Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 09:13 AM EDT

PDB ID	:	6MJ3
Title	:	CRYSTAL STRUCTURE OF RHESUS MACAQUE (MACACA MULATTA) IGG1 Fc Fragment-Fc-GAMMA RECEPTOR III complex
Authors	:	Gohain, N.; Tolbert, W.D.; Pazgier, M.
Deposited on	:	2018-09-20
Resolution	:	3.80 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:

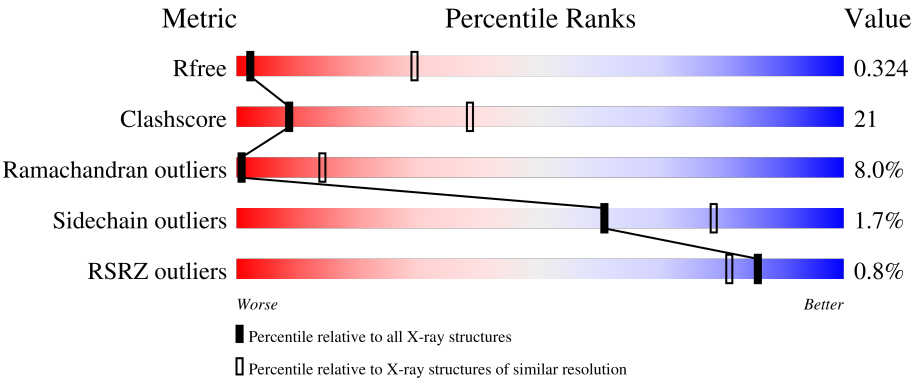
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 <=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	52% 38% · 8%
1	B	224	% 47% 40% 7% 6%
1	D	224	% 58% 30% · 7%
1	E	224	55% 33% 5% 6%
2	C	192	2% 47% 37% · 12%

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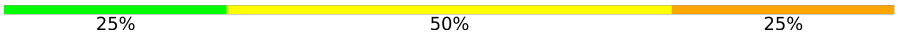
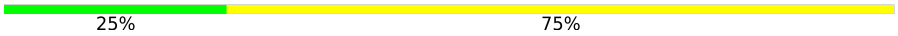
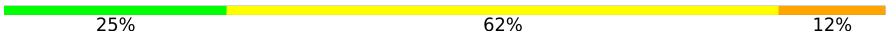
Mol	Chain	Length	Quality of chain
2	F	192	
3	G	8	
3	H	8	
3	I	8	
3	J	8	

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
3	NAG	H	5	-	-	-	X
3	NAG	J	5	-	-	-	X
4	NAG	C	202	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9856 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	207	Total	C	N	O	S	0	0	0
			1654	1050	278	320	6			
1	B	210	Total	C	N	O	S	0	0	0
			1674	1064	281	323	6			
1	D	208	Total	C	N	O	S	0	0	0
			1660	1053	279	322	6			
1	E	211	Total	C	N	O	S	0	0	0
			1680	1067	282	325	6			

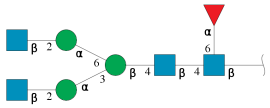
- Molecule 2 is a protein called Low affinity immunoglobulin gamma Fc region receptor III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	169	Total	C	N	O	S	0	0	0
			1375	875	238	258	4			
2	F	169	Total	C	N	O	S	0	0	0
			1375	875	238	258	4			

There are 4 discrepancies between the modelled and reference sequences:

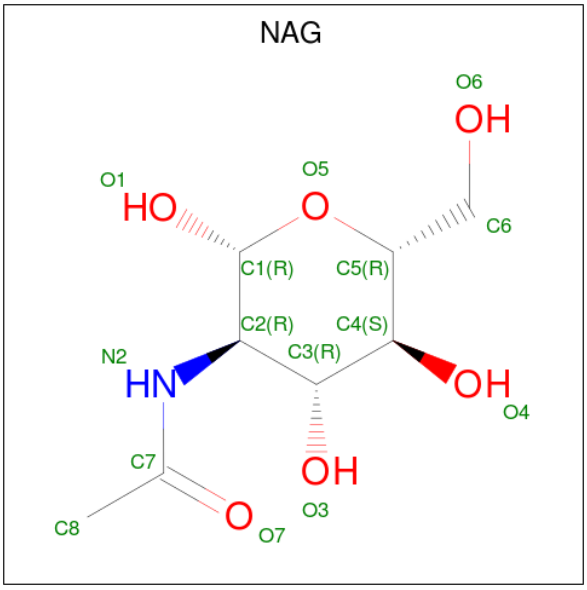
Chain	Residue	Modelled	Actual	Comment	Reference
C	38	GLN	ASN	engineered mutation	UNP A3RFZ7
C	169	GLN	ASN	engineered mutation	UNP A3RFZ7
F	38	GLN	ASN	engineered mutation	UNP A3RFZ7
F	169	GLN	ASN	engineered mutation	UNP A3RFZ7

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	G	8	Total C N O 99 56 4 39	0	0	0
3	H	8	Total C N O 99 56 4 39	0	0	0
3	I	8	Total C N O 99 56 4 39	0	0	0
3	J	8	Total C N O 99 56 4 39	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



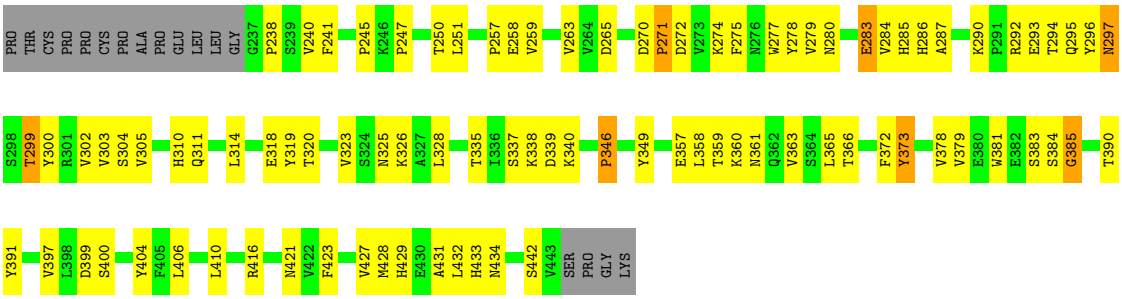
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0

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.

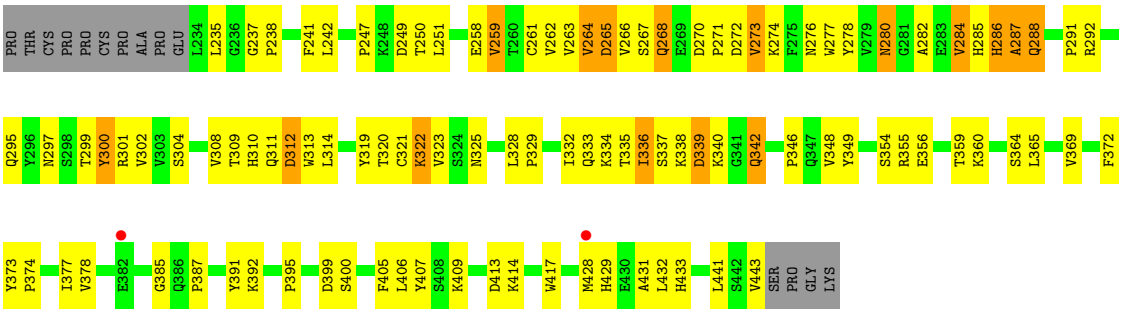
• Molecule 1: Igg1 Fc

Chain A:



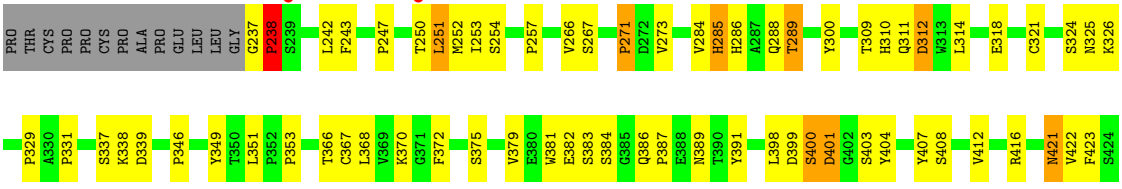
• Molecule 1: Igg1 Fc

Chain B:

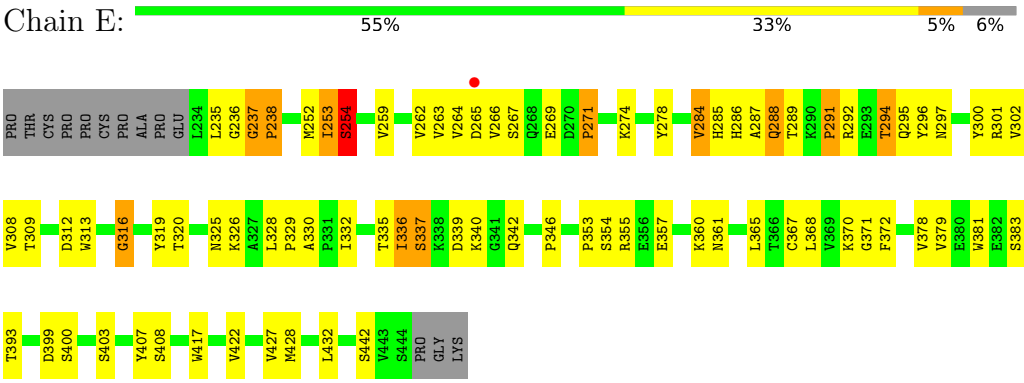


• Molecule 1: Igg1 Fc

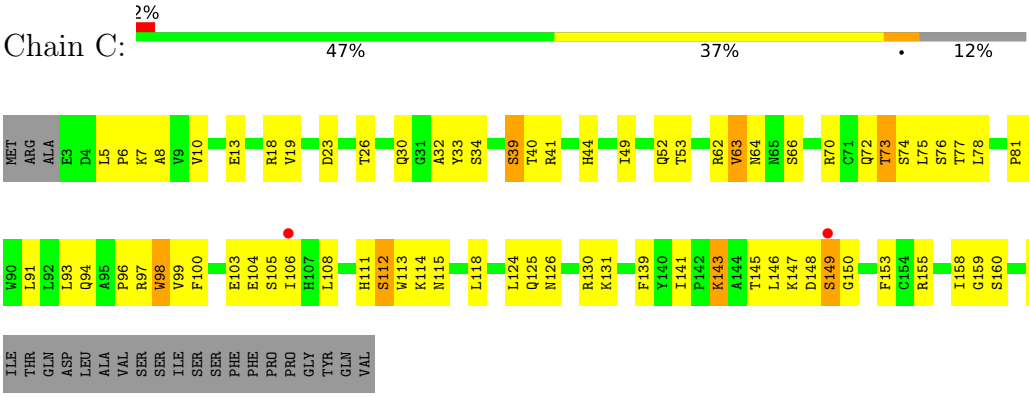
Chain D:



