W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2022 – 10:15 pm BST

PDB ID	:	7QQG
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)

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

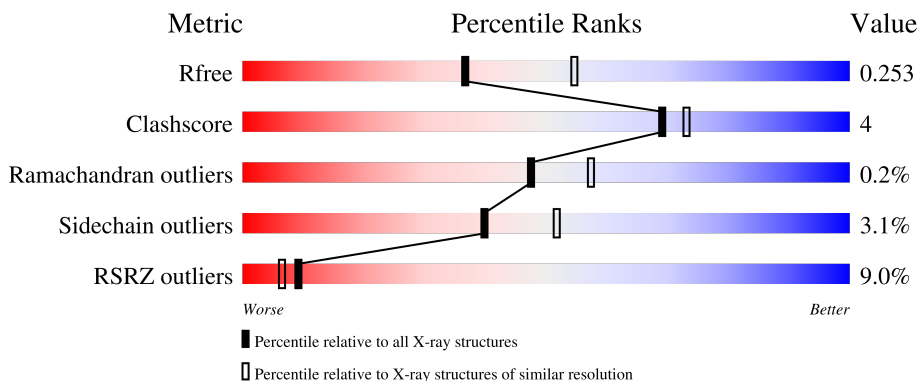|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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 2.43 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	Percentile Ranks	Value
Rfree		0.253
Clashscore		4
Ramachandran outliers		0.2%
Sidechain outliers		3.1%
RSRZ outliers		9.0%

Worse — *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (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 <=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	3% / 87% / 9% ·
1	B	636	3% / 87% / 10% ··
1	C	636	13% / 85% / 10% ··
1	D	636	15% / 69% / 8% / 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 28	C 16	N 2	O 10	0	0	0
2	J	2	Total 28	C 16	N 2	O 10	0	0	0
2	K	2	Total 28	C 16	N 2	O 10	0	0	0

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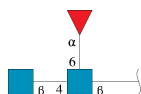
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	3	Total 38	C 22	N 2	O 14	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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

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

- Molecule 5 is (2R,3S,4R,5S)-2-(hydroxymethyl)piperidine-3,4,5-triol (three-letter code: DGJ) (formula: $C_6H_{13}NO_4$) (labeled as "Ligand of Interest" by depositor).
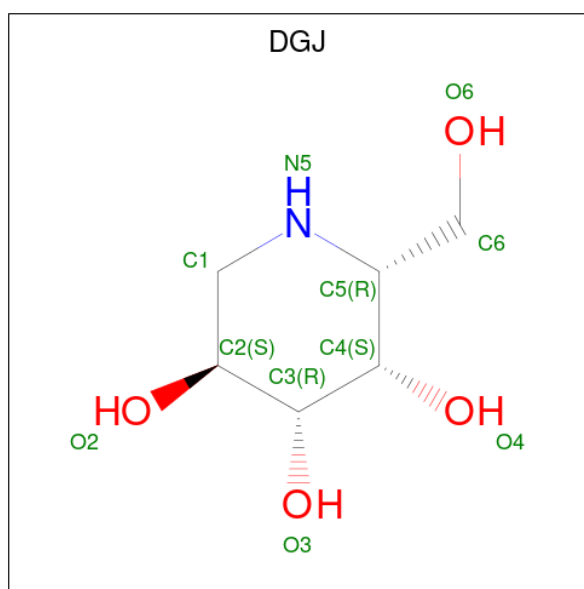
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 11	C 6	N 1	O 4	0	0
5	B	1	Total 11	C 6	N 1	O 4	0	0
5	C	1	Total 11	C 6	N 1	O 4	0	0

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

- Molecule 6 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).
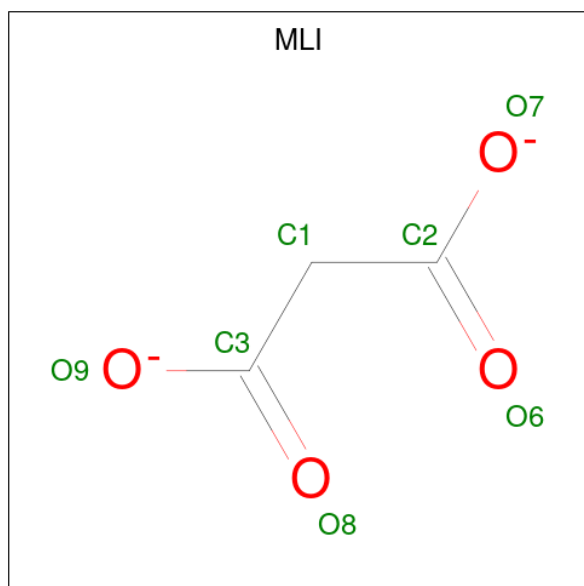
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 7	C 3	O 4	0	0
6	B	1	Total 7	C 3	O 4	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	86	Total 86	O 86	0	0
7	B	91	Total 91	O 91	0	0
7	C	33	Total 33	O 33	0	0
7	D	23	Total 23	O 23	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: Myogenesis-regulating glycosidase
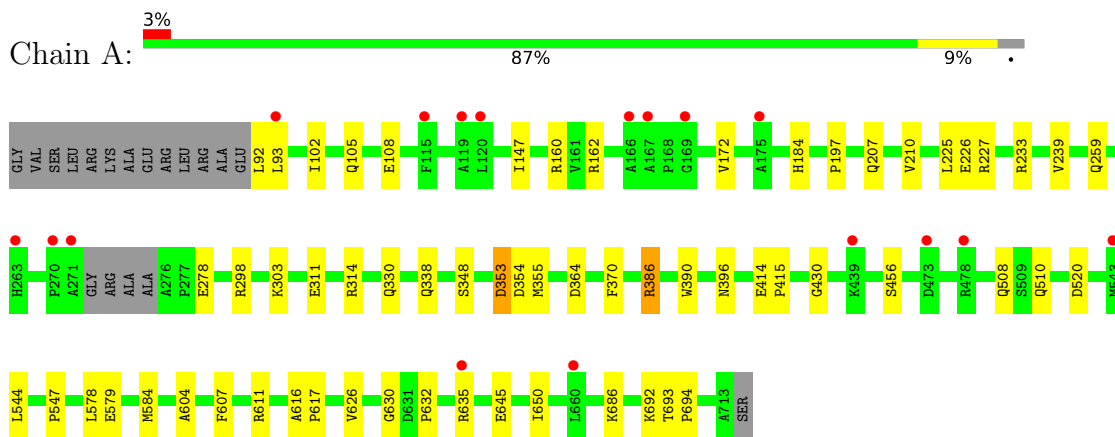
• Molecule 1: Myogenesis-regulating glycosidase
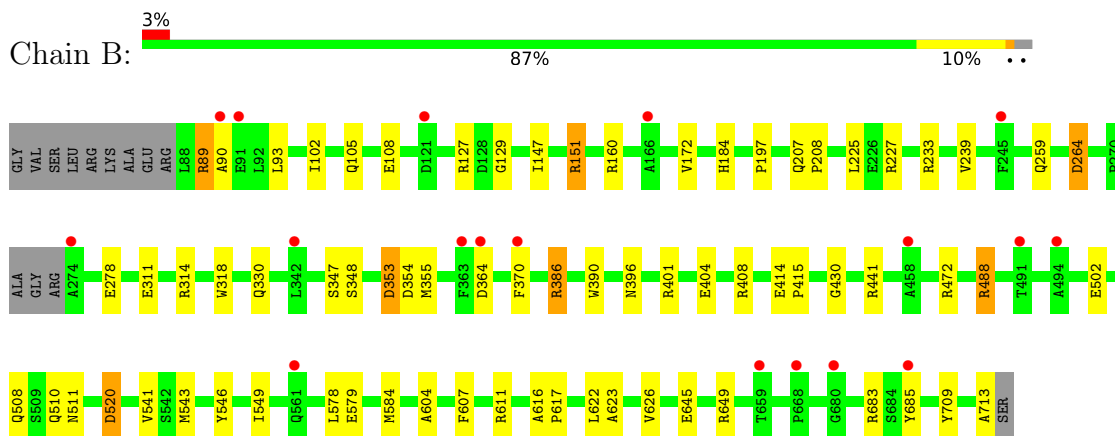
• Molecule 1: Myogenesis-regulating glycosidase
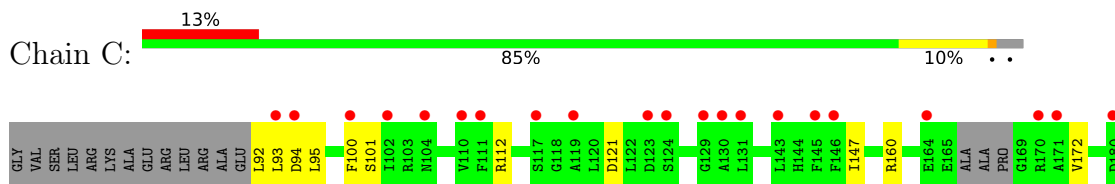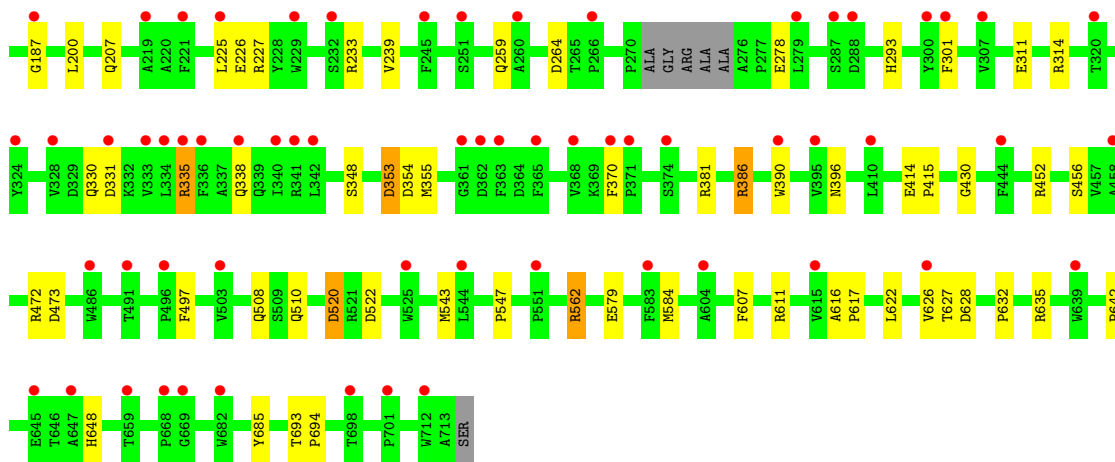
• Molecule 1: Myogenesis-regulating glycosidase
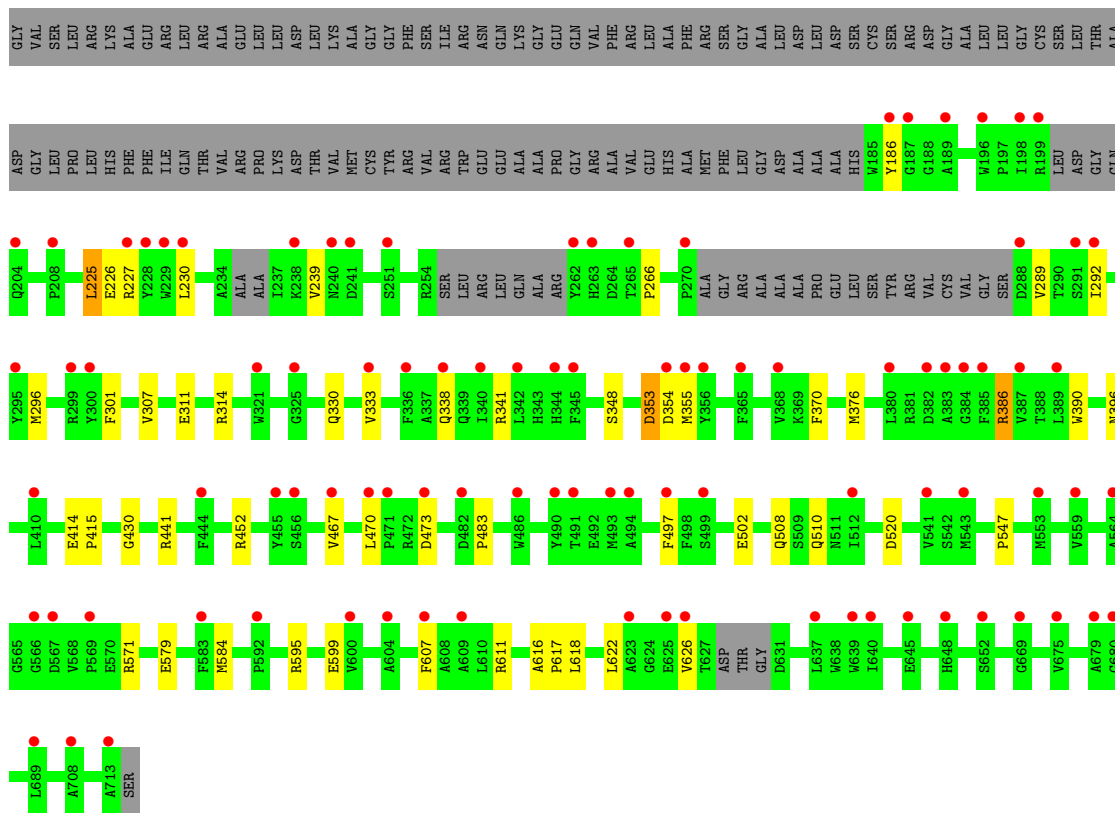
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose
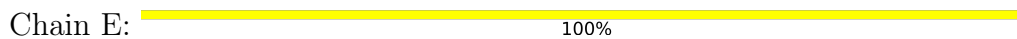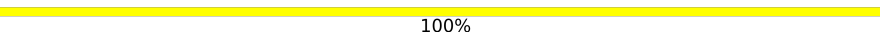
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

| 50% | 50% |

NAG1 NAG2

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

Chain H:

| 100% |

NAG1 NAG2

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

Chain I:

| 50% | 50% |

NAG1 NAG2

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

Chain J:

| 50% | 50% |

NAG1 NAG2

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

Chain K:

| 100% |

NAG1 NAG2

• 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% |

NAG1 NAG2 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) 97.0 (69.75-2.43)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.224 , 0.250 0.227 , 0.253	Depositor DCC
R_{free} test set	6013 reflections (4.80%)	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)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.92	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MLI, NAG, DGJ, FUC

