



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 09:42 AM BST

PDB ID : 6G4G
Title : Full length ectodomain of ectonucleotide phosphodiesterase/pyrophosphatase
-3 (NPP3) including the SMB domains but with a partially disordered active
site structure
Authors : Dohler, C.; Zebisch, M.; Strater, N.
Deposited on : 2018-03-27
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

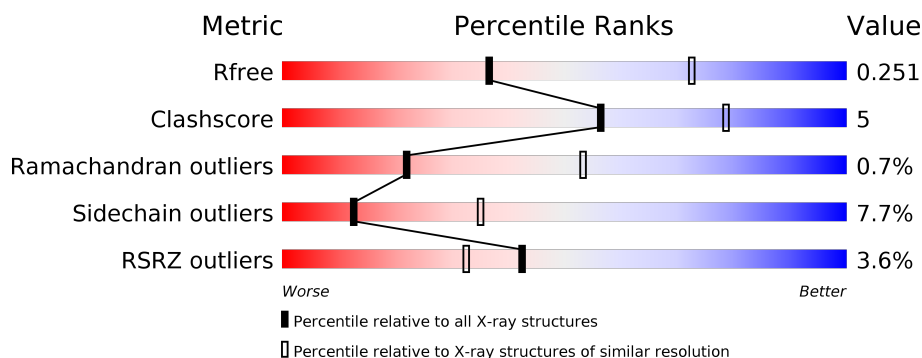
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



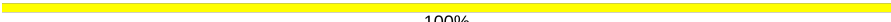
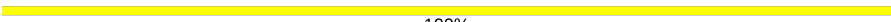
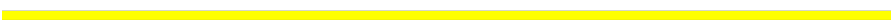
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	840	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>• 9%</div> </div> </div>
1	B	840	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>• 10%</div> </div> </div>
1	C	840	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>18%</div> <div>• 12%</div> </div> </div>
1	D	840	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>17%</div> <div>• 7%</div> </div> </div>
2	E	2	<div> <div></div> <div>100%</div> </div>
2	F	2	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	2	 100%
2	H	2	 100%
2	I	2	 100%
2	J	2	 100%
2	K	2	 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24786 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 Ectonucleotide pyrophosphatase/phosphodiesterase family member 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	765	Total	C	N	O	S	0	0	0
			6131	3903	1040	1140	48			
1	B	759	Total	C	N	O	S	0	0	0
			6087	3871	1035	1134	47			
1	C	742	Total	C	N	O	S	0	0	0
			5982	3818	1016	1102	46			
1	D	781	Total	C	N	O	S	0	0	0
			6274	3991	1064	1171	48			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	ALA	-	expression tag	UNP P97675
A	46	GLU	-	expression tag	UNP P97675
A	47	THR	-	expression tag	UNP P97675
A	48	GLY	-	expression tag	UNP P97675
A	201	VAL	MET	variant	UNP P97675
A	596	ASN	SER	variant	UNP P97675
A	597	ARG	GLY	variant	UNP P97675
A	876	GLY	-	expression tag	UNP P97675
A	877	THR	-	expression tag	UNP P97675
A	878	LYS	-	expression tag	UNP P97675
A	879	HIS	-	expression tag	UNP P97675
A	880	HIS	-	expression tag	UNP P97675
A	881	HIS	-	expression tag	UNP P97675
A	882	HIS	-	expression tag	UNP P97675
A	883	HIS	-	expression tag	UNP P97675
A	884	HIS	-	expression tag	UNP P97675
B	45	ALA	-	expression tag	UNP P97675
B	46	GLU	-	expression tag	UNP P97675
B	47	THR	-	expression tag	UNP P97675
B	48	GLY	-	expression tag	UNP P97675

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Chain	Residue	Modelled	Actual	Comment	Reference
B	201	VAL	MET	variant	UNP P97675
B	596	ASN	SER	variant	UNP P97675
B	597	ARG	GLY	variant	UNP P97675
B	876	GLY	-	expression tag	UNP P97675
B	877	THR	-	expression tag	UNP P97675
B	878	LYS	-	expression tag	UNP P97675
B	879	HIS	-	expression tag	UNP P97675
B	880	HIS	-	expression tag	UNP P97675
B	881	HIS	-	expression tag	UNP P97675
B	882	HIS	-	expression tag	UNP P97675
B	883	HIS	-	expression tag	UNP P97675
B	884	HIS	-	expression tag	UNP P97675
C	45	ALA	-	expression tag	UNP P97675
C	46	GLU	-	expression tag	UNP P97675
C	47	THR	-	expression tag	UNP P97675
C	48	GLY	-	expression tag	UNP P97675
C	201	VAL	MET	variant	UNP P97675
C	596	ASN	SER	variant	UNP P97675
C	597	ARG	GLY	variant	UNP P97675
C	876	GLY	-	expression tag	UNP P97675
C	877	THR	-	expression tag	UNP P97675
C	878	LYS	-	expression tag	UNP P97675
C	879	HIS	-	expression tag	UNP P97675
C	880	HIS	-	expression tag	UNP P97675
C	881	HIS	-	expression tag	UNP P97675
C	882	HIS	-	expression tag	UNP P97675
C	883	HIS	-	expression tag	UNP P97675
C	884	HIS	-	expression tag	UNP P97675
D	45	ALA	-	expression tag	UNP P97675
D	46	GLU	-	expression tag	UNP P97675
D	47	THR	-	expression tag	UNP P97675
D	48	GLY	-	expression tag	UNP P97675
D	201	VAL	MET	variant	UNP P97675
D	596	ASN	SER	variant	UNP P97675
D	597	ARG	GLY	variant	UNP P97675
D	876	GLY	-	expression tag	UNP P97675
D	877	THR	-	expression tag	UNP P97675
D	878	LYS	-	expression tag	UNP P97675
D	879	HIS	-	expression tag	UNP P97675
D	880	HIS	-	expression tag	UNP P97675
D	881	HIS	-	expression tag	UNP P97675
D	882	HIS	-	expression tag	UNP P97675

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Chain	Residue	Modelled	Actual	Comment	Reference
D	883	HIS	-	expression tag	UNP P97675
D	884	HIS	-	expression tag	UNP P97675

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

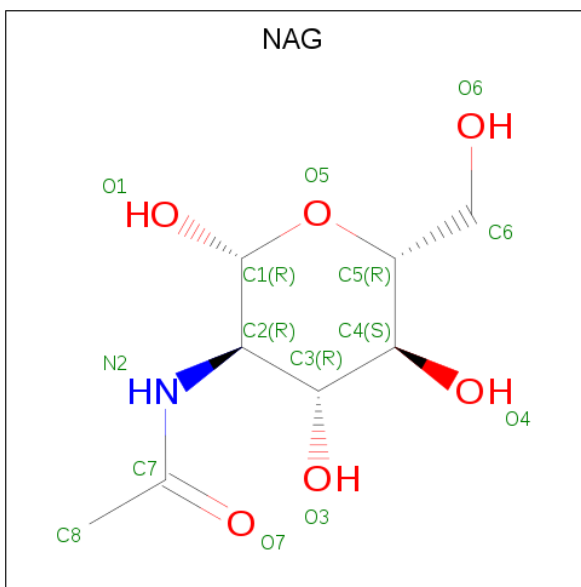


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

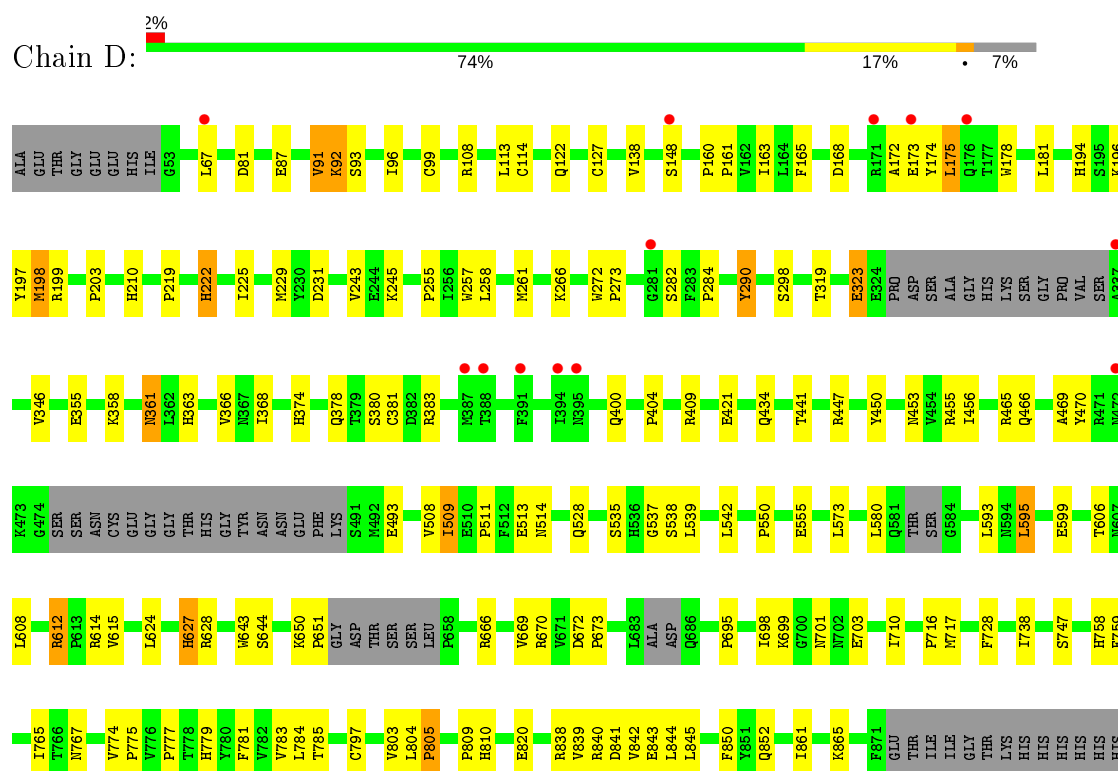
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: 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		
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	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 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 3



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

Chain E: 

NAG1
NAG2

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

Chain F: 

NAG1
NAG2

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

Chain G: 

NAG1
NAG2

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

Chain H: 

MAG1
MAG2

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

Chain I:  100%MAG1
MAG2

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

Chain J:  100%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

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.36 Å 116.30 Å 124.16 Å 86.77° 87.76° 88.20°	Depositor
Resolution (Å)	47.22 – 2.80 46.18 – 2.80	Depositor EDS
% Data completeness (in resolution range)	65.3 (47.22-2.80) 65.3 (46.18-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.81 Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.196 , 0.237 0.209 , 0.251	Depositor DCC
R_{free} test set	3360 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	59.9	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	24786	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.53	0/6303	0.72	0/8565
1	B	0.47	0/6254	0.70	0/8495
1	C	0.50	0/6148	0.70	0/8345
1	D	0.53	0/6449	0.75	1/8763 (0.0%)
All	All	0.51	0/25154	0.72	1/34168 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	99	CYS	C-N-CA	-5.60	107.69	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6131	0	5886	59	0
1	B	6087	0	5850	52	0
1	C	5982	0	5757	69	0
1	D	6274	0	6017	65	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	42	0	39	0	0
4	B	28	0	26	0	0
4	C	14	0	13	0	0
4	D	28	0	26	1	0
All	All	24786	0	23789	245	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 5.

