



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:50 AM UTC

PDB ID : 9ELU / pdb_00009elu
Title : CRYSTAL STRUCTURE OF RHESUS MACAQUE (MACACA MULATTA)
IGG1 FC FRAGMENT- FC-GAMMA RECEPTOR IIA COMPLEX P131
VARIANT
Authors : Tolbert, W.D.; Pazgier, M.
Deposited on : 2024-12-05
Resolution : 2.65 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

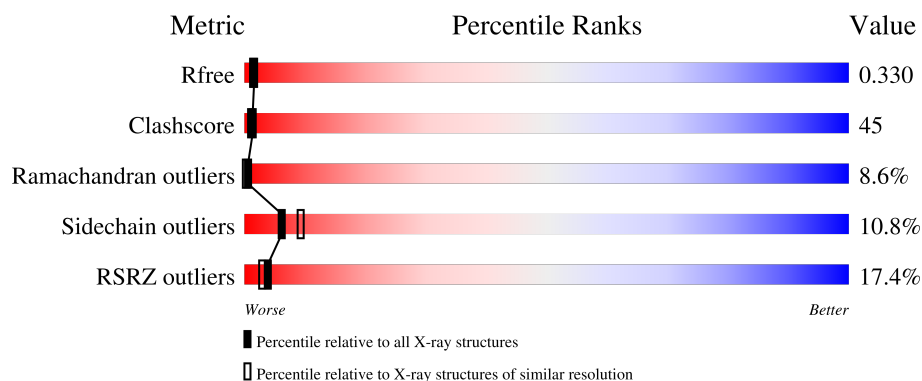
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	
1	B	224	
2	C	174	
3	D	9	
4	E	8	

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

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5058 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	215	Total	C	N	O	S	0	0	0
			1708	1085	286	331	6			
1	B	214	Total	C	N	O	S	0	0	0
			1701	1080	285	330	6			

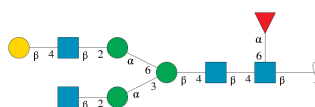
- Molecule 2 is a protein called IgG receptor IIA (CD32A) P131 variant Fc fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	173	Total	C	N	O	S	0	3	0
			1386	872	245	262	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	insertion	UNP F6TRF8
C	131	PRO	HIS	variant	UNP F6TRF8

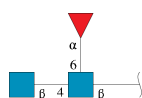
- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose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



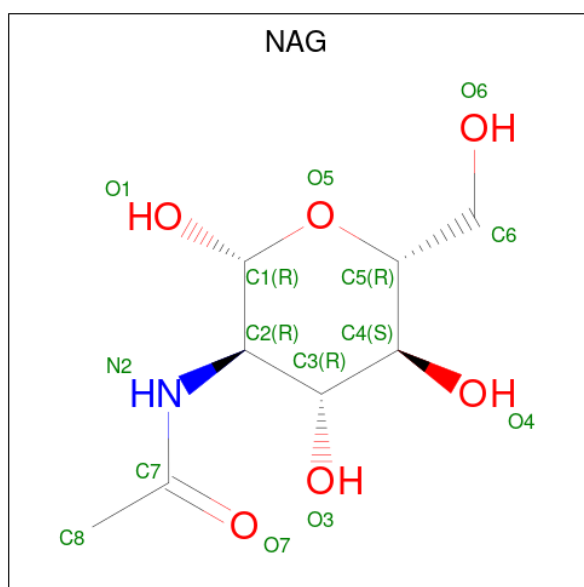
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	9	Total	C	N	O	0	0	0
			110	62	4	44			

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

- Molecule 5 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.



- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $\text{C}_8\text{H}_{15}\text{NO}_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		

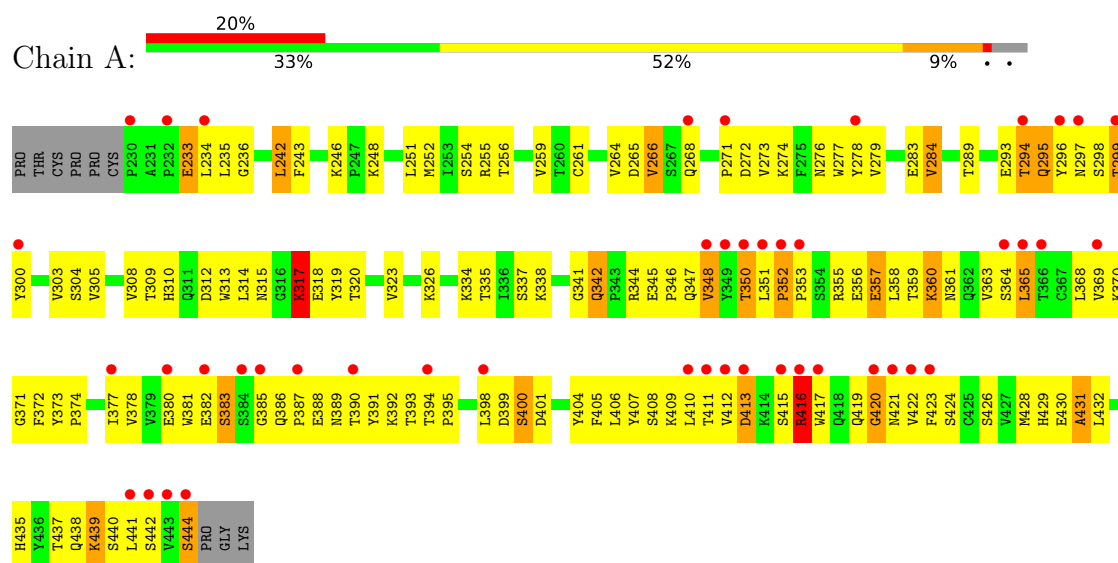
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			1	1		
7	C	1	Total	O	0	0
			1	1		

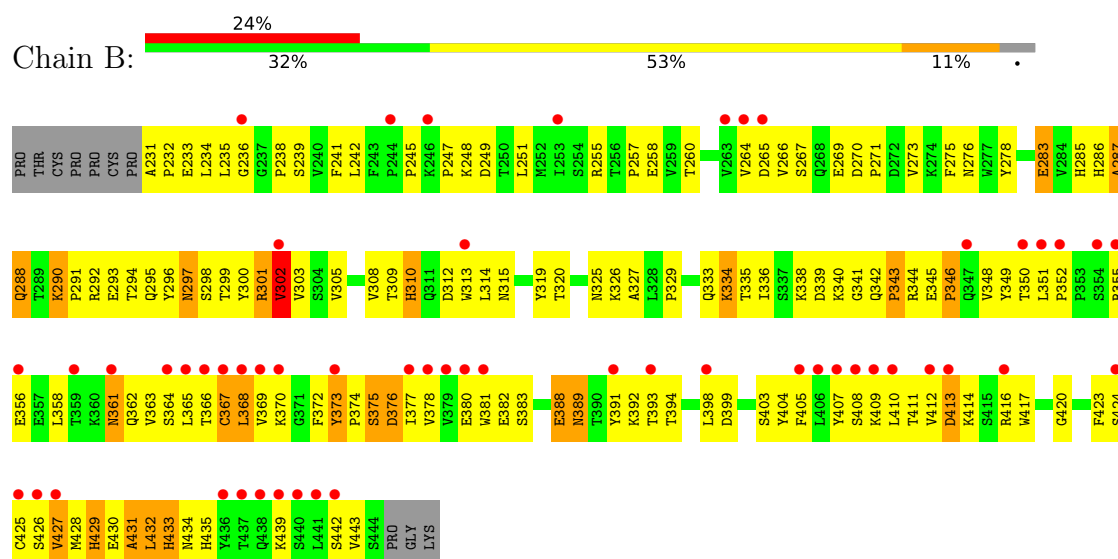
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

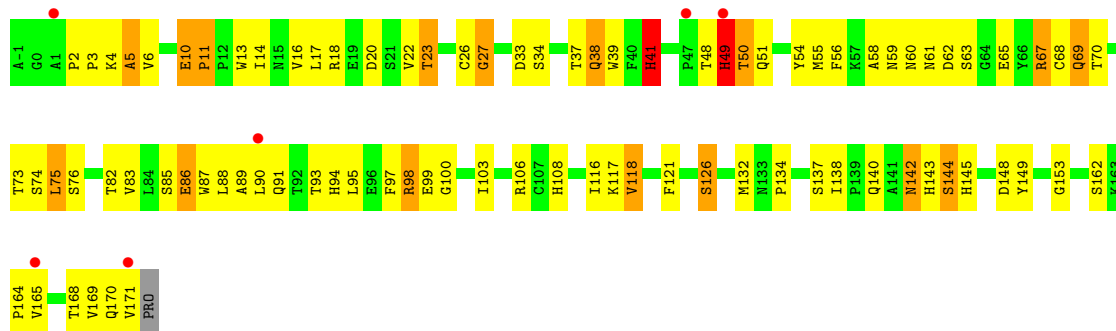
• Molecule 1: IgG1 Fc



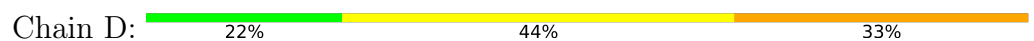
• Molecule 1: IgG1 Fc



• Molecule 2: IgG receptor IIA (CD32A) P131 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



- Molecule 4: 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 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[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, α , β , γ	127.53Å 127.53Å 256.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.37 – 2.65 46.37 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.37-2.65) 99.7 (46.37-2.65)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.277 , 0.327 0.281 , 0.330	Depositor DCC
R_{free} test set	1840 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	83.4	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 98.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5058	wwPDB-VP
Average B, all atoms (Å ²)	153.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: FUC, BMA, MAN, GAL, 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	0.49	0/1756	0.81	0/2398
1	B	0.44	0/1748	0.84	2/2387 (0.1%)
2	C	0.59	0/1430	0.92	2/1952 (0.1%)
All	All	0.51	0/4934	0.85	4/6737 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	302	VAL	CA-C-N	-6.83	114.43	123.17
1	B	302	VAL	C-N-CA	-6.83	114.43	123.17
2	C	142	ASN	CB-CA-C	-5.42	100.34	109.83
2	C	11	PRO	N-CA-C	-5.07	104.51	110.70

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	1708	0	1669	155	0
1	B	1701	0	1662	207	0
2	C	1386	0	1313	89	0
3	D	110	0	94	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	99	0	85	15	0
5	G	38	0	34	2	0
6	C	14	0	13	1	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
All	All	5058	0	4870	449	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 45.

