



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 02:28 AM UTC

PDB ID : 7UAJ / pdb_00007uaj
Title : Crystal structure of apo HPV16 E6
Authors : Shen, Q.; Leonard, P.G.; Cross, J.B.
Deposited on : 2022-03-13
Resolution : 3.25 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

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:

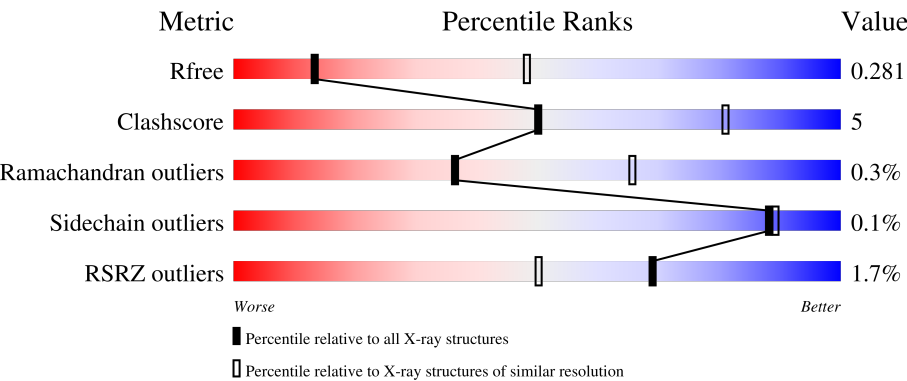
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	537	
1	B	537	
1	C	537	
1	D	537	
2	E	2	

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Mol	Chain	Length	Quality of chain
2	F	2	 100%
2	G	2	 100%
2	H	2	 100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16217 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 Maltose/maltodextrin-binding periplasmic protein, Protein E6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	511	Total	C	N	O	S	0	0	0
			4039	2579	676	766	18			
1	B	512	Total	C	N	O	S	0	0	0
			4033	2581	672	762	18			
1	C	509	Total	C	N	O	S	0	0	0
			4023	2569	674	762	18			
1	D	509	Total	C	N	O	S	0	0	0
			4022	2566	677	762	17			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP P0AEX9
A	-6	GLY	-	expression tag	UNP P0AEX9
A	-5	HIS	-	expression tag	UNP P0AEX9
A	-4	HIS	-	expression tag	UNP P0AEX9
A	-3	HIS	-	expression tag	UNP P0AEX9
A	-2	HIS	-	expression tag	UNP P0AEX9
A	-1	HIS	-	expression tag	UNP P0AEX9
A	0	HIS	-	expression tag	UNP P0AEX9
A	1	MET	-	expression tag	UNP P0AEX9
A	368	ASN	-	linker	UNP P0AEX9
A	369	SER	-	linker	UNP P0AEX9
A	370	SER	-	linker	UNP P0AEX9
A	371	SER	-	linker	UNP P0AEX9
A	372	GLU	-	linker	UNP P0AEX9
A	373	ASN	-	linker	UNP P0AEX9
A	374	LEU	-	linker	UNP P0AEX9
A	375	TYR	-	linker	UNP P0AEX9
A	376	PHE	-	linker	UNP P0AEX9
A	377	GLN	-	linker	UNP P0AEX9
A	378	GLY	-	linker	UNP P0AEX9
A	458	SER	CYS	conflict	UNP P03126

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Chain	Residue	Modelled	Actual	Comment	Reference
A	475	SER	CYS	conflict	UNP P03126
A	489	SER	CYS	conflict	UNP P03126
A	518	SER	CYS	conflict	UNP P03126
B	-7	MET	-	expression tag	UNP P0AEX9
B	-6	GLY	-	expression tag	UNP P0AEX9
B	-5	HIS	-	expression tag	UNP P0AEX9
B	-4	HIS	-	expression tag	UNP P0AEX9
B	-3	HIS	-	expression tag	UNP P0AEX9
B	-2	HIS	-	expression tag	UNP P0AEX9
B	-1	HIS	-	expression tag	UNP P0AEX9
B	0	HIS	-	expression tag	UNP P0AEX9
B	1	MET	-	expression tag	UNP P0AEX9
B	368	ASN	-	linker	UNP P0AEX9
B	369	SER	-	linker	UNP P0AEX9
B	370	SER	-	linker	UNP P0AEX9
B	371	SER	-	linker	UNP P0AEX9
B	372	GLU	-	linker	UNP P0AEX9
B	373	ASN	-	linker	UNP P0AEX9
B	374	LEU	-	linker	UNP P0AEX9
B	375	TYR	-	linker	UNP P0AEX9
B	376	PHE	-	linker	UNP P0AEX9
B	377	GLN	-	linker	UNP P0AEX9
B	378	GLY	-	linker	UNP P0AEX9
B	458	SER	CYS	conflict	UNP P03126
B	475	SER	CYS	conflict	UNP P03126
B	489	SER	CYS	conflict	UNP P03126
B	518	SER	CYS	conflict	UNP P03126
C	-7	MET	-	expression tag	UNP P0AEX9
C	-6	GLY	-	expression tag	UNP P0AEX9
C	-5	HIS	-	expression tag	UNP P0AEX9
C	-4	HIS	-	expression tag	UNP P0AEX9
C	-3	HIS	-	expression tag	UNP P0AEX9
C	-2	HIS	-	expression tag	UNP P0AEX9
C	-1	HIS	-	expression tag	UNP P0AEX9
C	0	HIS	-	expression tag	UNP P0AEX9
C	1	MET	-	expression tag	UNP P0AEX9
C	368	ASN	-	linker	UNP P0AEX9
C	369	SER	-	linker	UNP P0AEX9
C	370	SER	-	linker	UNP P0AEX9
C	371	SER	-	linker	UNP P0AEX9
C	372	GLU	-	linker	UNP P0AEX9
C	373	ASN	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	374	LEU	-	linker	UNP P0AEX9
C	375	TYR	-	linker	UNP P0AEX9
C	376	PHE	-	linker	UNP P0AEX9
C	377	GLN	-	linker	UNP P0AEX9
C	378	GLY	-	linker	UNP P0AEX9
C	458	SER	CYS	conflict	UNP P03126
C	475	SER	CYS	conflict	UNP P03126
C	489	SER	CYS	conflict	UNP P03126
C	518	SER	CYS	conflict	UNP P03126
D	-7	MET	-	expression tag	UNP P0AEX9
D	-6	GLY	-	expression tag	UNP P0AEX9
D	-5	HIS	-	expression tag	UNP P0AEX9
D	-4	HIS	-	expression tag	UNP P0AEX9
D	-3	HIS	-	expression tag	UNP P0AEX9
D	-2	HIS	-	expression tag	UNP P0AEX9
D	-1	HIS	-	expression tag	UNP P0AEX9
D	0	HIS	-	expression tag	UNP P0AEX9
D	1	MET	-	expression tag	UNP P0AEX9
D	368	ASN	-	linker	UNP P0AEX9
D	369	SER	-	linker	UNP P0AEX9
D	370	SER	-	linker	UNP P0AEX9
D	371	SER	-	linker	UNP P0AEX9
D	372	GLU	-	linker	UNP P0AEX9
D	373	ASN	-	linker	UNP P0AEX9
D	374	LEU	-	linker	UNP P0AEX9
D	375	TYR	-	linker	UNP P0AEX9
D	376	PHE	-	linker	UNP P0AEX9
D	377	GLN	-	linker	UNP P0AEX9
D	378	GLY	-	linker	UNP P0AEX9
D	458	SER	CYS	conflict	UNP P03126
D	475	SER	CYS	conflict	UNP P03126
D	489	SER	CYS	conflict	UNP P03126
D	518	SER	CYS	conflict	UNP P03126

