



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 09:30 AM BST

PDB ID : 5XBZ  
Title : Crystal structure of GH family 81 beta-1,3-glucanase from *Rhizomucor miehei* complexed with laminaripentaose  
Authors : Yang, S.; Qin, Z.; Zhou, P.; Yan, Q.; Jiang, Z.  
Deposited on : 2017-03-21  
Resolution : 2.70 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

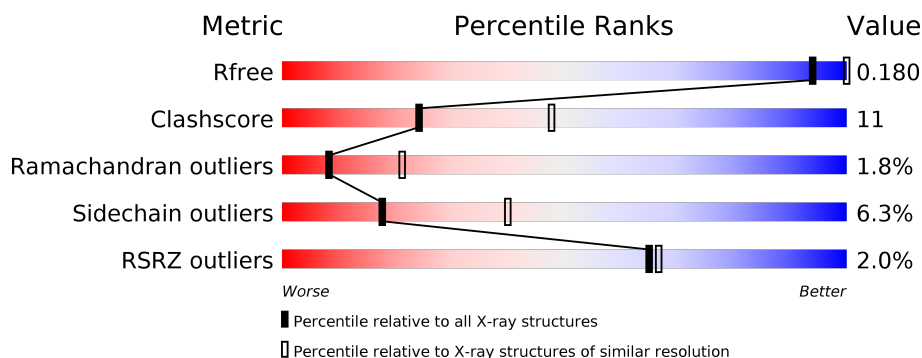
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



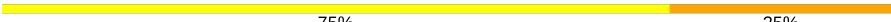

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	A	796	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	796	<div> <div>3%</div> <div> <div></div> <div>59%</div> <div>26%</div> <div>•</div> <div>11%</div> </div> </div>
2	C	5	<div> <div></div> <div>40%</div> <div>60%</div> </div>
2	F	5	<div> <div></div> <div>80%</div> <div>20%</div> </div>
2	G	5	<div> <div></div> <div>100%</div> </div>
3	D	4	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	4	 75%25%
4	E	3	 33%67%

## 2 Entry composition [i](#)

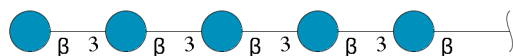
There are 5 unique types of molecules in this entry. The entry contains 11705 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Endo-beta-1,3-glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	710	Total	C	N	O	S	0	1	0
			5614	3594	934	1073	13			
1	B	705	Total	C	N	O	S	0	2	0
			5568	3567	929	1059	13			

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose.



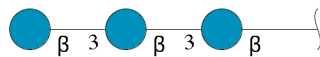
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	5	Total	C	O	0	0	0
			56	30	26			
2	F	5	Total	C	O	0	0	0
			56	30	26			
2	G	5	Total	C	O	0	0	0
			56	30	26			

- Molecule 3 is an oligosaccharide called beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	4	Total	C	O	0	0	0
			45	24	21			
3	H	4	Total	C	O	0	0	0
			45	24	21			

- Molecule 4 is an oligosaccharide called beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose.




Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	E	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 5 is water.

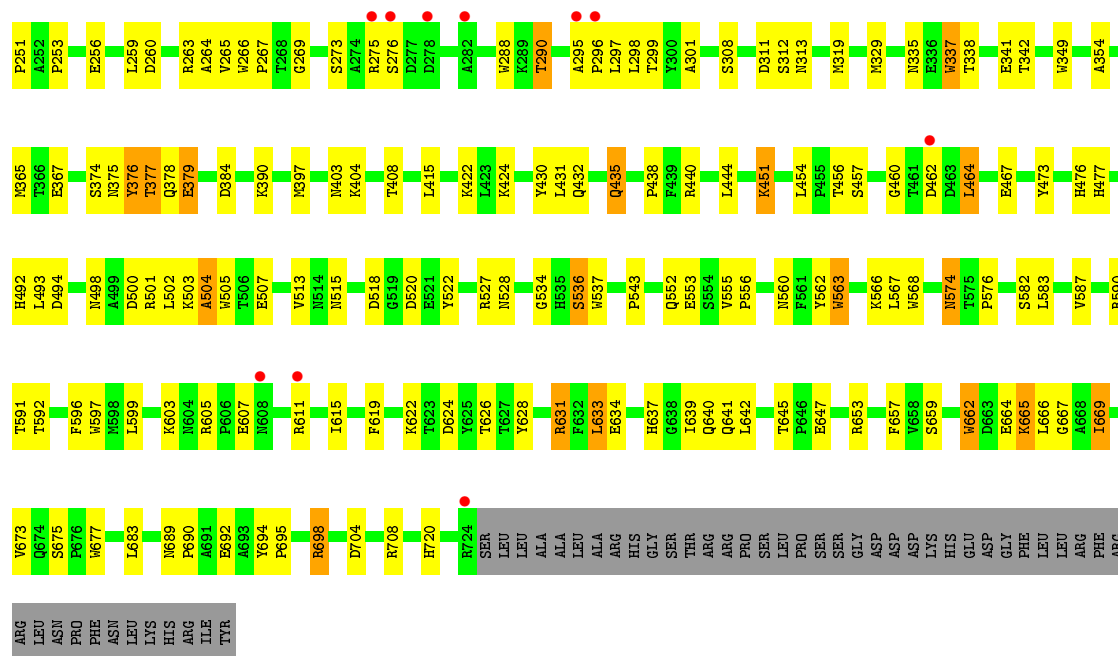
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	142	Total	O	0	0
			142	142		
5	B	89	Total	O	0	0
			89	89		

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.

- Chain A: 

Residue Type	Count	Percentage
Met	1	0.1%
Arg	1	0.1%
Phe	1	0.1%
Gln	1	0.1%
Val	1	0.1%
Ile	1	0.1%
Val	1	0.1%
Ala	1	0.1%
Ala	1	0.1%
Ala	1	0.1%
Thr	1	0.1%
Ile	1	0.1%
Thr	1	0.1%
Met	1	0.1%
Met	1	0.1%
Ile	1	0.1%
Thr	1	0.1%
Ser	1	0.1%
Tyr	1	0.1%
Ile	1	0.1%
Pro	1	0.1%
Gly	1	0.1%
Val	1	0.1%
Ala	1	0.1%
Gln	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Asp	1	0.1%
Gly	1	0.1%
Ala	1	0.1%
Val	1	0.1%
Gln	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Asp	1	0.1%
Gly	1	0.1%
Ala	1	0.1%
Gln	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Asp	1	0.1%
Gly	1	0.1%
Ala	1	0.1%
Gln	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Asp	1	0.1%
Gly	1	0.1%
Ala	1	0.1%
Gln	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Asp	1	0.1%
Gly	1	0.1%
Ala	1	0.1%
Gln	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Asp	1	0.1%
Gly	1	0.1%
Ala	1	0.1%
Gln	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Asp	1	0.1%
Gly	1	0.1%
Ala	1	0.1%
Gln	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Asp	1	0.1%
Gly	1	0.1%
Ala	1	0.1%
Gln	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Asp	1	0.1%
Gly	1	0.1%
Ala	1	0.1%
Gln	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Asp	1	0.1%
Gly	1	0.1%
Ala	1	0.1%
Gln	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Asp	1	0.1%
Gly	1	0.1%
Ala	1	0.1%
Gln	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Asp	1	0.1%
Gly	1	0.1%
Ala	1	0.1%
Gln	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Asp	1	0.1%
Gly	1	0.1%
Ala	1	0.1%
Gln	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Asp	1	0.1%
Gly	1	0.1%
Ala	1	0.1%
Gln	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Asp	1	0.1%
Gly	1	0.1%
Ala	1	0.1%
Gln	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Asp	1	0.1%
Gly	1	0.1%
Ala	1	0.1%
Gln	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Asp	1	0.1%
Gly	1	0.1%
Ala	1	0.1%
Gln	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Asp	1	0.1%
Gly	1	0.1%
Ala	1	0.1%
Gln	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Ser	1	0.1%
Asp	1	0.1%

- Chain B:
- 
- | Amino Acid | Category |
|------------|----------|
| MET        | Grey     |
| ARG        | Grey     |
| PHE        | Grey     |
| GLN        | Grey     |
| VAL        | Grey     |
| ILE        | Grey     |
| VAL        | Grey     |
| ALA        | Grey     |
| ALA        | Grey     |
| ALA        | Grey     |
| THR        | Grey     |
| ILE        | Grey     |
| MET        | Grey     |
| THR        | Grey     |
| ILE        | Grey     |
| THR        | Grey     |
| THR        | Grey     |
| THR        | Grey     |
| THR        | Grey     |
| ASP        | Grey     |
| G5         | Red      |
| D6         | Red      |
| F9         | Green    |
| V10        | Green    |
| P11        | Green    |
| V12        | Green    |
| S13        | Yellow   |
| N14        | Yellow   |
| F15        | Yellow   |
| D16        | Yellow   |
| K18        | Yellow   |
| S19        | Yellow   |
| I20        | Yellow   |
| E23        | Yellow   |
| H26        | Yellow   |
| M31        | Yellow   |
| Y32        | Yellow   |
| A33        | Yellow   |
| N34        | Yellow   |
| N37        | Yellow   |
| N44        | Yellow   |
| N49        | Yellow   |
| D64        | Yellow   |
| L80        | Yellow   |
| T81        | Yellow   |
| T82        | Yellow   |
| R83        | Yellow   |
| Q84        | Yellow   |
| L93        | Yellow   |
| P94        | Yellow   |
| P95        | Yellow   |
| THR        | Grey     |
| ASN        | Grey     |
| ASP        | Grey     |
| THR        | Grey     |
| VAL        | Grey     |
| THR        | Grey     |
| THR        | Grey     |
| THR        | Grey     |
| T98        | Grey     |
| F198       | Yellow   |
| S199       | Yellow   |
| G200       | Yellow   |
| R201       | Yellow   |
| K204       | Yellow   |
| M207       | Yellow   |
| N208       | Yellow   |
| D209       | Yellow   |
| D210       | Yellow   |
| P211       | Yellow   |
| T212       | Yellow   |
| S213       | Yellow   |
| Y218       | Yellow   |
| S219       | Yellow   |
| L220       | Yellow   |
| G221       | Yellow   |
| D222       | Yellow   |
| K223       | Yellow   |
| P224       | Yellow   |
| L225       | Yellow   |
| E226       | Yellow   |
| L227       | Yellow   |
| K228       | Yellow   |
| K229       | Yellow   |
| Q230       | Yellow   |
| D231       | Yellow   |
| N232       | Yellow   |
| S233       | Yellow   |
| M234       | Yellow   |
| L235       | Yellow   |
| V236       | Yellow   |
| A237       | Yellow   |
| S238       | Yellow   |
| K239       | Yellow   |
| P240       | Yellow   |
| I245       | Yellow   |
| R246       | Yellow   |
| V247       | Yellow   |
| A248       | Yellow   |



- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain C: 40%



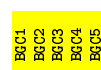
- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain F: 80%



- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain G: 100%

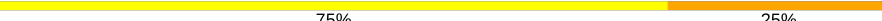


- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain D: 100%



- Molecule 3: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain H:  75% 25%

BGC1  
BGC2  
BGC3  
BGC4

- Molecule 4: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain E:  33% 67%

BGC1  
BGC2  
BGC3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.92Å 96.96Å 127.64Å 90.00° 93.91° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 47.63 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.70) 98.9 (47.63-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.174 , 0.190 0.177 , 0.180	Depositor DCC
$R_{free}$ test set	1765 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.8	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11705	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC

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	0.74	8/5776 (0.1%)	0.81	6/7890 (0.1%)
1	B	0.65	10/5731 (0.2%)	0.75	1/7826 (0.0%)
All	All	0.70	18/11507 (0.2%)	0.78	7/15716 (0.0%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	TRP	CD2-CE2	6.30	1.49	1.41
1	A	266	TRP	CD2-CE2	6.13	1.48	1.41
1	B	505	TRP	CD2-CE2	6.11	1.48	1.41
1	A	563	TRP	CD2-CE2	5.85	1.48	1.41
1	B	349	TRP	CD2-CE2	5.67	1.48	1.41
1	B	537	TRP	CD2-CE2	5.62	1.48	1.41
1	B	337	TRP	CD2-CE2	5.61	1.48	1.41
1	B	288	TRP	CD2-CE2	5.47	1.48	1.41
1	A	497	TRP	CD2-CE2	5.43	1.47	1.41
1	A	337	TRP	CD2-CE2	5.26	1.47	1.41
1	B	563	TRP	CD2-CE2	5.24	1.47	1.41
1	B	677	TRP	CD2-CE2	5.19	1.47	1.41
1	A	677	TRP	CD2-CE2	5.18	1.47	1.41
1	B	662	TRP	CD2-CE2	5.17	1.47	1.41
1	A	46	TRP	CD2-CE2	5.13	1.47	1.41
1	B	266	TRP	CD2-CE2	5.03	1.47	1.41
1	B	134	TRP	CD2-CE2	5.03	1.47	1.41
1	A	597	TRP	CD2-CE2	5.02	1.47	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	599	LEU	CA-CB-CG	7.08	131.59	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	A	464	LEU	CA-CB-CG	5.70	128.41	115.30
1	B	176	LEU	CA-CB-CG	5.63	128.26	115.30
1	A	16	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	698	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	A	298	LEU	CA-CB-CG	5.16	127.17	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	5614	0	5399	97	0
1	B	5568	0	5348	148	0
2	C	56	0	48	3	0
2	F	56	0	48	1	0
2	G	56	0	48	1	0
3	D	45	0	39	0	0
3	H	45	0	39	1	0
4	E	34	0	30	0	0
5	A	142	0	0	12	0
5	B	89	0	0	6	0
All	All	11705	0	10999	246	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 11.

