



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:06 PM UTC

PDB ID : 9ELZ / pdb\_00009elz  
Title : CRYSTAL STRUCTURE OF RHESUS MACAQUE (MACACA MULATTA)  
IGG2 FC FRAGMENT- FC-GAMMA RECEPTOR IIA COMPLEX H131  
VARIANT  
Authors : Tolbert, W.D.; Pazgier, M.  
Deposited on : 2024-12-05  
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

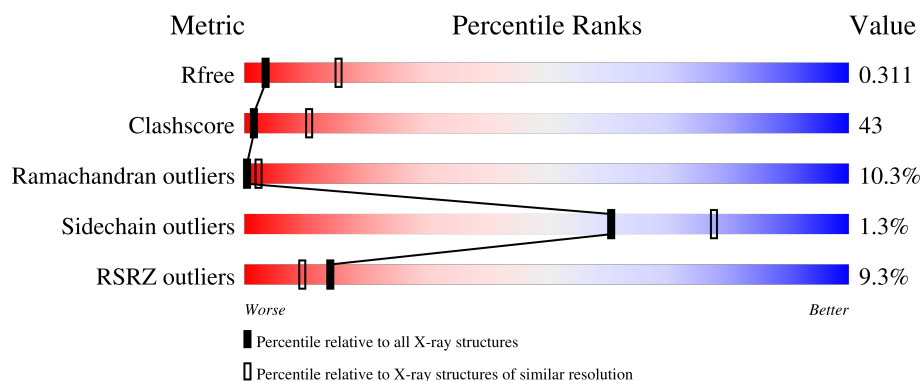
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	223	<div> <div>10%</div> <div>35%</div> <div>55%</div> <div>5%</div> <div>.</div> </div>
1	B	223	<div> <div>13%</div> <div>30%</div> <div>58%</div> <div>8%</div> <div>.</div> </div>
2	C	174	<div> <div>2%</div> <div>51%</div> <div>39%</div> <div>9%</div> <div>.</div> </div>
3	D	8	<div> <div>38%</div> <div>50%</div> <div>12%</div> </div>
3	E	8	<div> <div>25%</div> <div>62%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	3	 <div>33% 67%</div>
5	G	2	 <div>50% 50%</div>

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
5	FUC	G	2	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5035 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 IgG2 Fc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1697	1077	286	328	6			
1	B	215	Total	C	N	O	S	0	0	0
			1710	1085	288	330	7			

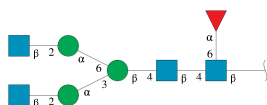
- Molecule 2 is a protein called IgG receptor IIA H131 variant Fc fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	173	Total	C	N	O	S	0	0	0
			1360	856	240	257	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	insertion	UNP F6TRF8

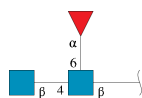
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	8	Total	C	N	O	0	0	0
			99	56	4	39			
3	E	8	Total	C	N	O	0	0	0
			99	56	4	39			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[al

pha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



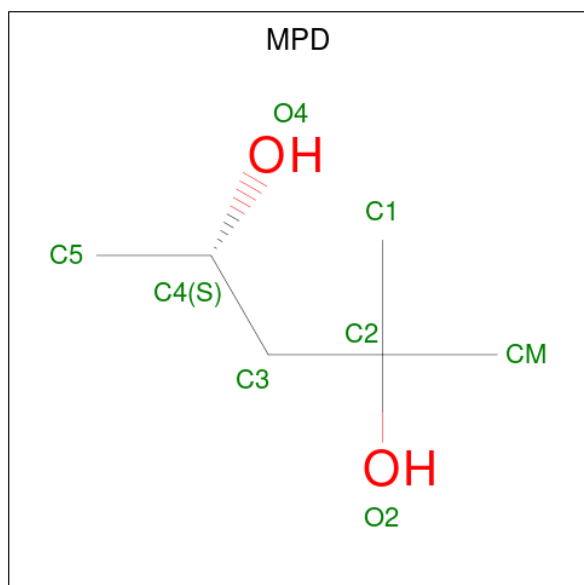
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



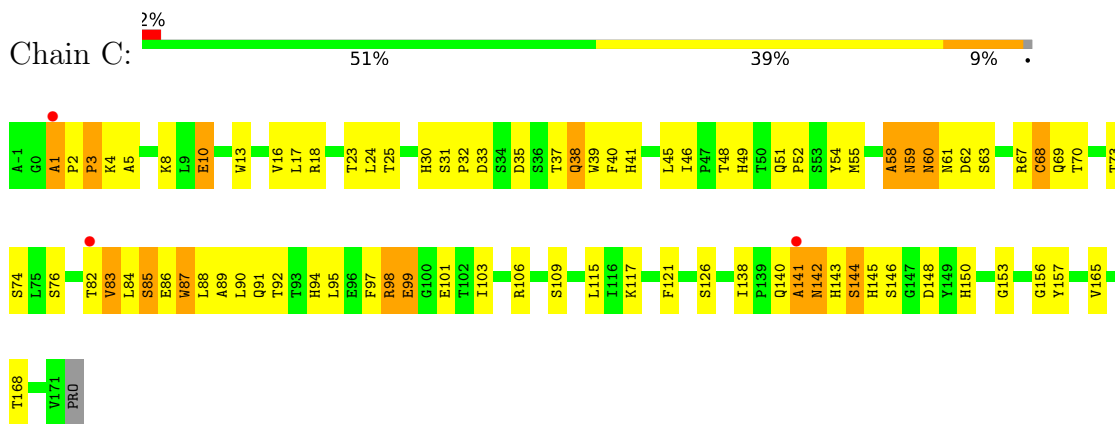
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		





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



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



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



- Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.12Å 128.12Å 253.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.92 – 3.20 28.92 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (28.92-3.20) 98.7 (28.92-3.20)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 3.18Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.275 , 0.306 0.281 , 0.311	Depositor DCC
$R_{free}$ test set	1057 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	105.7	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 105.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5035	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: MAN, BMA, MPD, FUC, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.38	0/1743	0.77	2/2379 (0.1%)
1	B	0.37	0/1757	0.82	4/2399 (0.2%)
2	C	0.40	0/1402	0.83	2/1912 (0.1%)
All	All	0.38	0/4902	0.80	8/6690 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	141	ALA	CA-C-N	-8.46	108.03	122.67
2	C	141	ALA	C-N-CA	-8.46	108.03	122.67
1	A	296	PHE	CA-C-N	5.61	128.57	120.38
1	A	296	PHE	C-N-CA	5.61	128.57	120.38
1	B	297	ASN	CA-C-N	5.30	131.66	121.54
1	B	297	ASN	C-N-CA	5.30	131.66	121.54
1	B	297	ASN	N-CA-CB	-5.13	101.81	110.49
1	B	385	GLY	N-CA-C	-5.08	108.32	114.92

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	1697	0	1662	160	0
1	B	1710	0	1674	174	0
2	C	1360	0	1296	102	0
3	D	99	0	85	3	0
3	E	99	0	85	8	0
4	F	38	0	34	4	0
5	G	24	0	22	7	0
6	A	8	0	14	0	0
All	All	5035	0	4872	422	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 43.

