



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 03:12 PM EDT

PDB ID : 3K8M
Title : Crystal structure of SusG with acarbose
Authors : Koropatkin, N.M.; Smith, T.J.
Deposited on : 2009-10-14
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

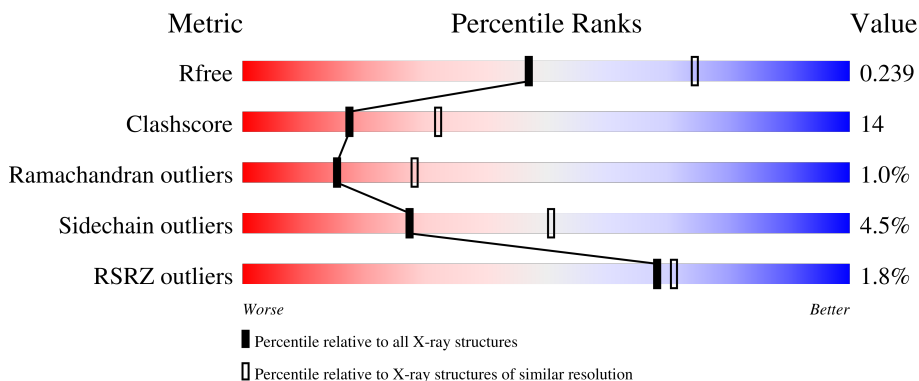
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	669	 3% 76% 18%
1	B	669	 3% 67% 27%
2	C	2	 100%
2	G	2	 50% 50%
3	D	3	 33% 67%

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	C	1	X	-	-	-
2	GLC	G	1	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10792 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 Alpha-amylase, susG.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	650	5178	3293	837	1032	5	11	0	0	0
1	B	646	5150	3279	833	1022	5	11	0	0	0

- Molecule 2 is an oligosaccharide called 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	32	19	1	12	0	0	0
2	G	2	32	19	1	12	0	0	0

- Molecule 3 is an oligosaccharide called 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- α -D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	3	44	25	1	18	0	0	0
3	E	3	44	25	1	18	0	0	0
3	H	3	44	25	1	18	0	0	0
3	I	3	44	25	1	18	0	0	0

- Molecule 4 is an oligosaccharide called α -D-glucopyranose-(1-4)- α -D-glucopyranose.

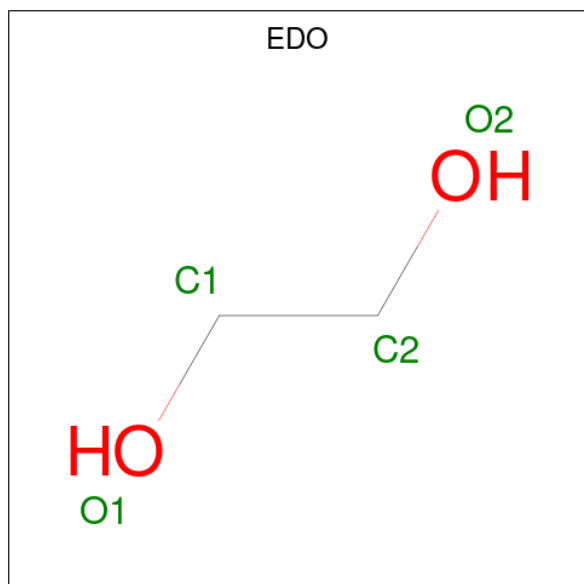


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	F	2	Total	C	O	0	0	0
			23	12	11			
4	J	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Ca	0	0
			2	2		
5	B	2	Total	Ca	0	0
			2	2		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		

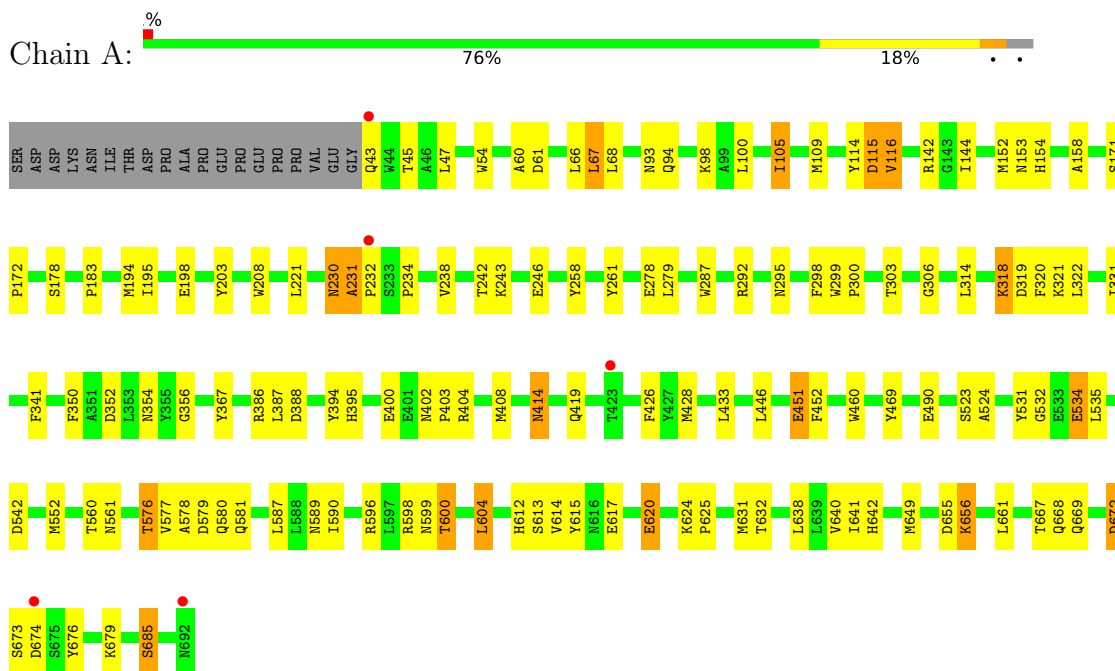
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	120	Total 120	O 120	0	0
7	B	50	Total 50	O 50	0	0

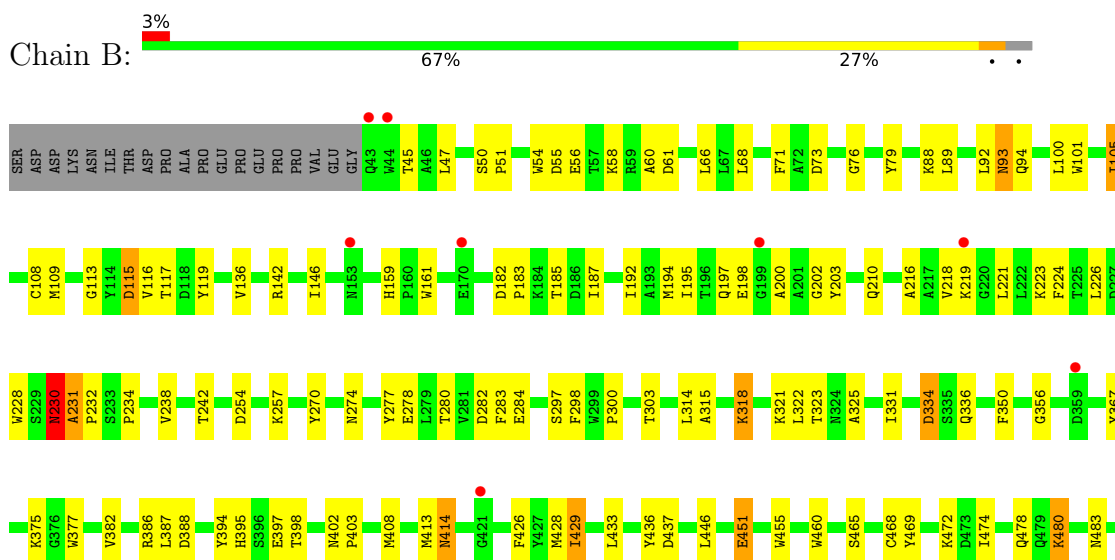
3 Residue-property plots

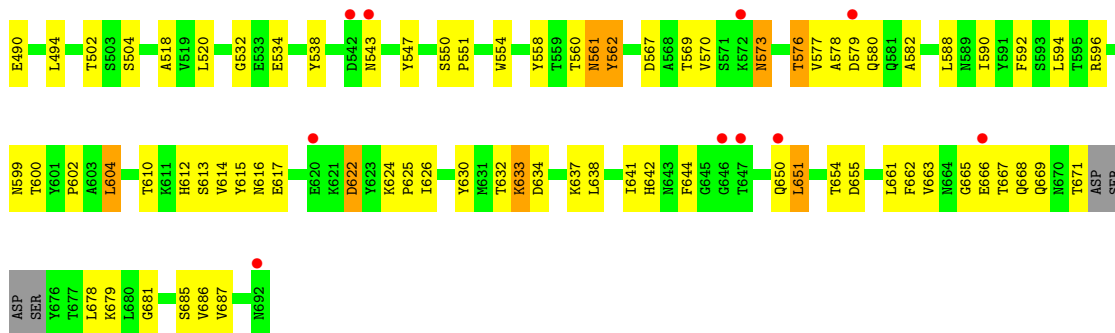
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Alpha-amylase, susG



- Molecule 1: Alpha-amylase, susG





- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose

Chain C: 100%

GLC1
AC12

- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose

Chain G: 50%

GLC1
AC12

- Molecule 3: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- α -D-glucopyranose

Chain D: 33% 67%

GLC1
GLC2
AC13

- Molecule 3: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- α -D-glucopyranose

Chain E: 67% 33%

GLC1
GLC2
AC13

- Molecule 3: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- α -D-glucopyranose

Chain H: 67% 33%

GLC1
GLC2
AC13

- Molecule 3: 4,6-dideoxy-4-{{(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl}amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain I:  33% 33% 33%

GLC1
GLC2
ACT3

- Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain F:  50% 50%

GLC1
GLC2

- Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain J:  100%

GLC1
GLC2

4 Data and refinement statistics i

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	127.71Å 127.71Å 127.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50 24.63 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.0 (25.00-2.50) 88.9 (24.63-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.201 , 0.247 0.195 , 0.239	Depositor DCC
R_{free} test set	7285 reflections (10.21%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.023 for -h,-l,-k 0.009 for -h,l,k 0.009 for l,-k,h 0.021 for -l,-k,-h 0.035 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10792	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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: GLC, AC1, EDO, CA

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	0.40	0/5306	0.62	0/7193
1	B	0.39	0/5277	0.61	0/7152
All	All	0.40	0/10583	0.62	0/14345

