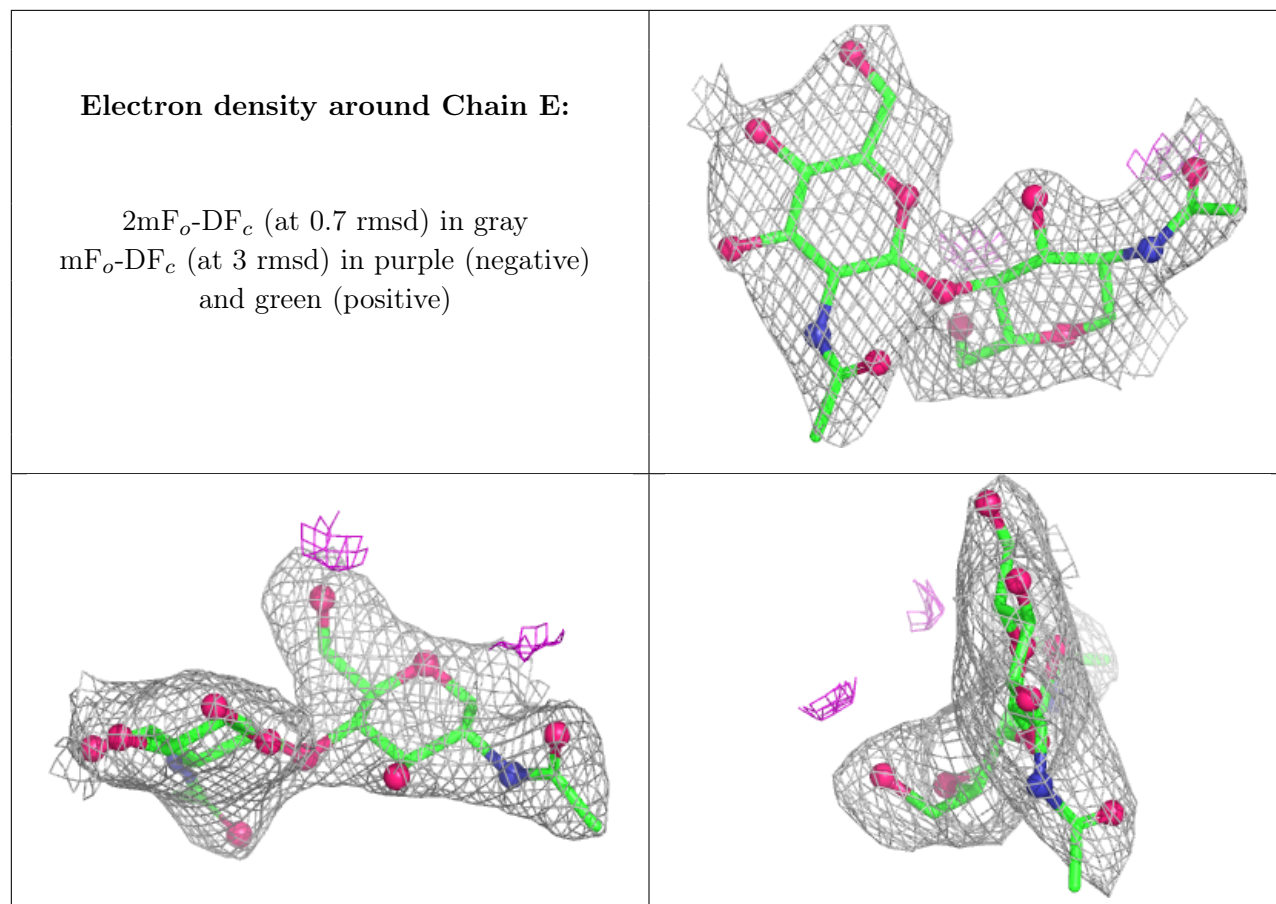
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	F	2	14/15	0.64	0.19	66,73,78,79	0
2	NAG	I	2	14/15	0.74	0.15	79,85,88,88	0
2	NAG	K	2	14/15	0.82	0.10	68,72,77,78	0
2	NAG	E	2	14/15	0.83	0.13	76,80,84,86	0
2	NAG	J	2	14/15	0.83	0.13	67,75,81,81	0
2	NAG	K	1	14/15	0.84	0.10	62,68,72,72	0