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	0.65	0/5129	0.81	0/6988
1	B	0.65	0/5169	0.80	0/7040
1	C	0.64	0/5067	0.78	0/6907
1	D	0.63	0/4097	0.76	0/5602
All	All	0.64	0/19462	0.79	0/26537

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 ⓘ

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	31	0
1	B	5013	0	4851	43	0
1	C	4913	0	4715	34	0
1	D	3964	0	3713	34	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	141	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 (141) 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
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:293:HIS:CE1	1:C:543:MET:HG2	2.32	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:D:330:GLN:HA	1:D:376:MET:HE1	1.83	0.59
1:D:225:LEU:HD12	1:D:225:LEU:O	2.02	0.58
1:D:330:GLN:HG3	1:D:376:MET:HE3	1.87	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:C:95:LEU:C	1:C:95:LEU:HD13	2.33	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
1:D:225:LEU:HD12	1:D:225:LEU:C	2.34	0.48
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:187:GLY:N	1:C:543:MET:HE1	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:GLU:HG2	1:D:301:PHE:CE1	2.51	0.46
1:D:333:VAL:HB	1:D:376:MET:HE1	1.97	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: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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:93:LEU:HD23	1:C:147:ILE:HG21	2.02	0.42
1:C:642:PRO:O	1:C:648:HIS:NE2	2.53	0.42
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: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:C:693:THR:HA	1:C:694:PRO:C	2.41	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:A:693:THR:HA	1:A:694:PRO:C	2.41	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:414:GLU:HB2	1:D:415:PRO:HD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:LEU:HD11	1:B:604:ALA:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3   Torsion angles (i)

5.3.1   Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	614/636 (96%)	586 (95%)	27 (4%)	1 (0%)	47	57
1	B	619/636 (97%)	592 (96%)	26 (4%)	1 (0%)	47	57
1	C	608/636 (96%)	579 (95%)	28 (5%)	1 (0%)	47	57
1	D	484/636 (76%)	455 (94%)	28 (6%)	1 (0%)	47	57
All	All	2325/2544 (91%)	2212 (95%)	109 (5%)	4 (0%)	47	57

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 (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	517/533 (97%)	502 (97%)	15 (3%)	42	54
1	B	519/533 (97%)	506 (98%)	13 (2%)	47	60
1	C	507/533 (95%)	486 (96%)	21 (4%)	30	40
1	D	402/533 (75%)	391 (97%)	11 (3%)	44	57
All	All	1945/2132 (91%)	1885 (97%)	60 (3%)	40	52

All (60) 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	364	ASP
1	A	386	ARG
1	A	456	SER
1	A	645	GLU
1	A	650	ILE
1	A	686	LYS
1	A	692	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	364	ASP
1	B	386	ARG
1	B	441	ARG
1	B	488	ARG
1	B	502	GLU
1	B	543	MET
1	C	92	LEU
1	C	112	ARG
1	C	121	ASP
1	C	200	LEU
1	C	207	GLN

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Mol	Chain	Res	Type
1	C	225	LEU
1	C	233	ARG
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	520	ASP
1	C	562	ARG
1	C	627	THR
1	C	685	TYR
1	D	225	LEU
1	D	296	MET
1	D	338	GLN
1	D	341	ARG
1	D	353	ASP
1	D	386	ARG
1	D	441	ARG
1	D	473	ASP
1	D	502	GLU
1	D	595	ARG
1	D	618	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	207	GLN
1	C	207	GLN
1	C	338	GLN

5.3.3 RNA (i)

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	2,1	14,14,15	0.50	0	17,19,21	1.39	2 (11%)
2	NAG	E	2	2	14,14,15	0.47	0	17,19,21	1.92	6 (35%)
3	NAG	F	1	3,1	14,14,15	0.42	0	17,19,21	1.27	2 (11%)
3	NAG	F	2	3	14,14,15	0.53	0	17,19,21	1.50	2 (11%)
3	FUC	F	3	3	10,10,11	0.89	1 (10%)	14,14,16	1.60	4 (28%)
2	NAG	G	1	2,1	14,14,15	0.50	0	17,19,21	1.03	0
2	NAG	G	2	2	14,14,15	0.80	0	17,19,21	1.16	2 (11%)
2	NAG	H	1	2,1	14,14,15	0.44	0	17,19,21	1.33	3 (17%)
2	NAG	H	2	2	14,14,15	0.67	0	17,19,21	1.10	1 (5%)
2	NAG	I	1	2,1	14,14,15	0.37	0	17,19,21	1.27	1 (5%)
2	NAG	I	2	2	14,14,15	0.42	0	17,19,21	1.08	0
2	NAG	J	1	2,1	14,14,15	0.49	0	17,19,21	0.90	0
2	NAG	J	2	2	14,14,15	0.25	0	17,19,21	0.96	1 (5%)
2	NAG	K	1	2,1	14,14,15	0.55	0	17,19,21	1.36	2 (11%)
2	NAG	K	2	2	14,14,15	0.40	0	17,19,21	0.96	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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	1	3,1	-	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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	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	2,1	-	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	2,1	-	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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	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	2.11	1.55	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	NAG	O5-C5-C6	4.23	113.84	107.20
2	E	2	NAG	C1-C2-N2	3.65	116.73	110.49
2	K	1	NAG	C1-C2-N2	-3.57	104.39	110.49
2	E	2	NAG	C4-C3-C2	-3.33	106.14	111.02
2	I	1	NAG	O5-C5-C6	3.29	112.37	107.20
3	F	3	FUC	O2-C2-C3	2.91	115.97	110.14
3	F	1	NAG	C2-N2-C7	-2.86	118.83	122.90
2	E	1	NAG	C2-N2-C7	2.80	126.90	122.90
2	E	2	NAG	O4-C4-C5	2.73	116.06	109.30
3	F	1	NAG	O3-C3-C2	-2.65	103.98	109.47
2	K	1	NAG	C4-C3-C2	2.65	114.90	111.02
2	E	2	NAG	C3-C4-C5	-2.64	105.53	110.24
2	H	1	NAG	O5-C5-C6	2.59	111.27	107.20
3	F	3	FUC	O3-C3-C2	2.57	114.91	109.99
2	G	2	NAG	C1-O5-C5	2.54	115.63	112.19
3	F	2	NAG	O5-C5-C4	-2.52	104.69	110.83
2	G	2	NAG	C3-C4-C5	-2.45	105.87	110.24
2	E	2	NAG	C1-O5-C5	2.37	115.40	112.19
3	F	3	FUC	O3-C3-C4	-2.32	104.98	110.35
2	H	1	NAG	O5-C1-C2	-2.29	107.67	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	2	NAG	C1-O5-C5	2.28	115.28	112.19
3	F	3	FUC	O5-C5-C6	2.26	112.19	107.33
2	E	1	NAG	O3-C3-C2	-2.23	104.86	109.47
2	E	2	NAG	O5-C5-C6	-2.19	103.77	107.20
2	K	2	NAG	C1-O5-C5	2.14	115.10	112.19
2	J	2	NAG	C1-O5-C5	2.07	115.00	112.19
2	H	1	NAG	C6-C5-C4	-2.06	108.19	113.00

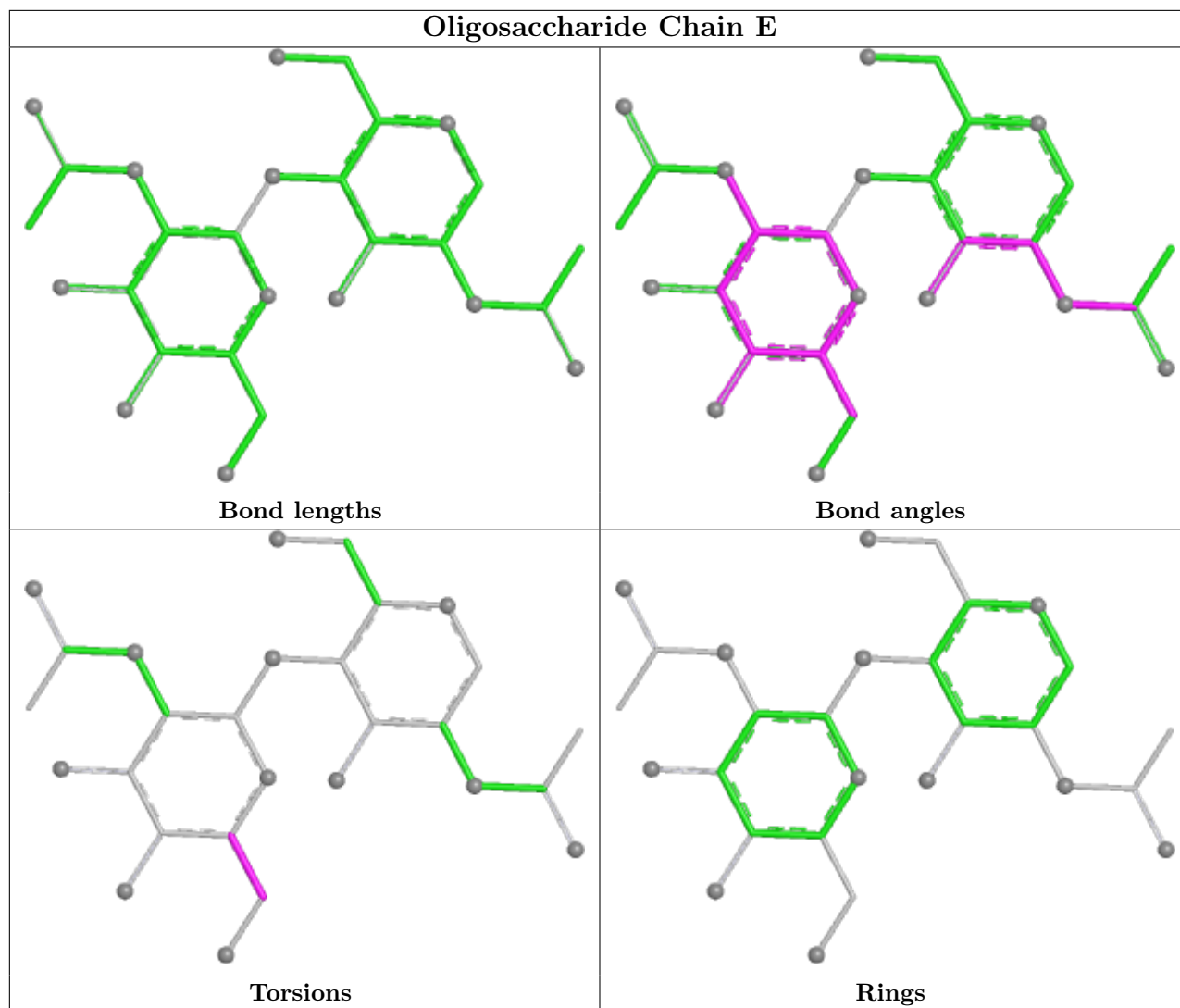There are no chirality outliers.

All (5) 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

There are no ring outliers.