All (449) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:LYS:HD2	1:B:291:PRO:CD	1.68	1.24
1:B:290:LYS:HE2	1:B:303:VAL:CG1	1.70	1.20
1:B:290:LYS:CD	1:B:291:PRO:HD2	1.75	1.15
1:B:288:GLN:HB2	1:B:305:VAL:O	1.49	1.13
1:B:409:LYS:HE3	1:B:411:THR:HG21	1.27	1.13
1:B:409:LYS:CE	1:B:411:THR:HG21	1.80	1.10
3:D:1:NAG:H82	3:D:1:NAG:O3	1.53	1.07
4:E:1:NAG:O3	4:E:1:NAG:H82	1.60	1.01
1:B:297:ASN:O	1:B:299:THR:HG23	1.63	0.97
1:B:409:LYS:CE	1:B:411:THR:CG2	2.42	0.97
1:B:248:LYS:HD2	1:B:255:ARG:HD2	1.47	0.97
1:B:409:LYS:HE2	1:B:411:THR:CG2	1.95	0.96
1:B:290:LYS:HE2	1:B:303:VAL:HG12	1.47	0.94
1:A:388:GLU:HG3	1:A:410:LEU:HD11	1.50	0.94
1:A:377:ILE:HD11	1:A:406:LEU:HD21	1.50	0.91
1:A:352:PRO:HB2	1:A:353:PRO:HD3	1.53	0.90
1:A:279:VAL:HG13	1:A:284:VAL:HG11	1.55	0.89
1:B:290:LYS:HG2	1:B:303:VAL:HG13	1.53	0.89
1:B:381:TRP:HZ2	1:B:408:SER:HB3	1.35	0.88
1:B:286:HIS:O	1:B:287:ALA:O	1.92	0.88
1:A:352:PRO:HB2	1:A:353:PRO:CD	2.04	0.87
1:B:290:LYS:CE	1:B:303:VAL:CG1	2.52	0.86
1:B:290:LYS:HD2	1:B:291:PRO:HD2	0.91	0.86
2:C:142:ASN:ND2	2:C:145:HIS:HE1	1.75	0.85
1:B:378:VAL:HB	1:B:428:MET:HB2	1.56	0.85
1:B:409:LYS:HE3	1:B:411:THR:CG2	2.05	0.84
1:B:248:LYS:HZ1	1:B:255:ARG:HG3	1.42	0.84
4:E:2:NAG:H83	4:E:8:FUC:H61	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:49[B]:HIS:HD2	2:C:54:TYR:HA	1.44	0.82
2:C:49[B]:HIS:CD2	2:C:54:TYR:HA	2.15	0.81
1:A:377:ILE:HG22	1:A:429:HIS:HD2	1.46	0.81
1:A:370:LYS:HE3	1:A:371:GLY:HA2	1.61	0.81
1:B:290:LYS:CE	1:B:303:VAL:HG12	2.12	0.80
1:B:288:GLN:CG	1:B:305:VAL:HB	2.12	0.80
1:B:290:LYS:HG2	1:B:303:VAL:CG1	2.11	0.79
1:B:248:LYS:NZ	1:B:255:ARG:HG3	1.97	0.79
1:B:288:GLN:CB	1:B:305:VAL:O	2.30	0.79
2:C:23:THR:HG22	2:C:55:MET:HG2	1.65	0.79
1:A:278:TYR:HD1	1:A:283:GLU:HA	1.49	0.78
1:A:380:GLU:HB2	1:A:426:SER:HB2	1.65	0.78
1:B:290:LYS:HE2	1:B:303:VAL:HG11	1.64	0.78
1:B:295:GLN:HG2	1:B:301:ARG:HB3	1.64	0.78
1:B:344:ARG:HH21	1:B:403:SER:HB3	1.47	0.78
1:A:377:ILE:HG22	1:A:429:HIS:CD2	2.19	0.77
1:B:372:PHE:HB2	1:B:429:HIS:CE1	2.19	0.77
1:B:295:GLN:OE1	1:B:301:ARG:HG2	1.84	0.77
1:B:248:LYS:HD2	1:B:255:ARG:CD	2.13	0.77
1:A:370:LYS:HD3	1:A:405:PHE:HB3	1.66	0.76
2:C:142:ASN:CG	2:C:145:HIS:CE1	2.64	0.76
1:B:288:GLN:HB2	1:B:305:VAL:C	2.09	0.76
1:B:295:GLN:CG	1:B:301:ARG:HB3	2.15	0.76
2:C:142:ASN:ND2	2:C:145:HIS:CE1	2.53	0.76
4:E:1:NAG:H61	4:E:2:NAG:HN2	1.50	0.75
2:C:91:GLN:HE22	2:C:106:ARG:NH1	1.85	0.75
1:B:381:TRP:CZ2	1:B:408:SER:HB3	2.21	0.75
1:B:355:ARG:HA	1:B:358:LEU:HG	1.69	0.74
1:B:288:GLN:OE1	1:B:288:GLN:HA	1.85	0.74
1:A:365:LEU:HB2	1:A:410:LEU:HB3	1.69	0.73
4:E:2:NAG:H83	4:E:8:FUC:O5	1.87	0.73
1:A:255:ARG:NH1	1:A:256:THR:OG1	2.21	0.73
1:B:248:LYS:HD3	1:B:248:LYS:C	2.14	0.73
1:B:301:ARG:HG3	1:B:301:ARG:O	1.87	0.73
2:C:142:ASN:OD1	2:C:144:SER:N	2.21	0.73
1:A:268:GLN:N	1:A:268:GLN:OE1	2.22	0.72
1:B:398:LEU:HD12	1:B:404:TYR:HE1	1.53	0.72
1:B:290:LYS:HG2	1:B:303:VAL:O	1.90	0.72
1:B:276:ASN:HB3	1:B:278:TYR:HE2	1.55	0.72
1:B:425:CYS:H	1:B:439:LYS:HB3	1.54	0.72
2:C:51:GLN:N	2:C:51:GLN:OE1	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:TYR:HB3	1:B:410:LEU:HD22	1.71	0.71
1:B:350:THR:HG22	1:B:439:LYS:HE3	1.71	0.71
2:C:142:ASN:CG	2:C:145:HIS:HE1	1.99	0.71
1:A:370:LYS:NZ	1:A:399:ASP:OD2	2.24	0.71
1:B:372:PHE:O	1:B:404:TYR:N	2.24	0.71
4:E:2:NAG:H83	4:E:8:FUC:C6	2.21	0.70
1:A:357:GLU:HG2	1:A:360:LYS:HG3	1.71	0.70
1:B:373:TYR:HD2	1:B:403:SER:HA	1.55	0.70
1:B:290:LYS:CG	1:B:303:VAL:HG13	2.21	0.70
1:B:238:PRO:HB3	1:B:265:ASP:O	1.91	0.70
1:B:248:LYS:CD	1:B:255:ARG:HD2	2.21	0.70
1:B:373:TYR:H	1:B:374:PRO:HD2	1.56	0.70
1:A:348:VAL:HG22	1:A:439:LYS:HD2	1.74	0.69
1:B:288:GLN:HG2	1:B:305:VAL:HB	1.74	0.69
1:A:392:LYS:HB3	1:B:405:PHE:HE2	1.57	0.69
1:B:320:THR:HA	1:B:335:THR:HG22	1.75	0.69
1:A:394:THR:HG23	1:A:406:LEU:HB2	1.75	0.69
4:E:1:NAG:H82	4:E:1:NAG:HO3	1.58	0.69
1:B:290:LYS:CB	1:B:303:VAL:O	2.42	0.68
4:E:2:NAG:C8	4:E:8:FUC:H61	2.22	0.68
1:B:248:LYS:CE	1:B:255:ARG:NE	2.55	0.68
1:B:348:VAL:HG22	1:B:369:VAL:HG12	1.76	0.68
2:C:33:ASP:N	2:C:33:ASP:OD2	2.27	0.68
1:A:398:LEU:HD22	1:A:399:ASP:H	1.59	0.67
1:A:370:LYS:CD	1:A:405:PHE:HB3	2.24	0.67
1:A:409:LYS:NZ	1:B:399:ASP:OD2	2.27	0.67
1:B:291:PRO:O	1:B:293:GLU:N	2.27	0.67
1:A:370:LYS:CE	1:A:399:ASP:OD2	2.41	0.67
5:G:1:NAG:O7	5:G:2:NAG:H82	1.95	0.67
1:A:278:TYR:HB2	1:A:320:THR:OG1	1.95	0.66
1:A:235:LEU:HD23	1:A:235:LEU:O	1.95	0.66
1:B:248:LYS:HE3	1:B:255:ARG:HE	1.59	0.66
1:A:357:GLU:OE2	1:A:364:SER:N	2.28	0.66
1:A:430:GLU:HA	1:A:435:HIS:CD2	2.31	0.65
1:A:294:THR:HA	1:A:300:TYR:CD1	2.31	0.65
1:A:265:ASP:HA	1:A:299:THR:HG21	1.79	0.65
1:A:294:THR:HA	1:A:300:TYR:CE1	2.31	0.65
1:A:357:GLU:HG3	1:B:349:TYR:HE2	1.62	0.65
2:C:67:ARG:NH1	2:C:76:SER:O	2.29	0.65
2:C:98:ARG:HA	2:C:170:GLN:O	1.97	0.65
1:A:353:PRO:HB3	1:A:363:VAL:HG11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:37:THR:HG22	2:C:70:THR:HG22	1.78	0.65
1:B:286:HIS:C	1:B:287:ALA:O	2.38	0.64
1:B:248:LYS:HE3	1:B:255:ARG:NE	2.11	0.64
3:D:1:NAG:O3	3:D:1:NAG:C8	2.39	0.64
1:A:357:GLU:HA	1:A:360:LYS:HZ3	1.63	0.64
1:A:394:THR:CG2	1:A:407:TYR:H	2.10	0.64
1:B:248:LYS:CE	1:B:255:ARG:HE	2.11	0.64
1:B:234:LEU:HD12	1:B:235:LEU:H	1.61	0.64
1:B:329:PRO:HB2	2:C:86:GLU:HA	1.80	0.64
1:A:370:LYS:HE2	1:A:399:ASP:OD2	1.98	0.64
1:B:288:GLN:HG3	1:B:305:VAL:HB	1.80	0.63
1:B:315:ASN:H	1:B:338:LYS:HZ3	1.46	0.63
1:A:357:GLU:OE1	1:A:363:VAL:HA	1.98	0.63
2:C:99:GLU:N	2:C:170:GLN:O	2.28	0.63
1:A:388:GLU:CD	1:A:389:ASN:H	2.07	0.63
2:C:142:ASN:OD1	2:C:142:ASN:O	2.17	0.62
2:C:100:GLY:HA2	2:C:140:GLN:HE22	1.62	0.62
1:B:266:VAL:CG1	1:B:271:PRO:HA	2.30	0.62
1:A:355:ARG:NH2	1:B:350:THR:OG1	2.33	0.62
1:B:409:LYS:HE2	1:B:411:THR:HG23	1.81	0.62
1:B:409:LYS:CE	1:B:411:THR:HG23	2.30	0.62
1:A:347:GLN:HG2	1:A:370:LYS:O	2.00	0.62
1:B:373:TYR:O	1:B:373:TYR:CD1	2.53	0.62
1:A:359:THR:OG1	1:A:360:LYS:NZ	2.31	0.61
2:C:18:ARG:HD3	2:C:85:SER:HB2	1.82	0.61
1:A:372:PHE:CE1	1:A:404:TYR:HB2	2.35	0.61
1:B:342:GLN:O	1:B:344:ARG:N	2.33	0.61
2:C:67:ARG:HG2	2:C:67:ARG:HH11	1.64	0.61
1:B:372:PHE:HB2	1:B:429:HIS:NE2	2.16	0.61
1:B:346:PRO:HD2	1:B:432:LEU:HD23	1.83	0.61
2:C:103:ILE:HB	2:C:138:ILE:CG1	2.31	0.60
1:A:415:SER:C	1:A:417:TRP:H	2.10	0.60
2:C:142:ASN:OD1	2:C:144:SER:HB3	2.02	0.60
1:A:233:GLU:O	1:A:235:LEU:N	2.31	0.60
1:A:265:ASP:HA	1:A:299:THR:CG2	2.31	0.60
1:A:372:PHE:HE1	1:A:404:TYR:HB2	1.67	0.60
1:B:432:LEU:CD1	1:B:433:HIS:H	2.15	0.59
4:E:1:NAG:O3	4:E:1:NAG:C8	2.46	0.59
1:A:394:THR:HG21	1:A:407:TYR:H	1.67	0.59
1:A:439:LYS:HD3	1:B:356:GLU:OE1	2.02	0.59
