



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 28, 2025 – 10:12 am BST

PDB ID : 9H0B / pdb\_00009h0b  
Title : Crystal structure of the Porcine Hemagglutinating Encephalomyelitis Virus (PHEV) receptor binding domain in complex with porcine DPEP1.  
Authors : Fernandez, I.; Rey, F.  
Deposited on : 2024-10-08  
Resolution : 2.25 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](mailto: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 Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

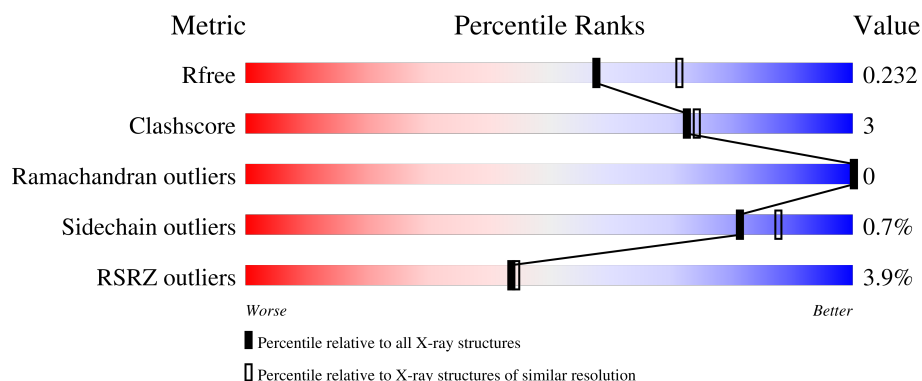
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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))
$R_{free}$	164625	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (2.26-2.26)

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  $\geq 3$ , 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	B	374	<div> <div>91%</div> <div>7%</div> <div>•</div> </div>
1	C	374	<div> <div>93%</div> <div>5%</div> <div>•</div> </div>
2	A	284	<div> <div>5%</div> <div>86%</div> <div>11%</div> <div>•</div> </div>
2	D	284	<div> <div>10%</div> <div>85%</div> <div>12%</div> <div>•</div> </div>
3	E	3	<div> <div>67%</div> <div>33%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	3	<div><div></div><div>33%</div><div>67%</div></div>
3	G	3	<div><div></div><div>33%</div><div>33%</div><div>33%</div></div>
3	H	3	<div><div></div><div>33%</div><div>67%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10626 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 Dipeptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	368	Total	C	N	O	S	0	0	0
			2834	1771	506	542	15			
1	C	368	Total	C	N	O	S	0	0	0
			2834	1771	506	542	15			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	386	ASP	-	expression tag	UNP P22412
B	387	ASP	-	expression tag	UNP P22412
B	388	ASP	-	expression tag	UNP P22412
B	389	ASP	-	expression tag	UNP P22412
B	390	LYS	-	expression tag	UNP P22412
C	386	ASP	-	expression tag	UNP P22412
C	387	ASP	-	expression tag	UNP P22412
C	388	ASP	-	expression tag	UNP P22412
C	389	ASP	-	expression tag	UNP P22412
C	390	LYS	-	expression tag	UNP P22412

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	277	Total	C	N	O	S	0	0	0
			2114	1312	369	408	25			
2	D	277	Total	C	N	O	S	0	0	0
			2114	1312	369	408	25			

There are 10 discrepancies between the modelled and reference sequences:

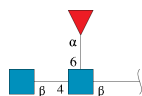
Chain	Residue	Modelled	Actual	Comment	Reference
A	606	ASP	-	expression tag	UNP Q2QKN3
A	607	ASP	-	expression tag	UNP Q2QKN3

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	608	ASP	-	expression tag	UNP Q2QKN3
A	609	ASP	-	expression tag	UNP Q2QKN3
A	610	LYS	-	expression tag	UNP Q2QKN3
D	606	ASP	-	expression tag	UNP Q2QKN3
D	607	ASP	-	expression tag	UNP Q2QKN3
D	608	ASP	-	expression tag	UNP Q2QKN3
D	609	ASP	-	expression tag	UNP Q2QKN3
D	610	LYS	-	expression tag	UNP Q2QKN3

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

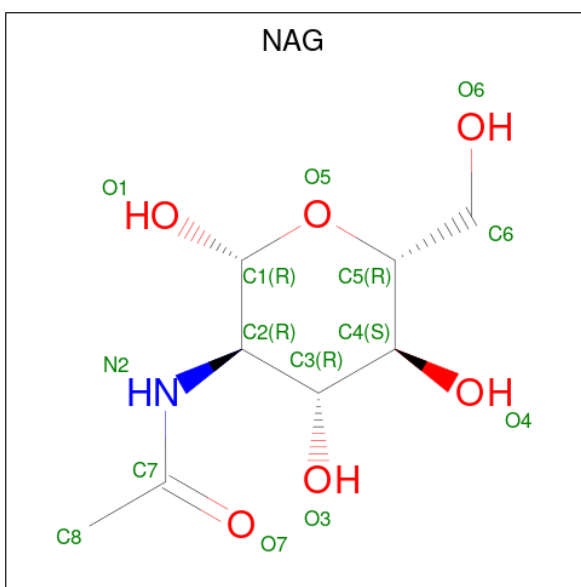


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	F	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	G	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	H	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	9	Total	Zn	0	0
			9	9		
4	C	5	Total	Zn	0	0
			5	5		
4	D	2	Total	Zn	0	0
			2	2		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

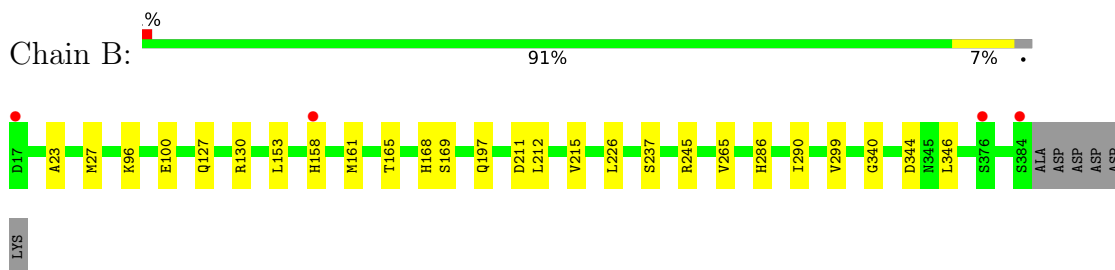
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	221	Total	O	0	0
			221	221		
6	A	77	Total	O	0	0
			77	77		
6	C	165	Total	O	0	0
			165	165		
6	D	43	Total	O	0	0
			43	43		

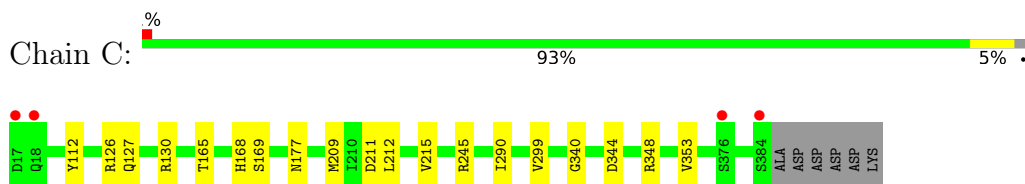
### 3 Residue-property plots [i](#)

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.