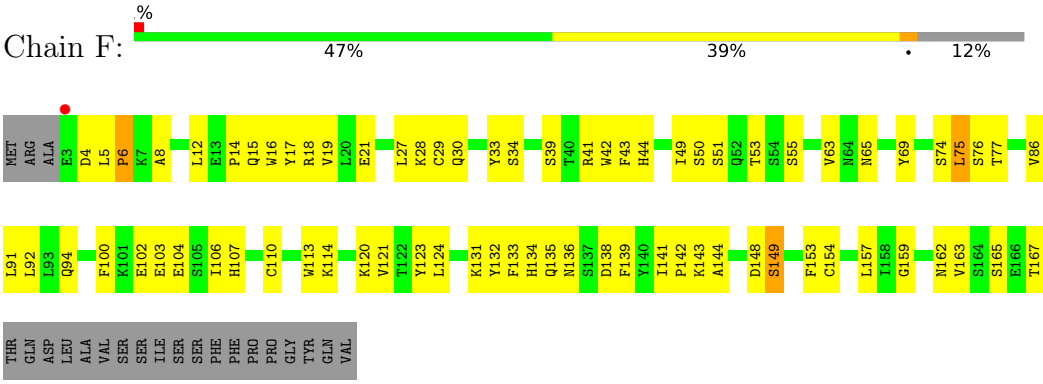
• Molecule 1: Igg1 Fc



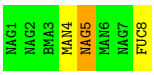
• Molecule 2: Low affinity immunoglobulin gamma Fc region receptor III



• Molecule 2: Low affinity immunoglobulin gamma Fc region receptor III

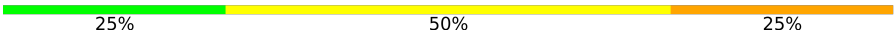


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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

Chain H:

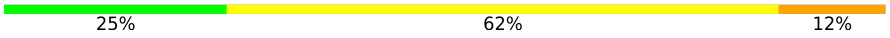


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

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

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	213.11Å 71.27Å 135.52Å 90.00° 119.72° 90.00°	Depositor
Resolution (Å)	66.51 – 3.80 101.05 – 3.80	Depositor EDS
% Data completeness (in resolution range)	75.3 (66.51-3.80) 82.7 (101.05-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 3.78Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.276 , 0.324 0.274 , 0.324	Depositor DCC
R_{free} test set	673 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å^2)	87.7	Xtriage
Anisotropy	0.805	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	9856	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BMA, NAG, FUC, MAN

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	0.30	0/1700	0.54	0/2321
1	B	0.33	0/1720	0.67	1/2348 (0.0%)
1	D	0.31	0/1706	0.61	2/2329 (0.1%)
1	E	0.30	0/1726	0.56	0/2356
2	C	0.29	0/1411	0.57	0/1913
2	F	0.31	0/1411	0.59	0/1913
All	All	0.31	0/9674	0.59	3/13180 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	238	PRO	N-CA-CB	-8.24	93.42	103.30
1	D	289	THR	C-N-CA	-5.18	108.74	121.70
1	B	265	ASP	CB-CG-OD1	-5.07	113.74	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1654	0	1614	66	0
1	B	1674	0	1639	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1660	0	1619	57	1
1	E	1680	0	1644	69	1
2	C	1375	0	1333	76	1
2	F	1375	0	1334	62	1
3	G	99	0	85	1	0
3	H	99	0	85	6	0
3	I	99	0	85	1	0
3	J	99	0	85	4	0
4	C	28	0	26	1	0
4	F	14	0	13	0	0
All	All	9856	0	9562	399	2

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 21.