All (245) 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:C:247:ASN:HD21	1:C:249:ALA:HB3	1.48	0.78
1:B:750:ILE:HD11	1:B:781:PHE:HB3	1.69	0.72
1:A:509:ILE:HD13	1:A:542:LEU:HD11	1.77	0.66
1:A:409:ARG:HH22	1:A:471:ARG:NE	1.94	0.66
1:A:550:PRO:HB2	1:A:858:VAL:HG12	1.78	0.65
1:D:840:ARG:O	1:D:844:LEU:HD12	1.97	0.65
1:B:688:ILE:HD11	1:B:716:PRO:HB2	1.79	0.65
1:C:231:ASP:HB2	1:C:455:ARG:HD2	1.79	0.64
1:B:231:ASP:HB2	1:B:455:ARG:HD2	1.79	0.64
1:A:409:ARG:HH22	1:A:471:ARG:HE	1.44	0.64
1:C:409:ARG:HH22	1:C:471:ARG:HE	1.45	0.64
1:B:509:ILE:HD13	1:B:542:LEU:HD11	1.78	0.64
1:A:231:ASP:HB2	1:A:455:ARG:HD2	1.79	0.64
1:C:409:ARG:HH22	1:C:471:ARG:NE	1.95	0.63
1:B:849:ASP:HB3	1:B:852:GLN:HE21	1.63	0.63
1:B:409:ARG:HH22	1:B:471:ARG:NE	1.96	0.63
1:B:409:ARG:HH22	1:B:471:ARG:HE	1.47	0.62
1:A:198:MET:CE	1:A:517:VAL:HG21	2.29	0.62
1:D:231:ASP:HB2	1:D:455:ARG:HD2	1.82	0.61
1:C:378:GLN:HB3	1:C:466:GLN:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:509:ILE:HD13	1:C:542:LEU:HD11	1.82	0.61
1:B:690:HIS:HB2	1:B:714:LEU:HD22	1.82	0.61
1:B:711:THR:HA	1:B:714:LEU:HD12	1.82	0.61
1:D:509:ILE:HD13	1:D:542:LEU:HD11	1.83	0.60
1:A:783:VAL:HG22	1:A:805:PRO:HB3	1.84	0.59
1:C:172:ALA:HA	1:C:175:LEU:HD12	1.84	0.59
1:B:270:TYR:CE1	1:B:299:ARG:HG2	2.37	0.59
1:B:608:LEU:HD11	1:B:631:VAL:HG11	1.84	0.58
1:D:666:ARG:HG3	1:D:710:ILE:HG22	1.86	0.58
1:D:172:ALA:HA	1:D:175:LEU:HD12	1.85	0.58
1:D:701:ASN:HD21	1:D:703:GLU:HG2	1.67	0.58
1:A:210:HIS:HB2	1:A:273:PRO:HG2	1.84	0.58
1:A:378:GLN:HB3	1:A:466:GLN:HG2	1.85	0.58
1:B:378:GLN:HB3	1:B:466:GLN:HG2	1.85	0.58
1:A:203:PRO:HD3	1:A:450:TYR:CE1	2.40	0.57
1:B:701:ASN:HD21	1:B:703:GLU:HG2	1.69	0.57
1:B:203:PRO:HD3	1:B:450:TYR:CE1	2.40	0.57
1:C:163:ILE:HD12	1:C:366:VAL:HG11	1.85	0.57
1:B:784:LEU:HB2	1:B:804:LEU:HB3	1.86	0.56
1:C:196:LYS:HB2	1:C:511:PRO:HG3	1.86	0.56
1:A:78:ASP:O	4:D:907:NAG:H4	2.05	0.56
1:A:860:GLU:O	1:A:863:GLN:HB2	2.05	0.56
1:C:638:MET:HE2	1:C:642:MET:HG2	1.88	0.56
1:A:849:ASP:HB3	1:A:852:GLN:HE21	1.70	0.56
1:C:400:GLN:HG2	1:C:470:TYR:HA	1.88	0.56
1:B:400:GLN:HG2	1:B:470:TYR:HA	1.88	0.56
1:C:638:MET:CE	1:C:642:MET:HG2	2.36	0.56
1:A:701:ASN:HD21	1:A:703:GLU:HG2	1.70	0.55
1:A:198:MET:HE1	1:A:517:VAL:HG21	1.87	0.55
1:B:89:THR:HG22	1:B:102:PHE:HB3	1.89	0.55
1:D:759:PHE:HB3	1:D:845:LEU:O	2.06	0.55
1:D:400:GLN:HG2	1:D:470:TYR:HA	1.89	0.55
1:D:203:PRO:HD3	1:D:450:TYR:CE1	2.42	0.55
1:D:378:GLN:HB3	1:D:466:GLN:HG2	1.88	0.55
1:A:400:GLN:HG2	1:A:470:TYR:HA	1.89	0.55
1:D:608:LEU:HD22	1:D:612:ARG:HA	1.89	0.55
1:C:225:ILE:HG12	1:C:455:ARG:HB3	1.89	0.54
1:D:163:ILE:HD12	1:D:366:VAL:HG11	1.90	0.54
1:A:642:MET:O	1:A:749:PRO:HD2	2.08	0.54
1:B:861:ILE:HG22	1:B:865:LYS:HE3	1.89	0.54
1:C:203:PRO:HD3	1:C:450:TYR:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:849:ASP:HB3	1:C:852:GLN:HE21	1.73	0.53
1:A:225:ILE:HG12	1:A:455:ARG:HB3	1.90	0.53
1:C:803:VAL:HG21	1:C:839:VAL:HG21	1.90	0.53
1:D:225:ILE:HG12	1:D:455:ARG:HB3	1.91	0.53
1:A:255:PRO:HD2	1:A:258:LEU:HD12	1.91	0.53
1:B:92:LYS:O	1:B:96:ILE:HG12	2.09	0.53
1:C:786:SER:HA	1:C:794:PRO:HG3	1.90	0.53
1:C:247:ASN:ND2	1:C:249:ALA:HB3	2.21	0.53
1:C:263:GLN:NE2	1:C:527:ILE:HB	2.24	0.53
1:C:96:ILE:HD11	1:C:103:ARG:HD2	1.91	0.53
1:B:750:ILE:HB	1:B:779:HIS:HB2	1.91	0.52
1:D:716:PRO:HG2	1:D:777:PRO:HD3	1.92	0.52
1:B:225:ILE:HG12	1:B:455:ARG:HB3	1.90	0.52
1:A:210:HIS:CB	1:A:273:PRO:HG2	2.40	0.52
1:D:698:ILE:HG23	1:D:699:LYS:HG3	1.91	0.51
1:D:839:VAL:O	1:D:842:VAL:HB	2.10	0.51
1:B:261:MET:HA	1:B:265:LEU:O	2.10	0.51
1:D:728:PHE:HZ	1:D:784:LEU:HD11	1.75	0.51
1:A:716:PRO:HG2	1:A:777:PRO:HD3	1.93	0.51
1:D:783:VAL:HG22	1:D:805:PRO:HB3	1.93	0.51
1:D:861:ILE:HG22	1:D:865:LYS:HE2	1.92	0.50
1:C:648:VAL:O	1:C:742:GLY:HA2	2.11	0.50
1:C:258:LEU:HA	1:C:261:MET:HE3	1.92	0.50
1:D:258:LEU:HA	1:D:261:MET:HE3	1.94	0.50
1:A:784:LEU:HD12	1:A:804:LEU:HD23	1.94	0.49
1:B:716:PRO:HG2	1:B:777:PRO:HD3	1.94	0.49
1:C:784:LEU:HB2	1:C:804:LEU:HB3	1.95	0.49
1:C:198:MET:HE1	1:C:371:LEU:HD22	1.95	0.49
1:D:537:GLY:HA3	1:D:550:PRO:HG3	1.95	0.49
1:D:651:PRO:HD2	1:D:738:ILE:HG13	1.94	0.49
1:A:453:ASN:OD1	1:A:455:ARG:HB2	2.13	0.49
1:C:747:SER:HA	1:C:781:PHE:O	2.13	0.49
1:C:784:LEU:HD12	1:C:804:LEU:HD23	1.94	0.49
1:B:258:LEU:HA	1:B:261:MET:HE3	1.93	0.48
1:B:580:LEU:HD23	1:B:586:GLU:HG3	1.95	0.48
1:A:784:LEU:HB2	1:A:804:LEU:HB3	1.94	0.48
1:A:71:ARG:CZ	1:A:79:ARG:HE	2.27	0.48
1:B:651:PRO:HD2	1:B:738:ILE:HG13	1.93	0.48
1:B:453:ASN:OD1	1:B:455:ARG:HB2	2.13	0.48
1:B:255:PRO:HD2	1:B:258:LEU:HD12	1.94	0.48
1:C:513:GLU:HG2	1:C:515:ILE:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:PRO:HD2	1:C:258:LEU:HD12	1.95	0.48
1:B:801:LEU:HB2	1:B:864:LEU:HD21	1.96	0.48
1:A:163:ILE:HD12	1:A:366:VAL:HG11	1.96	0.48
1:A:258:LEU:HA	1:A:261:MET:HE3	1.95	0.48
1:C:743:VAL:HG23	1:C:786:SER:HB3	1.96	0.48
1:A:651:PRO:HD2	1:A:738:ILE:HG13	1.96	0.47
1:C:765:ILE:HG21	1:C:775:PRO:HB3	1.96	0.47
1:D:765:ILE:HG21	1:D:775:PRO:HB3	1.96	0.47
1:A:550:PRO:HB2	1:A:858:VAL:CG1	2.45	0.47
1:D:255:PRO:HD2	1:D:258:LEU:HD12	1.97	0.47
1:A:270:TYR:CE1	1:A:299:ARG:HG2	2.49	0.47
1:C:404:PRO:HG2	1:C:469:ALA:HB3	1.97	0.47
1:C:174:TYR:HB3	1:C:181:LEU:HD12	1.95	0.47
1:A:441:THR:HG21	1:A:456:ILE:HG22	1.96	0.46
1:C:560:ALA:O	1:C:623:CYS:HB3	2.16	0.46
1:C:100:ASN:H	1:C:103:ARG:HB2	1.79	0.46
1:C:100:ASN:O	1:C:101:SER:C	2.54	0.46
1:A:747:SER:HA	1:A:781:PHE:O	2.15	0.46
1:A:743:VAL:HA	1:A:794:PRO:HG2	1.98	0.46
1:B:535:SER:HB3	1:B:862:LEU:HD22	1.98	0.46
1:D:290:TYR:OH	1:D:323:GLU:HG3	2.16	0.46
1:A:634:PHE:HA	1:A:641:PRO:HA	1.98	0.46
1:A:641:PRO:HG2	1:A:693:LEU:HD23	1.97	0.45
1:A:89:THR:HG22	1:A:102:PHE:HB3	1.98	0.45
1:C:750:ILE:HD11	1:C:781:PHE:HB3	1.99	0.45
1:C:695:PRO:HG3	1:C:729:HIS:HD2	1.82	0.45
1:C:838:ARG:O	1:C:841:ASP:HB2	2.17	0.45
1:C:839:VAL:HB	1:C:865:LYS:HA	1.99	0.45
1:D:361:ASN:HA	1:D:361:ASN:HD22	1.64	0.45
1:D:643:TRP:HA	1:D:747:SER:O	2.16	0.45
1:A:765:ILE:HG21	1:A:775:PRO:HB3	1.97	0.45
1:A:225:ILE:HG13	1:A:229:MET:SD	2.57	0.45
1:C:634:PHE:HA	1:C:641:PRO:HA	1.98	0.45
1:C:71:ARG:CZ	1:C:79:ARG:HE	2.30	0.45
1:D:779:HIS:CD2	1:D:809:PRO:HA	2.52	0.45
1:A:198:MET:CE	1:A:517:VAL:CG2	2.94	0.45
1:C:453:ASN:OD1	1:C:455:ARG:HB2	2.16	0.45
1:D:573:LEU:HD21	1:D:673:PRO:HB3	1.99	0.45
1:D:843:GLU:HG2	1:D:850:PHE:CD2	2.52	0.45
1:B:441:THR:HG21	1:B:456:ILE:HG22	1.99	0.44
1:B:71:ARG:CZ	1:B:79:ARG:HE	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:716:PRO:HG2	1:C:777:PRO:HD3	1.98	0.44
1:D:404:PRO:HG2	1:D:469:ALA:HB3	1.99	0.44
1:A:779:HIS:CD2	1:A:809:PRO:HA	2.52	0.44
1:A:785:THR:HG21	1:A:851:TYR:CE1	2.51	0.44
1:C:441:THR:HG21	1:C:456:ILE:HG22	2.00	0.44
1:D:441:THR:HG21	1:D:456:ILE:HG22	1.99	0.44
1:A:717:MET:HA	1:A:810:HIS:NE2	2.33	0.44
1:B:573:LEU:HD21	1:B:673:PRO:HB3	2.00	0.44
1:B:765:ILE:HG21	1:B:775:PRO:HB3	2.00	0.44
1:D:225:ILE:HG13	1:D:229:MET:SD	2.57	0.44
1:A:95:GLN:HB3	1:A:95:GLN:HE21	1.40	0.44
1:B:614:ARG:O	1:B:848:LEU:HA	2.17	0.44
1:D:380:SER:HB2	1:D:383:ARG:NH2	2.33	0.44
1:D:174:TYR:HB3	1:D:181:LEU:HD12	2.00	0.43
1:D:87:GLU:O	1:D:91:VAL:HG12	2.18	0.43
1:B:160:PRO:HA	1:B:161:PRO:HD3	1.95	0.43
1:C:717:MET:HA	1:C:810:HIS:NE2	2.33	0.43
1:A:861:ILE:HG22	1:A:865:LYS:HE3	1.99	0.43
1:C:225:ILE:HG13	1:C:229:MET:SD	2.58	0.43
1:C:695:PRO:HG3	1:C:729:HIS:CD2	2.53	0.43
1:D:595:LEU:HD13	1:D:599:GLU:HB3	2.00	0.43
1:D:198:MET:HE3	1:D:198:MET:HB2	1.76	0.43
1:D:555:GLU:HG3	1:D:615:VAL:N	2.34	0.43
1:D:717:MET:HA	1:D:810:HIS:NE2	2.33	0.43
1:D:160:PRO:HA	1:D:161:PRO:HD3	1.90	0.43
1:B:404:PRO:HG2	1:B:469:ALA:HB3	2.00	0.43
1:C:777:PRO:HG2	1:C:780:TYR:CZ	2.53	0.43
1:C:535:SER:HB3	1:C:862:LEU:HD22	2.00	0.43
1:B:198:MET:HG3	1:B:496:PHE:HB2	2.00	0.43
1:D:91:VAL:CG1	1:D:92:LYS:N	2.81	0.43
1:B:225:ILE:HG13	1:B:229:MET:SD	2.59	0.43
1:D:87:GLU:OE1	1:D:91:VAL:HG11	2.18	0.43
1:A:743:VAL:HG23	1:A:786:SER:HB3	2.01	0.43
1:B:199:ARG:HB3	1:B:513:GLU:HG3	2.00	0.43
1:D:196:LYS:HB2	1:D:511:PRO:HG3	1.99	0.43
1:A:268:ALA:HA	1:A:286:ILE:O	2.18	0.42
1:B:96:ILE:HG22	1:B:98:THR:H	1.83	0.42
1:B:268:ALA:HA	1:B:286:ILE:O	2.19	0.42
1:C:562:CYS:HB2	1:C:623:CYS:HB2	1.87	0.42
1:D:838:ARG:HG3	1:D:841:ASP:OD2	2.19	0.42
1:A:358:LYS:HA	1:A:363:HIS:ND1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:MET:CE	1:D:284:PRO:HA	2.49	0.42
1:A:261:MET:CE	1:A:284:PRO:HA	2.49	0.42
1:C:750:ILE:HB	1:C:779:HIS:HB2	2.00	0.42
1:D:861:ILE:O	1:D:865:LYS:HG3	2.20	0.42
1:C:199:ARG:HB3	1:C:513:GLU:HA	2.01	0.42
1:C:261:MET:HA	1:C:265:LEU:O	2.19	0.42
1:B:261:MET:CE	1:B:284:PRO:HA	2.50	0.42
1:C:688:ILE:HD11	1:C:716:PRO:HB2	2.01	0.42
1:D:627:HIS:CD2	1:D:670:ARG:HH12	2.37	0.42
1:C:182:LEU:HD21	1:C:343:LEU:HB3	2.01	0.42
1:C:87:GLU:O	1:C:91:VAL:HB	2.19	0.42
1:B:200:ALA:HA	1:B:514:ASN:ND2	2.34	0.42
1:D:650:LYS:HA	1:D:651:PRO:HD3	1.86	0.42
1:C:861:ILE:HG22	1:C:865:LYS:HE3	2.02	0.42
1:C:238:PHE:CE2	1:C:245:LYS:HA	2.55	0.42
1:C:695:PRO:O	1:C:698:ILE:HG22	2.20	0.42
1:D:539:LEU:HB3	1:D:542:LEU:HD13	2.02	0.42
1:B:717:MET:HA	1:B:810:HIS:NE2	2.34	0.41
1:C:358:LYS:HA	1:C:363:HIS:ND1	2.35	0.41
1:D:747:SER:HA	1:D:781:PHE:O	2.19	0.41
1:A:261:MET:HA	1:A:265:LEU:O	2.21	0.41
1:D:210:HIS:HB2	1:D:273:PRO:HG2	2.02	0.41
1:D:695:PRO:O	1:D:698:ILE:HG22	2.20	0.41
1:A:688:ILE:HD11	1:A:716:PRO:HB2	2.02	0.41
1:B:358:LYS:HA	1:B:363:HIS:ND1	2.35	0.41
1:A:271:TYR:CD1	1:A:290:TYR:HA	2.56	0.41
1:B:838:ARG:O	1:B:841:ASP:HB2	2.20	0.41
1:C:564:PHE:CE1	1:C:594:ASN:HB2	2.55	0.41
1:C:219:PRO:HA	1:C:222:HIS:CE1	2.56	0.41
1:B:196:LYS:HB2	1:B:511:PRO:HG3	2.03	0.41
1:C:257:TRP:O	1:C:261:MET:HG3	2.20	0.41
1:D:358:LYS:HA	1:D:363:HIS:ND1	2.35	0.41
1:A:247:ASN:HB3	1:A:250:TRP:HD1	1.86	0.41
1:C:361:ASN:HA	1:C:361:ASN:HD22	1.72	0.41
1:D:784:LEU:HD12	1:D:804:LEU:HD23	2.02	0.41
1:A:194:HIS:CE1	1:A:508:VAL:HG22	2.56	0.41
1:B:650:LYS:HA	1:B:651:PRO:HD3	1.86	0.41
1:D:535:SER:O	1:D:538:SER:HB3	2.20	0.41
1:A:573:LEU:HD21	1:A:673:PRO:HB3	2.03	0.41
1:D:194:HIS:CE1	1:D:508:VAL:HG22	2.56	0.41
1:D:197:TYR:HE1	1:D:374:HIS:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:LEU:HD23	1:B:261:MET:CE	2.51	0.41
1:C:342:ALA:HA	1:C:345:LEU:HD12	2.03	0.41
1:A:219:PRO:HA	1:A:222:HIS:CE1	2.56	0.40
1:A:217:LEU:HB2	1:A:222:HIS:HB3	2.03	0.40
1:A:258:LEU:HD23	1:A:261:MET:CE	2.51	0.40
1:C:261:MET:CE	1:C:284:PRO:HA	2.51	0.40
1:D:258:LEU:HD23	1:D:261:MET:CE	2.51	0.40
1:D:198:MET:HE1	1:D:514:ASN:HA	2.04	0.40
1:D:614:ARG:HD3	1:D:852:GLN:HG3	2.03	0.40
1:A:695:PRO:O	1:A:698:ILE:HG22	2.21	0.40
1:B:194:HIS:CE1	1:B:508:VAL:HG22	2.56	0.40
1:B:71:ARG:HH12	1:B:76:CYS:HA	1.87	0.40
1:D:219:PRO:HA	1:D:222:HIS:CE1	2.57	0.40
1:D:257:TRP:O	1:D:261:MET:HG3	2.22	0.40
1:A:257:TRP:O	1:A:261:MET:HG3	2.21	0.40
1:C:537:GLY:HA3	1:C:550:PRO:HG3	2.03	0.40
1:C:268:ALA:HA	1:C:286:ILE:O	2.21	0.40
1:C:595:LEU:HD13	1:C:599:GLU:HB3	2.04	0.40
1:D:199:ARG:HB3	1:D:513:GLU:HG3	2.03	0.40
1:D:453:ASN:OD1	1:D:455:ARG:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	751/840 (89%)	700 (93%)	47 (6%)	4 (0%)	29 61
1	B	745/840 (89%)	694 (93%)	44 (6%)	7 (1%)	17 46
1	C	724/840 (86%)	674 (93%)	44 (6%)	6 (1%)	19 49
1	D	769/840 (92%)	710 (92%)	54 (7%)	5 (1%)	22 53
All	All	2989/3360 (89%)	2778 (93%)	189 (6%)	22 (1%)	22 53

