



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:05 PM UTC

PDB ID : 8TOT / pdb_00008tot
Title : ACE2-peptide2 complex crystal form 2
Authors : Christie, M.; Payne, R.J.
Deposited on : 2023-08-03
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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

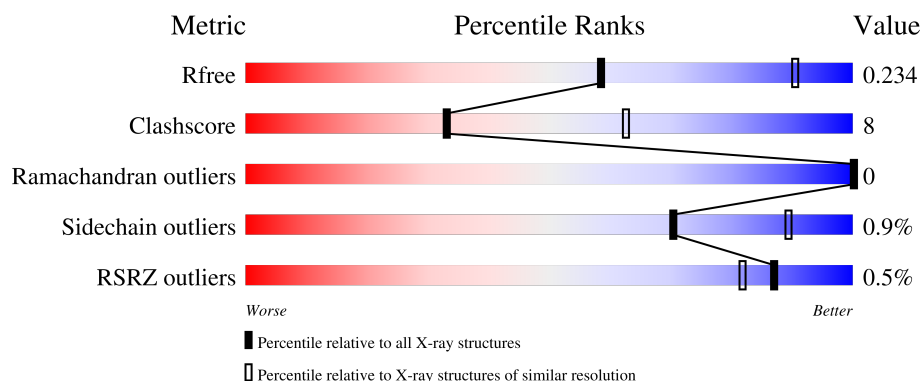
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

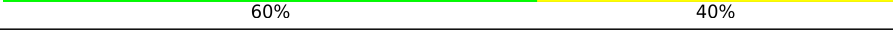
The reported resolution of this entry is 2.80 Å.

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.



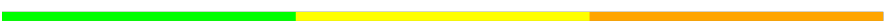
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 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	625	 78% 17% 5%
1	B	625	 76% 19% 5%
2	C	15	 73% 20% 7%
2	D	15	 60% 40%
3	E	2	 50% 50%

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Mol	Chain	Length	Quality of chain
3	F	2	 50%50%
3	G	2	 50%50%
3	H	2	 50%50%
4	I	3	 33%33%33%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10210 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	0	0
			4862	3111	805	917	29			
1	B	596	Total	C	N	O	S	0	0	0
			4862	3111	805	917	29			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	615	GLY	-	expression tag	UNP Q9BYF1
A	616	SER	-	expression tag	UNP Q9BYF1
A	617	HIS	-	expression tag	UNP Q9BYF1
A	618	HIS	-	expression tag	UNP Q9BYF1
A	619	HIS	-	expression tag	UNP Q9BYF1
A	620	HIS	-	expression tag	UNP Q9BYF1
A	621	HIS	-	expression tag	UNP Q9BYF1
A	622	HIS	-	expression tag	UNP Q9BYF1
A	623	HIS	-	expression tag	UNP Q9BYF1
A	624	HIS	-	expression tag	UNP Q9BYF1
A	625	HIS	-	expression tag	UNP Q9BYF1
A	626	HIS	-	expression tag	UNP Q9BYF1
A	627	SER	-	expression tag	UNP Q9BYF1
A	628	GLY	-	expression tag	UNP Q9BYF1
A	629	LEU	-	expression tag	UNP Q9BYF1
A	630	ASN	-	expression tag	UNP Q9BYF1
A	631	ASP	-	expression tag	UNP Q9BYF1
A	632	ILE	-	expression tag	UNP Q9BYF1
A	633	PHE	-	expression tag	UNP Q9BYF1
A	634	GLU	-	expression tag	UNP Q9BYF1
A	635	ALA	-	expression tag	UNP Q9BYF1
A	636	GLN	-	expression tag	UNP Q9BYF1
A	637	LYS	-	expression tag	UNP Q9BYF1
A	638	ILE	-	expression tag	UNP Q9BYF1
A	639	GLU	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	640	TRP	-	expression tag	UNP Q9BYF1
A	641	HIS	-	expression tag	UNP Q9BYF1
A	642	GLU	-	expression tag	UNP Q9BYF1
B	615	GLY	-	expression tag	UNP Q9BYF1
B	616	SER	-	expression tag	UNP Q9BYF1
B	617	HIS	-	expression tag	UNP Q9BYF1
B	618	HIS	-	expression tag	UNP Q9BYF1
B	619	HIS	-	expression tag	UNP Q9BYF1
B	620	HIS	-	expression tag	UNP Q9BYF1
B	621	HIS	-	expression tag	UNP Q9BYF1
B	622	HIS	-	expression tag	UNP Q9BYF1
B	623	HIS	-	expression tag	UNP Q9BYF1
B	624	HIS	-	expression tag	UNP Q9BYF1
B	625	HIS	-	expression tag	UNP Q9BYF1
B	626	HIS	-	expression tag	UNP Q9BYF1
B	627	SER	-	expression tag	UNP Q9BYF1
B	628	GLY	-	expression tag	UNP Q9BYF1
B	629	LEU	-	expression tag	UNP Q9BYF1
B	630	ASN	-	expression tag	UNP Q9BYF1
B	631	ASP	-	expression tag	UNP Q9BYF1
B	632	ILE	-	expression tag	UNP Q9BYF1
B	633	PHE	-	expression tag	UNP Q9BYF1
B	634	GLU	-	expression tag	UNP Q9BYF1
B	635	ALA	-	expression tag	UNP Q9BYF1
B	636	GLN	-	expression tag	UNP Q9BYF1
B	637	LYS	-	expression tag	UNP Q9BYF1
B	638	ILE	-	expression tag	UNP Q9BYF1
B	639	GLU	-	expression tag	UNP Q9BYF1
B	640	TRP	-	expression tag	UNP Q9BYF1
B	641	HIS	-	expression tag	UNP Q9BYF1
B	642	GLU	-	expression tag	UNP Q9BYF1

- Molecule 2 is a protein called Cyclic peptide 2.

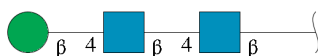
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	15	Total 123	C 80	N 24	O 18	S 1	0	0	1
2	D	15	Total 123	C 80	N 24	O 18	S 1	0	0	1

- Molecule 3 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
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		
7	B	1	Total	Cl	0	0
			1	1		

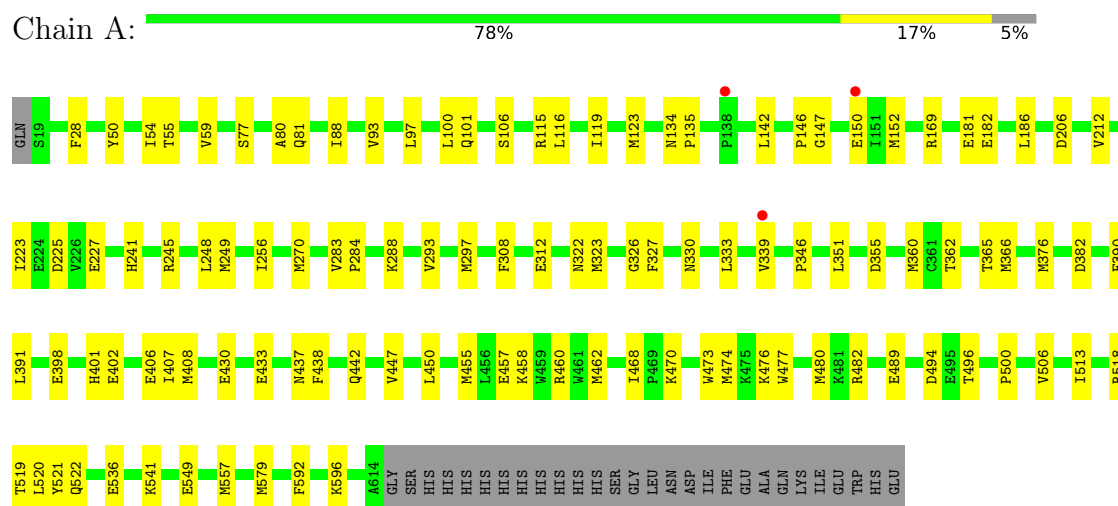
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	O	0	0
			1	1		