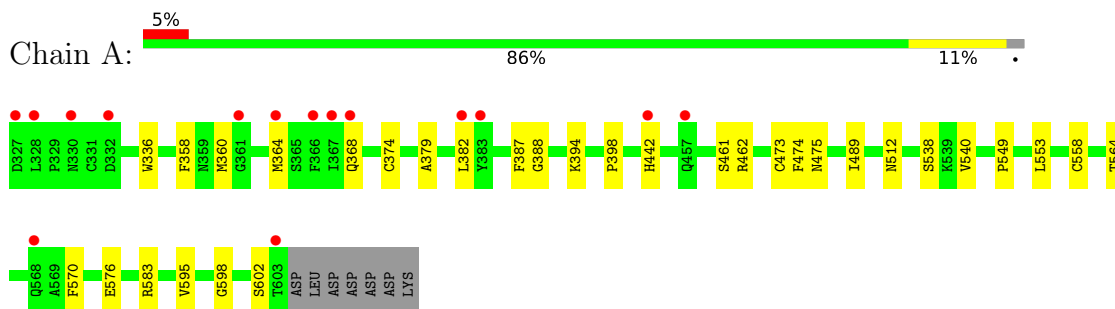
- Molecule 1: Dipeptidase 1



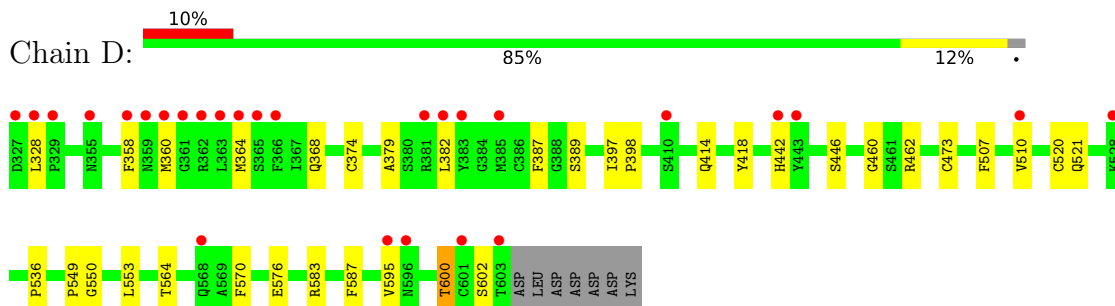
- Molecule 1: Dipeptidase 1



- Molecule 2: Spike glycoprotein



- Molecule 2: Spike glycoprotein




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

Chain E:  67% 33%



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

Chain F:  33% 67%




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

Chain G:  33% 33% 33%



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

Chain H:  33% 67%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.72Å 73.01Å 136.62Å 90.00° 91.94° 90.00°	Depositor
Resolution (Å)	48.33 – 2.25 48.33 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.33-2.25) 99.6 (48.33-2.25)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.198 , 0.235 0.197 , 0.232	Depositor DCC
$R_{free}$ test set	4506 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.8	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10626	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: FUC, ZN, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	B	0.28	0/2893	0.49	0/3932
1	C	0.26	0/2893	0.45	0/3932
2	A	0.21	0/2167	0.40	0/2948
2	D	0.20	0/2167	0.39	0/2948
All	All	0.24	0/10120	0.44	0/13760

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	B	2834	0	2754	15	0
1	C	2834	0	2754	13	0
2	A	2114	0	1977	18	0
2	D	2114	0	1977	21	0
3	E	38	0	34	0	0
3	F	38	0	34	0	0
3	G	38	0	34	1	0
3	H	38	0	34	0	0
4	B	9	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	5	0	0	0	0
4	D	2	0	0	0	0
5	A	28	0	26	0	0
5	D	28	0	26	0	0
6	A	77	0	0	0	0
6	B	221	0	0	0	0
6	C	165	0	0	0	0
6	D	43	0	0	0	0
All	All	10626	0	9650	62	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 3.