1:B:265:ASP:HA	1:B:299:THR:HB	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:HIS:O	1:B:287:ALA:C	2.47	0.58
1:A:341:GLY:HA3	1:A:373:TYR:CE1	2.38	0.58
1:A:398:LEU:HA	1:A:404:TYR:CD1	2.38	0.58
1:B:249:ASP:C	1:B:257:PRO:HG3	2.29	0.58
1:A:416:ARG:HH12	1:A:419:GLN:HE21	1.51	0.58
1:B:266:VAL:HB	1:B:300:TYR:HB2	1.86	0.58
1:B:290:LYS:CG	1:B:303:VAL:O	2.52	0.58
1:A:392:LYS:HB3	1:B:405:PHE:CE2	2.38	0.58
1:B:290:LYS:CD	1:B:303:VAL:HG13	2.33	0.57
1:B:314:LEU:HA	1:B:338:LYS:HD3	1.85	0.57
1:B:423:PHE:O	1:B:424:SER:OG	2.22	0.57
1:A:273:VAL:HG13	1:A:323:VAL:HG23	1.85	0.57
1:B:381:TRP:CE3	1:B:425:CYS:HB3	2.39	0.57
2:C:91:GLN:NE2	2:C:106:ARG:NH1	2.52	0.57
1:B:373:TYR:O	1:B:373:TYR:HD1	1.87	0.57
1:B:409:LYS:O	1:B:410:LEU:CD2	2.52	0.57
1:A:388:GLU:O	1:A:389:ASN:ND2	2.36	0.57
1:A:391:TYR:HA	1:A:409:LYS:O	2.05	0.57
1:B:409:LYS:HE2	1:B:411:THR:OG1	2.04	0.57
1:A:350:THR:HG22	1:A:441:LEU:HD23	1.86	0.57
1:B:413:ASP:HB2	1:B:416:ARG:HG2	1.86	0.57
2:C:17:LEU:HD21	2:C:89:ALA:HB2	1.86	0.57
2:C:142:ASN:OD1	2:C:145:HIS:CE1	2.58	0.56
1:B:361:ASN:O	1:B:414:LYS:HB2	2.05	0.56
1:A:391:TYR:HB3	1:A:410:LEU:HD12	1.87	0.56
2:C:91:GLN:NE2	2:C:106:ARG:HH11	2.03	0.56
2:C:142:ASN:OD1	2:C:142:ASN:C	2.48	0.56
1:A:355:ARG:HE	1:A:356:GLU:CD	2.14	0.56
3:D:8:NAG:O7	3:D:8:NAG:O3	2.19	0.56
2:C:48:THR:HG22	2:C:49[A]:HIS:H	1.70	0.56
1:B:343:PRO:HA	1:B:374:PRO:HD3	1.88	0.56
2:C:56:PHE:HE2	2:C:62:ASP:OD2	1.88	0.56
2:C:142:ASN:OD1	2:C:145:HIS:ND1	2.39	0.56
2:C:94:HIS:O	2:C:95:LEU:HD23	2.06	0.55
1:A:399:ASP:O	1:A:401:ASP:N	2.39	0.55
1:B:248:LYS:HZ1	1:B:255:ARG:CG	2.17	0.55
1:A:344:ARG:HD3	1:A:373:TYR:HB2	1.89	0.55
2:C:10[A]:GLU:HB3	2:C:11:PRO:CD	2.37	0.55
1:B:432:LEU:HD12	1:B:433:HIS:HB2	1.89	0.55
2:C:23:THR:HG22	2:C:55:MET:CG	2.36	0.55
2:C:67:ARG:HB3	2:C:75:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:LYS:O	1:B:410:LEU:HD22	2.07	0.55
1:B:325:ASN:OD1	1:B:326:LYS:N	2.40	0.55
1:A:246:LYS:HE3	3:D:6:GAL:H2	1.89	0.55
1:A:310:HIS:O	1:A:314:LEU:HD23	2.07	0.55
2:C:60:ASN:C	2:C:62:ASP:H	2.14	0.55
1:A:408:SER:O	1:B:407:TYR:OH	2.24	0.54
2:C:67:ARG:NH1	2:C:67:ARG:HG2	2.22	0.54
1:B:248:LYS:HD2	1:B:255:ARG:NE	2.21	0.54
1:A:318:GLU:OE1	1:A:337:SER:HB3	2.07	0.54
1:B:319:TYR:HB2	1:B:336:ILE:HD11	1.89	0.54
1:B:370:LYS:HA	1:B:405:PHE:HA	1.89	0.54
1:A:278:TYR:CD1	1:A:283:GLU:HA	2.36	0.54
2:C:48:THR:HG22	2:C:49[B]:HIS:H	1.73	0.54
1:A:341:GLY:HA3	1:A:373:TYR:HE1	1.72	0.54
1:A:372:PHE:HB2	1:A:429:HIS:NE2	2.23	0.54
1:A:374:PRO:HD3	1:A:430:GLU:OE2	2.07	0.54
1:A:388:GLU:O	1:A:391:TYR:HE1	1.90	0.54
1:B:248:LYS:NZ	1:B:255:ARG:CG	2.71	0.54
1:B:398:LEU:HA	1:B:404:TYR:CD1	2.43	0.54
2:C:56:PHE:CE2	2:C:62:ASP:OD2	2.61	0.54
1:A:416:ARG:NH1	1:A:419:GLN:HE21	2.06	0.54
1:B:270:ASP:OD2	1:B:326:LYS:HG3	2.07	0.54
1:B:389:ASN:HA	1:B:391:TYR:CE2	2.42	0.54
1:A:382:GLU:OE2	1:A:385:GLY:N	2.41	0.53
1:A:293:GLU:O	1:A:295:GLN:N	2.41	0.53
1:A:265:ASP:OD2	2:C:117:LYS:NZ	2.42	0.53
1:A:388:GLU:C	1:A:389:ASN:HD22	2.15	0.53
1:A:357:GLU:HG3	1:B:349:TYR:CE2	2.44	0.53
1:B:245:PRO:HB3	1:B:258:GLU:H	1.73	0.53
1:B:362:GLN:HA	1:B:362:GLN:OE1	2.07	0.53
2:C:59:ASN:ND2	6:C:201:NAG:H83	2.24	0.53
1:A:278:TYR:HE1	1:A:283:GLU:HB2	1.72	0.52
4:E:2:NAG:O7	4:E:2:NAG:O3	2.20	0.52
1:B:293:GLU:HG3	1:B:293:GLU:O	2.10	0.52
1:B:366:THR:OG1	1:B:367:CYS:N	2.43	0.52
1:B:374:PRO:HG2	1:B:429:HIS:CE1	2.44	0.52
1:A:242:LEU:O	1:A:242:LEU:HD23	2.09	0.52
1:A:420:GLY:HA3	1:A:442:SER:OG	2.10	0.52
1:B:391:TYR:O	1:B:392:LYS:HG3	2.10	0.52
1:B:432:LEU:CD1	1:B:433:HIS:HB2	2.40	0.52
1:A:415:SER:O	1:A:417:TRP:N	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:37:THR:OG1	2:C:50:THR:O	2.28	0.52
1:B:427:VAL:HG13	1:B:429:HIS:HB2	1.92	0.52
1:B:368:LEU:HD13	1:B:407:TYR:CZ	2.45	0.51
2:C:99:GLU:OE1	2:C:171:VAL:HG12	2.09	0.51
1:B:345:GLU:HA	1:B:431:ALA:HB1	1.93	0.51
1:A:381:TRP:HA	1:A:424:SER:O	2.11	0.51
1:B:290:LYS:CG	1:B:303:VAL:CG1	2.86	0.51
2:C:87:TRP:O	2:C:88:LEU:HD12	2.09	0.51
1:A:398:LEU:HA	1:A:404:TYR:HD1	1.74	0.51
1:B:346:PRO:HD3	1:B:431:ALA:HB3	1.93	0.51
1:B:374:PRO:O	1:B:376:ASP:N	2.44	0.51
2:C:100:GLY:HA2	2:C:140:GLN:NE2	2.25	0.51
1:B:301:ARG:HH21	4:E:2:NAG:C7	2.23	0.51
2:C:18:ARG:HG3	2:C:59:ASN:HA	1.92	0.51
1:A:251:LEU:HD23	1:A:428:MET:HB3	1.93	0.51
4:E:2:NAG:H83	4:E:8:FUC:C5	2.40	0.51
1:A:389:ASN:C	1:A:391:TYR:H	2.18	0.51
1:A:243:PHE:HE2	3:D:3:BMA:H62	1.75	0.50
2:C:20:ASP:OD1	2:C:108:HIS:HE1	1.94	0.50
1:B:329:PRO:O	2:C:85:SER:OG	2.29	0.50
1:A:233:GLU:C	1:A:235:LEU:H	2.18	0.50
1:A:278:TYR:CE1	1:A:283:GLU:HB2	2.47	0.50
1:A:357:GLU:HG2	1:A:360:LYS:CG	2.40	0.50
1:A:413:ASP:OD2	1:A:415:SER:OG	2.27	0.50
2:C:143:HIS:HA	2:C:169:VAL:HG13	1.92	0.50
1:B:248:LYS:HD3	1:B:248:LYS:O	2.10	0.50
1:B:312:ASP:O	1:B:319:TYR:OH	2.26	0.50
1:B:374:PRO:HG2	1:B:429:HIS:NE2	2.27	0.50
2:C:103:ILE:HB	2:C:138:ILE:HG13	1.92	0.50
1:A:255:ARG:HD2	1:A:256:THR:H	1.77	0.50
1:A:344:ARG:HH11	1:A:344:ARG:HG2	1.76	0.50
1:B:325:ASN:OD1	1:B:327:ALA:N	2.22	0.50
2:C:69:GLN:NE2	2:C:73:THR:O	2.46	0.49
2:C:91:GLN:HE22	2:C:106:ARG:HH11	1.58	0.49
1:B:247:PRO:O	1:B:251:LEU:HD12	2.13	0.49
1:B:340:LYS:HD2	1:B:340:LYS:C	2.37	0.49
2:C:13:TRP:HB3	2:C:91:GLN:HG2	1.94	0.49
1:A:442:SER:H	1:A:444:SER:HG	1.60	0.49
2:C:59:ASN:O	2:C:62:ASP:HB3	2.12	0.49
1:A:277:TRP:NE1	1:A:304:SER:OG	2.40	0.48
1:A:309:THR:HB	1:A:312:ASP:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:LEU:HD13	1:A:338:LYS:HD3	1.95	0.48
1:A:381:TRP:CG	1:A:410:LEU:HD13	2.48	0.48
1:B:248:LYS:C	1:B:248:LYS:CD	2.86	0.48
1:A:372:PHE:CE2	1:A:377:ILE:HG21	2.48	0.48
1:A:308:VAL:HG21	1:A:319:TYR:CZ	2.49	0.48
1:B:276:ASN:HB3	1:B:278:TYR:CE2	2.43	0.48
1:B:373:TYR:CD2	1:B:403:SER:HA	2.43	0.48
1:A:370:LYS:HD2	1:A:371:GLY:N	2.29	0.48
1:A:382:GLU:HB3	1:A:424:SER:HB2	1.96	0.48
1:B:388:GLU:O	1:B:389:ASN:CG	2.57	0.47
1:A:236:GLY:HA2	2:C:116:ILE:HD12	1.96	0.47
1:A:346:PRO:HD3	1:A:431:ALA:HB3	1.95	0.47
1:B:297:ASN:O	1:B:298:SER:C	2.56	0.47
1:B:309:THR:HB	1:B:312:ASP:HB2	1.96	0.47
1:B:375:SER:HA	1:B:404:TYR:CE2	2.49	0.47
2:C:2:PRO:HG2	2:C:74:SER:OG	2.14	0.47
1:B:290:LYS:CE	1:B:291:PRO:HD2	2.41	0.47
1:B:308:VAL:HG21	1:B:319:TYR:OH	2.14	0.47
1:A:342:GLN:OE1	1:A:342:GLN:N	2.32	0.47
1:A:442:SER:N	1:A:444:SER:OG	2.47	0.47
2:C:121:PHE:CD1	2:C:126:SER:HA	2.49	0.47
1:A:255:ARG:NH1	1:A:256:THR:O	2.47	0.47
1:B:283:GLU:HG2	1:B:285:HIS:CE1	2.50	0.47
1:B:381:TRP:CZ3	1:B:425:CYS:HB3	2.49	0.47
2:C:148:ASP:HB3	2:C:164:PRO:HB2	1.97	0.47
2:C:41:HIS:O	2:C:65:GLU:O	2.33	0.47
1:B:407:TYR:O	1:B:408:SER:HB2	2.15	0.46
1:B:334:LYS:HD2	1:B:334:LYS:HA	1.68	0.46
1:B:320:THR:HG22	1:B:335:THR:CG2	2.46	0.46
