



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:51 AM UTC

PDB ID : 9ELW / pdb_00009elw
Title : CRYSTAL STRUCTURE OF RHESUS MACAQUE (MACACA MULATTA)
IGG1 FC FRAGMENT- FC-GAMMA RECEPTOR IIA COMPLEX H131
VARIANT
Authors : Tolbert, W.D.; Pazgier, M.
Deposited on : 2024-12-05
Resolution : 3.55 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

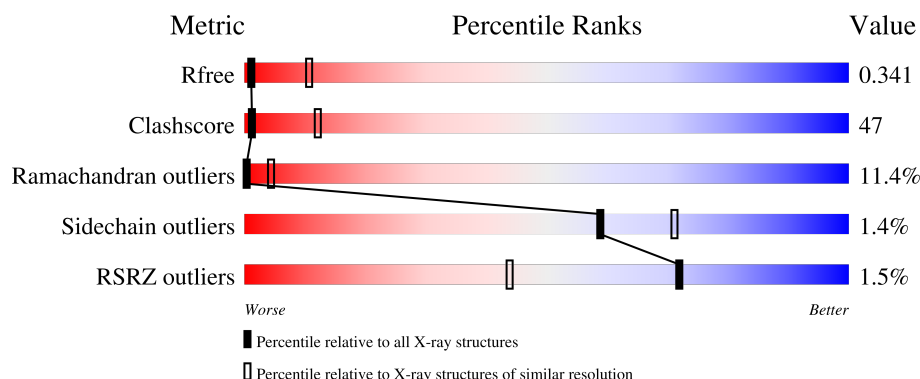
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	224	<div> <div>27%</div> <div>59%</div> <div>9%</div> <div>.</div> </div>
1	B	224	<div> <div>2%</div> <div>34%</div> <div>54%</div> <div>6%</div> <div>.</div> </div>
2	C	174	<div> <div>2%</div> <div>45%</div> <div>44%</div> <div>10%</div> <div>.</div> </div>
3	D	9	<div> <div>33%</div> <div>33%</div> <div>33%</div> </div>
3	E	9	<div> <div>22%</div> <div>56%</div> <div>22%</div> </div>

Continued on next page...

Continued from previous page...

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

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5051 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 IgG1 Fc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1701	1080	285	330	6			
1	B	214	Total	C	N	O	S	0	0	0
			1701	1080	285	330	6			

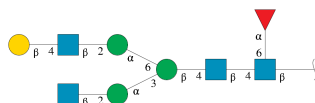
- Molecule 2 is a protein called IgG receptor IIA H131 variant Fc fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	174	Total	C	N	O	S	0	0	0
			1367	861	241	258	7			

There is a discrepancy between the modelled and reference sequences:

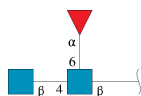
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	insertion	UNP F6TRF8

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]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	9	Total	C	N	O	0	0	0
			110	62	4	44			
3	E	9	Total	C	N	O	0	0	0
			110	62	4	44			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	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.

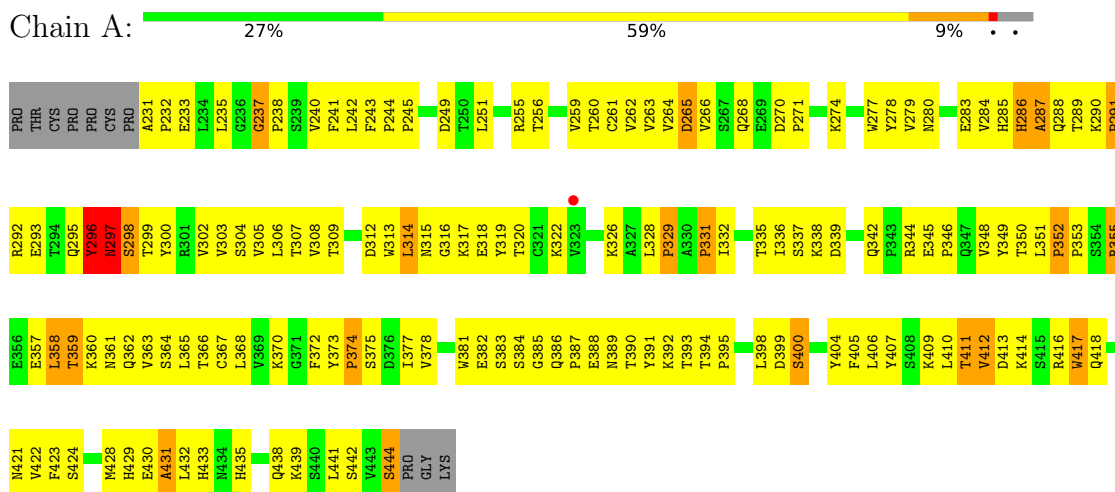


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	2	Total	C	N	O	0	0	0
			24	14	1	9			

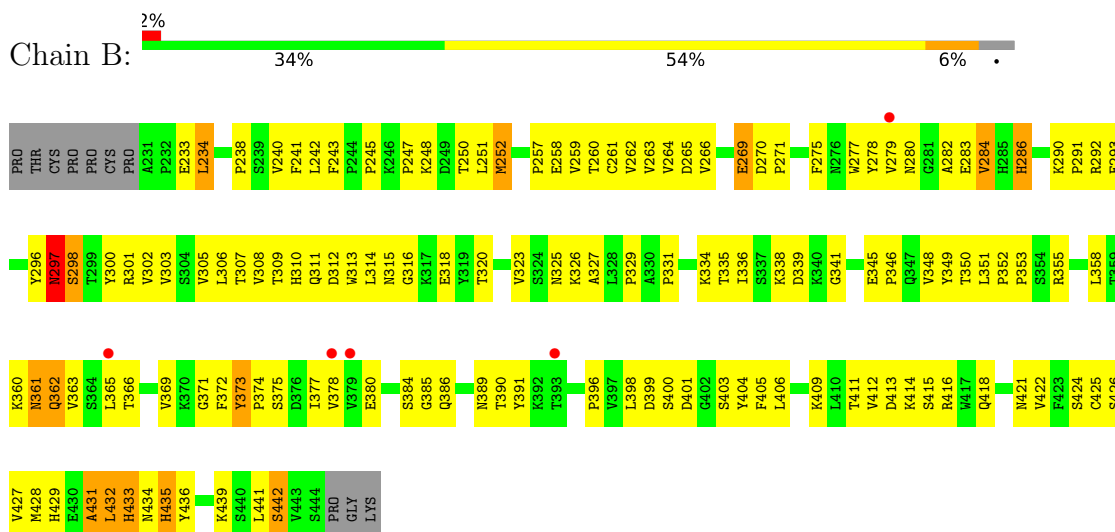
3 Residue-property plots

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.

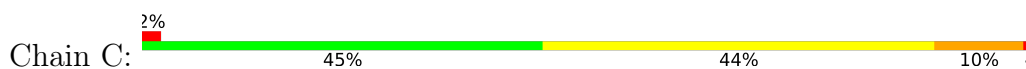
• Molecule 1: IgG1 Fc

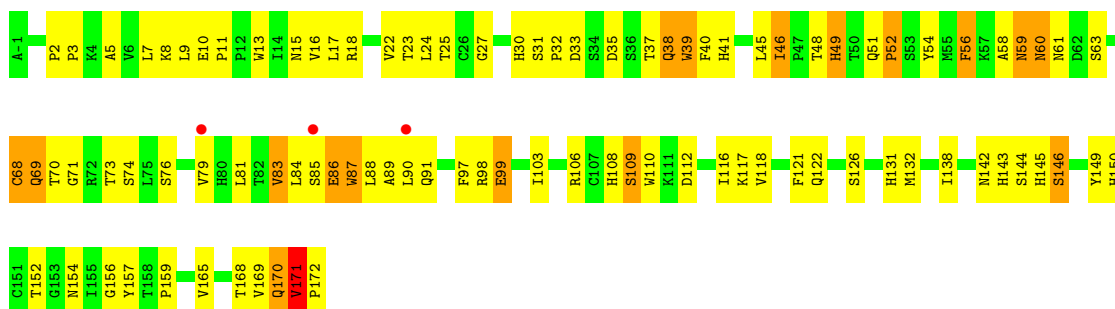


• Molecule 1: IgG1 Fc



• Molecule 2: IgG receptor IIA H131 variant Fc fragment





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

Chain D: 33% 33% 33%



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

Chain E: 22% 56% 22%



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

Chain G: 33% 67%



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

Chain F: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	127.16Å 127.16Å 254.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.17 – 3.55 46.17 – 3.55	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.17-3.55) 99.2 (46.17-3.55)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.293 , 0.337 0.298 , 0.341	Depositor DCC
R_{free} test set	747 reflections (3.44%)	wwPDB-VP
Wilson B-factor (Å ²)	147.8	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 143.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5051	wwPDB-VP
Average B, all atoms (Å ²)	197.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, FUC, BMA, GAL

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	0.53	1/1748 (0.1%)	1.04	9/2387 (0.4%)
1	B	0.42	0/1748	0.90	4/2387 (0.2%)
2	C	0.70	0/1410	1.08	0/1924
All	All	0.55	1/4906 (0.0%)	1.01	13/6698 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	GLY	C-N	-5.34	1.27	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	385	GLY	N-CA-C	-9.32	102.80	114.92
1	B	298	SER	N-CA-C	-9.19	103.17	114.75
1	A	297	ASN	CB-CA-C	-8.70	93.10	110.42
1	A	289	THR	CA-C-N	-7.80	112.82	122.42
1	A	289	THR	C-N-CA	-7.80	112.82	122.42
1	A	375	SER	CB-CA-C	-6.63	108.21	117.23
1	A	297	ASN	CA-C-N	6.35	132.57	121.52
1	A	297	ASN	C-N-CA	6.35	132.57	121.52
1	B	297	ASN	N-CA-CB	-5.90	100.52	110.49
1	A	286	HIS	CB-CA-C	-5.62	108.47	116.34
1	B	375	SER	CB-CA-C	-5.11	110.28	117.23
1	A	296	TYR	CA-C-N	-5.01	111.97	121.54
1	A	296	TYR	C-N-CA	-5.01	111.97	121.54

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	1701	0	1662	191	0
1	B	1701	0	1662	127	0
2	C	1367	0	1302	164	0
3	D	110	0	93	8	0
3	E	110	0	94	6	0
4	G	38	0	34	5	0
5	F	24	0	22	9	0
All	All	5051	0	4869	470	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 47.