All (62) 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)
2:A:473:CYS:HB3	2:A:549:PRO:HD2	1.66	0.77
2:D:473:CYS:HB3	2:D:549:PRO:HD2	1.74	0.70
1:C:348:ARG:HA	2:D:510:VAL:HG11	1.83	0.61
2:A:360:MET:O	2:A:364:MET:HG2	2.01	0.61
1:C:340:GLY:HA2	1:C:344:ASP:HB2	1.83	0.59
1:B:197:GLN:HG2	1:B:226:LEU:HD21	1.86	0.57
2:D:553:LEU:HD12	2:D:570:PHE:CE2	2.41	0.55
1:B:340:GLY:HA2	1:B:344:ASP:HB2	1.90	0.54
2:A:489:ILE:HD11	2:A:512:ASN:O	2.09	0.53
1:C:290:ILE:HG22	1:C:299:VAL:HG22	1.91	0.52
2:D:360:MET:O	2:D:364:MET:HG2	2.11	0.50
1:B:165:THR:HA	1:B:211:ASP:HB3	1.94	0.50
1:B:96:LYS:HE3	1:B:100:GLU:CD	2.37	0.49
2:A:553:LEU:HD12	2:A:570:PHE:CE2	2.47	0.49
2:D:389:SER:HA	2:D:600:THR:HG21	1.95	0.48
2:D:368:GLN:HG3	2:D:583:ARG:NH2	2.28	0.48
2:D:374:CYS:SG	2:D:379:ALA:HB2	2.54	0.48
1:C:112:TYR:CZ	3:G:1:NAG:H82	2.50	0.47
1:B:290:ILE:HG22	1:B:299:VAL:HG22	1.97	0.47
1:B:168:HIS:CG	1:B:169:SER:H	2.31	0.47
2:A:475:ASN:ND2	2:A:540:VAL:HG11	2.29	0.47
2:A:553:LEU:HD21	2:A:558:CYS:SG	2.55	0.46
2:A:388:GLY:HA2	2:A:598:GLY:HA3	1.98	0.46
2:A:475:ASN:HD22	2:A:540:VAL:HG11	1.81	0.46
2:A:358:PHE:O	2:A:602:SER:HA	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:ARG:NH2	2:D:521:GLN:HB3	2.31	0.45
1:C:168:HIS:CG	1:C:169:SER:H	2.32	0.45
2:A:462:ARG:HD3	2:A:462:ARG:HA	1.59	0.45
1:B:237:SER:HB3	1:B:286:HIS:ND1	2.31	0.45
1:B:127:GLN:HG2	1:B:130:ARG:NH2	2.32	0.44
2:D:398:PRO:HB3	2:D:576:GLU:HB3	1.98	0.44
2:D:387:PHE:CE2	2:D:595:VAL:HG13	2.52	0.44
2:D:462:ARG:HD3	2:D:462:ARG:HA	1.58	0.44
1:C:165:THR:HA	1:C:211:ASP:HB3	1.99	0.44
2:A:368:GLN:HG3	2:A:583:ARG:NH2	2.32	0.44
2:D:397:ILE:HD11	2:D:587:PHE:HB2	1.99	0.44
2:A:336:TRP:CH2	2:A:394:LYS:HG2	2.53	0.44
2:D:520:CYS:SG	2:D:536:PRO:HD2	2.58	0.44
2:A:387:PHE:CE2	2:A:595:VAL:HG22	2.53	0.44
2:A:398:PRO:HB3	2:A:576:GLU:HB3	2.00	0.43
1:B:346:LEU:C	1:B:346:LEU:HD13	2.43	0.43
1:C:245:ARG:HD3	1:C:245:ARG:HA	1.82	0.43
1:B:23:ALA:O	1:B:27:MET:HG3	2.19	0.43
2:D:358:PHE:O	2:D:602:SER:HA	2.18	0.43
1:B:153:LEU:HD12	1:B:161:MET:HE1	2.01	0.42
1:C:130:ARG:HH22	2:D:521:GLN:HB3	1.84	0.42
2:A:461:SER:HB2	2:D:460:GLY:C	2.44	0.42
1:C:126:ARG:HB3	2:D:507:PHE:CE2	2.54	0.42
1:C:127:GLN:HA	1:C:130:ARG:HD2	2.02	0.42
1:B:245:ARG:HD3	1:B:245:ARG:HA	1.89	0.42
1:B:265:VAL:HG22	1:B:290:ILE:HD12	2.01	0.41
1:B:212:LEU:O	1:B:215:VAL:HG22	2.20	0.41
2:A:379:ALA:HA	2:A:382:LEU:HD13	2.01	0.41
1:C:209:MET:HG2	1:C:353:VAL:HG21	2.02	0.41
2:D:379:ALA:HA	2:D:382:LEU:HD13	2.02	0.41
1:B:168:HIS:CG	1:B:169:SER:N	2.89	0.41
2:D:446:SER:HB2	2:D:550:GLY:HA2	2.02	0.41
2:A:374:CYS:SG	2:A:379:ALA:HB2	2.61	0.41
2:D:414:GLN:HA	2:D:418:TYR:O	2.21	0.41
2:A:474:PHE:HA	2:A:538:SER:O	2.21	0.40
1:C:212:LEU:O	1:C:215:VAL:HG22	2.21	0.40
2:D:387:PHE:O	2:D:600:THR:HG23	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	366/374 (98%)	355 (97%)	11 (3%)	0	100	100
1	C	366/374 (98%)	353 (96%)	13 (4%)	0	100	100
2	A	275/284 (97%)	264 (96%)	11 (4%)	0	100	100
2	D	275/284 (97%)	265 (96%)	10 (4%)	0	100	100
All	All	1282/1316 (97%)	1237 (96%)	45 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	B	307/312 (98%)	306 (100%)	1 (0%)	91	94
1	C	307/312 (98%)	306 (100%)	1 (0%)	91	94
2	A	240/247 (97%)	238 (99%)	2 (1%)	79	86
2	D	240/247 (97%)	236 (98%)	4 (2%)	56	66
All	All	1094/1118 (98%)	1086 (99%)	8 (1%)	81	88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	158	HIS
2	A	442	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	A	564	THR
1	C	177	ASN
2	D	328	LEU
2	D	442	HIS
2	D	564	THR
2	D	600	THR

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

Mol	Chain	Res	Type
2	A	472	GLN
2	A	593	ASN
2	D	472	GLN
2	D	475	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 ⓘ

12 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	0.76	0	17,19,21	1.20	3 (17%)
3	NAG	E	2	3	14,14,15	0.73	0	17,19,21	0.71	0
3	FUC	E	3	3	10,10,11	0.79	0	14,14,16	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	F	1	1,3	14,14,15	0.81	0	17,19,21	1.18	2 (11%)
3	NAG	F	2	3	14,14,15	0.75	0	17,19,21	0.83	0
3	FUC	F	3	3	10,10,11	0.75	0	14,14,16	1.12	1 (7%)
3	NAG	G	1	1,3	14,14,15	0.78	0	17,19,21	1.23	2 (11%)
3	NAG	G	2	3	14,14,15	0.70	0	17,19,21	0.91	1 (5%)
3	FUC	G	3	3	10,10,11	0.78	0	14,14,16	1.02	0
3	NAG	H	1	1,3	14,14,15	0.71	0	17,19,21	1.23	1 (5%)
3	NAG	H	2	3	14,14,15	0.77	0	17,19,21	0.82	0
3	FUC	H	3	3	10,10,11	0.72	0	14,14,16	1.08	2 (14%)

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	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	FUC	E	3	3	-	-	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	FUC	F	3	3	-	-	0/1/1/1
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	FUC	G	3	3	-	-	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	FUC	H	3	3	-	-	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	C1-O5-C5	3.06	116.33	112.19
3	E	1	NAG	C1-O5-C5	2.57	115.67	112.19
3	F	1	NAG	C1-O5-C5	2.53	115.62	112.19
3	E	1	NAG	O4-C4-C3	-2.31	105.01	110.35
3	G	1	NAG	C1-O5-C5	2.30	115.31	112.19
3	G	2	NAG	C1-O5-C5	2.28	115.28	112.19
3	H	3	FUC	C1-O5-C5	2.27	117.91	112.78

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	C2-N2-C7	2.12	125.93	122.90
3	F	1	NAG	O5-C1-C2	-2.09	107.99	111.29
3	G	1	NAG	O4-C4-C3	-2.07	105.56	110.35
3	F	3	FUC	O3-C3-C4	2.05	115.09	110.35
3	H	3	FUC	O3-C3-C4	2.04	115.07	110.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2