1:A:246:LYS:NZ	3:D:6:GAL:H2	2.30	0.46
1:A:344:ARG:HD3	1:A:373:TYR:CB	2.45	0.46
1:A:364:SER:O	1:A:364:SER:OG	2.33	0.46
1:B:301:ARG:NH2	4:E:2:NAG:O7	2.48	0.46
1:B:350:THR:CG2	1:B:439:LYS:HG3	2.45	0.46
1:B:310:HIS:O	1:B:314:LEU:HD23	2.16	0.46
1:A:389:ASN:O	1:A:391:TYR:N	2.49	0.46
1:A:317:LYS:HB3	1:A:319:TYR:CE1	2.49	0.46
1:A:365:LEU:O	1:A:409:LYS:HA	2.16	0.46
1:B:301:ARG:NH2	4:E:2:NAG:C7	2.79	0.46
2:C:10[A]:GLU:HB2	2:C:23:THR:OG1	2.16	0.46
2:C:10[B]:GLU:HB2	2:C:23:THR:OG1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:GLU:C	1:A:359:THR:H	2.24	0.46
1:A:261:CYS:HB2	1:A:277:TRP:CH2	2.50	0.46
1:B:258:GLU:HA	1:B:308:VAL:HG12	1.97	0.46
1:A:423:PHE:HB2	1:A:441:LEU:HD12	1.97	0.46
1:B:266:VAL:O	1:B:267:SER:HB3	2.16	0.46
2:C:14:ILE:HD13	2:C:93:THR:O	2.16	0.46
2:C:118:VAL:HG11	2:C:134:PRO:HA	1.98	0.46
1:B:248:LYS:CD	1:B:255:ARG:NE	2.79	0.45
1:B:409:LYS:HE2	1:B:411:THR:CB	2.46	0.45
2:C:23:THR:HA	2:C:54:TYR:O	2.16	0.45
2:C:121:PHE:HD1	2:C:126:SER:HA	1.80	0.45
2:C:170:GLN:OE1	2:C:171:VAL:HG22	2.17	0.45
1:A:255:ARG:HH11	1:A:256:THR:H	1.65	0.45
1:A:271:PRO:HB3	1:A:300:TYR:CD2	2.52	0.45
1:A:368:LEU:HD23	1:A:369:VAL:N	2.31	0.45
1:B:283:GLU:HG2	1:B:285:HIS:HE1	1.81	0.45
1:B:333:GLN:O	1:B:334:LYS:HB2	2.17	0.45
1:A:295:GLN:HG3	1:A:296:TYR:H	1.80	0.45
2:C:17:LEU:CD2	2:C:89:ALA:HB2	2.47	0.45
1:A:346:PRO:HG2	1:A:432:LEU:HD21	1.98	0.45
1:B:295:GLN:HB2	1:B:299:THR:O	2.17	0.45
1:B:409:LYS:O	1:B:410:LEU:HD23	2.16	0.45
2:C:4:LYS:O	2:C:5:ALA:CB	2.64	0.45
2:C:149:TYR:O	2:C:164:PRO:HA	2.15	0.45
1:A:409:LYS:HZ1	1:B:399:ASP:CG	2.24	0.45
1:B:241:PHE:CE2	4:E:3:BMA:H3	2.52	0.45
1:B:314:LEU:O	1:B:315:ASN:HB2	2.17	0.45
1:A:353:PRO:HB3	1:A:363:VAL:CG1	2.45	0.45
1:A:400:SER:OG	1:A:401:ASP:N	2.49	0.45
1:B:340:LYS:HD2	1:B:341:GLY:N	2.31	0.45
2:C:143:HIS:HA	2:C:169:VAL:CG1	2.47	0.45
1:A:378:VAL:HB	1:A:428:MET:HB2	1.98	0.44
1:A:415:SER:C	1:A:417:TRP:N	2.75	0.44
1:B:309:THR:HG22	1:B:312:ASP:H	1.81	0.44
1:A:274:LYS:HZ2	1:A:276:ASN:CG	2.25	0.44
1:B:248:LYS:NZ	1:B:255:ARG:CD	2.81	0.44
1:B:313:TRP:CH2	1:B:338:LYS:HG3	2.52	0.44
1:B:409:LYS:CG	1:B:411:THR:HG23	2.48	0.44
2:C:20:ASP:OD2	2:C:108:HIS:CE1	2.71	0.44
1:A:318:GLU:OE1	1:A:318:GLU:HA	2.17	0.44
1:A:370:LYS:HE3	1:A:371:GLY:CA	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:GLU:O	1:B:271:PRO:HD3	2.18	0.44
1:A:357:GLU:HA	1:A:360:LYS:NZ	2.32	0.44
1:B:248:LYS:HZ1	1:B:255:ARG:HE	1.64	0.44
1:B:248:LYS:CD	1:B:255:ARG:CD	2.88	0.44
1:B:372:PHE:HD2	1:B:429:HIS:HE2	1.66	0.44
1:A:246:LYS:CE	3:D:6:GAL:H2	2.45	0.44
1:A:271:PRO:HB3	1:A:300:TYR:HD2	1.83	0.44
1:A:313:TRP:NE1	1:A:338:LYS:HG2	2.33	0.44
1:A:432:LEU:HD12	1:A:435:HIS:C	2.43	0.44
1:B:363:VAL:HG22	1:B:365:LEU:HD22	2.00	0.43
1:B:382:GLU:OE2	1:B:424:SER:HB2	2.17	0.43
1:A:391:TYR:HA	1:A:410:LEU:HA	2.01	0.43
1:B:348:VAL:O	1:B:349:TYR:HD1	2.01	0.43
5:G:1:NAG:H62	5:G:3:FUC:O2	2.18	0.43
1:A:356:GLU:OE1	1:A:356:GLU:N	2.48	0.43
1:A:370:LYS:HZ3	1:A:399:ASP:CG	2.25	0.43
1:A:394:THR:OG1	1:A:395:PRO:HD2	2.19	0.43
1:A:320:THR:HG22	1:A:335:THR:HG22	2.00	0.43
2:C:4:LYS:O	2:C:74:SER:O	2.35	0.43
2:C:10[B]:GLU:CD	2:C:11:PRO:HD3	2.43	0.43
1:B:380:GLU:HB2	1:B:426:SER:HB2	2.01	0.43
1:B:366:THR:O	1:B:439:LYS:NZ	2.49	0.43
2:C:90:LEU:HD23	2:C:165:VAL:HG22	2.00	0.43
1:B:290:LYS:CD	1:B:303:VAL:CG1	2.93	0.43
1:B:320:THR:HG22	1:B:335:THR:HG21	2.01	0.43
1:A:370:LYS:HZ3	1:A:399:ASP:CB	2.32	0.43
1:B:432:LEU:HD13	1:B:433:HIS:N	2.34	0.43
1:A:344:ARG:HB3	1:A:345:GLU:H	1.66	0.42
1:B:374:PRO:CG	1:B:429:HIS:CE1	3.02	0.42
1:A:423:PHE:O	1:A:440:SER:HA	2.20	0.42
1:B:399:ASP:N	1:B:403:SER:O	2.46	0.42
1:A:386:GLN:HB3	1:A:387:PRO:HD2	2.02	0.42
1:B:251:LEU:HD21	1:B:430:GLU:OE2	2.20	0.42
1:B:329:PRO:CB	2:C:86:GLU:HA	2.48	0.42
1:B:377:ILE:HD12	1:B:429:HIS:CD2	2.55	0.42
1:B:242:LEU:HD22	1:B:260:THR:O	2.19	0.42
1:B:409:LYS:HG2	1:B:410:LEU:N	2.34	0.42
1:B:434:ASN:O	1:B:435:HIS:ND1	2.52	0.42
2:C:16:VAL:CG2	2:C:83:VAL:HG22	2.50	0.42
1:A:383:SER:O	1:A:422:VAL:HG13	2.20	0.42
1:B:290:LYS:HD2	1:B:291:PRO:HD3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:GLU:HG3	1:A:346:PRO:HD2	2.02	0.42
2:C:59:ASN:OD1	2:C:59:ASN:C	2.63	0.42
1:A:248:LYS:HD2	1:A:252:MET:SD	2.59	0.42
1:B:231:ALA:N	1:B:232:PRO:CD	2.83	0.42
1:B:278:TYR:O	1:B:320:THR:HG23	2.20	0.42
1:B:264:VAL:HG11	4:E:1:NAG:O4	2.21	0.41
2:C:88:LEU:HB3	2:C:162:SER:HB3	2.01	0.41
1:A:438:GLN:C	1:A:439:LYS:HZ1	2.26	0.41
1:B:308:VAL:CG2	1:B:319:TYR:OH	2.68	0.41
1:B:417:TRP:O	1:B:420:GLY:N	2.51	0.41
2:C:10[A]:GLU:HB3	2:C:11:PRO:HD2	2.02	0.41
2:C:97:PHE:CD2	2:C:97:PHE:N	2.89	0.41
2:C:103:ILE:O	2:C:137:SER:HA	2.19	0.41
2:C:148:ASP:N	2:C:148:ASP:OD2	2.53	0.41
2:C:10[B]:GLU:HB3	2:C:11:PRO:HD2	2.02	0.41
2:C:38:GLN:O	2:C:39:TRP:HB2	2.20	0.41
1:A:299:THR:O	1:A:300:TYR:CD1	2.74	0.41
1:A:357:GLU:CD	1:A:363:VAL:HA	2.44	0.41
1:A:409:LYS:NZ	1:B:399:ASP:CG	2.79	0.41
1:B:275:PHE:HE2	1:B:302:VAL:HG11	1.85	0.41
1:B:296:TYR:O	1:B:297:ASN:HB2	2.19	0.41
2:C:26:CYS:O	2:C:27:GLY:O	2.38	0.41
1:A:235:LEU:HA	2:C:132:MET:HE3	2.03	0.41
1:A:389:ASN:C	1:A:391:TYR:N	2.78	0.41
1:B:409:LYS:HG2	1:B:411:THR:HG23	2.01	0.41
1:A:388:GLU:C	1:A:389:ASN:ND2	2.78	0.41
1:B:288:GLN:CB	1:B:305:VAL:C	2.85	0.41
2:C:20:ASP:CG	2:C:108:HIS:HE1	2.29	0.41
1:A:236:GLY:CA	2:C:116:ILE:HD12	2.51	0.41
1:A:372:PHE:CD1	1:A:372:PHE:C	2.98	0.41
1:B:273:VAL:HG12	1:B:325:ASN:HD22	1.85	0.41
1:B:374:PRO:HD2	1:B:429:HIS:CE1	2.55	0.41
1:B:424:SER:OG	1:B:439:LYS:O	2.27	0.41
1:A:243:PHE:CZ	3:D:4:MAN:H2	2.56	0.41
1:A:264:VAL:O	1:A:265:ASP:HB2	2.21	0.41
1:A:266:VAL:CG1	1:A:300:TYR:HB2	2.50	0.41
1:B:296:TYR:O	1:B:297:ASN:CB	2.68	0.41
1:B:342:GLN:N	1:B:342:GLN:CD	2.79	0.41
1:B:363:VAL:O	1:B:411:THR:HG22	2.21	0.41
1:B:373:TYR:H	1:B:374:PRO:CD	2.29	0.41
1:B:442:SER:HB3	1:B:443:VAL:H	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:LYS:NZ	1:B:255:ARG:HE	2.18	0.40
1:B:269:GLU:C	1:B:271:PRO:HD3	2.46	0.40
1:B:308:VAL:HG21	1:B:319:TYR:CZ	2.56	0.40
1:B:290:LYS:HG2	1:B:303:VAL:C	2.46	0.40
1:B:291:PRO:C	1:B:293:GLU:N	2.79	0.40
1:B:290:LYS:HB2	1:B:303:VAL:O	2.17	0.40
1:B:320:THR:CA	1:B:335:THR:HG22	2.50	0.40
2:C:48:THR:O	2:C:49[B]:HIS:C	2.65	0.40
1:A:358:LEU:HD12	1:A:417:TRP:CH2	2.55	0.40
1:B:290:LYS:HG2	1:B:303:VAL:H	1.85	0.40
2:C:117:LYS:O	2:C:153:GLY:HA2	2.22	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	213/224 (95%)	150 (70%)	44 (21%)	19 (9%)	0	0
1	B	212/224 (95%)	150 (71%)	40 (19%)	22 (10%)	0	0
2	C	174/174 (100%)	144 (83%)	19 (11%)	11 (6%)	1	1
All	All	599/622 (96%)	444 (74%)	103 (17%)	52 (9%)	0	0