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	F	2	Total	C	O	0	0	0
			23	12	11			
2	G	2	Total	C	O	0	0	0
			23	12	11			
2	H	2	Total	C	O	0	0	0
			23	12	11			

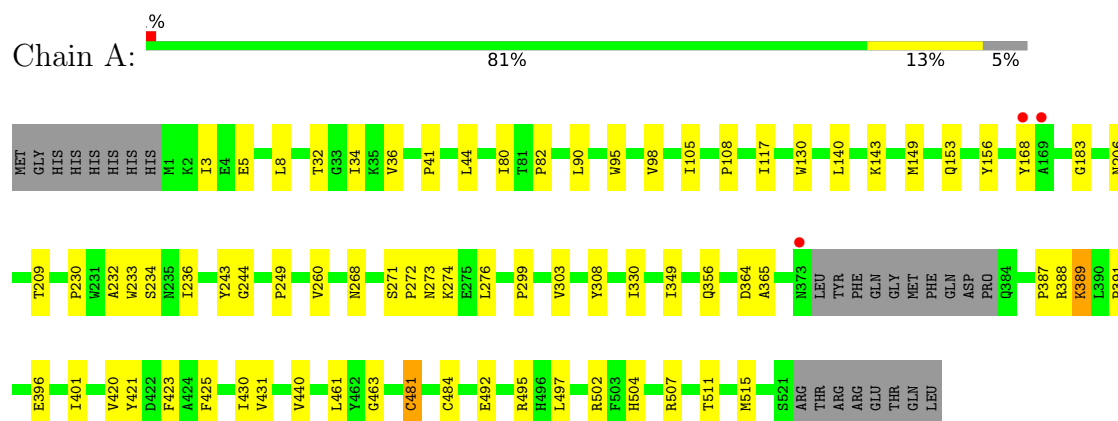
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		
3	B	2	Total	Zn	0	0
			2	2		
3	C	2	Total	Zn	0	0
			2	2		
3	D	2	Total	Zn	0	0
			2	2		

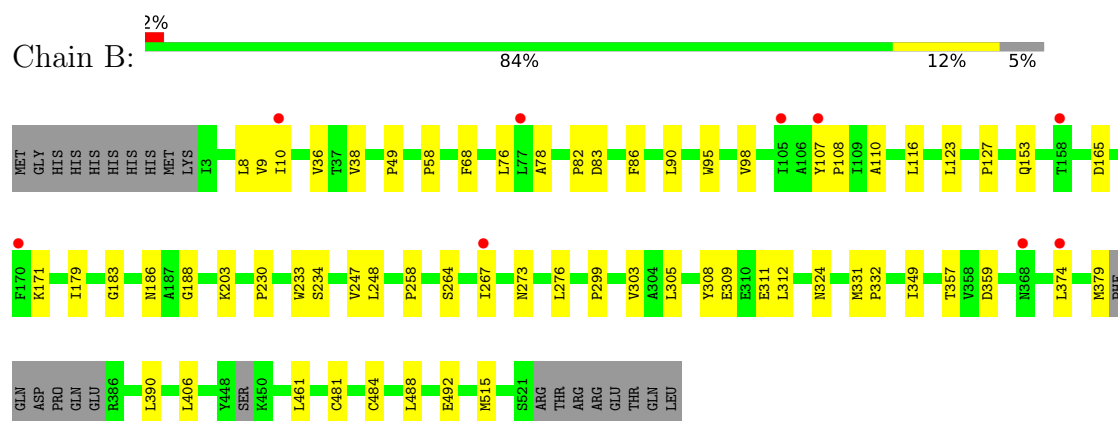
3 Residue-property plots [i](#)

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.

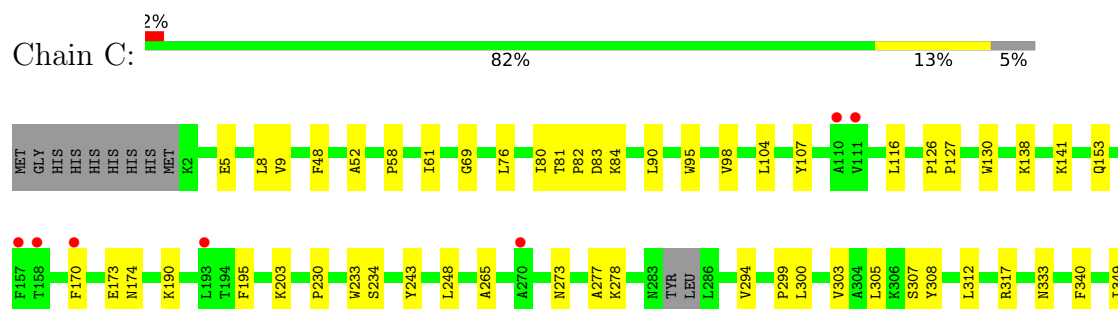
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Protein E6

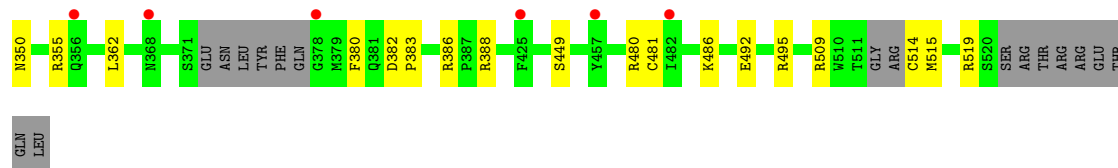


- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Protein E6

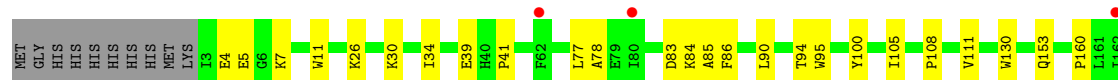
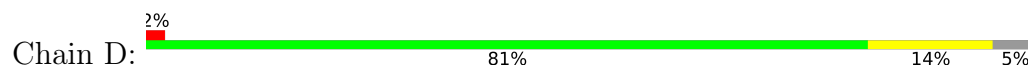


- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Protein E6





- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Protein E6



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.11Å 88.68Å 109.61Å 106.61° 90.16° 102.76°	Depositor
Resolution (Å)	52.39 – 3.25 52.39 – 3.25	Depositor EDS
% Data completeness (in resolution range)	91.5 (52.39-3.25) 91.8 (52.39-3.25)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.26Å)	Xtriage
Refinement program	PHENIX v 1.20.1-4887-000	Depositor
R, R_{free}	0.256 , 0.282 0.256 , 0.281	Depositor DCC
R_{free} test set	2139 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	106.4	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16217	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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: ZN, GLC

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	0.09	0/4133	0.26	1/5598 (0.0%)
1	B	0.08	0/4128	0.25	0/5595
1	C	0.09	0/4116	0.25	0/5572
1	D	0.08	0/4115	0.22	0/5576
All	All	0.08	0/16492	0.25	1/22341 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	THR	CB-CA-C	-5.89	107.94	116.54