All (470) 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:99:GLU:HB2	2:C:171:VAL:CG1	1.43	1.45
2:C:22:VAL:HG13	2:C:56:PHE:CE1	1.63	1.34
1:B:355:ARG:HA	1:B:358:LEU:CD2	1.58	1.32
5:F:1:NAG:O3	5:F:1:NAG:H82	1.39	1.23
1:A:328:LEU:HD21	1:A:332:ILE:CD1	1.67	1.23
1:B:355:ARG:CA	1:B:358:LEU:HD23	1.72	1.20
2:C:99:GLU:HB2	2:C:171:VAL:HG11	1.18	1.14
2:C:22:VAL:CG1	2:C:56:PHE:CE1	2.32	1.11
3:D:1:NAG:H82	3:D:1:NAG:O3	1.53	1.08
1:A:260:THR:HG22	1:A:305:VAL:HG12	1.34	1.08
2:C:59:ASN:HA	2:C:84:LEU:CD2	1.85	1.06
2:C:59:ASN:HA	2:C:84:LEU:HD22	1.34	1.05
1:A:260:THR:HG21	3:D:6:GAL:H5	1.35	1.04
2:C:99:GLU:CB	2:C:171:VAL:CG1	2.37	1.02
3:E:1:NAG:O3	3:E:1:NAG:H82	1.60	1.02
1:A:328:LEU:HD12	1:A:329:PRO:HD2	1.40	1.01
1:A:328:LEU:HD21	1:A:332:ILE:HD12	1.38	1.01
4:G:1:NAG:O7	4:G:2:NAG:H82	1.62	1.00
1:A:370:LYS:HD3	1:A:405:PHE:HB3	1.43	0.98
2:C:22:VAL:HG13	2:C:56:PHE:HE1	1.19	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:51:GLN:HG2	2:C:52:PRO:HD2	1.46	0.97
2:C:85:SER:O	2:C:86:GLU:HB3	1.63	0.96
1:A:309:THR:HB	1:A:312:ASP:HB2	1.48	0.95
2:C:99:GLU:HB2	2:C:171:VAL:HG13	1.51	0.93
2:C:18:ARG:HA	2:C:84:LEU:HD23	1.50	0.92
1:A:296:TYR:O	1:A:297:ASN:C	2.12	0.92
2:C:59:ASN:CA	2:C:84:LEU:HD22	1.98	0.92
1:A:242:LEU:HD11	1:A:336:ILE:HB	1.53	0.91
1:A:235:LEU:HB3	2:C:157:TYR:CZ	2.05	0.90
1:A:260:THR:CG2	3:D:6:GAL:H5	2.02	0.90
1:B:351:LEU:HB2	1:B:366:THR:HG21	1.53	0.90
1:A:358:LEU:O	1:A:359:THR:HG23	1.72	0.89
1:A:283:GLU:OE1	1:A:285:HIS:HB3	1.71	0.89
1:A:338:LYS:HG2	1:A:339:ASP:H	1.37	0.88
2:C:60:ASN:N	2:C:84:LEU:HD22	1.88	0.87
1:B:415:SER:HA	1:B:418:GLN:HB3	1.55	0.86
2:C:58:ALA:O	2:C:84:LEU:HD21	1.76	0.86
2:C:51:GLN:HG2	2:C:52:PRO:CD	2.05	0.85
1:A:237:GLY:HA3	1:A:328:LEU:HD13	1.57	0.85
2:C:22:VAL:HG13	2:C:56:PHE:CD1	2.10	0.85
2:C:85:SER:C	2:C:86:GLU:OE1	2.19	0.85
1:B:293:GLU:HA	1:B:302:VAL:HG22	1.59	0.84
2:C:99:GLU:CB	2:C:171:VAL:HG11	2.03	0.84
1:A:328:LEU:HD21	1:A:332:ILE:HD11	1.59	0.83
1:B:351:LEU:HB2	1:B:366:THR:CG2	2.08	0.83
1:B:355:ARG:HG3	1:B:358:LEU:HD21	1.60	0.82
5:F:1:NAG:O3	5:F:1:NAG:C8	2.26	0.82
2:C:60:ASN:H	2:C:84:LEU:HD22	1.45	0.81
2:C:48:THR:HG22	2:C:49:HIS:H	1.45	0.80
2:C:91:GLN:HE22	2:C:106:ARG:NH1	1.78	0.80
1:A:293:GLU:HA	1:A:302:VAL:HG22	1.64	0.80
2:C:8:LYS:HB2	2:C:25:THR:OG1	1.81	0.79
1:A:291:PRO:C	1:A:292:ARG:HG3	2.07	0.79
1:A:278:TYR:CE1	1:A:283:GLU:HG2	2.17	0.78
2:C:170:GLN:C	2:C:171:VAL:HG12	2.09	0.78
1:B:398:LEU:HA	1:B:404:TYR:HD1	1.46	0.78
2:C:85:SER:HB3	2:C:86:GLU:OE1	1.84	0.78
1:B:390:THR:HG21	1:B:412:VAL:HG13	1.65	0.78
2:C:59:ASN:CA	2:C:84:LEU:CD2	2.60	0.78
2:C:46:ILE:HD11	5:F:2:FUC:H4	1.65	0.77
1:B:384:SER:HB2	1:B:386:GLN:HB3	1.66	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:VAL:CG2	1:A:306:LEU:HB3	2.16	0.76
2:C:58:ALA:C	2:C:84:LEU:HD21	2.10	0.76
2:C:17:LEU:HD21	2:C:89:ALA:HB2	1.65	0.76
2:C:18:ARG:HA	2:C:84:LEU:CD2	2.16	0.76
2:C:169:VAL:O	2:C:170:GLN:HB2	1.85	0.76
2:C:99:GLU:HB2	2:C:171:VAL:HG12	1.61	0.75
2:C:35:ASP:O	2:C:37:THR:HG23	1.86	0.75
2:C:170:GLN:O	2:C:171:VAL:HG12	1.86	0.75
2:C:8:LYS:HB2	2:C:25:THR:HG1	1.52	0.75
1:B:242:LEU:HD22	1:B:336:ILE:HG12	1.69	0.74
1:B:269:GLU:CG	1:B:270:ASP:H	1.99	0.74
2:C:85:SER:O	2:C:86:GLU:CB	2.35	0.74
2:C:59:ASN:O	2:C:59:ASN:ND2	2.17	0.74
1:B:348:VAL:HG22	1:B:369:VAL:HG22	1.71	0.73
1:B:279:VAL:HB	1:B:282:ALA:HB3	1.71	0.73
2:C:59:ASN:C	2:C:59:ASN:HD22	1.96	0.73
1:B:269:GLU:HG2	1:B:270:ASP:H	1.52	0.73
1:A:388:GLU:HG2	1:A:410:LEU:HD11	1.70	0.72
1:A:328:LEU:CD2	1:A:332:ILE:HD12	2.18	0.72
2:C:63:SER:OG	2:C:83:VAL:HG23	1.89	0.72
1:B:269:GLU:HG2	1:B:270:ASP:N	2.03	0.72
1:B:309:THR:HB	1:B:312:ASP:HB2	1.72	0.72
1:B:421:ASN:OD1	1:B:422:VAL:N	2.23	0.72
2:C:9:LEU:HD21	2:C:79:VAL:HG21	1.72	0.72
2:C:37:THR:HG21	2:C:52:PRO:HG3	1.71	0.72
2:C:121:PHE:HD1	2:C:126:SER:HA	1.55	0.71
1:A:259:VAL:HG23	1:A:306:LEU:HB3	1.71	0.71
1:A:328:LEU:CD2	1:A:332:ILE:CD1	2.59	0.71
1:A:358:LEU:O	1:A:358:LEU:HG	1.90	0.71
1:B:240:VAL:HG23	1:B:263:VAL:HG22	1.72	0.71
1:B:355:ARG:HA	1:B:358:LEU:HD23	0.76	0.70
1:B:257:PRO:HG2	1:B:308:VAL:HG23	1.73	0.70
1:B:355:ARG:CA	1:B:358:LEU:CD2	2.46	0.70
2:C:116:ILE:HG13	2:C:117:LYS:HG3	1.71	0.70
1:A:296:TYR:O	1:A:298:SER:N	2.25	0.70
2:C:83:VAL:HG22	2:C:84:LEU:H	1.57	0.69
1:A:288:GLN:HB2	1:A:306:LEU:HD12	1.75	0.69
1:A:255:ARG:NH1	1:A:256:THR:OG1	2.26	0.69
1:A:398:LEU:HA	1:A:404:TYR:CD1	2.29	0.68
2:C:59:ASN:C	2:C:84:LEU:HD22	2.18	0.68
1:A:237:GLY:C	2:C:131:HIS:CE1	2.71	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:22:VAL:CG1	2:C:56:PHE:CD1	2.74	0.68
2:C:10:GLU:HB2	2:C:23:THR:OG1	1.94	0.67
1:A:255:ARG:NH1	1:A:256:THR:O	2.26	0.67
1:A:238:PRO:HD2	1:A:328:LEU:HB2	1.75	0.67
1:B:399:ASP:OD1	1:B:400:SER:N	2.25	0.66
2:C:30:HIS:ND1	2:C:35:ASP:HA	2.10	0.66
3:E:1:NAG:H82	3:E:1:NAG:HO3	1.57	0.65
1:A:242:LEU:HD11	1:A:336:ILE:CB	2.25	0.65
1:B:355:ARG:CG	1:B:358:LEU:HD21	2.27	0.65
2:C:91:GLN:NE2	2:C:106:ARG:NH1	2.43	0.64
2:C:70:THR:O	2:C:73:THR:HG22	1.97	0.64
1:A:398:LEU:HG	1:A:404:TYR:HE1	1.62	0.64
1:A:231:ALA:HB3	1:A:232:PRO:HD3	1.80	0.64
1:A:320:THR:HG22	1:A:335:THR:HA	1.78	0.64
1:A:278:TYR:HB2	1:A:320:THR:OG1	1.96	0.64
1:B:433:HIS:CG	1:B:434:ASN:H	2.16	0.63
1:A:242:LEU:HA	1:A:261:CYS:HA	1.79	0.63
1:A:364:SER:HA	1:A:411:THR:HA	1.80	0.63
2:C:9:LEU:HD21	2:C:79:VAL:CG2	2.28	0.63
1:B:264:VAL:HG12	1:B:301:ARG:HG3	1.80	0.63
1:B:325:ASN:OD1	1:B:326:LYS:N	2.31	0.63
2:C:48:THR:HG22	2:C:49:HIS:N	2.13	0.63
1:A:368:LEU:HD12	1:A:407:TYR:CE1	2.34	0.63
2:C:9:LEU:CD2	2:C:79:VAL:HG21	2.28	0.62
1:B:278:TYR:CE1	1:B:284:VAL:HG22	2.35	0.62
2:C:69:GLN:OE1	2:C:74:SER:C	2.43	0.62
1:B:242:LEU:CD2	1:B:336:ILE:HG12	2.30	0.62
1:B:262:VAL:HA	1:B:303:VAL:HG22	1.82	0.62
1:B:283:GLU:HG3	1:B:286:HIS:HB3	1.80	0.62
1:B:346:PRO:HG2	1:B:432:LEU:HD23	1.80	0.62
2:C:37:THR:HG21	2:C:52:PRO:CG	2.29	0.62
1:A:237:GLY:HA3	1:A:328:LEU:CD1	2.28	0.61
1:B:351:LEU:HB3	1:B:352:PRO:HD2	1.82	0.61
5:F:1:NAG:H82	5:F:1:NAG:HO3	1.59	0.61
2:C:10:GLU:HB3	2:C:11:PRO:CD	2.30	0.61
1:A:355:ARG:HD3	1:B:350:THR:HB	1.82	0.61
1:B:341:GLY:HA3	1:B:373:TYR:HE2	1.65	0.61
1:A:235:LEU:HB3	2:C:157:TYR:CE1	2.34	0.61
1:A:382:GLU:HB3	1:A:424:SER:HB2	1.81	0.61
1:A:392:LYS:HB2	1:B:405:PHE:HZ	1.66	0.61
1:B:360:LYS:HG3	1:B:361:ASN:H	1.65	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:171:VAL:O	2:C:171:VAL:HG22	2.01	0.61
3:D:1:NAG:O3	3:D:1:NAG:C8	2.39	0.61
1:A:362:GLN:HG3	1:A:413:ASP:HA	1.83	0.60
2:C:121:PHE:CD1	2:C:126:SER:HA	2.35	0.60
1:A:362:GLN:HB3	1:A:412:VAL:O	2.01	0.60
1:B:413:ASP:HB2	1:B:416:ARG:HG2	1.83	0.60
1:A:288:GLN:HG2	1:A:307:THR:OG1	2.01	0.60
1:B:278:TYR:HB2	1:B:320:THR:HB	1.82	0.60
2:C:18:ARG:CA	2:C:84:LEU:HD23	2.27	0.60
1:B:380:GLU:HB2	1:B:426:SER:HB2	1.84	0.60
1:A:268:GLN:OE1	1:A:268:GLN:N	2.23	0.59
1:B:374:PRO:HD2	1:B:429:HIS:CE1	2.36	0.59
1:A:416:ARG:NH2	1:A:421:ASN:HD22	2.00	0.59