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5178	0	4878	123	0
1	B	5150	0	4859	158	0
2	C	32	0	19	1	0
2	G	32	0	19	1	0
3	D	44	0	30	0	0
3	E	44	0	30	2	0
3	H	44	0	30	0	0
3	I	44	0	30	4	0
4	F	23	0	21	0	0
4	J	23	0	21	1	0
5	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	2	0	0	0	0
6	A	4	0	6	3	0
7	A	120	0	0	6	0
7	B	50	0	0	1	0
All	All	10792	0	9943	282	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (282) 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:B:159:HIS:HD2	1:B:161:TRP:H	1.14	0.96
1:B:238:VAL:HG21	1:B:314:LEU:HD21	1.48	0.92
1:A:318:LYS:HE2	1:A:318:LYS:HA	1.49	0.92
1:B:394:TYR:H	1:B:402:ASN:HD21	1.16	0.91
1:A:394:TYR:H	1:A:402:ASN:HD21	1.12	0.91
1:B:668:GLN:HB2	1:B:679:LYS:HB3	1.54	0.89
1:A:612:HIS:HD2	1:A:615:TYR:H	1.18	0.89
1:B:663:VAL:HG13	1:B:667:THR:HG21	1.55	0.88
1:B:219:LYS:HG2	1:B:284:GLU:HG3	1.56	0.86
1:B:480:LYS:HE3	1:B:483:ASN:HD22	1.43	0.84
1:B:651:LEU:HD12	1:B:678:LEU:HB3	1.60	0.84
1:B:387:LEU:HD11	1:B:428:MSE:HE3	1.60	0.83
1:A:94:GLN:HE22	1:A:581:GLN:HE22	1.24	0.82
1:B:596:ARG:O	1:B:600:THR:HG23	1.79	0.81
1:B:116:VAL:HG21	1:B:119:TYR:CZ	2.15	0.81
1:A:625:PRO:HB2	1:A:649:MSE:HE1	1.63	0.81
1:A:451:GLU:HG3	1:A:490:GLU:HG3	1.63	0.80
1:B:54:TRP:CD1	1:B:600:THR:HG22	2.17	0.79
1:B:624:LYS:HB3	1:B:625:PRO:HD3	1.65	0.78
1:A:238:VAL:HG21	1:A:314:LEU:HD21	1.65	0.78
1:B:54:TRP:CE2	1:B:56:GLU:HA	2.19	0.77
1:A:153:ASN:HD22	1:A:154:HIS:HD2	1.32	0.76
1:B:451:GLU:HG3	1:B:490:GLU:HG3	1.68	0.75
1:B:576:THR:HG22	1:B:579:ASP:H	1.52	0.74
1:A:47:LEU:HD21	1:A:669:GLN:HB2	1.69	0.74
1:B:159:HIS:CD2	1:B:161:TRP:H	2.01	0.74
1:B:238:VAL:CG2	1:B:314:LEU:HD21	2.18	0.74
1:A:300:PRO:HD2	1:A:303:THR:HG21	1.70	0.73
1:B:668:GLN:OE1	1:B:679:LYS:HG2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:SER:OG	1:B:538:TYR:HB2	1.88	0.72
1:A:152:MSE:HE2	1:A:387:LEU:HD13	1.71	0.72
1:B:300:PRO:O	1:B:303:THR:HB	1.89	0.72
1:A:587:LEU:O	1:A:590:ILE:HG22	1.90	0.72
1:A:94:GLN:HE22	1:A:581:GLN:NE2	1.88	0.71
1:B:318:LYS:HA	1:B:318:LYS:HE2	1.70	0.71
1:A:67:LEU:HD22	1:A:531:TYR:HE2	1.56	0.71
1:A:576:THR:HG23	1:A:578:ALA:H	1.55	0.70
1:B:94:GLN:HB3	1:B:592:PHE:HE1	1.54	0.70
1:B:465:SER:HA	1:B:644:PHE:O	1.93	0.69
1:A:576:THR:HG22	1:A:579:ASP:H	1.58	0.69
1:B:543:ASN:HB2	1:B:547:TYR:CE2	2.27	0.69
1:B:66:LEU:HD12	1:B:66:LEU:O	1.92	0.69
1:A:194:MSE:HE1	1:A:356:GLY:O	1.93	0.68
1:A:387:LEU:HD11	1:A:428:MSE:HE3	1.75	0.68
1:B:612:HIS:HD2	1:B:615:TYR:H	1.42	0.68
1:A:67:LEU:HD22	1:A:531:TYR:CE2	2.30	0.67
1:A:320:PHE:CE2	1:A:331:ILE:HD12	2.30	0.67
1:A:428:MSE:HE2	1:A:446:LEU:CD2	2.25	0.66
1:A:100:LEU:HD13	1:A:144:ILE:HG21	1.79	0.65
1:B:480:LYS:HE3	1:B:483:ASN:ND2	2.11	0.65
1:A:54:TRP:CD1	1:A:600:THR:HG22	2.32	0.65
1:B:616:ASN:HB2	1:B:617:GLU:OE1	1.97	0.65
7:A:767:HOH:O	1:B:321:LYS:HG2	1.97	0.64
1:A:596:ARG:O	1:A:600:THR:HG23	1.98	0.64
1:A:47:LEU:CD2	1:A:669:GLN:HB2	2.27	0.64
1:B:367:TYR:CZ	1:B:408:MSE:HE3	2.33	0.63
1:A:152:MSE:CE	1:A:387:LEU:HD13	2.29	0.63
1:A:198:GLU:OE1	1:A:395:HIS:HD2	1.82	0.62
1:A:640:VAL:O	1:A:641:ILE:HD13	1.98	0.62
1:A:672:ASP:O	1:A:674:ASP:N	2.31	0.62
1:B:455:TRP:CH2	1:B:502:THR:HG23	2.35	0.62
1:B:183:PRO:O	1:B:187:ILE:HG12	2.00	0.62
1:A:109:MSE:HE3	1:A:158:ALA:HB2	1.81	0.61
1:B:197:GLN:O	1:B:198:GLU:HG3	2.00	0.61
1:B:469:TYR:CE1	3:I:3:AC1:HCB1	2.35	0.61
1:B:474:ILE:HG22	1:B:478:GLN:HE21	1.66	0.61
1:A:142:ARG:HG3	1:A:142:ARG:HH11	1.65	0.61
1:A:523:SER:O	1:A:598:ARG:NH2	2.31	0.61
1:B:633:LYS:HE3	1:B:634:ASP:CG	2.21	0.61
1:B:654:THR:O	1:B:654:THR:HG22	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:VAL:CG2	1:A:314:LEU:HD21	2.30	0.61
1:A:115:ASP:HB3	1:A:350:PHE:CE1	2.36	0.60
1:B:79:TYR:CE1	1:B:562:TYR:HB2	2.36	0.60
1:B:663:VAL:CG1	1:B:667:THR:HG21	2.31	0.60
1:A:115:ASP:HB3	1:A:350:PHE:HE1	1.66	0.60
1:B:414:ASN:ND2	1:B:426:PHE:H	1.98	0.59
1:B:651:LEU:CD1	1:B:678:LEU:HB3	2.31	0.59
1:B:142:ARG:HG3	1:B:142:ARG:HH11	1.67	0.59
1:A:469:TYR:OH	1:A:620:GLU:HG3	2.02	0.59
1:A:612:HIS:CD2	1:A:615:TYR:H	2.10	0.59
1:B:474:ILE:HG22	1:B:478:GLN:NE2	2.17	0.59
1:A:208:TRP:HB2	6:A:750:EDO:H11	1.85	0.58
1:B:604:LEU:HD13	1:B:638:LEU:HD12	1.85	0.58
1:B:194:MSE:HE1	1:B:356:GLY:O	2.03	0.58
1:A:116:VAL:HG13	7:A:764:HOH:O	2.03	0.58
1:A:300:PRO:O	1:A:303:THR:HG22	2.04	0.58
1:B:668:GLN:HB2	1:B:679:LYS:CB	2.32	0.58
1:B:433:LEU:HD23	4:J:1:GLC:O4	2.03	0.58
1:B:428:MSE:HE2	1:B:446:LEU:CD2	2.34	0.57
1:B:651:LEU:HD11	1:B:678:LEU:HD23	1.85	0.57
1:B:602:PRO:HB3	1:B:633:LYS:HD3	1.86	0.57
1:A:234:PRO:HG2	1:A:322:LEU:HB2	1.86	0.57
1:A:668:GLN:HB2	1:A:679:LYS:HB3	1.86	0.57
1:A:321:LYS:H	1:A:321:LYS:HD2	1.68	0.57
1:A:194:MSE:HE3	1:A:354:ASN:OD1	2.05	0.57
1:A:625:PRO:CB	1:A:649:MSE:HE1	2.35	0.57
1:A:598:ARG:NH1	7:A:784:HOH:O	2.37	0.56
1:B:108:CYS:SG	1:B:113:GLY:HA2	2.46	0.56
1:B:115:ASP:HB3	1:B:350:PHE:HE1	1.70	0.56
1:B:576:THR:HG23	1:B:578:ALA:N	2.19	0.56
1:A:100:LEU:HD13	1:A:144:ILE:CG2	2.35	0.56
1:B:615:TYR:OH	1:B:651:LEU:HB2	2.05	0.56
1:B:68:LEU:HD11	1:B:105:ILE:HG22	1.87	0.56
1:B:494:LEU:HG	1:B:520:LEU:HD22	1.88	0.55
1:B:226:LEU:HB2	1:B:277:TYR:HB2	1.86	0.55
1:A:642:HIS:ND1	1:A:685:SER:HB3	2.21	0.55
1:B:60:ALA:H	1:B:599:ASN:ND2	2.04	0.55
1:B:633:LYS:HE3	1:B:634:ASP:CB	2.38	0.54
1:B:60:ALA:H	1:B:599:ASN:HD22	1.55	0.54
1:B:686:VAL:HG22	1:B:687:VAL:N	2.23	0.54
1:A:221:LEU:HD13	1:A:242:THR:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:LEU:HA	1:B:92:LEU:HD12	1.90	0.54
1:B:221:LEU:HD23	1:B:282:ASP:HA	1.89	0.54
1:B:231:ALA:O	1:B:234:PRO:HD3	2.08	0.54
1:B:230:ASN:C	1:B:232:PRO:HD2	2.28	0.53
1:A:612:HIS:HE1	1:A:655:ASP:OD2	1.90	0.53
1:B:612:HIS:CD2	1:B:614:VAL:H	2.25	0.53
1:B:610:THR:OG1	1:B:630:TYR:HB2	2.08	0.53
1:A:194:MSE:HE3	1:A:356:GLY:H	1.74	0.53
1:A:388:ASP:OD1	2:C:1:GLC:O5	2.19	0.53
1:A:386:ARG:NH1	1:A:388:ASP:HB2	2.24	0.53
1:B:115:ASP:HB3	1:B:350:PHE:CE1	2.43	0.53
1:B:231:ALA:N	1:B:232:PRO:HD2	2.24	0.52
1:A:68:LEU:CD1	1:A:105:ILE:HG22	2.39	0.52
1:A:47:LEU:HD12	1:A:667:THR:HB	1.90	0.52
1:B:195:ILE:HG12	1:B:395:HIS:HB2	1.91	0.52
1:B:388:ASP:OD1	2:G:1:GLC:O5	2.26	0.52
1:A:320:PHE:HE2	1:A:331:ILE:HD12	1.73	0.52
1:B:94:GLN:HB3	1:B:592:PHE:CE1	2.41	0.52
1:B:394:TYR:N	1:B:402:ASN:HD21	1.98	0.52
1:B:612:HIS:HE1	1:B:655:ASP:OD2	1.92	0.52
1:A:203:TYR:OH	6:A:750:EDO:H21	2.09	0.52
1:A:306:GLY:HA2	1:A:331:ILE:HD11	1.92	0.52
1:A:258:TYR:CE1	1:A:295:ASN:HB3	2.44	0.52
1:B:534:GLU:HB3	1:B:588:LEU:HD12	1.92	0.52
1:A:560:THR:HG23	7:A:694:HOH:O	2.10	0.51
1:B:460:TRP:CD2	3:I:2:GLC:H2	2.46	0.51