All (246) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:ASN:OD1	1:B:576:PRO:HD2	1.25	1.26
1:B:698:ARG:HG2	1:B:698:ARG:HH21	1.15	1.04
1:A:101:TYR:CZ	5:A:901:HOH:O	2.16	0.94
1:B:430:TYR:CD1	1:B:435:GLN:HG2	2.03	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:LYS:O	1:B:507:GLU:HG3	1.69	0.92
1:A:689:ASN:HD21	1:A:692:GLU:HG3	1.32	0.92
1:A:689:ASN:ND2	1:A:692:GLU:HG3	1.85	0.91
1:B:93:TYR:HB3	1:B:94:PRO:HD2	1.54	0.88
1:A:718:ARG:HD3	5:A:918:HOH:O	1.73	0.88
1:B:93:TYR:OH	1:B:624:ASP:OD1	1.91	0.88
1:B:229:LYS:HG3	1:B:229:LYS:O	1.75	0.85
1:A:92:SER:HB3	1:A:103:ASP:O	1.77	0.84
1:B:634:GLU:HG3	1:B:669:ILE:HD11	1.59	0.83
1:B:251:PRO:HG2	1:B:319:MET:HG3	1.62	0.81
1:B:592:THR:HA	1:B:596:PHE:HD2	1.48	0.79
1:B:689:ASN:OD1	1:B:692:GLU:HG2	1.83	0.79
1:B:182:ILE:O	1:B:183:SER:HB3	1.85	0.76
1:B:424:LYS:NZ	1:B:494:ASP:OD2	2.14	0.76
1:B:574:ASN:OD1	1:B:576:PRO:CD	2.22	0.75
1:A:311:ASP:CG	1:A:316:ARG:HH21	1.90	0.74
1:B:698:ARG:CG	1:B:698:ARG:HH21	1.96	0.74
2:G:3:BGC:H3	3:H:3:BGC:H2	1.70	0.74
1:B:227:LEU:HD12	1:B:235:LEU:HD13	1.70	0.73
1:B:208:ASN:ND2	5:B:902:HOH:O	2.21	0.72
1:A:698:ARG:HH21	1:A:698:ARG:HG2	1.54	0.71
1:B:26:HIS:HB3	1:B:444:LEU:HD23	1.72	0.70
1:B:220:LEU:HD11	1:B:246:ARG:HD3	1.74	0.69
1:B:18:LYS:HD3	1:B:23:GLU:OE1	1.92	0.69
1:B:633:LEU:HD12	1:B:669:ILE:HG21	1.75	0.68
1:A:615:ILE:HD11	1:A:623:THR:HG21	1.76	0.68
1:A:617:ILE:HG22	1:A:619:PHE:CE2	2.30	0.67
1:B:374:SER:O	1:B:422:LYS:NZ	2.28	0.67
1:B:377:THR:C	1:B:379:GLU:H	1.98	0.67
1:B:20:ILE:HD11	1:B:504:ALA:HB1	1.77	0.66
1:A:93:TYR:OH	1:A:624:ASP:OD1	2.11	0.66
1:B:187:ASP:O	1:B:188:GLU:HB2	1.96	0.66
1:A:28:PHE:CE1	1:A:543:PRO:HB3	2.32	0.65
1:B:454:LEU:O	1:B:460:GLY:HA3	1.97	0.65
1:A:313:ASN:OD1	5:A:902:HOH:O	2.14	0.65
1:B:31:MET:HG2	1:B:32:TYR:CE1	2.32	0.65
1:B:204:LYS:NZ	1:B:256:GLU:OE1	2.30	0.64
1:B:695:PRO:HA	1:B:698:ARG:HD3	1.80	0.63
1:B:515:ASN:HD21	1:B:520:ASP:HB3	1.63	0.63
1:A:390:LYS:HE2	1:A:704:ASP:OD1	1.99	0.63
1:B:698:ARG:NH2	1:B:698:ARG:HG2	1.96	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:PHE:HB2	1:B:622:LYS:O	1.99	0.62
1:B:513:VAL:HG13	1:B:528:ASN:HB2	1.80	0.62
1:B:536[A]:SER:OG	1:B:562:TYR:OH	2.14	0.61
1:A:480:GLN:HG2	1:A:509:LEU:HG	1.82	0.60
1:B:18:LYS:CD	1:B:23:GLU:OE1	2.49	0.60
1:A:390:LYS:NZ	2:C:4:BGC:O6	2.29	0.60
1:B:82:ILE:HD13	1:B:164:ILE:HD13	1.84	0.60
1:B:308:SER:HB3	1:B:590:ARG:CZ	2.32	0.59
1:B:432:GLN:HA	1:B:501:ARG:HH11	1.67	0.59
1:B:108:ILE:HG22	1:B:622:LYS:HB3	1.83	0.59
1:B:81:THR:HG23	1:B:113:VAL:HG13	1.85	0.59
1:B:592:THR:HA	1:B:596:PHE:CD2	2.36	0.57
1:B:184:VAL:HB	1:B:198:PHE:CE1	2.38	0.57
1:B:313:ASN:OD1	5:B:901:HOH:O	2.16	0.57
1:A:74:TYR:HB2	5:A:1013:HOH:O	2.04	0.56
1:B:295:ALA:HB1	1:B:296:PRO:CD	2.36	0.56
1:B:132:THR:OG1	1:B:140:ASN:ND2	2.26	0.56
1:B:198:PHE:CD2	1:B:198:PHE:N	2.74	0.55
1:B:17:PRO:HD2	1:B:522:TYR:CD1	2.42	0.55
1:A:698:ARG:NH2	1:A:698:ARG:HG2	2.21	0.55
1:A:228:ARG:NH1	5:A:907:HOH:O	2.40	0.55
1:A:555:VAL:N	1:A:556:PRO:CD	2.69	0.55
1:A:363:GLU:OE1	1:A:698:ARG:NH2	2.39	0.55
1:A:690:PRO:HG2	1:A:721:PHE:HA	1.89	0.54
1:B:295:ALA:HB1	1:B:296:PRO:HD2	1.89	0.54
1:B:536[B]:SER:HB3	1:B:562:TYR:HH	1.70	0.54
1:B:628:TYR:CD2	2:F:2:BGC:H3	2.42	0.54
1:A:448:ILE:HD13	1:A:509:LEU:HD12	1.88	0.54
1:B:566:LYS:NZ	1:B:647:GLU:OE2	2.28	0.54
1:A:92:SER:CB	1:A:103:ASP:O	2.53	0.54
1:A:690:PRO:HG3	1:A:718:ARG:HB2	1.90	0.54
1:A:277:ASP:OD2	1:A:277:ASP:C	2.46	0.54
1:A:20:ILE:HD11	1:A:504:ALA:HB1	1.90	0.53
1:A:446:LYS:O	1:A:523:PHE:HA	2.08	0.53
1:A:368:ILE:O	1:A:372:ILE:HD12	2.09	0.53
1:A:357:ASN:HD22	1:A:721:PHE:HD2	1.57	0.53
1:A:96:THR:HB	1:A:98:ASP:H	1.74	0.52
1:A:694:TYR:N	1:A:695:PRO:HD2	2.25	0.52
1:B:404:LYS:NZ	1:B:492:HIS:NE2	2.53	0.52
1:B:158:VAL:HG11	1:B:267:PRO:HB2	1.92	0.52
1:A:167:ASN:ND2	5:A:903:HOH:O	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:HIS:HB2	1:A:207:MET:HG3	1.92	0.51
1:B:260:ASP:O	1:B:263:ARG:HG2	2.10	0.51
1:B:263:ARG:HG3	1:B:264:ALA:N	2.24	0.51
1:B:690:PRO:HD3	1:B:720:HIS:NE2	2.24	0.51
1:B:201:ARG:NH1	1:B:222:ASP:O	2.36	0.51
1:A:177:SER:O	1:A:233:SER:HB3	2.11	0.51
1:A:163:TYR:CD1	1:A:248:ALA:HB2	2.46	0.51
1:B:534:GLY:O	1:B:591:THR:HG21	2.10	0.51
1:A:617:ILE:CG2	1:A:619:PHE:CE2	2.94	0.51
1:B:18:LYS:HZ3	1:B:522:TYR:HE1	1.57	0.51
1:B:163:TYR:CD1	1:B:248:ALA:HB2	2.47	0.50
1:A:231:ASP:CG	1:A:232:ASN:H	2.16	0.49
1:B:231:ASP:CG	1:B:232:ASN:N	2.66	0.49
1:A:125:VAL:HG22	1:A:126:VAL:N	2.28	0.49
1:A:172:THR:HG22	1:A:237:ALA:HB3	1.94	0.49
1:A:551:ASP:HA	1:A:618:TYR:O	2.13	0.49
1:B:49:ASN:HB2	5:B:915:HOH:O	2.13	0.49
1:A:197:THR:N	5:A:913:HOH:O	2.46	0.48
1:A:554:SER:OG	1:A:556:PRO:HD2	2.13	0.48
1:A:555:VAL:H	1:A:556:PRO:HD3	1.77	0.48
1:A:182:ILE:O	1:A:183:SER:HB3	2.13	0.48
1:A:420:LEU:O	1:A:424:LYS:HG3	2.14	0.48
1:B:384:ASP:HB2	1:B:467:GLU:OE2	2.13	0.48
1:B:376:TYR:CD1	1:B:422:LYS:HE2	2.49	0.48
1:B:503:LYS:HA	1:B:568:TRP:CZ2	2.48	0.48
1:A:363:GLU:CD	1:A:698:ARG:NH2	2.67	0.48
1:B:341:GLU:HA	5:B:914:HOH:O	2.13	0.48
1:B:377:THR:C	1:B:379:GLU:N	2.65	0.48
1:B:93:TYR:HB3	1:B:94:PRO:CD	2.36	0.48
1:A:555:VAL:N	1:A:556:PRO:HD3	2.29	0.48
1:A:720:HIS:ND1	1:A:720:HIS:N	2.61	0.48
1:B:64:ASP:HB3	1:B:329:MET:SD	2.53	0.47
1:B:367:GLU:OE1	1:B:708:ARG:HD2	2.14	0.47
1:A:339:LEU:N	1:A:339:LEU:HD22	2.29	0.47
1:A:431:LEU:HD11	1:A:501:ARG:HG3	1.95	0.47
1:B:231:ASP:C	1:B:233:SER:H	2.18	0.47
1:B:555:VAL:HB	1:B:556:PRO:HD3	1.95	0.47
1:B:251:PRO:CG	1:B:319:MET:HG3	2.39	0.47
1:B:637:HIS:HB3	1:B:666:LEU:HD11	1.96	0.47
1:A:448:ILE:CD1	1:A:509:LEU:HD12	2.45	0.47
1:B:227:LEU:CD1	1:B:235:LEU:HD13	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:PRO:O	1:A:544:ASP:CB	2.63	0.47
1:B:44:ASN:HB2	1:B:527:ARG:O	2.15	0.47
1:B:698:ARG:NH2	1:B:698:ARG:CG	2.65	0.47
1:B:144:SER:HB3	1:B:152:TYR:HB3	1.97	0.46
1:A:612:ASN:HA	1:A:665:LYS:HE2	1.98	0.46
1:B:556:PRO:HB2	1:B:642:LEU:O	2.15	0.46
1:B:597:TRP:HB3	1:B:657:PHE:CZ	2.50	0.46
1:A:177:SER:O	1:A:233:SER:CB	2.63	0.46
1:A:246:ARG:CZ	1:A:266:TRP:HB3	2.46	0.46
1:A:320:THR:HA	1:A:329:MET:O	2.14	0.46
1:B:301:ALA:HB2	1:B:337:TRP:CH2	2.50	0.46
1:A:146:PRO:HB2	5:A:988:HOH:O	2.15	0.46
1:A:30:PRO:HD3	1:A:445:TYR:OH	2.16	0.46
1:A:231:ASP:CG	1:A:232:ASN:N	2.69	0.46
1:A:28:PHE:CZ	1:A:543:PRO:HB3	2.51	0.46
1:A:639:ILE:HD11	5:A:990:HOH:O	2.15	0.46
1:B:187:ASP:O	1:B:188:GLU:CB	2.63	0.46
1:B:20:ILE:HD11	1:B:504:ALA:CB	2.45	0.46
1:A:600:ASP:OD1	1:A:613:LYS:NZ	2.49	0.46
1:A:168:TYR:O	1:A:242:THR:HA	2.16	0.46
1:B:552:GLN:HG3	1:B:553:GLU:N	2.31	0.46
1:B:220:LEU:CD1	1:B:246:ARG:HD3	2.45	0.46
1:A:696:ALA:O	1:A:700:VAL:HG22	2.16	0.45
1:A:77:ASN:OD1	1:A:123:SER:HA	2.17	0.45
1:B:80:LEU:HD23	1:B:155:PHE:CD2	2.50	0.45
1:A:223:LYS:NZ	1:A:239:LYS:NZ	2.64	0.45
1:B:397:MET:CE	1:B:645:THR:HG22	2.46	0.45
1:B:342:THR:N	5:B:914:HOH:O	2.49	0.45
1:B:440:ARG:CZ	1:B:451:LYS:HD3	2.47	0.45
1:B:473:TYR:HA	1:B:476:HIS:NE2	2.30	0.45
1:B:16:ASP:HA	1:B:17:PRO:HD2	1.65	0.45
1:B:210:ASP:HA	1:B:211:PRO:HA	1.74	0.45
1:B:354:ALA:O	1:B:408:THR:HA	2.16	0.45
1:B:390:LYS:HE2	1:B:704:ASP:OD1	2.16	0.45
1:B:639:ILE:HD12	1:B:640:GLN:NE2	2.31	0.45
1:A:171:LEU:O	1:A:173:PRO:HD3	2.16	0.45
1:A:467:GLU:HG3	1:A:467:GLU:O	2.17	0.45
1:B:298:LEU:HD21	1:B:319:MET:HE1	1.99	0.45
1:B:13:SER:OG	1:B:14:ASN:N	2.50	0.44
1:B:238:SER:OG	1:B:239:LYS:N	2.50	0.44
1:B:229:LYS:CG	1:B:229:LYS:O	2.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LYS:HZ3	1:A:239:LYS:HZ3	1.65	0.44
1:A:34:ASN:HD22	1:A:37:ASN:HD22	1.66	0.44
1:B:218:TYR:O	1:B:245:ILE:HA	2.17	0.44
1:B:583:LEU:O	1:B:587:VAL:HG23	2.18	0.44
1:B:694:TYR:HB3	1:B:695:PRO:CD	2.46	0.44
1:A:537:TRP:CE3	1:A:550:ARG:HB2	2.53	0.44
1:B:259:LEU:HA	1:B:259:LEU:HD23	1.75	0.44
1:B:641:GLN:HG2	1:B:653:ARG:CZ	2.48	0.44
1:B:6:ASP:O	1:B:275:ARG:HA	2.17	0.44
1:A:600:ASP:HB2	5:A:916:HOH:O	2.18	0.43
1:A:34:ASN:ND2	1:A:37:ASN:HB3	2.33	0.43
1:A:633:LEU:HD22	1:A:637:HIS:CD2	2.53	0.43
1:B:18:LYS:NZ	1:B:522:TYR:HE1	2.15	0.43
1:A:223:LYS:HZ3	1:A:239:LYS:NZ	2.16	0.43
1:B:120:SER:C	1:B:122:TRP:H	2.21	0.43
1:B:451:LYS:HB3	1:B:451:LYS:HE3	1.69	0.43
1:A:261:ALA:HB3	5:A:938:HOH:O	2.19	0.43
1:B:180:ALA:N	1:B:208:ASN:OD1	2.41	0.43
1:B:230:GLN:HB2	1:B:236:VAL:HG23	2.00	0.43
1:A:311:ASP:OD1	1:A:316:ARG:NH2	2.44	0.43
1:A:474:SER:HB3	2:C:2:BGC:H6C1	2.01	0.43
1:A:550:ARG:O	1:A:619:PHE:HA	2.19	0.43
1:B:432:GLN:CA	1:B:501:ARG:HH11	2.31	0.43
1:B:9:PHE:CD2	1:B:273:SER:HA	2.53	0.43
1:B:16:ASP:OD1	1:B:18:LYS:HG3	2.18	0.43
1:B:611:ARG:O	1:B:665:LYS:HE2	2.19	0.43
1:B:694:TYR:N	1:B:695:PRO:HD2	2.33	0.43
1:B:265:VAL:HG13	1:B:290:THR:CG2	2.49	0.43
1:A:692:GLU:O	1:A:695:PRO:HG2	2.19	0.43
1:B:560:ASN:HB3	5:B:939:HOH:O	2.18	0.43
1:B:174:GLN:HB2	1:B:236:VAL:HG13	2.00	0.43
1:A:42:PRO:HA	5:A:1034:HOH:O	2.19	0.42
1:A:174:GLN:HB2	1:A:174:GLN:HE21	1.67	0.42
1:A:697:LEU:HA	1:A:700:VAL:HG22	2.00	0.42
1:B:605:ARG:HE	1:B:615:ILE:HD13	1.83	0.42
1:A:537:TRP:CE3	1:A:550:ARG:CB	3.02	0.42
1:B:375:ASN:O	1:B:377:THR:N	2.52	0.42
1:B:673:VAL:CG1	1:B:675:SER:OG	2.68	0.42
1:A:258:LEU:HD11	1:A:298:LEU:HD11	2.00	0.42
1:A:464:LEU:HD23	1:A:465:SER:N	2.35	0.42
1:B:5:GLY:HA3	1:B:276:SER:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:PRO:O	1:A:698:ARG:HB2	2.20	0.42
1:B:138:SER:HA	1:B:157:ILE:O	2.20	0.42
1:B:376:TYR:CG	1:B:422:LYS:HE2	2.55	0.42
1:A:386:TYR:CD1	2:C:3:BGC:H6C2	2.54	0.42
1:B:376:TYR:CD2	1:B:422:LYS:HB3	2.55	0.42
1:B:297:LEU:HD23	1:B:335:ASN:HA	2.02	0.42
1:B:662:TRP:CE2	1:B:667:GLY:HA2	2.55	0.42
1:B:431:LEU:HD11	1:B:502:LEU:HA	2.01	0.41
1:B:515:ASN:ND2	1:B:520:ASP:HB3	2.33	0.41
1:A:530:ASP:OD1	1:A:530:ASP:C	2.59	0.41
1:B:377:THR:O	1:B:379:GLU:N	2.51	0.41
1:B:626:THR:OG1	1:B:631:ARG:HG2	2.20	0.41
1:B:464:LEU:HD12	1:B:543:PRO:HG2	2.02	0.41
1:A:89:VAL:HB	1:A:108:ILE:HG13	2.02	0.41
1:A:27:PRO:HG3	1:A:455:PRO:HD3	2.03	0.41
1:B:20:ILE:CD1	1:B:504:ALA:HB1	2.47	0.41
1:B:154:ASP:HB2	1:B:167:ASN:HB3	2.02	0.41
1:B:138:SER:OG	1:B:269:GLY:HA2	2.21	0.41
1:B:80:LEU:CD2	1:B:155:PHE:CD2	3.04	0.41
1:B:555:VAL:N	1:B:556:PRO:CD	2.84	0.41
1:A:575:THR:O	1:A:576:PRO:C	2.59	0.41
1:A:690:PRO:HG3	1:A:718:ARG:CB	2.51	0.41
1:A:314:VAL:HG21	1:A:332:LEU:HD13	2.03	0.41
1:A:428:LEU:HB3	1:A:429:PRO:HD3	2.02	0.41
1:A:646:PRO:HD3	1:A:710:TYR:OH	2.21	0.41
1:B:31:MET:HG2	1:B:32:TYR:CZ	2.55	0.41
1:A:464:LEU:HD12	1:A:543:PRO:HG2	2.03	0.40
1:B:186:ALA:C	1:B:188:GLU:H	2.25	0.40
1:B:231:ASP:CG	1:B:232:ASN:H	2.24	0.40
1:B:438:PRO:HG2	1:B:451:LYS:HE2	2.02	0.40
1:B:563:TRP:CZ2	1:B:567:LEU:HD11	2.57	0.40
1:B:403:ASN:HB2	1:B:493:LEU:HD13	2.02	0.40
1:B:673:VAL:HG12	1:B:675:SER:H	1.85	0.40
1:B:683:LEU:HA	1:B:683:LEU:HD12	1.87	0.40
1:B:556:PRO:HG2	1:B:640:GLN:C	2.42	0.40
1:B:11:PRO:HB2	1:B:13:SER:O	2.21	0.40
1:B:563:TRP:CD1	1:B:647:GLU:HB2	2.57	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	707/796 (89%)	654 (92%)	47 (7%)	6 (1%)	19	43
1	B	701/796 (88%)	611 (87%)	71 (10%)	19 (3%)	5	12
All	All	1408/1592 (88%)	1265 (90%)	118 (8%)	25 (2%)	8	21