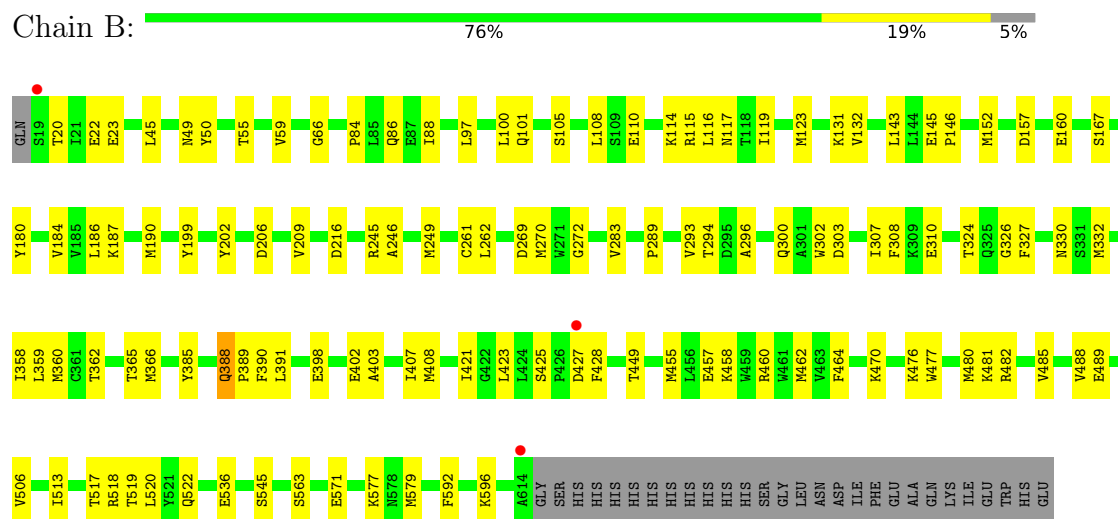
3 Residue-property plots

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: Angiotensin-converting enzyme 2



• Molecule 1: Angiotensin-converting enzyme 2

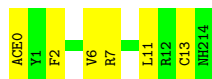


• Molecule 2: Cyclic peptide 2





- Molecule 2: Cyclic peptide 2



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



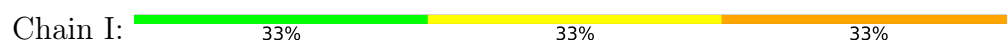
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.66Å 89.31Å 118.51Å 90.00° 116.93° 90.00°	Depositor
Resolution (Å)	49.24 – 2.80 49.24 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.24-2.80) 99.4 (49.24-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.210 , 0.242 0.200 , 0.234	Depositor DCC
R_{free} test set	2344 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	64.4	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10210	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: BMA, NAG, NH2, ACE, ZN, CL

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	0.38	0/4999	0.56	0/6792
1	B	0.39	0/4999	0.55	0/6792
2	C	0.49	0/123	0.66	0/165
2	D	0.44	0/123	0.64	0/165
All	All	0.39	0/10244	0.56	0/13914

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	4862	0	4633	74	0
1	B	4862	0	4633	78	0
2	C	123	0	124	4	0
2	D	123	0	124	5	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
4	I	39	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	28	0	26	0	0
6	B	56	0	52	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	1	0	0	0	0
All	All	10210	0	9726	155	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 8.