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	683	LEU
1	B	820	GLU
1	D	148	SER
1	A	820	GLU
1	C	820	GLU
1	D	290	TYR
1	A	148	SER
1	A	434	GLN
1	B	434	GLN
1	C	271	TYR
1	C	434	GLN
1	C	855	THR
1	D	434	GLN
1	B	373	ASP
1	B	684	ALA
1	C	821	ASN
1	D	93	SER
1	B	855	THR
1	D	272	TRP
1	C	669	VAL
1	A	616	ILE
1	B	272	TRP

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	686/749 (92%)	637 (93%)	49 (7%)	14	39
1	B	680/749 (91%)	631 (93%)	49 (7%)	14	38
1	C	665/749 (89%)	609 (92%)	56 (8%)	11	31
1	D	701/749 (94%)	645 (92%)	56 (8%)	12	34
All	All	2732/2996 (91%)	2522 (92%)	210 (8%)	13	35

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	81	ASP
1	A	92	LYS
1	A	95	GLN
1	A	96	ILE
1	A	113	LEU
1	A	127	CYS
1	A	138	VAL
1	A	155	GLU
1	A	165	PHE
1	A	168	ASP
1	A	222	HIS
1	A	245	LYS
1	A	298	SER
1	A	319	THR
1	A	323	GLU
1	A	346	VAL
1	A	355	GLU
1	A	361	ASN
1	A	368	ILE
1	A	376	MET
1	A	381	CYS
1	A	409	ARG
1	A	413	GLN
1	A	421	GLU
1	A	447	ARG
1	A	493	GLU
1	A	509	ILE
1	A	528	GLN
1	A	538	SER
1	A	593	LEU
1	A	595	LEU
1	A	610	PHE
1	A	612	ARG
1	A	624	LEU
1	A	627	HIS
1	A	628	ARG
1	A	644	SER
1	A	669	VAL
1	A	672	ASP
1	A	683	LEU
1	A	704	SER
1	A	774	VAL