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	4039	0	3974	42	0
1	B	4033	0	3953	42	0
1	C	4023	0	3949	44	0
1	D	4022	0	3953	45	0
2	E	23	0	21	1	0
2	F	23	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	23	0	21	0	0
2	H	23	0	21	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
All	All	16217	0	15913	171	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (171) 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:389:LYS:HG2	1:A:391:PRO:HD2	1.65	0.79
1:B:8:LEU:HB2	1:B:36:VAL:HG12	1.69	0.75
1:A:80:ILE:HG22	1:A:82:PRO:HD3	1.70	0.74
1:C:481:CYS:HB3	1:C:486:LYS:H	1.53	0.74
1:C:80:ILE:HG22	1:C:82:PRO:HD2	1.70	0.74
1:D:83:ASP:HB2	1:D:86:PHE:HB3	1.70	0.73
1:D:488:LEU:O	1:D:493:LYS:NZ	2.23	0.70
1:D:100:TYR:HB3	1:D:105:ILE:HD11	1.74	0.70
1:D:153:GLN:HA	1:D:349:ILE:HD11	1.73	0.70
1:A:156:TYR:HB2	2:E:2:GLC:H61	1.74	0.69
1:D:233:TRP:HB2	1:D:299:PRO:HG2	1.75	0.68
1:B:110:ALA:HA	1:B:303:VAL:HA	1.76	0.67
1:C:481:CYS:HB2	1:C:514:CYS:HB3	1.76	0.67
1:C:153:GLN:HA	1:C:349:ILE:HD11	1.77	0.67
1:A:273:ASN:HB3	1:A:276:LEU:HB2	1.78	0.66
1:C:234:SER:HB2	1:C:299:PRO:HD3	1.77	0.66
1:B:153:GLN:HA	1:B:349:ILE:HD11	1.77	0.66
1:B:481:CYS:HB3	1:B:484:CYS:HB2	1.78	0.66
1:A:8:LEU:HB2	1:A:36:VAL:HG12	1.78	0.65
1:A:168:TYR:HB2	1:A:183:GLY:HA3	1.80	0.63
1:C:480:ARG:HD2	1:C:509:ARG:HH11	1.64	0.62
1:A:492:GLU:HG2	1:A:515:MET:HG3	1.81	0.62
1:A:41:PRO:HG2	1:A:44:LEU:HB3	1.82	0.61
1:D:90:LEU:HB2	1:D:95:TRP:HE1	1.67	0.59
1:C:8:LEU:HD22	1:C:277:ALA:HB2	1.83	0.59
1:B:492:GLU:HG2	1:B:515:MET:HG2	1.83	0.58
1:C:81:THR:HG23	1:C:278:LYS:HE3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:PRO:HG3	1:D:258:PRO:HA	1.86	0.57
1:D:77:LEU:HD23	1:D:105:ILE:HG22	1.85	0.57
1:A:495:ARG:HD3	1:A:515:MET:HG2	1.85	0.57
1:A:431:VAL:HG13	1:B:374:LEU:HG	1.86	0.57
1:B:273:ASN:HB3	1:B:276:LEU:HB2	1.86	0.56
1:C:294:VAL:HB	1:C:300:LEU:HD11	1.88	0.56
1:B:123:LEU:HD21	1:B:127:PRO:HD3	1.88	0.56
1:C:308:TYR:HA	1:C:312:LEU:HB2	1.87	0.55
1:B:390:LEU:HD11	1:B:406:LEU:HD11	1.89	0.55
1:B:78:ALA:HB3	1:B:267:ILE:HG23	1.89	0.54
1:A:389:LYS:H	1:A:430:ILE:HG13	1.73	0.54
1:C:5:GLU:HA	1:C:273:ASN:HD21	1.73	0.54
1:D:77:LEU:HD21	1:D:266:GLY:HA3	1.89	0.54
1:A:140:LEU:HD23	1:A:143:LYS:HD3	1.90	0.53
1:A:206:ASN:HB3	1:A:209:THR:HG23	1.89	0.53
1:B:233:TRP:HB2	1:B:299:PRO:HG2	1.91	0.53
1:A:423:PHE:HE2	1:A:440:VAL:HG12	1.73	0.53
1:B:116:LEU:HB2	1:B:248:LEU:HD23	1.89	0.53
1:A:153:GLN:HA	1:A:349:ILE:HD11	1.91	0.52
1:D:94:THR:HB	1:D:108:PRO:HB3	1.91	0.52
1:B:82:PRO:HB3	1:B:107:TYR:HE1	1.74	0.52
1:D:34:ILE:HG13	1:D:276:LEU:HD21	1.92	0.51
1:B:8:LEU:HD21	1:B:273:ASN:HB2	1.92	0.51
1:C:492:GLU:HG2	1:C:495:ARG:HH12	1.76	0.51
1:A:234:SER:HB2	1:A:299:PRO:HD3	1.93	0.51
1:B:90:LEU:HB2	1:B:95:TRP:HE1	1.76	0.51
1:D:83:ASP:O	1:D:85:ALA:N	2.44	0.51
1:D:4:GLU:HG2	1:D:7:LYS:HB3	1.93	0.51
1:C:90:LEU:HB2	1:C:95:TRP:HE1	1.76	0.51
1:C:130:TRP:HB3	1:C:195:PHE:CE2	2.46	0.51
1:B:98:VAL:HG21	1:B:108:PRO:HD3	1.93	0.50
1:B:248:LEU:HD12	1:B:258:PRO:HG3	1.93	0.50
1:D:169:ALA:H	1:D:183:GLY:HA3	1.75	0.50
1:D:273:ASN:HB3	1:D:276:LEU:HB3	1.93	0.50
1:D:78:ALA:HB3	1:D:267:ILE:HG23	1.94	0.50
1:C:305:LEU:HG	1:C:307:SER:H	1.76	0.50
1:D:291:LEU:HD13	1:D:303:VAL:HG11	1.93	0.49
1:C:9:VAL:HB	1:C:58:PRO:HA	1.94	0.49
1:C:303:VAL:HG22	1:C:312:LEU:HD12	1.95	0.48
1:A:364:ASP:OD1	1:A:365:ALA:N	2.46	0.48
1:A:481:CYS:SG	1:A:484:CYS:N	2.84	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:ASP:N	1:C:383:PRO:HD2	2.28	0.48
1:C:515:MET:O	1:C:515:MET:HE3	2.14	0.48
1:C:107:TYR:HB2	1:C:265:ALA:HB3	1.97	0.47
1:C:98:VAL:HG23	1:C:104:LEU:HD12	1.97	0.47
1:D:280:PHE:O	1:D:284:TYR:HB2	2.15	0.47
1:D:232:ALA:O	1:D:236:ILE:HG12	2.15	0.47
1:A:423:PHE:CE2	1:A:440:VAL:HG12	2.50	0.46
1:D:5:GLU:HB3	1:D:272:PRO:HB2	1.97	0.46
1:D:305:LEU:HG	1:D:307:SER:H	1.80	0.46
1:B:49:PRO:HA	1:B:76:LEU:HD13	1.97	0.46
1:C:173:GLU:HG3	1:C:174:ASN:H	1.79	0.46
1:A:463:GLY:HA3	1:A:497:LEU:HD21	1.98	0.46
1:B:234:SER:HB3	1:B:299:PRO:HD3	1.98	0.46
1:A:401:ILE:HD11	1:A:420:VAL:HG12	1.98	0.46
1:A:5:GLU:HG2	1:A:272:PRO:HG3	1.98	0.45
1:B:247:VAL:HA	1:B:324:ASN:HD21	1.81	0.45
1:D:94:THR:HG21	1:D:304:ALA:HB2	1.97	0.45