All (422) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:46:ILE:CD1	5:G:2:FUC:H4	1.56	1.33
1:A:270:GLU:CD	1:A:326:LYS:HB2	1.56	1.30
2:C:1:ALA:HB1	2:C:2:PRO:HD3	1.27	1.15
1:A:350:THR:CG2	1:A:441:LEU:HB3	1.76	1.14
1:B:320:THR:HG22	1:B:335:THR:HG22	1.29	1.13
1:A:350:THR:HG22	1:A:441:LEU:HB3	1.31	1.06
1:B:351:LEU:HG	1:B:352:PRO:HD3	1.37	1.05
3:D:1:NAG:H82	3:D:1:NAG:O3	1.53	1.05
2:C:18:ARG:HA	2:C:84:LEU:HD23	1.40	1.04
1:A:270:GLU:CG	1:A:326:LYS:HB2	1.87	1.02
1:A:240:VAL:HG11	1:A:323:VAL:HG11	1.40	1.02
2:C:46:ILE:HD11	5:G:2:FUC:C4	1.90	1.02
3:E:1:NAG:O3	3:E:1:NAG:H82	1.60	1.01
1:B:263:VAL:HB	1:B:302:VAL:O	1.64	0.98
1:A:288:GLN:HB2	1:A:306:LEU:HD12	1.44	0.97
2:C:1:ALA:CB	2:C:2:PRO:HD3	1.96	0.95
2:C:46:ILE:HD11	5:G:2:FUC:H4	0.95	0.93
1:A:270:GLU:CD	1:A:326:LYS:CB	2.44	0.91
1:B:301:ARG:HH21	3:E:2:NAG:C7	1.82	0.91
1:B:380:GLU:HB2	1:B:426:SER:HB2	1.49	0.91
1:A:388:GLU:HG2	1:A:410:LEU:HD11	1.50	0.90
2:C:46:ILE:CD1	5:G:2:FUC:C4	2.49	0.90
2:C:1:ALA:CB	2:C:2:PRO:CD	2.51	0.89
1:B:357:GLU:HG2	1:B:360:LYS:HB3	1.56	0.87
1:B:374:PRO:HD2	1:B:429:HIS:CE1	2.09	0.86
1:B:396:PRO:HA	1:B:406:LEU:HD12	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:TYR:HB2	1:A:320:THR:HB	1.56	0.85
2:C:140:GLN:HG2	4:F:1:NAG:H83	1.58	0.85
1:A:235:LEU:HD21	2:C:157:TYR:CD1	2.13	0.84
1:B:262:VAL:HA	1:B:303:VAL:HG22	1.58	0.84
1:B:240:VAL:HG23	1:B:241:PHE:N	1.91	0.83
1:A:354:PRO:HG2	1:A:357:GLU:HB3	1.61	0.82
1:A:251:LEU:HD22	1:A:435:HIS:HB3	1.62	0.80
1:A:343:PRO:HB2	1:A:430:GLU:OE2	1.82	0.79
2:C:58:ALA:HB1	2:C:84:LEU:HD11	1.66	0.78
1:B:370:LYS:HG2	1:B:371:GLY:N	1.99	0.78
1:B:343:PRO:HA	1:B:374:PRO:HG3	1.66	0.77
1:B:239:SER:O	1:B:240:VAL:HG12	1.85	0.77
1:A:357:GLU:O	1:A:359:THR:N	2.18	0.77
1:B:389:ASN:O	1:B:389:ASN:ND2	2.17	0.77
1:A:270:GLU:HG2	1:A:326:LYS:HB2	1.66	0.76
1:B:354:PRO:HG2	1:B:357:GLU:HB3	1.69	0.75
1:A:238:PRO:HB3	1:A:265:ASP:O	1.87	0.74
2:C:91:GLN:HE22	2:C:106:ARG:NH1	1.84	0.74
1:A:370:LYS:HD2	1:A:371:GLY:H	1.53	0.73
1:B:246:LYS:HB2	1:B:249:ASP:HB2	1.71	0.73
2:C:4:LYS:O	2:C:73:THR:HG22	1.89	0.73
2:C:103:ILE:HD12	2:C:138:ILE:HD11	1.70	0.73
1:A:270:GLU:OE2	1:A:326:LYS:CG	2.35	0.73
1:A:270:GLU:OE2	1:A:326:LYS:HG3	1.88	0.72
1:B:372:PHE:HB2	1:B:429:HIS:NE2	2.04	0.72
1:B:240:VAL:HB	1:B:262:VAL:O	1.90	0.72
1:A:270:GLU:OE2	1:A:326:LYS:HB2	1.88	0.72
1:B:301:ARG:NH2	3:E:2:NAG:O7	2.23	0.72
1:B:372:PHE:CE2	1:B:404:TYR:HD2	2.07	0.72
1:A:308:VAL:HG11	1:A:313:TRP:CD1	2.25	0.71
2:C:142:ASN:H	2:C:142:ASN:HD22	1.37	0.71
1:A:375:SER:O	1:A:377:ILE:HG22	1.89	0.71
1:A:338:LYS:HG2	1:A:339:THR:H	1.53	0.71
1:B:360:LYS:HG3	1:B:361:ASN:H	1.55	0.71
1:A:236:GLY:O	1:A:332:ARG:NH2	2.23	0.70
1:B:347:GLN:HE21	1:B:370:LYS:HD3	1.55	0.70
1:A:270:GLU:HG2	1:A:327:ALA:N	2.06	0.70
1:A:280:ASP:HA	1:A:318:GLU:HB2	1.71	0.70
1:B:415:SER:HA	1:B:418:GLN:HB3	1.74	0.70
2:C:63:SER:HB3	2:C:83:VAL:HA	1.74	0.70
1:A:235:LEU:HD21	2:C:157:TYR:CE1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:SER:HB3	1:B:438:GLN:HG2	1.73	0.69
1:A:309:THR:CG2	1:A:312:ASP:HB2	2.23	0.69
1:B:374:PRO:HD2	1:B:429:HIS:HE1	1.57	0.69
1:B:354:PRO:CG	1:B:357:GLU:HB3	2.23	0.68
2:C:60:ASN:H	2:C:84:LEU:HD22	1.58	0.68
1:A:350:THR:HG22	1:A:441:LEU:CB	2.17	0.67
2:C:48:THR:HG22	2:C:49:HIS:H	1.58	0.67
1:B:301:ARG:NH2	3:E:2:NAG:C7	2.57	0.67
2:C:1:ALA:HB1	2:C:2:PRO:CD	2.09	0.67
1:A:308:VAL:HG11	1:A:313:TRP:HD1	1.58	0.67
2:C:51:GLN:HG2	2:C:52:PRO:HD2	1.77	0.67
1:A:375:SER:HG	1:A:404:TYR:HE2	1.43	0.67
1:A:363:VAL:HG23	1:A:414:LYS:HA	1.76	0.67
1:B:240:VAL:HG23	1:B:241:PHE:H	1.59	0.66
1:A:409:LYS:HD3	1:A:411:THR:OG1	1.95	0.66
1:B:278:TYR:O	1:B:282:VAL:N	2.24	0.66
1:B:386:GLN:NE2	1:B:387:PRO:HD2	2.11	0.66
1:A:417:TRP:O	1:A:420:GLY:N	2.29	0.66
1:A:392:LYS:HB2	1:B:405:PHE:CZ	2.31	0.66
1:B:240:VAL:CG1	1:B:263:VAL:HA	2.27	0.65
1:A:270:GLU:OE2	1:A:326:LYS:CB	2.42	0.65
2:C:10:GLU:HB2	2:C:23:THR:OG1	1.95	0.65
1:A:370:LYS:HD3	1:A:405:PHE:HB3	1.78	0.65
1:B:345:GLU:HG3	1:B:431:ALA:O	1.97	0.65
1:A:363:VAL:O	1:A:411:THR:HA	1.97	0.64
1:B:399:ASP:OD1	1:B:400:SER:N	2.29	0.64
1:A:409:LYS:HB2	1:B:407:TYR:OH	1.97	0.64
3:D:1:NAG:O3	3:D:1:NAG:C8	2.39	0.64
1:B:314:LEU:HA	1:B:338:LYS:HD2	1.80	0.63
1:B:346:PRO:HD2	1:B:432:LEU:HB3	1.79	0.63
1:A:262:VAL:HG12	1:A:303:VAL:HG12	1.79	0.62
2:C:46:ILE:HD13	5:G:2:FUC:H4	1.69	0.62
2:C:68:CYS:HB2	2:C:76:SER:OG	1.99	0.62
1:A:364:SER:C	1:A:365:LEU:HD12	2.25	0.62
1:A:353:PRO:HG2	1:A:417:TRP:CE2	2.34	0.62
1:A:358:LEU:HD11	1:A:417:TRP:CZ3	2.35	0.62
1:B:240:VAL:CG2	1:B:241:PHE:N	2.62	0.62
2:C:68:CYS:N	2:C:76:SER:OG	2.33	0.62
1:A:355:ARG:HH21	1:B:350:THR:CG2	2.12	0.61
1:A:368:LEU:HD12	1:A:407:TYR:CE2	2.36	0.61
1:A:368:LEU:HD12	1:A:407:TYR:CZ	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:140:GLN:HG2	4:F:1:NAG:C8	2.29	0.61
1:A:266:VAL:HB	1:A:300:TYR:HB2	1.82	0.61
2:C:48:THR:HG22	2:C:49:HIS:N	2.16	0.61
2:C:85:SER:HB3	2:C:86:GLU:OE1	2.00	0.61
1:B:373:TYR:H	1:B:374:PRO:CD	2.14	0.60
1:B:374:PRO:HB2	1:B:430:GLU:HB2	1.83	0.60
1:A:350:THR:O	1:A:351:LEU:HB2	2.00	0.60
2:C:70:THR:OG1	2:C:73:THR:HB	2.01	0.60
2:C:88:LEU:HD12	2:C:109:SER:HA	1.83	0.60
1:B:378:VAL:HB	1:B:428:MET:HB2	1.84	0.60
1:A:309:THR:HG23	1:A:312:ASP:HB2	1.83	0.60
1:B:313:TRP:HZ3	1:B:338:LYS:HG3	1.66	0.60
2:C:1:ALA:HB3	2:C:2:PRO:CD	2.32	0.60
1:B:425:CYS:H	1:B:439:LYS:HB3	1.66	0.60
1:A:372:PHE:O	1:A:403:SER:HB2	2.02	0.60
2:C:109:SER:HB3	2:C:115:LEU:HD13	1.82	0.59
1:B:239:SER:C	1:B:240:VAL:CG1	2.75	0.59
1:B:353:PRO:HD3	1:B:365:LEU:HD23	1.83	0.59
1:B:309:THR:HG22	1:B:312:ASP:HB2	1.83	0.59
2:C:23:THR:HG22	2:C:55:MET:HG3	1.84	0.59
1:B:413:ASP:OD1	1:B:414:LYS:N	2.35	0.59
2:C:59:ASN:O	2:C:61:ASN:N	2.36	0.59
1:A:397:VAL:HG21	1:B:395:PRO:HD2	1.83	0.59
1:A:252:MET:O	1:A:255:ARG:N	2.18	0.59
1:A:277:TRP:CE3	1:A:306:LEU:HD22	2.38	0.58
1:B:246:LYS:NZ	3:E:7:NAG:O4	2.36	0.58
1:B:250:THR:HA	1:B:310:HIS:HD2	1.68	0.58
2:C:90:LEU:HD23	2:C:165:VAL:HG22	1.85	0.58
1:A:276:ASN:HB2	1:A:322:LYS:HB3	1.85	0.58
1:A:370:LYS:HD2	1:A:371:GLY:N	2.18	0.58
1:A:265:ASP:HA	1:A:299:THR:OG1	2.04	0.58
1:B:313:TRP:CZ3	1:B:338:LYS:HA	2.39	0.58
1:A:353:PRO:HG2	1:A:417:TRP:CZ2	2.38	0.57
1:B:277:TRP:CD1	1:B:289:THR:HG21	2.39	0.57
1:B:343:PRO:CA	1:B:374:PRO:HG3	2.34	0.57
1:B:259:VAL:HB	1:B:306:LEU:HB3	1.86	0.57
1:B:240:VAL:HG11	1:B:263:VAL:HA	1.85	0.57
1:A:357:GLU:HB2	1:B:349:TYR:CZ	2.40	0.57
2:C:142:ASN:HD22	2:C:142:ASN:N	2.04	0.56
1:A:308:VAL:HG13	1:A:319:TYR:CZ	2.39	0.56
2:C:138:ILE:HD12	2:C:145:HIS:CD2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:TRP:CE3	1:A:410:LEU:HD12	2.40	0.56
1:A:238:PRO:HD3	1:A:328:LEU:HB3	1.88	0.56
1:A:288:GLN:CB	1:A:306:LEU:HD12	2.30	0.56
1:B:294:GLU:O	1:B:301:ARG:N	2.38	0.56
1:A:357:GLU:HB2	1:B:349:TYR:CE2	2.41	0.56
1:B:293:GLU:HB2	1:B:300:TYR:HE1	1.70	0.56
1:A:278:TYR:HE1	1:A:283:GLU:HG3	1.71	0.55
1:B:353:PRO:HG2	1:B:363:VAL:HG23	1.88	0.55
1:A:363:VAL:CG2	1:A:414:LYS:HA	2.37	0.55
1:B:301:ARG:NE	3:E:2:NAG:O7	2.38	0.55
1:B:311:GLN:O	1:B:311:GLN:NE2	2.39	0.55
1:B:432:LEU:HD11	1:B:436:TYR:N	2.21	0.55
1:A:270:GLU:HG2	1:A:327:ALA:H	1.72	0.55
1:B:424:SER:HB3	1:B:438:GLN:CG	2.36	0.55
2:C:38:GLN:O	2:C:39:TRP:HB2	2.06	0.55
1:B:396:PRO:CA	1:B:406:LEU:HD12	2.32	0.55
1:B:312:ASP:OD1	1:B:317:LYS:NZ	2.39	0.55
2:C:63:SER:CB	2:C:83:VAL:HA	2.37	0.55
1:A:378:VAL:HB	1:A:428:MET:HB2	1.89	0.54
2:C:83:VAL:HG23	2:C:84:LEU:O	2.07	0.54
3:E:1:NAG:O3	3:E:1:NAG:C8	2.46	0.54
1:A:235:LEU:CD1	2:C:156:GLY:HA2	2.38	0.54
1:A:268:GLN:OE1	1:A:268:GLN:N	2.36	0.54
1:A:290:LYS:HB2	1:A:305:VAL:HG22	1.89	0.54
1:A:291:PRO:HA	1:A:303:VAL:O	2.07	0.54
1:A:314:LEU:C	1:A:316:GLY:H	2.14	0.54
1:B:245:PRO:HB3	1:B:258:GLU:H	1.73	0.54
1:B:259:VAL:O	1:B:305:VAL:HA	2.08	0.54
1:B:301:ARG:HG2	1:B:302:VAL:N	2.22	0.54
1:A:278:TYR:HD1	1:A:283:GLU:HA	1.73	0.53
1:B:293:GLU:HB2	1:B:300:TYR:CE1	2.43	0.53
1:B:250:THR:HG23	1:B:251:LEU:HD12	1.91	0.53
1:A:354:PRO:HG3	1:A:364:SER:OG	2.08	0.53
1:A:388:GLU:O	1:A:391:TYR:HE2	1.91	0.53
1:A:295:GLN:HG3	1:A:300:TYR:CE1	2.44	0.53
1:B:425:CYS:SG	1:B:439:LYS:HD3	2.48	0.53
1:B:312:ASP:HB3	1:B:319:TYR:OH	2.09	0.53
1:B:357:GLU:HG2	1:B:360:LYS:CB	2.33	0.53
2:C:142:ASN:O	2:C:144:SER:N	2.41	0.53
1:A:278:TYR:CE1	1:A:283:GLU:CG	2.92	0.53
1:B:279:VAL:HG13	1:B:282:VAL:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LYS:NZ	1:A:403:SER:OG	2.39	0.52
1:B:258:GLU:HA	1:B:306:LEU:O	2.09	0.52
1:B:290:LYS:O	1:B:304:SER:HA	2.09	0.52
1:B:429:HIS:O	1:B:435:HIS:CD2	2.62	0.52
1:B:318:GLU:HG2	1:B:337:SER:HB3	1.91	0.52
1:A:364:SER:HA	1:A:411:THR:OG1	2.09	0.52
1:A:245:PRO:HG3	1:A:313:TRP:NE1	2.24	0.52
1:A:377:ILE:HD12	1:A:428:MET:O	2.10	0.52
2:C:121:PHE:HD1	2:C:126:SER:HA	1.74	0.52
1:B:249:ASP:HB3	1:B:256:THR:O	2.10	0.52
1:A:365:LEU:O	1:A:409:LYS:HA	2.09	0.52
1:B:240:VAL:CG2	1:B:262:VAL:O	2.58	0.52
1:B:275:PHE:O	1:B:276:ASN:ND2	2.43	0.52
1:B:295:GLN:HA	1:B:300:TYR:HA	1.90	0.52
1:B:416:ARG:O	1:B:421:ASN:HB2	2.10	0.52
2:C:46:ILE:HD13	5:G:2:FUC:C3	2.41	0.51
1:B:369:VAL:HG12	1:B:372:PHE:CD1	2.46	0.51
1:B:382:ALA:N	1:B:424:SER:O	2.44	0.51
2:C:60:ASN:H	2:C:84:LEU:HB2	1.76	0.51
1:A:270:GLU:HB3	1:A:327:ALA:HB2	1.93	0.51
1:B:293:GLU:OE1	1:B:300:TYR:OH	2.29	0.50
1:A:350:THR:HG21	1:A:441:LEU:HB3	1.87	0.50
1:A:413:ASP:OD1	1:A:414:LYS:N	2.40	0.50