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	376	TYR
1	B	498	ASN
1	A	188	GLU
1	A	544	ASP
1	B	182	ILE
1	B	183	SER
1	B	222	ASP
1	B	232	ASN
1	B	378	GLN
1	B	607	GLU
1	B	34	ASN
1	B	37	ASN
1	B	457	SER
1	B	574	ASN
1	A	55	ALA
1	A	147	GLN
1	A	278	ASP
1	B	64	ASP
1	B	187	ASP
1	B	379	GLU
1	B	504	ALA
1	A	64	ASP
1	B	121	GLU
1	B	240	PRO
1	B	253	PRO

### 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	599/685 (87%)	568 (95%)	31 (5%)	23	49
1	B	591/685 (86%)	546 (92%)	45 (8%)	13	30
All	All	1190/1370 (87%)	1114 (94%)	76 (6%)	18	39

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	88	LYS
1	A	92	SER
1	A	96	THR
1	A	150	ASN
1	A	163	TYR
1	A	169	ASN
1	A	207	MET
1	A	222	ASP
1	A	229	LYS
1	A	245	ILE
1	A	277	ASP
1	A	292	SER
1	A	311	ASP
1	A	315	LYS
1	A	342	THR
1	A	353	GLN
1	A	382	LYS
1	A	411	ARG
1	A	414	GLU
1	A	462	ASP
1	A	464	LEU
1	A	477	HIS
1	A	521	GLU
1	A	599	LEU
1	A	633	LEU
1	A	639	ILE

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Mol	Chain	Res	Type
1	A	649	MET
1	A	665	LYS
1	A	674	GLN
1	A	698	ARG
1	B	13	SER
1	B	19	SER
1	B	23	GLU
1	B	31	MET
1	B	84	GLN
1	B	108	ILE
1	B	129	ARG
1	B	163	TYR
1	B	181	ILE
1	B	182	ILE
1	B	198	PHE
1	B	207	MET
1	B	213	SER
1	B	219	SER
1	B	227	LEU
1	B	230	GLN
1	B	239	LYS
1	B	290	THR
1	B	299	THR
1	B	311	ASP
1	B	312	SER
1	B	338	THR
1	B	365	MET
1	B	377	THR
1	B	415	LEU
1	B	435	GLN
1	B	451	LYS
1	B	456	THR
1	B	462	ASP
1	B	464	LEU
1	B	477	HIS
1	B	500	ASP
1	B	518	ASP
1	B	536[A]	SER
1	B	536[B]	SER
1	B	582	SER
1	B	599	LEU
1	B	603	LYS

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Mol	Chain	Res	Type
1	B	631	ARG
1	B	633	LEU
1	B	659	SER
1	B	664	GLU
1	B	665	LYS
1	B	669	ILE
1	B	698	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	169	ASN
1	A	353	GLN
1	A	409	GLN
1	A	689	ASN
1	B	140	ASN
1	B	322	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