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Mol	Chain	Res	Type
1	A	797	CYS
1	A	817	SER
1	A	820	GLU
1	A	836	ILE
1	A	849	ASP
1	A	859	SER
1	B	65	ARG
1	B	77	THR
1	B	81	ASP
1	B	95	GLN
1	B	108	ARG
1	B	113	LEU
1	B	114	CYS
1	B	127	CYS
1	B	138	VAL
1	B	165	PHE
1	B	167	MET
1	B	168	ASP
1	B	198	MET
1	B	222	HIS
1	B	245	LYS
1	B	282	SER
1	B	298	SER
1	B	319	THR
1	B	323	GLU
1	B	355	GLU
1	B	361	ASN
1	B	368	ILE
1	B	376	MET
1	B	381	CYS
1	B	409	ARG
1	B	421	GLU
1	B	447	ARG
1	B	493	GLU
1	B	509	ILE
1	B	515	ILE
1	B	523	ASP
1	B	528	GLN
1	B	580	LEU
1	B	593	LEU
1	B	595	LEU
1	B	610	PHE

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Mol	Chain	Res	Type
1	B	612	ARG
1	B	624	LEU
1	B	627	HIS
1	B	628	ARG
1	B	672	ASP
1	B	683	LEU
1	B	687	ASN
1	B	767	ASN
1	B	774	VAL
1	B	797	CYS
1	B	817	SER
1	B	836	ILE
1	B	839	VAL
1	C	57	LYS
1	C	67	LEU
1	C	81	ASP
1	C	96	ILE
1	C	108	ARG
1	C	110	GLU
1	C	113	LEU
1	C	114	CYS
1	C	122	GLN
1	C	127	CYS
1	C	138	VAL
1	C	150	GLU
1	C	165	PHE
1	C	173	GLU
1	C	175	LEU
1	C	178	TRP
1	C	212	THR
1	C	222	HIS
1	C	245	LYS
1	C	270	TYR
1	C	282	SER
1	C	293	SER
1	C	298	SER
1	C	319	THR
1	C	323	GLU
1	C	346	VAL
1	C	355	GLU
1	C	361	ASN
1	C	368	ILE

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Mol	Chain	Res	Type
1	C	381	CYS
1	C	382	ASP
1	C	409	ARG
1	C	421	GLU
1	C	447	ARG
1	C	465	ARG
1	C	509	ILE
1	C	513	GLU
1	C	528	GLN
1	C	532	ASN
1	C	593	LEU
1	C	595	LEU
1	C	612	ARG
1	C	616	ILE
1	C	624	LEU
1	C	627	HIS
1	C	628	ARG
1	C	647	THR
1	C	669	VAL
1	C	710	ILE
1	C	767	ASN
1	C	774	VAL
1	C	785	THR
1	C	797	CYS
1	C	817	SER
1	C	822	LYS
1	C	859	SER
1	D	67	LEU
1	D	81	ASP
1	D	91	VAL
1	D	92	LYS
1	D	96	ILE
1	D	108	ARG
1	D	113	LEU
1	D	114	CYS
1	D	122	GLN
1	D	127	CYS
1	D	138	VAL
1	D	165	PHE
1	D	168	ASP
1	D	173	GLU
1	D	175	LEU

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Mol	Chain	Res	Type
1	D	178	TRP
1	D	198	MET
1	D	222	HIS
1	D	243	VAL
1	D	245	LYS
1	D	266	LYS
1	D	282	SER
1	D	298	SER
1	D	319	THR
1	D	323	GLU
1	D	346	VAL
1	D	355	GLU
1	D	361	ASN
1	D	368	ILE
1	D	381	CYS
1	D	409	ARG
1	D	421	GLU
1	D	447	ARG
1	D	465	ARG
1	D	493	GLU
1	D	509	ILE
1	D	528	GLN
1	D	580	LEU
1	D	593	LEU
1	D	595	LEU
1	D	606	THR
1	D	612	ARG
1	D	624	LEU
1	D	627	HIS
1	D	628	ARG
1	D	644	SER
1	D	669	VAL
1	D	672	ASP
1	D	758	HIS
1	D	767	ASN
1	D	774	VAL
1	D	785	THR
1	D	797	CYS
1	D	803	VAL
1	D	805	PRO
1	D	820	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	159	GLN
1	A	194	HIS
1	A	227	ASN
1	A	292	ASN
1	A	361	ASN
1	A	526	HIS
1	A	622	HIS
1	A	687	ASN
1	A	701	ASN
1	A	852	GLN
1	B	194	HIS
1	B	359	GLN
1	B	361	ASN
1	B	622	HIS
1	B	687	ASN
1	B	701	ASN
1	B	852	GLN
1	C	194	HIS
1	C	227	ASN
1	C	247	ASN
1	C	361	ASN
1	C	622	HIS
1	C	744	ASN
1	C	852	GLN
1	D	149	GLN
1	D	159	GLN
1	D	194	HIS
1	D	227	ASN
1	D	361	ASN
1	D	526	HIS
1	D	622	HIS
1	D	686	GLN
1	D	701	ASN
1	D	758	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 ⓘ

14 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	0.36	0	17,19,21	1.45	2 (11%)
2	NAG	E	2	2	14,14,15	0.33	0	17,19,21	1.07	1 (5%)
2	NAG	F	1	1,2	14,14,15	0.32	0	17,19,21	1.73	3 (17%)
2	NAG	F	2	2	14,14,15	0.37	0	17,19,21	1.12	1 (5%)
2	NAG	G	1	1,2	14,14,15	0.34	0	17,19,21	1.46	2 (11%)
2	NAG	G	2	2	14,14,15	0.31	0	17,19,21	1.03	1 (5%)
2	NAG	H	1	1,2	14,14,15	0.35	0	17,19,21	1.41	2 (11%)
2	NAG	H	2	2	14,14,15	0.32	0	17,19,21	0.99	1 (5%)
2	NAG	I	1	1,2	14,14,15	0.28	0	17,19,21	1.36	3 (17%)
2	NAG	I	2	2	14,14,15	0.33	0	17,19,21	0.81	1 (5%)
2	NAG	J	1	1,2	14,14,15	0.36	0	17,19,21	1.46	1 (5%)
2	NAG	J	2	2	14,14,15	0.33	0	17,19,21	1.04	1 (5%)
2	NAG	K	1	1,2	14,14,15	0.26	0	17,19,21	1.24	2 (11%)
2	NAG	K	2	2	14,14,15	0.34	0	17,19,21	1.20	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	-	0/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C1-O5-C5	5.78	120.02	112.19
2	G	1	NAG	O5-C1-C2	-5.22	103.05	111.29
2	J	1	NAG	O5-C1-C2	-5.18	103.11	111.29
2	E	1	NAG	O5-C1-C2	-4.89	103.57	111.29
2	H	1	NAG	O5-C1-C2	-4.73	103.81	111.29
2	E	2	NAG	C1-O5-C5	3.99	117.59	112.19
2	K	2	NAG	C1-O5-C5	3.92	117.51	112.19
2	G	2	NAG	C1-O5-C5	3.85	117.41	112.19
2	I	1	NAG	C1-O5-C5	3.64	117.12	112.19
2	J	2	NAG	C1-O5-C5	3.61	117.09	112.19
2	K	1	NAG	C1-O5-C5	3.56	117.01	112.19
2	H	2	NAG	C1-O5-C5	3.54	116.99	112.19
2	F	2	NAG	C1-O5-C5	3.47	116.89	112.19
2	E	1	NAG	C1-O5-C5	2.52	115.60	112.19
2	I	2	NAG	C1-O5-C5	2.51	115.59	112.19
2	I	1	NAG	O5-C1-C2	-2.41	107.48	111.29
2	F	1	NAG	C1-C2-N2	-2.33	106.51	110.49
2	H	1	NAG	C1-O5-C5	2.30	115.31	112.19
2	K	1	NAG	O5-C1-C2	-2.30	107.66	111.29
2	F	1	NAG	C3-C4-C5	2.28	114.31	110.24
2	G	1	NAG	C1-O5-C5	2.10	115.03	112.19
2	I	1	NAG	C1-C2-N2	-2.04	107.01	110.49

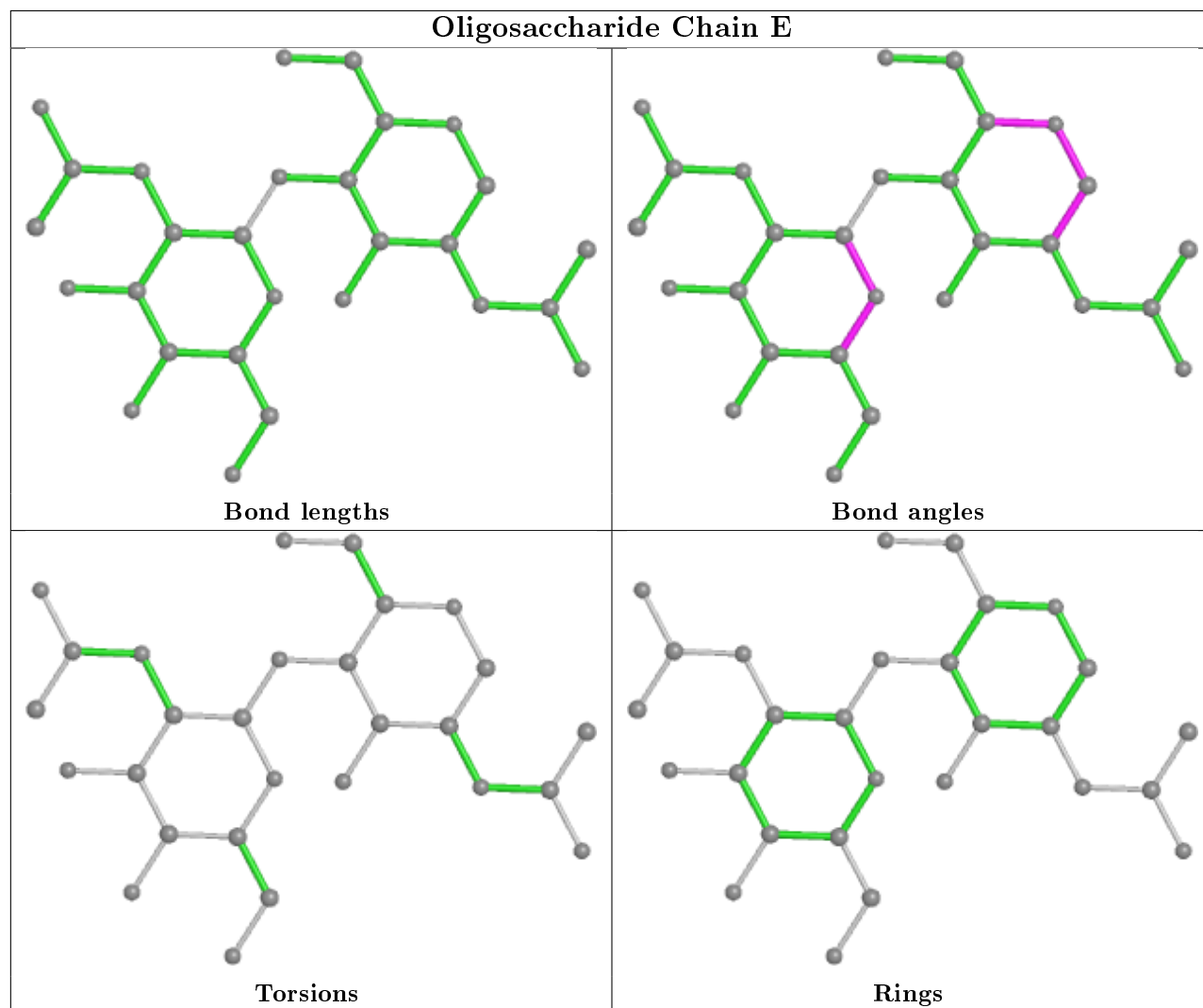
There are no chirality outliers.