1:B:351:LEU:CG	1:B:352:PRO:HD3	2.26	0.50
1:B:374:PRO:CB	1:B:430:GLU:HB2	2.41	0.50
1:B:433:HIS:CG	1:B:434:ASN:H	2.29	0.50
1:B:357:GLU:C	1:B:359:THR:H	2.20	0.50
1:B:369:VAL:HG11	1:B:377:ILE:CD1	2.41	0.50
1:A:391:TYR:HA	1:A:410:LEU:HA	1.93	0.50
1:A:430:GLU:O	1:A:435:HIS:HE1	1.94	0.50
1:A:280:ASP:N	1:A:318:GLU:O	2.25	0.50
1:B:424:SER:HA	1:B:439:LYS:HB3	1.94	0.50
2:C:17:LEU:HD21	2:C:89:ALA:HB2	1.94	0.50
1:A:280:ASP:HB2	1:A:318:GLU:H	1.76	0.50
1:B:278:TYR:HA	1:B:283:GLU:O	2.12	0.50
1:B:430:GLU:O	1:B:431:ALA:HB2	2.12	0.50
2:C:30:HIS:ND1	2:C:35:ASP:HA	2.27	0.50
2:C:138:ILE:HD12	2:C:145:HIS:HD2	1.77	0.50
1:A:366:THR:HG22	1:A:367:CYS:N	2.27	0.49
1:B:381:TRP:HA	1:B:425:CYS:HA	1.94	0.49
2:C:58:ALA:C	2:C:84:LEU:HD21	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:PHE:HB2	1:A:260:THR:OG1	2.12	0.49
1:B:239:SER:C	1:B:240:VAL:HG12	2.36	0.49
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.94	0.49
1:B:373:TYR:H	1:B:374:PRO:HD2	1.78	0.49
1:B:381:TRP:CE3	1:B:410:LEU:HD22	2.48	0.49
2:C:141:ALA:HB1	2:C:145:HIS:CG	2.48	0.49
2:C:24:LEU:N	2:C:54:TYR:O	2.39	0.49
2:C:13:TRP:NE1	2:C:106:ARG:HH11	2.09	0.49
2:C:67:ARG:NH1	2:C:76:SER:O	2.46	0.49
1:A:314:LEU:C	1:A:316:GLY:N	2.71	0.49
1:A:393:THR:HG22	1:A:406:LEU:HD13	1.95	0.49
1:B:242:LEU:HB2	1:B:260:THR:O	2.13	0.49
1:B:246:LYS:HB2	1:B:249:ASP:CB	2.42	0.49
1:B:346:PRO:HG2	1:B:432:LEU:HD23	1.95	0.49
2:C:46:ILE:HD13	5:G:2:FUC:C4	2.37	0.49
1:A:346:PRO:HD3	1:A:431:ALA:HB3	1.95	0.48
2:C:60:ASN:O	2:C:62:ASP:N	2.47	0.48
1:B:360:LYS:CG	1:B:361:ASN:H	2.24	0.48
1:B:333:GLN:OE1	1:B:333:GLN:HA	2.14	0.48
1:B:350:THR:OG1	1:B:441:LEU:HD12	2.14	0.48
2:C:35:ASP:O	2:C:37:THR:HG23	2.14	0.48
2:C:59:ASN:CA	2:C:84:LEU:HD22	2.43	0.48
2:C:140:GLN:O	4:F:1:NAG:H82	2.13	0.48
1:A:238:PRO:CD	1:A:328:LEU:HB3	2.44	0.48
1:B:357:GLU:C	1:B:359:THR:N	2.69	0.48
1:B:394:THR:O	1:B:406:LEU:HD11	2.13	0.48
2:C:8:LYS:HB2	2:C:25:THR:OG1	2.14	0.48
2:C:51:GLN:HG2	2:C:52:PRO:CD	2.43	0.48
2:C:86:GLU:O	2:C:88:LEU:N	2.43	0.48
1:A:429:HIS:O	1:A:435:HIS:ND1	2.38	0.48
1:A:278:TYR:CE1	1:A:283:GLU:HG2	2.48	0.47
1:B:329:PRO:HG3	2:C:87:TRP:CD1	2.49	0.47
1:B:369:VAL:HG11	1:B:377:ILE:HD11	1.95	0.47
1:A:389:ASN:OD1	1:A:390:THR:HG23	2.15	0.47
1:B:240:VAL:HG11	1:B:263:VAL:HG22	1.95	0.47
2:C:99:GLU:HG2	2:C:142:ASN:HA	1.96	0.47
2:C:37:THR:HG21	2:C:52:PRO:HG3	1.96	0.47
1:A:252:MET:HE2	1:A:252:MET:HB3	1.81	0.47
2:C:24:LEU:HB2	2:C:54:TYR:HB3	1.96	0.47
1:A:293:GLU:HA	1:A:302:VAL:HG22	1.97	0.47
1:A:392:LYS:CB	1:B:405:PHE:HZ	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:LYS:HA	1:B:332:ARG:O	2.15	0.47
2:C:58:ALA:CB	2:C:84:LEU:HD21	2.45	0.47
2:C:103:ILE:HB	2:C:138:ILE:HG12	1.97	0.47
1:A:251:LEU:HD22	1:A:435:HIS:CB	2.40	0.47
1:A:262:VAL:HG12	1:A:303:VAL:CG1	2.44	0.47
1:B:325:ASN:OD1	1:B:326:LYS:N	2.48	0.47
2:C:16:VAL:HG23	2:C:84:LEU:HG	1.97	0.47
1:A:310:HIS:O	1:A:314:LEU:HD12	2.15	0.46
1:A:392:LYS:CB	1:B:405:PHE:CZ	2.98	0.46
1:A:240:VAL:HG12	1:A:263:VAL:HG22	1.97	0.46
1:B:273:VAL:HB	1:B:275:PHE:HE1	1.79	0.46
1:A:240:VAL:HG11	1:A:323:VAL:CG1	2.29	0.46
1:B:240:VAL:HB	1:B:263:VAL:HA	1.96	0.46
1:B:427:VAL:HG12	1:B:429:HIS:H	1.80	0.46
2:C:60:ASN:C	2:C:62:ASP:H	2.24	0.46
1:A:278:TYR:HE1	1:A:283:GLU:CG	2.28	0.46
1:B:240:VAL:CB	1:B:262:VAL:O	2.60	0.46
1:A:243:PHE:CZ	3:D:6:MAN:H2	2.51	0.46
1:B:351:LEU:HG	1:B:352:PRO:CD	2.26	0.46
2:C:148:ASP:OD1	2:C:148:ASP:N	2.48	0.46
1:A:369:VAL:HG12	1:A:372:PHE:CE2	2.51	0.46
2:C:60:ASN:N	2:C:84:LEU:HD22	2.29	0.46
1:B:257:PRO:O	1:B:307:THR:HA	2.16	0.46
2:C:31:SER:O	2:C:33:ASP:N	2.49	0.46
2:C:117:LYS:O	2:C:153:GLY:HA2	2.16	0.45
1:A:344:ARG:HB3	1:A:371:GLY:O	2.16	0.45
1:A:407:TYR:CD2	1:B:407:TYR:HD2	2.35	0.45
1:B:328:LEU:HG	1:B:329:PRO:HD2	1.96	0.45
1:B:363:VAL:O	1:B:411:THR:HG22	2.16	0.45
1:B:386:GLN:HE21	1:B:387:PRO:HD2	1.80	0.45
2:C:10:GLU:OE1	2:C:10:GLU:HA	2.16	0.45
1:B:229:CYS:HB3	1:B:230:PRO:CD	2.47	0.45
1:A:309:THR:HG22	1:A:312:ASP:HB2	1.99	0.45
1:A:391:TYR:HA	1:A:409:LYS:O	2.17	0.45
1:B:258:GLU:O	1:B:258:GLU:HG2	2.16	0.45
1:A:252:MET:O	1:A:254:SER:N	2.50	0.44
1:A:279:VAL:HG23	1:A:284:VAL:HB	1.99	0.44
1:A:296:PHE:HB3	1:A:297:ASN:H	1.55	0.44
1:A:375:SER:OG	1:A:404:TYR:HE2	1.98	0.44
1:B:263:VAL:O	1:B:263:VAL:HG12	2.17	0.44
1:B:273:VAL:HG21	1:B:302:VAL:HG11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:91:GLN:NE2	2:C:106:ARG:NH1	2.61	0.44
1:B:240:VAL:CB	1:B:263:VAL:HA	2.48	0.44
1:B:311:GLN:NE2	1:B:315:ASN:OD1	2.50	0.44
1:B:290:LYS:HE2	1:B:305:VAL:HG23	2.00	0.44
1:B:291:PRO:O	1:B:292:ARG:HB3	2.18	0.44
2:C:86:GLU:OE1	2:C:86:GLU:N	2.50	0.44
1:A:245:PRO:CD	1:A:313:TRP:HE1	2.30	0.44
1:A:288:GLN:HG2	1:A:307:THR:OG1	2.17	0.44
1:B:363:VAL:HG22	1:B:365:LEU:HG	1.99	0.44
1:A:308:VAL:HG13	1:A:319:TYR:OH	2.17	0.44
1:A:278:TYR:CE1	1:A:283:GLU:HG3	2.52	0.44
1:A:412:VAL:HG22	1:A:413:ASP:N	2.33	0.44
1:B:392:LYS:HA	1:B:392:LYS:HD3	1.67	0.44
1:B:390:THR:HG21	1:B:411:THR:O	2.17	0.43
1:B:313:TRP:CH2	1:B:338:LYS:HA	2.52	0.43
1:B:368:LEU:HG	1:B:407:TYR:CE1	2.53	0.43
1:B:433:HIS:CG	1:B:434:ASN:N	2.84	0.43
1:B:433:HIS:ND1	1:B:434:ASN:N	2.66	0.43
1:A:352:PRO:O	1:B:351:LEU:HD21	2.18	0.43
1:A:359:THR:OG1	1:A:360:LYS:N	2.51	0.43
2:C:59:ASN:HA	2:C:84:LEU:HD22	1.99	0.43
1:A:235:LEU:CD1	2:C:156:GLY:C	2.91	0.43
1:B:425:CYS:H	1:B:439:LYS:CB	2.29	0.43
1:B:354:PRO:HG2	1:B:357:GLU:H	1.84	0.43
2:C:16:VAL:O	2:C:84:LEU:HA	2.18	0.43
1:A:245:PRO:HB3	1:A:258:GLU:O	2.19	0.43
2:C:48:THR:CG2	2:C:49:HIS:H	2.27	0.43
2:C:63:SER:HB3	2:C:83:VAL:HG12	1.99	0.43
1:B:274:LYS:HB2	1:B:324:SER:HB2	2.01	0.43
2:C:82:THR:O	2:C:83:VAL:HG22	2.19	0.43
1:A:430:GLU:HG3	1:A:431:ALA:N	2.33	0.42
1:B:290:LYS:HB2	1:B:305:VAL:HG22	2.00	0.42
2:C:23:THR:CG2	2:C:55:MET:HG3	2.46	0.42
4:F:1:NAG:H4	4:F:2:NAG:N2	2.34	0.42
1:A:245:PRO:HG3	1:A:313:TRP:HE1	1.84	0.42
1:A:436:TYR:CD1	1:A:436:TYR:C	2.96	0.42
1:B:264:VAL:HG12	1:B:265:ASP:N	2.35	0.42
1:A:286:ASN:HB3	1:A:287:ALA:H	1.71	0.42
1:B:279:VAL:N	1:B:320:THR:OG1	2.52	0.42
1:B:301:ARG:CZ	3:E:2:NAG:O7	2.66	0.42
2:C:48:THR:O	2:C:49:HIS:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:THR:HA	1:B:310:HIS:CD2	2.50	0.42
1:B:348:VAL:C	1:B:349:TYR:HD1	2.26	0.42
2:C:4:LYS:HA	2:C:4:LYS:HD3	1.88	0.42
1:A:313:TRP:CZ3	1:A:338:LYS:HG3	2.53	0.42
1:A:350:THR:H	1:A:351:LEU:HD12	1.85	0.42
2:C:10:GLU:C	2:C:10:GLU:CD	2.85	0.42
1:A:242:LEU:HD12	1:A:242:LEU:HA	1.71	0.42
1:A:365:LEU:HD13	1:A:412:VAL:H	1.84	0.42
1:A:407:TYR:CG	1:B:407:TYR:HD2	2.37	0.42
1:B:426:SER:HB3	1:B:436:TYR:CE2	2.53	0.42
2:C:13:TRP:HA	2:C:92:THR:O	2.19	0.42
1:A:261:CYS:HB2	1:A:277:TRP:CH2	2.55	0.42
1:A:388:GLU:HG3	1:A:389:ASN:H	1.85	0.42
1:A:398:LEU:HA	1:A:404:TYR:CD1	2.54	0.42
1:B:253:ILE:O	1:B:310:HIS:CE1	2.73	0.42
1:B:297:ASN:HB3	1:B:298:SER:H	1.45	0.42
1:B:374:PRO:CD	1:B:429:HIS:CE1	2.95	0.42
1:B:389:ASN:HD22	1:B:389:ASN:C	2.14	0.42
2:C:48:THR:CG2	2:C:49:HIS:N	2.83	0.42
2:C:33:ASP:N	2:C:33:ASP:OD1	2.52	0.42
1:A:249:ASP:OD1	1:A:255:ARG:HG2	2.20	0.42
1:A:344:ARG:O	1:A:431:ALA:HB2	2.20	0.42
1:A:392:LYS:HB2	1:B:405:PHE:CE2	2.55	0.42
1:A:392:LYS:HB2	1:B:405:PHE:HZ	1.79	0.42
1:B:398:LEU:HG	1:B:404:TYR:CE1	2.54	0.42
2:C:40:PHE:CD1	2:C:45:LEU:HA	2.55	0.42
1:A:295:GLN:OE1	1:A:295:GLN:N	2.46	0.42
1:A:299:THR:OG1	1:A:300:TYR:N	2.48	0.42
1:A:365:LEU:CD1	1:A:412:VAL:HG12	2.49	0.42
1:B:382:ALA:O	1:B:423:PHE:HA	2.20	0.42
1:B:432:LEU:HD13	1:B:437:THR:HG23	2.00	0.42
2:C:13:TRP:HE1	2:C:106:ARG:HH11	1.68	0.42
2:C:121:PHE:HB2	2:C:150:HIS:CE1	2.55	0.42
1:A:248:LYS:NZ	1:A:249:ASP:OD1	2.53	0.41
1:A:380:GLU:C	1:A:381:TRP:CD1	2.98	0.41
1:B:329:PRO:HG3	2:C:87:TRP:CG	2.54	0.41
1:B:348:VAL:O	1:B:349:TYR:HD1	2.02	0.41
1:B:404:TYR:O	1:B:405:PHE:HB3	2.20	0.41
1:A:290:LYS:O	1:A:304:SER:HA	2.20	0.41
1:A:345:GLU:HA	1:A:431:ALA:HB3	2.02	0.41
2:C:3:PRO:HG2	2:C:73:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:23:THR:HA	2:C:54:TYR:O	2.20	0.41
2:C:97:PHE:CD1	2:C:97:PHE:N	2.88	0.41
1:A:238:PRO:HG3	1:A:325:ASN:HD22	1.85	0.41
1:A:355:ARG:NH2	1:A:356:GLU:OE2	2.54	0.41
2:C:3:PRO:O	2:C:74:SER:HB2	2.20	0.41
1:A:430:GLU:HA	1:A:435:HIS:CE1	2.55	0.41
2:C:94:HIS:O	2:C:95:LEU:HD23	2.20	0.41
1:A:245:PRO:CG	1:A:313:TRP:HE1	2.34	0.41
1:B:309:THR:CG2	1:B:312:ASP:HB2	2.47	0.41
1:B:360:LYS:HG3	1:B:361:ASN:N	2.30	0.41
2:C:98:ARG:O	2:C:99:GLU:C	2.63	0.41
1:B:257:PRO:HG2	1:B:308:VAL:O	2.21	0.41
1:B:424:SER:HA	1:B:439:LYS:HE3	2.01	0.41
1:A:354:PRO:O	1:A:358:LEU:HB2	2.21	0.41
1:A:364:SER:O	1:A:365:LEU:HD12	2.20	0.41
1:B:277:TRP:NE1	1:B:289:THR:HG21	2.36	0.41
2:C:60:ASN:C	2:C:62:ASP:N	2.79	0.41
1:A:261:CYS:HB2	1:A:277:TRP:CZ2	2.56	0.41
1:B:239:SER:O	1:B:240:VAL:CG1	2.62	0.41
1:B:371:GLY:C	1:B:403:SER:HB2	2.46	0.40
1:B:374:PRO:CD	1:B:429:HIS:HE1	2.31	0.40
2:C:97:PHE:O	2:C:101:GLU:HB2	2.21	0.40
2:C:146:SER:OG	2:C:168:THR:HA	2.20	0.40
1:A:338:LYS:HG2	1:A:339:THR:N	2.29	0.40
1:A:234:LEU:HD12	1:A:235:LEU:H	1.86	0.40
1:A:266:VAL:HB	1:A:300:TYR:CB	2.52	0.40
1:B:369:VAL:HG12	1:B:372:PHE:CE1	2.56	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	211/223 (95%)	146 (69%)	43 (20%)	22 (10%)	0	2
1	B	213/223 (96%)	141 (66%)	50 (24%)	22 (10%)	0	2
2	C	171/174 (98%)	130 (76%)	24 (14%)	17 (10%)	0	2
All	All	595/620 (96%)	417 (70%)	117 (20%)	61 (10%)	0	2