1:B:68:PHE:HE2	1:B:264:SER:HB2	1.81	0.45
1:B:90:LEU:HB2	1:B:95:TRP:NE1	2.31	0.45
1:D:308:TYR:HD1	1:D:312:LEU:HB2	1.81	0.45
1:B:171:LYS:HD2	1:B:171:LYS:HA	1.69	0.45
1:A:507:ARG:HA	1:A:507:ARG:HD2	1.65	0.45
1:C:203:LYS:HA	1:C:203:LYS:HD2	1.62	0.45
1:A:230:PRO:HA	1:A:233:TRP:CE2	2.51	0.45
1:C:170:PHE:CD1	1:C:340:PHE:HB2	2.52	0.45
1:D:354:GLY:O	1:D:356:GLN:N	2.45	0.45
1:B:110:ALA:HB2	1:B:303:VAL:HG12	1.98	0.45
1:C:69:GLY:HA3	1:C:333:ASN:O	2.18	0.44
1:A:303:VAL:HG21	1:A:308:TYR:HB3	2.00	0.44
1:B:183:GLY:O	1:B:186:ASN:ND2	2.51	0.44
1:A:461:LEU:HD23	1:A:461:LEU:HA	1.82	0.44
1:A:34:ILE:HD12	1:A:276:LEU:HD13	1.99	0.44
1:C:90:LEU:HB2	1:C:95:TRP:NE1	2.32	0.44
1:C:233:TRP:HB2	1:C:299:PRO:HG2	1.98	0.44
1:D:479:ILE:HD12	1:D:493:LYS:HE3	1.99	0.44
1:A:90:LEU:HB2	1:A:95:TRP:HE1	1.81	0.44
1:C:48:PHE:CG	1:C:61:ILE:HD12	2.53	0.44
1:A:130:TRP:CD1	1:A:249:PRO:HB2	2.53	0.44
1:B:309:GLU:C	1:B:311:GLU:H	2.26	0.44
1:D:373:ASN:OD1	1:D:374:LEU:N	2.50	0.43
1:C:230:PRO:HA	1:C:233:TRP:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:LEU:O	1:B:308:TYR:HB3	2.18	0.43
1:C:116:LEU:HB2	1:C:248:LEU:HD23	2.00	0.43
1:D:459:TYR:HB3	1:D:505:ASN:HB3	2.01	0.43
2:H:1:GLC:H62	2:H:2:GLC:H5	2.00	0.43
1:B:165:ASP:HB3	1:B:188:GLY:HA2	2.00	0.43
1:D:474:LEU:H	1:D:474:LEU:HD23	1.84	0.43
1:A:502:ARG:H	1:A:502:ARG:HG2	1.70	0.42
1:C:380:PHE:HE1	1:C:388:ARG:HA	1.83	0.42
1:D:86:PHE:HE1	1:D:286:LEU:HD13	1.83	0.42
1:D:481:CYS:HB3	1:D:484:CYS:HB2	2.00	0.42
1:D:374:LEU:HD12	1:D:374:LEU:HA	1.89	0.42
1:C:449:SER:HA	1:D:374:LEU:HD11	2.00	0.42
1:A:3:ILE:HD13	1:A:271:SER:HA	2.02	0.42
1:B:82:PRO:HB2	1:B:86:PHE:HD2	1.85	0.42
1:D:11:TRP:CD2	1:D:41:PRO:HG3	2.54	0.42
1:D:111:VAL:HB	1:D:302:ALA:HB3	2.02	0.42
1:A:149:MET:HE2	1:A:149:MET:HB3	1.97	0.42
1:A:504:HIS:O	1:A:511:THR:N	2.45	0.42
1:B:230:PRO:HA	1:B:233:TRP:CE2	2.55	0.42
1:C:350:ASN:HB3	1:C:355:ARG:HB3	2.02	0.42
1:C:386:ARG:HG2	1:D:457:TYR:HB3	2.00	0.42
1:B:82:PRO:O	1:B:83:ASP:HB3	2.20	0.42
1:C:243:TYR:OH	1:C:317:ARG:NH1	2.52	0.42
1:B:9:VAL:HB	1:B:58:PRO:HA	2.02	0.42
1:B:203:LYS:HD2	1:B:203:LYS:C	2.45	0.42
1:C:138:LYS:HA	1:C:138:LYS:HD3	1.82	0.42
1:A:98:VAL:O	1:A:105:ILE:HG12	2.20	0.41
1:A:268:ASN:O	1:A:274:LYS:NZ	2.53	0.41
1:C:126:PRO:HA	1:C:127:PRO:HD3	1.97	0.41
1:C:190:LYS:HG2	1:C:362:LEU:HD12	2.01	0.41
1:D:26:LYS:O	1:D:30:LYS:HG2	2.21	0.41
1:D:387:PRO:HB3	1:D:392:GLN:HB2	2.01	0.41
1:B:203:LYS:HD2	1:B:203:LYS:O	2.20	0.41
1:A:260:VAL:HB	1:A:330:ILE:HA	2.03	0.41
1:A:421:TYR:HB3	1:A:425:PHE:CE2	2.55	0.41
1:B:379:MET:HE3	1:B:379:MET:HB2	1.84	0.41
1:D:461:LEU:HD23	1:D:461:LEU:HA	1.83	0.41
1:A:90:LEU:HD13	1:A:108:PRO:HG2	2.03	0.41
1:A:117:ILE:HA	1:A:244:GLY:O	2.21	0.41
1:C:141:LYS:HD3	1:C:141:LYS:HA	1.88	0.41
1:C:305:LEU:HD21	1:C:307:SER:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:TYR:CD1	1:B:312:LEU:HB2	2.56	0.41
1:B:461:LEU:HD23	1:B:461:LEU:HA	1.87	0.41
1:B:481:CYS:HB2	1:B:488:LEU:HD21	2.03	0.41
1:C:83:ASP:HB3	1:C:84:LYS:H	1.69	0.41
1:D:11:TRP:CD1	1:D:39:GLU:HB2	2.56	0.41
1:D:130:TRP:CD1	1:D:249:PRO:HB2	2.56	0.41
1:A:232:ALA:O	1:A:236:ILE:HG13	2.20	0.41
1:B:331:MET:HA	1:B:332:PRO:HD3	1.95	0.41
1:B:357:THR:O	1:B:359:ASP:N	2.47	0.41
1:A:44:LEU:H	1:A:44:LEU:HD23	1.85	0.40
1:C:515:MET:HE1	1:C:519:ARG:HG2	2.03	0.40
1:D:505:ASN:HB2	1:D:510:TRP:CD2	2.56	0.40
1:A:387:PRO:HG3	1:A:396:GLU:OE1	2.21	0.40
1:D:288:ASP:O	1:D:292:GLU:HG2	2.22	0.40
1:C:170:PHE:CE1	1:C:340:PHE:HB2	2.57	0.40
1:D:201:LYS:HA	1:D:201:LYS:HD3	1.90	0.40
1:B:303:VAL:HG22	1:B:308:TYR:HB2	2.04	0.40
1:D:218:PHE:HD2	1:D:236:ILE:HD12	1.87	0.40
1:B:10:ILE:HB	1:B:38:VAL:HG22	2.04	0.40
1:C:52:ALA:HB3	1:C:76:LEU:HD13	2.04	0.40
1:D:294:VAL:HB	1:D:300:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	507/537 (94%)	483 (95%)	20 (4%)	4 (1%)	16	44
1	B	508/537 (95%)	486 (96%)	21 (4%)	1 (0%)	43	70
1	C	501/537 (93%)	476 (95%)	25 (5%)	0	100	100
1	D	505/537 (94%)	481 (95%)	23 (5%)	1 (0%)	43	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2021/2148 (94%)	1926 (95%)	89 (4%)	6 (0%)	36	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	388	ARG
1	A	356	GLN
1	D	84	LYS
1	A	243	TYR
1	A	389	LYS
1	B	179	ILE