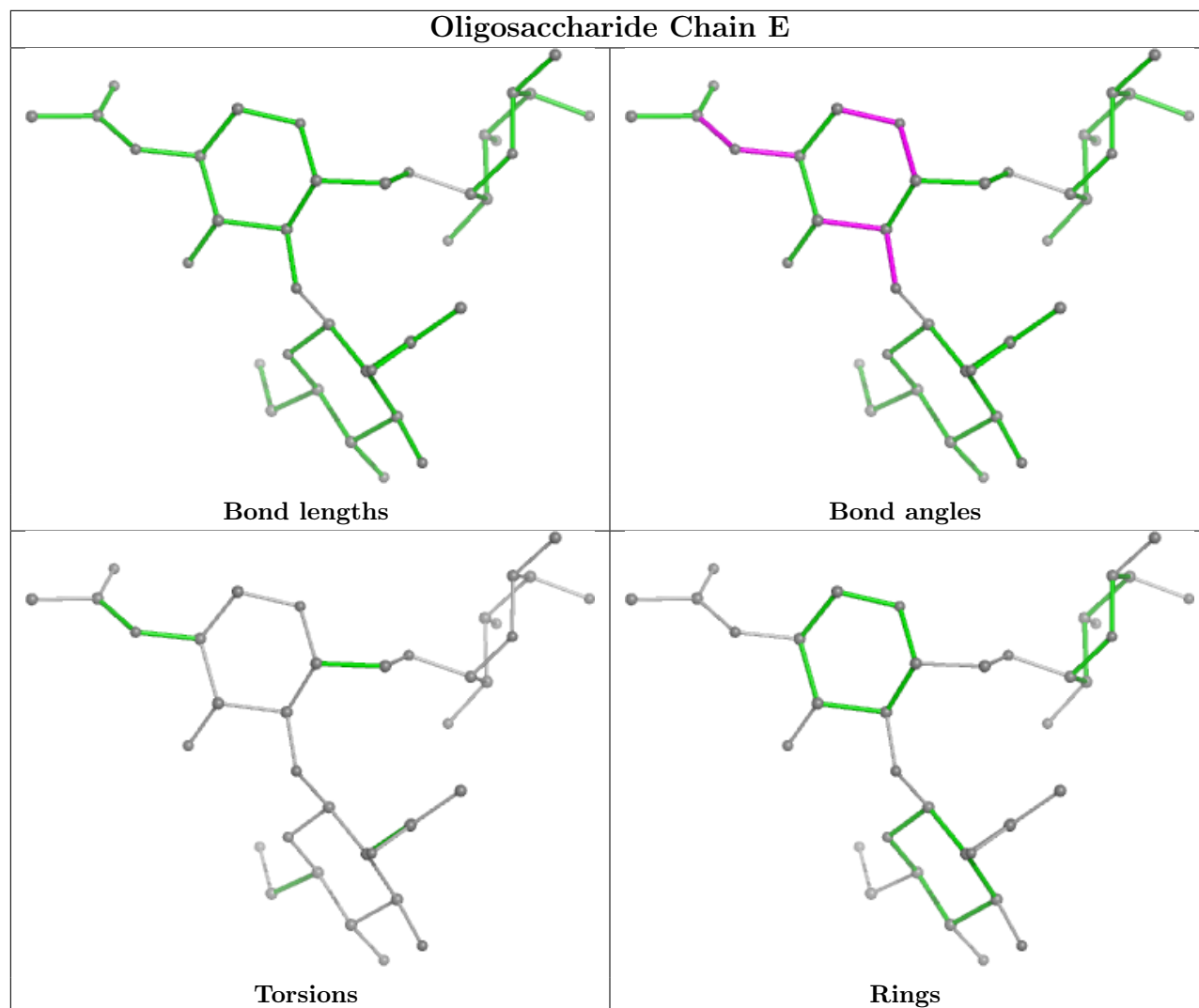
There are no ring outliers.

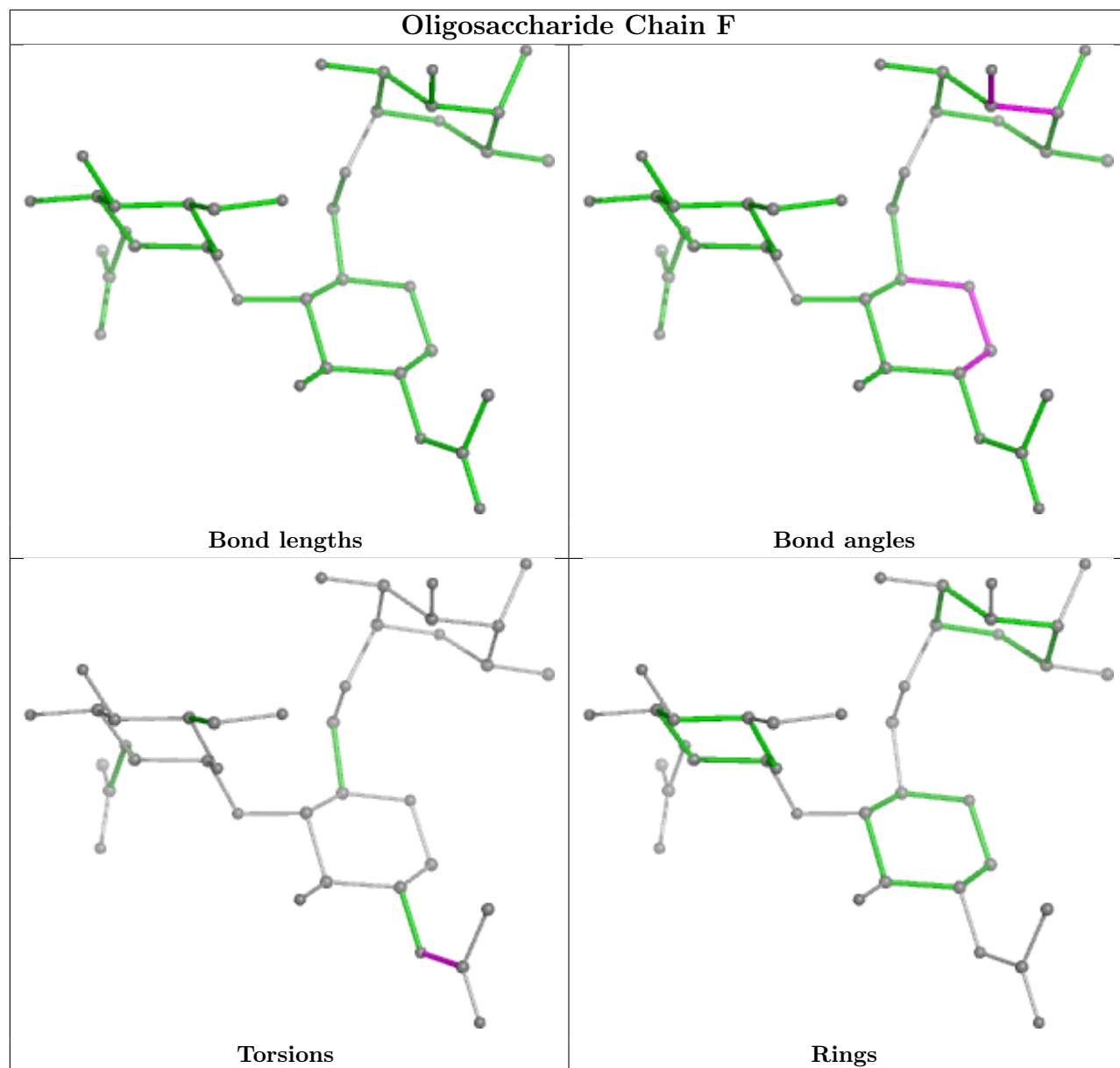
1 monomer is involved in 1 short contact:

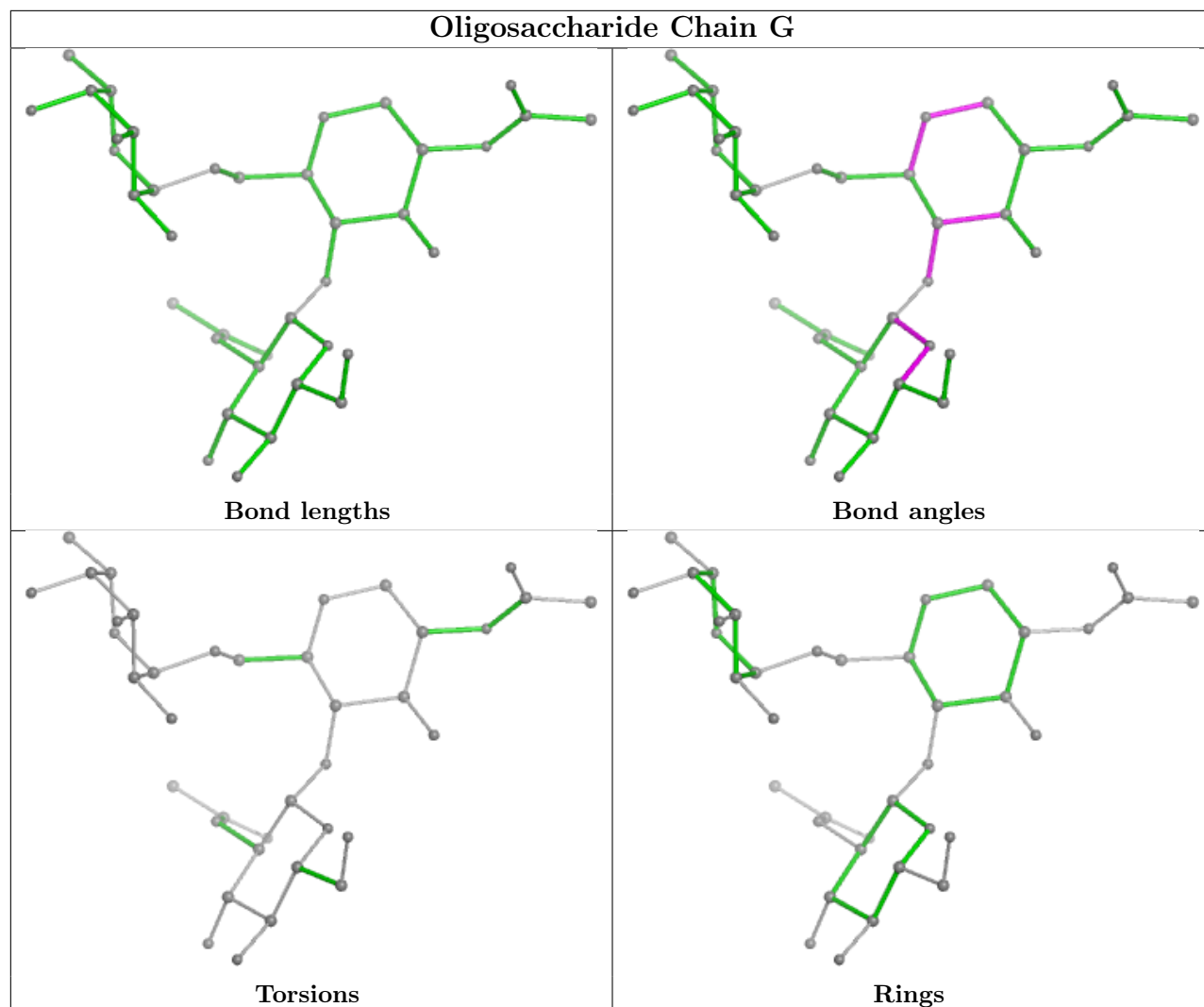
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	1	0