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	279	VAL
1	B	291	PRO
1	B	373	TYR
1	B	433	HIS
2	C	1	ALA
2	C	5	ALA
2	C	41	HIS
2	C	60	ASN
2	C	83	VAL
2	C	87	TRP
1	A	329	PRO
1	A	393	THR
1	A	442	SER
1	B	240	VAL
1	B	265	ASP
1	B	352	PRO
1	B	401	ASP
1	B	413	ASP
1	B	431	ALA
2	C	85	SER
2	C	143	HIS
1	A	236	GLY
1	A	271	PRO
1	A	291	PRO
1	A	298	SER
1	A	337	SER
1	A	383	SER
1	A	411	THR
1	A	443	LEU
1	B	253	ILE
1	B	375	SER
1	B	391	TYR
2	C	98	ARG
1	A	234	LEU

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Mol	Chain	Res	Type
1	A	350	THR
1	A	351	LEU
1	A	400	SER
1	B	231	ALA
1	B	432	LEU
2	C	3	PRO
2	C	32	PRO
2	C	99	GLU
1	A	334	LYS
1	A	358	LEU
1	A	359	THR
1	B	241	PHE
1	B	292	ARG
1	B	316	GLY
1	B	374	PRO
2	C	38	GLN
2	C	58	ALA
2	C	69	GLN
2	C	144	SER
1	A	253	ILE
1	A	315	ASN
1	A	418	GLN
1	B	377	ILE
1	A	352	PRO
1	B	346	PRO
1	B	282	VAL
2	C	10	GLU