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	LEU
1	A	272	ASP
1	A	295	GLN
1	A	411	THR
1	A	413	ASP
1	A	431	ALA

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Mol	Chain	Res	Type
1	B	287	ALA
1	B	297	ASN
1	B	361	ASN
1	B	373	TYR
1	B	375	SER
1	B	389	ASN
1	B	433	HIS
2	C	5	ALA
2	C	41	HIS
1	A	294	THR
1	A	361	ASN
1	A	390	THR
1	A	400	SER
1	A	416	ARG
1	B	383	SER
1	B	413	ASP
1	B	429	HIS
2	C	27	GLY
2	C	49[A]	HIS
2	C	49[B]	HIS
1	A	317	LYS
1	A	334	LYS
1	A	352	PRO
1	A	383	SER
1	B	292	ARG
1	B	310	HIS
1	B	352	PRO
1	B	367	CYS
1	B	432	LEU
2	C	69	GLN
2	C	98	ARG
1	A	351	LEU
1	A	420	GLY
1	B	236	GLY
1	B	431	ALA
2	C	3	PRO
2	C	38	GLN
2	C	58	ALA
1	A	360	LYS
1	A	421	ASN
1	B	233	GLU
1	B	334	LYS

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Mol	Chain	Res	Type
2	C	61	ASN
1	B	290	LYS
1	B	346	PRO
1	B	343	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	200/208 (96%)	174 (87%)	26 (13%)	4	6
1	B	199/208 (96%)	183 (92%)	16 (8%)	11	19
2	C	157/155 (101%)	137 (87%)	20 (13%)	4	6
All	All	556/571 (97%)	494 (89%)	62 (11%)	6	8

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	GLU
1	A	242	LEU
1	A	254	SER
1	A	259	VAL
1	A	266	VAL
1	A	284	VAL
1	A	289	THR
1	A	297	ASN
1	A	298	SER
1	A	299	THR
1	A	303	VAL
1	A	305	VAL
1	A	315	ASN
1	A	317	LYS
1	A	326	LYS
1	A	342	GLN
1	A	348	VAL
1	A	350	THR

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Mol	Chain	Res	Type
1	A	357	GLU
1	A	365	LEU
1	A	393	THR
1	A	412	VAL
1	A	416	ARG
1	A	437	THR
1	A	439	LYS
1	A	444	SER
1	B	239	SER
1	B	283	GLU
1	B	288	GLN
1	B	294	THR
1	B	301	ARG
1	B	302	VAL
1	B	339	ASP
1	B	351	LEU
1	B	364	SER
1	B	368	LEU
1	B	376	ASP
1	B	388	GLU
1	B	393	THR
1	B	394	THR
1	B	412	VAL
1	B	427	VAL
2	C	6	VAL
2	C	10[A]	GLU
2	C	10[B]	GLU
2	C	22	VAL
2	C	23	THR
2	C	34	SER
2	C	41	HIS
2	C	49[A]	HIS
2	C	49[B]	HIS
2	C	50	THR
2	C	63	SER
2	C	67	ARG
2	C	68	CYS
2	C	75	LEU
2	C	82	THR
2	C	86	GLU
2	C	118	VAL
2	C	126	SER

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Mol	Chain	Res	Type
2	C	144	SER
2	C	168	THR

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	285	HIS
1	A	389	ASN
1	A	435	HIS
1	A	438	GLN
1	B	276	ASN
1	B	285	HIS
1	B	347	GLN
1	B	418	GLN
2	C	15	ASN
2	C	69	GLN
2	C	91	GLN
2	C	108	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 ⓘ