2:C:22:VAL:HG11	2:C:56:PHE:CE1	2.35	0.59
1:B:398:LEU:HD12	1:B:404:TYR:HE1	1.67	0.59
2:C:49:HIS:CG	2:C:54:TYR:CE1	2.90	0.59
1:B:372:PHE:HB2	1:B:429:HIS:NE2	2.17	0.59
1:B:238:PRO:HB3	1:B:265:ASP:O	2.03	0.59
2:C:18:ARG:HG2	2:C:18:ARG:HH11	1.68	0.58
1:B:424:SER:HA	1:B:439:LYS:HB3	1.85	0.58
2:C:121:PHE:HE1	2:C:126:SER:HB2	1.69	0.58
1:A:251:LEU:HD11	1:A:428:MET:HB3	1.85	0.58
1:A:328:LEU:CD1	1:A:329:PRO:HD2	2.26	0.58
2:C:46:ILE:CD1	5:F:2:FUC:H4	2.34	0.58
1:A:381:TRP:CD2	1:A:410:LEU:HD12	2.39	0.58
1:B:258:GLU:HG3	1:B:307:THR:HG22	1.87	0.57
1:B:261:CYS:HB2	1:B:277:TRP:CH2	2.40	0.57
1:A:283:GLU:OE1	1:A:285:HIS:N	2.37	0.57
1:A:378:VAL:HB	1:A:428:MET:HB2	1.86	0.57
2:C:35:ASP:O	2:C:37:THR:CG2	2.51	0.57
2:C:48:THR:CG2	2:C:49:HIS:H	2.15	0.57
1:A:370:LYS:CD	1:A:405:PHE:HB3	2.28	0.57
1:B:391:TYR:HA	1:B:409:LYS:HG3	1.87	0.57
1:A:389:ASN:O	1:A:390:THR:OG1	2.21	0.57
2:C:103:ILE:HB	2:C:138:ILE:HG12	1.86	0.57
1:B:296:TYR:O	1:B:297:ASN:C	2.46	0.56
1:A:412:VAL:HG22	1:A:413:ASP:H	1.70	0.56
2:C:25:THR:O	2:C:39:TRP:HH2	1.87	0.56
2:C:103:ILE:HB	2:C:138:ILE:CG1	2.36	0.56
1:A:342:GLN:HG2	1:A:344:ARG:HH12	1.69	0.56
1:A:353:PRO:HB3	1:A:417:TRP:CZ2	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:GLU:CG	1:B:270:ASP:N	2.65	0.56
2:C:83:VAL:CG2	2:C:84:LEU:H	2.19	0.56
1:A:251:LEU:HD13	1:A:435:HIS:HB3	1.87	0.55
1:A:235:LEU:HD22	2:C:156:GLY:C	2.31	0.55
1:B:396:PRO:HA	1:B:406:LEU:HD12	1.88	0.55
1:A:355:ARG:HG2	1:B:350:THR:O	2.07	0.55
1:B:248:LYS:HE3	1:B:252:MET:SD	2.47	0.54
1:A:357:GLU:O	1:A:359:THR:N	2.40	0.54
1:B:280:ASN:C	1:B:280:ASN:HD22	2.15	0.54
1:B:341:GLY:HA3	1:B:373:TYR:CE2	2.41	0.54
2:C:97:PHE:CG	2:C:103:ILE:HG12	2.42	0.54
1:B:313:TRP:CH2	1:B:338:LYS:HG3	2.43	0.54
2:C:48:THR:O	2:C:49:HIS:C	2.51	0.54
2:C:59:ASN:O	2:C:61:ASN:N	2.41	0.54
2:C:122:GLN:NE2	2:C:146:SER:O	2.40	0.54
2:C:97:PHE:CD2	2:C:103:ILE:HG12	2.42	0.54
1:A:322:LYS:HZ2	1:A:331:PRO:HG2	1.73	0.54
2:C:56:PHE:HD1	2:C:56:PHE:H	1.54	0.54
2:C:83:VAL:HG22	2:C:84:LEU:N	2.21	0.54
1:A:262:VAL:HA	1:A:303:VAL:HB	1.89	0.54
1:A:346:PRO:HG2	1:A:432:LEU:HG	1.90	0.54
1:A:298:SER:HB2	2:C:126:SER:OG	2.09	0.53
1:B:242:LEU:HG	1:B:260:THR:O	2.07	0.53
2:C:59:ASN:HA	2:C:84:LEU:HD21	1.84	0.53
1:A:237:GLY:O	2:C:131:HIS:CE1	2.61	0.53
1:A:318:GLU:HB3	1:A:335:THR:OG1	2.07	0.53
1:B:369:VAL:HG12	1:B:372:PHE:CD2	2.42	0.53
1:B:241:PHE:HE1	3:E:8:NAG:HN2	1.56	0.53
2:C:90:LEU:HD23	2:C:165:VAL:HG22	1.90	0.53
1:A:249:ASP:OD1	1:A:255:ARG:HG2	2.08	0.53
1:A:360:LYS:HG2	1:A:361:ASN:H	1.73	0.53
2:C:99:GLU:CB	2:C:171:VAL:HG13	2.22	0.53
2:C:170:GLN:NE2	2:C:172:PRO:HD3	2.23	0.53
3:E:1:NAG:O3	3:E:1:NAG:C8	2.46	0.53
1:A:279:VAL:HG23	1:A:319:TYR:CE1	2.44	0.53
1:B:266:VAL:HB	1:B:300:TYR:HB2	1.91	0.53
2:C:99:GLU:CD	2:C:171:VAL:HG13	2.33	0.53
1:A:240:VAL:HG12	1:A:332:ILE:HG21	1.89	0.53
1:B:251:LEU:O	1:B:252:MET:HB3	2.07	0.53
1:B:389:ASN:HA	1:B:391:TYR:CE2	2.43	0.53
1:B:275:PHE:CD1	1:B:323:VAL:HG12	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLY:C	2:C:131:HIS:HE1	2.15	0.52
1:A:278:TYR:CD1	1:A:283:GLU:HA	2.43	0.52
1:B:270:ASP:HB2	1:B:327:ALA:HB2	1.90	0.52
1:A:382:GLU:OE1	1:A:422:VAL:HG12	2.09	0.52
2:C:54:TYR:OH	5:F:2:FUC:O4	2.27	0.52
2:C:48:THR:O	2:C:49:HIS:O	2.26	0.52
3:D:5:NAG:O3	3:D:5:NAG:H82	2.09	0.52
1:A:260:THR:HG21	3:D:6:GAL:C5	2.25	0.52
1:A:383:SER:OG	1:A:384:SER:N	2.43	0.52
2:C:11:PRO:C	2:C:13:TRP:H	2.16	0.52
2:C:59:ASN:ND2	2:C:59:ASN:C	2.67	0.52
2:C:23:THR:HA	2:C:54:TYR:O	2.10	0.52
1:A:286:HIS:O	1:A:288:GLN:N	2.42	0.52
1:B:338:LYS:HG2	1:B:339:ASP:H	1.75	0.52
1:A:365:LEU:HD23	1:A:441:LEU:HD11	1.92	0.52
1:B:245:PRO:HB3	1:B:258:GLU:O	2.10	0.52
2:C:18:ARG:HG2	2:C:18:ARG:NH1	2.24	0.51
1:B:398:LEU:HA	1:B:404:TYR:CD1	2.37	0.51
2:C:144:SER:OG	4:G:1:NAG:H83	2.10	0.51
1:A:394:THR:HG23	1:A:395:PRO:HD2	1.92	0.51
1:A:312:ASP:HB3	1:A:317:LYS:HD2	1.92	0.51
2:C:56:PHE:CD1	2:C:56:PHE:N	2.79	0.51
2:C:70:THR:OG1	2:C:73:THR:CG2	2.59	0.51
4:G:1:NAG:H62	4:G:3:FUC:O2	2.11	0.51
1:B:283:GLU:CG	1:B:286:HIS:HB3	2.40	0.51
1:A:349:TYR:HE2	1:A:368:LEU:HD22	1.75	0.51
1:B:278:TYR:HE1	1:B:284:VAL:HG22	1.74	0.51
2:C:142:ASN:OD1	2:C:144:SER:N	2.34	0.51
1:A:237:GLY:N	2:C:131:HIS:NE2	2.59	0.51
1:A:266:VAL:HB	1:A:300:TYR:HB2	1.92	0.51
1:B:266:VAL:HB	1:B:300:TYR:CB	2.40	0.51
1:B:351:LEU:HB3	1:B:352:PRO:CD	2.41	0.51
2:C:2:PRO:HG2	2:C:74:SER:OG	2.11	0.51
2:C:56:PHE:HD1	2:C:56:PHE:N	2.09	0.51
2:C:85:SER:O	2:C:86:GLU:OE1	2.28	0.51
1:A:349:TYR:CE2	1:A:368:LEU:HD22	2.46	0.50
1:B:247:PRO:O	1:B:250:THR:OG1	2.29	0.50
1:B:350:THR:O	1:B:351:LEU:HD12	2.12	0.50
1:B:374:PRO:HD2	1:B:429:HIS:HE1	1.76	0.50
2:C:46:ILE:HD12	5:F:2:FUC:O3	2.11	0.50
1:A:277:TRP:O	1:A:284:VAL:HG12	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:VAL:O	1:A:279:VAL:HG13	2.10	0.50
2:C:37:THR:CG2	2:C:52:PRO:HG3	2.40	0.50
1:B:296:TYR:HD1	1:B:297:ASN:N	2.10	0.50
1:B:259:VAL:CG1	1:B:306:LEU:HB3	2.41	0.50
1:A:348:VAL:HG13	1:A:439:LYS:CG	2.41	0.50
1:B:311:GLN:HA	1:B:314:LEU:HD12	1.93	0.50
2:C:168:THR:HG23	2:C:168:THR:O	2.12	0.50
1:A:377:ILE:HD12	1:A:429:HIS:CD2	2.47	0.49
1:A:391:TYR:HA	1:A:409:LYS:O	2.12	0.49
1:B:425:CYS:H	1:B:439:LYS:CB	2.25	0.49
1:A:238:PRO:HD2	1:A:328:LEU:HD13	1.92	0.49
1:A:299:THR:O	1:A:300:TYR:HD1	1.96	0.49
1:A:398:LEU:HA	1:A:404:TYR:HD1	1.76	0.49
2:C:13:TRP:NE1	2:C:106:ARG:HH11	2.10	0.49
1:B:280:ASN:O	1:B:280:ASN:ND2	2.45	0.49
1:A:392:LYS:HB2	1:B:405:PHE:CZ	2.47	0.49
1:A:284:VAL:HG13	1:A:284:VAL:O	2.13	0.49
1:B:358:LEU:O	1:B:414:LYS:HE2	2.13	0.49
1:A:357:GLU:HB2	1:B:349:TYR:CZ	2.48	0.49
1:B:283:GLU:OE2	1:B:286:HIS:HB3	2.12	0.49
1:B:296:TYR:O	1:B:298:SER:N	2.46	0.48
1:B:346:PRO:CG	1:B:432:LEU:HD23	2.43	0.48
1:B:346:PRO:HD2	1:B:432:LEU:HB3	1.95	0.48
1:B:427:VAL:HG12	1:B:429:HIS:H	1.78	0.48
2:C:40:PHE:CE1	2:C:45:LEU:HB2	2.48	0.48
1:A:355:ARG:HH11	1:B:350:THR:HB	1.78	0.48
1:A:358:LEU:O	1:A:359:THR:CG2	2.52	0.48
1:B:261:CYS:HB2	1:B:277:TRP:HH2	1.78	0.48
1:B:290:LYS:HB2	1:B:305:VAL:HB	1.94	0.48
2:C:60:ASN:HA	2:C:84:LEU:HB2	1.95	0.48
2:C:121:PHE:HB2	2:C:150:HIS:CE1	2.49	0.48
1:A:320:THR:HG22	1:A:335:THR:CA	2.41	0.48
1:B:433:HIS:CG	1:B:434:ASN:N	2.75	0.48
1:A:278:TYR:HD1	1:A:283:GLU:HA	1.79	0.48
1:A:352:PRO:HB2	1:A:353:PRO:HD2	1.94	0.48
1:A:417:TRP:CE3	1:A:444:SER:OG	2.67	0.48
1:A:261:CYS:HB3	1:A:277:TRP:CH2	2.49	0.48
1:B:384:SER:C	1:B:386:GLN:H	2.17	0.48
2:C:33:ASP:OD1	2:C:33:ASP:N	2.45	0.48
1:B:243:PHE:HZ	3:E:3:BMA:H5	1.78	0.47
1:B:373:TYR:H	1:B:374:PRO:HD2	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:GLU:HG2	1:A:410:LEU:CD1	2.42	0.47
2:C:169:VAL:O	2:C:170:GLN:CB	2.60	0.47
1:A:362:GLN:CG	1:A:413:ASP:HA	2.44	0.47
2:C:81:LEU:C	2:C:83:VAL:H	2.21	0.47
1:A:388:GLU:HG3	1:A:389:ASN:N	2.29	0.47
1:A:233:GLU:CB	2:C:157:TYR:OH	2.63	0.47
1:A:243:PHE:N	1:A:260:THR:O	2.48	0.47
1:B:264:VAL:O	1:B:265:ASP:HB2	2.15	0.47
1:A:235:LEU:HD23	2:C:157:TYR:CE2	2.49	0.47