26 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	BGC	C	1	2	12,12,12	0.91	0	17,17,17	1.25	3 (17%)
2	BGC	C	2	2	11,11,12	0.51	0	15,15,17	1.49	1 (6%)
2	BGC	C	3	2	11,11,12	0.71	0	15,15,17	3.09	7 (46%)
2	BGC	C	4	2	11,11,12	0.63	0	15,15,17	1.56	3 (20%)
2	BGC	C	5	2	11,11,12	0.66	0	15,15,17	1.85	3 (20%)
3	BGC	D	1	3	12,12,12	0.59	0	17,17,17	1.46	2 (11%)
3	BGC	D	2	3	11,11,12	0.43	0	15,15,17	2.06	3 (20%)
3	BGC	D	3	3	11,11,12	0.41	0	15,15,17	1.30	2 (13%)
3	BGC	D	4	3	11,11,12	0.64	0	15,15,17	2.72	5 (33%)
4	BGC	E	1	4	12,12,12	0.79	0	17,17,17	0.76	0
4	BGC	E	2	4	11,11,12	0.85	1 (9%)	15,15,17	1.77	3 (20%)
4	BGC	E	3	4	11,11,12	0.64	0	15,15,17	1.24	1 (6%)
2	BGC	F	1	2	12,12,12	0.58	0	17,17,17	0.93	1 (5%)
2	BGC	F	2	2	11,11,12	0.44	0	15,15,17	1.16	1 (6%)
2	BGC	F	3	2	11,11,12	0.60	0	15,15,17	3.44	7 (46%)
2	BGC	F	4	2	11,11,12	0.78	0	15,15,17	1.42	2 (13%)
2	BGC	F	5	2	11,11,12	0.75	0	15,15,17	3.03	7 (46%)
2	BGC	G	1	2	12,12,12	0.90	0	17,17,17	1.94	4 (23%)
2	BGC	G	2	2	11,11,12	0.37	0	15,15,17	1.49	3 (20%)
2	BGC	G	3	2	11,11,12	0.38	0	15,15,17	1.00	0
2	BGC	G	4	2	11,11,12	0.33	0	15,15,17	1.42	2 (13%)
2	BGC	G	5	2	11,11,12	0.55	0	15,15,17	1.22	1 (6%)
3	BGC	H	1	3	12,12,12	0.54	0	17,17,17	1.40	3 (17%)
3	BGC	H	2	3	11,11,12	0.60	0	15,15,17	1.28	1 (6%)
3	BGC	H	3	3	11,11,12	0.53	0	15,15,17	1.40	2 (13%)
3	BGC	H	4	3	11,11,12	0.58	0	15,15,17	1.64	3 (20%)

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	BGC	C	1	2	-	2/2/22/22	0/1/1/1
2	BGC	C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	C	3	2	-	2/2/19/22	0/1/1/1
2	BGC	C	4	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	C	5	2	-	2/2/19/22	0/1/1/1
3	BGC	D	1	3	-	0/2/22/22	0/1/1/1
3	BGC	D	2	3	-	0/2/19/22	0/1/1/1
3	BGC	D	3	3	-	0/2/19/22	0/1/1/1
3	BGC	D	4	3	-	1/2/19/22	0/1/1/1
4	BGC	E	1	4	-	0/2/22/22	0/1/1/1
4	BGC	E	2	4	-	0/2/19/22	0/1/1/1
4	BGC	E	3	4	-	0/2/19/22	0/1/1/1
2	BGC	F	1	2	-	2/2/22/22	0/1/1/1
2	BGC	F	2	2	-	1/2/19/22	0/1/1/1
2	BGC	F	3	2	-	2/2/19/22	0/1/1/1
2	BGC	F	4	2	-	0/2/19/22	0/1/1/1
2	BGC	F	5	2	-	2/2/19/22	0/1/1/1
2	BGC	G	1	2	-	1/2/22/22	0/1/1/1
2	BGC	G	2	2	-	0/2/19/22	0/1/1/1
2	BGC	G	3	2	-	0/2/19/22	0/1/1/1
2	BGC	G	4	2	-	0/2/19/22	0/1/1/1
2	BGC	G	5	2	-	0/2/19/22	0/1/1/1
3	BGC	H	1	3	-	2/2/22/22	0/1/1/1
3	BGC	H	2	3	-	0/2/19/22	0/1/1/1
3	BGC	H	3	3	-	2/2/19/22	0/1/1/1
3	BGC	H	4	3	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2	BGC	C2-C3	2.08	1.55	1.52

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	5	BGC	C1-O5-C5	9.24	124.72	112.19
2	F	3	BGC	C1-O5-C5	7.88	122.86	112.19
2	C	3	BGC	C1-C2-C3	7.11	118.41	109.67
3	D	4	BGC	C1-O5-C5	7.08	121.78	112.19
2	F	3	BGC	C1-C2-C3	6.15	117.23	109.67
3	D	2	BGC	C1-O5-C5	6.08	120.44	112.19
2	C	5	BGC	C1-O5-C5	5.90	120.19	112.19
2	F	3	BGC	O5-C1-C2	5.89	119.86	110.77
2	C	3	BGC	O5-C5-C6	5.85	116.38	107.20
4	E	2	BGC	C1-C2-C3	4.86	115.65	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	BGC	O3-C3-C2	-4.65	101.09	109.99
3	D	4	BGC	O5-C1-C2	4.51	117.73	110.77
2	C	2	BGC	C1-O5-C5	4.30	118.02	112.19
2	G	1	BGC	C3-C4-C5	-4.24	102.67	110.24
3	D	4	BGC	C2-C3-C4	-4.17	103.68	110.89
2	G	1	BGC	O5-C1-C2	4.11	117.61	110.28
2	C	3	BGC	C1-O5-C5	3.86	117.43	112.19
2	G	4	BGC	C1-O5-C5	3.61	117.09	112.19
2	G	5	BGC	O5-C5-C6	3.58	112.82	107.20
2	F	5	BGC	O5-C5-C6	3.56	112.78	107.20
4	E	3	BGC	C1-C2-C3	3.49	113.95	109.67
2	G	2	BGC	C1-O5-C5	3.41	116.81	112.19
2	F	4	BGC	C1-O5-C5	3.39	116.79	112.19
2	F	3	BGC	C3-C4-C5	3.36	116.24	110.24
2	F	3	BGC	O5-C5-C6	3.32	112.41	107.20
2	G	1	BGC	C1-C2-C3	3.25	117.05	110.31
2	C	4	BGC	C1-C2-C3	3.17	113.56	109.67
2	F	5	BGC	C3-C4-C5	3.07	115.72	110.24
3	D	2	BGC	C1-C2-C3	3.06	113.42	109.67
3	H	4	BGC	C1-O5-C5	3.04	116.31	112.19
2	G	2	BGC	C1-C2-C3	3.02	113.38	109.67
3	D	1	BGC	O5-C1-C2	-3.02	104.90	110.28
3	D	1	BGC	O4-C4-C5	-3.02	101.81	109.30
2	F	5	BGC	O3-C3-C4	-3.01	103.39	110.35
3	H	3	BGC	C1-O5-C5	2.99	116.24	112.19
3	D	3	BGC	O5-C5-C6	2.96	111.85	107.20
3	H	4	BGC	C3-C4-C5	2.92	115.45	110.24
2	F	3	BGC	C2-C3-C4	2.91	115.92	110.89
3	H	2	BGC	O3-C3-C2	-2.84	104.55	109.99
4	E	2	BGC	O5-C5-C6	2.80	111.60	107.20
3	D	4	BGC	O3-C3-C2	2.77	115.30	109.99
3	D	2	BGC	O3-C3-C2	-2.74	104.75	109.99
3	H	1	BGC	C1-C2-C3	-2.74	104.63	110.31
2	C	1	BGC	C1-C2-C3	-2.73	104.66	110.31
3	D	3	BGC	C1-C2-C3	2.72	113.01	109.67
3	H	3	BGC	C3-C4-C5	2.69	115.04	110.24
2	C	3	BGC	O5-C1-C2	2.69	114.92	110.77
2	F	3	BGC	O2-C2-C3	-2.60	104.94	110.14
2	F	5	BGC	O5-C1-C2	2.56	114.72	110.77
2	G	4	BGC	C1-C2-C3	2.47	112.71	109.67
2	C	5	BGC	O4-C4-C3	-2.45	104.67	110.35
2	C	3	BGC	C3-C4-C5	2.42	114.55	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	BGC	O3-C3-C2	-2.34	105.51	109.99
4	E	2	BGC	C2-C3-C4	2.34	114.94	110.89
2	C	4	BGC	C2-C3-C4	-2.33	106.87	110.89
2	F	5	BGC	O5-C5-C4	2.31	116.45	110.83
3	H	1	BGC	C4-C3-C2	-2.17	107.03	110.82
2	C	4	BGC	O3-C3-C2	2.17	114.15	109.99
2	F	2	BGC	O3-C3-C4	2.17	115.36	110.35
2	C	3	BGC	O2-C2-C1	-2.15	104.75	109.15
2	F	1	BGC	O4-C4-C5	2.14	114.61	109.30
2	F	4	BGC	O3-C3-C2	2.12	114.06	109.99
3	H	4	BGC	C1-C2-C3	2.12	112.27	109.67
2	C	5	BGC	O5-C1-C2	-2.09	107.55	110.77
2	C	1	BGC	O1-C1-O5	2.06	116.56	110.38
2	F	5	BGC	C6-C5-C4	-2.05	108.21	113.00
2	G	1	BGC	O5-C5-C6	2.05	111.52	106.44
3	H	1	BGC	O3-C3-C2	2.04	115.07	110.35
3	D	4	BGC	C3-C4-C5	-2.03	106.61	110.24
2	C	1	BGC	O5-C5-C6	2.03	111.48	106.44

There are no chirality outliers.