All (155) 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:421:ILE:HG13	1:B:423:LEU:HD23	1.57	0.87
1:B:571:GLU:OE2	1:B:577:LYS:NZ	2.15	0.79
1:A:407:ILE:HG13	1:A:408:MET:HE2	1.65	0.78
1:A:181:GLU:HG2	1:A:470:LYS:HD3	1.69	0.73
1:A:536:GLU:N	1:A:536:GLU:OE1	2.21	0.73
1:B:407:ILE:HG13	1:B:408:MET:HE2	1.71	0.73
1:B:97:LEU:O	1:B:101:GLN:HG3	1.88	0.72
1:A:458:LYS:O	1:A:462:MET:HG3	1.89	0.71
1:B:245:ARG:HB2	1:B:262:LEU:HD21	1.74	0.70
1:A:323:MET:HE3	1:A:327:PHE:CE2	2.28	0.69
1:A:402:GLU:HB3	1:A:518:ARG:HG3	1.76	0.67
1:A:55:THR:O	1:A:59:VAL:HG23	1.93	0.67
1:A:97:LEU:O	1:A:101:GLN:HG3	1.95	0.67
1:A:346:PRO:HB3	1:A:360:MET:HE2	1.75	0.67
1:B:308:PHE:HZ	1:B:360:MET:HE3	1.60	0.66
1:B:66:GLY:HA2	2:D:2:PHE:HE1	1.60	0.66
1:B:517:THR:HA	1:B:579:MET:HE1	1.78	0.63
1:B:55:THR:O	1:B:59:VAL:HG23	1.97	0.63
1:A:406:GLU:HG3	1:A:518:ARG:HD3	1.79	0.63
1:B:388:GLN:HG3	1:B:389:PRO:HD2	1.81	0.62
1:A:549:GLU:OE2	1:A:549:GLU:N	2.26	0.62
1:B:302:TRP:CZ2	1:B:423:LEU:HD21	2.35	0.62
1:A:297:MET:HE1	1:A:366:MET:HA	1.82	0.62
1:B:296:ALA:O	1:B:300:GLN:HG3	2.00	0.62
1:B:209:VAL:HG12	1:B:216:ASP:HA	1.82	0.61
1:B:294:THR:HG23	1:B:365:THR:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:MET:HE1	1:B:202:TYR:CZ	2.39	0.58
1:B:206:ASP:OD2	1:B:398:GLU:HG2	2.03	0.58
1:A:293:VAL:HG23	1:A:297:MET:HE2	1.86	0.58
1:B:132:VAL:HG11	1:B:167:SER:HB3	1.85	0.57
1:B:407:ILE:HG13	1:B:408:MET:CE	2.33	0.57
1:B:388:GLN:HE21	1:B:563:SER:HB3	1.69	0.57
1:B:86:GLN:OE1	1:B:86:GLN:N	2.26	0.57
1:A:474:MET:HE1	1:A:500:PRO:HD3	1.86	0.57
1:B:455:MET:HE2	1:B:485:VAL:HG21	1.86	0.57
1:A:288:LYS:NZ	1:A:433:GLU:OE1	2.38	0.57
1:A:460:ARG:NH2	1:A:506:VAL:HA	2.21	0.56
1:B:476:LYS:O	1:B:480:MET:HG3	2.06	0.56
1:B:308:PHE:CZ	1:B:360:MET:HE3	2.40	0.56
1:B:390:PHE:HD1	1:B:391:LEU:HD23	1.71	0.56
1:B:20:THR:HG22	1:B:23:GLU:HB2	1.88	0.56
1:B:116:LEU:HD12	1:B:186:LEU:HB3	1.89	0.55
1:A:477:TRP:CE3	1:A:500:PRO:HG3	2.43	0.54
1:A:407:ILE:CG1	1:A:408:MET:HE2	2.37	0.54
1:B:202:TYR:OH	2:D:7:ARG:HG2	2.08	0.54
1:A:152:MET:HG3	1:A:270:MET:HA	1.91	0.53
1:A:323:MET:HE2	1:A:376:MET:HE2	1.90	0.53
1:A:476:LYS:O	1:A:480:MET:HG3	2.09	0.53
1:A:482:ARG:NH1	1:A:489:GLU:OE2	2.40	0.53
1:B:86:GLN:H	1:B:86:GLN:CD	2.10	0.53
1:A:455:MET:HE3	1:A:480:MET:HB2	1.91	0.52
1:B:326:GLY:O	1:B:330:ASN:ND2	2.42	0.52
1:A:592:PHE:O	1:A:596:LYS:HG3	2.08	0.52
1:B:110:GLU:HG3	1:B:114:LYS:NZ	2.23	0.52
1:B:157:ASP:HB3	1:B:160:GLU:HB3	1.92	0.51
1:A:146:PRO:O	1:A:150:GLU:HG3	2.11	0.51
1:B:20:THR:HG23	1:B:23:GLU:H	1.75	0.51
1:A:50:TYR:CE1	1:A:54:ILE:HG23	2.46	0.51
1:A:430:GLU:HG2	1:A:541:LYS:NZ	2.26	0.50
1:A:457:GLU:HG2	1:A:513:ILE:HB	1.92	0.50
1:B:536:GLU:OE1	1:B:536:GLU:N	2.38	0.50
1:B:360:MET:HG2	1:B:362:THR:OG1	2.11	0.50
1:B:110:GLU:O	1:B:114:LYS:HG3	2.11	0.50
1:B:84:PRO:HB2	1:B:86:GLN:OE1	2.12	0.50
1:B:152:MET:HG3	1:B:270:MET:HA	1.94	0.49
1:A:468:ILE:HG22	1:A:473:TRP:HD1	1.77	0.49
1:A:115:ARG:NH2	1:A:182:GLU:OE1	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:PHE:CE2	1:B:358:ILE:HD12	2.48	0.49
1:A:390:PHE:CZ	2:C:4:ARG:HG2	2.47	0.49
1:A:447:VAL:HA	1:A:450:LEU:HD23	1.94	0.49
1:A:293:VAL:HG22	1:A:366:MET:SD	2.53	0.49
1:A:458:LYS:HE3	1:A:462:MET:HE3	1.95	0.49
1:B:246:ALA:HA	1:B:249:MET:HE2	1.94	0.49
1:A:519:THR:O	1:A:522:GLN:HG2	2.13	0.48
1:A:206:ASP:OD2	1:A:398:GLU:HG2	2.13	0.48
1:A:360:MET:HG2	1:A:362:THR:OG1	2.13	0.48
1:A:100:LEU:HD13	2:C:6:VAL:HG21	1.95	0.48
1:B:22:GLU:HG3	1:B:88:ILE:HG23	1.95	0.48
1:B:332:MET:HE2	1:B:359:LEU:HG	1.95	0.48
1:A:376:MET:HE3	1:A:376:MET:HB2	1.77	0.47
1:A:245:ARG:O	1:A:249:MET:HG3	2.14	0.47
1:B:123:MET:HE1	1:B:180:TYR:HA	1.97	0.47
1:A:169:ARG:NH2	1:A:270:MET:O	2.41	0.47
1:B:131:LYS:HB3	1:B:143:LEU:HD23	1.97	0.47
1:A:326:GLY:O	1:A:330:ASN:ND2	2.48	0.47
1:A:390:PHE:HD2	1:A:391:LEU:HD23	1.80	0.47
1:B:482:ARG:NH1	1:B:489:GLU:OE2	2.45	0.47
1:B:520:LEU:HD22	1:B:579:MET:HE2	1.96	0.47
1:A:181:GLU:CG	1:A:470:LYS:HD3	2.43	0.46
1:A:225:ASP:HB3	1:A:579:MET:CE	2.46	0.46
1:B:45:LEU:O	1:B:49:ASN:ND2	2.48	0.46
1:A:438:PHE:O	1:A:442:GLN:HG2	2.16	0.46
1:A:430:GLU:HG2	1:A:541:LYS:HZ1	1.81	0.46
1:B:293:VAL:HG22	1:B:366:MET:SD	2.55	0.46
1:B:302:TRP:CH2	1:B:310:GLU:HG3	2.51	0.46
1:A:297:MET:HE1	1:A:366:MET:CA	2.45	0.46
1:B:50:TYR:CE1	1:B:59:VAL:HG22	2.52	0.45
1:A:248:LEU:HB3	1:A:256:ILE:HD13	1.98	0.45
1:A:489:GLU:O	1:A:489:GLU:HG2	2.16	0.45
1:A:494:ASP:OD1	1:A:496:THR:OG1	2.29	0.45
1:B:289:PRO:HG2	1:B:428:PHE:CE2	2.52	0.45
1:B:390:PHE:CD1	1:B:391:LEU:HD23	2.52	0.44
1:A:223:ILE:O	1:A:227:GLU:HG3	2.16	0.44
1:A:212:VAL:HG12	1:A:212:VAL:O	2.18	0.44
1:A:450:LEU:HD21	1:A:519:THR:HG21	2.00	0.44
1:B:545:SER:HB2	4:I:1:NAG:H82	1.98	0.44
1:A:351:LEU:HB2	1:A:355:ASP:HB3	1.99	0.44
1:B:108:LEU:HD11	1:B:190:MET:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:0:ACE:H2	2:C:13:CYS:N	2.33	0.44
1:A:557:MET:HE3	1:A:557:MET:HB3	1.96	0.43
1:B:100:LEU:HA	2:D:6:VAL:HG21	1.98	0.43
1:B:519:THR:O	1:B:522:GLN:HG2	2.19	0.43
1:B:455:MET:HE3	1:B:455:MET:HB3	1.71	0.43
1:A:312:GLU:OE2	1:A:322:ASN:HB2	2.18	0.43
1:B:457:GLU:HG2	1:B:513:ILE:HB	2.01	0.43
1:A:100:LEU:CD1	2:C:6:VAL:HG21	2.49	0.43
1:B:458:LYS:O	1:B:462:MET:HG3	2.18	0.43
1:B:261:CYS:HB2	1:B:488:VAL:HG12	1.99	0.43
1:B:269:ASP:OD1	1:B:272:GLY:N	2.52	0.43
1:A:77:SER:O	1:A:81:GLN:HG2	2.19	0.43
1:A:88:ILE:HG21	1:A:93:VAL:HG12	2.00	0.43
1:A:518:ARG:HD2	1:A:519:THR:N	2.34	0.43
1:A:297:MET:HE1	1:A:365:THR:C	2.44	0.42
1:B:145:GLU:HA	1:B:146:PRO:HA	1.88	0.42
1:A:241:HIS:CD2	1:A:241:HIS:C	2.97	0.42
1:B:402:GLU:HB3	1:B:518:ARG:CD	2.49	0.42
1:A:119:ILE:O	1:A:123:MET:HG3	2.20	0.42
1:B:303:ASP:O	1:B:307:ILE:HG13	2.19	0.42
1:A:134:ASN:OD1	1:A:135:PRO:HD2	2.20	0.42
1:B:245:ARG:HB2	1:B:262:LEU:CD2	2.46	0.42
1:B:184:VAL:HG22	1:B:464:PHE:HE1	1.85	0.42
1:B:403:ALA:O	1:B:407:ILE:HG23	2.20	0.42
1:B:460:ARG:NH2	1:B:506:VAL:HA	2.35	0.42
2:D:11:LEU:HD23	2:D:11:LEU:HA	1.85	0.42
1:B:116:LEU:HD12	1:B:186:LEU:CB	2.50	0.42
1:A:116:LEU:HB2	1:A:186:LEU:HD13	2.02	0.42
1:A:28:PHE:HE2	1:A:80:ALA:HB2	1.85	0.41
1:B:388:GLN:HG3	1:B:389:PRO:CD	2.48	0.41
1:B:470:LYS:HB2	1:B:470:LYS:HE2	1.89	0.41
1:B:477:TRP:CZ2	1:B:481:LYS:HE2	2.56	0.41
1:B:187:LYS:HD2	1:B:199:TYR:CZ	2.56	0.41
1:B:302:TRP:CH2	1:B:423:LEU:HD21	2.55	0.41
1:B:425:SER:OG	1:B:427:ASP:OD1	2.25	0.41
2:D:0:ACE:H2	2:D:13:CYS:N	2.35	0.41
1:A:284:PRO:HD2	1:A:437:ASN:OD1	2.20	0.41
1:B:592:PHE:O	1:B:596:LYS:HG3	2.20	0.41
1:A:142:LEU:HD22	1:A:147:GLY:HA3	2.03	0.41
1:A:382:ASP:OD1	1:A:401:HIS:HE1	2.03	0.40
1:B:115:ARG:O	1:B:119:ILE:HG13	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:GLU:HB3	1:B:518:ARG:HD3	2.03	0.40
1:A:115:ARG:O	1:A:119:ILE:HG13	2.21	0.40
1:A:297:MET:HE1	1:A:366:MET:N	2.37	0.40
1:A:520:LEU:O	1:A:521:TYR:C	2.62	0.40
1:B:324:THR:O	1:B:327:PHE:HB3	2.21	0.40
1:A:308:PHE:CD1	1:A:333:LEU:HD13	2.56	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	594/625 (95%)	580 (98%)	14 (2%)	0	100	100
1	B	594/625 (95%)	587 (99%)	7 (1%)	0	100	100
2	C	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
2	D	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
All	All	1214/1280 (95%)	1191 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	526/552 (95%)	523 (99%)	3 (1%)	78	92
1	B	526/552 (95%)	520 (99%)	6 (1%)	65	87
2	C	13/13 (100%)	12 (92%)	1 (8%)	12	36
2	D	13/13 (100%)	13 (100%)	0	100	100
All	All	1078/1130 (95%)	1068 (99%)	10 (1%)	70	89