1 monomer is involved in 1 short contact:

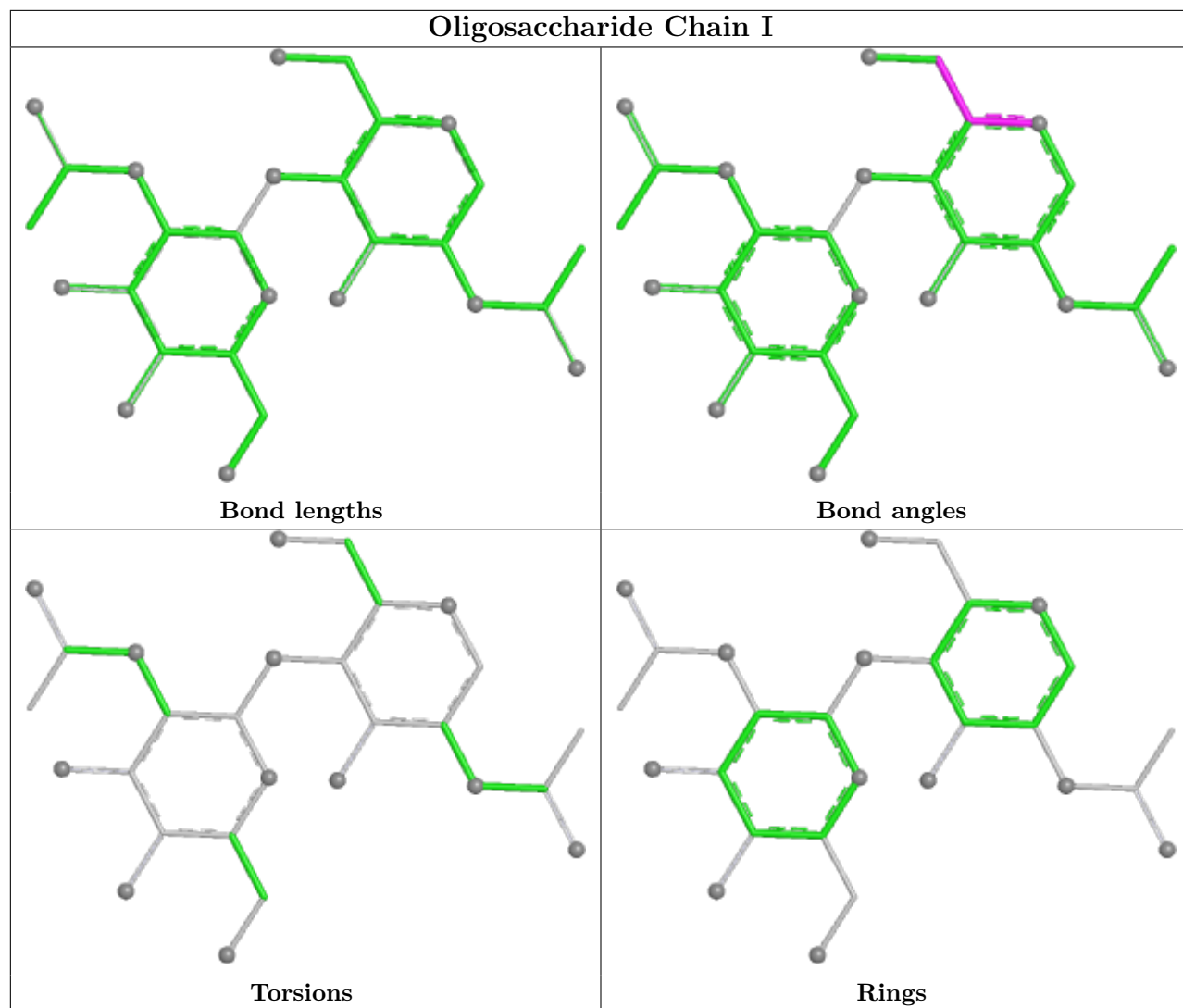| Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	3	FUC	1	0

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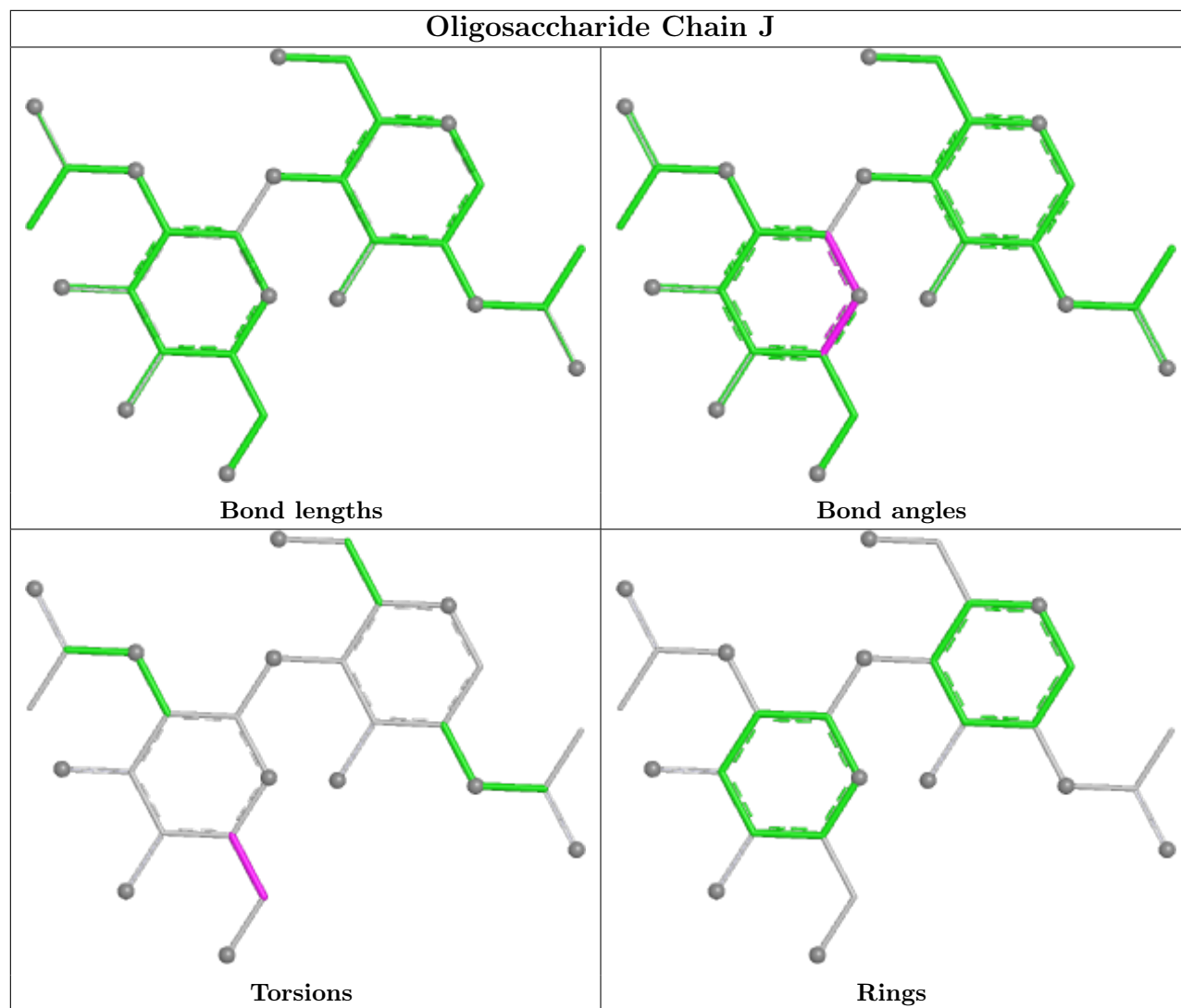
Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Full wwPDB X-ray Structure Validation Report

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain J

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain K

Bond lengths
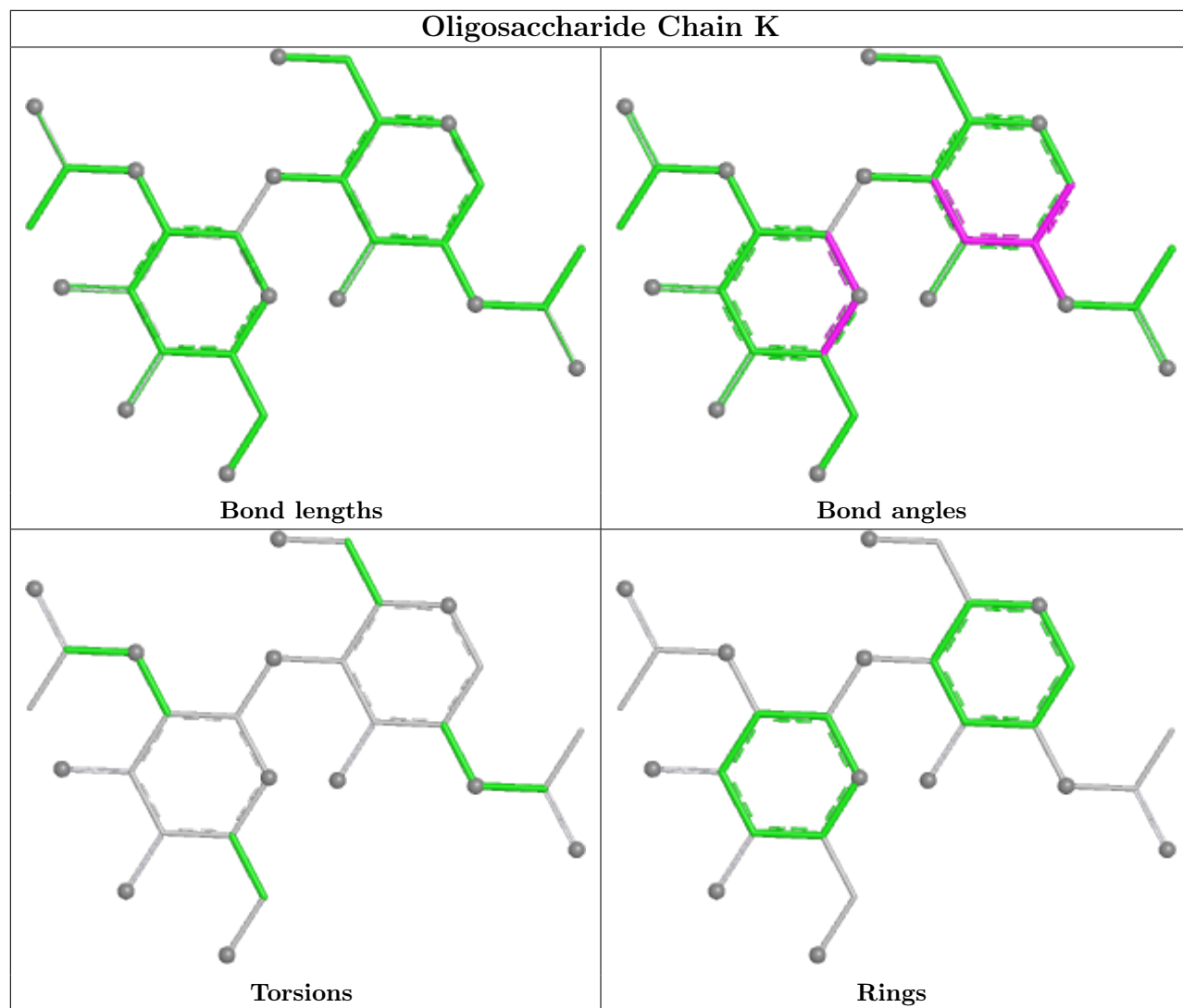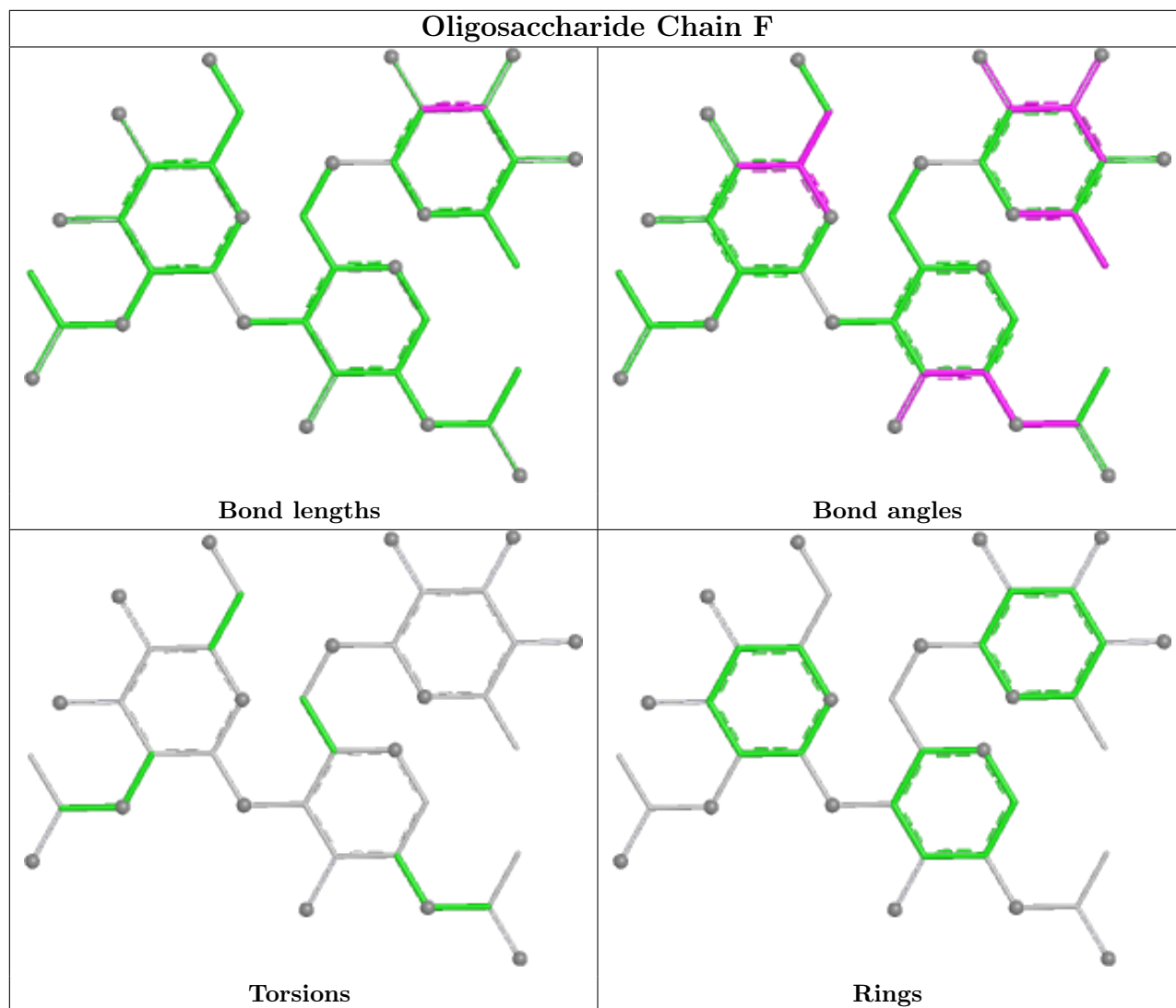