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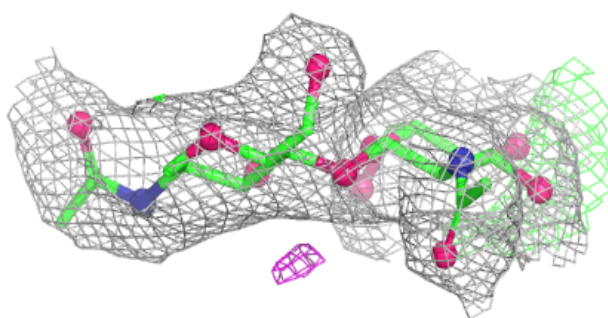
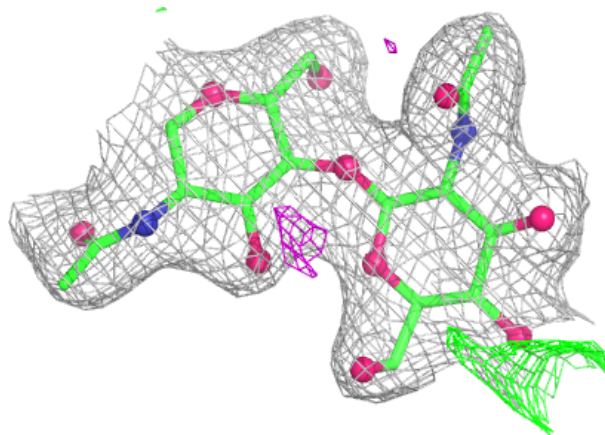
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	G	2	14/15	0.86	0.10	46,52,58,60	0
2	NAG	H	2	14/15	0.89	0.09	46,55,61,64	0
3	FUC	F	3	10/11	0.89	0.12	64,67,69,70	0
2	NAG	J	1	14/15	0.90	0.09	56,59,64,67	0
2	NAG	I	1	14/15	0.90	0.10	60,62,68,75	0
2	NAG	E	1	14/15	0.90	0.11	58,61,68,70	0
3	NAG	F	1	14/15	0.92	0.10	56,59,64,69	0
2	NAG	H	1	14/15	0.94	0.08	51,53,55,56	0
2	NAG	G	1	14/15	0.95	0.07	44,48,52,55	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.



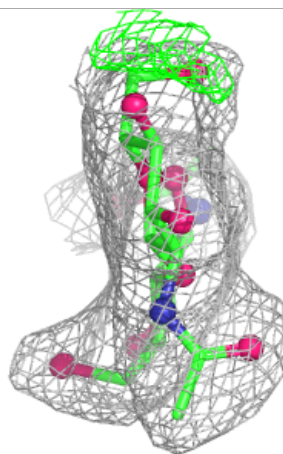
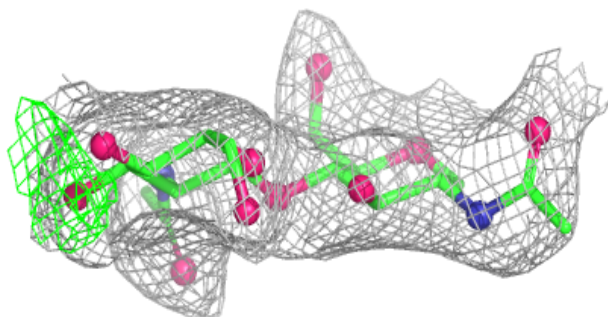
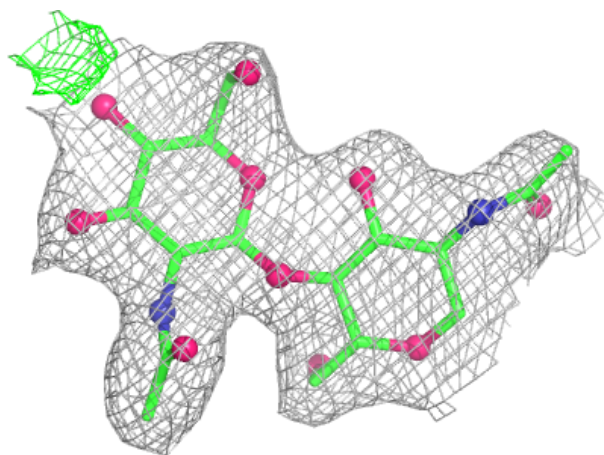
Electron density around Chain G:

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



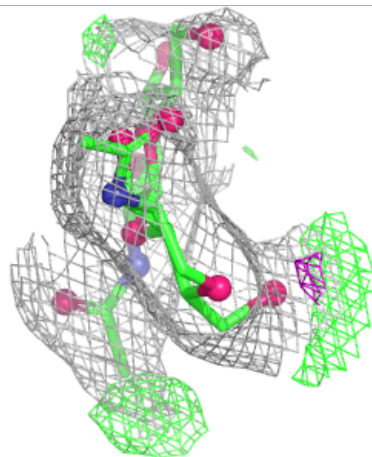
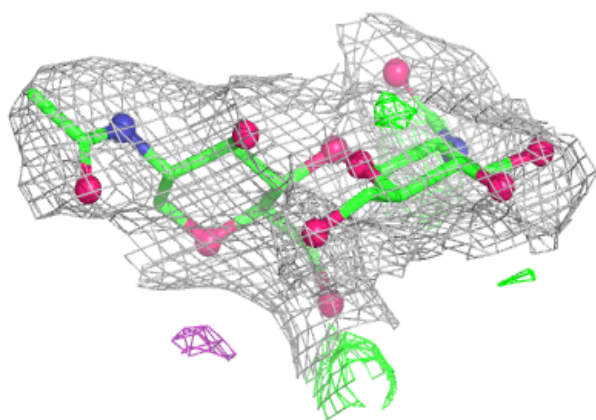
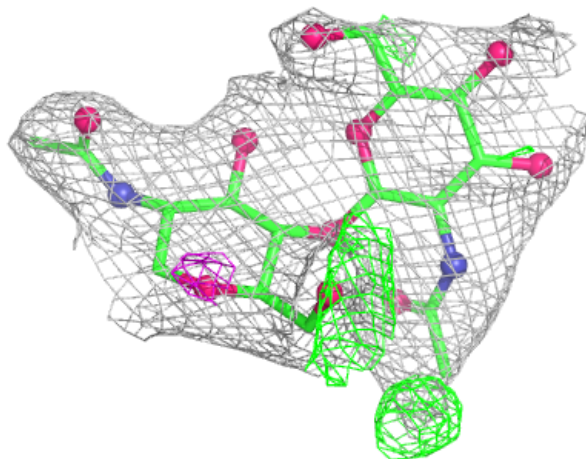
Electron density around Chain H:

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



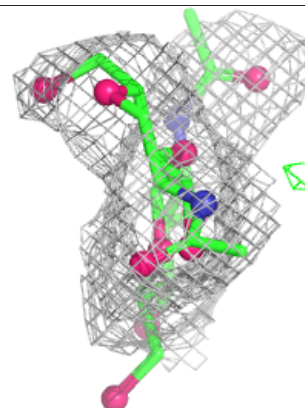
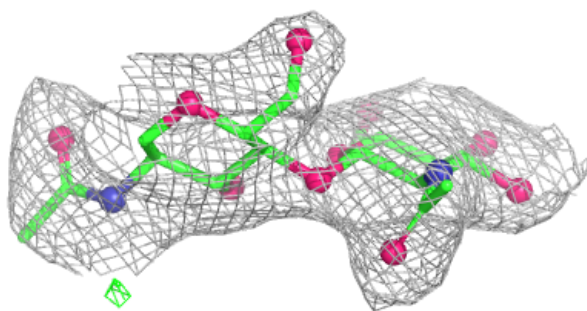
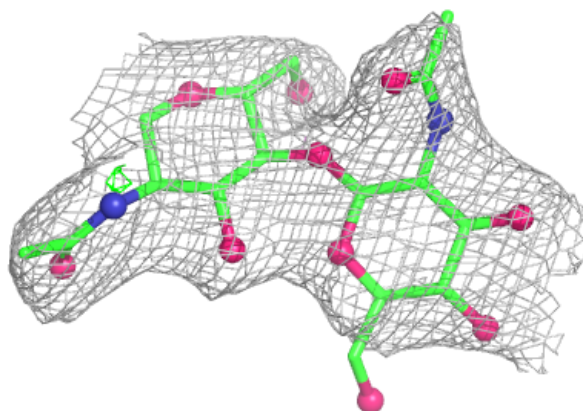
Electron density around Chain I:

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



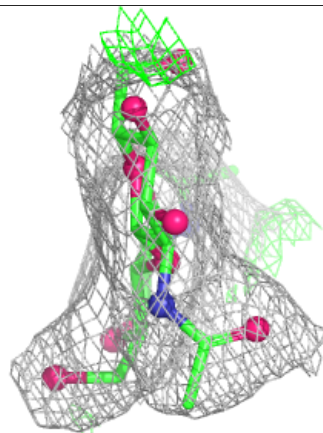
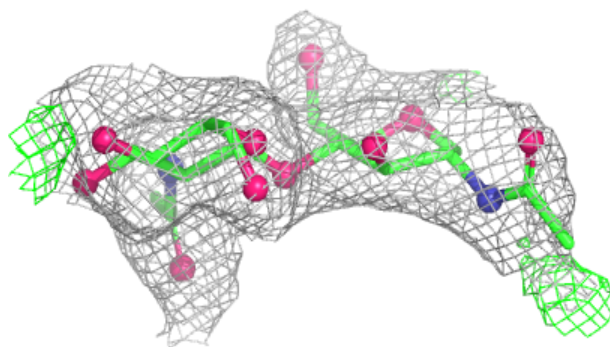
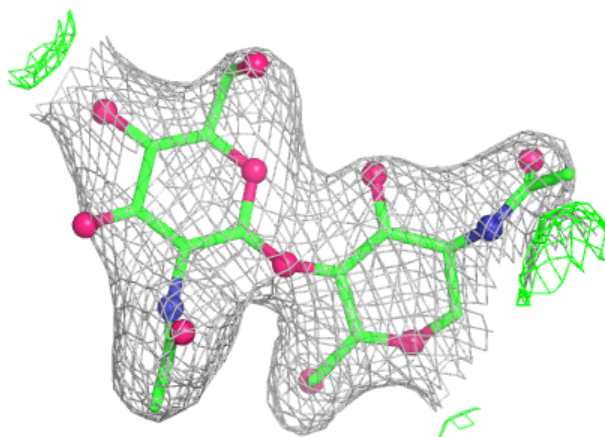
Electron density around Chain J:

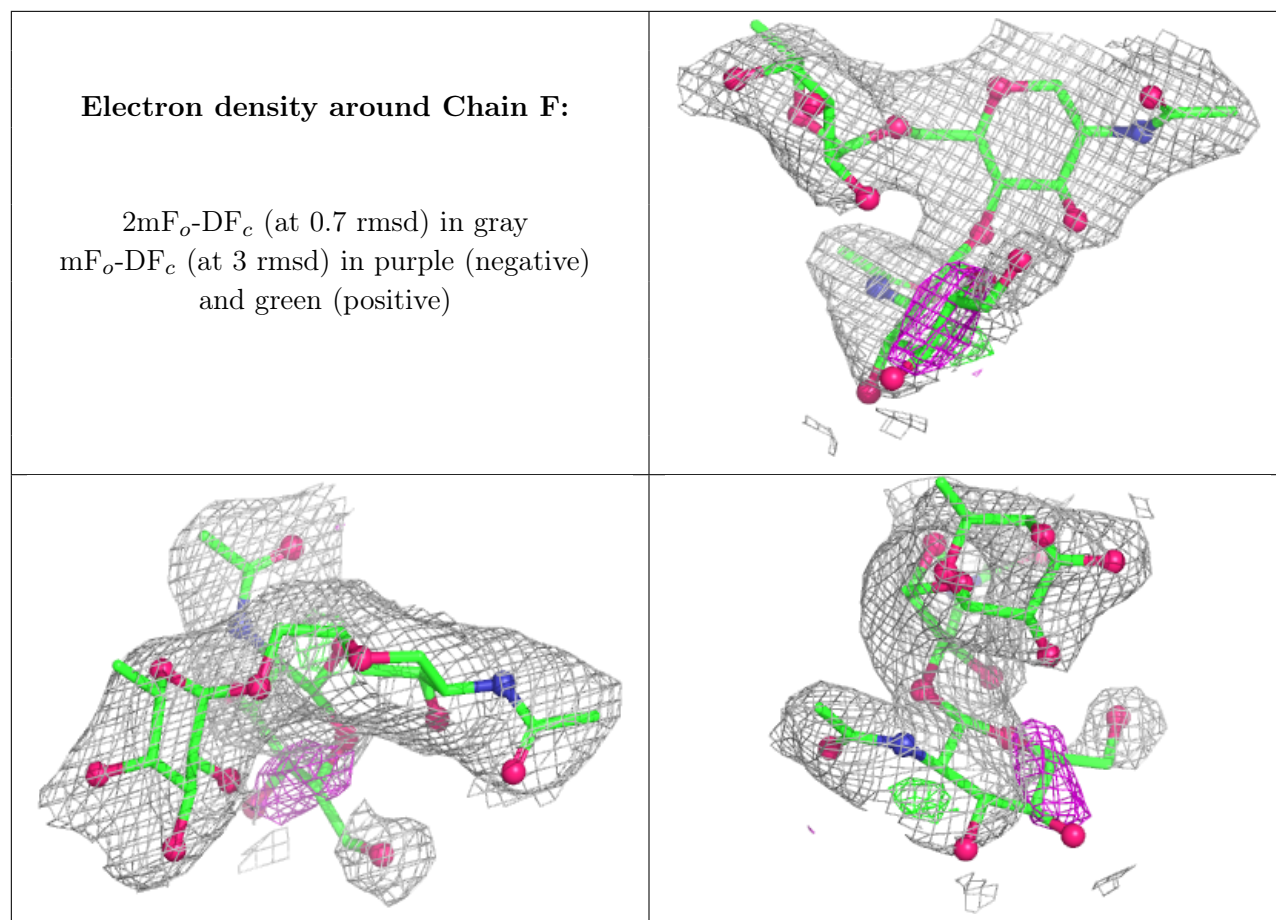
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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)