All (399) 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:266:VAL:CG1	1:B:300:TYR:O	1.85	1.23
1:B:266:VAL:HG11	1:B:300:TYR:O	1.34	1.21
1:B:247:PRO:O	1:B:251:LEU:HD12	1.45	1.16
2:C:32:ALA:HA	2:C:75:LEU:HD21	1.41	1.02
2:F:33:TYR:HB3	2:F:75:LEU:HD11	1.42	1.02
1:B:264:VAL:HG21	3:H:1:NAG:O4	1.61	0.99
1:E:346:PRO:HB3	1:E:372:PHE:HB3	1.47	0.94
1:D:379:VAL:HG12	1:D:427:VAL:HG12	1.48	0.93
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.52	0.91
2:C:32:ALA:CA	2:C:75:LEU:HD21	1.98	0.91
1:D:324:SER:HB3	1:D:331:PRO:HB3	1.52	0.90
1:D:318:GLU:HG2	1:D:337:SER:HB3	1.57	0.86
1:A:238:PRO:HD2	1:A:328:LEU:HG	1.55	0.86
1:B:235:LEU:HD23	1:B:237:GLY:H	1.41	0.84
1:E:360:LYS:HG3	1:E:361:ASN:H	1.40	0.84
2:C:73:THR:HG22	2:C:74:SER:H	1.42	0.83
1:A:240:VAL:HG11	1:A:323:VAL:HG11	1.62	0.82
1:E:294:THR:HG23	1:E:295:GLN:H	1.45	0.82
2:F:110:CYS:HB2	2:F:123:TYR:HE1	1.45	0.82
1:B:284:VAL:HG12	1:B:285:HIS:H	1.48	0.79
2:C:32:ALA:C	2:C:75:LEU:HD21	2.02	0.79
2:C:75:LEU:HG	2:C:76:SER:N	1.97	0.78
1:D:422:VAL:HG12	1:D:442:SER:HB3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:264:VAL:HG21	3:J:1:NAG:H3	1.64	0.78
1:B:309:THR:HB	1:B:312:ASP:HB3	1.67	0.77
2:C:32:ALA:HA	2:C:75:LEU:CD2	2.16	0.76
2:C:75:LEU:HG	2:C:76:SER:H	1.51	0.76
2:F:19:VAL:HG23	2:F:86:VAL:HG12	1.68	0.75
2:C:75:LEU:H	2:C:75:LEU:HD23	1.50	0.75
2:F:120:LYS:HD2	2:F:157:LEU:HD21	1.70	0.74
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.70	0.74
1:E:305:VAL:HG12	1:E:306:LEU:H	1.52	0.74
1:E:292:ARG:HG2	1:E:302:VAL:HG12	1.71	0.73
1:A:365:LEU:HD11	1:A:423:PHE:HD2	1.54	0.72
1:A:285:HIS:O	1:A:287:ALA:N	2.22	0.72
1:D:398:LEU:HA	1:D:404:TYR:HD1	1.53	0.72
1:A:340:LYS:O	1:A:373:TYR:OH	2.05	0.72
1:B:258:GLU:O	1:B:259:VAL:HG23	1.91	0.70
1:A:318:GLU:HG2	1:A:337:SER:HB3	1.72	0.70
2:C:32:ALA:HB1	2:C:73:THR:HB	1.73	0.70
1:A:294:THR:HG22	1:E:291:PRO:HG2	1.74	0.70
2:F:5:LEU:HB2	2:F:77:THR:CG2	2.22	0.69
1:B:320:THR:HG22	1:B:335:THR:HG22	1.73	0.69
1:B:277:TRP:NE1	1:B:321:CYS:SG	2.65	0.69
1:A:278:TYR:HB2	1:A:320:THR:HB	1.74	0.67
1:A:416:ARG:O	1:A:421:ASN:ND2	2.28	0.67
2:C:126:ASN:HD21	2:C:150:GLY:HA3	1.61	0.66
2:F:17:TYR:CE1	2:F:18:ARG:HG3	2.31	0.66
1:D:384:SER:OG	1:D:386:GLN:OE1	2.14	0.65
1:A:379:VAL:HG22	1:A:427:VAL:HG12	1.77	0.65
1:B:342:GLN:O	1:B:373:TYR:HB3	1.97	0.65
2:C:44:HIS:HB2	2:C:49:ILE:HD11	1.78	0.65
2:C:125:GLN:HG2	2:C:130:ARG:NH2	2.12	0.64
1:A:358:LEU:HD23	1:A:363:VAL:HG11	1.79	0.64
2:C:62:ARG:O	2:C:64:ASN:N	2.30	0.64
1:E:235:LEU:HD23	1:E:236:GLY:H	1.61	0.64
2:F:100:PHE:HD2	2:F:106:ILE:HD12	1.63	0.64
1:E:295:GLN:HG2	1:E:296:TYR:H	1.63	0.64
1:E:235:LEU:CD2	1:E:236:GLY:H	2.12	0.63
1:E:422:VAL:HG12	1:E:442:SER:HB3	1.80	0.63
2:C:13:GLU:HB2	2:C:26:THR:O	1.97	0.63
2:C:5:LEU:HG	2:C:6:PRO:HD2	1.81	0.63
1:A:365:LEU:HD12	1:A:410:LEU:HD23	1.81	0.63
1:B:278:TYR:HA	1:B:282:ALA:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:308:VAL:HG12	1:E:309:THR:O	1.99	0.63
2:F:5:LEU:HB2	2:F:77:THR:HG23	1.81	0.63
2:C:131:LYS:HD2	2:C:139:PHE:HE1	1.64	0.62
1:B:263:VAL:HG12	1:B:302:VAL:O	1.98	0.62
1:D:325:ASN:OD1	1:D:326:LYS:N	2.32	0.62
1:B:284:VAL:HG12	1:B:285:HIS:N	2.15	0.62
1:D:368:LEU:HD21	1:D:370:LYS:HB2	1.81	0.62
1:D:285:HIS:CG	1:D:286:HIS:H	2.18	0.62
1:A:432:LEU:O	1:A:434:ASN:N	2.33	0.61
1:B:265:ASP:OD1	3:H:1:NAG:N2	2.33	0.61
1:B:273:VAL:HG23	1:B:274:LYS:H	1.66	0.61
1:B:238:PRO:HB3	1:B:265:ASP:O	2.00	0.60
2:C:77:THR:O	2:C:78:LEU:HD12	2.00	0.60
1:A:240:VAL:HG12	1:A:263:VAL:HG13	1.84	0.60
1:D:309:THR:OG1	1:D:312:ASP:HB3	2.02	0.60
2:C:75:LEU:CG	2:C:76:SER:H	2.14	0.60
2:F:75:LEU:HD12	2:F:75:LEU:O	2.02	0.60
1:B:336:ILE:HG23	1:B:337:SER:H	1.67	0.59
1:E:264:VAL:CG2	3:J:1:NAG:H3	2.33	0.59
1:E:262:VAL:HG12	1:E:303:VAL:HG13	1.84	0.59
1:A:297:ASN:OD1	1:A:299:THR:HB	2.03	0.59
1:B:377:ILE:HG21	1:B:406:LEU:HD21	1.85	0.58
1:E:237:GLY:H	1:E:238:PRO:HD3	1.68	0.58
1:D:399:ASP:OD1	1:D:400:SER:N	2.35	0.58
2:F:33:TYR:HD2	2:F:75:LEU:HD21	1.68	0.58
1:B:263:VAL:HG13	1:B:263:VAL:O	2.03	0.58
2:C:131:LYS:HD2	2:C:139:PHE:CE1	2.39	0.58
1:E:313:TRP:CZ3	1:E:337:SER:HA	2.39	0.57
2:C:70:ARG:HE	2:C:81:PRO:HB3	1.69	0.57
2:C:73:THR:HG22	2:C:74:SER:N	2.16	0.57
2:F:113:TRP:CZ3	2:F:114:LYS:HE3	2.38	0.57
1:A:429:HIS:HB3	1:A:432:LEU:HD13	1.86	0.57
1:B:378:VAL:CG1	1:B:428:MET:HB2	2.34	0.57
2:C:19:VAL:O	2:C:86:VAL:HA	2.04	0.57
1:B:348:VAL:HG23	1:B:369:VAL:HG22	1.87	0.57
1:E:238:PRO:HG3	1:E:265:ASP:O	2.04	0.57
3:J:2:NAG:H83	3:J:2:NAG:H3	1.85	0.57
2:F:65:ASN:O	2:F:69:TYR:OH	2.15	0.56
1:B:333:GLN:N	1:B:333:GLN:OE1	2.39	0.56
1:D:237:GLY:CA	2:F:134:HIS:HB3	2.35	0.56
2:F:74:SER:O	2:F:75:LEU:HG	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:100:PHE:CE2	2:C:106:ILE:HG12	2.40	0.56
2:C:98:TRP:HD1	2:C:99:VAL:HG13	1.70	0.56
2:C:155:ARG:CZ	4:C:202:NAG:H62	2.36	0.56
2:F:16:TRP:CD1	2:F:94:GLN:HB3	2.40	0.56
2:C:91:LEU:HD21	2:C:118:LEU:HD21	1.86	0.56
1:D:266:VAL:HG23	1:D:300:TYR:HB2	1.87	0.55
1:D:267:SER:O	1:D:271:PRO:HB3	2.05	0.55
1:E:399:ASP:OD1	1:E:400:SER:N	2.39	0.55
2:F:44:HIS:HB3	2:F:49:ILE:HD11	1.88	0.55
1:E:297:ASN:OD1	1:E:297:ASN:N	2.38	0.55
1:B:264:VAL:HG22	3:H:1:NAG:H3	1.87	0.55
1:E:253:ILE:HG22	1:E:253:ILE:O	2.05	0.55
2:C:66:SER:HB2	2:C:86:VAL:HG22	1.89	0.55
1:D:429:HIS:HB3	1:D:432:LEU:HD13	1.89	0.55
2:F:100:PHE:CD2	2:F:106:ILE:HD12	2.42	0.55
1:A:258:GLU:HB3	1:A:305:VAL:HG13	1.89	0.55
1:B:242:LEU:HD12	1:B:261:CYS:SG	2.47	0.55
1:A:390:THR:O	1:A:410:LEU:HD12	2.06	0.55
1:B:334:LYS:HG2	1:B:335:THR:N	2.21	0.55
1:E:235:LEU:HD21	1:E:265:ASP:O	2.06	0.55
1:A:270:ASP:N	1:A:271:PRO:HD3	2.22	0.55
1:D:314:LEU:HA	1:D:338:LYS:HD3	1.89	0.55
1:E:360:LYS:CG	1:E:361:ASN:H	2.15	0.55
1:E:368:LEU:HD12	1:E:407:TYR:CE1	2.42	0.55
2:F:53:THR:HG22	2:F:55:SER:H	1.71	0.55
2:F:154:CYS:SG	2:F:165:SER:OG	2.65	0.55
2:C:72:GLN:HA	2:C:76:SER:OG	2.07	0.54
1:B:309:THR:HG22	1:B:310:HIS:H	1.72	0.54
1:B:372:PHE:HB2	1:B:429:HIS:CE1	2.42	0.54
1:E:325:ASN:OD1	1:E:326:LYS:N	2.41	0.54
2:F:102:GLU:HB3	2:F:103:GLU:OE1	2.08	0.54
2:F:148:ASP:OD1	2:F:149:SER:N	2.40	0.54
1:B:247:PRO:HA	1:B:250:THR:HG22	1.89	0.54
2:F:123:TYR:CE2	2:F:139:PHE:HB2	2.42	0.54
2:F:153:PHE:HB2	2:F:165:SER:HB2	1.89	0.54
1:E:284:VAL:HB	1:E:286:HIS:ND1	2.23	0.54
1:A:379:VAL:HG21	1:A:406:LEU:HD11	1.90	0.53
1:D:368:LEU:HD12	1:D:407:TYR:CZ	2.43	0.53
1:D:382:GLU:HB3	1:D:387:PRO:HA	1.89	0.53
1:D:429:HIS:CE1	1:D:430:GLU:HB3	2.43	0.53
2:C:145:THR:O	2:C:147:LYS:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:PHE:HB2	1:B:262:VAL:CG2	2.38	0.53
1:A:325:ASN:OD1	1:A:326:LYS:N	2.42	0.53
1:E:346:PRO:HD2	1:E:432:LEU:HD21	1.90	0.53
2:F:131:LYS:HD2	2:F:133:PHE:CZ	2.43	0.53
2:C:7:LYS:HA	2:C:77:THR:HB	1.91	0.53
2:F:110:CYS:HB2	2:F:123:TYR:CE1	2.35	0.53
1:E:296:TYR:OH	1:E:301:ARG:HD3	2.09	0.53
2:F:5:LEU:HB2	2:F:77:THR:HG21	1.90	0.53
1:A:292:ARG:HD2	1:E:288:GLN:HG3	1.90	0.52
1:E:284:VAL:HG23	1:E:285:HIS:N	2.24	0.52
2:C:100:PHE:CD2	2:C:106:ILE:HG12	2.44	0.52
1:A:357:GLU:HB2	1:B:349:TYR:CD1	2.44	0.52
1:A:429:HIS:HB3	1:A:432:LEU:CD1	2.39	0.52
1:D:243:PHE:HZ	3:I:3:BMA:H5	1.74	0.52
1:A:358:LEU:C	1:A:360:LYS:H	2.13	0.52
1:D:285:HIS:CG	1:D:286:HIS:N	2.77	0.52
1:B:354:SER:O	1:B:356:GLU:N	2.43	0.52
2:F:14:PRO:O	2:F:16:TRP:N	2.36	0.52
2:C:112:SER:OG	2:C:113:TRP:N	2.43	0.52
1:B:266:VAL:O	1:B:267:SER:HB3	2.10	0.52
1:B:399:ASP:HB2	1:B:405:PHE:HD2	1.74	0.52
1:A:290:LYS:HD2	1:A:303:VAL:CG1	2.40	0.51
2:C:106:ILE:HB	2:C:141:ILE:HG13	1.91	0.51
1:A:397:VAL:O	1:A:404:TYR:HA	2.10	0.51
1:B:270:ASP:N	1:B:271:PRO:HD3	2.26	0.51
1:D:266:VAL:CG2	1:D:300:TYR:HB2	2.40	0.51
1:D:346:PRO:HD3	1:D:432:LEU:HD11	1.93	0.51
1:D:367:CYS:HB2	1:D:381:TRP:CZ2	2.45	0.51
1:D:237:GLY:HA3	2:F:132:TYR:OH	2.11	0.51
2:C:103:GLU:O	2:C:104:GLU:HG3	2.10	0.51
1:E:252:MET:O	1:E:254:SER:N	2.44	0.51
1:B:266:VAL:HG13	1:B:300:TYR:HB3	1.93	0.51
1:D:375:SER:HB3	1:D:404:TYR:CE2	2.46	0.51
1:D:382:GLU:CB	1:D:387:PRO:HA	2.40	0.51
1:A:310:HIS:CD2	1:A:311:GLN:HG2	2.46	0.51
1:B:301:ARG:NH2	3:H:2:NAG:O7	2.44	0.51
2:F:33:TYR:CD2	2:F:75:LEU:HD21	2.46	0.51
1:D:398:LEU:HA	1:D:404:TYR:CD1	2.40	0.50
3:H:2:NAG:H3	3:H:2:NAG:H83	1.93	0.50
1:A:295:GLN:O	1:A:297:ASN:N	2.39	0.50
2:F:162:ASN:OD1	2:F:163:VAL:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:HIS:O	1:B:312:ASP:N	2.45	0.50
2:F:114:LYS:O	2:F:114:LYS:HG2	2.10	0.50
1:A:241:PHE:HE1	3:G:5:NAG:H81	1.77	0.50
2:C:103:GLU:HG2	2:C:143:LYS:HA	1.93	0.50
1:A:290:LYS:HD2	1:A:303:VAL:HG11	1.94	0.50
1:B:312:ASP:O	1:B:313:TRP:HB3	2.11	0.50
2:C:125:GLN:HG2	2:C:130:ARG:CZ	2.42	0.50
2:C:44:HIS:CB	2:C:49:ILE:HD11	2.42	0.49
2:F:43:PHE:O	2:F:69:TYR:HD1	1.93	0.49
1:B:313:TRP:CZ3	1:B:337:SER:HA	2.48	0.49
2:C:98:TRP:CD1	2:C:99:VAL:HG13	2.47	0.49
2:F:121:VAL:HG11	2:F:136:ASN:HA	1.93	0.49
1:B:276:ASN:OD1	1:B:284:VAL:HG22	2.11	0.49
