



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 08:09 PM BST

PDB ID : 1RZG  
Title : Crystal structure of Human anti-HIV-1 GP120 reactive antibody 412d  
Authors : Huang, C.C.; Venturi, M.; Majeed, S.; Moore, M.J.; Phogat, S.; Zhang, M.-Y.; Dimitrov, D.S.; Hendrickson, W.A.; Robinson, J.; Sodroski, J.; Wyatt, R.; Choe, H.; Farzan, M.; Kwong, P.D.  
Deposited on : 2003-12-24  
Resolution : 2.00 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

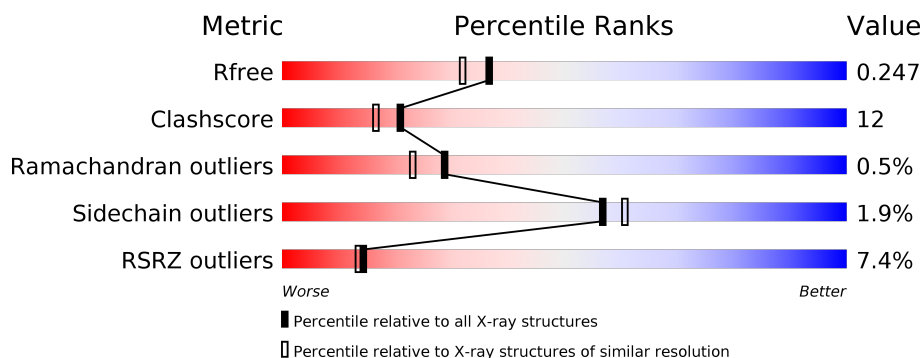
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	231	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div></div> </div> <div></div> </div>
1	C	231	<div> <div>20%</div> <div> <div></div> <div>58%</div> <div>32%</div> <div>7%</div> </div> <div></div> </div>
2	B	214	<div> <div></div> <div> <div></div> <div>81%</div> <div>18%</div> </div> </div>
2	D	214	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>20%</div> </div> <div></div> </div>
3	E	2	<div> <div></div> <div>100%</div> </div>
3	F	2	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	2	 100%
3	H	2	 50% 50%
3	I	2	 50% 50%
3	J	2	 100%
3	K	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	TYS	A	100	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7395 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.

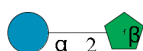
- Molecule 1 is a protein called Fab 412d light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1684	1066	278	332	8			
1	C	214	Total	C	N	O	S	0	0	0
			1617	1029	266	314	8			

- Molecule 2 is a protein called Fab 412d heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1642	1024	278	334	6			
2	D	214	Total	C	N	O	S	0	0	0
			1649	1027	279	336	7			

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



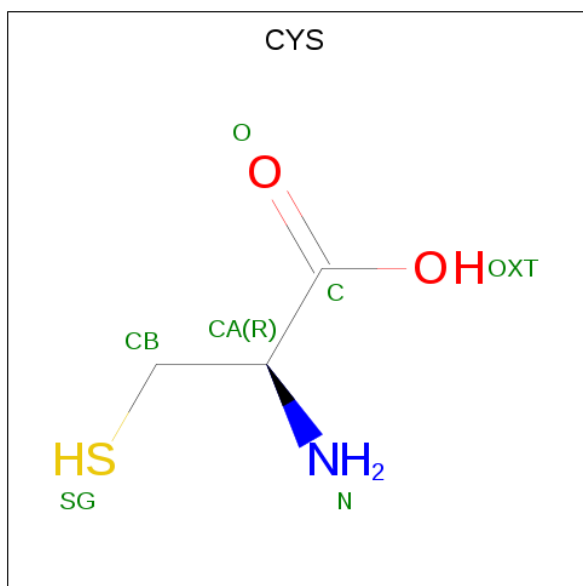
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	E	2	Total	C	O	0	0	0
			23	12	11			
3	F	2	Total	C	O	0	0	0
			23	12	11			
3	G	2	Total	C	O	0	0	0
			23	12	11			
3	H	2	Total	C	O	0	0	0
			23	12	11			
3	I	2	Total	C	O	0	0	0
			23	12	11			
3	J	2	Total	C	O	0	0	0
			23	12	11			

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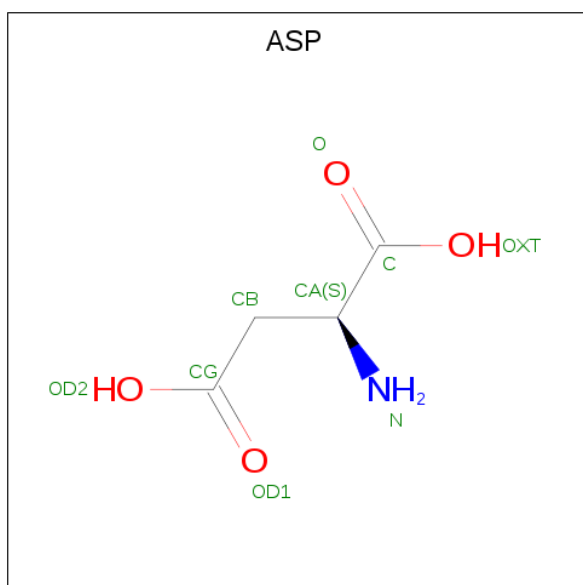
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	K	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is CYSTEINE (three-letter code: CYS) (formula:  $C_3H_7NO_2S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	S	0	0
			6	3	1	1	1		

- Molecule 5 is ASPARTIC ACID (three-letter code: ASP) (formula:  $C_4H_7NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			8	4	1	3		

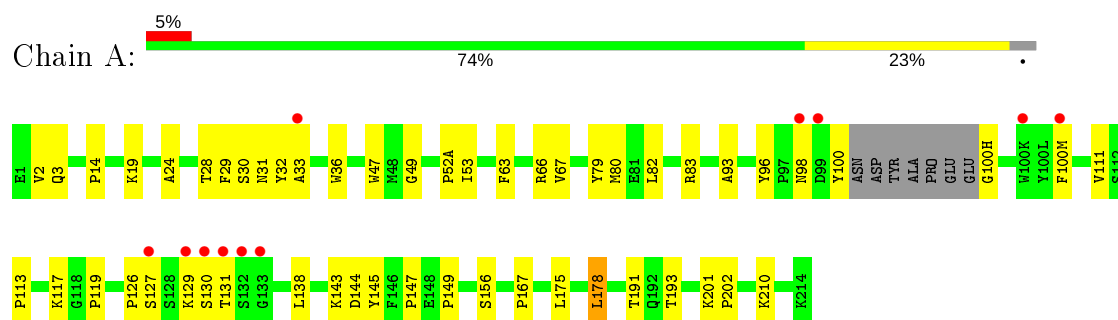
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	176	Total	O	0	0
			176	176		
6	B	193	Total	O	0	0
			193	193		
6	C	103	Total	O	0	0
			103	103		
6	D	156	Total	O	0	0
			156	156		

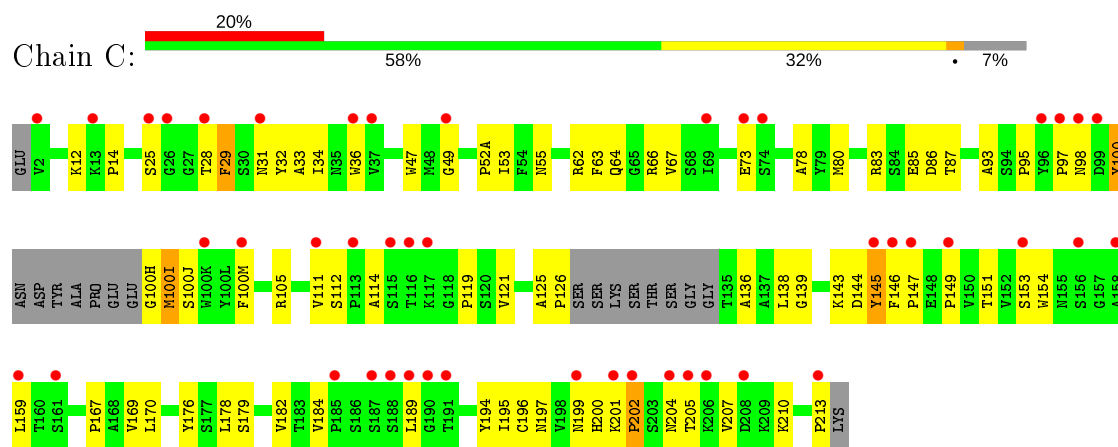
### 3 Residue-property plots [i](#)

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.

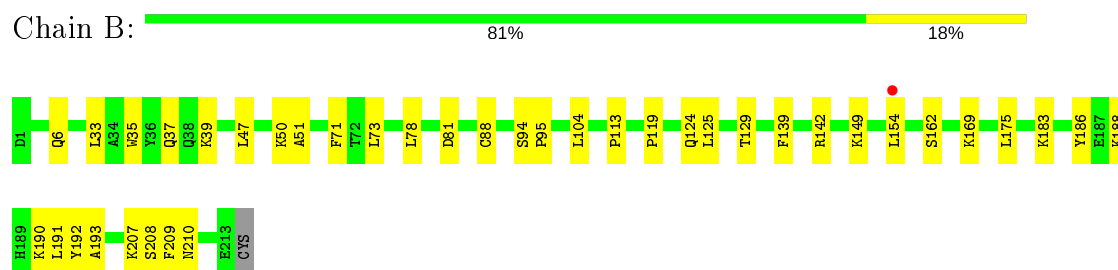
- Molecule 1: Fab 412d light chain



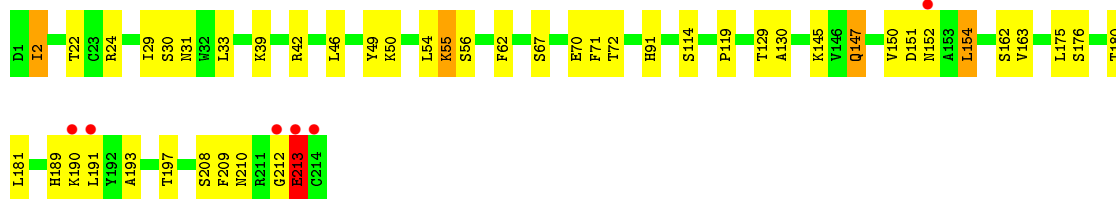
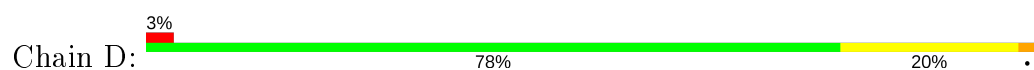
- Molecule 1: Fab 412d light chain