### 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	198/207 (96%)	195 (98%)	3 (2%)	57	76
1	B	200/207 (97%)	199 (100%)	1 (0%)	81	85
2	C	154/155 (99%)	151 (98%)	3 (2%)	50	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	552/569 (97%)	545 (99%)	7 (1%)	61 78

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	297	ASN
1	A	298	SER
1	A	350	THR
1	B	240	VAL
2	C	59	ASN
2	C	68	CYS
2	C	142	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	310	HIS
1	B	311	GLN
1	B	347	GLN
1	B	386	GLN
1	B	435	HIS
2	C	59	ASN
2	C	80	HIS
2	C	91	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](#)

21 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	D	1	1,3	14,14,15	0.47	0	17,19,21	0.52	0
3	NAG	D	2	3	14,14,15	0.28	0	17,19,21	0.43	0
3	BMA	D	3	3	11,11,12	0.95	0	15,15,17	1.35	2 (13%)
3	MAN	D	4	3	11,11,12	1.62	2 (18%)	15,15,17	1.56	2 (13%)
3	NAG	D	5	3	14,14,15	0.18	0	17,19,21	0.46	0
3	MAN	D	6	3	11,11,12	0.99	1 (9%)	15,15,17	0.99	0
3	NAG	D	7	3	14,14,15	1.19	1 (7%)	17,19,21	1.21	1 (5%)
3	FUC	D	8	3	10,10,11	0.75	0	14,14,16	0.85	0
3	NAG	E	1	1,3	14,14,15	0.46	0	17,19,21	0.50	0
3	NAG	E	2	3	14,14,15	0.54	0	17,19,21	0.69	0
3	BMA	E	3	3	11,11,12	0.69	0	15,15,17	1.40	4 (26%)
3	MAN	E	4	3	11,11,12	1.39	2 (18%)	15,15,17	1.20	2 (13%)
3	NAG	E	5	3	14,14,15	0.31	0	17,19,21	0.47	0
3	MAN	E	6	3	11,11,12	0.82	0	15,15,17	1.10	1 (6%)
3	NAG	E	7	3	14,14,15	0.63	1 (7%)	17,19,21	0.60	0
3	FUC	E	8	3	10,10,11	0.78	0	14,14,16	0.97	0
4	NAG	F	1	2,4	14,14,15	0.66	0	17,19,21	1.08	1 (5%)
4	NAG	F	2	4	14,14,15	0.81	1 (7%)	17,19,21	0.51	0
4	FUC	F	3	4	10,10,11	0.93	0	14,14,16	0.79	0
5	NAG	G	1	2,5	14,14,15	0.33	0	17,19,21	0.53	0
5	FUC	G	2	5	10,10,11	0.93	0	14,14,16	0.79	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	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
3	NAG	D	5	3	-	1/6/23/26	0/1/1/1
3	MAN	D	6	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	7	3	-	4/6/23/26	0/1/1/1
3	FUC	D	8	3	-	-	0/1/1/1
3	NAG	E	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	1/2/19/22	0/1/1/1
3	NAG	E	5	3	-	2/6/23/26	0/1/1/1
3	MAN	E	6	3	-	2/2/19/22	0/1/1/1
3	NAG	E	7	3	-	4/6/23/26	0/1/1/1
3	FUC	E	8	3	-	-	0/1/1/1
4	NAG	F	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	FUC	F	3	4	-	-	0/1/1/1
5	NAG	G	1	2,5	-	3/6/23/26	0/1/1/1
5	FUC	G	2	5	-	-	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4	MAN	O5-C1	-3.94	1.37	1.43
3	D	7	NAG	O5-C1	-3.71	1.37	1.43
3	E	4	MAN	C2-C3	2.91	1.56	1.52
4	F	2	NAG	C1-C2	2.63	1.55	1.52
3	E	4	MAN	O5-C1	-2.62	1.39	1.43
3	D	4	MAN	C2-C3	2.41	1.56	1.52
3	D	6	MAN	O5-C1	-2.13	1.40	1.43
3	E	7	NAG	C1-C2	2.01	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	MAN	O3-C3-C2	3.44	117.08	110.05
3	E	6	MAN	O2-C2-C3	-3.37	103.17	110.15
3	E	4	MAN	O3-C3-C2	3.33	116.86	110.05
3	D	7	NAG	C4-C3-C2	3.07	115.52	111.02
3	E	3	BMA	C1-C2-C3	2.75	113.65	109.64
3	D	4	MAN	C1-C2-C3	-2.69	105.73	109.64
3	E	4	MAN	C1-C2-C3	-2.66	105.78	109.64
3	E	3	BMA	C1-O5-C5	2.47	115.49	112.19
4	F	1	NAG	C1-O5-C5	2.42	115.44	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	BMA	O3-C3-C4	-2.17	105.27	110.38
3	D	3	BMA	O2-C2-C3	-2.13	105.74	110.15
3	E	3	BMA	O2-C2-C3	-2.10	105.79	110.15
3	E	3	BMA	C3-C4-C5	2.05	113.95	110.23

There are no chirality outliers.