20 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	0.45	0	17,19,21	0.51	0
3	NAG	D	2	3	14,14,15	0.71	1 (7%)	17,19,21	0.80	0
3	BMA	D	3	3	11,11,12	1.40	1 (9%)	15,15,17	1.23	3 (20%)
3	MAN	D	4	3	11,11,12	1.35	1 (9%)	15,15,17	0.90	1 (6%)
3	NAG	D	5	3	14,14,15	0.54	0	17,19,21	1.67	3 (17%)
3	GAL	D	6	3	11,11,12	0.90	1 (9%)	15,15,17	2.29	3 (20%)
3	MAN	D	7	3	11,11,12	0.25	0	15,15,17	0.49	0
3	NAG	D	8	3	14,14,15	0.29	0	17,19,21	0.55	0
3	FUC	D	9	3	10,10,11	0.76	0	14,14,16	0.84	0
4	NAG	E	1	1,4	14,14,15	0.44	0	17,19,21	0.50	0
4	NAG	E	2	4	14,14,15	0.54	0	17,19,21	0.74	0
4	BMA	E	3	4	11,11,12	1.01	1 (9%)	15,15,17	1.45	2 (13%)
4	MAN	E	4	4	11,11,12	1.20	2 (18%)	15,15,17	1.24	2 (13%)
4	NAG	E	5	4	14,14,15	0.22	0	17,19,21	0.31	0
4	MAN	E	6	4	11,11,12	0.82	0	15,15,17	0.90	0
4	NAG	E	7	4	14,14,15	0.40	0	17,19,21	0.40	0
4	FUC	E	8	4	10,10,11	0.82	1 (10%)	14,14,16	0.96	0
5	NAG	G	1	5,2	14,14,15	0.66	0	17,19,21	1.07	1 (5%)
5	NAG	G	2	5	14,14,15	0.49	0	17,19,21	0.64	1 (5%)
5	FUC	G	3	5	10,10,11	0.94	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	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
3	NAG	D	5	3	-	4/6/23/26	0/1/1/1
3	GAL	D	6	3	-	2/2/19/22	0/1/1/1
3	MAN	D	7	3	-	2/2/19/22	0/1/1/1
3	NAG	D	8	3	-	4/6/23/26	0/1/1/1
3	FUC	D	9	3	-	-	0/1/1/1
4	NAG	E	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	4	MAN	O5-C1	-2.82	1.39	1.43
3	D	4	MAN	O5-C1	-2.69	1.39	1.43
4	E	3	BMA	O5-C1	-2.54	1.39	1.43
3	D	2	NAG	O5-C1	-2.47	1.39	1.43
3	D	3	BMA	O5-C5	2.45	1.48	1.43
3	D	6	GAL	C1-C2	2.43	1.58	1.52
4	E	8	FUC	O5-C5	2.05	1.47	1.43
4	E	4	MAN	O5-C5	2.02	1.47	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	6	GAL	C1-O5-C5	6.05	120.30	112.19
3	D	6	GAL	C1-C2-C3	4.61	116.36	109.64
3	D	5	NAG	C1-O5-C5	4.54	118.27	112.19
3	D	5	NAG	O4-C4-C5	3.35	117.57	109.32
4	E	3	BMA	C1-C2-C3	2.85	113.80	109.64
4	E	4	MAN	C1-C2-C3	-2.78	105.59	109.64
3	D	6	GAL	O5-C1-C2	2.57	116.93	110.79
4	E	3	BMA	C1-O5-C5	2.54	115.59	112.19
3	D	3	BMA	C1-O5-C5	2.54	115.59	112.19
5	G	1	NAG	C1-O5-C5	2.41	115.42	112.19
4	E	4	MAN	O3-C3-C2	2.35	114.86	110.05
3	D	5	NAG	C3-C4-C5	-2.34	105.99	110.23
3	D	4	MAN	O6-C6-C5	-2.14	104.06	111.33
5	G	2	NAG	C1-O5-C5	2.09	114.98	112.19
3	D	3	BMA	O2-C2-C3	-2.06	105.89	110.15
3	D	3	BMA	C6-C5-C4	-2.02	108.05	113.02

There are no chirality outliers.

All (35) torsion outliers are listed below:

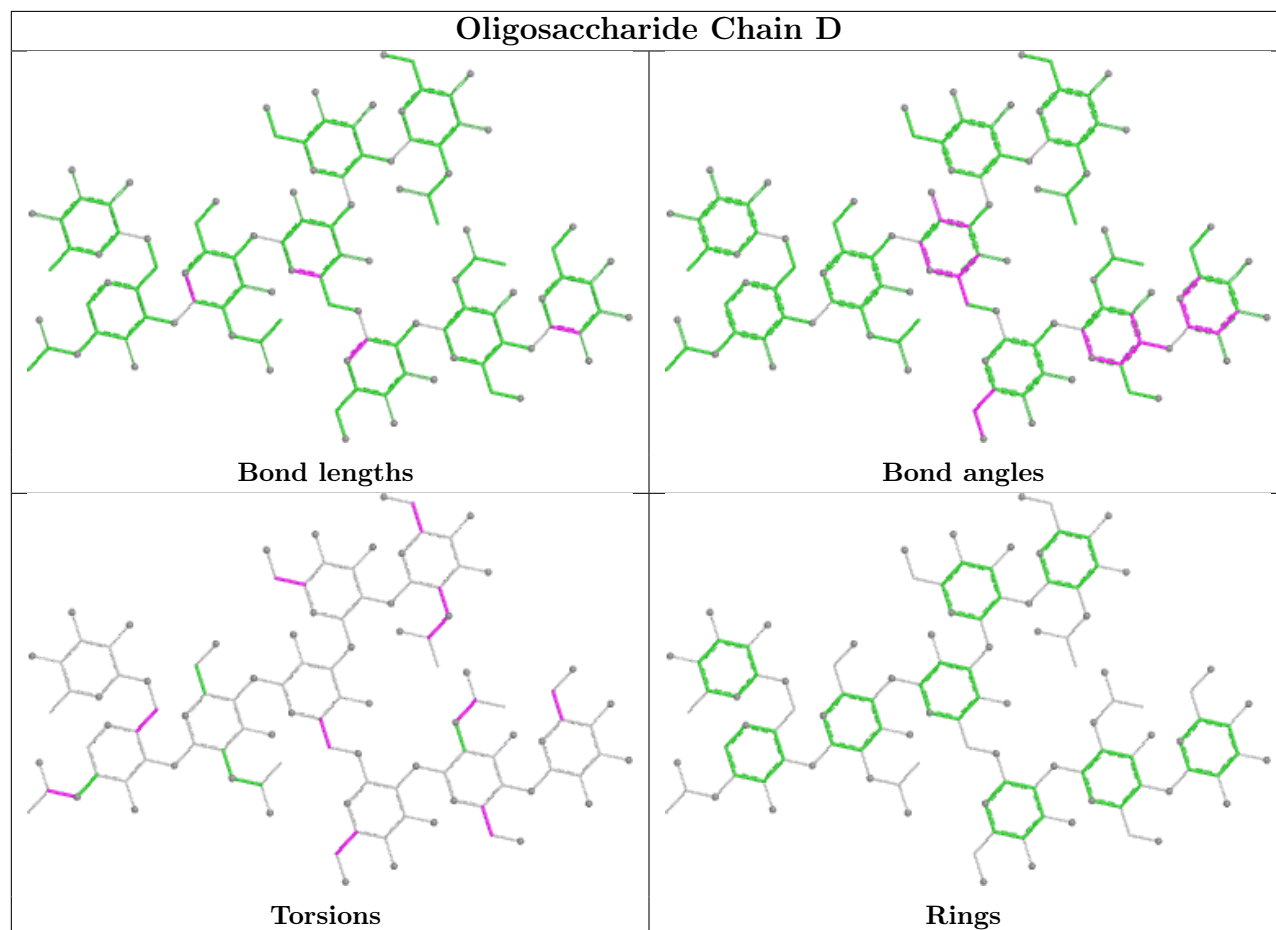
Mol	Chain	Res	Type	Atoms
5	G	2	NAG	O5-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6
3	D	7	MAN	O5-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
4	E	5	NAG	O5-C5-C6-O6
4	E	6	MAN	C4-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
4	E	4	MAN	O5-C5-C6-O6
3	D	6	GAL	O5-C5-C6-O6
4	E	6	MAN	O5-C5-C6-O6
4	E	4	MAN	C4-C5-C6-O6
3	D	6	GAL	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6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

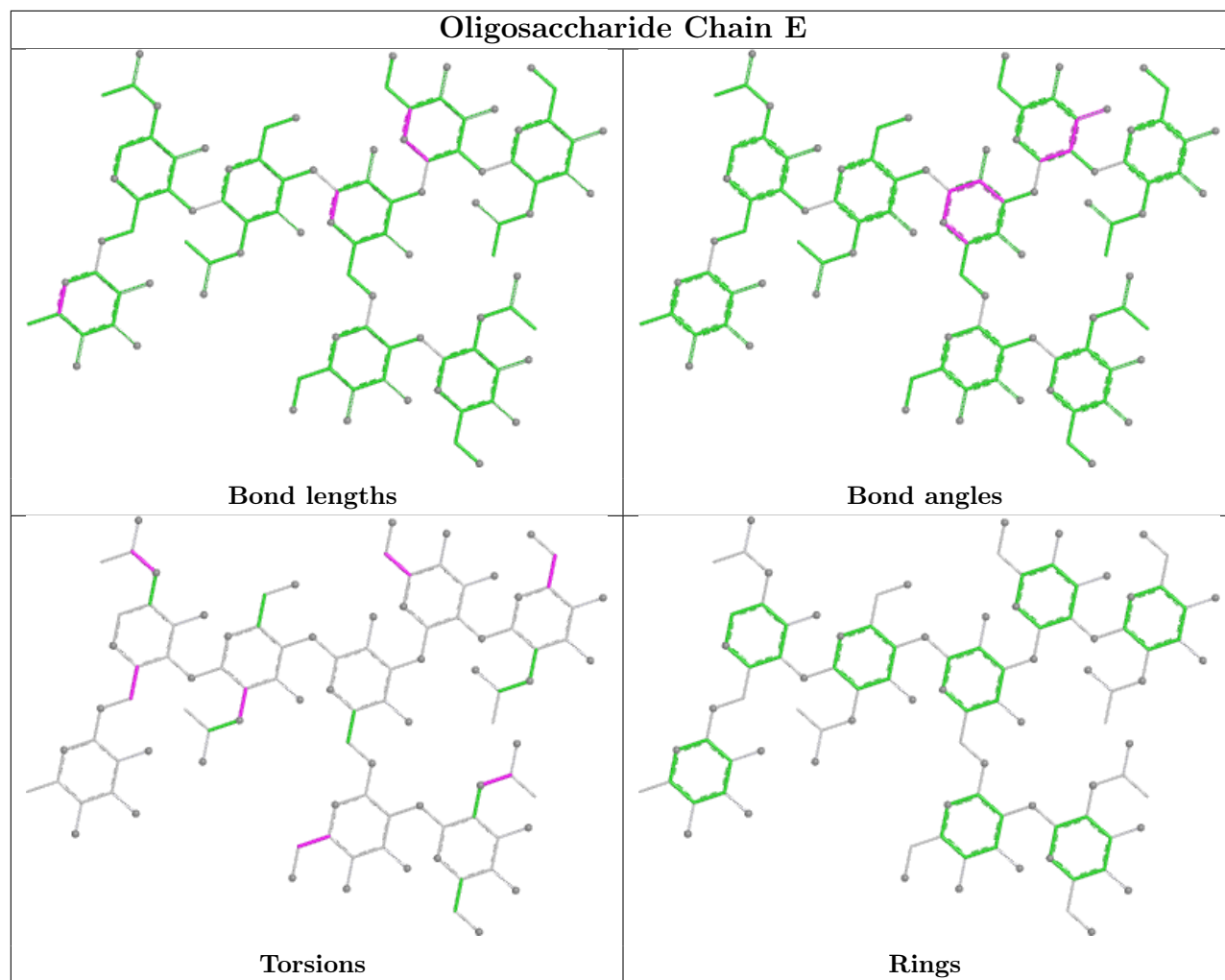
There are no ring outliers.