1:A:363:VAL:HG23	1:A:414:LYS:HA	1.97	0.47
1:A:421:ASN:OD1	1:A:422:VAL:HG23	2.16	0.47
1:B:425:CYS:SG	1:B:439:LYS:HD2	2.55	0.47
2:C:13:TRP:HA	2:C:13:TRP:CE3	2.50	0.47
1:A:238:PRO:CD	1:A:328:LEU:HB2	2.42	0.46
1:B:296:TYR:HD1	1:B:297:ASN:H	1.62	0.46
1:A:295:GLN:OE1	1:A:295:GLN:N	2.44	0.46
1:A:373:TYR:CE1	1:A:374:PRO:HB3	2.51	0.46
1:B:369:VAL:O	1:B:405:PHE:HA	2.16	0.46
1:B:425:CYS:H	1:B:439:LYS:HB3	1.81	0.46
1:A:283:GLU:OE1	1:A:285:HIS:CB	2.53	0.46
1:A:283:GLU:CD	1:A:285:HIS:HB3	2.37	0.46
1:B:260:THR:HB	3:E:6:GAL:H2	1.97	0.46
2:C:87:TRP:CE3	2:C:87:TRP:HA	2.50	0.46
2:C:11:PRO:O	2:C:13:TRP:N	2.49	0.46
1:A:344:ARG:HG2	1:A:373:TYR:HB3	1.97	0.46
1:A:381:TRP:CG	1:A:410:LEU:HD12	2.51	0.46
2:C:142:ASN:OD1	2:C:144:SER:HB2	2.16	0.46
2:C:143:HIS:O	2:C:143:HIS:CG	2.68	0.46
1:B:390:THR:HG23	1:B:390:THR:O	2.15	0.46
2:C:85:SER:CB	2:C:86:GLU:OE1	2.60	0.46
1:A:372:PHE:HB2	1:A:429:HIS:NE2	2.31	0.45
1:B:242:LEU:HD21	1:B:259:VAL:CG2	2.46	0.45
1:A:386:GLN:HB2	1:A:387:PRO:CD	2.46	0.45
1:A:417:TRP:CZ3	1:A:444:SER:OG	2.66	0.45
1:B:318:GLU:HB3	1:B:335:THR:CG2	2.46	0.45
1:A:240:VAL:HG22	1:A:241:PHE:N	2.30	0.45
1:A:338:LYS:HG2	1:A:339:ASP:N	2.18	0.45
2:C:15:ASN:O	2:C:91:GLN:HG2	2.16	0.45
1:A:274:LYS:HD3	1:A:274:LYS:HA	1.79	0.45
1:A:286:HIS:HB3	1:A:287:ALA:H	1.47	0.45
1:B:362:GLN:HG3	1:B:412:VAL:HA	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:VAL:O	1:B:411:THR:HG22	2.16	0.45
2:C:170:GLN:C	2:C:171:VAL:CG1	2.81	0.45
1:A:322:LYS:NZ	1:A:331:PRO:HG2	2.31	0.45
1:A:348:VAL:HG13	1:A:439:LYS:HG3	1.98	0.45
1:A:237:GLY:CA	2:C:131:HIS:NE2	2.79	0.45
1:A:352:PRO:CB	1:A:353:PRO:CD	2.95	0.45
1:B:378:VAL:HG11	1:B:428:MET:HE3	1.99	0.45
1:A:240:VAL:CG1	1:A:332:ILE:HG21	2.46	0.45
1:A:242:LEU:HD12	1:A:242:LEU:O	2.16	0.45
1:A:388:GLU:HG3	1:A:389:ASN:H	1.81	0.45
1:B:432:LEU:HD11	1:B:436:TYR:N	2.31	0.45
2:C:154:ASN:OD1	2:C:159:PRO:HB3	2.17	0.45
2:C:63:SER:OG	2:C:83:VAL:HA	2.16	0.45
1:A:251:LEU:CD1	1:A:428:MET:HB3	2.47	0.45
2:C:10:GLU:OE2	2:C:11:PRO:HD3	2.17	0.45
2:C:91:GLN:HE22	2:C:108:HIS:HB2	1.82	0.45
2:C:121:PHE:CE1	2:C:126:SER:HB2	2.52	0.44
1:A:411:THR:O	1:A:411:THR:HG23	2.18	0.44
1:A:237:GLY:O	2:C:131:HIS:HE1	1.99	0.44
1:A:264:VAL:HG22	1:A:265:ASP:N	2.33	0.44
1:A:278:TYR:HB2	1:A:320:THR:HG1	1.81	0.44
1:A:295:GLN:HG3	1:A:300:TYR:CE1	2.52	0.44
1:A:362:GLN:HB3	1:A:412:VAL:C	2.43	0.44
1:A:417:TRP:HZ3	1:A:418:GLN:NE2	2.16	0.44
1:B:350:THR:CG2	1:B:441:LEU:HD12	2.47	0.44
2:C:10:GLU:HB3	2:C:11:PRO:HD3	1.99	0.44
1:A:314:LEU:O	1:A:316:GLY:N	2.50	0.44
2:C:70:THR:OG1	2:C:73:THR:HG22	2.18	0.44
1:A:337:SER:OG	1:A:338:LYS:N	2.51	0.44
1:A:393:THR:HG23	1:A:406:LEU:HD13	2.00	0.44
1:B:346:PRO:HG3	1:B:429:HIS:HB3	1.99	0.44
2:C:145:HIS:O	2:C:149:TYR:OH	2.20	0.44
1:A:242:LEU:HD12	1:A:242:LEU:C	2.43	0.44
1:B:310:HIS:O	1:B:314:LEU:HG	2.18	0.44
1:B:363:VAL:CG1	1:B:365:LEU:HG	2.47	0.44
1:A:424:SER:HB3	1:A:438:GLN:HG3	1.99	0.44
2:C:46:ILE:HD11	5:F:2:FUC:C4	2.41	0.44
1:A:357:GLU:HB2	1:B:349:TYR:CE2	2.53	0.44
1:A:412:VAL:HG22	1:A:413:ASP:N	2.32	0.44
2:C:116:ILE:HG13	2:C:117:LYS:CG	2.45	0.44
1:A:373:TYR:HA	1:A:374:PRO:HA	1.69	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:TYR:CD1	1:B:297:ASN:N	2.86	0.43
1:B:355:ARG:CA	1:B:358:LEU:HD21	2.45	0.43
2:C:16:VAL:C	2:C:17:LEU:HD23	2.43	0.43
1:A:270:ASP:OD2	1:A:326:LYS:HB3	2.17	0.43
1:A:298:SER:HB2	2:C:126:SER:CB	2.48	0.43
1:A:368:LEU:HD12	1:A:407:TYR:CZ	2.52	0.43
1:A:399:ASP:OD1	1:B:409:LYS:NZ	2.48	0.43
2:C:109:SER:HB2	2:C:110:TRP:H	1.52	0.43
1:A:278:TYR:CE1	1:A:283:GLU:CG	2.95	0.43
1:A:359:THR:OG1	1:A:360:LYS:N	2.51	0.43
2:C:30:HIS:CE1	2:C:52:PRO:HG3	2.53	0.43
1:A:233:GLU:HB3	2:C:157:TYR:OH	2.19	0.43
1:A:308:VAL:HG12	1:A:309:THR:N	2.34	0.43
2:C:54:TYR:HH	5:F:2:FUC:HO4	1.66	0.43
2:C:86:GLU:O	2:C:88:LEU:N	2.51	0.43
2:C:132:MET:HE3	2:C:132:MET:HB2	1.97	0.43
1:A:350:THR:H	1:A:351:LEU:HD12	1.84	0.43
2:C:170:GLN:CD	2:C:172:PRO:HD3	2.44	0.43
1:A:409:LYS:NZ	1:A:411:THR:HG21	2.34	0.43
2:C:7:LEU:HD11	2:C:24:LEU:HD22	2.00	0.43
1:A:308:VAL:CG1	1:A:313:TRP:HB2	2.49	0.42
1:A:364:SER:C	1:A:365:LEU:HD12	2.44	0.42
1:B:369:VAL:HG12	1:B:372:PHE:CE2	2.54	0.42
2:C:59:ASN:ND2	2:C:61:ASN:OD1	2.51	0.42
2:C:59:ASN:CA	2:C:84:LEU:HD21	2.45	0.42
2:C:70:THR:OG1	2:C:73:THR:HG21	2.19	0.42
2:C:122:GLN:HE22	2:C:145:HIS:HA	1.84	0.42
1:A:382:GLU:CB	1:A:424:SER:HB2	2.47	0.42
1:A:398:LEU:HA	1:A:404:TYR:CE1	2.54	0.42
1:A:422:VAL:O	1:A:423:PHE:CD1	2.72	0.42
1:B:398:LEU:HD23	1:B:399:ASP:N	2.35	0.42
2:C:13:TRP:HA	2:C:13:TRP:HE3	1.84	0.42
2:C:38:GLN:O	2:C:39:TRP:HB2	2.19	0.42
1:A:237:GLY:CA	2:C:131:HIS:CE1	3.03	0.42
1:A:365:LEU:O	1:A:409:LYS:HA	2.19	0.42
2:C:87:TRP:O	2:C:88:LEU:HD12	2.20	0.42
1:B:360:LYS:CG	1:B:361:ASN:H	2.31	0.42
1:A:430:GLU:O	1:A:435:HIS:NE2	2.53	0.42
2:C:142:ASN:O	2:C:169:VAL:HG11	2.20	0.42
1:A:243:PHE:HE1	3:D:3:BMA:H62	1.85	0.41
1:A:280:ASN:N	1:A:318:GLU:O	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:ASN:O	1:A:361:ASN:ND2	2.42	0.41
1:A:373:TYR:CD1	1:A:374:PRO:HB3	2.55	0.41
1:B:362:GLN:HE21	1:B:412:VAL:C	2.28	0.41
1:B:233:GLU:O	1:B:234:LEU:HG	2.20	0.41
2:C:91:GLN:NE2	2:C:108:HIS:HB2	2.35	0.41
2:C:31:SER:O	2:C:33:ASP:N	2.52	0.41
2:C:68:CYS:HB2	2:C:76:SER:HB3	2.02	0.41
2:C:37:THR:HG21	2:C:52:PRO:N	2.34	0.41
1:A:399:ASP:O	1:A:400:SER:C	2.63	0.41
2:C:10:GLU:HB2	2:C:23:THR:HG1	1.85	0.41
2:C:11:PRO:C	2:C:13:TRP:N	2.78	0.41
2:C:118:VAL:HA	2:C:152:THR:O	2.20	0.41
1:B:345:GLU:HA	1:B:431:ALA:CB	2.50	0.41
1:B:350:THR:C	1:B:351:LEU:HD12	2.46	0.41
1:A:240:VAL:HG11	1:A:332:ILE:CG2	2.51	0.41
1:A:241:PHE:CE1	3:D:8:NAG:H82	2.56	0.41
1:A:244:PRO:HB2	1:A:245:PRO:HD2	2.02	0.41
1:A:259:VAL:HG23	1:A:259:VAL:O	2.20	0.41
1:A:290:LYS:H	1:A:304:SER:HB2	1.84	0.41
1:A:290:LYS:O	1:A:304:SER:HA	2.20	0.41
1:A:348:VAL:HG13	1:A:439:LYS:HG2	2.01	0.41
1:A:364:SER:HA	1:A:411:THR:CA	2.50	0.41
1:B:371:GLY:C	1:B:403:SER:HB2	2.45	0.41
1:B:441:LEU:O	1:B:442:SER:OG	2.34	0.41
1:A:260:THR:HG22	1:A:305:VAL:CG1	2.26	0.41
1:A:366:THR:HG22	1:A:367:CYS:N	2.36	0.41
1:B:283:GLU:HG3	1:B:286:HIS:CB	2.51	0.41
1:B:428:MET:HA	1:B:435:HIS:O	2.21	0.41
2:C:144:SER:OG	4:G:1:NAG:C8	2.68	0.41
1:B:323:VAL:O	1:B:331:PRO:HB3	2.21	0.40
2:C:63:SER:HB3	2:C:83:VAL:HB	2.02	0.40
1:A:263:VAL:O	1:A:263:VAL:HG12	2.21	0.40
1:A:264:VAL:O	1:A:265:ASP:HB2	2.21	0.40
1:A:345:GLU:HA	1:A:431:ALA:HB3	2.04	0.40
4:G:1:NAG:H4	4:G:2:NAG:N2	2.36	0.40
1:A:235:LEU:N	2:C:157:TYR:OH	2.55	0.40
1:A:241:PHE:HB2	1:A:262:VAL:HG23	2.03	0.40
1:A:259:VAL:HG13	1:A:308:VAL:HG21	2.03	0.40
1:A:277:TRP:C	1:A:284:VAL:HG12	2.47	0.40
1:A:391:TYR:HB3	1:A:410:LEU:HA	2.04	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	212/224 (95%)	144 (68%)	46 (22%)	22 (10%)	0	5
1	B	212/224 (95%)	143 (68%)	45 (21%)	24 (11%)	0	4
2	C	172/174 (99%)	131 (76%)	19 (11%)	22 (13%)	0	3
All	All	596/622 (96%)	418 (70%)	110 (18%)	68 (11%)	0	4