2:C:91:LEU:HD23	2:C:112:SER:HA	1.94	0.49
1:B:277:TRP:HH2	1:B:304:SER:HG	1.60	0.49
2:C:10:VAL:HG21	2:C:82:VAL:HB	1.95	0.49
2:C:91:LEU:CD2	2:C:118:LEU:HD21	2.42	0.49
2:C:158:ILE:O	2:C:160:SER:N	2.46	0.49
2:F:107:HIS:CE1	2:F:138:ASP:HB3	2.47	0.49
1:B:292:ARG:HB2	1:B:300:TYR:CD1	2.48	0.49
1:E:367:CYS:HB3	1:E:408:SER:OG	2.12	0.49
2:C:149:SER:HA	2:C:170:ILE:O	2.12	0.49
1:A:279:VAL:HG12	1:A:319:TYR:CD1	2.47	0.49
1:A:294:THR:H	1:E:291:PRO:HG2	1.75	0.49
1:A:383:SER:O	1:A:385:GLY:N	2.46	0.49
1:B:278:TYR:HE2	1:B:322:LYS:HD2	1.77	0.49
2:C:32:ALA:O	2:C:75:LEU:HD21	2.12	0.49
1:D:247:PRO:HA	1:D:250:THR:HG22	1.95	0.49
1:D:416:ARG:O	1:D:421:ASN:HB2	2.12	0.49
1:E:309:THR:HB	1:E:312:ASP:HB2	1.95	0.49
2:F:4:ASP:O	2:F:5:LEU:HD12	2.12	0.49
1:A:357:GLU:HG3	1:B:349:TYR:CE2	2.48	0.49
1:B:413:ASP:OD1	1:B:414:LYS:N	2.46	0.49
1:E:263:VAL:HB	1:E:302:VAL:HG23	1.95	0.49
1:E:264:VAL:HG22	1:E:265:ASP:N	2.28	0.49
1:E:360:LYS:HG3	1:E:361:ASN:N	2.19	0.49
1:B:399:ASP:OD1	1:B:400:SER:N	2.38	0.48
2:C:63:VAL:HA	2:C:86:VAL:HG21	1.94	0.48
2:F:103:GLU:O	2:F:104:GLU:HG3	2.13	0.48
1:E:278:TYR:H	1:E:320:THR:HG1	1.58	0.48
2:C:40:THR:HG21	2:C:53:THR:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:148:ASP:OD1	2:C:149:SER:N	2.47	0.48
1:B:399:ASP:HB2	1:B:405:PHE:CD2	2.48	0.48
2:C:18:ARG:O	2:C:94:GLN:HG2	2.13	0.48
2:F:12:LEU:HD23	2:F:27:LEU:HG	1.95	0.48
2:F:18:ARG:HB3	2:F:92:LEU:HD21	1.95	0.48
1:D:372:PHE:H	1:D:403:SER:HB2	1.79	0.48
1:A:293:GLU:HA	1:E:291:PRO:HG3	1.96	0.48
1:E:267:SER:HB3	1:E:271:PRO:HG3	1.95	0.48
2:F:88:ILE:HG13	2:F:88:ILE:O	2.14	0.48
1:D:252:MET:HG3	1:D:253:ILE:HG23	1.96	0.48
1:E:367:CYS:HB2	1:E:381:TRP:CH2	2.48	0.48
1:A:399:ASP:OD1	1:A:400:SER:N	2.41	0.48
1:B:264:VAL:O	1:B:265:ASP:HB2	2.13	0.47
1:D:237:GLY:N	2:F:132:TYR:HE2	2.12	0.47
2:C:32:ALA:CB	2:C:73:THR:HB	2.44	0.47
2:C:23:ASP:OD2	2:C:111:HIS:NE2	2.47	0.47
1:B:292:ARG:O	1:B:292:ARG:HG3	2.14	0.47
2:C:77:THR:HG22	2:C:78:LEU:N	2.29	0.47
2:C:97:ARG:HB2	2:C:100:PHE:CE1	2.49	0.47
2:F:143:LYS:HG2	2:F:144:ALA:O	2.15	0.47
1:A:265:ASP:HA	1:A:299:THR:HG23	1.96	0.47
1:B:285:HIS:O	1:B:285:HIS:ND1	2.47	0.47
2:C:39:SER:O	2:C:73:THR:HG23	2.15	0.47
1:E:368:LEU:HD21	1:E:370:LYS:HB2	1.96	0.47
1:E:379:VAL:HG13	1:E:393:THR:HG21	1.97	0.46
1:A:378:VAL:CG1	1:A:428:MET:HB2	2.45	0.46
1:D:288:GLN:HG2	1:D:289:THR:N	2.31	0.46
1:E:296:TYR:HB3	1:E:297:ASN:OD1	2.16	0.46
1:E:371:GLY:HA2	1:E:403:SER:HB3	1.97	0.46
2:C:77:THR:HG22	2:C:78:LEU:H	1.80	0.46
1:D:257:PRO:HG3	1:D:310:HIS:HA	1.97	0.46
1:A:366:THR:HG22	1:B:407:TYR:OH	2.15	0.46
1:A:292:ARG:HD3	1:A:300:TYR:CE2	2.51	0.46
1:B:338:LYS:HG2	1:B:339:ASP:N	2.31	0.46
1:D:242:LEU:HD12	1:D:321:CYS:HB3	1.98	0.46
1:D:349:TYR:CG	1:E:357:GLU:HB3	2.51	0.46
2:F:33:TYR:CG	2:F:34:SER:N	2.82	0.46
2:F:134:HIS:CG	2:F:135:GLN:H	2.34	0.46
1:B:273:VAL:HG23	1:B:274:LYS:N	2.28	0.46
1:E:383:SER:O	1:E:385:GLY:N	2.49	0.45
1:B:365:LEU:HD23	1:B:441:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:PHE:N	1:D:403:SER:HB2	2.31	0.45
1:E:385:GLY:O	1:E:387:PRO:HD3	2.15	0.45
1:A:263:VAL:HB	1:A:302:VAL:CG1	2.45	0.45
1:B:336:ILE:HG23	1:B:337:SER:N	2.29	0.45
1:E:378:VAL:CG1	1:E:428:MET:HB2	2.47	0.45
2:C:5:LEU:CD2	2:C:75:LEU:HB2	2.47	0.45
1:A:346:PRO:HB3	1:A:372:PHE:CB	2.35	0.45
1:B:308:VAL:HG12	1:B:309:THR:O	2.17	0.45
1:A:247:PRO:O	1:A:251:LEU:HG	2.17	0.45
1:B:431:ALA:O	1:B:432:LEU:HD12	2.17	0.45
1:E:367:CYS:HB2	1:E:381:TRP:CZ2	2.51	0.45
1:B:374:PRO:HD2	1:B:429:HIS:HE1	1.82	0.45
2:C:147:LYS:O	2:C:147:LYS:HG3	2.16	0.45
2:C:63:VAL:HA	2:C:86:VAL:CG2	2.47	0.44
1:B:313:TRP:O	1:B:314:LEU:HG	2.17	0.44
1:A:357:GLU:HB2	1:B:349:TYR:CE1	2.53	0.44
1:B:284:VAL:CG1	1:B:285:HIS:H	2.15	0.44
1:B:364:SER:HB2	1:B:409:LYS:HG3	1.99	0.44
1:D:383:SER:HB2	1:D:423:PHE:CE1	2.53	0.44
2:C:124:LEU:HD12	2:C:153:PHE:CE1	2.53	0.44
2:C:166:GLU:HG3	2:C:167:THR:N	2.33	0.44
2:F:90:TRP:HB3	2:F:163:VAL:HG11	1.98	0.44
1:B:287:ALA:HB1	1:B:304:SER:HB2	1.99	0.44
2:F:5:LEU:HB3	2:F:6:PRO:HD2	1.98	0.44
2:F:123:TYR:CD2	2:F:139:PHE:HB2	2.52	0.44
1:B:417:TRP:CZ2	1:B:443:VAL:HG22	2.52	0.44
1:B:284:VAL:O	1:B:286:HIS:ND1	2.51	0.44
1:E:264:VAL:HG21	3:J:1:NAG:C3	2.43	0.44
1:E:305:VAL:HG12	1:E:306:LEU:N	2.28	0.44
1:A:275:PHE:CE2	1:A:304:SER:HB2	2.53	0.44
1:D:351:LEU:HD23	1:E:354:SER:HB3	2.00	0.44
1:D:372:PHE:HE1	1:D:375:SER:HA	1.82	0.44
1:D:429:HIS:CG	1:D:430:GLU:N	2.86	0.44
1:E:235:LEU:HD23	1:E:236:GLY:N	2.32	0.44
1:B:266:VAL:HG13	1:B:300:TYR:O	1.99	0.43
2:F:49:ILE:O	2:F:51:SER:N	2.50	0.43
2:F:91:LEU:HD13	2:F:163:VAL:HG11	1.99	0.43
1:D:252:MET:HB2	1:D:435:HIS:CD2	2.52	0.43
1:D:422:VAL:HG12	1:D:442:SER:CB	2.44	0.43
2:C:149:SER:HA	2:C:171:THR:HA	2.00	0.43
1:B:263:VAL:CG1	1:B:302:VAL:HB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:412:VAL:HG11	1:D:423:PHE:CZ	2.53	0.43
2:C:8:ALA:CB	2:C:76:SER:HB2	2.48	0.43
1:A:290:LYS:HB2	1:A:303:VAL:HB	1.99	0.43
1:E:252:MET:O	1:E:252:MET:HG3	2.19	0.43
1:E:379:VAL:HA	1:E:427:VAL:HG12	2.01	0.43
2:C:32:ALA:CA	2:C:75:LEU:CD2	2.82	0.43
2:C:114:LYS:O	2:C:114:LYS:HG3	2.19	0.43
1:D:389:ASN:HA	1:D:391:TYR:HD2	1.83	0.43
1:E:294:THR:HG23	1:E:295:GLN:N	2.24	0.43
2:F:27:LEU:HB3	2:F:42:TRP:CH2	2.54	0.43
1:A:245:PRO:HG3	1:A:259:VAL:HG22	2.00	0.43
1:D:242:LEU:HD12	1:D:321:CYS:CB	2.49	0.43
2:F:29:CYS:O	2:F:30:GLN:NE2	2.51	0.43
1:D:309:THR:HG1	1:D:312:ASP:HB3	1.83	0.43
2:F:8:ALA:HB2	2:F:76:SER:HB2	2.01	0.43
1:A:297:ASN:C	1:A:299:THR:H	2.19	0.42
1:A:381:TRP:CD2	1:A:410:LEU:HD22	2.54	0.42
2:C:34:SER:HB2	2:C:39:SER:H	1.84	0.42
1:B:266:VAL:CG1	1:B:300:TYR:C	2.76	0.42
2:F:28:LYS:HG2	2:F:55:SER:OG	2.19	0.42
1:B:266:VAL:O	1:B:299:THR:HA	2.18	0.42
1:B:272:ASP:N	1:B:325:ASN:HD21	2.16	0.42
1:D:311:GLN:OE1	1:D:311:GLN:N	2.53	0.42
1:D:366:THR:HA	1:D:408:SER:O	2.20	0.42
2:F:120:LYS:HG2	2:F:132:TYR:OH	2.19	0.42
1:A:263:VAL:HB	1:A:302:VAL:HG13	2.00	0.42
1:A:279:VAL:O	1:A:280:ASN:HB2	2.20	0.42
1:A:349:TYR:HB3	1:B:354:SER:HB3	2.01	0.42
1:B:336:ILE:HG13	1:B:337:SER:N	2.34	0.42
2:C:125:GLN:HE21	2:C:126:ASN:HD22	1.65	0.42
1:E:328:LEU:HD21	1:E:332:ILE:HG13	2.01	0.42
2:C:99:VAL:HG23	2:C:99:VAL:O	2.20	0.42
1:B:247:PRO:C	1:B:251:LEU:HD12	2.30	0.42
1:E:266:VAL:HG21	1:E:300:TYR:HB2	2.02	0.42
2:C:97:ARG:HH22	2:C:105:SER:H	1.66	0.42
1:A:250:THR:HA	1:A:257:PRO:HG3	2.01	0.42
1:A:278:TYR:HE1	1:A:283:GLU:HG3	1.85	0.42
1:E:287:ALA:O	1:E:289:THR:N	2.48	0.42
2:C:106:ILE:HB	2:C:141:ILE:CG1	2.50	0.42
1:A:292:ARG:HD3	1:A:300:TYR:HE2	1.85	0.42
1:A:319:TYR:O	1:A:335:THR:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:VAL:CG1	1:A:323:VAL:HG11	2.42	0.42
1:A:431:ALA:C	1:A:432:LEU:HD12	2.40	0.42
1:D:273:VAL:HG12	1:D:325:ASN:HB2	2.01	0.42
1:E:336:ILE:HG22	1:E:337:SER:N	2.34	0.42
1:A:397:VAL:HG11	1:B:395:PRO:HD3	2.01	0.41
1:B:322:LYS:HA	1:B:333:GLN:HB3	2.02	0.41
1:E:263:VAL:O	1:E:301:ARG:HG3	2.20	0.41
1:E:325:ASN:HB3	1:E:328:LEU:HB3	2.01	0.41
2:F:121:VAL:HG12	2:F:133:PHE:O	2.20	0.41
1:A:277:TRP:O	1:A:283:GLU:HA	2.20	0.41
1:A:297:ASN:O	1:A:299:THR:N	2.43	0.41
1:E:360:LYS:HD2	1:E:361:ASN:OD1	2.19	0.41
1:E:365:LEU:HD21	1:E:417:TRP:CZ3	2.54	0.41
2:C:72:GLN:HG3	2:C:76:SER:OG	2.21	0.41
2:F:134:HIS:CG	2:F:135:GLN:N	2.88	0.41
1:B:264:VAL:CG2	3:H:1:NAG:H3	2.48	0.41
1:D:379:VAL:HA	1:D:426:SER:O	2.21	0.41
1:D:399:ASP:O	1:D:401:ASP:N	2.52	0.41
1:A:314:LEU:O	1:A:338:LYS:HD3	2.20	0.41
1:B:241:PHE:HB2	1:B:262:VAL:HG22	2.02	0.41
2:F:149:SER:HA	2:F:170:ILE:O	2.19	0.41
1:E:313:TRP:HZ3	1:E:337:SER:HA	1.83	0.41
2:C:39:SER:OG	2:C:40:THR:N	2.54	0.41
1:B:323:VAL:HG12	1:B:332:ILE:O	2.21	0.41
2:C:32:ALA:HA	2:C:75:LEU:CG	2.51	0.41
2:C:93:LEU:HD11	2:C:108:LEU:HB3	2.02	0.41
2:F:16:TRP:NE1	2:F:94:GLN:HB3	2.36	0.41
1:A:365:LEU:HD11	1:A:423:PHE:CD2	2.44	0.41
1:E:267:SER:OG	1:E:269:GLU:N	2.54	0.41
1:E:329:PRO:HG3	2:F:113:TRP:CD2	2.55	0.41
2:C:40:THR:OG1	2:C:41:ARG:N	2.54	0.41
2:F:124:LEU:HD22	2:F:153:PHE:CZ	2.55	0.41
1:B:288:GLN:HA	1:B:288:GLN:OE1	2.21	0.41
1:B:328:LEU:HA	1:B:329:PRO:HD3	1.95	0.41
1:B:359:THR:HG23	1:B:360:LYS:N	2.36	0.41
2:F:153:PHE:HB3	2:F:167:THR:HA	2.02	0.41
1:D:288:GLN:HG2	1:D:289:THR:H	1.86	0.40
2:C:30:GLN:O	2:C:32:ALA:N	2.54	0.40
2:C:76:SER:O	2:C:77:THR:C	2.59	0.40
1:A:238:PRO:HD2	1:A:328:LEU:CG	2.38	0.40
1:D:237:GLY:N	2:F:134:HIS:HB3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:335:THR:O	1:E:336:ILE:HD13	2.22	0.40
2:F:19:VAL:CG2	2:F:86:VAL:HG12	2.46	0.40
1:B:391:TYR:O	1:B:392:LYS:HD2	2.22	0.40
1:D:389:ASN:HA	1:D:391:TYR:CD2	2.56	0.40
1:E:353:PRO:HD2	1:E:417:TRP:CZ2	2.56	0.40
1:D:251:LEU:HD12	1:D:253:ILE:H	1.87	0.40
2:C:63:VAL:HG23	2:C:64:ASN:H	1.85	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:GLU:OE1	2:C:33:TYR:OH[1_565]	2.05	0.15
1:E:316:GLY:O	2:F:171:THR:OG1[4_446]	2.11	0.09