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	NAG	A	805	14/15	0.55	0.23	87,95,100,101	0
4	NAG	D	1001	14/15	0.69	0.17	86,91,94,95	0
4	NAG	B	802	14/15	0.73	0.17	96,101,103,103	0
4	NAG	A	802	14/15	0.73	0.15	73,76,81,81	0
4	NAG	D	1002	14/15	0.73	0.15	77,87,92,92	0
4	NAG	C	803	14/15	0.80	0.14	73,77,79,79	0
4	NAG	C	801	14/15	0.82	0.14	81,84,88,88	0
4	NAG	C	802	14/15	0.85	0.12	74,76,78,78	0
6	MLI	B	804	7/7	0.88	0.11	52,53,54,55	0
4	NAG	A	801	14/15	0.90	0.09	50,54,56,58	0
5	DGJ	C	804	11/11	0.91	0.09	48,49,51,52	0
4	NAG	B	801	14/15	0.91	0.09	52,54,58,58	0

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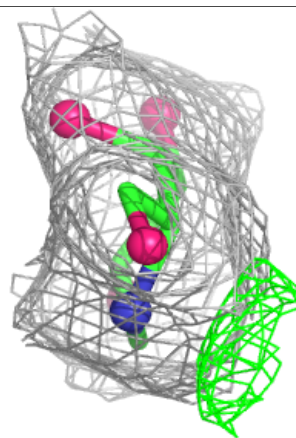
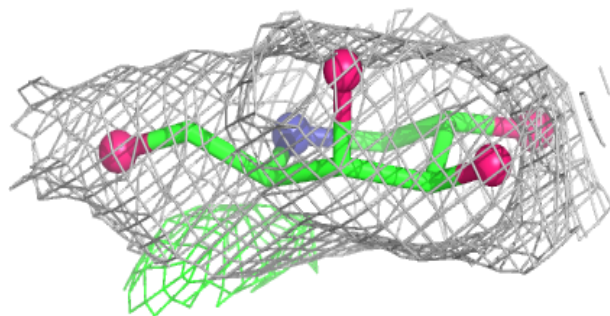
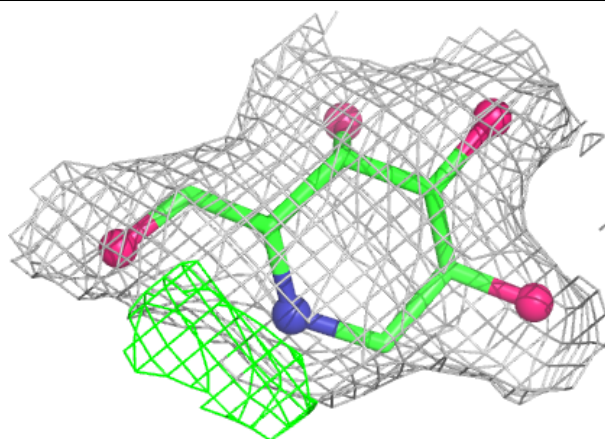
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MLI	A	804	7/7	0.92	0.13	51,53,55,56	0
5	DGJ	D	1000	11/11	0.92	0.09	50,52,53,54	0
5	DGJ	B	803	11/11	0.95	0.06	39,40,43,44	0
5	DGJ	A	803	11/11	0.96	0.07	35,36,39,41	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