Bond angles

Torsions

Rings

Oligosaccharide Chain F

5.6 Ligand geometry ⓘ

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	#$|Z| > 2$
5	DGJ	D	1000	-	11,11,11	1.45	1 (9%)	13,15,15	0.93	0
4	NAG	D	1001	1	14,14,15	0.59	0	17,19,21	1.47	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	NAG	A	801	1	14,14,15	0.55	0	17,19,21	2.11	4 (23%)
4	NAG	A	805	1	14,14,15	0.56	0	17,19,21	1.04	0
4	NAG	C	802	1	14,14,15	0.32	0	17,19,21	1.35	3 (17%)
4	NAG	C	801	1	14,14,15	0.71	0	17,19,21	1.44	2 (11%)
4	NAG	D	1002	1	14,14,15	0.60	0	17,19,21	1.61	2 (11%)
4	NAG	C	803	1	14,14,15	0.90	0	17,19,21	2.13	2 (11%)
6	MLI	B	804	-	6,6,6	1.25	0	7,7,7	1.56	1 (14%)
4	NAG	B	802	1	14,14,15	0.47	0	17,19,21	1.11	1 (5%)
5	DGJ	A	803	-	11,11,11	1.42	3 (27%)	13,15,15	1.92	3 (23%)
5	DGJ	B	803	-	11,11,11	1.47	3 (27%)	13,15,15	0.95	0
4	NAG	B	801	1	14,14,15	0.60	0	17,19,21	1.21	4 (23%)
5	DGJ	C	804	-	11,11,11	1.87	3 (27%)	13,15,15	1.72	4 (30%)
6	MLI	A	804	-	6,6,6	1.82	2 (33%)	7,7,7	1.37	0
4	NAG	A	802	1	14,14,15	0.56	0	17,19,21	1.66	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
5	DGJ	D	1000	-	-	0/2/19/19	0/1/1/1
4	NAG	D	1001	1	-	0/6/23/26	0/1/1/1
4	NAG	A	801	1	-	0/6/23/26	0/1/1/1
4	NAG	A	805	1	-	0/6/23/26	0/1/1/1
4	NAG	C	802	1	-	0/6/23/26	0/1/1/1
4	NAG	C	801	1	-	2/6/23/26	0/1/1/1
4	NAG	D	1002	1	-	1/6/23/26	0/1/1/1
4	NAG	C	803	1	-	0/6/23/26	0/1/1/1
6	MLI	B	804	-	-	0/4/4/4	-
4	NAG	B	802	1	-	0/6/23/26	0/1/1/1
5	DGJ	A	803	-	-	0/2/19/19	0/1/1/1
5	DGJ	B	803	-	-	0/2/19/19	0/1/1/1
4	NAG	B	801	1	-	1/6/23/26	0/1/1/1
5	DGJ	C	804	-	-	0/2/19/19	0/1/1/1
6	MLI	A	804	-	-	0/4/4/4	-
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	3.85	1.56	1.52
5	C	804	DGJ	C1-C2	3.82	1.56	1.52
5	C	804	DGJ	C5-N5	3.11	1.52	1.47
5	B	803	DGJ	C1-N5	2.90	1.51	1.47
5	A	803	DGJ	C1-N5	2.75	1.51	1.47
5	B	803	DGJ	C5-N5	2.74	1.51	1.47
6	A	804	MLI	C1-C2	2.61	1.55	1.51
5	C	804	DGJ	C1-N5	2.49	1.50	1.47
6	A	804	MLI	C1-C3	2.32	1.54	1.51
5	B	803	DGJ	C1-C2	2.27	1.54	1.52
5	A	803	DGJ	C1-C2	2.24	1.54	1.52
5	A	803	DGJ	C5-N5	2.05	1.50	1.47

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	803	NAG	C1-O5-C5	7.30	122.09	112.19
4	A	801	NAG	C3-C4-C5	-5.19	100.98	110.24
4	D	1002	NAG	C1-O5-C5	4.86	118.78	112.19
4	A	802	NAG	C1-O5-C5	4.46	118.24	112.19
4	C	801	NAG	C1-O5-C5	4.35	118.09	112.19
5	A	803	DGJ	C1-N5-C5	3.76	117.74	109.61
5	A	803	DGJ	O2-C2-C3	3.62	117.40	110.14
4	A	801	NAG	O4-C4-C5	3.55	118.11	109.30
5	C	804	DGJ	C1-N5-C5	3.25	116.64	109.61
4	A	801	NAG	O3-C3-C2	3.25	116.18	109.47
4	C	803	NAG	C8-C7-N2	-3.15	110.76	116.10
4	D	1002	NAG	C1-C2-N2	-3.10	105.19	110.49
4	D	1001	NAG	O3-C3-C2	-2.97	103.32	109.47
4	B	802	NAG	C1-O5-C5	2.74	115.91	112.19
4	C	802	NAG	C1-O5-C5	2.62	115.74	112.19
5	C	804	DGJ	C4-C5-N5	2.55	114.24	109.14
4	B	801	NAG	C3-C4-C5	-2.46	105.85	110.24
4	B	801	NAG	O4-C4-C5	2.44	115.35	109.30
5	A	803	DGJ	O3-C3-C2	2.43	114.64	109.99
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
4	C	802	NAG	O5-C1-C2	-2.37	107.55	111.29
6	B	804	MLI	O9-C3-C1	2.24	121.70	114.54
4	A	802	NAG	C4-C3-C2	-2.24	107.73	111.02
4	C	801	NAG	O5-C5-C6	2.21	110.68	107.20
4	B	801	NAG	C1-O5-C5	2.18	115.15	112.19
5	C	804	DGJ	O4-C4-C3	-2.17	105.34	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1001	NAG	C6-C5-C4	2.12	117.98	113.00
4	B	801	NAG	O3-C3-C2	-2.03	105.26	109.47
4	A	801	NAG	O5-C5-C4	-2.03	105.89	110.83
4	C	802	NAG	C2-N2-C7	-2.03	120.02	122.90

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:

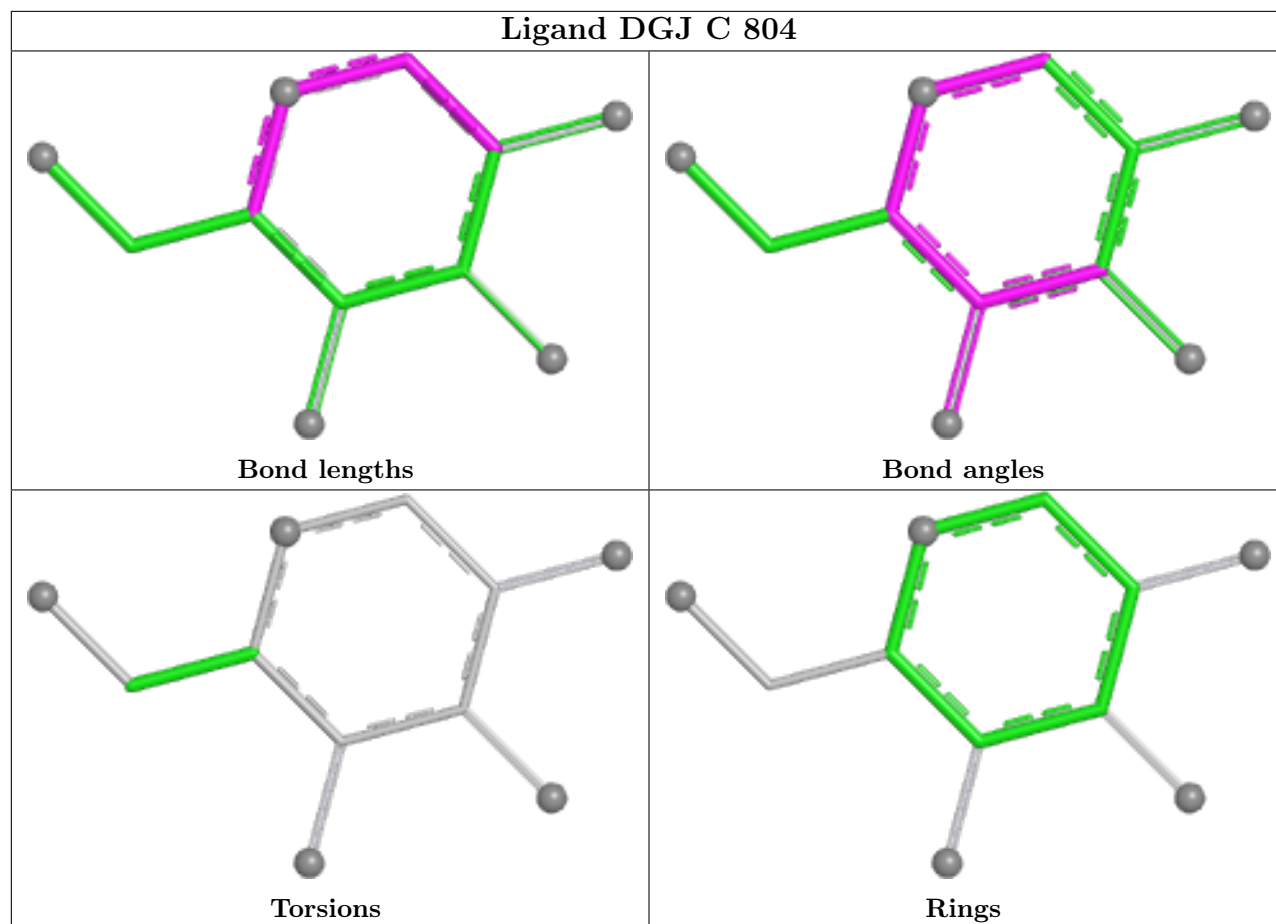| Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	NAG	1	0
5	B	803	DGJ	1	0

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 then 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.