- Molecule 2: Fab 412d heavy chain



- Molecule 2: Fab 412d heavy chain



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



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



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



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



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



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



Chain K:

100%

GLA1  
FRU2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.09 Å   89.31 Å   85.86 Å 90.00°   110.31°   90.00°	Depositor
Resolution (Å)	20.00 – 2.00 29.15 – 1.88	Depositor EDS
% Data completeness (in resolution range)	94.1 (20.00-2.00) 86.2 (29.15-1.88)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.06 (at 1.88 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.201   ,   0.251 0.196   ,   0.247	Depositor DCC
$R_{free}$ test set	6757 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 57.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7395	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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: GLC, FRU, TYS

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	0.34	0/1711	0.67	1/2331 (0.0%)
1	C	0.31	0/1643	0.62	0/2242
2	B	0.33	0/1677	0.65	0/2273
2	D	0.32	0/1684	0.64	1/2281 (0.0%)
All	All	0.33	0/6715	0.65	2/9127 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	ALA	N-CA-C	-5.16	97.06	111.00
2	D	114	SER	N-CA-C	-5.02	97.44	111.00

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	1684	0	1639	47	0
1	C	1617	0	1571	60	0
2	B	1642	0	1596	31	0
2	D	1649	0	1600	34	0
3	E	23	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	23	0	21	0	0
3	G	23	0	21	0	0
3	H	23	0	21	1	0
3	I	23	0	21	2	0
3	J	23	0	21	0	0
3	K	23	0	21	0	0
4	D	6	0	3	1	0
5	D	8	0	4	0	0
6	A	176	0	0	4	0
6	B	193	0	0	2	0
6	C	103	0	0	3	0
6	D	156	0	0	2	0
All	All	7395	0	6560	163	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 12.

All (163) 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:129:LYS:HE2	2:B:208:SER:H	1.16	1.03
1:A:126:PRO:HG3	1:A:138:LEU:HB3	1.41	0.97
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.59	0.84
1:C:126:PRO:HG3	1:C:138:LEU:HB3	1.59	0.84
1:C:195:ILE:HG12	1:C:210:LYS:HG2	1.60	0.83
1:C:119:PRO:HD2	1:C:205:THR:HG21	1.64	0.78
2:D:55:LYS:HA	2:D:55:LYS:HE2	1.66	0.78
2:D:193:ALA:HB2	2:D:208:SER:HB3	1.68	0.75
2:D:147:GLN:HG2	2:D:154:LEU:HD21	1.67	0.74
1:A:127:SER:H	1:A:130:SER:HB3	1.52	0.74
1:C:83:ARG:HB2	1:C:85:GLU:HG2	1.69	0.73
1:A:193:THR:HG23	1:A:210:LYS:HE3	1.70	0.72
2:B:188:LYS:HE3	6:B:394:HOH:O	1.91	0.70
1:A:129:LYS:HE3	2:B:207:LYS:HD3	1.76	0.68
1:A:129:LYS:HE2	2:B:208:SER:N	2.00	0.67
1:C:200:HIS:CD2	1:C:202:PRO:HD2	2.30	0.66
2:B:78:LEU:HD11	2:B:104:LEU:HD21	1.77	0.66
1:C:153:SER:HB3	1:C:197:ASN:HB2	1.76	0.65
1:A:67:VAL:HG22	1:A:82:LEU:HD13	1.79	0.65
2:D:46:LEU:HD23	2:D:55:LYS:HD2	1.78	0.65
1:A:2:VAL:HG11	1:A:96:TYR:OH	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:PRO:HG3	1:C:145:TYR:CB	2.27	0.64
1:A:2:VAL:HG13	1:A:2:VAL:O	1.98	0.64
2:B:193:ALA:HB2	2:B:208:SER:HB3	1.78	0.64
1:A:98:ASN:HB2	6:A:9034:HOH:O	1.99	0.63
2:B:190:LYS:HE3	2:B:191:LEU:HD11	1.84	0.60
1:C:145:TYR:HD2	1:C:145:TYR:H	1.47	0.60
1:C:33:ALA:HB3	1:C:95:PRO:HD2	1.85	0.59
1:C:100:TYS:O1	1:C:100(I):MET:HB2	2.01	0.59
2:B:191:LEU:HG	2:B:210:ASN:OD1	2.03	0.59
1:A:30:SER:HB3	1:A:53:ILE:HD12	1.82	0.59
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.84	0.59
1:C:67:VAL:O	3:I:1:GLC:H2	2.03	0.59
1:A:127:SER:O	1:A:131:THR:HG23	2.03	0.58
1:A:178:LEU:C	1:A:178:LEU:HD12	2.25	0.57
1:C:29:PHE:CD2	1:C:52(A):PRO:HB3	2.40	0.57
1:A:28:THR:OG1	1:A:31:ASN:ND2	2.38	0.56
1:C:119:PRO:HG3	1:C:145:TYR:HB3	1.87	0.56
1:A:100(H):GLY:HA3	3:H:1:GLC:H2	1.87	0.56
1:C:100(J):SER:HB3	2:D:91:HIS:HD2	1.69	0.56
2:B:142:ARG:HH11	2:B:142:ARG:HG2	1.70	0.56
2:D:30:SER:C	2:D:31:ASN:HD22	2.09	0.56
2:D:193:ALA:CB	2:D:208:SER:HB3	2.34	0.56
1:C:200:HIS:HB3	1:C:205:THR:HB	1.88	0.56
1:C:167:PRO:HD2	2:D:162:SER:OG	2.06	0.55
1:A:14:PRO:HG2	1:A:113:PRO:HG3	1.88	0.55
2:D:212:GLY:O	2:D:213:GLU:C	2.45	0.55
2:B:169:LYS:C	2:B:169:LYS:HD2	2.28	0.55
1:A:129:LYS:HE3	2:B:207:LYS:HA	1.89	0.55
1:C:143:LYS:HG2	1:C:144:ASP:OD2	2.07	0.55
1:C:33:ALA:HB3	1:C:95:PRO:CD	2.38	0.54
2:B:193:ALA:CB	2:B:208:SER:HB3	2.38	0.54
1:A:66:ARG:CZ	1:A:83:ARG:HH22	2.22	0.53
1:C:93:ALA:HB1	1:C:100(M):PHE:HB3	1.91	0.53
2:D:145:LYS:HB3	2:D:197:THR:HB	1.90	0.53
1:A:167:PRO:HD2	2:B:162:SER:OG	2.09	0.53
2:D:55:LYS:HA	2:D:55:LYS:CE	2.38	0.52
1:A:2:VAL:HG13	6:A:9031:HOH:O	2.09	0.52
2:B:191:LEU:N	2:B:191:LEU:HD12	2.25	0.52
1:C:126:PRO:CG	1:C:138:LEU:HB3	2.37	0.52
1:A:93:ALA:HB1	1:A:100(M):PHE:HB3	1.91	0.51
2:B:149:LYS:HG2	2:B:154:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:SER:O	1:C:14:PRO:HB2	2.11	0.51
2:B:125:LEU:O	2:B:183:LYS:HD2	2.11	0.50
2:D:119:PRO:HB3	2:D:209:PHE:CE2	2.47	0.50
2:D:31:ASN:N	2:D:31:ASN:HD22	2.10	0.50
1:C:139:GLY:HA2	1:C:154:TRP:CH2	2.47	0.50
4:D:9004:CYS:HA	6:D:9161:HOH:O	2.11	0.50
1:C:119:PRO:HG3	1:C:145:TYR:HB2	1.92	0.49
1:C:28:THR:OG1	1:C:31:ASN:ND2	2.45	0.49
2:D:190:LYS:O	2:D:210:ASN:HA	2.12	0.49
1:A:47:TRP:CZ2	1:A:49:GLY:HA2	2.47	0.49
2:D:33:LEU:HD22	2:D:71:PHE:CG	2.47	0.49
1:A:29:PHE:CE2	1:A:52(A):PRO:HB3	2.48	0.49
2:B:6:GLN:HG3	2:B:88:CYS:SG	2.53	0.49
1:C:119:PRO:CB	1:C:145:TYR:HB3	2.43	0.48
1:C:32:TYR:CZ	1:C:97:PRO:HG2	2.47	0.48
1:C:36:TRP:CE2	1:C:80:MET:HB2	2.49	0.48
1:C:105:ARG:NH1	6:C:9063:HOH:O	2.47	0.48
1:C:184:VAL:HG11	1:C:194:TYR:CE2	2.47	0.48
2:D:2:ILE:HD13	2:D:29:ILE:HG22	1.96	0.48
1:A:126:PRO:CG	1:A:138:LEU:HB3	2.29	0.48
2:D:54:LEU:HD21	2:D:62:PHE:O	2.14	0.48
1:A:144:ASP:HB3	1:A:175:LEU:HD13	1.96	0.48
1:A:36:TRP:CE2	1:A:80:MET:HB2	2.49	0.48
2:B:186:TYR:HA	2:B:192:TYR:OH	2.14	0.48
1:C:136:ALA:CB	1:C:189:LEU:HD11	2.44	0.47
1:A:117:LYS:NZ	6:A:9135:HOH:O	2.47	0.47
2:B:124:GLN:HG2	2:B:129:THR:O	2.14	0.47
1:A:83:ARG:C	1:A:111:VAL:HG11	2.35	0.47
2:B:39:LYS:NZ	2:B:81:ASP:OD1	2.47	0.47
2:D:129:THR:HG22	2:D:130:ALA:N	2.31	0.47
1:A:119:PRO:CB	1:A:145:TYR:HB3	2.40	0.46
2:B:113:PRO:HB3	2:B:139:PHE:HB3	1.98	0.46
2:D:55:LYS:NZ	2:D:56:SER:H	2.12	0.46
2:B:175:LEU:HD23	2:B:175:LEU:C	2.36	0.46
2:D:39:LYS:HB2	2:D:42:ARG:HD2	1.96	0.46
1:C:202:PRO:HB3	6:C:9080:HOH:O	2.16	0.46
2:D:180:THR:O	2:D:181:LEU:HD23	2.16	0.46
1:A:67:VAL:CG2	1:A:82:LEU:HD13	2.45	0.46
1:A:191:THR:HG23	6:D:9104:HOH:O	2.16	0.46
2:D:190:LYS:HD2	2:D:213:GLU:OE2	2.16	0.46
2:D:31:ASN:ND2	2:D:67:SER:HB2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:PRO:HB2	6:A:9032:HOH:O	2.16	0.45
1:C:178:LEU:C	1:C:178:LEU:HD23	2.37	0.45
2:D:22:THR:HG22	2:D:72:THR:HG22	1.99	0.45
2:B:50:LYS:O	2:B:51:ALA:HB3	2.16	0.45
1:C:126:PRO:HB2	1:C:213:PRO:HB3	1.98	0.45
1:A:127:SER:N	1:A:130:SER:HB3	2.26	0.45
1:A:19:LYS:HE2	1:A:79:TYR:CD2	2.52	0.45
1:C:34:ILE:HG21	1:C:78:ALA:HB3	1.98	0.45
1:A:63:PHE:HB3	1:A:67:VAL:CG2	2.46	0.45
1:A:66:ARG:NE	1:A:83:ARG:HH22	2.15	0.45
1:C:31:ASN:ND2	1:C:98:ASN:O	2.50	0.45
1:C:87:THR:HB	6:C:9101:HOH:O	2.17	0.45
1:C:66:ARG:HH22	1:C:86:ASP:CG	2.19	0.45
2:D:151:ASP:OD2	2:D:189:HIS:HB3	2.16	0.44
1:A:143:LYS:HE2	6:B:230:HOH:O	2.18	0.44
1:A:129:LYS:HE3	2:B:207:LYS:CD	2.47	0.44
1:C:12:LYS:O	1:C:111:VAL:HA	2.17	0.44
1:C:159:LEU:HD21	1:C:182:VAL:HG21	2.00	0.44
1:A:31:ASN:ND2	1:A:98:ASN:O	2.50	0.43
1:C:119:PRO:CG	1:C:145:TYR:HB3	2.48	0.43
1:C:151:THR:OG1	1:C:199:ASN:HB3	2.18	0.43
1:C:178:LEU:HD23	1:C:179:SER:N	2.33	0.43
1:C:47:TRP:CZ2	1:C:49:GLY:HA2	2.53	0.43
1:C:201:LYS:O	1:C:202:PRO:C	2.57	0.43
1:C:63:PHE:O	1:C:67:VAL:HG12	2.19	0.43
1:C:154:TRP:CH2	1:C:196:CYS:HB3	2.54	0.43
2:D:151:ASP:HA	2:D:191:LEU:HB2	2.00	0.43
1:C:119:PRO:HB3	1:C:145:TYR:HB3	2.00	0.43
1:C:86:ASP:O	1:C:87:THR:C	2.57	0.42
2:D:49:TYR:HD1	2:D:50:LYS:HG3	1.83	0.42
2:D:150:VAL:O	2:D:151:ASP:HB2	2.19	0.42
2:D:31:ASN:N	2:D:31:ASN:ND2	2.66	0.42
1:C:169:VAL:O	1:C:176:TYR:HD1	2.02	0.42
1:C:112:SER:C	1:C:114:ALA:H	2.22	0.42
1:A:147:PRO:HD2	1:A:202:PRO:HB3	2.02	0.42
1:C:146:PHE:HA	1:C:147:PRO:HA	1.88	0.42
2:B:94:SER:HA	2:B:95:PRO:C	2.40	0.42
2:B:35:TRP:CE2	2:B:73:LEU:HB2	2.55	0.42
2:D:163:VAL:HG22	2:D:175:LEU:HD12	2.01	0.42
1:A:2:VAL:C	1:A:3:GLN:HG2	2.40	0.41
2:D:175:LEU:HD23	2:D:176:SER:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:LEU:HD22	2:B:71:PHE:CG	2.54	0.41
1:C:31:ASN:CG	1:C:98:ASN:O	2.59	0.41
1:A:201:LYS:N	1:A:202:PRO:CD	2.83	0.41
2:B:142:ARG:HG2	2:B:142:ARG:NH1	2.34	0.41
1:C:170:LEU:HD13	1:C:176:TYR:CE1	2.55	0.41
1:A:66:ARG:CZ	1:A:83:ARG:NH2	2.84	0.41
2:B:119:PRO:HB3	2:B:209:PHE:CZ	2.55	0.41
1:C:125:ALA:HA	1:C:126:PRO:HD3	1.82	0.41
1:C:53:ILE:HD12	1:C:73:GLU:OE2	2.19	0.41
1:C:55:ASN:HA	1:C:55:ASN:HD22	1.68	0.41
2:D:193:ALA:HB2	2:D:208:SER:CB	2.45	0.41
2:D:31:ASN:HD21	2:D:67:SER:HB2	1.85	0.41
1:C:100(H):GLY:O	1:C:100(I):MET:C	2.58	0.41
2:D:24:ARG:HG2	2:D:70:GLU:OE2	2.20	0.41
1:A:24:ALA:HB1	1:A:32:TYR:CZ	2.55	0.40
1:C:64:GLN:HA	3:I:1:GLC:O2	2.21	0.40
1:C:145:TYR:CD2	1:C:145:TYR:N	2.89	0.40
1:A:129:LYS:CE	2:B:207:LYS:HA	2.51	0.40
1:C:121:VAL:HG21	1:C:207:VAL:CG1	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	220/231 (95%)	211 (96%)	9 (4%)	0	100	100
1	C	208/231 (90%)	180 (86%)	26 (12%)	2 (1%)	15	9
2	B	211/214 (99%)	202 (96%)	9 (4%)	0	100	100
2	D	212/214 (99%)	203 (96%)	7 (3%)	2 (1%)	17	11
All	All	851/890 (96%)	796 (94%)	51 (6%)	4 (0%)	29	23