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	SER
1	A	283	VAL
1	A	339	VAL
1	B	105	SER
1	B	117	ASN
1	B	283	VAL
1	B	385	TYR
1	B	388	GLN
1	B	449	THR
2	C	13	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	241	HIS
1	A	429	GLN
1	A	472	GLN
1	A	535	HIS
1	A	540	HIS
1	B	24	GLN
1	B	76	GLN
1	B	98	GLN
1	B	300	GLN
1	B	330	ASN
1	B	388	GLN
1	B	535	HIS
2	C	3	GLN
2	D	3	GLN

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 ⓘ

11 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$
3	NAG	E	1	1,3	14,14,15	0.39	0	17,19,21	0.89	0
3	NAG	E	2	3	14,14,15	0.44	0	17,19,21	0.72	1 (5%)
3	NAG	F	1	1,3	14,14,15	0.43	0	17,19,21	0.59	0
3	NAG	F	2	3	14,14,15	1.68	1 (7%)	17,19,21	2.06	3 (17%)
3	NAG	G	1	1,3	14,14,15	0.41	0	17,19,21	0.95	1 (5%)
3	NAG	G	2	3	14,14,15	0.61	0	17,19,21	1.08	0
3	NAG	H	1	1,3	14,14,15	0.37	0	17,19,21	0.88	0
3	NAG	H	2	3	14,14,15	0.34	0	17,19,21	1.08	1 (5%)
4	NAG	I	1	1,4	14,14,15	0.82	1 (7%)	17,19,21	1.04	1 (5%)
4	NAG	I	2	4	14,14,15	0.32	0	17,19,21	0.73	0
4	BMA	I	3	4	11,11,12	0.98	1 (9%)	15,15,17	1.14	1 (6%)

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
3	NAG	E	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	BMA	I	3	4	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	NAG	O5-C1	5.94	1.53	1.43
4	I	1	NAG	O5-C1	2.93	1.48	1.43
4	I	3	BMA	C1-C2	2.26	1.57	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	NAG	C1-O5-C5	7.16	121.78	112.19
4	I	3	BMA	C1-O5-C5	3.73	117.19	112.19
3	H	2	NAG	C1-O5-C5	3.72	117.17	112.19
4	I	1	NAG	C1-O5-C5	3.15	116.41	112.19
3	F	2	NAG	C2-N2-C7	2.87	126.74	122.90
3	E	2	NAG	C1-O5-C5	2.29	115.26	112.19
3	F	2	NAG	C1-C2-N2	2.08	113.71	110.43
3	G	1	NAG	C1-O5-C5	2.06	114.94	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	NAG	C4-C5-C6-O6
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
3	F	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6

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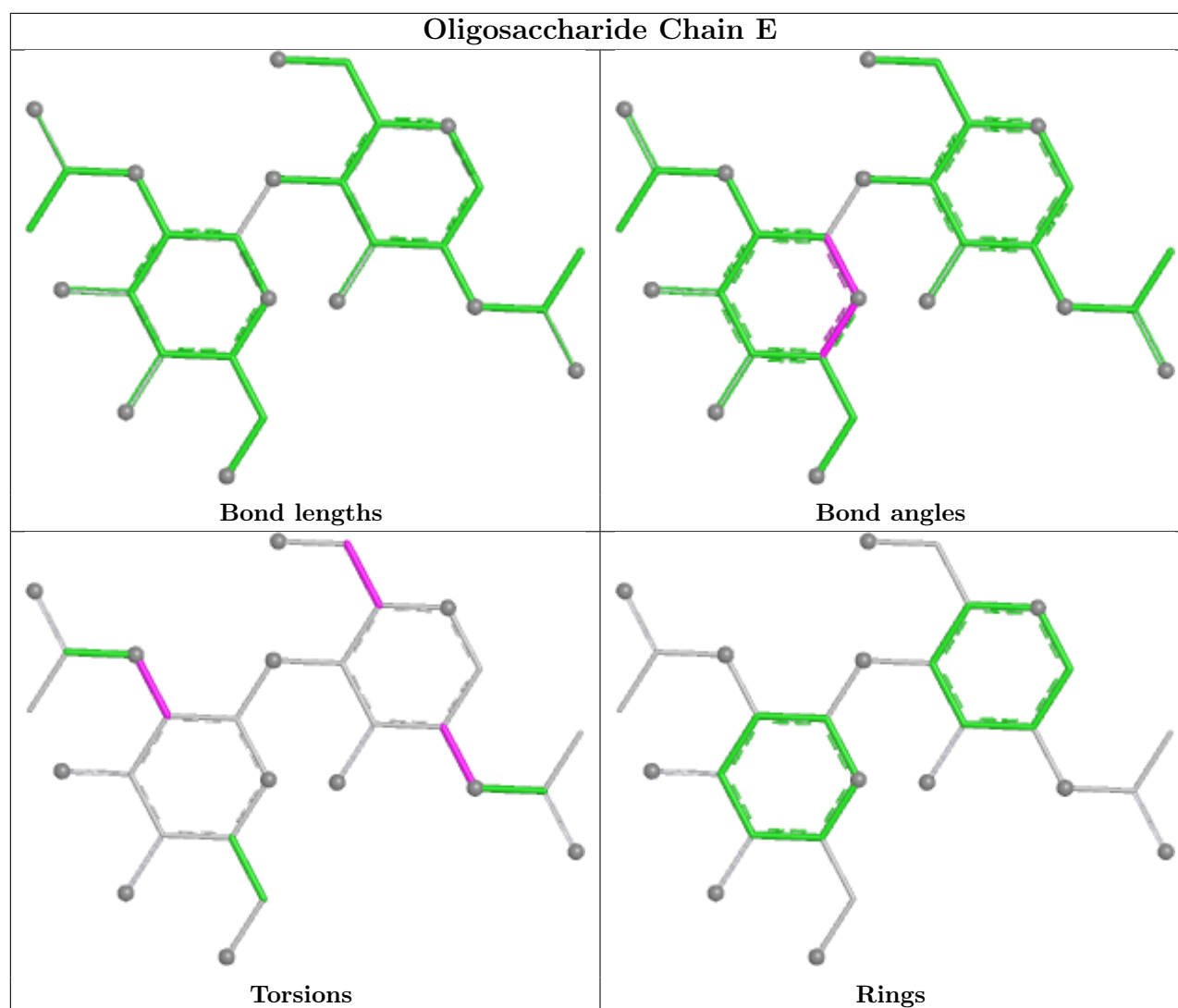
Mol	Chain	Res	Type	Atoms
4	I	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C3-C2-N2-C7
3	E	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C1-C2-N2-C7
3	E	2	NAG	C1-C2-N2-C7
3	F	2	NAG	C1-C2-N2-C7
3	F	1	NAG	C4-C5-C6-O6