Full wwPDB X-ray Structure Validation Report

Ligand DGJ D 1000

Bond lengths

Bond angles

Torsions

Rings

Ligand DGJ A 803

Bond lengths

Bond angles

Torsions

Rings

Ligand DGJ B 803

Bond lengths

Bond angles

Torsions

Rings

Ligand DGJ C 804
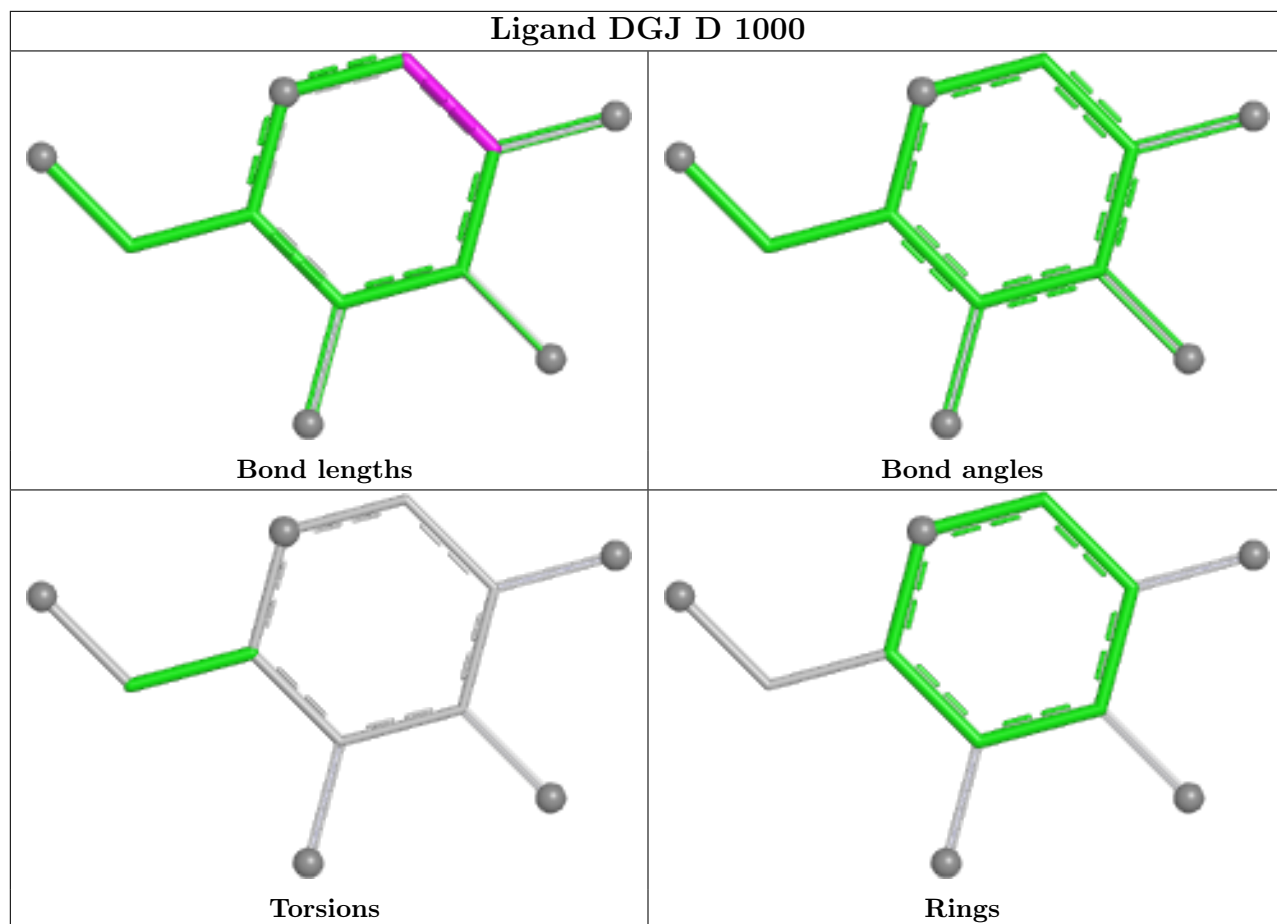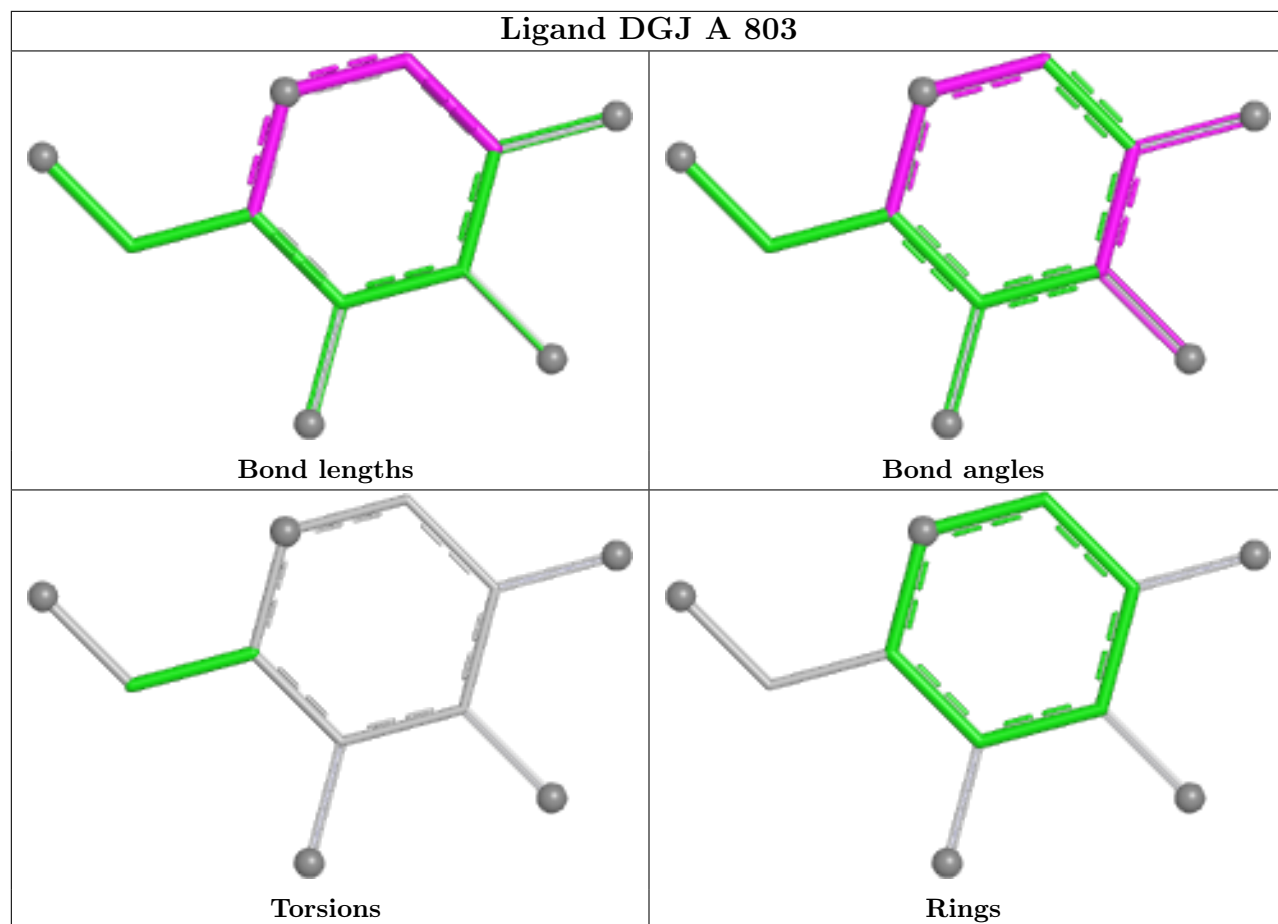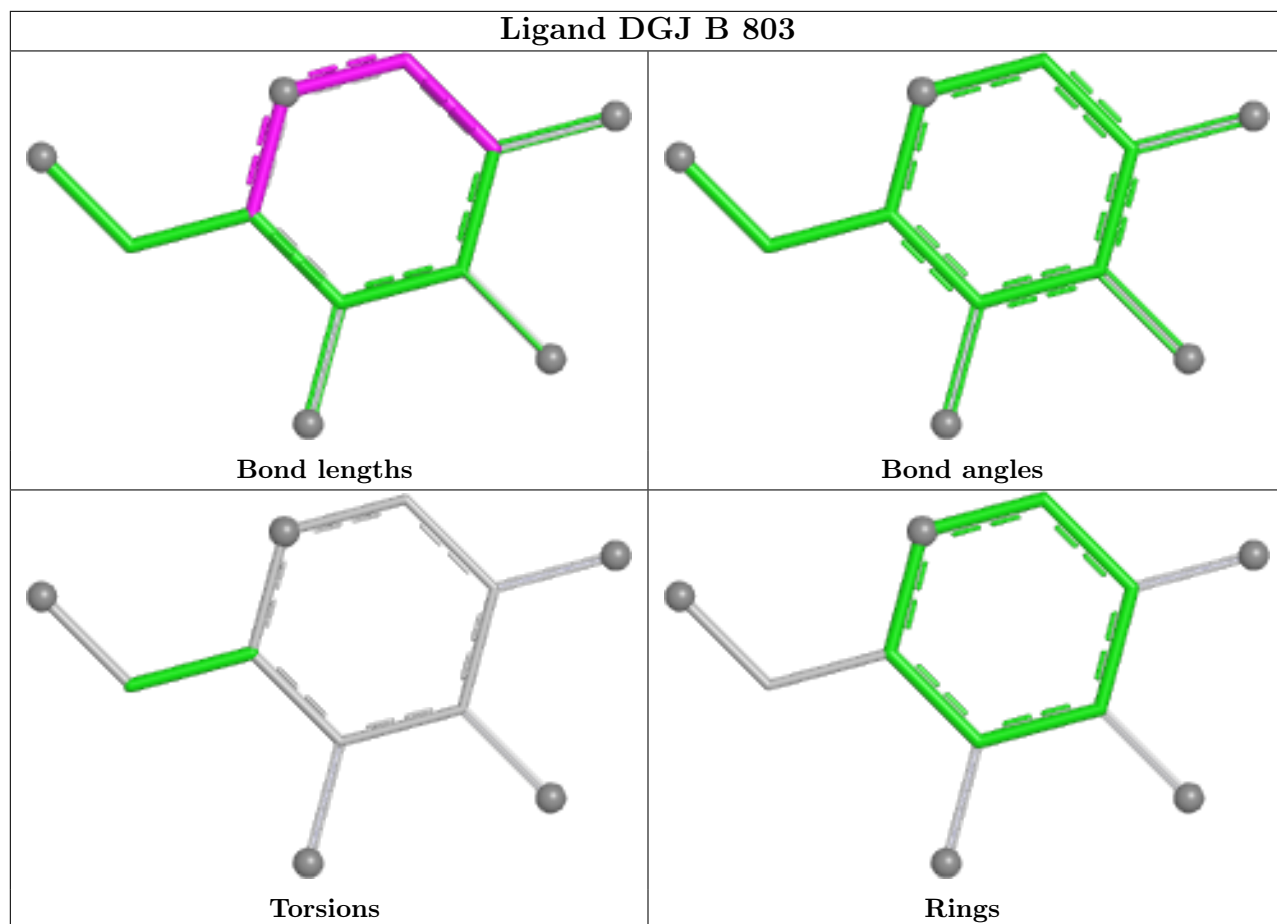
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	618/636 (97%)	0.76	17 (2%)	53	49	29, 45, 66, 95	0
1	B	623/636 (97%)	0.72	18 (2%)	51	47	32, 50, 72, 100	0
1	C	614/636 (96%)	1.01	83 (13%)	3	1	50, 70, 94, 110	0
1	D	496/636 (77%)	1.27	94 (18%)	1	0	52, 75, 101, 116	0
All	All	2351/2544 (92%)	0.92	212 (9%)	9	6	29, 60, 92, 116	0