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	PRO
1	A	287	ALA
1	A	297	ASN
1	A	314	LEU
1	A	315	ASN
1	A	358	LEU
1	A	359	THR
1	A	411	THR
1	A	417	TRP
1	B	433	HIS
2	C	5	ALA
2	C	32	PRO
2	C	60	ASN
2	C	83	VAL
2	C	86	GLU
2	C	87	TRP
2	C	112	ASP
1	A	329	PRO
1	A	355	ARG
1	A	442	SER
1	B	252	MET
1	B	269	GLU
1	B	271	PRO
1	B	286	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	329	PRO
1	B	361	ASN
1	B	362	GLN
1	B	431	ALA
1	B	435	HIS
2	C	27	GLY
2	C	41	HIS
2	C	49	HIS
2	C	71	GLY
2	C	99	GLU
2	C	170	GLN
1	A	385	GLY
1	A	433	HIS
1	B	292	ARG
1	B	315	ASN
1	B	316	GLY
1	B	373	TYR
1	B	401	ASP
1	B	432	LEU
2	C	3	PRO
1	A	400	SER
1	B	234	LEU
1	B	297	ASN
1	B	334	LYS
1	B	377	ILE
2	C	38	GLN
2	C	98	ARG
2	C	109	SER
2	C	171	VAL
1	A	352	PRO
1	B	284	VAL
2	C	39	TRP
2	C	52	PRO
2	C	69	GLN
1	A	265	ASP
1	A	431	ALA
1	B	442	SER
2	C	146	SER
1	A	412	VAL
1	B	291	PRO
1	A	291	PRO
1	B	353	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	331	PRO
1	A	374	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	199/208 (96%)	196 (98%)	3 (2%)	57	70
1	B	199/208 (96%)	199 (100%)	0	100	100
2	C	155/155 (100%)	150 (97%)	5 (3%)	34	58
All	All	553/571 (97%)	545 (99%)	8 (1%)	59	71