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	429/456 (94%)	428 (100%)	1 (0%)	87	87
1	B	425/456 (93%)	425 (100%)	0	100	100
1	C	427/456 (94%)	427 (100%)	0	100	100
1	D	426/456 (93%)	426 (100%)	0	100	100
All	All	1707/1824 (94%)	1706 (100%)	1 (0%)	88	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	481	CYS

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	40	HIS
1	A	87	GLN
1	A	295	ASN

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Mol	Chain	Res	Type
1	A	456	HIS
1	A	501	GLN
1	B	119	ASN
1	B	125	ASN
1	B	283	ASN
1	C	456	HIS
1	D	228	ASN
1	D	326	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GLC	E	1	2	12,12,12	0.53	0	17,17,17	0.53	0
2	GLC	E	2	2	11,11,12	0.61	0	15,15,17	0.56	0
2	GLC	F	1	2	12,12,12	0.52	0	17,17,17	0.47	0
2	GLC	F	2	2	11,11,12	0.61	0	15,15,17	0.57	0
2	GLC	G	1	2	12,12,12	0.54	0	17,17,17	0.47	0
2	GLC	G	2	2	11,11,12	0.63	0	15,15,17	0.50	0
2	GLC	H	1	2	12,12,12	0.52	0	17,17,17	0.53	0
2	GLC	H	2	2	11,11,12	0.58	0	15,15,17	0.53	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	E	1	2	-	0/2/22/22	0/1/1/1
2	GLC	E	2	2	-	2/2/19/22	0/1/1/1
2	GLC	F	1	2	-	0/2/22/22	0/1/1/1
2	GLC	F	2	2	-	0/2/19/22	0/1/1/1
2	GLC	G	1	2	-	2/2/22/22	0/1/1/1
2	GLC	G	2	2	-	0/2/19/22	0/1/1/1
2	GLC	H	1	2	-	2/2/22/22	0/1/1/1
2	GLC	H	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

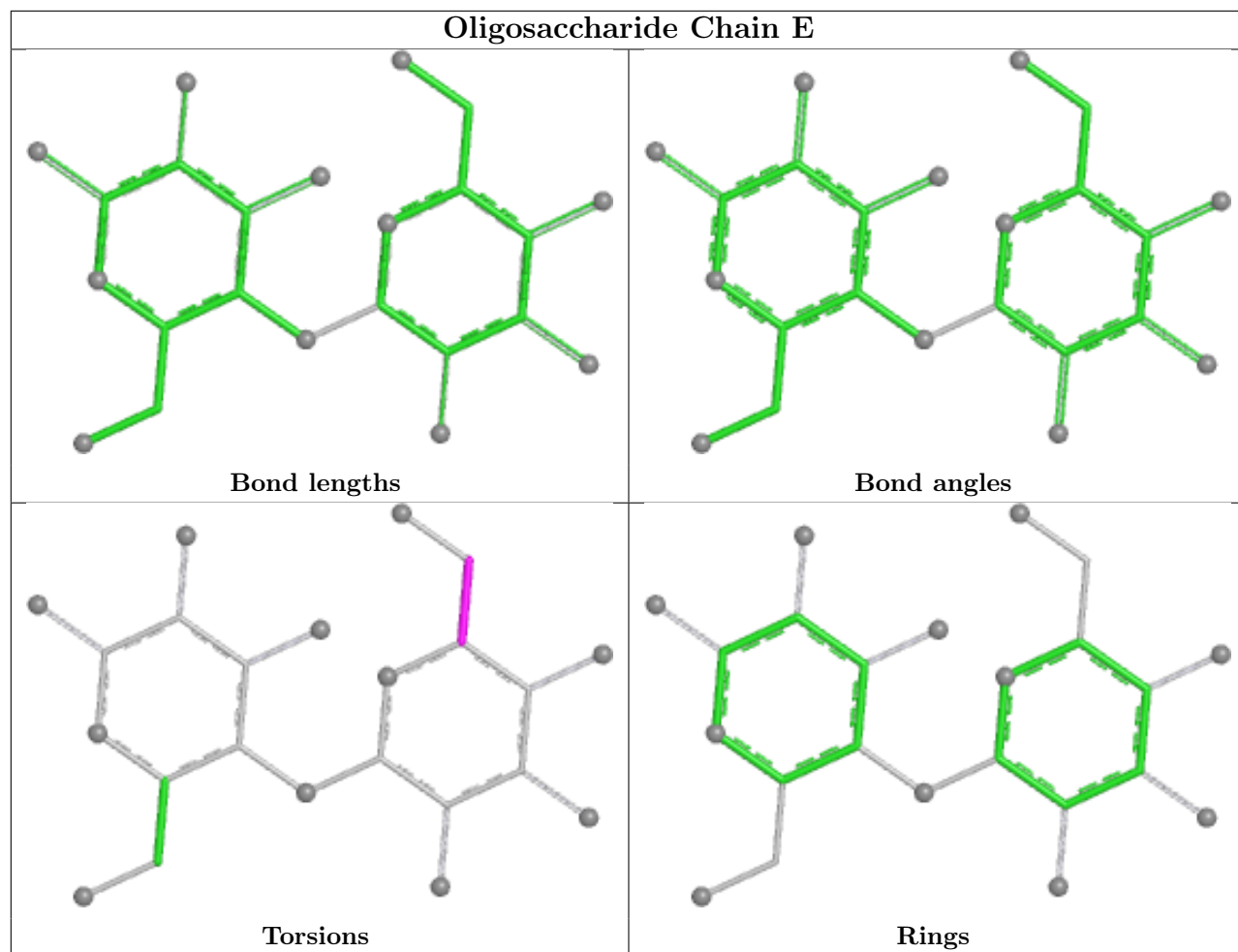
Mol	Chain	Res	Type	Atoms
2	G	1	GLC	O5-C5-C6-O6
2	E	2	GLC	O5-C5-C6-O6
2	G	1	GLC	C4-C5-C6-O6
2	H	1	GLC	C4-C5-C6-O6
2	H	1	GLC	O5-C5-C6-O6
2	E	2	GLC	C4-C5-C6-O6

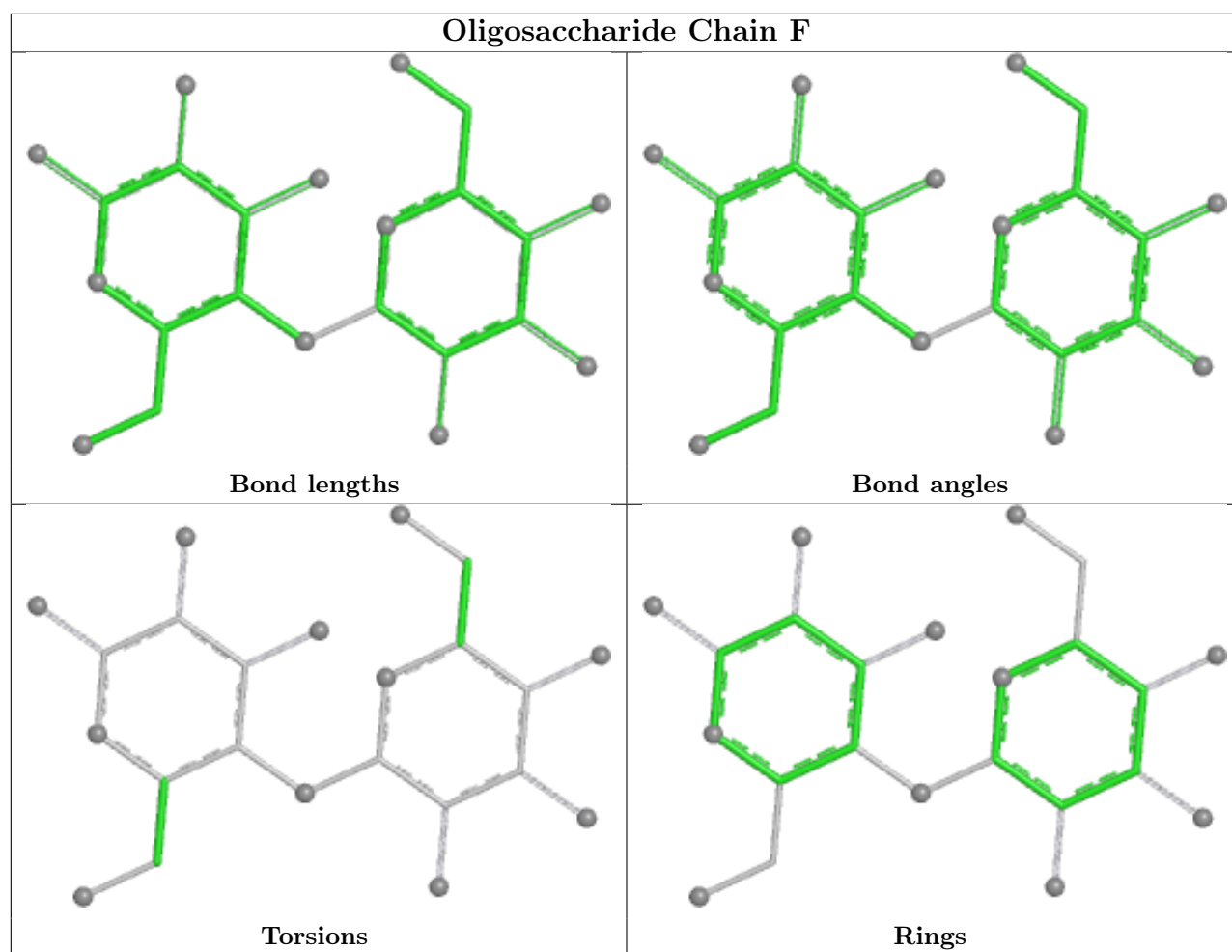
There are no ring outliers.