All (33) torsion outliers are listed below:

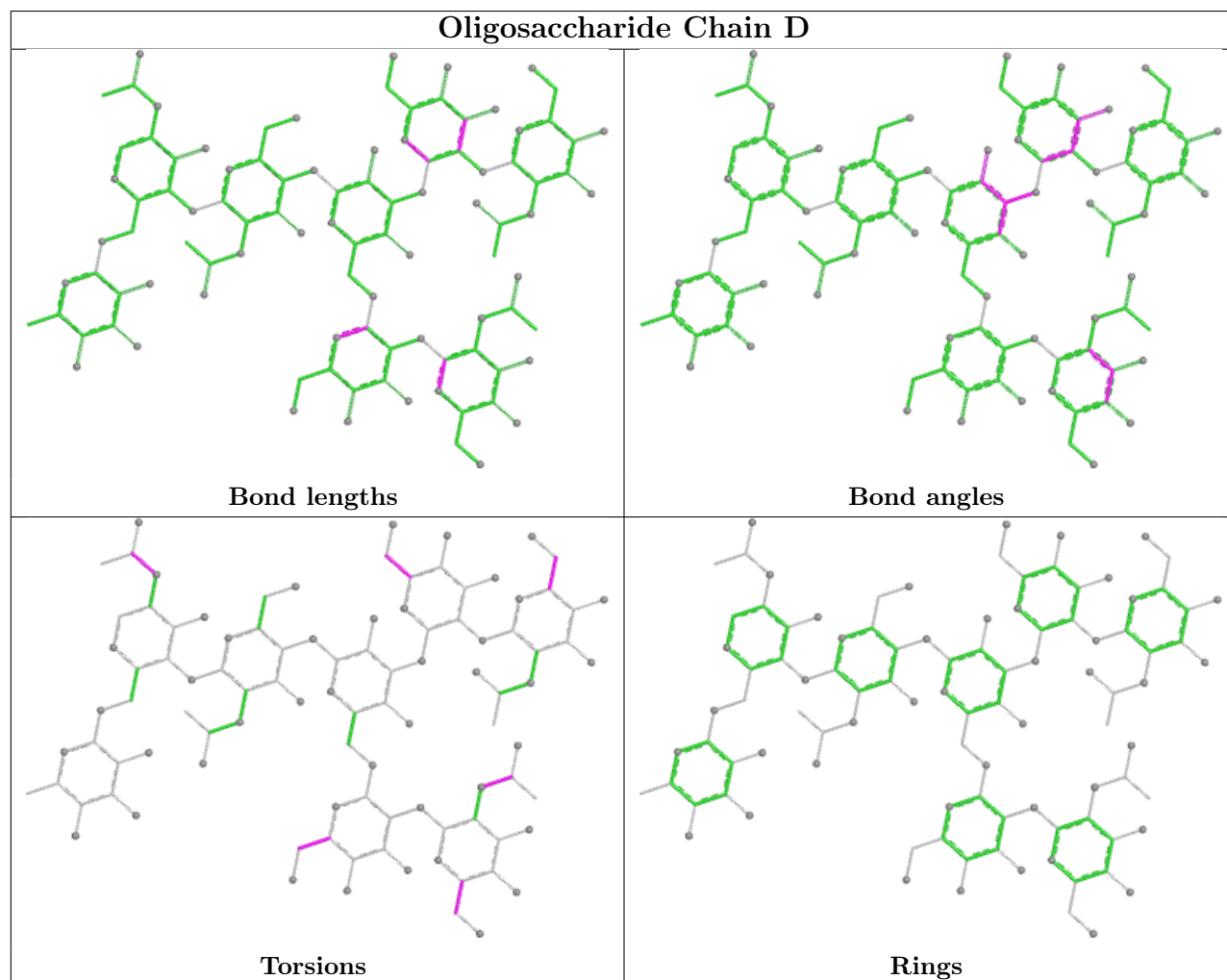
Mol	Chain	Res	Type	Atoms
4	F	1	NAG	C3-C2-N2-C7
4	F	2	NAG	O5-C5-C6-O6
3	E	7	NAG	O5-C5-C6-O6
3	E	5	NAG	O5-C5-C6-O6
3	E	6	MAN	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	D	6	MAN	C4-C5-C6-O6
3	E	7	NAG	C4-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6
3	D	7	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
3	D	6	MAN	O5-C5-C6-O6
3	E	6	MAN	O5-C5-C6-O6
3	E	5	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	7	NAG	C8-C7-N2-C2
3	D	7	NAG	O7-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	7	NAG	C8-C7-N2-C2
3	E	7	NAG	O7-C7-N2-C2
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
3	D	7	NAG	C4-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
3	D	5	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6

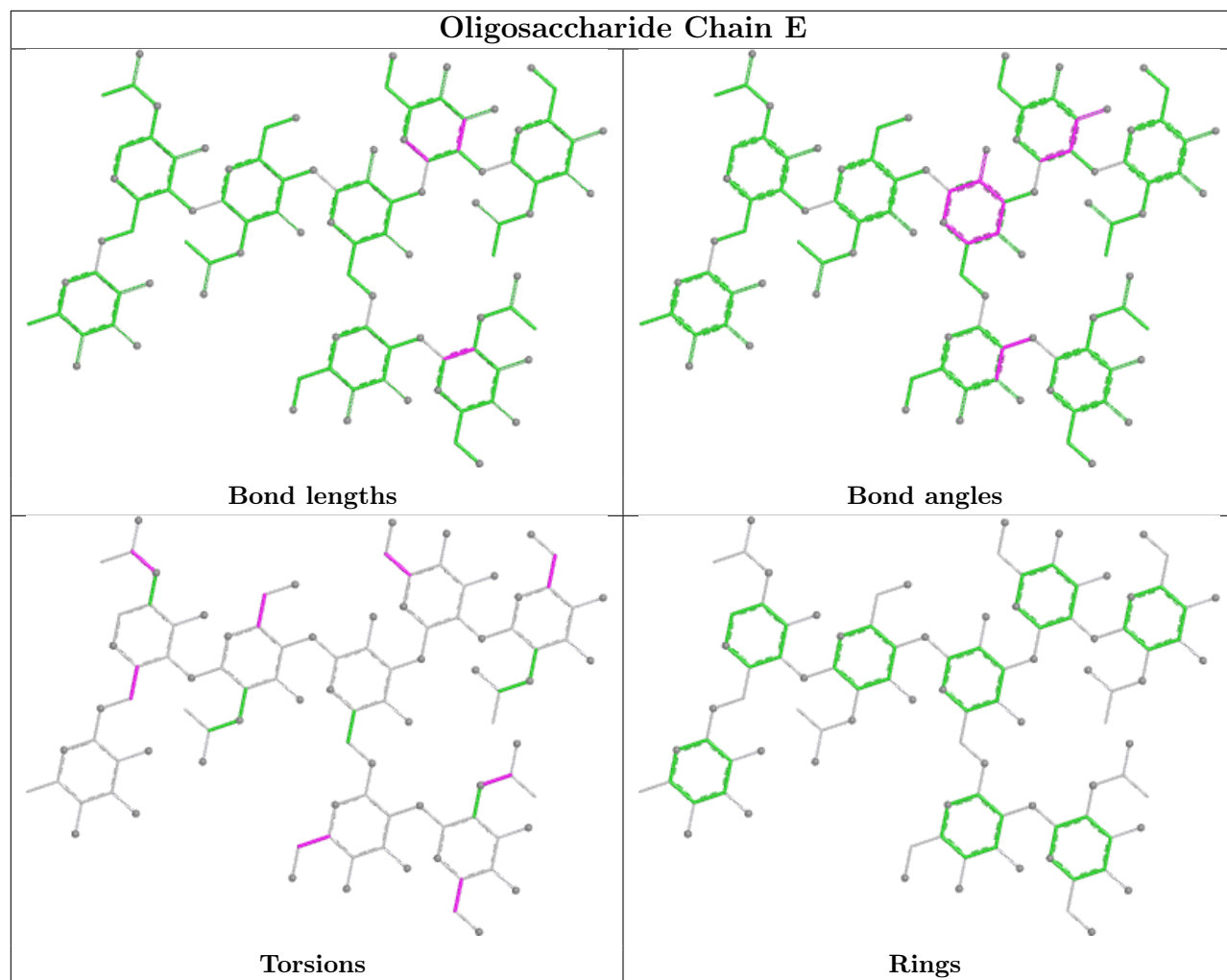
There are no ring outliers.

