



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:36 PM UTC

PDB ID : 9O5V / pdb_00009o5v
Title : Crystal structure of chimeric BANAL-52 RBD complexed with chimeric Rhinolophus sinicus ACE2
Authors : Hsueh, F.-C.; Shi, K.; Aihara, H.; Li, F.
Deposited on : 2025-04-10
Resolution : 3.35 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

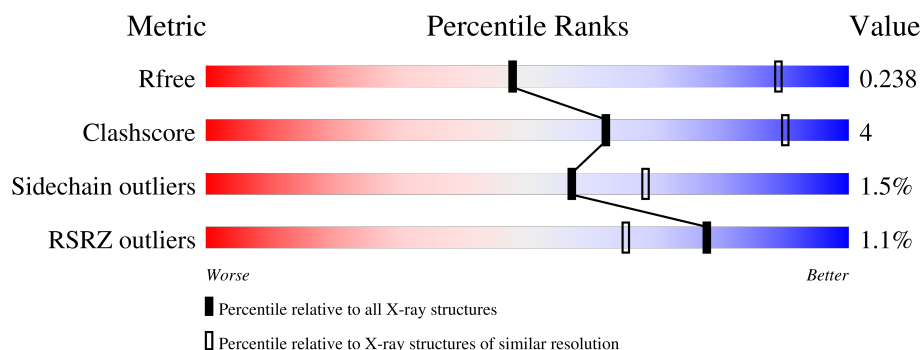
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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.



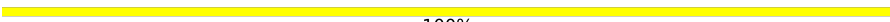
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	603	% 85% 13% ..
1	B	603	% 87% 11% .
2	E	232	76% 5% 19%
2	F	232	% 72% 9% 19%
3	C	2	100%
3	D	2	100%

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Mol	Chain	Length	Quality of chain
3	H	2	 100%
4	G	5	 100%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 12922 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 ACE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	0	0
			4847	3095	808	915	29			
1	B	595	Total	C	N	O	S	0	0	0
			4847	3095	808	915	29			

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	188	Total	C	N	O	S	0	1	0
			1499	964	243	282	10			
2	F	188	Total	C	N	O	S	0	0	0
			1496	962	243	282	9			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	321	VAL	GLN	conflict	UNP P0DTC2
E	323	SER	THR	conflict	UNP P0DTC2
E	324	GLY	GLU	conflict	UNP P0DTC2
E	325	ASP	SER	conflict	UNP P0DTC2
E	326	VAL	ILE	conflict	UNP P0DTC2
E	346	LYS	ARG	variant	UNP P0DTC2
E	348	PRO	ALA	conflict	UNP P0DTC2
E	354	GLU	ASN	conflict	UNP P0DTC2
E	357	LYS	ARG	conflict	UNP P0DTC2
E	372	THR	ALA	conflict	UNP P0DTC2
E	373	PHE	SER	conflict	UNP P0DTC2
E	384	ALA	PRO	conflict	UNP P0DTC2
E	393	SER	THR	conflict	UNP P0DTC2
E	402	VAL	ILE	conflict	UNP P0DTC2
E	403	LYS	ARG	conflict	UNP P0DTC2
E	406	ASP	GLU	conflict	UNP P0DTC2

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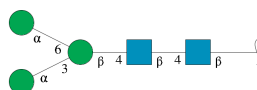
Chain	Residue	Modelled	Actual	Comment	Reference
E	417	VAL	LYS	conflict	UNP P0DTC2
E	430	MET	THR	conflict	UNP P0DTC2
E	434	LEU	ILE	conflict	UNP P0DTC2
E	438	THR	SER	conflict	UNP P0DTC2
E	439	ARG	ASN	conflict	UNP P0DTC2
E	441	ILE	LEU	conflict	UNP P0DTC2
E	443	ALA	SER	conflict	UNP P0DTC2
E	444	THR	LYS	variant	UNP P0DTC2
E	445	SER	VAL	conflict	UNP P0DTC2
E	446	THR	GLY	conflict	UNP P0DTC2
E	452	LYS	LEU	conflict	UNP P0DTC2
E	498	HIS	GLN	conflict	UNP P0DTC2
E	519	ASN	HIS	conflict	UNP P0DTC2
E	529	LEU	LYS	conflict	UNP P0DTC2
E	532	ASP	ASN	conflict	UNP P0DTC2
E	534	ILE	VAL	conflict	UNP P0DTC2
E	536	SER	ASN	conflict	UNP P0DTC2

- 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	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	D	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 alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

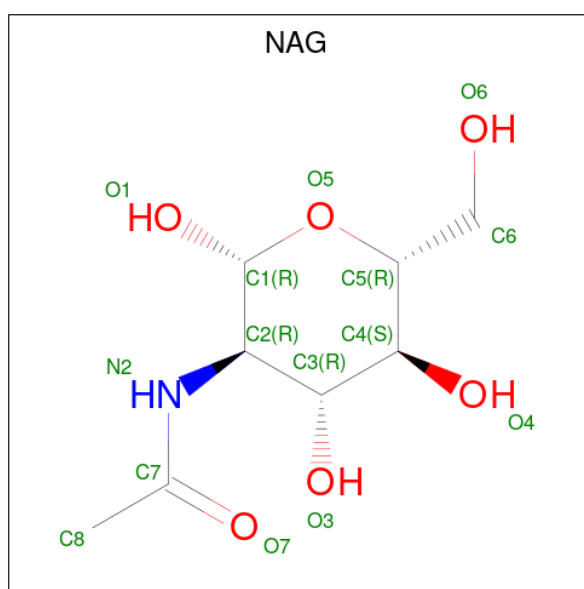
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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 SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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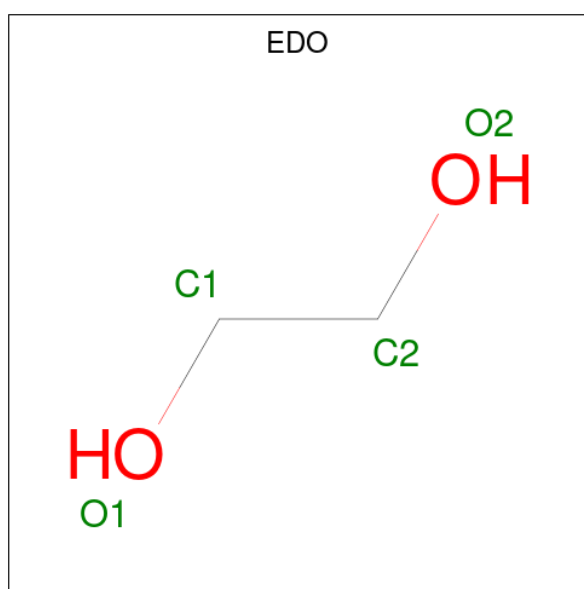
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total	Cl	0	0
			2	2		