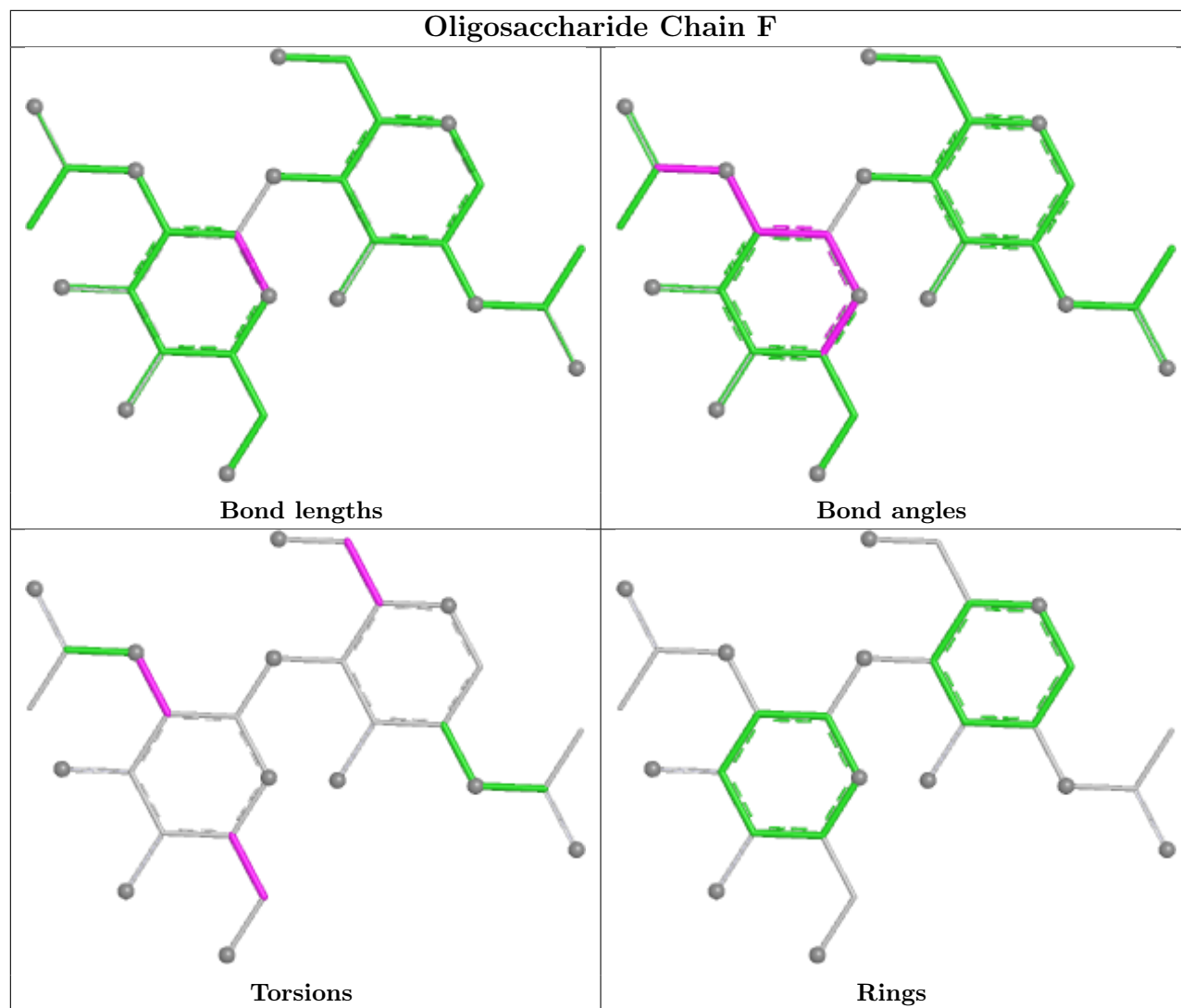
There are no ring outliers.

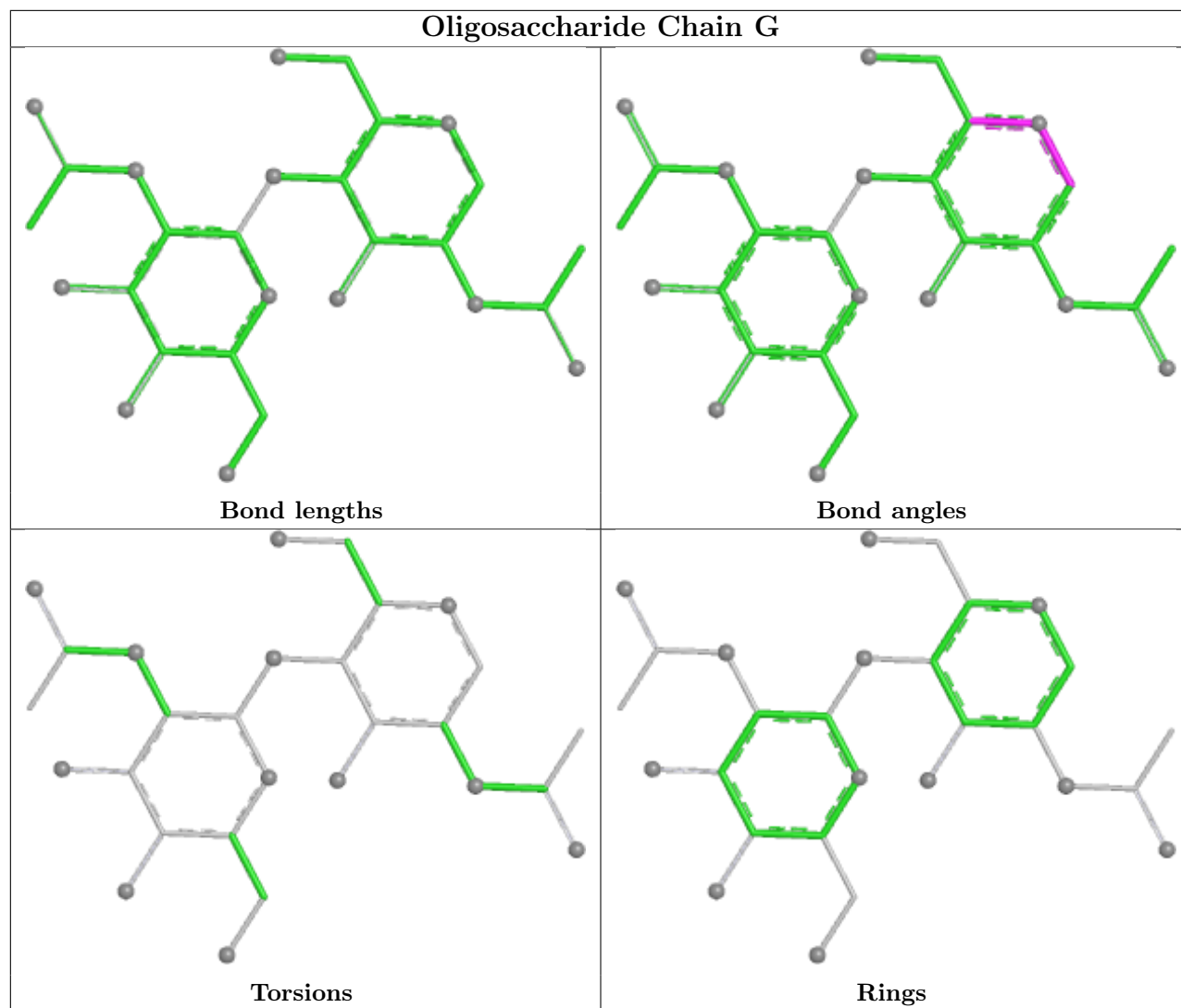
1 monomer is involved in 1 short contact:

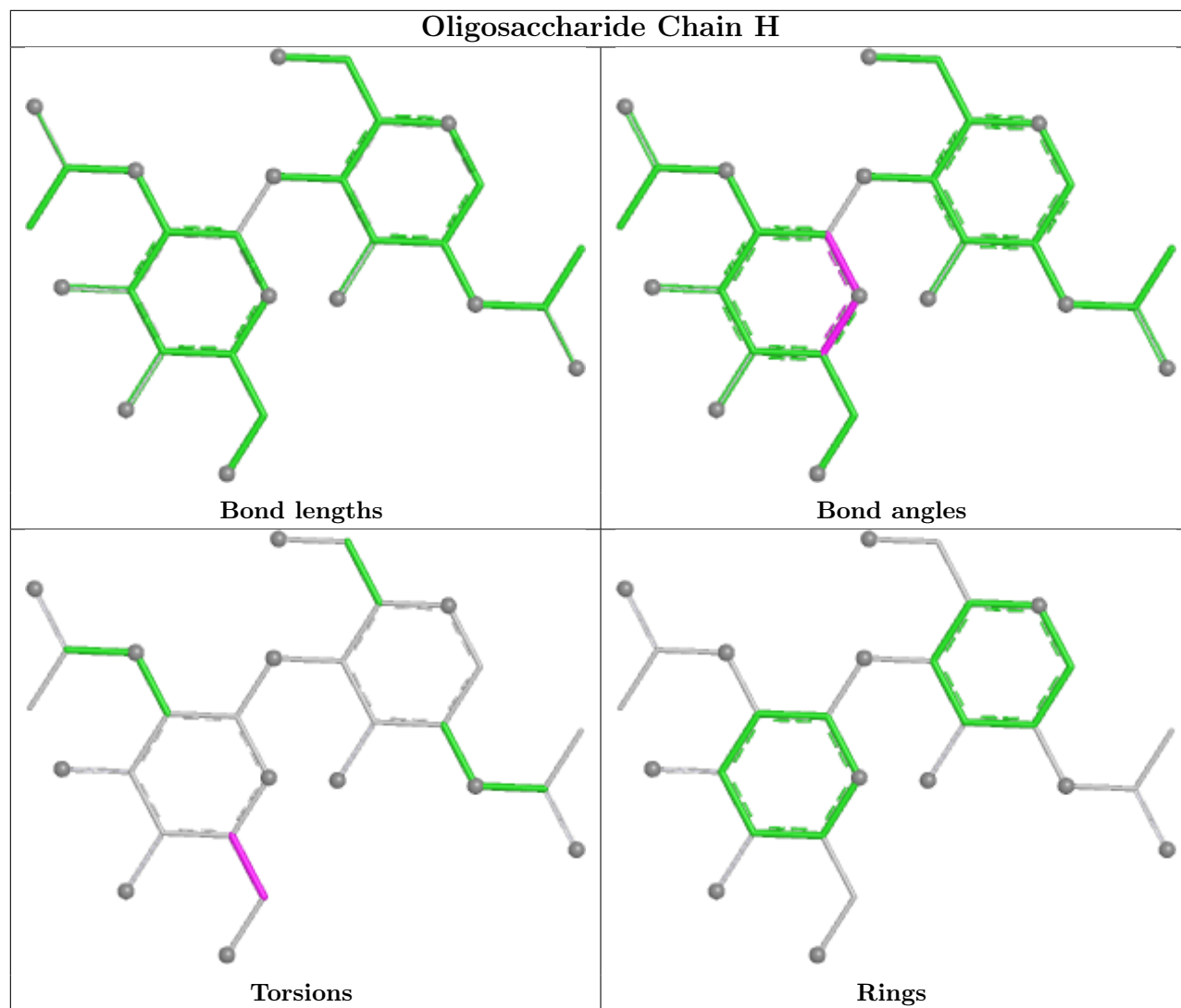
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	1	0

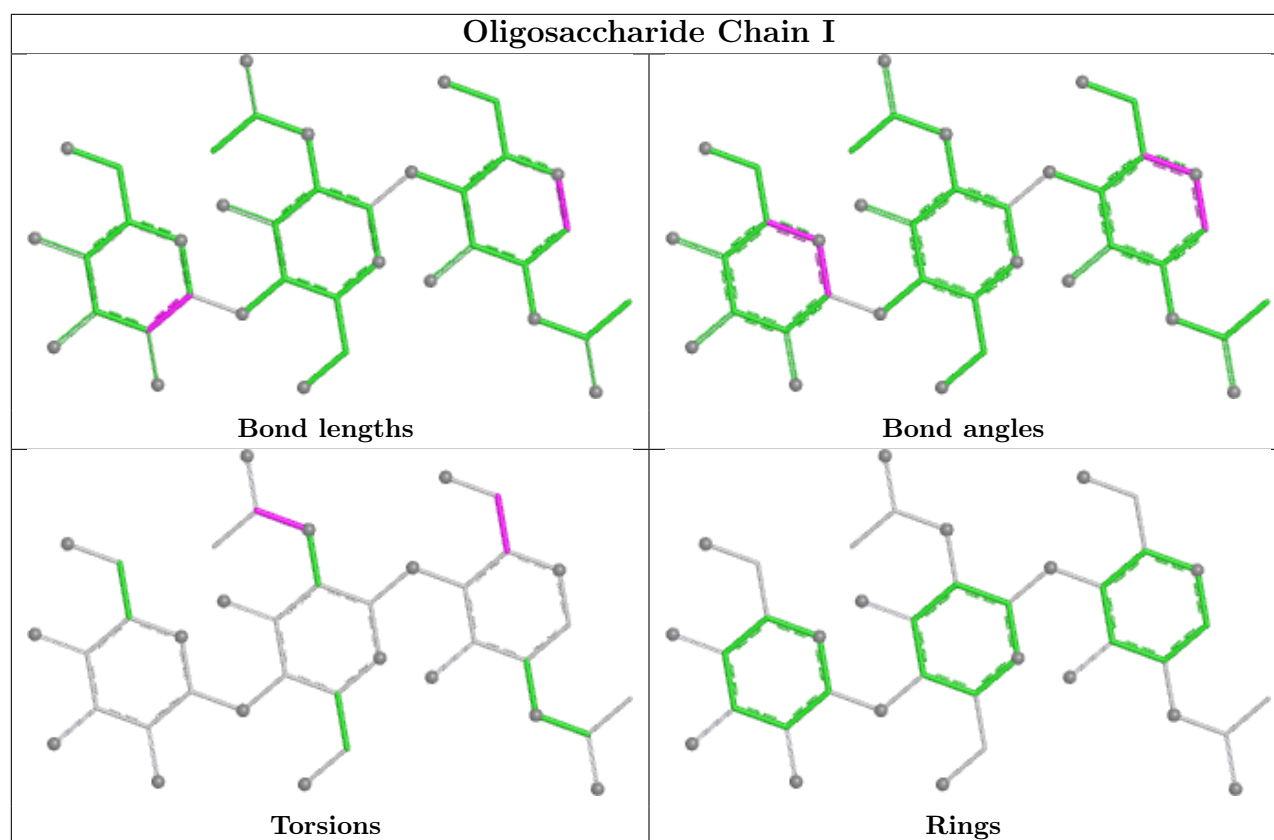
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	NAG	A	703	1	14,14,15	1.63	2 (14%)	17,19,21	1.14	1 (5%)
6	NAG	B	701	1	14,14,15	0.47	0	17,19,21	0.70	0
6	NAG	B	702	1	14,14,15	0.38	0	17,19,21	0.57	0
6	NAG	A	702	1	14,14,15	0.36	0	17,19,21	0.56	0
6	NAG	B	703	1	14,14,15	1.07	1 (7%)	17,19,21	0.67	0
6	NAG	B	704	1	14,14,15	0.37	0	17,19,21	0.57	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	NAG	A	703	1	-	1/6/23/26	0/1/1/1
6	NAG	B	701	1	-	3/6/23/26	0/1/1/1
6	NAG	B	702	1	-	0/6/23/26	0/1/1/1
6	NAG	A	702	1	-	2/6/23/26	0/1/1/1
6	NAG	B	703	1	-	2/6/23/26	0/1/1/1
6	NAG	B	704	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	703	NAG	C1-C2	4.94	1.59	1.52
6	B	703	NAG	C1-C2	3.12	1.56	1.52
6	A	703	NAG	C3-C2	2.55	1.57	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	703	NAG	C2-N2-C7	2.34	126.03	122.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	702	NAG	O5-C5-C6-O6
6	A	702	NAG	C4-C5-C6-O6
6	B	701	NAG	C4-C5-C6-O6
6	A	703	NAG	C3-C2-N2-C7
6	B	701	NAG	O5-C5-C6-O6
6	B	701	NAG	C3-C2-N2-C7
6	B	703	NAG	O5-C5-C6-O6
6	B	703	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	596/625 (95%)	-0.21	3 (0%) 87 82	48, 65, 91, 144	0
1	B	596/625 (95%)	-0.17	3 (0%) 87 82	49, 67, 93, 147	0
2	C	13/15 (86%)	-0.23	0 100 100	53, 59, 67, 78	0
2	D	13/15 (86%)	0.05	0 100 100	57, 63, 78, 81	0
All	All	1218/1280 (95%)	-0.19	6 (0%) 87 82	48, 66, 91, 147	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	339	VAL	4.2
1	B	427	ASP	2.5
1	A	150	GLU	2.5
1	B	19	SER	2.4
1	A	138	PRO	2.2
1	B	614	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