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

Mol	Chain	Res	Type
1	A	296	TYR
1	A	298	SER
1	A	444	SER
2	C	46	ILE
2	C	56	PHE
2	C	59	ASN
2	C	68	CYS
2	C	171	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	HIS
1	A	418	GLN
1	B	361	ASN
1	B	362	GLN
2	C	15	ASN
2	C	30	HIS
2	C	60	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	91	GLN
2	C	94	HIS
2	C	122	GLN
2	C	135	ASN
2	C	145	HIS

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 ⓘ

23 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	0.36	0	17,19,21	0.62	0
3	BMA	D	3	3	11,11,12	1.29	1 (9%)	15,15,17	1.34	2 (13%)
3	MAN	D	4	3	11,11,12	0.88	0	15,15,17	0.75	0
3	NAG	D	5	3	14,14,15	1.25	1 (7%)	17,19,21	2.61	7 (41%)
3	GAL	D	6	3	11,11,12	3.87	9 (81%)	15,15,17	2.20	4 (26%)
3	MAN	D	7	3	11,11,12	1.50	2 (18%)	15,15,17	1.26	2 (13%)
3	NAG	D	8	3	14,14,15	0.37	0	17,19,21	0.55	0
3	FUC	D	9	3	10,10,11	0.76	0	14,14,16	0.84	0
3	NAG	E	1	1,3	14,14,15	0.45	0	17,19,21	0.50	0
3	NAG	E	2	3	14,14,15	0.29	0	17,19,21	0.39	0
3	BMA	E	3	3	11,11,12	1.14	2 (18%)	15,15,17	1.35	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	E	4	3	11,11,12	1.08	1 (9%)	15,15,17	0.84	0
3	NAG	E	5	3	14,14,15	1.60	1 (7%)	17,19,21	1.76	4 (23%)
3	GAL	E	6	3	11,11,12	5.08	9 (81%)	15,15,17	2.17	6 (40%)
3	MAN	E	7	3	11,11,12	1.47	2 (18%)	15,15,17	1.20	2 (13%)
3	NAG	E	8	3	14,14,15	0.38	0	17,19,21	0.54	0
3	FUC	E	9	3	10,10,11	0.79	0	14,14,16	0.97	0
5	NAG	F	1	5,2	14,14,15	0.36	0	17,19,21	0.67	0
5	FUC	F	2	5	10,10,11	0.44	0	14,14,16	1.41	1 (7%)
4	NAG	G	1	4,2	14,14,15	0.67	0	17,19,21	1.07	1 (5%)
4	NAG	G	2	4	14,14,15	0.71	1 (7%)	17,19,21	0.58	0
4	FUC	G	3	4	10,10,11	0.91	0	14,14,16	0.80	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	-	5/6/23/26	0/1/1/1
3	GAL	D	6	3	-	0/2/19/22	0/1/1/1
3	MAN	D	7	3	-	2/2/19/22	0/1/1/1
3	NAG	D	8	3	-	2/6/23/26	0/1/1/1
3	FUC	D	9	3	-	-	0/1/1/1
3	NAG	E	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	2/2/19/22	0/1/1/1
3	NAG	E	5	3	-	4/6/23/26	0/1/1/1
3	GAL	E	6	3	-	2/2/19/22	0/1/1/1
3	MAN	E	7	3	-	2/2/19/22	0/1/1/1
3	NAG	E	8	3	-	2/6/23/26	0/1/1/1
3	FUC	E	9	3	-	-	0/1/1/1
5	NAG	F	1	5,2	-	4/6/23/26	0/1/1/1
5	FUC	F	2	5	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	FUC	G	3	4	-	-	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	6	GAL	C2-C3	8.70	1.65	1.52
3	E	6	GAL	O5-C1	-8.25	1.29	1.43
3	D	6	GAL	C2-C3	7.00	1.63	1.52
3	E	6	GAL	O2-C2	6.36	1.56	1.43
3	D	6	GAL	O5-C5	5.96	1.55	1.43
3	E	6	GAL	O4-C4	5.71	1.57	1.43
3	E	5	NAG	O5-C1	-5.62	1.34	1.43
3	E	6	GAL	C1-C2	4.42	1.62	1.52
3	E	6	GAL	C4-C3	4.16	1.63	1.52
3	D	5	NAG	C1-C2	3.99	1.57	1.52
3	D	6	GAL	C4-C5	3.95	1.61	1.53
3	D	6	GAL	O4-C4	3.86	1.52	1.43
3	D	6	GAL	O5-C1	-3.68	1.37	1.43
3	E	7	MAN	O5-C1	-3.66	1.37	1.43
3	E	6	GAL	C4-C5	3.51	1.60	1.53
3	D	7	MAN	O5-C1	-3.38	1.38	1.43
3	D	6	GAL	O3-C3	3.32	1.51	1.43
3	D	6	GAL	O2-C2	-3.11	1.36	1.43
3	D	7	MAN	C2-C3	2.84	1.56	1.52
3	E	4	MAN	C2-C3	2.78	1.56	1.52
3	E	6	GAL	O5-C5	2.67	1.48	1.43
3	E	6	GAL	O6-C6	2.63	1.53	1.42
3	D	3	BMA	O5-C1	-2.52	1.39	1.43
4	G	2	NAG	C1-C2	2.50	1.55	1.52
3	E	7	MAN	C2-C3	2.50	1.56	1.52
3	E	3	BMA	O5-C1	-2.47	1.39	1.43
3	D	6	GAL	C4-C3	2.21	1.58	1.52
3	E	3	BMA	C2-C3	2.17	1.55	1.52
3	D	6	GAL	C6-C5	2.15	1.59	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5	NAG	C2-N2-C7	6.12	131.10	122.90
3	D	6	GAL	C1-C2-C3	5.11	117.08	109.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	6	GAL	O5-C5-C6	-4.65	98.62	107.66
3	E	6	GAL	C1-C2-C3	4.62	116.36	109.64
3	D	6	GAL	C1-O5-C5	-4.59	106.04	112.19
3	D	5	NAG	O4-C4-C5	4.39	120.14	109.32
5	F	2	FUC	C1-C2-C3	3.89	115.31	109.64
3	E	5	NAG	C1-O5-C5	-3.76	107.15	112.19
3	D	5	NAG	O5-C5-C4	-3.67	101.91	110.83
3	D	5	NAG	O4-C4-C3	-3.56	101.99	110.38
3	D	5	NAG	O3-C3-C4	-3.34	102.50	110.38
3	E	5	NAG	C3-C4-C5	3.13	115.91	110.23
3	D	7	MAN	O3-C3-C2	3.03	116.25	110.05
3	E	5	NAG	O4-C4-C5	-3.03	101.86	109.32
3	D	6	GAL	O5-C5-C4	2.89	117.87	110.83
3	E	5	NAG	O4-C4-C3	-2.89	103.56	110.38
3	D	5	NAG	C1-C2-N2	-2.83	105.97	110.43
3	E	7	MAN	O3-C3-C2	2.82	115.81	110.05
3	D	5	NAG	C1-O5-C5	2.73	115.84	112.19
3	E	6	GAL	O2-C2-C3	2.64	115.62	110.15
3	D	6	GAL	O5-C1-C2	-2.58	104.63	110.79
3	E	7	MAN	C1-C2-C3	-2.42	106.12	109.64
4	G	1	NAG	C1-O5-C5	2.41	115.42	112.19
3	E	3	BMA	C1-C2-C3	2.41	113.15	109.64
3	E	6	GAL	C3-C4-C5	-2.39	105.91	110.23
3	E	3	BMA	C2-C3-C4	2.26	114.84	110.86
3	E	6	GAL	O2-C2-C1	2.19	114.23	109.22
3	D	7	MAN	C1-C2-C3	-2.14	106.53	109.64
3	D	3	BMA	C2-C3-C4	2.05	114.47	110.86
3	D	3	BMA	C1-C2-C3	2.04	112.61	109.64
3	E	6	GAL	C2-C3-C4	-2.04	107.28	110.86
3	E	3	BMA	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	7	MAN	O5-C5-C6-O6
3	D	7	MAN	O5-C5-C6-O6
3	E	6	GAL	O5-C5-C6-O6
3	D	5	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	G	2	NAG	C4-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
3	D	5	NAG	C4-C5-C6-O6
3	E	6	GAL	C4-C5-C6-O6
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	5	NAG	C8-C7-N2-C2
3	D	5	NAG	O7-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	5	NAG	C8-C7-N2-C2
3	E	5	NAG	O7-C7-N2-C2
5	F	1	NAG	C8-C7-N2-C2
5	F	1	NAG	O7-C7-N2-C2
3	E	8	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
3	E	7	MAN	C4-C5-C6-O6
3	D	7	MAN	C4-C5-C6-O6
3	D	8	NAG	O5-C5-C6-O6
3	E	5	NAG	C4-C5-C6-O6
3	E	8	NAG	C4-C5-C6-O6
3	D	5	NAG	C3-C2-N2-C7
5	F	1	NAG	C3-C2-N2-C7
5	F	1	NAG	O5-C5-C6-O6
3	E	5	NAG	O5-C5-C6-O6
3	D	8	NAG	C4-C5-C6-O6

There are no ring outliers.