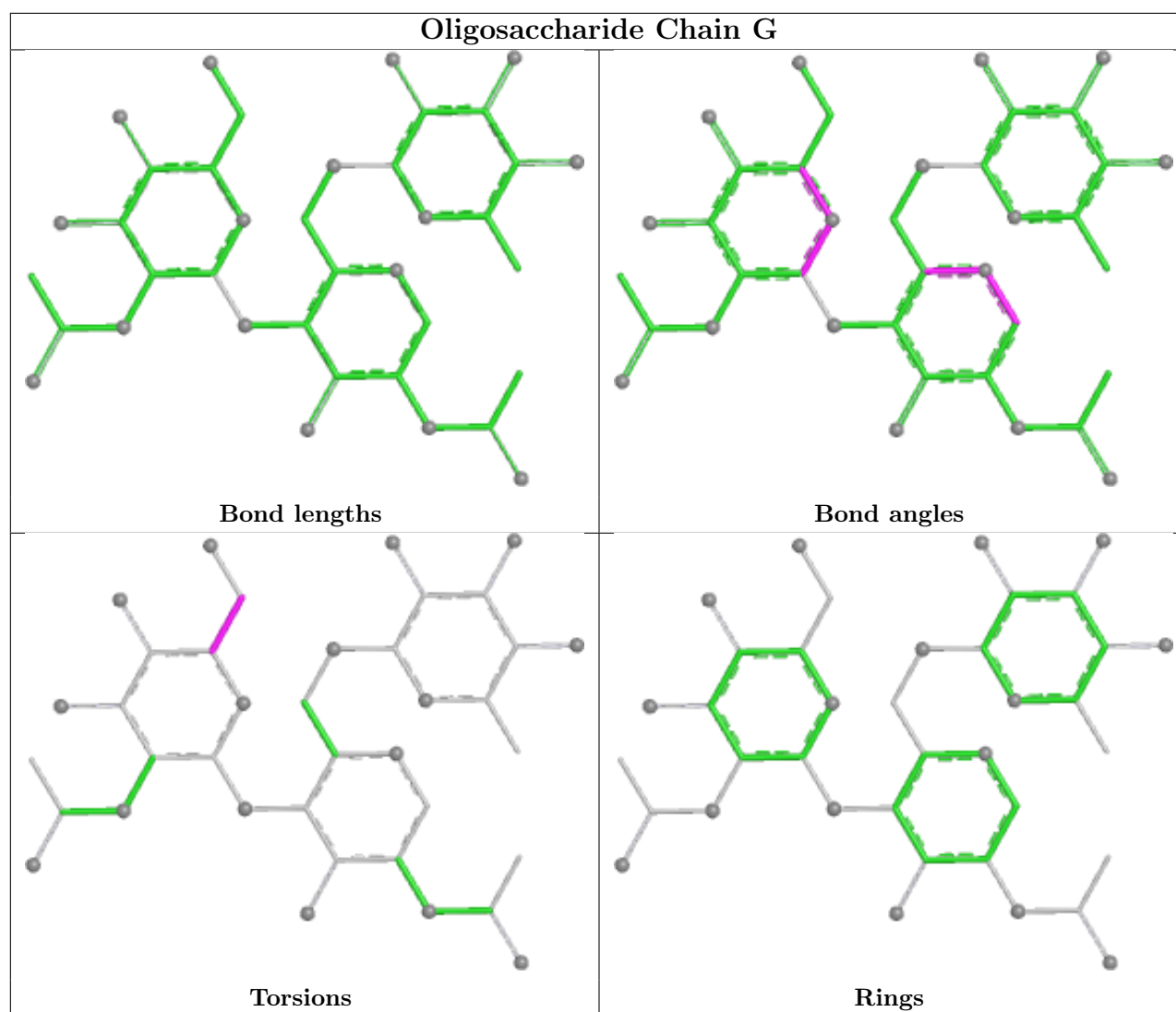
12 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	8	NAG	1	0
4	E	8	FUC	5	0
4	E	1	NAG	5	0
4	E	3	BMA	1	0
5	G	3	FUC	1	0
3	D	3	BMA	1	0
3	D	1	NAG	2	0
3	D	4	MAN	1	0
4	E	2	NAG	10	0
5	G	2	NAG	1	0
3	D	6	GAL	3	0
5	G	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 [i](#)

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	NAG	C	201	2	14,14,15	0.41	0	17,19,21	0.51	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	NAG	C	201	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	201	NAG	O5-C5-C6-O6
6	C	201	NAG	C4-C5-C6-O6
6	C	201	NAG	C8-C7-N2-C2
6	C	201	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	201	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	215/224 (95%)	1.09	45 (20%) 2 1	58, 136, 256, 303	0
1	B	214/224 (95%)	1.38	54 (25%) 1 1	101, 194, 295, 336	0
2	C	173/174 (99%)	0.54	6 (3%) 47 38	46, 93, 159, 198	3 (1%)
All	All	602/622 (96%)	1.04	105 (17%) 4 3	46, 141, 271, 336	3 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	426	SER	8.9
1	B	427	VAL	8.2
1	B	378	VAL	7.7
1	B	425	CYS	7.3
1	B	379	VAL	6.7
1	B	368	LEU	5.9
1	B	437	THR	5.7
1	B	302	VAL	5.5
1	B	440	SER	5.2
1	A	443	VAL	5.2
1	B	424	SER	4.8
1	B	366	THR	4.6
1	B	393	THR	4.6
1	B	439	LYS	4.5
1	A	416	ARG	4.2
1	A	390	THR	4.2
1	A	364	SER	4.2
1	A	365	LEU	4.1
1	B	365	LEU	4.1
1	B	381	TRP	3.9
1	B	377	ILE	3.9
1	A	366	THR	3.8
2	C	171	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
2	C	49[A]	HIS	3.7
1	A	412	VAL	3.7
1	B	359	THR	3.6
2	C	1	ALA	3.6
1	B	369	VAL	3.6
1	A	350	THR	3.5
1	A	444	SER	3.5
1	B	313	TRP	3.3
1	B	355	ARG	3.3
1	A	352	PRO	3.3
1	B	409	LYS	3.3
1	B	370	LYS	3.1
1	A	369	VAL	3.1
1	B	405	PHE	3.1
1	B	244	PRO	3.0
1	B	412	VAL	3.0
2	C	90	LEU	3.0
1	A	300	TYR	2.9
1	A	380	GLU	2.9
1	A	385	GLY	2.9
1	B	361	ASN	2.9
1	A	423	PHE	2.9
1	B	441	LEU	2.8
1	A	232	PRO	2.8
1	A	353	PRO	2.8
1	A	297	ASN	2.8
1	A	411	THR	2.8
1	B	373	TYR	2.8
1	B	367	CYS	2.8
1	A	384	SER	2.8
1	A	234	LEU	2.7
1	B	416	ARG	2.7
1	A	351	LEU	2.7
1	B	408	SER	2.7
1	A	382	GLU	2.7
1	B	364	SER	2.7
1	B	413	ASP	2.7
1	A	422	VAL	2.6
1	B	406	LEU	2.6
1	B	436	TYR	2.6
1	A	294	THR	2.6
1	B	356	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	271	PRO	2.6
1	B	350	THR	2.5
1	A	442	SER	2.5
1	B	398	LEU	2.5
1	A	230	PRO	2.5
1	A	417	TRP	2.5
1	A	413	ASP	2.5
1	A	421	ASN	2.5
1	A	410	LEU	2.5
1	B	253	ILE	2.4
1	A	278	TYR	2.4
1	A	296	TYR	2.4
1	A	398	LEU	2.4
1	B	352	PRO	2.4
1	B	380	GLU	2.3
1	A	415	SER	2.3
1	A	299	THR	2.3
1	B	438	GLN	2.3
1	A	387	PRO	2.3
1	B	391	TYR	2.2
1	A	441	LEU	2.2
1	A	268	GLN	2.2
1	B	236	GLY	2.2
1	B	264	VAL	2.2
2	C	165	VAL	2.2
1	A	394	THR	2.2
1	B	407	TYR	2.2
2	C	47	PRO	2.2
1	B	265	ASP	2.2
1	B	442	SER	2.2
1	B	246	LYS	2.1
1	B	263	VAL	2.1
1	B	354	SER	2.1
1	B	347	GLN	2.1
1	A	377	ILE	2.1
1	B	351	LEU	2.1
1	A	348	VAL	2.1
1	A	420	GLY	2.0
1	B	410	LEU	2.0
1	A	349	TYR	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 ⓘ