All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	25	SER
1	C	100(I)	MET
2	D	213	GLU
2	D	2	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	187/193 (97%)	185 (99%)	2 (1%)	73	78
1	C	179/193 (93%)	173 (97%)	6 (3%)	37	36
2	B	188/189 (100%)	188 (100%)	0	100	100
2	D	189/189 (100%)	184 (97%)	5 (3%)	46	48
All	All	743/764 (97%)	730 (98%)	13 (2%)	57	65

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	PRO
1	A	178	LEU
1	C	29	PHE
1	C	62	ARG
1	C	145	TYR
1	C	149	PRO
1	C	202	PRO
1	C	204	ASN
2	D	55	LYS
2	D	147	GLN
2	D	152	ASN
2	D	154	LEU
2	D	213	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	55	ASN
1	A	58	HIS
2	B	3	GLN
2	B	27	GLN
2	B	31	ASN
2	B	79	GLN
2	B	91	HIS
1	C	31	ASN
1	C	55	ASN
2	D	31	ASN
2	D	91	HIS
2	D	138	ASN
2	D	210	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	TYS	A	100	1	15,16,17	1.80	2 (13%)	18,22,24	0.59	0
1	TYS	C	100	1	15,16,17	1.81	2 (13%)	18,22,24	0.61	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
1	TYS	A	100	1	-	2/10/11/13	0/1/1/1
1	TYS	C	100	1	-	7/10/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	TYS	OH-S	-6.29	1.48	1.58
1	C	100	TYS	OH-S	-6.22	1.48	1.58
1	C	100	TYS	OH-CZ	-2.73	1.38	1.42
1	A	100	TYS	OH-CZ	-2.35	1.38	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	100	TYS	CE1-CZ-OH-S
1	A	100	TYS	CE2-CZ-OH-S
1	C	100	TYS	C-CA-CB-CG
1	C	100	TYS	CZ-OH-S-O1
1	C	100	TYS	N-CA-CB-CG
1	C	100	TYS	CA-CB-CG-CD2
1	C	100	TYS	CA-CB-CG-CD1
1	C	100	TYS	CZ-OH-S-O3
1	C	100	TYS	CZ-OH-S-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	100	TYS	1	0