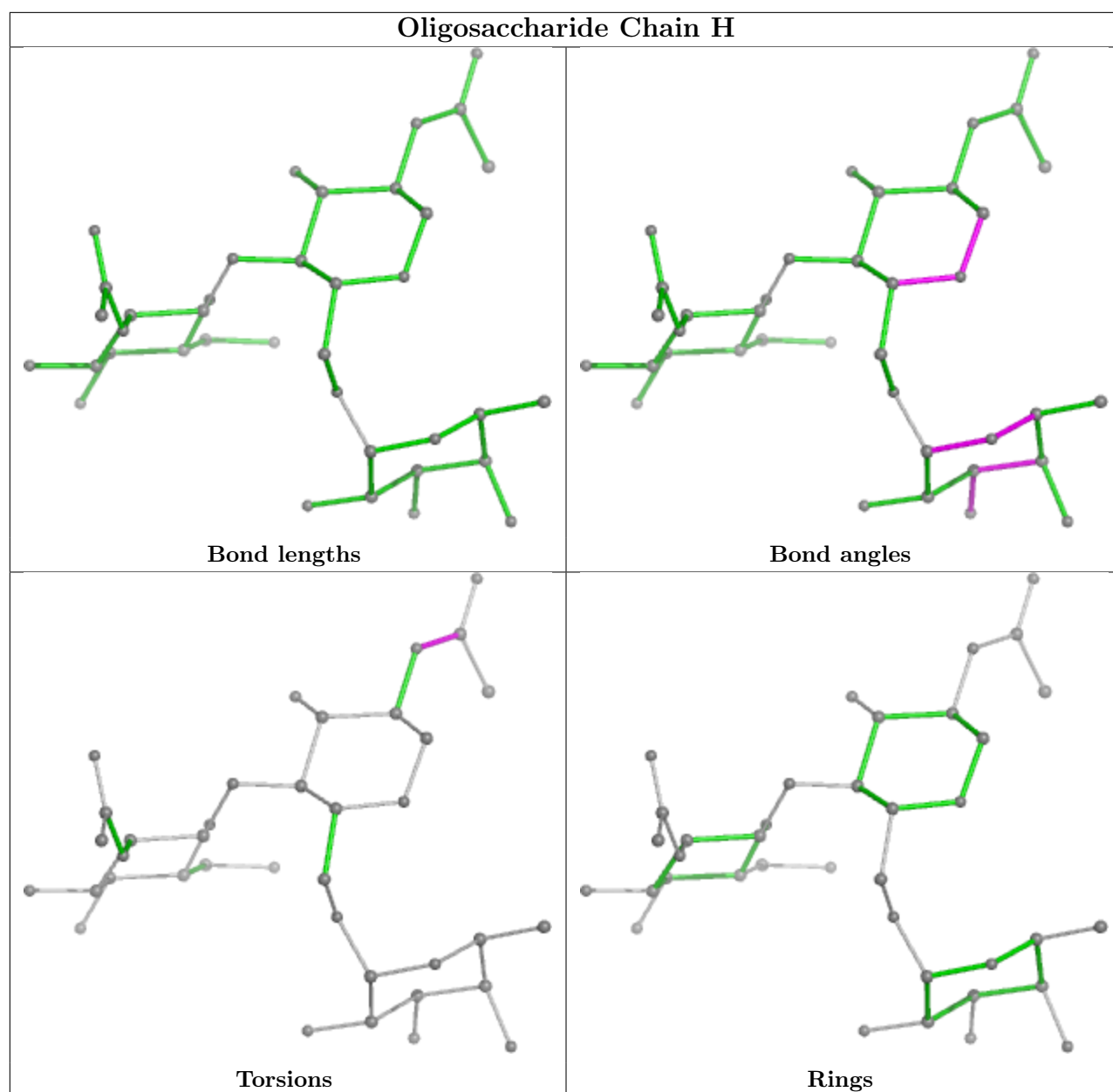
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 16 are monoatomic - leaving 4 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
5	NAG	D	701	2	14,14,15	0.61	0	17,19,21	1.03	0
5	NAG	A	702	2	14,14,15	0.70	0	17,19,21	0.77	0
5	NAG	D	702	2	14,14,15	0.70	0	17,19,21	0.83	0
5	NAG	A	701	2	14,14,15	0.76	0	17,19,21	0.99	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
5	NAG	D	701	2	-	0/6/23/26	0/1/1/1
5	NAG	A	702	2	-	2/6/23/26	0/1/1/1
5	NAG	D	702	2	-	2/6/23/26	0/1/1/1
5	NAG	A	701	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	702	NAG	O5-C5-C6-O6
5	A	702	NAG	O5-C5-C6-O6
5	A	702	NAG	C4-C5-C6-O6
5	D	702	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	368/374 (98%)	-0.56	4 (1%) 77 79	25, 32, 47, 77	0
1	C	368/374 (98%)	-0.31	4 (1%) 77 79	27, 39, 54, 101	0
2	A	277/284 (97%)	0.27	15 (5%) 32 32	36, 50, 73, 92	0
2	D	277/284 (97%)	0.52	27 (9%) 15 14	42, 56, 83, 111	0
All	All	1290/1316 (98%)	-0.08	50 (3%) 44 44	25, 43, 71, 111	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	327	ASP	4.1
2	D	442	HIS	4.1
2	A	327	ASP	4.1
2	D	361	GLY	3.8
1	C	17	ASP	3.8
2	D	382	LEU	3.7
1	C	18	GLN	3.6
2	D	328	LEU	3.6
1	C	384	SER	3.6
2	A	332	ASP	3.5
1	B	384	SER	3.5
2	D	360	MET	3.4
2	D	359	ASN	3.3
2	D	362	ARG	3.2
2	D	366	PHE	3.2
2	D	443	TYR	3.2
2	D	603	THR	3.2
2	D	381	ARG	3.1
2	D	510	VAL	2.9
2	A	364	MET	2.9
2	D	601	CYS	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	A	568	GLN	2.7
2	D	365	SER	2.7
2	A	366	PHE	2.7
2	A	382	LEU	2.7
2	A	442	HIS	2.6
2	D	355	ASN	2.6
2	A	368	GLN	2.5
2	A	457	GLN	2.5
2	D	358	PHE	2.5
2	A	603	THR	2.5
2	D	528	LYS	2.5
2	D	383	TYR	2.4
2	D	595	VAL	2.3
2	A	383	TYR	2.3
2	D	568	GLN	2.3
2	A	330	ASN	2.3
2	D	363	LEU	2.3
1	B	158	HIS	2.3
2	D	364	MET	2.2
1	B	376	SER	2.2
1	C	376	SER	2.1
2	A	361	GLY	2.1
2	A	367	ILE	2.1
2	A	328	LEU	2.1
2	D	385	MET	2.1
2	D	596	ASN	2.1
1	B	17	ASP	2.1
2	D	410	SER	2.1
2	D	329	PRO	2.0