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	623	ALA	7.2
1	B	166	ALA	6.4
1	D	497	PHE	6.1
1	A	167	ALA	5.9
1	D	187	GLY	5.9
1	D	669	GLY	5.8
1	D	680	GLY	5.6
1	D	342	LEU	5.1
1	D	186	TYR	5.1
1	C	342	LEU	5.0
1	D	380	LEU	5.0
1	D	340	ILE	5.0
1	C	170	ARG	5.0
1	D	336	PHE	4.8
1	C	93	LEU	4.5
1	D	543	MET	4.5
1	D	227	ARG	4.5
1	D	385	PHE	4.5
1	C	129	GLY	4.5
1	C	124	SER	4.2
1	D	292	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	637	LEU	4.2
1	C	334	LEU	4.2
1	D	383	ALA	4.2
1	D	564	ALA	4.1
1	D	241	ASP	4.1
1	C	146	PHE	4.1
1	D	204	GLN	4.0
1	C	626	VAL	4.0
1	D	583	PHE	4.0
1	C	701	PRO	4.0
1	D	270	PRO	3.9
1	D	494	ALA	3.9
1	D	592	PRO	3.8
1	D	230	LEU	3.8
1	C	171	ALA	3.8
1	A	166	ALA	3.8
1	D	389	LEU	3.8
1	D	198	ILE	3.8
1	C	187	GLY	3.8
1	C	94	ASP	3.7
1	D	604	ALA	3.6
1	D	228	TYR	3.6
1	D	333	VAL	3.6
1	C	338	GLN	3.6
1	C	100	PHE	3.5
1	D	491	THR	3.5
1	D	295	TYR	3.5
1	C	668	PRO	3.5
1	C	145	PHE	3.5
1	C	335	ARG	3.5
1	D	455	TYR	3.5
1	C	669	GLY	3.5
1	C	221	PHE	3.4
1	C	229	TRP	3.4
1	A	115	PHE	3.4
1	C	365	PHE	3.4
1	C	340	ILE	3.4
1	D	512	ILE	3.4
1	D	338	GLN	3.3
1	D	240	ASN	3.3
1	C	131	LEU	3.3
1	D	345	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	444	PHE	3.3
1	D	288	ASP	3.3
1	C	117	SER	3.3
1	C	458	ALA	3.2
1	C	328	VAL	3.2
1	C	111	PHE	3.2
1	C	410	LEU	3.2
1	C	363	PHE	3.2
1	C	219	ALA	3.2
1	D	569	PRO	3.2
1	C	307	VAL	3.2
1	C	320	THR	3.1
1	D	410	LEU	3.1
1	A	543	MET	3.1
1	A	473	ASP	3.1
1	B	274	ALA	3.1
1	D	467	VAL	3.1
1	D	679	ALA	3.1
1	D	493	MET	3.0
1	D	291	SER	3.0
1	D	456	SER	3.0
1	C	119	ALA	3.0
1	C	104	ASN	3.0
1	D	387	VAL	3.0
1	D	263	HIS	3.0
1	C	225	LEU	2.9
1	B	680	GLY	2.9
1	C	300	TYR	2.9
1	C	324	TYR	2.9
1	C	368	VAL	2.9
1	C	245	PHE	2.9
1	D	559	VAL	2.9
1	D	473	ASP	2.9
1	C	371	PRO	2.8
1	C	682	TRP	2.8
1	D	708	ALA	2.8
1	C	615	VAL	2.8
1	D	265	THR	2.8
1	B	91	GLU	2.8
1	A	271	ALA	2.7
1	C	525	TRP	2.7
1	D	321	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	713	ALA	2.7
1	C	503	VAL	2.7
1	D	626	VAL	2.7
1	A	169	GLY	2.7
1	C	362	ASP	2.7
1	B	342	LEU	2.7
1	D	645	GLU	2.6
1	D	251	SER	2.6
1	B	364	ASP	2.6
1	D	344	HIS	2.6
1	C	544	LEU	2.6
1	D	208	PRO	2.6
1	D	648	HIS	2.6
1	B	245	PHE	2.6
1	D	384	GLY	2.6
1	D	471	PRO	2.5
1	C	444	PHE	2.5
1	C	583	PHE	2.5
1	C	361	GLY	2.5
1	C	712	TRP	2.5
1	A	270	PRO	2.5
1	D	482	ASP	2.5
1	D	300	TYR	2.5
1	D	625	GLU	2.5
1	C	301	PHE	2.5
1	D	607	PHE	2.5
1	C	251	SER	2.5
1	C	551	PRO	2.5
1	C	279	LEU	2.5
1	C	491	THR	2.5
1	C	110	VAL	2.4
1	C	130	ALA	2.4
1	D	640	ILE	2.4
1	C	333	VAL	2.4
1	D	354	ASP	2.4
1	C	604	ALA	2.4
1	A	478	ARG	2.4
1	D	365	PHE	2.4
1	B	668	PRO	2.4
1	C	698	THR	2.4
1	A	119	ALA	2.4
1	A	93	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	336	PHE	2.4
1	A	175	ALA	2.4
1	D	262	TYR	2.3
1	D	499	SER	2.3
1	D	600	VAL	2.3
1	C	341	ARG	2.3
1	D	566	GLY	2.3
1	D	382	ASP	2.3
1	C	287	SER	2.3
1	D	470	LEU	2.3
1	D	229	TRP	2.3
1	B	685	TYR	2.3
1	C	180	ASP	2.3
1	C	266	PRO	2.3
1	D	675	VAL	2.3
1	B	370	PHE	2.3
1	C	260	ALA	2.3
1	D	609	ALA	2.3
1	D	356	TYR	2.3
1	C	645	GLU	2.3
1	B	121	ASP	2.3
1	B	494	ALA	2.3
1	B	561	GLN	2.3
1	C	123	ASP	2.3
1	C	659	THR	2.3
1	D	325	GLY	2.2
1	C	370	PHE	2.2
1	B	458	ALA	2.2
1	D	689	LEU	2.2
1	D	553	MET	2.2
1	C	102	ILE	2.2
1	D	299	ARG	2.2
1	C	288	ASP	2.2
1	A	439	LYS	2.2
1	C	496	PRO	2.2
1	C	232	SER	2.2
1	B	90	ALA	2.2
1	D	567	ASP	2.2
1	C	390	TRP	2.2
1	D	541	VAL	2.2
1	C	647	ALA	2.2
1	C	395	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	639	TRP	2.1
1	C	374	SER	2.1
1	D	199	ARG	2.1
1	D	368	VAL	2.1
1	D	486	TRP	2.1
1	A	660	LEU	2.1
1	D	490	TYR	2.1
1	A	120	LEU	2.1
1	C	143	LEU	2.1
1	D	355	MET	2.1
1	C	331	ASP	2.1
1	A	263	HIS	2.1
1	B	363	PHE	2.1
1	A	635	ARG	2.0
1	C	486	TRP	2.0
1	C	639	TRP	2.0
1	B	659	THR	2.0
1	D	238	LYS	2.0
1	D	652	SER	2.0
1	C	164	GLU	2.0
1	D	189	ALA	2.0
1	D	196	TRP	2.0
1	B	491	THR	2.0