## 5.5 Carbohydrates

14 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	GLC	E	1	3	11,11,12	1.37	1 (9%)	15,15,17	1.67	2 (13%)
3	FRU	E	2	3	11,12,12	1.37	2 (18%)	10,18,18	0.50	0
3	GLC	F	1	3	11,11,12	1.34	1 (9%)	15,15,17	1.56	2 (13%)
3	FRU	F	2	3	11,12,12	1.50	2 (18%)	10,18,18	0.53	0
3	GLC	G	1	3	11,11,12	1.51	2 (18%)	15,15,17	1.55	2 (13%)
3	FRU	G	2	3	11,12,12	1.33	2 (18%)	10,18,18	0.74	0
3	GLC	H	1	3	11,11,12	1.45	1 (9%)	15,15,17	1.68	2 (13%)
3	FRU	H	2	3	11,12,12	1.41	2 (18%)	10,18,18	0.58	0
3	GLC	I	1	3	11,11,12	1.35	1 (9%)	15,15,17	1.62	2 (13%)
3	FRU	I	2	3	11,12,12	1.37	2 (18%)	10,18,18	0.56	0
3	GLC	J	1	3	11,11,12	1.48	1 (9%)	15,15,17	1.65	2 (13%)
3	FRU	J	2	3	11,12,12	1.45	2 (18%)	10,18,18	0.66	0
3	GLC	K	1	3	11,11,12	1.39	1 (9%)	15,15,17	1.69	2 (13%)
3	FRU	K	2	3	11,12,12	1.40	2 (18%)	10,18,18	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
3	GLC	E	1	3	-	0/2/19/22	0/1/1/1
3	FRU	E	2	3	-	0/5/24/24	0/1/1/1
3	GLC	F	1	3	-	0/2/19/22	0/1/1/1
3	FRU	F	2	3	-	0/5/24/24	0/1/1/1
3	GLC	G	1	3	-	0/2/19/22	0/1/1/1
3	FRU	G	2	3	-	0/5/24/24	0/1/1/1
3	GLC	H	1	3	-	0/2/19/22	0/1/1/1
3	FRU	H	2	3	-	2/5/24/24	0/1/1/1
3	GLC	I	1	3	-	0/2/19/22	0/1/1/1
3	FRU	I	2	3	-	0/5/24/24	0/1/1/1
3	GLC	J	1	3	-	0/2/19/22	0/1/1/1
3	FRU	J	2	3	-	0/5/24/24	0/1/1/1
3	GLC	K	1	3	-	0/2/19/22	0/1/1/1
3	FRU	K	2	3	-	0/5/24/24	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	2	FRU	O2-C2	3.78	1.47	1.40
3	J	2	FRU	O2-C2	3.76	1.47	1.40
3	F	2	FRU	O2-C2	3.76	1.47	1.40
3	K	2	FRU	O2-C2	3.72	1.47	1.40
3	G	2	FRU	O2-C2	3.54	1.46	1.40
3	I	2	FRU	O2-C2	3.39	1.46	1.40
3	E	2	FRU	O2-C2	3.29	1.46	1.40
3	J	1	GLC	C4-C5	2.93	1.59	1.53
3	F	1	GLC	C4-C5	2.88	1.59	1.53
3	G	1	GLC	C4-C5	2.87	1.59	1.53
3	E	1	GLC	C4-C5	2.80	1.58	1.53
3	H	1	GLC	C4-C5	2.78	1.58	1.53
3	K	1	GLC	C4-C5	2.75	1.58	1.53
3	I	1	GLC	C4-C5	2.69	1.58	1.53
3	F	2	FRU	C1-C2	2.55	1.56	1.52
3	I	2	FRU	C1-C2	2.43	1.56	1.52
3	E	2	FRU	C1-C2	2.35	1.56	1.52
3	G	1	GLC	C2-C3	2.32	1.55	1.52
3	H	2	FRU	C1-C2	2.31	1.56	1.52
3	J	2	FRU	C1-C2	2.30	1.56	1.52
3	G	2	FRU	C1-C2	2.26	1.56	1.52
3	K	2	FRU	C1-C2	2.14	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	1	GLC	C1-O5-C5	5.04	119.02	112.19
3	E	1	GLC	C1-O5-C5	5.03	119.01	112.19
3	H	1	GLC	C1-O5-C5	4.94	118.89	112.19
3	J	1	GLC	C1-O5-C5	4.92	118.85	112.19
3	G	1	GLC	C1-O5-C5	4.76	118.64	112.19
3	I	1	GLC	C1-O5-C5	4.69	118.54	112.19
3	F	1	GLC	C1-O5-C5	4.67	118.52	112.19
3	J	1	GLC	C6-C5-C4	2.54	118.95	113.00
3	K	1	GLC	C6-C5-C4	2.50	118.85	113.00
3	H	1	GLC	C6-C5-C4	2.48	118.82	113.00
3	F	1	GLC	C6-C5-C4	2.43	118.69	113.00
3	E	1	GLC	C6-C5-C4	2.36	118.53	113.00
3	I	1	GLC	C6-C5-C4	2.31	118.42	113.00
3	G	1	GLC	C6-C5-C4	2.27	118.33	113.00

There are no chirality outliers.

All (2) torsion outliers are listed below:

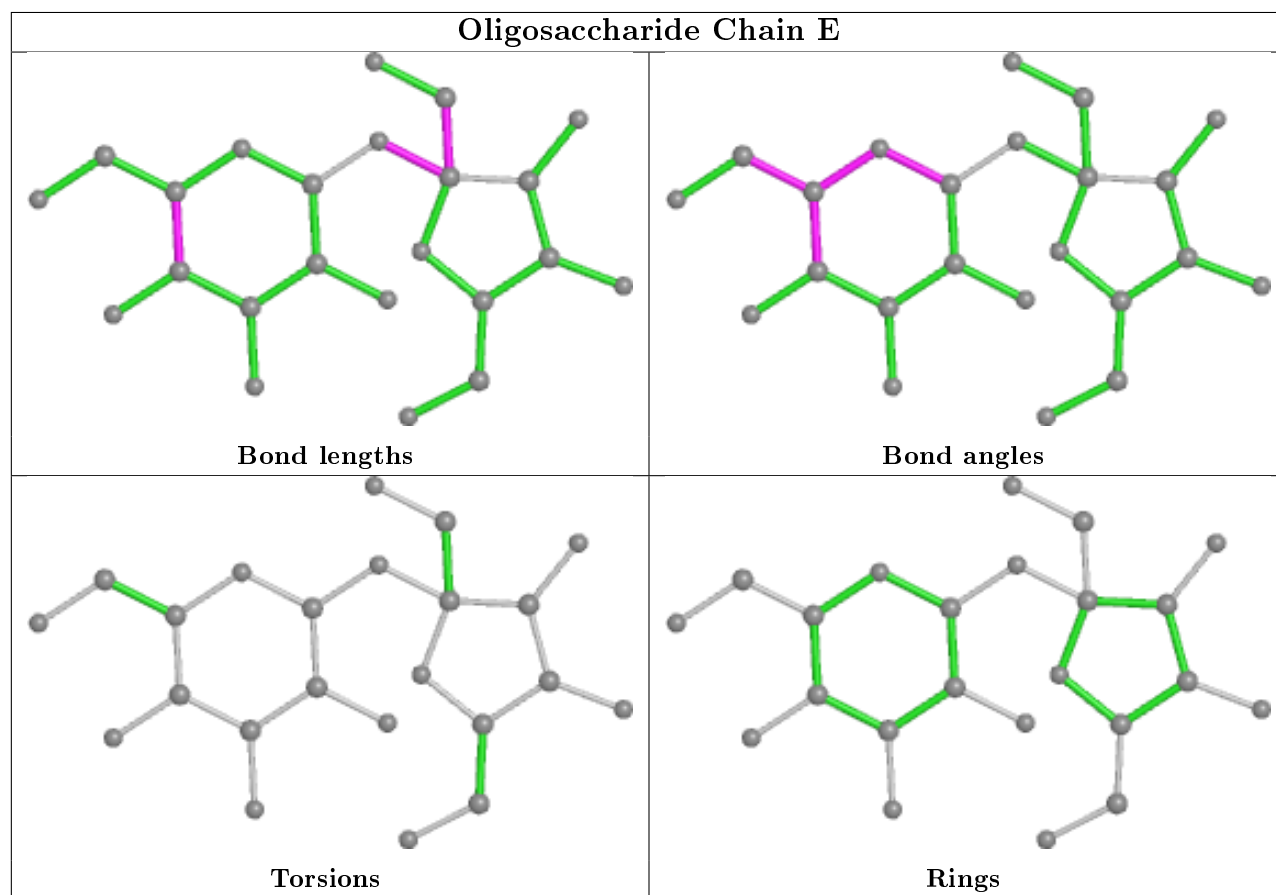
Mol	Chain	Res	Type	Atoms
3	H	2	FRU	O5-C5-C6-O6
3	H	2	FRU	C4-C5-C6-O6