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	205/224 (92%)	161 (78%)	28 (14%)	16 (8%)	1 15
1	B	208/224 (93%)	139 (67%)	48 (23%)	21 (10%)	0 9
1	D	206/224 (92%)	161 (78%)	31 (15%)	14 (7%)	1 18
1	E	209/224 (93%)	148 (71%)	40 (19%)	21 (10%)	0 9
2	C	167/192 (87%)	131 (78%)	26 (16%)	10 (6%)	1 20
2	F	167/192 (87%)	134 (80%)	22 (13%)	11 (7%)	1 19
All	All	1162/1280 (91%)	874 (75%)	195 (17%)	93 (8%)	1 14

All (93) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	PRO
1	A	286	HIS
1	A	433	HIS
1	B	268	GLN
1	B	280	ASN
1	B	284	VAL
1	B	291	PRO
1	B	297	ASN
1	B	300	TYR
1	B	312	ASP
1	B	339	ASP
1	B	355	ARG
1	D	238	PRO
1	D	254	SER
1	D	271	PRO
1	D	284	VAL
1	D	285	HIS
1	D	430	GLU
1	E	253	ILE
2	C	63	VAL
2	C	146	LEU
2	F	63	VAL
1	A	272	ASP
1	A	296	TYR
1	A	361	ASN
1	A	384	SER
1	B	259	VAL
1	B	273	VAL
1	B	288	GLN
1	B	336	ILE
1	D	251	LEU
1	D	312	ASP
1	D	353	PRO
1	D	401	ASP
1	D	421	ASN
1	D	443	VAL
1	E	237	GLY
1	E	259	VAL
1	E	337	SER
1	E	355	ARG
1	E	384	SER
2	C	115	ASN
2	C	149	SER

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Mol	Chain	Res	Type
2	C	159	GLY
2	F	21	GLU
2	F	39	SER
2	F	149	SER
1	A	283	GLU
1	A	359	THR
1	A	442	SER
1	B	287	ALA
1	B	385	GLY
1	D	400	SER
1	E	274	LYS
1	E	288	GLN
1	E	294	THR
1	E	316	GLY
1	E	336	ILE
2	C	73	THR
2	C	96	PRO
2	C	143	LYS
2	F	15	GLN
2	F	50	SER
2	F	159	GLY
1	A	297	ASN
1	A	299	THR
1	B	295	GLN
1	B	311	GLN
1	B	322	LYS
1	B	342	GLN
1	E	339	ASP
2	C	112	SER
2	F	41	ARG
2	F	142	PRO
1	A	284	VAL
1	A	339	ASP
1	B	319	TYR
1	D	329	PRO
1	E	319	TYR
1	E	342	GLN
2	C	52	GLN
1	A	346	PRO
1	E	254	SER
1	E	271	PRO
1	E	291	PRO

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Mol	Chain	Res	Type
2	F	6	PRO
1	B	387	PRO
1	A	385	GLY
1	E	238	PRO
1	E	284	VAL
1	E	330	ALA
1	E	385	GLY
2	F	141	ILE

5.3.2 Protein sidechains (i)

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	194/208 (93%)	191 (98%)	3 (2%)	65	81
1	B	196/208 (94%)	189 (96%)	7 (4%)	35	63
1	D	195/208 (94%)	192 (98%)	3 (2%)	65	81
1	E	197/208 (95%)	195 (99%)	2 (1%)	76	86
2	C	154/174 (88%)	152 (99%)	2 (1%)	69	82
2	F	154/174 (88%)	153 (99%)	1 (1%)	86	92
All	All	1090/1180 (92%)	1072 (98%)	18 (2%)	60	78

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	274	LYS
1	A	373	TYR
1	A	391	TYR
1	B	249	ASP
1	B	264	VAL
1	B	268	GLN
1	B	280	ASN
1	B	286	HIS
1	B	340	LYS
1	B	433	HIS

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Mol	Chain	Res	Type
1	D	238	PRO
1	D	339	ASP
1	D	425	CYS
1	E	254	SER
1	E	340	LYS
2	C	39	SER
2	C	98	TRP
2	F	75	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

32 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	G	1	1,3	14,14,15	0.30	0	17,19,21	0.66	0
3	NAG	G	2	3	14,14,15	0.33	0	17,19,21	0.50	0
3	BMA	G	3	3	11,11,12	0.58	0	15,15,17	0.94	0
3	MAN	G	4	3	11,11,12	1.02	1 (9%)	15,15,17	1.13	2 (13%)
3	NAG	G	5	3	14,14,15	0.45	0	17,19,21	1.08	2 (11%)
3	MAN	G	6	3	11,11,12	0.85	0	15,15,17	1.03	0
3	NAG	G	7	3	14,14,15	0.28	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	FUC	G	8	3	10,10,11	0.95	0	14,14,16	1.06	2 (14%)
3	NAG	H	1	1,3	14,14,15	1.08	1 (7%)	17,19,21	1.70	1 (5%)
3	NAG	H	2	3	14,14,15	0.44	0	17,19,21	1.35	2 (11%)
3	BMA	H	3	3	11,11,12	0.65	0	15,15,17	0.90	1 (6%)
3	MAN	H	4	3	11,11,12	1.06	1 (9%)	15,15,17	1.34	3 (20%)
3	NAG	H	5	3	14,14,15	0.68	1 (7%)	17,19,21	1.12	2 (11%)
3	MAN	H	6	3	11,11,12	0.69	0	15,15,17	1.13	2 (13%)
3	NAG	H	7	3	14,14,15	0.36	0	17,19,21	0.46	0
3	FUC	H	8	3	10,10,11	0.72	0	14,14,16	0.83	0
3	NAG	I	1	1,3	14,14,15	0.35	0	17,19,21	0.85	1 (5%)
3	NAG	I	2	3	14,14,15	0.26	0	17,19,21	0.49	0
3	BMA	I	3	3	11,11,12	0.85	0	15,15,17	0.88	0
3	MAN	I	4	3	11,11,12	1.05	1 (9%)	15,15,17	1.13	1 (6%)
3	NAG	I	5	3	14,14,15	0.63	1 (7%)	17,19,21	0.92	1 (5%)
3	MAN	I	6	3	11,11,12	0.65	0	15,15,17	0.90	1 (6%)
3	NAG	I	7	3	14,14,15	0.23	0	17,19,21	0.45	0
3	FUC	I	8	3	10,10,11	1.11	1 (10%)	14,14,16	1.06	1 (7%)
3	NAG	J	1	1,3	14,14,15	0.19	0	17,19,21	0.58	0
3	NAG	J	2	3	14,14,15	0.47	0	17,19,21	1.37	2 (11%)
3	BMA	J	3	3	11,11,12	0.68	0	15,15,17	0.90	1 (6%)
3	MAN	J	4	3	11,11,12	1.01	0	15,15,17	1.50	3 (20%)
3	NAG	J	5	3	14,14,15	0.63	1 (7%)	17,19,21	1.06	2 (11%)
3	MAN	J	6	3	11,11,12	1.07	2 (18%)	15,15,17	1.38	2 (13%)
3	NAG	J	7	3	14,14,15	0.33	0	17,19,21	0.42	0
3	FUC	J	8	3	10,10,11	0.95	0	14,14,16	0.98	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	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	MAN	G	4	3	-	0/2/19/22	0/1/1/1
3	NAG	G	5	3	-	3/6/23/26	0/1/1/1
3	MAN	G	6	3	-	2/2/19/22	0/1/1/1

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	NAG	O5-C1	3.94	1.50	1.43
3	I	4	MAN	O5-C1	-2.69	1.39	1.43
3	G	4	MAN	O5-C1	-2.55	1.39	1.43
3	I	8	FUC	C1-C2	2.45	1.57	1.52
3	J	6	MAN	C2-C3	2.39	1.56	1.52
3	J	6	MAN	C1-C2	2.37	1.57	1.52
3	H	5	NAG	O5-C1	-2.28	1.40	1.43
3	I	5	NAG	O5-C1	-2.16	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	5	NAG	O5-C1	-2.11	1.40	1.43
3	H	4	MAN	O5-C1	-2.03	1.40	1.43