14 monomers are involved in 28 short contacts:

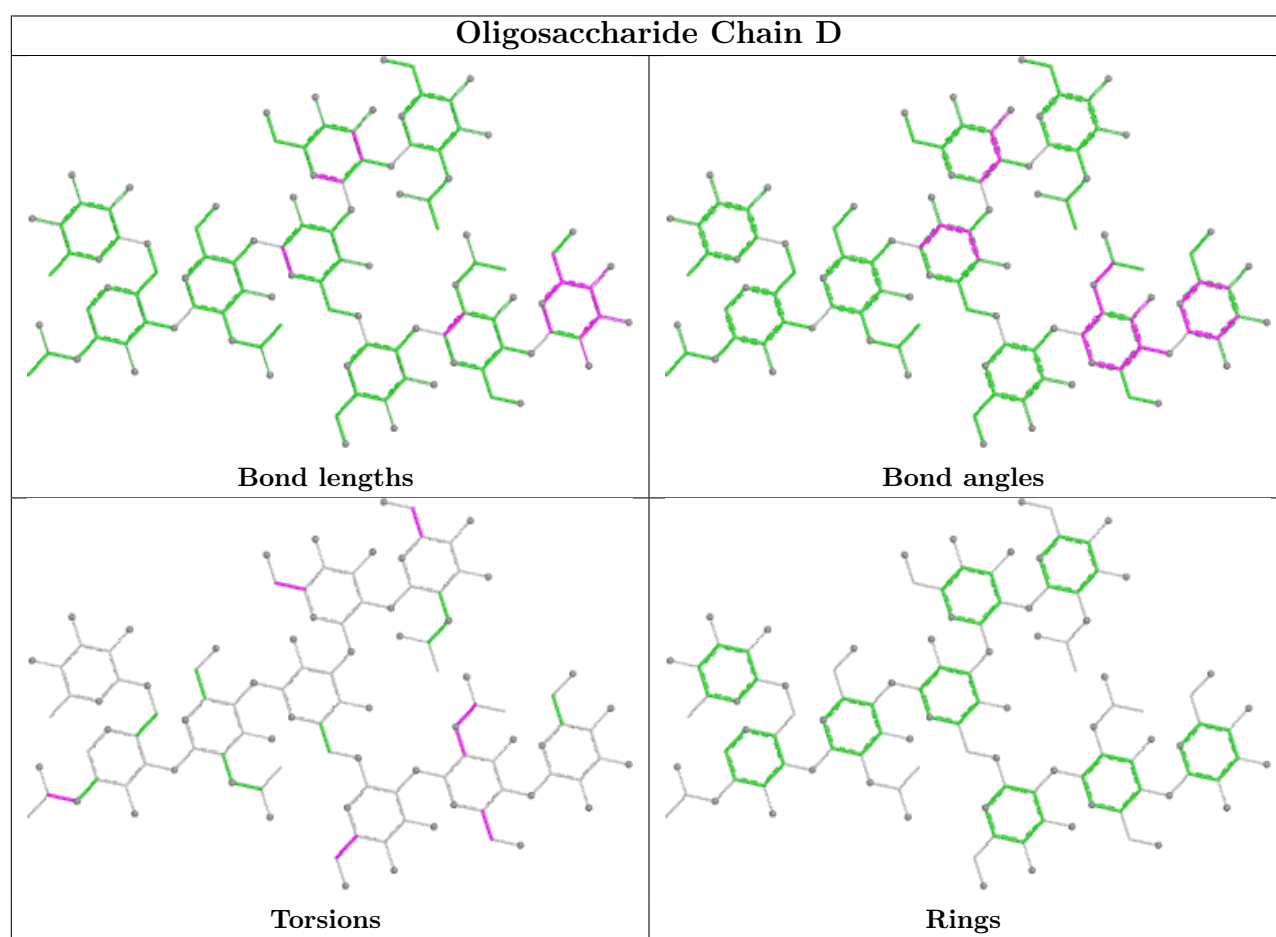
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	6	GAL	1	0
4	G	3	FUC	1	0
3	D	6	GAL	3	0
4	G	2	NAG	2	0
3	E	3	BMA	1	0
3	D	1	NAG	2	0
3	D	5	NAG	1	0

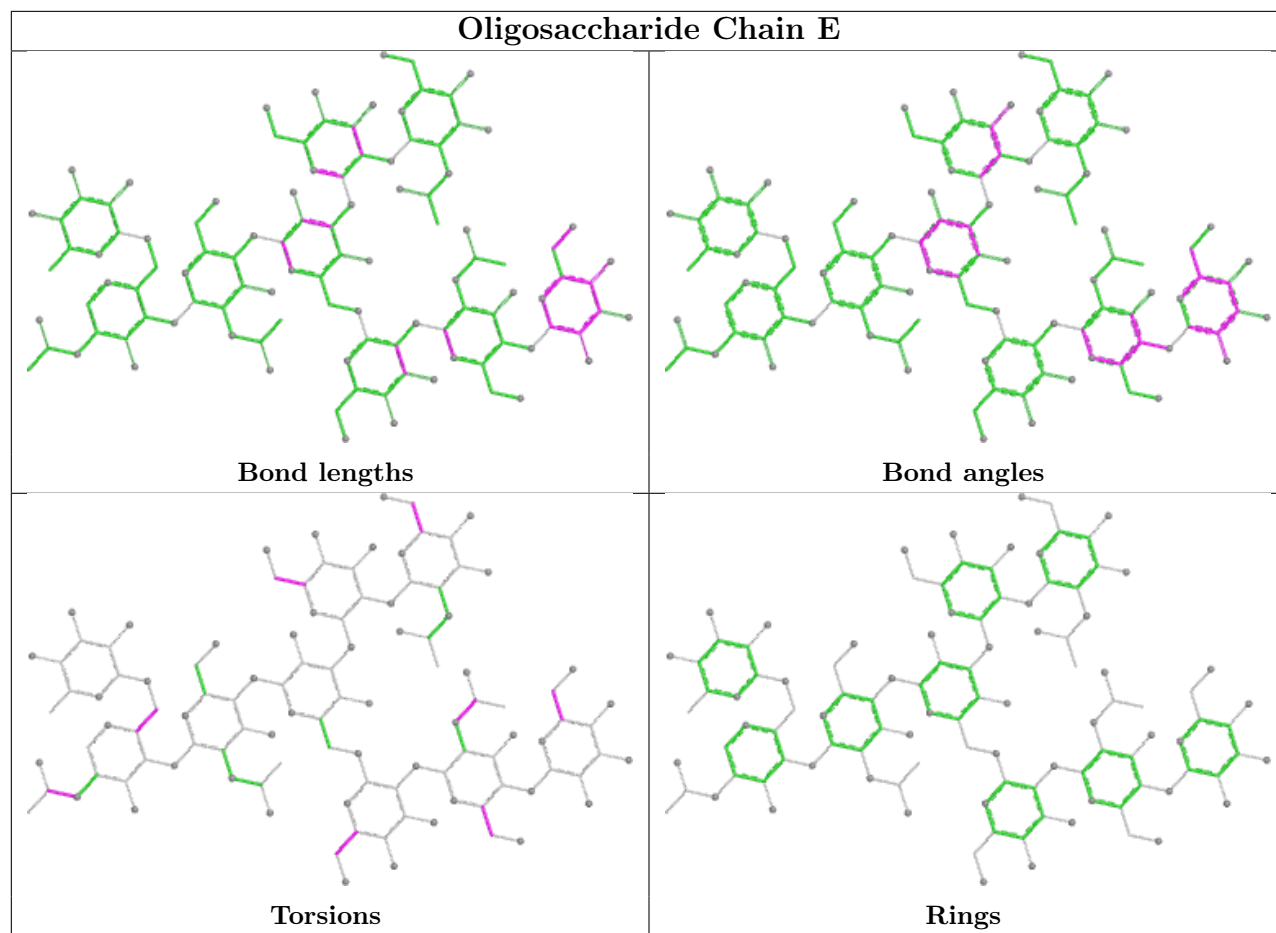
Continued on next page...

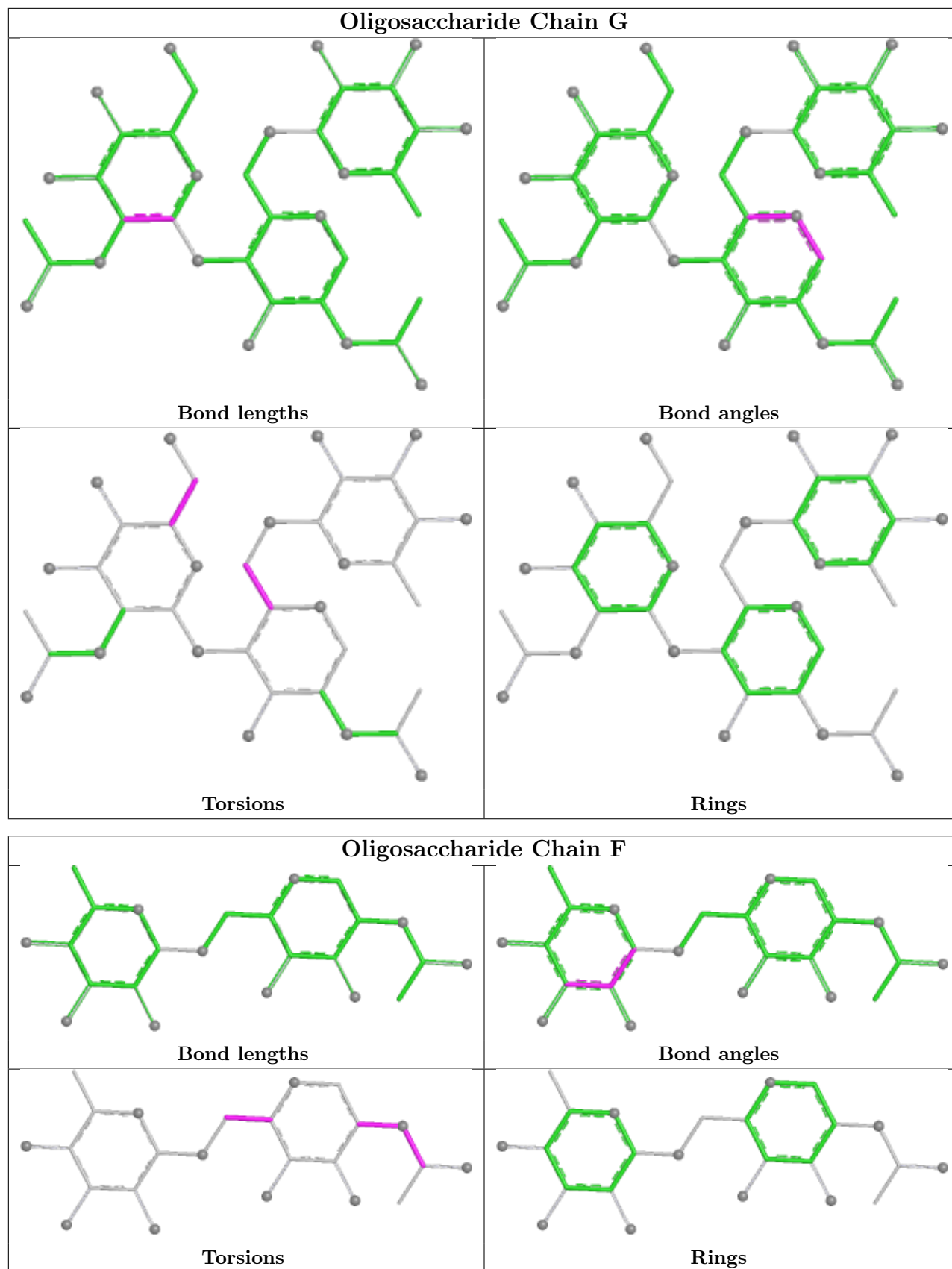
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1	NAG	3	0
4	G	1	NAG	5	0
3	D	8	NAG	1	0
3	D	3	BMA	1	0
3	E	8	NAG	1	0
3	E	1	NAG	3	0
5	F	2	FUC	6	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