1:B:375:LYS:HE3	1:B:413:MSE:HE1	1.92	0.51
1:A:617:GLU:O	1:A:620:GLU:HB3	2.10	0.51
1:B:79:TYR:CD1	1:B:562:TYR:HB2	2.46	0.51
1:A:433:LEU:HD13	1:A:452:PHE:CE2	2.46	0.50
1:A:402:ASN:HB2	1:A:403:PRO:HD3	1.94	0.50
1:B:54:TRP:CD2	1:B:56:GLU:HA	2.46	0.50
1:B:665:GLY:O	1:B:667:THR:HG23	2.12	0.50
1:A:414:ASN:ND2	1:A:426:PHE:H	2.10	0.50
1:B:532:GLY:N	1:B:534:GLU:OE2	2.43	0.50
1:A:142:ARG:HG3	1:A:142:ARG:NH1	2.27	0.49
1:B:105:ILE:HD13	1:B:105:ILE:H	1.77	0.49
1:B:624:LYS:CB	1:B:625:PRO:HD3	2.40	0.49
1:B:633:LYS:HE3	1:B:634:ASP:HB2	1.93	0.49
1:A:604:LEU:HD13	1:A:638:LEU:HD12	1.94	0.49
1:A:576:THR:HG23	1:A:578:ALA:N	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:GLU:O	1:A:620:GLU:HG2	2.10	0.49
1:B:50:SER:N	1:B:51:PRO:CD	2.76	0.49
1:B:136:VAL:HA	1:B:146:ILE:HD12	1.94	0.49
1:B:270:TYR:HB2	1:B:278:GLU:O	2.13	0.49
1:A:195:ILE:HG12	1:A:395:HIS:HB2	1.95	0.48
1:B:47:LEU:HD12	1:B:667:THR:HB	1.95	0.48
1:B:480:LYS:HA	1:B:483:ASN:ND2	2.28	0.48
1:A:367:TYR:CZ	1:A:408:MSE:HE3	2.48	0.48
1:A:404:ARG:HG3	1:A:404:ARG:HH11	1.79	0.48
1:A:612:HIS:CD2	1:A:614:VAL:H	2.32	0.48
1:B:187:ILE:HD13	1:B:192:ILE:HD12	1.95	0.48
1:A:194:MSE:CE	1:A:356:GLY:H	2.27	0.48
1:B:66:LEU:HD12	1:B:66:LEU:C	2.34	0.48
3:E:1:GLC:H62	3:E:2:GLC:H5	1.95	0.48
1:A:620:GLU:O	1:A:624:LYS:NZ	2.47	0.47
1:A:576:THR:HG23	1:A:577:VAL:N	2.28	0.47
1:B:662:PHE:HB3	1:B:687:VAL:HB	1.94	0.47
1:A:669:GLN:HE21	1:A:676:TYR:HE1	1.60	0.47
1:B:402:ASN:HB2	1:B:403:PRO:HD3	1.96	0.47
1:B:315:ALA:HA	1:B:334:ASP:OD2	2.14	0.47
1:B:323:THR:HG22	1:B:325:ALA:H	1.80	0.47
1:B:254:ASP:OD2	1:B:254:ASP:N	2.48	0.47
1:A:292:ARG:HD2	1:A:299:TRP:CH2	2.50	0.46
1:B:624:LYS:HB3	1:B:625:PRO:CD	2.41	0.46
1:A:183:PRO:HD2	7:A:20:HOH:O	2.15	0.46
1:A:306:GLY:C	1:A:331:ILE:HD11	2.36	0.46
1:A:318:LYS:NZ	1:A:319:ASP:H	2.13	0.46
1:A:60:ALA:O	1:A:98:LYS:HD2	2.15	0.46
1:A:278:GLU:HG2	1:A:279:LEU:N	2.30	0.46
1:B:480:LYS:HA	1:B:483:ASN:HD22	1.80	0.46
1:A:318:LYS:HE2	1:A:318:LYS:CA	2.35	0.46
1:B:641:ILE:HB	1:B:686:VAL:HG12	1.98	0.46
1:B:387:LEU:CD1	1:B:428:MSE:HE3	2.40	0.45
1:B:642:HIS:ND1	1:B:685:SER:CB	2.79	0.45
1:A:230:ASN:O	1:A:231:ALA:C	2.54	0.45
1:B:219:LYS:HA	1:B:283:PHE:O	2.16	0.45
1:B:573:ASN:N	1:B:573:ASN:OD1	2.49	0.45
1:B:666:GLU:HB3	1:B:681:GLY:HA3	1.98	0.45
1:B:386:ARG:HA	1:B:429:ILE:HG22	1.97	0.45
1:B:576:THR:HG23	1:B:577:VAL:N	2.31	0.45
1:B:626:ILE:HG12	1:B:651:LEU:CD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:THR:CG2	1:B:579:ASP:H	2.26	0.45
1:A:194:MSE:HE1	1:A:356:GLY:N	2.31	0.45
1:A:43:GLN:CD	1:A:43:GLN:N	2.70	0.45
1:A:400:GLU:O	1:A:403:PRO:HD2	2.17	0.45
1:B:51:PRO:HD3	1:B:661:LEU:O	2.17	0.45
1:B:58:LYS:HE2	1:B:93:ASN:HD21	1.81	0.45
1:A:60:ALA:H	1:A:599:ASN:HD22	1.63	0.45
1:A:524:ALA:HA	1:A:631:MSE:HE1	1.98	0.44
1:B:194:MSE:HE3	1:B:356:GLY:H	1.82	0.44
1:B:223:LYS:HG2	1:B:280:THR:OG1	2.18	0.44
1:B:429:ILE:CG2	1:B:429:ILE:O	2.65	0.44
1:A:460:TRP:CG	3:E:2:GLC:H2	2.52	0.44
1:B:322:LEU:CD2	1:B:331:ILE:HD11	2.47	0.44
1:A:404:ARG:HG3	1:A:404:ARG:NH1	2.32	0.44
1:A:535:LEU:HD21	1:A:577:VAL:HG22	1.99	0.44
1:B:68:LEU:CD1	1:B:105:ILE:HG22	2.47	0.44
1:B:88:LYS:HD2	1:B:554:TRP:CZ3	2.53	0.44
1:B:223:LYS:NZ	1:B:242:THR:H	2.16	0.44
1:B:224:PHE:CD2	1:B:238:VAL:HG22	2.52	0.44
1:A:194:MSE:CE	1:A:356:GLY:N	2.81	0.44
1:A:428:MSE:HE2	1:A:446:LEU:HD21	1.98	0.44
1:A:656:LYS:HD2	1:A:656:LYS:N	2.33	0.44
1:B:460:TRP:CG	3:I:2:GLC:H2	2.52	0.44
1:A:178:SER:O	1:A:341:PHE:HA	2.18	0.43
1:B:116:VAL:HG21	1:B:119:TYR:CE2	2.51	0.43
1:A:532:GLY:N	1:A:534:GLU:OE2	2.50	0.43
1:B:567:ASP:OD1	1:B:569:THR:HG23	2.18	0.43
1:B:183:PRO:HB2	1:B:203:TYR:CE1	2.54	0.43
1:B:394:TYR:HB2	1:B:402:ASN:ND2	2.34	0.43
1:B:580:GLN:C	1:B:582:ALA:H	2.21	0.43
1:A:153:ASN:ND2	1:A:154:HIS:HD2	2.08	0.43
1:A:261:TYR:HA	1:A:287:TRP:CZ2	2.53	0.43
1:A:230:ASN:N	1:A:230:ASN:HD22	2.17	0.43
1:A:318:LYS:HA	1:A:318:LYS:CE	2.35	0.43
1:B:414:ASN:HD21	1:B:426:PHE:H	1.66	0.43
1:B:182:ASP:OD2	1:B:185:THR:HG23	2.18	0.43
1:B:200:ALA:C	1:B:202:GLY:H	2.22	0.43
1:A:669:GLN:NE2	1:A:676:TYR:HE1	2.17	0.43
1:B:218:VAL:O	1:B:284:GLU:HA	2.19	0.43
1:B:228:TRP:CE2	1:B:257:LYS:HE3	2.54	0.43
1:B:538:TYR:OH	1:B:570:VAL:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:THR:OG1	1:A:243:LYS:N	2.52	0.43
1:A:367:TYR:CE1	1:A:408:MSE:HE3	2.54	0.43
1:A:394:TYR:N	1:A:402:ASN:HD21	1.96	0.43
1:B:576:THR:HG23	1:B:578:ALA:H	1.84	0.43
1:A:433:LEU:HD13	1:A:452:PHE:CD2	2.54	0.43
1:B:142:ARG:HG3	1:B:142:ARG:NH1	2.32	0.43
1:B:298:PHE:O	1:B:300:PRO:HD3	2.19	0.43
1:B:588:LEU:HG	1:B:592:PHE:CE2	2.53	0.43
1:A:171:SER:HA	1:A:172:PRO:HD3	1.87	0.42
1:A:298:PHE:O	1:A:300:PRO:HD3	2.19	0.42
1:B:234:PRO:HG2	1:B:322:LEU:HB2	2.00	0.42
1:A:419:GLN:O	1:A:419:GLN:HG2	2.18	0.42
1:A:231:ALA:N	1:A:232:PRO:HD2	2.34	0.42
1:B:650:GLN:HA	1:B:678:LEU:O	2.19	0.42
1:A:451:GLU:HG2	7:A:769:HOH:O	2.18	0.42
1:B:567:ASP:HB3	1:B:570:VAL:HG23	2.02	0.42
1:B:377:TRP:HB3	1:B:382:VAL:HG21	2.02	0.42
1:A:68:LEU:HD11	1:A:105:ILE:HG22	2.02	0.42
1:A:230:ASN:C	1:A:232:PRO:HD2	2.41	0.41
1:B:551:PRO:HB3	1:B:560:THR:OG1	2.20	0.41
1:B:617:GLU:OE1	1:B:617:GLU:N	2.45	0.41
1:B:45:THR:HG22	1:B:669:GLN:O	2.20	0.41
1:B:436:TYR:CG	1:B:437:ASP:N	2.88	0.41
1:B:622:ASP:OD2	1:B:622:ASP:N	2.54	0.41
1:A:300:PRO:O	1:A:303:THR:CG2	2.68	0.41
1:A:640:VAL:C	1:A:641:ILE:HD13	2.41	0.41
1:B:580:GLN:NE2	1:B:588:LEU:H	2.19	0.41
1:B:602:PRO:CB	1:B:633:LYS:HD3	2.48	0.41
1:B:210:GLN:HG2	7:B:710:HOH:O	2.20	0.41
1:B:472:LYS:NZ	3:I:3:AC1:O3B	2.52	0.41
1:B:518:ALA:HA	1:B:594:LEU:HD13	2.02	0.41
1:B:55:ASP:O	1:B:56:GLU:HB2	2.20	0.41
1:B:73:ASP:HB2	1:B:560:THR:HG22	2.03	0.41
1:B:109:MSE:H	1:B:109:MSE:HG2	1.72	0.41
1:B:367:TYR:CE1	1:B:408:MSE:HE3	2.55	0.41
1:B:414:ASN:HD22	1:B:414:ASN:HA	1.66	0.41
1:B:632:THR:HB	1:B:637:LYS:HG3	2.03	0.41
1:A:114:TYR:O	1:A:154:HIS:HE1	2.04	0.41
1:A:208:TRP:CB	6:A:750:EDO:H11	2.50	0.41
1:A:306:GLY:CA	1:A:331:ILE:HD11	2.51	0.40
1:A:668:GLN:OE1	1:A:679:LYS:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:GLN:HE21	1:A:580:GLN:HB3	1.72	0.40
1:A:589:ASN:HD22	1:A:589:ASN:HA	1.74	0.40
1:B:101:TRP:C	1:B:101:TRP:CD1	2.92	0.40
1:B:397:GLU:HG3	1:B:398:THR:HG23	2.03	0.40
1:A:534:GLU:OE1	1:A:552:MSE:HE1	2.21	0.40
1:A:66:LEU:HD12	1:A:66:LEU:C	2.42	0.40
1:B:216:ALA:O	1:B:336:GLN:HG2	2.22	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	648/669 (97%)	611 (94%)	33 (5%)	4 (1%)	25 43
1	B	642/669 (96%)	573 (89%)	60 (9%)	9 (1%)	11 20
All	All	1290/1338 (96%)	1184 (92%)	93 (7%)	13 (1%)	15 28