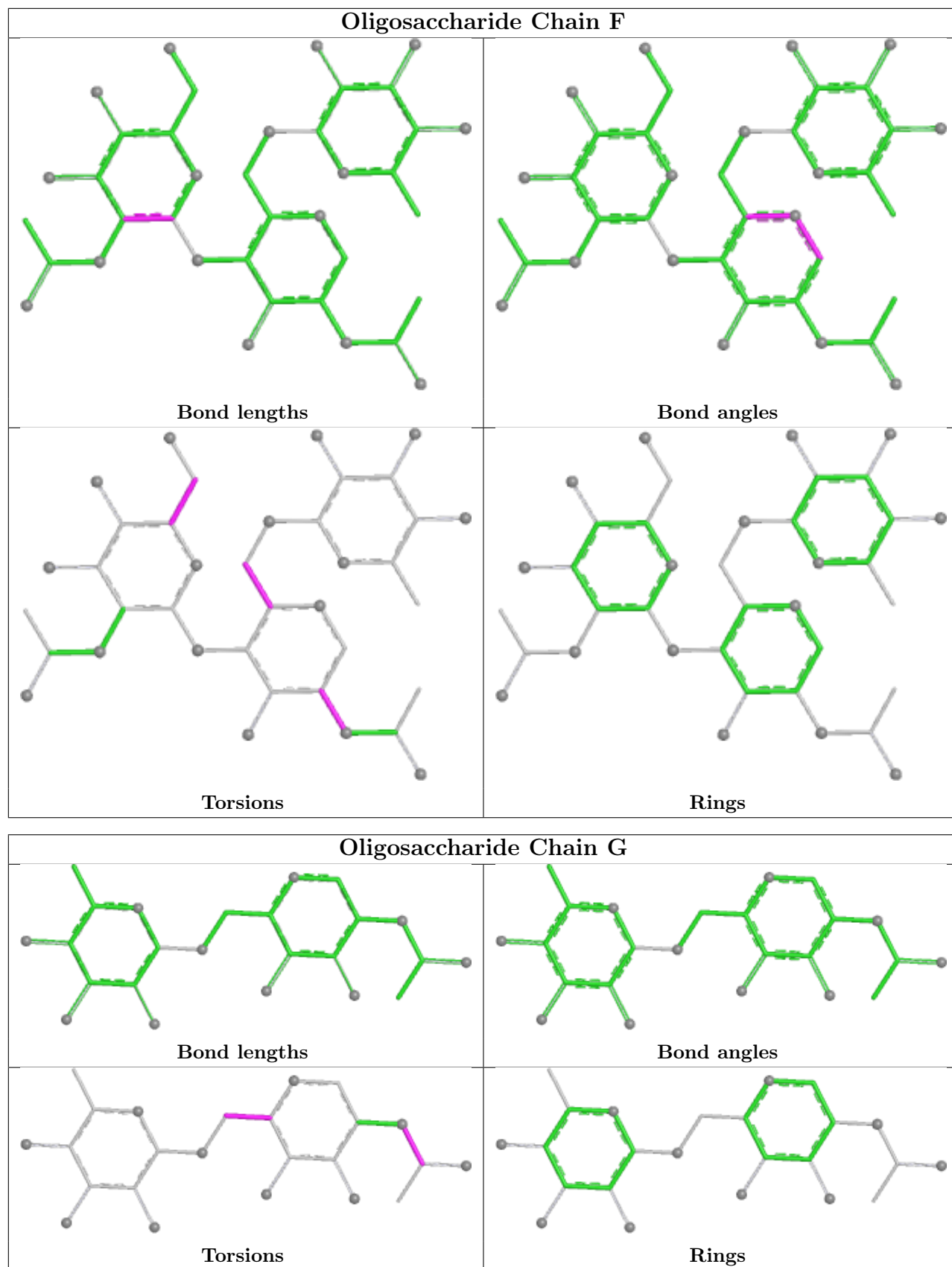
8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2	NAG	1	0
4	F	1	NAG	4	0
3	E	2	NAG	5	0
3	E	7	NAG	1	0
3	D	1	NAG	2	0
3	D	6	MAN	1	0
5	G	2	FUC	7	0
3	E	1	NAG	2	0

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







## 5.6 Ligand geometry

1 ligand is 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	$\# Z  > 2$
6	MPD	A	501	-	7,7,7	0.27	0	9,10,10	0.36	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
6	MPD	A	501	-	-	3/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	501	MPD	C1-C2-C3-C4
6	A	501	MPD	O2-C2-C3-C4
6	A	501	MPD	CM-C2-C3-C4

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	213/223 (95%)	0.73	23 (10%) 11 7	55, 141, 254, 290	0
1	B	215/223 (96%)	0.97	30 (13%) 6 5	92, 182, 258, 287	0
2	C	173/174 (99%)	0.20	3 (1%) 69 49	61, 89, 152, 196	0
All	All	601/620 (96%)	0.66	56 (9%) 14 9	55, 141, 251, 290	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	426	SER	5.2
1	B	425	CYS	4.8
1	A	352	PRO	4.5
1	B	379	VAL	3.8
1	A	412	VAL	3.7
1	A	351	LEU	3.6
1	B	365	LEU	3.4
1	A	385	GLY	3.4
1	B	412	VAL	3.2
2	C	1	ALA	3.2
1	B	378	VAL	3.2
1	A	287	ALA	3.2
1	B	368	LEU	3.1
1	B	366	THR	3.0
1	A	440	SER	3.0
1	A	270	GLU	2.9
1	A	366	THR	2.9
1	B	408	SER	2.9
1	B	406	LEU	2.9
1	B	364	SER	2.8
1	B	437	THR	2.7
2	C	141	ALA	2.6
1	A	364	SER	2.6

*Continued on next page...*



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Mol	Chain	Res	Type	RSRZ
1	B	391	TYR	2.6
1	B	427	VAL	2.5
1	B	369	VAL	2.5
1	A	297	ASN	2.5
1	A	442	SER	2.5
1	A	411	THR	2.5
1	A	286	ASN	2.4
1	B	394	THR	2.4
1	A	298	SER	2.4
1	A	441	LEU	2.4
1	B	367	CYS	2.4
1	B	359	THR	2.3
1	B	441	LEU	2.3
1	A	248	LYS	2.3
1	B	348	VAL	2.3
1	A	354	PRO	2.2
1	B	398	LEU	2.2
1	A	369	VAL	2.2
1	A	378	VAL	2.2
1	A	395	PRO	2.2
1	B	381	TRP	2.2
1	B	409	LYS	2.2
2	C	82	THR	2.2
1	A	406	LEU	2.2
1	B	346	PRO	2.2
1	B	389	ASN	2.2
1	A	353	PRO	2.2
1	B	236	GLY	2.2
1	B	433	HIS	2.2
1	B	424	SER	2.1
1	B	352	PRO	2.1
1	A	368	LEU	2.1
1	B	260	THR	2.0

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

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

### 6.3 Carbohydrates ⓘ

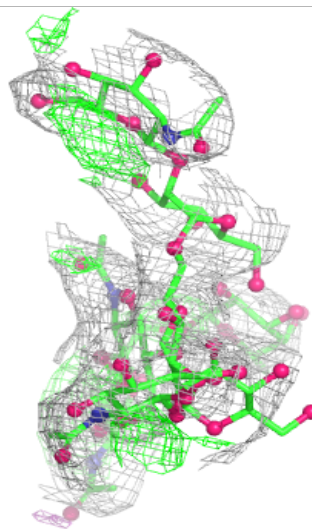
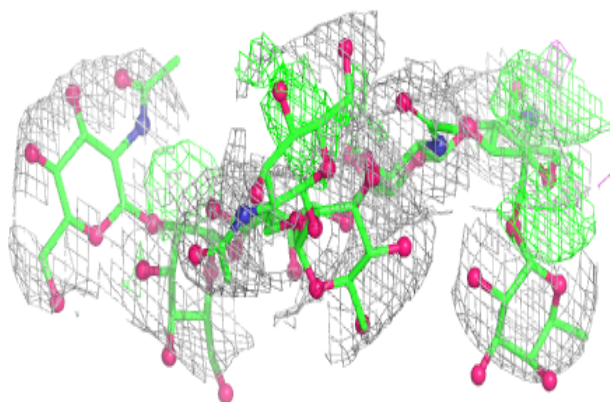
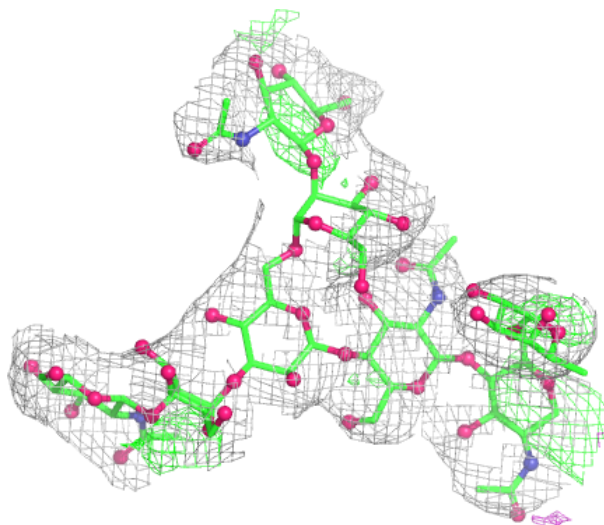
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	E	7	14/15	0.46	0.15	124,152,161,177	0
4	NAG	F	2	14/15	0.48	0.14	205,258,288,301	0
4	NAG	F	1	14/15	0.51	0.15	141,200,229,252	0
3	NAG	E	1	14/15	0.53	0.16	134,156,179,200	0
4	FUC	F	3	10/11	0.53	0.11	235,246,255,261	0
5	NAG	G	1	14/15	0.58	0.10	136,178,191,197	0
3	FUC	E	8	10/11	0.59	0.13	154,179,192,212	0
3	MAN	D	4	11/12	0.65	0.18	117,147,168,170	0
5	FUC	G	2	10/11	0.68	0.35	171,197,209,210	0
3	MAN	E	4	11/12	0.76	0.15	148,179,211,213	0
3	NAG	E	5	14/15	0.77	0.10	143,168,190,193	0
3	NAG	D	5	14/15	0.78	0.11	127,144,162,163	0
3	BMA	E	3	11/12	0.80	0.10	127,142,151,163	0
3	FUC	D	8	10/11	0.80	0.20	77,107,140,178	0
3	MAN	E	6	11/12	0.81	0.09	122,129,143,145	0
3	NAG	E	2	14/15	0.81	0.12	112,141,161,165	0
3	NAG	D	7	14/15	0.82	0.15	83,118,134,135	0
3	NAG	D	1	14/15	0.86	0.17	65,87,123,139	0
3	NAG	D	2	14/15	0.92	0.12	72,90,105,105	0
3	BMA	D	3	11/12	0.93	0.07	75,83,104,106	0
3	MAN	D	6	11/12	0.94	0.09	49,65,113,115	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.