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1	NAG	C1-O5-C5	6.59	121.11	112.19
3	J	2	NAG	C2-N2-C7	4.42	129.19	122.90
3	H	2	NAG	C2-N2-C7	4.36	129.11	122.90
3	J	4	MAN	O2-C2-C3	-3.31	103.51	110.14
3	J	4	MAN	C1-O5-C5	3.31	116.67	112.19
3	H	4	MAN	O2-C2-C3	-3.26	103.60	110.14
3	I	4	MAN	O2-C2-C3	-3.19	103.75	110.14
3	G	5	NAG	C1-O5-C5	3.11	116.41	112.19
3	H	5	NAG	C1-O5-C5	2.97	116.21	112.19
3	J	6	MAN	C1-C2-C3	2.90	113.23	109.67
3	J	5	NAG	C1-O5-C5	2.79	115.97	112.19
3	G	4	MAN	O2-C2-C3	-2.70	104.74	110.14
3	J	4	MAN	C1-C2-C3	-2.60	106.48	109.67
3	I	1	NAG	C1-O5-C5	2.58	115.68	112.19
3	H	5	NAG	C3-C4-C5	2.50	114.70	110.24
3	H	4	MAN	C1-O5-C5	2.49	115.57	112.19
3	H	4	MAN	C1-C2-C3	-2.49	106.61	109.67
3	J	5	NAG	C3-C4-C5	2.42	114.56	110.24
3	H	2	NAG	C1-C2-N2	2.42	114.62	110.49
3	H	6	MAN	C1-O5-C5	2.39	115.44	112.19
3	G	5	NAG	C3-C4-C5	2.32	114.37	110.24
3	I	6	MAN	C1-O5-C5	2.31	115.33	112.19
3	I	8	FUC	O2-C2-C1	2.29	113.84	109.15
3	G	8	FUC	C1-C2-C3	2.27	112.46	109.67
3	H	6	MAN	O2-C2-C3	-2.26	105.62	110.14
3	I	5	NAG	C3-C4-C5	2.21	114.18	110.24
3	J	6	MAN	O5-C1-C2	2.19	114.15	110.77
3	G	4	MAN	C1-O5-C5	2.15	115.11	112.19
3	J	2	NAG	C1-C2-N2	2.13	114.13	110.49
3	H	3	BMA	C1-O5-C5	2.13	115.07	112.19
3	J	3	BMA	C1-O5-C5	2.11	115.05	112.19
3	G	8	FUC	O5-C5-C4	2.04	113.18	109.52

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	6	MAN	O5-C5-C6-O6
3	H	7	NAG	C4-C5-C6-O6
3	I	5	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	H	7	NAG	O5-C5-C6-O6
3	I	7	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	J	7	NAG	O5-C5-C6-O6
3	I	5	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	G	7	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	I	7	NAG	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	J	6	MAN	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	G	7	NAG	C4-C5-C6-O6
3	I	6	MAN	C4-C5-C6-O6
3	J	6	MAN	C4-C5-C6-O6
3	G	5	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	J	2	NAG	C8-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2
3	H	6	MAN	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	H	5	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	J	7	NAG	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	H	6	MAN	C4-C5-C6-O6
3	G	5	NAG	C4-C5-C6-O6
3	H	4	MAN	C4-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	H	4	MAN	O5-C5-C6-O6
3	G	6	MAN	O5-C5-C6-O6
3	G	5	NAG	C3-C2-N2-C7
3	H	2	NAG	C3-C2-N2-C7
3	H	5	NAG	C3-C2-N2-C7
3	J	2	NAG	C3-C2-N2-C7
3	G	6	MAN	C4-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	I	5	NAG	C3-C2-N2-C7
3	J	5	NAG	C3-C2-N2-C7
3	H	5	NAG	C4-C5-C6-O6
3	I	5	NAG	C1-C2-N2-C7
3	J	5	NAG	C1-C2-N2-C7

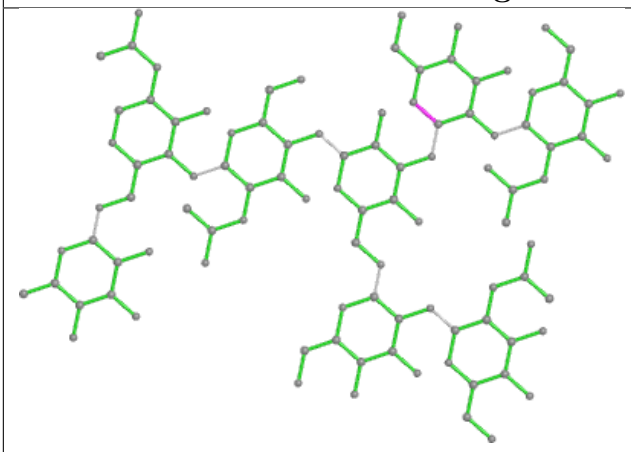
There are no ring outliers.

6 monomers are involved in 12 short contacts:

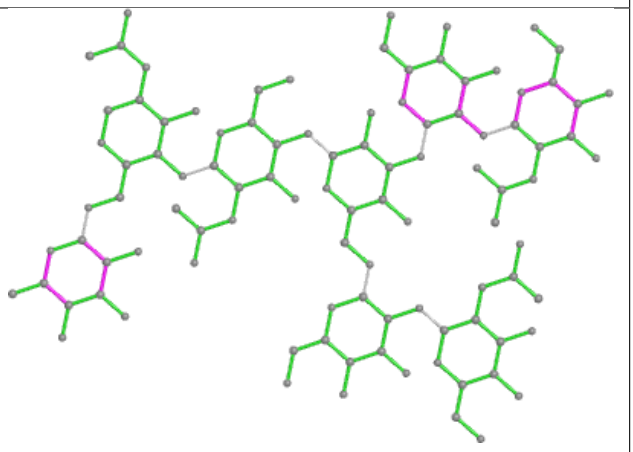
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	3	BMA	1	0
3	H	2	NAG	2	0
3	G	5	NAG	1	0
3	H	1	NAG	4	0
3	J	2	NAG	1	0
3	J	1	NAG	3	0