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	673	SER
1	A	542	ASP
1	B	230	ASN
1	B	558	TYR
1	B	468	CYS
1	B	561	ASN
1	B	562	TYR
1	B	71	PHE
1	A	672	ASP
1	B	231	ALA
1	B	76	GLY

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Mol	Chain	Res	Type
1	A	231	ALA
1	B	550	SER

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	551/557 (99%)	527 (96%)	24 (4%)	28	52
1	B	547/557 (98%)	522 (95%)	25 (5%)	27	50
All	All	1098/1114 (99%)	1049 (96%)	49 (4%)	27	51

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR
1	A	61	ASP
1	A	67	LEU
1	A	93	ASN
1	A	105	ILE
1	A	115	ASP
1	A	116	VAL
1	A	230	ASN
1	A	246	GLU
1	A	318	LYS
1	A	352	ASP
1	A	414	ASN
1	A	451	GLU
1	A	534	GLU
1	A	561	ASN
1	A	576	THR
1	A	600	THR
1	A	604	LEU
1	A	613	SER
1	A	620	GLU
1	A	632	THR

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Mol	Chain	Res	Type
1	A	656	LYS
1	A	661	LEU
1	A	685	SER
1	B	61	ASP
1	B	93	ASN
1	B	100	LEU
1	B	105	ILE
1	B	115	ASP
1	B	117	THR
1	B	230	ASN
1	B	274	ASN
1	B	297	SER
1	B	318	LYS
1	B	334	ASP
1	B	414	ASN
1	B	429	ILE
1	B	451	GLU
1	B	480	LYS
1	B	561	ASN
1	B	573	ASN
1	B	576	THR
1	B	590	ILE
1	B	604	LEU
1	B	613	SER
1	B	622	ASP
1	B	633	LYS
1	B	651	LEU
1	B	671	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	106	HIS
1	A	154	HIS
1	A	230	ASN
1	A	395	HIS
1	A	402	ASN
1	A	414	ASN
1	A	543	ASN
1	A	561	ASN
1	A	573	ASN

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Mol	Chain	Res	Type
1	A	580	GLN
1	A	581	GLN
1	A	589	ASN
1	A	599	ASN
1	A	608	ASN
1	A	612	HIS
1	A	669	GLN
1	A	670	ASN
1	B	93	ASN
1	B	154	HIS
1	B	159	HIS
1	B	230	ASN
1	B	274	ASN
1	B	395	HIS
1	B	402	ASN
1	B	414	ASN
1	B	478	GLN
1	B	483	ASN
1	B	543	ASN
1	B	561	ASN
1	B	580	GLN
1	B	599	ASN
1	B	612	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

20 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	GLC	C	1	2,1	11,11,12	0.53	0	15,15,17	0.98	0
2	AC1	C	2	2	21,22,23	1.47	3 (14%)	22,32,34	0.90	1 (4%)
3	GLC	D	1	3	12,12,12	1.11	0	17,17,17	0.83	0
3	GLC	D	2	3	11,11,12	1.30	2 (18%)	15,15,17	0.89	0
3	AC1	D	3	3	21,22,23	1.38	3 (14%)	22,32,34	0.91	1 (4%)
3	GLC	E	1	3	12,12,12	1.14	0	17,17,17	0.84	0
3	GLC	E	2	3	11,11,12	1.13	0	15,15,17	1.06	1 (6%)
3	AC1	E	3	3	21,22,23	1.59	4 (19%)	22,32,34	0.91	1 (4%)
4	GLC	F	1	4	12,12,12	1.00	0	17,17,17	0.72	0
4	GLC	F	2	4	11,11,12	1.19	2 (18%)	15,15,17	0.80	0
2	GLC	G	1	2,1	11,11,12	0.56	0	15,15,17	1.12	1 (6%)
2	AC1	G	2	2	21,22,23	1.59	3 (14%)	22,32,34	0.90	2 (9%)
3	GLC	H	1	3	12,12,12	1.25	0	17,17,17	0.81	0
3	GLC	H	2	3	11,11,12	1.00	0	15,15,17	0.77	0
3	AC1	H	3	3	21,22,23	1.37	3 (14%)	22,32,34	0.90	1 (4%)
3	GLC	I	1	3	12,12,12	1.08	0	17,17,17	0.77	0
3	GLC	I	2	3	11,11,12	1.28	0	15,15,17	0.80	0
3	AC1	I	3	3	21,22,23	1.44	3 (14%)	22,32,34	0.92	1 (4%)
4	GLC	J	1	4	12,12,12	1.16	0	17,17,17	0.73	0
4	GLC	J	2	4	11,11,12	1.36	2 (18%)	15,15,17	0.82	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	C	1	2,1	1/1/4/5	0/2/19/22	0/1/1/1
2	AC1	C	2	2	-	2/6/43/46	0/2/2/2
3	GLC	D	1	3	-	0/2/22/22	0/1/1/1
3	GLC	D	2	3	-	0/2/19/22	0/1/1/1
3	AC1	D	3	3	-	1/6/43/46	0/2/2/2
3	GLC	E	1	3	-	0/2/22/22	0/1/1/1
3	GLC	E	2	3	-	0/2/19/22	0/1/1/1
3	AC1	E	3	3	-	3/6/43/46	0/2/2/2
4	GLC	F	1	4	-	0/2/22/22	0/1/1/1
4	GLC	F	2	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	G	1	2,1	1/1/4/5	0/2/19/22	0/1/1/1
2	AC1	G	2	2	-	1/6/43/46	0/2/2/2
3	GLC	H	1	3	-	0/2/22/22	0/1/1/1
3	GLC	H	2	3	-	0/2/19/22	0/1/1/1
3	AC1	H	3	3	-	1/6/43/46	0/2/2/2
3	GLC	I	1	3	-	0/2/22/22	0/1/1/1
3	GLC	I	2	3	-	0/2/19/22	0/1/1/1
3	AC1	I	3	3	-	2/6/43/46	0/2/2/2
4	GLC	J	1	4	-	0/2/22/22	0/1/1/1
4	GLC	J	2	4	-	0/2/19/22	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	AC1	C4A-C5B	4.01	1.54	1.51
3	E	3	AC1	C4A-C5B	3.55	1.54	1.51
2	C	2	AC1	C4A-C5B	3.52	1.54	1.51
2	C	2	AC1	C3B-C4A	3.50	1.58	1.53
2	G	2	AC1	C3B-C4A	3.25	1.57	1.53
3	D	3	AC1	C4A-C5B	3.23	1.54	1.51
3	I	3	AC1	C4A-C5B	3.03	1.53	1.51
3	I	3	AC1	C3B-C4A	3.02	1.57	1.53
3	E	3	AC1	C2B-C1B	2.99	1.56	1.52
2	G	2	AC1	C2B-C1B	2.92	1.56	1.52
3	H	3	AC1	C4A-C5B	2.76	1.53	1.51
3	E	3	AC1	C3B-C4A	2.75	1.57	1.53
3	D	2	GLC	O5-C1	2.74	1.48	1.43
3	D	3	AC1	C3B-C4A	2.52	1.56	1.53
3	H	3	AC1	C3B-C4A	2.50	1.56	1.53
4	J	2	GLC	O5-C1	2.43	1.47	1.43
3	H	3	AC1	C2B-C1B	2.29	1.55	1.52
3	D	3	AC1	C2B-C1B	2.28	1.55	1.52
2	C	2	AC1	C2B-C1B	2.21	1.55	1.52
3	E	3	AC1	O5-C1	2.20	1.47	1.43
3	I	3	AC1	C2B-C1B	2.17	1.55	1.52
4	J	2	GLC	O5-C5	2.16	1.47	1.43
4	F	2	GLC	O5-C1	2.11	1.47	1.43
4	F	2	GLC	O5-C5	2.05	1.47	1.43
3	D	2	GLC	C2-C3	2.04	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	3	AC1	C2-C3-C4	-2.83	108.13	110.63
3	E	3	AC1	C2-C3-C4	-2.81	108.15	110.63
3	D	3	AC1	C2-C3-C4	-2.71	108.23	110.63
3	H	3	AC1	C2-C3-C4	-2.63	108.31	110.63
3	E	2	GLC	C1-C2-C3	-2.36	106.77	109.67
2	C	2	AC1	C2-C3-C4	-2.29	108.61	110.63
2	G	2	AC1	C2-C3-C4	-2.21	108.68	110.63
2	G	2	AC1	C7B-C1B-N4A	-2.19	107.39	110.68
2	G	1	GLC	C1-O5-C5	-2.03	109.44	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	GLC	C1
2	G	1	GLC	C1

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	AC1	C2B-C1B-N4A-C4
3	E	3	AC1	C3-C4-N4A-C1B
3	E	3	AC1	C5-C4-N4A-C1B
3	E	3	AC1	C2B-C1B-N4A-C4
3	H	3	AC1	C3-C4-N4A-C1B
3	I	3	AC1	C2B-C1B-N4A-C4
2	C	2	AC1	C5-C4-N4A-C1B
3	D	3	AC1	C3-C4-N4A-C1B
3	I	3	AC1	C5-C4-N4A-C1B
2	G	2	AC1	C5-C4-N4A-C1B