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	5	Total	O	0	0
			5	5		

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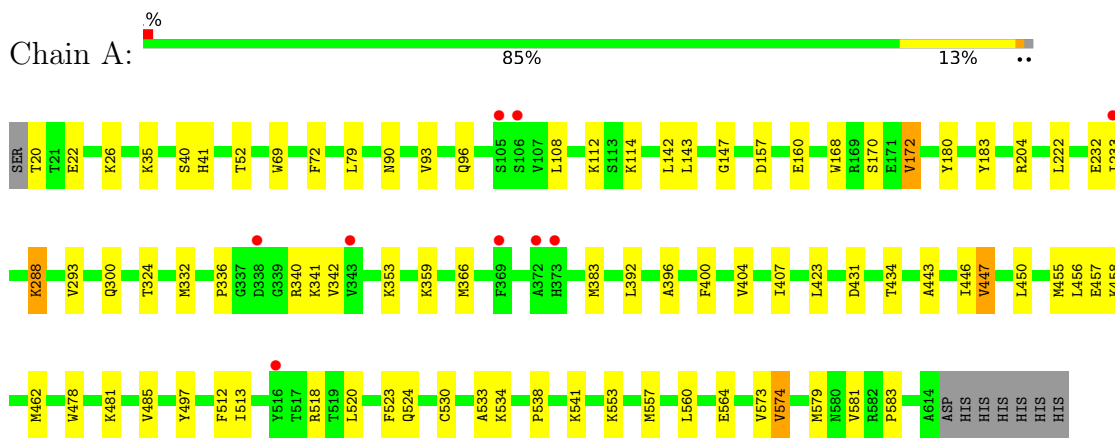
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	5	Total	O	0	0
			5	5		
10	F	1	Total	O	0	0
			1	1		

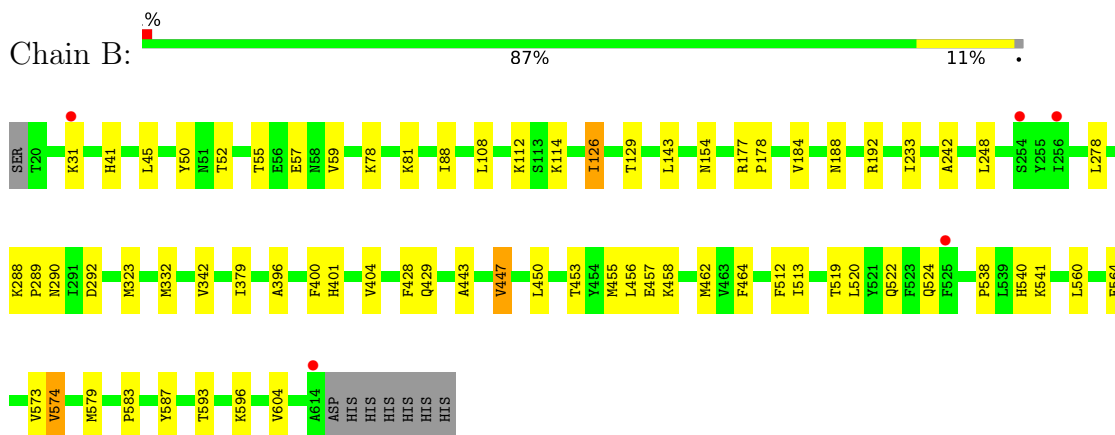
3 Residue-property plots

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.

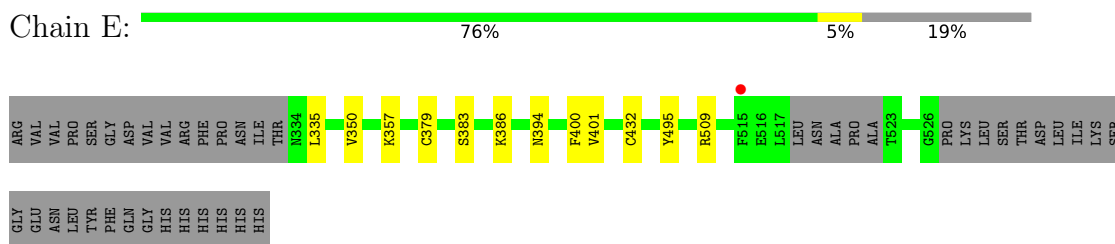
• Molecule 1: ACE2



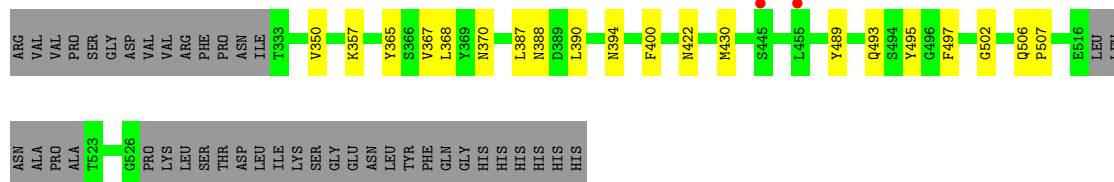
• Molecule 1: ACE2



• Molecule 2: Spike protein S1



- Molecule 2: Spike protein S1



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



MAG1
MAG2

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



MAG1
MAG2

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



MAG1
MAG2

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



MAG1
MAG2
BMA3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.90Å 117.35Å 108.45Å 90.00° 95.79° 90.00°	Depositor
Resolution (Å)	34.39 – 3.35 34.39 – 3.35	Depositor EDS
% Data completeness (in resolution range)	68.7 (34.39-3.35) 59.2 (34.39-3.35)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.34 (at 3.32Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.227 , 0.266 (Not available) , 0.238	Depositor DCC
R_{free} test set	1010 reflections (3.53%)	wwPDB-VP
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	12922	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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: NA, MAN, NAG, BMA, CL, EDO, ZN

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	0.08	0/4981	0.24	0/6761
1	B	0.08	0/4981	0.23	0/6761
2	E	0.09	0/1541	0.24	0/2095
2	F	0.11	0/1538	0.29	0/2090
All	All	0.09	0/13041	0.24	0/17707