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

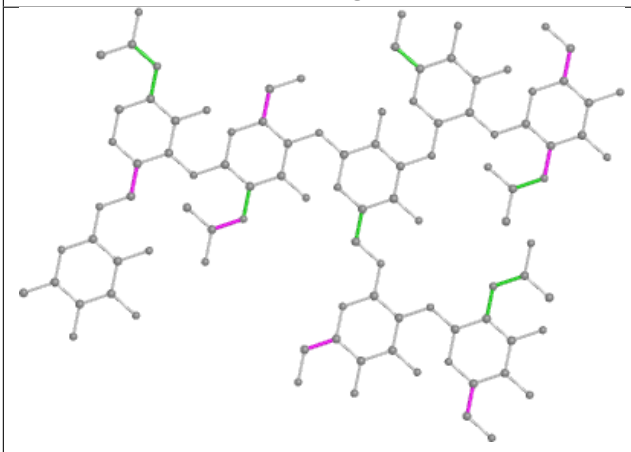
Oligosaccharide Chain G



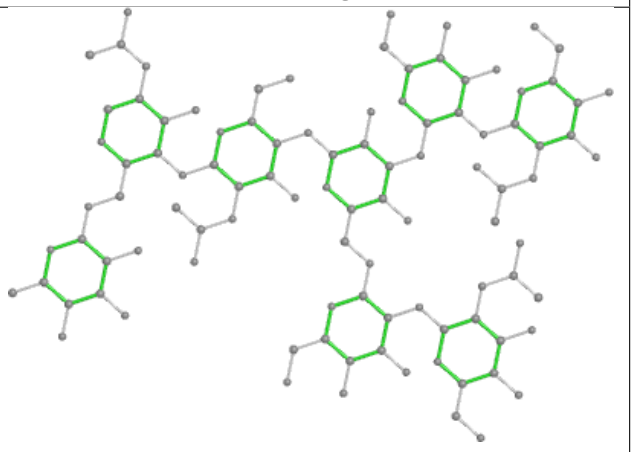
Bond lengths



Bond angles

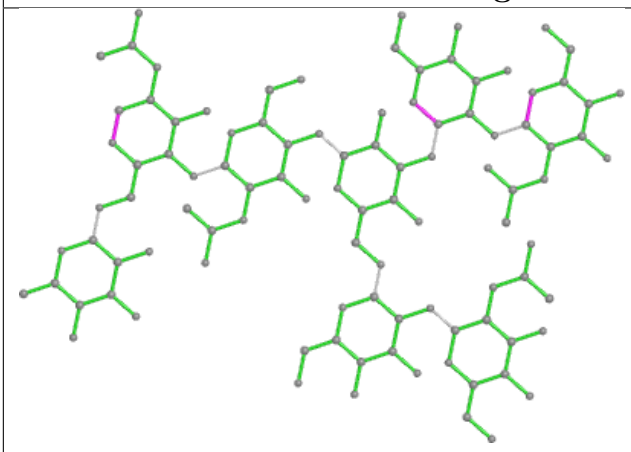


Torsions

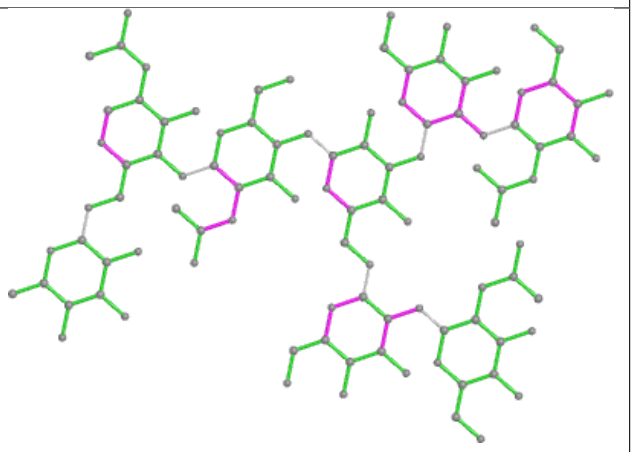


Rings

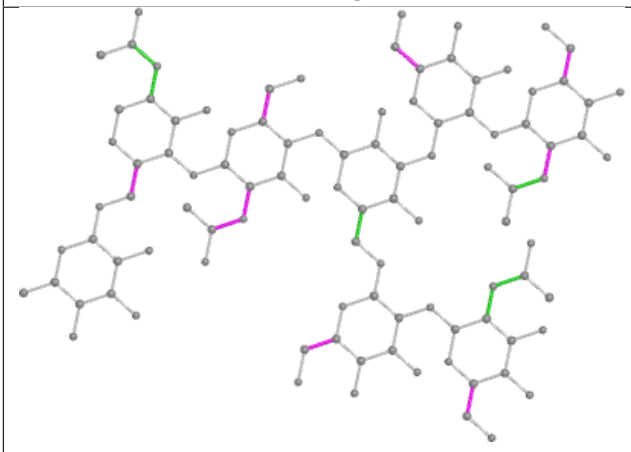
Oligosaccharide Chain H



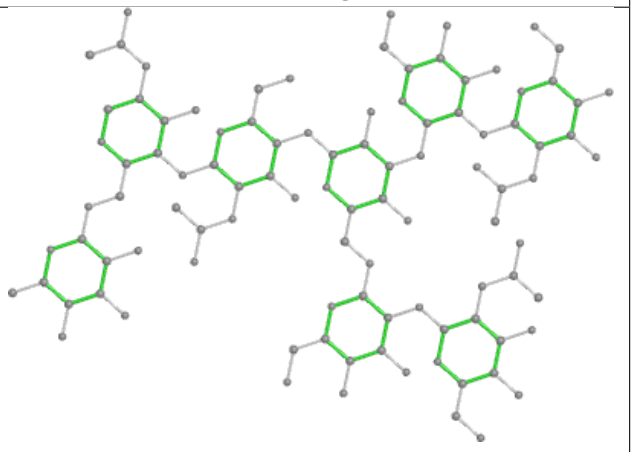
Bond lengths



Bond angles

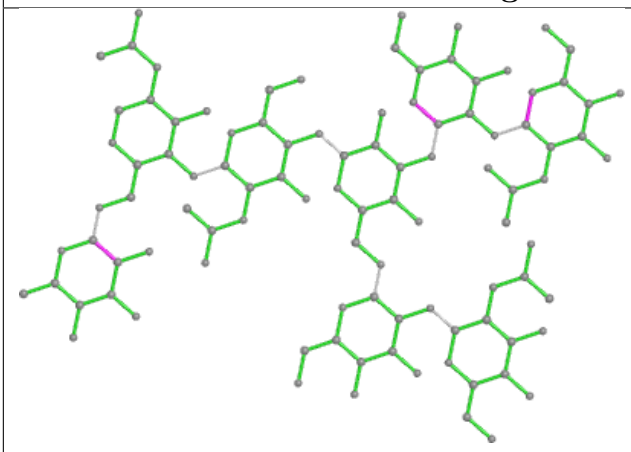


Torsions

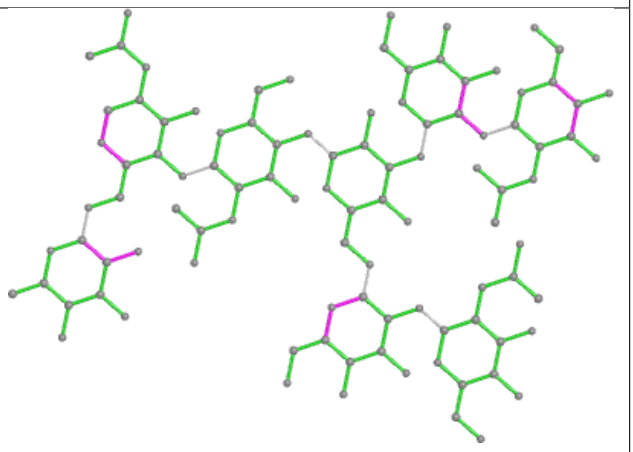


Rings

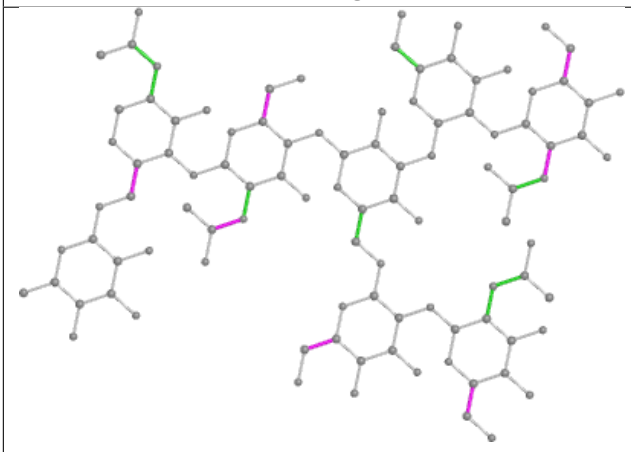
Oligosaccharide Chain I



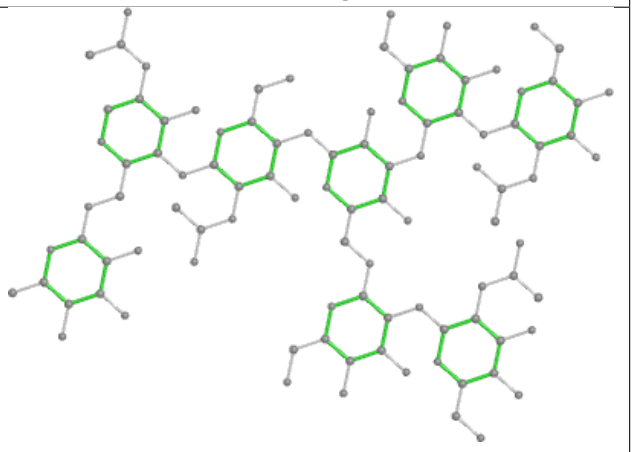
Bond lengths



Bond angles

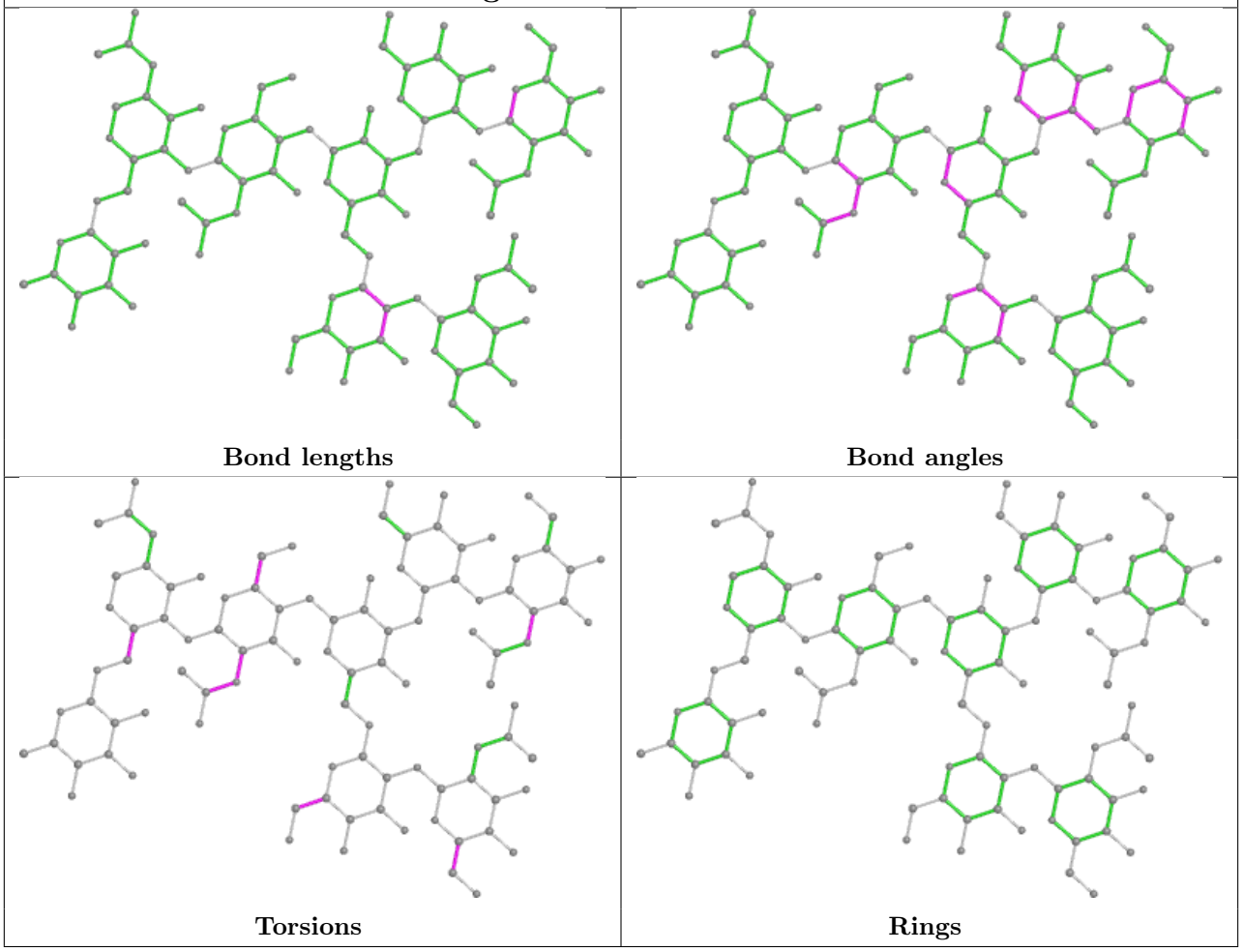


Torsions



Rings

Oligosaccharide Chain J



5.6 Ligand geometry

3 ligands 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	$\#\|Z\| > 2$
4	NAG	C	201	2	14,14,15	0.35	0	17,19,21	0.47	0
4	NAG	C	202	2	14,14,15	1.36	2 (14%)	17,19,21	1.20	2 (11%)
4	NAG	F	201	2	14,14,15	0.51	0	17,19,21	0.63	1 (5%)

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
4	NAG	C	201	2	-	2/6/23/26	0/1/1/1
4	NAG	C	202	2	-	2/6/23/26	0/1/1/1
4	NAG	F	201	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	202	NAG	O5-C1	-3.48	1.38	1.43
4	C	202	NAG	C1-C2	-3.08	1.47	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	202	NAG	C3-C4-C5	3.36	116.22	110.24
4	F	201	NAG	C1-O5-C5	2.23	115.21	112.19
4	C	202	NAG	O5-C5-C4	2.19	116.16	110.83

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	202	NAG	O5-C5-C6-O6
4	F	201	NAG	O5-C5-C6-O6
4	F	201	NAG	C4-C5-C6-O6
4	C	202	NAG	C4-C5-C6-O6
4	C	201	NAG	O5-C5-C6-O6
4	C	201	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	202	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	207/224 (92%)	-0.13	0	100	100	50, 84, 109, 135	0
1	B	210/224 (93%)	0.05	2 (0%)	82	76	63, 92, 119, 144	0
1	D	208/224 (92%)	0.11	2 (0%)	82	76	63, 93, 113, 132	0
1	E	211/224 (94%)	-0.00	1 (0%)	91	87	64, 103, 132, 152	0
2	C	169/192 (88%)	0.02	3 (1%)	68	61	69, 97, 139, 152	0
2	F	169/192 (88%)	-0.07	1 (0%)	89	85	67, 96, 134, 152	0
All	All	1174/1280 (91%)	-0.00	9 (0%)	86	81	50, 94, 129, 152	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	265	ASP	4.3
2	F	3	GLU	2.7
1	D	250	THR	2.3
1	B	428	MET	2.3
2	C	106	ILE	2.3
1	B	382	GLU	2.2
1	D	239	SER	2.2
2	C	89	GLY	2.0
2	C	149	SER	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 (i)

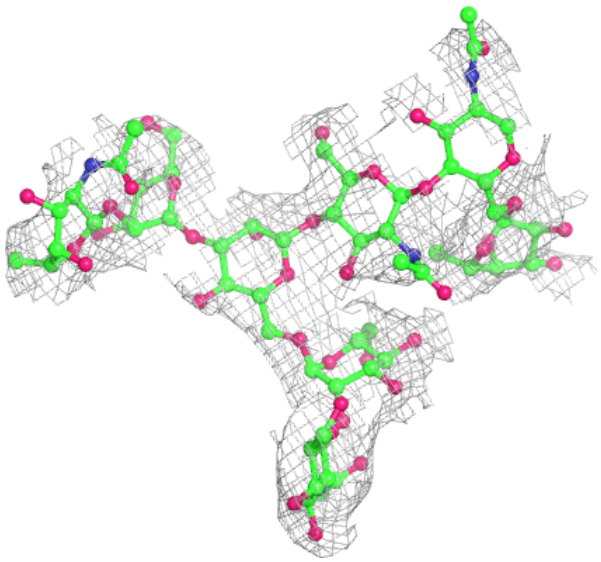
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