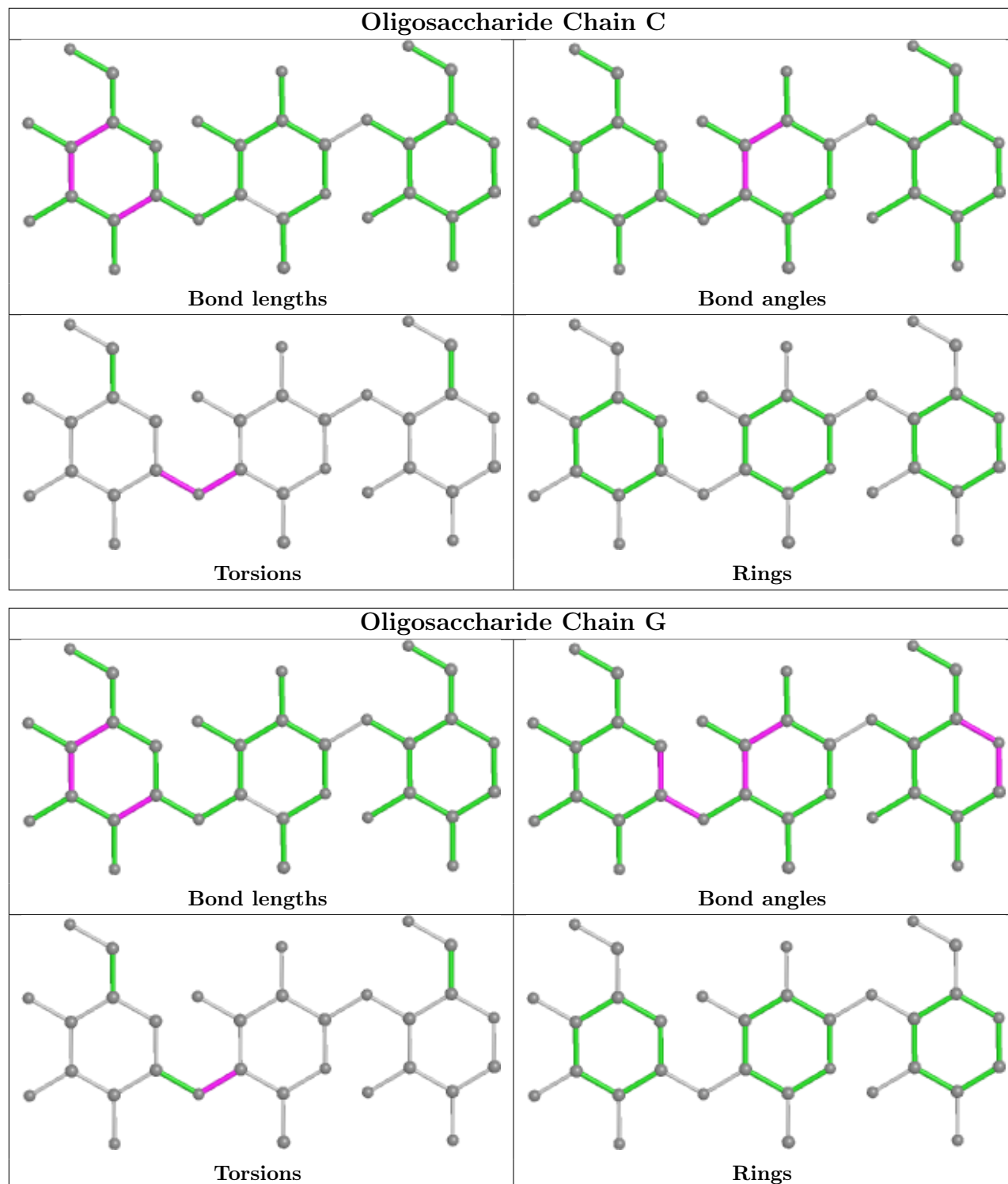
There are no ring outliers.

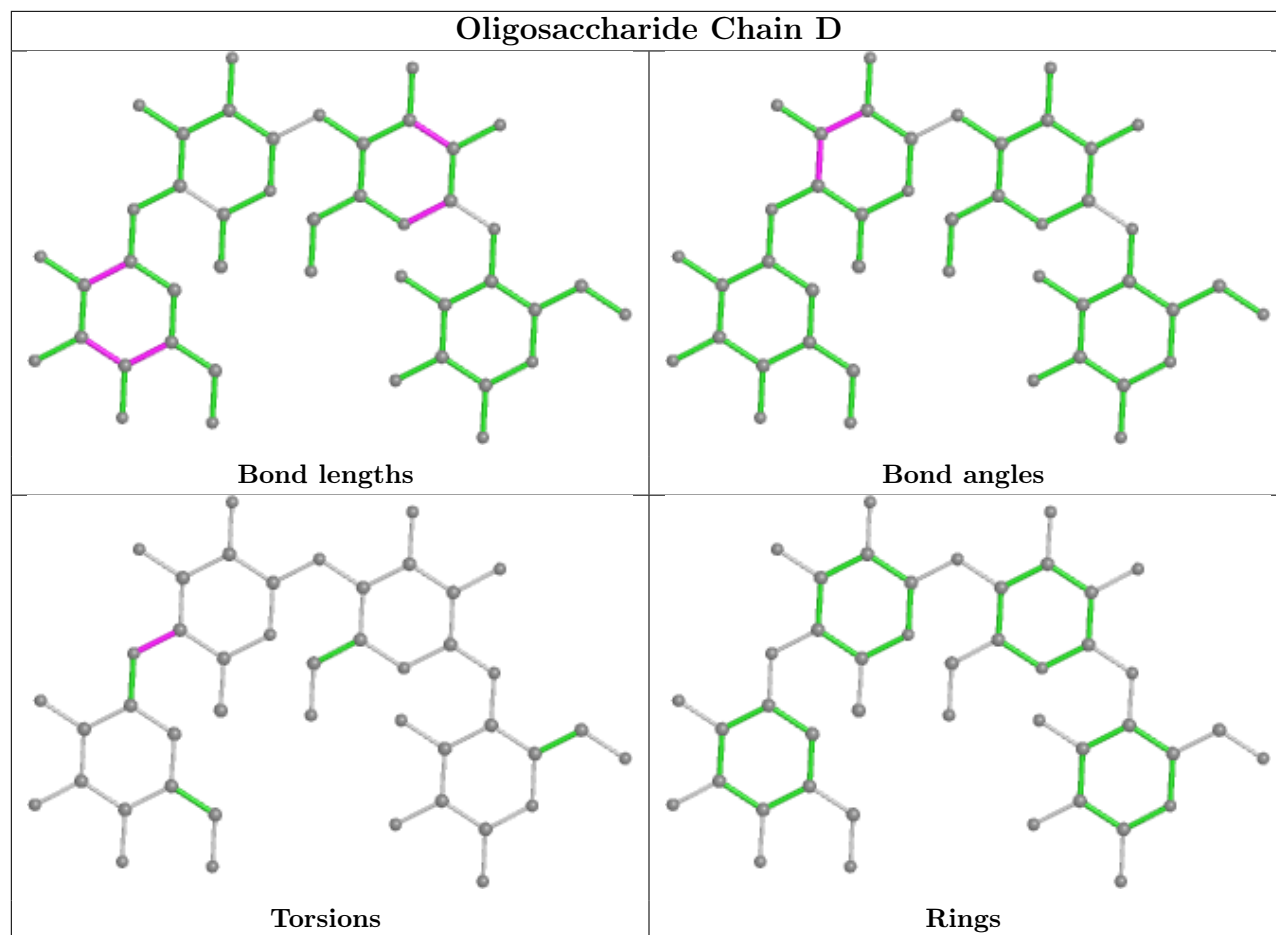
7 monomers are involved in 9 short contacts:

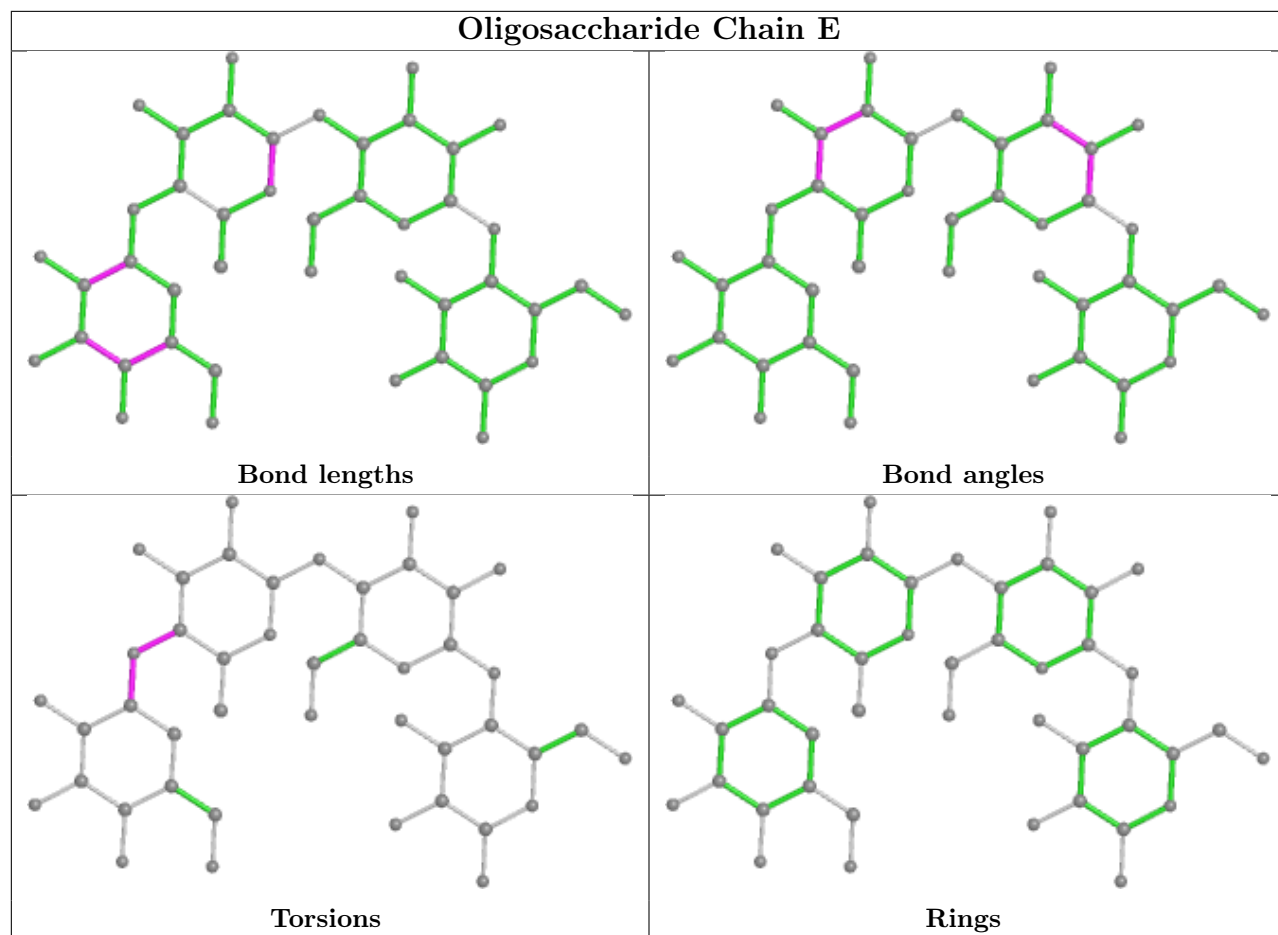
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	3	AC1	2	0
2	G	1	GLC	1	0
3	E	1	GLC	1	0
2	C	1	GLC	1	0
3	E	2	GLC	2	0
4	J	1	GLC	1	0
3	I	2	GLC	2	0