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	4847	0	4633	48	0
1	B	4847	0	4632	40	0
2	E	1499	0	1404	5	0
2	F	1496	0	1409	11	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0
3	H	28	0	25	2	0
4	G	61	0	52	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
6	A	1	0	0	0	0
7	A	14	0	13	0	0
7	B	28	0	26	0	0
7	F	14	0	13	0	0
8	B	2	0	0	0	0
9	B	16	0	23	1	0
10	A	5	0	0	0	0
10	B	5	0	0	0	0
10	F	1	0	0	0	0
All	All	12922	0	12280	104	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (104) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:PRO:HD2	1:A:541:LYS:HD3	1.69	0.73
1:A:457:GLU:HG2	1:A:513:ILE:HB	1.75	0.66
1:A:336:PRO:HG3	1:A:340:ARG:HH11	1.61	0.64
1:B:560:LEU:HD13	1:B:564:GLU:HG3	1.81	0.62
2:E:350:VAL:HA	2:E:400:PHE:HB2	1.83	0.61
1:A:534:LYS:HB3	1:B:429:GLN:OE1	2.01	0.61
2:E:357:LYS:HE3	2:E:394:ASN:HD22	1.65	0.61
1:B:108:LEU:HD23	1:B:112:LYS:HB3	1.84	0.58
1:B:520:LEU:HD22	1:B:579:MET:HE2	1.86	0.57
1:A:520:LEU:HD22	1:A:579:MET:HE2	1.87	0.57
1:A:52:THR:HB	1:A:340:ARG:HH22	1.70	0.57
1:B:573:VAL:HG13	1:B:574:VAL:HG13	1.86	0.57
1:B:233:ILE:HD13	1:B:450:LEU:HD13	1.88	0.56
1:A:108:LEU:HD23	1:A:112:LYS:HB3	1.87	0.56
1:B:289:PRO:HB2	1:B:428:PHE:HE1	1.71	0.55
2:E:379:CYS:HA	2:E:432:CYS:HA	1.88	0.55
1:B:443:ALA:HA	1:B:447:VAL:HG13	1.88	0.55
1:A:573:VAL:HG13	1:A:574:VAL:HG13	1.89	0.53
1:B:524:GLN:HG2	1:B:583:PRO:HG2	1.89	0.53
1:B:538:PRO:HD2	1:B:541:LYS:HD3	1.89	0.53
1:A:142:LEU:HB3	1:A:147:GLY:HA3	1.91	0.53
2:F:350:VAL:HA	2:F:400:PHE:HB2	1.90	0.53
1:B:457:GLU:HG2	1:B:513:ILE:HB	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:THR:HA	1:A:342:VAL:HG22	1.92	0.52
1:A:446:ILE:HD13	1:A:523:PHE:HZ	1.75	0.52
1:A:431:ASP:HB2	1:A:434:THR:HG23	1.91	0.52
1:A:288:LYS:HD3	1:A:434:THR:HG22	1.92	0.51
1:A:96:GLN:HG2	1:A:392:LEU:HD13	1.92	0.51
2:F:497:PHE:CG	2:F:507:PRO:HG3	2.45	0.51
1:A:20:THR:HG22	1:A:22:GLU:H	1.76	0.51
2:F:365:TYR:HB2	2:F:388:ASN:HA	1.92	0.50
1:B:78:LYS:HA	1:B:81:LYS:HD2	1.93	0.50
1:A:443:ALA:HA	1:A:447:VAL:HG13	1.94	0.49
1:A:560:LEU:HD22	1:A:564:GLU:HG3	1.94	0.49
1:B:289:PRO:HB2	1:B:428:PHE:CE1	2.46	0.49
1:B:290:ASN:ND2	1:B:292:ASP:HB3	2.27	0.49
1:B:52:THR:HA	1:B:342:VAL:HG22	1.95	0.49
2:F:387:LEU:HA	2:F:390:LEU:HD12	1.95	0.49
1:B:396:ALA:HB3	1:B:400:PHE:CG	2.48	0.48
2:F:367:VAL:HG13	2:F:368:LEU:HD13	1.93	0.48
1:A:232:GLU:HB2	1:A:581:VAL:HG11	1.95	0.48
1:B:332:MET:SD	1:B:342:VAL:HG11	2.53	0.48
1:B:31:LYS:HD2	2:F:489:TYR:HB3	1.96	0.47
1:B:593:THR:HA	1:B:596:LYS:HE2	1.95	0.47
1:A:157:ASP:HB3	1:A:160:GLU:HB3	1.95	0.47
1:B:323:MET:HE1	1:B:379:ILE:HG21	1.97	0.47
1:A:180:TYR:HA	1:A:183:TYR:HB3	1.97	0.47
1:A:524:GLN:HG2	1:A:583:PRO:HG2	1.95	0.47
1:B:55:THR:O	1:B:59:VAL:HG23	2.14	0.47
1:A:41:HIS:CD2	1:A:353:LYS:HD2	2.50	0.46
2:E:383:SER:HB2	2:E:386:LYS:HB2	1.96	0.46
1:A:300:GLN:HE22	1:A:423:LEU:HA	1.79	0.46
1:B:143:LEU:HD23	1:B:143:LEU:H	1.80	0.46
1:B:188:ASN:HB3	1:B:192:ARG:HE	1.80	0.46
2:E:401:VAL:HG22	2:E:509:ARG:HG2	1.96	0.46
1:B:242:ALA:HB2	1:B:604:VAL:HA	1.96	0.46
1:B:50:TYR:CE1	1:B:59:VAL:HG22	2.51	0.46
1:B:519:THR:O	1:B:522:GLN:HG2	2.16	0.46
1:B:184:VAL:HG22	1:B:464:PHE:HE1	1.81	0.45
1:A:530:CYS:HA	1:A:533:ALA:HB3	1.99	0.45
1:B:455:MET:HE3	1:B:455:MET:HB3	1.83	0.45
1:B:450:LEU:HD21	1:B:519:THR:HG21	1.97	0.45
1:A:26:LYS:HG2	1:A:93:VAL:HG11	1.99	0.45
1:A:204:ARG:HG2	1:A:222:LEU:HD23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:TRP:O	1:A:172:VAL:HG22	2.17	0.44
2:F:350:VAL:HG22	2:F:422:ASN:HB3	1.97	0.44
2:F:357:LYS:HE3	2:F:394:ASN:HD22	1.82	0.44
1:A:35:LYS:HG2	1:A:72:PHE:CE1	2.52	0.44
2:F:367:VAL:O	2:F:368:LEU:HB2	2.17	0.44
3:H:1:NAG:H61	3:H:2:NAG:O5	2.17	0.44
3:H:1:NAG:H4	3:H:2:NAG:H2	1.70	0.44
1:A:324:THR:HG23	1:A:383:MET:HE2	1.99	0.44
1:A:404:VAL:O	1:A:407:ILE:HG12	2.18	0.44
1:B:540:HIS:HA	1:B:587:TYR:CE2	2.53	0.44
1:A:143:LEU:H	1:A:143:LEU:HD23	1.81	0.44
1:B:41:HIS:O	1:B:45:LEU:HB2	2.18	0.44
1:A:455:MET:HE3	1:A:455:MET:HB3	1.81	0.44
1:A:341:LYS:HD2	1:A:341:LYS:HA	1.73	0.43
1:A:90:ASN:HB3	1:A:93:VAL:HG22	2.00	0.43
1:A:455:MET:HE2	1:A:485:VAL:HG21	2.00	0.43
1:A:233:ILE:HD13	1:A:450:LEU:HD13	1.99	0.43
1:A:396:ALA:HB3	1:A:400:PHE:CG	2.54	0.43
1:A:332:MET:SD	1:A:342:VAL:HG21	2.59	0.42
1:B:456:LEU:HD23	1:B:512:PHE:CD2	2.54	0.42
1:A:170:SER:HB3	1:A:497:TYR:HE2	1.84	0.42
1:A:332:MET:SD	1:A:342:VAL:HG11	2.60	0.42
1:A:456:LEU:HD23	1:A:512:PHE:CD2	2.54	0.42
1:A:553:LYS:HE3	1:A:573:VAL:O	2.20	0.42
1:B:154:ASN:HA	9:B:703:EDO:H12	2.01	0.42
1:A:40:SER:HB2	1:A:69:TRP:CZ3	2.55	0.42
1:B:248:LEU:HD21	1:B:278:LEU:HD22	2.02	0.42
1:B:126:ILE:HA	1:B:129:THR:HG22	2.02	0.41
1:A:458:LYS:NZ	1:A:462:MET:HE3	2.35	0.41
2:F:430:MET:HE3	2:F:430:MET:HB2	1.98	0.41
1:A:359:LYS:HE3	1:A:359:LYS:HB3	1.92	0.41
1:B:453:THR:HG23	1:B:512:PHE:CD2	2.56	0.41
1:B:114:LYS:HA	1:B:114:LYS:HD2	1.90	0.41
1:B:458:LYS:NZ	1:B:462:MET:HE3	2.34	0.41
2:F:502:GLY:O	2:F:506:GLN:HG3	2.21	0.41
1:B:177:ARG:HB3	1:B:178:PRO:HD3	2.03	0.41
1:A:114:LYS:HA	1:A:114:LYS:HD2	1.95	0.41
1:A:478:TRP:HA	1:A:481:LYS:HB2	2.02	0.41
1:B:400:PHE:O	1:B:404:VAL:HG23	2.21	0.40
1:A:293:VAL:HG22	1:A:366:MET:SD	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