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

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
3	NAG	F	2	14/15	0.62	0.26	66,73,78,79	0
2	NAG	J	2	14/15	0.75	0.32	67,75,81,81	0
2	NAG	I	2	14/15	0.75	0.18	79,85,88,88	0
2	NAG	E	2	14/15	0.80	0.29	76,80,84,86	0
2	NAG	E	1	14/15	0.82	0.26	58,61,68,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
2	NAG	K	1	14/15	0.83	0.17	62,68,72,72	0
2	NAG	J	1	14/15	0.83	0.17	56,59,64,67	0
3	FUC	F	3	10/11	0.84	0.26	64,67,69,70	0
2	NAG	G	2	14/15	0.85	0.18	46,52,58,60	0
2	NAG	H	2	14/15	0.87	0.15	46,55,61,64	0
2	NAG	K	2	14/15	0.87	0.14	68,72,77,78	0
3	NAG	F	1	14/15	0.88	0.18	56,59,64,69	0
2	NAG	H	1	14/15	0.89	0.18	51,53,55,56	0
2	NAG	G	1	14/15	0.90	0.17	44,48,52,55	0
2	NAG	I	1	14/15	0.91	0.13	60,62,68,75	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:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
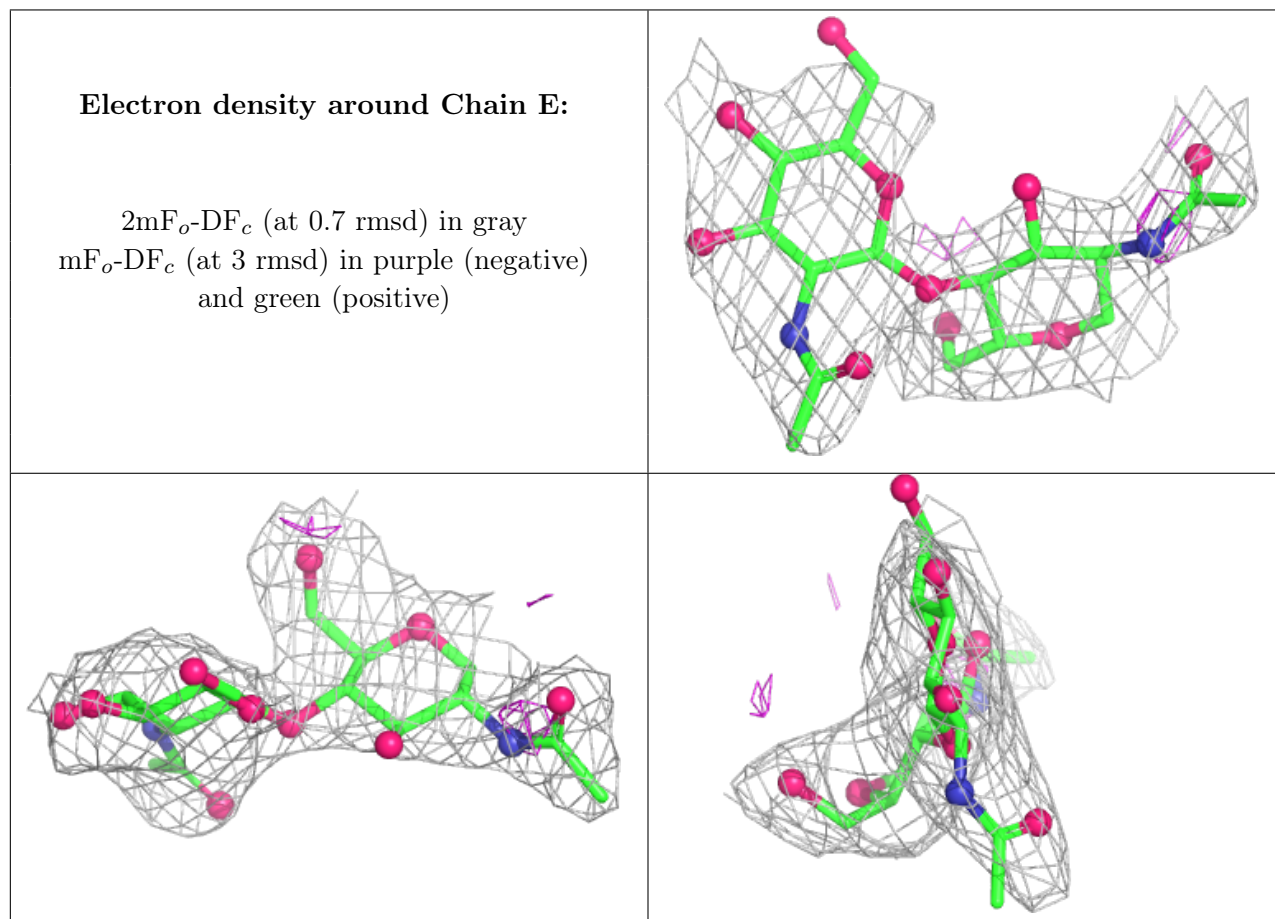
Electron density around Chain G:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
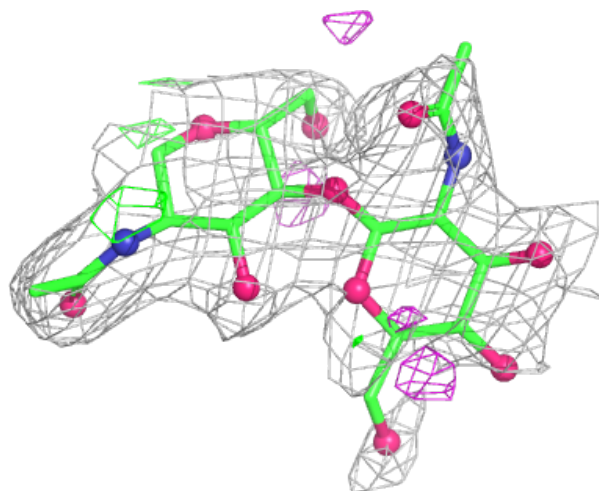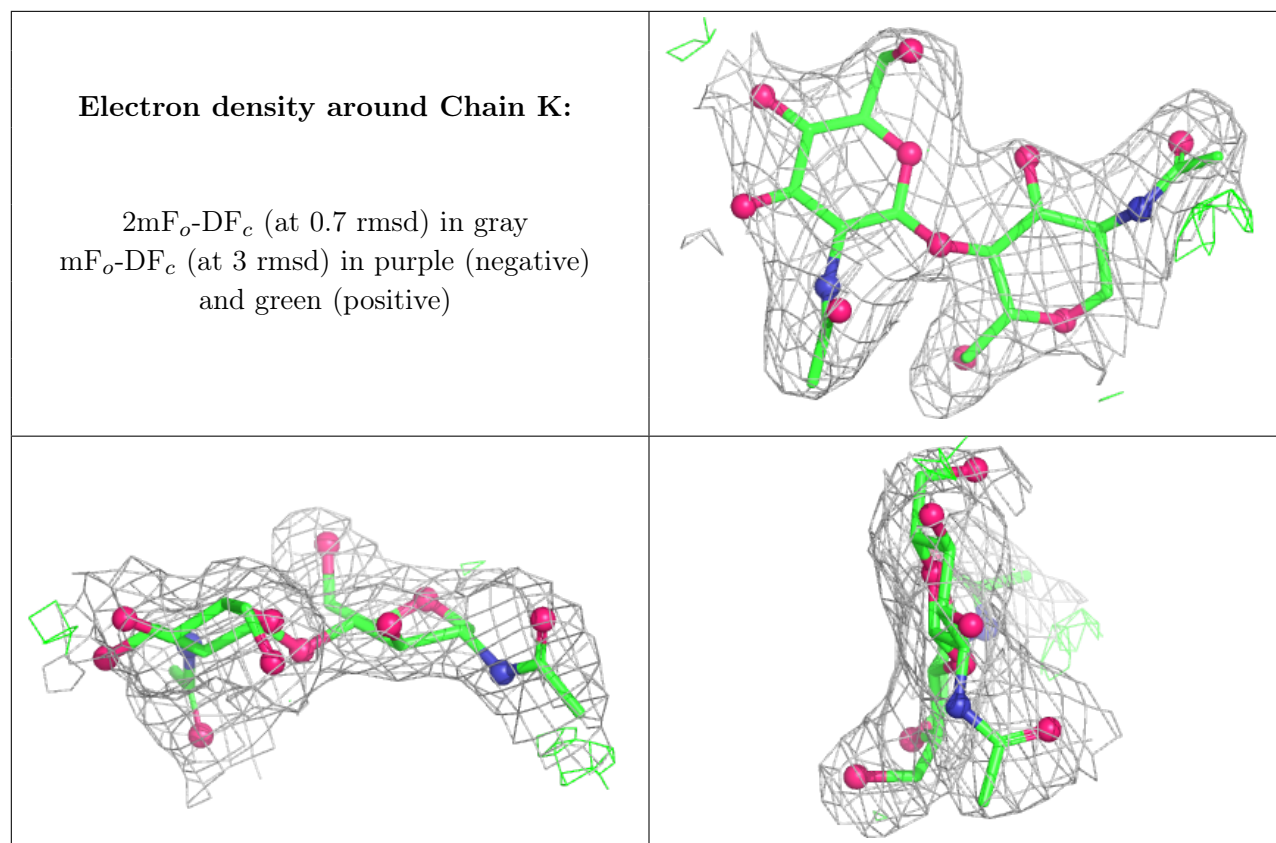and green (positive)
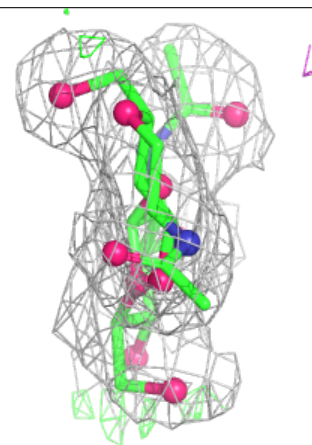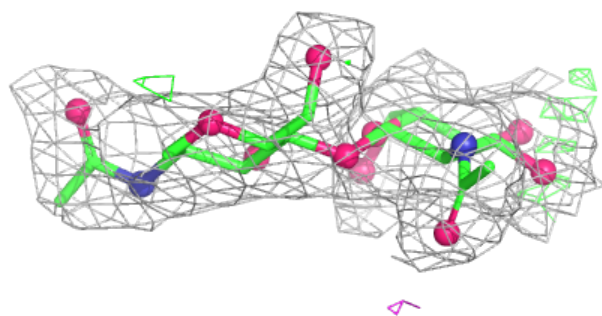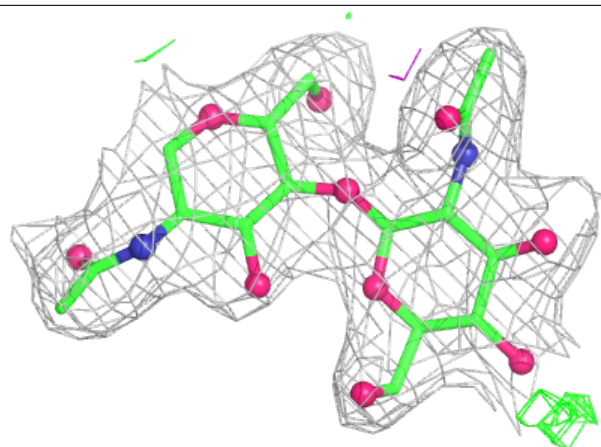
Electron density around Chain H:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
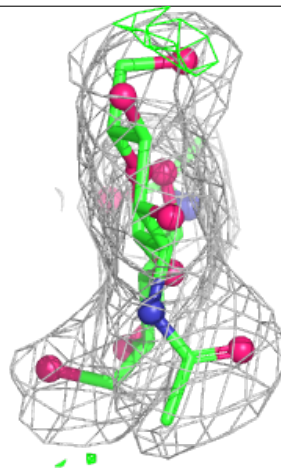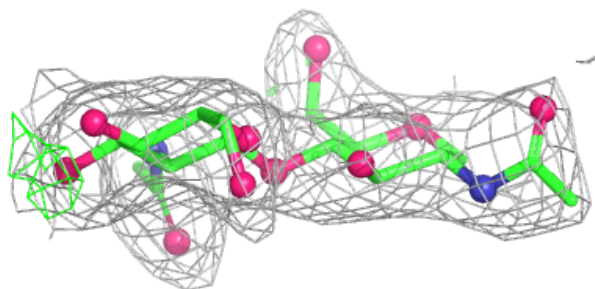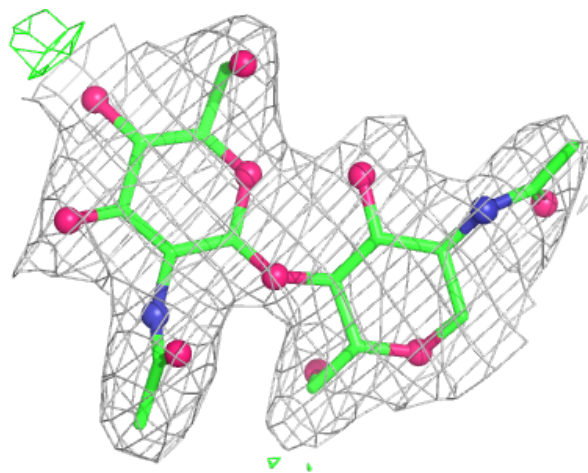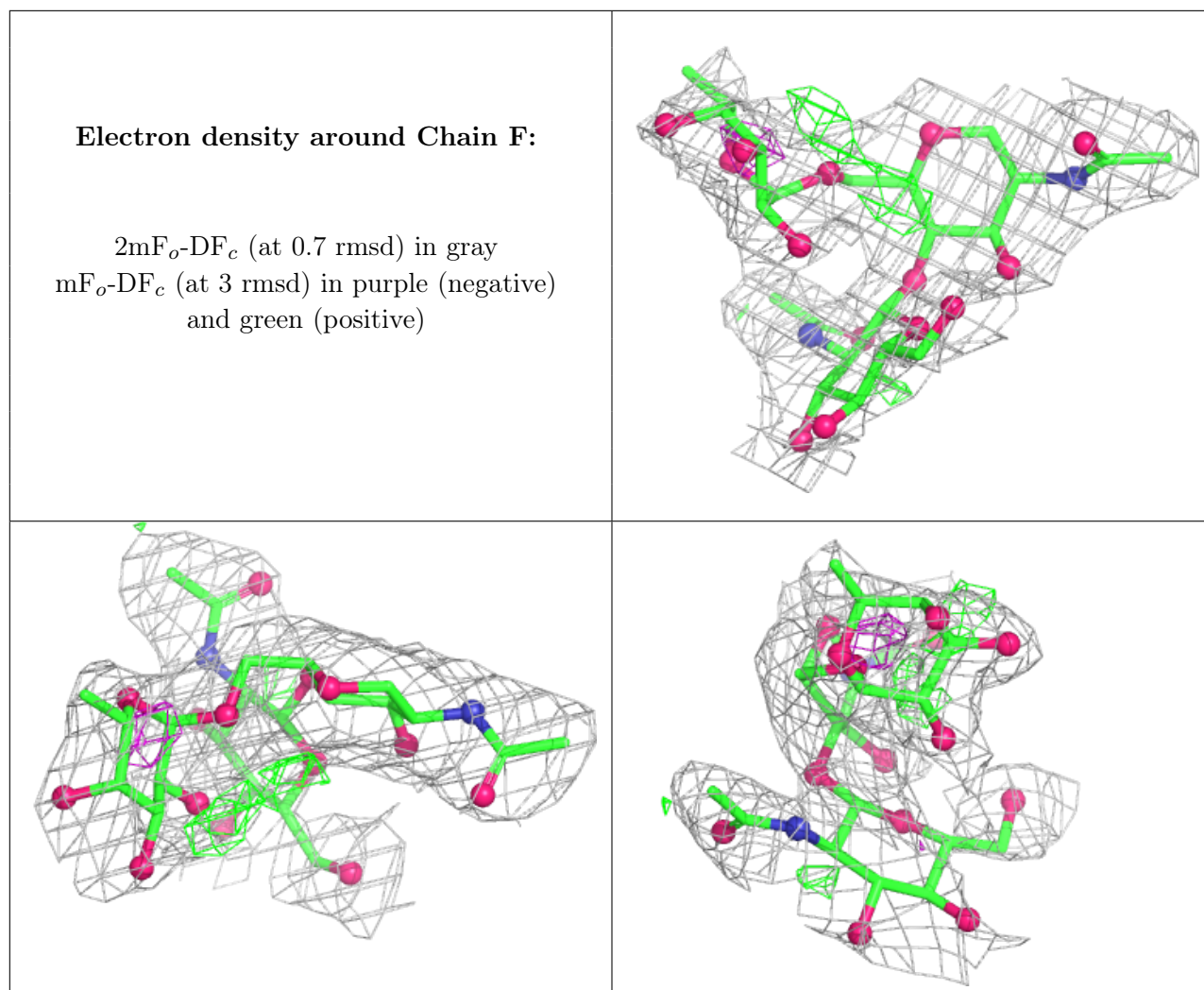
Electron density around Chain I:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
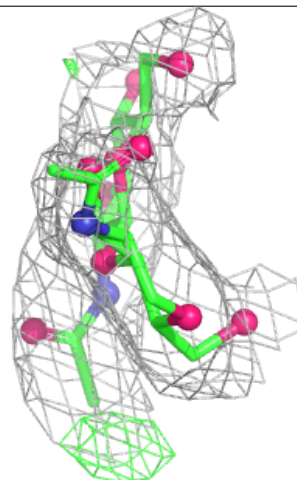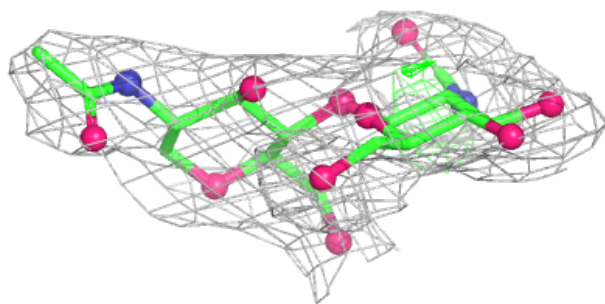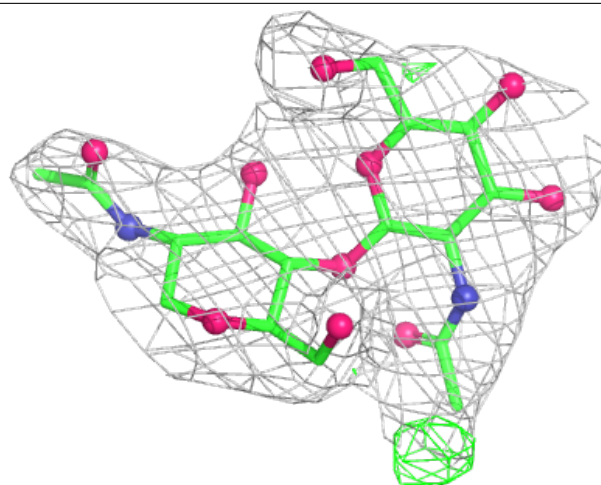
Electron density around Chain J:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
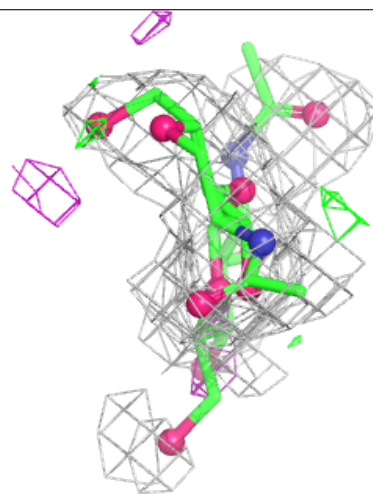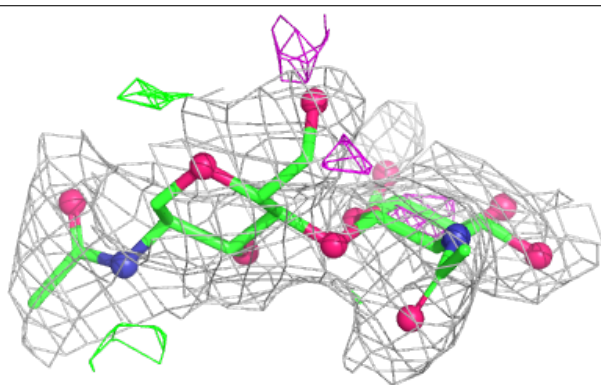
Electron density around Chain K:

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

Electron density around Chain F:

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

6.4 Ligands ⓘ

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
4	NAG	B	802	14/15	0.45	0.37	96,101,103,103	0
4	NAG	D	1001	14/15	0.64	0.17	86,91,94,95	0
4	NAG	A	802	14/15	0.68	0.21	73,76,81,81	0
4	NAG	A	805	14/15	0.68	0.24	87,95,100,101	0
4	NAG	D	1002	14/15	0.68	0.25	77,87,92,92	0
4	NAG	C	803	14/15	0.75	0.16	73,77,79,79	0
4	NAG	C	802	14/15	0.76	0.30	74,76,78,78	0
4	NAG	C	801	14/15	0.80	0.15	81,84,88,88	0
5	DGJ	C	804	11/11	0.84	0.17	48,49,51,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\mathring{A}^2$)	Q<0.9
5	DGJ	D	1000	11/11	0.84	0.19	50,52,53,54	0
4	NAG	B	801	14/15	0.89	0.16	52,54,58,58	0
6	MLI	A	804	7/7	0.89	0.15	51,53,55,56	0
6	MLI	B	804	7/7	0.89	0.20	52,53,54,55	0
4	NAG	A	801	14/15	0.91	0.17	50,54,56,58	0
5	DGJ	A	803	11/11	0.92	0.20	35,36,39,41	0
5	DGJ	B	803	11/11	0.94	0.19	39,40,43,44	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)
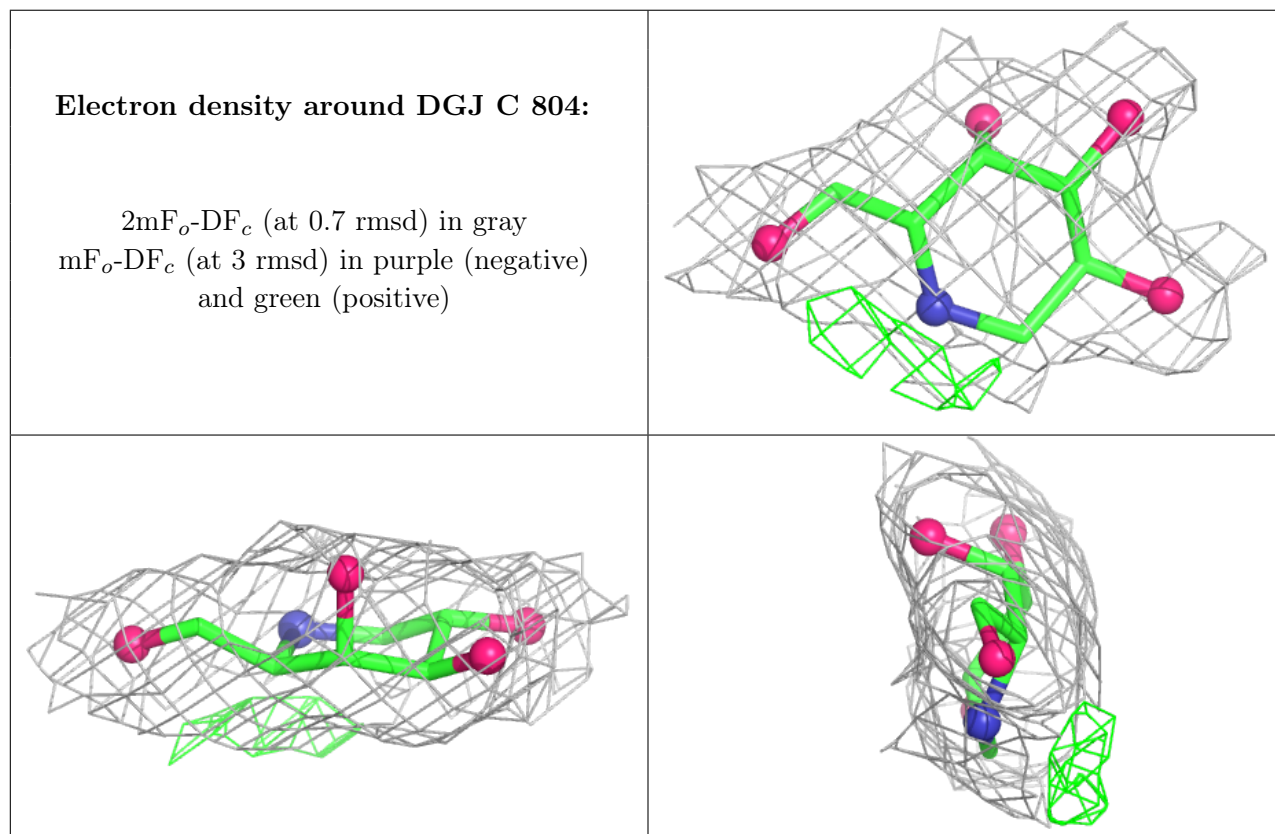
Electron density around DGJ D 1000:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
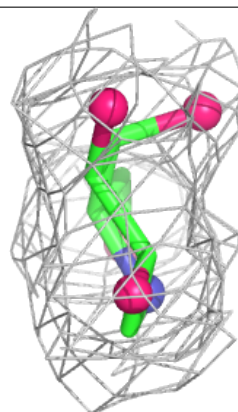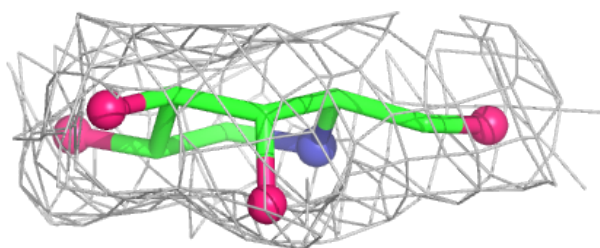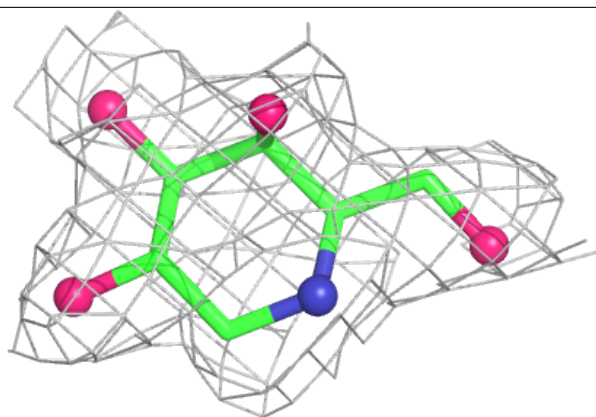
Electron density around DGJ A 803:

$2mF_o$-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)
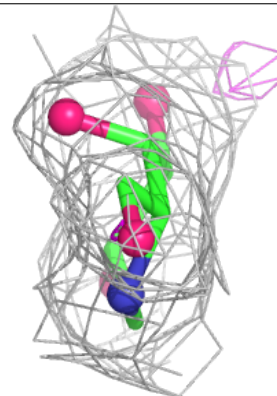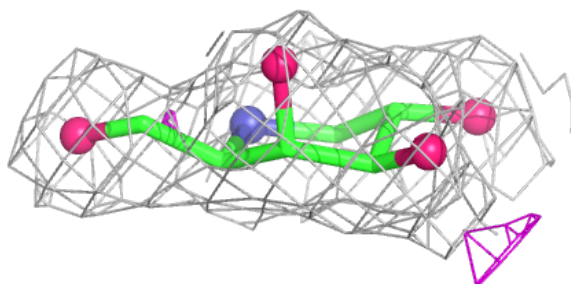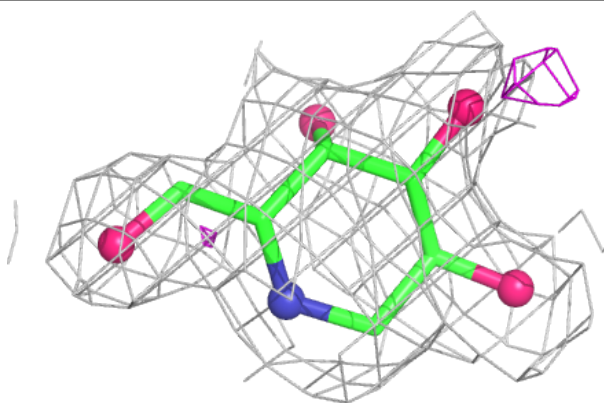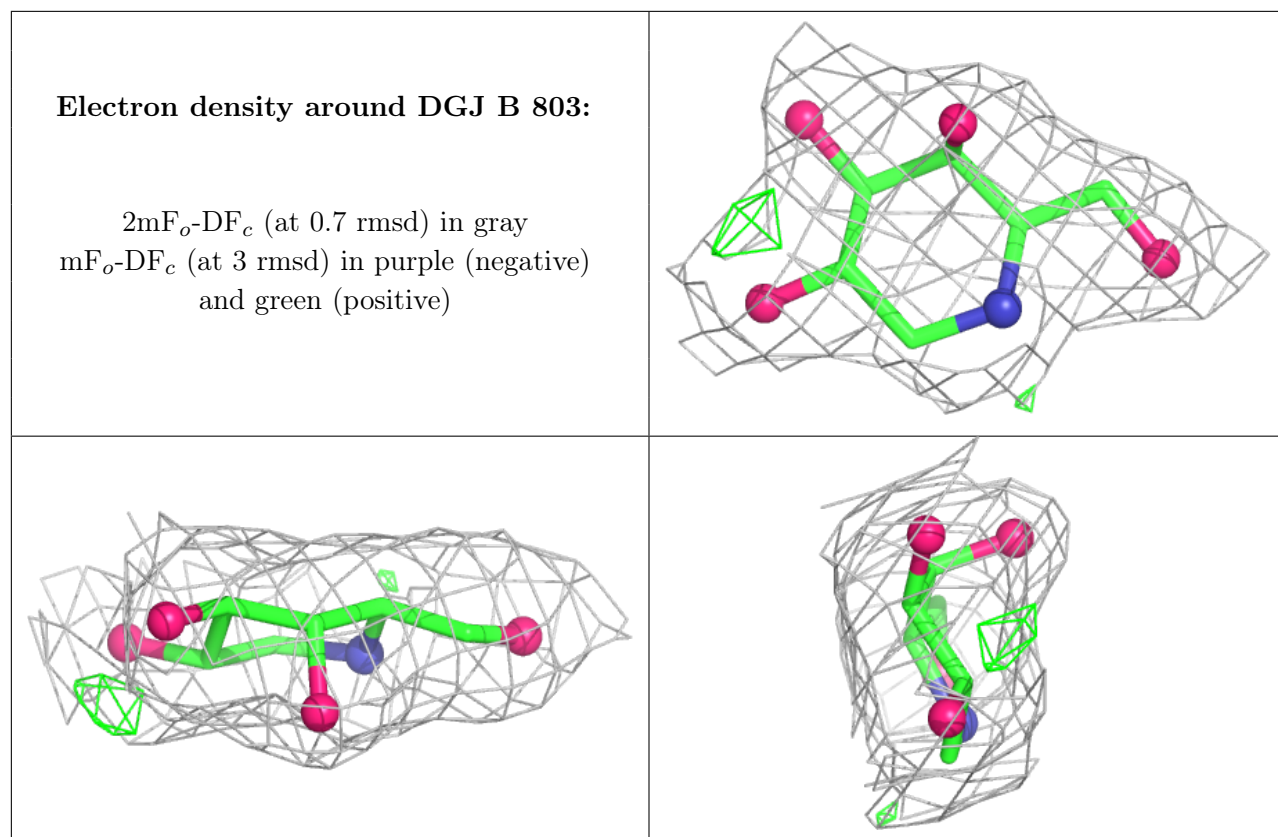
6.5 Other polymers (i)

There are no such residues in this entry.