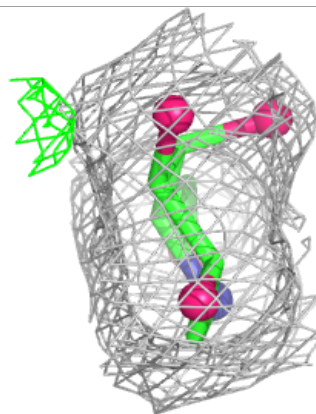
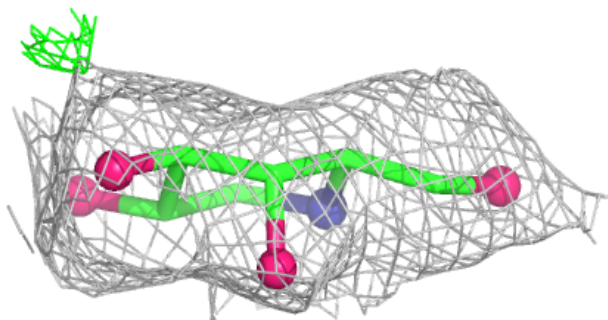
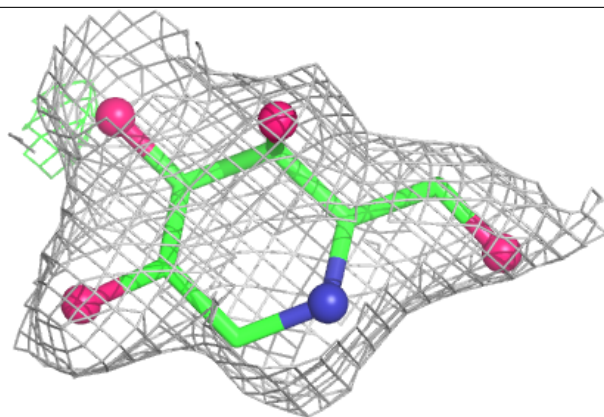
Electron density around DGJ C 804:

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



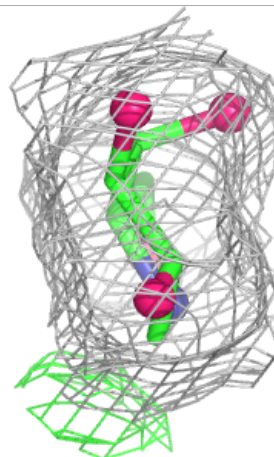
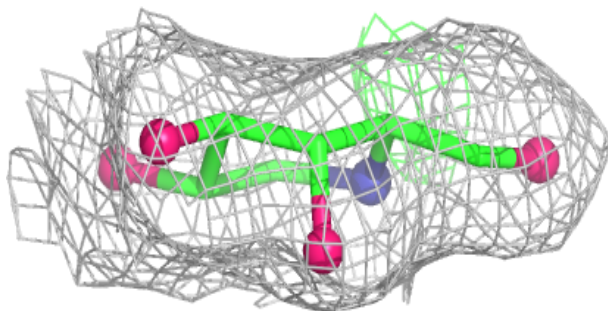
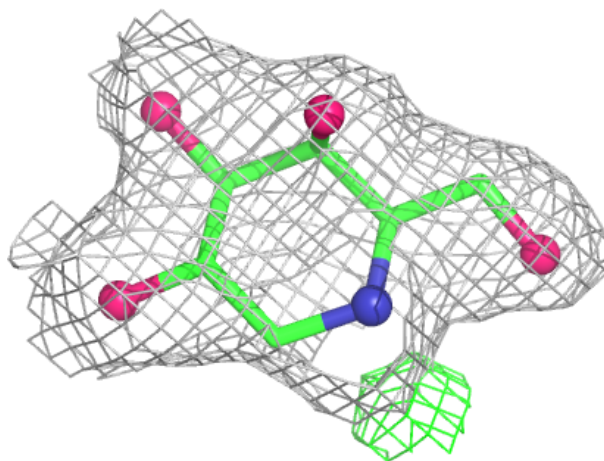
Electron density around DGJ D 1000:

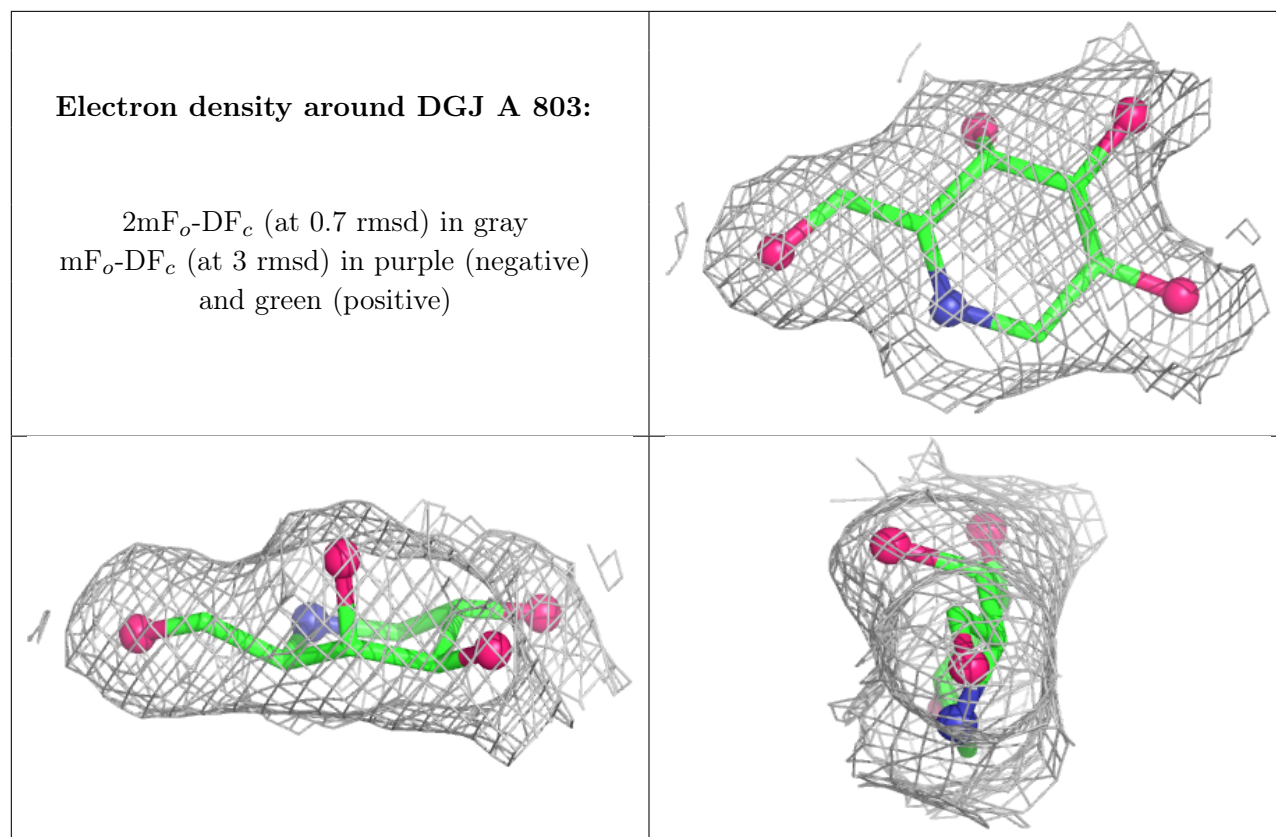
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around DGJ B 803:

$2mF_o-DF_c$ (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.