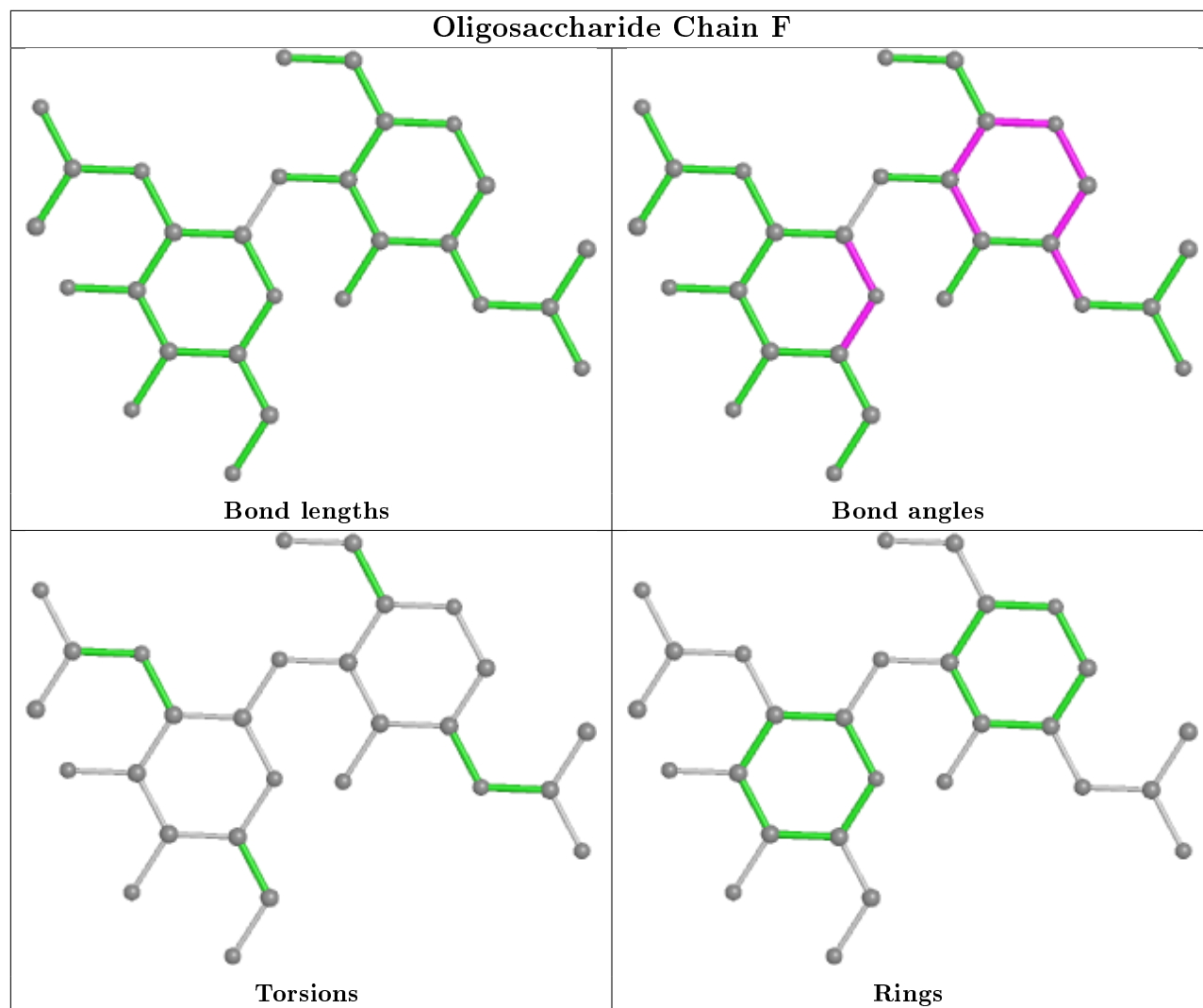
There are no torsion outliers.

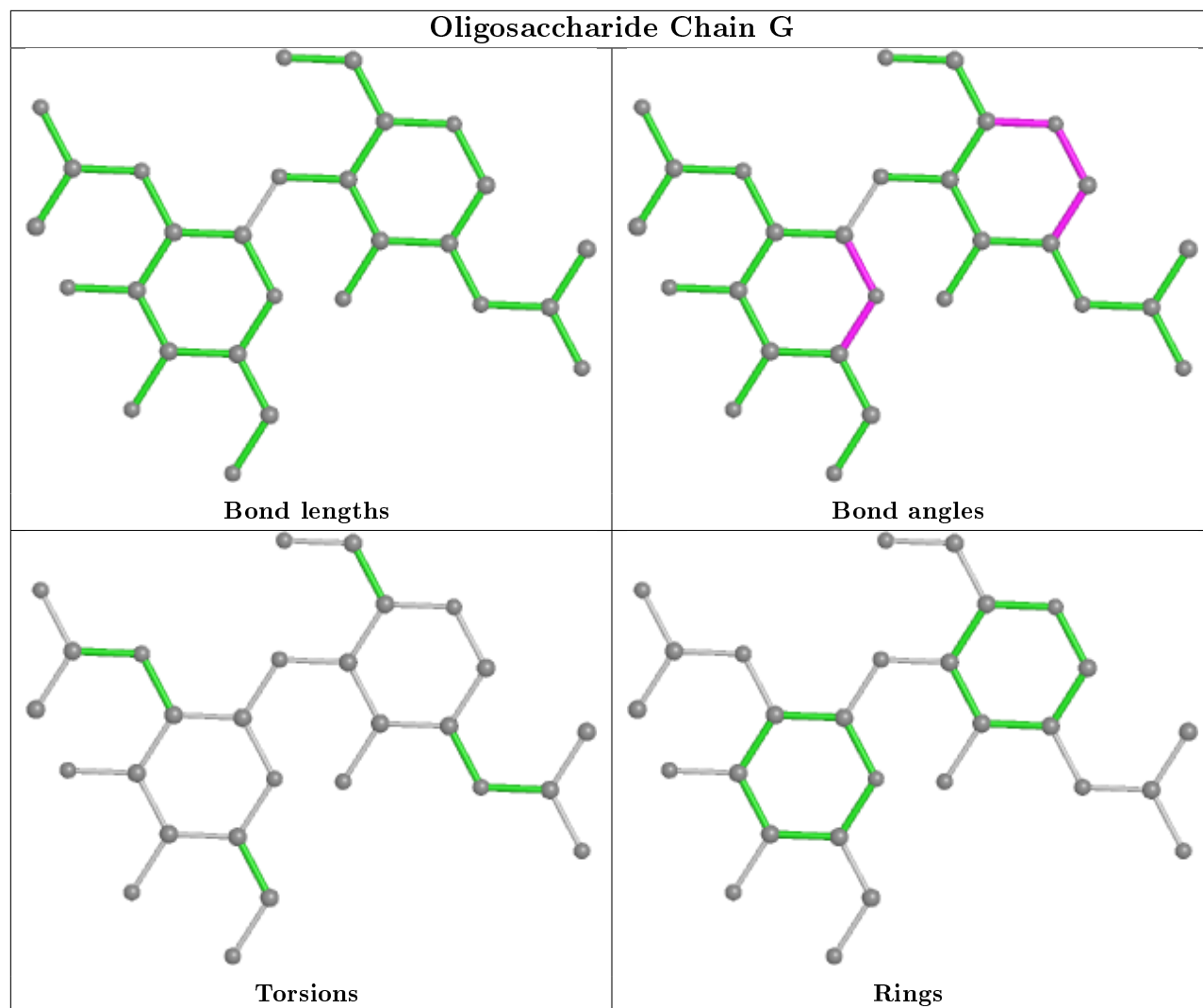
There are no ring outliers.

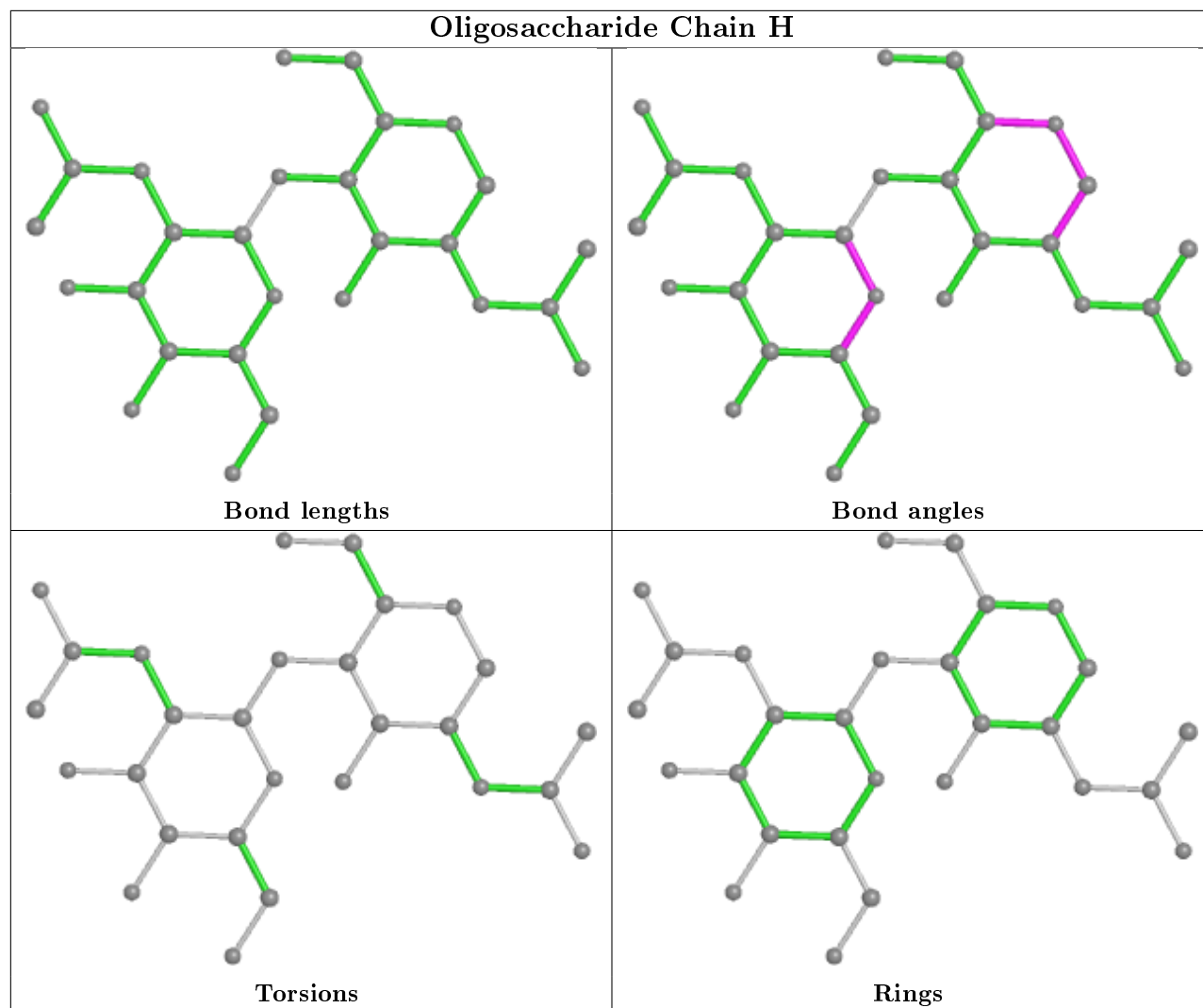
No monomer is involved in short contacts.