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	214/224 (95%)	0.04	1 (0%) 87 66	96, 193, 325, 385	0
1	B	214/224 (95%)	0.03	5 (2%) 61 34	151, 231, 301, 341	0
2	C	174/174 (100%)	-0.09	3 (1%) 69 40	96, 138, 187, 221	0
All	All	602/622 (96%)	-0.00	9 (1%) 72 44	96, 191, 301, 385	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	90	LEU	3.2
2	C	79	VAL	2.9
1	B	393	THR	2.7
1	B	379	VAL	2.7
1	A	323	VAL	2.5
1	B	378	VAL	2.2
1	B	365	LEU	2.1
1	B	279	VAL	2.1
2	C	85	SER	2.0

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

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

6.3 Carbohydrates [i](#)

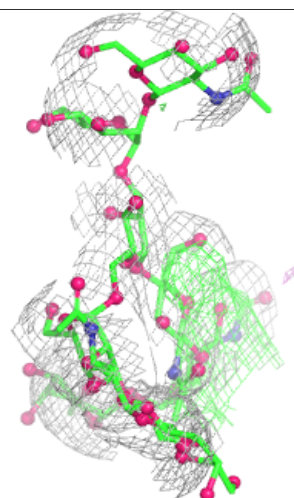
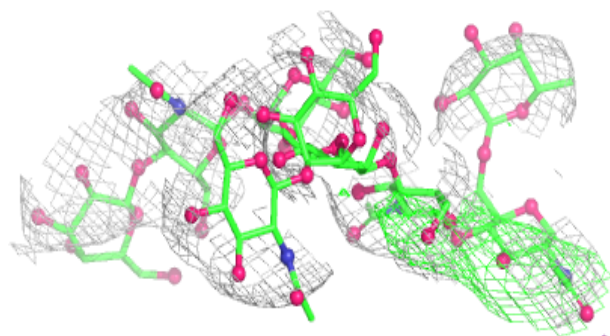
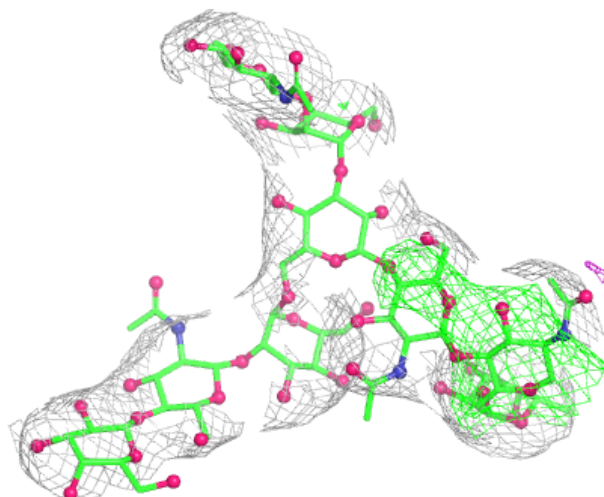
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	G	1	14/15	0.12	0.11	199,236,266,274	0
3	FUC	E	9	10/11	0.46	0.12	214,237,251,263	0
5	NAG	F	1	14/15	0.46	0.09	196,221,240,243	0
3	BMA	E	3	11/12	0.61	0.09	207,212,238,238	0
3	NAG	E	8	14/15	0.66	0.11	201,222,246,261	0
3	FUC	D	9	10/11	0.67	0.18	155,177,221,230	0
3	GAL	E	6	11/12	0.72	0.28	190,216,225,241	0
3	MAN	E	4	11/12	0.75	0.10	198,226,238,251	0
3	NAG	E	5	14/15	0.78	0.15	171,196,211,221	0
3	NAG	E	1	14/15	0.78	0.08	194,212,227,231	0
3	NAG	D	8	14/15	0.83	0.07	162,194,208,212	0
3	MAN	E	7	11/12	0.83	0.11	203,225,239,245	0
3	NAG	E	2	14/15	0.85	0.09	198,208,217,223	0
3	NAG	D	1	14/15	0.85	0.20	137,147,171,175	0
3	MAN	D	7	11/12	0.87	0.13	174,192,229,251	0
3	MAN	D	4	11/12	0.87	0.09	106,139,175,196	0
3	NAG	D	5	14/15	0.92	0.10	163,186,203,209	0
3	BMA	D	3	11/12	0.93	0.07	125,156,169,173	0
3	GAL	D	6	11/12	0.94	0.21	136,194,227,237	0
4	NAG	G	2	14/15	-	-	252,291,311,314	0
4	FUC	G	3	10/11	-	-	279,293,302,304	0
3	NAG	D	2	14/15	0.95	0.12	128,147,155,174	0
5	FUC	F	2	10/11	-	-	223,246,263,263	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.

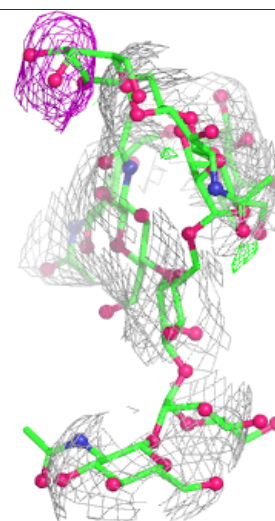
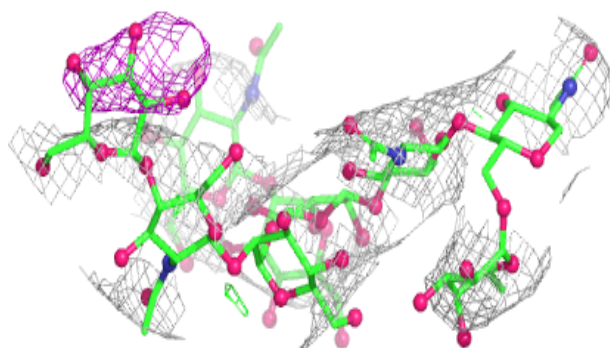
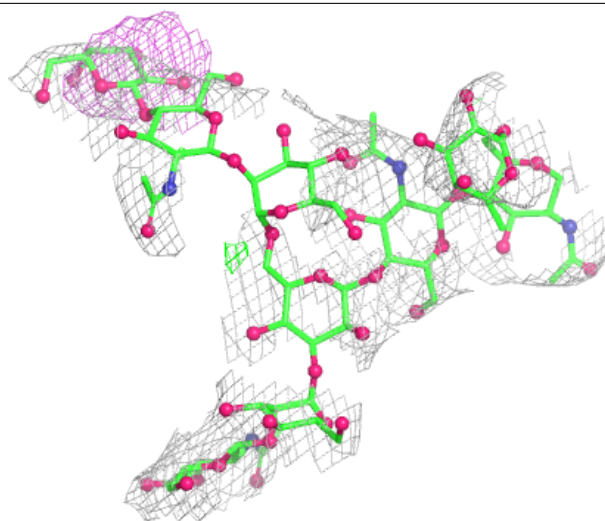
Electron density around Chain D:

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



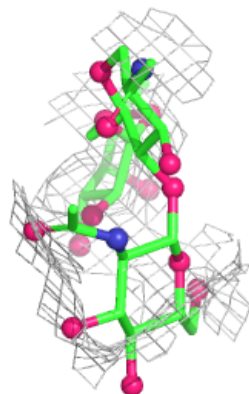
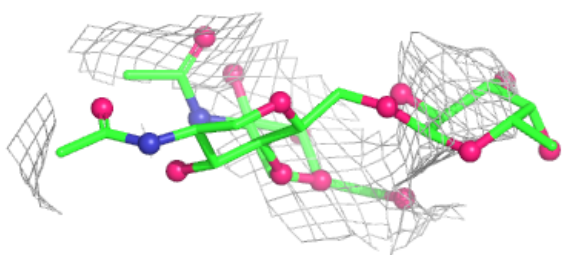
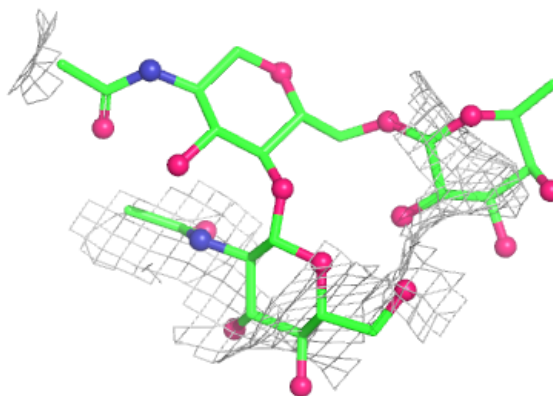
Electron density around Chain E:

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

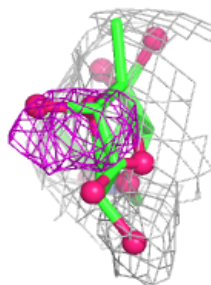
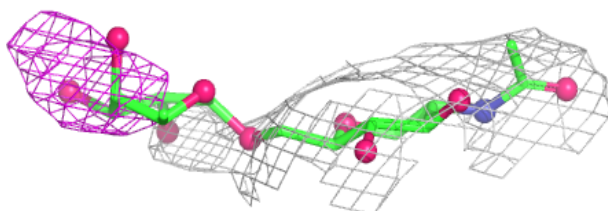
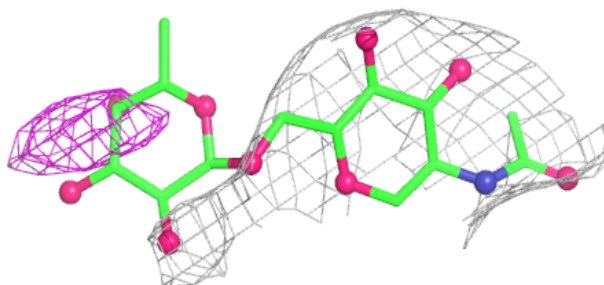


Electron density around Chain G:

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

**Electron density around Chain 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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.