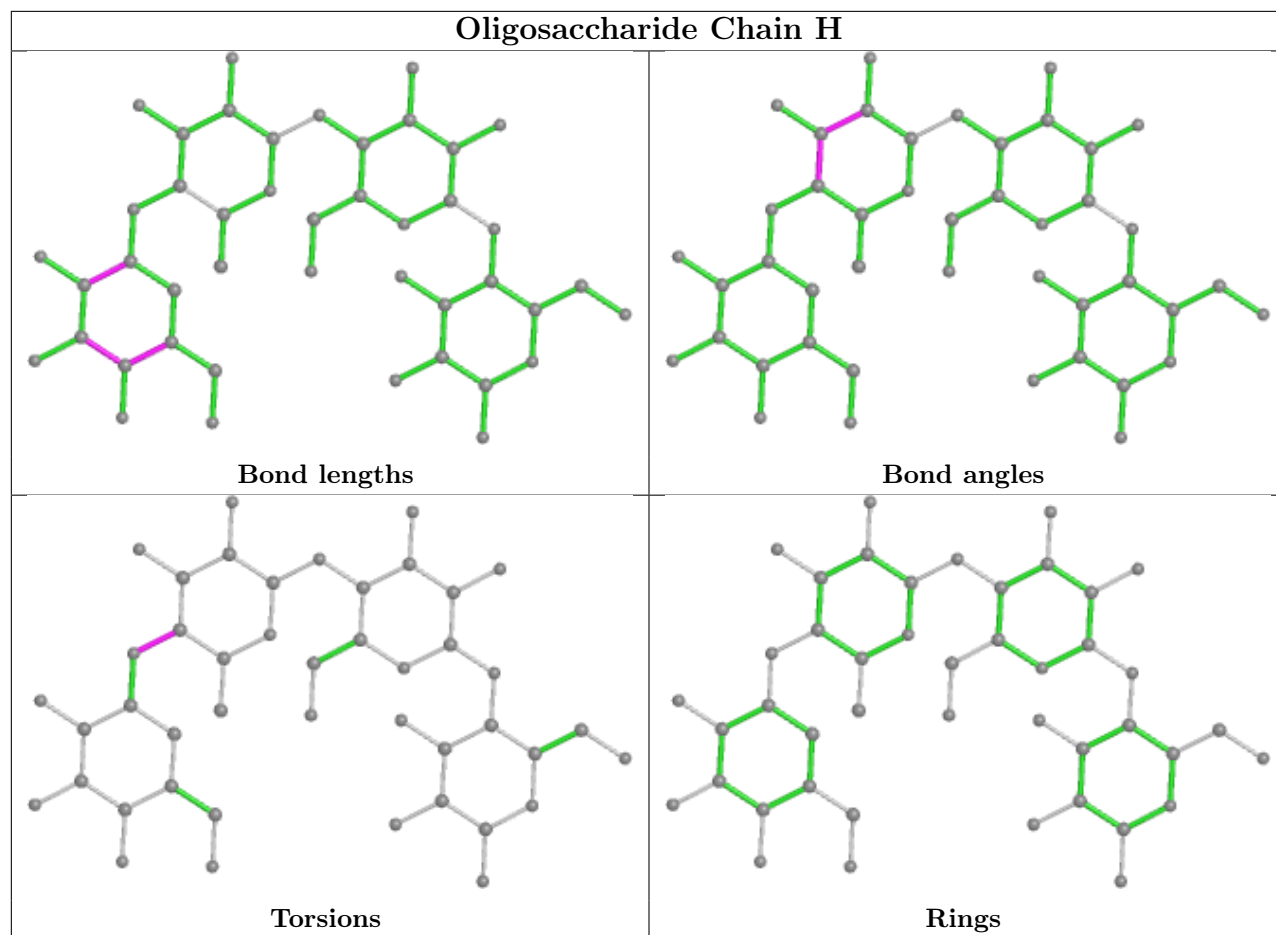
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

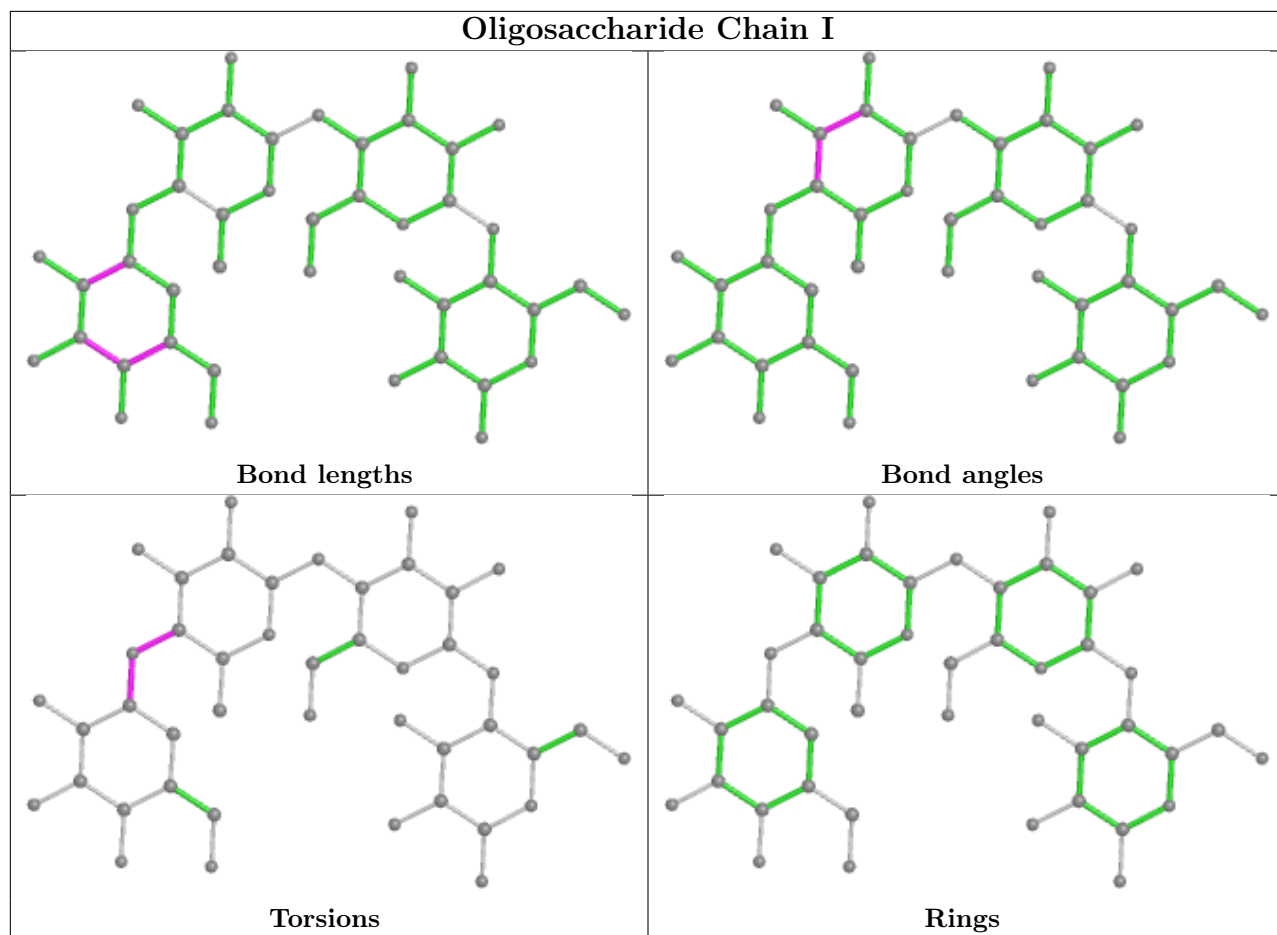
bond angles, torsion angles, and ring geometry for oligosaccharide.