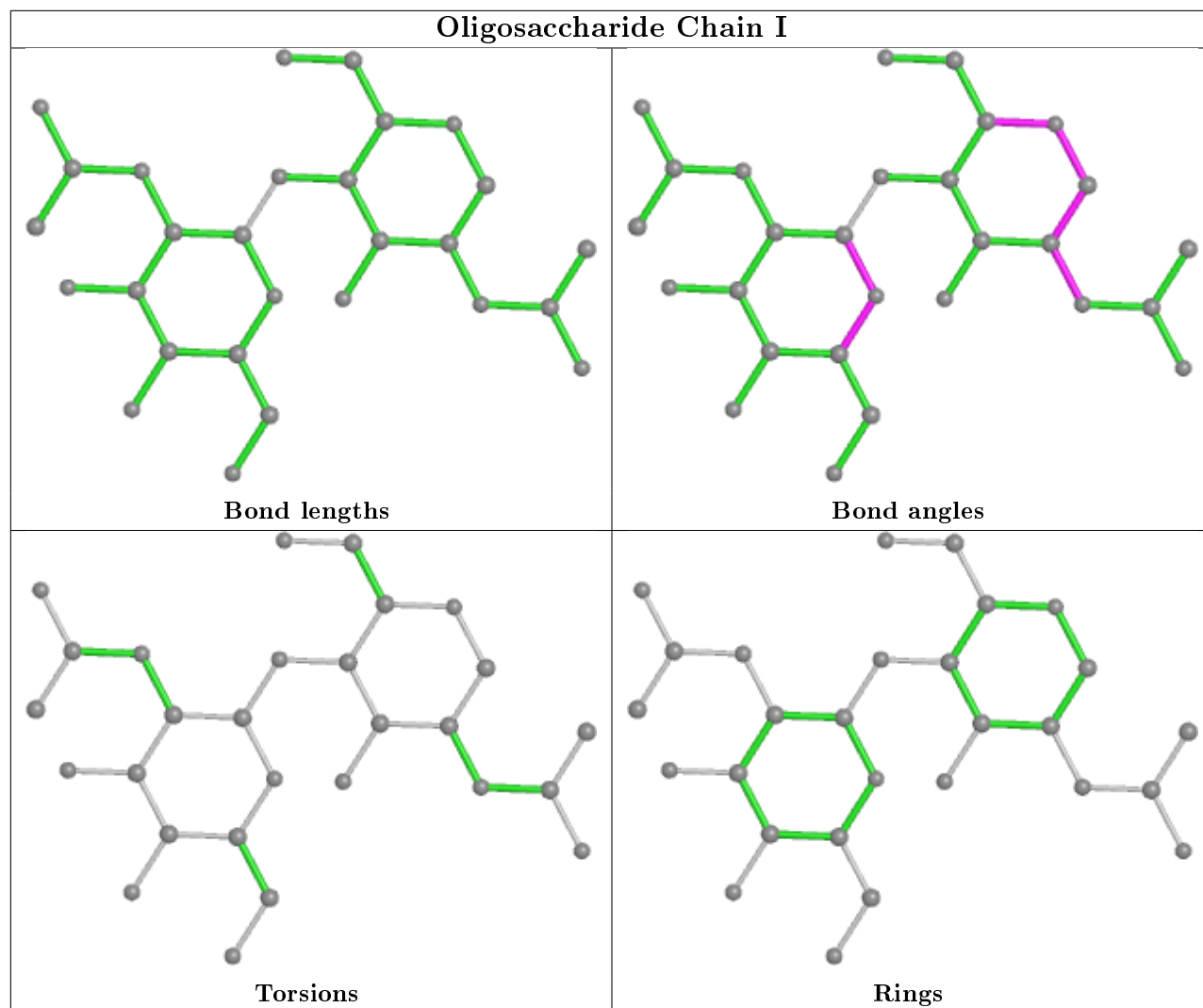
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