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

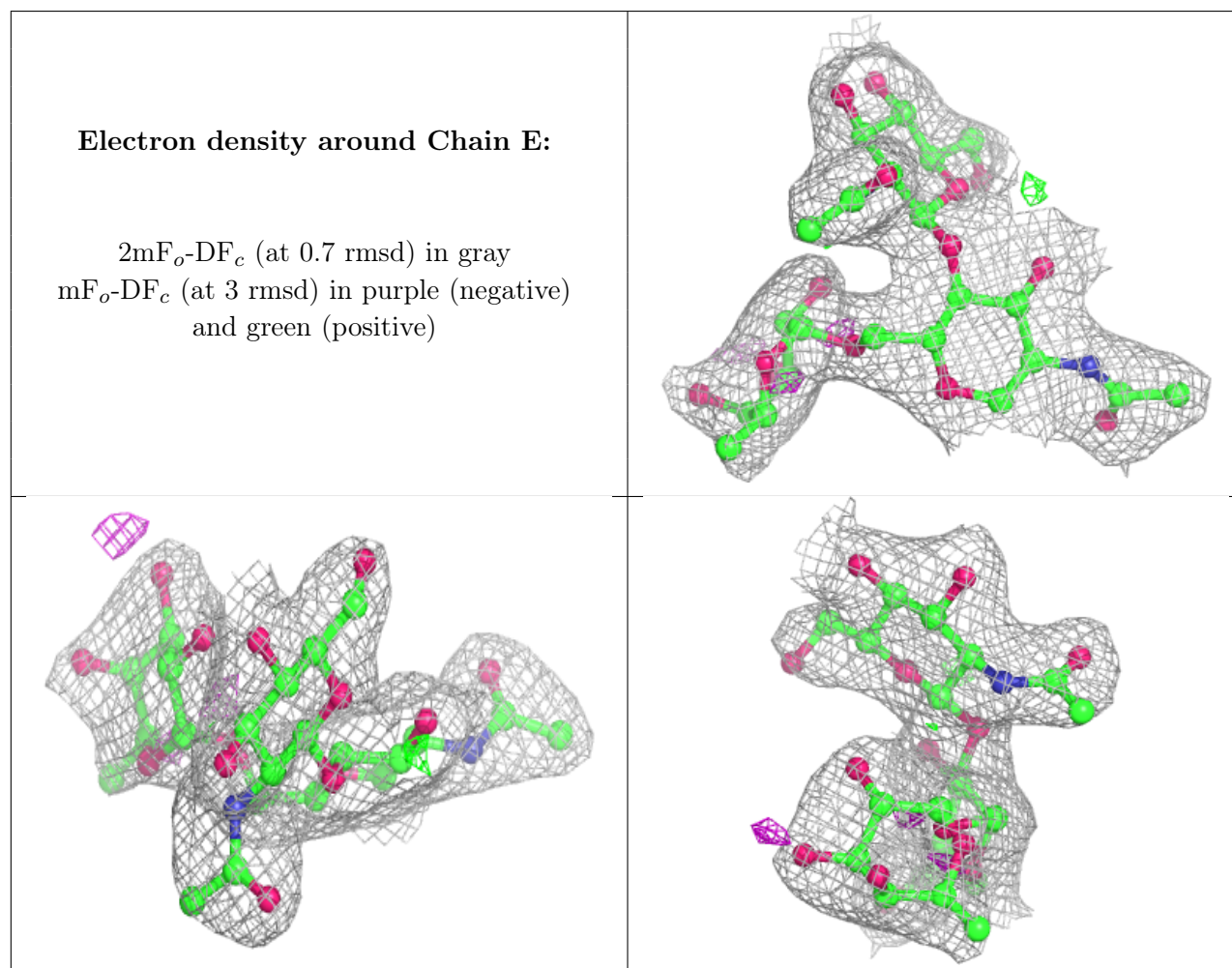
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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
3	FUC	G	3	10/11	0.63	0.19	70,80,85,85	0
3	NAG	H	2	14/15	0.64	0.18	79,87,91,92	0
3	NAG	F	2	14/15	0.66	0.17	63,77,87,90	0
3	NAG	G	2	14/15	0.76	0.14	63,79,82,83	0
3	FUC	E	3	10/11	0.80	0.14	51,62,64,66	0
3	FUC	H	3	10/11	0.80	0.15	58,70,77,79	0
3	NAG	H	1	14/15	0.83	0.12	50,61,72,82	0
3	NAG	E	2	14/15	0.85	0.12	57,61,67,70	0
3	FUC	F	3	10/11	0.88	0.11	44,56,64,64	0
3	NAG	G	1	14/15	0.92	0.08	36,49,66,67	0
3	NAG	F	1	14/15	0.93	0.09	41,47,57,67	0
3	NAG	E	1	14/15	0.95	0.07	33,46,55,58	0

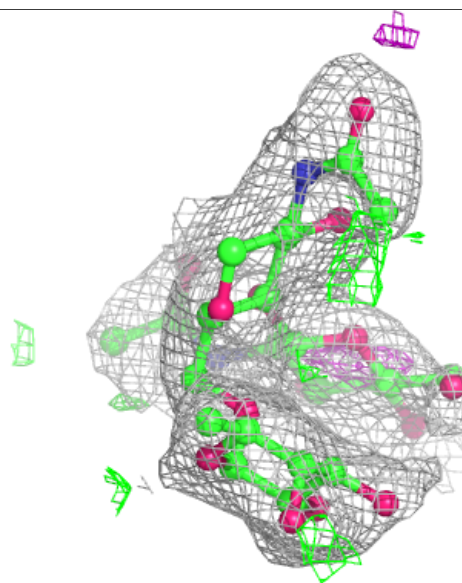
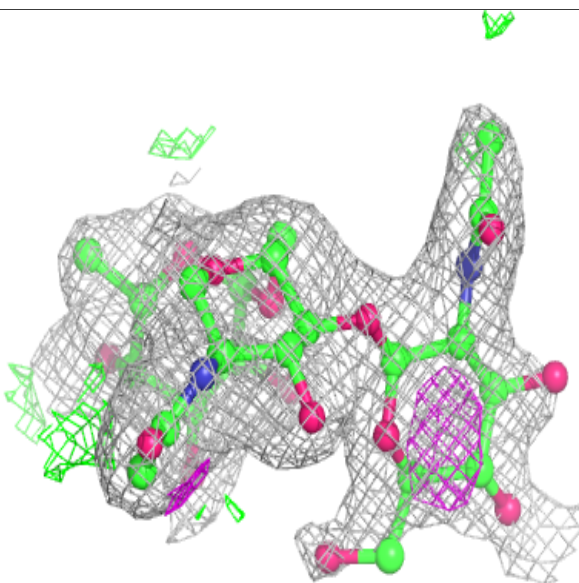
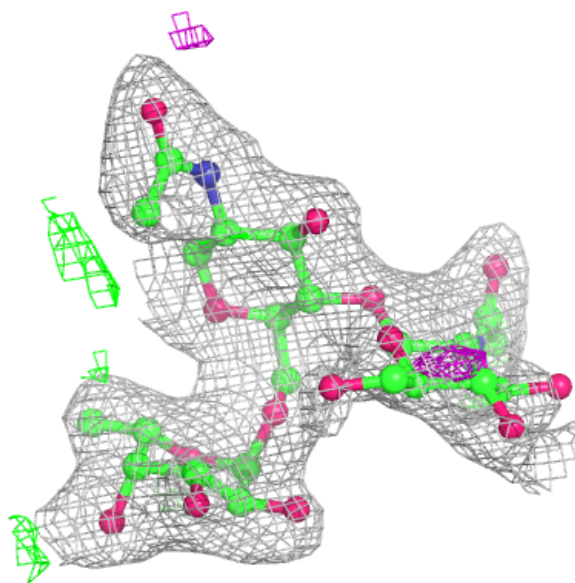
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