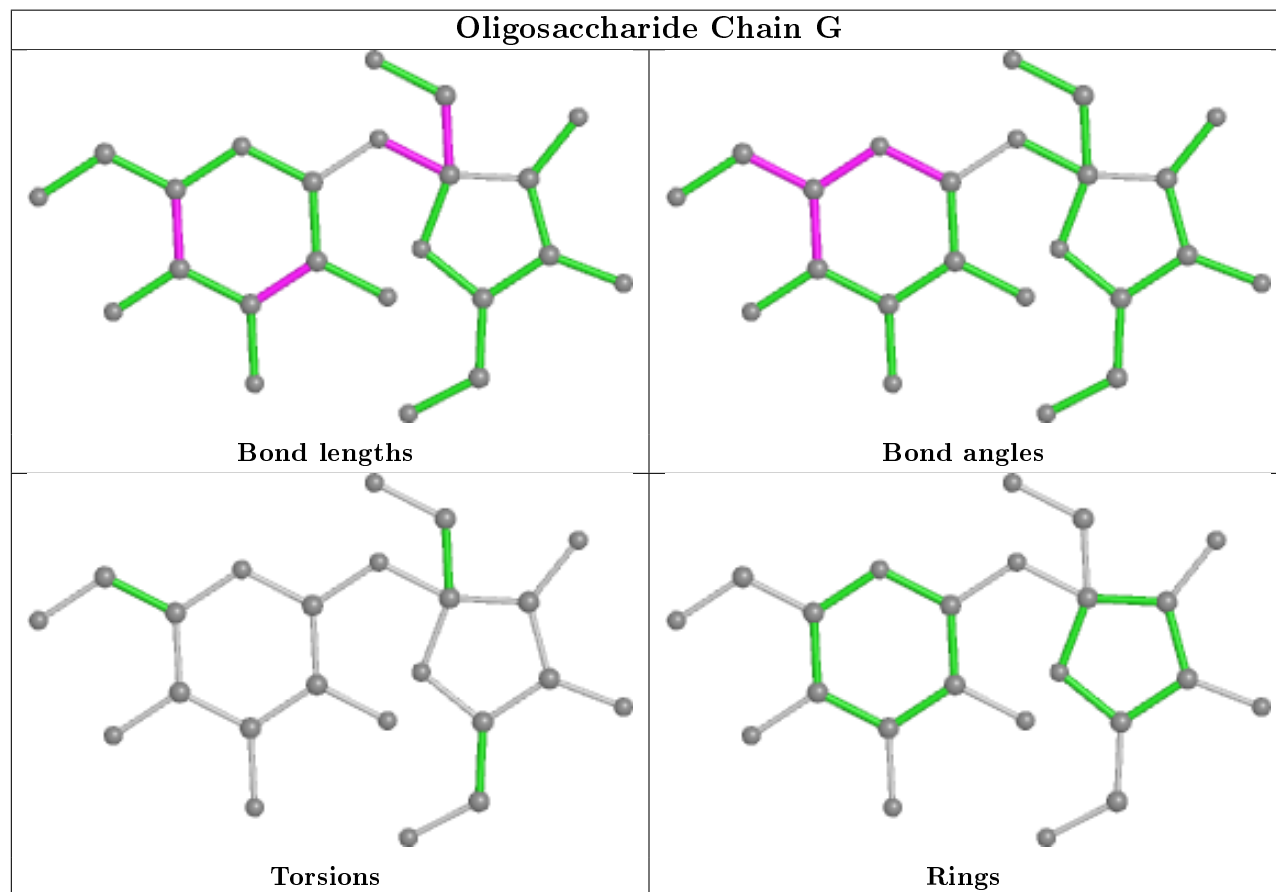
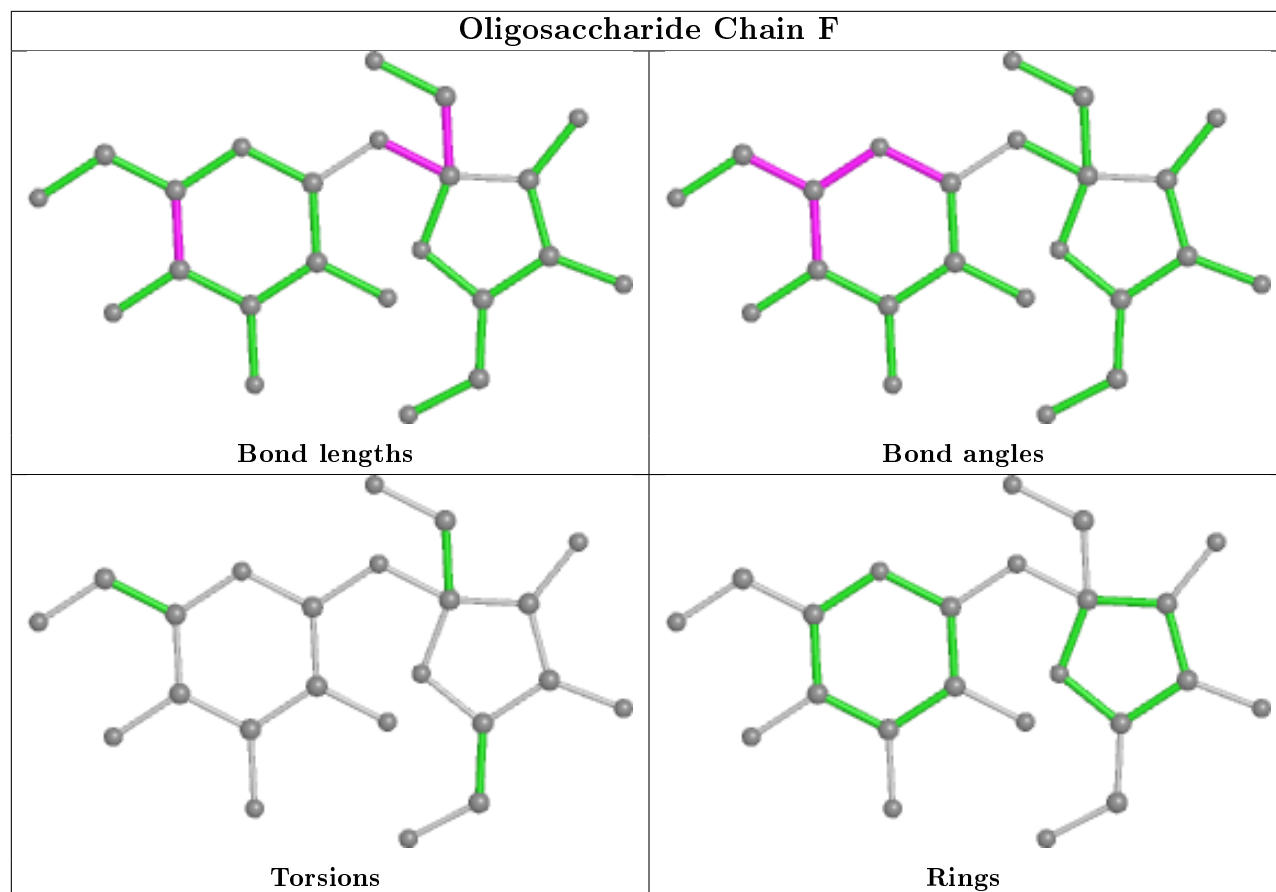
There are no ring outliers.

2 monomers are involved in 3 short contacts:

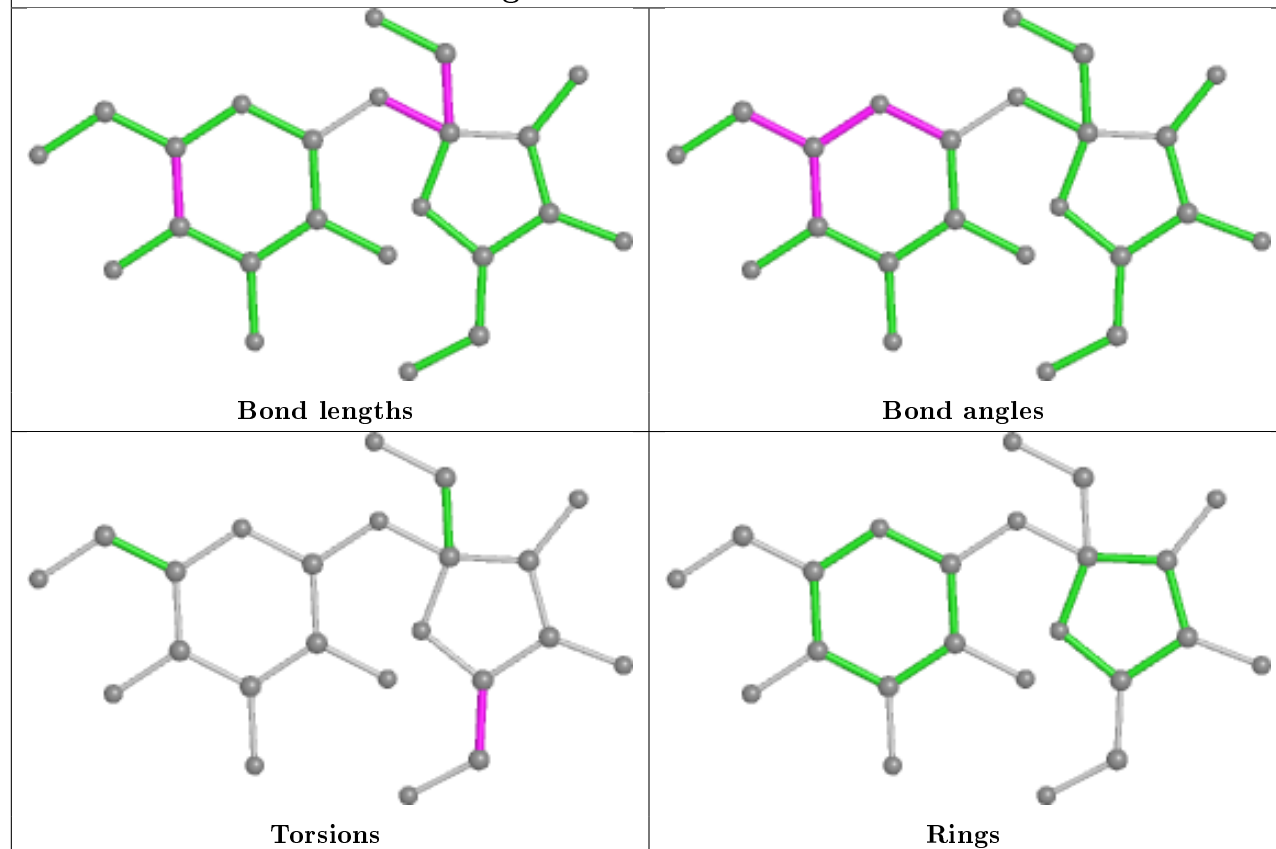
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	GLC	1	0
3	I	1	GLC	2	0