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	435/533 (82%)	428 (98%)	7 (2%)	55	67
1	B	519/533 (97%)	512 (99%)	7 (1%)	61	70
2	E	164/203 (81%)	162 (99%)	2 (1%)	63	72
2	F	164/203 (81%)	161 (98%)	3 (2%)	51	66
All	All	1282/1472 (87%)	1263 (98%)	19 (2%)	57	68

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LEU
1	A	172	VAL
1	A	288	LYS
1	A	447	VAL
1	A	518	ARG
1	A	557	MET
1	A	574	VAL
1	B	57	GLU
1	B	88	ILE
1	B	126	ILE
1	B	288	LYS
1	B	401	HIS
1	B	447	VAL
1	B	574	VAL
2	E	335	LEU
2	E	495	TYR
2	F	370	ASN
2	F	493	GLN

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Mol	Chain	Res	Type
2	F	495	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	277	ASN
1	A	472	GLN
1	A	599	ASN
1	B	58	ASN
1	B	290	ASN
2	E	370	ASN
2	E	437	ASN
2	E	506	GLN
2	F	394	ASN
2	F	437	ASN

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	C	1	1,3	14,14,15	0.78	0	17,19,21	1.24	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	2	3	14,14,15	0.69	0	17,19,21	0.86	1 (5%)
3	NAG	D	1	1,3	14,14,15	0.74	0	17,19,21	0.86	1 (5%)
3	NAG	D	2	3	14,14,15	0.69	0	17,19,21	1.24	1 (5%)
4	NAG	G	1	4,1	14,14,15	0.63	0	17,19,21	1.01	1 (5%)
4	NAG	G	2	4	14,14,15	0.73	0	17,19,21	1.01	1 (5%)
4	BMA	G	3	4	11,11,12	0.81	0	15,15,17	2.36	5 (33%)
4	MAN	G	4	4	11,11,12	0.64	0	15,15,17	1.38	1 (6%)
4	MAN	G	5	4	11,11,12	0.73	0	15,15,17	1.03	1 (6%)
3	NAG	H	1	1,3	14,14,15	0.72	0	17,19,21	1.49	3 (17%)
3	NAG	H	2	3	14,14,15	0.83	0	17,19,21	1.10	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
3	NAG	C	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	3/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	1/2/19/22	0/1/1/1
4	MAN	G	5	4	-	2/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	3	BMA	C1-O5-C5	6.82	121.32	112.19
4	G	4	MAN	C1-O5-C5	4.52	118.25	112.19
3	D	2	NAG	C2-N2-C7	3.63	127.77	122.90
3	H	1	NAG	O4-C4-C3	-3.41	102.34	110.38
4	G	5	MAN	C1-O5-C5	2.91	116.09	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	O5-C1-C2	-2.78	106.99	111.29
4	G	3	BMA	C2-C3-C4	2.74	115.68	110.86
3	H	2	NAG	C2-N2-C7	2.71	126.54	122.90
3	C	1	NAG	C2-N2-C7	2.68	126.49	122.90
4	G	2	NAG	O5-C1-C2	-2.52	107.39	111.29
3	H	1	NAG	C1-O5-C5	2.41	115.42	112.19
4	G	3	BMA	C3-C4-C5	2.36	114.50	110.23
4	G	3	BMA	O4-C4-C3	-2.17	105.27	110.38
3	C	1	NAG	O4-C4-C3	-2.17	105.27	110.38
4	G	3	BMA	O3-C3-C2	-2.12	105.72	110.05
4	G	1	NAG	C1-O5-C5	2.04	114.92	112.19
3	D	1	NAG	C2-N2-C7	2.03	125.62	122.90
3	C	2	NAG	O5-C1-C2	-2.02	108.17	111.29

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
3	C	1	NAG	O5-C5-C6-O6
4	G	5	MAN	O5-C5-C6-O6
4	G	4	MAN	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	D	2	NAG	C1-C2-N2-C7
4	G	5	MAN	C4-C5-C6-O6
3	D	2	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