All (19) torsion outliers are listed below:

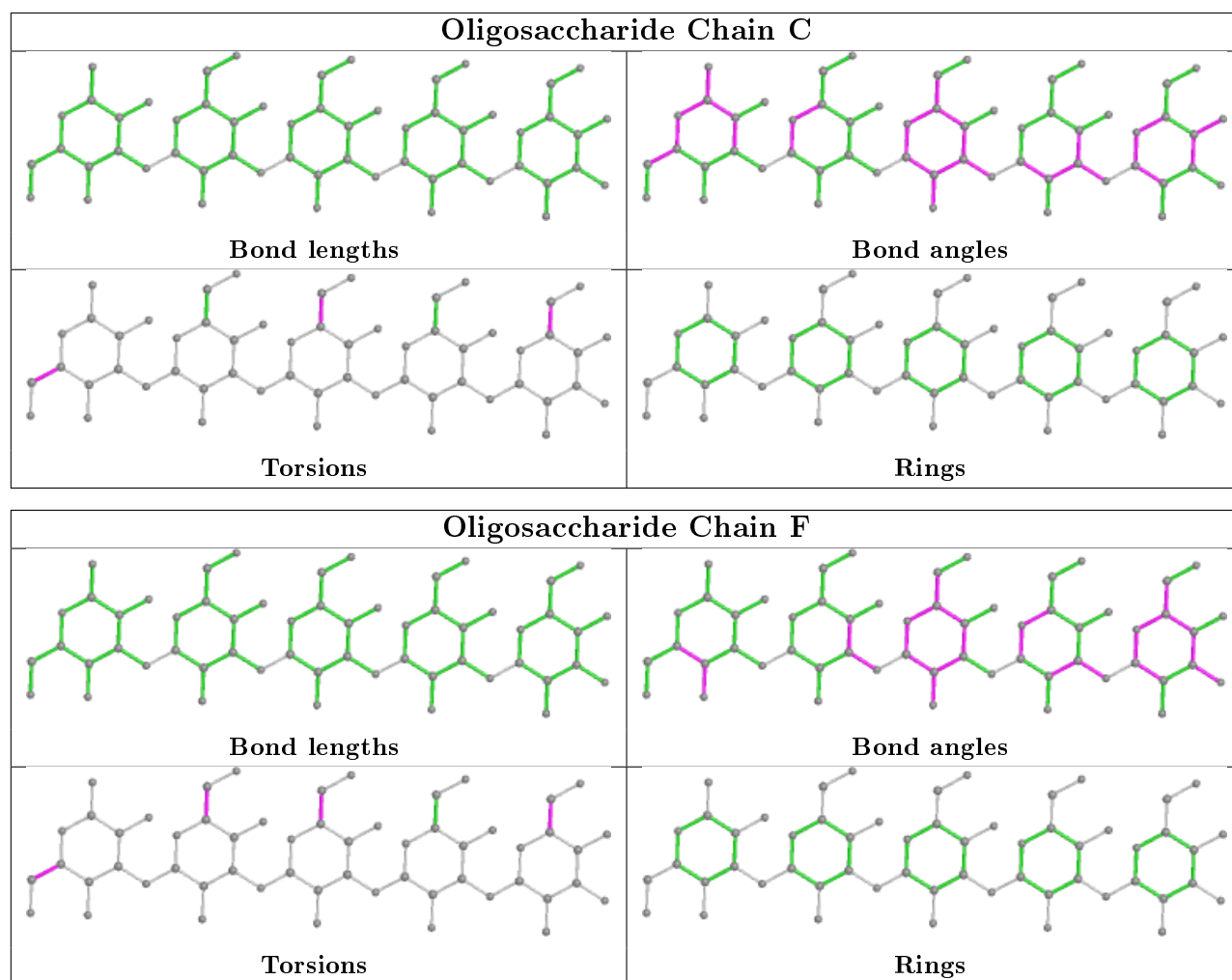
Mol	Chain	Res	Type	Atoms
2	F	3	BGC	O5-C5-C6-O6
2	F	1	BGC	O5-C5-C6-O6
2	F	1	BGC	C4-C5-C6-O6
3	H	1	BGC	C4-C5-C6-O6
2	C	5	BGC	O5-C5-C6-O6
2	F	3	BGC	C4-C5-C6-O6
2	C	1	BGC	O5-C5-C6-O6
2	C	5	BGC	C4-C5-C6-O6
2	C	3	BGC	O5-C5-C6-O6
3	H	1	BGC	O5-C5-C6-O6
3	H	3	BGC	O5-C5-C6-O6
2	F	5	BGC	C4-C5-C6-O6
2	G	1	BGC	O5-C5-C6-O6
2	C	1	BGC	C4-C5-C6-O6
3	H	3	BGC	C4-C5-C6-O6
2	F	2	BGC	O5-C5-C6-O6
2	C	3	BGC	C4-C5-C6-O6
3	D	4	BGC	C4-C5-C6-O6
2	F	5	BGC	O5-C5-C6-O6

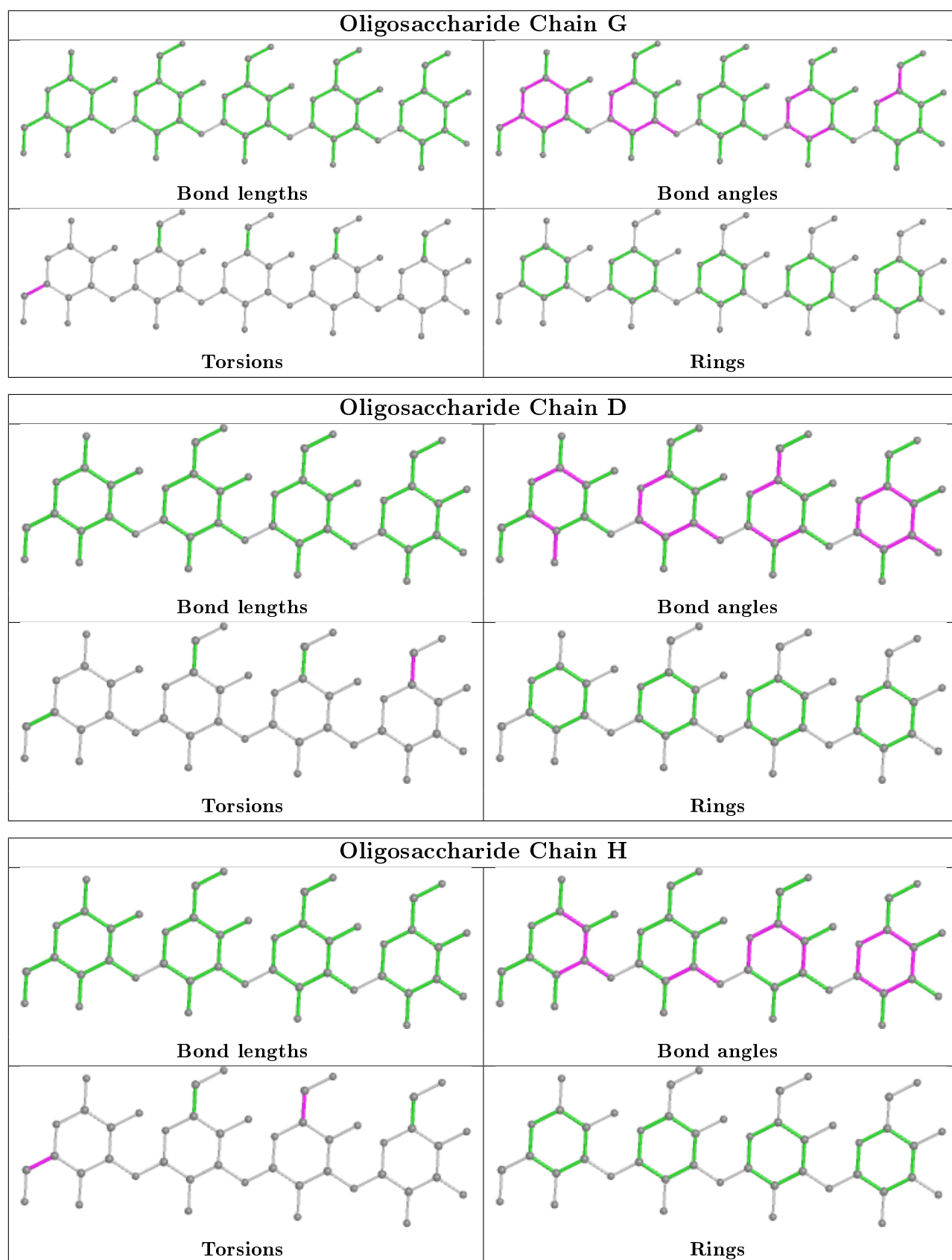
There are no ring outliers.