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

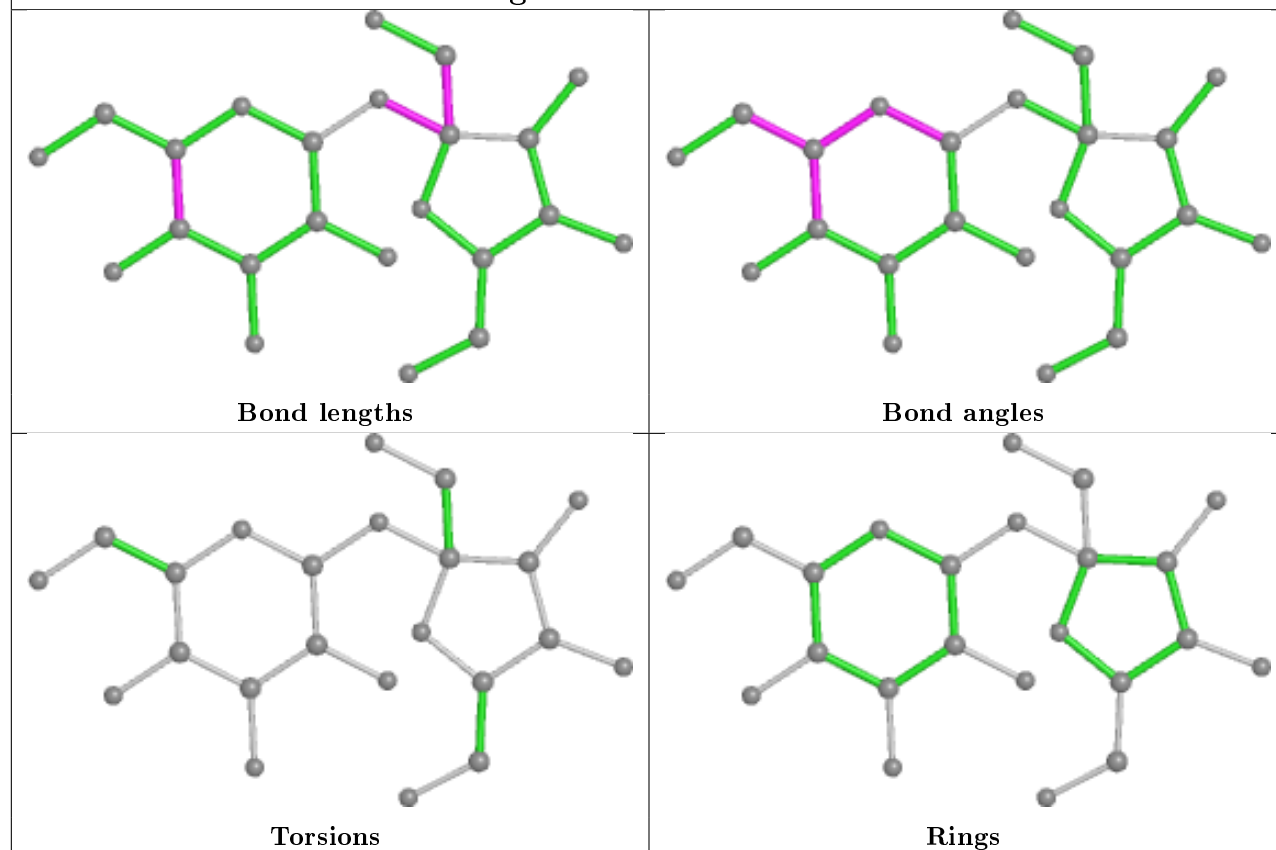




## Oligosaccharide Chain H

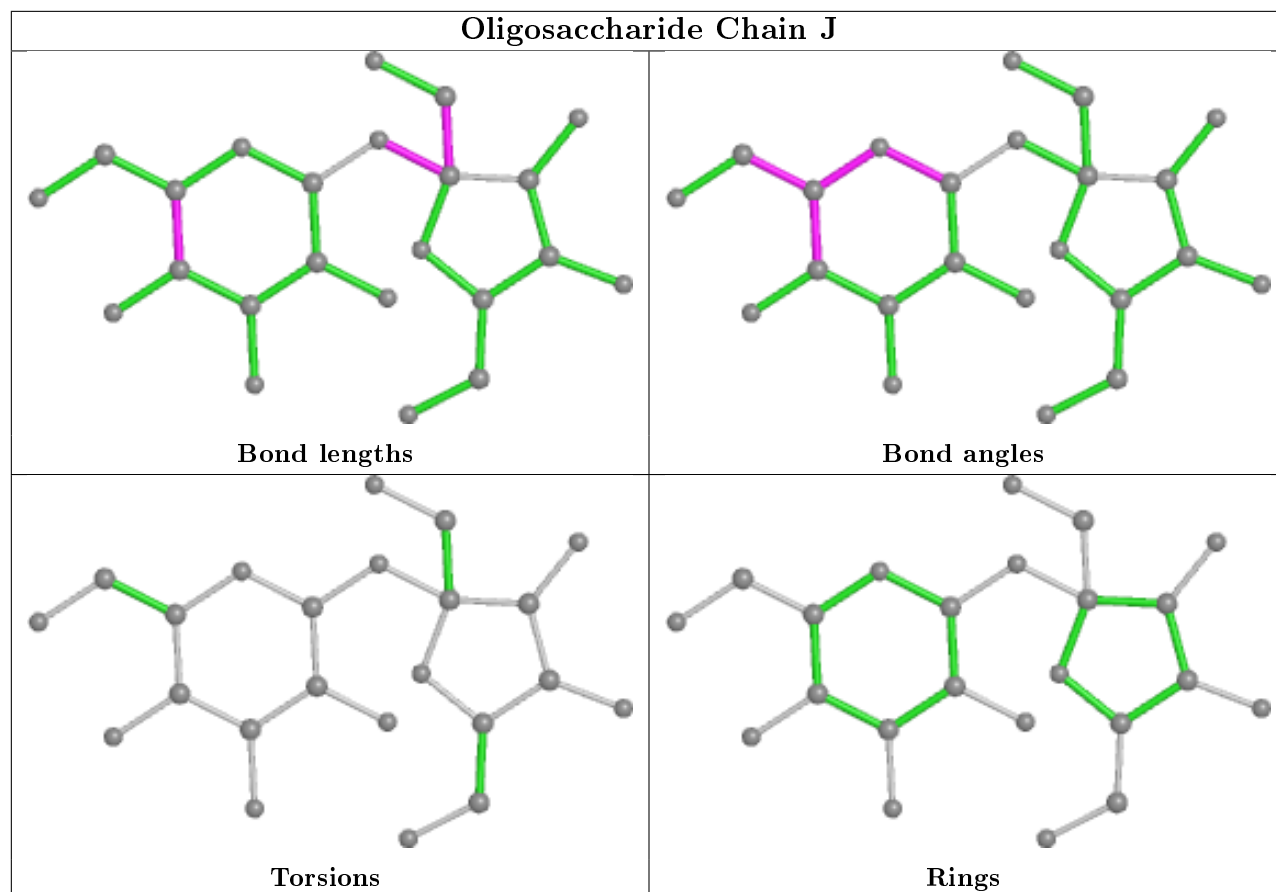


## Oligosaccharide Chain I

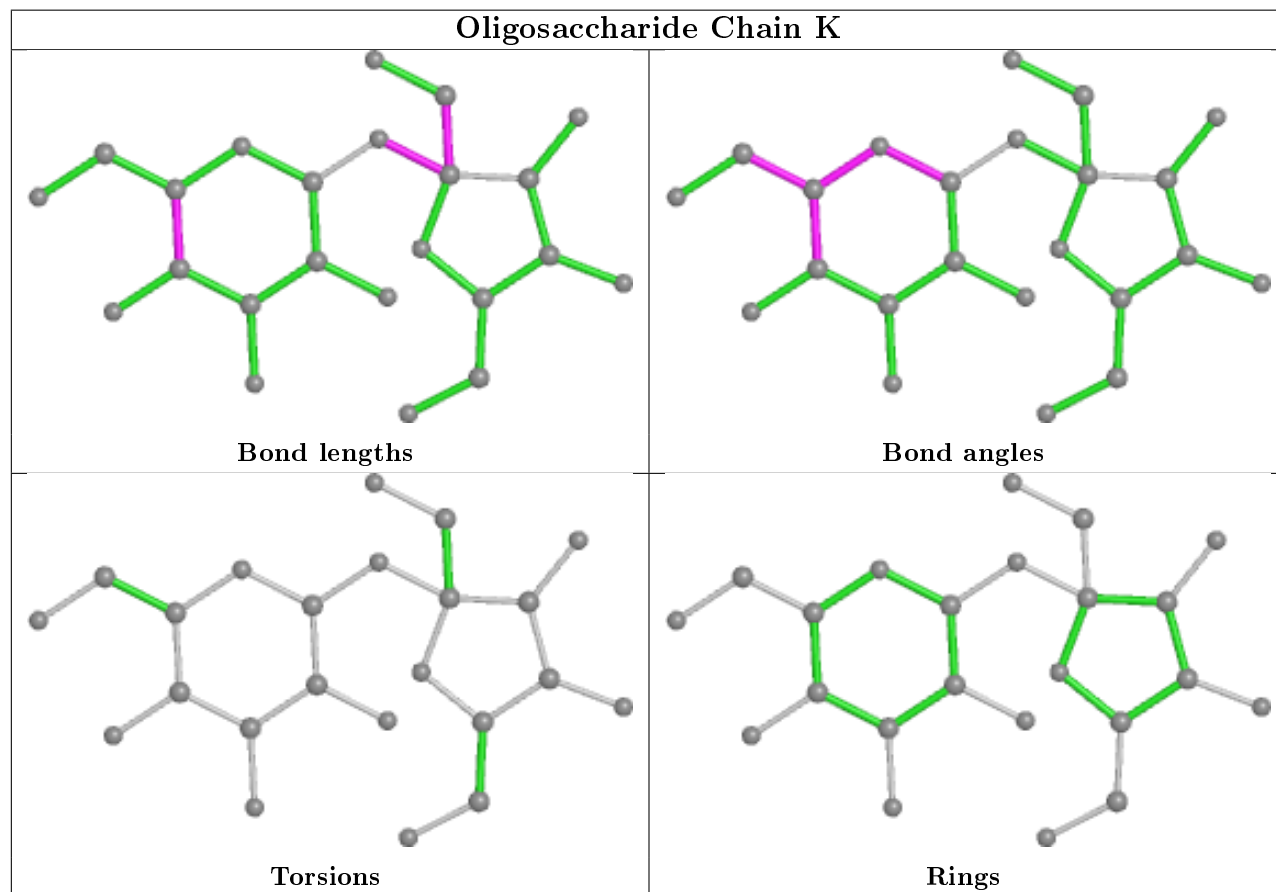




## Oligosaccharide Chain J



## Oligosaccharide Chain K



## 5.6 Ligand geometry

2 ligands are modelled in this entry.

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

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, 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	223/231 (96%)	0.01	11 (4%) 29 28	17, 29, 50, 72	0
1	C	213/231 (92%)	0.92	46 (21%) 0 0	22, 45, 67, 76	0
2	B	213/214 (99%)	-0.28	1 (0%) 91 90	16, 27, 42, 65	0
2	D	214/214 (100%)	-0.12	6 (2%) 53 51	22, 32, 49, 87	0
All	All	863/890 (96%)	0.13	64 (7%) 14 13	16, 32, 58, 87	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	98	ASN	7.0
1	C	99	ASP	5.5
1	A	129	LYS	5.4
1	A	130	SER	5.3
2	D	214	CYS	5.0
1	C	25	SER	5.0
1	C	191	THR	4.9
1	A	132	SER	4.9
1	C	201	LYS	4.5
1	C	113	PRO	4.5
1	A	131	THR	4.5
2	D	213	GLU	4.4
1	C	74	SER	4.0
1	A	99	ASP	4.0
2	D	212	GLY	3.8
1	A	133	GLY	3.7
1	C	149	PRO	3.7
1	C	187	SER	3.4
1	C	115	SER	3.2
1	C	36	TRP	3.2
2	D	191	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	26	GLY	3.1
1	C	28	THR	3.1
1	C	189	LEU	3.0
1	C	204	ASN	3.0
1	C	147	PRO	3.0
1	C	206	LYS	2.9
1	C	205	THR	2.9
1	C	116	THR	2.9
1	A	100(M)	PHE	2.8
1	C	202	PRO	2.8
2	B	154	LEU	2.8
1	C	156	SER	2.8
1	C	97	PRO	2.8
1	C	96	TYR	2.7
1	C	159	LEU	2.7
1	C	208	ASP	2.7
1	C	199	ASN	2.7
1	C	190	GLY	2.6
1	C	2	VAL	2.6
1	C	158	ALA	2.6
1	C	100(M)	PHE	2.5
1	C	146	PHE	2.5
1	A	100(K)	TRP	2.5
1	C	49	GLY	2.4
1	C	188	SER	2.4
2	D	190	LYS	2.4
1	C	37	VAL	2.4
1	C	69	ILE	2.3
1	C	100(K)	TRP	2.3
1	C	117	LYS	2.2
1	C	31	ASN	2.2
1	C	185	PRO	2.2
1	C	73	GLU	2.2
1	C	153	SER	2.1
1	A	98	ASN	2.1
1	C	111	VAL	2.1
1	C	213	PRO	2.1
1	A	33	ALA	2.0
1	C	145	TYR	2.0
2	D	152	ASN	2.0
1	A	127	SER	2.0
1	C	161	SER	2.0