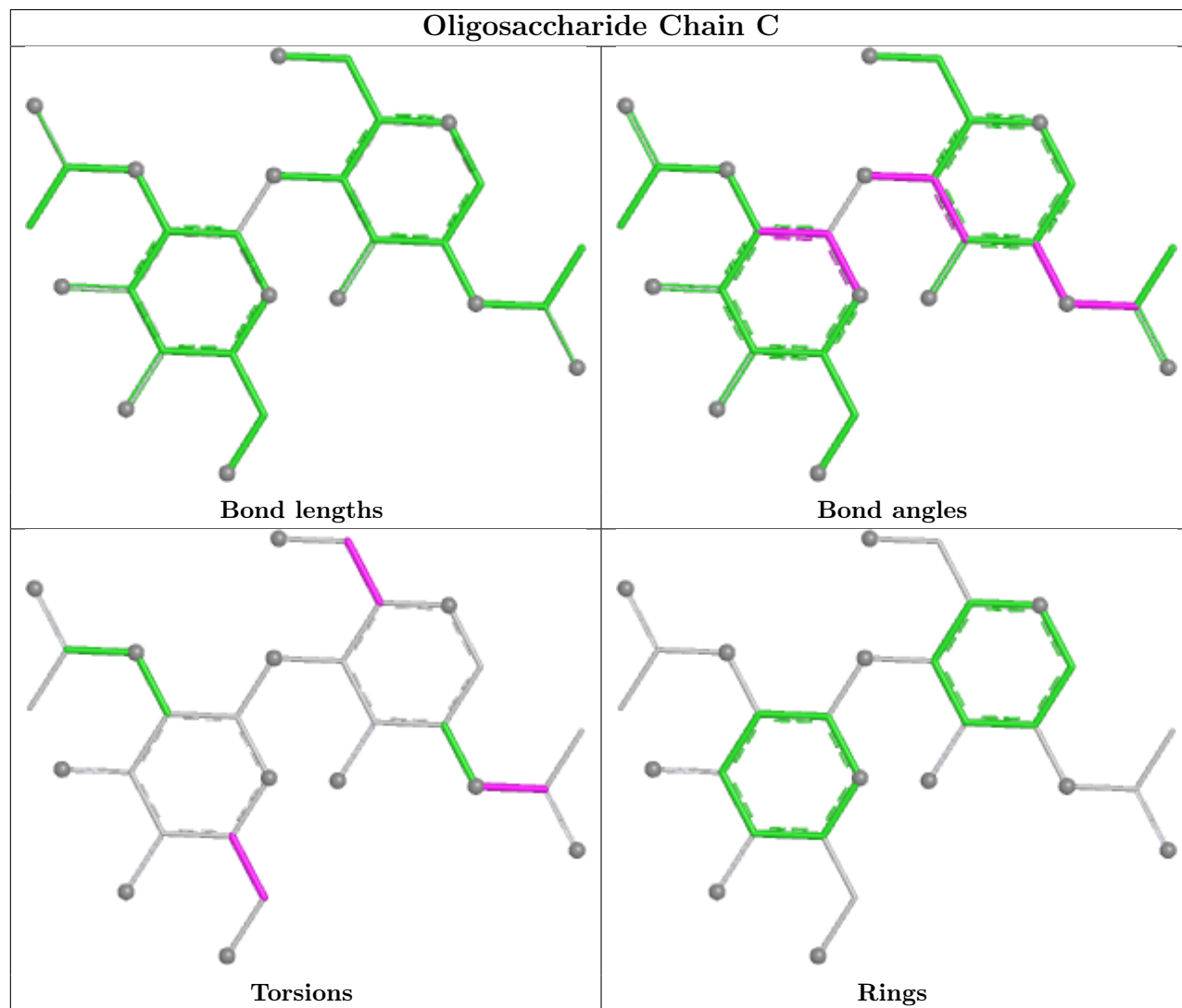
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	2	0