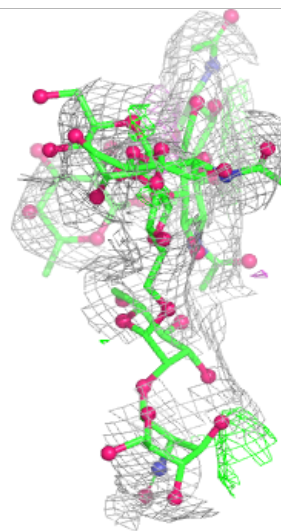
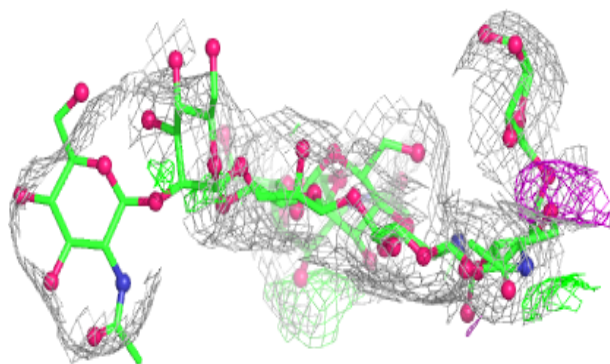
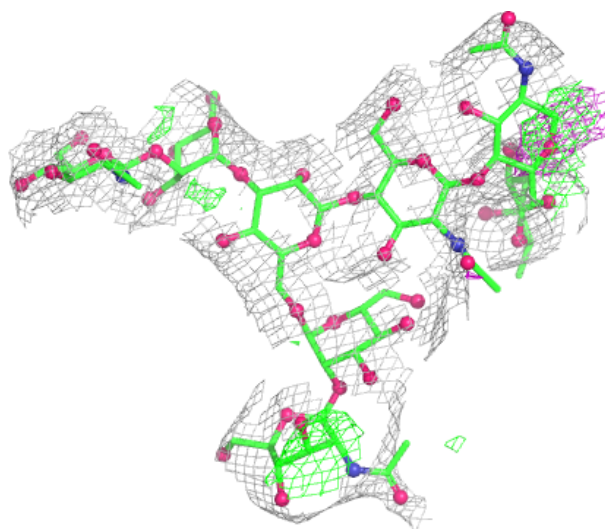
**Electron density around Chain D:**

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



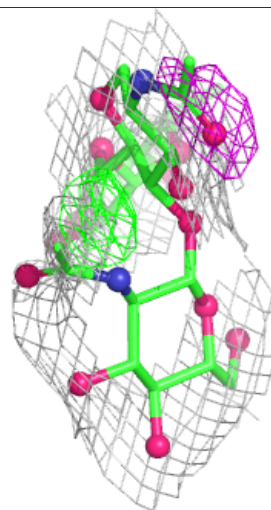
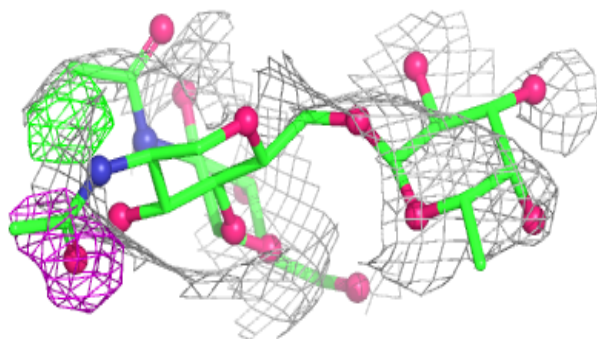
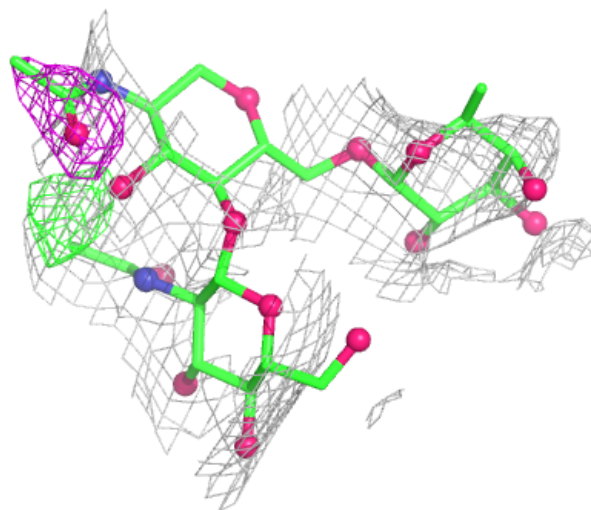
**Electron density around Chain E:**

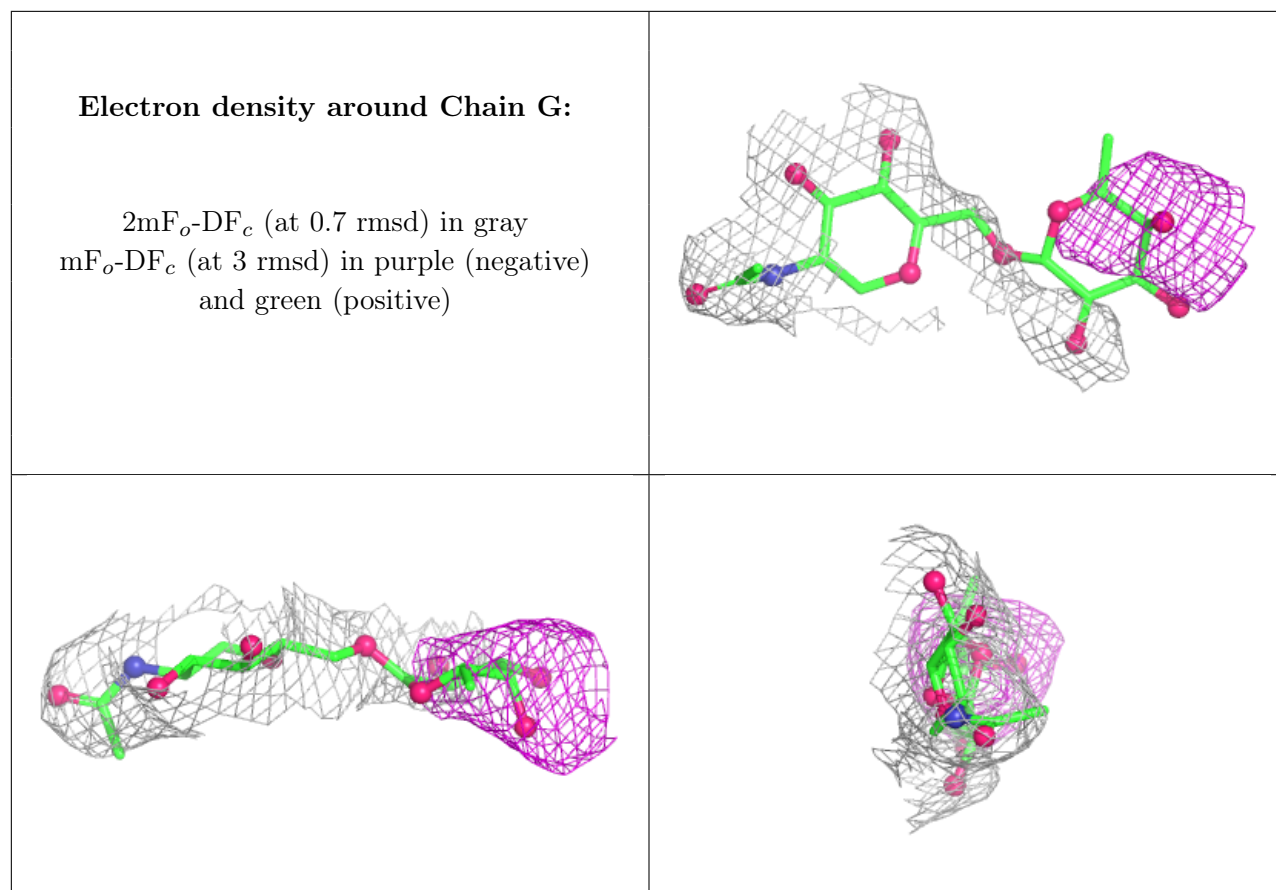
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 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
6	MPD	A	501	8/8	0.86	0.23	20,20,20,20	8

## 6.5 Other polymers [i](#)

There are no such residues in this entry.