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	C	13	LYS	2.0

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

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
1	TYS	A	100	16/17	0.73	0.43	72,81,89,89	0
1	TYS	C	100	16/17	0.84	0.51	78,86,95,96	0

## 6.3 Carbohydrates ⓘ

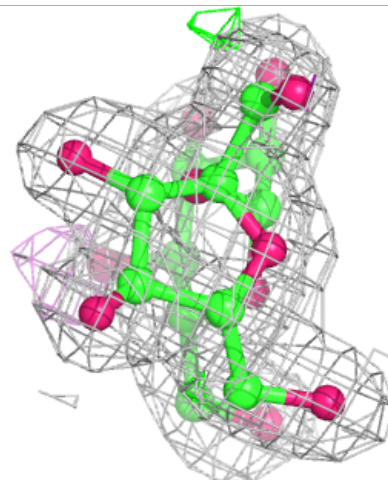
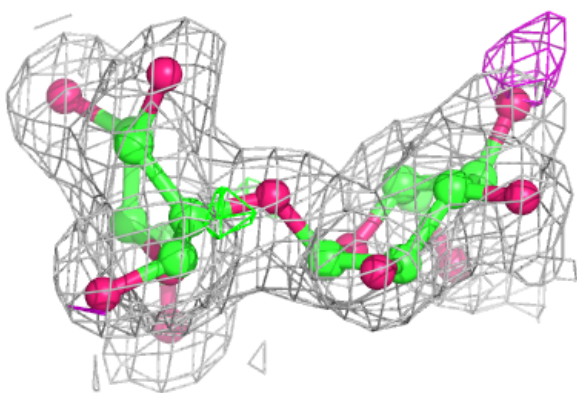
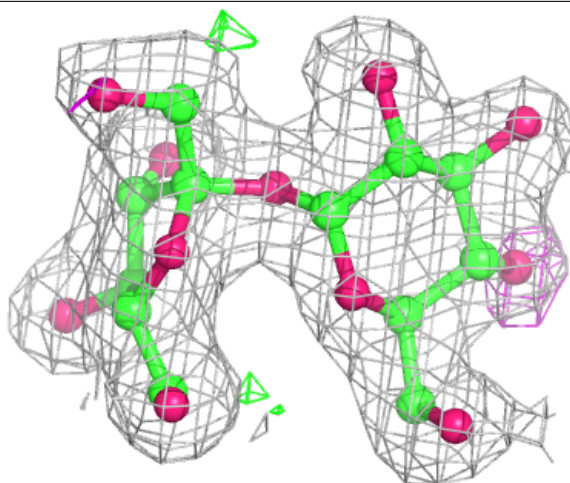
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	FRU	H	2	12/12	0.51	0.26	82,83,84,85	0
3	FRU	J	2	12/12	0.51	0.26	67,70,71,72	0
3	GLC	H	1	11/12	0.78	0.19	85,86,86,86	0
3	FRU	G	2	12/12	0.82	0.15	30,35,36,38	0
3	FRU	K	2	12/12	0.84	0.13	42,45,46,47	0
3	GLC	J	1	11/12	0.87	0.23	71,72,73,73	0
3	FRU	F	2	12/12	0.88	0.11	22,28,31,33	0
3	FRU	I	2	12/12	0.88	0.13	43,46,48,48	0
3	GLC	K	1	11/12	0.89	0.22	45,47,48,49	0
3	GLC	G	1	11/12	0.90	0.13	37,39,40,42	0
3	GLC	I	1	11/12	0.91	0.12	44,46,48,49	0
3	GLC	F	1	11/12	0.93	0.09	29,31,33,36	0
3	FRU	E	2	12/12	0.94	0.08	26,27,29,32	0
3	GLC	E	1	11/12	0.94	0.09	27,29,32,34	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.

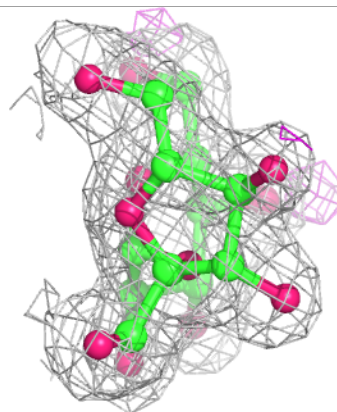
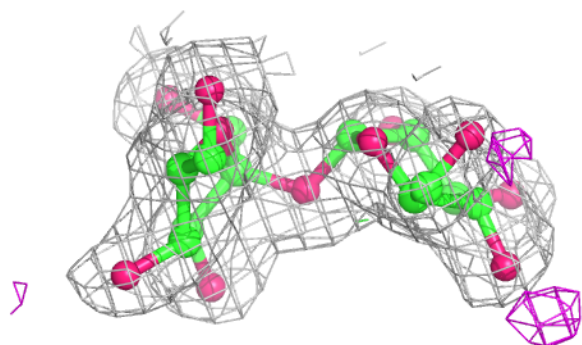
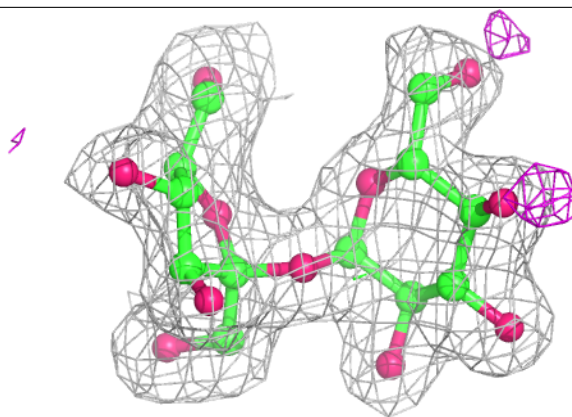
**Electron density around Chain E:**

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



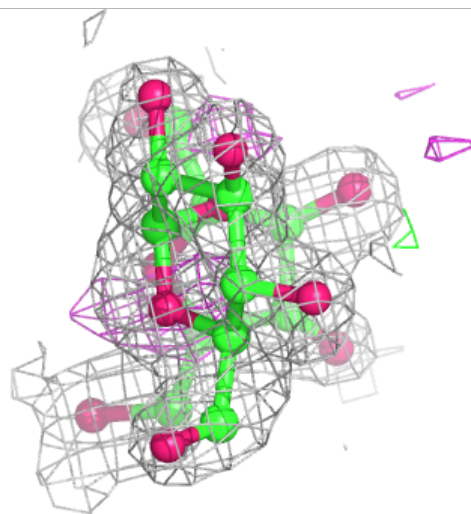
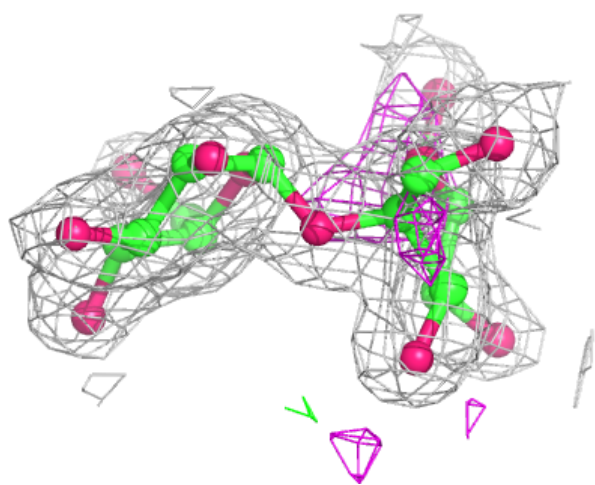
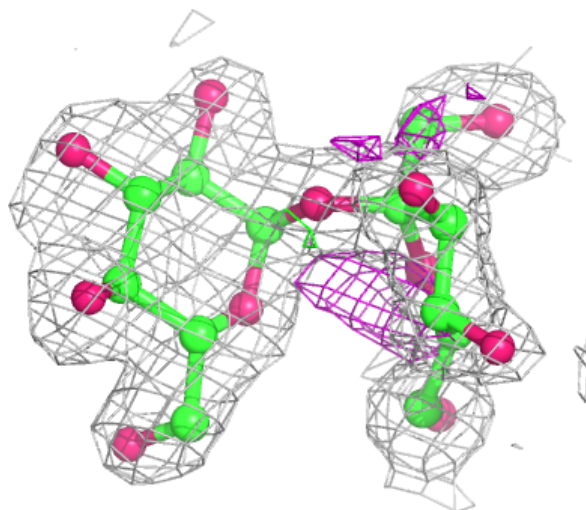
**Electron density around Chain F:**