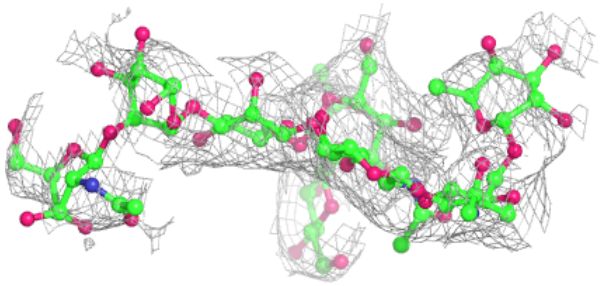
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FUC	G	8	10/11	0.59	0.39	161,169,173,176	0
3	NAG	J	5	14/15	0.66	0.51	164,171,175,176	0
3	FUC	I	8	10/11	0.70	0.25	114,120,126,130	0
3	NAG	H	5	14/15	0.71	0.46	155,166,172,174	0
3	FUC	H	8	10/11	0.73	0.28	134,140,145,147	0
3	FUC	J	8	10/11	0.77	0.26	126,128,133,138	0
3	NAG	G	5	14/15	0.79	0.32	149,151,155,160	0
3	NAG	I	7	14/15	0.83	0.30	98,101,106,106	0
3	NAG	G	1	14/15	0.87	0.21	94,105,129,144	0
3	NAG	I	5	14/15	0.87	0.21	116,120,131,135	0
3	NAG	G	2	14/15	0.88	0.33	119,121,126,129	0
3	NAG	H	1	14/15	0.88	0.20	75,84,105,123	0
3	NAG	J	2	14/15	0.88	0.18	89,99,101,101	0
3	NAG	I	2	14/15	0.88	0.18	100,104,109,117	0
3	NAG	J	7	14/15	0.88	0.25	84,91,110,112	0
3	MAN	H	4	11/12	0.88	0.15	122,127,133,143	0
3	NAG	I	1	14/15	0.89	0.18	79,84,96,104	0
3	NAG	J	1	14/15	0.89	0.15	91,99,116,122	0
3	BMA	H	3	11/12	0.89	0.15	87,91,97,110	0
3	MAN	G	6	11/12	0.90	0.14	105,107,109,109	0
3	BMA	J	3	11/12	0.90	0.17	100,102,108,120	0
3	MAN	J	4	11/12	0.90	0.17	134,140,144,154	0
3	NAG	G	7	14/15	0.91	0.21	92,97,100,101	0
3	NAG	H	2	14/15	0.91	0.19	79,86,93,96	0
3	MAN	G	4	11/12	0.91	0.17	138,140,144,146	0
3	NAG	H	7	14/15	0.92	0.17	91,94,95,100	0
3	MAN	I	4	11/12	0.93	0.16	111,112,117,117	0
3	BMA	G	3	11/12	0.93	0.18	111,121,124,131	0
3	MAN	I	6	11/12	0.93	0.15	101,103,106,109	0
3	BMA	I	3	11/12	0.94	0.13	100,102,104,107	0
3	MAN	H	6	11/12	0.95	0.13	76,82,88,90	0
3	MAN	J	6	11/12	0.95	0.21	99,102,107,112	0

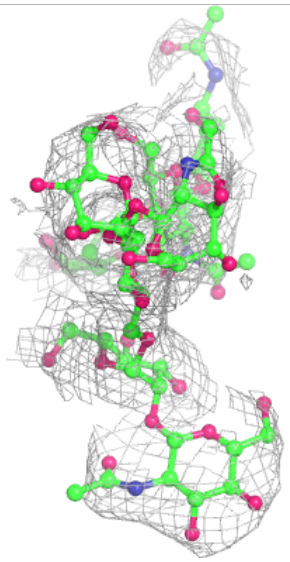
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

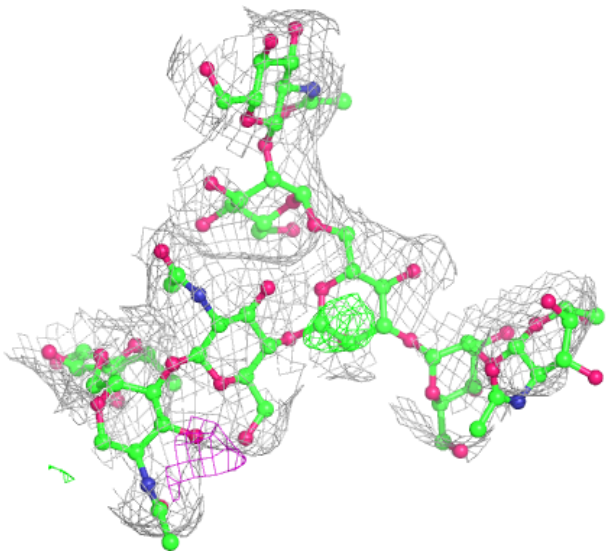


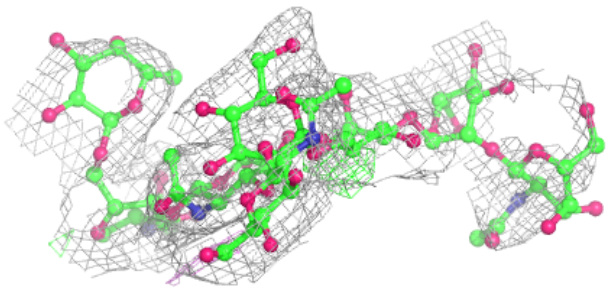


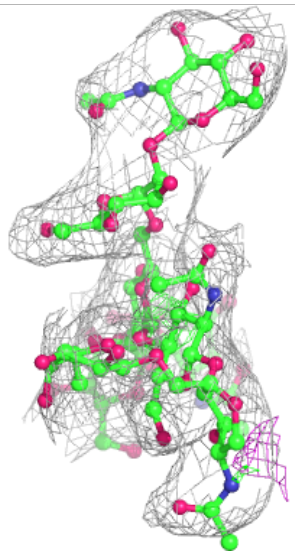


Electron density around Chain H:

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

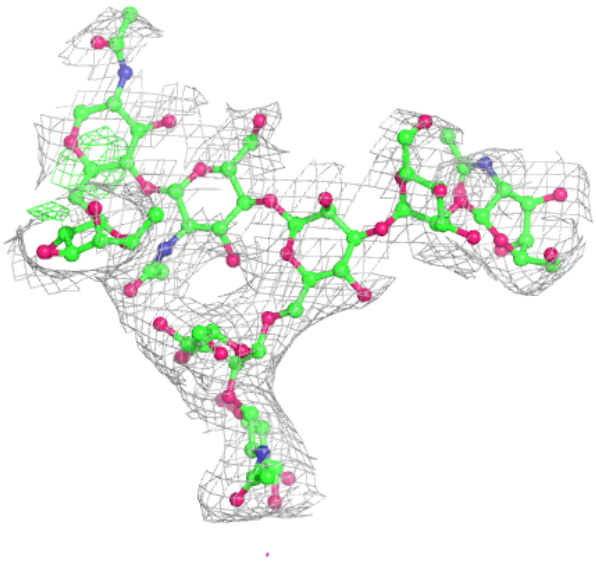


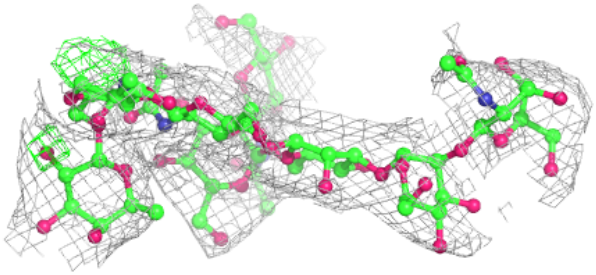


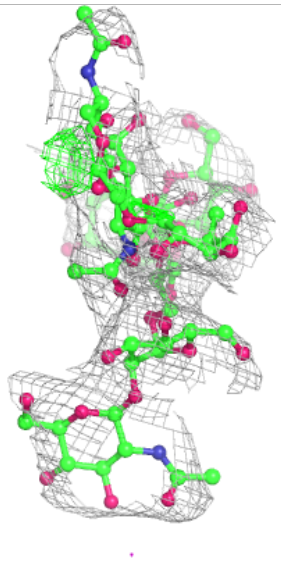


Electron density around Chain I:

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

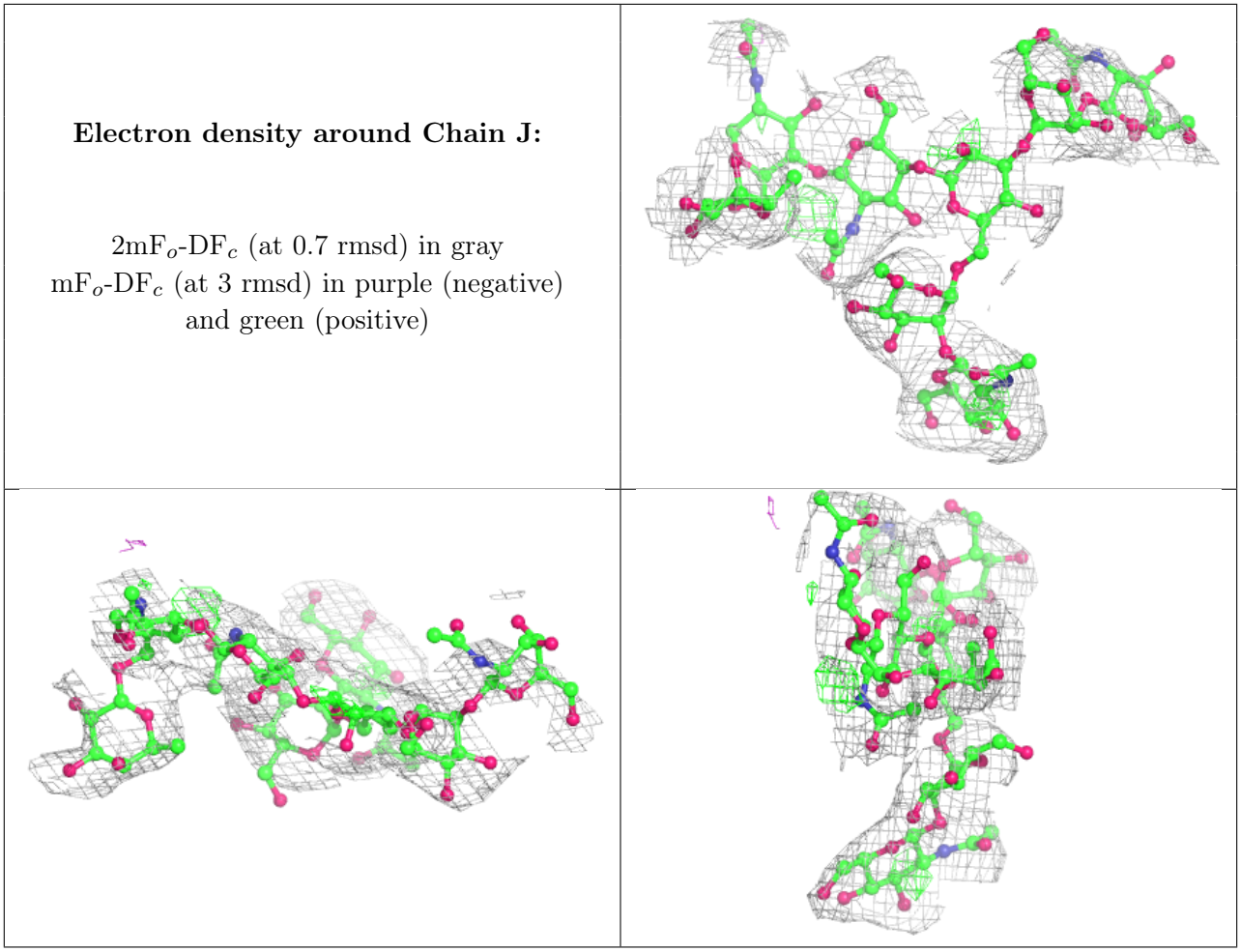






Electron density around Chain J:

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



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	NAG	C	202	14/15	0.54	0.62	136,148,171,171	0
4	NAG	F	201	14/15	0.83	0.28	142,151,153,157	0
4	NAG	C	201	14/15	0.89	0.17	40,59,74,75	0

6.5 Other polymers

There are no such residues in this entry.