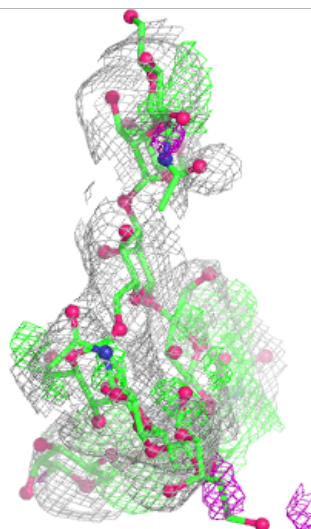
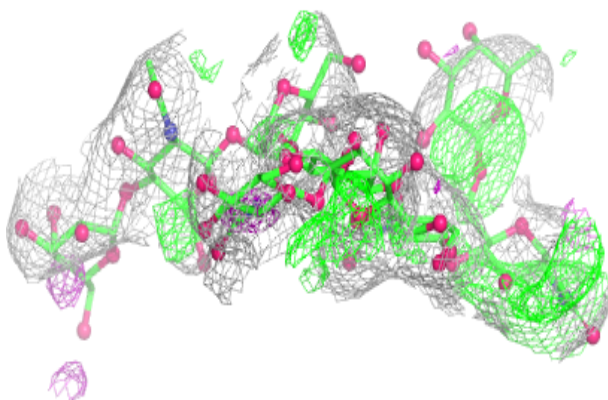
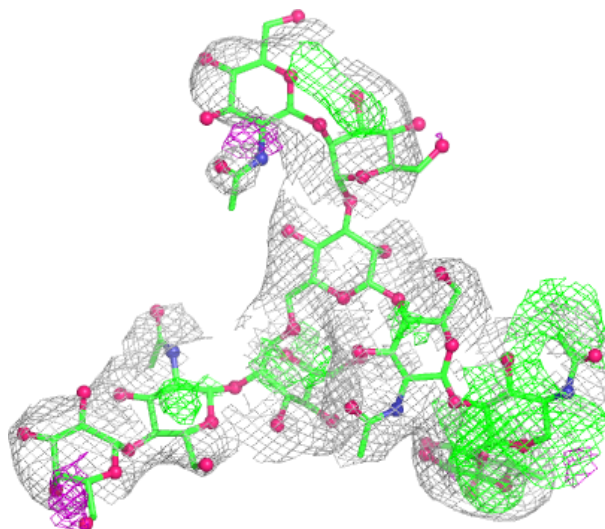
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FUC	E	8	10/11	0.61	0.15	176,177,190,194	0
4	NAG	E	1	14/15	0.66	0.17	150,169,185,205	0
4	NAG	E	5	14/15	0.69	0.15	184,194,214,224	0
3	FUC	D	9	10/11	0.72	0.23	108,127,170,177	0
3	NAG	D	8	14/15	0.72	0.21	174,197,229,241	0
4	NAG	E	7	14/15	0.73	0.18	144,152,161,162	0
3	NAG	D	1	14/15	0.75	0.22	88,106,118,149	0
4	MAN	E	4	11/12	0.76	0.21	168,197,230,258	0
4	MAN	E	6	11/12	0.78	0.10	161,166,185,190	0
3	MAN	D	7	11/12	0.85	0.20	139,156,184,184	0
3	GAL	D	6	11/12	0.86	0.28	131,177,243,292	0
3	NAG	D	5	14/15	0.86	0.15	108,144,165,175	0
4	BMA	E	3	11/12	0.90	0.09	139,151,163,166	0
4	NAG	E	2	14/15	0.90	0.10	136,151,164,169	0
3	MAN	D	4	11/12	0.91	0.13	87,98,124,147	0
3	BMA	D	3	11/12	0.93	0.09	99,108,111,116	0
3	NAG	D	2	14/15	0.95	0.10	74,98,107,115	0
5	NAG	G	1	14/15	-	-	169,215,253,269	0
5	NAG	G	2	14/15	-	-	226,268,308,315	0
5	FUC	G	3	10/11	-	-	286,301,317,328	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.

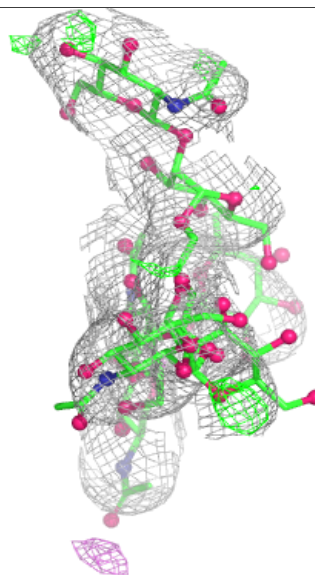
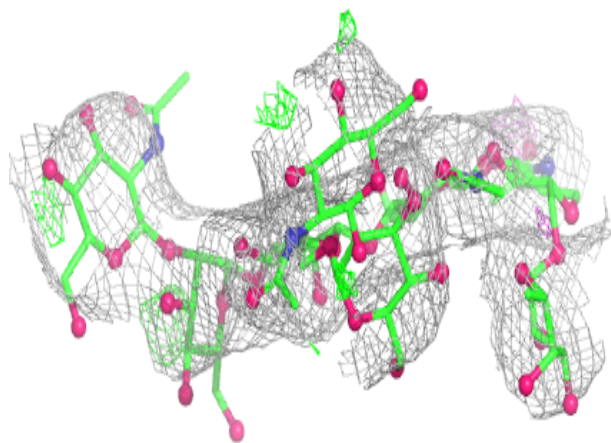
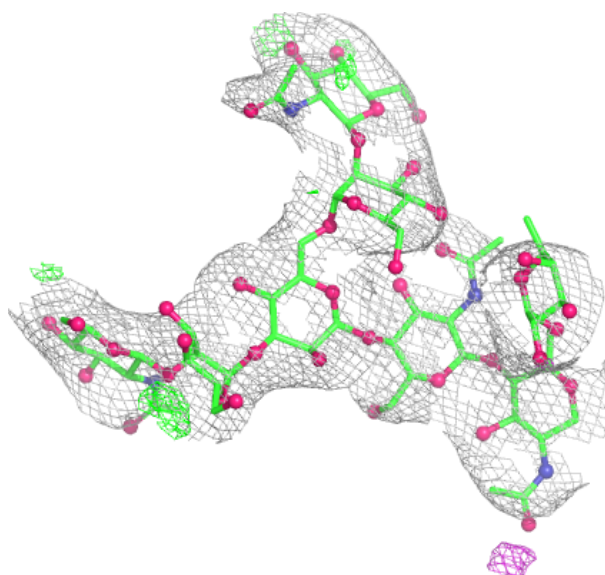
Electron density around Chain D:

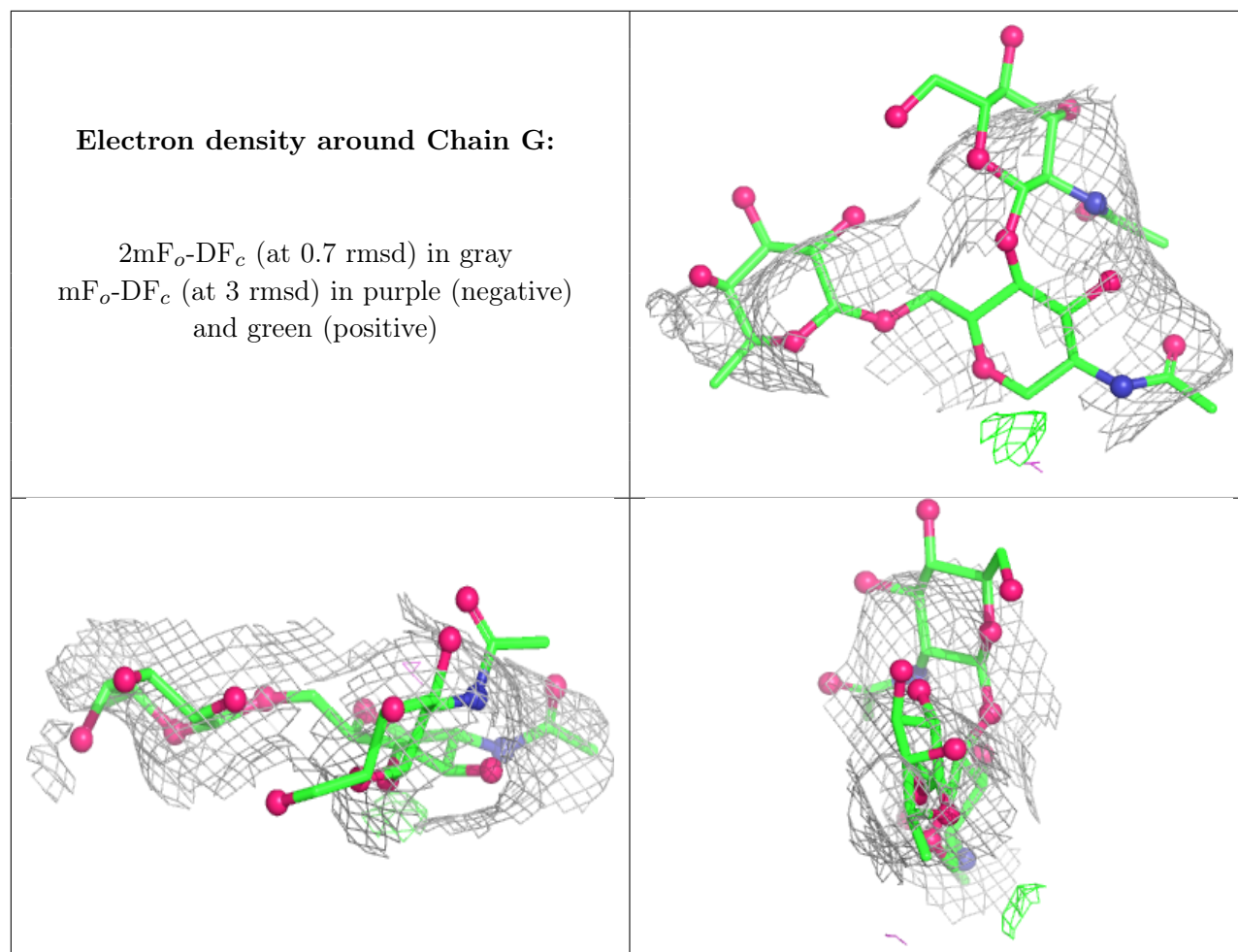
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NAG	C	201	14/15	0.59	0.12	185,210,223,223	0

6.5 Other polymers [i](#)

There are no such residues in this entry.