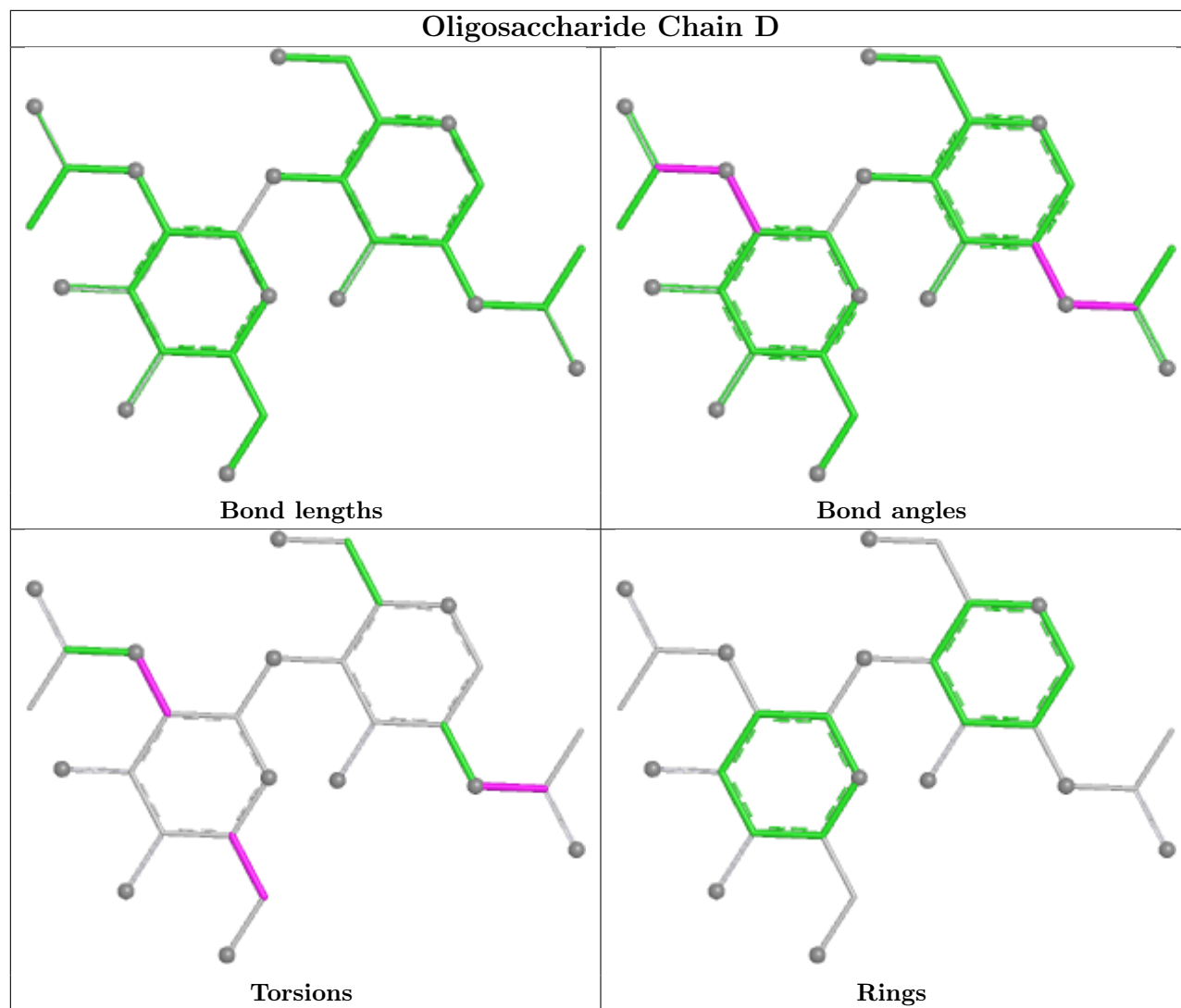
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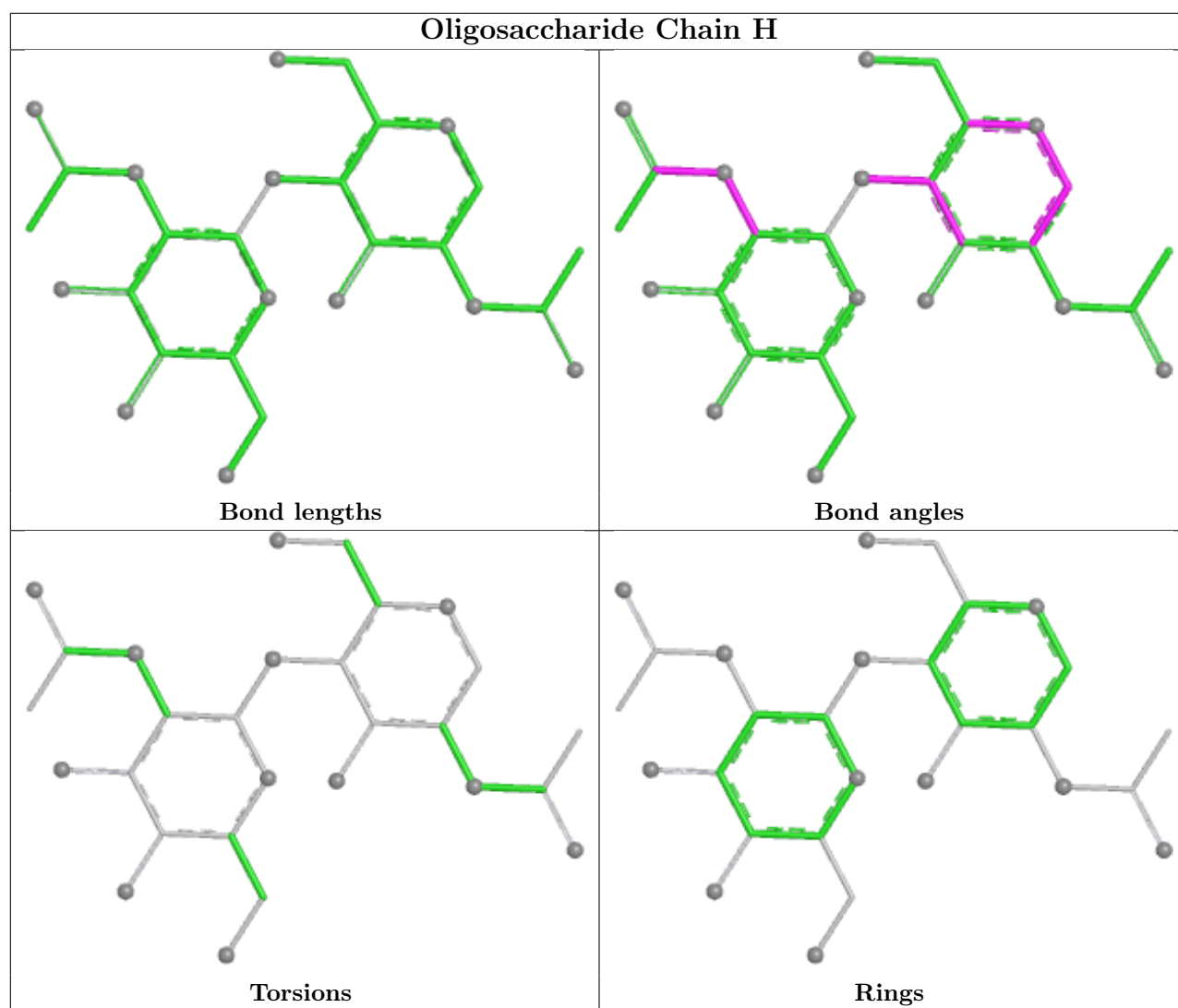
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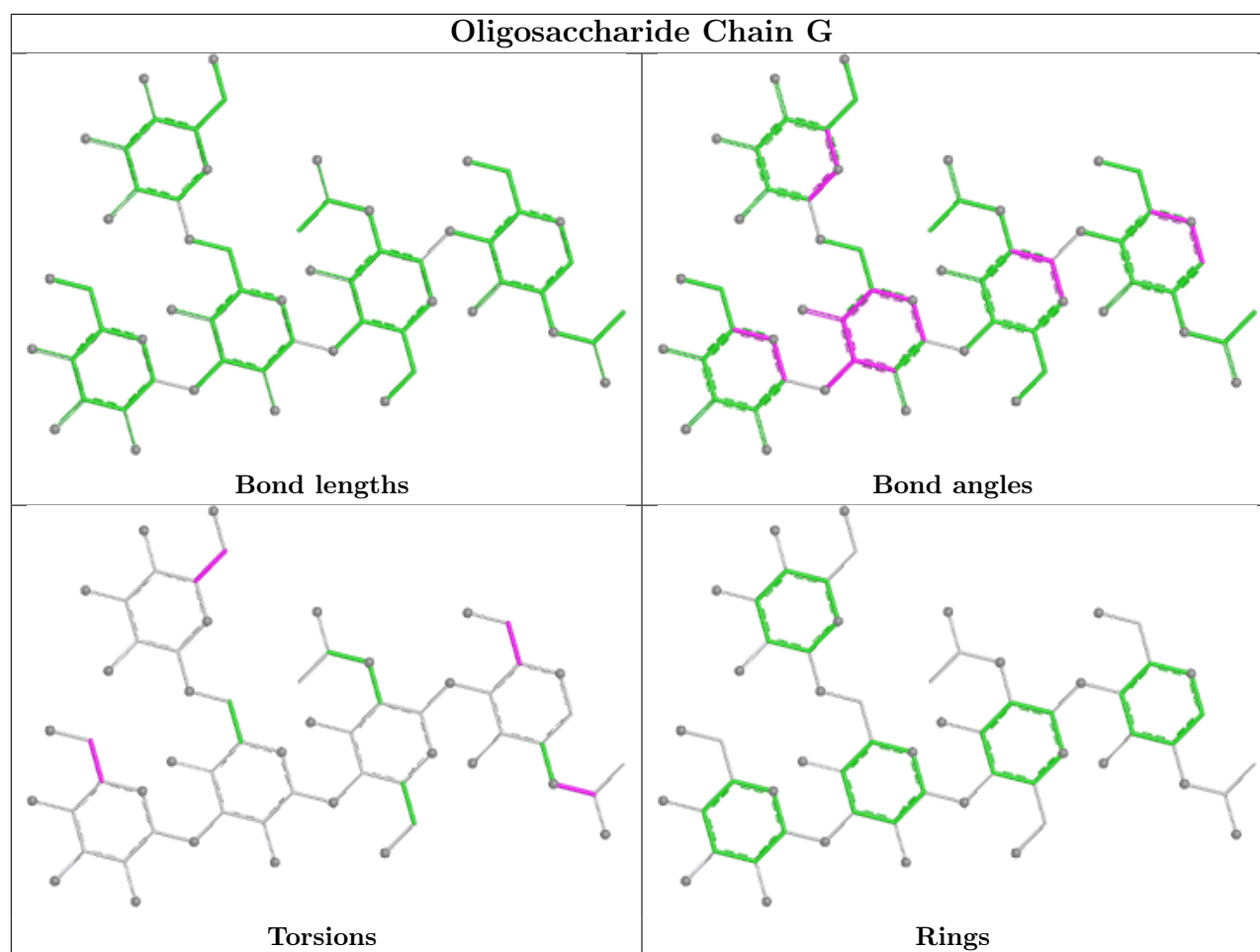
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	2	NAG	2	0