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



**Electron density around Chain G:**

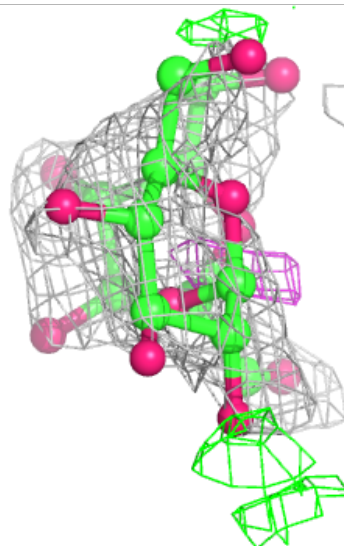
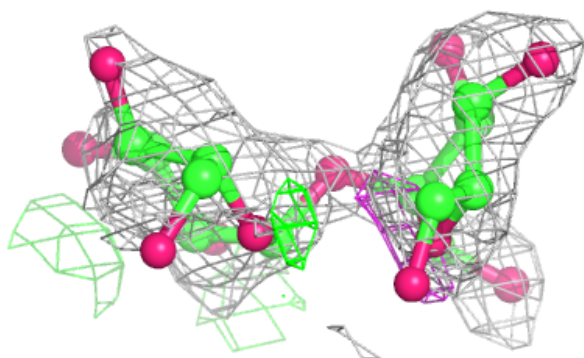
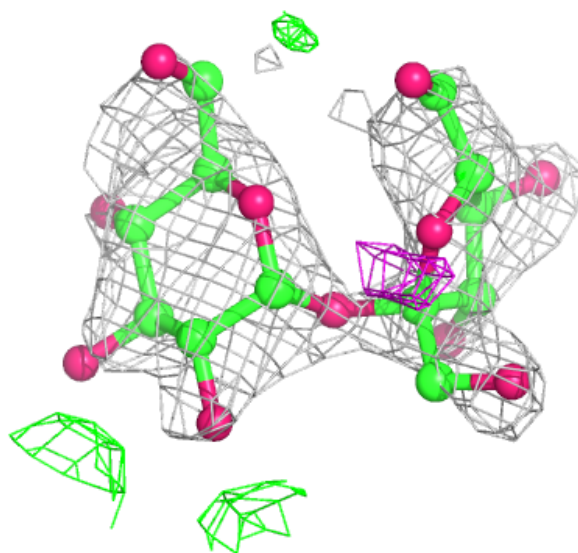
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





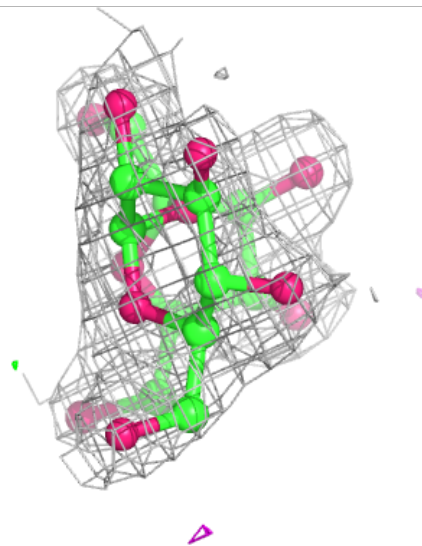
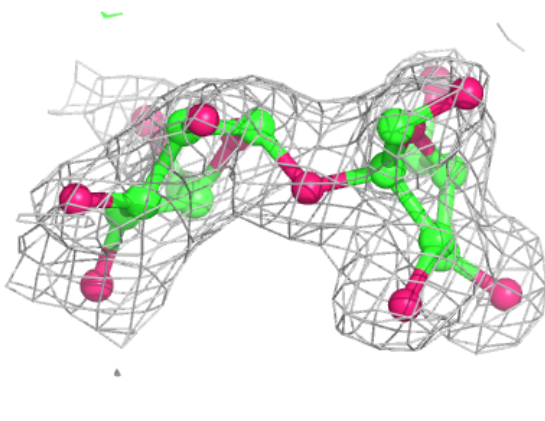
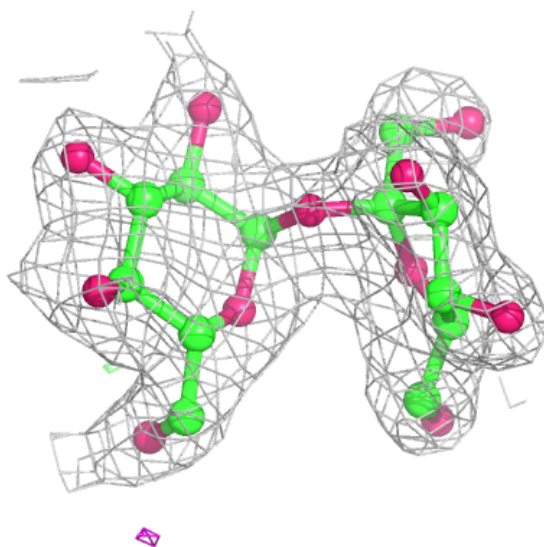
**Electron density around Chain H:**

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



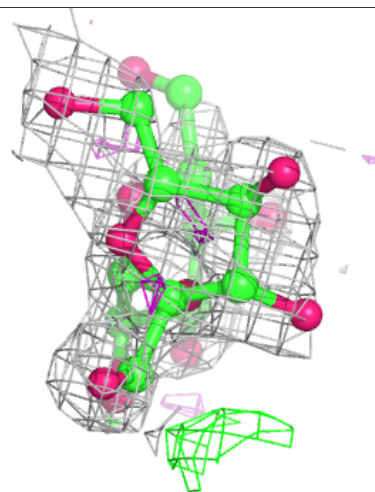
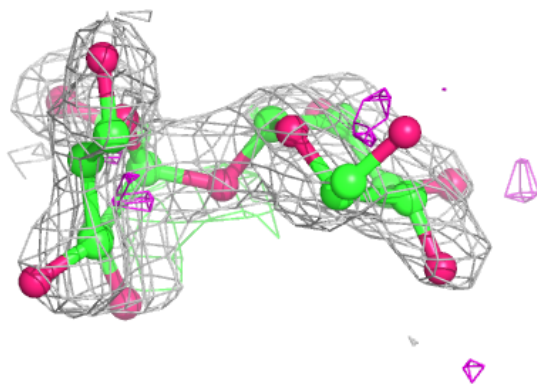
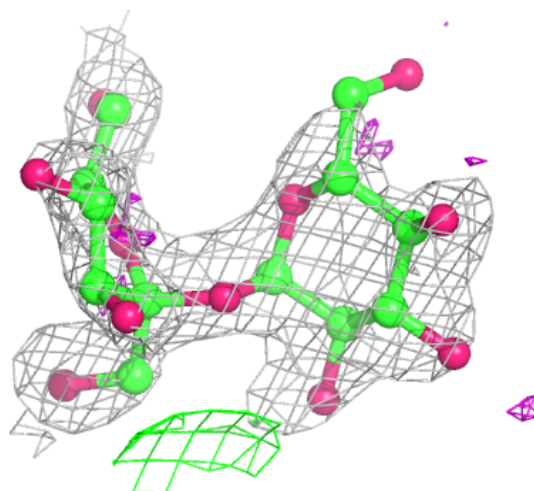
**Electron density around Chain I:**

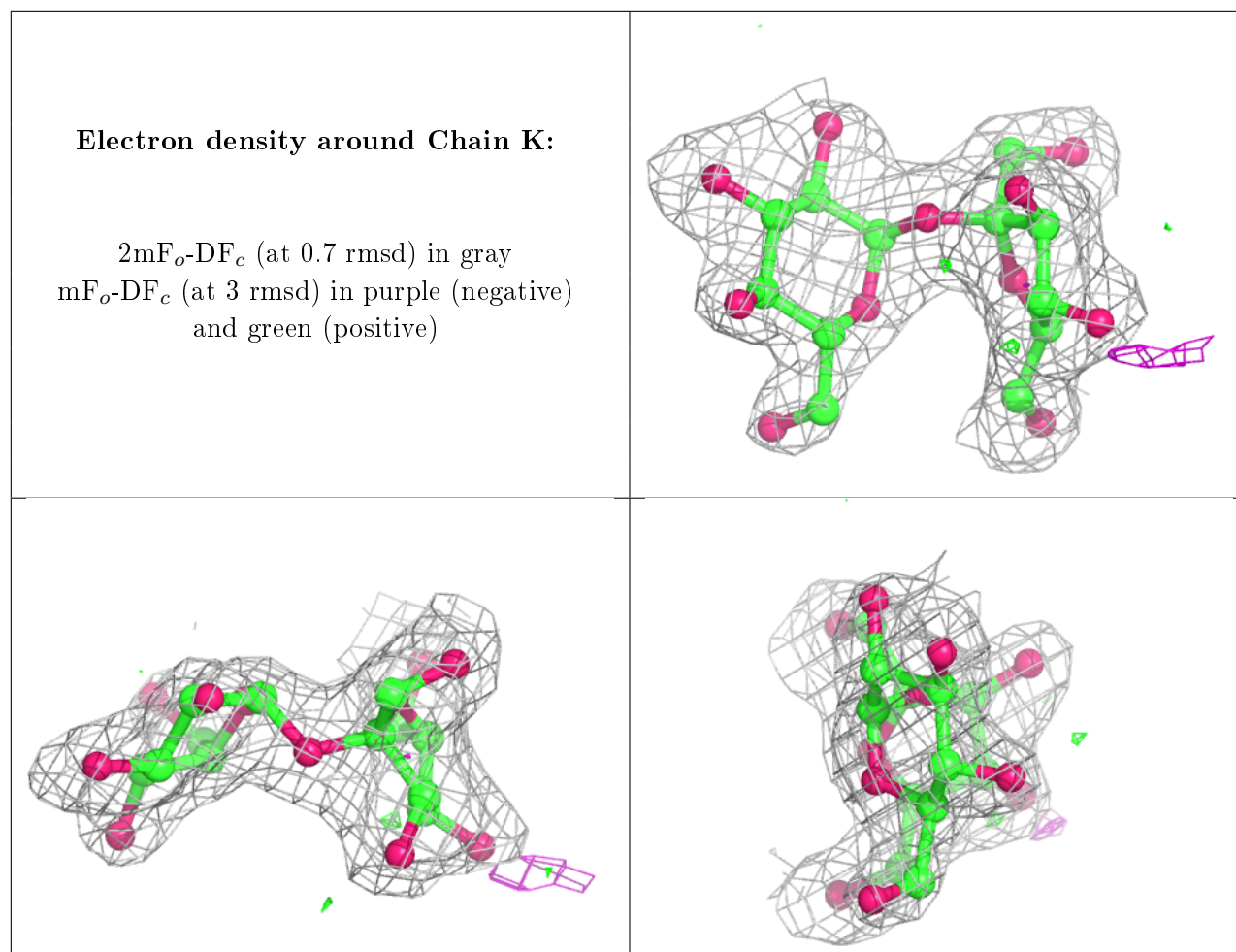
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain J:**

$2mF_o-DF_c$  (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( $\text{\AA}^2$ )	Q<0.9
4	CYS	D	9004	6/7	0.54	0.27	87,87,87,89	0
5	ASP	D	9005	8/9	0.62	0.20	86,86,87,87	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.