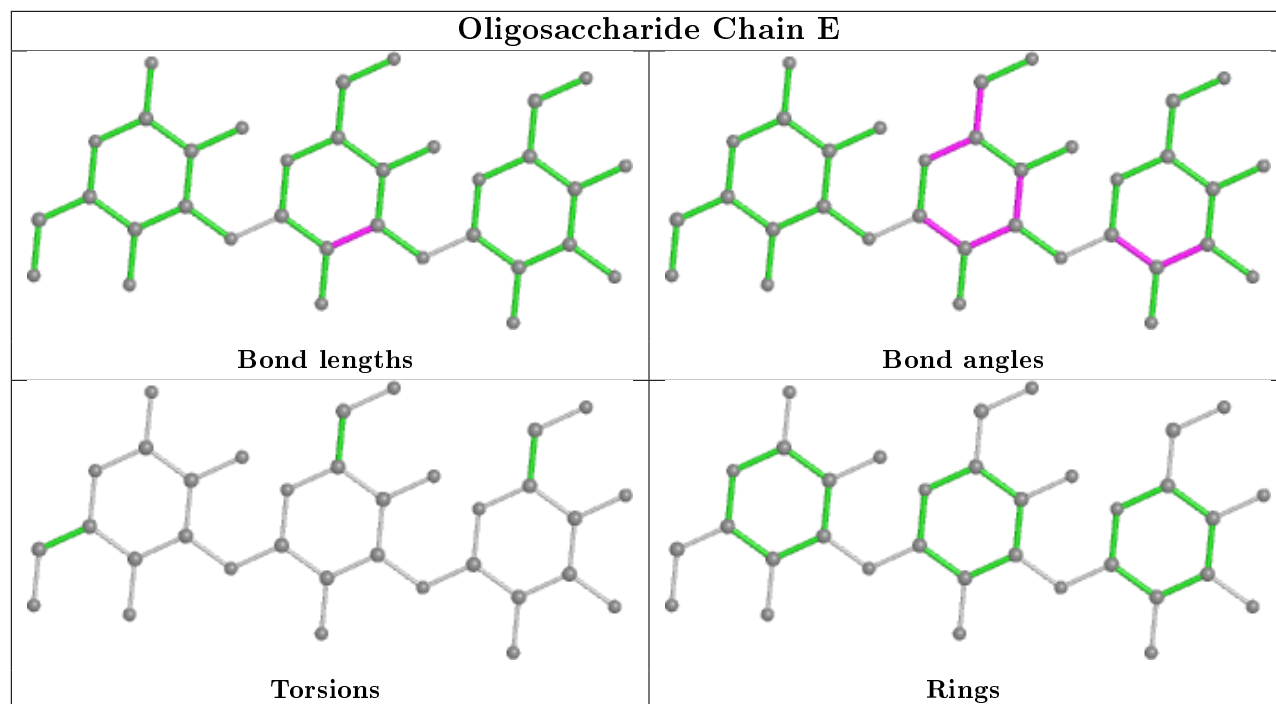
6 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	BGC	1	0
2	G	3	BGC	1	0
2	C	3	BGC	1	0
2	C	2	BGC	1	0
3	H	3	BGC	1	0
2	C	4	BGC	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](#)

There are no ligands in this entry.

## 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	A	710/796 (89%)	-0.63	4 (0%) 89 91	7, 15, 37, 82	0
1	B	705/796 (88%)	-0.02	24 (3%) 45 45	15, 36, 67, 87	0
All	All	1415/1592 (88%)	-0.32	28 (1%) 65 67	7, 25, 58, 87	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	ASP	4.1
1	B	5	GLY	4.0
1	B	724	ARG	4.0
1	A	74	TYR	3.7
1	B	462	ASP	3.5
1	A	5	GLY	3.2
1	B	200	GLY	3.0
1	B	240	PRO	2.9
1	B	275	ARG	2.8
1	B	184	VAL	2.7
1	B	278	ASP	2.6
1	B	102	THR	2.5
1	B	295	ALA	2.3
1	B	93	TYR	2.3
1	B	296	PRO	2.3
1	B	223	LYS	2.3
1	A	75	GLY	2.1
1	B	199	SER	2.1
1	B	276	SER	2.1
1	B	126	VAL	2.1
1	B	225	LEU	2.1
1	B	282	ALA	2.1
1	B	238	SER	2.1
1	B	611	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	608	ASN	2.0
1	B	230	GLN	2.0
1	B	226	GLU	2.0
1	A	147	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

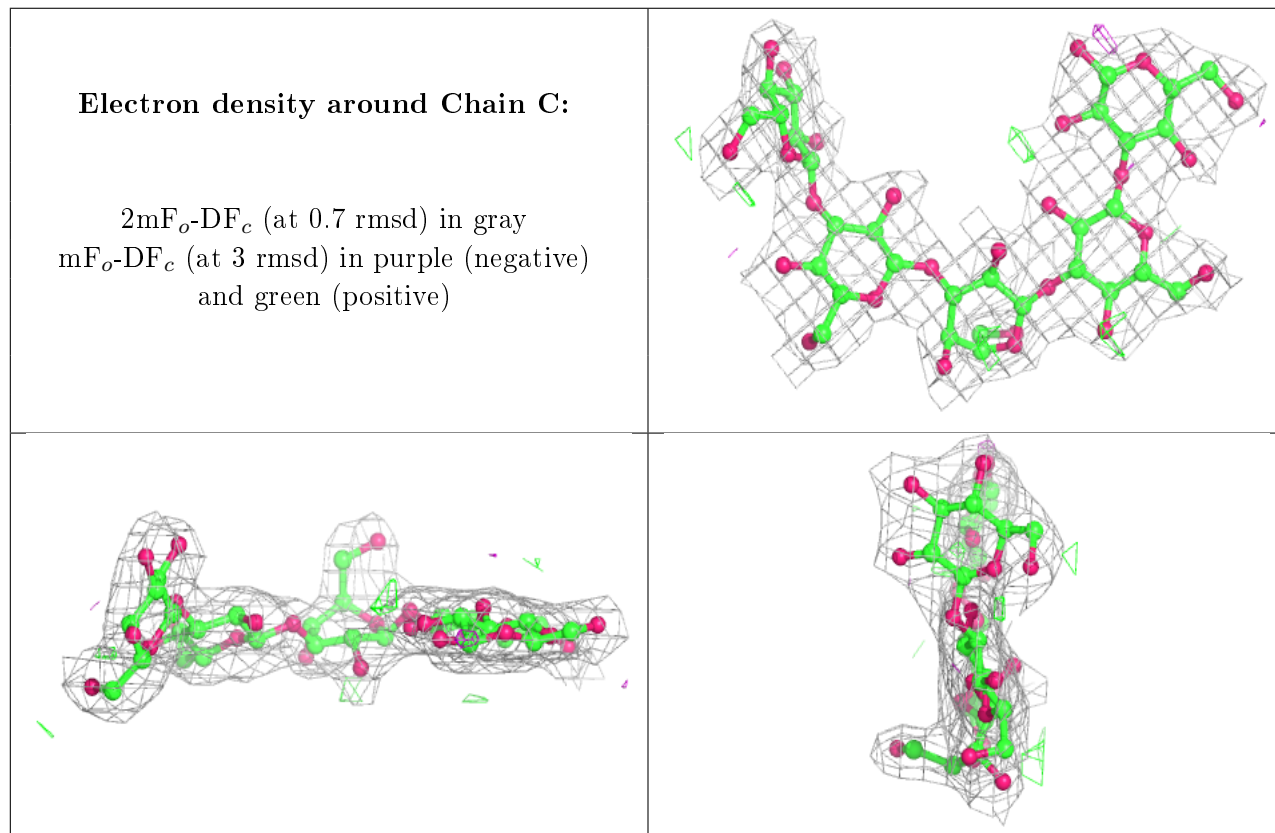
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BGC	G	1	12/12	0.71	0.35	54,62,68,68	0
3	BGC	H	4	11/12	0.76	0.37	78,81,84,84	0
2	BGC	G	5	11/12	0.77	0.35	58,72,77,80	0
3	BGC	H	1	12/12	0.82	0.29	46,59,65,67	0
4	BGC	E	1	12/12	0.83	0.21	37,44,50,51	0
3	BGC	H	3	11/12	0.86	0.23	68,72,75,78	0
3	BGC	D	4	11/12	0.87	0.29	44,47,56,59	0
3	BGC	H	2	11/12	0.88	0.15	44,54,63,66	0
4	BGC	E	3	11/12	0.88	0.18	30,41,45,52	0
2	BGC	F	1	12/12	0.88	0.19	48,54,59,61	0
2	BGC	F	5	11/12	0.89	0.18	35,40,40,46	0
4	BGC	E	2	11/12	0.91	0.17	34,41,42,42	0
2	BGC	C	5	11/12	0.92	0.13	18,19,21,22	0
2	BGC	G	2	11/12	0.92	0.17	48,54,57,58	0
2	BGC	F	4	11/12	0.93	0.13	35,38,39,40	0
3	BGC	D	1	12/12	0.93	0.18	26,29,32,32	0
2	BGC	G	4	11/12	0.93	0.21	53,57,61,63	0
2	BGC	G	3	11/12	0.94	0.15	44,47,49,52	0
2	BGC	C	1	12/12	0.94	0.18	17,23,28,28	0
2	BGC	F	3	11/12	0.94	0.14	35,40,43,44	0
3	BGC	D	3	11/12	0.95	0.17	26,29,33,39	0
2	BGC	F	2	11/12	0.96	0.12	35,44,47,49	0
2	BGC	C	3	11/12	0.97	0.12	13,13,14,14	0
3	BGC	D	2	11/12	0.97	0.14	24,26,28,29	0