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

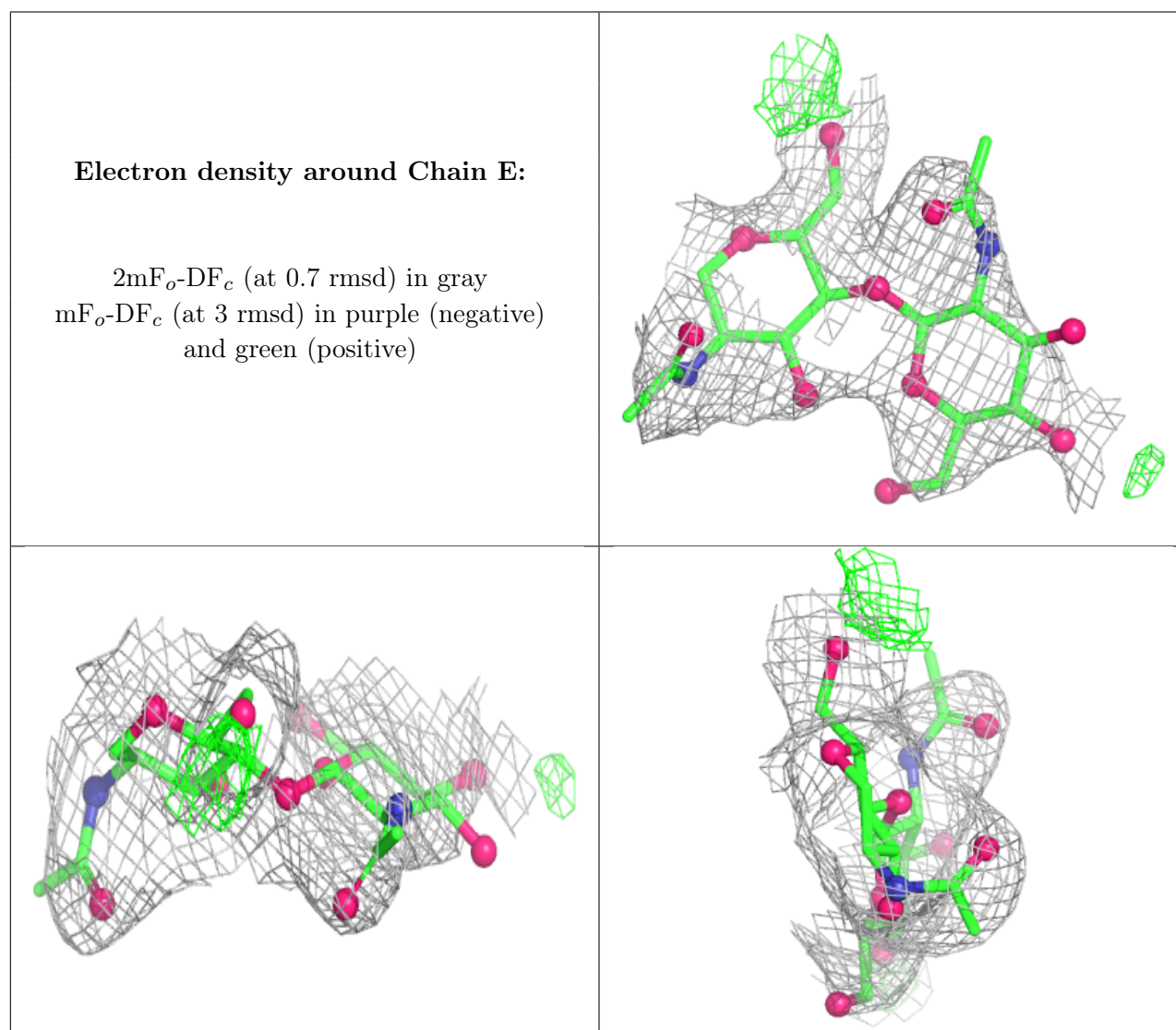
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	E	2	14/15	0.71	0.13	106,108,111,111	0

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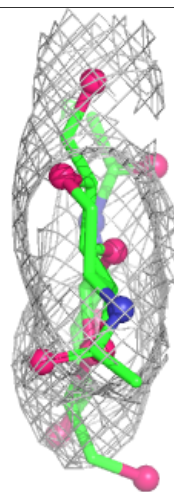
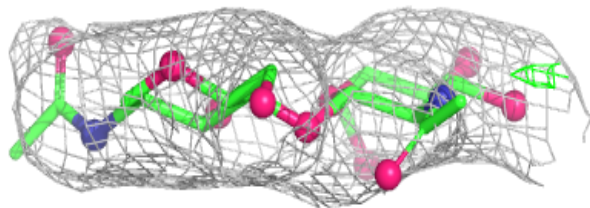
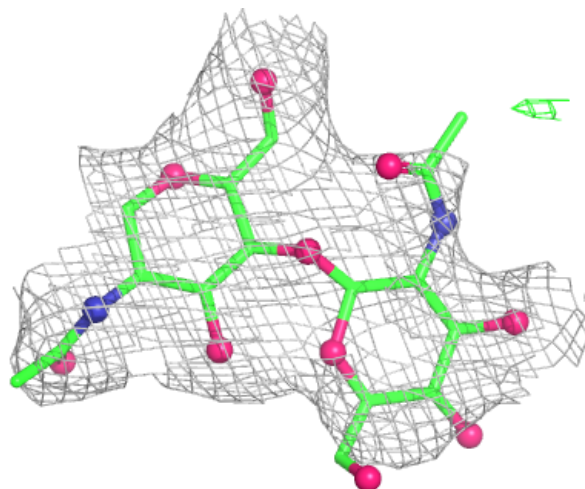
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BMA	I	3	11/12	0.71	0.12	105,107,109,111	0
3	NAG	H	2	14/15	0.73	0.14	116,120,122,122	0
3	NAG	F	2	14/15	0.75	0.13	113,116,118,118	0
3	NAG	H	1	14/15	0.75	0.15	101,103,106,107	0
3	NAG	G	2	14/15	0.76	0.12	97,99,101,102	0
3	NAG	E	1	14/15	0.76	0.13	96,97,100,102	0
4	NAG	I	2	14/15	0.78	0.11	98,99,102,102	0
3	NAG	G	1	14/15	0.81	0.11	80,84,87,88	0
4	NAG	I	1	14/15	0.84	0.10	81,86,89,90	0
3	NAG	F	1	14/15	0.90	0.11	99,101,102,104	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.