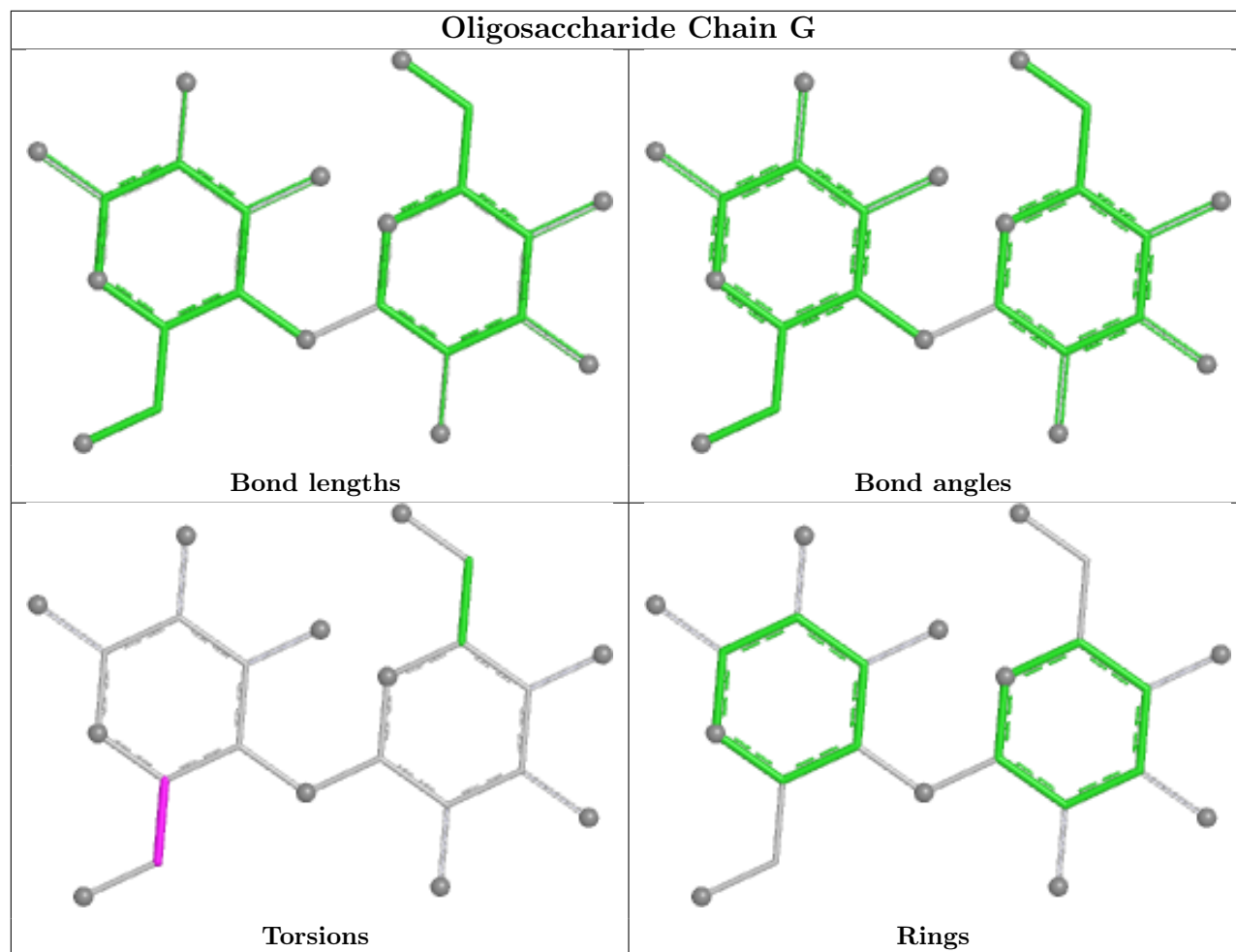
3 monomers are involved in 2 short contacts:

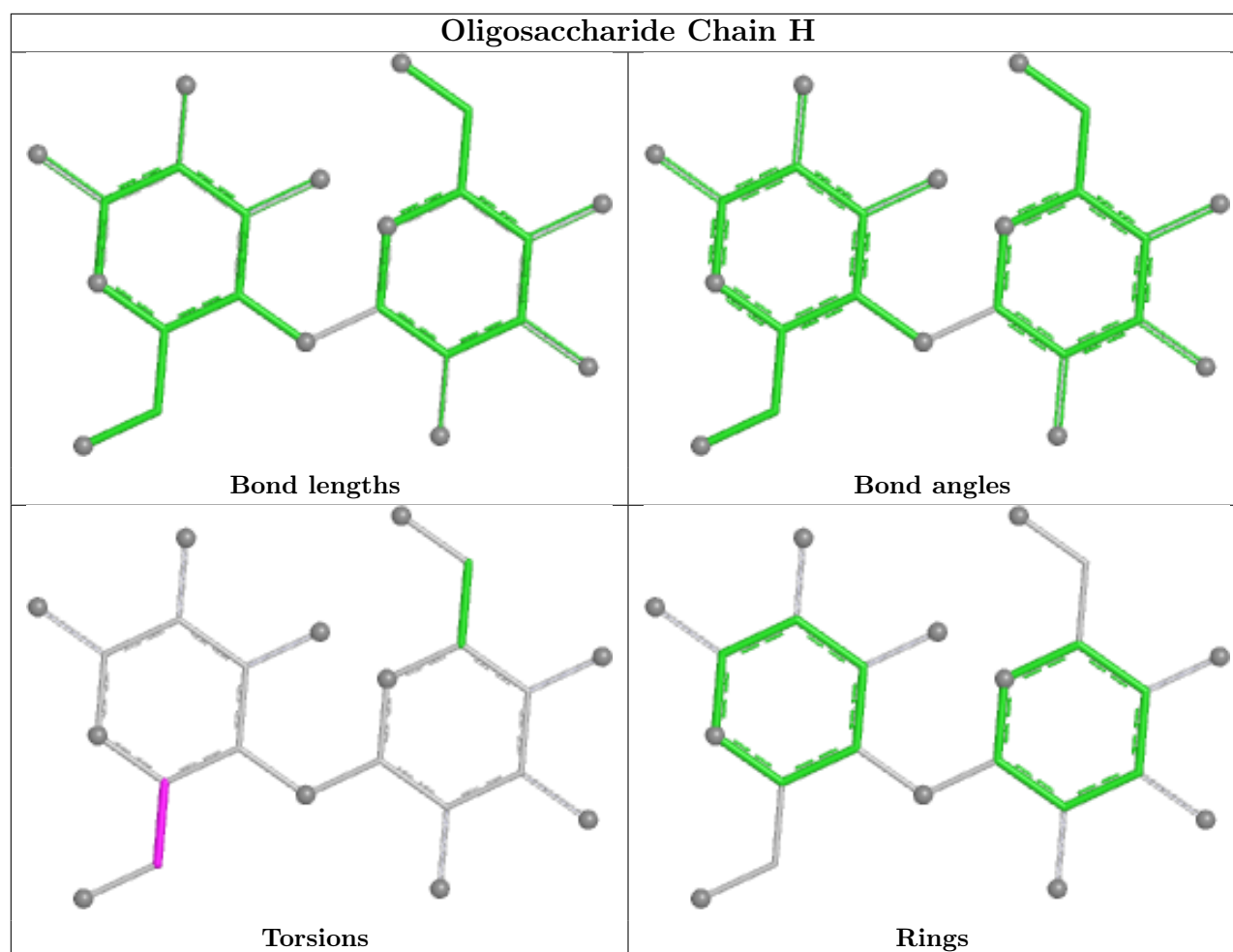
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	GLC	1	0
2	E	2	GLC	1	0
2	H	2	GLC	1	0