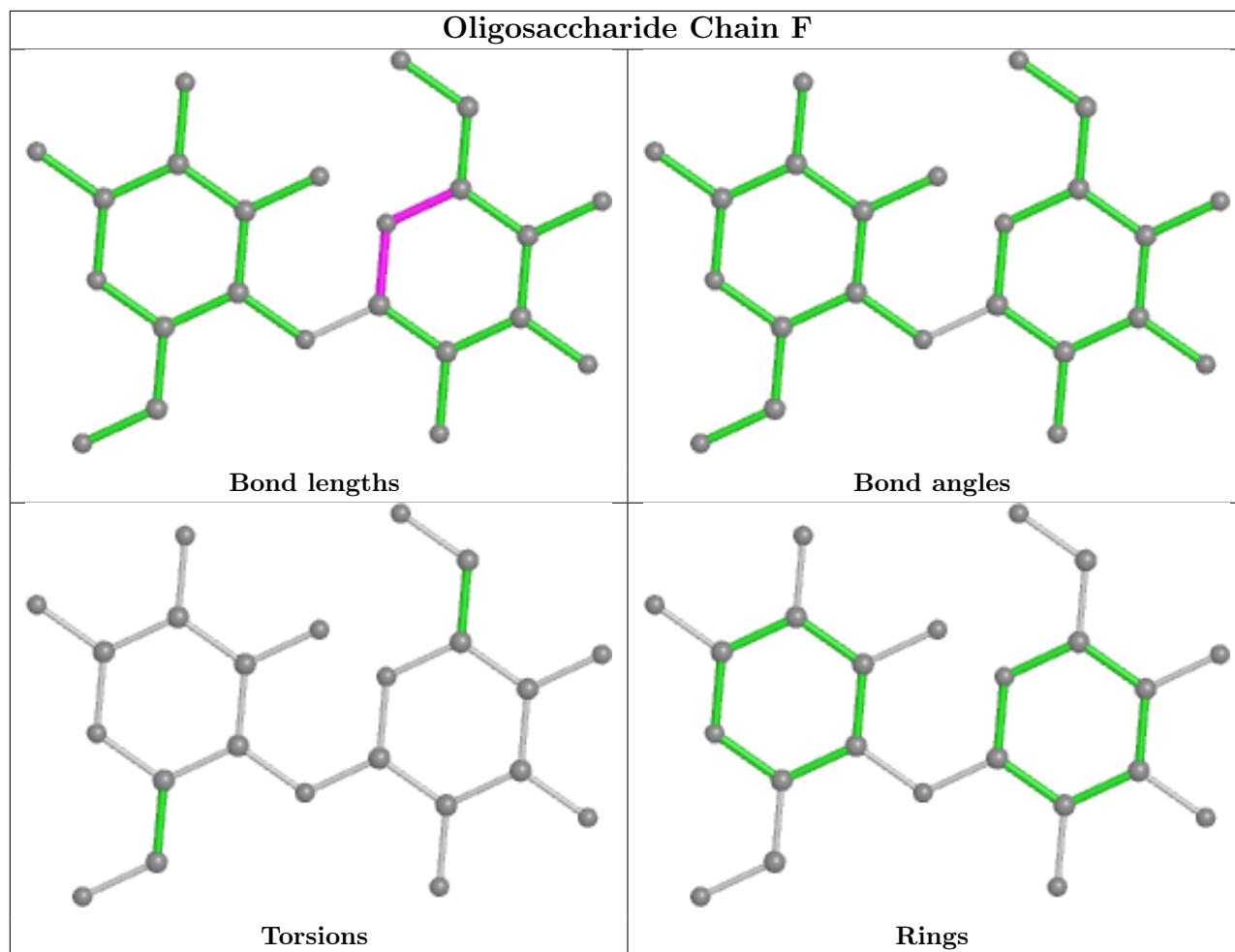


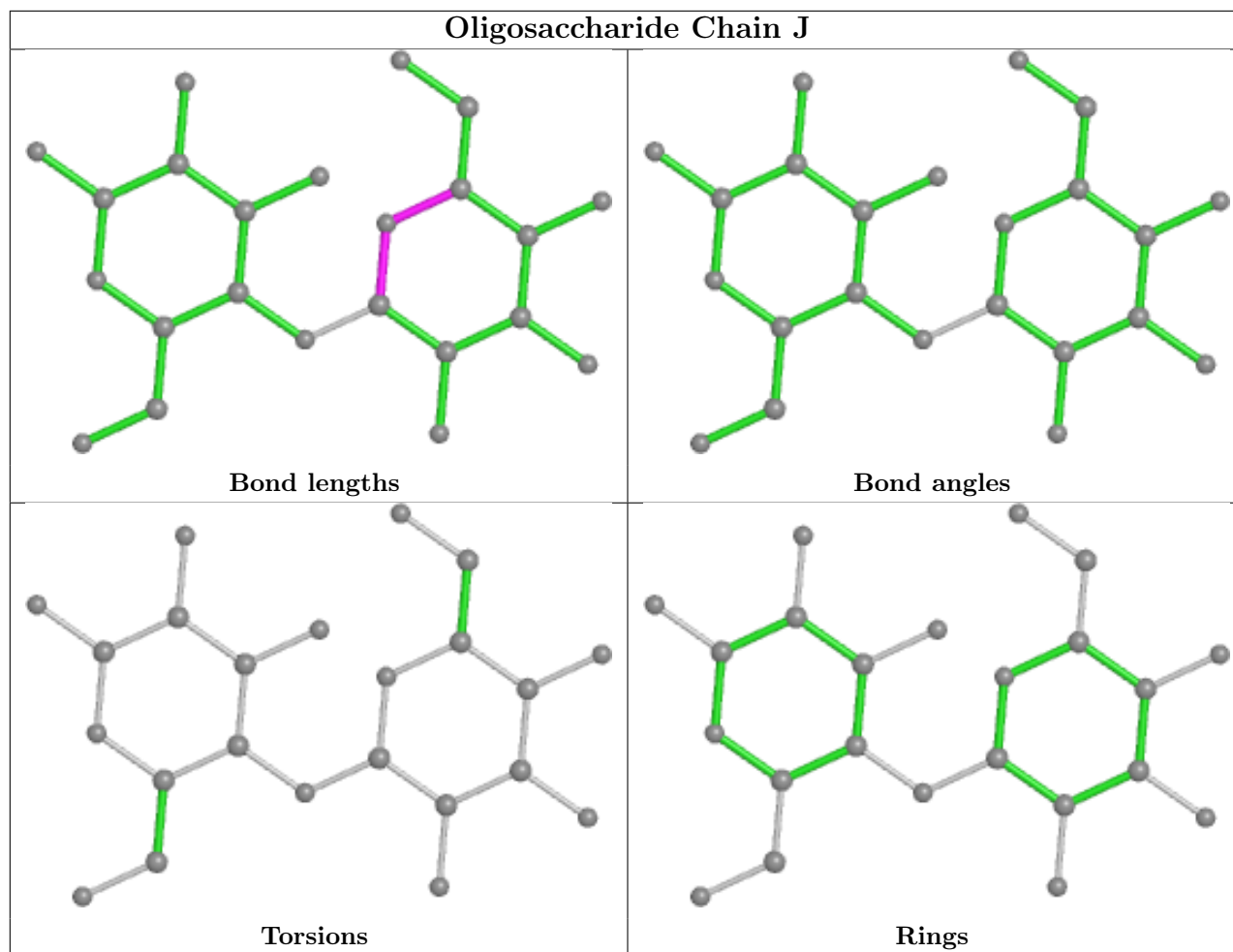












5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	EDO	A	750	-	3,3,3	0.73	0	2,2,2	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	750	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	750	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	750	EDO	3	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	639/669 (95%)	-0.30	5 (0%) 86 87	19, 35, 56, 71	0
1	B	635/669 (94%)	0.06	18 (2%) 53 56	23, 48, 65, 79	0
All	All	1274/1338 (95%)	-0.12	23 (1%) 68 71	19, 41, 63, 79	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	692	ASN	4.5
1	B	692	ASN	4.0
1	B	43	GLN	3.5
1	B	579	ASP	2.6
1	B	666	GLU	2.6
1	A	232	PRO	2.5
1	B	572	LYS	2.5
1	B	543	ASN	2.4
1	B	646	GLY	2.4
1	B	421	GLY	2.3
1	B	542	ASP	2.3
1	B	650	GLN	2.2
1	B	359	ASP	2.2
1	A	423	THR	2.2
1	B	153	ASN	2.1
1	B	647	THR	2.1
1	A	674	ASP	2.1
1	B	170	GLU	2.1
1	B	620	GLU	2.1
1	B	219	LYS	2.1
1	B	44	TRP	2.1
1	B	199	GLY	2.0
1	A	43	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

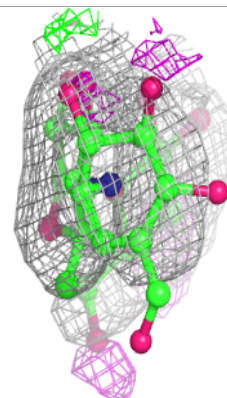
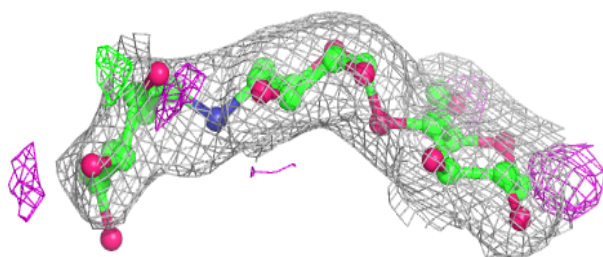
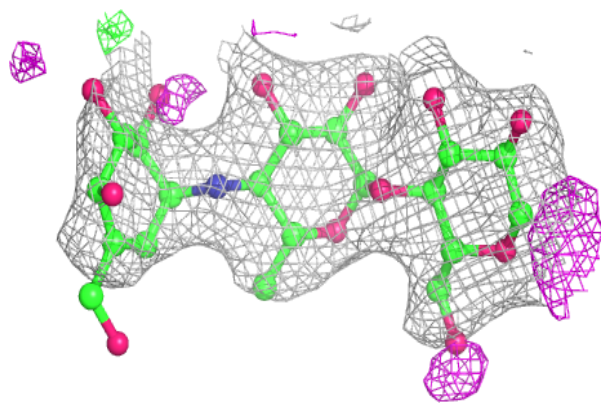
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	AC1	G	2	21/22	0.79	0.25	53,58,67,67	0
3	AC1	I	3	21/22	0.79	0.32	75,79,82,83	0
3	GLC	I	2	11/12	0.80	0.17	75,76,77,77	0
3	AC1	E	3	21/22	0.84	0.25	43,57,70,74	0
2	AC1	C	2	21/22	0.86	0.24	39,51,67,70	0
3	GLC	I	1	12/12	0.87	0.32	77,78,79,80	0
4	GLC	J	1	12/12	0.87	0.26	71,74,75,76	0
3	GLC	E	2	11/12	0.89	0.14	45,48,51,54	0
3	GLC	H	1	12/12	0.90	0.21	51,61,63,66	0
4	GLC	J	2	11/12	0.90	0.19	64,66,69,71	0
3	AC1	H	3	21/22	0.91	0.16	37,47,59,60	0
3	AC1	D	3	21/22	0.91	0.15	37,45,55,58	0
3	GLC	E	1	12/12	0.92	0.20	54,63,63,66	0
3	GLC	D	1	12/12	0.92	0.16	45,49,53,55	0
2	GLC	G	1	11/12	0.93	0.14	52,54,56,59	0
4	GLC	F	2	11/12	0.94	0.14	50,53,57,61	0
2	GLC	C	1	11/12	0.94	0.14	40,43,46,50	0
4	GLC	F	1	12/12	0.94	0.23	57,59,61,62	0
3	GLC	D	2	11/12	0.95	0.10	37,40,42,44	0
3	GLC	H	2	11/12	0.96	0.11	32,38,43,44	0

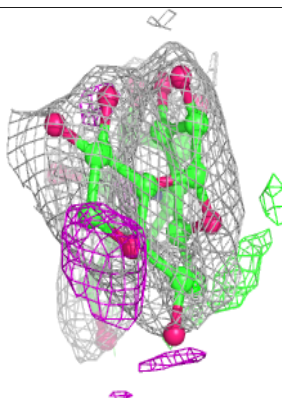
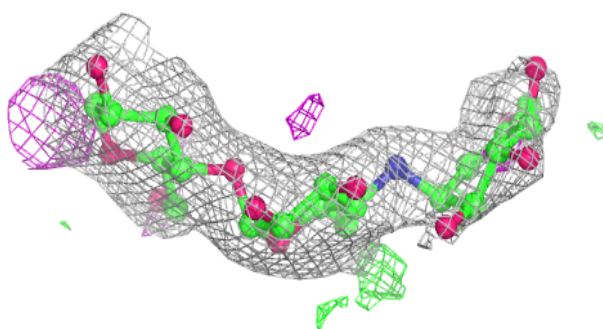
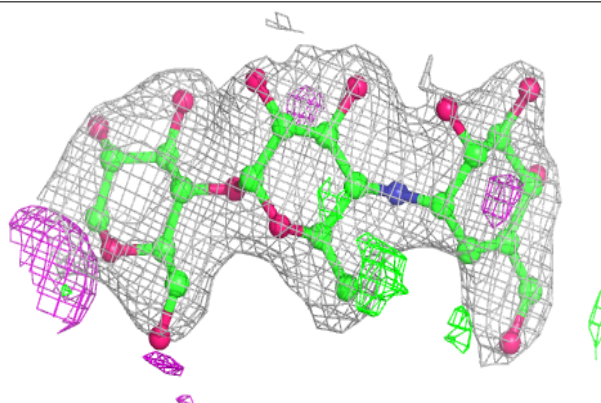
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

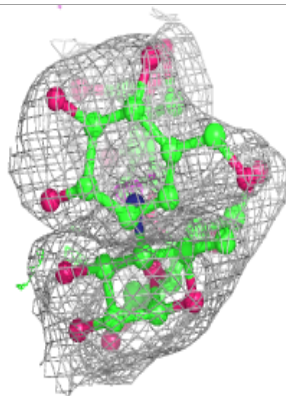
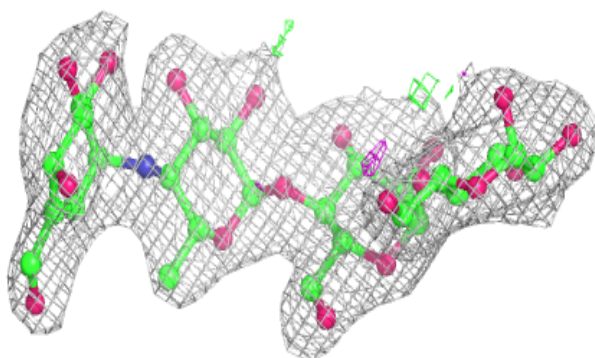
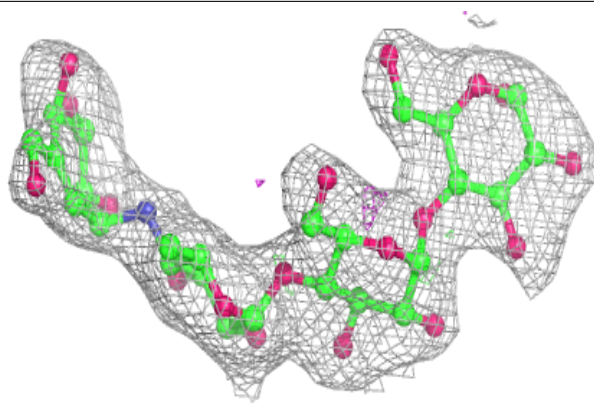
**Electron density around Chain G:**