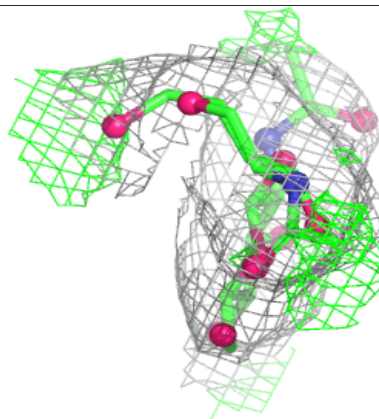
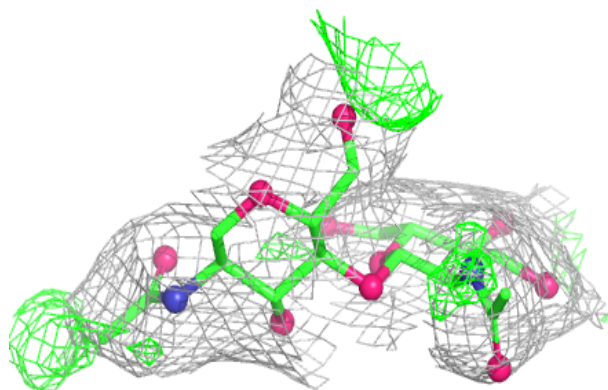
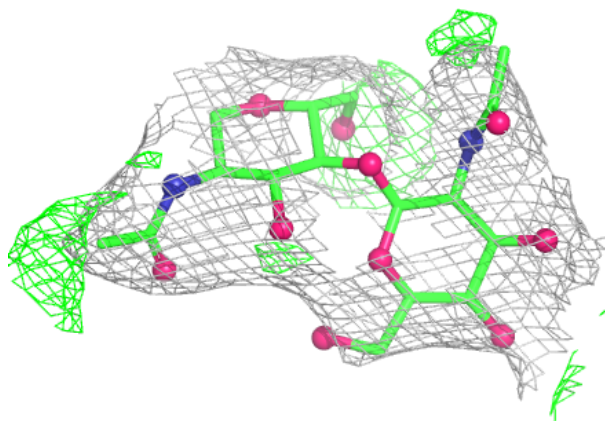
Electron density around Chain F:

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



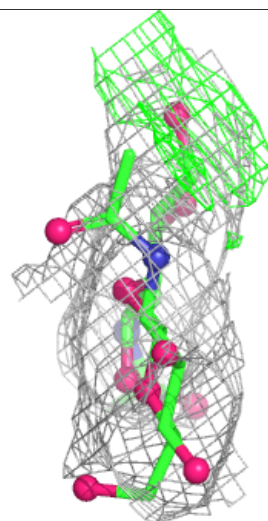
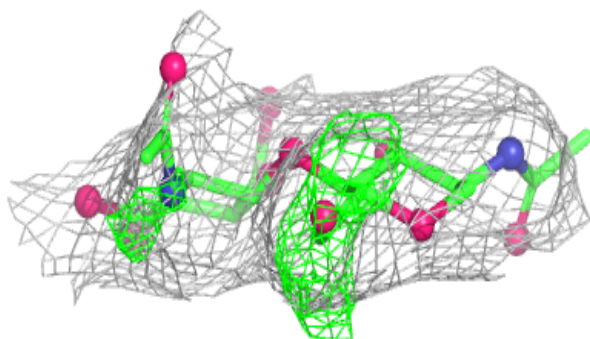
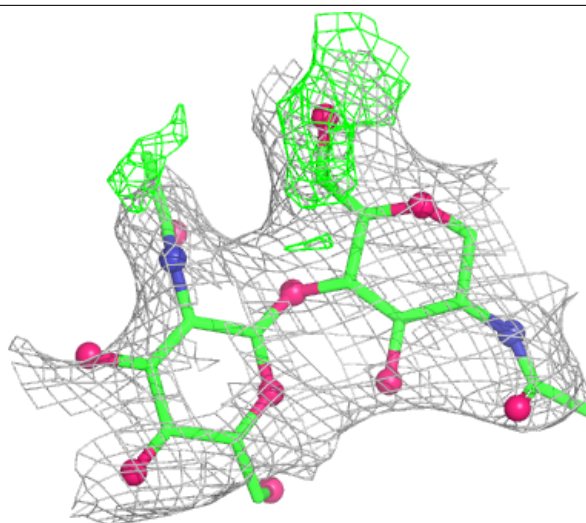
Electron density around Chain G:

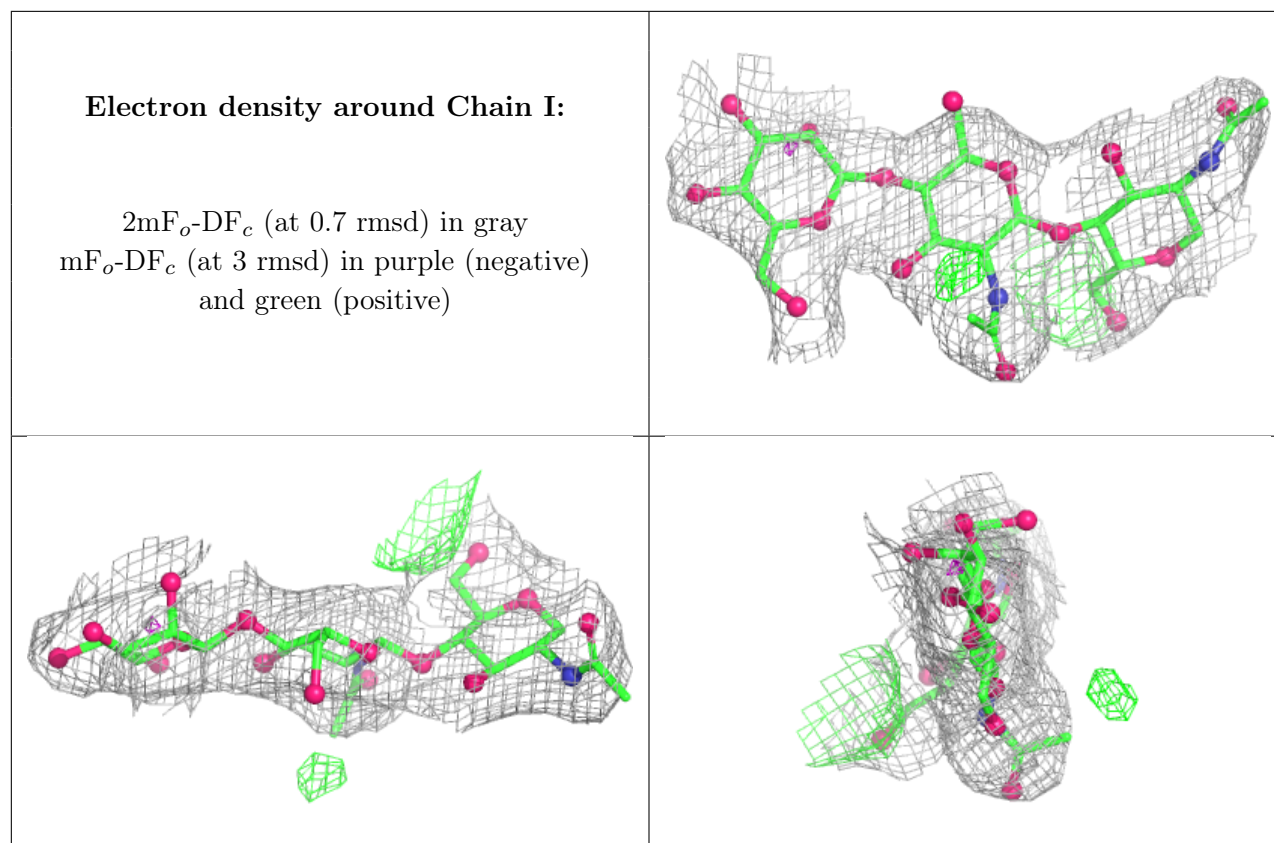
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	A	703	14/15	0.40	0.17	96,97,99,100	0
6	NAG	A	702	14/15	0.60	0.15	99,103,106,107	0
6	NAG	B	701	14/15	0.66	0.15	98,100,103,104	0
6	NAG	B	702	14/15	0.68	0.14	96,100,103,104	0
6	NAG	B	703	14/15	0.74	0.14	101,104,107,109	0
5	ZN	A	701	1/1	0.77	0.22	114,114,114,114	0
6	NAG	B	704	14/15	0.78	0.12	85,89,92,93	0
5	ZN	B	705	1/1	0.80	0.19	116,116,116,116	0
7	CL	A	704	1/1	0.95	0.09	61,61,61,61	0
7	CL	B	706	1/1	0.96	0.10	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.