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 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	511/537 (95%)	-0.17	3 (0%) 85 73	64, 103, 145, 173	0
1	B	512/537 (95%)	-0.05	9 (1%) 67 48	71, 111, 154, 176	0
1	C	509/537 (94%)	0.03	13 (2%) 57 38	76, 120, 175, 223	0
1	D	509/537 (94%)	-0.03	10 (1%) 65 46	82, 141, 181, 218	0
All	All	2041/2148 (95%)	-0.05	35 (1%) 69 50	64, 117, 171, 223	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	267	ILE	3.9
1	B	170	PHE	3.8
1	B	107	TYR	3.6
1	C	110	ALA	3.0
1	D	80	ILE	3.0
1	C	158	THR	2.9
1	C	378	GLY	2.8
1	B	105	ILE	2.8
1	C	457	TYR	2.8
1	C	368	ASN	2.7
1	D	62	PHE	2.7
1	C	170	PHE	2.7
1	D	474	LEU	2.6
1	D	286	LEU	2.5
1	C	425	PHE	2.4
1	D	178	ASP	2.4
1	A	168	TYR	2.3
1	D	227	ILE	2.3
1	D	430	ILE	2.3
1	B	77	LEU	2.3
1	C	111	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	270	ALA	2.3
1	B	158	THR	2.3
1	C	356	GLN	2.3
1	B	374	LEU	2.3
1	C	482	ILE	2.3
1	C	193	LEU	2.3
1	D	390	LEU	2.3
1	B	368	ASN	2.3
1	D	162	ILE	2.1
1	D	410	TYR	2.1
1	A	169	ALA	2.1
1	A	373	ASN	2.1
1	B	10	ILE	2.0
1	C	157	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

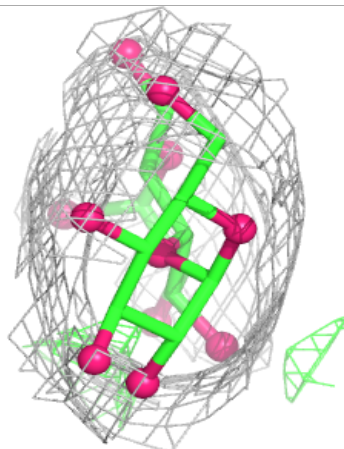
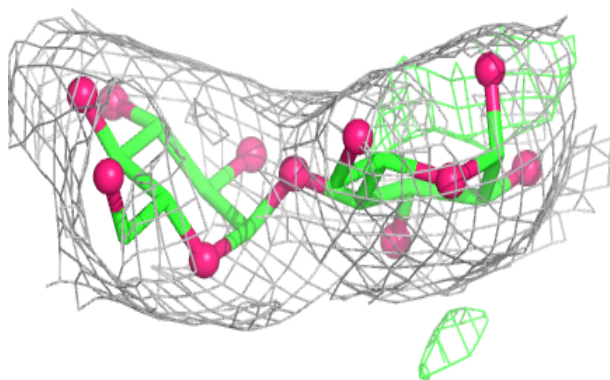
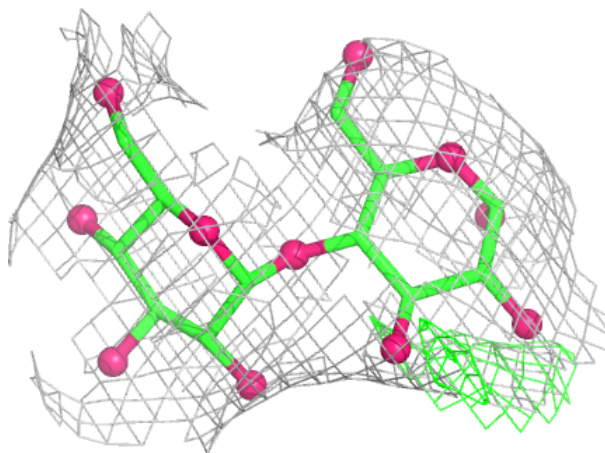
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	H	1	12/12	0.85	0.10	98,116,123,126	0
2	GLC	F	2	11/12	0.87	0.09	84,96,108,109	0
2	GLC	F	1	12/12	0.87	0.10	101,104,110,111	0
2	GLC	H	2	11/12	0.88	0.08	115,120,129,129	0
2	GLC	E	1	12/12	0.92	0.09	63,70,75,80	0
2	GLC	G	1	12/12	0.92	0.10	91,101,107,113	0
2	GLC	E	2	11/12	0.93	0.07	69,74,76,76	0
2	GLC	G	2	11/12	0.95	0.05	98,102,107,115	0

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

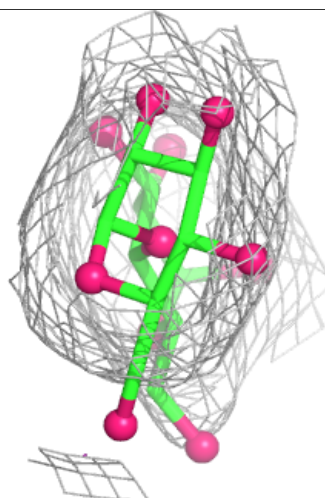
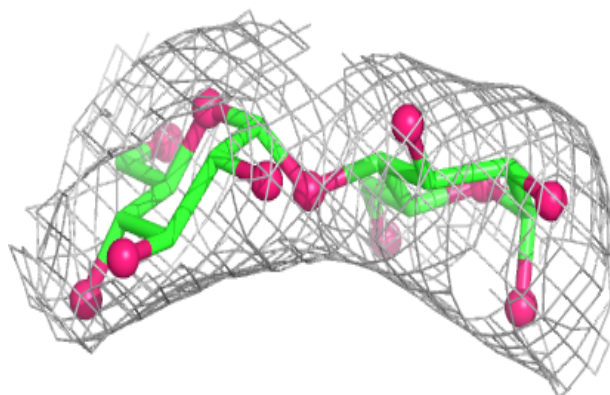
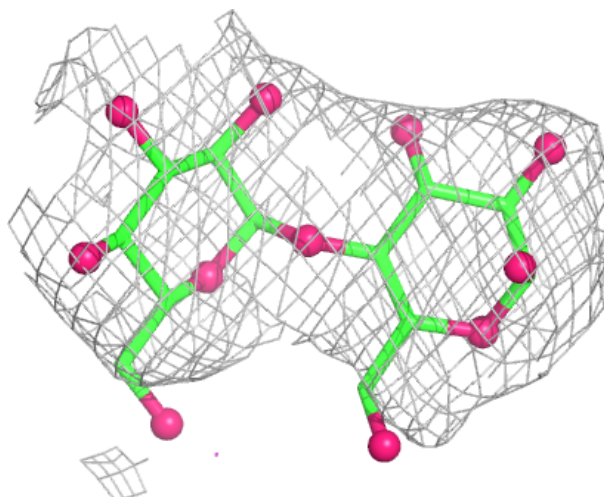
Electron density around Chain E:

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



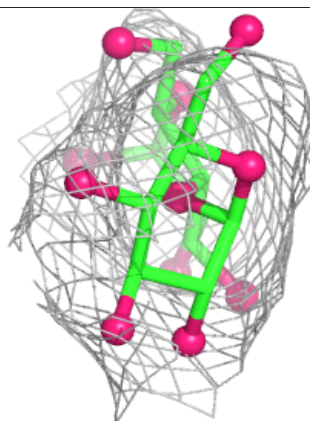
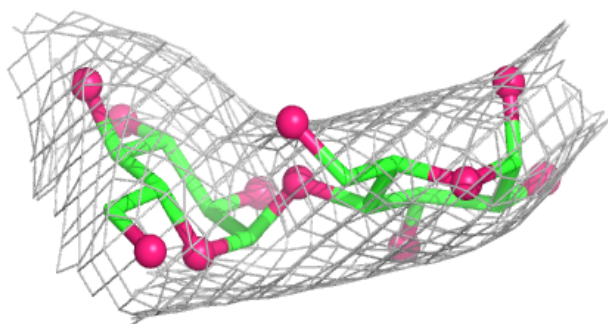
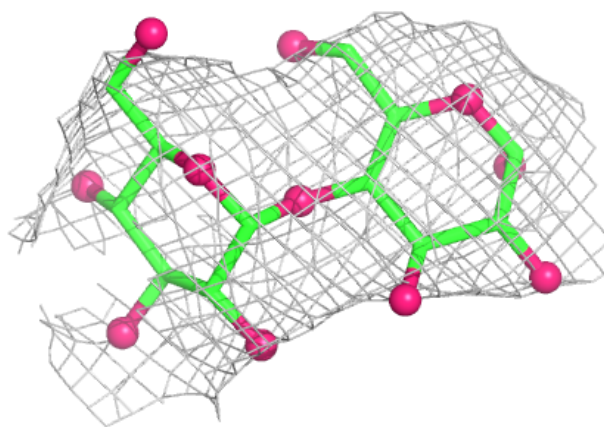
Electron density around Chain F:

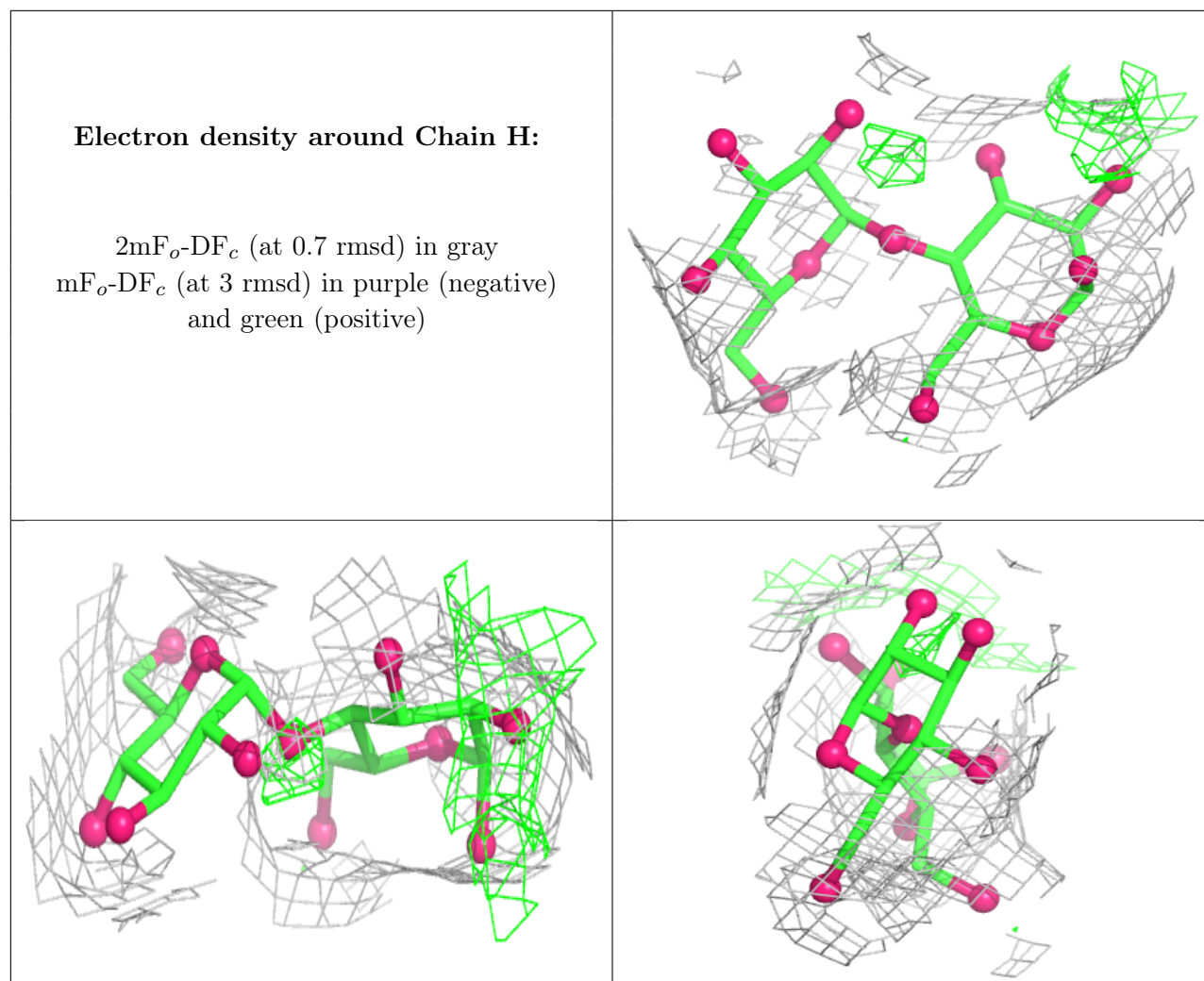
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

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





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
3	ZN	C	601	1/1	0.89	0.08	220,220,220,220	0
3	ZN	D	601	1/1	0.90	0.06	218,218,218,218	0
3	ZN	A	601	1/1	0.91	0.07	141,141,141,141	0
3	ZN	B	601	1/1	0.97	0.04	127,127,127,127	0
3	ZN	C	600	1/1	1.00	0.01	80,80,80,80	0
3	ZN	B	600	1/1	1.00	0.05	74,74,74,74	0
3	ZN	D	600	1/1	1.00	0.03	80,80,80,80	0
3	ZN	A	600	1/1	1.00	0.04	73,73,73,73	0

6.5 Other polymers ⓘ

There are no such residues in this entry.