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

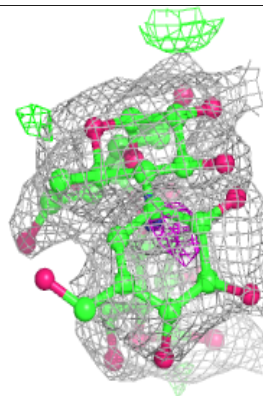
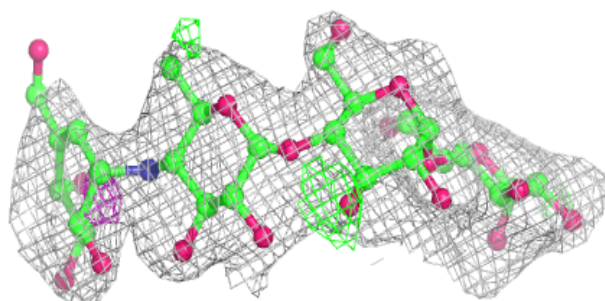
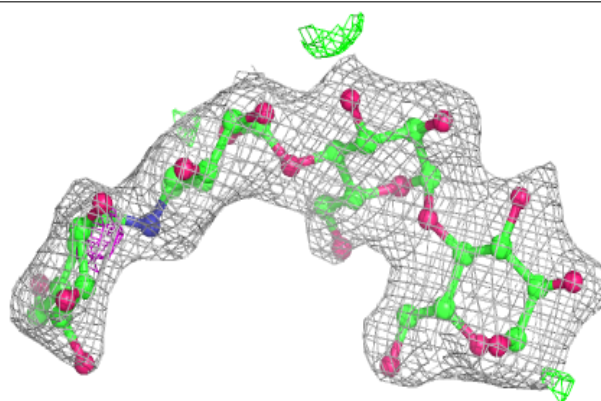


Electron density around Chain D:

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

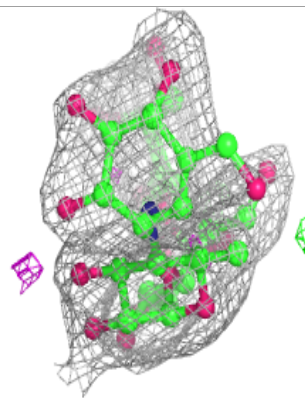
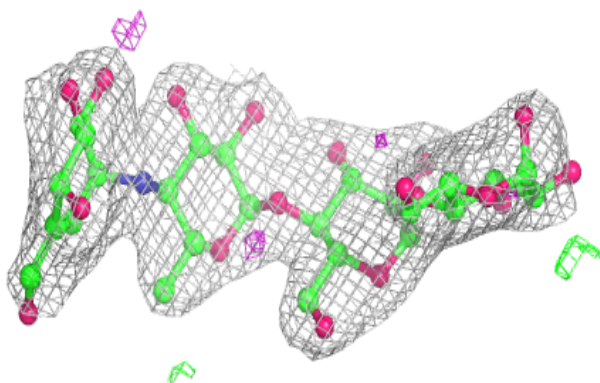
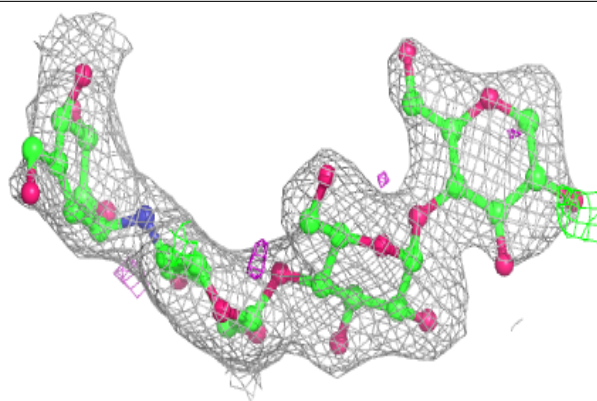
**Electron density around Chain E:**

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

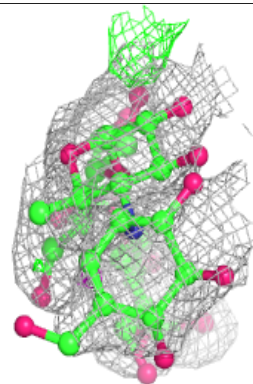
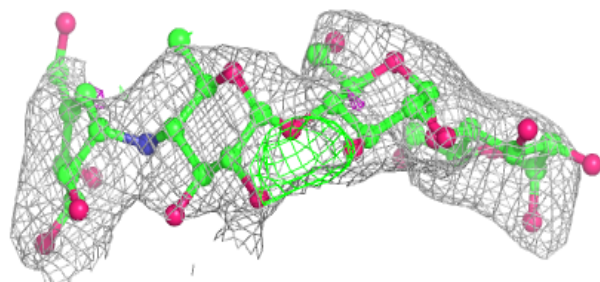
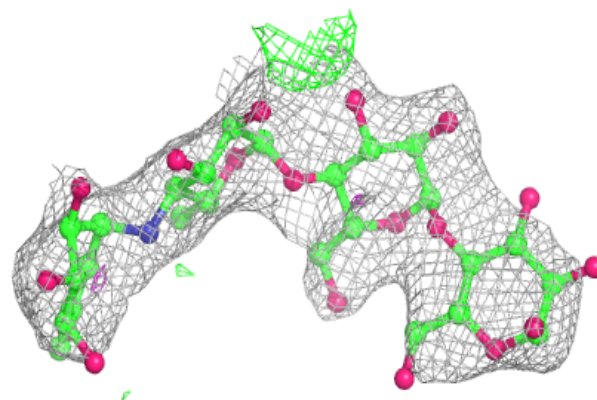


Electron density around Chain H:

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

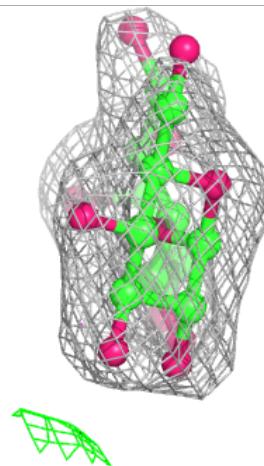
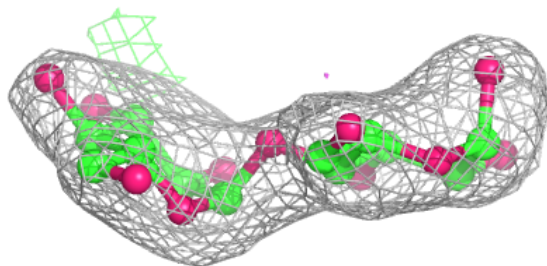
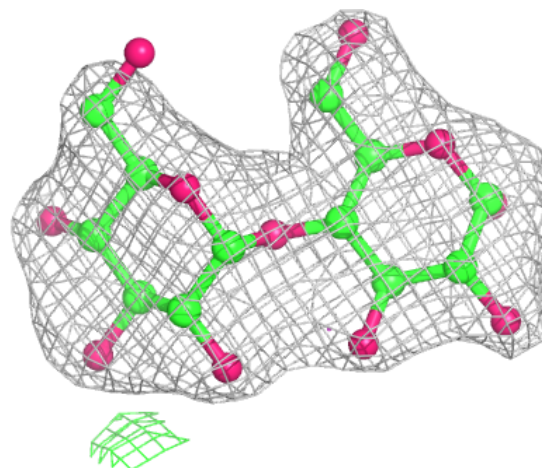
**Electron density around Chain I:**

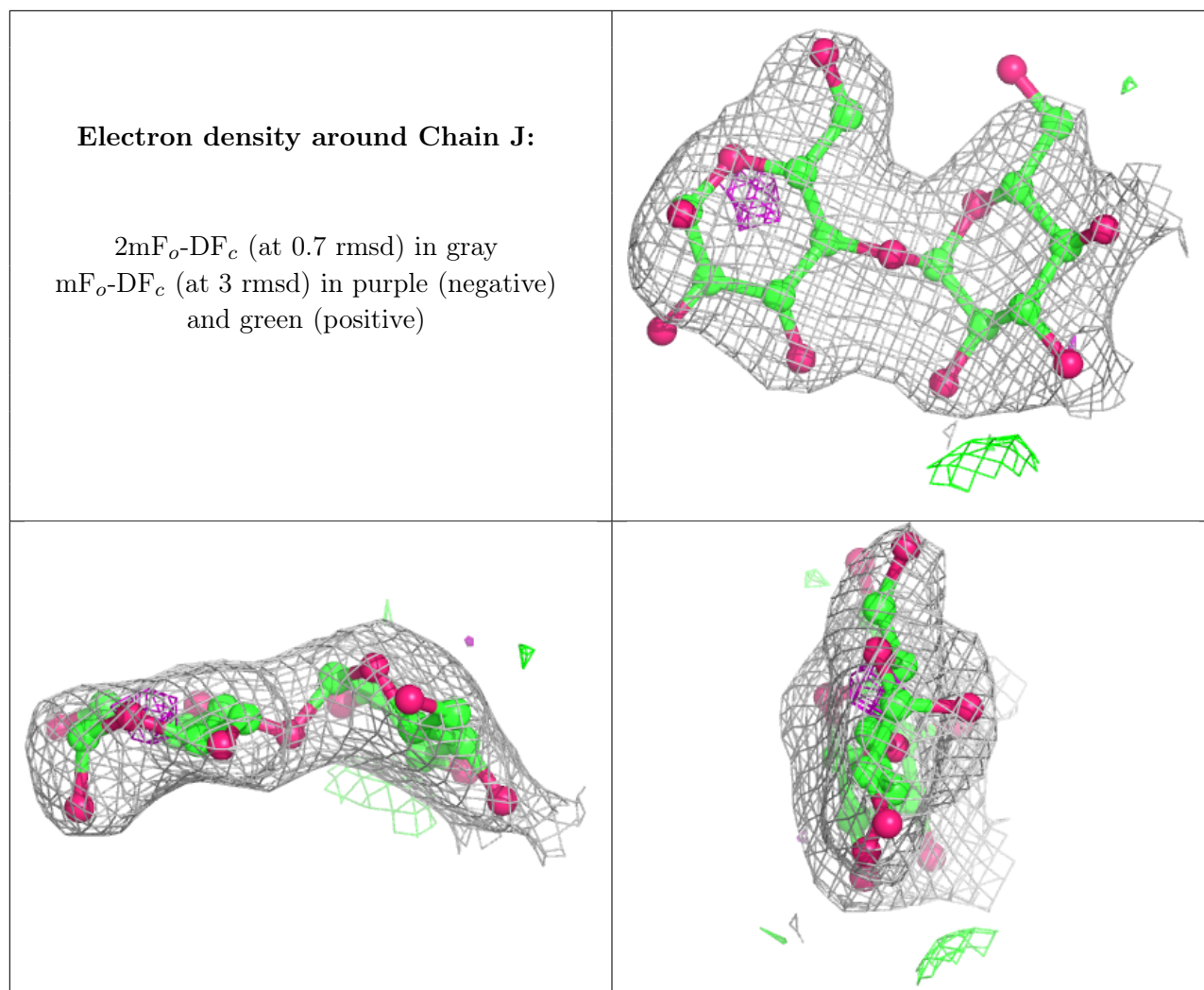
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain F:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CA	B	810	1/1	0.80	0.18	72,72,72,72	0
5	CA	B	800	1/1	0.93	0.08	72,72,72,72	0
6	EDO	A	750	4/4	0.93	0.13	44,44,45,46	0
5	CA	A	710	1/1	0.96	0.08	50,50,50,50	0
5	CA	A	700	1/1	0.97	0.09	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.