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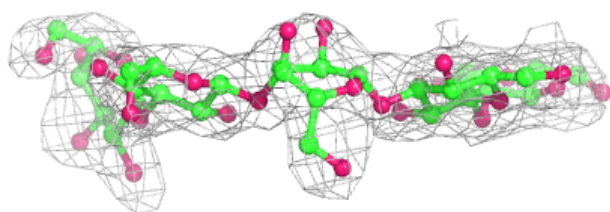
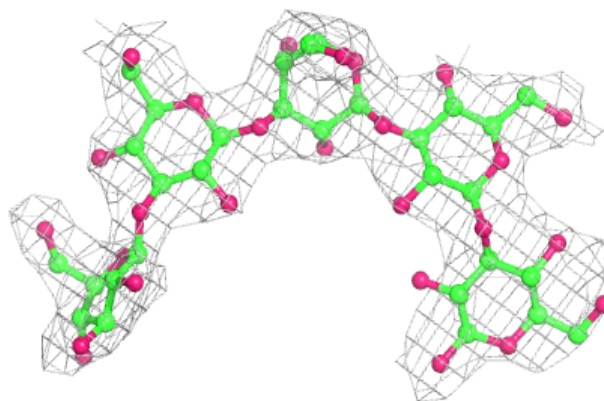
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BGC	C	2	11/12	0.98	0.12	12,13,14,15	0
2	BGC	C	4	11/12	0.99	0.10	11,12,13,15	0

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

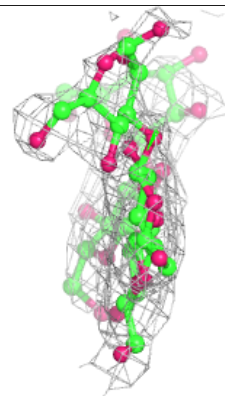
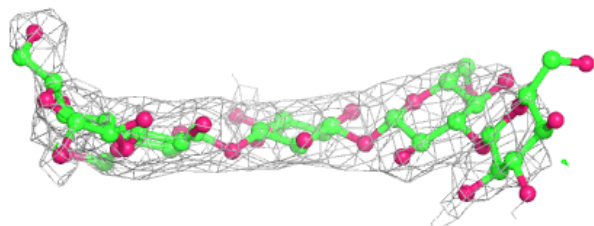
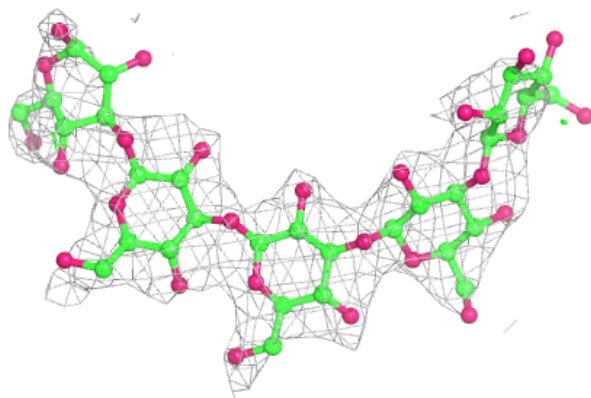


**Electron density around Chain F:**

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

**Electron density around Chain G:**

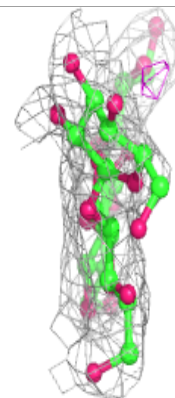
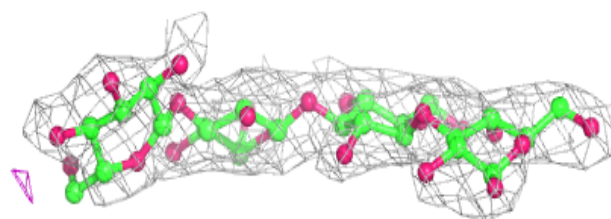
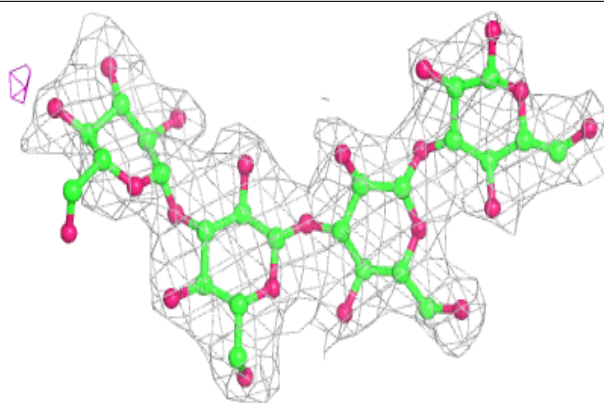
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



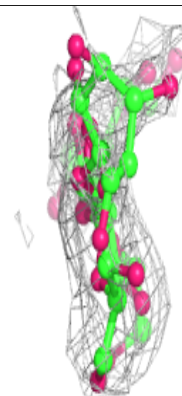
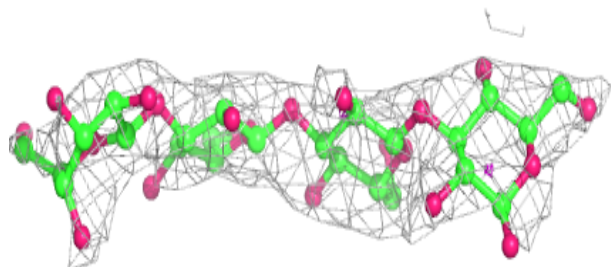
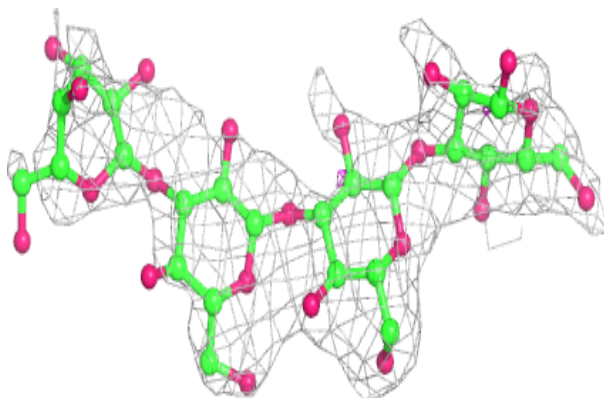


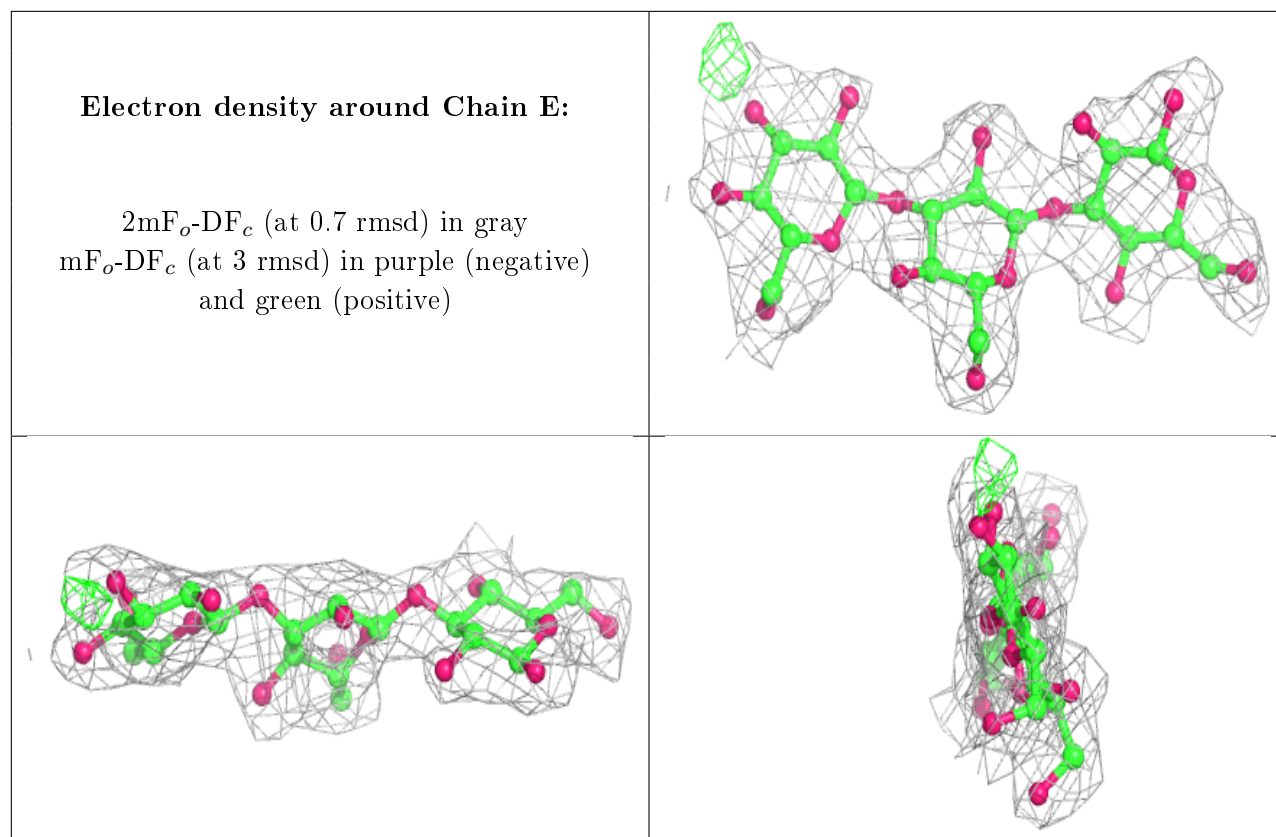
**Electron density around Chain D:**

$2mF_o-DF_c$  (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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.