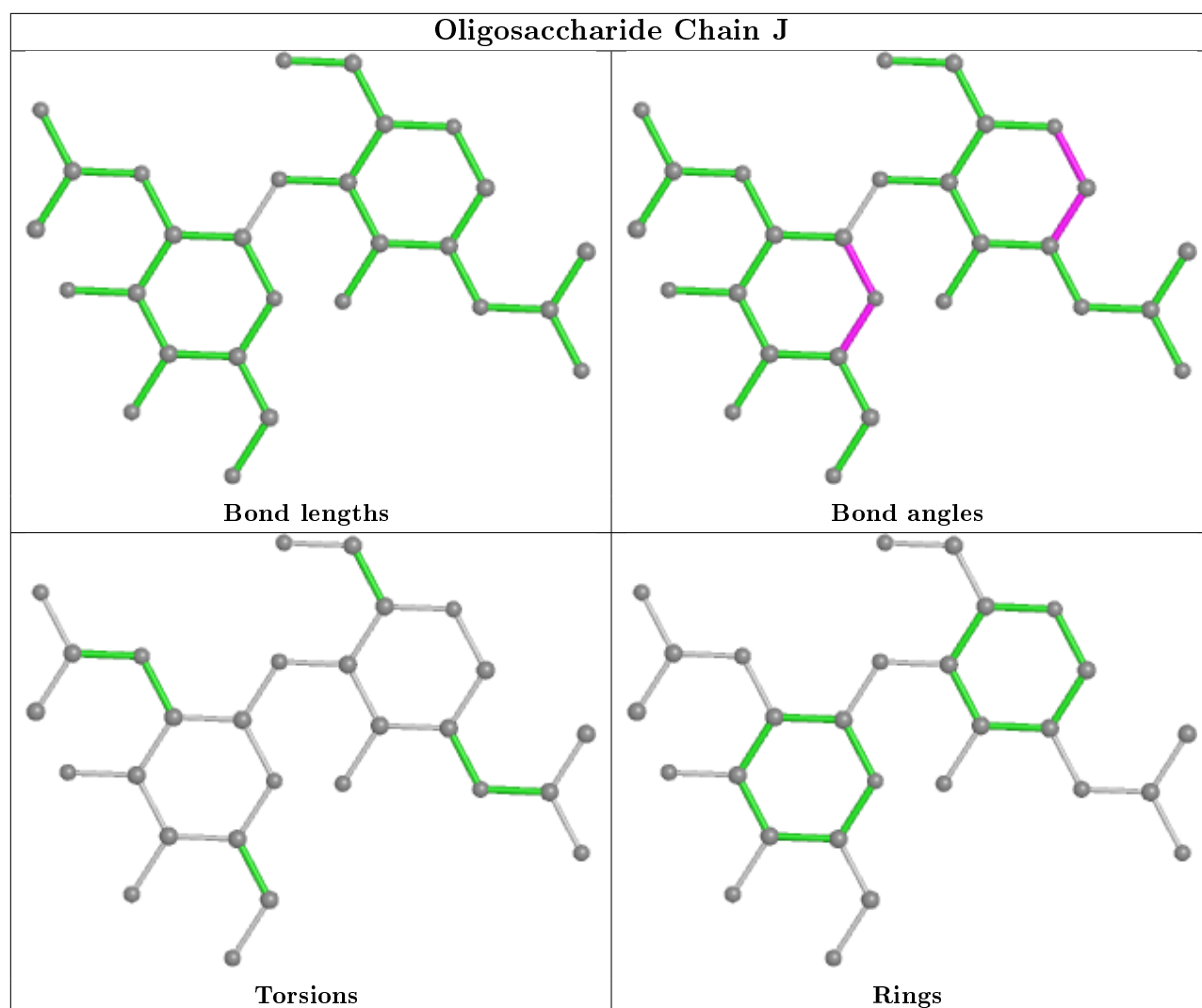


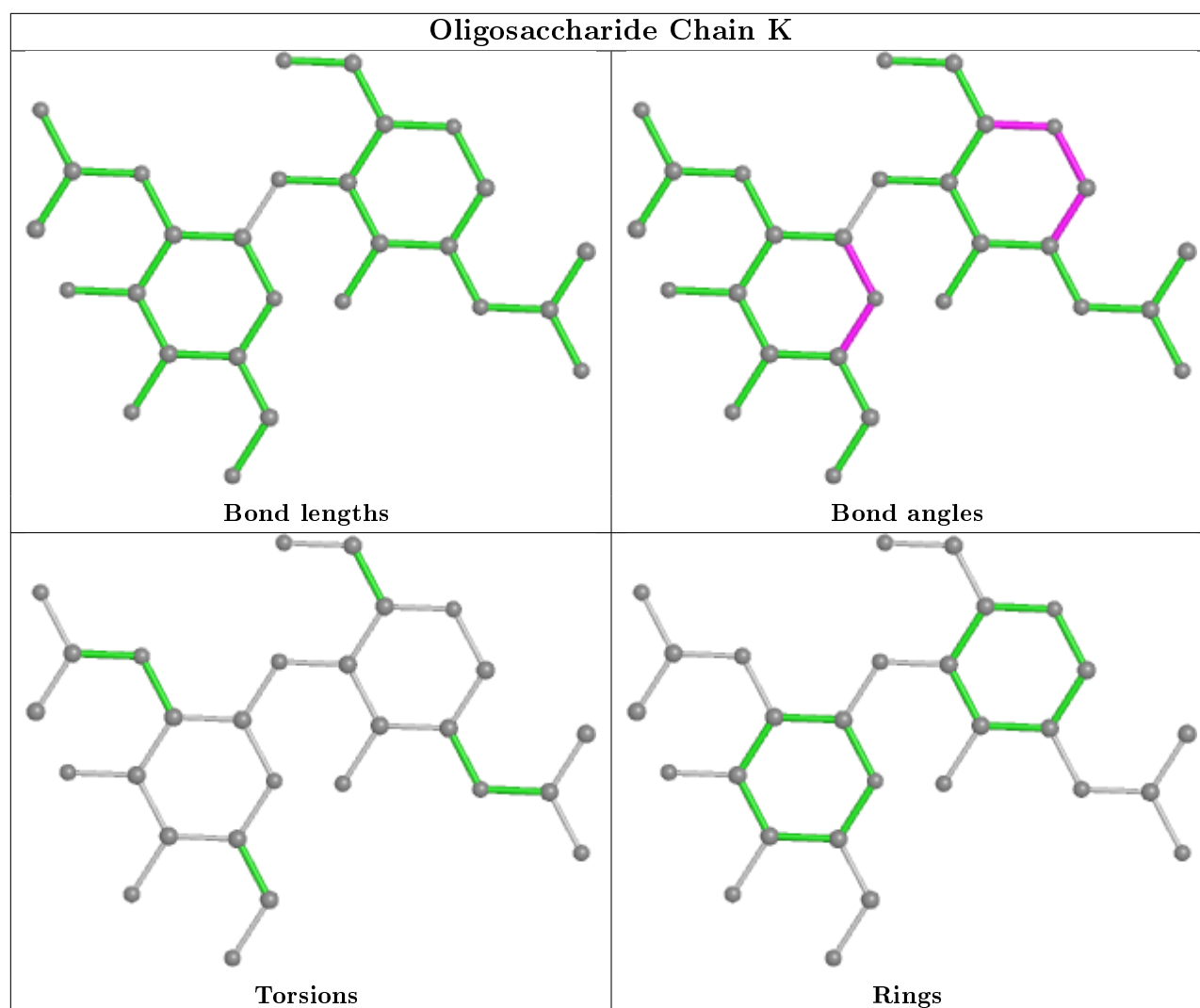












5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	904	1	14,14,15	0.31	0	17,19,21	1.07	2 (11%)
4	NAG	A	904	1	14,14,15	0.32	0	17,19,21	1.15	2 (11%)
4	NAG	D	904	1	14,14,15	0.29	0	17,19,21	1.11	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	904	1	14,14,15	0.32	0	17,19,21	1.08	2 (11%)
4	NAG	A	908	1	14,14,15	0.40	0	17,19,21	1.25	3 (17%)
4	NAG	B	905	1	14,14,15	0.32	0	17,19,21	1.07	1 (5%)
4	NAG	A	905	1	14,14,15	0.38	0	17,19,21	1.18	1 (5%)
4	NAG	D	907	1	14,14,15	0.40	0	17,19,21	1.36	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
4	NAG	B	904	1	-	1/6/23/26	0/1/1/1
4	NAG	A	904	1	-	1/6/23/26	0/1/1/1
4	NAG	D	904	1	-	1/6/23/26	0/1/1/1
4	NAG	C	904	1	-	1/6/23/26	0/1/1/1
4	NAG	A	908	1	-	1/6/23/26	0/1/1/1
4	NAG	B	905	1	-	0/6/23/26	0/1/1/1
4	NAG	A	905	1	-	2/6/23/26	0/1/1/1
4	NAG	D	907	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	907	NAG	C1-O5-C5	4.54	118.35	112.19
4	A	908	NAG	O5-C1-C2	-3.91	105.11	111.29
4	A	905	NAG	C1-O5-C5	3.60	117.07	112.19
4	D	904	NAG	O5-C1-C2	-3.18	106.26	111.29
4	A	904	NAG	O5-C1-C2	-3.10	106.40	111.29
4	C	904	NAG	O5-C1-C2	-2.97	106.60	111.29
4	B	905	NAG	C1-O5-C5	2.93	116.16	112.19
4	B	904	NAG	O5-C1-C2	-2.77	106.92	111.29
4	A	904	NAG	C1-O5-C5	2.62	115.75	112.19
4	B	904	NAG	C1-O5-C5	2.53	115.62	112.19
4	C	904	NAG	C1-O5-C5	2.48	115.55	112.19
4	D	904	NAG	C1-O5-C5	2.47	115.54	112.19
4	A	908	NAG	C1-O5-C5	2.08	115.01	112.19
4	A	908	NAG	C1-C2-N2	2.00	113.91	110.49

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	907	NAG	O5-C5-C6-O6
4	D	907	NAG	C4-C5-C6-O6
4	A	905	NAG	O5-C5-C6-O6
4	A	905	NAG	C4-C5-C6-O6
4	A	908	NAG	O5-C5-C6-O6
4	B	904	NAG	O5-C5-C6-O6
4	C	904	NAG	O5-C5-C6-O6
4	D	904	NAG	O5-C5-C6-O6
4	A	904	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
4	D	907	NAG	1	0

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	765/840 (91%)	-0.09	22 (2%)	51	41	28, 66, 114, 148	1 (0%)
1	B	759/840 (90%)	0.25	39 (5%)	28	19	56, 93, 127, 150	1 (0%)
1	C	742/840 (88%)	0.09	37 (4%)	28	19	43, 82, 126, 168	1 (0%)
1	D	781/840 (92%)	-0.22	13 (1%)	70	63	30, 61, 102, 130	1 (0%)
All	All	3047/3360 (90%)	0.01	111 (3%)	42	32	28, 76, 121, 168	4 (0%)

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	669	VAL	6.2
1	C	766	THR	5.0
1	A	65	ARG	5.0
1	C	731	VAL	4.6
1	C	394	ILE	4.6
1	C	739	GLU	4.6
1	C	101	SER	4.6
1	A	67	LEU	4.5
1	A	78	ASP	4.2
1	C	391	PHE	4.2
1	B	64	HIS	4.2
1	C	431	LYS	4.0
1	A	706	TYR	3.9
1	B	185	ILE	3.9
1	B	589	VAL	3.9
1	C	707	ASP	3.9
1	C	471	ARG	3.8
1	D	394	ILE	3.7
1	B	528	GLN	3.6
1	B	390	TYR	3.4
1	D	171	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	149	GLN	3.4
1	B	129	ASP	3.4
1	B	67	LEU	3.4
1	B	826	LEU	3.4
1	A	68	GLU	3.3
1	C	393	GLU	3.3
1	C	74	SER	3.3
1	C	64	HIS	3.3
1	A	578	LEU	3.3
1	A	661	VAL	3.3
1	A	66	GLY	3.3
1	C	388	THR	3.3
1	C	569	PRO	3.3
1	B	66	GLY	3.2
1	B	138	VAL	3.2
1	B	68	GLU	3.2
1	D	176	GLN	3.2
1	A	573	LEU	3.1
1	B	392	PRO	3.1
1	C	648	VAL	3.1
1	B	384	VAL	3.0
1	C	392	PRO	2.9
1	B	565	THR	2.9
1	C	426	ASP	2.8
1	C	380	SER	2.8
1	C	706	TYR	2.8
1	D	395	ASN	2.8
1	A	565	THR	2.8
1	B	554	GLU	2.8
1	B	53	GLY	2.8
1	C	395	ASN	2.7
1	C	102	PHE	2.7
1	C	738	ILE	2.7
1	C	688	ILE	2.7
1	A	64	HIS	2.7
1	C	422	GLU	2.7
1	C	708	ALA	2.7
1	B	386	TYR	2.7
1	B	871	PHE	2.7
1	B	472	ASN	2.7
1	C	698	ILE	2.6
1	A	572	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	380	SER	2.6
1	D	281	GLY	2.6
1	B	91	VAL	2.6
1	C	667	ALA	2.6
1	A	821	ASN	2.5
1	A	567	PRO	2.5
1	B	188	LEU	2.5
1	A	376	MET	2.5
1	A	53	GLY	2.5
1	A	702	ASN	2.5
1	A	79	ARG	2.4
1	D	337	ALA	2.4
1	A	568	LEU	2.4
1	C	67	LEU	2.4
1	B	282	SER	2.4
1	B	706	TYR	2.4
1	C	727	TYR	2.4
1	B	98	THR	2.4
1	B	65	ARG	2.4
1	B	548	TYR	2.3
1	C	472	ASN	2.3
1	A	554	GLU	2.3
1	D	148	SER	2.2
1	B	391	PHE	2.2
1	D	67	LEU	2.2
1	B	54	SER	2.2
1	A	81	ASP	2.2
1	C	595	LEU	2.2
1	B	365	CYS	2.2
1	A	393	GLU	2.2
1	B	363	HIS	2.1
1	D	391	PHE	2.1
1	B	62	SER	2.1
1	D	388	THR	2.1
1	C	150	GLU	2.1
1	C	382	ASP	2.1
1	B	621	ASP	2.1
1	D	173	GLU	2.1
1	B	233	TYR	2.1
1	B	377	ASP	2.1
1	C	711	THR	2.1
1	B	578	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	472	ASN	2.1
1	B	556	LEU	2.0
1	B	137	GLU	2.0
1	B	566	THR	2.0
1	D	387	MET	2.0
1	C	641	PRO	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](#)

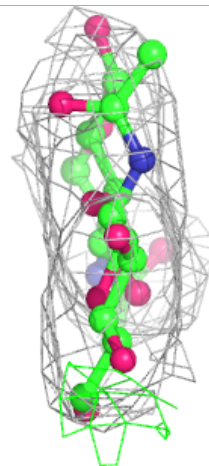
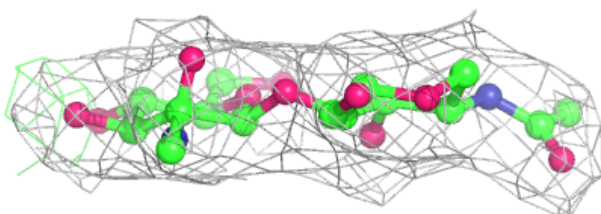
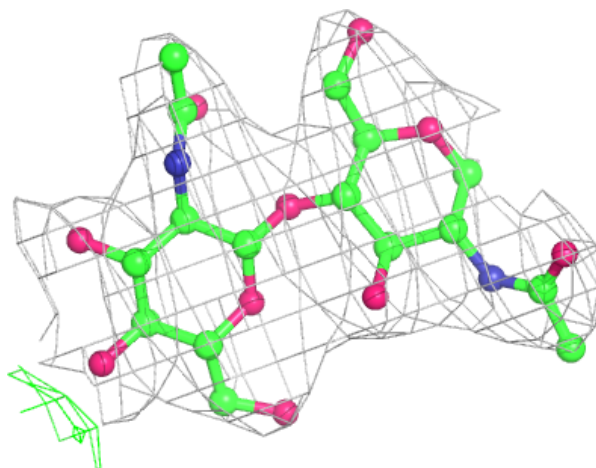
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	J	2	14/15	0.80	0.20	109,112,119,119	0
2	NAG	E	2	14/15	0.85	0.21	79,86,96,98	0
2	NAG	H	2	14/15	0.88	0.23	103,108,111,113	0
2	NAG	K	2	14/15	0.88	0.17	63,71,78,82	0
2	NAG	G	2	14/15	0.89	0.26	112,115,124,125	0
2	NAG	I	2	14/15	0.92	0.13	68,72,82,87	0
2	NAG	J	1	14/15	0.93	0.21	90,96,100,103	0
2	NAG	G	1	14/15	0.94	0.14	95,101,108,111	0
2	NAG	F	2	14/15	0.94	0.15	49,61,67,67	0
2	NAG	H	1	14/15	0.96	0.15	87,92,99,101	0
2	NAG	K	1	14/15	0.96	0.15	43,55,60,63	0
2	NAG	E	1	14/15	0.97	0.15	56,62,69,74	0
2	NAG	I	1	14/15	0.98	0.13	53,58,62,63	0
2	NAG	F	1	14/15	0.98	0.12	36,43,51,57	0

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

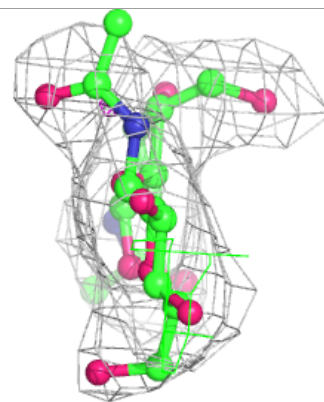
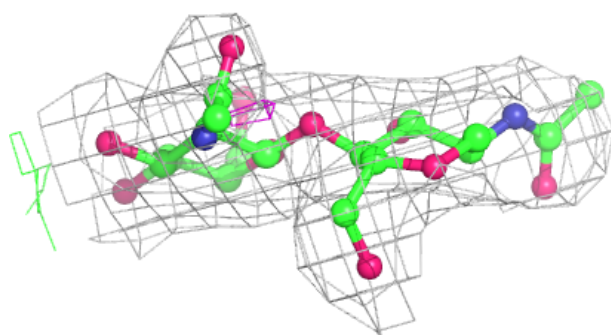
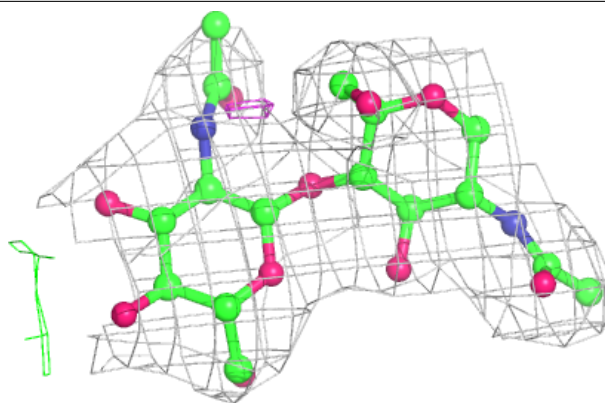
Electron density around Chain E:

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

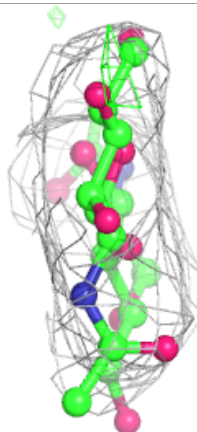
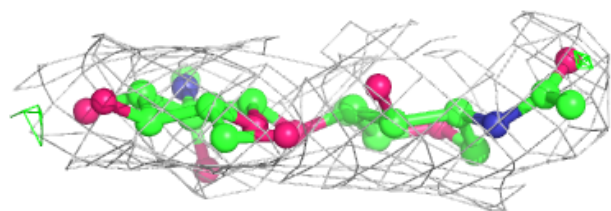
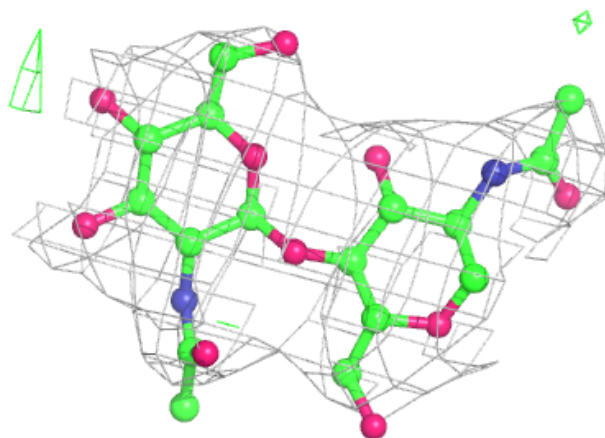


Electron density around Chain F:

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

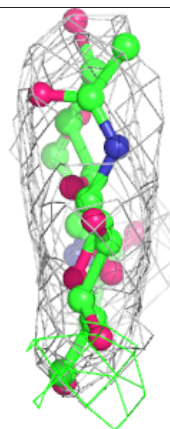
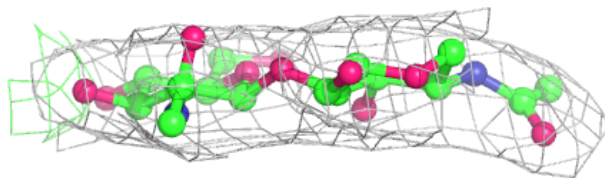
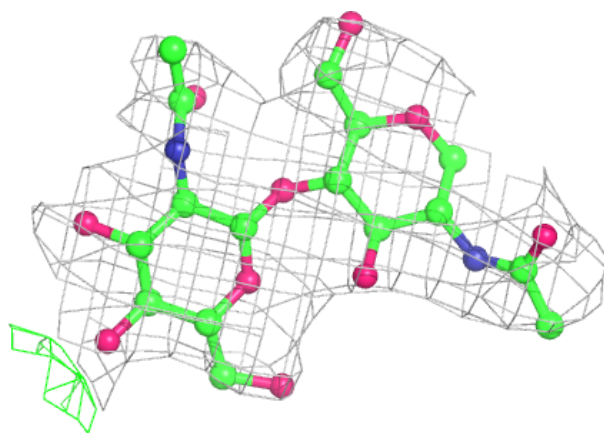
**Electron density around Chain G:**

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



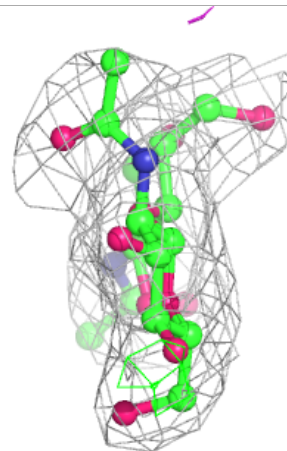
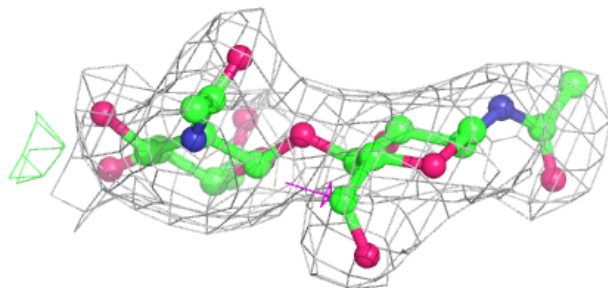
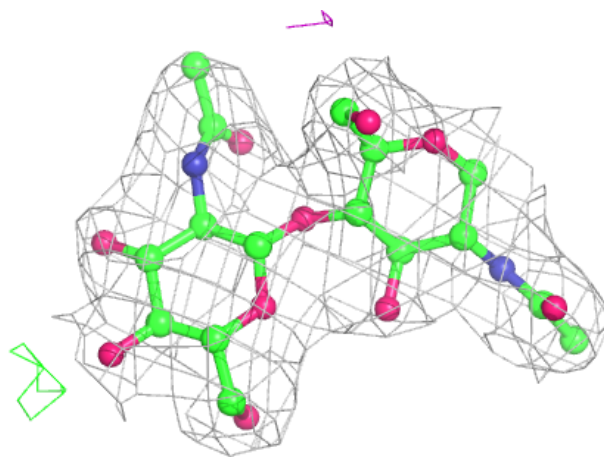
Electron density around Chain H:

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



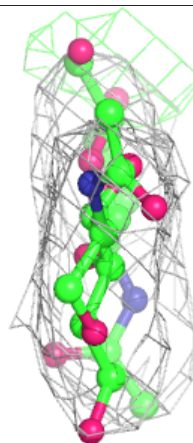
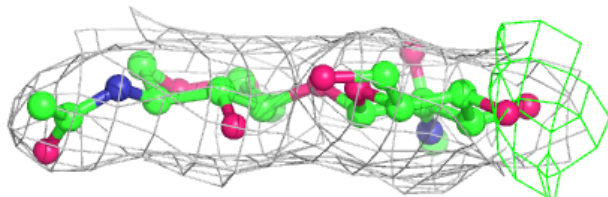
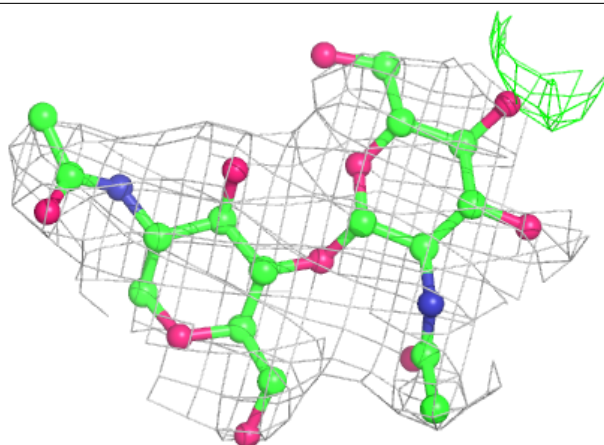
Electron density around Chain I:

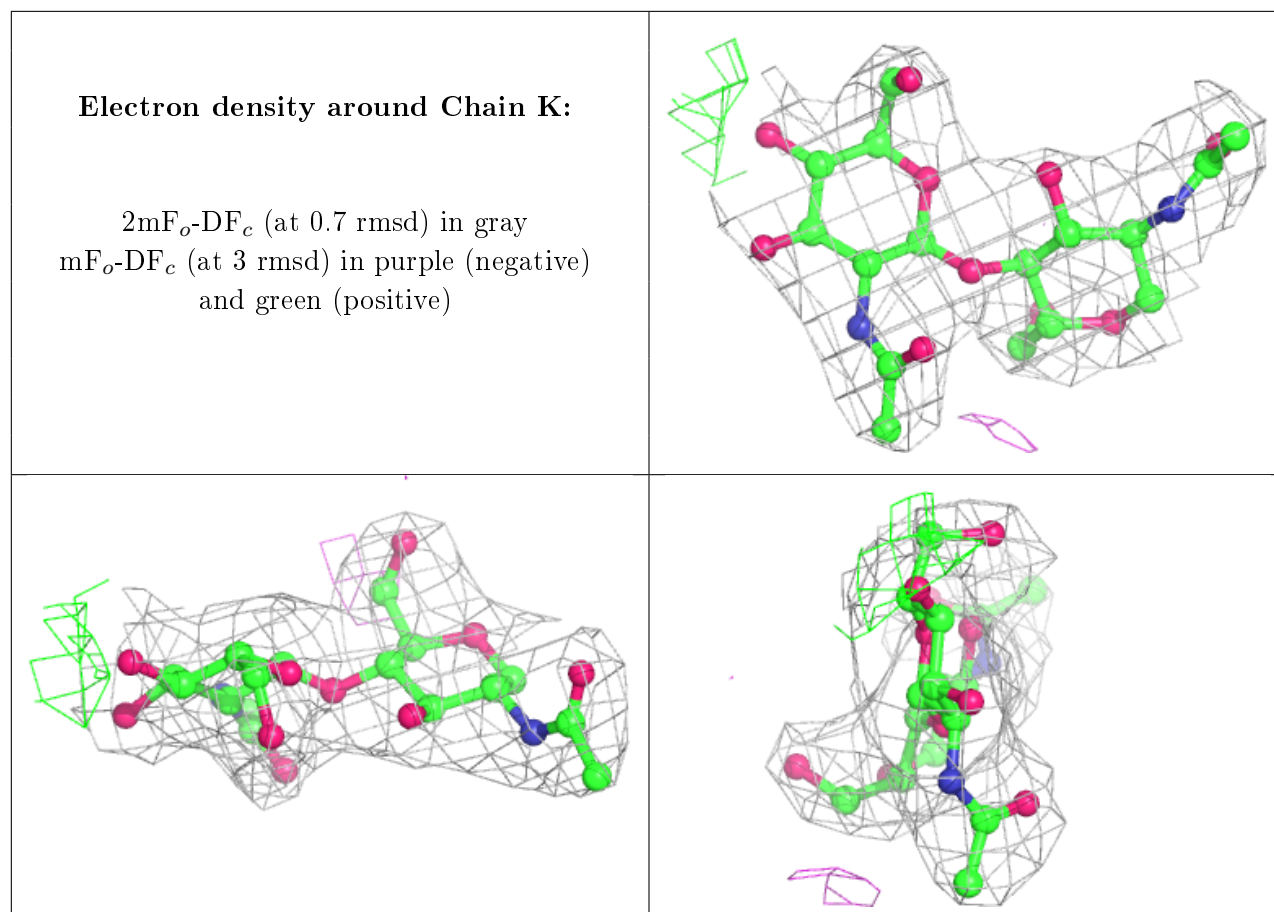
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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	A	908	14/15	0.84	0.18	96,103,112,113	0
4	NAG	B	904	14/15	0.85	0.34	117,120,124,124	0
4	NAG	B	905	14/15	0.88	0.20	79,85,91,92	0
4	NAG	D	904	14/15	0.89	0.22	58,65,73,76	0
4	NAG	A	905	14/15	0.89	0.15	45,62,74,75	0
4	NAG	C	904	14/15	0.90	0.35	74,86,94,97	0
4	NAG	A	904	14/15	0.90	0.20	63,70,73,75	0
4	NAG	D	907	14/15	0.91	0.26	77,84,89,91	0
3	CA	D	901	1/1	0.94	0.07	102,102,102,102	0
3	CA	C	901	1/1	0.97	0.07	87,87,87,87	0
3	CA	B	901	1/1	0.98	0.08	95,95,95,95	0
3	CA	A	901	1/1	0.99	0.11	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.