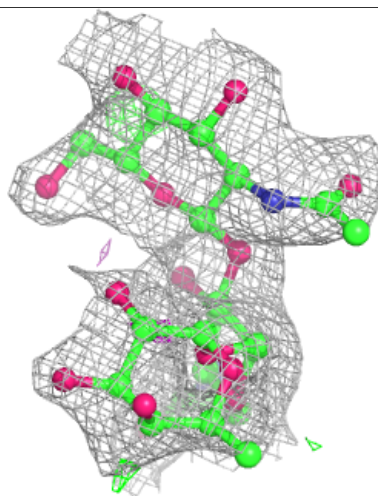
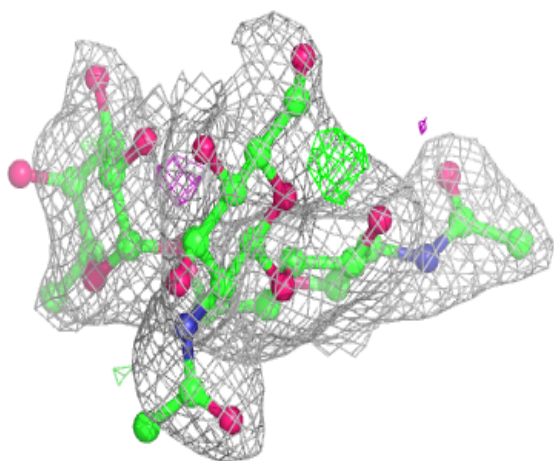
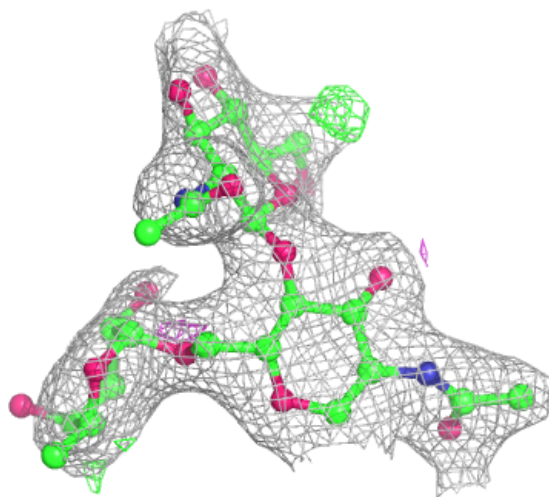
**Electron density around Chain F:**

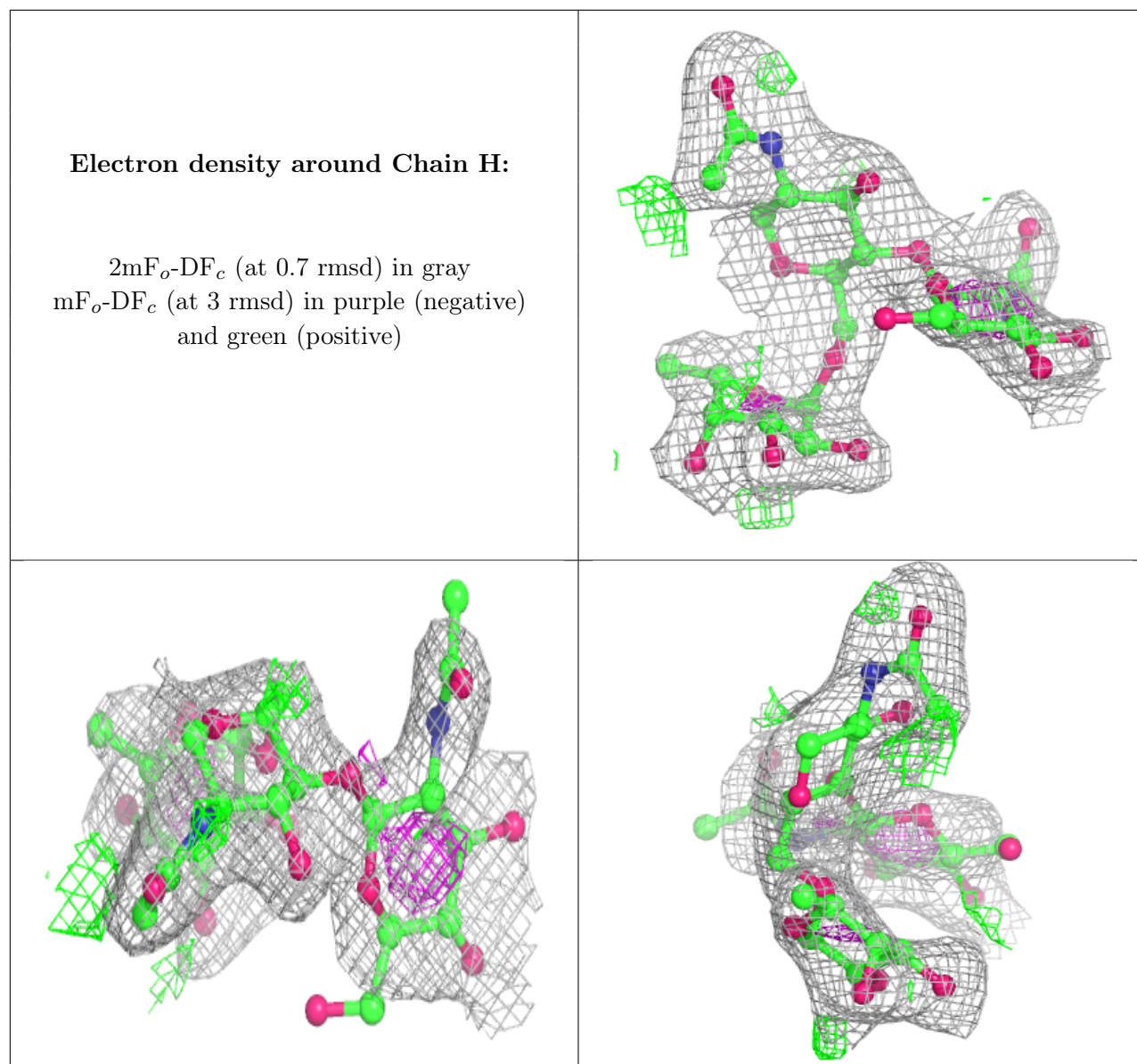
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	NAG	D	701	14/15	0.29	0.33	74,95,103,105	0
5	NAG	A	702	14/15	0.31	0.24	103,119,125,130	0
5	NAG	D	702	14/15	0.37	0.24	121,131,134,137	0
5	NAG	A	701	14/15	0.82	0.14	53,69,74,75	0
4	ZN	D	703	1/1	0.94	0.07	75,75,75,75	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ZN	D	704	1/1	0.94	0.08	111,111,111,111	0
4	ZN	B	405	1/1	0.94	0.08	85,85,85,85	0
4	ZN	B	403	1/1	0.95	0.07	63,63,63,63	0
4	ZN	C	401	1/1	0.96	0.16	58,58,58,58	0
4	ZN	C	402	1/1	0.96	0.08	94,94,94,94	0
4	ZN	B	404	1/1	0.96	0.14	64,64,64,64	0
4	ZN	B	402	1/1	0.96	0.14	58,58,58,58	0
4	ZN	B	409	1/1	0.97	0.04	41,41,41,41	0
4	ZN	B	401	1/1	0.97	0.06	60,60,60,60	0
4	ZN	B	408	1/1	0.97	0.08	73,73,73,73	0
4	ZN	C	403	1/1	0.98	0.06	45,45,45,45	0
4	ZN	C	404	1/1	0.99	0.05	37,37,37,37	0
4	ZN	C	405	1/1	0.99	0.05	38,38,38,38	0
4	ZN	B	407	1/1	0.99	0.06	31,31,31,31	0
4	ZN	B	406	1/1	0.99	0.06	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.