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 13 ligands modelled in this entry, 5 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	$\# Z > 2$
7	NAG	F	601	2	14,14,15	0.71	0	17,19,21	2.41	4 (23%)
9	EDO	B	704	-	3,3,3	0.25	0	2,2,2	0.32	0
9	EDO	B	703	-	3,3,3	0.25	0	2,2,2	0.31	0
7	NAG	A	703	1	14,14,15	0.71	0	17,19,21	0.86	0
7	NAG	B	707	1	14,14,15	0.70	0	17,19,21	0.93	1 (5%)
7	NAG	B	706	1	14,14,15	0.71	0	17,19,21	0.93	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	EDO	B	705	-	3,3,3	0.24	0	2,2,2	0.30	0
9	EDO	B	708	-	3,3,3	0.25	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
7	NAG	F	601	2	-	5/6/23/26	0/1/1/1
9	EDO	B	704	-	-	0/1/1/1	-
9	EDO	B	703	-	-	1/1/1/1	-
7	NAG	A	703	1	-	2/6/23/26	0/1/1/1
7	NAG	B	707	1	-	2/6/23/26	0/1/1/1
7	NAG	B	706	1	-	2/6/23/26	0/1/1/1
9	EDO	B	705	-	-	0/1/1/1	-
9	EDO	B	708	-	-	0/1/1/1	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	601	NAG	C2-N2-C7	8.38	134.13	122.90
7	F	601	NAG	C8-C7-N2	2.59	120.41	116.12
7	F	601	NAG	C1-O5-C5	2.36	115.35	112.19
7	F	601	NAG	C1-C2-N2	2.35	114.14	110.43
7	B	706	NAG	C2-N2-C7	2.24	125.91	122.90
7	B	707	NAG	C1-O5-C5	2.14	115.05	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	703	NAG	C4-C5-C6-O6
7	A	703	NAG	O5-C5-C6-O6
7	B	706	NAG	C8-C7-N2-C2
7	B	706	NAG	O7-C7-N2-C2
7	F	601	NAG	C8-C7-N2-C2
7	F	601	NAG	O7-C7-N2-C2
7	B	707	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	F	601	NAG	O5-C5-C6-O6
7	B	707	NAG	C4-C5-C6-O6
9	B	703	EDO	O1-C1-C2-O2
7	F	601	NAG	C1-C2-N2-C7
7	F	601	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	703	EDO	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 [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	595/603 (98%)	0.38	9 (1%) 72 57	40, 77, 127, 169	0
1	B	595/603 (98%)	0.12	5 (0%) 82 71	29, 63, 132, 177	0
2	E	188/232 (81%)	0.24	1 (0%) 87 78	38, 74, 137, 186	1 (0%)
2	F	188/232 (81%)	0.35	2 (1%) 78 65	60, 95, 145, 177	0
All	All	1566/1670 (93%)	0.26	17 (1%) 78 65	29, 75, 134, 186	1 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	372	ALA	4.0
2	E	515	PHE	3.1
1	A	516	TYR	3.0
1	B	254	SER	2.6
2	F	455	LEU	2.6
2	F	445	SER	2.6
1	B	525	PHE	2.6
1	B	31	LYS	2.5
1	A	373	HIS	2.4
1	B	614	ALA	2.3
1	A	106	SER	2.3
1	A	338	ASP	2.2
1	A	105	SER	2.1
1	B	256	ILE	2.1
1	A	369	PHE	2.1
1	A	343	VAL	2.1
1	A	233	ILE	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

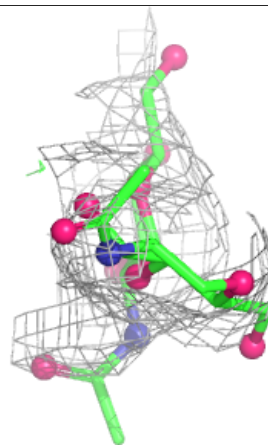
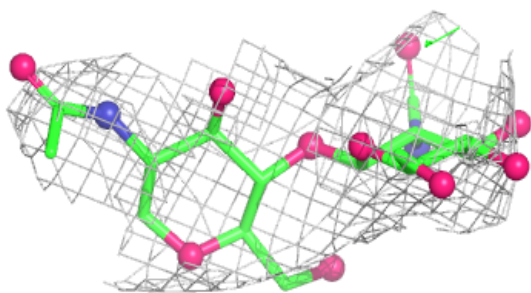
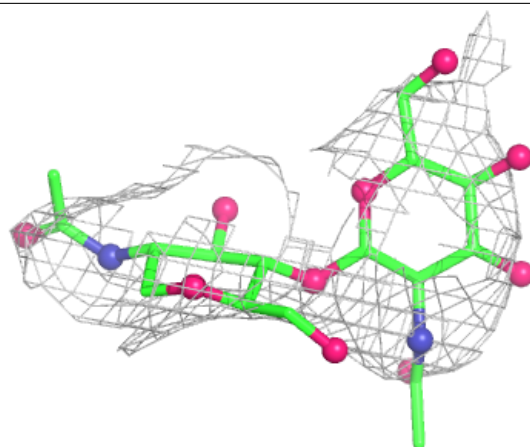
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	C	1	14/15	-	-	92,96,103,116	0
3	NAG	C	2	14/15	-	-	100,106,112,113	0
3	NAG	D	1	14/15	-	-	100,105,121,123	0
3	NAG	D	2	14/15	-	-	99,115,125,126	0
4	MAN	G	5	11/12	0.53	0.11	107,125,130,136	0
4	BMA	G	3	11/12	0.67	0.12	110,116,125,127	0
3	NAG	H	2	14/15	0.68	0.12	108,120,132,136	0
4	MAN	G	4	11/12	0.73	0.14	94,130,138,141	0
4	NAG	G	2	14/15	0.76	0.10	86,108,123,127	0
3	NAG	H	1	14/15	0.78	0.11	91,99,110,121	0
4	NAG	G	1	14/15	0.79	0.10	56,75,97,106	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.

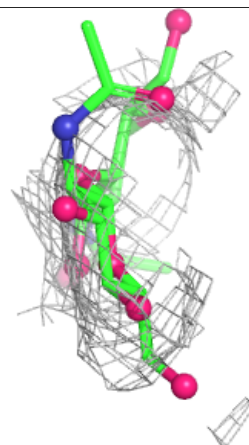
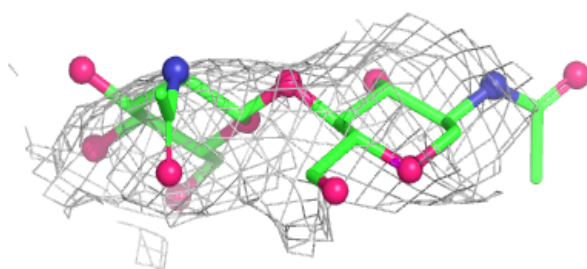
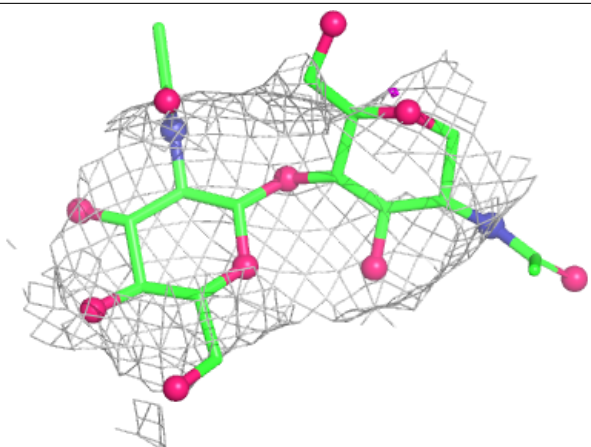
Electron density around Chain C:

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



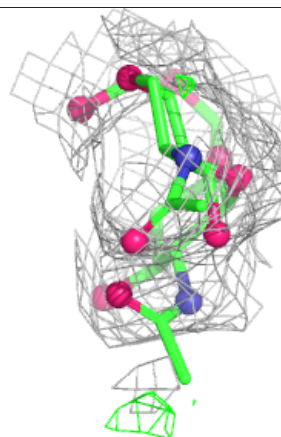
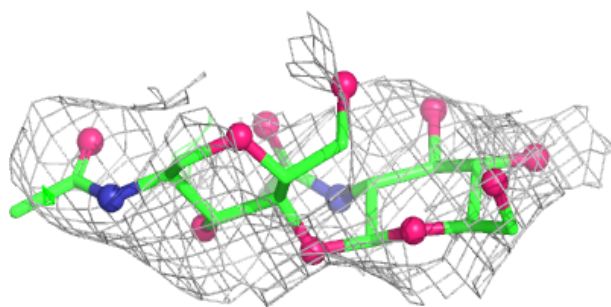
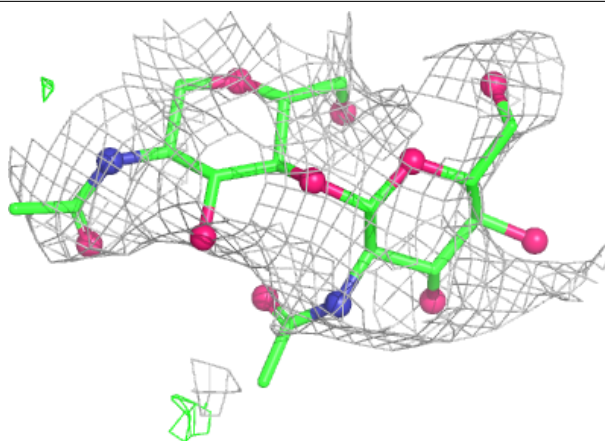
Electron density around Chain D:

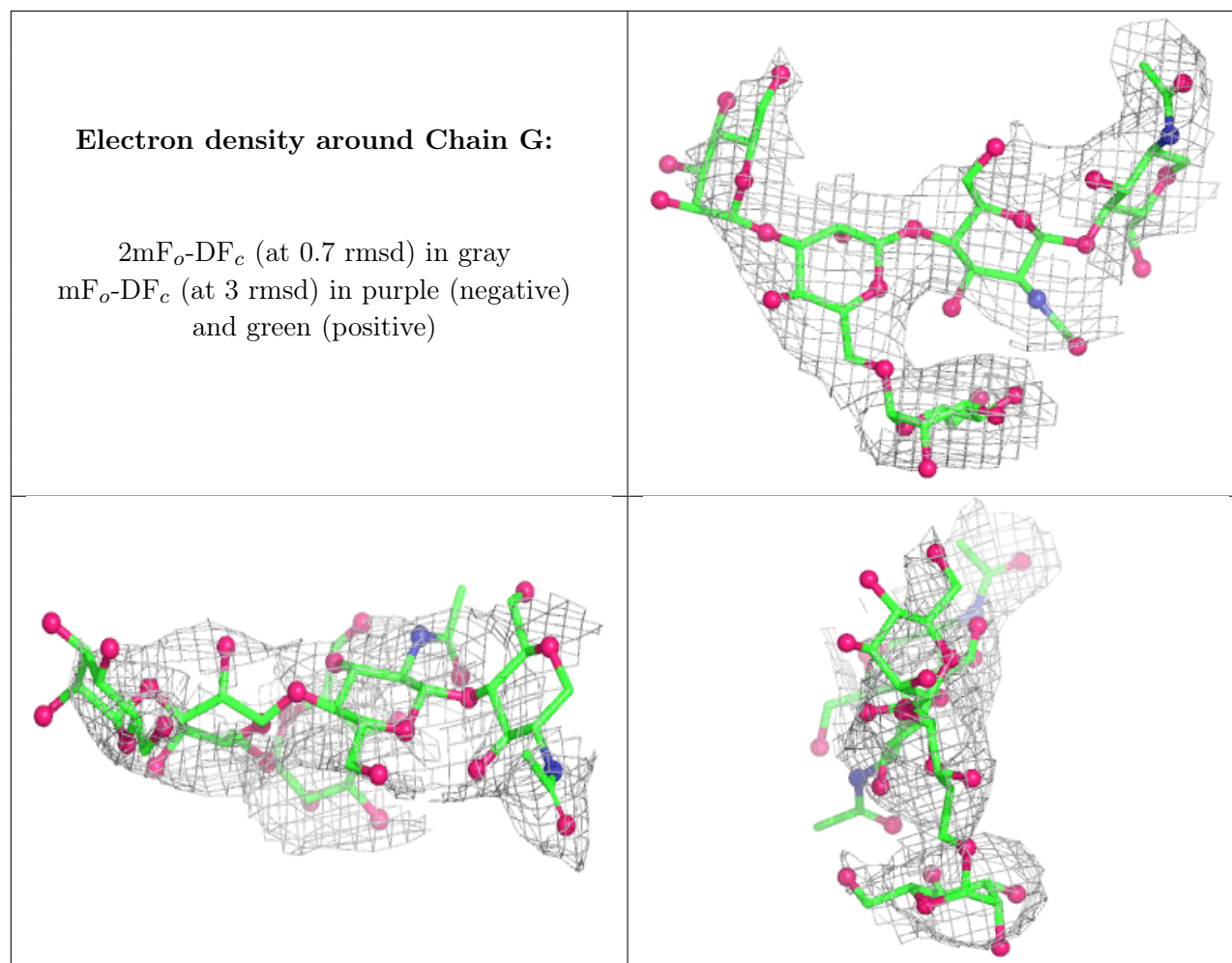
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain 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($\text{\AA}^2$)	Q<0.9
7	NAG	A	703	14/15	0.57	0.14	100,118,129,132	0
8	CL	B	702	1/1	0.61	0.32	107,107,107,107	0
7	NAG	B	706	14/15	0.64	0.13	79,124,136,145	0
7	NAG	B	707	14/15	0.70	0.11	71,78,86,91	0
7	NAG	F	601	14/15	0.72	0.12	97,104,113,126	0
9	EDO	B	704	4/4	0.74	0.15	34,46,59,62	0
9	EDO	B	705	4/4	0.76	0.13	54,55,56,71	0
9	EDO	B	708	4/4	0.80	0.09	46,47,49,50	0
9	EDO	B	703	4/4	0.83	0.13	44,45,46,46	0
8	CL	B	709	1/1	0.90	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ZN	A	701	1/1	0.93	0.04	84,84,84,84	0
6	NA	A	702	1/1	0.93	0.06	56,56,56,56	0
5	ZN	B	701	1/1	0.98	0.05	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.